Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2016 – 03:33 PM EST

PDB ID	:	5B1A
Title	:	Bovine heart cytochrome c oxidase in the fully oxidized state at 1.5 angstrom resolution
Authors	:	Yano, N.; Muramoto, K.; Shimada, A.; Takemura, S.; Baba, J.; Fujisawa, H.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on	:	2015-12-01
Resolution	:	1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

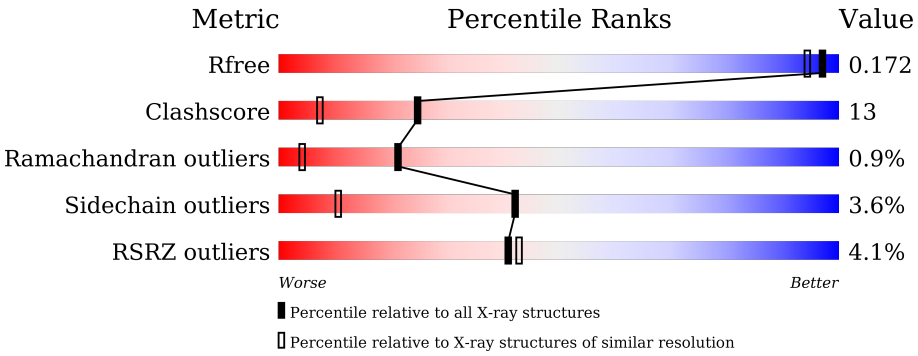
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	73% 22% •
1	N	514	73% 24% •
2	B	227	2% 65% 29% • •
2	O	227	2% 69% 26% • •
3	C	261	72% 25% • •
3	P	261	% 71% 22% 6% •

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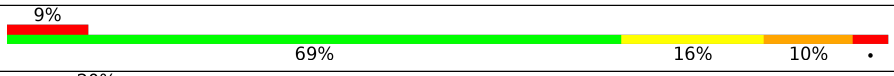
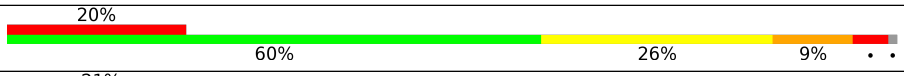
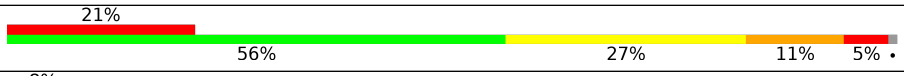
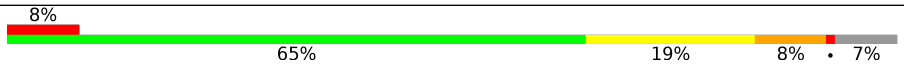
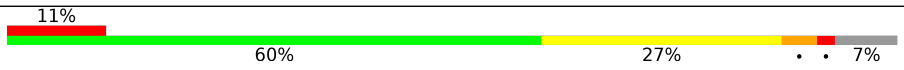
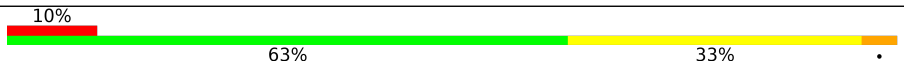
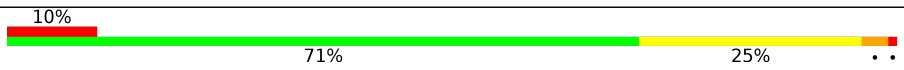
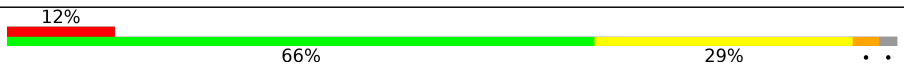
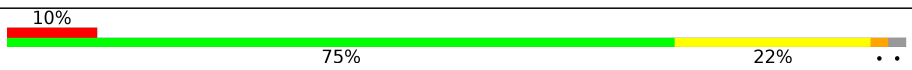
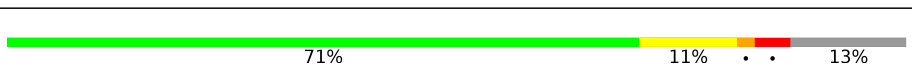
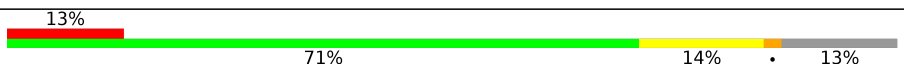
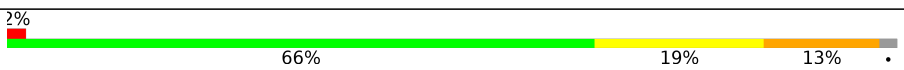
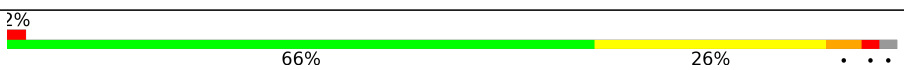
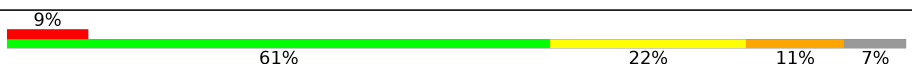
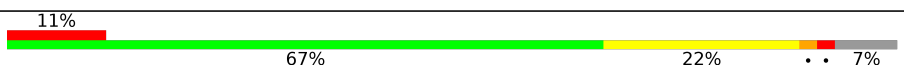
Mol	Chain	Length	Quality of chain
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	601	X	-	-	-
14	HEA	A	602	X	-	-	-
14	HEA	N	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	602	X	-	-	-
18	PER	A	606	-	-	-	X
18	PER	N	606	-	-	-	X
19	PGV	A	608	-	-	-	X
19	PGV	C	307	-	-	-	X
19	PGV	Q	201	-	-	-	X
2	FME	B	1	-	-	X	-
20	TGL	B	301	-	-	-	X
20	TGL	D	201	-	-	X	X
20	TGL	L	101	-	-	-	X
20	TGL	N	608	-	-	-	X
20	TGL	Q	202	-	-	-	X
20	TGL	Y	101	-	-	X	X
22	CHD	C	304	-	-	-	X
22	CHD	J	102	-	-	-	X
22	CHD	P	305	-	-	-	X
22	CHD	W	101	-	-	-	X
23	PSC	B	304	-	-	-	X
25	CDL	C	303	-	-	X	X
25	CDL	G	102	-	-	X	X
25	CDL	P	304	-	-	X	X
25	CDL	T	103	-	-	X	X
28	DMU	J	101	-	-	-	X
28	DMU	M	101	-	-	-	X
28	DMU	P	306	-	-	-	X
28	DMU	Z	101	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 35054 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	18	0
			4168	2778	645	704	41			
1	N	514	Total	C	N	O	S	0	16	0
			4154	2771	643	699	41			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	9	0
			1899	1234	292	353	20			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	288	347	20			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	9	0
			2185	1457	349	363	16			
3	P	259	Total	C	N	O	S	0	9	0
			2185	1457	349	363	16			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	5	0
			1242	809	206	223	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1224	797	202	221	4			

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	1	0
			863	550	148	163	2			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	4	0
			778	481	139	152	6			
6	S	98	Total	C	N	O	S	0	2	0
			763	473	136	148	6			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	1	0
			686	440	130	114	1	1			
7	T	84	Total	C	N	O	P	S	0	1	0
			686	440	130	114	1	1			

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	1	0
			469	302	79	85	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			

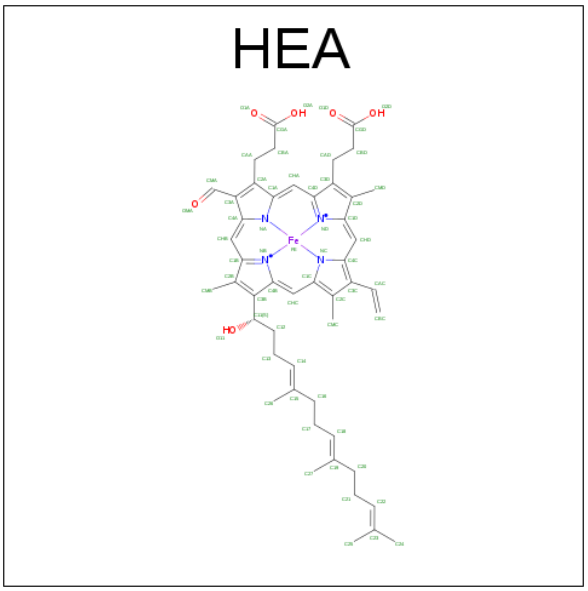
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	1	0
			388	259	65	61	3			

- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
14	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Cu	0	0
			1	1		
15	N	1	Total	Cu	0	0
			1	1		

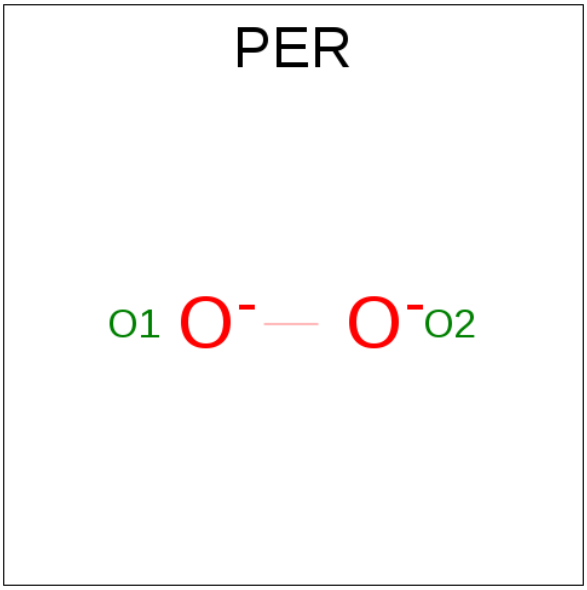
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		
16	N	1	Total	Mg	0	0
			1	1		

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

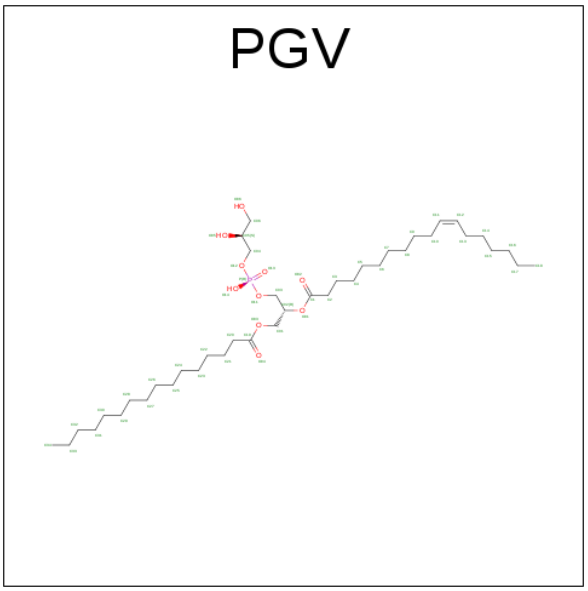
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is PEROXIDE ION (three-letter code: PER) (formula: O_2).



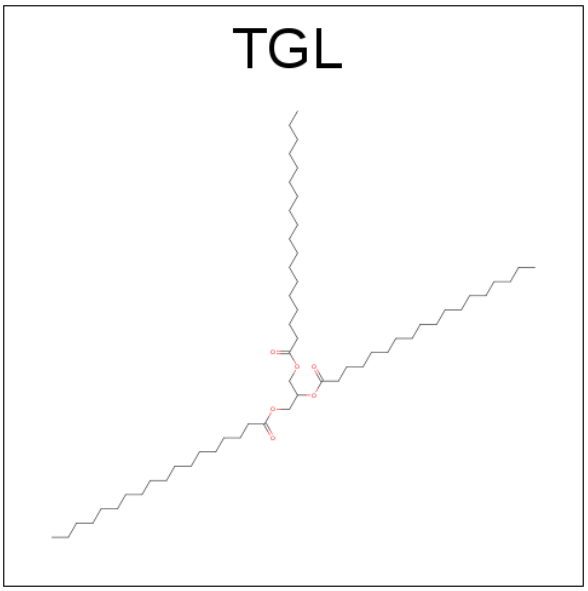
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total O 2 2	0	0
18	N	1	Total O 2 2	0	0

- Molecule 19 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



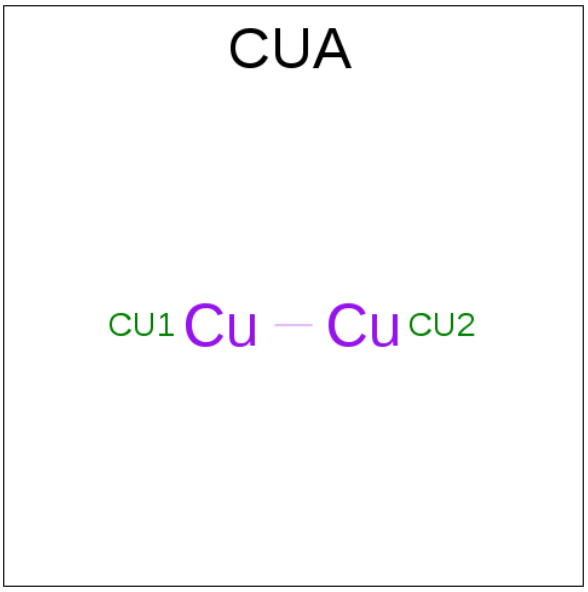
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	Q	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 20 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



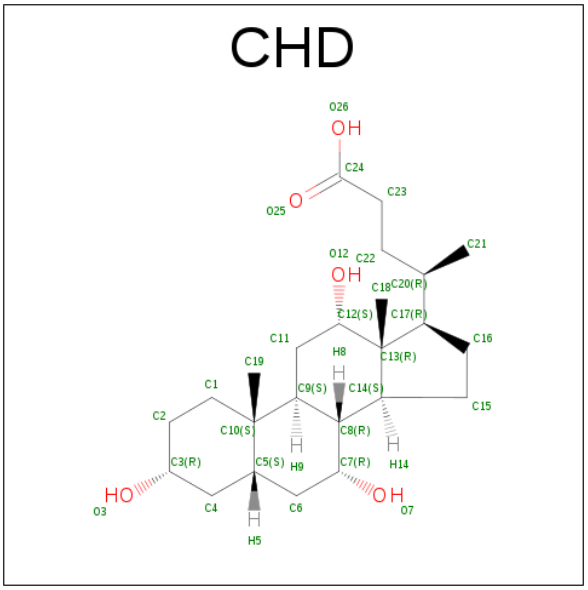
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	B	1	Total C O 63 57 6	0	0
20	D	1	Total C O 63 57 6	0	0
20	L	1	Total C O 63 57 6	0	0
20	N	1	Total C O 63 57 6	0	0
20	Q	1	Total C O 63 57 6	0	0
20	Y	1	Total C O 63 57 6	0	0

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	B	1	Total Cu 2 2	0	0
21	O	1	Total Cu 2 2	0	0

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0

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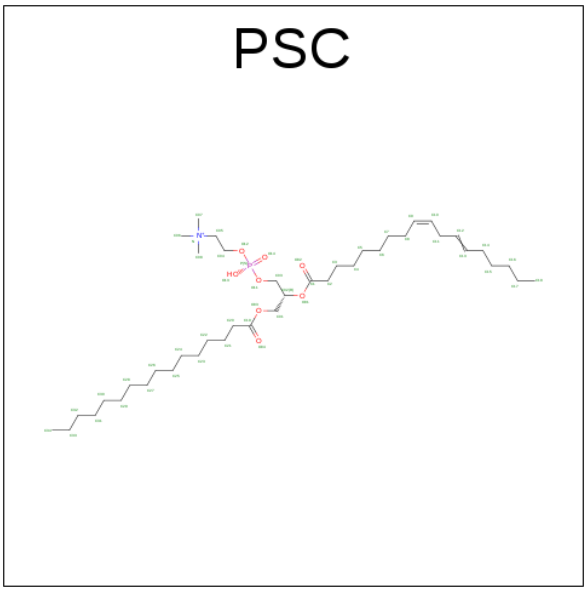
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	O	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).

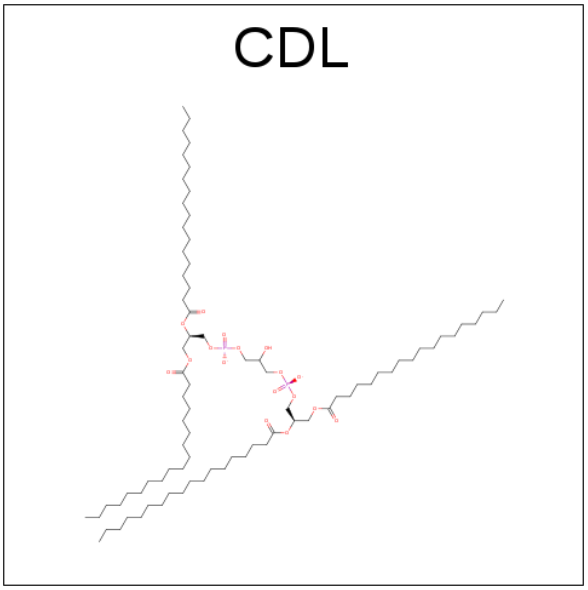


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C N O P 52 42 1 8 1	0	0
23	O	1	Total C N O P 52 42 1 8 1	0	0

- Molecule 24 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

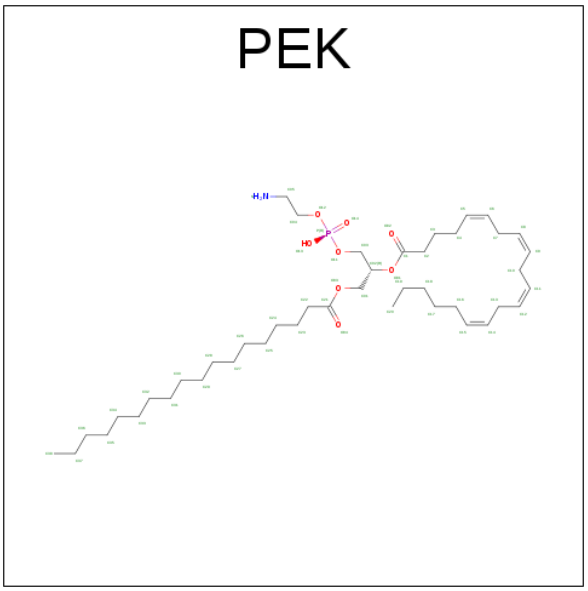
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	P	1	Total X 1 1	0	0
24	C	1	Total X 1 1	0	0

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	C	1	Total C O P 100 81 17 2	0	0
25	G	1	Total C O P 100 81 17 2	0	0
25	P	1	Total C O P 100 81 17 2	0	0
25	T	1	Total C O P 100 81 17 2	0	0

- Molecule 26 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: $C_{43}H_{78}NO_8P$).

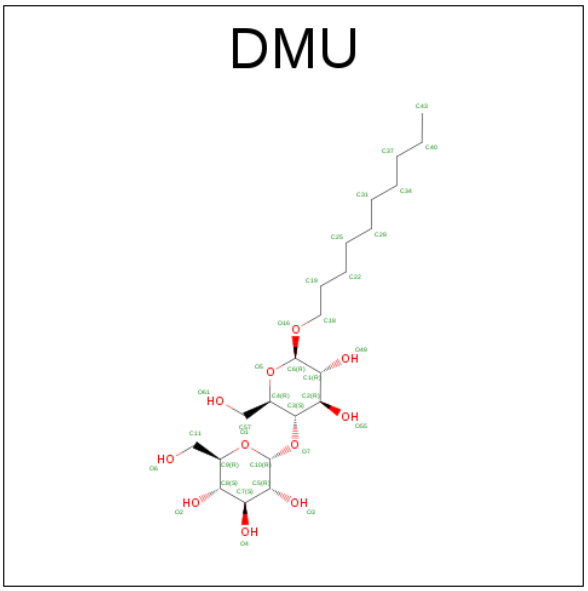


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	S	1	Total	Zn	0	0
			1	1		
27	F	1	Total	Zn	0	0
			1	1		

- Molecule 28 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	J	1	Total C O 33 22 11	0	0
28	M	1	Total C O 33 22 11	0	0
28	P	1	Total C O 33 22 11	0	0
28	Z	1	Total C O 33 22 11	0	0

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	297	Total O 297 297	0	0
29	B	273	Total O 274 274	0	1
29	C	176	Total O 176 176	0	0
29	D	266	Total O 266 266	0	0
29	E	178	Total O 178 178	0	0
29	F	199	Total O 199 199	0	0
29	G	100	Total O 100 100	0	0
29	H	122	Total O 122 122	0	0

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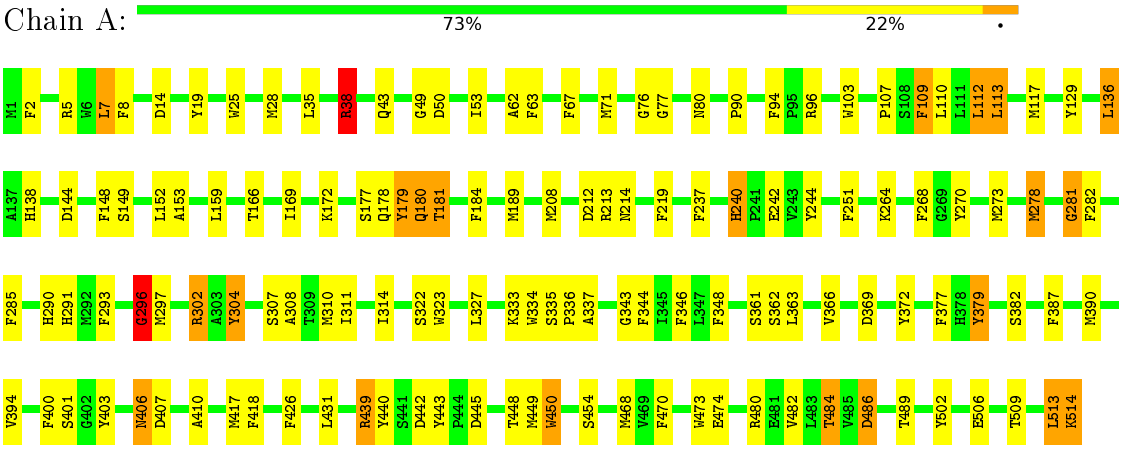
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	I	88	Total O 88 88	0	0
29	J	63	Total O 63 63	0	0
29	K	69	Total O 69 69	0	0
29	L	48	Total O 48 48	0	0
29	M	47	Total O 47 47	0	0
29	N	290	Total O 290 290	0	0
29	O	242	Total O 243 243	0	1
29	P	173	Total O 173 173	0	0
29	Q	164	Total O 164 164	0	0
29	R	151	Total O 151 151	0	0
29	S	186	Total O 186 186	0	0
29	T	94	Total O 94 94	0	0
29	U	110	Total O 110 110	0	0
29	V	71	Total O 71 71	0	0
29	W	58	Total O 58 58	0	0
29	X	57	Total O 57 57	0	0
29	Y	40	Total O 40 40	0	0
29	Z	37	Total O 37 37	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

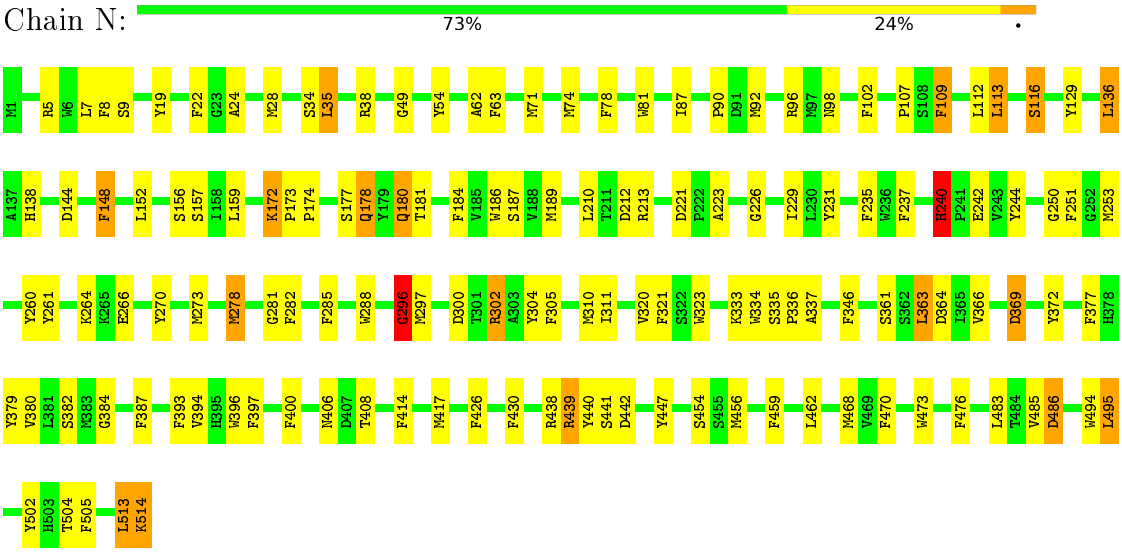
- Molecule 1: Cytochrome c oxidase subunit 1

Chain A:



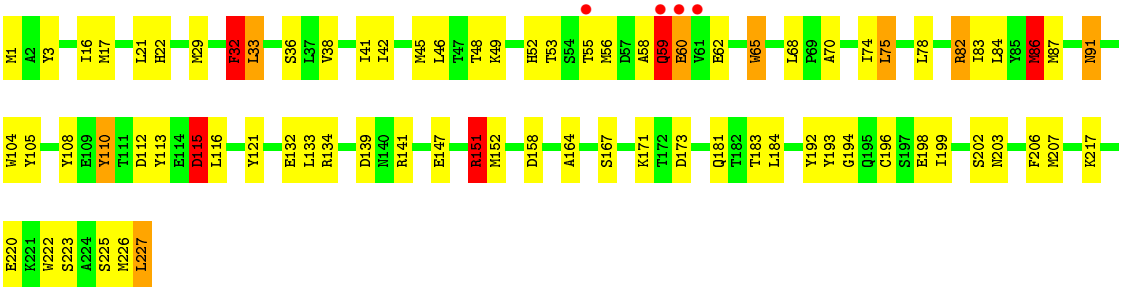
- Molecule 1: Cytochrome c oxidase subunit 1

Chain N:

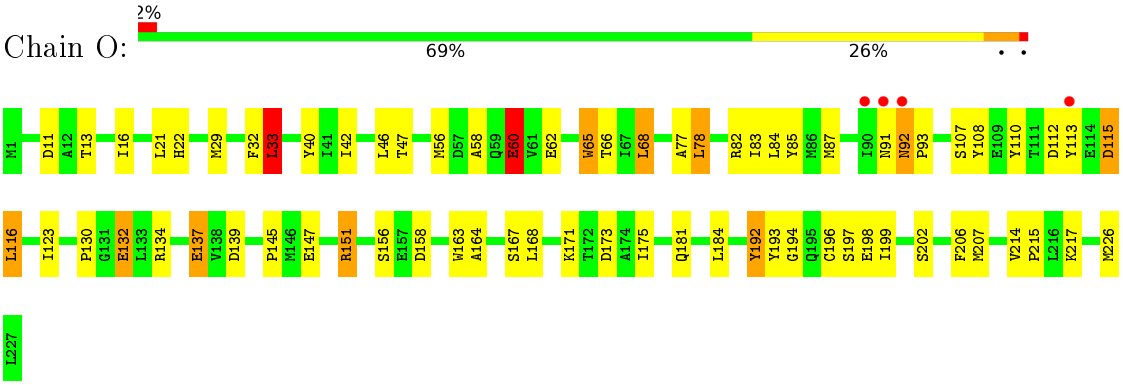


- Molecule 2: Cytochrome c oxidase subunit 2

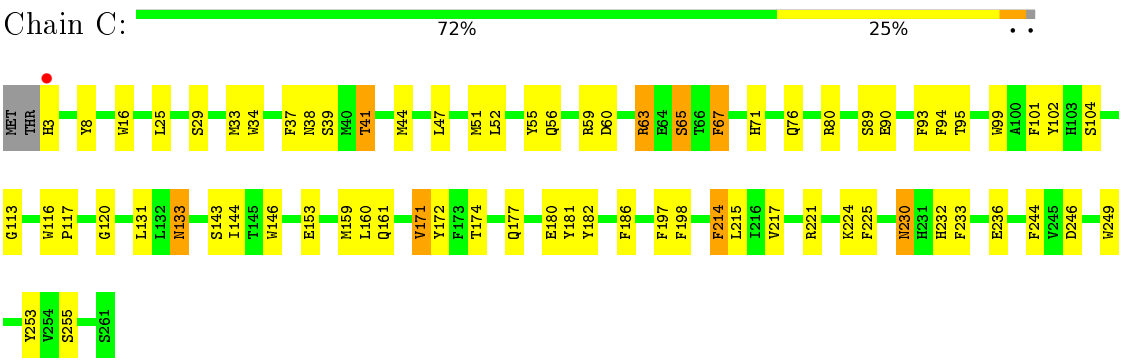
Chain B:



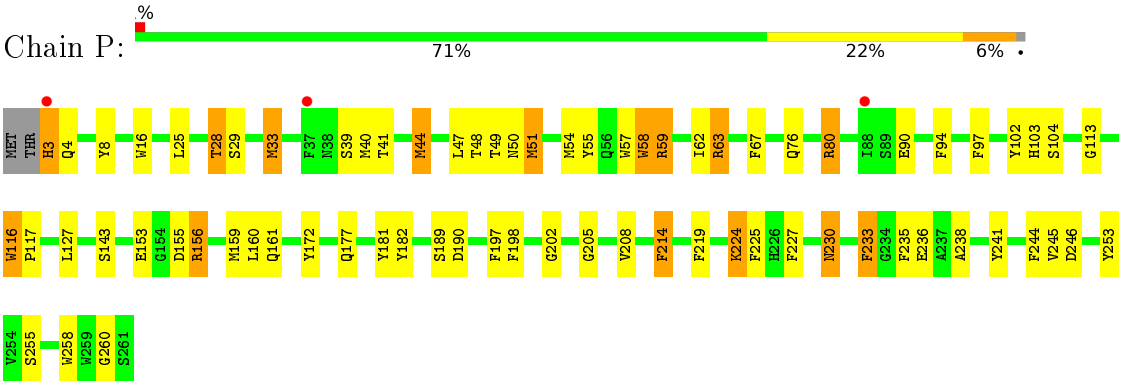
• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 3: Cytochrome c oxidase subunit 3

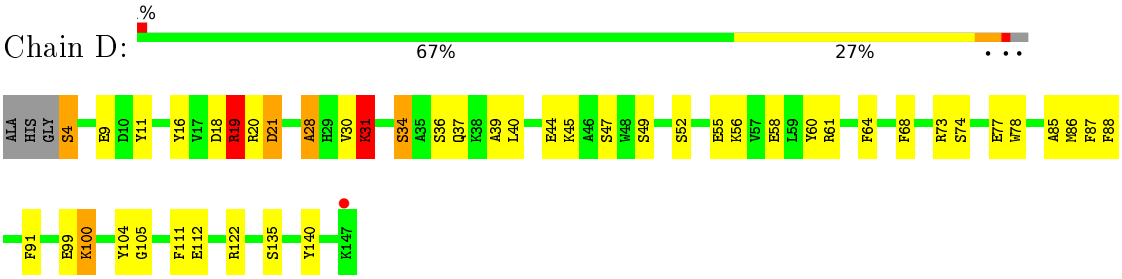


• Molecule 3: Cytochrome c oxidase subunit 3



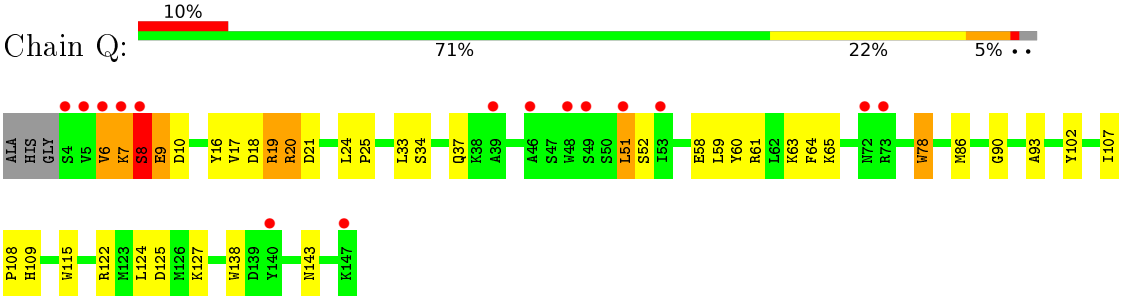
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:



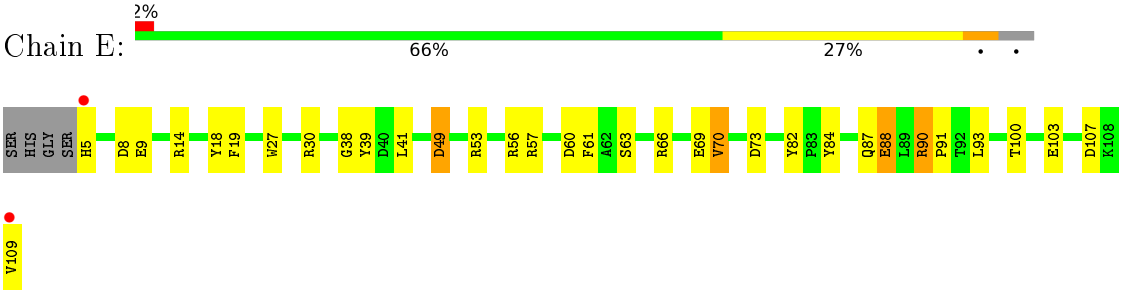
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q:



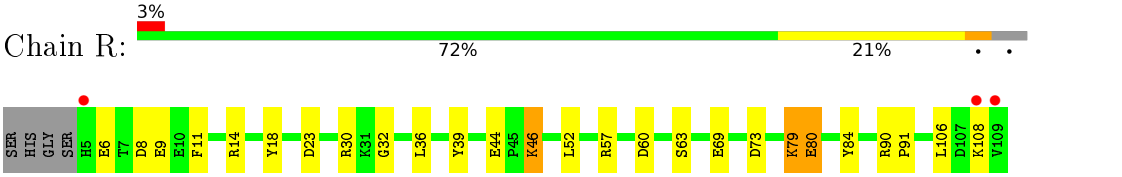
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain E:



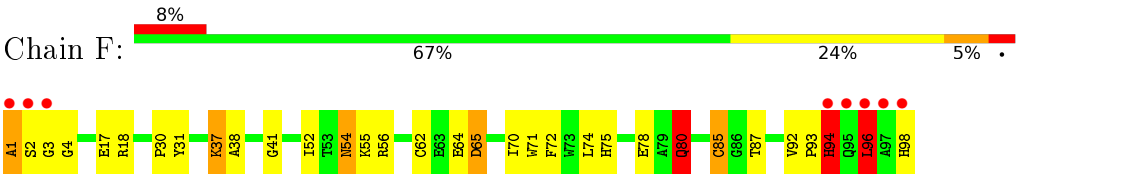
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

Chain R:



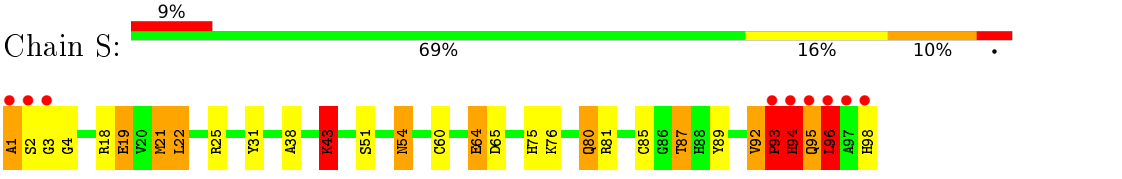
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain F:



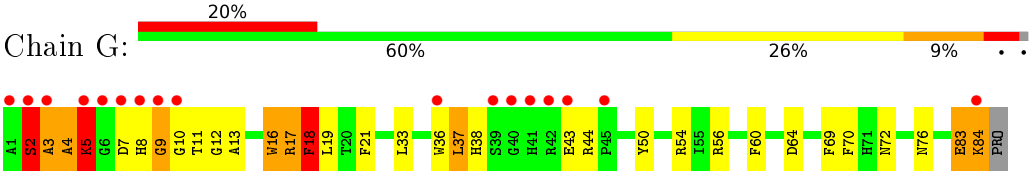
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

Chain S:



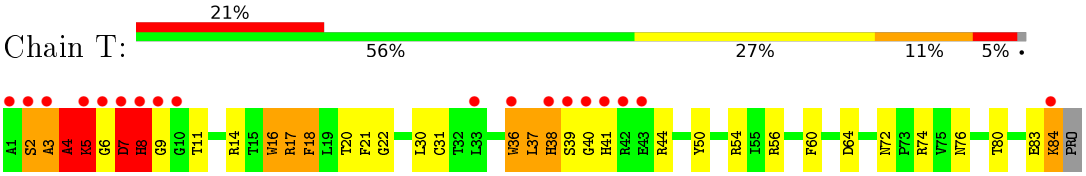
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain G:



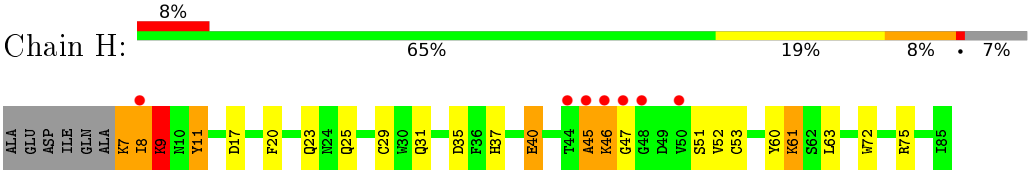
• Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

Chain T:



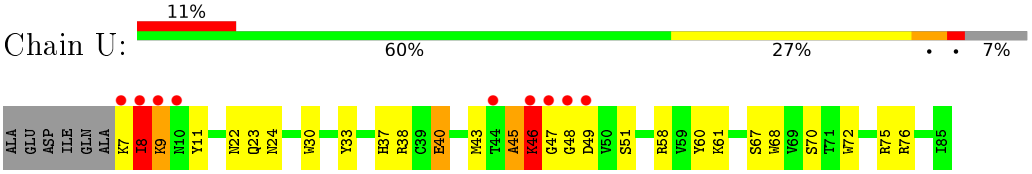
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain H:



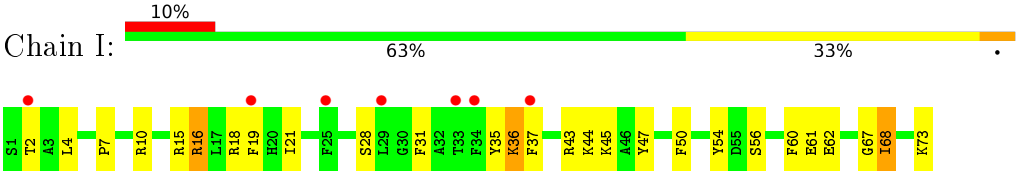
• Molecule 8: Cytochrome c oxidase subunit 6B1

Chain U:



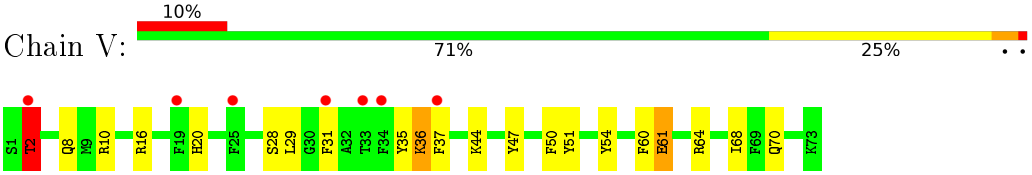
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain I:



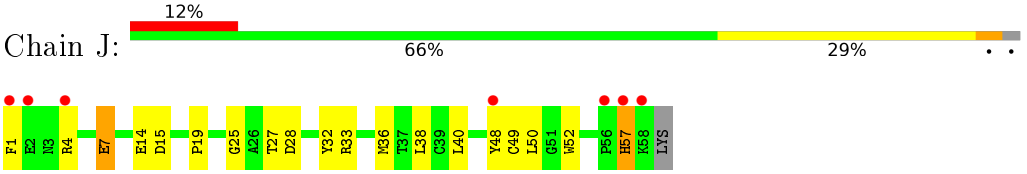
• Molecule 9: Cytochrome c oxidase subunit 6C

Chain V:



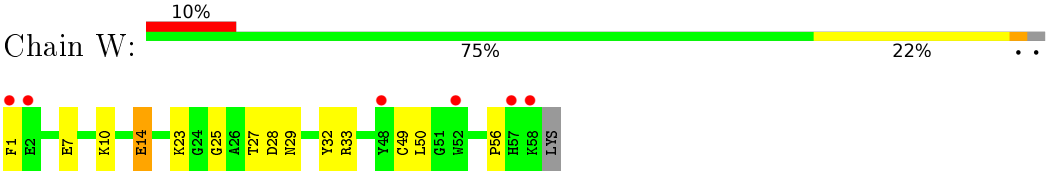
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain J:



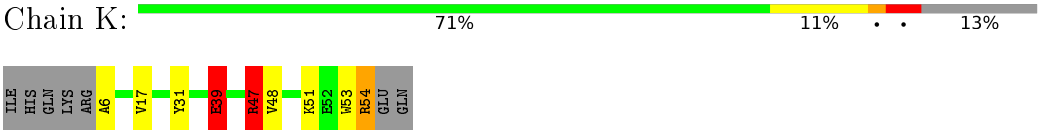
• Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain W:



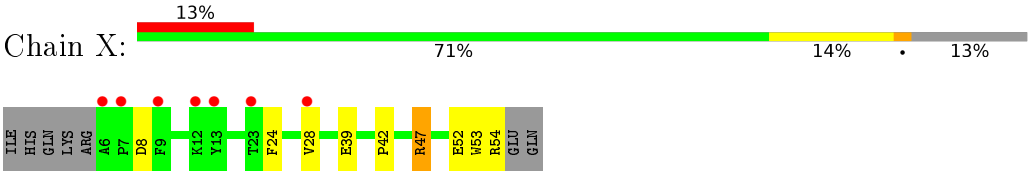
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain K:



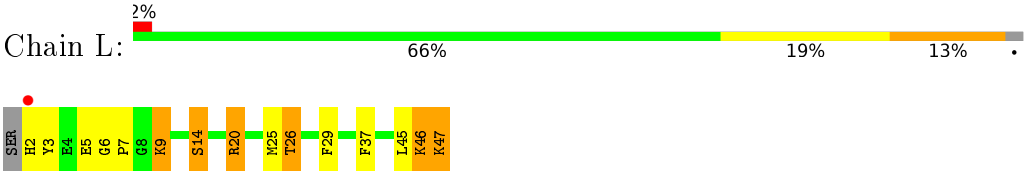
• Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

Chain X:



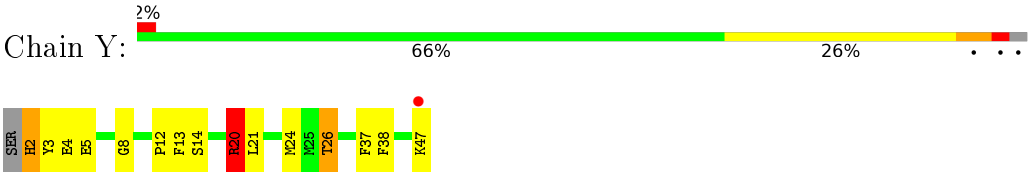
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain L:



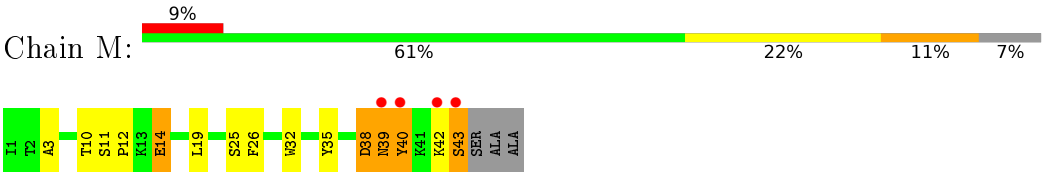
• Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:



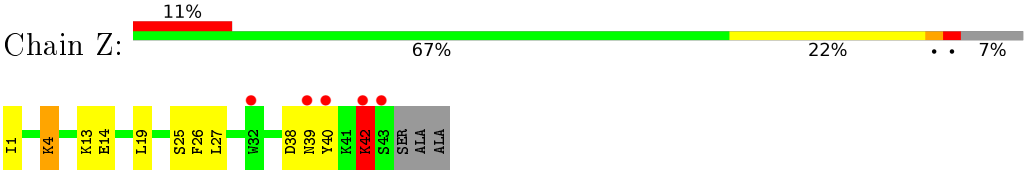
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:



• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	181.94Å 204.40Å 177.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.50 89.10 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (40.00-1.50) 98.2 (89.10-1.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.149 , 0.172 0.149 , 0.172	Depositor DCC
R_{free} test set	51654 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	20.6	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 66.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	35054	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CHD, HEA, SAC, CDL, PSC, PEK, MG, PER, PGV, TPO, UNX, CUA, NA, FME, TGL, CU, DMU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.84	54/4297 (1.3%)	1.89	89/5864 (1.5%)
1	N	1.85	57/4283 (1.3%)	1.76	84/5845 (1.4%)
2	B	1.94	37/1937 (1.9%)	1.80	32/2637 (1.2%)
2	O	1.82	30/1908 (1.6%)	1.57	23/2597 (0.9%)
3	C	1.91	41/2272 (1.8%)	1.79	46/3102 (1.5%)
3	P	1.91	37/2272 (1.6%)	1.77	52/3102 (1.7%)
4	D	2.05	31/1277 (2.4%)	1.87	40/1720 (2.3%)
4	Q	1.67	17/1259 (1.4%)	1.88	23/1698 (1.4%)
5	E	2.01	24/871 (2.8%)	2.45	41/1182 (3.5%)
5	R	1.89	18/882 (2.0%)	1.60	14/1196 (1.2%)
6	F	1.96	16/795 (2.0%)	1.65	7/1079 (0.6%)
6	S	1.89	17/780 (2.2%)	1.69	14/1058 (1.3%)
7	G	2.03	15/702 (2.1%)	1.87	19/953 (2.0%)
7	T	1.95	14/702 (2.0%)	1.59	9/953 (0.9%)
8	H	1.77	7/682 (1.0%)	1.52	9/921 (1.0%)
8	U	1.74	10/682 (1.5%)	1.36	5/921 (0.5%)
9	I	1.96	13/605 (2.1%)	1.73	13/802 (1.6%)
9	V	1.70	7/605 (1.2%)	1.85	9/802 (1.1%)
10	J	1.80	6/471 (1.3%)	1.54	4/636 (0.6%)
10	W	1.65	4/480 (0.8%)	1.36	2/648 (0.3%)
11	K	2.09	14/398 (3.5%)	1.91	7/546 (1.3%)
11	X	1.63	7/405 (1.7%)	1.47	5/556 (0.9%)
12	L	2.01	6/393 (1.5%)	1.76	11/526 (2.1%)
12	Y	1.97	11/401 (2.7%)	1.52	3/536 (0.6%)
13	M	1.80	6/345 (1.7%)	1.68	5/470 (1.1%)
13	Z	1.70	4/345 (1.2%)	1.43	3/470 (0.6%)
All	All	1.87	503/30049 (1.7%)	1.77	569/40820 (1.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	N	0	3
2	B	0	3
3	C	0	1
4	Q	0	1
5	E	0	2
6	F	0	1
6	S	0	2
7	G	0	1
7	T	0	1
10	J	0	1
11	K	0	1
13	M	0	1
All	All	0	22

All (503) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	65	TRP	CB-CG	-17.96	1.18	1.50
2	B	65	TRP	CB-CG	-17.06	1.19	1.50
4	D	58	GLU	CD-OE1	15.90	1.43	1.25
11	K	47	ARG	CZ-NH2	14.60	1.52	1.33
7	T	36	TRP	CB-CG	13.34	1.74	1.50
2	O	60	GLU	CD-OE1	12.69	1.39	1.25
11	X	54	ARG	CZ-NH2	12.54	1.49	1.33
5	R	90	ARG	NE-CZ	12.50	1.49	1.33
7	G	36	TRP	CB-CG	11.64	1.71	1.50
2	O	167	SER	CB-OG	-11.38	1.27	1.42
3	P	224	LYS	CE-NZ	11.24	1.77	1.49
11	K	54	ARG	NE-CZ	11.17	1.47	1.33
4	D	44	GLU	CD-OE1	10.96	1.37	1.25
12	L	26	THR	CB-CG2	-10.21	1.18	1.52
12	L	5	GLU	CD-OE2	-10.04	1.14	1.25
2	B	115	ASP	CB-CG	9.99	1.72	1.51
6	F	1	ALA	C-O	9.89	1.42	1.23
5	R	46	LYS	CE-NZ	9.87	1.73	1.49
7	T	17	ARG	CZ-NH2	9.84	1.45	1.33
1	N	242	GLU	CD-OE1	9.65	1.36	1.25
8	H	40	GLU	CD-OE2	9.63	1.36	1.25
3	P	104	SER	CB-OG	9.56	1.54	1.42
3	C	172	TYR	CG-CD1	9.45	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	8	GLN	CG-CD	-9.33	1.29	1.51
13	Z	40	TYR	CE1-CZ	9.31	1.50	1.38
8	U	40	GLU	CD-OE2	9.23	1.35	1.25
12	Y	4	GLU	CD-OE1	9.23	1.35	1.25
9	I	61	GLU	CD-OE1	-9.21	1.15	1.25
3	C	90	GLU	CD-OE1	9.20	1.35	1.25
5	E	39	TYR	CG-CD2	-9.10	1.27	1.39
3	C	104	SER	CB-OG	9.10	1.54	1.42
1	A	96	ARG	CZ-NH1	8.97	1.44	1.33
2	B	132	GLU	CD-OE2	8.96	1.35	1.25
6	S	1	ALA	C-O	8.84	1.40	1.23
3	C	63	ARG	CZ-NH2	8.79	1.44	1.33
2	O	60	GLU	CD-OE2	8.76	1.35	1.25
5	R	84	TYR	CG-CD1	8.70	1.50	1.39
1	N	278[A]	MET	SD-CE	-8.67	1.29	1.77
1	N	278[B]	MET	SD-CE	-8.67	1.29	1.77
3	P	172	TYR	CG-CD1	8.67	1.50	1.39
11	X	52	GLU	CD-OE1	8.67	1.35	1.25
6	F	4	GLY	N-CA	8.66	1.59	1.46
12	L	29	PHE	CD2-CE2	-8.45	1.22	1.39
3	P	102	TYR	CG-CD1	-8.36	1.28	1.39
6	S	4	GLY	N-CA	8.36	1.58	1.46
7	T	80	THR	C-O	-8.33	1.07	1.23
3	P	182	TYR	CD2-CE2	-8.29	1.26	1.39
4	Q	20	ARG	CD-NE	-8.26	1.32	1.46
9	I	28	SER	CB-OG	8.26	1.52	1.42
7	G	16	TRP	CZ3-CH2	8.18	1.53	1.40
1	A	382	SER	CA-CB	8.15	1.65	1.52
1	N	382	SER	CB-OG	-8.13	1.31	1.42
2	O	147	GLU	CD-OE1	-8.12	1.16	1.25
2	O	132	GLU	CD-OE2	8.08	1.34	1.25
2	B	223	SER	CA-CB	8.03	1.65	1.52
2	O	197	SER	CB-OG	8.03	1.52	1.42
10	J	48	TYR	CG-CD2	8.01	1.49	1.39
4	D	60	TYR	CE1-CZ	7.98	1.49	1.38
5	E	9	GLU	CG-CD	7.97	1.64	1.51
4	D	77	GLU	CD-OE1	7.96	1.34	1.25
4	Q	20	ARG	CZ-NH2	-7.96	1.22	1.33
2	O	65	TRP	CE3-CZ3	7.93	1.51	1.38
3	P	153	GLU	CG-CD	7.92	1.63	1.51
11	K	31	TYR	CE1-CZ	7.89	1.48	1.38
4	Q	6	VAL	C-O	7.88	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	244	PHE	CD1-CE1	7.88	1.55	1.39
6	F	56	ARG	CZ-NH1	7.88	1.43	1.33
3	P	76	GLN	CB-CG	-7.80	1.31	1.52
6	S	18	ARG	CZ-NH1	7.78	1.43	1.33
9	I	62	GLU	CD-OE1	7.76	1.34	1.25
1	N	439	ARG	CZ-NH1	7.75	1.43	1.33
4	D	135	SER	CA-CB	7.73	1.64	1.52
6	F	17	GLU	CD-OE1	7.68	1.34	1.25
13	M	40	TYR	CE1-CZ	7.67	1.48	1.38
1	A	19	TYR	CG-CD2	7.62	1.49	1.39
1	A	514	LYS	N-CA	7.57	1.61	1.46
9	V	47	TYR	CE1-CZ	7.56	1.48	1.38
1	N	441	SER	CA-CB	7.54	1.64	1.52
13	M	14	GLU	CD-OE2	7.53	1.33	1.25
5	E	90	ARG	CZ-NH1	7.51	1.42	1.33
11	K	39	GLU	CG-CD	-7.51	1.40	1.51
5	E	103	GLU	CD-OE2	7.46	1.33	1.25
7	T	21	PHE	CG-CD1	-7.44	1.27	1.38
2	B	59	GLN	CD-OE1	7.41	1.40	1.24
2	B	36	SER	CB-OG	7.40	1.51	1.42
3	C	253	TYR	CG-CD2	-7.35	1.29	1.39
11	K	47	ARG	CD-NE	7.34	1.58	1.46
5	R	32	GLY	N-CA	7.32	1.57	1.46
1	A	189	MET	CG-SD	-7.32	1.62	1.81
2	B	59	GLN	CG-CD	7.31	1.67	1.51
3	C	230	ASN	CB-CG	-7.30	1.34	1.51
1	N	323	TRP	CZ3-CH2	7.29	1.51	1.40
2	O	198	GLU	CD-OE2	-7.28	1.17	1.25
3	C	182	TYR	CZ-OH	-7.26	1.25	1.37
2	O	60	GLU	CG-CD	7.20	1.62	1.51
1	A	322	SER	CA-CB	7.19	1.63	1.52
10	J	25	GLY	N-CA	7.18	1.56	1.46
5	E	9	GLU	CD-OE2	7.17	1.33	1.25
9	I	60	PHE	CG-CD2	7.17	1.49	1.38
9	I	4	LEU	CA-CB	7.14	1.70	1.53
1	N	226	GLY	N-CA	7.13	1.56	1.46
6	S	92	VAL	C-O	-7.13	1.09	1.23
1	A	401	SER	CA-CB	7.12	1.63	1.52
4	D	100[A]	LYS	CE-NZ	7.11	1.66	1.49
4	D	100[B]	LYS	CE-NZ	7.11	1.66	1.49
3	C	102	TYR	CG-CD1	-7.11	1.29	1.39
2	B	113	TYR	CG-CD2	7.09	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	16	TRP	CE3-CZ3	7.07	1.50	1.38
4	D	47	SER	CA-CB	7.07	1.63	1.52
1	N	470	PHE	CE2-CZ	7.03	1.50	1.37
2	O	65	TRP	CD2-CE3	7.01	1.50	1.40
3	C	65	SER	CA-CB	6.99	1.63	1.52
5	E	56	ARG	CZ-NH2	6.99	1.42	1.33
3	C	94	PHE	CG-CD2	6.99	1.49	1.38
6	F	18	ARG	CZ-NH2	6.99	1.42	1.33
7	G	17	ARG	CZ-NH2	6.98	1.42	1.33
4	D	61	ARG	CZ-NH2	6.97	1.42	1.33
5	E	9	GLU	CA-CB	6.94	1.69	1.53
3	P	182	TYR	CE1-CZ	6.92	1.47	1.38
5	R	39	TYR	CG-CD2	-6.91	1.30	1.39
3	C	113	GLY	N-CA	6.91	1.56	1.46
1	A	242	GLU	CD-OE1	6.88	1.33	1.25
3	C	29	SER	CB-OG	-6.86	1.33	1.42
1	A	49	GLY	C-O	6.86	1.34	1.23
7	G	83	GLU	CD-OE1	6.86	1.33	1.25
3	P	258	TRP	CG-CD1	6.84	1.46	1.36
1	A	149	SER	CB-OG	6.83	1.51	1.42
1	N	335	SER	CB-OG	6.83	1.51	1.42
1	N	49	GLY	C-O	6.83	1.34	1.23
1	N	514	LYS	N-CA	6.82	1.59	1.46
5	E	109	VAL	N-CA	6.82	1.59	1.46
12	L	14	SER	CB-OG	6.77	1.51	1.42
2	B	167	SER	CB-OG	-6.76	1.33	1.42
2	O	193	TYR	CG-CD1	6.75	1.48	1.39
5	E	84	TYR	CG-CD1	6.74	1.48	1.39
12	Y	5	GLU	CD-OE2	-6.74	1.18	1.25
1	A	450	TRP	CE3-CZ3	6.71	1.49	1.38
1	A	480	ARG	CZ-NH2	6.69	1.41	1.33
2	B	82	ARG	CZ-NH1	6.69	1.41	1.33
10	W	25	GLY	N-CA	6.69	1.56	1.46
3	C	8	TYR	CG-CD2	6.69	1.47	1.39
12	Y	26	THR	CB-CG2	-6.67	1.30	1.52
6	S	89	TYR	CE1-CZ	6.64	1.47	1.38
13	M	40	TYR	CG-CD1	6.62	1.47	1.39
1	N	270	TYR	CE1-CZ	6.62	1.47	1.38
11	K	47	ARG	CG-CD	6.60	1.68	1.51
1	N	281	GLY	N-CA	6.60	1.55	1.46
5	R	39	TYR	CE2-CZ	-6.59	1.29	1.38
1	N	514	LYS	CA-CB	6.54	1.68	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	12	GLY	CA-C	6.54	1.62	1.51
6	S	93	PRO	CA-CB	6.54	1.66	1.53
1	N	502	TYR	CG-CD2	6.54	1.47	1.39
2	B	223	SER	CB-OG	-6.53	1.33	1.42
5	E	73	ASP	CB-CG	6.52	1.65	1.51
7	G	5	LYS	CA-CB	6.50	1.68	1.53
5	E	38	GLY	N-CA	6.49	1.55	1.46
11	K	17	VAL	N-CA	6.49	1.59	1.46
1	A	382	SER	CB-OG	-6.46	1.33	1.42
3	P	233	PHE	CD2-CE2	6.45	1.52	1.39
5	E	84	TYR	CE1-CZ	-6.44	1.30	1.38
2	B	108	TYR	CE2-CZ	6.43	1.47	1.38
8	U	33	TYR	CG-CD1	6.42	1.47	1.39
3	P	143	SER	CA-CB	6.42	1.62	1.52
11	K	39	GLU	CD-OE2	6.42	1.32	1.25
8	H	72	TRP	CD2-CE2	6.41	1.49	1.41
12	Y	4	GLU	CG-CD	6.41	1.61	1.51
4	D	88	PHE	CE2-CZ	6.39	1.49	1.37
3	C	143	SER	CA-CB	6.38	1.62	1.52
2	B	65	TRP	CD2-CE3	6.38	1.50	1.40
11	K	39	GLU	CB-CG	6.38	1.64	1.52
7	G	56	ARG	CZ-NH1	6.37	1.41	1.33
6	F	3	GLY	CA-C	6.36	1.62	1.51
4	D	52	SER	CB-OG	6.34	1.50	1.42
1	N	264	LYS	CD-CE	6.33	1.67	1.51
1	N	187	SER	CA-CB	6.33	1.62	1.52
6	S	19	GLU	CD-OE1	6.33	1.32	1.25
2	B	65	TRP	CD2-CE2	6.32	1.49	1.41
2	B	113	TYR	CB-CG	-6.31	1.42	1.51
12	Y	5	GLU	CD-OE1	-6.31	1.18	1.25
2	O	123	ILE	N-CA	6.28	1.58	1.46
7	T	17	ARG	CZ-NH1	6.27	1.41	1.33
4	D	34	SER	CB-OG	6.27	1.50	1.42
1	A	450	TRP	CG-CD1	6.26	1.45	1.36
3	C	41	THR	C-O	6.24	1.35	1.23
5	E	103	GLU	CB-CG	6.22	1.64	1.52
7	G	21	PHE	CG-CD1	-6.22	1.29	1.38
5	R	80	GLU	CD-OE1	6.21	1.32	1.25
9	I	56	SER	CB-OG	6.18	1.50	1.42
4	Q	18	ASP	N-CA	6.17	1.58	1.46
3	C	99	TRP	CE3-CZ3	6.17	1.49	1.38
3	C	120	GLY	N-CA	6.17	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	W	14[A]	GLU	CD-OE1	-6.17	1.18	1.25
10	W	14[B]	GLU	CD-OE1	-6.17	1.18	1.25
4	Q	64	PHE	CG-CD2	6.16	1.48	1.38
3	P	116	TRP	CZ3-CH2	6.16	1.49	1.40
1	A	242	GLU	CD-OE2	-6.14	1.18	1.25
2	B	152	MET	CB-CG	-6.14	1.31	1.51
1	A	335	SER	CB-OG	6.14	1.50	1.42
5	E	41	LEU	C-O	6.14	1.35	1.23
4	Q	78	TRP	CE3-CZ3	6.14	1.48	1.38
7	G	13	ALA	N-CA	6.13	1.58	1.46
3	C	255	SER	CA-CB	6.13	1.62	1.52
5	R	80	GLU	CG-CD	6.11	1.61	1.51
8	U	72	TRP	CD1-NE1	6.11	1.48	1.38
5	R	84	TYR	CE1-CZ	-6.11	1.30	1.38
1	N	116	SER	CB-OG	6.11	1.50	1.42
2	O	115	ASP	CB-CG	6.10	1.64	1.51
5	R	18	TYR	CG-CD2	6.10	1.47	1.39
2	B	225	SER	CA-CB	6.09	1.62	1.52
6	F	72	PHE	CD1-CE1	6.09	1.51	1.39
3	C	153	GLU	CD-OE2	-6.09	1.19	1.25
3	C	171	VAL	CB-CG1	6.09	1.65	1.52
3	C	34	TRP	CE3-CZ3	6.08	1.48	1.38
1	A	213	ARG	CZ-NH2	6.08	1.41	1.33
1	A	363	LEU	CB-CG	-6.08	1.34	1.52
3	C	249	TRP	CE3-CZ3	6.08	1.48	1.38
12	Y	2	HIS	N-CA	6.07	1.58	1.46
1	N	96	ARG	CZ-NH1	6.07	1.41	1.33
5	E	91	PRO	CA-C	6.06	1.65	1.52
5	E	84	TYR	CE2-CZ	6.05	1.46	1.38
2	B	167	SER	CA-CB	-6.02	1.44	1.52
3	P	59	ARG	CZ-NH1	6.02	1.40	1.33
13	Z	40	TYR	CG-CD2	6.01	1.47	1.39
7	T	14	ARG	CZ-NH1	6.01	1.40	1.33
6	F	78	GLU	CD-OE2	-6.00	1.19	1.25
4	D	68	PHE	CG-CD1	5.98	1.47	1.38
5	R	84	TYR	CE2-CZ	5.97	1.46	1.38
1	A	400	PHE	CD2-CE2	5.97	1.51	1.39
1	N	441	SER	CB-OG	5.96	1.50	1.42
6	S	43	LYS	CB-CG	5.96	1.68	1.52
6	F	2	SER	N-CA	5.95	1.58	1.46
10	J	7	GLU	CD-OE1	5.95	1.32	1.25
3	C	76	GLN	CB-CG	-5.95	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	105	GLY	N-CA	5.95	1.54	1.46
3	P	198	PHE	CG-CD2	5.93	1.47	1.38
4	D	9	GLU	CG-CD	5.92	1.60	1.51
3	C	233	PHE	CD1-CE1	5.92	1.51	1.39
5	E	19	PHE	CE1-CZ	5.92	1.48	1.37
6	F	62	CYS	N-CA	5.92	1.58	1.46
6	S	3	GLY	C-O	5.91	1.33	1.23
13	M	40	TYR	CG-CD2	5.91	1.46	1.39
11	X	53	TRP	CE3-CZ3	5.91	1.48	1.38
3	C	225	PHE	CG-CD1	5.90	1.47	1.38
3	P	16	TRP	CG-CD1	5.88	1.45	1.36
3	C	181	TYR	CE2-CZ	-5.87	1.30	1.38
7	G	18	PHE	CG-CD2	-5.87	1.29	1.38
3	P	253	TYR	CZ-OH	5.86	1.47	1.37
2	O	163	TRP	CG-CD1	5.85	1.45	1.36
1	N	19	TYR	CG-CD2	5.85	1.46	1.39
11	X	47	ARG	NE-CZ	5.84	1.40	1.33
12	Y	38	PHE	CG-CD1	5.83	1.47	1.38
1	A	214	ASN	C-O	5.83	1.34	1.23
9	V	51	TYR	CG-CD1	5.83	1.46	1.39
7	G	5	LYS	CA-C	5.83	1.68	1.52
1	N	129	TYR	CD2-CE2	5.83	1.48	1.39
1	A	281	GLY	N-CA	5.81	1.54	1.46
2	B	222	TRP	CE3-CZ3	5.81	1.48	1.38
6	F	80	GLN	CD-OE1	5.80	1.36	1.24
10	J	19	PRO	CA-CB	5.79	1.65	1.53
2	B	55	THR	C-O	5.79	1.34	1.23
13	Z	4	LYS	N-CA	5.78	1.57	1.46
3	C	177	GLN	CB-CG	-5.78	1.36	1.52
10	J	14	GLU	CD-OE2	5.78	1.32	1.25
1	A	90	PRO	N-CD	5.77	1.55	1.47
4	D	36	SER	CB-OG	-5.76	1.34	1.42
4	D	49	SER	CA-CB	5.75	1.61	1.52
1	A	474	GLU	CD-OE1	5.75	1.31	1.25
5	R	11	PHE	CG-CD2	5.74	1.47	1.38
1	A	43	GLN	CG-CD	5.73	1.64	1.51
5	E	27	TRP	CE3-CZ3	5.73	1.48	1.38
1	N	454	SER	CA-CB	5.73	1.61	1.52
4	D	91	PHE	CG-CD1	5.73	1.47	1.38
2	B	55	THR	CB-CG2	5.73	1.71	1.52
11	K	54	ARG	CZ-NH2	5.72	1.40	1.33
13	M	11	SER	CB-OG	5.72	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	384	GLY	N-CA	5.72	1.54	1.46
4	Q	125	ASP	CB-CG	5.72	1.63	1.51
2	B	198	GLU	CB-CG	5.71	1.62	1.52
1	N	250	GLY	CA-C	5.69	1.60	1.51
8	U	30	TRP	CG-CD1	5.69	1.44	1.36
11	K	31	TYR	CG-CD2	5.68	1.46	1.39
9	I	7	PRO	CA-C	-5.68	1.41	1.52
1	A	179	TYR	CG-CD1	5.67	1.46	1.39
9	I	68	ILE	CB-CG1	-5.67	1.38	1.54
9	V	50	PHE	CG-CD1	5.66	1.47	1.38
9	I	54	TYR	CD2-CE2	5.65	1.47	1.39
7	G	3	ALA	N-CA	5.64	1.57	1.46
2	O	21	LEU	CA-CB	5.64	1.66	1.53
8	U	67	SER	CA-CB	5.63	1.61	1.52
2	O	192	TYR	CE2-CZ	5.63	1.45	1.38
11	K	53	TRP	CE3-CZ3	5.63	1.48	1.38
1	A	448	THR	C-O	5.62	1.34	1.23
2	B	21	LEU	CA-CB	5.62	1.66	1.53
3	C	101	PHE	CD1-CE1	5.62	1.50	1.39
5	R	9	GLU	CG-CD	5.62	1.60	1.51
12	Y	20	ARG	CZ-NH1	5.62	1.40	1.33
7	T	83	GLU	CD-OE1	5.61	1.31	1.25
6	S	89	TYR	CG-CD2	5.61	1.46	1.39
2	O	110	TYR	CG-CD2	5.61	1.46	1.39
12	Y	8	GLY	N-CA	5.61	1.54	1.46
5	R	69	GLU	CB-CG	5.60	1.62	1.52
6	S	3	GLY	CA-C	5.60	1.60	1.51
4	D	85	ALA	C-O	5.59	1.33	1.23
3	C	253	TYR	CE1-CZ	-5.59	1.31	1.38
9	V	28	SER	CB-OG	5.58	1.49	1.42
2	O	66	THR	CB-OG1	5.58	1.54	1.43
2	O	107	SER	CA-CB	5.57	1.61	1.52
2	B	82	ARG	CZ-NH2	5.56	1.40	1.33
4	D	64	PHE	CA-CB	5.56	1.66	1.53
12	Y	3	TYR	CG-CD1	5.56	1.46	1.39
4	D	58	GLU	CB-CG	5.56	1.62	1.52
1	N	231	TYR	CE1-CZ	5.55	1.45	1.38
12	L	6	GLY	CA-C	5.55	1.60	1.51
4	Q	102	TYR	CG-CD2	5.55	1.46	1.39
2	B	121	TYR	CE2-CZ	5.55	1.45	1.38
6	F	18	ARG	CZ-NH1	5.55	1.40	1.33
1	N	382	SER	CA-CB	5.55	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	10	ARG	CZ-NH1	5.53	1.40	1.33
1	A	307	SER	CB-OG	5.52	1.49	1.42
1	A	506	GLU	CD-OE2	5.52	1.31	1.25
1	A	77	GLY	N-CA	5.51	1.54	1.46
3	C	172	TYR	CE2-CZ	5.51	1.45	1.38
5	E	69	GLU	CA-CB	5.51	1.66	1.53
3	P	94	PHE	CE1-CZ	5.51	1.47	1.37
3	C	233	PHE	CD2-CE2	5.50	1.50	1.39
1	N	9	SER	CB-OG	5.50	1.49	1.42
1	A	362[A]	SER	CA-CB	5.50	1.61	1.52
1	A	362[B]	SER	CA-CB	5.50	1.61	1.52
11	X	39	GLU	CD-OE1	5.50	1.31	1.25
1	A	410	ALA	CA-CB	5.50	1.64	1.52
1	N	494	TRP	CE3-CZ3	5.50	1.47	1.38
3	P	102	TYR	CG-CD2	5.50	1.46	1.39
1	A	184	PHE	CG-CD1	5.49	1.47	1.38
1	A	333	LYS	C-O	5.49	1.33	1.23
6	F	85	CYS	C-O	5.49	1.33	1.23
1	N	440	TYR	CE1-CZ	5.48	1.45	1.38
1	N	486	ASP	CG-OD1	5.48	1.38	1.25
1	N	144	ASP	CB-CG	5.47	1.63	1.51
1	N	189	MET	CG-SD	-5.47	1.67	1.81
1	N	92	MET	CB-CG	5.46	1.68	1.51
3	P	230	ASN	CB-CG	-5.46	1.38	1.51
2	B	110	TYR	CD1-CE1	5.45	1.47	1.39
3	P	80[A]	ARG	CZ-NH1	-5.45	1.25	1.33
3	P	80[B]	ARG	CZ-NH1	-5.45	1.25	1.33
1	A	418	PHE	CD2-CE2	5.44	1.50	1.39
1	N	156	SER	CB-OG	5.44	1.49	1.42
11	K	39	GLU	CD-OE1	5.44	1.31	1.25
11	K	47	ARG	NE-CZ	5.43	1.40	1.33
1	N	320	VAL	CB-CG1	5.42	1.64	1.52
3	C	146	TRP	CE3-CZ3	5.42	1.47	1.38
3	C	198	PHE	CG-CD2	5.42	1.46	1.38
5	R	63	SER	CB-OG	5.42	1.49	1.42
2	B	220	GLU	CD-OE1	-5.41	1.19	1.25
7	T	56	ARG	CZ-NH1	5.41	1.40	1.33
4	D	28	ALA	C-O	5.41	1.33	1.23
1	N	305	PHE	CG-CD2	5.41	1.46	1.38
2	B	60	GLU	CG-CD	5.41	1.60	1.51
5	R	57	ARG	CZ-NH1	5.41	1.40	1.33
1	A	426	PHE	CG-CD1	5.41	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	U	76	ARG	CZ-NH1	5.40	1.40	1.33
1	A	296	GLY	N-CA	5.39	1.54	1.46
8	H	20	PHE	CG-CD1	5.39	1.46	1.38
2	O	85	TYR	CG-CD2	5.39	1.46	1.39
2	O	137	GLU	CD-OE1	5.39	1.31	1.25
7	T	16	TRP	CD2-CE2	5.39	1.47	1.41
1	N	157	SER	CB-OG	5.38	1.49	1.42
1	N	71	MET	CG-SD	5.37	1.95	1.81
4	Q	90	GLY	N-CA	5.37	1.54	1.46
2	O	202	SER	CA-CB	5.37	1.61	1.52
1	N	502	TYR	CE1-CZ	5.36	1.45	1.38
3	P	153	GLU	CD-OE1	-5.36	1.19	1.25
5	E	88	GLU	CG-CD	5.36	1.59	1.51
3	P	255	SER	C-O	5.36	1.33	1.23
2	B	65	TRP	CZ2-CH2	5.36	1.47	1.37
5	E	57	ARG	CZ-NH1	5.36	1.40	1.33
4	D	140	TYR	CB-CG	5.35	1.59	1.51
3	P	198	PHE	CE2-CZ	5.35	1.47	1.37
3	C	89	SER	CB-OG	5.34	1.49	1.42
12	L	5	GLU	CD-OE1	-5.34	1.19	1.25
13	M	26	PHE	CE1-CZ	5.34	1.47	1.37
4	Q	6	VAL	CA-CB	5.33	1.66	1.54
5	E	61	PHE	CG-CD1	5.33	1.46	1.38
2	O	145	PRO	C-O	5.33	1.33	1.23
4	D	60	TYR	CG-CD1	5.33	1.46	1.39
3	P	90	GLU	CD-OE2	5.33	1.31	1.25
3	C	221	ARG	CZ-NH2	5.32	1.40	1.33
3	C	181	TYR	CB-CG	5.32	1.59	1.51
6	S	3	GLY	N-CA	5.32	1.54	1.46
6	F	31	TYR	CE1-CZ	5.31	1.45	1.38
8	U	70	SER	CB-OG	-5.31	1.35	1.42
3	P	182	TYR	CE2-CZ	5.31	1.45	1.38
5	R	30	ARG	CZ-NH2	5.30	1.40	1.33
6	S	21[A]	MET	C-O	5.30	1.33	1.23
6	S	21[B]	MET	C-O	5.30	1.33	1.23
8	U	22	ASN	CG-OD1	5.30	1.35	1.24
11	X	53	TRP	CB-CG	5.30	1.59	1.50
1	A	103	TRP	CE3-CZ3	5.30	1.47	1.38
3	P	235	PHE	CD1-CE1	5.30	1.49	1.39
1	A	264	LYS	CD-CE	5.29	1.64	1.51
6	S	60	CYS	CB-SG	5.29	1.91	1.82
9	I	18	ARG	C-O	5.28	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	14	GLU	CD-OE1	5.28	1.31	1.25
1	N	81	TRP	CG-CD1	5.27	1.44	1.36
1	A	406	ASN	C-O	5.27	1.33	1.23
2	O	156	SER	CA-CB	5.26	1.60	1.52
7	T	5	LYS	CA-CB	5.26	1.65	1.53
1	N	266	GLU	CD-OE2	5.25	1.31	1.25
2	B	192	TYR	CD1-CE1	5.25	1.47	1.39
2	O	40	TYR	CG-CD1	5.25	1.46	1.39
2	O	65	TRP	CD2-CE2	5.25	1.47	1.41
7	T	4	ALA	C-O	-5.25	1.13	1.23
3	P	253	TYR	CD2-CE2	5.25	1.47	1.39
1	N	184	PHE	CG-CD1	5.24	1.46	1.38
4	D	111	PHE	CD1-CE1	5.24	1.49	1.39
3	P	16	TRP	CE3-CZ3	5.24	1.47	1.38
1	N	235	PHE	CG-CD2	5.23	1.46	1.38
4	Q	138	TRP	CE3-CZ3	5.23	1.47	1.38
1	A	5	ARG	CZ-NH1	5.23	1.39	1.33
3	C	94	PHE	CE1-CZ	5.23	1.47	1.37
12	Y	13	PHE	CG-CD1	5.22	1.46	1.38
1	A	71	MET	CG-SD	5.21	1.94	1.81
3	P	55	TYR	CE1-CZ	5.21	1.45	1.38
1	A	509	THR	C-O	5.21	1.33	1.23
5	E	87	GLN	N-CA	5.21	1.56	1.46
1	A	443	TYR	CB-CG	5.21	1.59	1.51
2	B	198	GLU	CD-OE2	-5.20	1.20	1.25
8	H	11	TYR	N-CA	5.20	1.56	1.46
1	A	278[A]	MET	SD-CE	-5.20	1.48	1.77
1	A	278[B]	MET	SD-CE	-5.20	1.48	1.77
5	E	82	TYR	CD1-CE1	5.20	1.47	1.39
4	D	87[A]	PHE	CG-CD1	5.20	1.46	1.38
4	D	87[B]	PHE	CG-CD1	5.20	1.46	1.38
8	U	40	GLU	CD-OE1	-5.19	1.20	1.25
4	Q	18	ASP	CB-CG	-5.18	1.40	1.51
1	A	343	GLY	N-CA	5.17	1.53	1.46
1	A	482	VAL	CA-CB	5.17	1.65	1.54
4	D	58	GLU	CD-OE2	5.17	1.31	1.25
3	P	3	HIS	C-O	5.17	1.33	1.23
7	T	22	GLY	N-CA	5.17	1.53	1.46
6	F	70	ILE	N-CA	5.16	1.56	1.46
1	N	92	MET	CG-SD	-5.16	1.67	1.81
1	N	387	PHE	CE1-CZ	5.16	1.47	1.37
11	X	53	TRP	CG-CD1	5.15	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	35	TYR	CG-CD1	5.15	1.45	1.39
1	N	396	TRP	CD2-CE2	5.14	1.47	1.41
3	P	113	GLY	N-CA	5.14	1.53	1.46
8	U	68	TRP	CZ3-CH2	5.14	1.48	1.40
2	B	147	GLU	CD-OE2	-5.14	1.20	1.25
6	S	43	LYS	CG-CD	5.14	1.70	1.52
2	B	220	GLU	CG-CD	5.13	1.59	1.51
1	N	513	LEU	C-O	5.13	1.33	1.23
9	I	47	TYR	CE1-CZ	5.13	1.45	1.38
2	B	38	VAL	CA-CB	5.12	1.65	1.54
4	Q	60	TYR	CE2-CZ	5.12	1.45	1.38
7	T	64	ASP	CG-OD1	5.12	1.37	1.25
7	T	44	ARG	CZ-NH2	5.12	1.39	1.33
1	A	403	TYR	CG-CD2	-5.12	1.32	1.39
4	D	40	LEU	C-O	5.11	1.33	1.23
1	N	485	VAL	CA-CB	5.11	1.65	1.54
4	D	11	TYR	CE1-CZ	-5.10	1.31	1.38
1	A	38	ARG	CZ-NH2	5.09	1.39	1.33
3	C	65	SER	CB-OG	5.09	1.48	1.42
9	I	19	PHE	CG-CD2	5.09	1.46	1.38
1	A	379	TYR	CZ-OH	5.08	1.46	1.37
3	P	260	GLY	N-CA	5.08	1.53	1.46
1	N	476	PHE	CG-CD2	5.08	1.46	1.38
3	P	244	PHE	CD1-CE1	5.08	1.49	1.39
2	B	202	SER	CB-OG	5.08	1.48	1.42
3	C	56	GLN	CB-CG	5.08	1.66	1.52
2	B	198	GLU	CD-OE1	-5.08	1.20	1.25
10	W	1	PHE	N-CA	5.08	1.56	1.46
4	Q	25	PRO	N-CA	5.07	1.55	1.47
1	N	90	PRO	N-CD	5.07	1.54	1.47
7	G	69	PHE	CG-CD2	5.07	1.46	1.38
8	H	75	ARG	NE-CZ	5.07	1.39	1.33
2	O	202	SER	CB-OG	-5.06	1.35	1.42
3	P	58	TRP	CZ3-CH2	5.06	1.48	1.40
4	Q	6	VAL	C-N	5.06	1.45	1.34
13	Z	14	GLU	CD-OE2	5.05	1.31	1.25
2	B	147	GLU	CD-OE1	-5.05	1.20	1.25
1	A	144	ASP	CB-CG	5.04	1.62	1.51
4	D	56	LYS	CE-NZ	5.04	1.61	1.49
1	N	261	TYR	CD1-CE1	5.04	1.47	1.39
2	O	65	TRP	CG-CD2	5.04	1.52	1.43
2	O	82	ARG	CZ-NH1	5.04	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	244	TYR	CE1-CZ	5.04	1.45	1.38
1	A	94	PHE	CG-CD2	5.04	1.46	1.38
3	P	189	SER	CB-OG	5.03	1.48	1.42
9	V	54	TYR	CG-CD2	5.03	1.45	1.39
1	A	502	TYR	CD1-CE1	5.03	1.46	1.39
1	N	223	ALA	N-CA	5.02	1.56	1.46
1	N	5	ARG	CZ-NH2	5.02	1.39	1.33
7	G	69	PHE	C-O	5.02	1.32	1.23
5	R	73	ASP	CG-OD2	-5.02	1.13	1.25
8	H	40	GLU	CG-CD	5.01	1.59	1.51
6	S	93	PRO	CA-C	5.01	1.62	1.52
6	F	3	GLY	N-CA	5.01	1.53	1.46
1	N	473	TRP	CE3-CZ3	5.01	1.47	1.38
8	H	53	CYS	C-O	5.00	1.32	1.23
3	P	227	PHE	CE1-CZ	5.00	1.46	1.37
4	Q	138	TRP	CD1-NE1	5.00	1.46	1.38
7	G	17	ARG	CZ-NH1	5.00	1.39	1.33
4	Q	6	VAL	CA-C	5.00	1.66	1.52

All (569) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	90	ARG	NE-CZ-NH1	35.49	138.05	120.30
4	Q	20	ARG	NE-CZ-NH1	32.93	136.77	120.30
4	Q	20	ARG	NE-CZ-NH2	-31.64	104.48	120.30
5	E	90	ARG	NE-CZ-NH2	-24.93	107.83	120.30
9	V	10	ARG	NE-CZ-NH2	-21.32	109.64	120.30
9	V	10	ARG	NE-CZ-NH1	21.08	130.84	120.30
11	K	47	ARG	NE-CZ-NH1	-19.70	110.45	120.30
2	B	151	ARG	NE-CZ-NH1	18.72	129.66	120.30
1	A	213	ARG	NE-CZ-NH2	-17.11	111.75	120.30
1	N	189	MET	CG-SD-CE	-16.98	73.03	100.20
1	A	38	ARG	NE-CZ-NH1	16.94	128.77	120.30
1	A	38	ARG	NE-CZ-NH2	-15.95	112.32	120.30
2	B	151	ARG	NE-CZ-NH2	-14.92	112.84	120.30
11	K	54	ARG	NE-CZ-NH1	-14.87	112.87	120.30
11	K	47	ARG	NE-CZ-NH2	14.80	127.70	120.30
3	C	181	TYR	CB-CG-CD2	-14.70	112.18	121.00
11	X	54	ARG	NE-CZ-NH1	-14.52	113.04	120.30
1	A	189	MET	CG-SD-CE	-14.16	77.54	100.20
3	P	153	GLU	OE1-CD-OE2	14.02	140.12	123.30
4	D	20	ARG	NE-CZ-NH1	-13.88	113.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	82	ARG	NE-CZ-NH2	-13.82	113.39	120.30
7	G	64	ASP	CB-CG-OD2	-13.77	105.91	118.30
5	E	56	ARG	NE-CZ-NH1	13.70	127.15	120.30
2	B	134	ARG	NE-CZ-NH2	-13.46	113.57	120.30
1	A	8	PHE	CB-CG-CD2	-13.38	111.43	120.80
1	A	129	TYR	CB-CG-CD1	-13.09	113.15	121.00
3	C	63	ARG	NE-CZ-NH2	-12.99	113.81	120.30
2	O	82	ARG	NE-CZ-NH2	-12.95	113.83	120.30
12	L	20	ARG	NE-CZ-NH2	-12.94	113.83	120.30
5	E	66	ARG	NE-CZ-NH2	-12.77	113.91	120.30
1	N	144	ASP	CB-CG-OD1	-12.54	107.02	118.30
5	E	56	ARG	NE-CZ-NH2	-12.19	114.20	120.30
1	N	71	MET	CG-SD-CE	-11.76	81.38	100.20
3	P	156	ARG	NE-CZ-NH1	11.57	126.08	120.30
2	B	115	ASP	CB-CG-OD1	11.25	128.43	118.30
4	Q	122	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	N	440	TYR	CB-CG-CD1	-11.11	114.33	121.00
7	G	56	ARG	NE-CZ-NH2	11.09	125.84	120.30
1	A	14	ASP	CB-CG-OD1	-11.01	108.39	118.30
1	N	302[A]	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	N	302[B]	ARG	NE-CZ-NH1	10.84	125.72	120.30
5	E	70	VAL	CA-CB-CG1	-10.57	95.04	110.90
5	E	84	TYR	CZ-CE2-CD2	-10.52	110.33	119.80
11	K	47	ARG	CG-CD-NE	10.50	133.85	111.80
1	A	8	PHE	CB-CG-CD1	10.47	128.13	120.80
10	J	28	ASP	CB-CG-OD2	-10.40	108.94	118.30
9	V	8	GLN	CB-CA-C	10.31	131.02	110.40
9	V	8	GLN	CB-CG-CD	-10.28	84.88	111.60
1	A	400	PHE	CB-CG-CD2	-10.23	113.64	120.80
1	N	372	TYR	CB-CG-CD1	-10.15	114.91	121.00
5	E	73	ASP	CB-CG-OD2	-10.12	109.19	118.30
1	N	486	ASP	CB-CG-OD1	10.11	127.40	118.30
3	P	253	TYR	CB-CG-CD2	-10.09	114.94	121.00
5	E	90	ARG	CD-NE-CZ	10.05	137.68	123.60
5	E	61	PHE	CB-CG-CD1	-9.99	113.81	120.80
1	N	8	PHE	CB-CG-CD2	-9.95	113.84	120.80
6	S	43	LYS	CB-CG-CD	9.91	137.38	111.60
9	I	10	ARG	NE-CZ-NH1	9.84	125.22	120.30
3	C	181	TYR	CZ-CE2-CD2	-9.79	110.99	119.80
11	X	54	ARG	NE-CZ-NH2	9.66	125.13	120.30
1	A	71	MET	CG-SD-CE	-9.62	84.82	100.20
10	W	28	ASP	CB-CG-OD2	-9.61	109.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	366	VAL	CG1-CB-CG2	-9.52	95.66	110.90
9	I	10	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	N	400	PHE	CB-CG-CD2	-9.46	114.17	120.80
4	D	58	GLU	OE1-CD-OE2	9.35	134.52	123.30
5	E	49	ASP	CB-CG-OD2	9.33	126.69	118.30
3	C	181	TYR	CD1-CE1-CZ	-9.22	111.50	119.80
1	N	251	PHE	CB-CG-CD1	-9.21	114.35	120.80
1	A	372	TYR	CB-CG-CD1	-9.20	115.48	121.00
3	C	181	TYR	CE1-CZ-CE2	9.15	134.45	119.80
5	R	90	ARG	NE-CZ-NH1	-9.09	115.76	120.30
1	A	442	ASP	CB-CG-OD1	-9.06	110.15	118.30
1	A	442	ASP	CB-CG-OD2	9.05	126.44	118.30
4	D	58	GLU	CG-CD-OE2	-9.00	100.31	118.30
1	A	387	PHE	CB-CG-CD1	-8.97	114.52	120.80
2	O	134	ARG	NE-CZ-NH2	-8.90	115.85	120.30
5	E	84	TYR	CG-CD1-CE1	-8.89	114.19	121.30
2	O	33	LEU	CB-CG-CD1	8.87	126.07	111.00
1	N	270	TYR	CB-CG-CD2	-8.81	115.71	121.00
2	O	21	LEU	CB-CG-CD1	-8.78	96.08	111.00
5	E	53	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	N	414	PHE	CB-CG-CD1	-8.72	114.70	120.80
11	X	47	ARG	NE-CZ-NH1	8.71	124.65	120.30
3	C	63	ARG	NE-CZ-NH1	8.69	124.65	120.30
3	C	244	PHE	CD1-CE1-CZ	-8.68	109.69	120.10
1	A	439	ARG	NE-CZ-NH1	8.67	124.64	120.30
3	P	233	PHE	CB-CG-CD2	-8.66	114.74	120.80
7	T	60	PHE	CB-CG-CD2	-8.60	114.78	120.80
2	B	3	TYR	CB-CG-CD2	-8.57	115.86	121.00
9	V	68	ILE	CB-CG1-CD1	-8.57	89.91	113.90
5	E	14	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	302[A]	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	302[B]	ARG	NE-CZ-NH1	8.52	124.56	120.30
3	C	233	PHE	CB-CG-CD2	-8.50	114.85	120.80
5	R	8	ASP	CB-CG-OD2	-8.50	110.65	118.30
7	T	60	PHE	CB-CG-CD1	8.48	126.74	120.80
4	Q	61	ARG	NE-CZ-NH1	8.47	124.53	120.30
3	P	155	ASP	CB-CG-OD1	8.41	125.87	118.30
2	B	206	PHE	CB-CG-CD1	-8.33	114.97	120.80
3	C	172	TYR	CG-CD2-CE2	8.32	127.96	121.30
7	G	5	LYS	CB-CA-C	8.30	127.00	110.40
4	D	19[A]	ARG	CG-CD-NE	8.28	129.18	111.80
4	D	19[B]	ARG	CG-CD-NE	8.28	129.18	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	156	ARG	NE-CZ-NH2	-8.22	116.19	120.30
5	R	30	ARG	NE-CZ-NH1	8.18	124.39	120.30
3	P	214	PHE	CB-CG-CD2	-8.17	115.08	120.80
1	A	366	VAL	CG1-CB-CG2	-8.10	97.94	110.90
5	R	30	ARG	NE-CZ-NH2	-8.08	116.26	120.30
2	B	75	LEU	CB-CG-CD2	-8.08	97.27	111.00
1	A	450	TRP	CB-CG-CD1	-8.04	116.54	127.00
1	N	363	LEU	CB-CG-CD2	8.00	124.61	111.00
1	A	440	TYR	CB-CG-CD1	-7.96	116.22	121.00
3	C	153	GLU	OE1-CD-OE2	7.96	132.85	123.30
1	N	430	PHE	CB-CG-CD2	-7.95	115.23	120.80
2	B	134	ARG	NE-CZ-NH1	7.95	124.27	120.30
2	B	141	ARG	NE-CZ-NH2	-7.93	116.34	120.30
3	P	33[A]	MET	CG-SD-CE	7.91	112.86	100.20
3	P	33[B]	MET	CG-SD-CE	7.91	112.86	100.20
2	B	105	TYR	CD1-CE1-CZ	-7.88	112.71	119.80
1	A	7	LEU	CB-CG-CD1	7.84	124.32	111.00
1	A	470	PHE	CB-CG-CD2	-7.76	115.37	120.80
3	P	197	PHE	CB-CG-CD1	-7.71	115.40	120.80
6	F	1	ALA	C-N-CA	7.68	140.91	121.70
3	C	186	PHE	CG-CD1-CE1	-7.66	112.38	120.80
2	O	151	ARG	NE-CZ-NH2	-7.66	116.47	120.30
7	G	56	ARG	NH1-CZ-NH2	-7.64	111.00	119.40
12	L	20	ARG	NE-CZ-NH1	7.63	124.11	120.30
3	P	63	ARG	NE-CZ-NH1	7.63	124.11	120.30
3	C	244	PHE	CB-CG-CD1	-7.62	115.47	120.80
3	C	67	PHE	CB-CG-CD1	-7.60	115.48	120.80
12	Y	20	ARG	NE-CZ-NH1	7.59	124.09	120.30
7	G	60	PHE	CB-CG-CD2	-7.58	115.50	120.80
1	N	439	ARG	NE-CZ-NH1	7.53	124.06	120.30
5	E	57	ARG	NE-CZ-NH1	-7.52	116.54	120.30
2	O	11	ASP	CB-CG-OD2	7.51	125.06	118.30
5	E	100	THR	CA-CB-CG2	-7.51	101.89	112.40
1	N	231	TYR	CB-CG-CD1	-7.42	116.55	121.00
4	Q	127	LYS	CD-CE-NZ	7.42	128.78	111.70
3	P	90	GLU	OE1-CD-OE2	7.41	132.19	123.30
3	P	244	PHE	CD1-CE1-CZ	-7.40	111.22	120.10
1	N	129	TYR	CB-CG-CD1	-7.40	116.56	121.00
4	D	111	PHE	CB-CG-CD1	-7.39	115.62	120.80
5	E	66	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	N	442	ASP	CB-CG-OD2	7.38	124.94	118.30
1	N	129	TYR	CG-CD2-CE2	-7.36	115.41	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	8	PHE	CB-CG-CD1	7.33	125.93	120.80
1	N	486	ASP	CB-CG-OD2	-7.32	111.71	118.30
7	G	19	LEU	CB-CG-CD1	-7.24	98.69	111.00
4	D	20	ARG	NE-CZ-NH2	7.23	123.92	120.30
9	I	54	TYR	CB-CG-CD1	-7.22	116.67	121.00
2	O	173	ASP	CB-CG-OD1	7.22	124.80	118.30
1	N	212	ASP	CB-CG-OD2	7.21	124.79	118.30
4	Q	19[A]	ARG	NE-CZ-NH2	-7.21	116.70	120.30
4	Q	19[B]	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	A	270	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	A	35	LEU	CB-CG-CD2	7.19	123.23	111.00
3	P	219	PHE	CB-CG-CD2	-7.17	115.78	120.80
9	I	43	ARG	NE-CZ-NH1	7.14	123.87	120.30
3	P	8	TYR	CZ-CE2-CD2	-7.14	113.37	119.80
4	D	122	ARG	NE-CZ-NH2	-7.13	116.74	120.30
11	K	51	LYS	CD-CE-NZ	-7.12	95.32	111.70
10	J	4	ARG	NE-CZ-NH1	7.10	123.85	120.30
5	E	82	TYR	CB-CG-CD2	-7.09	116.75	121.00
3	P	181	TYR	CB-CG-CD2	-7.06	116.77	121.00
5	R	23	ASP	CB-CG-OD2	7.05	124.65	118.30
1	N	513	LEU	C-N-CA	-7.05	104.08	121.70
4	Q	8	SER	N-CA-C	7.04	130.02	111.00
3	P	198	PHE	CB-CG-CD2	-7.03	115.88	120.80
2	O	206	PHE	CB-CG-CD1	-7.00	115.90	120.80
2	O	147	GLU	OE1-CD-OE2	-6.99	114.91	123.30
1	A	251	PHE	CB-CG-CD1	-6.99	115.91	120.80
9	I	61	GLU	OE1-CD-OE2	-6.99	114.92	123.30
3	P	102	TYR	CB-CG-CD2	-6.97	116.82	121.00
4	Q	19[A]	ARG	CB-CG-CD	6.97	129.73	111.60
4	Q	19[B]	ARG	CB-CG-CD	6.97	129.73	111.60
7	G	50	TYR	CG-CD2-CE2	-6.96	115.73	121.30
4	Q	6	VAL	CB-CA-C	6.96	124.62	111.40
3	C	233	PHE	CD1-CG-CD2	6.96	127.34	118.30
6	S	25	ARG	NE-CZ-NH1	6.96	123.78	120.30
13	M	38	ASP	CB-CG-OD2	-6.94	112.05	118.30
2	O	134	ARG	NE-CZ-NH1	6.91	123.76	120.30
5	E	103	GLU	OE1-CD-OE2	-6.89	115.03	123.30
1	N	213	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	N	63	PHE	CB-CG-CD2	-6.88	115.98	120.80
1	A	270	TYR	CD1-CE1-CZ	-6.86	113.63	119.80
2	O	108	TYR	CZ-CE2-CD2	-6.85	113.63	119.80
1	A	377	PHE	CB-CG-CD2	-6.85	116.01	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	253	TYR	CZ-CE2-CD2	-6.85	113.64	119.80
5	R	69	GLU	OE1-CD-OE2	6.84	131.51	123.30
4	D	4	SER	N-CA-C	6.83	129.44	111.00
5	E	103	GLU	O-C-N	6.83	133.62	122.70
3	C	146	TRP	CD1-CG-CD2	-6.81	100.85	106.30
1	A	5	ARG	NE-CZ-NH1	-6.79	116.91	120.30
8	H	63	LEU	CB-CG-CD1	-6.78	99.48	111.00
3	P	214	PHE	CB-CG-CD1	6.77	125.54	120.80
6	F	1	ALA	O-C-N	6.76	133.52	122.70
2	O	65	TRP	CB-CA-C	6.76	123.93	110.40
2	B	133	LEU	CB-CG-CD1	-6.74	99.54	111.00
1	A	109	PHE	CB-CG-CD1	-6.74	116.08	120.80
3	P	97	PHE	CB-CG-CD2	-6.74	116.08	120.80
6	S	25	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	A	484	THR	CA-CB-CG2	-6.72	102.99	112.40
3	C	94	PHE	CB-CG-CD2	-6.71	116.10	120.80
5	R	60	ASP	CB-CG-OD2	6.68	124.31	118.30
5	E	90	ARG	CB-CG-CD	6.68	128.96	111.60
7	G	18	PHE	CB-CG-CD1	-6.67	116.13	120.80
3	C	101	PHE	CG-CD1-CE1	-6.67	113.46	120.80
4	D	34	SER	O-C-N	-6.67	112.03	122.70
8	H	52	VAL	CB-CA-C	-6.67	98.73	111.40
1	N	7	LEU	CB-CG-CD1	6.65	122.31	111.00
6	F	96	LEU	CA-CB-CG	6.64	130.58	115.30
7	T	7	ASP	N-CA-C	6.64	128.92	111.00
1	N	74	MET	CA-CB-CG	-6.63	102.02	113.30
9	I	15	ARG	NE-CZ-NH2	-6.63	116.99	120.30
4	D	112	GLU	OE1-CD-OE2	-6.62	115.35	123.30
7	T	44	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	N	296	GLY	O-C-N	-6.59	112.16	122.70
3	P	241	TYR	CB-CG-CD1	-6.59	117.05	121.00
1	A	129	TYR	CD1-CG-CD2	6.57	125.13	117.90
9	I	50	PHE	CB-CG-CD1	-6.57	116.20	120.80
1	N	505	PHE	CB-CG-CD2	-6.56	116.21	120.80
1	N	438	ARG	NE-CZ-NH2	-6.53	117.03	120.30
5	E	8	ASP	CB-CG-OD2	-6.53	112.42	118.30
2	O	151	ARG	NE-CZ-NH1	6.53	123.57	120.30
4	Q	124	LEU	CB-CG-CD2	6.52	122.09	111.00
1	A	63	PHE	CB-CG-CD2	-6.52	116.24	120.80
1	A	240	HIS	CA-CB-CG	-6.51	102.53	113.60
5	E	60	ASP	CB-CG-OD1	-6.50	112.45	118.30
6	S	92	VAL	C-N-CD	6.48	142.01	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	346	PHE	CB-CG-CD2	-6.48	116.27	120.80
3	C	90	GLU	OE1-CD-OE2	6.47	131.07	123.30
1	A	50	ASP	CB-CG-OD2	6.46	124.12	118.30
9	I	4	LEU	CB-CG-CD1	-6.46	100.02	111.00
4	Q	16	TYR	CB-CG-CD1	-6.45	117.13	121.00
4	D	74	SER	CA-CB-OG	-6.45	93.80	111.20
13	M	35	TYR	CG-CD2-CE2	-6.44	116.15	121.30
3	C	146	TRP	CD1-NE1-CE2	-6.43	103.21	109.00
4	D	61	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	480	ARG	NE-CZ-NH1	6.43	123.52	120.30
3	C	52	LEU	CB-CG-CD1	-6.43	100.07	111.00
1	N	38	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	N	144	ASP	OD1-CG-OD2	6.41	135.47	123.30
1	N	393	PHE	CB-CG-CD2	-6.39	116.33	120.80
4	Q	51	LEU	CB-CG-CD1	6.38	121.84	111.00
11	X	47	ARG	CD-NE-CZ	6.37	132.51	123.60
1	N	136[A]	LEU	CB-CG-CD2	-6.36	100.19	111.00
1	N	136[B]	LEU	CB-CG-CD2	-6.36	100.19	111.00
2	O	132	GLU	CG-CD-OE1	-6.35	105.61	118.30
3	P	233	PHE	CZ-CE2-CD2	-6.34	112.49	120.10
1	A	344	PHE	CB-CG-CD2	-6.34	116.36	120.80
4	D	99	GLU	OE1-CD-OE2	-6.34	115.69	123.30
7	T	20	THR	CA-CB-CG2	-6.33	103.54	112.40
5	E	84	TYR	CB-CG-CD1	-6.30	117.22	121.00
1	N	364	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	N	35	LEU	CB-CG-CD1	-6.29	100.31	111.00
2	O	132	GLU	CG-CD-OE2	6.29	130.88	118.30
8	H	61	LYS	CD-CE-NZ	6.28	126.15	111.70
8	H	17	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	285	PHE	CB-CG-CD2	-6.26	116.42	120.80
12	Y	37	PHE	CB-CG-CD2	-6.25	116.43	120.80
5	E	49	ASP	OD1-CG-OD2	-6.25	111.43	123.30
2	B	158	ASP	CB-CG-OD2	-6.24	112.69	118.30
6	S	96	LEU	CB-CG-CD2	6.24	121.60	111.00
9	I	47	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	N	235	PHE	CB-CG-CD2	-6.23	116.44	120.80
4	D	91	PHE	CB-CG-CD2	-6.22	116.45	120.80
1	A	251	PHE	CB-CG-CD2	6.21	125.15	120.80
8	U	75	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	67	PHE	CB-CG-CD1	-6.19	116.47	120.80
1	N	260	TYR	CB-CG-CD2	-6.17	117.30	121.00
12	L	29	PHE	CB-CG-CD2	6.16	125.11	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	148	PHE	CB-CG-CD2	-6.16	116.49	120.80
6	S	1	ALA	C-N-CA	6.15	137.07	121.70
1	N	387	PHE	CB-CG-CD1	-6.13	116.51	120.80
1	A	213	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	372	TYR	CG-CD1-CE1	-6.12	116.41	121.30
1	N	213	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	N	113[A]	LEU	CB-CG-CD1	6.12	121.40	111.00
1	N	113[B]	LEU	CB-CG-CD1	6.12	121.40	111.00
13	M	10	THR	CA-CB-CG2	-6.11	103.84	112.40
3	C	214	PHE	CB-CG-CD1	6.09	125.07	120.80
6	S	94	HIS	N-CA-C	6.09	127.45	111.00
3	P	63	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	N	240	HIS	CA-CB-CG	-6.07	103.28	113.60
2	O	112	ASP	CB-CG-OD1	6.06	123.75	118.30
10	J	38	LEU	CB-CG-CD1	-6.05	100.71	111.00
6	S	96	LEU	CB-CG-CD1	-6.04	100.73	111.00
3	C	181	TYR	CD1-CG-CD2	6.04	124.54	117.90
5	E	82	TYR	CD1-CE1-CZ	-6.03	114.38	119.80
1	N	476	PHE	CB-CG-CD1	-6.03	116.58	120.80
3	C	233	PHE	CB-CG-CD1	-6.02	116.58	120.80
4	Q	18	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	2	PHE	CB-CG-CD1	-6.01	116.59	120.80
5	E	70	VAL	CB-CA-C	6.00	122.80	111.40
7	G	3	ALA	N-CA-C	6.00	127.19	111.00
5	R	36	LEU	CB-CG-CD2	-6.00	100.81	111.00
3	C	59	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	N	253	MET	CA-CB-CG	-5.98	103.13	113.30
3	C	102	TYR	CB-CG-CD2	-5.98	117.41	121.00
12	L	45	LEU	CB-CG-CD1	-5.97	100.85	111.00
1	A	513	LEU	C-N-CA	-5.96	106.79	121.70
4	Q	20	ARG	CD-NE-CZ	5.96	131.94	123.60
1	A	152	LEU	CB-CG-CD2	5.94	121.10	111.00
12	L	46	LYS	CB-CG-CD	-5.94	96.17	111.60
2	B	65	TRP	CB-CA-C	5.93	122.25	110.40
6	F	3	GLY	C-N-CA	5.93	134.74	122.30
1	A	327	LEU	CB-CG-CD1	-5.91	100.95	111.00
2	B	45	MET	CG-SD-CE	5.91	109.66	100.20
2	B	184	LEU	N-CA-CB	-5.90	98.60	110.40
6	S	1	ALA	O-C-N	5.89	132.13	122.70
3	C	197	PHE	CB-CG-CD1	-5.88	116.68	120.80
1	A	450	TRP	CG-CD1-NE1	-5.88	104.22	110.10
5	E	70	VAL	CA-CB-CG2	-5.87	102.09	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	18	TYR	CB-CG-CD1	-5.87	117.48	121.00
4	D	21	ASP	CB-CG-OD2	5.87	123.58	118.30
1	N	251	PHE	CB-CG-CD2	5.86	124.91	120.80
5	E	61	PHE	CB-CG-CD2	5.86	124.90	120.80
1	A	372	TYR	CD1-CG-CD2	5.85	124.34	117.90
3	P	8	TYR	CB-CG-CD2	-5.85	117.49	121.00
11	K	47	ARG	CB-CG-CD	5.84	126.78	111.60
5	R	52	LEU	CB-CG-CD2	5.83	120.92	111.00
3	P	233	PHE	CD1-CG-CD2	5.82	125.86	118.30
4	Q	63	LYS	CD-CE-NZ	-5.82	98.32	111.70
1	A	486[A]	ASP	CB-CG-OD1	-5.82	113.07	118.30
1	A	486[B]	ASP	CB-CG-OD1	-5.82	113.07	118.30
12	L	29	PHE	CG-CD2-CE2	5.82	127.20	120.80
7	G	19	LEU	CA-CB-CG	-5.81	101.93	115.30
4	D	31[A]	LYS	C-N-CA	-5.81	107.17	121.70
4	D	31[B]	LYS	C-N-CA	-5.81	107.17	121.70
9	V	10	ARG	CG-CD-NE	-5.81	99.60	111.80
1	A	270	TYR	CG-CD2-CE2	-5.81	116.65	121.30
3	C	214	PHE	CB-CG-CD2	-5.81	116.73	120.80
1	A	112	LEU	CD1-CG-CD2	-5.79	93.12	110.50
2	O	158	ASP	CB-CG-OD1	5.79	123.51	118.30
3	P	80[A]	ARG	CD-NE-CZ	-5.78	115.50	123.60
3	P	80[B]	ARG	CD-NE-CZ	-5.78	115.50	123.60
12	L	9	LYS	CD-CE-NZ	-5.78	98.42	111.70
5	E	19	PHE	CB-CG-CD2	-5.77	116.76	120.80
12	L	37	PHE	CB-CG-CD1	-5.76	116.76	120.80
1	N	152	LEU	CD1-CG-CD2	5.76	127.79	110.50
2	B	82	ARG	NH1-CZ-NH2	5.75	125.73	119.40
3	C	172	TYR	CG-CD1-CE1	-5.75	116.70	121.30
6	S	22	LEU	CB-CG-CD1	5.75	120.78	111.00
1	A	136[A]	LEU	CB-CG-CD2	-5.75	101.22	111.00
1	A	136[B]	LEU	CB-CG-CD2	-5.75	101.22	111.00
2	B	32[A]	PHE	O-C-N	5.75	131.90	122.70
2	B	32[B]	PHE	O-C-N	5.75	131.90	122.70
1	N	397	PHE	CB-CG-CD2	-5.74	116.78	120.80
1	A	407	ASP	CB-CG-OD2	5.74	123.46	118.30
1	N	237	PHE	CB-CG-CD2	-5.74	116.79	120.80
3	C	93	PHE	CG-CD1-CE1	5.73	127.10	120.80
1	N	109	PHE	CB-CG-CD2	5.73	124.81	120.80
6	F	3	GLY	N-CA-C	-5.72	98.80	113.10
3	C	16	TRP	NE1-CE2-CD2	5.71	113.00	107.30
1	A	304	TYR	CB-CG-CD2	-5.69	117.58	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	233	PHE	CG-CD1-CE1	-5.69	114.54	120.80
13	M	26	PHE	CB-CG-CD2	-5.68	116.82	120.80
7	T	18	PHE	CB-CG-CD1	-5.68	116.82	120.80
8	H	75	ARG	NE-CZ-NH2	-5.68	117.46	120.30
9	I	16	ARG	NE-CZ-NH2	-5.68	117.46	120.30
4	D	74	SER	N-CA-CB	-5.67	101.99	110.50
12	L	26	THR	CA-CB-OG1	-5.67	97.09	109.00
3	P	57	TRP	CD1-CG-CD2	5.67	110.84	106.30
5	E	19	PHE	CD1-CE1-CZ	-5.66	113.30	120.10
8	H	9	LYS	CD-CE-NZ	5.66	124.73	111.70
7	G	18	PHE	CB-CG-CD2	5.66	124.76	120.80
5	E	90	ARG	NH1-CZ-NH2	-5.66	113.17	119.40
3	C	146	TRP	CG-CD1-NE1	5.66	115.76	110.10
2	B	112	ASP	CB-CG-OD2	5.65	123.39	118.30
4	D	91	PHE	CG-CD2-CE2	-5.65	114.59	120.80
11	K	54	ARG	CA-C-O	5.65	131.96	120.10
13	M	3	ALA	O-C-N	5.65	131.74	122.70
1	A	403	TYR	CZ-CE2-CD2	-5.65	114.72	119.80
8	H	25	GLN	CA-C-O	5.64	131.95	120.10
1	A	449	MET	CA-CB-CG	-5.64	103.72	113.30
3	P	253	TYR	CD1-CE1-CZ	-5.64	114.73	119.80
6	S	3	GLY	N-CA-C	-5.61	99.08	113.10
1	A	237	PHE	CD1-CG-CD2	5.59	125.57	118.30
4	Q	86	MET	CG-SD-CE	-5.59	91.26	100.20
5	E	61	PHE	CG-CD1-CE1	-5.58	114.66	120.80
9	V	68	ILE	CA-CB-CG2	5.58	122.06	110.90
4	D	122	ARG	NE-CZ-NH1	5.57	123.09	120.30
2	O	108	TYR	CG-CD1-CE1	-5.57	116.84	121.30
1	N	96	ARG	NE-CZ-NH1	5.57	123.09	120.30
4	D	64	PHE	CB-CG-CD1	-5.57	116.90	120.80
8	H	35	ASP	CB-CG-OD1	-5.57	113.29	118.30
4	D	39	ALA	O-C-N	5.56	131.60	122.70
1	N	78	PHE	CB-CG-CD2	-5.56	116.91	120.80
3	P	253	TYR	CD1-CG-CD2	5.56	124.02	117.90
1	A	113[A]	LEU	O-C-N	-5.56	113.80	122.70
1	A	113[B]	LEU	O-C-N	-5.56	113.80	122.70
3	C	146	TRP	CG-CD2-CE3	-5.56	128.90	133.90
3	P	236	GLU	CA-CB-CG	-5.56	101.17	113.40
3	C	16	TRP	CD1-NE1-CE2	-5.56	104.00	109.00
5	E	30	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	148	PHE	CB-CG-CD2	-5.54	116.92	120.80
9	I	47	TYR	CB-CG-CD1	5.54	124.32	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	S	92	VAL	CB-CA-C	5.54	121.92	111.40
1	A	310	MET	CA-CB-CG	-5.54	103.89	113.30
1	N	456	MET	CA-CB-CG	-5.52	103.91	113.30
5	R	106	LEU	CB-CG-CD2	-5.51	101.63	111.00
1	A	348	PHE	CB-CG-CD2	-5.50	116.95	120.80
7	G	56	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	212	ASP	CB-CG-OD2	5.50	123.25	118.30
4	D	16	TYR	CB-CG-CD2	-5.50	117.70	121.00
4	D	55	GLU	OE1-CD-OE2	-5.49	116.72	123.30
8	H	35	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	110	LEU	CB-CG-CD2	-5.48	101.68	111.00
1	N	379	TYR	CB-CG-CD2	-5.48	117.71	121.00
2	O	139	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	390	MET	CG-SD-CE	5.47	108.95	100.20
2	B	59	GLN	N-CA-CB	5.47	120.44	110.60
2	O	116	LEU	CB-CG-CD2	-5.46	101.72	111.00
7	T	8	HIS	N-CA-C	5.46	125.74	111.00
8	U	38	ARG	NE-CZ-NH2	-5.46	117.57	120.30
7	G	44	ARG	CB-CG-CD	-5.46	97.42	111.60
1	N	98	ASN	N-CA-CB	-5.45	100.78	110.60
1	A	296	GLY	O-C-N	-5.45	113.98	122.70
9	V	29	LEU	CB-CG-CD1	5.45	120.26	111.00
5	R	84	TYR	CG-CD1-CE1	-5.44	116.95	121.30
1	N	310	MET	CG-SD-CE	-5.44	91.50	100.20
1	N	159	LEU	CB-CG-CD1	-5.43	101.76	111.00
7	T	5	LYS	CB-CA-C	5.42	121.23	110.40
3	C	95	THR	OG1-CB-CG2	-5.42	97.54	110.00
4	Q	6	VAL	CA-CB-CG1	5.42	119.03	110.90
1	A	159	LEU	CB-CG-CD1	-5.42	101.79	111.00
1	N	430	PHE	CD1-CG-CD2	5.41	125.33	118.30
12	L	20	ARG	CG-CD-NE	-5.40	100.47	111.80
1	N	212	ASP	CB-CG-OD1	-5.40	113.44	118.30
1	N	96	ARG	N-CA-CB	-5.39	100.89	110.60
4	D	16	TYR	CG-CD2-CE2	-5.38	117.00	121.30
4	D	86	MET	CA-CB-CG	-5.38	104.16	113.30
7	G	16	TRP	O-C-N	5.38	131.30	122.70
9	I	45	LYS	CD-CE-NZ	-5.37	99.36	111.70
1	N	102	PHE	CB-CG-CD1	-5.36	117.05	120.80
1	A	445	ASP	CB-CG-OD1	-5.35	113.48	118.30
3	C	233	PHE	CG-CD2-CE2	-5.35	114.92	120.80
1	N	221	ASP	CB-CG-OD2	-5.35	113.48	118.30
11	X	47	ARG	NH1-CZ-NH2	-5.34	113.52	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	103	TRP	CD1-CG-CD2	5.34	110.57	106.30
4	Q	125	ASP	CB-CG-OD1	-5.34	113.49	118.30
3	C	233	PHE	CG-CD1-CE1	-5.33	114.94	120.80
5	E	8	ASP	CB-CG-OD1	5.32	123.09	118.30
7	G	16	TRP	CD1-CG-CD2	5.32	110.56	106.30
1	A	237	PHE	CB-CG-CD1	-5.32	117.08	120.80
1	N	253	MET	CG-SD-CE	-5.31	91.70	100.20
12	Y	21	LEU	CB-CG-CD2	-5.31	101.97	111.00
3	P	51[A]	MET	CA-CB-CG	-5.31	104.27	113.30
3	P	51[B]	MET	CA-CB-CG	-5.31	104.27	113.30
4	D	18	ASP	CB-CG-OD1	5.30	123.07	118.30
6	S	81	ARG	NE-CZ-NH2	-5.30	117.65	120.30
5	E	107	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	372	TYR	CZ-CE2-CD2	-5.28	115.04	119.80
3	P	244	PHE	CG-CD2-CE2	-5.28	114.99	120.80
1	A	237	PHE	CB-CG-CD2	-5.27	117.11	120.80
1	N	172	LYS	CD-CE-NZ	-5.27	99.57	111.70
1	N	210	LEU	CB-CG-CD2	-5.27	102.04	111.00
1	N	288	TRP	CD1-NE1-CE2	-5.27	104.25	109.00
1	A	363	LEU	CB-CG-CD1	5.27	119.96	111.00
2	B	139	ASP	CB-CG-OD2	5.26	123.04	118.30
4	D	31[A]	LYS	CD-CE-NZ	-5.26	99.59	111.70
4	D	31[B]	LYS	CD-CE-NZ	-5.26	99.59	111.70
6	S	64	GLU	CA-C-N	-5.26	105.62	117.20
8	U	76	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	473	TRP	CD1-CG-CD2	5.26	110.51	106.30
2	B	32[A]	PHE	CB-CG-CD1	-5.26	117.12	120.80
2	B	32[B]	PHE	CB-CG-CD1	-5.26	117.12	120.80
7	G	17	ARG	NE-CZ-NH1	5.26	122.93	120.30
4	D	31[A]	LYS	CA-CB-CG	5.26	124.96	113.40
4	D	31[B]	LYS	CA-CB-CG	5.26	124.96	113.40
3	P	28	THR	CA-CB-CG2	-5.25	105.05	112.40
9	V	10	ARG	CD-NE-CZ	5.25	130.95	123.60
3	C	76	GLN	CB-CG-CD	5.25	125.25	111.60
1	N	495	LEU	CB-CG-CD1	5.25	119.92	111.00
3	P	16	TRP	CG-CD1-NE1	-5.24	104.86	110.10
2	B	86	MET	CG-SD-CE	5.24	108.58	100.20
3	P	227	PHE	CB-CG-CD1	-5.24	117.13	120.80
2	B	65	TRP	CA-CB-CG	5.24	123.65	113.70
2	B	91	ASN	N-CA-C	5.24	125.14	111.00
1	A	445	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	502	TYR	CB-CG-CD2	-5.23	117.86	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	63	SER	O-C-N	5.23	131.07	122.70
5	R	44	GLU	OE1-CD-OE2	-5.23	117.02	123.30
1	A	129	TYR	CG-CD2-CE2	-5.23	117.12	121.30
1	N	54	TYR	CG-CD2-CE2	-5.23	117.12	121.30
2	O	184	LEU	N-CA-CB	-5.23	99.95	110.40
1	N	514	LYS	CA-C-O	-5.22	109.14	120.10
1	N	447	TYR	CB-CG-CD1	5.22	124.13	121.00
3	C	197	PHE	CG-CD1-CE1	-5.20	115.08	120.80
3	P	253	TYR	CE1-CZ-CE2	5.20	128.12	119.80
3	C	80[A]	ARG	NE-CZ-NH1	-5.19	117.70	120.30
3	C	80[B]	ARG	NE-CZ-NH1	-5.19	117.70	120.30
3	C	215	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	A	244	TYR	CB-CG-CD2	-5.18	117.89	121.00
4	D	16	TYR	CE1-CZ-CE2	5.17	128.08	119.80
1	N	156	SER	N-CA-CB	-5.17	102.74	110.50
1	A	366	VAL	CA-CB-CG2	-5.17	103.14	110.90
2	B	141	ARG	NE-CZ-NH1	5.16	122.88	120.30
3	P	182	TYR	CZ-CE2-CD2	5.16	124.45	119.80
5	R	23	ASP	CB-CG-OD1	-5.16	113.66	118.30
3	C	8	TYR	CZ-CE2-CD2	-5.15	115.16	119.80
3	C	41	THR	CA-CB-CG2	-5.14	105.20	112.40
6	F	94	HIS	C-N-CA	5.14	134.56	121.70
1	N	270	TYR	CD1-CE1-CZ	-5.14	115.17	119.80
3	C	244	PHE	CE1-CZ-CE2	5.14	129.25	120.00
5	E	73	ASP	OD1-CG-OD2	5.14	133.06	123.30
1	A	454	SER	N-CA-CB	-5.14	102.80	110.50
7	G	2	SER	CA-CB-OG	5.14	125.07	111.20
1	N	346	PHE	CG-CD2-CE2	-5.14	115.15	120.80
4	D	45	LYS	CG-CD-CE	5.13	127.30	111.90
1	N	35	LEU	CA-CB-CG	-5.13	103.49	115.30
1	A	323	TRP	CD1-NE1-CE2	-5.13	104.38	109.00
13	Z	27	LEU	CB-CG-CD2	5.13	119.72	111.00
2	B	227	LEU	CB-CG-CD2	-5.13	102.28	111.00
6	F	65	ASP	CB-CG-OD1	-5.13	113.69	118.30
3	P	190	ASP	CB-CG-OD2	-5.12	113.69	118.30
4	D	104	TYR	CG-CD2-CE2	-5.12	117.21	121.30
1	N	285	PHE	CB-CG-CD2	-5.11	117.22	120.80
7	G	64	ASP	OD1-CG-OD2	5.11	133.01	123.30
4	Q	16	TYR	CE1-CZ-CE2	5.11	127.98	119.80
4	D	61	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	153	ALA	N-CA-CB	-5.10	102.96	110.10
1	A	166	THR	CA-CB-CG2	-5.10	105.26	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	225	PHE	CB-CG-CD1	-5.09	117.23	120.80
2	B	133	LEU	CB-CG-CD2	-5.09	102.35	111.00
7	T	50	TYR	CB-CG-CD2	-5.09	117.95	121.00
4	D	73	ARG	CB-CG-CD	-5.09	98.37	111.60
1	N	54	TYR	CD1-CE1-CZ	-5.09	115.22	119.80
8	U	8	ILE	CB-CA-C	5.09	121.77	111.60
3	C	60	ASP	CB-CG-OD2	-5.08	113.72	118.30
4	D	30	VAL	O-C-N	-5.08	114.58	122.70
10	W	23	LYS	CD-CE-NZ	-5.07	100.03	111.70
5	E	103	GLU	CG-CD-OE1	5.07	128.43	118.30
1	N	189	MET	CB-CG-SD	-5.06	97.21	112.40
2	O	214	VAL	CG1-CB-CG2	5.06	119.00	110.90
4	D	19[A]	ARG	CD-NE-CZ	5.06	130.69	123.60
4	D	19[B]	ARG	CD-NE-CZ	5.06	130.69	123.60
5	E	93	LEU	CB-CG-CD1	-5.06	102.40	111.00
5	E	18	TYR	N-CA-CB	-5.06	101.50	110.60
9	I	35	TYR	CB-CG-CD2	-5.05	117.97	121.00
3	P	44[A]	MET	CG-SD-CE	5.05	108.28	100.20
3	P	44[B]	MET	CG-SD-CE	5.05	108.28	100.20
3	P	181	TYR	CD1-CE1-CZ	-5.05	115.25	119.80
1	A	379	TYR	CZ-CE2-CD2	-5.05	115.26	119.80
4	Q	59	LEU	CB-CG-CD2	-5.05	102.42	111.00
3	C	236	GLU	CA-CB-CG	-5.04	102.31	113.40
13	Z	1	ILE	CG1-CB-CG2	-5.04	100.31	111.40
3	P	49	THR	CA-CB-CG2	-5.04	105.34	112.40
13	Z	26	PHE	CB-CG-CD2	-5.04	117.27	120.80
8	U	46	LYS	CB-CA-C	5.04	120.47	110.40
1	A	450	TRP	CB-CG-CD2	5.03	133.14	126.60
10	J	15	ASP	CB-CG-OD2	5.03	122.83	118.30
1	N	300	ASP	CB-CG-OD1	5.03	122.83	118.30
3	P	244	PHE	CB-CG-CD1	-5.03	117.28	120.80
4	Q	24	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	A	237	PHE	CG-CD1-CE1	-5.03	115.27	120.80
2	O	68	LEU	CB-CG-CD1	5.02	119.54	111.00
7	G	2	SER	C-N-CA	5.02	134.25	121.70
3	P	80[A]	ARG	NE-CZ-NH1	-5.02	117.79	120.30
3	P	80[B]	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	A	181	THR	OG1-CB-CG2	-5.02	98.46	110.00
1	N	346	PHE	CD1-CE1-CZ	-5.01	114.08	120.10
2	B	173	ASP	CB-CG-OD1	5.01	122.81	118.30
12	L	14	SER	N-CA-CB	-5.01	102.98	110.50
2	B	151	ARG	CD-NE-CZ	-5.01	116.59	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	369	ASP	CB-CG-OD2	-5.00	113.80	118.30
3	P	238	ALA	N-CA-CB	-5.00	103.09	110.10
3	P	181	TYR	CE1-CZ-CE2	5.00	127.80	119.80

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	GLY	Mainchain
1	A	304	TYR	Sidechain
1	A	379	TYR	Sidechain
1	A	38	ARG	Sidechain
2	B	110	TYR	Sidechain
2	B	151	ARG	Sidechain
2	B	68	LEU	Mainchain
3	C	133	ASN	Sidechain
5	E	49	ASP	Sidechain
5	E	88	GLU	Sidechain
6	F	93	PRO	Peptide
7	G	18	PHE	Sidechain
10	J	57	HIS	Peptide
11	K	39	GLU	Mainchain
13	M	14	GLU	Sidechain
1	N	240	HIS	Sidechain
1	N	296	GLY	Mainchain
1	N	304	TYR	Sidechain
4	Q	8	SER	Peptide
6	S	92	VAL	Mainchain
6	S	93	PRO	Peptide
7	T	40	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4168	0	4137	74	0
1	N	4154	0	4129	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1899	0	1898	65	0
2	O	1870	0	1868	40	0
3	C	2185	0	2097	38	0
3	P	2185	0	2097	51	0
4	D	1242	0	1235	19	0
4	Q	1224	0	1211	25	0
5	E	852	0	845	1	0
5	R	863	0	857	8	2
6	F	778	0	754	27	0
6	S	763	0	742	42	0
7	G	686	0	651	42	0
7	T	686	0	651	45	0
8	H	662	0	623	24	0
8	U	662	0	623	15	0
9	I	601	0	613	17	2
9	V	601	0	613	13	0
10	J	460	0	459	13	0
10	W	469	0	464	9	0
11	K	384	0	366	6	0
11	X	391	0	374	4	0
12	L	380	0	380	19	0
12	Y	388	0	388	29	0
13	M	335	0	352	7	0
13	Z	335	0	352	5	0
14	A	120	0	107	10	0
14	N	120	0	107	11	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	1	0
18	N	2	0	0	1	0
19	A	102	0	152	11	0
19	C	102	0	152	8	0
19	N	51	0	76	1	0
19	P	102	0	152	9	0
19	Q	51	0	76	11	0
20	B	63	0	109	3	0
20	D	63	0	106	21	0
20	L	63	0	110	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	N	63	0	110	6	0
20	Q	63	0	110	15	0
20	Y	63	0	110	23	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	0	0
22	C	58	0	77	3	0
22	J	29	0	37	6	0
22	O	29	0	39	0	0
22	P	58	0	77	7	0
22	W	29	0	38	6	0
23	B	52	0	80	13	0
23	O	52	0	80	19	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	C	100	0	154	26	0
25	G	100	0	156	37	0
25	P	100	0	156	24	0
25	T	100	0	156	28	0
26	C	53	0	77	13	0
26	G	106	0	154	16	0
26	P	53	0	77	16	0
26	T	106	0	154	18	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	J	33	0	42	5	0
28	M	33	0	42	0	0
28	P	33	0	42	10	0
28	Z	33	0	42	0	0
29	A	297	0	0	17	0
29	B	274	0	0	13	0
29	C	176	0	0	8	0
29	D	266	0	0	5	0
29	E	178	0	0	2	0
29	F	199	0	0	9	0
29	G	100	0	0	7	0
29	H	122	0	0	8	0
29	I	88	0	0	2	0
29	J	63	0	0	2	0
29	K	69	0	0	4	0
29	L	48	0	0	2	0
29	M	47	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	N	290	0	0	12	0
29	O	243	0	0	4	0
29	P	173	0	0	8	0
29	Q	164	0	0	8	0
29	R	151	0	0	4	0
29	S	186	0	0	9	0
29	T	94	0	0	3	0
29	U	110	0	0	5	0
29	V	71	0	0	2	0
29	W	58	0	0	1	0
29	X	57	0	0	1	0
29	Y	40	0	0	3	0
29	Z	37	0	0	0	0
All	All	35054	0	31975	816	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (816) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:C:302:PGV:C21	19:C:302:PGV:C22	1.77	1.62
26:T:101:PEK:C2	26:T:101:PEK:C3	1.76	1.56
2:B:1:FME:CN	2:B:1:FME:N	1.70	1.53
3:P:224:LYS:NZ	3:P:224:LYS:CE	1.77	1.47
20:D:201:TGL:OG2	20:D:201:TGL:CB1	1.63	1.47
1:N:302[B]:ARG:NH1	1:N:361:SER:CB	1.76	1.47
1:N:302[B]:ARG:HH12	1:N:361:SER:CB	1.27	1.45
5:R:46:LYS:CE	5:R:46:LYS:NZ	1.73	1.45
12:Y:20:ARG:HH22	12:Y:24[B]:MET:CE	1.36	1.37
12:Y:20:ARG:NH2	20:Y:101:TGL:HC32	1.35	1.37
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE3	1.65	1.31
12:L:20:ARG:NH2	20:L:101:TGL:HC32	1.43	1.31
26:C:306:PEK:H383	25:G:102:CDL:C27	1.62	1.26
2:O:22[B]:HIS:CE1	9:V:44:LYS:HE2	1.70	1.25
18:A:606:PER:O1	18:A:606:PER:O2	1.55	1.24
2:B:115:ASP:HB3	29:B:601:HOH:O	1.34	1.23
1:N:302[B]:ARG:NH1	1:N:361:SER:HB2	0.92	1.22
6:S:76:LYS:CE	6:S:93:PRO:HG2	1.68	1.22
18:N:606:PER:O1	18:N:606:PER:O2	1.55	1.21
4:D:100[B]:LYS:HE2	29:D:401:HOH:O	1.40	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:20:ARG:NH2	12:Y:24[B]:MET:CE	2.07	1.17
12:L:9:LYS:HE3	29:L:224:HOH:O	1.42	1.15
7:G:5:LYS:HG3	26:G:103:PEK:H371	1.28	1.15
2:B:1:FME:O1	2:B:1:FME:N	1.80	1.14
29:P:436:HOH:O	6:S:1:ALA:HB2	1.45	1.14
23:O:303:PSC:H12	23:O:303:PSC:C34	1.77	1.13
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	1.88	1.13
20:Q:202:TGL:H362	9:V:20:HIS:HE1	1.12	1.12
11:K:54:ARG:HD2	29:K:141:HOH:O	1.45	1.12
8:H:9:LYS:HA	8:H:9:LYS:CE	1.79	1.11
26:C:306:PEK:H383	25:G:102:CDL:H273	1.13	1.11
26:P:308:PEK:H383	25:T:103:CDL:H273	1.21	1.10
26:P:308:PEK:C38	25:T:103:CDL:H273	1.82	1.09
7:G:84:LYS:HD2	7:G:84:LYS:H	1.11	1.09
1:A:136[B]:LEU:HD11	29:A:988:HOH:O	1.52	1.09
20:D:201:TGL:CB2	20:D:201:TGL:OG2	2.01	1.08
8:H:9:LYS:HA	8:H:9:LYS:HE2	1.33	1.08
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:HD2	1.52	1.08
12:Y:20:ARG:HH22	12:Y:24[B]:MET:HE1	0.90	1.07
6:S:19:GLU:HG2	29:S:314:HOH:O	1.54	1.07
1:A:513:LEU:O	1:A:514:LYS:HB2	1.54	1.06
26:T:102:PEK:H361	25:T:103:CDL:H872	1.32	1.06
1:N:513:LEU:O	1:N:514:LYS:HB2	1.52	1.06
23:O:303:PSC:H12	23:O:303:PSC:H342	1.34	1.06
6:S:76:LYS:HE2	6:S:93:PRO:HG2	1.11	1.05
12:Y:20:ARG:NH2	12:Y:24[B]:MET:HE1	1.69	1.05
26:C:306:PEK:C38	25:G:102:CDL:C27	2.33	1.05
19:Q:201:PGV:H011	19:Q:201:PGV:C2	1.84	1.05
2:B:22[B]:HIS:CE1	9:I:44:LYS:CE	2.40	1.04
12:Y:24[B]:MET:SD	20:Y:101:TGL:HC21	1.97	1.04
12:L:14:SER:H	20:L:101:TGL:HC31	1.17	1.04
1:N:417[A]:MET:HE2	29:N:880:HOH:O	1.56	1.04
4:Q:9:GLU:HB3	29:Q:427:HOH:O	1.54	1.03
20:Y:101:TGL:OC1	20:Y:101:TGL:HC41	1.21	1.03
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.41	1.03
12:Y:20:ARG:HH21	20:Y:101:TGL:CC3	1.72	1.02
19:A:608:PGV:H311	13:M:19:LEU:HD23	1.41	1.02
1:N:513:LEU:O	1:N:514:LYS:CB	2.04	1.02
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.39	1.02
4:Q:65:LYS:HE3	29:Q:421:HOH:O	1.55	1.02
12:Y:20:ARG:NH2	20:Y:101:TGL:CC3	2.23	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:90:ARG:HD2	29:E:311:HOH:O	1.58	1.01
26:P:308:PEK:C38	25:T:103:CDL:C27	2.39	1.01
1:N:302[B]:ARG:HH11	1:N:361:SER:HB2	1.19	1.01
20:Q:202:TGL:H362	9:V:20:HIS:CE1	1.97	0.99
7:G:5:LYS:HB2	26:G:103:PEK:H351	1.45	0.98
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.28	0.98
29:A:964:HOH:O	20:D:201:TGL:HC31	1.62	0.98
1:N:486:ASP:OD2	4:Q:19[B]:ARG:HD2	1.64	0.97
2:B:49:LYS:HE2	29:B:609:HOH:O	1.65	0.97
12:Y:14:SER:H	20:Y:101:TGL:HC31	1.31	0.95
6:F:1:ALA:HB3	6:S:65:ASP:OD1	1.67	0.95
1:A:178[B]:GLN:NE2	29:A:701:HOH:O	1.97	0.95
25:G:102:CDL:H541	25:G:102:CDL:C24	1.96	0.94
26:C:306:PEK:C38	25:G:102:CDL:H273	1.93	0.94
26:P:308:PEK:H382	25:T:103:CDL:C27	1.98	0.94
7:G:4:ALA:CB	1:N:282:PHE:HA	1.98	0.94
23:O:303:PSC:H342	23:O:303:PSC:C12	1.96	0.94
26:P:308:PEK:H051	29:P:476:HOH:O	1.67	0.93
6:S:76:LYS:HE2	6:S:93:PRO:CG	1.99	0.93
3:C:67:PHE:HE1	25:C:303:CDL:H1	1.35	0.92
12:L:20:ARG:HH22	20:L:101:TGL:CC3	1.81	0.92
2:O:22[B]:HIS:HE1	9:V:44:LYS:HE2	1.27	0.92
1:N:178[B]:GLN:HG3	1:N:186:TRP:CZ2	2.04	0.92
25:T:103:CDL:H541	25:T:103:CDL:H242	1.48	0.92
2:B:56:MET:HA	23:B:304:PSC:H201	1.51	0.91
2:B:22[B]:HIS:HE1	9:I:44:LYS:HE3	1.11	0.91
3:C:180[B]:GLU:HG2	29:C:422:HOH:O	1.70	0.91
19:Q:201:PGV:H011	19:Q:201:PGV:H22	1.51	0.91
3:C:51[B]:MET:HE2	25:C:303:CDL:H391	1.53	0.90
23:O:303:PSC:H71	29:V:170:HOH:O	1.69	0.90
3:C:224:LYS:CD	25:C:303:CDL:HB31	2.00	0.90
2:B:1:FME:CN	2:B:1:FME:CA	2.49	0.90
1:A:282:PHE:HA	7:T:4:ALA:CB	2.01	0.89
8:U:9:LYS:HG2	29:U:187:HOH:O	1.71	0.89
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:CD	2.20	0.89
7:G:72:ASN:H	7:G:76:ASN:HD22	1.17	0.89
19:A:607:PGV:H343	26:G:101:PEK:H382	1.55	0.88
12:L:20:ARG:HH22	20:L:101:TGL:HC32	1.12	0.88
1:A:417[B]:MET:CE	29:A:816:HOH:O	2.21	0.88
12:Y:20:ARG:NH2	12:Y:24[B]:MET:SD	2.47	0.88
23:B:304:PSC:H212	23:B:304:PSC:H02	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:156:ARG:HE	22:P:305:CHD:H232	1.38	0.88
3:P:67:PHE:HE1	25:P:304:CDL:H1	1.39	0.87
4:D:19[A]:ARG:NH2	4:D:21:ASP:OD1	2.07	0.87
20:Y:101:TGL:OC1	20:Y:101:TGL:CC4	2.17	0.87
12:L:20:ARG:NH2	20:L:101:TGL:CC3	2.34	0.86
4:Q:6:VAL:HG12	4:Q:10:ASP:OD2	1.74	0.86
7:T:72:ASN:H	7:T:76:ASN:HD22	1.19	0.86
4:Q:9:GLU:HA	4:Q:9:GLU:OE2	1.76	0.86
2:B:22[B]:HIS:HE1	9:I:44:LYS:CE	1.79	0.85
25:G:102:CDL:H212	1:N:311[A]:ILE:CD1	2.07	0.85
23:O:303:PSC:H12	23:O:303:PSC:H343	1.58	0.85
6:S:75:HIS:H	6:S:80:GLN:HE22	1.21	0.85
1:A:178[B]:GLN:HG3	7:T:7:ASP:OD2	1.77	0.85
10:J:49:CYS:HB3	28:J:101:DMU:H9	1.58	0.84
6:S:94:HIS:CD2	6:S:95:GLN:H	1.93	0.84
1:N:136[B]:LEU:HD11	29:N:976:HOH:O	1.77	0.84
7:G:84:LYS:H	7:G:84:LYS:CD	1.89	0.84
2:O:29[B]:MET:SD	2:O:33:LEU:HD22	2.18	0.83
7:G:4:ALA:HB1	1:N:282:PHE:HA	1.59	0.83
1:N:417[A]:MET:CE	29:N:880:HOH:O	2.19	0.83
6:F:75:HIS:H	6:F:80:GLN:HE22	1.26	0.83
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.61	0.83
1:N:321:PHE:CD2	23:O:303:PSC:H341	2.12	0.83
1:A:513:LEU:O	1:A:514:LYS:CB	2.27	0.82
3:C:224:LYS:HE3	25:C:303:CDL:HB31	1.61	0.82
12:Y:24[B]:MET:HG2	20:Y:101:TGL:HA22	1.61	0.82
25:G:102:CDL:H352	2:O:78:LEU:HD12	1.59	0.82
19:Q:201:PGV:H011	19:Q:201:PGV:H21	1.61	0.82
1:N:28:MET:CE	14:N:601:HEA:H271	2.10	0.81
25:G:102:CDL:H241	25:G:102:CDL:H541	1.61	0.81
20:D:201:TGL:CB1	20:D:201:TGL:CG2	2.57	0.81
26:P:308:PEK:H383	25:T:103:CDL:C27	2.04	0.81
7:T:30:LEU:HD21	25:T:103:CDL:H471	1.61	0.81
19:Q:201:PGV:H311	13:Z:19:LEU:HD23	1.63	0.81
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.21	0.81
6:S:94:HIS:HA	29:S:318:HOH:O	1.81	0.81
12:L:20:ARG:HH21	20:L:101:TGL:HC32	1.42	0.81
3:P:63:ARG:HE	25:P:304:CDL:CA2	1.93	0.80
8:H:9:LYS:CA	8:H:9:LYS:CE	2.53	0.80
3:C:161[A]:GLN:HE22	26:C:306:PEK:C2	1.95	0.80
2:B:16[B]:ILE:HG23	29:B:523:HOH:O	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:103:CDL:H511	25:T:103:CDL:H181	1.61	0.79
7:G:37:LEU:HD21	25:G:102:CDL:H361	1.65	0.79
6:F:54[A]:ASN:H	6:F:54[A]:ASN:HD22	1.29	0.79
20:Q:202:TGL:H352	9:V:16:ARG:HE	1.46	0.79
4:Q:19[A]:ARG:HG2	4:Q:21:ASP:OD1	1.81	0.79
26:P:308:PEK:H382	25:T:103:CDL:H272	1.64	0.79
3:P:160:LEU:HD13	22:P:305:CHD:H181	1.65	0.79
12:Y:20:ARG:HH21	20:Y:101:TGL:HC32	0.89	0.79
3:C:67:PHE:CE1	25:C:303:CDL:H1	2.18	0.78
12:Y:24[B]:MET:SD	20:Y:101:TGL:CC2	2.72	0.78
2:B:87[B]:MET:HE2	29:B:417:HOH:O	1.80	0.78
3:C:224:LYS:CE	25:C:303:CDL:HB31	2.11	0.78
3:P:156:ARG:HE	22:P:305:CHD:C23	1.96	0.78
3:C:63:ARG:HE	25:C:303:CDL:CA2	1.96	0.78
8:H:9:LYS:CA	8:H:9:LYS:HE2	2.13	0.78
1:A:178[B]:GLN:H	1:A:178[B]:GLN:CD	1.87	0.78
2:B:82:ARG:HD2	29:B:403:HOH:O	1.82	0.78
26:P:308:PEK:N	26:P:308:PEK:O02	2.16	0.78
26:C:306:PEK:H383	25:G:102:CDL:H271	1.63	0.77
7:T:36:TRP:HE3	7:T:39:SER:HB3	1.47	0.77
3:C:63:ARG:HE	25:C:303:CDL:HA21	1.48	0.77
26:T:101:PEK:C3	26:T:101:PEK:C1	2.62	0.77
1:N:28:MET:CE	14:N:601:HEA:C27	2.63	0.77
4:D:34:SER:H	4:D:37:GLN:HE21	1.33	0.77
19:C:302:PGV:H221	19:C:302:PGV:C21	2.12	0.77
25:G:102:CDL:H332	29:O:488:HOH:O	1.85	0.77
25:G:102:CDL:OA7	25:G:102:CDL:H342	1.84	0.77
3:P:67:PHE:CE1	25:P:304:CDL:H1	2.20	0.77
20:N:608:TGL:H281	20:N:608:TGL:HB91	1.68	0.76
19:P:303:PGV:H172	25:P:304:CDL:H642	1.65	0.76
23:O:303:PSC:C12	23:O:303:PSC:C34	2.59	0.76
4:D:78:TRP:CA	20:D:201:TGL:HB21	2.15	0.75
6:S:43:LYS:H	6:S:43:LYS:HD2	1.52	0.75
2:B:74:ILE:O	2:B:78:LEU:HD13	1.85	0.75
12:L:20:ARG:HH22	20:L:101:TGL:HC52	1.52	0.75
1:A:53:ILE:HG13	29:A:980:HOH:O	1.87	0.75
2:B:56:MET:HG2	23:B:304:PSC:H211	1.68	0.75
20:L:101:TGL:H312	20:L:101:TGL:H362	1.67	0.75
20:N:608:TGL:H281	20:N:608:TGL:CB9	2.17	0.75
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.69	0.75
1:N:297[B]:MET:SD	1:N:302[B]:ARG:HG3	2.27	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.69	0.74
2:B:53:THR:HG21	29:D:305:HOH:O	1.88	0.74
26:P:308:PEK:H041	7:T:17:ARG:HH22	1.52	0.74
3:C:224:LYS:HD2	25:C:303:CDL:HB31	1.68	0.74
1:N:406:ASN:HD21	19:Q:201:PGV:H21	1.52	0.73
3:C:161[A]:GLN:HE22	26:C:306:PEK:H22	1.50	0.73
25:C:303:CDL:H522	25:C:303:CDL:OB9	1.88	0.73
3:C:33[B]:MET:HG2	3:C:39:SER:O	1.88	0.73
25:T:103:CDL:H762	25:T:103:CDL:H562	1.69	0.73
6:S:43:LYS:CD	6:S:43:LYS:H	2.00	0.73
25:G:102:CDL:H212	1:N:311[A]:ILE:HD12	1.69	0.73
3:P:33[A]:MET:HB2	28:P:306:DMU:H8	1.70	0.73
25:G:102:CDL:H201	25:G:102:CDL:H522	1.71	0.73
7:G:76:ASN:HD21	26:G:101:PEK:HN2	1.37	0.72
23:O:303:PSC:H02	23:O:303:PSC:H212	1.71	0.72
1:N:28:MET:HE1	14:N:601:HEA:H271	1.70	0.72
3:P:156:ARG:NE	22:P:305:CHD:H232	2.05	0.72
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.55	0.72
3:P:33[A]:MET:HB2	28:P:306:DMU:C19	2.20	0.71
19:A:607:PGV:H183	26:G:101:PEK:H322	1.71	0.71
12:L:20:ARG:HH22	20:L:101:TGL:CC5	2.03	0.71
7:T:30:LEU:CD2	25:T:103:CDL:H471	2.20	0.70
2:B:49:LYS:HD3	20:D:201:TGL:HC71	1.73	0.70
7:T:36:TRP:CE3	7:T:39:SER:HB3	2.26	0.70
8:U:45:ALA:O	8:U:47:GLY:N	2.25	0.70
1:N:302[B]:ARG:HH12	1:N:361:SER:CA	2.04	0.70
3:P:63:ARG:HE	25:P:304:CDL:HA22	1.54	0.70
1:A:112:LEU:HG	29:A:937:HOH:O	1.90	0.70
14:N:601:HEA:HMC1	14:N:601:HEA:HBC1	1.74	0.70
2:O:22[B]:HIS:CE1	9:V:44:LYS:CE	2.63	0.70
1:N:178[B]:GLN:CG	1:N:186:TRP:CZ2	2.73	0.70
4:Q:6:VAL:CG1	4:Q:10:ASP:OD2	2.40	0.70
12:Y:14:SER:N	20:Y:101:TGL:HC31	2.06	0.70
4:D:31[A]:LYS:CG	29:D:301:HOH:O	2.40	0.70
25:G:102:CDL:H241	25:G:102:CDL:C54	2.21	0.70
20:Q:202:TGL:CA9	20:Q:202:TGL:H231	2.21	0.70
19:C:302:PGV:H222	19:C:302:PGV:C21	2.12	0.70
2:B:29[B]:MET:SD	2:B:33:LEU:HD22	2.32	0.69
1:A:406:ASN:HD21	19:A:608:PGV:H22	1.56	0.69
10:J:33:ARG:HG2	22:J:102:CHD:H152	1.75	0.69
1:A:28:MET:CE	14:A:601:HEA:C27	2.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:56:MET:HG2	23:O:303:PSC:H211	1.75	0.69
3:P:127:LEU:HD13	25:T:103:CDL:OB3	1.92	0.69
7:T:76:ASN:HD21	26:T:101:PEK:HN2	1.36	0.69
11:K:47:ARG:HD3	29:K:160:HOH:O	1.91	0.69
1:A:177:SER:H	1:A:180:GLN:HE21	1.40	0.69
19:P:301:PGV:H32	29:P:523:HOH:O	1.91	0.69
6:S:94:HIS:HD2	6:S:95:GLN:O	1.76	0.68
25:T:103:CDL:H511	25:T:103:CDL:C18	2.23	0.68
26:P:308:PEK:H042	6:S:1:ALA:N	2.08	0.68
6:F:92:VAL:HG21	29:F:387:HOH:O	1.94	0.68
1:N:178[B]:GLN:HG3	1:N:186:TRP:CE2	2.29	0.67
3:P:63:ARG:HE	25:P:304:CDL:HA21	1.59	0.67
10:W:10:LYS:O	10:W:14[B]:GLU:HG3	1.94	0.67
7:T:38:HIS:HD2	29:T:210:HOH:O	1.76	0.67
25:P:304:CDL:OB9	25:P:304:CDL:H522	1.94	0.67
1:A:484:THR:HG22	29:A:972:HOH:O	1.94	0.67
8:U:48:GLY:HA2	29:U:176:HOH:O	1.94	0.67
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.77	0.67
8:U:43:MET:HE3	8:U:49:ASP:N	2.09	0.67
1:N:302[B]:ARG:NH1	1:N:361:SER:OG	2.28	0.67
2:O:60:GLU:CD	2:O:60:GLU:H	1.97	0.67
19:P:303:PGV:H172	25:P:304:CDL:C64	2.25	0.67
1:A:273:MET:HE2	29:A:888:HOH:O	1.94	0.66
7:G:72:ASN:H	7:G:76:ASN:ND2	1.93	0.66
25:P:304:CDL:HB21	25:P:304:CDL:OB6	1.95	0.66
7:T:5:LYS:HG3	26:T:102:PEK:H351	1.76	0.66
7:G:11:TPO:HG21	29:G:280:HOH:O	1.96	0.66
8:H:23:GLN:HG3	29:H:166:HOH:O	1.95	0.66
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.30	0.66
10:W:33:ARG:HG2	22:W:101:CHD:H182	1.76	0.66
12:L:14:SER:N	20:L:101:TGL:HC31	2.01	0.66
6:S:43:LYS:HE2	29:S:342:HOH:O	1.95	0.66
3:P:4:GLN:N	29:P:401:HOH:O	2.29	0.66
7:T:37:LEU:HD23	25:T:103:CDL:H361	1.77	0.66
29:C:541:HOH:O	10:J:1:PHE:HE2	1.79	0.65
23:O:303:PSC:C02	23:O:303:PSC:H212	2.26	0.65
4:Q:78:TRP:N	20:Q:202:TGL:HB21	2.11	0.65
4:D:31[A]:LYS:HG2	29:D:301:HOH:O	1.95	0.65
7:G:3:ALA:HB3	26:G:103:PEK:H362	1.79	0.65
2:O:29[B]:MET:SD	2:O:33:LEU:CD2	2.84	0.65
6:S:94:HIS:CD2	6:S:95:GLN:N	2.64	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:28:MET:HE2	14:N:601:HEA:H273	1.78	0.65
26:T:102:PEK:C36	25:T:103:CDL:H872	2.20	0.65
12:Y:20:ARG:CZ	12:Y:24[B]:MET:CE	2.75	0.65
7:G:3:ALA:CB	26:G:103:PEK:H383	2.27	0.64
29:N:703:HOH:O	4:Q:6:VAL:HG11	1.97	0.64
10:J:32:TYR:OH	22:J:102:CHD:H213	1.97	0.64
5:R:46:LYS:CD	5:R:46:LYS:NZ	2.56	0.64
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.80	0.64
7:G:5:LYS:CG	26:G:103:PEK:H371	2.17	0.64
23:O:303:PSC:H322	23:O:303:PSC:C28	2.27	0.64
1:A:468:MET:HG3	29:A:957:HOH:O	1.97	0.64
1:N:302[B]:ARG:HH11	1:N:361:SER:CB	1.87	0.64
5:R:80:GLU:CD	5:R:80:GLU:H	2.00	0.64
4:D:28:ALA:H	4:D:31[B]:LYS:NZ	1.95	0.63
8:H:47:GLY:HA2	29:H:180:HOH:O	1.97	0.63
1:N:177:SER:H	1:N:180:GLN:HE21	1.46	0.63
1:N:297[B]:MET:HB3	1:N:302[B]:ARG:HD2	1.79	0.63
2:O:22[B]:HIS:HE1	9:V:44:LYS:CE	2.06	0.63
19:A:608:PGV:H061	19:A:608:PGV:O11	1.99	0.63
7:G:3:ALA:HB1	26:G:103:PEK:H383	1.79	0.63
7:T:84:LYS:H	7:T:84:LYS:NZ	1.96	0.63
2:B:83:ILE:O	2:B:87[A]:MET:HG3	1.99	0.62
13:M:39:ASN:O	13:M:43:SER:HB3	1.99	0.62
7:T:72:ASN:H	7:T:76:ASN:ND2	1.94	0.62
2:B:1:FME:HCN	2:B:193:TYR:H	1.64	0.62
3:C:51[B]:MET:CE	25:C:303:CDL:H391	2.29	0.62
6:S:22:LEU:HD12	29:S:329:HOH:O	1.99	0.62
20:Q:202:TGL:HA92	20:Q:202:TGL:H231	1.81	0.62
13:Z:42:LYS:HG3	13:Z:42:LYS:O	1.99	0.62
1:A:28:MET:HE2	14:A:601:HEA:H273	1.81	0.62
2:O:92:ASN:HB3	29:U:128:HOH:O	1.99	0.62
7:T:11:TPO:O	7:T:11:TPO:CG2	2.48	0.62
20:D:201:TGL:CG3	20:D:201:TGL:CB1	2.77	0.62
25:G:102:CDL:H541	25:G:102:CDL:H242	1.80	0.62
20:N:608:TGL:HB91	20:N:608:TGL:C28	2.30	0.61
1:A:417[B]:MET:HE2	29:A:816:HOH:O	1.92	0.61
26:P:308:PEK:H042	6:S:1:ALA:H1	1.64	0.61
6:S:94:HIS:CG	6:S:95:GLN:H	2.14	0.61
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.35	0.61
2:O:47:THR:HB	20:Q:202:TGL:H181	1.81	0.61
2:B:32[B]:PHE:CD2	9:I:31:PHE:CZ	2.89	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:78:TRP:HB3	20:Q:202:TGL:HB22	1.83	0.61
6:S:43:LYS:HD3	29:S:251:HOH:O	1.99	0.61
20:Y:101:TGL:HG31	29:Y:221:HOH:O	2.00	0.61
7:T:84:LYS:H	7:T:84:LYS:HZ3	1.48	0.61
23:B:304:PSC:H212	23:B:304:PSC:C02	2.28	0.61
20:D:201:TGL:HG12	20:D:201:TGL:HC32	1.82	0.60
5:R:46:LYS:NZ	29:R:202:HOH:O	2.34	0.60
6:S:76:LYS:NZ	6:S:93:PRO:HG2	2.15	0.60
1:A:278[B]:MET:HE3	7:T:5:LYS:HB3	1.83	0.60
2:B:183[A]:THR:HG22	29:B:462:HOH:O	2.00	0.60
26:G:101:PEK:C12	26:G:101:PEK:H161	2.30	0.60
14:A:601:HEA:HBC1	14:A:601:HEA:HMC1	1.83	0.60
19:A:608:PGV:H311	13:M:19:LEU:CD2	2.26	0.60
7:T:3:ALA:O	7:T:4:ALA:HB2	2.02	0.60
19:C:302:PGV:H161	19:C:302:PGV:H12	1.84	0.60
6:F:94:HIS:CE1	29:F:203:HOH:O	2.53	0.60
1:N:468:MET:HG3	29:N:943:HOH:O	2.00	0.60
3:P:50:ASN:HD22	3:P:51[A]:MET:HE2	1.65	0.60
1:N:28:MET:HE2	14:N:601:HEA:C27	2.27	0.60
20:D:201:TGL:HA91	20:D:201:TGL:H231	1.84	0.60
1:A:278[B]:MET:CE	7:T:5:LYS:HB3	2.31	0.60
6:S:19:GLU:OE1	6:S:31:TYR:OH	2.17	0.60
7:T:38:HIS:CD2	29:T:210:HOH:O	2.50	0.60
8:U:43:MET:CE	8:U:49:ASP:H	2.15	0.59
1:A:514:LYS:HD2	29:F:252:HOH:O	2.02	0.59
2:B:52:HIS:HE1	23:B:304:PSC:H212	1.66	0.59
6:F:54[A]:ASN:H	6:F:54[A]:ASN:ND2	1.99	0.59
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.37	0.59
3:P:224:LYS:CD	25:P:304:CDL:HB32	2.32	0.59
6:S:43:LYS:CE	29:S:342:HOH:O	2.48	0.59
3:C:161[A]:GLN:HE22	26:C:306:PEK:H21	1.66	0.59
4:D:78:TRP:HA	20:D:201:TGL:HB21	1.84	0.59
26:C:306:PEK:H382	25:G:102:CDL:C27	2.29	0.59
3:C:224:LYS:CD	25:C:303:CDL:CB3	2.77	0.58
6:F:54[A]:ASN:N	6:F:54[A]:ASN:HD22	2.00	0.58
2:B:52:HIS:CE1	23:B:304:PSC:H211	2.38	0.58
6:F:30:PRO:O	6:F:96:LEU:HD11	2.02	0.58
29:C:541:HOH:O	10:J:1:PHE:CE2	2.52	0.58
25:G:102:CDL:HA21	25:G:102:CDL:H111	1.86	0.58
20:Y:101:TGL:CG3	29:Y:221:HOH:O	2.52	0.58
23:O:303:PSC:H012	23:O:303:PSC:P	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:31:CYS:SG	25:T:103:CDL:H532	2.43	0.58
8:U:43:MET:HE3	8:U:49:ASP:H	1.68	0.58
12:Y:24[B]:MET:CG	20:Y:101:TGL:HA22	2.32	0.58
1:N:273:MET:HE2	29:N:749:HOH:O	2.03	0.58
4:D:78:TRP:N	20:D:201:TGL:HB21	2.17	0.58
12:L:2:HIS:CG	12:L:3:TYR:H	2.21	0.58
12:Y:20:ARG:NH2	12:Y:24[B]:MET:HE2	2.14	0.58
1:A:113[B]:LEU:HD11	1:A:117[B]:MET:SD	2.43	0.58
7:G:4:ALA:HB1	1:N:282:PHE:CA	2.32	0.58
1:N:302[B]:ARG:HH11	1:N:302[B]:ARG:HG2	1.66	0.58
3:C:55:TYR:CE1	25:C:303:CDL:H532	2.38	0.58
7:G:84:LYS:N	7:G:84:LYS:HD2	1.97	0.58
1:A:302[B]:ARG:NE	1:A:361[B]:SER:OG	2.35	0.58
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.81	0.58
7:T:2:SER:OG	26:T:102:PEK:H302	2.04	0.58
6:F:87[A]:THR:HG21	29:F:324:HOH:O	2.03	0.57
2:B:70:ALA:HB1	25:T:103:CDL:H461	1.86	0.57
10:J:50:LEU:HB2	28:J:101:DMU:H20	1.86	0.57
19:P:301:PGV:H062	8:U:24:ASN:HB3	1.86	0.57
2:B:1:FME:CN	2:B:1:FME:HA	2.35	0.57
2:O:42:ILE:HG21	20:Q:202:TGL:H232	1.86	0.57
19:A:607:PGV:C18	26:G:101:PEK:H322	2.34	0.57
25:G:102:CDL:HA31	29:G:267:HOH:O	2.04	0.57
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.87	0.57
3:P:51[A]:MET:HE1	3:P:54[A]:MET:HE1	1.87	0.57
1:A:281:GLY:C	7:T:4:ALA:HB1	2.25	0.57
7:G:9:GLY:HA3	29:N:797:HOH:O	2.05	0.57
3:C:224:LYS:HE3	25:C:303:CDL:CB3	2.32	0.57
20:Y:101:TGL:HC42	29:Y:225:HOH:O	2.04	0.56
1:A:177:SER:H	1:A:180:GLN:NE2	2.03	0.56
12:L:46:LYS:HA	29:L:217:HOH:O	2.04	0.56
1:N:116:SER:HB3	29:N:931:HOH:O	2.05	0.56
3:C:63:ARG:HE	25:C:303:CDL:HA22	1.69	0.56
6:F:94:HIS:HE1	29:F:203:HOH:O	1.85	0.56
1:A:302[B]:ARG:NE	2:B:84:LEU:HD11	2.20	0.56
3:C:174:THR:HG21	25:C:303:CDL:H861	1.88	0.56
1:N:177:SER:H	1:N:180:GLN:NE2	2.04	0.56
2:B:52:HIS:HE1	23:B:304:PSC:C21	2.18	0.56
6:F:54[B]:ASN:ND2	29:F:203:HOH:O	2.39	0.56
20:N:608:TGL:H281	20:N:608:TGL:HB92	1.88	0.56
1:N:136[B]:LEU:CD1	29:N:976:HOH:O	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:304:PSC:H032	29:E:275:HOH:O	2.05	0.56
25:G:102:CDL:H182	25:G:102:CDL:H511	1.87	0.56
26:T:101:PEK:C2	26:T:101:PEK:H32	2.19	0.55
2:B:29[B]:MET:SD	2:B:33:LEU:CD2	2.93	0.55
4:D:34:SER:H	4:D:37:GLN:NE2	2.03	0.55
8:H:8:ILE:HG22	8:H:8:ILE:O	2.06	0.55
1:A:311[B]:ILE:HG13	1:A:314:ILE:HD12	1.87	0.55
10:J:27:THR:HG22	29:J:205:HOH:O	2.06	0.55
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.88	0.55
4:D:100[B]:LYS:CE	29:D:401:HOH:O	2.18	0.55
2:B:49:LYS:HD3	20:D:201:TGL:CC7	2.36	0.55
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.24	0.55
6:S:94:HIS:N	29:S:204:HOH:O	2.38	0.55
12:Y:20:ARG:NH1	12:Y:24[B]:MET:HE2	2.22	0.55
1:A:172:LYS:NZ	1:A:178[A]:GLN:HE22	2.05	0.55
6:S:94:HIS:CD2	6:S:95:GLN:O	2.59	0.55
23:B:304:PSC:H21	23:B:304:PSC:H011	1.88	0.55
3:P:246:ASP:HB2	29:P:522:HOH:O	2.06	0.54
8:U:9:LYS:HA	29:U:129:HOH:O	2.07	0.54
7:T:5:LYS:HB2	26:T:102:PEK:H331	1.88	0.54
25:G:102:CDL:H632	29:G:258:HOH:O	2.07	0.54
19:P:303:PGV:H182	25:P:304:CDL:H662	1.89	0.54
7:T:5:LYS:HG3	26:T:102:PEK:H371	1.88	0.54
2:B:83:ILE:O	2:B:87[B]:MET:HB2	2.07	0.54
2:B:227:LEU:HD21	29:B:548:HOH:O	2.06	0.54
23:O:303:PSC:H22	23:O:303:PSC:H201	1.89	0.54
19:N:607:PGV:H61	3:P:54[A]:MET:HG2	1.89	0.54
2:B:217:LYS:HD3	29:B:615:HOH:O	2.08	0.54
19:C:302:PGV:H211	19:C:302:PGV:C22	2.17	0.54
1:A:28:MET:CE	14:A:601:HEA:H271	2.35	0.54
2:O:58:ALA:O	2:O:62:GLU:HG3	2.08	0.54
4:Q:17[A]:VAL:CG1	29:Q:419:HOH:O	2.56	0.54
25:C:303:CDL:H672	25:C:303:CDL:H811	1.89	0.53
3:P:29:SER:HB2	28:P:306:DMU:H21	1.90	0.53
2:B:16[A]:ILE:HD12	2:B:87[A]:MET:HG2	1.89	0.53
2:B:52:HIS:CE1	23:B:304:PSC:C21	2.91	0.53
4:Q:19[B]:ARG:NH2	29:Q:302:HOH:O	2.39	0.53
1:N:172:LYS:NZ	1:N:178[A]:GLN:HE22	2.06	0.53
1:N:459:PHE:HE2	29:Q:311:HOH:O	1.92	0.53
12:Y:20:ARG:CZ	12:Y:24[B]:MET:HE2	2.38	0.53
26:T:101:PEK:H31	26:T:101:PEK:C1	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:TRP:CZ3	20:D:201:TGL:HA52	2.43	0.53
20:B:301:TGL:HC22	29:I:173:HOH:O	2.08	0.53
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.38	0.53
25:P:304:CDL:OB9	25:P:304:CDL:HB4	2.09	0.53
2:B:183[A]:THR:HG23	29:B:622:HOH:O	2.08	0.53
3:P:161[A]:GLN:HE22	26:P:308:PEK:H21	1.74	0.53
19:Q:201:PGV:C01	19:Q:201:PGV:C2	2.67	0.53
6:S:76:LYS:CE	6:S:93:PRO:CG	2.62	0.53
7:G:2:SER:OG	26:G:103:PEK:C29	2.56	0.53
6:F:1:ALA:HA	7:G:17:ARG:NH1	2.24	0.53
2:O:87[B]:MET:HE2	29:O:411:HOH:O	2.09	0.53
1:A:514:LYS:HE2	29:F:223:HOH:O	2.09	0.53
3:C:246:ASP:HB2	29:C:531:HOH:O	2.09	0.53
3:C:171:VAL:HG22	25:C:303:CDL:H851	1.90	0.53
3:C:51[B]:MET:HE2	25:C:303:CDL:C39	2.34	0.53
25:G:102:CDL:H761	1:N:282:PHE:HZ	1.74	0.53
19:Q:201:PGV:H162	19:Q:201:PGV:H321	1.91	0.53
1:A:25:TRP:CE3	20:L:101:TGL:HB92	2.44	0.53
23:O:303:PSC:H22	23:O:303:PSC:H231	1.91	0.53
19:P:303:PGV:H11	19:P:303:PGV:C15	2.40	0.52
2:B:41[B]:ILE:HD11	9:I:21:ILE:HD13	1.90	0.52
3:P:33[A]:MET:HB2	28:P:306:DMU:H9	1.91	0.52
7:T:2:SER:OG	26:T:102:PEK:H291	2.09	0.52
4:Q:93:ALA:HB3	11:X:28[B]:VAL:HG12	1.91	0.52
9:I:67:GLY:HA3	11:K:54:ARG:HD3	1.91	0.52
25:G:102:CDL:H611	25:G:102:CDL:H652	1.92	0.52
28:P:306:DMU:H11	10:W:49:CYS:HB3	1.91	0.52
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE2	2.41	0.52
25:C:303:CDL:OB6	25:C:303:CDL:HB22	2.10	0.52
20:B:301:TGL:HC21	29:B:589:HOH:O	2.10	0.52
3:P:80[A]:ARG:HG2	3:P:233:PHE:CE2	2.45	0.52
12:Y:20:ARG:NH1	12:Y:24[B]:MET:CE	2.73	0.52
25:G:102:CDL:C18	25:G:102:CDL:H511	2.40	0.52
6:F:1:ALA:CB	6:S:65:ASP:OD1	2.50	0.52
8:U:9:LYS:HG3	8:U:11:TYR:H	1.76	0.52
1:A:486[A]:ASP:OD1	4:D:19[A]:ARG:HD2	2.10	0.51
8:U:7:LYS:O	8:U:8:ILE:HB	2.10	0.51
19:Q:201:PGV:H301	19:Q:201:PGV:H142	1.92	0.51
1:A:281:GLY:O	7:T:4:ALA:HB1	2.10	0.51
12:L:20:ARG:HH22	20:L:101:TGL:CC4	2.22	0.51
7:G:5:LYS:CB	26:G:103:PEK:H351	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:9:LYS:HD3	8:H:11:TYR:H	1.75	0.51
4:D:100[B]:LYS:HD2	4:D:100[B]:LYS:O	2.10	0.51
5:R:14[B]:ARG:HG2	29:R:228:HOH:O	2.11	0.51
12:Y:24[B]:MET:SD	20:Y:101:TGL:CC3	2.99	0.51
20:Y:101:TGL:OA1	20:Y:101:TGL:H162	2.11	0.51
20:L:101:TGL:H292	20:L:101:TGL:H102	1.92	0.51
7:G:11:TPO:CG2	7:G:16:TRP:HE1	2.12	0.51
19:Q:201:PGV:H22	19:Q:201:PGV:C01	2.32	0.51
10:W:33:ARG:HG2	22:W:101:CHD:C18	2.39	0.51
1:A:28:MET:CE	14:A:601:HEA:H273	2.38	0.51
2:O:113:TYR:HD1	8:U:58:ARG:HH22	1.59	0.51
1:N:112:LEU:HD23	1:N:112:LEU:C	2.32	0.50
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.41	0.50
3:P:40:MET:O	3:P:44[B]:MET:HG3	2.10	0.50
7:T:5:LYS:HB2	26:T:102:PEK:H351	1.94	0.50
1:A:514:LYS:HA	6:F:38:ALA:CB	2.39	0.50
7:G:5:LYS:HB3	1:N:278[B]:MET:HE3	1.93	0.50
29:O:571:HOH:O	20:Q:202:TGL:HC61	2.12	0.50
4:Q:33:LEU:HD22	4:Q:37:GLN:HB3	1.94	0.50
12:Y:20:ARG:HH12	12:Y:24[B]:MET:CE	2.23	0.50
2:O:113:TYR:HD1	8:U:58:ARG:NH2	2.10	0.50
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.93	0.50
3:P:54[A]:MET:HB3	3:P:58:TRP:CZ3	2.46	0.50
4:Q:7:LYS:N	4:Q:10:ASP:OD2	2.44	0.50
10:W:32:TYR:OH	22:W:101:CHD:H213	2.11	0.50
12:Y:20:ARG:NH2	12:Y:24[A]:MET:HG3	2.27	0.50
23:O:303:PSC:C2	23:O:303:PSC:H201	2.42	0.50
1:A:28:MET:HE1	14:A:601:HEA:H271	1.94	0.50
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.11	0.50
6:S:54:ASN:HD22	6:S:54:ASN:C	2.15	0.50
12:Y:24[B]:MET:HG2	20:Y:101:TGL:CA2	2.39	0.50
12:L:26:THR:HG23	13:M:25:SER:HB3	1.92	0.50
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.10	0.50
6:S:64:GLU:O	6:S:65:ASP:HB2	2.11	0.50
19:P:303:PGV:H11	19:P:303:PGV:H151	1.94	0.49
7:G:37:LEU:HD21	25:G:102:CDL:C36	2.37	0.49
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.94	0.49
4:Q:78:TRP:CA	20:Q:202:TGL:HB21	2.43	0.49
20:N:608:TGL:C28	20:N:608:TGL:CB9	2.86	0.49
20:D:201:TGL:H342	9:I:16:ARG:HH21	1.76	0.49
1:A:28:MET:HE1	14:A:601:HEA:C27	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:11:TPO:HG22	7:G:16:TRP:NE1	2.12	0.49
20:L:101:TGL:H362	20:L:101:TGL:C31	2.39	0.49
25:P:304:CDL:H392	25:P:304:CDL:H271	1.95	0.49
6:S:85:CYS:SG	6:S:87[A]:THR:CG2	2.82	0.49
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.95	0.49
11:X:42:PRO:O	11:X:47:ARG:NH2	2.45	0.49
2:B:16[B]:ILE:HG13	2:B:17:MET:N	2.27	0.49
1:N:178[B]:GLN:HA	1:N:181:THR:HG23	1.95	0.49
22:P:307:CHD:H12	22:P:307:CHD:H212	1.95	0.48
2:B:41[A]:ILE:HD13	23:B:304:PSC:H342	1.94	0.48
8:H:8:ILE:O	8:H:9:LYS:HE2	2.13	0.48
8:H:9:LYS:N	8:H:9:LYS:HE2	2.28	0.48
12:L:47:LYS:NZ	12:L:47:LYS:HB3	2.28	0.48
3:P:33[B]:MET:CE	28:P:306:DMU:H6	2.43	0.48
3:P:33[B]:MET:HA	28:P:306:DMU:H9	1.96	0.48
3:P:59:ARG:HA	25:P:304:CDL:H512	1.94	0.48
12:Y:20:ARG:CZ	12:Y:24[B]:MET:HE1	2.40	0.48
6:S:1:ALA:HA	7:T:17:ARG:NH1	2.29	0.48
2:B:86:MET:HE1	29:B:403:HOH:O	2.13	0.48
19:C:302:PGV:H212	19:C:302:PGV:C22	2.17	0.48
7:G:70[B]:PHE:HB2	26:G:101:PEK:H041	1.94	0.48
8:H:9:LYS:CE	29:H:103:HOH:O	2.60	0.48
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.94	0.48
10:W:56:PRO:HG3	12:Y:47:LYS:HE2	1.96	0.48
4:D:78:TRP:HB3	20:D:201:TGL:CB2	2.44	0.48
2:O:29[A]:MET:HB2	9:V:35:TYR:CE2	2.49	0.48
20:D:201:TGL:CB3	20:D:201:TGL:OG2	2.61	0.48
25:G:102:CDL:C33	29:O:488:HOH:O	2.50	0.48
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:HD3	2.12	0.48
8:H:45:ALA:O	8:H:47:GLY:N	2.47	0.48
6:F:64:GLU:O	6:F:65:ASP:HB2	2.15	0.47
2:O:83:ILE:O	2:O:87[A]:MET:HG3	2.13	0.47
6:S:94:HIS:HD2	6:S:95:GLN:N	2.10	0.47
8:H:37:HIS:HE1	29:H:111:HOH:O	1.96	0.47
3:P:33[A]:MET:CB	28:P:306:DMU:H9	2.44	0.47
7:T:8:HIS:O	7:T:9:GLY:C	2.51	0.47
1:N:408:THR:HB	19:Q:201:PGV:H51	1.96	0.47
3:P:3:HIS:C	29:P:401:HOH:O	2.52	0.47
4:Q:52:SER:HB2	29:Q:316:HOH:O	2.12	0.47
22:C:305:CHD:H212	22:C:305:CHD:H12	1.95	0.47
20:Q:202:TGL:HA91	20:Q:202:TGL:H231	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:HIS:N	29:C:406:HOH:O	2.46	0.47
5:R:79:LYS:HD2	5:R:79:LYS:HA	1.71	0.47
1:N:22:PHE:HA	20:Y:101:TGL:HB61	1.95	0.47
2:B:1:FME:CN	2:B:193:TYR:H	2.27	0.47
26:C:306:PEK:H382	25:G:102:CDL:H272	1.97	0.47
2:B:41[B]:ILE:HD11	9:I:21:ILE:CD1	2.44	0.47
1:N:113[A]:LEU:HD12	20:Y:101:TGL:C13	2.44	0.47
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.96	0.47
3:P:62:ILE:HD12	25:P:304:CDL:H511	1.97	0.47
1:N:513:LEU:O	1:N:514:LYS:CG	2.63	0.47
25:P:304:CDL:H411	25:P:304:CDL:H452	1.96	0.47
19:A:608:PGV:H231	13:M:12:PRO:HG3	1.97	0.47
11:K:47:ARG:HG2	11:K:48:VAL:HG23	1.95	0.47
7:G:5:LYS:HB3	1:N:278[B]:MET:CE	2.44	0.47
2:O:60:GLU:CD	2:O:60:GLU:N	2.68	0.47
3:P:205:GLY:HA3	26:T:101:PEK:H181	1.95	0.47
25:P:304:CDL:H242	25:P:304:CDL:H652	1.96	0.47
20:Y:101:TGL:HC52	20:Y:101:TGL:HC22	1.45	0.47
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.15	0.47
6:F:87[A]:THR:HG21	29:F:223:HOH:O	2.14	0.47
25:G:102:CDL:H201	25:G:102:CDL:C52	2.42	0.47
10:J:40:LEU:HD12	22:J:102:CHD:O12	2.15	0.47
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.82	0.47
19:A:607:PGV:H343	26:G:101:PEK:C38	2.36	0.47
2:B:58:ALA:O	2:B:62:GLU:HG3	2.15	0.47
1:A:240:HIS:C	1:A:240:HIS:CD2	2.88	0.46
8:H:9:LYS:CA	8:H:9:LYS:HE3	2.42	0.46
25:G:102:CDL:C44	1:N:311[B]:ILE:HG22	2.45	0.46
25:T:103:CDL:H561	25:T:103:CDL:H592	1.52	0.46
1:A:308:ALA:O	1:A:311[B]:ILE:HG22	2.16	0.46
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.50	0.46
2:B:42:ILE:HG21	20:D:201:TGL:H232	1.97	0.46
3:P:224:LYS:CE	25:P:304:CDL:HB32	2.45	0.46
23:B:304:PSC:H221	23:B:304:PSC:H251	1.36	0.46
4:D:78:TRP:CB	20:D:201:TGL:HB21	2.45	0.46
1:N:112:LEU:HG	29:N:921:HOH:O	2.15	0.46
6:S:2:SER:HB2	29:S:309:HOH:O	2.16	0.46
25:T:103:CDL:H142	25:T:103:CDL:H362	1.98	0.46
1:A:282:PHE:CA	7:T:4:ALA:CB	2.85	0.46
9:I:73:LYS:HD3	9:I:73:LYS:HA	1.54	0.46
11:K:39:GLU:HB3	29:K:112:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:156:ARG:HE	22:P:305:CHD:C24	2.28	0.46
7:G:84:LYS:NZ	29:G:203:HOH:O	2.49	0.46
1:N:148:PHE:HB3	3:P:28:THR:HB	1.98	0.46
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.98	0.46
3:P:3:HIS:HD2	29:P:534:HOH:O	1.97	0.46
7:G:3:ALA:O	7:G:4:ALA:CB	2.64	0.46
8:H:7:LYS:HG3	8:H:8:ILE:HD12	1.97	0.46
1:A:136[B]:LEU:CD1	29:A:988:HOH:O	2.33	0.46
10:J:36:MET:HB3	22:J:102:CHD:H183	1.97	0.46
1:N:34:SER:HB2	14:N:601:HEA:C2B	2.46	0.46
2:O:116:LEU:HD13	2:O:226:MET:CG	2.46	0.46
19:A:608:PGV:P	19:A:608:PGV:H061	2.55	0.46
3:C:133:ASN:ND2	29:C:402:HOH:O	2.39	0.46
3:P:103:HIS:HA	19:P:301:PGV:H012	1.98	0.46
19:P:303:PGV:C18	25:P:304:CDL:H662	2.46	0.46
12:Y:12:PRO:HB2	20:Y:101:TGL:HG2	1.97	0.46
3:C:160:LEU:HD13	22:C:304:CHD:H181	1.96	0.45
3:P:208:VAL:HG22	3:P:245:VAL:CG1	2.46	0.45
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.98	0.45
29:A:703:HOH:O	6:F:37:LYS:HE2	2.17	0.45
7:G:33:LEU:O	7:G:37:LEU:HB2	2.15	0.45
3:P:33[B]:MET:HG2	3:P:39:SER:O	2.14	0.45
7:T:3:ALA:O	7:T:4:ALA:CB	2.63	0.45
9:V:61:GLU:OE1	9:V:64:ARG:NE	2.46	0.45
10:J:49:CYS:HB3	28:J:101:DMU:C19	2.40	0.45
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.04	0.45
1:A:297[A]:MET:HG2	29:A:933:HOH:O	2.15	0.45
3:C:41:THR:HA	3:C:44[B]:MET:HE2	1.98	0.45
7:T:31:CYS:SG	25:T:103:CDL:H551	2.56	0.45
1:N:240:HIS:CD2	1:N:240:HIS:C	2.90	0.45
25:C:303:CDL:OB6	25:C:303:CDL:CB2	2.65	0.45
4:D:78:TRP:HB3	20:D:201:TGL:HB21	1.98	0.45
1:N:136[B]:LEU:HD11	29:T:280:HOH:O	2.16	0.45
3:P:116:TRP:HA	3:P:117:PRO:C	2.37	0.45
8:H:31:GLN:NE2	29:H:101:HOH:O	2.37	0.45
20:L:101:TGL:H222	20:L:101:TGL:HA91	1.63	0.45
26:C:306:PEK:H331	26:C:306:PEK:H362	1.72	0.45
6:F:87[B]:THR:HG21	29:F:304:HOH:O	2.16	0.45
8:H:9:LYS:HD3	8:H:11:TYR:HB2	1.98	0.45
2:O:32[B]:PHE:CD2	9:V:31:PHE:CZ	3.05	0.45
2:B:22[B]:HIS:CE1	29:B:461:HOH:O	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:304:CHD:H231	22:C:304:CHD:H162	1.98	0.45
2:B:116:LEU:HD11	2:B:226:MET:HB3	1.99	0.45
12:L:20:ARG:NH2	20:L:101:TGL:HC52	2.27	0.45
3:P:33[A]:MET:CB	28:P:306:DMU:C19	2.94	0.45
5:R:108:LYS:NZ	29:R:203:HOH:O	2.48	0.44
1:A:178[B]:GLN:HG2	1:A:179:TYR:CE2	2.52	0.44
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.72	0.44
25:T:103:CDL:H612	25:T:103:CDL:H672	1.99	0.44
9:V:36:LYS:NZ	9:V:36:LYS:HB2	2.32	0.44
2:B:78:LEU:CD1	2:B:78:LEU:N	2.81	0.44
8:H:37:HIS:HD2	8:H:40:GLU:OE2	2.00	0.44
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.18	0.44
26:T:101:PEK:H203	26:T:101:PEK:H171	1.71	0.44
7:G:2:SER:OG	26:G:103:PEK:H292	2.17	0.44
10:J:7:GLU:HG3	29:J:238:HOH:O	2.16	0.44
20:L:101:TGL:H312	20:L:101:TGL:C36	2.43	0.44
1:N:336:PRO:HB2	1:N:394[B]:VAL:HG11	2.00	0.44
1:N:483:LEU:HD21	13:Z:4:LYS:HE3	1.99	0.44
10:J:52:TRP:O	10:J:57:HIS:HE1	2.00	0.44
1:N:178[B]:GLN:HG3	1:N:178[B]:GLN:O	2.18	0.44
3:P:80[A]:ARG:HH11	3:P:80[A]:ARG:HD3	1.49	0.44
6:S:21[B]:MET:HE2	6:S:21[B]:MET:HB2	1.64	0.44
25:T:103:CDL:H382	25:T:103:CDL:H161	1.98	0.44
7:T:37:LEU:HD12	7:T:37:LEU:HA	1.89	0.44
23:O:303:PSC:H242	23:O:303:PSC:H272	1.66	0.44
25:P:304:CDL:H132	25:P:304:CDL:OA6	2.17	0.44
7:T:38:HIS:CE1	25:T:103:CDL:H122	2.52	0.44
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.99	0.44
1:A:28:MET:HE2	14:A:601:HEA:C27	2.41	0.44
7:G:38:HIS:CD2	29:G:209:HOH:O	2.71	0.44
7:G:84:LYS:N	7:G:84:LYS:CD	2.69	0.44
26:P:308:PEK:C04	6:S:1:ALA:N	2.78	0.44
7:T:11:TPO:O	7:T:11:TPO:HG22	2.18	0.44
2:B:164:ALA:O	2:B:194:GLY:HA3	2.18	0.44
20:B:301:TGL:H252	20:B:301:TGL:H221	1.76	0.44
29:A:703:HOH:O	6:F:37:LYS:HG3	2.17	0.44
25:P:304:CDL:H261	25:P:304:CDL:H672	1.99	0.44
3:P:41:THR:HA	3:P:44[B]:MET:HE2	2.00	0.44
5:R:6:GLU:HA	29:R:308:HOH:O	2.17	0.44
11:K:6:ALA:N	29:K:103:HOH:O	2.51	0.44
26:P:308:PEK:H042	6:S:1:ALA:H2	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:6:VAL:HG13	29:Q:446:HOH:O	2.18	0.44
1:A:302[B]:ARG:NH1	29:A:705:HOH:O	2.51	0.43
2:B:32[B]:PHE:CE2	9:I:31:PHE:CZ	3.06	0.43
20:Y:101:TGL:H283	20:Y:101:TGL:H252	1.53	0.43
25:C:303:CDL:H671	25:C:303:CDL:H641	1.87	0.43
7:G:5:LYS:HA	1:N:278[B]:MET:HE3	2.00	0.43
8:H:9:LYS:NZ	29:H:103:HOH:O	2.45	0.43
3:C:55:TYR:CD1	25:C:303:CDL:H532	2.54	0.43
19:C:302:PGV:H172	25:C:303:CDL:C65	2.48	0.43
12:L:26:THR:HG23	13:M:25:SER:CB	2.47	0.43
14:N:601:HEA:HHC	14:N:601:HEA:H122	2.01	0.43
2:O:215:PRO:HD3	9:V:60:PHE:CD2	2.53	0.43
1:N:514:LYS:HG2	6:S:38:ALA:CB	2.48	0.43
7:T:8:HIS:CD2	7:T:8:HIS:O	2.71	0.43
1:A:334:TRP:HB2	20:D:201:TGL:HG11	2.00	0.43
2:B:41[B]:ILE:HA	2:B:41[B]:ILE:HD13	1.72	0.43
7:G:83:GLU:OE2	29:G:201:HOH:O	2.21	0.43
8:H:8:ILE:C	8:H:9:LYS:HE2	2.38	0.43
10:J:32:TYR:CE2	22:J:102:CHD:H213	2.54	0.43
1:N:426:PHE:HZ	20:N:608:TGL:HA42	1.83	0.43
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.84	0.43
26:P:308:PEK:C1	29:P:441:HOH:O	2.67	0.43
6:S:87[A]:THR:HG21	29:S:266:HOH:O	2.19	0.43
7:T:5:LYS:CG	26:T:102:PEK:H351	2.46	0.43
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	2.00	0.43
7:G:10:GLY:HA3	29:G:272:HOH:O	2.19	0.43
1:N:377:PHE:HA	1:N:380:VAL:HG22	2.00	0.43
1:N:514:LYS:NZ	29:N:704:HOH:O	2.50	0.43
23:O:303:PSC:H322	23:O:303:PSC:H281	1.99	0.43
3:P:63:ARG:NE	25:P:304:CDL:HA22	2.29	0.43
29:C:401:HOH:O	6:F:52:ILE:HD11	2.18	0.43
25:G:102:CDL:H441	1:N:311[B]:ILE:HG22	2.01	0.43
4:Q:17[B]:VAL:HG22	4:Q:19[B]:ARG:HG3	2.00	0.43
1:A:112:LEU:HD23	1:A:112:LEU:C	2.38	0.43
25:G:102:CDL:H401	2:O:77:ALA:CB	2.48	0.43
9:I:36:LYS:HZ2	9:I:36:LYS:HB2	1.84	0.43
10:W:27:THR:HG22	29:W:208:HOH:O	2.18	0.43
29:A:763:HOH:O	12:L:7:PRO:HG3	2.19	0.43
1:N:24:ALA:HB2	14:N:601:HEA:H253	2.01	0.43
23:O:303:PSC:H292	23:O:303:PSC:H262	1.04	0.43
20:Q:202:TGL:CA9	20:Q:202:TGL:C23	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:103:CDL:H631	25:T:103:CDL:H661	1.77	0.43
2:B:41[A]:ILE:O	2:B:42:ILE:C	2.56	0.42
7:G:5:LYS:HD3	1:N:278[B]:MET:HE3	2.00	0.42
23:O:303:PSC:H291	23:O:303:PSC:H261	0.86	0.42
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.01	0.42
1:A:76:GLY:O	1:A:80:ASN:HB2	2.20	0.42
26:C:306:PEK:C38	25:G:102:CDL:H271	2.30	0.42
7:G:3:ALA:O	7:G:4:ALA:HB2	2.19	0.42
6:S:51:SER:O	6:S:93:PRO:HA	2.19	0.42
22:W:101:CHD:H111	22:W:101:CHD:H12A	1.90	0.42
12:L:25:MET:HG2	20:L:101:TGL:HA62	2.01	0.42
19:Q:201:PGV:H22	19:Q:201:PGV:H202	2.01	0.42
25:T:103:CDL:H541	25:T:103:CDL:C24	2.34	0.42
3:C:37:PHE:CG	28:J:101:DMU:H6	2.54	0.42
2:B:16[A]:ILE:HD11	2:B:86:MET:HG2	2.00	0.42
3:C:33[A]:MET:HB2	28:J:101:DMU:C22	2.49	0.42
1:N:302[B]:ARG:HG2	1:N:302[B]:ARG:NH1	2.35	0.42
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.50	0.42
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.85	0.42
9:I:73:LYS:HD3	29:I:125:HOH:O	2.18	0.42
1:N:87:ILE:O	1:N:173:PRO:HD3	2.20	0.42
25:T:103:CDL:HA21	25:T:103:CDL:H111	2.02	0.42
1:A:169:ILE:HA	1:A:169:ILE:HD13	1.87	0.42
19:A:608:PGV:O06	29:A:702:HOH:O	2.18	0.42
19:C:307:PGV:H72	19:C:307:PGV:H42	1.77	0.42
3:P:177:GLN:HA	3:P:177:GLN:OE1	2.20	0.42
10:W:32:TYR:CE2	22:W:101:CHD:H213	2.55	0.42
1:A:172:LYS:HD2	1:A:181:THR:HG22	2.01	0.41
3:C:144[B]:ILE:HA	3:C:144[B]:ILE:HD12	1.93	0.41
1:N:62:ALA:HB2	14:N:601:HEA:HBD1	2.01	0.41
20:Q:202:TGL:HG31	20:Q:202:TGL:HC21	1.55	0.41
3:C:217:VAL:HG22	25:C:303:CDL:H732	2.02	0.41
20:D:201:TGL:HB92	20:D:201:TGL:H132	2.02	0.41
7:G:5:LYS:CB	1:N:278[B]:MET:HE3	2.50	0.41
1:A:336:PRO:HB2	1:A:394[B]:VAL:HG11	2.02	0.41
1:A:489:THR:HA	6:F:71:TRP:O	2.20	0.41
2:O:16:ILE:HD12	2:O:87[A]:MET:HG2	2.03	0.41
3:P:33[B]:MET:HE3	28:P:306:DMU:H6	2.02	0.41
2:O:130:PRO:HA	4:Q:115:TRP:CZ3	2.55	0.41
2:B:56:MET:HA	23:B:304:PSC:C20	2.37	0.41
9:I:68:ILE:HD13	9:I:68:ILE:HG21	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:G:102:CDL:H371	2:O:78:LEU:CD1	2.51	0.41
3:C:116:TRP:HA	3:C:117:PRO:C	2.40	0.41
25:G:102:CDL:H201	25:G:102:CDL:H511	2.03	0.41
1:N:439:ARG:HD3	2:O:199:ILE:HB	2.03	0.41
25:T:103:CDL:H581	25:T:103:CDL:H782	2.03	0.41
3:C:65:SER:HB3	3:C:71:HIS:CE1	2.56	0.41
6:F:55:LYS:HA	6:F:74:LEU:O	2.20	0.41
1:N:333:LYS:CD	29:N:988:HOH:O	2.68	0.41
25:G:102:CDL:H541	25:G:102:CDL:C23	2.47	0.41
8:H:8:ILE:CG2	8:H:8:ILE:O	2.69	0.41
13:M:32:TRP:CZ3	13:M:40:TYR:OH	2.74	0.41
1:N:107:PRO:HB3	3:P:25:LEU:HB2	2.01	0.41
1:N:361:SER:OG	2:O:84:LEU:HD13	2.20	0.41
7:T:38:HIS:ND1	7:T:38:HIS:N	2.69	0.41
2:B:1:FME:HCN	2:B:193:TYR:HB2	2.02	0.41
1:A:268:PHE:CZ	2:B:58:ALA:HA	2.55	0.41
3:C:131:LEU:CD2	25:G:102:CDL:HB61	2.51	0.41
22:J:102:CHD:H193	22:J:102:CHD:H111	1.60	0.41
2:O:164:ALA:O	2:O:194:GLY:HA3	2.21	0.41
22:P:305:CHD:H222	22:P:305:CHD:H162	1.50	0.41
11:X:24:PHE:O	11:X:28[A]:VAL:HG12	2.21	0.41
11:X:8:ASP:HB2	29:X:111:HOH:O	2.20	0.41
4:Q:107:ILE:HB	4:Q:108:PRO:CD	2.51	0.41
7:T:41:HIS:HB3	7:T:74:ARG:NH1	2.36	0.41
8:U:37:HIS:HD2	8:U:40:GLU:OE2	2.04	0.41
29:H:145:HOH:O	8:U:46:LYS:HD3	2.19	0.41
8:H:46:LYS:HD2	29:U:155:HOH:O	2.20	0.41
6:F:54[A]:ASN:N	6:F:54[A]:ASN:ND2	2.65	0.41
25:G:102:CDL:C24	25:G:102:CDL:C54	2.80	0.41
2:O:13:THR:HG21	2:O:192:TYR:CZ	2.55	0.41
2:O:84:LEU:HA	2:O:87[A]:MET:HE2	2.03	0.41
3:P:50:ASN:HD22	3:P:51[A]:MET:CE	2.33	0.41
4:Q:109:HIS:HD2	29:Q:401:HOH:O	2.03	0.41
9:V:2:THR:HG22	29:V:137:HOH:O	2.19	0.41
2:B:48:THR:HB	9:I:16:ARG:CZ	2.51	0.40
20:L:101:TGL:HB62	20:L:101:TGL:HB31	1.80	0.40
3:P:202:GLY:HA3	26:T:101:PEK:H21	2.03	0.40
1:A:172:LYS:HZ2	1:A:178[A]:GLN:HE22	1.69	0.40
1:A:439:ARG:HD3	2:B:199:ILE:HB	2.03	0.40
8:H:46:LYS:HG2	29:H:171:HOH:O	2.20	0.40
3:P:48:THR:HG23	25:P:304:CDL:H401	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:94:HIS:CG	6:S:95:GLN:N	2.84	0.40
1:A:208[B]:MET:HB3	1:A:219:PHE:CD1	2.57	0.40
1:A:293:PHE:CE1	1:A:361[B]:SER:HB2	2.57	0.40
1:A:361[A]:SER:OG	2:B:84:LEU:HD13	2.21	0.40
2:O:13:THR:HB	2:O:168:LEU:HD23	2.03	0.40
4:Q:78:TRP:CB	20:Q:202:TGL:HB22	2.50	0.40
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.22	0.40
25:P:304:CDL:H631	25:P:304:CDL:H222	2.02	0.40
7:T:5:LYS:CB	26:T:102:PEK:H351	2.51	0.40
2:B:59:GLN:HG2	29:B:468:HOH:O	2.20	0.40
25:C:303:CDL:H201	25:C:303:CDL:H621	2.03	0.40
3:C:38:ASN:HA	29:C:450:HOH:O	2.21	0.40
26:C:306:PEK:H041	7:G:17:ARG:HH22	1.87	0.40
26:P:308:PEK:C04	6:S:1:ALA:H2	2.33	0.40
1:A:278[B]:MET:HE1	7:T:5:LYS:HB3	2.02	0.40
22:W:101:CHD:H212	22:W:101:CHD:H162	1.82	0.40
10:W:29:ASN:H	10:W:29:ASN:HD22	1.69	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:2:THR:CB	5:R:80:GLU:OE1[3_647]	2.00	0.20
9:I:2:THR:CG2	5:R:80:GLU:OE1[3_647]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/514 (103%)	515 (97%)	15 (3%)	0	100	100
1	N	528/514 (103%)	511 (97%)	17 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	234/227 (103%)	230 (98%)	4 (2%)	0	100 100
2	O	230/227 (101%)	225 (98%)	4 (2%)	1 (0%)	39 14
3	C	266/261 (102%)	261 (98%)	4 (2%)	1 (0%)	39 14
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100 100
4	D	147/147 (100%)	143 (97%)	4 (3%)	0	100 100
4	Q	145/147 (99%)	139 (96%)	5 (3%)	1 (1%)	26 6
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100 100
5	R	104/109 (95%)	104 (100%)	0	0	100 100
6	F	100/98 (102%)	95 (95%)	3 (3%)	2 (2%)	9 1
6	S	98/98 (100%)	92 (94%)	2 (2%)	4 (4%)	3 0
7	G	82/85 (96%)	68 (83%)	8 (10%)	6 (7%)	1 0
7	T	82/85 (96%)	71 (87%)	5 (6%)	6 (7%)	1 0
8	H	77/85 (91%)	68 (88%)	6 (8%)	3 (4%)	4 0
8	U	77/85 (91%)	68 (88%)	5 (6%)	4 (5%)	2 0
9	I	71/73 (97%)	71 (100%)	0	0	100 100
9	V	71/73 (97%)	69 (97%)	1 (1%)	1 (1%)	14 2
10	J	56/59 (95%)	56 (100%)	0	0	100 100
10	W	57/59 (97%)	57 (100%)	0	0	100 100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100 100
11	X	48/56 (86%)	46 (96%)	2 (4%)	0	100 100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100 100
12	Y	45/47 (96%)	43 (96%)	2 (4%)	0	100 100
13	M	41/46 (89%)	39 (95%)	2 (5%)	0	100 100
13	Z	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	7 1
All	All	3590/3614 (99%)	3460 (96%)	100 (3%)	30 (1%)	21 5

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
6	F	96	LEU
7	G	4	ALA
7	G	5	LYS
7	G	8	HIS

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Mol	Chain	Res	Type
8	H	8	ILE
8	H	45	ALA
4	Q	8	SER
6	S	94	HIS
6	S	95	GLN
7	T	3	ALA
7	T	4	ALA
7	T	5	LYS
7	T	7	ASP
7	T	8	HIS
8	U	8	ILE
8	U	45	ALA
8	U	46	LYS
8	H	46	LYS
6	S	96	LEU
9	V	2	THR
13	Z	42	LYS
7	G	37	LEU
7	G	7	ASP
8	U	51	SER
3	C	232	HIS
2	O	92	ASN
7	T	6	GLY
6	S	93	PRO
7	G	9	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	444/426 (104%)	438 (99%)	6 (1%)	74 47
1	N	442/426 (104%)	432 (98%)	10 (2%)	58 24
2	B	219/210 (104%)	208 (95%)	11 (5%)	30 5
2	O	215/210 (102%)	206 (96%)	9 (4%)	36 7
3	C	233/226 (103%)	230 (99%)	3 (1%)	76 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	P	233/226 (103%)	230 (99%)	3 (1%)	76 50
4	D	133/129 (103%)	128 (96%)	5 (4%)	40 9
4	Q	131/129 (102%)	124 (95%)	7 (5%)	28 4
5	E	92/95 (97%)	90 (98%)	2 (2%)	60 25
5	R	93/95 (98%)	91 (98%)	2 (2%)	60 25
6	F	85/81 (105%)	79 (93%)	6 (7%)	18 1
6	S	83/81 (102%)	75 (90%)	8 (10%)	10 0
7	G	68/68 (100%)	63 (93%)	5 (7%)	17 1
7	T	68/68 (100%)	61 (90%)	7 (10%)	9 0
8	H	71/75 (95%)	65 (92%)	6 (8%)	13 1
8	U	71/75 (95%)	67 (94%)	4 (6%)	26 3
9	I	57/57 (100%)	55 (96%)	2 (4%)	43 11
9	V	57/57 (100%)	52 (91%)	5 (9%)	12 1
10	J	49/50 (98%)	49 (100%)	0	100 100
10	W	50/50 (100%)	48 (96%)	2 (4%)	38 8
11	K	39/46 (85%)	38 (97%)	1 (3%)	54 19
11	X	40/46 (87%)	40 (100%)	0	100 100
12	L	39/40 (98%)	38 (97%)	1 (3%)	54 19
12	Y	40/40 (100%)	38 (95%)	2 (5%)	30 5
13	M	37/38 (97%)	33 (89%)	4 (11%)	8 0
13	Z	37/38 (97%)	33 (89%)	4 (11%)	8 0
All	All	3126/3082 (101%)	3011 (96%)	115 (4%)	42 10

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	369	ASP
2	B	32[A]	PHE
2	B	32[B]	PHE
2	B	33	LEU

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Mol	Chain	Res	Type
2	B	59	GLN
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	86	MET
2	B	91	ASN
2	B	115	ASP
2	B	171	LYS
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	19[A]	ARG
4	D	19[B]	ARG
4	D	31[A]	LYS
4	D	31[B]	LYS
5	E	5	HIS
5	E	70	VAL
6	F	37	LYS
6	F	54[A]	ASN
6	F	54[B]	ASN
6	F	80	GLN
6	F	94	HIS
6	F	98	HIS
7	G	2	SER
7	G	18	PHE
7	G	43	GLU
7	G	54	ARG
7	G	84	LYS
8	H	7	LYS
8	H	9	LYS
8	H	29	CYS
8	H	51	SER
8	H	60	TYR
8	H	61	LYS
9	I	36	LYS
9	I	37	PHE
11	K	47	ARG
12	L	47	LYS
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS

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Mol	Chain	Res	Type
13	M	43	SER
1	N	109	PHE
1	N	138	HIS
1	N	174	PRO
1	N	178[A]	GLN
1	N	178[B]	GLN
1	N	180	GLN
1	N	363	LEU
1	N	369	ASP
1	N	495	LEU
1	N	504	THR
2	O	33	LEU
2	O	60	GLU
2	O	65	TRP
2	O	68	LEU
2	O	78	LEU
2	O	91	ASN
2	O	115	ASP
2	O	171	LYS
2	O	217	LYS
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	7	LYS
4	Q	8	SER
4	Q	9	GLU
4	Q	20	ARG
4	Q	51	LEU
4	Q	58	GLU
4	Q	143	ASN
5	R	79	LYS
5	R	91	PRO
6	S	43	LYS
6	S	54	ASN
6	S	80	GLN
6	S	87[A]	THR
6	S	87[B]	THR
6	S	94	HIS
6	S	96	LEU
6	S	98	HIS
7	T	2	SER
7	T	7	ASP

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Mol	Chain	Res	Type
7	T	18	PHE
7	T	37	LEU
7	T	38	HIS
7	T	54	ARG
7	T	84	LYS
8	U	8	ILE
8	U	9	LYS
8	U	60	TYR
8	U	61	LYS
9	V	2	THR
9	V	36	LYS
9	V	37	PHE
9	V	61	GLU
9	V	70	GLN
10	W	7	GLU
10	W	50	LEU
12	Y	2	HIS
12	Y	20	ARG
13	Z	13	LYS
13	Z	38	ASP
13	Z	39	ASN
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
2	B	10	GLN
2	B	52	HIS
2	B	59	GLN
2	B	181	GLN
2	B	195	GLN
3	C	3	HIS
3	C	68	GLN
3	C	76	GLN
4	D	37	GLN
4	D	109	HIS
4	D	143	ASN
5	E	94	ASN
6	F	80	GLN
7	G	76	ASN
8	H	31	GLN

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Mol	Chain	Res	Type
8	H	37	HIS
10	J	29	ASN
10	J	57	HIS
1	N	180	GLN
2	O	10	GLN
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
7	T	8	HIS
7	T	76	ASN
8	U	31	GLN
8	U	37	HIS
9	V	20	HIS
10	W	29	ASN
10	W	57	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	FME	A	1	1	8,9,10	1.62	2 (25%)	5,9,11	2.16	3 (60%)
2	FME	B	1	2	8,9,10	5.44	6 (75%)	5,9,11	13.37	2 (40%)
7	TPO	G	11	7	7,10,11	2.16	3 (42%)	10,14,16	2.41	3 (30%)
9	SAC	I	1	9	7,8,9	2.62	3 (42%)	7,9,11	1.49	1 (14%)
1	FME	N	1	1	8,9,10	1.22	1 (12%)	5,9,11	2.22	3 (60%)
2	FME	O	1	2	8,9,10	1.83	4 (50%)	5,9,11	2.07	2 (40%)
7	TPO	T	11	7	7,10,11	1.65	2 (28%)	10,14,16	1.70	2 (20%)
9	SAC	V	1	9	7,8,9	2.28	2 (28%)	7,9,11	2.29	4 (57%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	0/6/9/11	0/0/0/0
2	FME	B	1	2	-	1/6/9/11	0/0/0/0
7	TPO	G	11	7	-	0/8/11/13	0/0/0/0
9	SAC	I	1	9	-	0/6/8/10	0/0/0/0
1	FME	N	1	1	-	0/6/9/11	0/0/0/0
2	FME	O	1	2	-	0/6/9/11	0/0/0/0
7	TPO	T	11	7	-	0/8/11/13	0/0/0/0
9	SAC	V	1	9	-	0/6/8/10	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-8.24	0.95	1.22
2	B	1	FME	CG-SD	-4.18	1.59	1.81
2	O	1	FME	CG-SD	-3.02	1.65	1.81
1	N	1	FME	CB-CG	2.03	1.59	1.51
9	I	1	SAC	O-C	2.05	1.29	1.19
2	O	1	FME	CB-CG	2.08	1.60	1.51
2	O	1	FME	CN-N	2.08	1.40	1.33
7	T	11	TPO	P-O3P	2.18	1.62	1.54
7	G	11	TPO	P-O2P	2.28	1.62	1.54
1	A	1	FME	O-C	2.49	1.31	1.19
7	G	11	TPO	CG2-CB	2.60	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1	FME	CB-CA	2.71	1.58	1.53
7	T	11	TPO	P-O1P	2.95	1.60	1.50
7	G	11	TPO	P-O1P	3.36	1.61	1.50
9	I	1	SAC	CA-N	3.39	1.51	1.46
2	B	1	FME	CB-CG	3.45	1.65	1.51
1	A	1	FME	CA-N	3.48	1.51	1.46
2	B	1	FME	CA-N	3.82	1.51	1.46
9	V	1	SAC	CA-N	3.90	1.51	1.46
2	B	1	FME	CB-CA	4.27	1.61	1.53
9	V	1	SAC	OAC-C1A	4.42	1.33	1.23
9	I	1	SAC	OAC-C1A	5.17	1.35	1.23
2	B	1	FME	CN-N	10.25	1.71	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	FME	O1-CN-N	-29.38	79.86	124.80
2	B	1	FME	CG-CB-CA	-5.24	97.31	113.07
7	G	11	TPO	C-CA-N	-4.14	100.81	109.95
2	O	1	FME	CG-CB-CA	-4.03	100.96	113.07
1	A	1	FME	O1-CN-N	-3.19	119.92	124.80
1	N	1	FME	O-C-CA	-2.91	117.75	125.69
7	G	11	TPO	O-C-CA	-2.91	117.75	125.69
1	A	1	FME	O-C-CA	-2.82	117.97	125.69
9	V	1	SAC	OAC-C1A-N	-2.74	116.26	121.84
9	V	1	SAC	O-C-CA	-2.17	119.75	125.69
2	O	1	FME	O-C-CA	-2.13	119.86	125.69
7	T	11	TPO	O-C-CA	-2.04	120.11	125.69
1	A	1	FME	CE-SD-CG	2.05	107.50	100.36
1	N	1	FME	CB-CG-SD	2.16	122.53	113.07
9	V	1	SAC	CA-N-C1A	2.59	130.21	121.32
1	N	1	FME	CE-SD-CG	3.11	111.16	100.36
9	I	1	SAC	CB-CA-N	3.15	117.60	110.70
9	V	1	SAC	C2A-C1A-N	3.45	122.70	116.10
7	T	11	TPO	O3P-P-OG1	4.27	119.39	106.62
7	G	11	TPO	CG2-CB-CA	5.11	123.35	113.15

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	FME	O1-CN-N-CA

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FME	7	0
7	G	11	TPO	4	0
7	T	11	TPO	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 46 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	HEA	A	601	1	40,67,67	2.58	16 (40%)	36,103,103	3.14	15 (41%)
14	HEA	A	602	1,18	40,67,67	1.76	7 (17%)	36,103,103	2.44	12 (33%)
18	PER	A	606	15,14	0,1,1	0.00	-	0,0,0	0.00	-
19	PGV	A	607	-	50,50,50	1.50	8 (16%)	51,56,56	1.54	11 (21%)
19	PGV	A	608	-	50,50,50	1.94	6 (12%)	51,56,56	2.45	14 (27%)
20	TGL	B	301	-	62,62,62	1.70	8 (12%)	65,65,65	2.94	21 (32%)
21	CUA	B	302	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	B	303	-	29,32,32	2.70	17 (58%)	48,51,51	2.70	23 (47%)
23	PSC	B	304	-	51,51,51	1.29	3 (5%)	55,59,59	1.80	14 (25%)
19	PGV	C	302	-	50,50,50	1.40	5 (10%)	51,56,56	2.04	5 (9%)
25	CDL	C	303	-	99,99,99	1.77	20 (20%)	101,111,111	2.29	30 (29%)
22	CHD	C	304	-	29,32,32	1.46	5 (17%)	48,51,51	3.86	27 (56%)
22	CHD	C	305	-	29,32,32	2.39	13 (44%)	48,51,51	2.85	20 (41%)
26	PEK	C	306	-	51,52,52	1.60	5 (9%)	52,57,57	2.24	19 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	PGV	C	307	-	50,50,50	1.26	4 (8%)	51,56,56	1.60	7 (13%)
20	TGL	D	201	-	62,62,62	2.74	11 (17%)	65,65,65	3.32	25 (38%)
26	PEK	G	101	-	51,52,52	1.18	4 (7%)	52,57,57	1.73	13 (25%)
25	CDL	G	102	-	99,99,99	1.46	14 (14%)	101,111,111	1.85	23 (22%)
26	PEK	G	103	-	51,52,52	1.27	3 (5%)	52,57,57	1.86	12 (23%)
28	DMU	J	101	-	34,34,34	0.96	1 (2%)	45,45,45	1.60	7 (15%)
22	CHD	J	102	-	29,32,32	1.82	8 (27%)	48,51,51	4.74	32 (66%)
20	TGL	L	101	-	62,62,62	2.06	13 (20%)	65,65,65	2.84	26 (40%)
28	DMU	M	101	-	34,34,34	1.47	5 (14%)	45,45,45	2.25	17 (37%)
14	HEA	N	601	1	40,67,67	2.25	11 (27%)	36,103,103	3.61	16 (44%)
14	HEA	N	602	1,18	40,67,67	1.53	8 (20%)	36,103,103	2.51	16 (44%)
18	PER	N	606	15,14	0,1,1	0.00	-	0,0,0	0.00	-
19	PGV	N	607	-	50,50,50	1.48	7 (14%)	51,56,56	1.49	10 (19%)
20	TGL	N	608	-	62,62,62	1.43	8 (12%)	65,65,65	2.22	12 (18%)
21	CUA	O	301	2	0,1,1	0.00	-	0,0,0	0.00	-
22	CHD	O	302	-	29,32,32	2.43	10 (34%)	48,51,51	2.50	21 (43%)
23	PSC	O	303	-	51,51,51	1.42	3 (5%)	55,59,59	1.75	11 (20%)
19	PGV	P	301	-	50,50,50	1.08	2 (4%)	51,56,56	1.69	8 (15%)
19	PGV	P	303	-	50,50,50	1.08	3 (6%)	51,56,56	1.53	13 (25%)
25	CDL	P	304	-	99,99,99	2.00	24 (24%)	101,111,111	2.15	31 (30%)
22	CHD	P	305	-	29,32,32	1.38	5 (17%)	48,51,51	3.61	28 (58%)
28	DMU	P	306	-	34,34,34	0.84	1 (2%)	45,45,45	1.90	9 (20%)
22	CHD	P	307	-	29,32,32	1.86	9 (31%)	48,51,51	2.62	17 (35%)
26	PEK	P	308	-	51,52,52	1.66	6 (11%)	52,57,57	1.94	14 (26%)
19	PGV	Q	201	-	50,50,50	1.29	3 (6%)	51,56,56	1.78	10 (19%)
20	TGL	Q	202	-	62,62,62	2.32	10 (16%)	65,65,65	2.70	14 (21%)
26	PEK	T	101	-	51,52,52	1.59	5 (9%)	52,57,57	2.27	11 (21%)
26	PEK	T	102	-	51,52,52	1.29	2 (3%)	52,57,57	1.65	8 (15%)
25	CDL	T	103	-	99,99,99	1.49	12 (12%)	101,111,111	1.72	19 (18%)
22	CHD	W	101	-	29,32,32	1.95	10 (34%)	48,51,51	4.72	30 (62%)
20	TGL	Y	101	-	62,62,62	2.01	12 (19%)	65,65,65	3.08	27 (41%)
28	DMU	Z	101	-	34,34,34	1.25	5 (14%)	45,45,45	1.90	14 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	A	601	1	3/3/7/16	0/24/76/76	0/0/8/8
14	HEA	A	602	1,18	3/3/7/16	0/24/76/76	0/0/8/8
18	PER	A	606	15,14	-	0/0/0/0	0/0/0/0
19	PGV	A	607	-	-	0/55/55/55	0/0/0/0
19	PGV	A	608	-	-	0/55/55/55	0/0/0/0
20	TGL	B	301	-	-	0/65/65/65	0/0/0/0
21	CUA	B	302	2	-	0/0/0/0	0/0/0/0
22	CHD	B	303	-	-	0/7/74/74	0/4/4/4
23	PSC	B	304	-	-	0/55/55/55	0/0/0/0
19	PGV	C	302	-	-	0/55/55/55	0/0/0/0
25	CDL	C	303	-	-	0/110/110/110	0/0/0/0
22	CHD	C	304	-	-	0/7/74/74	0/4/4/4
22	CHD	C	305	-	-	0/7/74/74	0/4/4/4
26	PEK	C	306	-	-	0/56/56/56	0/0/0/0
19	PGV	C	307	-	-	0/55/55/55	0/0/0/0
20	TGL	D	201	-	-	0/65/65/65	0/0/0/0
26	PEK	G	101	-	-	0/56/56/56	0/0/0/0
25	CDL	G	102	-	-	1/110/110/110	0/0/0/0
26	PEK	G	103	-	-	0/56/56/56	0/0/0/0
28	DMU	J	101	-	-	0/19/59/59	0/2/2/2
22	CHD	J	102	-	-	0/7/74/74	0/4/4/4
20	TGL	L	101	-	-	0/65/65/65	0/0/0/0
28	DMU	M	101	-	-	0/19/59/59	0/2/2/2
14	HEA	N	601	1	2/2/7/16	0/24/76/76	0/0/8/8
14	HEA	N	602	1,18	3/3/7/16	0/24/76/76	0/0/8/8
18	PER	N	606	15,14	-	0/0/0/0	0/0/0/0
19	PGV	N	607	-	-	0/55/55/55	0/0/0/0
20	TGL	N	608	-	-	0/65/65/65	0/0/0/0
21	CUA	O	301	2	-	0/0/0/0	0/0/0/0
22	CHD	O	302	-	-	0/7/74/74	0/4/4/4
23	PSC	O	303	-	-	0/55/55/55	0/0/0/0
19	PGV	P	301	-	-	1/55/55/55	0/0/0/0
19	PGV	P	303	-	-	0/55/55/55	0/0/0/0
25	CDL	P	304	-	-	0/110/110/110	0/0/0/0
22	CHD	P	305	-	-	0/7/74/74	0/4/4/4
28	DMU	P	306	-	-	0/19/59/59	0/2/2/2
22	CHD	P	307	-	-	0/7/74/74	0/4/4/4
26	PEK	P	308	-	-	0/56/56/56	0/0/0/0
19	PGV	Q	201	-	-	2/55/55/55	0/0/0/0
20	TGL	Q	202	-	-	0/65/65/65	0/0/0/0
26	PEK	T	101	-	-	0/56/56/56	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEK	T	102	-	-	0/56/56/56	0/0/0/0
25	CDL	T	103	-	-	0/110/110/110	0/0/0/0
22	CHD	W	101	-	-	0/7/74/74	0/4/4/4
20	TGL	Y	101	-	-	0/65/65/65	0/0/0/0
28	DMU	Z	101	-	-	0/19/59/59	0/2/2/2

All (332) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	C18-C19	-7.80	1.12	1.32
20	B	301	TGL	OC1-CC1	-6.22	1.04	1.22
14	A	601	HEA	C16-C17	-5.95	1.32	1.53
14	N	601	HEA	C18-C19	-5.85	1.17	1.32
14	A	602	HEA	C3C-C2C	-5.29	1.33	1.40
22	O	302	CHD	C10-C5	-5.27	1.46	1.55
22	B	303	CHD	C13-C14	-5.02	1.46	1.55
14	N	601	HEA	C3C-C2C	-4.51	1.34	1.40
14	A	601	HEA	C3C-C2C	-4.33	1.34	1.40
14	N	601	HEA	C16-C17	-4.16	1.39	1.53
20	D	201	TGL	C10-CB9	-4.00	1.28	1.51
25	C	303	CDL	C79-C78	-3.98	1.28	1.51
14	A	601	HEA	C3A-C2A	-3.91	1.35	1.40
20	B	301	TGL	CB2-CB1	-3.89	1.39	1.50
25	T	103	CDL	C42-C41	-3.63	1.30	1.51
14	A	601	HEA	C14-C15	-3.58	1.23	1.32
20	L	101	TGL	C20-CA9	-3.45	1.31	1.51
25	P	304	CDL	C79-C78	-3.40	1.32	1.51
25	P	304	CDL	C59-C58	-3.38	1.32	1.51
22	B	303	CHD	C10-C5	-3.36	1.49	1.55
20	L	101	TGL	C10-CB9	-3.30	1.32	1.51
25	G	102	CDL	C59-C58	-3.30	1.32	1.51
20	Q	202	TGL	C10-CB9	-3.22	1.33	1.51
25	G	102	CDL	C62-C61	-3.21	1.33	1.51
20	N	608	TGL	OC1-CC1	-3.19	1.13	1.22
26	G	101	PEK	C23-C22	-3.17	1.40	1.52
25	T	103	CDL	C62-C61	-3.17	1.33	1.51
20	Y	101	TGL	C20-CA9	-3.16	1.33	1.51
19	N	607	PGV	O01-C02	-3.14	1.38	1.46
25	P	304	CDL	C19-C18	-3.06	1.34	1.51
25	P	304	CDL	C62-C61	-3.04	1.34	1.51
25	T	103	CDL	C22-C21	-3.03	1.34	1.51
25	G	102	CDL	C82-C81	-3.01	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	304	CDL	C22-C21	-2.98	1.34	1.51
20	Y	101	TGL	C10-CB9	-2.97	1.34	1.51
25	C	303	CDL	C82-C81	-2.95	1.34	1.51
25	T	103	CDL	C59-C58	-2.94	1.34	1.51
25	C	303	CDL	C59-C58	-2.91	1.34	1.51
25	C	303	CDL	C62-C61	-2.89	1.35	1.51
20	N	608	TGL	C20-CA9	-2.86	1.35	1.51
25	T	103	CDL	C19-C18	-2.85	1.35	1.51
19	P	303	PGV	P-O14	-2.83	1.43	1.55
22	B	303	CHD	C8-C7	-2.82	1.48	1.53
25	T	103	CDL	C39-C38	-2.80	1.35	1.51
25	C	303	CDL	C19-C18	-2.79	1.35	1.51
20	B	301	TGL	C20-CA9	-2.78	1.35	1.51
20	N	608	TGL	C10-CB9	-2.78	1.35	1.51
20	D	201	TGL	C15-CC9	-2.75	1.35	1.51
25	P	304	CDL	C39-C38	-2.74	1.35	1.51
14	A	601	HEA	C3B-C2B	-2.72	1.31	1.41
20	D	201	TGL	C20-CA9	-2.71	1.36	1.51
22	C	305	CHD	C13-C12	-2.70	1.50	1.54
25	G	102	CDL	C39-C38	-2.69	1.36	1.51
20	Q	202	TGL	C20-CA9	-2.67	1.36	1.51
25	G	102	CDL	C19-C18	-2.66	1.36	1.51
26	T	101	PEK	C23-C22	-2.66	1.42	1.52
25	C	303	CDL	C22-C21	-2.66	1.36	1.51
20	N	608	TGL	C15-CC9	-2.63	1.36	1.51
25	P	304	CDL	C82-C81	-2.62	1.36	1.51
20	Y	101	TGL	C15-CC9	-2.52	1.37	1.51
25	T	103	CDL	C82-C81	-2.47	1.37	1.51
25	C	303	CDL	C39-C38	-2.47	1.37	1.51
25	G	102	CDL	C79-C78	-2.46	1.37	1.51
14	A	601	HEA	C4A-NA	-2.46	1.33	1.36
25	C	303	CDL	C42-C41	-2.46	1.37	1.51
22	O	302	CHD	C13-C14	-2.42	1.51	1.55
25	P	304	CDL	C42-C41	-2.41	1.37	1.51
22	B	303	CHD	C10-C9	-2.40	1.51	1.56
25	G	102	CDL	C42-C41	-2.38	1.37	1.51
20	Q	202	TGL	C15-CC9	-2.37	1.38	1.51
20	B	301	TGL	C10-CB9	-2.36	1.38	1.51
25	P	304	CDL	OA2-CA2	-2.34	1.35	1.44
20	L	101	TGL	C15-CC9	-2.34	1.38	1.51
20	L	101	TGL	CA6-CA5	-2.26	1.38	1.51
20	B	301	TGL	C15-CC9	-2.23	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	102	CDL	C22-C21	-2.23	1.38	1.51
19	A	608	PGV	C3-C2	-2.22	1.43	1.52
14	A	602	HEA	CAD-C3D	-2.21	1.48	1.52
25	T	103	CDL	C79-C78	-2.21	1.38	1.51
14	N	601	HEA	C14-C15	-2.20	1.27	1.32
19	Q	201	PGV	C3-C2	-2.18	1.43	1.52
19	C	307	PGV	C21-C20	-2.02	1.44	1.52
22	J	102	CHD	C6-C5	2.00	1.57	1.53
22	B	303	CHD	C1-C10	2.00	1.57	1.54
25	P	304	CDL	CA3-CA4	2.00	1.56	1.50
22	C	304	CHD	C20-C17	2.00	1.58	1.54
20	Y	101	TGL	CG1-CG2	2.01	1.56	1.50
25	C	303	CDL	CA2-C1	2.02	1.59	1.51
22	P	305	CHD	C13-C14	2.03	1.59	1.55
26	T	101	PEK	C3-C4	2.03	1.60	1.52
25	G	102	CDL	C71-CB7	2.03	1.56	1.50
22	P	307	CHD	C8-C14	2.03	1.57	1.53
19	C	302	PGV	C01-C02	2.06	1.56	1.50
20	D	201	TGL	CB2-CB1	2.06	1.56	1.50
25	P	304	CDL	CA6-CA4	2.07	1.56	1.50
22	C	304	CHD	C11-C9	2.07	1.57	1.53
26	G	101	PEK	C38-C37	2.08	1.67	1.49
19	A	607	PGV	C25-C24	2.10	1.63	1.51
28	Z	101	DMU	O3-C5	2.11	1.47	1.43
25	P	304	CDL	C11-CA5	2.12	1.56	1.50
20	Q	202	TGL	CC2-CC1	2.12	1.56	1.50
19	A	607	PGV	O06-C06	2.14	1.51	1.42
19	P	303	PGV	C01-C02	2.16	1.56	1.50
22	W	101	CHD	C16-C17	2.16	1.59	1.54
28	M	101	DMU	C3-C4	2.17	1.58	1.52
22	O	302	CHD	C4-C5	2.17	1.57	1.53
22	W	101	CHD	C6-C7	2.18	1.56	1.52
14	A	601	HEA	CMC-C2C	2.19	1.56	1.51
26	G	103	PEK	C01-C02	2.21	1.57	1.50
19	N	607	PGV	C8-C7	2.22	1.64	1.51
26	P	308	PEK	P-O12	2.23	1.68	1.59
22	P	305	CHD	C8-C14	2.23	1.58	1.53
19	A	607	PGV	C8-C7	2.24	1.64	1.51
28	Z	101	DMU	O16-C6	2.24	1.44	1.40
19	C	307	PGV	P-O11	2.26	1.68	1.59
22	P	307	CHD	C2-C3	2.27	1.57	1.51
22	B	303	CHD	O3-C3	2.27	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	C13-C14	2.27	1.58	1.50
28	Z	101	DMU	O1-C10	2.28	1.47	1.41
19	A	607	PGV	C29-C28	2.28	1.64	1.51
14	A	602	HEA	CMC-C2C	2.29	1.56	1.51
19	C	302	PGV	O06-C06	2.30	1.52	1.42
25	P	304	CDL	C31-CA7	2.30	1.57	1.50
22	J	102	CHD	C6-C7	2.32	1.56	1.52
20	Q	202	TGL	CB3-CB2	2.33	1.61	1.52
20	N	608	TGL	CG1-CG2	2.34	1.57	1.50
19	A	607	PGV	O01-C1	2.35	1.41	1.34
26	P	308	PEK	C03-C02	2.35	1.57	1.50
14	N	602	HEA	C4D-CHA	2.36	1.46	1.40
26	C	306	PEK	O04-C21	2.36	1.29	1.22
22	P	305	CHD	C10-C5	2.37	1.59	1.55
25	G	102	CDL	CB6-CB4	2.37	1.57	1.50
20	B	301	TGL	CG1-CG2	2.38	1.57	1.50
22	B	303	CHD	C8-C9	2.38	1.58	1.53
22	J	102	CHD	C13-C12	2.39	1.58	1.54
28	M	101	DMU	O16-C6	2.40	1.44	1.40
20	Y	101	TGL	OG2-CG2	2.42	1.53	1.46
22	B	303	CHD	C21-C20	2.49	1.59	1.53
25	C	303	CDL	PA1-OA5	2.52	1.69	1.59
20	Y	101	TGL	CC2-CC1	2.52	1.58	1.50
20	L	101	TGL	CG1-CG2	2.53	1.58	1.50
14	N	601	HEA	CMD-C2D	2.54	1.57	1.51
20	Y	101	TGL	CB2-CB1	2.57	1.58	1.50
26	G	101	PEK	O11-C03	2.58	1.55	1.44
22	P	307	CHD	C11-C9	2.59	1.58	1.53
22	P	307	CHD	C6-C5	2.59	1.58	1.53
22	W	101	CHD	C11-C9	2.60	1.58	1.53
22	C	305	CHD	C8-C7	2.61	1.58	1.53
25	C	303	CDL	OB2-CB2	2.61	1.55	1.44
26	G	101	PEK	O01-C02	2.61	1.53	1.46
28	M	101	DMU	C2-C1	2.61	1.59	1.52
28	M	101	DMU	O5-C4	2.61	1.50	1.44
14	N	602	HEA	CMB-C2B	2.62	1.57	1.51
28	Z	101	DMU	O7-C3	2.63	1.50	1.43
22	C	305	CHD	C11-C9	2.63	1.58	1.53
22	C	305	CHD	C10-C9	2.64	1.61	1.56
22	W	101	CHD	C8-C7	2.66	1.58	1.53
22	P	307	CHD	C16-C17	2.69	1.60	1.54
14	A	601	HEA	CMB-C2B	2.71	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	C12-C13	2.72	1.62	1.53
14	A	602	HEA	C12-C13	2.73	1.62	1.53
19	N	607	PGV	O01-C1	2.73	1.42	1.34
20	Y	101	TGL	CC3-CC2	2.74	1.62	1.52
14	N	601	HEA	C12-C13	2.74	1.62	1.53
26	C	306	PEK	P-O11	2.75	1.70	1.59
19	A	607	PGV	O03-C01	2.76	1.51	1.45
19	A	607	PGV	C3-C2	2.77	1.62	1.52
20	D	201	TGL	CG3-CG2	2.80	1.58	1.50
14	A	601	HEA	C4C-CHD	2.80	1.47	1.40
22	W	101	CHD	C13-C14	2.81	1.60	1.55
14	A	601	HEA	C12-C13	2.82	1.62	1.53
25	P	304	CDL	PA1-OA5	2.82	1.71	1.59
22	J	102	CHD	C8-C7	2.85	1.58	1.53
22	C	304	CHD	C10-C5	2.86	1.60	1.55
20	L	101	TGL	OB1-CB1	2.87	1.31	1.22
28	Z	101	DMU	O55-C2	2.88	1.49	1.43
26	P	308	PEK	P-O11	2.92	1.71	1.59
25	C	303	CDL	OB8-CB6	2.92	1.51	1.45
22	O	302	CHD	C4-C3	2.93	1.57	1.51
22	C	304	CHD	C8-C14	2.93	1.59	1.53
19	P	303	PGV	C20-C19	2.93	1.59	1.50
14	A	601	HEA	C22-C23	2.94	1.41	1.32
22	C	305	CHD	C2-C3	2.95	1.59	1.51
22	O	302	CHD	C8-C9	2.96	1.59	1.53
25	C	303	CDL	OB6-CB5	2.96	1.43	1.34
20	L	101	TGL	OG2-CG2	2.97	1.54	1.46
14	N	602	HEA	C20-C19	2.97	1.58	1.51
14	N	602	HEA	O11-C11	2.97	1.49	1.42
22	C	305	CHD	C16-C15	2.97	1.62	1.54
19	N	607	PGV	C03-C02	2.98	1.59	1.50
26	P	308	PEK	C22-C21	2.99	1.59	1.50
22	J	102	CHD	C13-C17	3.00	1.60	1.55
22	P	307	CHD	C16-C15	3.00	1.62	1.54
19	C	302	PGV	C21-C20	3.00	1.63	1.52
14	A	601	HEA	CAA-C2A	3.02	1.56	1.52
26	C	306	PEK	C22-C21	3.02	1.59	1.50
22	O	302	CHD	C13-C12	3.03	1.59	1.54
22	P	305	CHD	C8-C9	3.05	1.59	1.53
14	A	601	HEA	CAD-C3D	3.05	1.57	1.52
14	A	602	HEA	C24-C23	3.06	1.59	1.50
20	Y	101	TGL	CG3-CG2	3.07	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	305	CHD	C13-C17	3.07	1.61	1.55
22	J	102	CHD	C8-C9	3.08	1.59	1.53
19	N	607	PGV	C3-C2	3.09	1.63	1.52
22	W	101	CHD	C20-C17	3.09	1.60	1.54
20	Q	202	TGL	OC1-CC1	3.11	1.31	1.22
22	W	101	CHD	C8-C9	3.11	1.60	1.53
14	N	602	HEA	C14-C15	3.13	1.40	1.32
25	C	303	CDL	PB2-OB2	3.16	1.72	1.59
14	N	601	HEA	C16-C15	3.16	1.58	1.51
25	P	304	CDL	PB2-OB2	3.17	1.72	1.59
26	T	101	PEK	O11-C03	3.18	1.57	1.44
22	C	304	CHD	C8-C9	3.19	1.60	1.53
22	B	303	CHD	C6-C5	3.19	1.59	1.53
22	C	305	CHD	O12-C12	3.19	1.49	1.43
22	P	307	CHD	C22-C20	3.20	1.63	1.54
22	P	305	CHD	C11-C9	3.25	1.59	1.53
22	B	303	CHD	C18-C13	3.27	1.59	1.54
20	L	101	TGL	CG3-CG2	3.33	1.60	1.50
19	N	607	PGV	O03-C01	3.33	1.52	1.45
25	P	304	CDL	OB2-CB2	3.33	1.58	1.44
14	A	601	HEA	C16-C15	3.34	1.59	1.51
22	C	305	CHD	C16-C17	3.39	1.61	1.54
28	P	306	DMU	O16-C6	3.40	1.46	1.40
14	N	601	HEA	CMB-C2B	3.41	1.58	1.51
20	L	101	TGL	CB2-CB1	3.41	1.60	1.50
14	N	602	HEA	C1A-NA	3.44	1.41	1.36
22	J	102	CHD	C8-C14	3.45	1.60	1.53
22	W	101	CHD	C8-C14	3.49	1.60	1.53
20	N	608	TGL	OG2-CB1	3.54	1.44	1.34
14	N	601	HEA	C1A-NA	3.59	1.41	1.36
19	A	608	PGV	O01-C1	3.59	1.44	1.34
22	C	305	CHD	C6-C5	3.60	1.59	1.53
22	B	303	CHD	C6-C7	3.62	1.58	1.52
19	A	608	PGV	P-O12	3.63	1.74	1.59
22	P	307	CHD	C6-C7	3.64	1.58	1.52
22	B	303	CHD	O7-C7	3.64	1.51	1.43
22	C	305	CHD	C11-C12	3.71	1.59	1.53
25	C	303	CDL	CB2-C1	3.74	1.66	1.51
22	C	305	CHD	C4-C3	3.74	1.59	1.51
14	A	602	HEA	C1A-NA	3.77	1.41	1.36
20	L	101	TGL	CC2-CC1	3.79	1.61	1.50
28	J	101	DMU	O16-C6	3.80	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	304	CDL	OB6-CB5	3.81	1.45	1.34
28	M	101	DMU	O7-C3	3.82	1.53	1.43
14	N	601	HEA	CMC-C2C	3.84	1.59	1.51
22	B	303	CHD	C4-C5	3.84	1.60	1.53
23	B	304	PSC	C13-C12	3.85	1.54	1.31
22	W	101	CHD	C13-C12	3.86	1.60	1.54
22	B	303	CHD	C15-C14	3.92	1.62	1.54
14	A	601	HEA	C1A-NA	3.93	1.42	1.36
19	C	307	PGV	O03-C19	3.99	1.45	1.33
23	O	303	PSC	C13-C12	3.99	1.55	1.31
22	O	302	CHD	C16-C17	4.00	1.62	1.54
22	O	302	CHD	C6-C7	4.04	1.59	1.52
22	B	303	CHD	C16-C17	4.05	1.63	1.54
22	W	101	CHD	C13-C17	4.07	1.62	1.55
25	P	304	CDL	CB2-C1	4.07	1.67	1.51
23	O	303	PSC	O03-C19	4.09	1.45	1.33
20	B	301	TGL	OG3-CC1	4.11	1.45	1.33
19	N	607	PGV	C01-C02	4.16	1.62	1.50
19	P	301	PGV	O01-C1	4.17	1.46	1.34
20	N	608	TGL	OG3-CC1	4.24	1.45	1.33
20	D	201	TGL	OG3-CC1	4.29	1.46	1.33
19	C	302	PGV	C20-C19	4.29	1.63	1.50
22	B	303	CHD	C4-C3	4.33	1.60	1.51
23	B	304	PSC	O03-C19	4.35	1.46	1.33
22	J	102	CHD	C20-C17	4.35	1.62	1.54
19	P	301	PGV	O03-C19	4.47	1.46	1.33
22	P	307	CHD	C11-C12	4.49	1.61	1.53
25	G	102	CDL	OA8-CA7	4.50	1.46	1.33
19	A	607	PGV	C01-C02	4.50	1.63	1.50
19	C	302	PGV	C22-C21	4.51	1.77	1.51
25	P	304	CDL	OB8-CB6	4.53	1.55	1.45
19	Q	201	PGV	O01-C1	4.55	1.47	1.34
19	A	608	PGV	P-O13	4.57	1.68	1.51
20	D	201	TGL	CC2-CC1	4.61	1.63	1.50
14	A	602	HEA	C18-C19	4.63	1.44	1.32
19	C	307	PGV	O01-C1	4.65	1.48	1.34
25	T	103	CDL	OA8-CA7	4.72	1.47	1.33
25	C	303	CDL	O1-C1	4.73	1.57	1.43
22	B	303	CHD	C19-C10	4.76	1.63	1.54
22	O	302	CHD	C15-C14	4.80	1.64	1.54
22	C	305	CHD	C22-C20	4.84	1.67	1.54
22	O	302	CHD	C19-C10	4.84	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	601	HEA	O11-C11	4.85	1.54	1.42
20	Q	202	TGL	OG1-CA1	4.98	1.48	1.33
25	C	303	CDL	OA6-CA5	4.98	1.49	1.34
20	Q	202	TGL	OG3-CC1	5.01	1.48	1.33
25	T	103	CDL	OB6-CB5	5.05	1.49	1.34
25	G	102	CDL	OA6-CA5	5.05	1.49	1.34
25	G	102	CDL	OB6-CB5	5.19	1.49	1.34
26	T	102	PEK	O03-C21	5.25	1.49	1.33
25	G	102	CDL	OB8-CB7	5.29	1.49	1.33
20	L	101	TGL	OG1-CA1	5.34	1.49	1.33
26	G	103	PEK	O03-C21	5.36	1.49	1.33
26	T	102	PEK	O01-C1	5.40	1.50	1.34
20	N	608	TGL	OG1-CA1	5.40	1.49	1.33
25	T	103	CDL	OA6-CA5	5.42	1.50	1.34
23	B	304	PSC	O01-C1	5.46	1.50	1.34
25	P	304	CDL	OA6-CA5	5.53	1.50	1.34
20	D	201	TGL	OG1-CA1	5.62	1.50	1.33
25	P	304	CDL	O1-C1	5.65	1.60	1.43
25	C	303	CDL	OA8-CA7	5.66	1.50	1.33
25	T	103	CDL	OB8-CB7	5.71	1.50	1.33
20	L	101	TGL	OG3-CC1	5.77	1.50	1.33
19	Q	201	PGV	O03-C19	5.78	1.50	1.33
26	G	103	PEK	O01-C1	5.80	1.51	1.34
26	T	101	PEK	C2-C1	5.85	1.67	1.50
25	P	304	CDL	OA8-CA7	5.92	1.50	1.33
25	C	303	CDL	PB2-OB3	5.93	1.72	1.51
23	O	303	PSC	O01-C1	5.95	1.51	1.34
25	C	303	CDL	OB8-CB7	6.02	1.51	1.33
26	C	306	PEK	O03-C21	6.06	1.51	1.33
26	P	308	PEK	O03-C21	6.09	1.51	1.33
20	Y	101	TGL	OG1-CA1	6.09	1.51	1.33
26	C	306	PEK	O01-C1	6.11	1.52	1.34
26	T	101	PEK	C3-C2	6.37	1.76	1.52
25	P	304	CDL	PB2-OB3	6.44	1.74	1.51
20	D	201	TGL	OC1-CC1	6.49	1.41	1.22
26	P	308	PEK	O01-C1	6.70	1.54	1.34
19	A	608	PGV	O03-C19	6.87	1.53	1.33
20	Y	101	TGL	OG3-CC1	6.89	1.53	1.33
25	P	304	CDL	OB8-CB7	6.93	1.54	1.33
20	B	301	TGL	OG1-CA1	7.14	1.54	1.33
20	Y	101	TGL	OG2-CB1	7.39	1.56	1.34
19	A	608	PGV	O02-C1	7.56	1.44	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	101	TGL	OG2-CB1	7.94	1.57	1.34
20	Q	202	TGL	OG2-CB1	9.03	1.60	1.34
20	D	201	TGL	OG2-CB1	9.96	1.63	1.34
20	Q	202	TGL	OB1-CB1	11.27	1.55	1.22
20	D	201	TGL	OB1-CB1	13.02	1.61	1.22

All (712) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	D	201	TGL	OG2-CB1-CB2	-16.01	77.78	111.53
22	W	101	CHD	C18-C13-C12	-14.04	95.04	109.09
20	Q	202	TGL	OG2-CB1-CB2	-12.80	84.54	111.53
14	N	601	HEA	C27-C19-C18	-10.34	103.56	123.58
22	P	305	CHD	C18-C13-C12	-10.24	98.84	109.09
20	Y	101	TGL	CC4-CC3-CC2	-9.49	78.17	113.30
22	C	304	CHD	C18-C13-C12	-9.42	99.66	109.09
20	L	101	TGL	CC4-CC3-CC2	-9.23	79.13	113.30
25	C	303	CDL	C52-C51-CB5	-9.22	77.62	113.57
14	A	602	HEA	C13-C12-C11	-8.39	104.87	114.74
22	C	305	CHD	C23-C22-C20	-8.23	104.61	114.79
25	P	304	CDL	C52-C51-CB5	-8.00	82.38	113.57
26	C	306	PEK	C36-C35-C34	-7.37	76.28	114.54
22	C	305	CHD	C17-C13-C12	-7.28	111.30	117.68
19	A	608	PGV	O01-C1-C2	-6.98	96.82	111.53
22	P	307	CHD	C6-C7-C8	-6.97	104.08	111.46
22	C	304	CHD	C6-C5-C4	-6.89	103.68	111.07
22	P	307	CHD	C23-C22-C20	-6.87	106.30	114.79
28	M	101	DMU	C22-C25-C28	-6.81	79.15	114.54
22	J	102	CHD	C18-C13-C12	-6.64	102.45	109.09
22	B	303	CHD	C11-C12-C13	-6.63	104.53	111.22
14	N	602	HEA	C13-C12-C11	-6.63	106.94	114.74
14	A	601	HEA	C27-C19-C18	-6.62	110.76	123.58
22	W	101	CHD	C17-C13-C14	-6.52	93.48	100.08
20	Y	101	TGL	C26-C25-C24	-6.51	80.72	114.54
22	C	305	CHD	C6-C7-C8	-6.31	104.77	111.46
20	B	301	TGL	OG3-CG3-CG2	-6.27	91.79	108.70
22	P	305	CHD	O7-C7-C6	-6.05	95.25	110.02
22	C	304	CHD	O7-C7-C6	-5.98	95.42	110.02
20	Q	202	TGL	CG3-CG2-CG1	-5.98	98.15	112.08
14	N	602	HEA	CAD-CBD-CGD	-5.78	101.53	112.78
22	P	307	CHD	C17-C13-C12	-5.62	112.75	117.68
22	C	304	CHD	C19-C10-C1	-5.49	98.93	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	601	HEA	CMB-C2B-C1B	-5.48	118.98	128.31
22	B	303	CHD	C5-C4-C3	-5.45	104.81	112.88
22	P	305	CHD	C6-C5-C4	-5.29	105.39	111.07
22	O	302	CHD	C5-C4-C3	-5.27	105.08	112.88
22	P	307	CHD	C21-C20-C22	-5.24	101.81	110.33
22	O	302	CHD	C6-C5-C4	-5.19	105.50	111.07
28	M	101	DMU	O5-C4-C3	-5.15	98.79	109.78
22	B	303	CHD	C19-C10-C1	-4.98	99.79	108.23
26	C	306	PEK	O03-C21-O04	-4.93	110.58	123.51
20	L	101	TGL	C22-C21-C20	-4.84	89.39	114.54
14	A	601	HEA	C13-C12-C11	-4.81	109.09	114.74
19	C	302	PGV	C30-C29-C28	-4.77	89.77	114.54
22	O	302	CHD	C2-C1-C10	-4.72	104.34	112.81
22	J	102	CHD	C1-C10-C9	-4.68	104.00	111.43
22	C	304	CHD	C17-C13-C14	-4.65	95.37	100.08
23	O	303	PSC	C28-C27-C26	-4.61	90.61	114.54
22	P	307	CHD	C22-C20-C17	-4.60	100.55	110.24
22	O	302	CHD	C15-C14-C8	-4.59	111.55	118.34
14	A	601	HEA	CMB-C2B-C1B	-4.57	120.53	128.31
22	J	102	CHD	C6-C5-C4	-4.57	106.16	111.07
25	C	303	CDL	CB6-CB4-CB3	-4.56	101.46	112.08
20	L	101	TGL	OG3-CC1-OC1	-4.54	111.62	123.51
22	P	305	CHD	C14-C8-C9	-4.53	103.24	109.63
22	B	303	CHD	C6-C5-C4	-4.53	106.20	111.07
25	C	303	CDL	OB8-CB6-CB4	-4.53	96.47	108.70
28	Z	101	DMU	C22-C25-C28	-4.52	91.06	114.54
19	Q	201	PGV	C5-C4-C3	-4.50	91.17	114.54
25	C	303	CDL	C53-C52-C51	-4.49	96.69	113.30
22	O	302	CHD	C19-C10-C1	-4.48	100.64	108.23
22	J	102	CHD	C14-C13-C12	-4.43	103.37	107.37
20	B	301	TGL	CB4-CB3-CB2	-4.41	96.99	113.30
25	C	303	CDL	C76-C75-C74	-4.38	91.79	114.54
20	N	608	TGL	OG1-CA1-OA1	-4.37	112.06	123.51
22	B	303	CHD	O3-C3-C4	-4.37	101.03	109.86
20	B	301	TGL	CB3-CB2-CB1	-4.35	96.59	113.57
14	A	602	HEA	CAD-CBD-CGD	-4.35	104.32	112.78
14	A	602	HEA	C20-C19-C18	-4.32	112.94	120.98
26	P	308	PEK	O03-C21-O04	-4.30	112.25	123.51
14	N	602	HEA	C1A-C2A-C3A	-4.24	102.83	107.07
26	C	306	PEK	C03-C02-C01	-4.22	102.25	112.08
20	D	201	TGL	OG3-CC1-OC1	-4.22	112.46	123.51
28	P	306	DMU	O1-C10-C5	-4.21	101.52	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	C	302	PGV	C28-C27-C26	-4.20	92.74	114.54
22	J	102	CHD	C17-C13-C14	-4.18	95.85	100.08
22	B	303	CHD	C2-C1-C10	-4.18	105.31	112.81
22	C	305	CHD	C16-C17-C13	-4.17	99.56	103.59
22	J	102	CHD	C9-C11-C12	-4.16	109.16	114.38
26	G	101	PEK	C24-C23-C22	-4.15	97.93	113.30
20	Y	101	TGL	CA4-CA3-CA2	-4.10	98.13	113.30
20	Y	101	TGL	CA8-CA7-CA6	-4.08	93.33	114.54
22	P	305	CHD	C19-C10-C9	-4.08	105.80	111.20
22	C	305	CHD	C11-C9-C10	-4.08	109.53	113.77
28	Z	101	DMU	O55-C2-C1	-4.04	101.25	110.36
22	C	305	CHD	C22-C20-C17	-4.02	101.77	110.24
22	O	302	CHD	C16-C17-C13	-4.02	99.71	103.59
20	B	301	TGL	OG3-CC1-OC1	-4.01	113.00	123.51
28	M	101	DMU	O5-C6-O16	-4.01	100.38	109.99
28	M	101	DMU	C18-O16-C6	-3.98	107.05	114.00
22	B	303	CHD	C15-C14-C8	-3.97	112.46	118.34
20	L	101	TGL	C20-CA9-CA8	-3.97	93.93	114.54
23	B	304	PSC	C32-C31-C30	-3.94	94.07	114.54
20	L	101	TGL	CA4-CA3-CA2	-3.92	98.80	113.30
19	Q	201	PGV	C8-C7-C6	-3.91	94.25	114.54
22	C	304	CHD	C22-C23-C24	-3.88	97.24	113.05
19	P	301	PGV	O04-C19-C20	-3.87	108.94	123.76
22	P	307	CHD	C14-C8-C7	-3.81	106.33	111.77
22	C	305	CHD	C22-C23-C24	-3.80	97.56	113.05
25	C	303	CDL	C77-C76-C75	-3.80	94.82	114.54
28	Z	101	DMU	C6-C1-C2	-3.78	102.49	109.98
28	Z	101	DMU	O49-C1-C6	-3.78	101.63	110.01
20	B	301	TGL	CB5-CB4-CB3	-3.76	95.03	114.54
14	N	602	HEA	CAA-CBA-CGA	-3.74	105.51	112.78
14	N	602	HEA	CBA-CAA-C2A	-3.72	105.94	112.47
22	B	303	CHD	O12-C12-C13	-3.71	104.92	111.12
25	C	303	CDL	OB4-PB2-OB5	-3.70	90.60	108.24
20	Q	202	TGL	OG3-CC1-OC1	-3.70	113.81	123.51
25	C	303	CDL	C73-C72-C71	-3.69	99.65	113.30
20	L	101	TGL	C24-C23-C22	-3.67	95.47	114.54
19	Q	201	PGV	C3-C2-C1	-3.65	99.31	113.57
19	A	607	PGV	C34-C33-C32	-3.65	84.93	113.49
28	M	101	DMU	O16-C6-C1	-3.62	103.54	108.00
19	A	608	PGV	C23-C22-C21	-3.62	95.75	114.54
14	A	601	HEA	C20-C21-C22	-3.61	102.12	111.61
19	P	301	PGV	C03-C02-C01	-3.61	103.66	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	M	101	DMU	C25-C28-C31	-3.57	95.98	114.54
22	C	305	CHD	C14-C8-C7	-3.55	106.70	111.77
25	G	102	CDL	OA6-CA5-OA7	-3.54	114.03	123.67
14	A	602	HEA	C16-C15-C14	-3.54	114.39	120.98
20	Y	101	TGL	CB5-CB4-CB3	-3.54	96.17	114.54
26	T	101	PEK	C3-C2-C1	-3.53	99.78	113.57
25	C	303	CDL	OB6-CB4-CB3	-3.52	95.99	108.36
22	P	305	CHD	O3-C3-C4	-3.52	102.75	109.86
23	B	304	PSC	C28-C27-C26	-3.52	96.27	114.54
14	N	601	HEA	C1A-C2A-C3A	-3.52	103.55	107.07
22	C	305	CHD	C9-C11-C12	-3.51	109.98	114.38
28	P	306	DMU	O6-C11-C9	-3.50	99.61	111.30
20	B	301	TGL	OA1-CA1-CA2	-3.50	110.35	123.76
25	G	102	CDL	OA8-CA7-OA9	-3.50	114.34	123.51
28	Z	101	DMU	O16-C6-C1	-3.50	103.70	108.00
22	P	305	CHD	C19-C10-C1	-3.49	102.31	108.23
22	O	302	CHD	O3-C3-C4	-3.49	102.81	109.86
20	L	101	TGL	C26-C25-C24	-3.48	96.47	114.54
20	Y	101	TGL	OB1-CB1-CB2	-3.48	110.44	123.76
26	P	308	PEK	C36-C35-C34	-3.46	96.55	114.54
20	N	608	TGL	OG2-CB1-OB1	-3.45	114.28	123.67
22	J	102	CHD	C14-C8-C9	-3.41	104.82	109.63
28	Z	101	DMU	C18-O16-C6	-3.41	108.05	114.00
20	L	101	TGL	CA5-CA4-CA3	-3.40	96.89	114.54
19	P	303	PGV	C03-C02-C01	-3.36	104.25	112.08
19	A	608	PGV	O04-C19-C20	-3.34	110.96	123.76
23	B	304	PSC	C08-N-C07	-3.34	100.31	108.96
25	P	304	CDL	CB4-OB6-CB5	-3.33	109.67	117.91
22	O	302	CHD	C14-C13-C12	-3.33	104.36	107.37
25	T	103	CDL	CA6-CA4-CA3	-3.31	104.36	112.08
14	A	601	HEA	C27-C19-C20	-3.31	110.33	115.37
20	B	301	TGL	OG2-CB1-OB1	-3.27	114.76	123.67
28	Z	101	DMU	O5-C6-O16	-3.26	102.17	109.99
22	C	305	CHD	C15-C14-C8	-3.25	113.53	118.34
23	B	304	PSC	C29-C28-C27	-3.23	97.74	114.54
22	O	302	CHD	C14-C8-C9	-3.23	105.07	109.63
19	P	303	PGV	C27-C26-C25	-3.23	97.78	114.54
22	P	307	CHD	C11-C12-C13	-3.22	107.97	111.22
25	C	303	CDL	OB6-CB5-OB7	-3.22	114.92	123.67
28	M	101	DMU	C22-C19-C18	-3.20	99.01	113.47
22	P	307	CHD	C22-C23-C24	-3.20	100.00	113.05
25	P	304	CDL	C78-C77-C76	-3.17	98.07	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	A	608	PGV	O14-P-O11	-3.16	93.15	108.24
20	D	201	TGL	OG3-CC1-CC2	-3.16	102.12	111.85
25	C	303	CDL	OB9-CB7-C71	-3.14	111.72	123.76
14	A	601	HEA	CBA-CAA-C2A	-3.13	106.98	112.47
23	O	303	PSC	C29-C28-C27	-3.13	98.30	114.54
14	A	601	HEA	CAA-CBA-CGA	-3.12	106.71	112.78
14	N	602	HEA	C16-C15-C14	-3.09	115.22	120.98
19	A	608	PGV	C27-C26-C25	-3.08	98.56	114.54
14	N	601	HEA	OMA-CMA-C3A	-3.06	118.02	125.03
25	P	304	CDL	OB6-CB4-CB3	-3.05	97.63	108.36
26	G	101	PEK	O03-C21-C22	-3.05	102.45	111.85
22	B	303	CHD	C5-C6-C7	-3.05	110.97	114.44
14	N	601	HEA	CAA-CBA-CGA	-3.04	106.88	112.78
14	N	602	HEA	CBD-CAD-C3D	-3.02	107.18	112.49
20	L	101	TGL	C12-C11-C10	-2.99	99.00	114.54
23	B	304	PSC	C27-C26-C25	-2.99	99.02	114.54
22	C	304	CHD	C9-C11-C12	-2.98	110.64	114.38
25	P	304	CDL	C73-C72-C71	-2.94	102.42	113.30
19	C	307	PGV	O03-C19-O04	-2.94	115.81	123.51
25	P	304	CDL	OB8-CB7-OB9	-2.93	115.82	123.51
22	B	303	CHD	C11-C9-C8	-2.93	106.55	110.77
20	Q	202	TGL	OG3-CG3-CG2	-2.92	100.82	108.70
22	P	307	CHD	C13-C17-C20	-2.90	115.91	119.44
20	Y	101	TGL	C23-C22-C21	-2.89	99.54	114.54
19	N	607	PGV	O01-C1-C2	-2.88	105.46	111.53
25	C	303	CDL	OB4-PB2-OB2	-2.87	94.58	108.24
14	A	601	HEA	CMC-C2C-C1C	-2.86	123.45	128.31
22	W	101	CHD	C19-C10-C1	-2.85	103.41	108.23
22	C	305	CHD	C14-C8-C9	-2.85	105.62	109.63
23	O	303	PSC	C27-C26-C25	-2.84	99.77	114.54
28	M	101	DMU	C6-C1-C2	-2.84	104.34	109.98
28	M	101	DMU	O49-C1-C2	-2.84	103.96	110.36
26	T	101	PEK	O01-C1-C2	-2.82	105.58	111.53
22	J	102	CHD	C13-C14-C8	-2.81	111.03	114.73
20	D	201	TGL	CG2-OG2-CB1	-2.80	110.98	117.91
25	C	303	CDL	C75-C74-C73	-2.80	99.98	114.54
19	P	303	PGV	O03-C01-C02	-2.79	101.16	108.70
19	A	607	PGV	C31-C30-C29	-2.79	100.04	114.54
14	A	602	HEA	C13-C14-C15	-2.78	121.62	127.75
20	B	301	TGL	OB1-CB1-CB2	-2.78	113.13	123.76
20	B	301	TGL	CB6-CB5-CB4	-2.77	100.14	114.54
19	C	307	PGV	O04-C19-C20	-2.77	113.15	123.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	O	302	CHD	C18-C13-C12	-2.76	106.33	109.09
28	M	101	DMU	O7-C3-C4	-2.76	101.97	109.33
14	N	602	HEA	C12-C13-C14	-2.76	104.56	112.42
26	G	101	PEK	C02-O01-C1	-2.76	111.09	117.91
19	P	301	PGV	C21-C20-C19	-2.75	102.82	113.57
19	A	608	PGV	C8-C9-C10	-2.75	102.60	113.79
26	C	306	PEK	C33-C32-C31	-2.75	100.28	114.54
22	C	305	CHD	C1-C2-C3	-2.72	106.79	110.41
22	P	307	CHD	C10-C9-C8	-2.71	108.92	111.86
25	G	102	CDL	C43-C42-C41	-2.71	100.46	114.54
22	P	307	CHD	C16-C17-C13	-2.71	100.98	103.59
20	Y	101	TGL	OC1-CC1-CC2	-2.70	113.41	123.76
28	Z	101	DMU	O61-C57-C4	-2.69	102.32	111.30
19	A	607	PGV	C01-O03-C19	-2.68	109.00	117.00
20	L	101	TGL	OB1-CB1-CB2	-2.68	113.50	123.76
20	B	301	TGL	CB8-CB7-CB6	-2.65	100.76	114.54
19	P	303	PGV	C24-C23-C22	-2.65	100.77	114.54
26	G	103	PEK	C13-C14-C15	-2.65	108.40	124.38
25	P	304	CDL	OB9-CB7-C71	-2.64	113.64	123.76
20	N	608	TGL	OG3-CC1-OC1	-2.63	116.61	123.51
26	T	101	PEK	C24-C23-C22	-2.62	103.59	113.30
22	C	305	CHD	C19-C10-C1	-2.62	103.80	108.23
23	O	303	PSC	O01-C1-O02	-2.61	116.58	123.67
28	M	101	DMU	O1-C9-C8	-2.60	104.70	109.67
19	N	607	PGV	C3-C2-C1	-2.60	103.42	113.57
22	P	307	CHD	C16-C17-C20	-2.60	107.97	112.12
20	Y	101	TGL	CA7-CA6-CA5	-2.59	101.08	114.54
19	N	607	PGV	C14-C13-C12	-2.59	96.53	112.08
25	P	304	CDL	CA6-CA4-CA3	-2.58	106.07	112.08
19	N	607	PGV	O03-C19-O04	-2.58	116.76	123.51
26	G	101	PEK	O01-C02-C01	-2.58	99.31	108.36
26	G	103	PEK	O02-C1-C2	-2.56	113.94	123.76
22	C	305	CHD	O3-C3-C2	-2.54	103.90	110.04
26	G	103	PEK	C2-C3-C4	-2.54	109.00	113.65
26	T	102	PEK	O01-C1-O02	-2.52	116.80	123.67
20	B	301	TGL	C14-C13-C12	-2.52	101.45	114.54
23	B	304	PSC	O01-C1-O02	-2.52	116.82	123.67
22	C	304	CHD	C19-C10-C9	-2.51	107.88	111.20
22	B	303	CHD	C18-C13-C12	-2.51	106.58	109.09
14	A	602	HEA	CBA-CAA-C2A	-2.50	108.08	112.47
19	P	303	PGV	O03-C19-C20	-2.48	104.21	111.85
14	A	602	HEA	C12-C13-C14	-2.47	105.38	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	303	CHD	C16-C15-C14	-2.47	100.15	105.11
22	W	101	CHD	C19-C10-C5	-2.47	105.91	110.28
25	T	103	CDL	OB7-CB5-C51	-2.46	114.35	123.76
28	Z	101	DMU	O49-C1-C2	-2.46	104.82	110.36
14	N	601	HEA	C13-C12-C11	-2.44	111.87	114.74
14	N	601	HEA	C25-C23-C22	-2.43	114.77	122.63
19	N	607	PGV	C03-C02-C01	-2.43	106.42	112.08
22	P	307	CHD	C4-C5-C10	-2.43	110.05	112.66
26	G	101	PEK	O03-C21-O04	-2.43	117.15	123.51
19	P	303	PGV	C21-C20-C19	-2.42	104.12	113.57
28	M	101	DMU	O2-C8-C9	-2.41	102.88	109.23
22	C	305	CHD	C4-C5-C10	-2.40	110.08	112.66
26	G	103	PEK	C24-C23-C22	-2.40	104.40	113.30
20	Y	101	TGL	OG3-CC1-OC1	-2.40	117.22	123.51
25	P	304	CDL	C76-C75-C74	-2.40	102.09	114.54
20	D	201	TGL	C12-C11-C10	-2.39	102.14	114.54
22	W	101	CHD	C9-C8-C7	-2.38	109.01	111.89
22	O	302	CHD	C17-C13-C12	-2.38	115.59	117.68
28	M	101	DMU	O4-C7-C5	-2.38	105.00	110.36
26	C	306	PEK	O02-C1-C2	-2.38	114.66	123.76
14	A	601	HEA	CBD-CAD-C3D	-2.37	108.32	112.49
19	A	607	PGV	C4-C3-C2	-2.37	104.52	113.30
26	C	306	PEK	O12-P-O14	-2.37	99.51	109.21
25	C	303	CDL	CA6-CA4-CA3	-2.37	106.57	112.08
20	D	201	TGL	OG3-CG3-CG2	-2.36	102.32	108.70
14	N	602	HEA	C13-C14-C15	-2.36	122.54	127.75
22	B	303	CHD	C9-C8-C7	-2.36	109.03	111.89
20	Y	101	TGL	C22-C21-C20	-2.36	102.30	114.54
25	P	304	CDL	OA8-CA7-OA9	-2.35	117.36	123.51
25	T	103	CDL	OA6-CA5-OA7	-2.34	117.30	123.67
22	O	302	CHD	C16-C15-C14	-2.34	100.42	105.11
20	B	301	TGL	CG3-CG2-CG1	-2.33	106.66	112.08
28	J	101	DMU	O1-C10-C5	-2.32	105.46	110.28
25	T	103	CDL	CB2-C1-CA2	-2.31	105.06	112.42
19	N	607	PGV	O01-C1-O02	-2.31	117.40	123.67
28	J	101	DMU	C18-O16-C6	-2.30	109.97	114.00
19	A	607	PGV	O01-C1-O02	-2.30	117.40	123.67
22	C	304	CHD	C21-C20-C22	-2.30	106.59	110.33
22	O	302	CHD	C19-C10-C9	-2.28	108.18	111.20
22	C	304	CHD	O3-C3-C4	-2.28	105.26	109.86
19	A	607	PGV	O01-C02-C01	-2.26	100.41	108.36
25	T	103	CDL	OA9-CA7-C31	-2.25	115.15	123.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	102	CDL	OB7-CB5-C51	-2.23	115.22	123.76
23	O	303	PSC	C21-C20-C19	-2.23	104.88	113.57
23	O	303	PSC	C08-N-C06	-2.23	103.19	108.96
22	C	305	CHD	C16-C15-C14	-2.22	100.66	105.11
14	A	601	HEA	C1A-C2A-C3A	-2.21	104.85	107.07
20	D	201	TGL	CB7-CB6-CB5	-2.21	103.05	114.54
28	M	101	DMU	O3-C5-C10	-2.21	105.10	110.01
22	O	302	CHD	C13-C17-C20	-2.21	116.75	119.44
28	M	101	DMU	C19-C22-C25	-2.20	103.13	114.54
26	T	101	PEK	O01-C1-O02	-2.19	117.71	123.67
20	L	101	TGL	C25-C24-C23	-2.19	103.16	114.54
23	B	304	PSC	C26-C25-C24	-2.19	103.19	114.54
20	D	201	TGL	CC3-CC2-CC1	-2.18	105.08	113.57
26	C	306	PEK	C2-C3-C4	-2.17	109.67	113.65
14	N	602	HEA	C17-C18-C19	-2.17	122.96	127.75
22	P	305	CHD	C11-C12-C13	-2.17	109.03	111.22
20	Y	101	TGL	CG3-CG2-CG1	-2.17	107.03	112.08
20	Y	101	TGL	CB8-CB7-CB6	-2.16	103.33	114.54
20	D	201	TGL	OG1-CA1-OA1	-2.16	117.86	123.51
22	O	302	CHD	O12-C12-C13	-2.16	107.52	111.12
20	L	101	TGL	OC1-CC1-CC2	-2.15	115.51	123.76
26	T	101	PEK	O11-P-O14	-2.15	100.40	109.21
19	A	607	PGV	C5-C4-C3	-2.15	103.36	114.54
22	W	101	CHD	C6-C5-C4	-2.15	108.76	111.07
26	G	101	PEK	C25-C24-C23	-2.13	103.47	114.54
19	P	303	PGV	C10-C11-C12	-2.12	107.98	124.66
28	Z	101	DMU	O7-C10-O1	-2.12	105.17	110.69
23	B	304	PSC	C11-C12-C13	-2.12	111.61	124.38
19	A	608	PGV	C10-C11-C12	-2.09	108.17	124.66
25	G	102	CDL	C61-C60-C59	-2.09	103.71	114.54
14	N	601	HEA	CMC-C2C-C1C	-2.08	124.77	128.31
19	N	607	PGV	C18-C17-C16	-2.08	97.19	113.49
20	B	301	TGL	C27-C26-C25	-2.08	95.07	115.41
22	P	307	CHD	C19-C10-C1	-2.08	104.71	108.23
14	A	602	HEA	C1A-C2A-C3A	-2.07	105.00	107.07
22	B	303	CHD	C18-C13-C17	-2.06	107.96	111.20
19	N	607	PGV	C32-C31-C30	-2.06	103.86	114.54
23	O	303	PSC	O02-C1-C2	-2.06	115.89	123.76
14	N	601	HEA	C16-C15-C14	-2.06	117.15	120.98
20	D	201	TGL	CG3-CG2-CG1	-2.05	107.31	112.08
28	J	101	DMU	O6-C11-C9	-2.03	104.52	111.30
20	Y	101	TGL	OG2-CB1-OB1	-2.02	118.19	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	601	HEA	C3C-CAC-CBC	-2.01	122.35	126.40
20	D	201	TGL	CC6-CC5-CC4	-2.01	104.10	114.54
19	P	303	PGV	C22-C21-C20	-2.01	105.87	113.30
22	W	101	CHD	C21-C20-C17	-2.01	109.89	112.99
26	P	308	PEK	C03-C02-C01	-2.00	107.42	112.08
25	T	103	CDL	C22-C21-C20	2.02	125.02	114.54
25	P	304	CDL	C43-C42-C41	2.02	125.05	114.54
23	O	303	PSC	C04-C05-N	2.02	122.66	116.04
26	C	306	PEK	C31-C30-C29	2.03	125.07	114.54
14	N	602	HEA	C3A-C4A-NA	2.03	114.78	110.94
26	C	306	PEK	O13-P-O11	2.03	117.91	108.24
25	T	103	CDL	CA6-OA8-CA7	2.03	123.05	117.00
22	B	303	CHD	O7-C7-C8	2.03	113.91	109.28
22	W	101	CHD	C14-C8-C9	2.03	112.50	109.63
20	D	201	TGL	C22-C21-C20	2.04	125.14	114.54
28	Z	101	DMU	C11-C9-C8	2.05	118.11	112.99
25	C	303	CDL	C59-C58-C57	2.05	125.19	114.54
22	J	102	CHD	C18-C13-C17	2.06	114.45	111.20
19	P	303	PGV	C33-C32-C31	2.06	135.59	115.41
28	M	101	DMU	O4-C7-C8	2.08	115.06	110.36
28	Z	101	DMU	O16-C18-C19	2.09	115.64	109.63
25	G	102	CDL	C39-C38-C37	2.09	125.40	114.54
22	J	102	CHD	C15-C14-C13	2.09	105.60	103.59
22	C	305	CHD	C2-C1-C10	2.09	116.56	112.81
20	L	101	TGL	CC7-CC6-CC5	2.10	125.44	114.54
22	O	302	CHD	C23-C22-C20	2.10	117.40	114.79
26	T	101	PEK	C3-C4-C5	2.11	124.73	112.08
19	C	307	PGV	C26-C25-C24	2.11	125.50	114.54
26	C	306	PEK	C3-C2-C1	2.13	121.87	113.57
19	P	303	PGV	C9-C10-C11	2.13	124.85	112.08
26	G	103	PEK	O01-C02-C01	2.13	115.85	108.36
25	P	304	CDL	C63-C62-C61	2.14	125.66	114.54
20	Q	202	TGL	CG2-OG2-CB1	2.15	123.22	117.91
19	P	301	PGV	C24-C23-C22	2.17	125.79	114.54
20	Y	101	TGL	C30-C29-C14	2.17	125.82	114.54
20	D	201	TGL	C11-C10-CB9	2.17	125.82	114.54
22	C	304	CHD	C22-C20-C17	2.17	114.82	110.24
25	C	303	CDL	OB2-PB2-OB3	2.18	118.12	109.21
19	C	307	PGV	C25-C24-C23	2.18	125.88	114.54
23	B	304	PSC	C16-C15-C14	2.18	122.67	113.79
22	W	101	CHD	C18-C13-C14	2.19	114.65	111.20
25	G	102	CDL	C22-C21-C20	2.20	125.96	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	L	101	TGL	OG3-CG3-CG2	2.21	114.68	108.70
19	A	607	PGV	C32-C31-C30	2.22	126.05	114.54
14	A	601	HEA	C3C-C4C-NC	2.22	112.08	109.21
22	C	304	CHD	C18-C13-C14	2.22	114.70	111.20
19	P	303	PGV	C26-C25-C24	2.23	126.10	114.54
26	P	308	PEK	C3-C2-C1	2.23	122.28	113.57
26	T	101	PEK	C11-C10-C9	2.24	119.62	112.17
28	J	101	DMU	O55-C2-C3	2.25	115.23	109.89
19	N	607	PGV	O03-C19-C20	2.26	118.79	111.85
20	D	201	TGL	C16-C15-CC9	2.26	126.26	114.54
20	L	101	TGL	CC6-CC5-CC4	2.26	126.26	114.54
25	C	303	CDL	C22-C21-C20	2.26	126.30	114.54
26	G	101	PEK	C03-C02-C01	2.27	117.36	112.08
22	O	302	CHD	C4-C3-C2	2.27	113.43	110.53
26	G	101	PEK	C38-C37-C36	2.27	131.26	113.49
26	C	306	PEK	C34-C33-C32	2.27	126.35	114.54
20	Q	202	TGL	C15-CC9-CC8	2.28	126.39	114.54
28	P	306	DMU	O5-C6-O16	2.28	115.46	109.99
20	Y	101	TGL	C15-CC9-CC8	2.29	126.44	114.54
22	P	307	CHD	C18-C13-C12	2.29	111.39	109.09
20	L	101	TGL	C15-CC9-CC8	2.30	126.47	114.54
25	C	303	CDL	C87-C86-C85	2.30	131.51	113.49
22	W	101	CHD	C16-C17-C13	2.30	105.81	103.59
25	T	103	CDL	C23-C22-C21	2.31	126.52	114.54
28	M	101	DMU	O16-C18-C19	2.31	116.27	109.63
25	C	303	CDL	C58-C57-C56	2.31	126.54	114.54
14	N	602	HEA	C25-C23-C24	2.32	120.24	114.61
28	Z	101	DMU	O3-C5-C7	2.33	115.62	110.36
25	G	102	CDL	CA6-OA8-CA7	2.34	123.96	117.00
14	A	601	HEA	CMD-C2D-C3D	2.34	130.13	125.24
28	Z	101	DMU	O5-C4-C57	2.34	112.45	106.38
14	N	602	HEA	C21-C20-C19	2.34	120.36	112.61
23	B	304	PSC	C07-N-C06	2.35	115.05	108.96
26	G	103	PEK	O03-C21-C22	2.36	119.11	111.85
19	P	301	PGV	C15-C14-C13	2.36	123.38	113.79
14	A	602	HEA	C26-C15-C14	2.37	128.17	123.58
25	P	304	CDL	C56-C55-C54	2.37	126.85	114.54
25	C	303	CDL	C57-C56-C55	2.38	126.91	114.54
23	B	304	PSC	C01-O03-C19	2.40	124.14	117.00
19	A	608	PGV	O12-P-O13	2.40	119.03	109.21
26	P	308	PEK	C29-C28-C27	2.40	127.01	114.54
25	T	103	CDL	OA6-CA4-CA6	2.41	116.83	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	O	302	CHD	C1-C10-C9	2.42	115.27	111.43
25	P	304	CDL	C82-C81-C80	2.42	127.12	114.54
25	T	103	CDL	C19-C18-C17	2.43	127.15	114.54
26	P	308	PEK	C26-C25-C24	2.43	127.19	114.54
22	P	305	CHD	C9-C10-C5	2.43	112.14	108.68
25	P	304	CDL	CB6-CB4-CB3	2.44	117.78	112.08
20	Y	101	TGL	CC7-CC6-CC5	2.45	127.25	114.54
22	W	101	CHD	C11-C9-C8	2.46	114.31	110.77
25	G	102	CDL	C79-C78-C77	2.46	127.31	114.54
22	B	303	CHD	C4-C3-C2	2.46	113.68	110.53
14	A	602	HEA	C21-C20-C19	2.47	120.78	112.61
19	A	607	PGV	O02-C1-C2	2.47	133.21	123.76
20	D	201	TGL	C20-CA9-CA8	2.47	127.39	114.54
19	P	303	PGV	C32-C31-C30	2.48	127.42	114.54
26	C	306	PEK	C29-C28-C27	2.49	127.48	114.54
26	T	102	PEK	C02-O01-C1	2.50	124.08	117.91
25	P	304	CDL	C83-C82-C81	2.50	127.54	114.54
25	G	102	CDL	C44-C43-C42	2.51	127.58	114.54
25	G	102	CDL	C84-C83-C82	2.52	127.63	114.54
26	G	101	PEK	C01-O03-C21	2.52	124.51	117.00
19	Q	201	PGV	C7-C6-C5	2.53	127.69	114.54
22	C	304	CHD	C15-C14-C13	2.53	106.03	103.59
26	C	306	PEK	O03-C01-C02	2.54	115.56	108.70
14	A	602	HEA	C3C-C4C-NC	2.55	112.51	109.21
19	C	307	PGV	O01-C1-C2	2.56	116.92	111.53
22	P	305	CHD	C2-C1-C10	2.56	117.39	112.81
22	J	102	CHD	C21-C20-C22	2.56	114.49	110.33
19	Q	201	PGV	C32-C31-C30	2.57	127.86	114.54
26	G	101	PEK	C10-C9-C8	2.57	139.87	124.38
26	T	101	PEK	C25-C24-C23	2.57	127.89	114.54
22	C	304	CHD	C14-C8-C7	2.58	115.46	111.77
25	G	102	CDL	C72-C71-CB7	2.59	123.66	113.57
28	P	306	DMU	C1-C2-C3	2.59	115.35	109.63
25	T	103	CDL	C72-C71-CB7	2.59	123.69	113.57
25	G	102	CDL	C83-C82-C81	2.60	128.03	114.54
20	Q	202	TGL	C10-CB9-CB8	2.60	128.03	114.54
20	Q	202	TGL	CG1-OG1-CA1	2.60	124.74	117.00
22	B	303	CHD	C1-C10-C5	2.62	110.65	107.76
22	W	101	CHD	C15-C14-C13	2.63	106.12	103.59
14	N	602	HEA	C27-C19-C18	2.64	128.70	123.58
23	O	303	PSC	C02-O01-C1	2.65	124.45	117.91
19	P	303	PGV	C15-C14-C13	2.66	124.58	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Y	101	TGL	CC3-CC2-CC1	2.68	124.02	113.57
25	P	304	CDL	C42-C41-C40	2.68	128.47	114.54
20	L	101	TGL	OG1-CA1-CA2	2.69	120.14	111.85
25	C	303	CDL	CA4-OA6-CA5	2.69	124.57	117.91
25	C	303	CDL	OA8-CA6-CA4	2.71	116.03	108.70
20	N	608	TGL	C15-CC9-CC8	2.72	128.67	114.54
20	Q	202	TGL	CB5-CB4-CB3	2.73	128.72	114.54
25	T	103	CDL	C76-C75-C74	2.73	128.72	114.54
22	P	305	CHD	C1-C2-C3	2.73	114.05	110.41
28	J	101	DMU	O16-C18-C19	2.74	117.51	109.63
25	G	102	CDL	C19-C18-C17	2.75	128.81	114.54
26	P	308	PEK	C01-O03-C21	2.75	125.20	117.00
19	A	607	PGV	C27-C26-C25	2.75	128.84	114.54
22	C	305	CHD	C11-C9-C8	2.77	114.76	110.77
26	T	102	PEK	O03-C01-C02	2.77	116.19	108.70
22	P	305	CHD	C13-C14-C8	2.78	118.38	114.73
20	L	101	TGL	CC3-CC2-CC1	2.78	124.42	113.57
22	B	303	CHD	C1-C10-C9	2.78	115.85	111.43
19	C	302	PGV	C15-C14-C13	2.79	125.12	113.79
22	W	101	CHD	C6-C7-C8	2.79	114.42	111.46
20	L	101	TGL	C13-C12-C11	2.80	129.07	114.54
25	P	304	CDL	C72-C71-CB7	2.81	124.52	113.57
25	P	304	CDL	C39-C38-C37	2.81	129.13	114.54
22	P	305	CHD	C11-C9-C8	2.82	114.84	110.77
26	G	103	PEK	C02-O01-C1	2.83	124.90	117.91
22	J	102	CHD	O7-C7-C8	2.83	115.73	109.28
26	C	306	PEK	C14-C13-C12	2.84	121.59	112.17
22	C	304	CHD	O7-C7-C8	2.84	115.76	109.28
25	P	304	CDL	OA8-CA7-C31	2.85	120.62	111.85
22	J	102	CHD	C4-C5-C10	2.91	115.78	112.66
23	B	304	PSC	C22-C21-C20	2.92	124.11	113.30
25	G	102	CDL	C23-C22-C21	2.92	129.70	114.54
25	P	304	CDL	C32-C31-CA7	2.92	124.96	113.57
20	Y	101	TGL	OG2-CG2-CG3	2.92	118.64	108.36
20	N	608	TGL	C11-C10-CB9	2.93	129.74	114.54
19	Q	201	PGV	O03-C19-C20	2.95	120.91	111.85
26	T	101	PEK	O02-C1-C2	2.96	135.10	123.76
25	P	304	CDL	OA8-CA6-CA4	2.97	116.71	108.70
19	Q	201	PGV	C4-C3-C2	2.98	124.34	113.30
20	B	301	TGL	OG1-CG1-CG2	2.98	116.75	108.70
20	Q	202	TGL	OC1-CC1-CC2	2.99	135.21	123.76
26	G	101	PEK	C30-C29-C28	3.00	130.13	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	304	PSC	C31-C30-C29	3.00	130.13	114.54
14	N	601	HEA	C3C-C4C-NC	3.01	113.10	109.21
25	T	103	CDL	C83-C82-C81	3.01	130.18	114.54
22	P	305	CHD	C18-C13-C14	3.02	115.96	111.20
20	D	201	TGL	C14-C13-C12	3.02	130.25	114.54
14	N	602	HEA	C3C-C4C-NC	3.03	113.12	109.21
26	T	102	PEK	C11-C10-C9	3.03	122.23	112.17
25	C	303	CDL	C42-C41-C40	3.03	130.28	114.54
22	C	304	CHD	C18-C13-C17	3.04	116.00	111.20
22	C	304	CHD	C4-C3-C2	3.05	114.43	110.53
20	B	301	TGL	C15-CC9-CC8	3.05	130.38	114.54
25	G	102	CDL	C40-C39-C38	3.05	130.40	114.54
28	J	101	DMU	C22-C25-C28	3.05	130.40	114.54
26	T	101	PEK	O03-C21-C22	3.06	121.27	111.85
20	Q	202	TGL	C21-C20-CA9	3.07	130.48	114.54
25	C	303	CDL	OA8-CA7-C31	3.08	121.33	111.85
26	T	102	PEK	C01-O03-C21	3.08	126.18	117.00
20	D	201	TGL	OG1-CA1-CA2	3.09	121.36	111.85
22	W	101	CHD	O7-C7-C8	3.09	116.31	109.28
26	P	308	PEK	C27-C26-C25	3.10	130.62	114.54
22	B	303	CHD	O3-C3-C2	3.10	117.52	110.04
19	P	301	PGV	O01-C1-C2	3.11	118.07	111.53
26	G	101	PEK	C11-C10-C9	3.12	122.53	112.17
23	O	303	PSC	O01-C02-C03	3.12	119.33	108.36
25	P	304	CDL	OB2-PB2-OB3	3.12	122.00	109.21
26	P	308	PEK	O03-C01-C02	3.13	117.14	108.70
22	W	101	CHD	C13-C14-C8	3.14	118.85	114.73
22	P	305	CHD	C15-C14-C8	3.15	123.00	118.34
22	P	305	CHD	C21-C20-C22	3.15	115.44	110.33
20	Q	202	TGL	C16-C15-CC9	3.15	130.91	114.54
22	P	305	CHD	C5-C6-C7	3.17	118.05	114.44
22	P	307	CHD	O7-C7-C8	3.19	116.54	109.28
26	T	102	PEK	O03-C21-C22	3.20	121.69	111.85
22	P	305	CHD	O12-C12-C13	3.20	116.46	111.12
20	N	608	TGL	OG1-CG1-CG2	3.21	117.37	108.70
25	P	304	CDL	OA6-CA4-CA3	3.21	119.65	108.36
22	B	303	CHD	C6-C7-C8	3.23	114.88	111.46
20	D	201	TGL	CA4-CA3-CA2	3.24	125.29	113.30
28	P	306	DMU	O16-C18-C19	3.25	118.97	109.63
22	P	305	CHD	C17-C13-C12	3.26	120.54	117.68
19	P	301	PGV	C02-O01-C1	3.26	125.97	117.91
22	W	101	CHD	C21-C20-C22	3.28	115.66	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	G	102	CDL	C80-C79-C78	3.29	131.62	114.54
22	O	302	CHD	O7-C7-C8	3.29	116.77	109.28
19	A	607	PGV	C30-C29-C28	3.32	131.76	114.54
26	P	308	PEK	C35-C34-C33	3.35	131.91	114.54
25	G	102	CDL	CA4-OA6-CA5	3.35	126.20	117.91
26	T	102	PEK	C2-C3-C4	3.36	119.81	113.65
26	G	103	PEK	C11-C10-C9	3.43	123.58	112.17
19	N	607	PGV	O02-C1-C2	3.46	137.01	123.76
25	P	304	CDL	C54-C53-C52	3.47	132.57	114.54
14	N	602	HEA	C26-C15-C16	3.47	120.66	115.37
25	P	304	CDL	O1-C1-CB2	3.47	122.31	109.32
25	C	303	CDL	C39-C38-C37	3.48	132.61	114.54
26	C	306	PEK	C26-C25-C24	3.48	132.63	114.54
25	P	304	CDL	OA4-PA1-OA3	3.54	130.96	112.56
22	J	102	CHD	C6-C7-C8	3.57	115.24	111.46
19	Q	201	PGV	O01-C1-C2	3.64	119.20	111.53
22	B	303	CHD	C14-C13-C12	3.66	110.68	107.37
28	P	306	DMU	O1-C9-C8	3.68	116.69	109.67
22	C	304	CHD	C1-C10-C5	3.68	111.82	107.76
20	L	101	TGL	OG2-CG2-CG3	3.71	121.40	108.36
26	C	306	PEK	O03-C21-C22	3.74	123.37	111.85
22	P	305	CHD	C14-C13-C12	3.77	110.78	107.37
22	J	102	CHD	C22-C20-C17	3.81	118.26	110.24
26	G	103	PEK	O03-C01-C02	3.82	119.02	108.70
22	W	101	CHD	C4-C3-C2	3.83	115.43	110.53
19	A	608	PGV	O01-C02-C01	3.84	121.84	108.36
28	P	306	DMU	O3-C5-C10	3.85	118.54	110.01
28	P	306	DMU	O7-C10-C5	3.85	117.69	108.12
22	O	302	CHD	C1-C10-C5	3.86	112.01	107.76
20	Y	101	TGL	OG1-CA1-CA2	3.86	123.73	111.85
22	W	101	CHD	C22-C20-C17	3.88	118.40	110.24
25	P	304	CDL	CA6-OA8-CA7	3.88	128.55	117.00
22	W	101	CHD	C11-C9-C10	3.89	117.81	113.77
22	W	101	CHD	C5-C4-C3	3.90	118.66	112.88
26	G	103	PEK	C01-O03-C21	3.90	128.62	117.00
25	G	102	CDL	CB6-OB8-CB7	3.94	128.73	117.00
14	N	601	HEA	C20-C21-C22	3.94	121.95	111.61
25	G	102	CDL	OA8-CA7-C31	3.96	124.03	111.85
22	J	102	CHD	C4-C3-C2	3.96	115.60	110.53
25	C	303	CDL	CA6-OA8-CA7	3.97	128.82	117.00
26	P	308	PEK	C24-C23-C22	3.98	128.02	113.30
19	Q	201	PGV	O01-C02-C01	3.99	122.37	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	P	308	PEK	O01-C1-C2	3.99	119.94	111.53
20	N	608	TGL	CB3-CB2-CB1	4.00	129.15	113.57
25	T	103	CDL	CB6-OB8-CB7	4.01	128.94	117.00
22	P	305	CHD	C1-C10-C5	4.07	112.24	107.76
26	C	306	PEK	C02-O01-C1	4.09	128.01	117.91
22	C	305	CHD	C1-C10-C5	4.12	112.30	107.76
25	C	303	CDL	OB5-PB2-OB3	4.14	126.15	109.21
22	J	102	CHD	C1-C2-C3	4.14	115.93	110.41
22	B	303	CHD	C9-C11-C12	4.15	119.59	114.38
25	T	103	CDL	OA8-CA7-C31	4.15	124.64	111.85
26	G	103	PEK	C14-C13-C12	4.16	125.97	112.17
25	G	102	CDL	OB8-CB6-CB4	4.16	119.94	108.70
22	J	102	CHD	C5-C4-C3	4.18	119.07	112.88
20	L	101	TGL	CB3-CB2-CB1	4.19	129.92	113.57
22	J	102	CHD	C9-C10-C5	4.22	114.68	108.68
19	A	608	PGV	O03-C19-C20	4.22	124.83	111.85
22	J	102	CHD	C2-C1-C10	4.26	120.45	112.81
22	W	101	CHD	C10-C9-C8	4.28	116.49	111.86
26	C	306	PEK	C24-C23-C22	4.31	129.26	113.30
22	W	101	CHD	C15-C14-C8	4.31	124.73	118.34
22	O	302	CHD	C17-C13-C14	4.31	104.44	100.08
26	G	101	PEK	O04-C21-C22	4.32	140.28	123.76
14	A	601	HEA	CMB-C2B-C3B	4.35	134.03	125.14
25	T	103	CDL	CA4-OA6-CA5	4.35	128.67	117.91
14	N	601	HEA	C20-C19-C18	4.39	129.15	120.98
20	D	201	TGL	CB5-CB4-CB3	4.39	137.35	114.54
14	A	602	HEA	C27-C19-C20	4.44	122.14	115.37
26	P	308	PEK	C02-O01-C1	4.46	128.93	117.91
20	Y	101	TGL	CG1-OG1-CA1	4.48	130.34	117.00
22	P	305	CHD	C4-C5-C10	4.48	117.47	112.66
25	T	103	CDL	OB8-CB6-CB4	4.51	120.88	108.70
28	P	306	DMU	O16-C6-C1	4.52	113.56	108.00
22	J	102	CHD	O12-C12-C13	4.52	118.67	111.12
20	B	301	TGL	CG2-OG2-CB1	4.54	129.15	117.91
20	D	201	TGL	CG3-OG3-CC1	4.54	130.54	117.00
22	C	304	CHD	C5-C6-C7	4.55	119.61	114.44
14	N	601	HEA	CMB-C2B-C3B	4.57	134.48	125.14
19	A	608	PGV	C01-O03-C19	4.59	130.69	117.00
22	B	303	CHD	C15-C14-C13	4.60	108.02	103.59
19	Q	201	PGV	C01-O03-C19	4.61	130.72	117.00
19	C	307	PGV	O03-C01-C02	4.61	121.16	108.70
25	C	303	CDL	OB6-CB5-C51	4.61	121.25	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	W	101	CHD	C1-C10-C5	4.73	112.97	107.76
20	L	101	TGL	CG3-OG3-CC1	4.77	131.20	117.00
22	P	305	CHD	C16-C17-C13	4.81	108.23	103.59
20	N	608	TGL	OG2-CB1-CB2	4.87	121.79	111.53
26	C	306	PEK	O01-C1-C2	4.88	121.80	111.53
20	D	201	TGL	C21-C20-CA9	4.89	139.94	114.54
22	J	102	CHD	C23-C22-C20	4.89	120.84	114.79
22	P	305	CHD	C10-C9-C8	4.90	117.16	111.86
22	W	101	CHD	C4-C5-C10	4.91	117.93	112.66
20	B	301	TGL	OG3-CC1-CC2	4.92	126.98	111.85
20	L	101	TGL	OG1-CG1-CG2	5.01	122.21	108.70
20	Y	101	TGL	OG3-CG3-CG2	5.09	122.43	108.70
20	Y	101	TGL	CG3-OG3-CC1	5.14	132.31	117.00
22	J	102	CHD	C9-C8-C7	5.14	118.10	111.89
20	L	101	TGL	OG2-CB1-CB2	5.22	122.53	111.53
22	W	101	CHD	C23-C22-C20	5.23	121.25	114.79
19	A	608	PGV	O01-C1-O02	5.27	138.00	123.67
20	Y	101	TGL	CB3-CB2-CB1	5.29	134.20	113.57
22	P	305	CHD	C15-C14-C13	5.34	108.74	103.59
22	J	102	CHD	C1-C10-C5	5.35	113.65	107.76
25	P	304	CDL	CA4-OA6-CA5	5.41	131.29	117.91
22	C	304	CHD	C16-C17-C13	5.45	108.85	103.59
25	T	103	CDL	OB6-CB5-C51	5.48	123.07	111.53
26	P	308	PEK	O03-C21-C22	5.49	128.74	111.85
22	C	305	CHD	C18-C13-C12	5.51	114.61	109.09
20	N	608	TGL	OG1-CA1-CA2	5.58	129.03	111.85
20	D	201	TGL	OC1-CC1-CC2	5.60	145.21	123.76
19	A	608	PGV	C02-O01-C1	5.67	131.93	117.91
28	J	101	DMU	O16-C6-C1	5.67	114.98	108.00
20	Y	101	TGL	OG3-CC1-CC2	5.68	129.34	111.85
20	D	201	TGL	CB3-CB2-CB1	5.75	136.00	113.57
25	C	303	CDL	OB8-CB7-C71	5.77	129.62	111.85
25	T	103	CDL	OA6-CA5-C11	5.84	123.83	111.53
22	P	307	CHD	C1-C10-C5	5.90	114.26	107.76
22	C	304	CHD	C4-C5-C10	5.92	119.00	112.66
25	C	303	CDL	OA6-CA5-C11	5.95	124.06	111.53
22	J	102	CHD	C6-C5-C10	5.95	119.05	112.66
25	P	304	CDL	OA6-CA5-C11	5.99	124.15	111.53
20	N	608	TGL	OG2-CG2-CG3	6.00	129.44	108.36
20	D	201	TGL	CG1-OG1-CA1	6.00	134.88	117.00
22	C	304	CHD	C15-C14-C8	6.07	127.33	118.34
25	P	304	CDL	OB8-CB7-C71	6.07	130.54	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	C	307	PGV	O03-C19-C20	6.16	130.82	111.85
20	B	301	TGL	OG1-CA1-CA2	6.17	130.84	111.85
22	J	102	CHD	C5-C6-C7	6.19	121.49	114.44
20	N	608	TGL	CG2-OG2-CB1	6.28	133.44	117.91
20	Q	202	TGL	CB3-CB2-CB1	6.30	138.13	113.57
22	C	304	CHD	C10-C9-C8	6.34	118.71	111.86
22	P	305	CHD	C4-C3-C2	6.38	118.69	110.53
22	C	304	CHD	C6-C5-C10	6.40	119.52	112.66
22	W	101	CHD	C14-C8-C7	6.50	121.06	111.77
23	B	304	PSC	O01-C1-C2	6.52	125.26	111.53
19	P	301	PGV	O03-C19-C20	6.53	131.96	111.85
26	T	102	PEK	O01-C1-C2	6.55	125.34	111.53
22	J	102	CHD	C11-C12-C13	6.63	117.91	111.22
22	W	101	CHD	C11-C12-C13	6.63	117.91	111.22
25	G	102	CDL	OB6-CB5-C51	6.70	125.65	111.53
19	A	608	PGV	C3-C2-C1	6.74	139.87	113.57
20	L	101	TGL	OG3-CC1-CC2	6.83	132.86	111.85
22	P	305	CHD	C6-C5-C10	6.87	120.02	112.66
22	C	304	CHD	C14-C13-C12	6.89	113.61	107.37
26	G	103	PEK	O01-C1-C2	7.03	126.35	111.53
20	N	608	TGL	CG3-OG3-CC1	7.06	138.02	117.00
22	C	304	CHD	C16-C17-C20	7.10	123.47	112.12
25	G	102	CDL	OA6-CA5-C11	7.25	126.81	111.53
22	W	101	CHD	O12-C12-C13	7.28	123.27	111.12
22	C	304	CHD	C6-C7-C8	7.42	119.33	111.46
23	O	303	PSC	O01-C1-C2	7.59	127.53	111.53
14	N	601	HEA	C27-C19-C20	7.74	127.16	115.37
22	P	305	CHD	C6-C7-C8	7.79	119.71	111.46
20	B	301	TGL	OG2-CG2-CG3	7.82	135.85	108.36
19	C	302	PGV	C22-C21-C20	7.91	142.59	113.30
20	Y	101	TGL	CG2-OG2-CB1	7.95	137.57	117.91
19	C	302	PGV	C23-C22-C21	8.11	156.69	114.54
14	A	601	HEA	C20-C19-C18	8.22	136.29	120.98
20	L	101	TGL	CG2-OG2-CB1	8.27	138.36	117.91
22	J	102	CHD	C10-C9-C8	8.60	121.16	111.86
14	A	601	HEA	C17-C18-C19	9.01	147.62	127.75
22	J	102	CHD	C15-C14-C8	9.12	131.85	118.34
20	Y	101	TGL	OG2-CB1-CB2	9.13	130.76	111.53
22	W	101	CHD	C13-C17-C20	9.13	130.57	119.44
22	J	102	CHD	C14-C8-C7	9.31	125.09	111.77
22	J	102	CHD	C13-C17-C20	9.44	130.94	119.44
20	B	301	TGL	OG2-CB1-CB2	9.44	131.43	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	301	TGL	CG3-OG3-CC1	9.97	146.69	117.00
20	Q	202	TGL	OG2-CB1-OB1	10.04	150.99	123.67
14	N	601	HEA	C17-C18-C19	11.38	152.85	127.75
20	D	201	TGL	OG2-CB1-OB1	12.05	156.45	123.67
26	T	101	PEK	C2-C3-C4	12.61	136.78	113.65
22	J	102	CHD	C17-C13-C12	14.23	130.16	117.68
22	W	101	CHD	C17-C13-C12	17.77	133.26	117.68

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	602	HEA	ND
14	A	602	HEA	NA
14	A	602	HEA	NB
14	N	601	HEA	ND
14	N	601	HEA	NB
14	A	601	HEA	ND
14	A	601	HEA	NA
14	A	601	HEA	NB
14	N	602	HEA	ND
14	N	602	HEA	NA
14	N	602	HEA	NB

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	G	102	CDL	CA4-OA6-CA5-C11
19	P	301	PGV	P-O11-C03-C02
19	Q	201	PGV	C02-O01-C1-O02
19	Q	201	PGV	C02-O01-C1-C2

There are no ring outliers.

40 monomers are involved in 372 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	601	HEA	9	0
14	A	602	HEA	1	0
18	A	606	PER	1	0
19	A	607	PGV	4	0
19	A	608	PGV	7	0
20	B	301	TGL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	304	PSC	13	0
19	C	302	PGV	7	0
25	C	303	CDL	26	0
22	C	304	CHD	2	0
22	C	305	CHD	1	0
26	C	306	PEK	13	0
19	C	307	PGV	1	0
20	D	201	TGL	21	0
26	G	101	PEK	7	0
25	G	102	CDL	37	0
26	G	103	PEK	9	0
28	J	101	DMU	5	0
22	J	102	CHD	6	0
20	L	101	TGL	19	0
14	N	601	HEA	10	0
14	N	602	HEA	1	0
18	N	606	PER	1	0
19	N	607	PGV	1	0
20	N	608	TGL	6	0
23	O	303	PSC	19	0
19	P	301	PGV	3	0
19	P	303	PGV	6	0
25	P	304	CDL	24	0
22	P	305	CHD	6	0
28	P	306	DMU	10	0
22	P	307	CHD	1	0
26	P	308	PEK	16	0
19	Q	201	PGV	11	0
20	Q	202	TGL	15	0
26	T	101	PEK	8	0
26	T	102	PEK	10	0
25	T	103	CDL	28	0
22	W	101	CHD	6	0
20	Y	101	TGL	23	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	513/514 (99%)	-0.46	0 100 100	17, 21, 29, 68	0
1	N	513/514 (99%)	-0.38	0 100 100	18, 25, 33, 63	0
2	B	226/227 (99%)	-0.51	4 (1%) 71 75	20, 28, 49, 71	0
2	O	226/227 (99%)	-0.50	4 (1%) 71 75	25, 34, 60, 90	0
3	C	259/261 (99%)	-0.78	1 (0%) 93 94	19, 25, 37, 77	0
3	P	259/261 (99%)	-0.69	3 (1%) 81 83	20, 26, 39, 70	0
4	D	144/147 (97%)	-0.79	1 (0%) 89 91	23, 29, 44, 76	0
4	Q	144/147 (97%)	0.57	15 (10%) 8 8	29, 43, 76, 153	0
5	E	105/109 (96%)	-0.63	2 (1%) 70 73	23, 30, 53, 136	0
5	R	105/109 (96%)	-0.12	3 (2%) 55 58	26, 38, 61, 149	0
6	F	98/98 (100%)	0.06	8 (8%) 14 14	21, 31, 94, 141	0
6	S	98/98 (100%)	0.07	9 (9%) 11 11	22, 30, 80, 126	0
7	G	83/85 (97%)	0.59	17 (20%) 1 1	23, 32, 110, 158	0
7	T	83/85 (97%)	0.56	18 (21%) 1 1	23, 36, 112, 154	0
8	H	79/85 (92%)	-0.18	7 (8%) 12 11	25, 36, 92, 133	0
8	U	79/85 (92%)	-0.21	9 (11%) 7 6	31, 40, 103, 127	0
9	I	72/73 (98%)	0.26	7 (9%) 10 9	27, 41, 63, 82	0
9	V	72/73 (98%)	0.55	7 (9%) 10 9	27, 47, 69, 143	0
10	J	58/59 (98%)	0.33	7 (12%) 6 5	25, 35, 65, 134	0
10	W	58/59 (98%)	0.04	6 (10%) 9 8	27, 38, 69, 158	0
11	K	49/56 (87%)	-0.54	0 100 100	28, 35, 49, 58	0
11	X	49/56 (87%)	1.03	7 (14%) 4 3	36, 47, 68, 81	0
12	L	46/47 (97%)	-0.72	1 (2%) 65 68	22, 27, 53, 95	0
12	Y	46/47 (97%)	-0.60	1 (2%) 65 68	27, 34, 58, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	43/46 (93%)	-0.24	4 (9%) 11 10	24, 28, 64, 118	0
13	Z	43/46 (93%)	0.04	5 (11%) 6 6	31, 38, 79, 145	0
All	All	3550/3614 (98%)	-0.29	146 (4%) 41 43	17, 29, 61, 158	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	37.2
4	Q	5	VAL	33.5
4	Q	6	VAL	14.8
6	F	97	ALA	13.2
6	F	98	HIS	11.7
5	R	109	VAL	11.1
4	Q	7	LYS	10.4
10	J	1	PHE	10.3
4	Q	4	SER	10.2
9	V	37	PHE	9.5
6	F	96	LEU	9.3
6	S	98	HIS	9.0
10	J	58	LYS	8.9
7	G	1	ALA	8.2
9	I	37	PHE	7.9
7	T	36	TRP	7.8
8	U	8	ILE	7.4
8	U	7	LYS	7.3
13	Z	42	LYS	7.3
9	V	2	THR	7.1
11	X	6	ALA	7.1
5	R	5	HIS	6.8
6	F	1	ALA	6.6
6	S	2	SER	6.3
8	H	47	GLY	6.1
10	W	58	LYS	6.0
7	G	40	GLY	6.0
6	S	1	ALA	5.9
7	T	8	HIS	5.9
8	H	45	ALA	5.9
4	Q	8	SER	5.9
6	S	96	LEU	5.8
3	P	3	HIS	5.8
6	F	2	SER	5.6

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Mol	Chain	Res	Type	RSRZ
13	M	40	TYR	5.6
7	T	1	ALA	5.6
11	X	13	TYR	5.6
11	X	7	PRO	5.6
5	E	5	HIS	5.5
4	Q	51	LEU	5.5
10	W	1	PHE	5.5
6	S	94	HIS	5.3
7	G	3	ALA	5.3
8	H	44	THR	5.3
7	T	3	ALA	5.2
7	T	84	LYS	5.0
13	Z	43	SER	5.0
2	O	90	ILE	5.0
9	I	25	PHE	4.9
7	G	84	LYS	4.9
13	M	42	LYS	4.8
7	T	42	ARG	4.7
8	H	46	LYS	4.6
7	G	36	TRP	4.6
6	F	95	GLN	4.5
7	T	40	GLY	4.4
6	F	94	HIS	4.3
13	M	43	SER	4.3
4	Q	147	LYS	4.3
4	Q	53	ILE	4.3
7	T	10	GLY	4.3
8	H	8	ILE	4.2
9	V	34	PHE	4.2
9	V	25	PHE	4.2
7	G	2	SER	4.1
7	T	2	SER	4.1
12	Y	47	LYS	4.0
7	G	8	HIS	4.0
8	U	10	ASN	4.0
10	W	57	HIS	4.0
5	E	109	VAL	3.9
7	T	5	LYS	3.9
7	T	9	GLY	3.9
7	G	7	ASP	3.8
7	T	41	HIS	3.8
7	G	42	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
10	W	48	TYR	3.7
13	Z	40	TYR	3.7
6	S	95	GLN	3.7
7	G	39	SER	3.6
7	G	41	HIS	3.6
8	U	48	GLY	3.5
7	T	39	SER	3.3
7	G	9	GLY	3.2
9	V	31	PHE	3.1
4	Q	39	ALA	3.1
9	V	19	PHE	3.1
7	G	10	GLY	3.1
4	D	147	LYS	3.1
8	H	48	GLY	3.1
10	W	52	TRP	3.0
13	M	39	ASN	3.0
9	I	29	LEU	3.0
2	O	113	TYR	2.9
7	G	6	GLY	2.9
4	Q	48	TRP	2.9
7	G	45	PRO	2.9
13	Z	39	ASN	2.9
7	G	5	LYS	2.9
2	B	55	THR	2.8
10	J	48	TYR	2.8
7	T	6	GLY	2.8
10	J	57	HIS	2.8
8	U	49	ASP	2.8
7	T	7	ASP	2.8
4	Q	140	TYR	2.7
11	X	12	LYS	2.7
3	C	3	HIS	2.7
6	S	93	PRO	2.7
9	I	19	PHE	2.7
2	B	59	GLN	2.7
8	U	46	LYS	2.7
7	T	33	LEU	2.7
10	J	2	GLU	2.6
5	R	108	LYS	2.6
4	Q	46	ALA	2.6
8	H	50	VAL	2.6
9	I	2	THR	2.5

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Mol	Chain	Res	Type	RSRZ
7	T	38	HIS	2.5
11	X	28[A]	VAL	2.5
2	O	91	ASN	2.4
8	U	47	GLY	2.4
7	T	43	GLU	2.4
12	L	2	HIS	2.4
4	Q	72	ASN	2.4
10	J	56	PRO	2.4
2	B	61	VAL	2.3
3	P	37	PHE	2.3
9	I	33	THR	2.3
2	B	60	GLU	2.3
4	Q	73	ARG	2.3
6	F	3	GLY	2.3
10	W	2	GLU	2.2
8	U	9	LYS	2.2
9	V	33	THR	2.2
13	Z	32	TRP	2.2
9	I	34	PHE	2.1
6	S	3	GLY	2.1
11	X	9	PHE	2.1
11	X	23	THR	2.1
3	P	88	ILE	2.1
8	U	44	THR	2.0
4	Q	49	SER	2.0
10	J	4	ARG	2.0
2	O	92	ASN	2.0
7	G	43	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FME	O	1	10/11	0.97	0.06	-	29,34,48,59	0
7	TPO	G	11	11/12	0.49	0.31	-	61,102,165,180	0
1	FME	A	1	10/11	0.97	0.10	-	31,39,64,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FME	B	1	10/11	0.97	0.08	-	22,27,48,55	0
9	SAC	I	1	9/10	0.91	0.31	-	54,70,75,82	0
1	FME	N	1	10/11	0.98	0.09	-	33,40,72,74	0
9	SAC	V	1	9/10	0.52	0.37	-	114,126,154,162	0
7	TPO	T	11	11/12	0.62	0.24	-	75,96,179,187	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	CHD	W	101	29/29	0.45	0.43	13.85	59,136,161,164	0
22	CHD	J	102	29/29	0.57	0.44	10.79	57,133,165,172	0
25	CDL	P	304	100/100	0.86	0.27	10.35	32,78,140,149	0
25	CDL	C	303	100/100	0.85	0.32	6.72	29,72,127,137	0
18	PER	N	606	2/2	0.96	0.18	6.23	20,20,20,26	0
19	PGV	A	608	51/51	0.87	0.17	6.09	31,68,107,120	0
19	PGV	Q	201	51/51	0.85	0.26	5.71	42,79,161,191	0
20	TGL	N	608	63/63	0.86	0.20	5.68	47,76,120,136	0
25	CDL	T	103	100/100	0.69	0.28	5.27	50,91,168,202	0
20	TGL	D	201	63/63	0.85	0.14	4.98	30,55,90,101	0
25	CDL	G	102	100/100	0.70	0.30	4.80	51,96,162,187	0
18	PER	A	606	2/2	0.97	0.18	4.78	17,17,17,22	0
22	CHD	P	305	29/29	0.79	0.35	4.34	47,91,109,111	0
20	TGL	L	101	63/63	0.87	0.17	3.98	30,58,96,101	0
28	DMU	Z	101	33/33	0.85	0.20	3.69	41,47,61,63	0
20	TGL	Y	101	63/63	0.83	0.18	3.36	37,64,106,120	0
28	DMU	J	101	33/33	0.77	0.25	3.36	44,65,156,176	0
22	CHD	C	304	29/29	0.79	0.40	2.88	46,96,116,118	0
20	TGL	B	301	63/63	0.90	0.12	2.82	40,65,90,103	0
28	DMU	M	101	33/33	0.90	0.14	2.51	33,38,51,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
19	PGV	C	307	51/51	0.81	0.25	2.42	47,85,169,181	0
23	PSC	B	304	52/52	0.81	0.24	2.41	39,107,190,207	0
20	TGL	Q	202	63/63	0.79	0.17	2.35	40,62,99,110	0
28	DMU	P	306	33/33	0.80	0.20	2.12	36,105,192,198	0
23	PSC	O	303	52/52	0.84	0.23	1.82	37,75,191,211	0
26	PEK	T	102	53/53	0.73	0.28	1.57	44,95,159,176	0
26	PEK	G	103	53/53	0.83	0.25	1.34	46,93,150,158	0
19	PGV	P	301	51/51	0.81	0.21	1.27	45,85,147,177	0
19	PGV	C	302	51/51	0.98	0.07	1.20	22,29,81,98	0
26	PEK	P	308	53/53	0.77	0.21	1.20	38,79,120,144	0
26	PEK	C	306	53/53	0.77	0.17	1.17	34,78,128,158	0
16	MG	N	604	1/1	0.99	0.09	0.96	25,25,25,25	0
26	PEK	G	101	53/53	0.97	0.08	0.78	23,40,82,96	0
26	PEK	T	101	53/53	0.97	0.08	0.76	26,42,83,92	0
19	PGV	A	607	51/51	0.98	0.07	0.71	20,29,56,65	0
14	HEA	N	601	60/60	0.99	0.08	0.70	21,23,43,51	0
19	PGV	P	303	51/51	0.98	0.06	0.58	21,30,71,79	0
14	HEA	N	602	60/60	0.99	0.08	0.11	19,21,28,31	0
22	CHD	C	305	29/29	0.94	0.07	0.03	26,28,31,34	0
19	PGV	N	607	51/51	0.98	0.07	-0.14	22,32,67,68	0
22	CHD	O	302	29/29	0.95	0.07	-0.23	23,26,29,34	0
21	CUA	O	301	2/2	1.00	0.08	-0.25	27,27,27,27	0
14	HEA	A	601	60/60	0.99	0.07	-0.28	17,19,37,48	0
27	ZN	S	101	1/1	1.00	0.04	-0.39	26,26,26,26	0
22	CHD	B	303	29/29	0.95	0.06	-0.40	24,26,29,37	0
27	ZN	F	101	1/1	1.00	0.04	-0.51	26,26,26,26	0
21	CUA	B	302	2/2	1.00	0.08	-0.54	21,21,21,21	0
14	HEA	A	602	60/60	0.99	0.07	-0.68	17,18,25,30	0
22	CHD	P	307	29/29	0.94	0.06	-0.89	25,29,32,35	0
17	NA	N	605	1/1	1.00	0.03	-2.21	30,30,30,30	0
16	MG	A	604	1/1	0.99	0.04	-2.60	19,19,19,19	0
17	NA	A	605	1/1	1.00	0.02	-3.05	23,23,23,23	0
15	CU	A	603	1/1	1.00	0.07	-	19,19,19,19	0
24	UNX	P	302	1/1	0.81	0.39	-	38,38,38,38	0
24	UNX	C	301	1/1	0.89	0.23	-	39,39,39,39	0
15	CU	N	603	1/1	1.00	0.08	-	21,21,21,21	0

6.5 Other polymers

There are no such residues in this entry.