Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:15 AM GMT

PDB ID	:	3L71
Title	:	Cytochrome BC1 complex from chicken with azoxystrobin bound
Authors	:	Huang, L.; Berry, E.A.
Deposited on	:	2009-12-27
Resolution	:	2.84 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:

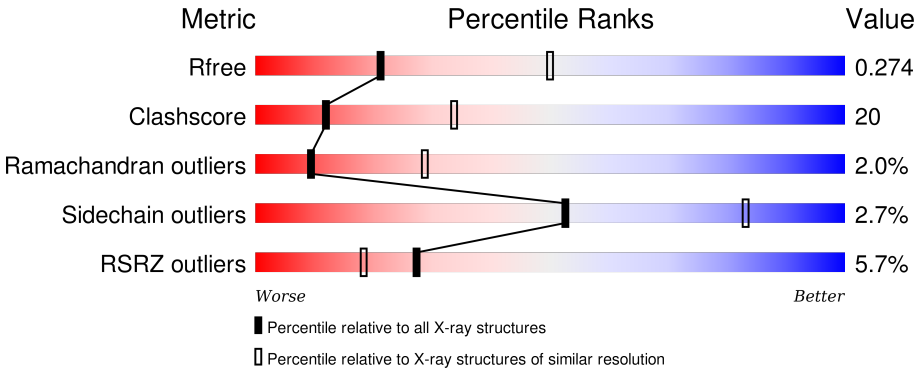
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.84 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	3170 (2.88-2.80)
Clashscore	102246	3658 (2.88-2.80)
Ramachandran outliers	100387	3591 (2.88-2.80)
Sidechain outliers	100360	3594 (2.88-2.80)
RSRZ outliers	91569	3184 (2.88-2.80)

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	446	3% 65% 32%
1	N	446	3% 60% 36%
2	B	441	5% 51% 40% 5%
2	O	441	4% 54% 37%
3	C	380	2% 78% 21%

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Mol	Chain	Length	Quality of chain
3	P	380	4% 75% 23%
4	D	241	2% 73% 25%
4	Q	241	2% 69% 30%
5	E	196	37% 47% 46% 6%
5	R	196	5% 52% 44%
6	F	110	67% 23% 8%
6	S	110	60% 29% 8%
7	G	81	2% 64% 32%
7	T	81	7% 63% 32%
8	H	77	% 57% 34% 9%
8	U	77	6% 51% 35% 13%
9	I	47	28% 45% 49%
9	V	47	32% 30% 60% 9%
10	J	61	3% 77% 20%
10	W	61	3% 74% 25%

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
11	PEE	A	2005	-	-	-	X
11	PEE	A	2008	-	-	-	X
11	PEE	C	2007	-	-	-	X
11	PEE	N	3008	-	X	-	-
11	PEE	P	3005	-	-	-	X
11	PEE	P	3007	-	-	-	X
14	UQ	C	2002	-	-	-	X
14	UQ	P	3002	-	-	-	X
15	GOL	P	3011	-	-	-	X
19	FES	E	501	-	-	X	-
19	FES	R	501	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32655 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 Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3447	2160	607	659	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

- Molecule 2 is a protein called Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3133	1968	544	612	9			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	614	10			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3017	2022	478	505	12			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

- Molecule 4 is a protein called Mitochondrial cytochrome c1, heme protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			
4	Q	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1509	950	263	290	6			

- Molecule 6 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			
6	S	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			

- Molecule 7 is a protein called Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	80	Total	C	N	O	0	0	0
			672	437	119	116			
7	T	79	Total	C	N	O	0	0	0
			662	432	117	113			

- Molecule 8 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total	C	N	O	S	0	0	0
			574	350	105	114	5			
8	U	67	Total	C	N	O	S	0	0	0
			553	338	103	107	5			

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			287	171	58	56	2			
9	V	43	Total	C	N	O	S	0	0	0
			277	167	55	53	2			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	28	UNK	-	INSERTION	UNP Q5ZLR5

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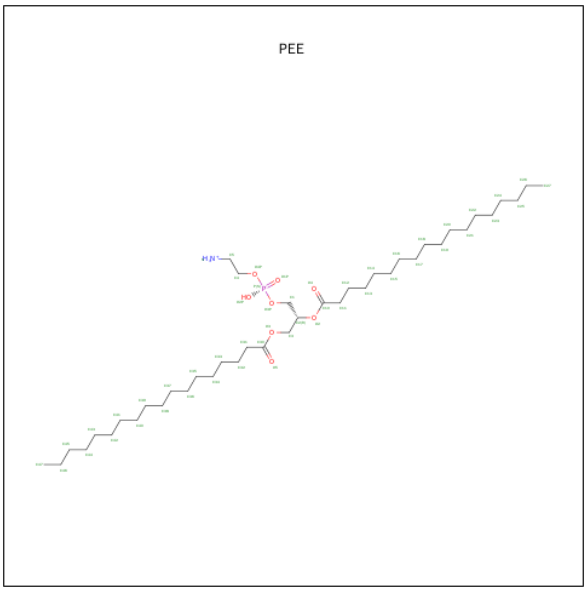
Chain	Residue	Modelled	Actual	Comment	Reference
I	29	UNK	-	INSERTION	UNP Q5ZLR5
I	30	UNK	-	INSERTION	UNP Q5ZLR5
I	31	UNK	-	INSERTION	UNP Q5ZLR5
I	32	UNK	-	INSERTION	UNP Q5ZLR5
I	33	UNK	-	INSERTION	UNP Q5ZLR5
I	34	UNK	-	INSERTION	UNP Q5ZLR5
I	35	UNK	-	INSERTION	UNP Q5ZLR5
I	36	UNK	-	INSERTION	UNP Q5ZLR5
I	37	UNK	-	INSERTION	UNP Q5ZLR5
I	38	UNK	-	INSERTION	UNP Q5ZLR5
I	39	UNK	-	INSERTION	UNP Q5ZLR5
I	40	UNK	-	INSERTION	UNP Q5ZLR5
I	41	UNK	-	INSERTION	UNP Q5ZLR5
I	42	UNK	-	INSERTION	UNP Q5ZLR5
V	25	UNK	-	INSERTION	UNP Q5ZLR5
V	26	UNK	-	INSERTION	UNP Q5ZLR5
V	27	UNK	-	INSERTION	UNP Q5ZLR5
V	28	UNK	-	INSERTION	UNP Q5ZLR5
V	29	UNK	-	INSERTION	UNP Q5ZLR5
V	30	UNK	-	INSERTION	UNP Q5ZLR5
V	31	UNK	-	INSERTION	UNP Q5ZLR5
V	32	UNK	-	INSERTION	UNP Q5ZLR5
V	33	UNK	-	INSERTION	UNP Q5ZLR5
V	35	UNK	-	INSERTION	UNP Q5ZLR5
V	36	UNK	-	INSERTION	UNP Q5ZLR5
V	37	UNK	-	INSERTION	UNP Q5ZLR5
V	38	UNK	-	INSERTION	UNP Q5ZLR5
V	39	UNK	-	INSERTION	UNP Q5ZLR5
V	40	UNK	-	INSERTION	UNP Q5ZLR5

- Molecule 10 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein.

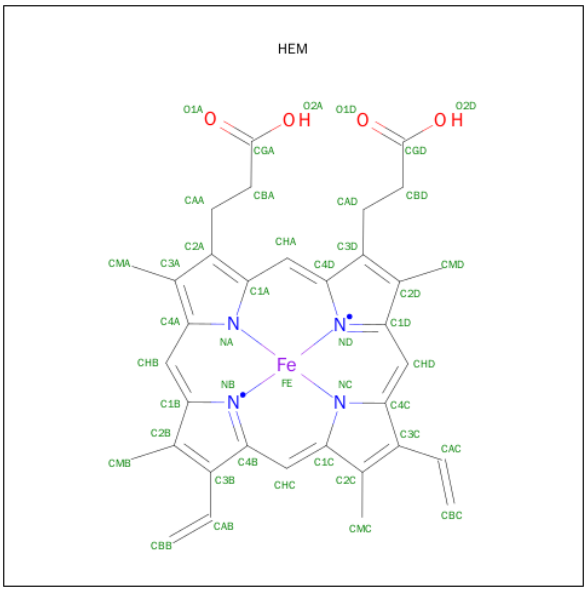
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	60	Total	C	N	O	0	0	1
			479	311	86	82			

- Molecule 11 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



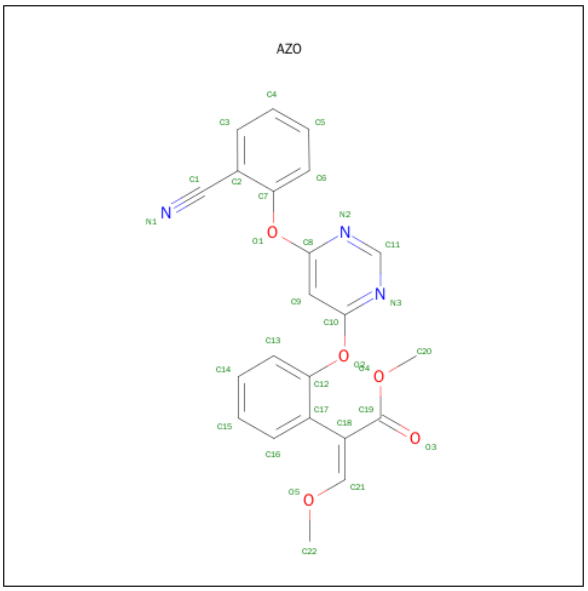
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C N O P 50 40 1 8 1	0	0
11	A	1	Total C O P 21 12 8 1	0	0
11	C	1	Total C N O P 49 39 1 8 1	0	0
11	N	1	Total O P 5 4 1	0	0
11	P	1	Total C N O P 50 40 1 8 1	0	0
11	P	1	Total C N O P 49 39 1 8 1	0	0

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



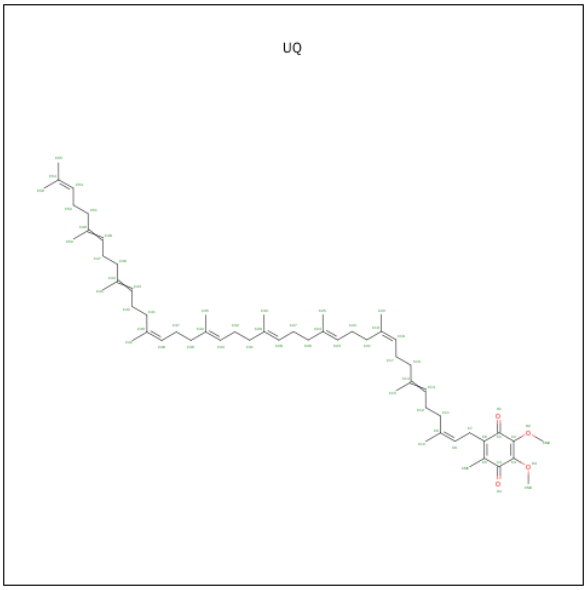
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is METHYL (2Z)-2-(2-{[6-(2-CYANOPHENOXY)PYRIMIDIN-4-YL]OXY}PHENYL)-3-METHOXYACRYLATE (three-letter code: AZO) (formula: $C_{22}H_{17}N_3O_5$).



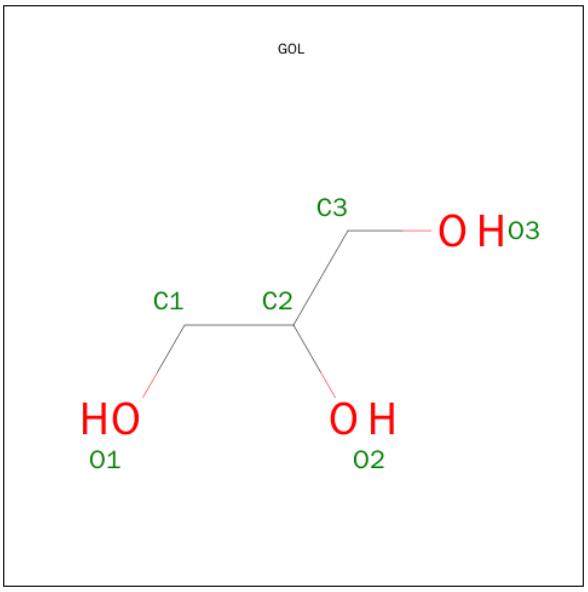
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	N	O	0	0
			30	22	3	5		
13	P	1	Total	C	N	O	0	0
			30	22	3	5		

- Molecule 14 is COENZYME Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-ISOMER (three-letter code: UQ) (formula: $C_{59}H_{90}O_4$).



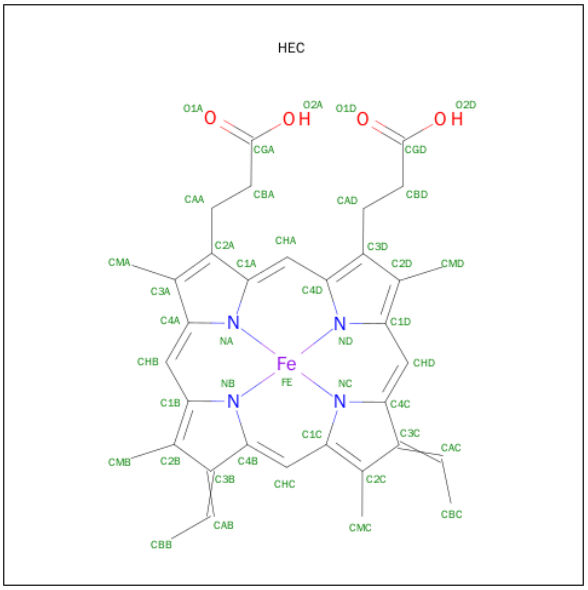
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			19	15	4		
14	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 15 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



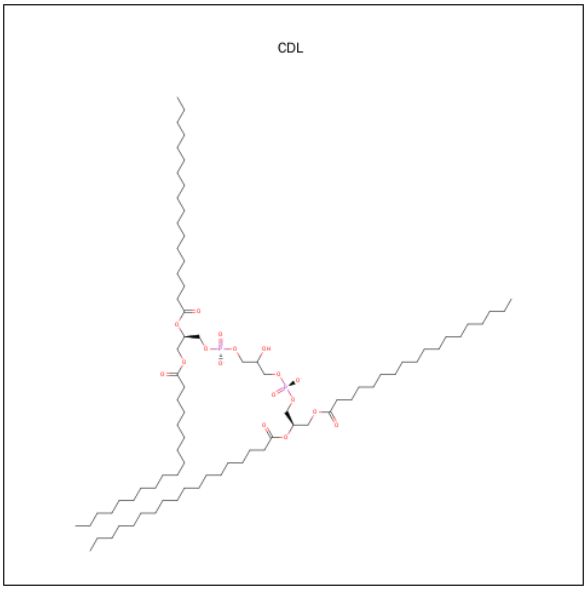
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			6	3	3		
15	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 16 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



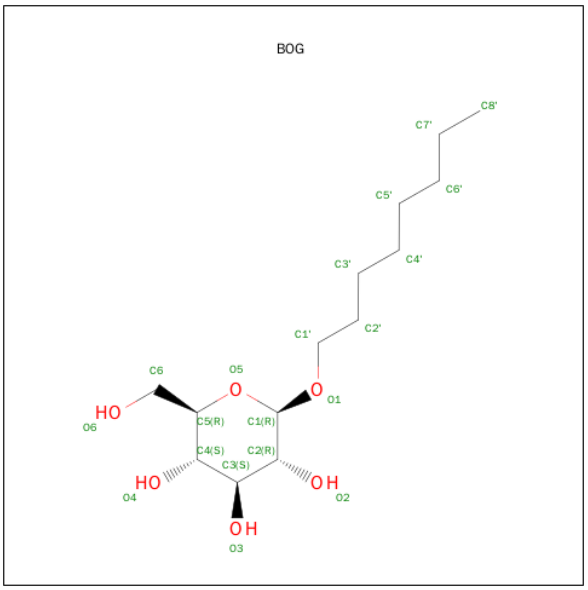
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
16	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



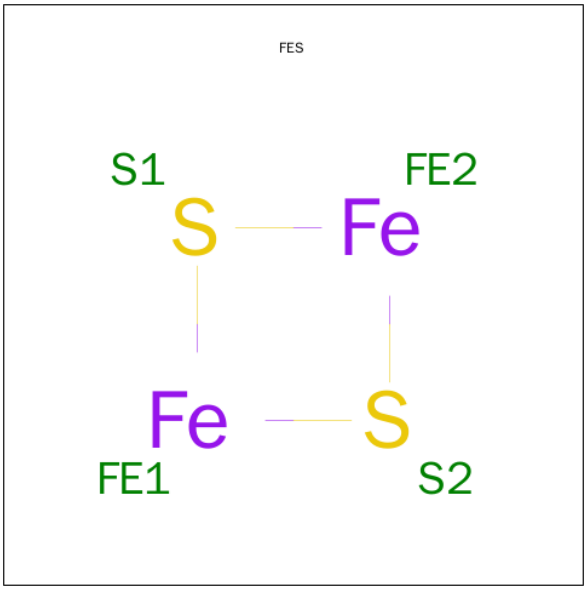
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	C	O	P	0	0
			42	23	17	2		
17	G	1	Total	C	O	P	0	0
			40	21	17	2		
17	Q	1	Total	C	O	P	0	0
			42	23	17	2		
17	T	1	Total	C	O	P	0	0
			40	21	17	2		

- Molecule 18 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	D	1	Total C O 20 14 6	0	0
18	D	1	Total C O 13 7 6	0	0
18	P	1	Total C O 12 6 6	0	0
18	Q	1	Total C O 20 14 6	0	0
18	Q	1	Total C O 13 7 6	0	0

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	E	1	Total Fe S 4 2 2	0	0
19	R	1	Total Fe S 4 2 2	0	0

- Molecule 20 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	C	8	Total O 8 8	0	0
20	E	1	Total O 1 1	0	0
20	P	9	Total O 9 9	0	0

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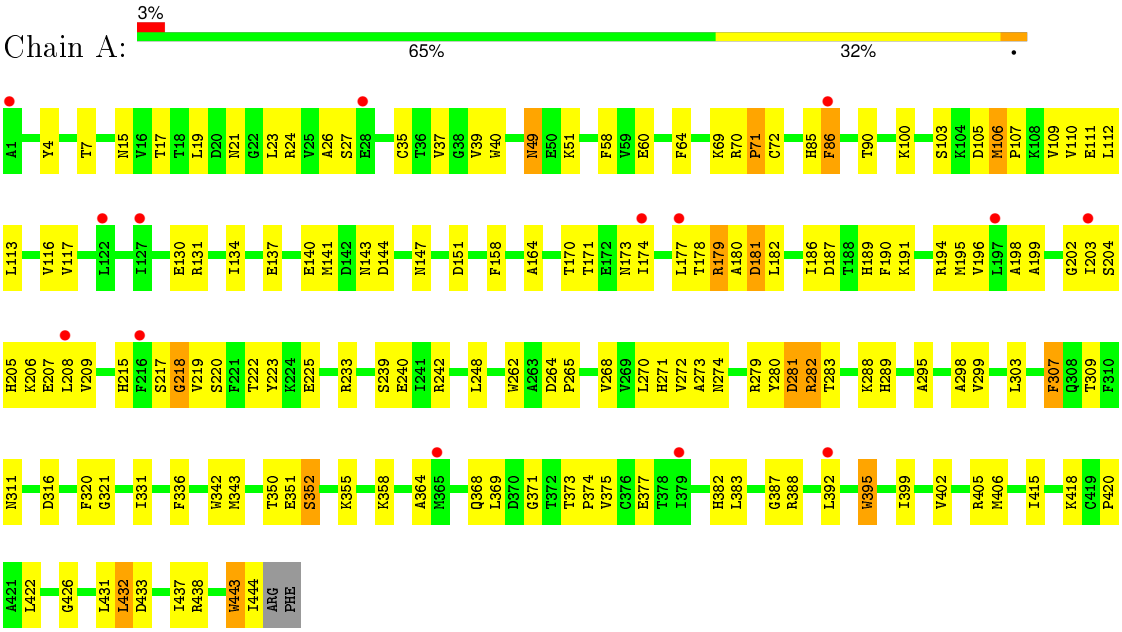
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	R	1	Total O 1 1	0	0

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.

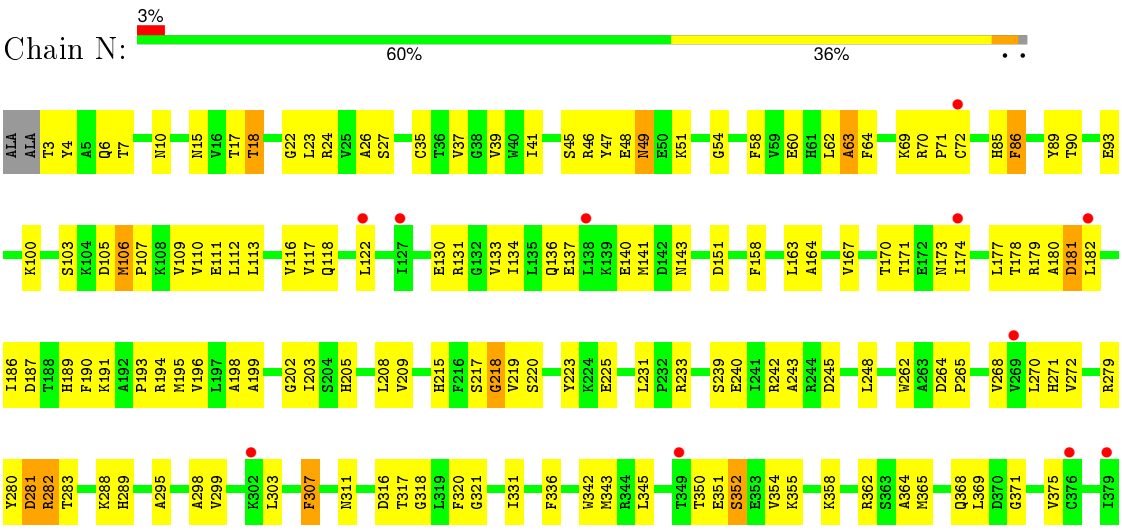
• Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

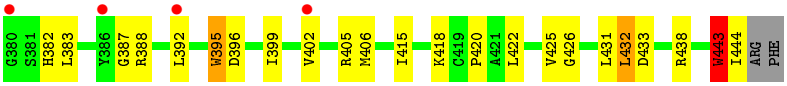
Chain A:



• Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

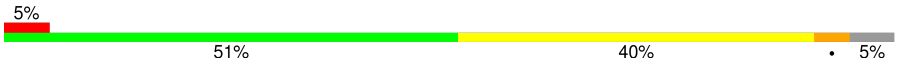
Chain N:

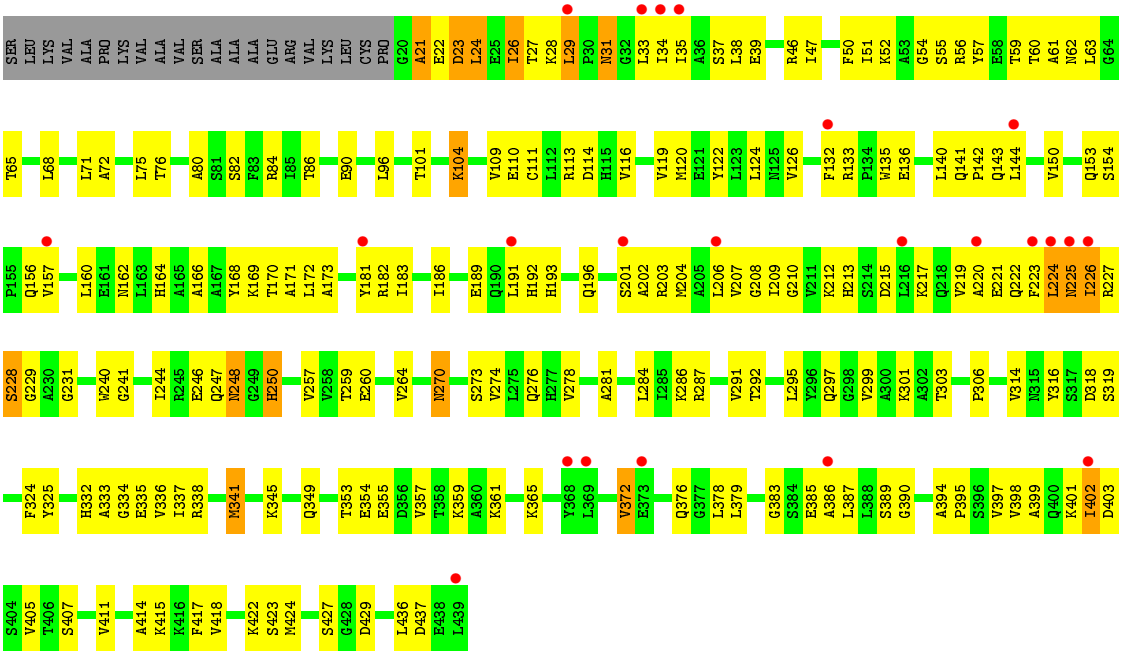




• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

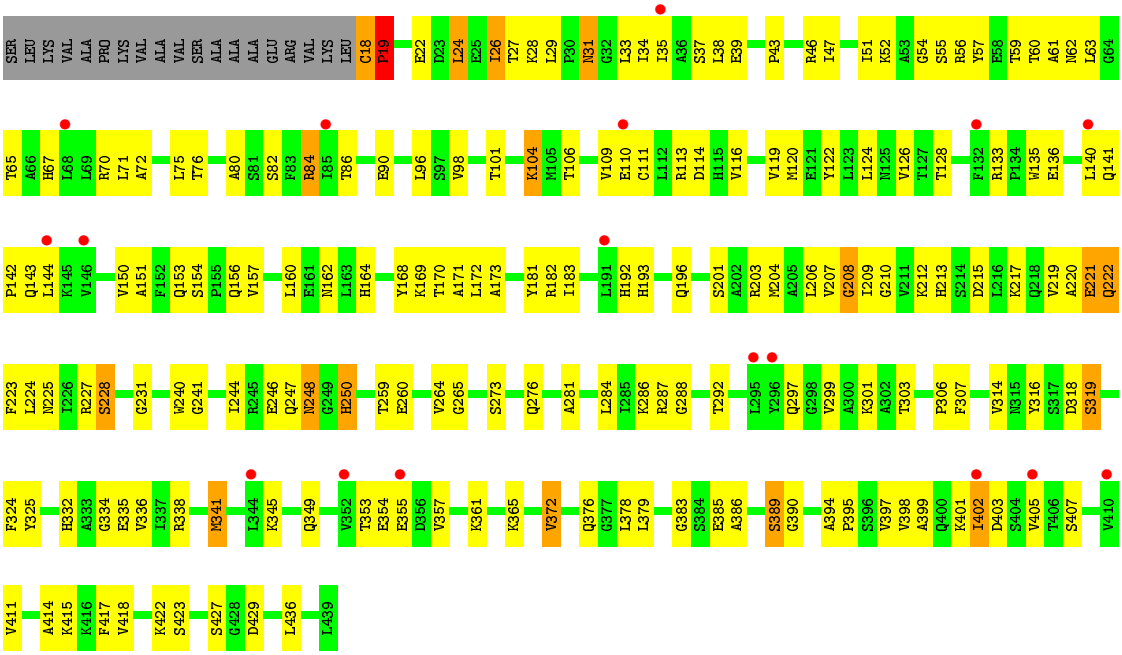
Chain B:





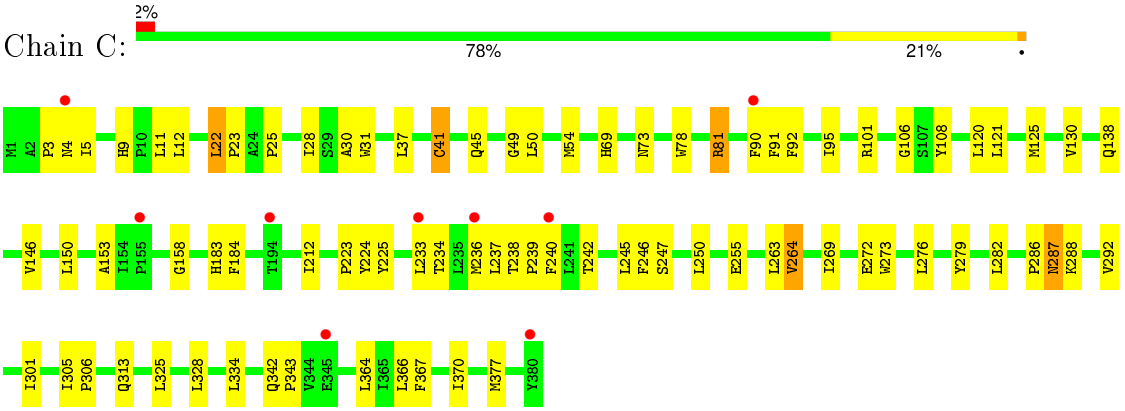
• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

Chain O:



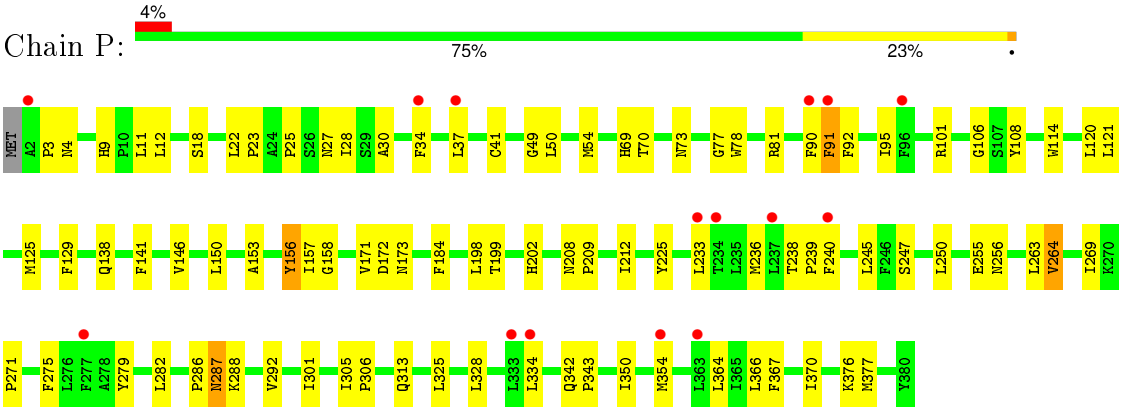
• Molecule 3: Cytochrome b

Chain C:



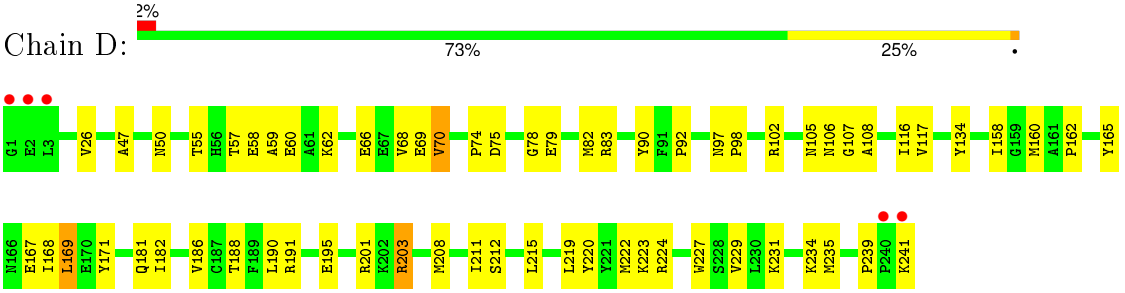
• Molecule 3: Cytochrome b

Chain P:



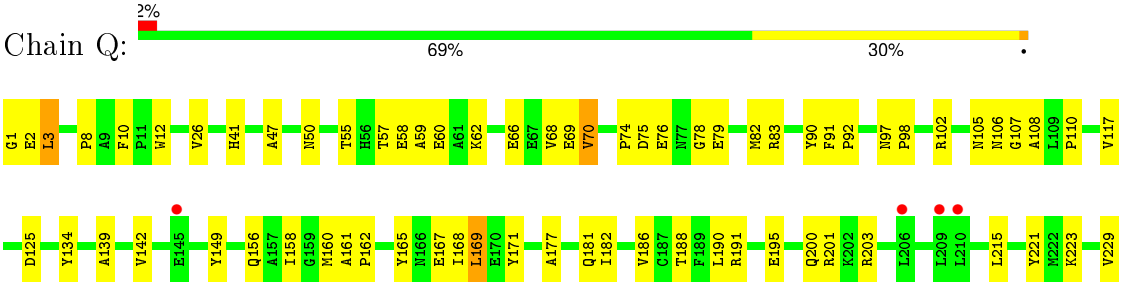
• Molecule 4: Mitochondrial cytochrome c1, heme protein

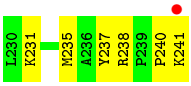
Chain D:



• Molecule 4: Mitochondrial cytochrome c1, heme protein

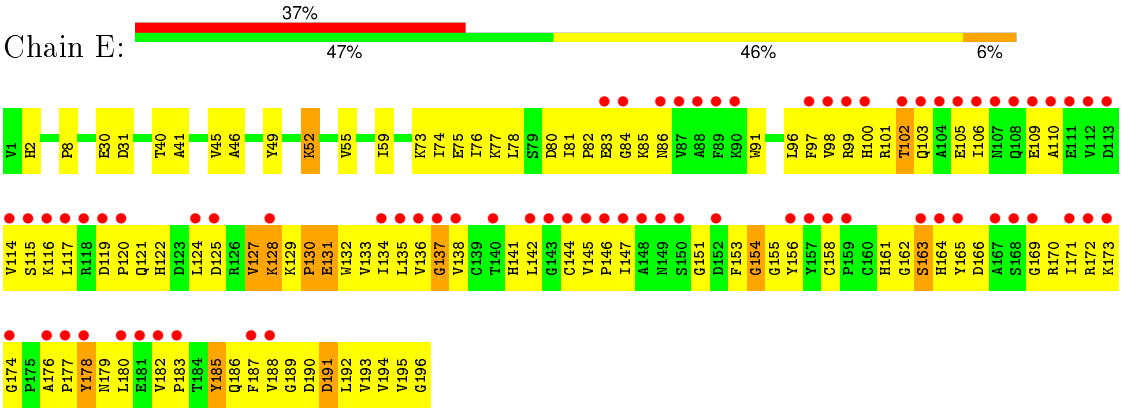
Chain Q:





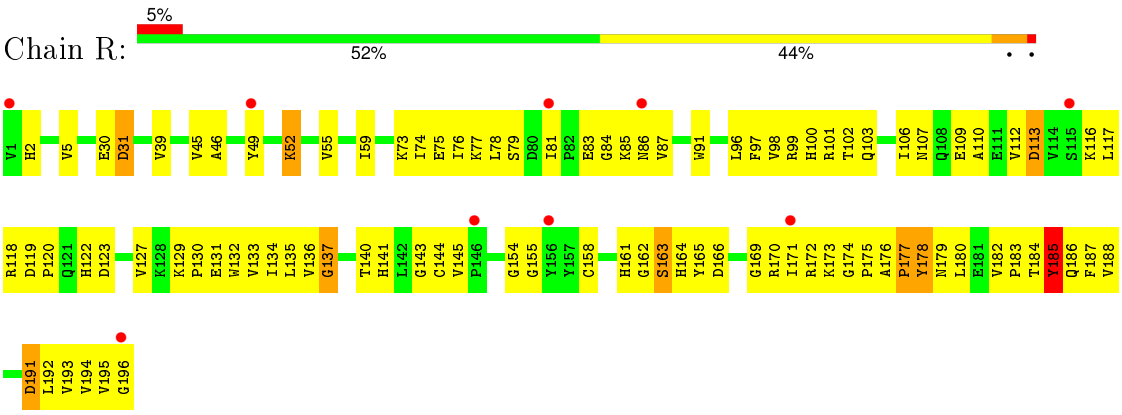
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



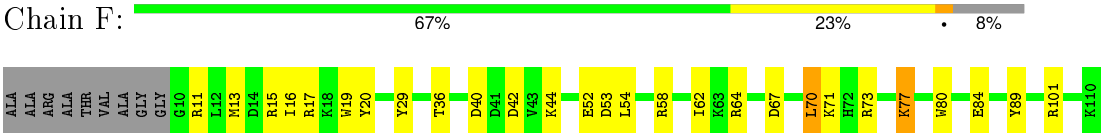
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain R:



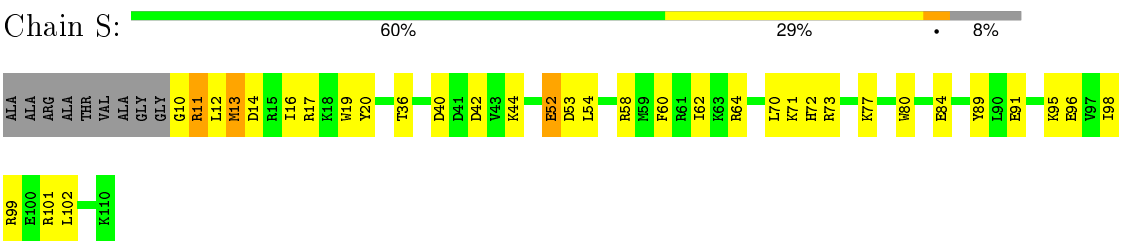
• Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein

Chain F:



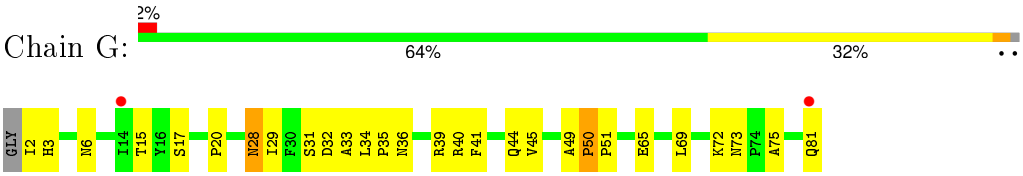
• Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein

Chain S:



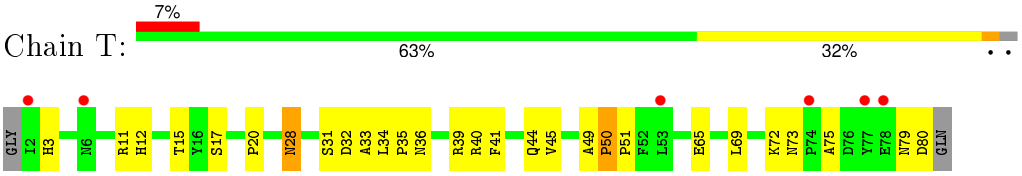
• Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c

Chain G:



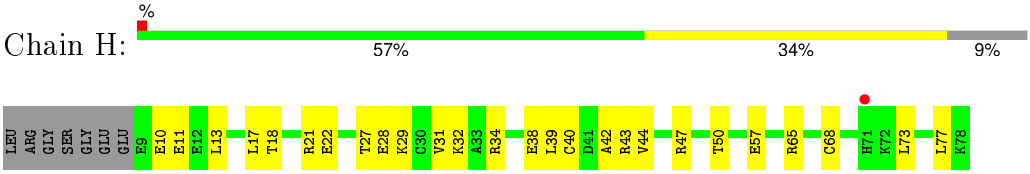
• Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c

Chain T:



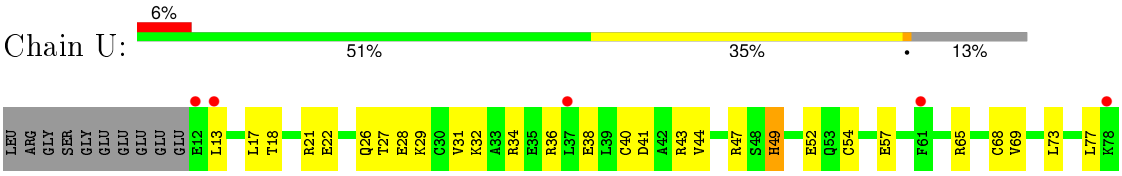
• Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii

Chain H:



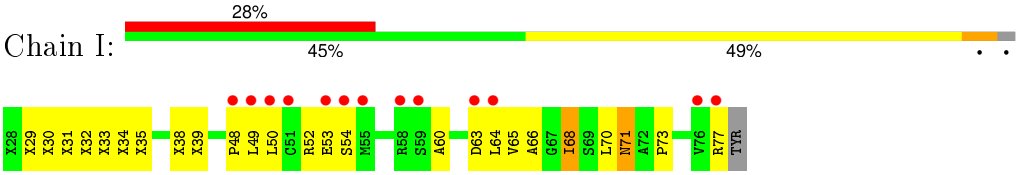
• Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii

Chain U:



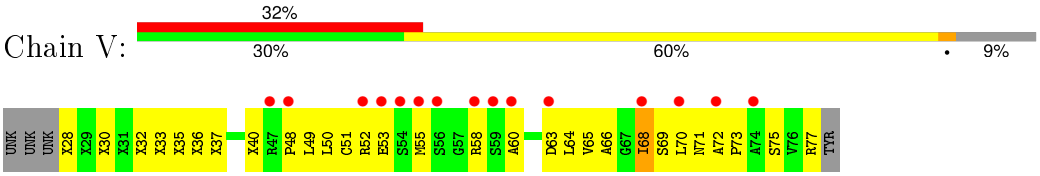
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I:



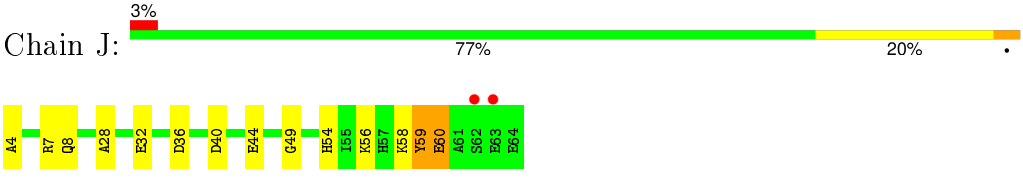
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain V:



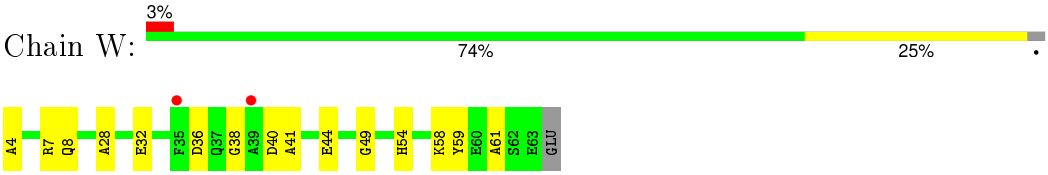
• Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein

Chain J:



• Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	170.15Å 181.31Å 240.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.94 – 2.84 144.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (24.94-2.84) 93.6 (144.78-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.82Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.281 0.239 , 0.274	Depositor DCC
R_{free} test set	3237 reflections (2.00%)	DCC
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 55.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 170949 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	32655	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, AZO, CDL, UQ, FES, HEC, PEE, HEM, BOG

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	0.44	0/3518	0.66	0/4767
1	N	0.42	0/3508	0.65	0/4753
2	B	0.39	0/3187	0.62	0/4321
2	O	0.40	0/3202	0.63	0/4343
3	C	0.51	0/3119	0.67	0/4270
3	P	0.46	0/3114	0.65	0/4263
4	D	0.47	0/1956	0.63	0/2658
4	Q	0.38	0/1956	0.61	0/2658
5	E	0.37	0/1547	0.59	0/2103
5	R	0.37	0/1543	0.60	1/2098 (0.0%)
6	F	0.53	0/911	0.65	0/1219
6	S	0.44	0/911	0.60	0/1219
7	G	0.49	0/694	0.66	0/941
7	T	0.42	0/684	0.62	0/929
8	H	0.42	0/582	0.63	0/779
8	U	0.32	0/561	0.57	0/751
9	I	0.39	0/218	0.58	0/293
9	V	0.37	0/218	0.59	0/293
10	J	0.43	0/508	0.60	0/682
10	W	0.40	0/490	0.60	0/660
All	All	0.43	0/32427	0.63	1/44000 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	R	143	GLY	N-CA-C	5.62	127.15	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3447	0	3362	125	0
1	N	3437	0	3349	148	0
2	B	3133	0	3130	192	0
2	O	3147	0	3146	189	0
3	C	3017	0	3063	69	0
3	P	3012	0	3058	85	0
4	D	1898	0	1846	54	0
4	Q	1898	0	1846	66	0
5	E	1513	0	1478	114	0
5	R	1509	0	1474	101	0
6	F	891	0	893	20	0
6	S	891	0	893	31	0
7	G	672	0	653	30	0
7	T	662	0	645	34	0
8	H	574	0	548	20	0
8	U	553	0	535	27	0
9	I	287	0	250	38	0
9	V	277	0	249	38	0
10	J	497	0	490	16	0
10	W	479	0	478	16	0
11	A	71	0	90	0	0
11	C	49	0	72	5	0
11	N	5	0	0	0	0
11	P	99	0	149	3	0
12	C	86	0	60	5	0
12	P	86	0	60	4	0
13	C	30	0	17	0	0
13	P	30	0	17	2	0
14	C	19	0	17	4	0
14	P	19	0	17	6	0
15	C	6	0	8	1	0
15	P	6	0	8	0	0
16	D	43	0	30	3	0
16	Q	43	0	30	2	0
17	D	42	0	28	4	0
17	G	40	0	24	4	0
17	Q	42	0	28	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	T	40	0	24	3	0
18	D	33	0	39	1	0
18	P	12	0	11	1	0
18	Q	33	0	39	1	0
19	E	4	0	0	2	0
19	R	4	0	0	2	0
20	C	8	0	0	0	0
20	E	1	0	0	0	0
20	P	9	0	0	1	0
20	R	1	0	0	0	0
All	All	32655	0	32154	1295	0

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 20.

All (1295) 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)
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.14	1.11
9:I:33:UNK:HG2	9:I:73:PRO:HB3	1.12	1.09
2:O:353:THR:HG22	2:O:355:GLU:H	1.14	1.07
2:O:76:THR:HG22	2:O:82:SER:H	1.16	1.07
2:B:353:THR:HG22	2:B:355:GLU:H	1.17	1.07
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.37	1.04
2:B:76:THR:HG22	2:B:82:SER:H	1.17	1.03
2:O:338:ARG:HH11	2:O:338:ARG:HG3	1.24	0.99
1:A:178:THR:HG22	1:A:180:ALA:H	1.24	0.98
1:N:178:THR:HG22	1:N:180:ALA:H	1.24	0.97
2:B:338:ARG:HG3	2:B:338:ARG:HH11	1.26	0.97
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.07	0.96
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.45	0.96
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.49	0.95
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.47	0.95
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.81	0.94
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.49	0.94
4:D:57:THR:HG22	4:D:59:ALA:H	1.32	0.93
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.51	0.92
4:D:47:ALA:H	4:D:50:ASN:HD22	1.05	0.92
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.50	0.92
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.31	0.92
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:27:THR:HG22	2:O:28:LYS:H	1.33	0.90
9:I:33:UNK:HG2	9:I:73:PRO:CB	2.00	0.89
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.57	0.87
7:T:41:PHE:O	7:T:45:VAL:HG23	1.74	0.87
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.40	0.86
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.39	0.86
9:V:64:LEU:HD12	9:V:77:ARG:O	1.75	0.86
1:N:10:ASN:ND2	2:O:19:PRO:HD2	1.91	0.86
9:I:32:UNK:N	9:I:73:PRO:HG2	1.90	0.85
7:G:41:PHE:O	7:G:45:VAL:HG23	1.76	0.85
5:E:127:VAL:HG12	5:E:128:LYS:H	1.40	0.85
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.57	0.85
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.58	0.84
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.42	0.84
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.43	0.84
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.60	0.84
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.60	0.84
2:O:248:ASN:HD22	2:O:248:ASN:C	1.81	0.83
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.05	0.83
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.78	0.82
3:P:238:THR:HB	3:P:239:PRO:HD3	1.61	0.82
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.62	0.82
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.45	0.82
2:O:160:LEU:HD12	9:V:64:LEU:HD13	1.62	0.81
1:N:331:ILE:HG21	1:N:431:LEU:HB2	1.61	0.81
3:C:9:HIS:HD2	3:C:12:LEU:H	1.26	0.81
2:B:27:THR:HG22	2:B:28:LYS:H	1.43	0.81
3:P:9:HIS:HD2	3:P:12:LEU:H	1.25	0.81
2:O:47:ILE:HD13	2:O:120:MET:HE2	1.62	0.81
2:O:338:ARG:NH1	2:O:338:ARG:HG3	1.95	0.80
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.63	0.80
3:C:238:THR:HB	3:C:239:PRO:HD3	1.63	0.80
1:A:443:TRP:CE3	1:A:443:TRP:HA	2.17	0.79
3:P:69:HIS:CD2	3:P:73:ASN:HD22	1.99	0.79
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.63	0.79
3:C:22:LEU:HD21	14:C:2002:UQ:HM32	1.65	0.79
2:B:338:ARG:HG3	2:B:338:ARG:NH1	1.98	0.78
1:N:282:ARG:HH21	9:V:36:UNK:HA	1.48	0.78
2:B:248:ASN:HD22	2:B:248:ASN:C	1.85	0.78
2:B:37:SER:HB3	2:B:213:HIS:ND1	1.98	0.78
1:N:10:ASN:HD21	2:O:18:CYS:N	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:141:HIS:HB2	5:E:176:ALA:HB2	1.66	0.78
1:A:178:THR:HB	1:A:181:ASP:OD1	1.83	0.78
2:B:47:ILE:HD13	2:B:120:MET:CE	2.14	0.78
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.66	0.78
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.66	0.77
2:O:18:CYS:HB2	2:O:19:PRO:HD3	1.66	0.77
1:N:143:ASN:HD22	9:V:48:PRO:HD3	1.50	0.77
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.66	0.77
2:B:47:ILE:HD13	2:B:120:MET:HE2	1.66	0.77
1:A:331:ILE:HG21	1:A:431:LEU:HB2	1.67	0.77
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.48	0.77
4:D:47:ALA:H	4:D:50:ASN:ND2	1.82	0.77
2:B:31:ASN:ND2	2:B:31:ASN:H	1.83	0.77
5:E:121:GLN:CG	5:E:170:ARG:HD3	2.06	0.76
2:B:76:THR:HG22	2:B:82:SER:N	1.99	0.76
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.65	0.76
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.19	0.76
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.67	0.76
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.67	0.76
2:O:76:THR:HG22	2:O:82:SER:N	1.99	0.76
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.51	0.75
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.66	0.75
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.52	0.74
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.68	0.74
2:O:399:ALA:O	2:O:402:ILE:HG22	1.86	0.74
3:C:81:ARG:HH22	15:C:2011:GOL:H11	1.51	0.74
9:V:35:UNK:HG3	9:V:36:UNK:N	2.01	0.74
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.68	0.74
5:E:84:GLY:N	5:E:102:THR:HG23	2.02	0.74
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.69	0.74
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.70	0.74
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.04	0.74
9:I:34:UNK:HG3	9:I:35:UNK:N	2.03	0.74
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.19	0.74
7:T:72:LYS:HE2	8:U:57:GLU:OE1	1.87	0.74
2:O:27:THR:HG22	2:O:28:LYS:N	2.03	0.74
2:B:399:ALA:O	2:B:402:ILE:HG22	1.86	0.74
1:A:443:TRP:HE3	1:A:443:TRP:HA	1.52	0.73
5:R:186:GLN:HE21	5:R:188:VAL:HG13	1.53	0.73
5:R:31:ASP:OD2	10:W:7:ARG:HG3	1.88	0.73
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ASP:OD2	9:I:33:UNK:HB2	1.88	0.73
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.68	0.73
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.69	0.73
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.19	0.73
1:N:105:ASP:O	1:N:109:VAL:HG23	1.88	0.73
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.72	0.72
5:R:135:LEU:HD23	5:R:182:VAL:HG22	1.72	0.72
1:A:343:MET:HB3	1:A:444:ILE:HA	1.72	0.72
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.54	0.72
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.70	0.72
4:D:57:THR:HG22	4:D:59:ALA:N	2.04	0.72
2:O:62:ASN:O	2:O:65:THR:HG22	1.88	0.72
5:E:31:ASP:OD2	10:J:7:ARG:HG3	1.89	0.72
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.71	0.72
2:O:217:LYS:O	2:O:221:GLU:HG2	1.90	0.72
5:E:86:ASN:OD1	5:E:99:ARG:HB2	1.90	0.71
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.91	0.71
2:B:27:THR:HG22	2:B:28:LYS:N	2.03	0.71
7:T:80:ASP:HB3	8:U:47:ARG:HH11	1.55	0.71
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.90	0.71
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.19	0.71
2:B:31:ASN:HD22	2:B:31:ASN:H	1.37	0.71
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.25	0.71
2:B:38:LEU:HD12	2:B:39:GLU:N	2.06	0.71
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.26	0.71
1:A:103:SER:HB3	1:A:202:GLY:O	1.90	0.71
6:S:91:GLU:O	6:S:95:LYS:HG3	1.91	0.71
1:N:182:LEU:O	1:N:186:ILE:HG13	1.91	0.71
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.26	0.71
4:D:62:LYS:O	4:D:66:GLU:HG3	1.91	0.71
2:B:76:THR:CG2	2:B:82:SER:H	2.00	0.70
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.73	0.70
2:O:154:SER:O	2:O:157:VAL:HG12	1.91	0.70
9:I:70:LEU:HD23	9:I:71:ASN:H	1.56	0.70
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.74	0.70
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.55	0.70
3:P:247:SER:OG	3:P:250:LEU:HB2	1.92	0.70
1:N:178:THR:HB	1:N:181:ASP:OD1	1.89	0.70
2:O:221:GLU:HG3	2:O:222:GLN:H	1.57	0.70
2:B:31:ASN:N	2:B:31:ASN:HD22	1.90	0.70
1:A:282:ARG:HH21	9:I:35:UNK:HA	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:47:ILE:HD13	2:O:120:MET:CE	2.21	0.70
10:J:7:ARG:NH1	10:J:7:ARG:HB3	2.07	0.69
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.73	0.69
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.91	0.69
1:A:281:ASP:CG	9:I:33:UNK:HB2	2.13	0.69
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.57	0.69
2:O:361:LYS:O	2:O:365:LYS:HG3	1.93	0.69
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.74	0.69
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.74	0.69
8:H:10:GLU:O	8:H:11:GLU:HG3	1.92	0.69
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.75	0.69
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.07	0.69
8:U:28:GLU:HG2	8:U:32:LYS:HE3	1.75	0.68
3:C:41:CYS:HG	3:C:90:PHE:HD2	1.41	0.68
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.76	0.68
2:O:225:ASN:O	2:O:227:ARG:HG3	1.93	0.68
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.28	0.68
1:N:402:VAL:HG22	1:N:406:MET:CE	2.23	0.68
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.73	0.68
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.59	0.68
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.24	0.68
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.23	0.68
8:U:27:THR:O	8:U:31:VAL:HG23	1.94	0.68
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.29	0.68
2:B:124:LEU:HD11	2:B:223:PHE:CB	2.23	0.68
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.75	0.68
4:D:231:LYS:O	6:F:71:LYS:HE3	1.93	0.68
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.28	0.68
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.09	0.67
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.75	0.67
2:O:341:MET:HE2	2:O:341:MET:HA	1.74	0.67
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.76	0.67
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.29	0.67
4:Q:62:LYS:O	4:Q:66:GLU:HG3	1.94	0.67
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.30	0.67
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.29	0.67
5:R:102:THR:O	5:R:106:ILE:HG13	1.94	0.67
5:E:122:HIS:HB3	5:E:125:ASP:CG	2.14	0.67
2:B:154:SER:O	2:B:157:VAL:HG12	1.95	0.67
5:R:166:ASP:OD2	5:R:170:ARG:HB2	1.95	0.67
5:E:127:VAL:HG12	5:E:128:LYS:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.95	0.67
4:Q:57:THR:HG22	4:Q:59:ALA:N	2.10	0.66
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.76	0.66
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.25	0.66
1:A:350:THR:HG22	1:A:352:SER:H	1.60	0.66
3:P:41:CYS:HG	3:P:90:PHE:HD2	1.43	0.66
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.76	0.66
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.78	0.66
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.77	0.66
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.76	0.66
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.77	0.66
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.10	0.66
10:W:7:ARG:HB3	10:W:7:ARG:NH1	2.10	0.66
5:E:52:LYS:C	5:E:52:LYS:HD3	2.15	0.66
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.78	0.65
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.76	0.65
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.78	0.65
5:E:130:PRO:HG2	5:E:131:GLU:CD	2.17	0.65
1:N:112:LEU:O	1:N:116:VAL:HG23	1.96	0.65
5:R:83:GLU:HA	5:R:100:HIS:HB3	1.77	0.65
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.61	0.65
5:E:130:PRO:HG2	5:E:131:GLU:H	1.61	0.65
2:O:299:VAL:HG11	2:O:336:VAL:HG13	1.76	0.65
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.30	0.65
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.77	0.65
2:B:306:PRO:HA	9:I:52:ARG:CG	2.26	0.65
5:E:190:ASP:C	5:E:192:LEU:H	1.98	0.65
4:D:235:MET:HB3	7:G:15:THR:HG22	1.78	0.65
8:H:28:GLU:HG2	8:H:32:LYS:HE3	1.77	0.65
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.78	0.65
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.32	0.65
2:O:150:VAL:O	2:O:153:GLN:HG3	1.97	0.65
2:O:422:LYS:O	2:O:436:LEU:HD21	1.95	0.65
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.27	0.64
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.63	0.64
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.31	0.64
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.78	0.64
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.79	0.64
6:S:53:ASP:OD1	6:S:54:LEU:N	2.30	0.64
2:B:270:ASN:ND2	2:B:270:ASN:H	1.94	0.64
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ARG:NH2	9:I:35:UNK:HA	2.12	0.64
8:H:27:THR:O	8:H:31:VAL:HG23	1.97	0.64
2:O:353:THR:HG22	2:O:355:GLU:N	2.00	0.64
5:R:86:ASN:OD1	5:R:99:ARG:HB2	1.97	0.64
3:C:49:GLY:C	12:C:501:HEM:HAC	2.17	0.64
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.12	0.64
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.12	0.64
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.79	0.64
2:B:422:LYS:O	2:B:436:LEU:HD21	1.98	0.64
6:F:53:ASP:OD1	6:F:54:LEU:N	2.30	0.64
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.33	0.64
3:P:25:PRO:HB2	3:P:28:ILE:HG23	1.78	0.64
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.13	0.64
1:N:282:ARG:NH2	9:V:37:UNK:N	2.45	0.64
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.31	0.64
1:N:350:THR:HG22	1:N:352:SER:H	1.62	0.64
1:A:182:LEU:O	1:A:186:ILE:HG13	1.98	0.64
5:R:52:LYS:HD3	5:R:52:LYS:C	2.18	0.64
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.79	0.63
2:B:46:ARG:HD2	2:B:110:GLU:CG	2.28	0.63
3:C:247:SER:OG	3:C:250:LEU:HB2	1.99	0.63
1:N:143:ASN:HD22	9:V:48:PRO:CD	2.11	0.63
8:H:28:GLU:O	8:H:32:LYS:HG3	1.97	0.63
8:U:43:ARG:O	8:U:47:ARG:HG3	1.97	0.63
2:O:192:HIS:O	2:O:196:GLN:HG3	1.98	0.63
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.81	0.63
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.63	0.63
2:B:341:MET:HE2	2:B:341:MET:HA	1.81	0.63
2:O:219:VAL:O	2:O:223:PHE:HB2	1.98	0.63
7:T:79:ASN:O	7:T:80:ASP:HB2	1.97	0.63
6:S:91:GLU:HG2	6:S:95:LYS:HE3	1.80	0.63
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.80	0.63
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.80	0.63
1:N:343:MET:HB3	1:N:444:ILE:HA	1.81	0.63
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.81	0.63
2:B:341:MET:HA	2:B:341:MET:CE	2.29	0.62
1:N:15:ASN:O	1:N:26:ALA:HA	1.98	0.62
10:J:7:ARG:HH11	10:J:7:ARG:CB	2.11	0.62
5:R:109:GLU:HG2	5:R:123:ASP:HB2	1.81	0.62
5:R:78:LEU:HD11	5:R:187:PHE:CD1	2.33	0.62
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.34	0.62
3:P:342:GLN:NE2	3:P:343:PRO:HD2	2.14	0.62
2:B:150:VAL:O	2:B:153:GLN:HG3	1.99	0.62
2:O:207:VAL:HG12	2:O:208:GLY:H	1.64	0.62
1:N:233:ARG:HH21	1:N:316:ASP:HB2	1.64	0.62
2:O:273:SER:O	2:O:276:GLN:HB3	1.99	0.62
3:P:101:ARG:C	3:P:101:ARG:HD2	2.20	0.62
3:C:236:MET:O	3:C:239:PRO:HD2	1.99	0.62
2:B:361:LYS:O	2:B:365:LYS:HG3	2.00	0.62
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.80	0.62
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.29	0.62
3:P:49:GLY:C	12:P:501:HEM:HAC	2.19	0.62
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.32	0.62
5:E:55:VAL:O	5:E:59:ILE:HG12	2.00	0.62
3:P:22:LEU:HD21	14:P:3002:UQ:HM32	1.81	0.62
2:B:207:VAL:HG12	2:B:208:GLY:H	1.64	0.62
5:E:101:ARG:HA	5:E:105:GLU:OE1	1.99	0.62
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.80	0.62
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.82	0.62
2:O:38:LEU:HD12	2:O:39:GLU:N	2.15	0.62
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.34	0.61
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.64	0.61
5:E:147:ILE:O	5:E:156:TYR:HA	1.99	0.61
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.24	0.61
1:N:106:MET:O	1:N:110:VAL:HG23	2.00	0.61
2:O:46:ARG:HD2	2:O:110:GLU:CG	2.30	0.61
2:B:62:ASN:O	2:B:65:THR:HG22	2.00	0.61
2:B:201:SER:OG	2:B:228:SER:HA	1.99	0.61
5:E:106:ILE:C	5:E:110:ALA:HB3	2.20	0.61
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.82	0.61
3:P:236:MET:O	3:P:239:PRO:HD2	2.00	0.61
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.83	0.61
5:E:136:VAL:CG2	5:E:183:PRO:HD3	2.28	0.61
3:C:37:LEU:O	3:C:41:CYS:HB2	2.01	0.61
2:B:207:VAL:HG21	2:B:383:GLY:HA3	1.83	0.61
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.00	0.61
8:U:28:GLU:O	8:U:32:LYS:HG3	2.01	0.60
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.36	0.60
5:E:78:LEU:HD12	5:E:190:ASP:O	2.01	0.60
5:R:83:GLU:HG3	5:R:100:HIS:CE1	2.36	0.60
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.17	0.60
1:A:402:VAL:HG22	1:A:406:MET:CE	2.32	0.60
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.00	0.60
2:O:397:VAL:O	2:O:401:LYS:HG2	2.02	0.60
3:P:146:VAL:HG21	3:P:269:ILE:HG21	1.83	0.60
1:N:170:THR:HG22	1:N:171:THR:N	2.16	0.60
3:C:146:VAL:HG21	3:C:269:ILE:HG21	1.84	0.60
9:I:31:UNK:C	9:I:73:PRO:HG2	2.31	0.60
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.31	0.60
5:R:117:LEU:HD21	5:R:172:ARG:NH1	2.17	0.60
2:O:76:THR:HG23	2:O:136:GLU:OE1	2.01	0.60
2:O:341:MET:HA	2:O:341:MET:CE	2.31	0.60
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.17	0.60
2:B:299:VAL:CG1	2:B:336:VAL:HG13	2.31	0.60
2:B:192:HIS:O	2:B:196:GLN:HG3	2.01	0.60
10:W:7:ARG:HH11	10:W:7:ARG:CB	2.15	0.60
2:B:202:ALA:HB3	2:B:229:GLY:O	2.02	0.60
2:O:18:CYS:HB2	2:O:19:PRO:CD	2.32	0.59
2:O:248:ASN:C	2:O:248:ASN:ND2	2.55	0.59
2:O:299:VAL:CG1	2:O:336:VAL:HG13	2.32	0.59
5:E:122:HIS:HE1	5:E:124:LEU:HD12	1.66	0.59
1:N:136:GLN:OE1	9:V:50:LEU:HB3	2.03	0.59
1:A:15:ASN:O	1:A:26:ALA:HA	2.02	0.59
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.37	0.59
3:P:37:LEU:O	3:P:41:CYS:HB2	2.02	0.59
2:O:248:ASN:HD21	2:O:250:HIS:HB2	1.68	0.59
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.37	0.59
16:Q:501:HEC:HMB1	16:Q:501:HEC:HBB3	1.85	0.59
5:E:101:ARG:HB2	5:E:131:GLU:HA	1.82	0.59
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.02	0.59
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.84	0.59
2:O:372:VAL:O	2:O:372:VAL:HG12	2.02	0.59
2:O:76:THR:CG2	2:O:82:SER:H	2.04	0.59
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.84	0.59
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.03	0.59
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.36	0.59
6:S:11:ARG:HA	6:S:14:ASP:HB2	1.85	0.59
1:A:105:ASP:O	1:A:109:VAL:HG23	2.03	0.58
3:C:245:LEU:O	4:D:201:ARG:HD2	2.02	0.58
3:P:199:THR:HA	18:P:2010:BOG:O1	2.03	0.58
4:Q:12:TRP:NE1	4:Q:125:ASP:OD2	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:TYR:CG	1:A:281:ASP:N	2.71	0.58
8:H:40:CYS:O	8:H:44:VAL:HG23	2.03	0.58
5:R:186:GLN:NE2	5:R:188:VAL:HG13	2.17	0.58
2:O:124:LEU:HD11	2:O:223:PHE:HB3	1.84	0.58
5:E:106:ILE:O	5:E:110:ALA:HB3	2.03	0.58
2:B:33:LEU:CD2	2:B:224:LEU:HD12	2.32	0.58
9:I:70:LEU:HD23	9:I:71:ASN:N	2.19	0.58
1:A:49:ASN:HD21	1:A:51:LYS:HE3	1.69	0.58
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.70	0.58
8:U:27:THR:HG22	8:U:29:LYS:H	1.66	0.58
1:N:69:LYS:HD2	1:N:70:ARG:NH2	2.18	0.58
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.84	0.58
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.86	0.58
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.85	0.58
5:E:114:VAL:HG21	5:E:172:ARG:NH1	2.19	0.58
2:B:207:VAL:HG12	2:B:208:GLY:N	2.19	0.58
2:O:101:THR:HG23	2:O:104:LYS:HE3	1.85	0.58
2:B:248:ASN:HD21	2:B:250:HIS:HB2	1.69	0.58
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.71	0.58
4:D:167:GLU:HG3	8:H:13:LEU:CD2	2.34	0.58
5:E:163:SER:HA	5:E:174:GLY:HA3	1.86	0.58
1:N:178:THR:HG22	1:N:180:ALA:N	2.08	0.57
1:A:69:LYS:HD2	1:A:70:ARG:NH2	2.18	0.57
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.44	0.57
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.86	0.57
1:A:178:THR:CG2	1:A:179:ARG:N	2.67	0.57
1:N:331:ILE:CG2	1:N:431:LEU:HB2	2.34	0.57
6:S:99:ARG:NH1	6:S:99:ARG:HB3	2.20	0.57
1:N:173:ASN:O	1:N:177:LEU:HG	2.04	0.57
1:N:371:GLY:O	1:N:375:VAL:HG23	2.05	0.57
2:B:372:VAL:O	2:B:372:VAL:HG12	2.04	0.57
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.37	0.57
1:A:131:ARG:NH2	1:A:177:LEU:O	2.37	0.57
2:O:27:THR:CG2	2:O:28:LYS:H	2.11	0.57
9:V:65:VAL:HG12	9:V:66:ALA:N	2.19	0.57
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.20	0.57
5:E:109:GLU:OE2	5:E:153:PHE:HB3	2.03	0.57
3:C:9:HIS:CD2	3:C:12:LEU:H	2.15	0.57
9:V:70:LEU:HD23	9:V:71:ASN:N	2.20	0.57
2:O:334:GLY:O	2:O:338:ARG:HG2	2.05	0.57
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:317:THR:HG23	1:N:318:GLY:N	2.19	0.57
2:O:318:ASP:O	2:O:319:SER:HB2	2.05	0.57
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.87	0.57
5:R:163:SER:H	5:R:175:PRO:HD2	1.70	0.57
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.87	0.56
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.39	0.56
5:R:188:VAL:HG23	5:R:192:LEU:HB2	1.86	0.56
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.85	0.56
1:A:130:GLU:O	1:A:134:ILE:HG13	2.04	0.56
2:B:24:LEU:HD12	2:B:37:SER:O	2.05	0.56
2:O:407:SER:O	2:O:411:VAL:HG23	2.05	0.56
1:N:178:THR:CG2	1:N:179:ARG:N	2.67	0.56
3:P:9:HIS:CD2	3:P:12:LEU:H	2.15	0.56
1:A:106:MET:O	1:A:110:VAL:HG23	2.04	0.56
2:O:357:VAL:O	2:O:361:LYS:HG3	2.05	0.56
3:P:153:ALA:HB2	3:P:288:LYS:HG2	1.87	0.56
1:A:395:TRP:CE3	1:A:395:TRP:HA	2.40	0.56
1:N:10:ASN:HD21	2:O:19:PRO:HD2	1.70	0.56
6:S:17:ARG:HG2	6:S:17:ARG:HH11	1.71	0.56
11:P:3007:PEE:H50	17:T:3004:CDL:H712	1.88	0.56
2:B:225:ASN:O	2:B:227:ARG:N	2.38	0.56
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.20	0.56
5:R:161:HIS:HB2	5:R:175:PRO:HG3	1.88	0.56
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.87	0.56
8:U:21:ARG:HG3	8:U:21:ARG:HH11	1.69	0.56
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.87	0.56
7:G:40:ARG:HB3	17:G:2004:CDL:HA32	1.86	0.56
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.87	0.56
1:N:131:ARG:NH2	1:N:177:LEU:O	2.37	0.56
2:O:31:ASN:H	2:O:31:ASN:ND2	2.04	0.56
1:A:178:THR:HG22	1:A:180:ALA:N	2.07	0.56
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.88	0.56
1:N:103:SER:HB3	1:N:202:GLY:O	2.06	0.56
2:B:71:LEU:HD12	2:B:144:LEU:HD23	1.87	0.55
1:A:17:THR:HG23	1:A:205:HIS:NE2	2.21	0.55
2:O:221:GLU:C	2:O:223:PHE:H	2.10	0.55
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.53	0.55
2:O:207:VAL:HG21	2:O:383:GLY:HA3	1.89	0.55
5:R:73:LYS:HB3	5:R:196:GLY:O	2.05	0.55
1:A:7:THR:HG21	2:B:113:ARG:CD	2.32	0.55
2:B:122:TYR:O	2:B:126:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:49:GLY:N	10:W:54:HIS:ND1	2.54	0.55
5:E:135:LEU:HD11	5:E:169:GLY:HA3	1.89	0.55
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.36	0.55
1:N:130:GLU:O	1:N:134:ILE:HG13	2.07	0.55
5:E:116:LYS:HD2	5:E:116:LYS:N	2.22	0.55
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.41	0.55
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.25	0.55
2:O:402:ILE:HD13	2:O:402:ILE:C	2.27	0.55
2:O:207:VAL:HG12	2:O:208:GLY:N	2.22	0.55
2:O:156:GLN:HE22	9:V:77:ARG:C	2.09	0.55
5:E:131:GLU:H	5:E:131:GLU:CD	2.10	0.55
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.71	0.55
5:R:55:VAL:O	5:R:59:ILE:HG12	2.06	0.55
1:A:369:LEU:HD12	1:A:392:LEU:HD11	1.89	0.55
1:A:106:MET:O	1:A:106:MET:HE2	2.07	0.55
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.50	0.55
5:R:81:ILE:HG12	5:R:87:VAL:HG21	1.87	0.55
3:P:313:GLN:NE2	6:S:36:THR:OG1	2.40	0.55
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.89	0.55
2:O:221:GLU:O	2:O:223:PHE:N	2.40	0.55
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.72	0.55
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.37	0.55
1:A:170:THR:HG22	1:A:171:THR:N	2.23	0.55
2:O:71:LEU:HD12	2:O:144:LEU:HD23	1.89	0.54
9:I:65:VAL:HG12	9:I:66:ALA:N	2.22	0.54
5:E:84:GLY:CA	5:E:102:THR:HG23	2.37	0.54
5:E:99:ARG:HD3	5:E:105:GLU:OE2	2.08	0.54
10:J:7:ARG:HB3	10:J:7:ARG:HH11	1.72	0.54
2:B:397:VAL:O	2:B:401:LYS:HG2	2.07	0.54
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.71	0.54
1:A:4:TYR:HB3	2:B:114:ASP:OD2	2.07	0.54
2:O:24:LEU:HD12	2:O:37:SER:O	2.08	0.54
2:B:357:VAL:O	2:B:361:LYS:HG3	2.06	0.54
17:Q:3003:CDL:HB22	7:T:40:ARG:NH2	2.22	0.54
2:B:264:VAL:HG23	2:B:316:TYR:C	2.28	0.54
1:A:23:LEU:HD23	1:A:24:ARG:N	2.22	0.54
1:N:187:ASP:O	1:N:191:LYS:HE3	2.07	0.54
5:R:49:TYR:CE1	10:W:32:GLU:HG3	2.43	0.54
2:B:96:LEU:H	9:I:70:LEU:HD22	1.72	0.54
2:O:59:THR:HG22	2:O:61:ALA:H	1.73	0.54
5:E:130:PRO:HG2	5:E:131:GLU:OE1	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:202:HIS:NE2	14:P:3002:UQ:O4	2.36	0.54
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.41	0.54
1:A:191:LYS:CA	1:A:195:MET:HE2	2.38	0.54
2:O:140:LEU:O	2:O:143:GLN:HB3	2.07	0.54
8:H:18:THR:O	8:H:22:GLU:HG3	2.08	0.54
3:C:150:LEU:HB3	3:C:292:VAL:HG22	1.90	0.54
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.90	0.54
8:U:28:GLU:CG	8:U:32:LYS:HE3	2.38	0.54
2:O:276:GLN:HG2	2:O:281:ALA:HB2	1.90	0.54
2:O:31:ASN:N	2:O:31:ASN:HD22	2.06	0.54
1:A:288:LYS:HE3	1:A:289:HIS:CE1	2.43	0.54
1:N:295:ALA:O	1:N:299:VAL:HG23	2.08	0.54
1:N:4:TYR:HB3	2:O:114:ASP:OD2	2.08	0.54
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.72	0.54
3:P:245:LEU:O	4:Q:201:ARG:HD2	2.08	0.54
2:B:212:LYS:HB3	2:B:215:ASP:OD2	2.08	0.54
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.43	0.54
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.07	0.54
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.44	0.53
9:V:70:LEU:HD23	9:V:71:ASN:OD1	2.08	0.53
7:T:40:ARG:HB3	17:T:3004:CDL:HA32	1.89	0.53
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.23	0.53
1:N:49:ASN:ND2	1:N:51:LYS:H	2.04	0.53
5:E:83:GLU:HB3	5:E:102:THR:CG2	2.38	0.53
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.43	0.53
10:J:56:LYS:O	10:J:60:GLU:HB2	2.09	0.53
3:P:121:LEU:O	3:P:125:MET:HG3	2.07	0.53
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.89	0.53
3:C:263:LEU:O	3:C:264:VAL:HG23	2.08	0.53
2:B:248:ASN:ND2	2:B:248:ASN:C	2.58	0.53
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.90	0.53
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.89	0.53
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.89	0.53
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.43	0.53
5:R:77:LYS:HA	5:R:191:ASP:O	2.09	0.53
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.44	0.53
12:C:502:HEM:HMC2	12:C:502:HEM:HBC2	1.89	0.53
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.90	0.53
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.48	0.53
3:C:334:LEU:HD21	11:C:2007:PEE:H65	1.89	0.53
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:11:ARG:O	6:F:15:ARG:HG3	2.08	0.53
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.90	0.53
4:D:47:ALA:HA	4:D:90:TYR:HA	1.90	0.53
3:P:150:LEU:HB3	3:P:292:VAL:HG22	1.90	0.53
5:E:135:LEU:HD23	5:E:182:VAL:HG22	1.91	0.53
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.42	0.53
8:H:27:THR:HG22	8:H:29:LYS:H	1.74	0.53
2:B:273:SER:O	2:B:276:GLN:HB3	2.08	0.53
4:D:102:ARG:HA	4:D:108:ALA:O	2.08	0.53
1:N:49:ASN:HD21	1:N:51:LYS:HE3	1.73	0.53
10:J:49:GLY:N	10:J:54:HIS:ND1	2.57	0.53
9:I:29:UNK:O	9:I:30:UNK:HB2	2.08	0.53
7:T:80:ASP:HB3	8:U:47:ARG:NH1	2.24	0.52
2:B:21:ALA:O	2:B:22:GLU:HB3	2.08	0.52
2:B:101:THR:HG23	2:B:104:LYS:HE3	1.90	0.52
2:O:72:ALA:HB1	2:O:75:LEU:HD12	1.92	0.52
3:C:28:ILE:HG12	3:C:225:TYR:OH	2.09	0.52
2:B:153:GLN:HE22	9:I:34:UNK:CG	2.22	0.52
4:D:79:GLU:HA	4:D:79:GLU:OE2	2.09	0.52
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.27	0.52
2:B:140:LEU:O	2:B:143:GLN:HB3	2.08	0.52
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.24	0.52
3:P:28:ILE:HG12	3:P:225:TYR:OH	2.09	0.52
3:P:78:TRP:CZ3	4:Q:201:ARG:HG3	2.44	0.52
2:B:318:ASP:O	2:B:319:SER:HB2	2.09	0.52
1:A:268:VAL:O	1:A:272:VAL:HG23	2.10	0.52
7:G:65:GLU:O	7:G:69:LEU:HG	2.09	0.52
9:I:38:UNK:O	9:I:39:UNK:C	2.56	0.52
5:R:188:VAL:HG23	5:R:192:LEU:CB	2.40	0.52
1:N:26:ALA:HB2	1:N:383:LEU:HD11	1.92	0.52
3:P:138:GLN:HB2	3:P:255:GLU:O	2.10	0.52
6:S:40:ASP:O	6:S:44:LYS:HG3	2.10	0.52
2:O:34:ILE:HD13	2:O:390:GLY:HA2	1.91	0.52
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.45	0.52
2:O:338:ARG:NH1	2:O:338:ARG:CG	2.67	0.52
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.92	0.52
10:J:60:GLU:HA	10:J:60:GLU:OE2	2.10	0.52
5:R:178:TYR:N	5:R:178:TYR:CD1	2.78	0.52
2:B:59:THR:HG22	2:B:60:THR:N	2.25	0.52
8:U:18:THR:O	8:U:22:GLU:HG3	2.10	0.52
2:B:402:ILE:HD13	2:B:402:ILE:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.37	0.52
5:E:178:TYR:H	5:E:178:TYR:HD1	1.58	0.52
5:E:187:PHE:C	5:E:189:GLY:H	2.13	0.52
6:S:99:ARG:HB3	6:S:99:ARG:HH11	1.75	0.52
2:B:334:GLY:O	2:B:338:ARG:HG2	2.10	0.51
2:B:27:THR:CG2	2:B:28:LYS:H	2.17	0.51
2:O:361:LYS:HA	2:O:402:ILE:HD11	1.91	0.51
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.90	0.51
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.40	0.51
4:Q:70:VAL:HG21	4:Q:83:ARG:CZ	2.40	0.51
2:O:259:THR:HG22	2:O:260:GLU:N	2.24	0.51
5:E:146:PRO:HG2	5:E:180:LEU:HD21	1.91	0.51
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.55	0.51
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.39	0.51
2:B:189:GLU:OE1	2:B:189:GLU:N	2.42	0.51
1:N:402:VAL:HG22	1:N:406:MET:HE1	1.91	0.51
14:P:3002:UQ:HM51	14:P:3002:UQ:C8	2.41	0.51
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.73	0.51
2:B:57:TYR:CD1	2:B:57:TYR:N	2.78	0.51
5:E:74:ILE:HG22	5:E:91:TRP:CD1	2.44	0.51
1:N:364:ALA:O	1:N:368:GLN:HG3	2.10	0.51
2:O:259:THR:CG2	2:O:260:GLU:N	2.74	0.51
2:B:407:SER:O	2:B:411:VAL:HG23	2.11	0.51
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.93	0.51
4:Q:167:GLU:CG	8:U:13:LEU:HD12	2.40	0.51
6:F:84:GLU:CD	6:F:84:GLU:H	2.14	0.51
5:R:134:ILE:HD12	5:R:185:TYR:HD1	1.74	0.51
1:N:63:ALA:O	1:N:116:VAL:HG13	2.11	0.51
9:V:70:LEU:HD23	9:V:71:ASN:H	1.74	0.51
8:U:22:GLU:O	8:U:26:GLN:HG2	2.10	0.51
3:C:101:ARG:C	3:C:101:ARG:HD2	2.30	0.51
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.91	0.51
3:C:153:ALA:HB2	3:C:288:LYS:HG2	1.93	0.51
2:B:76:THR:HG23	2:B:82:SER:HB2	1.92	0.51
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.26	0.51
3:P:138:GLN:OE1	3:P:138:GLN:HA	2.11	0.51
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.50	0.51
10:W:4:ALA:O	10:W:8:GLN:HG3	2.10	0.51
8:U:40:CYS:O	8:U:44:VAL:HG23	2.11	0.51
4:D:57:THR:HB	4:D:60:GLU:HG3	1.92	0.51
7:T:36:ASN:O	7:T:40:ARG:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.40	0.51
1:A:187:ASP:O	1:A:191:LYS:HE3	2.10	0.51
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.91	0.51
17:D:2003:CDL:HB22	7:G:40:ARG:NH2	2.26	0.51
4:Q:2:GLU:O	4:Q:3:LEU:O	2.29	0.51
8:H:21:ARG:HG3	8:H:21:ARG:HH11	1.76	0.51
5:E:155:GLY:HA3	5:E:166:ASP:O	2.11	0.51
9:I:64:LEU:HD12	9:I:77:ARG:O	2.11	0.51
2:B:361:LYS:HA	2:B:402:ILE:HD11	1.92	0.51
2:O:164:HIS:O	2:O:173:ALA:HA	2.11	0.51
17:D:2003:CDL:HA61	17:D:2003:CDL:H721	1.93	0.51
2:B:345:LYS:O	2:B:349:GLN:HG3	2.10	0.51
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.11	0.51
2:B:292:THR:O	2:B:292:THR:HG22	2.11	0.51
3:P:212:ILE:CD1	6:S:62:ILE:HG23	2.40	0.50
3:P:106:GLY:HA2	3:P:108:TYR:CZ	2.46	0.50
2:O:57:TYR:N	2:O:57:TYR:CD1	2.79	0.50
2:O:31:ASN:HB2	2:O:201:SER:OG	2.11	0.50
5:R:110:ALA:HA	5:R:122:HIS:NE2	2.25	0.50
5:E:135:LEU:CD1	5:E:169:GLY:HA3	2.41	0.50
1:N:137:GLU:O	1:N:141:MET:HG3	2.10	0.50
2:O:122:TYR:O	2:O:126:VAL:HG23	2.10	0.50
3:P:350:ILE:O	3:P:354:MET:HG2	2.11	0.50
5:E:141:HIS:HB2	5:E:176:ALA:CB	2.40	0.50
10:W:7:ARG:HB3	10:W:7:ARG:HH11	1.73	0.50
7:T:40:ARG:HD2	17:T:3004:CDL:OA4	2.12	0.50
1:A:112:LEU:O	1:A:116:VAL:HG23	2.11	0.50
1:N:140:GLU:HG3	9:V:50:LEU:HD12	1.93	0.50
3:P:313:GLN:HE21	6:S:36:THR:CB	2.24	0.50
1:A:191:LYS:C	1:A:195:MET:HE2	2.32	0.50
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.94	0.50
2:B:28:LYS:O	2:B:29:LEU:O	2.29	0.50
2:B:46:ARG:HD2	2:B:110:GLU:CD	2.32	0.50
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.47	0.50
2:B:332:HIS:O	2:B:336:VAL:HG23	2.12	0.50
2:B:395:PRO:O	2:B:398:VAL:HG12	2.11	0.50
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.93	0.50
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	1.93	0.50
2:B:259:THR:HG22	2:B:260:GLU:N	2.26	0.50
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.93	0.50
14:C:2002:UQ:HM51	14:C:2002:UQ:C8	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.41	0.50
2:O:52:LYS:O	2:O:203:ARG:NH2	2.35	0.50
12:C:502:HEM:HMC2	12:C:502:HEM:CBC	2.41	0.50
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.94	0.50
2:B:338:ARG:CG	2:B:338:ARG:NH1	2.69	0.50
5:E:189:GLY:O	5:E:192:LEU:N	2.45	0.50
8:H:28:GLU:CG	8:H:32:LYS:HE3	2.42	0.50
2:B:287:ARG:HB3	9:I:53:GLU:HG3	1.93	0.50
3:P:34:PHE:HB2	20:P:381:HOH:O	2.10	0.50
3:C:328:LEU:HD12	7:G:51:PRO:CB	2.32	0.50
5:R:131:GLU:N	5:R:131:GLU:OE1	2.45	0.50
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.27	0.50
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.42	0.50
3:C:78:TRP:CZ3	4:D:201:ARG:HG3	2.47	0.50
2:B:59:THR:HG22	2:B:61:ALA:H	1.75	0.50
3:C:313:GLN:HE21	6:F:36:THR:CB	2.25	0.50
1:N:279:ARG:HH22	9:V:30:UNK:C	2.23	0.50
1:N:281:ASP:O	1:N:283:THR:N	2.45	0.50
3:C:41:CYS:SG	3:C:90:PHE:HD2	2.35	0.50
5:E:190:ASP:O	5:E:192:LEU:N	2.44	0.50
2:B:52:LYS:O	2:B:203:ARG:NH2	2.41	0.50
1:N:280:TYR:CG	1:N:281:ASP:N	2.79	0.50
3:P:156:TYR:C	3:P:158:GLY:H	2.13	0.50
1:A:307:PHE:CD1	1:A:307:PHE:C	2.85	0.50
5:R:165:TYR:HA	5:R:170:ARG:O	2.12	0.49
5:E:130:PRO:HG2	5:E:131:GLU:OE2	2.11	0.49
5:E:82:PRO:HG2	5:E:85:LYS:HB2	1.94	0.49
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.94	0.49
4:D:102:ARG:HB3	4:D:107:GLY:HA2	1.94	0.49
3:C:286:PRO:O	3:C:287:ASN:HB2	2.12	0.49
2:O:345:LYS:O	2:O:349:GLN:HG3	2.12	0.49
4:D:169:LEU:HD23	4:D:169:LEU:C	2.32	0.49
5:E:165:TYR:HA	5:E:170:ARG:O	2.12	0.49
1:N:7:THR:HG21	2:O:113:ARG:CD	2.39	0.49
2:O:286:LYS:HE2	2:O:287:ARG:HH12	1.77	0.49
5:R:97:PHE:O	5:R:134:ILE:HA	2.13	0.49
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.93	0.49
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.26	0.49
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.48	0.49
1:A:137:GLU:O	1:A:141:MET:HG3	2.12	0.49
1:A:158:PHE:O	1:A:164:ALA:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:382:HIS:HB3	1:N:388:ARG:O	2.12	0.49
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.51	0.49
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.48	0.49
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.40	0.49
5:E:106:ILE:O	5:E:106:ILE:HG22	2.11	0.49
8:U:21:ARG:HG3	8:U:21:ARG:NH1	2.27	0.49
2:O:212:LYS:HB3	2:O:215:ASP:OD2	2.12	0.49
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.93	0.49
4:Q:79:GLU:HA	4:Q:79:GLU:OE2	2.13	0.49
3:P:334:LEU:HD21	11:P:3007:PEE:H65	1.93	0.49
1:A:49:ASN:ND2	1:A:51:LYS:H	2.10	0.49
1:A:173:ASN:O	1:A:177:LEU:HG	2.12	0.49
4:D:169:LEU:HD23	4:D:169:LEU:O	2.11	0.49
1:A:371:GLY:O	1:A:375:VAL:HG23	2.12	0.49
1:N:10:ASN:ND2	2:O:19:PRO:CD	2.71	0.49
3:C:263:LEU:O	3:C:264:VAL:CG2	2.61	0.49
3:P:263:LEU:O	3:P:264:VAL:CG2	2.61	0.49
1:A:220:SER:HB2	1:A:225:GLU:HB2	1.95	0.49
3:P:286:PRO:O	3:P:287:ASN:HB2	2.13	0.49
4:Q:47:ALA:HA	4:Q:90:TYR:HA	1.95	0.49
1:N:10:ASN:CG	2:O:19:PRO:HD2	2.33	0.49
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.43	0.49
3:P:198:LEU:HD21	12:P:502:HEM:HMA3	1.93	0.49
5:R:177:PRO:HG2	5:R:178:TYR:H	1.77	0.49
5:E:97:PHE:O	5:E:134:ILE:HA	2.12	0.49
5:E:188:VAL:HG12	5:E:188:VAL:O	2.12	0.49
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.95	0.49
5:R:118:ARG:NH1	5:R:174:GLY:O	2.45	0.49
10:W:40:ASP:O	10:W:44:GLU:HG3	2.11	0.49
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.95	0.49
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.48	0.49
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	1.95	0.49
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.13	0.49
3:C:50:LEU:O	3:C:54:MET:HG3	2.12	0.49
2:B:27:THR:CG2	2:B:28:LYS:N	2.74	0.49
4:D:165:TYR:CZ	4:D:168:ILE:HG13	2.48	0.49
2:O:292:THR:HG22	2:O:292:THR:O	2.13	0.49
2:B:353:THR:HG22	2:B:355:GLU:N	2.03	0.48
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.13	0.48
2:B:164:HIS:O	2:B:173:ALA:HA	2.13	0.48
2:O:59:THR:HG22	2:O:60:THR:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:220:SER:HB2	1:N:225:GLU:HB2	1.94	0.48
1:A:64:PHE:HE2	1:A:86:PHE:CE1	2.31	0.48
4:Q:1:GLY:O	4:Q:2:GLU:HB2	2.13	0.48
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.47	0.48
4:D:70:VAL:HG21	4:D:83:ARG:CZ	2.43	0.48
2:O:402:ILE:HG23	2:O:403:ASP:N	2.28	0.48
8:U:43:ARG:HD2	8:U:47:ARG:NH2	2.28	0.48
5:R:129:LYS:HB3	5:R:131:GLU:OE1	2.13	0.48
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.48	0.48
5:E:73:LYS:HB3	5:E:196:GLY:O	2.12	0.48
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.94	0.48
8:U:17:LEU:HD13	8:U:73:LEU:HD22	1.96	0.48
4:D:171:TYR:OH	4:D:182:ILE:HA	2.13	0.48
2:O:395:PRO:HA	2:O:398:VAL:HG12	1.95	0.48
4:D:57:THR:CG2	4:D:58:GLU:N	2.75	0.48
2:B:324:PHE:HE2	2:B:341:MET:HE3	1.79	0.48
5:R:155:GLY:HA3	5:R:166:ASP:O	2.13	0.48
5:R:186:GLN:O	5:R:193:VAL:HG23	2.14	0.48
9:I:34:UNK:CG	9:I:35:UNK:N	2.76	0.48
5:R:78:LEU:HD11	5:R:187:PHE:HD1	1.77	0.48
1:N:64:PHE:HE2	1:N:86:PHE:CE1	2.32	0.48
3:P:263:LEU:O	3:P:264:VAL:HG23	2.13	0.48
1:N:219:VAL:HG12	1:N:220:SER:N	2.27	0.48
8:H:17:LEU:HD13	8:H:73:LEU:HD22	1.94	0.48
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.93	0.48
6:F:58:ARG:HD2	6:F:89:TYR:OH	2.13	0.48
6:S:84:GLU:H	6:S:84:GLU:CD	2.16	0.48
2:B:353:THR:HG22	2:B:354:GLU:N	2.28	0.48
5:R:170:ARG:HA	5:R:179:ASN:CB	2.39	0.48
1:A:27:SER:HA	1:A:199:ALA:O	2.13	0.48
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.48	0.48
5:E:178:TYR:CD1	5:E:178:TYR:N	2.82	0.48
3:P:325:LEU:HD22	3:P:370:ILE:HG13	1.96	0.48
5:R:119:ASP:HB3	5:R:179:ASN:HD21	1.77	0.48
2:O:170:THR:O	2:O:172:LEU:N	2.47	0.48
3:C:45:GLN:HB3	12:C:501:HEM:HAB	1.94	0.48
2:O:31:ASN:ND2	2:O:31:ASN:N	2.58	0.48
5:E:189:GLY:O	5:E:192:LEU:O	2.32	0.48
5:E:83:GLU:C	5:E:85:LYS:H	2.16	0.48
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.95	0.48
2:B:56:ARG:HG3	2:B:56:ARG:HH11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.43	0.48
2:B:264:VAL:HG23	2:B:316:TYR:O	2.13	0.48
3:P:279:TYR:O	3:P:282:LEU:HB3	2.14	0.48
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.44	0.48
2:B:110:GLU:O	2:B:111:CYS:HB3	2.14	0.48
3:P:28:ILE:HD11	3:P:225:TYR:CE2	2.48	0.48
2:B:259:THR:CG2	2:B:260:GLU:N	2.77	0.48
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.79	0.48
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.96	0.48
3:P:30:ALA:HB1	17:Q:3003:CDL:H111	1.95	0.48
5:R:162:GLY:O	5:R:163:SER:C	2.51	0.48
1:A:364:ALA:O	1:A:368:GLN:HG3	2.14	0.48
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.96	0.48
1:A:223:TYR:HD2	1:A:223:TYR:H	1.60	0.48
7:T:65:GLU:O	7:T:69:LEU:HG	2.13	0.48
5:R:135:LEU:HD13	5:R:180:LEU:HD12	1.95	0.48
5:E:77:LYS:HA	5:E:192:LEU:HD23	1.96	0.48
1:A:248:LEU:HD12	1:A:426:GLY:HA2	1.94	0.48
1:N:45:SER:HA	1:N:48:GLU:HG3	1.95	0.48
5:E:190:ASP:C	5:E:192:LEU:N	2.67	0.47
2:O:71:LEU:CD2	9:V:68:ILE:HG13	2.44	0.47
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.78	0.47
8:U:65:ARG:O	8:U:68:CYS:HB3	2.14	0.47
1:A:358:LYS:HE3	1:A:399:ILE:O	2.14	0.47
10:J:40:ASP:O	10:J:44:GLU:HG3	2.14	0.47
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.95	0.47
4:Q:195:GLU:OE1	4:Q:201:ARG:NH2	2.47	0.47
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.37	0.47
6:S:95:LYS:O	6:S:99:ARG:HG3	2.14	0.47
5:R:178:TYR:N	5:R:178:TYR:HD1	2.12	0.47
1:N:358:LYS:HE3	1:N:399:ILE:O	2.14	0.47
6:F:77:LYS:HE2	6:F:77:LYS:HB3	1.74	0.47
2:B:28:LYS:HG2	2:B:28:LYS:O	2.14	0.47
5:E:75:GLU:HB3	5:E:194:VAL:HG22	1.95	0.47
2:O:227:ARG:HB3	2:O:228:SER:H	1.52	0.47
2:O:56:ARG:HG3	2:O:56:ARG:NH1	2.28	0.47
1:N:191:LYS:CA	1:N:195:MET:HE2	2.44	0.47
5:R:49:TYR:HE1	10:W:32:GLU:HG3	1.79	0.47
2:O:414:ALA:O	2:O:418:VAL:HG23	2.14	0.47
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.49	0.47
1:A:320:PHE:CE2	1:A:415:ILE:HD11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:121:LEU:O	3:C:125:MET:HG3	2.14	0.47
1:N:151:ASP:OD2	5:R:2:HIS:NE2	2.31	0.47
3:P:92:PHE:O	3:P:95:ILE:HG22	2.14	0.47
4:Q:240:PRO:O	4:Q:241:LYS:C	2.53	0.47
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.49	0.47
2:B:47:ILE:CD1	2:B:120:MET:HE2	2.42	0.47
2:O:29:LEU:HB2	2:O:31:ASN:HD21	1.79	0.47
2:B:215:ASP:O	2:B:219:VAL:HG23	2.15	0.47
9:I:49:LEU:HD22	9:I:54:SER:HB3	1.96	0.47
10:W:7:ARG:NH1	10:W:7:ARG:CB	2.75	0.47
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.14	0.47
1:A:151:ASP:OD2	5:E:2:HIS:NE2	2.33	0.47
1:N:320:PHE:CE2	1:N:415:ILE:HD11	2.49	0.47
1:N:248:LEU:HD12	1:N:426:GLY:HA2	1.97	0.47
3:C:92:PHE:O	3:C:95:ILE:HG22	2.13	0.47
1:N:288:LYS:HE3	1:N:289:HIS:CE1	2.49	0.47
2:O:76:THR:HG23	2:O:82:SER:HB2	1.97	0.47
5:E:127:VAL:O	5:E:128:LYS:HB2	2.15	0.47
5:R:185:TYR:HB3	5:R:195:VAL:HA	1.96	0.47
5:R:185:TYR:O	5:R:186:GLN:HB3	2.14	0.47
2:O:303:THR:HA	2:O:335:GLU:OE1	2.15	0.47
1:A:217:SER:O	1:A:218:GLY:C	2.53	0.47
2:O:325:TYR:CD1	9:V:60:ALA:HB3	2.50	0.47
5:R:113:ASP:HB2	5:R:116:LYS:HB2	1.96	0.47
5:R:75:GLU:O	5:R:75:GLU:HG3	2.15	0.47
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.50	0.47
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.50	0.47
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.15	0.47
2:B:402:ILE:HG23	2:B:403:ASP:N	2.30	0.47
1:N:281:ASP:HB2	9:V:33:UNK:HB2	1.95	0.47
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.50	0.47
2:O:385:GLU:O	2:O:389:SER:HB3	2.14	0.47
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.45	0.47
3:P:108:TYR:HB3	3:P:114:TRP:CE3	2.50	0.47
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.95	0.47
4:D:208:MET:O	4:D:212:SER:HB2	2.15	0.47
4:D:69:GLU:OE1	4:D:82:MET:HB3	2.15	0.47
8:U:34:ARG:O	8:U:38:GLU:HG3	2.15	0.47
5:R:135:LEU:CD2	5:R:182:VAL:HG22	2.42	0.47
5:E:122:HIS:HB3	5:E:125:ASP:OD1	2.14	0.47
1:A:70:ARG:HA	1:A:71:PRO:HD2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:235:MET:CB	7:G:15:THR:HG22	2.45	0.47
3:P:50:LEU:O	3:P:54:MET:HG3	2.15	0.47
1:N:205:HIS:O	1:N:208:LEU:HB3	2.15	0.47
3:C:224:TYR:HB3	4:D:227:TRP:CZ2	2.50	0.47
5:R:84:GLY:O	5:R:85:LYS:HD3	2.14	0.47
3:P:238:THR:HB	3:P:239:PRO:CD	2.40	0.46
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.44	0.46
7:G:36:ASN:O	7:G:40:ARG:HG3	2.15	0.46
3:P:156:TYR:CD2	3:P:156:TYR:N	2.80	0.46
1:A:204:SER:HB3	1:A:207:GLU:HB2	1.97	0.46
4:D:57:THR:HG22	4:D:58:GLU:N	2.29	0.46
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.46	0.46
5:E:75:GLU:HG3	5:E:75:GLU:O	2.15	0.46
2:O:332:HIS:O	2:O:336:VAL:HG23	2.15	0.46
4:Q:68:VAL:HG11	4:Q:92:PRO:HG3	1.97	0.46
8:H:43:ARG:O	8:H:47:ARG:HG3	2.15	0.46
2:O:156:GLN:NE2	9:V:77:ARG:C	2.68	0.46
7:T:80:ASP:OD1	8:U:47:ARG:HD3	2.15	0.46
3:P:22:LEU:HD21	14:P:3002:UQ:CM3	2.45	0.46
2:B:101:THR:OG1	2:B:104:LYS:HG3	2.15	0.46
2:B:402:ILE:O	2:B:405:VAL:HG23	2.16	0.46
10:W:32:GLU:HG2	10:W:36:ASP:OD2	2.15	0.46
4:D:203:ARG:NH1	18:D:2091:BOG:O3	2.49	0.46
1:N:245:ASP:OD1	7:T:11:ARG:NE	2.44	0.46
3:P:90:PHE:CE1	3:P:236:MET:HB3	2.51	0.46
2:B:24:LEU:O	2:B:24:LEU:HG	2.16	0.46
5:E:187:PHE:C	5:E:189:GLY:N	2.68	0.46
5:E:191:ASP:N	5:E:191:ASP:OD2	2.48	0.46
9:I:71:ASN:HD22	9:I:71:ASN:H	1.64	0.46
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.81	0.46
1:N:307:PHE:CD1	1:N:307:PHE:C	2.88	0.46
3:P:328:LEU:CD1	7:T:51:PRO:HB3	2.35	0.46
1:N:282:ARG:NH2	9:V:36:UNK:HA	2.24	0.46
2:B:411:VAL:O	2:B:415:LYS:HG3	2.15	0.46
4:Q:3:LEU:N	4:Q:3:LEU:HD12	2.31	0.46
2:B:414:ALA:O	2:B:418:VAL:HG23	2.15	0.46
9:V:51:CYS:HB2	9:V:53:GLU:OE1	2.16	0.46
1:N:158:PHE:O	1:N:164:ALA:HB2	2.15	0.46
4:Q:69:GLU:OE1	4:Q:82:MET:HB3	2.16	0.46
9:V:70:LEU:CD2	9:V:71:ASN:OD1	2.64	0.46
5:E:91:TRP:HZ2	5:E:196:GLY:HA2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:117:VAL:HG21	4:D:191:ARG:HA	1.97	0.46
2:B:385:GLU:O	2:B:387:LEU:N	2.49	0.46
1:N:27:SER:HA	1:N:199:ALA:O	2.16	0.46
2:O:110:GLU:O	2:O:111:CYS:HB3	2.15	0.46
4:Q:139:ALA:HB2	8:U:41:ASP:OD1	2.16	0.46
2:B:225:ASN:O	2:B:226:ILE:C	2.53	0.46
2:B:274:VAL:O	2:B:278:VAL:HG23	2.15	0.46
3:C:279:TYR:O	3:C:282:LEU:HB3	2.16	0.46
4:Q:57:THR:HB	4:Q:60:GLU:HG3	1.98	0.46
5:R:106:ILE:HG21	5:R:130:PRO:HB3	1.97	0.46
3:P:153:ALA:CB	3:P:288:LYS:HG2	2.45	0.46
1:N:22:GLY:O	1:N:193:PRO:HA	2.15	0.46
5:E:141:HIS:HB3	19:E:501:FES:S2	2.55	0.46
5:R:76:ILE:O	5:R:193:VAL:HG12	2.16	0.46
1:A:26:ALA:O	1:A:198:ALA:HA	2.16	0.46
1:A:239:SER:HB2	7:G:17:SER:O	2.16	0.46
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.51	0.46
3:C:138:GLN:HB2	3:C:255:GLU:O	2.16	0.46
5:R:137:GLY:O	5:R:145:VAL:HG13	2.15	0.46
2:O:353:THR:HG22	2:O:354:GLU:N	2.31	0.45
2:O:46:ARG:HD2	2:O:110:GLU:CD	2.36	0.45
5:R:106:ILE:O	5:R:109:GLU:HB3	2.15	0.45
1:N:383:LEU:O	1:N:387:GLY:HA2	2.16	0.45
5:E:41:ALA:O	5:E:45:VAL:HG23	2.16	0.45
6:S:52:GLU:OE2	7:T:11:ARG:NH1	2.49	0.45
6:S:16:ILE:O	6:S:19:TRP:HB3	2.16	0.45
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.51	0.45
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.98	0.45
5:R:140:THR:OG1	5:R:176:ALA:HB1	2.16	0.45
5:R:96:LEU:HD12	5:R:135:LEU:O	2.16	0.45
1:A:49:ASN:HD21	1:A:51:LYS:CE	2.28	0.45
2:B:156:GLN:HE22	9:I:77:ARG:C	2.20	0.45
4:Q:57:THR:CG2	4:Q:58:GLU:N	2.79	0.45
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.98	0.45
5:R:188:VAL:O	5:R:192:LEU:HB2	2.16	0.45
1:A:402:VAL:HA	1:A:406:MET:CE	2.46	0.45
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.47	0.45
4:D:102:ARG:NH1	4:D:102:ARG:HG2	2.31	0.45
2:B:104:LYS:C	2:B:104:LYS:HD2	2.37	0.45
10:W:59:TYR:N	10:W:59:TYR:CD1	2.84	0.45
6:F:13:MET:O	6:F:17:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:223:TYR:HD2	1:N:223:TYR:H	1.64	0.45
1:A:233:ARG:HH21	1:A:316:ASP:HB2	1.81	0.45
1:N:106:MET:HE2	1:N:106:MET:O	2.17	0.45
5:R:184:THR:O	5:R:185:TYR:HB3	2.16	0.45
5:R:77:LYS:HA	5:R:192:LEU:HD23	1.97	0.45
1:N:122:LEU:HD11	1:N:186:ILE:HD12	1.99	0.45
5:E:76:ILE:O	5:E:193:VAL:HG12	2.17	0.45
4:Q:102:ARG:HG2	4:Q:102:ARG:HH11	1.80	0.45
1:N:240:GLU:HA	1:N:422:LEU:O	2.17	0.45
1:A:178:THR:HG22	1:A:179:ARG:N	2.31	0.45
2:O:169:LYS:O	2:O:170:THR:HG23	2.15	0.45
11:C:2007:PEE:H11	6:F:29:TYR:OH	2.16	0.45
3:P:18:SER:CB	3:P:202:HIS:HE1	2.30	0.45
1:A:144:ASP:OD2	1:A:147:ASN:ND2	2.49	0.45
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.82	0.45
7:G:81:GLN:HG3	7:G:81:GLN:OXT	2.17	0.45
11:P:3007:PEE:H7	7:T:44:GLN:HE21	1.81	0.45
2:O:307:PHE:H	9:V:52:ARG:HG2	1.82	0.45
2:B:86:THR:O	2:B:90:GLU:HG3	2.17	0.45
4:Q:168:ILE:O	4:Q:168:ILE:HG12	2.16	0.45
1:A:382:HIS:HB3	1:A:388:ARG:O	2.17	0.45
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.52	0.45
1:N:143:ASN:ND2	9:V:48:PRO:HD3	2.25	0.45
5:R:112:VAL:HG21	5:R:170:ARG:NH2	2.32	0.45
5:E:84:GLY:N	5:E:100:HIS:O	2.44	0.45
1:N:26:ALA:O	1:N:198:ALA:HA	2.17	0.45
1:N:49:ASN:HD21	1:N:51:LYS:CE	2.30	0.45
2:O:345:LYS:HG2	2:O:418:VAL:CG1	2.46	0.45
3:P:208:ASN:HB2	3:P:209:PRO:HD2	1.99	0.45
7:G:28:ASN:HB3	7:G:31:SER:OG	2.17	0.45
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.99	0.45
2:B:303:THR:HA	2:B:335:GLU:OE1	2.17	0.45
2:B:72:ALA:HB1	2:B:75:LEU:HD12	1.97	0.45
2:O:46:ARG:HD2	2:O:110:GLU:HG2	1.99	0.45
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.99	0.45
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.98	0.45
2:O:54:GLY:C	2:O:56:ARG:H	2.20	0.45
2:O:286:LYS:C	2:O:288:GLY:H	2.20	0.45
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.47	0.45
2:O:345:LYS:HG2	2:O:418:VAL:HG13	1.99	0.45
2:O:86:THR:O	2:O:90:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:ASP:O	6:F:44:LYS:HG3	2.17	0.45
1:A:222:THR:OG1	1:A:225:GLU:HG3	2.17	0.45
4:Q:200:GLN:NE2	18:Q:3091:BOG:H5	2.32	0.45
5:E:137:GLY:O	5:E:145:VAL:HG13	2.16	0.45
1:N:106:MET:HE2	1:N:110:VAL:CG2	2.47	0.45
3:P:376:LYS:O	6:S:17:ARG:NH1	2.47	0.45
1:N:23:LEU:HD23	1:N:24:ARG:N	2.31	0.45
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.46	0.44
5:R:163:SER:HA	5:R:174:GLY:HA3	1.99	0.44
1:N:191:LYS:C	1:N:195:MET:HE2	2.37	0.44
5:E:73:LYS:HB2	5:E:195:VAL:O	2.16	0.44
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.99	0.44
5:R:169:GLY:O	5:R:179:ASN:HB3	2.17	0.44
5:R:161:HIS:CB	5:R:175:PRO:HG3	2.47	0.44
6:F:13:MET:HA	6:F:13:MET:HE2	1.98	0.44
4:D:222:MET:HE3	5:E:40:THR:HG23	1.99	0.44
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.83	0.44
10:J:32:GLU:HG2	10:J:36:ASP:OD2	2.17	0.44
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.99	0.44
5:E:127:VAL:CG1	5:E:128:LYS:H	2.13	0.44
9:I:68:ILE:HD13	9:I:68:ILE:HA	1.85	0.44
1:A:205:HIS:O	1:A:208:LEU:HB3	2.18	0.44
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.65	0.44
5:R:179:ASN:O	5:R:180:LEU:C	2.56	0.44
10:J:56:LYS:HE2	10:J:56:LYS:HB3	1.82	0.44
4:Q:161:ALA:O	4:Q:162:PRO:C	2.56	0.44
5:E:136:VAL:O	5:E:138:VAL:N	2.44	0.44
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.32	0.44
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.57	0.44
5:R:171:ILE:HG12	5:R:176:ALA:O	2.18	0.44
2:B:402:ILE:HG23	2:B:403:ASP:H	1.83	0.44
2:O:26:ILE:O	2:O:26:ILE:HG12	2.16	0.44
9:V:64:LEU:HD12	9:V:77:ARG:C	2.36	0.44
2:B:295:LEU:O	2:B:299:VAL:HG23	2.18	0.44
17:Q:3003:CDL:H721	17:Q:3003:CDL:HA61	1.99	0.44
11:C:2007:PEE:H7	7:G:44:GLN:HE21	1.81	0.44
4:D:168:ILE:HG12	4:D:168:ILE:O	2.18	0.44
2:B:170:THR:O	2:B:172:LEU:N	2.50	0.44
3:C:286:PRO:O	3:C:287:ASN:CB	2.65	0.44
3:P:275:PHE:HB3	13:P:3001:AZO:C11	2.48	0.44
16:D:501:HEC:HBB3	16:D:501:HEC:HMB1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:438:ARG:HH11	1:N:438:ARG:HG3	1.83	0.44
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.53	0.44
2:O:221:GLU:CG	2:O:222:GLN:H	2.25	0.44
1:N:402:VAL:HA	1:N:406:MET:CE	2.48	0.44
3:P:28:ILE:HD11	3:P:225:TYR:CZ	2.53	0.44
3:P:18:SER:HB2	3:P:202:HIS:HE1	1.82	0.44
2:O:411:VAL:O	2:O:415:LYS:HG3	2.18	0.44
9:V:33:UNK:HA	9:V:73:PRO:HB3	2.00	0.44
2:O:162:ASN:O	2:O:244:ILE:HD12	2.18	0.44
3:C:49:GLY:O	12:C:501:HEM:HAC	2.17	0.44
2:B:333:ALA:O	2:B:337:ILE:HG13	2.18	0.44
3:P:41:CYS:SG	3:P:91:PHE:HA	2.58	0.43
5:E:133:VAL:HG13	5:E:133:VAL:O	2.18	0.43
5:E:129:LYS:HG3	5:E:187:PHE:CE2	2.53	0.43
3:C:106:GLY:HA2	3:C:108:TYR:CZ	2.53	0.43
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.46	0.43
1:A:26:ALA:HB2	1:A:383:LEU:HD11	1.99	0.43
2:B:56:ARG:HG3	2:B:56:ARG:NH1	2.33	0.43
5:E:114:VAL:HG21	5:E:172:ARG:HH12	1.83	0.43
5:E:96:LEU:HD12	5:E:135:LEU:O	2.18	0.43
4:Q:2:GLU:HB3	4:Q:3:LEU:HD12	2.00	0.43
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.32	0.43
5:E:49:TYR:CE1	10:J:32:GLU:HG3	2.53	0.43
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.53	0.43
6:S:58:ARG:HD2	6:S:89:TYR:OH	2.18	0.43
8:H:34:ARG:O	8:H:38:GLU:HG3	2.18	0.43
1:A:217:SER:O	1:A:219:VAL:HG23	2.18	0.43
1:N:239:SER:HB2	7:T:17:SER:O	2.18	0.43
5:R:103:GLN:O	5:R:107:ASN:ND2	2.51	0.43
1:A:205:HIS:O	1:A:209:VAL:HG12	2.18	0.43
3:C:153:ALA:CB	3:C:288:LYS:HG2	2.49	0.43
3:P:286:PRO:O	3:P:287:ASN:CB	2.66	0.43
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.53	0.43
4:D:105:ASN:O	4:D:106:ASN:HB2	2.18	0.43
2:O:324:PHE:HE2	2:O:341:MET:HE3	1.83	0.43
2:B:220:ALA:O	2:B:224:LEU:HB2	2.18	0.43
3:P:101:ARG:O	3:P:101:ARG:HD2	2.18	0.43
1:N:134:ILE:HG22	1:N:174:ILE:HD13	2.00	0.43
3:P:263:LEU:C	3:P:264:VAL:HG23	2.39	0.43
4:D:234:LYS:HD2	5:E:8:PRO:HB2	2.00	0.43
2:B:68:LEU:HD23	2:B:186:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:33:LEU:HD12	2:O:204:MET:O	2.17	0.43
2:B:33:LEU:HD12	2:B:204:MET:O	2.19	0.43
2:B:46:ARG:HD2	2:B:110:GLU:HG2	2.00	0.43
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.83	0.43
1:N:362:ARG:O	1:N:365:MET:HG2	2.18	0.43
4:Q:238:ARG:CZ	5:R:5:VAL:HG22	2.48	0.43
4:D:223:LYS:HD3	4:D:223:LYS:C	2.38	0.43
5:R:101:ARG:HH21	5:R:130:PRO:HA	1.83	0.43
2:B:168:TYR:HB2	2:B:173:ALA:HB2	2.00	0.43
2:B:54:GLY:C	2:B:56:ARG:H	2.21	0.43
1:N:17:THR:HG23	1:N:205:HIS:NE2	2.34	0.43
5:R:96:LEU:HD21	5:R:195:VAL:HG21	2.00	0.43
5:R:79:SER:OG	5:R:191:ASP:HB2	2.18	0.43
2:O:222:GLN:HG2	2:O:222:GLN:O	2.19	0.43
11:C:2007:PEE:H50	17:G:2004:CDL:H712	2.01	0.43
3:P:198:LEU:HD13	14:P:3002:UQ:HM53	2.01	0.43
1:A:274:ASN:ND2	1:A:309:THR:HB	2.34	0.43
3:C:273:TRP:HA	3:C:276:LEU:CD1	2.48	0.43
3:C:120:LEU:HD23	3:C:120:LEU:HA	1.87	0.43
1:N:178:THR:HG22	1:N:179:ARG:N	2.33	0.43
1:A:331:ILE:CG2	1:A:431:LEU:HB2	2.41	0.43
5:E:162:GLY:O	5:E:163:SER:C	2.57	0.43
9:I:39:UNK:HA	9:V:40:UNK:O	2.19	0.43
1:N:354:VAL:HG23	1:N:355:LYS:N	2.34	0.43
8:H:21:ARG:HG3	8:H:21:ARG:NH1	2.34	0.43
2:O:141:GLN:N	2:O:142:PRO:HD2	2.34	0.43
1:A:21:ASN:N	1:A:21:ASN:OD1	2.49	0.43
7:T:28:ASN:HB3	7:T:31:SER:OG	2.19	0.43
2:B:297:GLN:O	2:B:301:LYS:HG3	2.18	0.43
1:A:106:MET:HE2	1:A:106:MET:C	2.39	0.43
4:Q:235:MET:CB	7:T:15:THR:HG22	2.45	0.43
5:R:133:VAL:HG13	5:R:133:VAL:O	2.19	0.43
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.48	0.43
8:U:21:ARG:HD2	8:U:65:ARG:NH1	2.33	0.43
2:O:395:PRO:O	2:O:398:VAL:HG12	2.18	0.43
1:A:418:LYS:O	1:A:420:PRO:HD3	2.19	0.43
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.54	0.43
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.84	0.43
1:N:106:MET:N	1:N:107:PRO:HD2	2.34	0.42
2:B:209:ILE:HG22	2:B:210:GLY:N	2.34	0.42
5:R:184:THR:HG22	5:R:185:TYR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:402:ILE:HG23	2:O:403:ASP:H	1.84	0.42
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.84	0.42
2:B:395:PRO:O	2:B:398:VAL:CG1	2.67	0.42
4:D:239:PRO:C	4:D:241:LYS:H	2.20	0.42
2:B:35:ILE:HD13	2:B:217:LYS:HA	2.01	0.42
2:O:18:CYS:CB	2:O:19:PRO:CD	2.97	0.42
5:E:130:PRO:C	5:E:132:TRP:H	2.21	0.42
2:B:399:ALA:O	2:B:402:ILE:CG2	2.63	0.42
1:N:170:THR:HG22	1:N:171:THR:H	1.84	0.42
6:F:16:ILE:O	6:F:19:TRP:HB3	2.19	0.42
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.62	0.42
5:E:171:ILE:HG23	5:E:171:ILE:O	2.18	0.42
5:E:77:LYS:HG3	5:E:191:ASP:O	2.18	0.42
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.53	0.42
8:U:65:ARG:O	8:U:69:VAL:HG23	2.20	0.42
2:O:264:VAL:HG12	2:O:265:GLY:N	2.34	0.42
5:E:151:GLY:O	5:E:154:GLY:N	2.52	0.42
3:P:9:HIS:CD2	3:P:11:LEU:HB2	2.54	0.42
14:C:2002:UQ:HM51	14:C:2002:UQ:H8	2.01	0.42
5:R:100:HIS:HD2	5:R:131:GLU:O	2.02	0.42
17:D:2003:CDL:OB3	6:F:73:ARG:NH2	2.52	0.42
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.19	0.42
1:N:271:HIS:CE1	1:N:311:ASN:HD22	2.37	0.42
6:S:98:ILE:O	6:S:102:LEU:HG	2.20	0.42
2:B:353:THR:CG2	2:B:354:GLU:N	2.82	0.42
1:A:191:LYS:N	1:A:195:MET:HE2	2.35	0.42
3:P:129:PHE:CE1	13:P:3001:AZO:H223	2.55	0.42
1:N:351:GLU:O	1:N:355:LYS:HB2	2.20	0.42
1:A:143:ASN:HB2	9:I:48:PRO:HD2	2.01	0.42
5:R:74:ILE:HG22	5:R:91:TRP:CD1	2.54	0.42
4:Q:169:LEU:O	4:Q:169:LEU:HD23	2.20	0.42
2:O:222:GLN:O	2:O:223:PHE:CD2	2.72	0.42
7:G:40:ARG:HD2	17:G:2004:CDL:OA4	2.19	0.42
12:P:502:HEM:HMC2	12:P:502:HEM:HBC2	2.01	0.42
1:N:170:THR:CG2	1:N:171:THR:N	2.82	0.42
2:O:96:LEU:HD13	2:O:109:VAL:HG12	2.01	0.42
1:A:140:GLU:OE2	9:I:50:LEU:N	2.39	0.42
4:D:186:VAL:O	4:D:190:LEU:HG	2.19	0.42
8:H:50:THR:HG23	8:H:50:THR:O	2.19	0.42
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.50	0.42
4:D:211:ILE:HD13	4:D:211:ILE:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:270:LEU:HD23	1:N:270:LEU:HA	1.88	0.42
5:E:161:HIS:HB2	19:E:501:FES:S1	2.60	0.42
5:E:81:ILE:HG22	5:E:100:HIS:HB2	2.00	0.42
2:O:399:ALA:HA	2:O:402:ILE:HG22	2.01	0.42
1:A:206:LYS:HA	1:A:209:VAL:HG12	2.01	0.42
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.37	0.42
10:W:38:GLY:O	10:W:41:ALA:HB3	2.19	0.42
3:P:70:THR:O	3:P:77:GLY:HA3	2.20	0.42
2:B:26:ILE:HG12	2:B:26:ILE:O	2.20	0.42
2:O:341:MET:CE	2:O:417:PHE:HE2	2.23	0.42
3:C:9:HIS:CD2	3:C:11:LEU:HB2	2.55	0.42
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.55	0.42
2:O:54:GLY:O	2:O:56:ARG:N	2.53	0.42
3:P:288:LYS:O	3:P:292:VAL:HG23	2.19	0.42
1:A:240:GLU:HA	1:A:422:LEU:O	2.20	0.42
4:Q:41:HIS:CE1	4:Q:110:PRO:HB2	2.54	0.42
2:B:162:ASN:O	2:B:244:ILE:HD12	2.20	0.42
3:P:342:GLN:NE2	3:P:342:GLN:HA	2.35	0.42
1:N:111:GLU:HG3	1:N:215:HIS:NE2	2.35	0.42
2:O:54:GLY:C	2:O:56:ARG:N	2.73	0.42
1:N:51:LYS:HB2	1:N:51:LYS:HE3	1.91	0.42
2:B:345:LYS:HG2	2:B:418:VAL:HG13	2.02	0.42
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.20	0.42
2:B:166:ALA:HB2	2:B:244:ILE:HG13	2.02	0.42
2:B:50:PHE:CD1	2:B:50:PHE:N	2.88	0.42
2:B:169:LYS:O	2:B:170:THR:HG23	2.19	0.41
9:V:52:ARG:HG3	9:V:52:ARG:HH11	1.85	0.41
10:J:4:ALA:O	10:J:8:GLN:HG3	2.20	0.41
1:N:418:LYS:O	1:N:420:PRO:HD3	2.20	0.41
1:N:243:ALA:O	1:N:425:VAL:HA	2.20	0.41
2:B:246:GLU:HB3	2:B:427:SER:HB3	2.01	0.41
2:O:67:HIS:O	2:O:70:ARG:HB3	2.19	0.41
5:E:117:LEU:HD23	5:E:119:ASP:O	2.20	0.41
5:E:179:ASN:O	5:E:180:LEU:C	2.57	0.41
1:A:281:ASP:O	1:A:283:THR:N	2.53	0.41
3:C:28:ILE:CD1	14:C:2002:UQ:HM21	2.50	0.41
3:C:31:TRP:NE1	11:C:2007:PEE:O4	2.53	0.41
2:B:54:GLY:C	2:B:56:ARG:N	2.73	0.41
4:Q:68:VAL:HG11	4:Q:92:PRO:CG	2.50	0.41
16:D:501:HEC:HAD1	16:D:501:HEC:HMD1	1.88	0.41
1:A:271:HIS:CE1	1:A:311:ASN:HD22	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:THR:HB	1:A:374:PRO:CD	2.50	0.41
3:C:130:VAL:HG23	3:C:183:HIS:HB2	2.01	0.41
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.41	0.41
3:C:233:LEU:O	3:C:237:LEU:HB2	2.20	0.41
2:B:399:ALA:HA	2:B:402:ILE:HG22	2.02	0.41
10:J:7:ARG:NH1	10:J:7:ARG:CB	2.71	0.41
9:V:69:SER:HB2	9:V:72:ALA:H	1.84	0.41
1:A:206:LYS:HA	1:A:209:VAL:CG1	2.51	0.41
2:B:59:THR:CG2	2:B:60:THR:N	2.83	0.41
3:P:271:PRO:HB2	3:P:275:PHE:HB2	2.02	0.41
6:S:13:MET:HA	6:S:16:ILE:HD12	2.02	0.41
9:V:35:UNK:CG	9:V:36:UNK:N	2.75	0.41
2:B:361:LYS:HD3	2:B:403:ASP:HA	2.02	0.41
5:R:83:GLU:CD	5:R:102:THR:HA	2.40	0.41
1:N:117:VAL:HG23	1:N:118:GLN:HG3	2.03	0.41
2:B:54:GLY:O	2:B:56:ARG:N	2.54	0.41
3:C:325:LEU:HD22	3:C:370:ILE:HG13	2.03	0.41
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.20	0.41
1:N:217:SER:O	1:N:218:GLY:C	2.59	0.41
2:O:37:SER:CB	2:O:213:HIS:ND1	2.68	0.41
1:N:106:MET:CE	1:N:110:VAL:HG21	2.50	0.41
5:R:185:TYR:CD2	5:R:185:TYR:N	2.88	0.41
1:N:90:THR:O	1:N:167:VAL:HG11	2.21	0.41
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.48	0.41
5:E:185:TYR:O	5:E:186:GLN:HB3	2.21	0.41
4:D:68:VAL:HG11	4:D:92:PRO:HG3	2.03	0.41
1:A:295:ALA:O	1:A:299:VAL:HG23	2.21	0.41
1:N:163:LEU:HA	1:N:163:LEU:HD23	1.93	0.41
2:B:29:LEU:HD12	2:B:33:LEU:HD23	2.02	0.41
1:N:70:ARG:HA	1:N:71:PRO:HD2	1.80	0.41
3:P:49:GLY:O	12:P:501:HEM:HAC	2.20	0.41
5:R:161:HIS:HB2	19:R:501:FES:S1	2.61	0.41
8:H:21:ARG:HD2	8:H:65:ARG:NH1	2.36	0.41
8:H:65:ARG:O	8:H:68:CYS:HB3	2.20	0.41
1:N:133:VAL:O	1:N:137:GLU:HG3	2.21	0.41
9:V:32:UNK:N	9:V:73:PRO:HG2	2.36	0.41
3:P:271:PRO:HD2	3:P:279:TYR:CD2	2.55	0.41
2:B:385:GLU:C	2:B:387:LEU:H	2.24	0.41
3:C:242:THR:O	3:C:246:PHE:HB2	2.20	0.41
1:A:106:MET:N	1:A:107:PRO:HD2	2.35	0.41
5:R:76:ILE:CD1	5:R:98:VAL:HG21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:74:PRO:HA	4:Q:79:GLU:O	2.21	0.41
2:O:227:ARG:O	2:O:228:SER:O	2.39	0.41
2:O:101:THR:OG1	2:O:104:LYS:HG3	2.20	0.41
1:A:279:ARG:HH22	9:I:30:UNK:C	2.33	0.41
5:R:75:GLU:HB3	5:R:194:VAL:HG22	2.01	0.41
7:G:2:ILE:HG22	7:G:6:ASN:HD21	1.86	0.41
1:N:47:TYR:CZ	1:N:231:LEU:HD11	2.55	0.41
5:E:119:ASP:O	5:E:121:GLN:N	2.53	0.41
2:O:248:ASN:ND2	2:O:250:HIS:H	2.18	0.41
5:E:102:THR:C	5:E:103:GLN:HG3	2.41	0.41
2:O:399:ALA:O	2:O:402:ILE:CG2	2.63	0.41
1:N:342:TRP:O	1:N:345:LEU:HB2	2.20	0.41
1:N:205:HIS:O	1:N:209:VAL:HG12	2.20	0.41
4:Q:165:TYR:CZ	4:Q:168:ILE:HG13	2.56	0.41
4:D:220:TYR:O	4:D:224:ARG:HG2	2.20	0.41
3:P:141:PHE:HE1	3:P:171:VAL:O	2.04	0.41
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.50	0.41
2:O:98:VAL:HA	2:O:106:THR:O	2.21	0.41
2:B:355:GLU:CD	2:B:359:LYS:HE3	2.41	0.41
2:O:341:MET:HE2	2:O:341:MET:CA	2.45	0.41
1:A:106:MET:CE	1:A:110:VAL:HG21	2.50	0.41
5:R:185:TYR:HD2	5:R:185:TYR:N	2.19	0.41
6:S:17:ARG:NH1	6:S:17:ARG:HG2	2.35	0.41
2:B:287:ARG:CB	9:I:53:GLU:HG3	2.51	0.41
2:B:22:GLU:O	2:B:23:ASP:CG	2.59	0.41
2:O:306:PRO:HA	9:V:52:ARG:CG	2.50	0.41
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.36	0.41
8:H:39:LEU:O	8:H:42:ALA:HB3	2.20	0.41
3:C:5:ILE:O	3:C:5:ILE:HG22	2.21	0.41
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.20	0.41
6:S:10:GLY:C	6:S:12:LEU:H	2.24	0.41
1:A:351:GLU:O	1:A:355:LYS:HB2	2.20	0.41
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.65	0.41
1:N:268:VAL:O	1:N:272:VAL:HG23	2.21	0.41
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.35	0.41
2:O:43:PRO:O	2:O:113:ARG:HG3	2.21	0.41
6:S:71:LYS:O	6:S:72:HIS:HB2	2.21	0.41
5:E:75:GLU:HA	5:E:193:VAL:O	2.21	0.41
2:O:225:ASN:C	2:O:227:ARG:HG3	2.41	0.41
1:A:402:VAL:HG22	1:A:406:MET:HE1	2.01	0.41
1:N:4:TYR:HE2	1:N:396:ASP:OD2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LEU:HD22	1:A:437:ILE:HD13	2.03	0.41
1:N:46:ARG:NH1	1:N:93:GLU:OE2	2.50	0.41
2:B:257:VAL:HG22	2:B:424:MET:HG3	2.03	0.41
3:P:172:ASP:OD1	3:P:173:ASN:N	2.52	0.41
2:O:209:ILE:HG22	2:O:210:GLY:N	2.36	0.40
1:N:402:VAL:HA	1:N:406:MET:HE1	2.02	0.40
14:P:3002:UQ:HM51	14:P:3002:UQ:H8	2.02	0.40
4:D:116:ILE:HG12	16:D:501:HEC:HMA3	2.03	0.40
3:C:272:GLU:O	3:C:273:TRP:C	2.59	0.40
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.82	0.40
1:N:106:MET:HE2	1:N:110:VAL:HG23	2.02	0.40
1:A:37:VAL:HG22	1:A:109:VAL:HG11	2.03	0.40
2:O:150:VAL:CG2	2:O:151:ALA:N	2.84	0.40
1:A:422:LEU:HD22	1:A:437:ILE:CD1	2.51	0.40
2:B:141:GLN:N	2:B:142:PRO:HD2	2.35	0.40
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.85	0.40
4:D:158:ILE:HG12	4:D:160:MET:H	1.86	0.40
2:O:403:ASP:C	2:O:405:VAL:H	2.24	0.40
6:S:96:GLU:OE1	6:S:99:ARG:NH2	2.54	0.40
3:C:31:TRP:HE1	17:G:2004:CDL:H1	1.87	0.40
5:E:172:ARG:HB2	5:E:173:LYS:H	1.74	0.40
1:N:48:GLU:CD	1:N:54:GLY:H	2.24	0.40
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.76	0.40
2:O:297:GLN:O	2:O:301:LYS:HG3	2.21	0.40
1:A:270:LEU:O	1:A:273:ALA:HB3	2.20	0.40
5:R:164:HIS:CD2	5:R:173:LYS:HB3	2.56	0.40
5:E:101:ARG:NH2	5:E:130:PRO:O	2.55	0.40
2:O:168:TYR:HB2	2:O:173:ALA:HB2	2.04	0.40
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.56	0.40
3:C:30:ALA:HB1	17:D:2003:CDL:H111	2.02	0.40
1:A:383:LEU:O	1:A:387:GLY:HA2	2.22	0.40
1:A:51:LYS:HB2	1:A:51:LYS:HE3	1.89	0.40
5:R:141:HIS:HB3	19:R:501:FES:S2	2.62	0.40
1:N:62:LEU:O	1:N:64:PHE:N	2.55	0.40
1:A:320:PHE:HE2	1:A:415:ILE:HD11	1.86	0.40
2:O:307:PHE:HE2	9:V:52:ARG:HE	1.69	0.40
2:O:246:GLU:HB3	2:O:427:SER:HB3	2.02	0.40
2:B:206:LEU:HG	2:B:206:LEU:O	2.22	0.40
1:N:233:ARG:NH2	1:N:316:ASP:O	2.53	0.40
16:Q:501:HEC:CMB	16:Q:501:HEC:HBB3	2.51	0.40
7:G:29:ILE:HA	7:G:33:ALA:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:120:LEU:HA	3:P:120:LEU:HD23	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	442/446 (99%)	411 (93%)	25 (6%)	6 (1%)	14 40
1	N	440/446 (99%)	408 (93%)	25 (6%)	7 (2%)	12 36
2	B	418/441 (95%)	353 (84%)	50 (12%)	15 (4%)	4 13
2	O	420/441 (95%)	364 (87%)	42 (10%)	14 (3%)	5 15
3	C	378/380 (100%)	360 (95%)	14 (4%)	4 (1%)	17 47
3	P	377/380 (99%)	353 (94%)	19 (5%)	5 (1%)	15 42
4	D	239/241 (99%)	223 (93%)	16 (7%)	0	100 100
4	Q	239/241 (99%)	221 (92%)	16 (7%)	2 (1%)	24 56
5	E	194/196 (99%)	148 (76%)	34 (18%)	12 (6%)	2 4
5	R	194/196 (99%)	162 (84%)	23 (12%)	9 (5%)	3 9
6	F	99/110 (90%)	96 (97%)	2 (2%)	1 (1%)	19 50
6	S	99/110 (90%)	90 (91%)	8 (8%)	1 (1%)	19 50
7	G	78/81 (96%)	70 (90%)	7 (9%)	1 (1%)	15 42
7	T	77/81 (95%)	69 (90%)	6 (8%)	2 (3%)	7 21
8	H	68/77 (88%)	65 (96%)	3 (4%)	0	100 100
8	U	65/77 (84%)	61 (94%)	2 (3%)	2 (3%)	5 16
9	I	29/47 (62%)	27 (93%)	2 (7%)	0	100 100
9	V	29/47 (62%)	28 (97%)	1 (3%)	0	100 100
10	J	59/61 (97%)	56 (95%)	3 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	W	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	11 34
All	All	4002/4160 (96%)	3619 (90%)	301 (8%)	82 (2%)	9 29

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ALA
2	B	24	LEU
2	B	29	LEU
2	B	171	ALA
2	B	226	ILE
2	B	228	SER
3	C	287	ASN
5	E	102	THR
5	E	127	VAL
5	E	128	LYS
5	E	130	PRO
5	E	163	SER
1	N	282	ARG
2	O	171	ALA
2	O	222	GLN
2	O	228	SER
3	P	287	ASN
4	Q	3	LEU
5	R	163	SER
8	U	49	HIS
8	U	52	GLU
1	A	218	GLY
1	A	262	TRP
1	A	282	ARG
2	B	26	ILE
2	B	231	GLY
2	B	386	ALA
2	B	389	SER
5	E	80	ASP
5	E	177	PRO
5	E	191	ASP
1	N	218	GLY
1	N	262	TRP
2	O	26	ILE
2	O	231	GLY
2	O	372	VAL

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Mol	Chain	Res	Type
2	O	389	SER
3	P	157	ILE
10	W	61	ALA
1	A	72	CYS
1	A	433	ASP
2	B	221	GLU
2	B	372	VAL
3	C	264	VAL
1	N	72	CYS
1	N	433	ASP
2	O	19	PRO
2	O	24	LEU
5	R	185	TYR
5	R	191	ASP
6	S	11	ARG
2	B	222	GLN
2	B	224	LEU
3	C	3	PRO
5	E	115	SER
1	N	63	ALA
2	O	319	SER
2	O	386	ALA
3	P	156	TYR
3	P	264	VAL
2	B	55	SER
1	N	443	TRP
2	O	55	SER
2	O	221	GLU
3	P	3	PRO
4	Q	177	ALA
5	R	127	VAL
7	T	33	ALA
5	E	137	GLY
6	F	77	LYS
5	R	113	ASP
5	R	120	PRO
5	R	177	PRO
7	T	50	PRO
3	C	158	GLY
5	E	120	PRO
5	R	137	GLY
7	G	50	PRO

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Mol	Chain	Res	Type
2	O	208	GLY
1	A	71	PRO
5	E	154	GLY
5	R	154	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	365/368 (99%)	352 (96%)	13 (4%)	42	75
1	N	365/368 (99%)	352 (96%)	13 (4%)	42	75
2	B	331/347 (95%)	320 (97%)	11 (3%)	45	77
2	O	333/347 (96%)	323 (97%)	10 (3%)	48	80
3	C	328/329 (100%)	320 (98%)	8 (2%)	57	86
3	P	328/329 (100%)	322 (98%)	6 (2%)	66	90
4	D	200/200 (100%)	197 (98%)	3 (2%)	72	92
4	Q	200/200 (100%)	197 (98%)	3 (2%)	72	92
5	E	166/166 (100%)	162 (98%)	4 (2%)	57	86
5	R	165/166 (99%)	161 (98%)	4 (2%)	57	86
6	F	93/96 (97%)	90 (97%)	3 (3%)	46	79
6	S	93/96 (97%)	89 (96%)	4 (4%)	35	69
7	G	71/71 (100%)	70 (99%)	1 (1%)	74	93
7	T	70/71 (99%)	69 (99%)	1 (1%)	74	93
8	H	65/71 (92%)	65 (100%)	0	100	100
8	U	63/71 (89%)	62 (98%)	1 (2%)	70	91
9	I	23/26 (88%)	21 (91%)	2 (9%)	13	33
9	V	23/26 (88%)	20 (87%)	3 (13%)	5	14
10	J	49/49 (100%)	47 (96%)	2 (4%)	37	70
10	W	47/49 (96%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3378/3446 (98%)	3286 (97%)	92 (3%)	52 83

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	58	PHE
1	A	86	PHE
1	A	106	MET
1	A	179	ARG
1	A	181	ASP
1	A	281	ASP
1	A	307	PHE
1	A	352	SER
1	A	395	TRP
1	A	405	ARG
1	A	432	LEU
1	A	443	TRP
2	B	23	ASP
2	B	31	ASN
2	B	104	LYS
2	B	193	HIS
2	B	225	ASN
2	B	248	ASN
2	B	250	HIS
2	B	270	ASN
2	B	341	MET
2	B	402	ILE
2	B	437	ASP
3	C	22	LEU
3	C	41	CYS
3	C	81	ARG
3	C	91	PHE
3	C	184	PHE
3	C	223	PRO
3	C	240	PHE
3	C	367	PHE
4	D	70	VAL
4	D	169	LEU
4	D	203	ARG
5	E	52	LYS
5	E	131	GLU

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Mol	Chain	Res	Type
5	E	178	TYR
5	E	185	TYR
6	F	52	GLU
6	F	64	ARG
6	F	70	LEU
7	G	28	ASN
9	I	68	ILE
9	I	71	ASN
10	J	59	TYR
10	J	60	GLU
1	N	18	THR
1	N	49	ASN
1	N	58	PHE
1	N	86	PHE
1	N	106	MET
1	N	181	ASP
1	N	281	ASP
1	N	307	PHE
1	N	352	SER
1	N	395	TRP
1	N	405	ARG
1	N	432	LEU
1	N	443	TRP
2	O	18	CYS
2	O	19	PRO
2	O	31	ASN
2	O	84	ARG
2	O	104	LYS
2	O	193	HIS
2	O	248	ASN
2	O	250	HIS
2	O	341	MET
2	O	402	ILE
3	P	81	ARG
3	P	91	PHE
3	P	184	PHE
3	P	240	PHE
3	P	256	ASN
3	P	367	PHE
4	Q	70	VAL
4	Q	169	LEU
4	Q	203	ARG

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Mol	Chain	Res	Type
5	R	31	ASP
5	R	52	LYS
5	R	178	TYR
5	R	185	TYR
6	S	13	MET
6	S	52	GLU
6	S	64	ARG
6	S	70	LEU
7	T	28	ASN
8	U	49	HIS
9	V	58	ARG
9	V	68	ILE
9	V	75	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	49	ASN
1	A	85	HIS
1	A	118	GLN
1	A	173	ASN
1	A	267	ASN
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
1	A	311	ASN
1	A	339	GLN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	247	GLN
2	B	248	ASN
2	B	270	ASN
2	B	276	GLN
2	B	297	GLN
2	B	329	GLN
2	B	343	GLN
2	B	362	ASN
2	B	363	GLN
3	C	9	HIS
3	C	17	ASN

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Mol	Chain	Res	Type
3	C	69	HIS
3	C	82	ASN
3	C	207	ASN
3	C	313	GLN
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	148	HIS
5	E	3	ASN
5	E	122	HIS
5	E	149	ASN
5	E	164	HIS
7	G	6	ASN
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
9	I	71	ASN
1	N	32	GLN
1	N	49	ASN
1	N	85	HIS
1	N	118	GLN
1	N	143	ASN
1	N	173	ASN
1	N	267	ASN
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
1	N	311	ASN
1	N	339	GLN
2	O	31	ASN
2	O	153	GLN
2	O	156	GLN
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	297	GLN
2	O	329	GLN
2	O	343	GLN
2	O	362	ASN
2	O	363	GLN
3	P	9	HIS

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Mol	Chain	Res	Type
3	P	17	ASN
3	P	69	HIS
3	P	82	ASN
3	P	207	ASN
3	P	313	GLN
3	P	332	ASN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	148	HIS
4	Q	200	GLN
5	R	57	GLN
5	R	107	ASN
5	R	164	HIS
5	R	186	GLN
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

29 ligands 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	$\#\|Z\| > 2$
11	PEE	A	2005	-	49,49,50	1.43	9 (18%)	50,54,55	0.93	5 (10%)
11	PEE	A	2008	-	20,20,50	1.80	6 (30%)	21,25,55	0.69	0
13	AZO	C	2001	-	32,32,32	2.92	15 (46%)	38,42,42	3.36	11 (28%)
14	UQ	C	2002	-	19,19,63	2.51	11 (57%)	23,26,79	1.37	4 (17%)
11	PEE	C	2007	-	48,48,50	1.29	7 (14%)	49,53,55	0.91	4 (8%)
15	GOL	C	2011	-	5,5,5	1.33	0	5,5,5	0.67	0
12	HEM	C	501	3	30,50,50	2.92	11 (36%)	24,82,82	2.47	9 (37%)
12	HEM	C	502	3	30,50,50	2.47	8 (26%)	24,82,82	2.30	8 (33%)
17	CDL	D	2003	-	41,41,99	1.16	2 (4%)	43,53,111	1.06	2 (4%)
18	BOG	D	2009	-	20,20,20	1.01	1 (5%)	25,25,25	0.91	2 (8%)
18	BOG	D	2091	-	13,13,20	1.27	2 (15%)	18,18,25	1.07	2 (11%)
16	HEC	D	501	4	24,50,50	2.41	4 (16%)	19,82,82	3.12	5 (26%)
19	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
17	CDL	G	2004	-	39,39,99	1.19	2 (5%)	41,51,111	1.13	3 (7%)
11	PEE	N	3008	-	4,4,50	3.74	4 (100%)	6,6,55	0.55	0
18	BOG	P	2010	-	12,12,20	1.38	3 (25%)	17,17,25	0.63	0
13	AZO	P	3001	-	32,32,32	3.12	16 (50%)	38,42,42	3.40	15 (39%)
14	UQ	P	3002	-	19,19,63	2.50	11 (57%)	23,26,79	1.34	3 (13%)
11	PEE	P	3005	-	49,49,50	1.41	9 (18%)	50,54,55	0.93	5 (10%)
11	PEE	P	3007	-	48,48,50	1.23	7 (14%)	49,53,55	0.87	4 (8%)
15	GOL	P	3011	-	5,5,5	1.35	0	5,5,5	0.69	0
12	HEM	P	501	3	30,50,50	2.59	9 (30%)	24,82,82	2.29	8 (33%)
12	HEM	P	502	3	30,50,50	2.67	10 (33%)	24,82,82	2.34	9 (37%)
17	CDL	Q	3003	-	41,41,99	1.17	2 (4%)	43,53,111	1.08	4 (9%)
18	BOG	Q	3009	-	20,20,20	0.97	1 (5%)	25,25,25	0.86	2 (8%)
18	BOG	Q	3091	-	13,13,20	1.33	2 (15%)	18,18,25	1.09	2 (11%)
16	HEC	Q	501	4	24,50,50	2.44	3 (12%)	19,82,82	3.13	6 (31%)
19	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
17	CDL	T	3004	-	39,39,99	1.18	2 (5%)	41,51,111	1.14	4 (9%)

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
11	PEE	A	2005	-	-	0/53/53/54	0/0/0/0
11	PEE	A	2008	-	-	0/24/24/54	0/0/0/0
13	AZO	C	2001	-	-	0/23/23/23	0/3/3/3
14	UQ	C	2002	-	-	0/11/35/87	0/1/1/1
11	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
15	GOL	C	2011	-	-	0/4/4/4	0/0/0/0
12	HEM	C	501	3	-	0/10/54/54	0/0/8/8
12	HEM	C	502	3	-	0/10/54/54	0/0/8/8
17	CDL	D	2003	-	-	0/51/51/110	0/0/0/0
18	BOG	D	2009	-	-	0/11/31/31	0/1/1/1
18	BOG	D	2091	-	-	0/4/24/31	0/1/1/1
16	HEC	D	501	4	-	0/6/54/54	0/0/8/8
19	FES	E	501	5	-	0/0/4/4	0/1/1/1
17	CDL	G	2004	-	-	0/49/49/110	0/0/0/0
11	PEE	N	3008	-	-	0/0/0/54	0/0/0/0
18	BOG	P	2010	-	-	0/2/22/31	0/1/1/1
13	AZO	P	3001	-	-	0/23/23/23	0/3/3/3
14	UQ	P	3002	-	-	0/11/35/87	0/1/1/1
11	PEE	P	3005	-	-	0/53/53/54	0/0/0/0
11	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
15	GOL	P	3011	-	-	0/4/4/4	0/0/0/0
12	HEM	P	501	3	-	0/10/54/54	0/0/8/8
12	HEM	P	502	3	-	0/10/54/54	0/0/8/8
17	CDL	Q	3003	-	-	0/51/51/110	0/0/0/0
18	BOG	Q	3009	-	-	0/11/31/31	0/1/1/1
18	BOG	Q	3091	-	-	0/4/24/31	0/1/1/1
16	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
19	FES	R	501	5	-	0/0/4/4	0/1/1/1
17	CDL	T	3004	-	-	0/49/49/110	0/0/0/0

All (157) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	501	HEC	C3B-C2B	-8.76	1.31	1.40
16	Q	501	HEC	C3B-C2B	-8.73	1.31	1.40
16	Q	501	HEC	C3C-C2C	-6.84	1.33	1.40
12	C	501	HEM	C3B-CAB	-6.59	1.39	1.51
12	P	502	HEM	C3B-CAB	-6.53	1.39	1.51
13	P	3001	AZO	C18-C19	-6.38	1.32	1.48
12	C	502	HEM	C3B-CAB	-6.23	1.39	1.51
12	C	501	HEM	C3B-C4B	-6.21	1.46	1.51
12	P	501	HEM	C2D-C3D	-6.21	1.35	1.54
12	P	502	HEM	C2D-C3D	-6.19	1.35	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	502	HEM	C3C-CAC	-6.18	1.39	1.51
12	C	501	HEM	C2D-C3D	-6.10	1.36	1.54
13	C	2001	AZO	C18-C19	-6.08	1.33	1.48
16	D	501	HEC	C3C-C2C	-6.08	1.34	1.40
12	C	501	HEM	C3C-CAC	-6.07	1.39	1.51
12	P	502	HEM	C3C-CAC	-6.03	1.40	1.51
12	P	501	HEM	C3B-CAB	-5.77	1.40	1.51
12	P	501	HEM	C3C-CAC	-5.51	1.41	1.51
12	C	502	HEM	C2D-C3D	-5.44	1.38	1.54
12	C	501	HEM	C2C-C1C	-4.28	1.44	1.52
12	C	501	HEM	C3D-C4D	-4.22	1.46	1.51
12	P	501	HEM	C3B-C4B	-4.12	1.48	1.51
12	P	502	HEM	C2C-C1C	-3.84	1.45	1.52
12	P	501	HEM	C3D-C4D	-3.67	1.46	1.51
12	P	501	HEM	C2C-C1C	-3.41	1.46	1.52
12	P	502	HEM	C3B-C4B	-3.22	1.49	1.51
12	C	502	HEM	C3D-C4D	-3.11	1.47	1.51
12	P	502	HEM	C2D-C1D	-3.01	1.42	1.51
12	C	502	HEM	C2C-C1C	-2.98	1.46	1.52
12	P	502	HEM	C3D-C4D	-2.97	1.47	1.51
11	P	3005	PEE	C19-C18	-2.96	1.34	1.51
11	A	2005	PEE	C19-C18	-2.91	1.34	1.51
11	P	3007	PEE	C22-C21	-2.84	1.35	1.51
11	P	3007	PEE	C19-C18	-2.78	1.35	1.51
11	P	3005	PEE	C22-C21	-2.77	1.35	1.51
11	C	2007	PEE	C19-C18	-2.76	1.35	1.51
11	A	2005	PEE	C22-C21	-2.72	1.35	1.51
11	C	2007	PEE	C22-C21	-2.62	1.36	1.51
16	D	501	HEC	C1D-CHD	-2.47	1.33	1.39
12	C	501	HEM	C2D-C1D	-2.34	1.44	1.51
16	Q	501	HEC	C1D-CHD	-2.31	1.33	1.39
13	C	2001	AZO	O5-C22	-2.24	1.40	1.44
16	D	501	HEC	C4C-NC	-2.14	1.33	1.36
17	T	3004	CDL	OB2-CB2	-2.06	1.36	1.44
12	C	501	HEM	C2B-C1B	-2.05	1.45	1.51
11	P	3007	PEE	C31-C30	2.01	1.56	1.50
13	C	2001	AZO	C17-C18	2.02	1.51	1.49
13	P	3001	AZO	C17-C18	2.02	1.51	1.49
17	D	2003	CDL	O1-C1	2.03	1.49	1.43
11	N	3008	PEE	P-O2P	2.04	1.61	1.54
11	C	2007	PEE	O2-C2	2.04	1.51	1.46
13	C	2001	AZO	O5-C21	2.04	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	3007	PEE	C3-C2	2.05	1.56	1.50
17	D	2003	CDL	CA3-CA4	2.07	1.56	1.50
17	G	2004	CDL	O1-C1	2.08	1.49	1.43
17	Q	3003	CDL	CA3-CA4	2.09	1.56	1.50
13	P	3001	AZO	C9-C10	2.13	1.42	1.38
13	P	3001	AZO	C13-C12	2.14	1.44	1.39
11	A	2008	PEE	C11-C10	2.14	1.57	1.50
17	T	3004	CDL	O1-C1	2.15	1.50	1.43
17	G	2004	CDL	CB3-CB4	2.17	1.56	1.50
17	Q	3003	CDL	O1-C1	2.21	1.50	1.43
18	P	2010	BOG	C1-C2	2.21	1.57	1.52
18	D	2091	BOG	C4-C5	2.22	1.57	1.53
11	P	3005	PEE	C11-C10	2.22	1.57	1.50
13	P	3001	AZO	C15-C16	2.25	1.43	1.38
18	Q	3091	BOG	C4-C5	2.26	1.57	1.53
18	P	2010	BOG	C4-C5	2.26	1.57	1.53
11	A	2005	PEE	C11-C10	2.26	1.57	1.50
11	P	3005	PEE	C31-C30	2.27	1.57	1.50
11	C	2007	PEE	C3-C2	2.30	1.57	1.50
13	P	3001	AZO	C4-C3	2.30	1.43	1.38
13	P	3001	AZO	O2-C10	2.31	1.39	1.36
14	P	3002	UQ	C8-C9	2.33	1.37	1.33
18	D	2091	BOG	O5-C1	2.34	1.47	1.41
13	C	2001	AZO	C15-C16	2.35	1.43	1.38
18	Q	3009	BOG	O5-C1	2.35	1.47	1.41
14	C	2002	UQ	C8-C9	2.36	1.37	1.33
11	P	3005	PEE	C1-C2	2.39	1.57	1.50
18	D	2009	BOG	O5-C1	2.39	1.48	1.41
14	P	3002	UQ	O2-C2	2.40	1.43	1.37
18	P	2010	BOG	O5-C1	2.43	1.47	1.43
14	C	2002	UQ	O2-C2	2.44	1.43	1.37
14	P	3002	UQ	C5-C4	2.45	1.56	1.47
13	P	3001	AZO	C6-C7	2.46	1.44	1.39
14	C	2002	UQ	C5-C4	2.47	1.56	1.47
18	Q	3091	BOG	O5-C1	2.48	1.48	1.41
13	C	2001	AZO	C5-C4	2.48	1.44	1.38
14	C	2002	UQ	C7-C8	2.48	1.54	1.50
13	P	3001	AZO	C5-C4	2.51	1.44	1.38
11	P	3007	PEE	O2-C10	2.51	1.41	1.34
11	A	2005	PEE	C1-C2	2.53	1.57	1.50
11	A	2005	PEE	C31-C30	2.54	1.58	1.50
14	P	3002	UQ	C7-C8	2.55	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	3002	UQ	CM5-C5	2.56	1.56	1.50
11	A	2008	PEE	C1-C2	2.57	1.58	1.50
14	C	2002	UQ	C3-C4	2.58	1.56	1.48
11	A	2005	PEE	C3-C2	2.61	1.58	1.50
11	A	2008	PEE	C3-C2	2.61	1.58	1.50
13	C	2001	AZO	C6-C7	2.63	1.45	1.39
14	P	3002	UQ	C3-C4	2.64	1.56	1.48
11	P	3005	PEE	C3-C2	2.65	1.58	1.50
14	C	2002	UQ	CM5-C5	2.66	1.56	1.50
11	P	3007	PEE	P-O1P	2.67	1.60	1.51
13	C	2001	AZO	C13-C12	2.71	1.45	1.39
11	C	2007	PEE	O2-C10	2.72	1.42	1.34
11	N	3008	PEE	P-O3P	2.74	1.64	1.54
14	P	3002	UQ	C2-C1	2.75	1.56	1.48
13	C	2001	AZO	C4-C3	2.82	1.44	1.38
14	C	2002	UQ	O3-C3	2.84	1.44	1.37
11	C	2007	PEE	P-O1P	2.85	1.61	1.51
11	N	3008	PEE	P-O4P	2.93	1.65	1.54
11	A	2008	PEE	P-O1P	2.94	1.61	1.51
12	C	502	HEM	C4C-NC	2.95	1.39	1.36
12	C	502	HEM	CBC-CAC	2.99	1.46	1.29
13	P	3001	AZO	O5-C21	2.99	1.40	1.34
11	A	2008	PEE	O2-C10	2.99	1.43	1.34
11	P	3007	PEE	O3-C30	2.99	1.42	1.33
11	A	2005	PEE	P-O1P	3.01	1.62	1.51
11	P	3005	PEE	P-O1P	3.02	1.62	1.51
14	P	3002	UQ	O3-C3	3.05	1.45	1.37
14	C	2002	UQ	C2-C1	3.06	1.57	1.48
11	C	2007	PEE	O3-C30	3.07	1.42	1.33
12	P	501	HEM	C4C-NC	3.10	1.39	1.36
11	A	2005	PEE	O2-C10	3.10	1.43	1.34
11	A	2008	PEE	O3-C30	3.17	1.42	1.33
12	C	501	HEM	C4C-NC	3.21	1.40	1.36
11	P	3005	PEE	O3-C30	3.24	1.43	1.33
11	P	3005	PEE	O2-C10	3.32	1.44	1.34
11	A	2005	PEE	O3-C30	3.43	1.43	1.33
12	P	502	HEM	CBC-CAC	3.44	1.49	1.29
14	P	3002	UQ	C6-C5	3.65	1.43	1.35
13	C	2001	AZO	C8-N2	3.68	1.37	1.32
12	C	501	HEM	CBB-CAB	3.68	1.50	1.29
12	P	502	HEM	C4C-NC	3.73	1.40	1.36
12	C	501	HEM	CBC-CAC	3.74	1.50	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	2002	UQ	C6-C1	3.76	1.57	1.46
14	C	2002	UQ	C6-C5	3.81	1.44	1.35
14	P	3002	UQ	C6-C1	3.85	1.57	1.46
12	P	501	HEM	CBC-CAC	3.89	1.51	1.29
13	C	2001	AZO	C10-N3	3.91	1.38	1.32
12	P	502	HEM	CBB-CAB	3.91	1.51	1.29
12	P	501	HEM	CBB-CAB	3.94	1.52	1.29
13	P	3001	AZO	C8-N2	4.31	1.38	1.32
12	C	502	HEM	CBB-CAB	4.52	1.55	1.29
14	C	2002	UQ	C7-C6	5.02	1.60	1.51
13	C	2001	AZO	C2-C7	5.02	1.52	1.40
14	P	3002	UQ	C7-C6	5.11	1.60	1.51
13	P	3001	AZO	C10-N3	5.14	1.39	1.32
13	C	2001	AZO	C17-C12	5.22	1.50	1.40
13	P	3001	AZO	O4-C19	5.33	1.45	1.33
13	P	3001	AZO	C2-C7	5.34	1.53	1.40
13	C	2001	AZO	O4-C19	5.70	1.46	1.33
13	P	3001	AZO	C17-C12	5.91	1.51	1.40
11	N	3008	PEE	P-O1P	5.97	1.62	1.50
13	C	2001	AZO	C21-C18	7.11	1.50	1.35
13	P	3001	AZO	C21-C18	7.45	1.51	1.35

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	D	501	HEC	CBB-CAB-C3B	-8.84	107.70	127.35
16	Q	501	HEC	CBB-CAB-C3B	-8.61	108.22	127.35
13	C	2001	AZO	C22-O5-C21	-7.23	108.29	115.90
13	P	3001	AZO	C22-O5-C21	-7.23	108.29	115.90
16	Q	501	HEC	CBC-CAC-C3C	-6.34	113.25	127.35
16	D	501	HEC	CBC-CAC-C3C	-6.28	113.39	127.35
13	C	2001	AZO	N2-C11-N3	-6.04	118.50	128.67
13	P	3001	AZO	N2-C11-N3	-5.78	118.93	128.67
13	P	3001	AZO	C9-C10-N3	-3.79	119.36	124.88
13	C	2001	AZO	C9-C10-N3	-3.49	119.79	124.88
14	C	2002	UQ	C7-C6-C1	-3.42	114.54	118.56
12	C	501	HEM	CAA-C2A-C1A	-3.37	123.35	127.01
17	T	3004	CDL	CB4-OB6-CB5	-3.32	109.91	117.89
13	P	3001	AZO	C9-C8-N2	-3.24	120.15	124.88
16	D	501	HEC	CAA-C2A-C3A	-3.16	119.98	129.00
17	G	2004	CDL	CA4-OA6-CA5	-3.12	110.39	117.89
17	G	2004	CDL	CB4-OB6-CB5	-3.08	110.50	117.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	501	HEC	CAA-C2A-C3A	-3.07	120.23	129.00
14	P	3002	UQ	C7-C6-C1	-3.07	114.95	118.56
12	P	501	HEM	CAA-C2A-C1A	-3.00	123.75	127.01
12	C	501	HEM	C3C-CAC-CBC	-2.96	119.92	124.46
13	C	2001	AZO	C9-C8-N2	-2.89	120.67	124.88
14	P	3002	UQ	C10-C9-C8	-2.86	117.89	123.50
14	C	2002	UQ	C10-C9-C8	-2.76	118.09	123.50
17	T	3004	CDL	CA4-OA6-CA5	-2.70	111.41	117.89
17	D	2003	CDL	CB4-OB6-CB5	-2.56	111.74	117.89
17	Q	3003	CDL	CB4-OB6-CB5	-2.43	112.05	117.89
17	T	3004	CDL	CA6-CA4-CA3	-2.39	106.47	112.07
17	D	2003	CDL	CA6-CA4-CA3	-2.39	106.48	112.07
17	Q	3003	CDL	CA6-CA4-CA3	-2.35	106.58	112.07
12	C	501	HEM	CMA-C3A-C4A	-2.30	124.57	128.36
17	G	2004	CDL	CA6-CA4-CA3	-2.26	106.78	112.07
17	Q	3003	CDL	CA4-OA6-CA5	-2.15	112.73	117.89
17	T	3004	CDL	CB6-CB4-CB3	-2.12	107.11	112.07
13	P	3001	AZO	O4-C19-O3	-2.08	119.41	123.56
17	Q	3003	CDL	CB6-CB4-CB3	-2.07	107.24	112.07
12	P	501	HEM	C3C-CAC-CBC	-2.05	121.32	124.46
14	C	2002	UQ	C11-C9-C8	2.03	125.27	120.74
13	C	2001	AZO	O2-C10-N3	2.04	122.51	118.98
13	P	3001	AZO	O1-C8-N2	2.10	122.61	118.98
13	P	3001	AZO	C7-C2-C1	2.15	120.87	119.43
12	P	502	HEM	C3B-C4B-CHC	2.16	126.20	123.16
16	Q	501	HEC	CAD-C3D-C4D	2.16	129.35	127.01
16	Q	501	HEC	CBA-CAA-C2A	2.19	116.45	112.53
12	P	502	HEM	C2D-C3D-C4D	2.27	105.35	101.50
13	C	2001	AZO	C20-O4-C19	2.30	120.23	115.90
11	A	2005	PEE	O3-C3-C2	2.31	114.91	108.69
11	P	3005	PEE	C23-C22-C21	2.32	126.51	114.53
11	P	3007	PEE	C22-C21-C20	2.35	126.66	114.53
13	P	3001	AZO	O2-C10-N3	2.35	123.04	118.98
11	P	3007	PEE	C23-C22-C21	2.35	126.68	114.53
11	A	2005	PEE	C23-C22-C21	2.38	126.80	114.53
11	P	3005	PEE	O3-C3-C2	2.40	115.14	108.69
13	P	3001	AZO	C10-C9-C8	2.41	117.67	115.18
11	C	2007	PEE	C22-C21-C20	2.42	127.05	114.53
18	Q	3091	BOG	O1-C1-C2	2.43	111.08	108.21
12	C	502	HEM	C2D-C3D-C4D	2.48	105.70	101.50
11	C	2007	PEE	C23-C22-C21	2.49	127.39	114.53
11	C	2007	PEE	C19-C18-C17	2.50	127.44	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	D	2091	BOG	O1-C1-C2	2.50	111.16	108.21
11	P	3005	PEE	C22-C21-C20	2.51	127.47	114.53
11	A	2005	PEE	C22-C21-C20	2.52	127.56	114.53
11	P	3007	PEE	C19-C18-C17	2.53	127.57	114.53
18	Q	3009	BOG	O1-C1-C2	2.53	111.23	108.04
11	P	3005	PEE	C19-C18-C17	2.53	127.61	114.53
11	A	2005	PEE	C19-C18-C17	2.58	127.83	114.53
13	P	3001	AZO	C12-O2-C10	2.59	124.74	118.73
18	D	2009	BOG	C1'-O1-C1	2.61	118.50	113.94
11	A	2005	PEE	C20-C19-C18	2.62	128.03	114.53
11	P	3005	PEE	C20-C19-C18	2.64	128.19	114.53
18	Q	3009	BOG	C1'-O1-C1	2.64	118.56	113.94
12	C	501	HEM	CMD-C2D-C3D	2.69	126.25	114.35
13	P	3001	AZO	C7-O1-C8	2.70	124.99	118.73
13	P	3001	AZO	C20-O4-C19	2.72	121.01	115.90
13	C	2001	AZO	C7-O1-C8	2.73	125.06	118.73
11	P	3007	PEE	C20-C19-C18	2.74	128.68	114.53
13	C	2001	AZO	C12-O2-C10	2.78	125.16	118.73
11	C	2007	PEE	C20-C19-C18	2.78	128.87	114.53
18	D	2009	BOG	O1-C1-C2	2.84	111.63	108.04
12	C	502	HEM	CMC-C2C-C3C	2.93	123.84	116.53
12	P	501	HEM	CMD-C2D-C3D	3.01	127.67	114.35
12	P	501	HEM	CAD-C3D-C2D	3.04	121.97	113.22
12	P	502	HEM	CAA-C2A-C1A	3.07	130.34	127.01
12	C	502	HEM	CMD-C2D-C3D	3.17	128.36	114.35
18	D	2091	BOG	C1'-O1-C1	3.18	118.50	113.29
12	P	502	HEM	CMD-C2D-C3D	3.21	128.54	114.35
18	Q	3091	BOG	C1'-O1-C1	3.36	118.80	113.29
12	C	501	HEM	CAD-C3D-C2D	3.43	123.09	113.22
16	D	501	HEC	CAD-C3D-C4D	3.50	130.81	127.01
12	C	502	HEM	CAD-C3D-C2D	3.50	123.28	113.22
14	P	3002	UQ	C8-C7-C6	3.70	122.76	111.64
12	C	502	HEM	CAA-C2A-C1A	3.71	131.03	127.01
14	C	2002	UQ	C8-C7-C6	3.76	122.94	111.64
12	C	501	HEM	C2D-C3D-C4D	3.81	107.96	101.50
12	P	502	HEM	C3B-CAB-CBB	3.89	130.43	124.46
12	P	501	HEM	CMC-C2C-C3C	3.92	126.31	116.53
12	P	502	HEM	CAD-C3D-C2D	3.96	124.59	113.22
12	P	501	HEM	C2D-C3D-C4D	4.05	108.37	101.50
12	C	502	HEM	C3B-CAB-CBB	4.06	130.69	124.46
12	P	502	HEM	CMC-C2C-C3C	4.16	126.92	116.53
12	P	502	HEM	CMB-C2B-C3B	4.49	127.75	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	P	3001	AZO	O4-C19-C18	4.65	119.53	111.82
12	C	501	HEM	CAD-C3D-C4D	4.67	128.96	112.47
12	C	501	HEM	CMC-C2C-C3C	4.68	128.21	116.53
13	C	2001	AZO	O4-C19-C18	4.70	119.61	111.82
12	P	501	HEM	CAD-C3D-C4D	4.87	129.64	112.47
12	C	502	HEM	CMB-C2B-C3B	4.96	128.91	116.53
12	P	502	HEM	CAD-C3D-C4D	4.98	130.03	112.47
12	P	501	HEM	CMB-C2B-C3B	5.10	129.27	116.53
12	C	502	HEM	CAD-C3D-C4D	5.18	130.73	112.47
12	C	501	HEM	CMB-C2B-C3B	5.46	130.16	116.53
16	D	501	HEC	CAA-C2A-C1A	6.20	133.75	127.01
16	Q	501	HEC	CAA-C2A-C1A	6.85	134.44	127.01
13	C	2001	AZO	C11-N2-C8	10.97	121.79	114.31
13	P	3001	AZO	C11-N2-C8	11.09	121.88	114.31
13	P	3001	AZO	C11-N3-C10	11.28	122.00	114.31
13	C	2001	AZO	C11-N3-C10	11.51	122.16	114.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	2002	UQ	4	0
11	C	2007	PEE	5	0
15	C	2011	GOL	1	0
12	C	501	HEM	3	0
12	C	502	HEM	2	0
17	D	2003	CDL	4	0
18	D	2091	BOG	1	0
16	D	501	HEC	3	0
19	E	501	FES	2	0
17	G	2004	CDL	4	0
18	P	2010	BOG	1	0
13	P	3001	AZO	2	0
14	P	3002	UQ	6	0
11	P	3007	PEE	3	0
12	P	501	HEM	2	0
12	P	502	HEM	2	0
17	Q	3003	CDL	3	0
18	Q	3091	BOG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	Q	501	HEC	2	0
19	R	501	FES	2	0
17	T	3004	CDL	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	444/446 (99%)	0.37	14 (3%) 51 40	41, 68, 96, 110	0
1	N	442/446 (99%)	0.36	15 (3%) 49 38	48, 80, 103, 110	0
2	B	420/441 (95%)	0.40	23 (5%) 29 19	57, 87, 120, 142	0
2	O	422/441 (95%)	0.39	17 (4%) 42 31	49, 85, 113, 129	0
3	C	380/380 (100%)	0.36	9 (2%) 62 52	30, 48, 88, 132	0
3	P	379/380 (99%)	0.38	15 (3%) 42 31	33, 63, 94, 132	0
4	D	241/241 (100%)	0.29	5 (2%) 67 57	36, 51, 88, 109	0
4	Q	241/241 (100%)	0.27	5 (2%) 67 57	56, 76, 106, 127	0
5	E	196/196 (100%)	1.72	72 (36%) 0 0	41, 144, 176, 184	0
5	R	196/196 (100%)	0.30	9 (4%) 36 26	51, 97, 144, 156	0
6	F	101/110 (91%)	0.22	0 100 100	38, 52, 70, 104	0
6	S	101/110 (91%)	0.09	0 100 100	60, 74, 107, 131	0
7	G	80/81 (98%)	0.47	2 (2%) 61 50	42, 61, 106, 117	0
7	T	79/81 (97%)	0.59	6 (7%) 17 9	56, 85, 150, 159	0
8	H	70/77 (90%)	0.41	1 (1%) 78 71	45, 68, 91, 128	0
8	U	67/77 (87%)	0.31	5 (7%) 17 9	90, 117, 137, 141	0
9	I	31/47 (65%)	1.86	13 (41%) 0 0	80, 115, 142, 143	0
9	V	31/47 (65%)	1.76	15 (48%) 0 0	78, 115, 140, 145	0
10	J	61/61 (100%)	0.20	2 (3%) 50 39	52, 65, 103, 147	0
10	W	60/61 (98%)	0.37	2 (3%) 50 39	63, 79, 109, 119	0
All	All	4042/4160 (97%)	0.44	230 (5%) 27 18	30, 73, 131, 184	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	157	TYR	7.9
5	E	109	GLU	7.4
5	E	188	VAL	7.1
5	E	116	LYS	6.8
5	E	98	VAL	6.5
9	I	63	ASP	6.5
5	E	117	LEU	6.1
9	V	63	ASP	5.9
9	I	48	PRO	5.7
5	E	84	GLY	5.7
5	E	159	PRO	5.7
2	B	220	ALA	5.6
4	D	241	LYS	5.6
5	R	196	GLY	5.6
2	B	33	LEU	5.5
7	T	78	GLU	5.4
9	I	50	LEU	5.3
5	E	163	SER	5.2
5	E	171	ILE	5.2
5	E	183	PRO	5.2
5	E	114	VAL	5.2
5	R	81	ILE	5.0
5	E	120	PRO	5.0
5	E	138	VAL	5.0
7	T	2	ILE	4.9
5	E	102	THR	4.8
5	E	107	ASN	4.8
5	E	115	SER	4.8
5	E	149	ASN	4.8
2	B	224	LEU	4.8
5	E	103	GLN	4.8
5	E	112	VAL	4.6
9	V	68	ILE	4.5
5	E	148	ALA	4.4
2	B	226	ILE	4.4
5	E	156	TYR	4.4
5	E	158	CYS	4.4
5	E	174	GLY	4.4
5	E	113	ASP	4.2
5	E	124	LEU	4.2
1	N	379	ILE	4.2
5	E	86	ASN	4.2
5	E	167	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
5	E	173	LYS	4.1
5	E	152	ASP	4.1
5	E	150	SER	4.0
5	E	165	TYR	4.0
5	E	180	LEU	4.0
5	E	108	GLN	4.0
1	N	127	ILE	4.0
7	T	77	TYR	3.8
5	E	178	TYR	3.8
10	J	63	GLU	3.8
9	I	76	VAL	3.7
9	I	55	MET	3.7
4	Q	206	LEU	3.7
9	I	51	CYS	3.7
5	E	104	ALA	3.6
8	U	13	LEU	3.6
4	D	240	PRO	3.5
4	Q	210	LEU	3.5
5	E	145	VAL	3.5
2	B	225	ASN	3.5
2	B	29	LEU	3.5
5	E	146	PRO	3.4
2	O	410	VAL	3.4
5	E	169	GLY	3.4
9	V	53	GLU	3.4
5	E	177	PRO	3.3
5	E	111	GLU	3.3
3	C	380	TYR	3.3
2	O	402	ILE	3.3
9	I	54	SER	3.3
9	V	54	SER	3.3
5	R	86	ASN	3.3
1	N	122	LEU	3.3
5	E	134	ILE	3.2
5	E	97	PHE	3.2
9	V	56	SER	3.2
5	E	168	SER	3.1
1	A	392	LEU	3.1
2	B	439	LEU	3.1
3	P	237	LEU	3.1
5	E	83	GLU	3.1
5	E	172	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
5	E	187	PHE	3.1
9	V	48	PRO	3.1
2	O	144	LEU	3.1
5	E	105	GLU	3.1
1	A	365	MET	3.0
5	E	125	ASP	3.0
2	B	35	ILE	3.0
4	Q	209	LEU	3.0
2	O	132	PHE	3.0
1	A	197	LEU	3.0
2	O	191	LEU	3.0
1	N	138	LEU	3.0
7	T	53	LEU	3.0
3	P	233	LEU	2.9
3	P	363	LEU	2.9
7	T	6	ASN	2.9
5	E	87	VAL	2.9
2	B	201	SER	2.9
7	G	14	ILE	2.9
1	N	376	CYS	2.9
1	A	379	ILE	2.9
1	N	386	TYR	2.8
1	A	216	PHE	2.8
3	C	345	GLU	2.8
2	O	352	VAL	2.8
5	E	118	ARG	2.8
3	C	236	MET	2.8
9	I	64	LEU	2.8
5	E	181	GLU	2.8
5	E	119	ASP	2.7
2	B	216	LEU	2.7
2	O	344	LEU	2.7
5	E	90	LYS	2.7
4	D	3	LEU	2.7
2	O	296	TYR	2.7
3	P	34	PHE	2.6
5	E	144	CYS	2.6
5	E	143	GLY	2.6
9	I	77	ARG	2.6
3	P	277	PHE	2.6
2	B	402	ILE	2.6
4	D	1	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
5	R	171	ILE	2.6
1	N	174	ILE	2.6
3	C	4	ASN	2.6
5	E	106	ILE	2.6
1	N	302	LYS	2.6
5	E	147	ILE	2.5
5	E	136	VAL	2.5
2	O	68	LEU	2.5
9	I	59	SER	2.5
2	O	355	GLU	2.5
1	A	28	GLU	2.5
9	V	55	MET	2.5
3	C	155	PRO	2.5
1	N	392	LEU	2.5
2	B	369	LEU	2.5
9	V	74	ALA	2.5
1	N	182	LEU	2.5
2	B	368	TYR	2.5
9	V	58	ARG	2.5
8	U	37	LEU	2.4
1	A	86	PHE	2.4
3	C	90	PHE	2.4
1	A	208	LEU	2.4
2	B	223	PHE	2.4
5	R	1	VAL	2.4
1	A	203	ILE	2.4
2	B	386	ALA	2.4
2	O	405	VAL	2.4
2	B	144	LEU	2.4
9	V	60	ALA	2.4
9	I	53	GLU	2.4
1	A	177	LEU	2.4
3	P	334	LEU	2.4
5	E	135	LEU	2.4
10	W	39	ALA	2.4
5	E	140	THR	2.4
1	A	122	LEU	2.4
5	R	49	TYR	2.4
1	N	349	THR	2.4
9	V	72	ALA	2.3
3	C	233	LEU	2.3
5	E	176	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
3	P	91	PHE	2.3
2	B	157	VAL	2.3
5	E	89	PHE	2.3
10	W	35	PHE	2.3
8	H	71	HIS	2.3
1	A	174	ILE	2.3
3	P	96	PHE	2.3
7	G	81	GLN	2.3
2	B	34	ILE	2.3
2	B	206	LEU	2.2
8	U	12	GLU	2.2
2	B	132	PHE	2.2
5	E	182	VAL	2.2
5	E	88	ALA	2.2
4	Q	145	GLU	2.2
8	U	78	LYS	2.2
3	P	90	PHE	2.2
10	J	62	SER	2.2
1	N	269	VAL	2.2
5	E	99	ARG	2.2
9	I	49	LEU	2.2
1	A	1	ALA	2.2
1	N	72	CYS	2.2
9	V	47	ARG	2.2
2	O	140	LEU	2.2
5	E	137	GLY	2.2
3	P	37	LEU	2.2
1	A	127	ILE	2.1
7	T	74	PRO	2.1
3	P	2	ALA	2.1
2	O	146	VAL	2.1
1	N	380	GLY	2.1
9	V	59	SER	2.1
2	O	85	ILE	2.1
2	O	295	LEU	2.1
3	C	194	THR	2.1
5	R	115	SER	2.1
3	C	240	PHE	2.1
2	B	191	LEU	2.1
3	P	234	THR	2.1
4	Q	241	LYS	2.1
5	E	128	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
8	U	61	PHE	2.1
9	V	52	ARG	2.1
2	O	35	ILE	2.1
2	O	110	GLU	2.1
5	R	156	TYR	2.1
9	V	70	LEU	2.1
3	P	333	LEU	2.0
3	P	240	PHE	2.0
4	D	2	GLU	2.0
5	E	110	ALA	2.0
5	R	146	PRO	2.0
2	B	373	GLU	2.0
5	E	100	HIS	2.0
5	E	164	HIS	2.0
2	B	181	TYR	2.0
3	P	354	MET	2.0
9	I	58	ARG	2.0
1	N	402	VAL	2.0
5	E	142	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
15	GOL	P	3011	6/6	0.88	0.45	7.31	84,86,87,88	0
11	PEE	A	2005	50/51	0.85	0.55	6.55	79,96,106,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
14	UQ	P	3002	19/63	0.75	0.54	5.94	126,136,137,137	0
14	UQ	C	2002	19/63	0.86	0.47	5.26	91,92,94,95	0
11	PEE	C	2007	49/51	0.95	0.41	4.48	46,67,84,85	0
11	PEE	P	3007	49/51	0.90	0.59	3.85	74,88,100,101	0
11	PEE	P	3005	50/51	0.80	0.54	3.55	92,105,114,115	0
11	PEE	A	2008	21/51	0.72	0.31	3.33	132,136,139,140	0
18	BOG	Q	3009	20/20	0.83	0.40	1.78	74,89,91,93	0
17	CDL	D	2003	42/100	0.89	0.27	1.72	92,101,111,114	0
12	HEM	P	501	43/43	0.98	0.32	1.47	42,49,60,64	0
12	HEM	C	502	43/43	0.98	0.31	1.38	32,37,47,54	0
13	AZO	C	2001	30/30	0.96	0.26	1.36	36,39,41,41	0
17	CDL	G	2004	40/100	0.93	0.28	1.12	73,85,100,101	0
17	CDL	Q	3003	42/100	0.85	0.27	1.08	117,129,145,145	0
18	BOG	P	2010	12/20	0.57	0.25	0.96	140,143,144,145	0
18	BOG	D	2009	20/20	0.91	0.28	0.94	60,72,75,76	0
12	HEM	C	501	43/43	0.98	0.29	0.91	35,40,50,55	0
15	GOL	C	2011	6/6	0.91	0.22	0.68	80,84,85,86	0
13	AZO	P	3001	30/30	0.95	0.26	0.54	52,60,66,67	0
16	HEC	Q	501	43/43	0.96	0.23	0.35	60,65,71,72	0
12	HEM	P	502	43/43	0.98	0.26	0.19	38,47,58,60	0
16	HEC	D	501	43/43	0.98	0.22	0.11	31,37,45,48	0
17	CDL	T	3004	40/100	0.91	0.22	-0.01	97,104,113,114	0
19	FES	R	501	4/4	0.99	0.14	-0.85	88,89,90,91	0
19	FES	E	501	4/4	0.95	0.13	-1.73	153,153,154,154	0
18	BOG	D	2091	13/20	0.41	0.33	-	207,208,208,208	0
18	BOG	Q	3091	13/20	0.16	0.44	-	192,194,195,195	0
11	PEE	N	3008	5/51	0.85	0.21	-	110,111,112,112	0

6.5 Other polymers

There are no such residues in this entry.