Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:15 AM GMT

PDB ID	:	3L75
Title	:	Cytochrome BC1 complex from chicken with fenamidone bound
Authors	:	Huang, L.; Berry, E.A.
Deposited on	:	2009-12-28
Resolution	:	2.79 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:

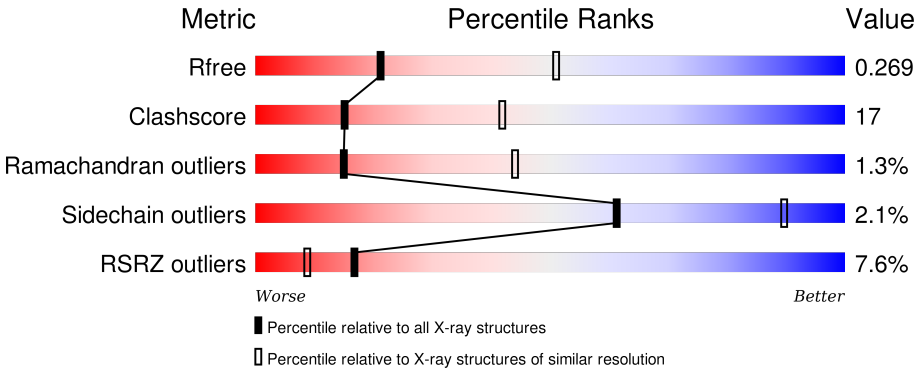
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.79 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	2% 65% 31%
1	N	446	5% 67% 29%
2	B	441	5% 55% 38% 5%
2	O	441	4% 55% 39%
3	C	380	80% 20%

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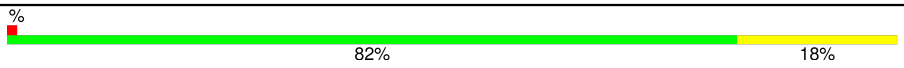
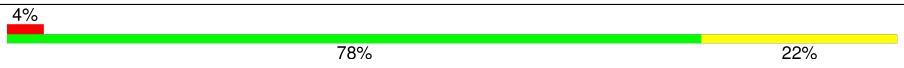
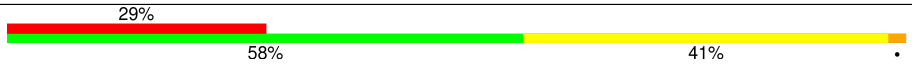
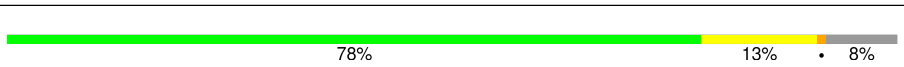
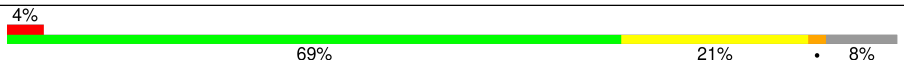
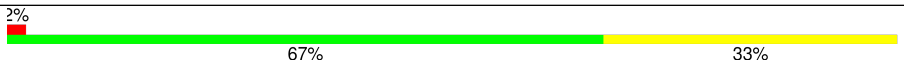
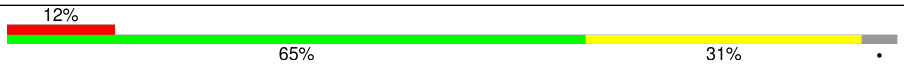
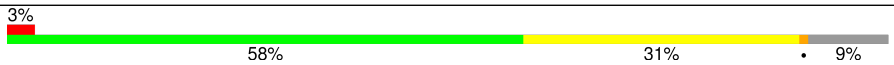
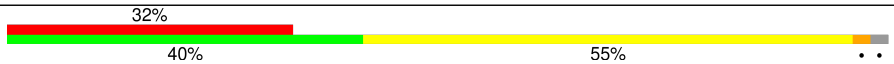
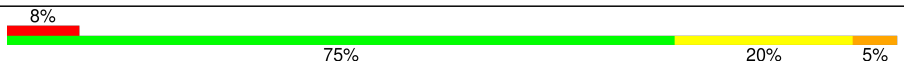
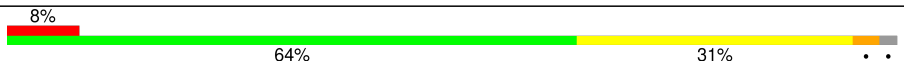
Mol	Chain	Length	Quality of chain
3	P	380	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	47	
9	V	47	
10	J	61	
10	W	61	

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	C	2005	-	-	-	X
11	PEE	C	2007	-	-	-	X
11	PEE	N	3008	-	X	-	-
11	PEE	P	3005	-	-	-	X
11	PEE	P	3007	-	-	-	X
12	UNL	C	2046	-	-	-	X
12	UNL	C	2048	-	-	-	X
12	UNL	P	3046	-	-	-	X
15	UQ	C	2002	-	-	-	X
15	UQ	P	3002	-	-	-	X
16	AZI	C	2011	-	-	-	X
16	AZI	P	3011	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	BOG	D	2091	-	-	-	X
17	BOG	P	2010	-	-	-	X
19	CDL	G	2004	-	-	-	X
20	FES	R	501	-	-	X	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32691 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	443	Total	C	N	O	S	0	0	1
			3440	2155	606	658	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	421	Total	C	N	O	S	0	0	0
			3141	1974	545	613	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 5, RIESKE IRONSULFUR PROTEIN, 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
			1512	952	262	292	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	81	Total	C	N	O	0	0	0
			676	439	120	117			
7	T	78	Total	C	N	O	0	0	0
			654	428	116	110			

- 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			

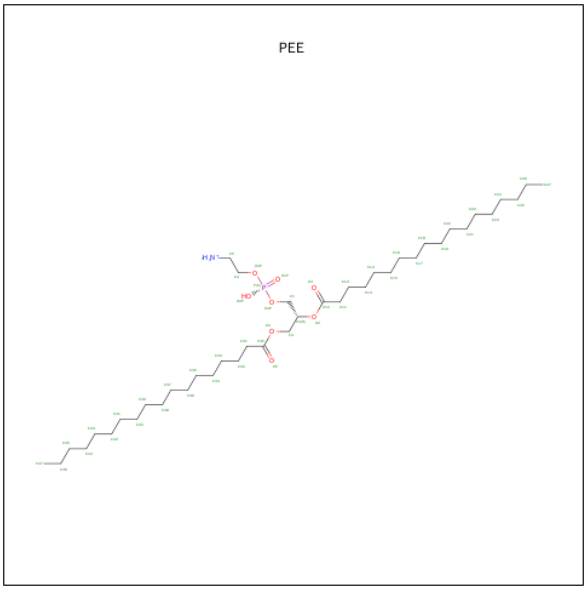
- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			288	172	58	56	2			
9	V	44	Total	C	N	O	S	0	0	1
			278	167	56	53	2			

- 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 497 321 87 89	0	0	0
10	W	60	Total C N O 479 311 86 82	0	0	1

- 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 O P 21 12 8 1	0	0
11	C	1	Total C N O P 50 40 1 8 1	0	0
11	C	1	Total C N O P 48 38 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 48 38 1 8 1	0	0

- Molecule 12 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	P	5	Total O 7 7	0	0

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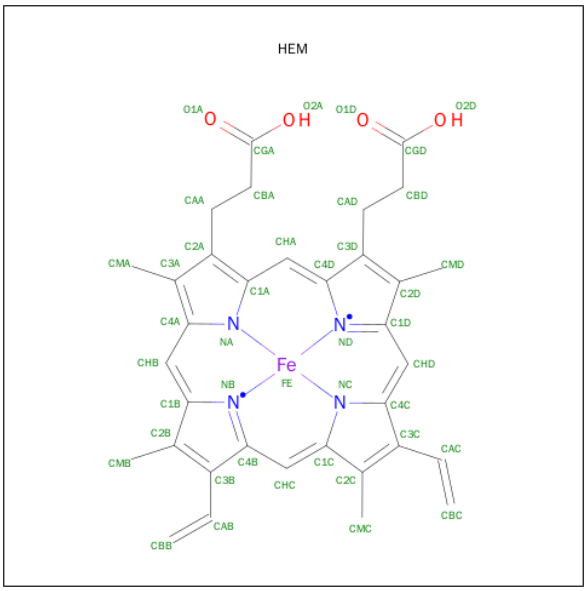
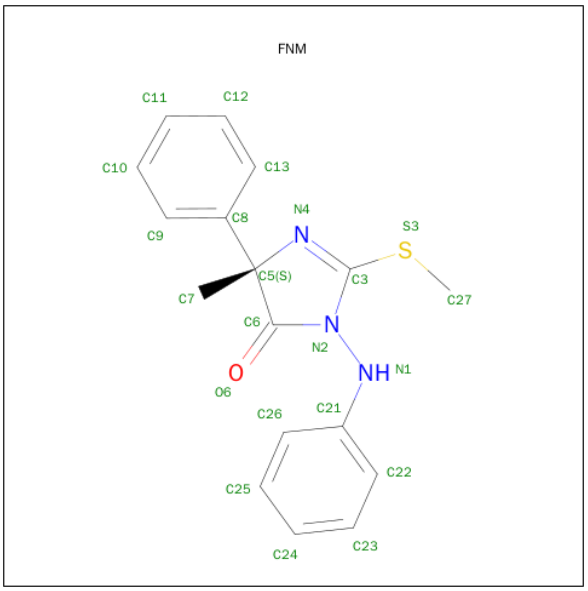
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	R	1	Total O 1 1	0	0
12	A	1	Total O 1 1	0	0
12	D	1	Total O 2 2	0	0
12	C	3	Total O 5 5	0	0

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



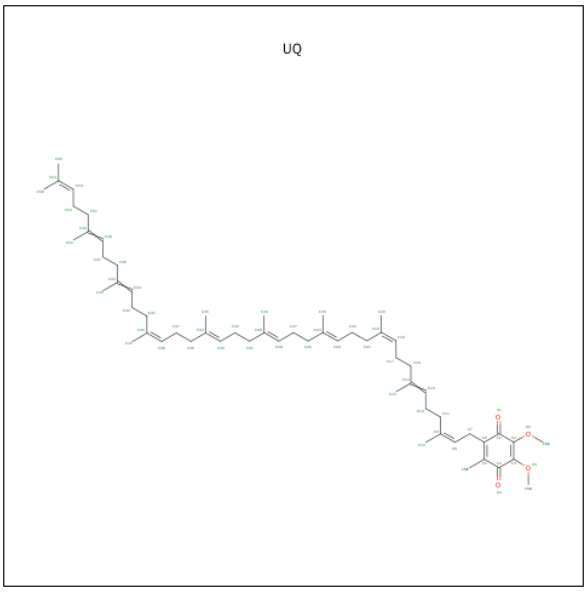
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C Fe N O 43 34 1 4 4	0	0
13	C	1	Total C Fe N O 43 34 1 4 4	0	0
13	P	1	Total C Fe N O 43 34 1 4 4	0	0
13	P	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 14 is (5S)-5-METHYL-2-(METHYLSULFANYL)-5-PHENYL-3-(PHENYLAMINO)-3,5-DIHYDRO-4H-IMIDAZOL-4-ONE (three-letter code: FNM) (formula: $C_{17}H_{17}N_3OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	N	O	S	0	0
			22	17	3	1	1		
14	P	1	Total	C	N	O	S	0	0
			22	17	3	1	1		

- Molecule 15 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
15	C	1	Total	C	O	0	0
			19	15	4		

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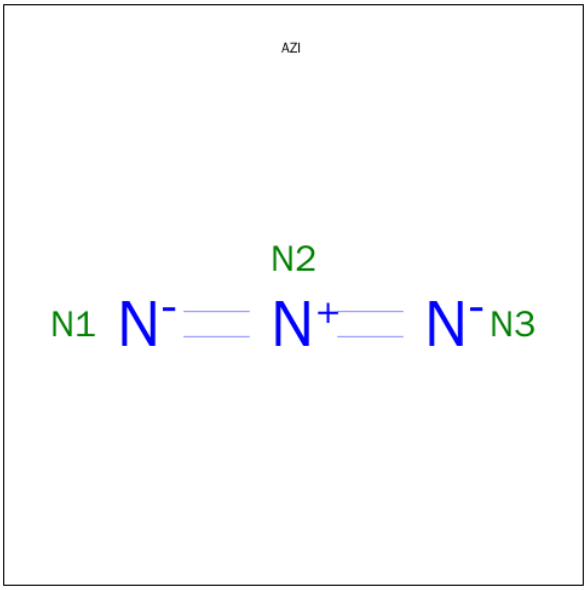
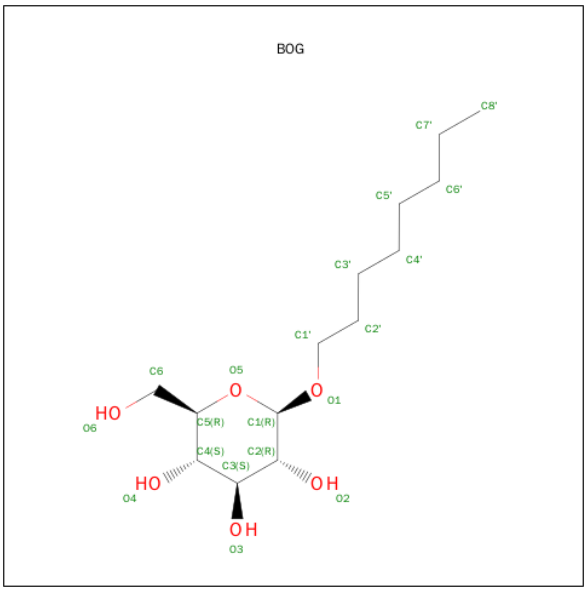
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	P	1	Total C O 19 15 4	0	0

- Molecule 16 is AZIDE ION (three-letter code: AZI) (formula: N_3).



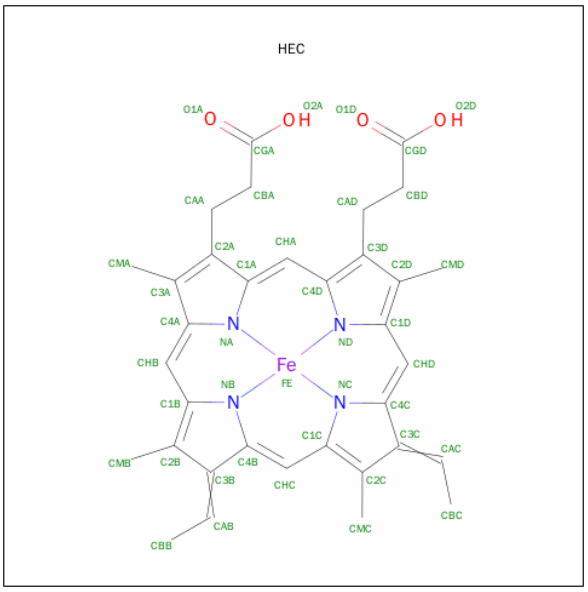
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total N 3 3	0	0
16	P	1	Total N 3 3	0	0

- Molecule 17 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



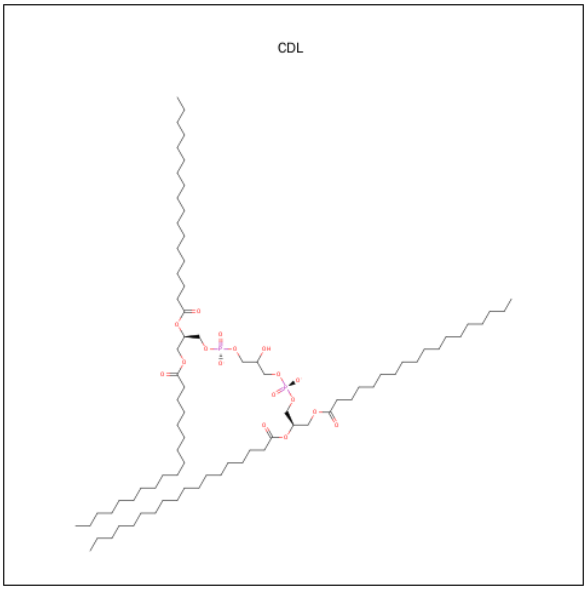
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	C	1	Total C O 12 10 2	0	0
17	D	1	Total C O 20 14 6	0	0
17	D	1	Total C O 20 14 6	0	0
17	P	1	Total C O 19 13 6	0	0
17	Q	1	Total C O 20 14 6	0	0
17	Q	1	Total C O 20 14 6	0	0

- Molecule 18 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

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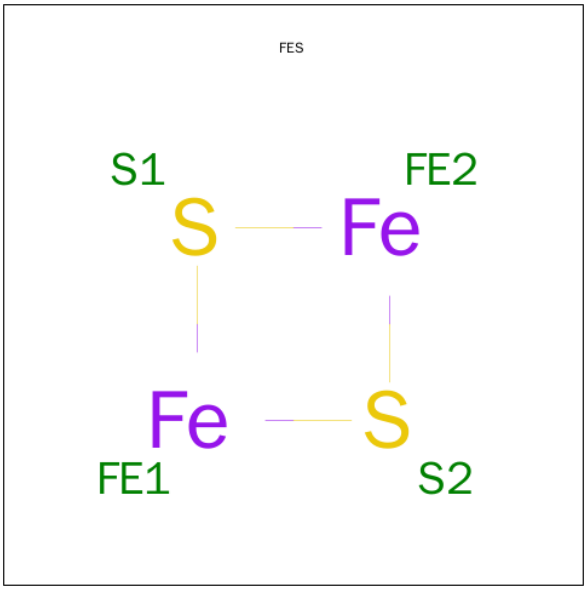
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	Q	1	Total C O P 42 23 17 2	0	0
19	T	1	Total C O P 40 21 17 2	0	0

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 21 is water.

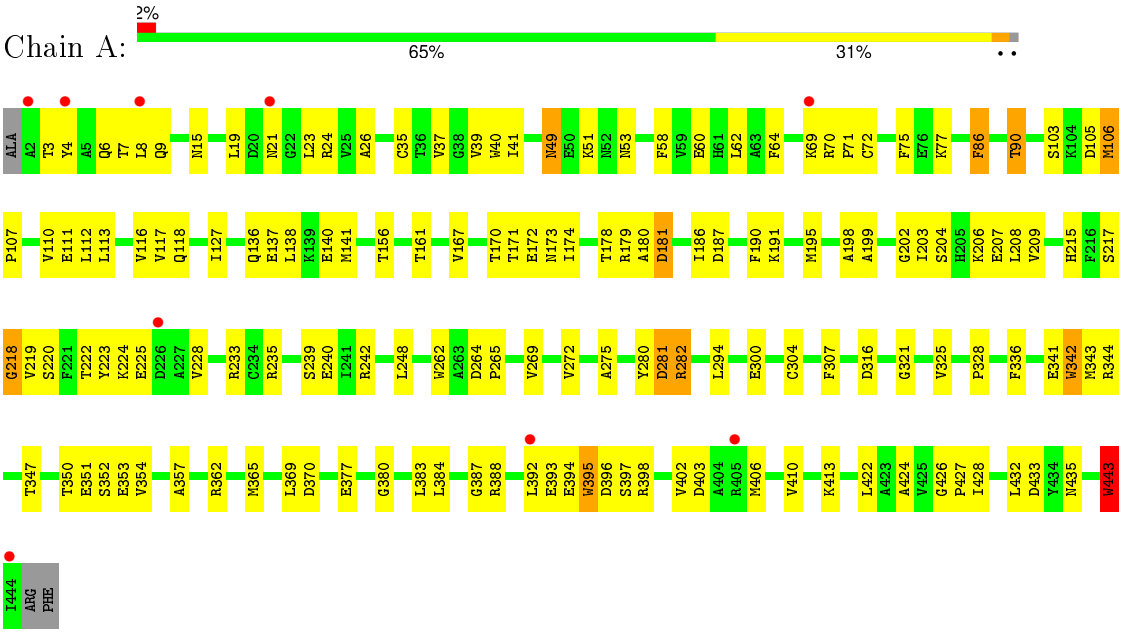
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	2	Total O 2 2	0	0
21	C	9	Total O 9 9	0	0
21	E	3	Total O 3 3	0	0
21	P	10	Total O 10 10	0	0
21	R	4	Total O 4 4	0	0

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.

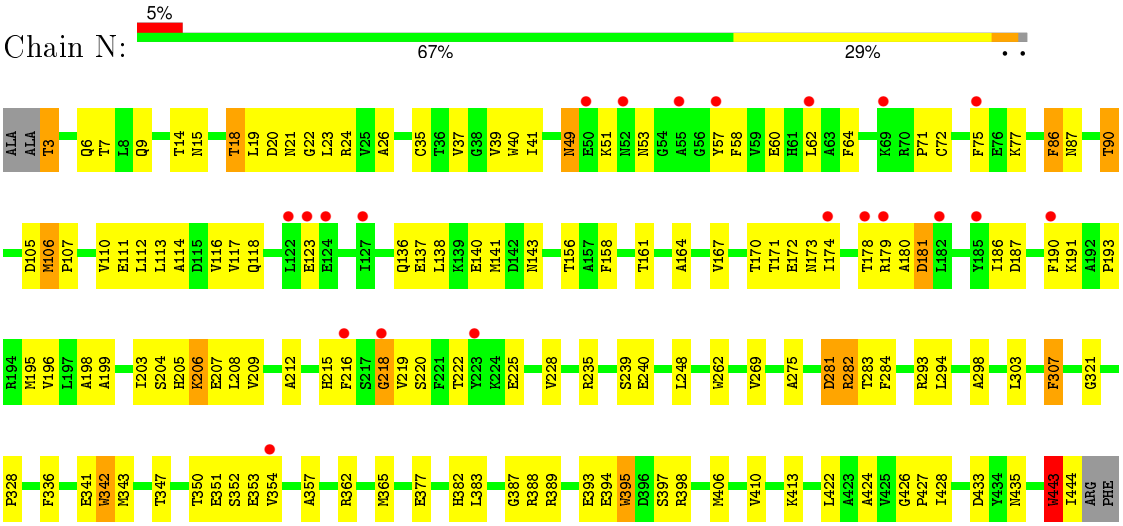
• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

Chain A:



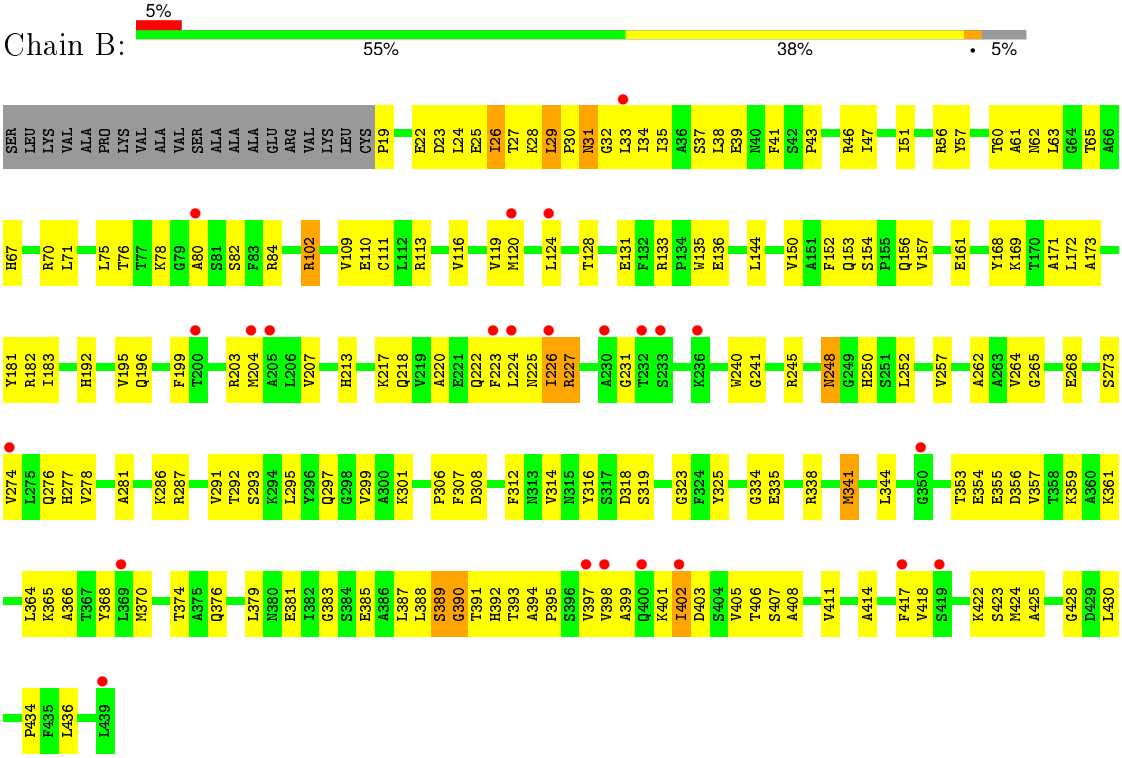
• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

Chain N:



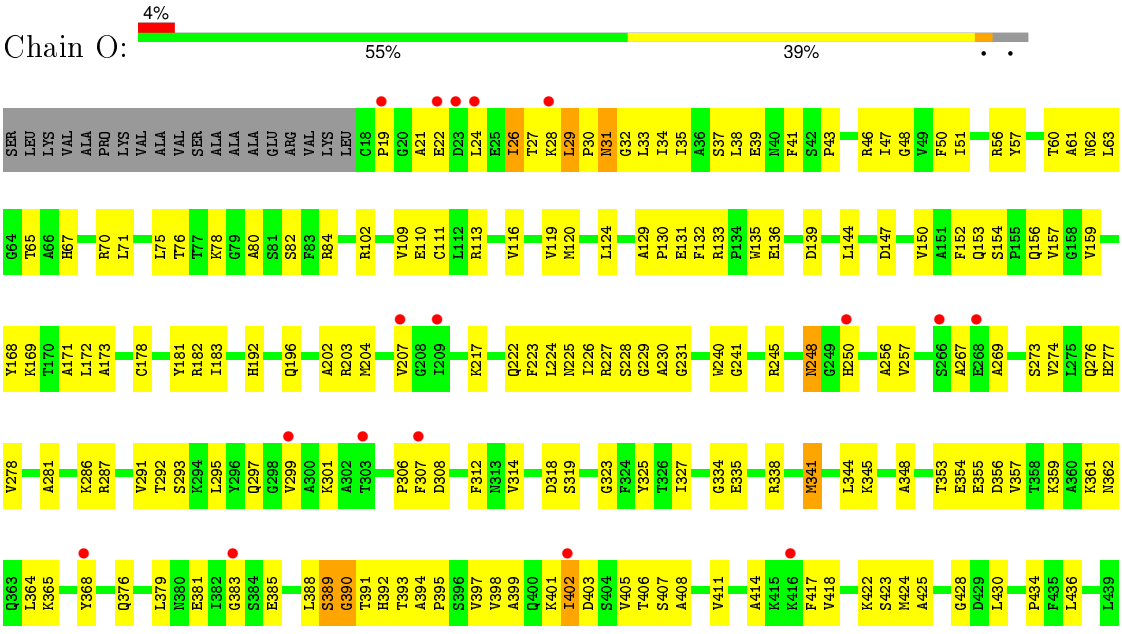
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

Chain B:



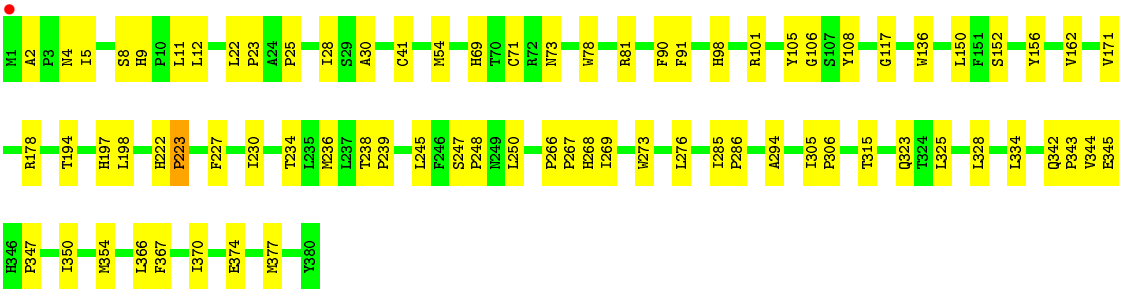
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

Chain O:

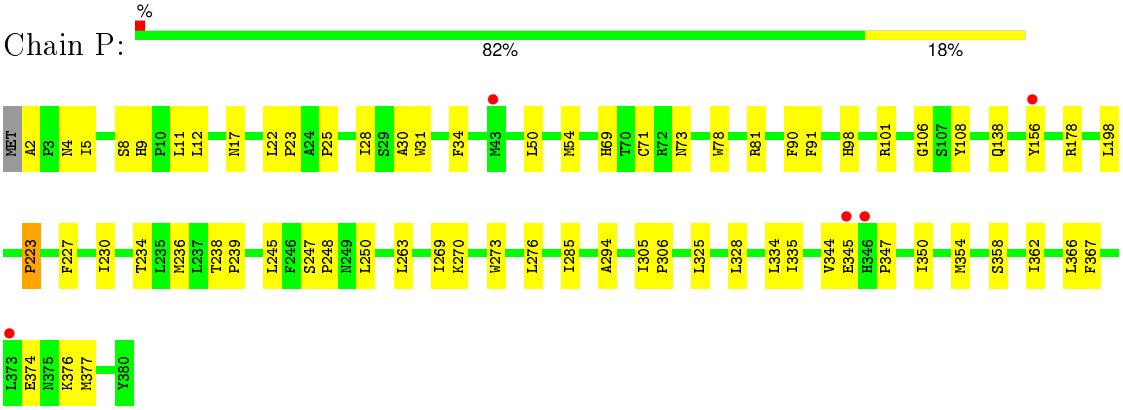


• Molecule 3: CYTOCHROME B

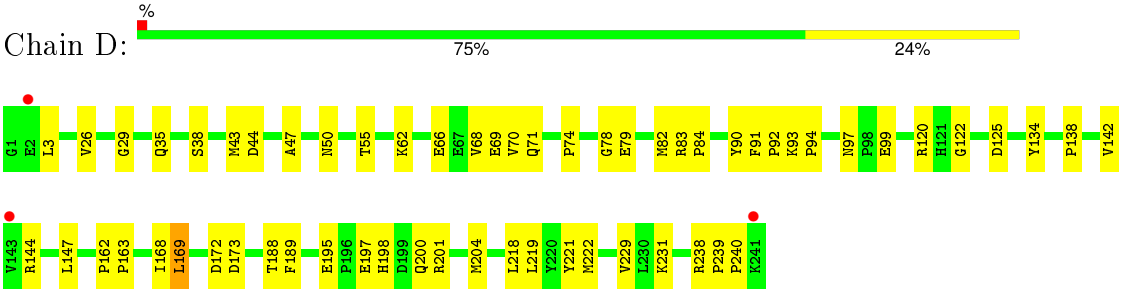
Chain C:



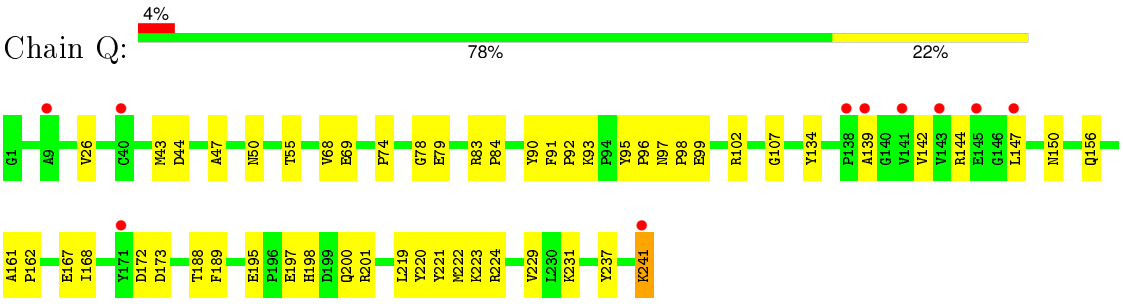
• Molecule 3: CYTOCHROME B



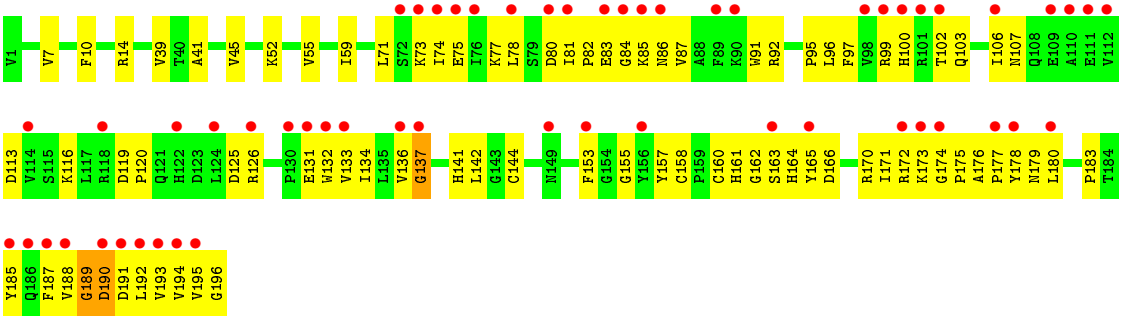
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN



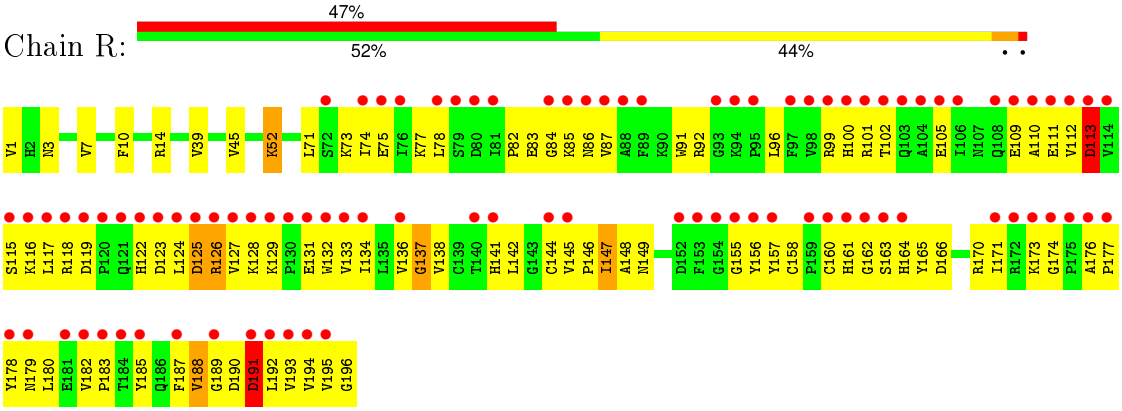
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN



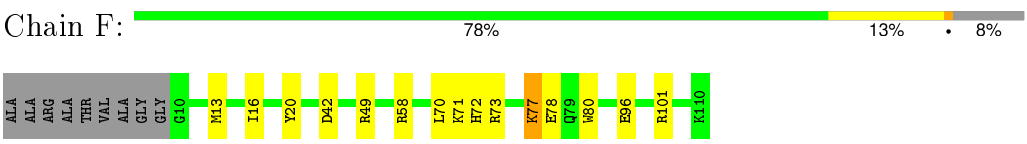
• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL



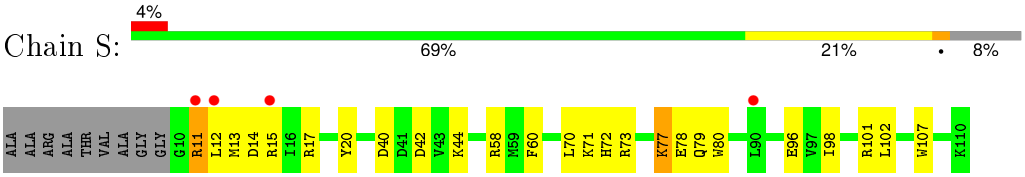
• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL



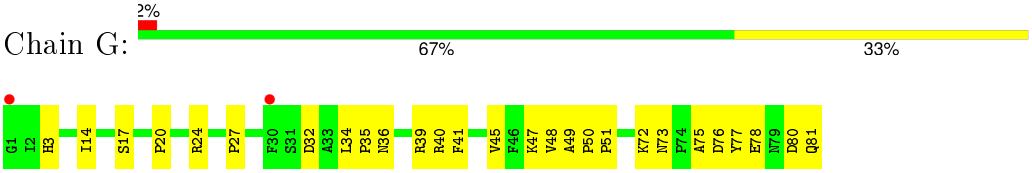
• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN



• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

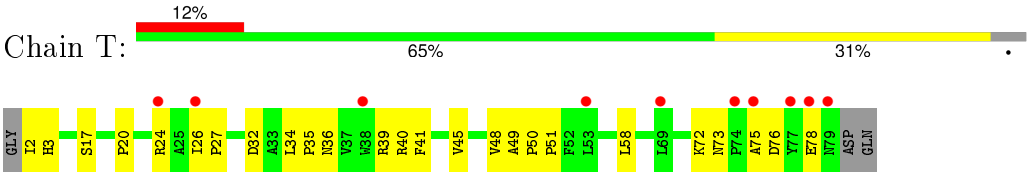


• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C



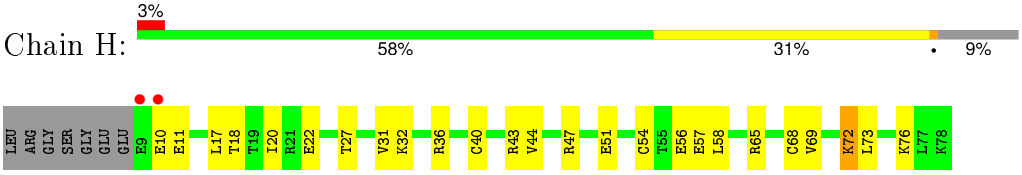
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain T:



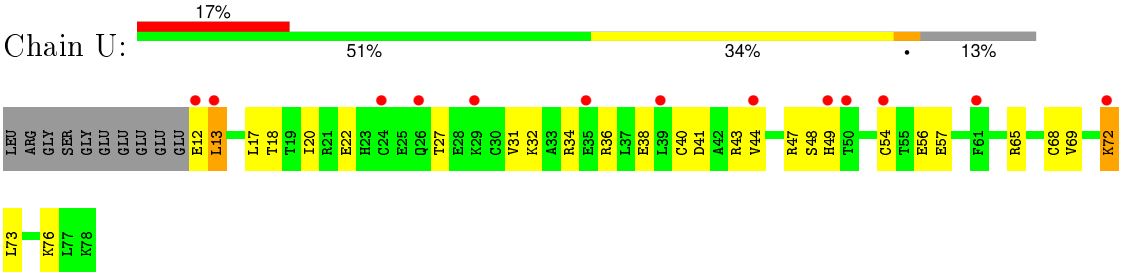
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain H:



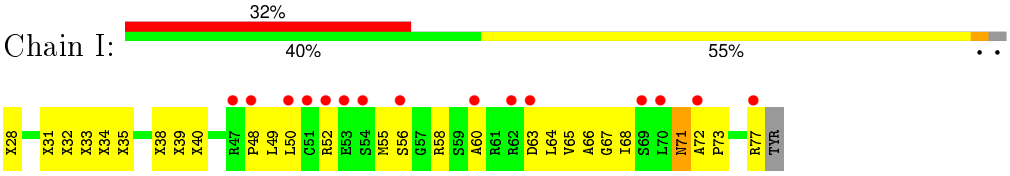
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain U:



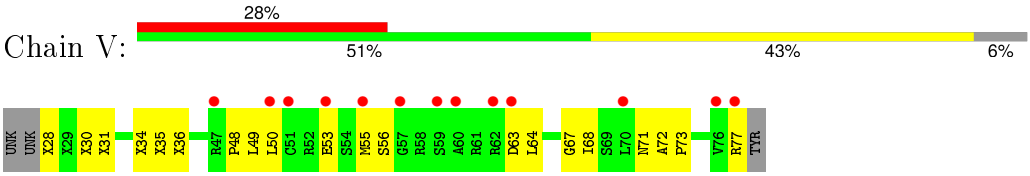
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain I:



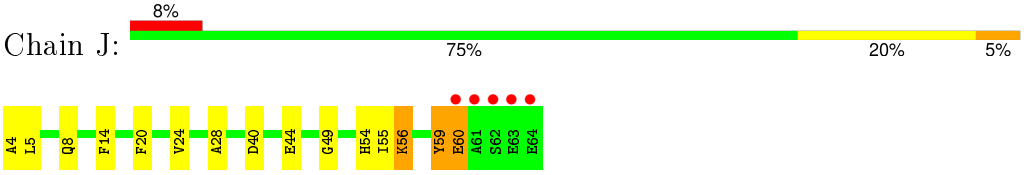
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain V:

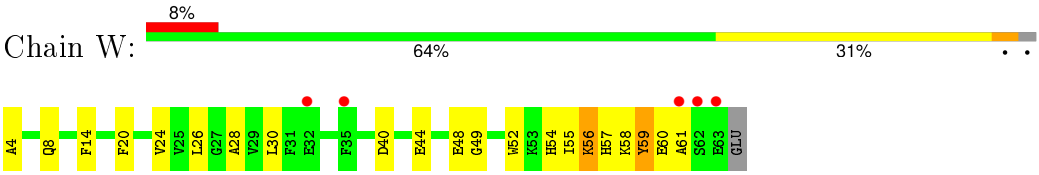


• Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN

Chain J:



• Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	172.28Å 182.14Å 241.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.78 – 2.79 58.78 – 2.79	Depositor EDS
% Data completeness (in resolution range)	97.6 (58.78-2.79) 97.3 (58.78-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.248 , 0.275 0.243 , 0.269	Depositor DCC
R_{free} test set	3610 reflections (2.00%)	DCC
Wilson B-factor (Å^2)	64.6	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 183994 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	32691	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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: AZI, CDL, UQ, FES, HEC, PEE, FNM, UNL, 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	0.43	0/3511	0.63	0/4757
1	N	0.42	0/3508	0.63	0/4753
2	B	0.37	0/3196	0.60	0/4334
2	O	0.38	0/3202	0.62	1/4343 (0.0%)
3	C	0.52	0/3119	0.65	0/4270
3	P	0.46	0/3114	0.63	0/4263
4	D	0.47	0/1956	0.63	0/2658
4	Q	0.39	0/1956	0.60	0/2658
5	E	0.37	0/1547	0.59	0/2103
5	R	0.35	0/1545	0.57	0/2098
6	F	0.51	0/911	0.65	0/1219
6	S	0.42	0/911	0.61	0/1219
7	G	0.49	0/698	0.66	0/946
7	T	0.44	0/676	0.65	0/918
8	H	0.43	0/582	0.59	0/779
8	U	0.31	0/561	0.55	0/751
9	I	0.36	0/218	0.61	0/293
9	V	0.36	0/218	0.58	0/293
10	J	0.43	0/508	0.59	0/682
10	W	0.42	0/490	0.57	0/660
All	All	0.43	0/32427	0.62	1/43997 (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})
2	O	227	ARG	N-CA-C	5.48	125.81	111.00

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	3440	0	3353	135	0
1	N	3437	0	3349	137	0
2	B	3141	0	3142	187	0
2	O	3147	0	3146	178	0
3	C	3017	0	3063	69	0
3	P	3012	0	3058	60	0
4	D	1898	0	1846	48	0
4	Q	1898	0	1846	47	0
5	E	1513	0	1478	67	0
5	R	1512	0	1476	95	0
6	F	891	0	893	15	0
6	S	891	0	893	22	0
7	G	676	0	659	26	0
7	T	654	0	641	24	0
8	H	574	0	548	17	0
8	U	553	0	535	23	0
9	I	288	0	254	42	0
9	V	278	0	252	31	0
10	J	497	0	490	11	0
10	W	479	0	478	14	0
11	A	21	0	13	1	0
11	C	98	0	147	0	0
11	N	5	0	0	0	0
11	P	98	0	147	1	0
12	A	1	0	0	0	0
12	C	5	0	0	0	0
12	D	2	0	0	0	0
12	P	7	0	0	0	0
12	R	1	0	0	0	0
13	C	86	0	60	5	0
13	P	86	0	60	5	0
14	C	22	0	17	2	0
14	P	22	0	17	1	0
15	C	19	0	17	4	0
15	P	19	0	17	3	0
16	C	3	0	0	0	0
16	P	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	C	12	0	18	0	0
17	D	40	0	56	2	0
17	P	19	0	24	1	0
17	Q	40	0	56	1	0
18	D	43	0	30	3	0
18	Q	43	0	30	1	0
19	D	42	0	28	2	0
19	G	40	0	24	1	0
19	Q	42	0	28	3	0
19	T	40	0	24	1	0
20	E	4	0	0	1	0
20	R	4	0	0	2	0
21	A	2	0	0	0	0
21	C	9	0	0	1	0
21	E	3	0	0	0	0
21	P	10	0	0	1	0
21	R	4	0	0	0	0
All	All	32691	0	32213	1132	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 17.

All (1132) 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)
2:O:353:THR:HG22	2:O:355:GLU:H	1.16	1.11
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.33	1.07
2:B:353:THR:HG22	2:B:355:GLU:H	1.20	1.06
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.38	1.03
1:N:178:THR:HG22	1:N:180:ALA:H	1.22	1.02
7:T:72:LYS:HG2	8:U:56:GLU:OE2	1.62	1.00
1:A:343:MET:O	1:A:347:THR:HG22	1.62	1.00
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.08	0.99
1:A:178:THR:HG22	1:A:180:ALA:H	1.24	0.99
1:N:343:MET:O	1:N:347:THR:HG22	1.63	0.98
2:B:76:THR:HG22	2:B:82:SER:H	1.25	0.97
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.47	0.95
4:D:47:ALA:H	4:D:50:ASN:HD22	1.11	0.95
8:U:20:ILE:HD11	8:U:76:LYS:HD2	1.49	0.94
1:N:206:LYS:H	1:N:206:LYS:HD2	1.32	0.94
1:A:344:ARG:HB2	1:A:344:ARG:NH1	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:23:PRO:HG2	7:G:3:HIS:HB2	1.49	0.93
8:H:20:ILE:HD11	8:H:76:LYS:HD2	1.49	0.91
1:N:206:LYS:H	1:N:206:LYS:CD	1.84	0.91
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.56	0.88
1:A:178:THR:HB	1:A:181:ASP:OD1	1.74	0.87
9:I:71:ASN:HD22	9:I:71:ASN:H	1.19	0.87
3:P:23:PRO:HG2	7:T:3:HIS:HB2	1.55	0.87
1:N:178:THR:HB	1:N:181:ASP:OD1	1.75	0.85
2:B:27:THR:HG22	2:B:28:LYS:H	1.39	0.85
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.74	0.85
9:I:32:UNK:N	9:I:73:PRO:HG2	1.93	0.83
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.44	0.83
9:I:64:LEU:HD12	9:I:77:ARG:O	1.78	0.83
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.59	0.83
1:N:282:ARG:HH21	9:V:36:UNK:CB	1.91	0.82
4:D:47:ALA:H	4:D:50:ASN:ND2	1.76	0.82
5:R:85:LYS:HE2	5:R:87:VAL:HG22	1.62	0.82
5:R:101:ARG:HH22	5:R:127:VAL:HG11	1.45	0.81
2:O:76:THR:HG22	2:O:82:SER:H	1.43	0.81
1:A:344:ARG:HB2	1:A:344:ARG:HH11	1.44	0.81
5:E:134:ILE:HB	5:E:185:TYR:CE2	2.15	0.81
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.61	0.81
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.45	0.80
5:E:85:LYS:HE2	5:E:87:VAL:HG22	1.64	0.80
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.64	0.80
5:R:188:VAL:HG11	5:R:192:LEU:HD12	1.62	0.80
1:N:22:GLY:O	1:N:193:PRO:HA	1.82	0.80
1:N:205:HIS:HB3	1:N:206:LYS:NZ	1.97	0.80
9:I:71:ASN:N	9:I:71:ASN:HD22	1.79	0.79
2:B:153:GLN:HE22	9:I:34:UNK:CG	1.95	0.79
2:B:153:GLN:NE2	9:I:34:UNK:CG	2.45	0.79
2:O:27:THR:HG22	2:O:28:LYS:H	1.46	0.79
1:N:204:SER:HB3	1:N:207:GLU:HB2	1.63	0.78
2:B:153:GLN:HE22	9:I:34:UNK:HG2	1.48	0.78
1:A:281:ASP:CG	9:I:33:UNK:HB1	2.03	0.78
2:O:192:HIS:O	2:O:196:GLN:HG3	1.83	0.78
1:A:204:SER:HB3	1:A:207:GLU:HB2	1.64	0.77
2:O:62:ASN:O	2:O:65:THR:HG22	1.83	0.77
2:B:22:GLU:HG2	2:B:39:GLU:HB3	1.66	0.77
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.20	0.76
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.02	0.76
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.67	0.76
1:N:49:ASN:HD22	1:N:51:LYS:H	1.32	0.76
9:I:49:LEU:HD13	9:I:55:MET:HG2	1.66	0.76
1:N:362:ARG:O	1:N:365:MET:HG2	1.86	0.75
3:P:238:THR:HB	3:P:239:PRO:HD3	1.69	0.75
1:N:143:ASN:HD22	9:V:48:PRO:HD2	1.53	0.74
10:W:40:ASP:O	10:W:44:GLU:HG3	1.87	0.74
3:C:30:ALA:HB1	19:D:2003:CDL:H111	1.69	0.74
2:B:27:THR:HG22	2:B:28:LYS:N	2.01	0.74
2:B:153:GLN:NE2	9:I:34:UNK:HG2	2.01	0.74
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.23	0.73
2:B:47:ILE:HD13	2:B:120:MET:CE	2.18	0.73
2:B:154:SER:O	2:B:157:VAL:HG12	1.88	0.73
2:B:62:ASN:O	2:B:65:THR:HG22	1.88	0.73
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.06	0.73
2:B:76:THR:HG22	2:B:82:SER:N	2.03	0.73
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.18	0.73
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.18	0.73
3:P:247:SER:OG	3:P:250:LEU:HB2	1.89	0.72
2:B:227:ARG:NE	2:B:227:ARG:HA	2.04	0.72
1:N:49:ASN:ND2	1:N:51:LYS:H	1.86	0.72
1:A:362:ARG:O	1:A:365:MET:HG2	1.89	0.72
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.04	0.72
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.71	0.72
7:T:73:ASN:HB3	7:T:76:ASP:OD2	1.89	0.71
2:O:76:THR:HG22	2:O:82:SER:HB2	1.72	0.71
3:C:238:THR:HB	3:C:239:PRO:HD3	1.73	0.71
1:A:49:ASN:HD22	1:A:51:LYS:H	1.38	0.71
8:U:47:ARG:HD3	8:U:48:SER:H	1.54	0.71
2:O:297:GLN:O	2:O:301:LYS:HG3	1.91	0.71
3:P:9:HIS:HD2	3:P:12:LEU:H	1.37	0.71
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.31	0.71
10:J:40:ASP:O	10:J:44:GLU:HG3	1.90	0.70
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.26	0.70
1:A:178:THR:HG22	1:A:180:ALA:N	2.03	0.70
2:O:376:GLN:HE22	9:V:77:ARG:NH2	1.89	0.70
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.22	0.70
2:O:76:THR:HG23	2:O:136:GLU:OE1	1.91	0.70
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.55	0.70
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:CYS:SG	3:C:90:PHE:HD2	2.15	0.70
3:C:328:LEU:HD23	7:G:51:PRO:HB3	1.72	0.70
2:O:47:ILE:HD13	2:O:120:MET:CE	2.21	0.69
2:O:248:ASN:HD22	2:O:248:ASN:C	1.95	0.69
2:B:71:LEU:HD23	9:I:68:ILE:HG13	1.73	0.69
3:C:269:ILE:HD12	5:R:160:CYS:SG	2.33	0.69
5:R:101:ARG:HG2	5:R:105:GLU:OE1	1.93	0.69
3:P:30:ALA:HB1	19:Q:3003:CDL:H111	1.75	0.69
2:B:248:ASN:HD22	2:B:248:ASN:C	1.96	0.69
7:G:73:ASN:HB3	7:G:76:ASP:OD2	1.92	0.69
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.58	0.69
2:B:153:GLN:NE2	9:I:34:UNK:HG1	2.09	0.68
8:U:27:THR:O	8:U:31:VAL:HG23	1.93	0.68
10:J:55:ILE:HG22	10:J:59:TYR:HE1	1.58	0.68
10:W:55:ILE:HG22	10:W:59:TYR:HE1	1.58	0.68
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.34	0.68
1:N:187:ASP:O	1:N:191:LYS:HE3	1.94	0.68
3:P:101:ARG:C	3:P:101:ARG:HD2	2.14	0.68
3:C:9:HIS:HD2	3:C:12:LEU:H	1.41	0.68
2:O:27:THR:HG22	2:O:28:LYS:N	2.07	0.67
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.56	0.67
2:B:192:HIS:O	2:B:196:GLN:HG3	1.94	0.67
8:U:47:ARG:HG3	8:U:49:HIS:H	1.59	0.67
2:B:297:GLN:O	2:B:301:LYS:HG3	1.93	0.67
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.77	0.67
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.75	0.67
1:N:178:THR:HG22	1:N:180:ALA:N	2.03	0.67
2:B:156:GLN:HE22	9:I:77:ARG:C	1.98	0.67
1:A:350:THR:HG22	1:A:352:SER:H	1.59	0.67
1:A:398:ARG:HH11	1:A:398:ARG:HG2	1.59	0.67
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.10	0.67
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.77	0.66
5:R:129:LYS:HB3	5:R:131:GLU:OE1	1.95	0.66
1:N:206:LYS:HA	1:N:209:VAL:HG12	1.77	0.66
2:O:43:PRO:O	2:O:113:ARG:HG3	1.95	0.66
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.78	0.66
2:O:407:SER:O	2:O:411:VAL:HG23	1.95	0.66
2:O:154:SER:O	2:O:157:VAL:HG12	1.96	0.66
2:B:264:VAL:HG23	2:B:316:TYR:C	2.16	0.66
2:O:399:ALA:O	2:O:402:ILE:HG22	1.96	0.66
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:19:LEU:O	1:N:21:ASN:N	2.29	0.66
3:C:344:VAL:O	3:C:345:GLU:HG3	1.95	0.65
9:I:28:UNK:HA	9:I:72:ALA:HB2	1.77	0.65
4:Q:241:LYS:HA	4:Q:241:LYS:HE3	1.78	0.65
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.77	0.65
3:P:273:TRP:HA	3:P:276:LEU:CD1	2.26	0.65
5:E:163:SER:OG	5:E:175:PRO:HD2	1.96	0.65
5:E:73:LYS:HG2	5:E:196:GLY:HA3	1.78	0.65
2:B:381:GLU:OE1	2:B:381:GLU:HA	1.96	0.65
3:C:22:LEU:HD21	15:C:2002:UQ:HM32	1.78	0.65
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.60	0.65
9:I:31:UNK:C	9:I:73:PRO:HG2	2.27	0.65
5:R:147:ILE:HG22	5:R:148:ALA:N	2.12	0.65
5:R:10:PHE:O	5:R:14:ARG:HG3	1.96	0.64
1:A:222:THR:OG1	1:A:225:GLU:HG3	1.96	0.64
2:O:381:GLU:OE1	2:O:381:GLU:HA	1.97	0.64
2:O:31:ASN:ND2	2:O:33:LEU:H	1.94	0.64
1:N:350:THR:HG22	1:N:352:SER:H	1.61	0.64
5:R:116:LYS:HA	5:R:116:LYS:HE2	1.79	0.64
1:A:398:ARG:NH1	1:A:398:ARG:HG2	2.11	0.64
1:N:106:MET:HE1	1:N:107:PRO:HA	1.79	0.64
1:A:443:TRP:CE3	1:A:443:TRP:HA	2.32	0.64
1:N:21:ASN:HB2	1:N:218:GLY:O	1.97	0.64
2:B:27:THR:HG21	2:B:217:LYS:HE3	1.81	0.63
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.32	0.63
1:N:222:THR:OG1	1:N:225:GLU:HG3	1.98	0.63
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.63	0.63
3:P:269:ILE:HG23	14:P:3001:FNM:H23	1.81	0.63
1:A:49:ASN:ND2	1:A:51:LYS:H	1.96	0.63
1:N:26:ALA:HB2	1:N:383:LEU:HD11	1.81	0.63
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.34	0.63
3:P:273:TRP:HA	3:P:276:LEU:HD12	1.79	0.63
1:A:350:THR:HB	1:A:353:GLU:HG3	1.81	0.63
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.80	0.63
1:N:49:ASN:C	1:N:49:ASN:HD22	2.02	0.63
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.14	0.63
2:O:71:LEU:HD23	9:V:68:ILE:HG13	1.81	0.63
1:A:77:LYS:HE3	2:B:359:LYS:NZ	2.14	0.63
9:I:71:ASN:N	9:I:71:ASN:ND2	2.40	0.63
5:E:164:HIS:HB2	5:E:173:LYS:HB3	1.79	0.63
5:R:164:HIS:HB2	5:R:173:LYS:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:LYS:HD3	2:B:403:ASP:HA	1.81	0.62
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.80	0.62
1:A:187:ASP:O	1:A:191:LYS:HE3	1.98	0.62
1:N:60:GLU:OE2	1:N:90:THR:HG22	2.00	0.62
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.00	0.62
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.34	0.62
5:E:78:LEU:HD11	5:E:187:PHE:HE1	1.64	0.62
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.40	0.62
7:T:41:PHE:O	7:T:45:VAL:HG23	1.99	0.62
2:B:389:SER:O	2:B:391:THR:HG23	1.99	0.62
5:R:142:LEU:HD12	5:R:161:HIS:CE1	2.35	0.62
5:R:190:ASP:O	5:R:191:ASP:HB2	2.00	0.62
1:N:205:HIS:HB3	1:N:206:LYS:HZ1	1.65	0.62
2:B:31:ASN:ND2	2:B:33:LEU:H	1.98	0.62
2:B:113:ARG:O	2:B:116:VAL:HG23	2.00	0.61
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.65	0.61
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.81	0.61
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.30	0.61
7:G:41:PHE:O	7:G:45:VAL:HG23	2.00	0.61
5:E:171:ILE:HG12	5:E:176:ALA:O	2.00	0.61
1:N:77:LYS:HE3	2:O:359:LYS:NZ	2.15	0.61
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.36	0.61
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.66	0.61
5:R:82:PRO:HD2	5:R:85:LYS:CD	2.30	0.61
1:A:443:TRP:HE3	1:A:443:TRP:HA	1.63	0.61
1:N:114:ALA:HB2	1:N:216:PHE:CE1	2.35	0.61
2:O:388:LEU:O	2:O:389:SER:HB3	1.99	0.61
1:A:60:GLU:OE2	1:A:90:THR:HG22	2.00	0.61
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.82	0.61
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.81	0.61
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.35	0.61
8:H:27:THR:O	8:H:31:VAL:HG23	2.01	0.60
3:P:347:PRO:O	3:P:350:ILE:HG22	2.01	0.60
9:V:34:UNK:N	9:V:35:UNK:N	2.48	0.60
8:H:40:CYS:O	8:H:44:VAL:HG23	2.02	0.60
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.16	0.60
2:B:38:LEU:HD12	2:B:39:GLU:N	2.17	0.60
2:B:157:VAL:CG2	9:I:64:LEU:HD21	2.24	0.60
4:D:47:ALA:N	4:D:50:ASN:HD22	1.92	0.60
5:R:188:VAL:HB	5:R:192:LEU:HB2	1.82	0.60
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:LEU:O	2:B:389:SER:HB3	2.02	0.60
1:A:7:THR:HG21	2:B:113:ARG:CD	2.31	0.60
3:P:22:LEU:HD21	15:P:3002:UQ:HM32	1.84	0.60
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.32	0.60
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.82	0.60
2:O:124:LEU:HD21	2:O:223:PHE:HB3	1.82	0.60
2:O:33:LEU:HD21	2:O:224:LEU:HD12	1.84	0.59
1:A:248:LEU:HD12	1:A:426:GLY:HA2	1.83	0.59
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.85	0.59
1:A:106:MET:HE1	1:A:107:PRO:HA	1.85	0.59
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.83	0.59
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.70	0.59
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.44	0.59
2:O:56:ARG:HG3	2:O:56:ARG:NH1	2.17	0.59
3:C:227:PHE:HE1	4:D:222:MET:HE2	1.68	0.59
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.38	0.59
4:Q:241:LYS:HG3	4:Q:241:LYS:OXT	2.03	0.59
2:B:399:ALA:O	2:B:402:ILE:HG22	2.03	0.59
5:R:164:HIS:CD2	5:R:173:LYS:HD3	2.38	0.59
2:B:226:ILE:O	2:B:226:ILE:HG23	2.02	0.59
9:V:31:UNK:C	9:V:73:PRO:HG2	2.32	0.59
2:O:353:THR:HG22	2:O:354:GLU:N	2.18	0.59
2:O:38:LEU:HD12	2:O:39:GLU:N	2.17	0.59
1:A:170:THR:HG22	1:A:171:THR:N	2.18	0.59
2:O:335:GLU:HA	2:O:338:ARG:HH12	1.68	0.59
2:O:385:GLU:OE1	2:O:392:HIS:HA	2.02	0.59
3:C:269:ILE:HG23	14:C:2001:FNM:H23	1.83	0.59
2:O:306:PRO:HG2	9:V:50:LEU:O	2.03	0.59
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.91	0.58
2:B:43:PRO:O	2:B:113:ARG:HG3	2.03	0.58
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.85	0.58
5:R:82:PRO:HG2	5:R:85:LYS:HB2	1.85	0.58
1:N:350:THR:HB	1:N:353:GLU:HG3	1.85	0.58
3:C:41:CYS:SG	3:C:90:PHE:CD2	2.96	0.58
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.33	0.58
2:O:353:THR:HG22	2:O:355:GLU:N	2.01	0.58
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.44	0.58
1:N:205:HIS:HB3	1:N:206:LYS:HZ2	1.68	0.58
5:E:160:CYS:SG	3:P:269:ILE:HD12	2.44	0.58
9:V:30:UNK:HG3	9:V:31:UNK:N	2.18	0.58
7:G:72:LYS:HG2	8:H:56:GLU:OE2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:328:LEU:HD23	7:T:51:PRO:HB3	1.86	0.58
5:R:122:HIS:O	5:R:125:ASP:HB2	2.04	0.58
3:C:273:TRP:HA	3:C:276:LEU:CD1	2.34	0.58
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.85	0.58
2:O:402:ILE:HD13	2:O:402:ILE:C	2.24	0.58
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.86	0.58
5:R:82:PRO:HD2	5:R:85:LYS:HD2	1.86	0.58
1:N:383:LEU:O	1:N:387:GLY:HA2	2.03	0.58
4:D:200:GLN:NE2	17:D:2091:BOG:H5	2.19	0.58
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.39	0.58
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.37	0.57
10:W:55:ILE:CG2	10:W:59:TYR:HE1	2.16	0.57
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.33	0.57
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.03	0.57
5:E:77:LYS:HE2	5:E:80:ASP:OD2	2.04	0.57
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.37	0.57
2:B:353:THR:HG22	2:B:354:GLU:N	2.18	0.57
10:J:55:ILE:CG2	10:J:59:TYR:HE1	2.17	0.57
7:T:72:LYS:HG2	8:U:56:GLU:CD	2.24	0.57
1:N:140:GLU:HG3	9:V:50:LEU:HD12	1.86	0.57
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.37	0.57
2:O:157:VAL:CG2	9:V:64:LEU:HD21	2.28	0.57
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.39	0.57
6:S:11:ARG:O	6:S:15:ARG:HG3	2.05	0.57
1:N:206:LYS:N	1:N:206:LYS:HD2	2.13	0.57
3:C:245:LEU:O	4:D:201:ARG:HD2	2.04	0.57
5:E:103:GLN:O	5:E:107:ASN:ND2	2.37	0.57
2:O:338:ARG:HB2	2:O:338:ARG:HH11	1.70	0.57
2:B:292:THR:O	2:B:292:THR:HG22	2.05	0.57
2:B:56:ARG:NH1	2:B:56:ARG:HG3	2.18	0.57
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.87	0.57
2:B:414:ALA:O	2:B:418:VAL:HG23	2.05	0.57
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.87	0.57
2:B:407:SER:O	2:B:411:VAL:HG23	2.05	0.57
3:C:247:SER:OG	3:C:250:LEU:HB2	2.05	0.57
5:E:99:ARG:HB3	5:E:133:VAL:HG13	1.87	0.56
1:A:49:ASN:C	1:A:49:ASN:HD22	2.08	0.56
10:W:4:ALA:O	10:W:8:GLN:HG3	2.05	0.56
2:B:385:GLU:OE1	2:B:392:HIS:HA	2.04	0.56
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.87	0.56
1:N:161:THR:HG21	1:N:235:ARG:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.87	0.56
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.32	0.56
1:A:219:VAL:HG12	1:A:220:SER:N	2.20	0.56
2:B:402:ILE:HD13	2:B:402:ILE:C	2.26	0.56
5:R:126:ARG:HB3	5:R:182:VAL:HG21	1.88	0.56
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.70	0.56
3:C:71:CYS:SG	3:C:81:ARG:HD2	2.45	0.56
2:O:389:SER:O	2:O:391:THR:HG23	2.05	0.56
1:A:15:ASN:O	1:A:26:ALA:HA	2.05	0.56
4:Q:47:ALA:HA	4:Q:90:TYR:HA	1.87	0.56
2:B:341:MET:CE	2:B:417:PHE:HE2	2.17	0.56
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.88	0.56
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.41	0.56
2:O:414:ALA:O	2:O:418:VAL:HG23	2.06	0.56
2:B:76:THR:HG22	2:B:82:SER:HB2	1.88	0.56
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.87	0.56
1:N:347:THR:HG21	1:N:444:ILE:C	2.26	0.56
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.40	0.56
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.71	0.56
1:N:170:THR:HG22	1:N:171:THR:N	2.21	0.56
5:R:99:ARG:HB3	5:R:133:VAL:HG13	1.88	0.55
19:D:2003:CDL:OB3	6:F:73:ARG:NH2	2.39	0.55
3:C:28:ILE:HD11	15:C:2002:UQ:HM21	1.88	0.55
1:A:26:ALA:HB2	1:A:383:LEU:HD11	1.87	0.55
2:O:308:ASP:OD2	9:V:56:SER:HA	2.05	0.55
1:A:350:THR:HG22	1:A:351:GLU:N	2.21	0.55
2:B:27:THR:CG2	2:B:28:LYS:H	2.14	0.55
2:O:341:MET:CE	2:O:417:PHE:HE2	2.17	0.55
2:O:76:THR:CG2	2:O:136:GLU:OE1	2.54	0.55
7:T:48:VAL:O	7:T:51:PRO:HD2	2.05	0.55
2:B:338:ARG:HB2	2:B:338:ARG:HH11	1.72	0.55
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.89	0.55
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.42	0.55
2:B:124:LEU:HD21	2:B:223:PHE:HB3	1.88	0.55
9:I:38:UNK:O	9:I:39:UNK:C	2.55	0.55
5:E:85:LYS:HG2	5:E:86:ASN:N	2.22	0.55
5:R:131:GLU:CD	5:R:131:GLU:H	2.10	0.55
2:B:46:ARG:HH21	2:B:376:GLN:HG3	1.72	0.55
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.41	0.55
5:R:52:LYS:HD3	5:R:52:LYS:C	2.27	0.55
5:R:85:LYS:HG2	5:R:86:ASN:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.21	0.55
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.42	0.55
18:D:501:HEC:HMC1	18:D:501:HEC:HBC3	1.89	0.55
5:R:74:ILE:HD11	5:R:96:LEU:HD23	1.88	0.55
3:P:270:LYS:O	3:P:270:LYS:HG3	2.07	0.55
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.71	0.55
1:N:15:ASN:O	1:N:26:ALA:HA	2.07	0.55
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.37	0.55
1:N:248:LEU:HD12	1:N:426:GLY:HA2	1.88	0.55
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.89	0.55
1:N:106:MET:HE2	1:N:110:VAL:CG2	2.36	0.55
2:O:150:VAL:O	2:O:153:GLN:HG3	2.07	0.55
1:A:4:TYR:HE2	1:A:396:ASP:OD2	1.90	0.55
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.42	0.55
3:C:101:ARG:C	3:C:101:ARG:HD2	2.26	0.55
5:R:128:LYS:O	5:R:129:LYS:HG3	2.07	0.55
1:N:350:THR:HG22	1:N:351:GLU:N	2.22	0.55
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.42	0.55
1:A:106:MET:N	1:A:107:PRO:HD2	2.22	0.54
7:G:48:VAL:O	7:G:51:PRO:HD2	2.07	0.54
5:R:126:ARG:H	5:R:126:ARG:HD3	1.72	0.54
1:N:398:ARG:HG2	1:N:398:ARG:HH11	1.72	0.54
1:N:191:LYS:C	1:N:195:MET:HE2	2.28	0.54
2:B:368:TYR:HE1	2:B:381:GLU:OE2	1.90	0.54
5:R:137:GLY:O	5:R:145:VAL:HG22	2.07	0.54
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.08	0.54
2:O:368:TYR:HE1	2:O:381:GLU:OE2	1.91	0.54
5:R:122:HIS:HB3	5:R:125:ASP:OD1	2.08	0.54
3:C:377:MET:HE1	6:F:20:TYR:CD1	2.43	0.54
2:O:292:THR:HG22	2:O:292:THR:O	2.08	0.54
5:E:119:ASP:OD2	5:E:179:ASN:ND2	2.40	0.54
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.90	0.54
3:C:285:ILE:HD12	3:C:294:ALA:HB2	1.89	0.54
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.23	0.54
9:I:71:ASN:H	9:I:71:ASN:ND2	1.94	0.54
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.37	0.54
1:N:398:ARG:HG2	1:N:398:ARG:NH1	2.22	0.54
8:U:47:ARG:CD	8:U:48:SER:H	2.21	0.54
2:B:335:GLU:HA	2:B:338:ARG:HH12	1.72	0.54
3:P:230:ILE:HG22	4:Q:219:LEU:HD13	1.89	0.54
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:33:LEU:CD2	2:O:224:LEU:HD12	2.36	0.54
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.90	0.54
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.37	0.54
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.43	0.54
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.54	0.54
2:B:34:ILE:HD13	2:B:390:GLY:CA	2.38	0.54
1:A:239:SER:HB2	7:G:17:SER:O	2.08	0.54
4:Q:195:GLU:HG3	4:Q:198:HIS:HB2	1.89	0.54
3:P:227:PHE:HE1	4:Q:222:MET:HE2	1.73	0.54
5:E:177:PRO:HB2	5:E:178:TYR:CD1	2.43	0.54
2:O:46:ARG:HD2	2:O:110:GLU:CD	2.28	0.54
2:B:150:VAL:O	2:B:153:GLN:HG3	2.08	0.54
2:B:156:GLN:NE2	9:I:77:ARG:C	2.60	0.53
2:B:227:ARG:HE	2:B:227:ARG:HA	1.72	0.53
1:A:395:TRP:CE3	1:A:395:TRP:HA	2.43	0.53
3:P:9:HIS:CD2	3:P:11:LEU:H	2.26	0.53
1:N:106:MET:N	1:N:107:PRO:HD2	2.23	0.53
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.42	0.53
5:R:115:SER:O	5:R:116:LYS:HG2	2.08	0.53
2:O:248:ASN:ND2	2:O:250:HIS:H	2.06	0.53
3:C:78:TRP:CD2	4:D:197:GLU:HG3	2.44	0.53
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.89	0.53
5:R:134:ILE:HD11	5:R:193:VAL:HG21	1.89	0.53
5:E:165:TYR:HA	5:E:170:ARG:O	2.08	0.53
2:B:46:ARG:HH11	2:B:110:GLU:HG3	1.73	0.53
8:U:12:GLU:O	8:U:13:LEU:HB2	2.08	0.53
1:N:53:ASN:H	1:N:173:ASN:ND2	2.07	0.53
2:O:46:ARG:HH11	2:O:110:GLU:HG3	1.72	0.53
1:N:106:MET:HE2	1:N:110:VAL:HG23	1.89	0.53
3:P:198:LEU:HD13	15:P:3002:UQ:HM53	1.91	0.53
1:N:90:THR:O	1:N:167:VAL:HG11	2.09	0.53
2:O:353:THR:HB	2:O:356:ASP:CG	2.29	0.53
2:O:76:THR:HG22	2:O:82:SER:CB	2.38	0.53
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.91	0.53
19:Q:3003:CDL:OB3	6:S:73:ARG:NH2	2.42	0.53
3:C:273:TRP:HA	3:C:276:LEU:HD12	1.90	0.53
8:U:40:CYS:O	8:U:44:VAL:HG23	2.07	0.53
1:A:383:LEU:O	1:A:387:GLY:HA2	2.09	0.52
2:B:306:PRO:HA	9:I:52:ARG:CG	2.38	0.52
3:P:376:LYS:O	6:S:17:ARG:NH1	2.40	0.52
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:MET:HE2	1:A:110:VAL:HG23	1.90	0.52
1:A:170:THR:HG22	1:A:172:GLU:H	1.73	0.52
3:C:28:ILE:CD1	15:C:2002:UQ:HM21	2.39	0.52
2:B:128:THR:HG21	2:B:224:LEU:HD23	1.92	0.52
2:O:46:ARG:HD2	2:O:110:GLU:OE2	2.09	0.52
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.90	0.52
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.38	0.52
2:O:31:ASN:HD22	2:O:32:GLY:N	2.07	0.52
5:R:190:ASP:O	5:R:191:ASP:CB	2.58	0.52
1:N:170:THR:HG22	1:N:172:GLU:H	1.74	0.52
8:H:65:ARG:O	8:H:69:VAL:HG23	2.10	0.52
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.39	0.52
2:B:78:LYS:HA	2:B:131:GLU:OE2	2.09	0.52
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.91	0.52
2:B:286:LYS:HE2	2:B:287:ARG:HH12	1.74	0.52
3:P:223:PRO:HB2	3:P:227:PHE:CD2	2.44	0.52
1:N:112:LEU:O	1:N:116:VAL:HG23	2.09	0.52
3:C:347:PRO:O	3:C:350:ILE:HG22	2.09	0.52
9:I:49:LEU:O	9:I:50:LEU:HD23	2.10	0.52
3:C:150:LEU:HD23	5:R:142:LEU:HD21	1.92	0.52
11:A:2008:PEE:H13	3:C:222:HIS:HE1	1.73	0.52
5:E:113:ASP:OD1	5:E:116:LYS:HG2	2.10	0.52
5:R:91:TRP:CE2	5:R:92:ARG:HG3	2.44	0.52
1:A:344:ARG:HH11	1:A:344:ARG:CB	2.17	0.52
9:I:64:LEU:HA	9:I:77:ARG:O	2.10	0.52
5:E:83:GLU:HG2	5:E:102:THR:HA	1.92	0.52
4:Q:97:ASN:OD1	4:Q:99:GLU:HB2	2.10	0.52
2:B:353:THR:HB	2:B:356:ASP:CG	2.30	0.52
2:O:203:ARG:HD2	2:O:230:ALA:O	2.10	0.52
2:O:273:SER:O	2:O:276:GLN:HB3	2.10	0.52
4:Q:231:LYS:O	6:S:71:LYS:HE3	2.10	0.52
2:B:264:VAL:HG23	2:B:316:TYR:O	2.10	0.52
1:N:136:GLN:OE1	9:V:50:LEU:HB3	2.10	0.52
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.92	0.52
1:N:206:LYS:CE	1:N:206:LYS:H	2.23	0.51
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.74	0.51
2:B:46:ARG:HD2	2:B:110:GLU:OE2	2.10	0.51
2:O:335:GLU:HA	2:O:338:ARG:NH1	2.24	0.51
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.45	0.51
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.92	0.51
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:387:GLY:O	1:N:388:ARG:HB3	2.09	0.51
3:C:223:PRO:HB2	3:C:227:PHE:CD2	2.46	0.51
2:B:307:PHE:CD1	2:B:308:ASP:N	2.79	0.51
2:B:318:ASP:O	2:B:319:SER:HB2	2.09	0.51
3:P:344:VAL:O	3:P:345:GLU:HG3	2.09	0.51
1:A:106:MET:HE2	1:A:110:VAL:CG2	2.40	0.51
3:C:9:HIS:CD2	3:C:11:LEU:H	2.28	0.51
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.46	0.51
8:H:43:ARG:O	8:H:47:ARG:HG3	2.10	0.51
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.78	0.51
1:A:344:ARG:HB2	1:A:344:ARG:CZ	2.40	0.51
2:B:25:GLU:HB2	2:B:213:HIS:CG	2.45	0.51
8:U:65:ARG:O	8:U:68:CYS:HB3	2.09	0.51
2:B:248:ASN:ND2	2:B:250:HIS:H	2.08	0.51
5:E:74:ILE:HD11	5:E:96:LEU:HD23	1.92	0.51
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.41	0.51
1:A:106:MET:HG3	1:A:203:ILE:HG21	1.93	0.51
8:U:54:CYS:HA	8:U:57:GLU:OE2	2.11	0.51
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.45	0.51
2:B:361:LYS:O	2:B:365:LYS:HG3	2.10	0.51
10:W:49:GLY:N	10:W:54:HIS:ND1	2.59	0.51
5:R:83:GLU:HG2	5:R:102:THR:CG2	2.23	0.51
2:B:27:THR:CG2	2:B:28:LYS:N	2.72	0.51
5:E:133:VAL:HG13	5:E:133:VAL:O	2.11	0.51
2:B:46:ARG:HD2	2:B:110:GLU:CD	2.31	0.51
2:O:287:ARG:HD3	9:V:53:GLU:HG2	1.92	0.51
1:N:106:MET:HG3	1:N:203:ILE:HG21	1.93	0.51
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.50	0.51
2:B:334:GLY:HA2	2:B:434:PRO:HD3	1.92	0.51
2:O:308:ASP:OD2	9:V:55:MET:O	2.29	0.51
1:A:424:ALA:HB1	1:A:428:ILE:HG21	1.93	0.51
2:O:422:LYS:O	2:O:436:LEU:HD21	2.11	0.51
3:P:245:LEU:O	4:Q:201:ARG:HD2	2.11	0.51
2:B:274:VAL:O	2:B:278:VAL:HG23	2.11	0.51
1:N:206:LYS:HA	1:N:209:VAL:CG1	2.41	0.50
2:B:31:ASN:HD22	2:B:32:GLY:N	2.08	0.50
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.93	0.50
1:N:106:MET:CE	1:N:110:VAL:HG21	2.41	0.50
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.93	0.50
10:J:4:ALA:O	10:J:8:GLN:HG3	2.11	0.50
5:R:84:GLY:N	5:R:100:HIS:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:29:LEU:HB3	2:O:30:PRO:HD2	1.93	0.50
1:A:21:ASN:HB3	1:A:219:VAL:HG22	1.92	0.50
1:A:220:SER:HB2	1:A:225:GLU:HB2	1.93	0.50
1:N:9:GLN:HG2	1:N:393:GLU:OE2	2.10	0.50
2:O:402:ILE:HG23	2:O:403:ASP:N	2.26	0.50
5:R:116:LYS:O	5:R:117:LEU:HD23	2.11	0.50
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.46	0.50
2:B:225:ASN:O	2:B:226:ILE:C	2.48	0.50
2:O:144:LEU:CB	2:O:183:ILE:HD12	2.41	0.50
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.93	0.50
3:C:98:HIS:CD2	13:C:502:HEM:NC	2.78	0.50
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.93	0.50
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.46	0.50
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.41	0.50
3:P:98:HIS:CD2	13:P:502:HEM:NC	2.79	0.50
5:E:190:ASP:CG	5:E:191:ASP:H	2.15	0.50
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.93	0.50
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.46	0.50
5:E:52:LYS:C	5:E:52:LYS:HD3	2.31	0.50
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.94	0.50
2:B:273:SER:O	2:B:276:GLN:HB3	2.11	0.50
5:R:78:LEU:HD22	5:R:132:TRP:CZ3	2.46	0.50
2:B:308:ASP:OD2	9:I:56:SER:HA	2.11	0.50
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.47	0.50
1:A:380:GLY:O	1:A:384:LEU:HB2	2.12	0.50
2:O:26:ILE:O	2:O:26:ILE:HG12	2.11	0.50
3:P:377:MET:HE1	6:S:20:TYR:CD1	2.47	0.50
1:N:209:VAL:O	1:N:212:ALA:HB3	2.11	0.50
2:O:361:LYS:O	2:O:365:LYS:HG3	2.11	0.50
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.27	0.50
2:B:424:MET:HG2	2:B:425:ALA:N	2.27	0.50
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.94	0.50
1:N:220:SER:HB2	1:N:225:GLU:HB2	1.92	0.49
5:R:101:ARG:HB3	5:R:105:GLU:HB2	1.93	0.49
2:O:307:PHE:CD1	2:O:308:ASP:N	2.80	0.49
1:N:410:VAL:O	1:N:413:LYS:HB3	2.11	0.49
2:O:225:ASN:O	2:O:226:ILE:C	2.50	0.49
1:A:23:LEU:HD23	1:A:24:ARG:N	2.26	0.49
3:C:230:ILE:HG22	4:D:219:LEU:HD13	1.93	0.49
5:R:109:GLU:C	5:R:111:GLU:H	2.15	0.49
1:N:219:VAL:HG12	1:N:220:SER:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:67:GLY:O	9:V:68:ILE:HD13	2.13	0.49
3:P:335:ILE:HD13	7:T:58:LEU:HD23	1.93	0.49
5:R:82:PRO:HD2	5:R:85:LYS:HD3	1.94	0.49
9:I:67:GLY:O	9:I:68:ILE:HD13	2.12	0.49
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.47	0.49
3:P:156:TYR:CD2	3:P:156:TYR:N	2.79	0.49
4:D:43:MET:HE2	4:D:91:PHE:CE2	2.47	0.49
1:N:138:LEU:HD11	1:N:174:ILE:HD12	1.95	0.49
1:N:156:THR:HA	5:R:7:VAL:HG21	1.94	0.49
1:A:156:THR:HA	5:E:7:VAL:HG21	1.93	0.49
4:Q:68:VAL:HG11	4:Q:92:PRO:HG3	1.94	0.49
2:O:274:VAL:O	2:O:278:VAL:HG23	2.13	0.49
1:A:300:GLU:OE1	1:A:300:GLU:HA	2.12	0.49
1:A:138:LEU:HD11	1:A:174:ILE:HD12	1.95	0.49
2:O:113:ARG:O	2:O:116:VAL:HG23	2.12	0.49
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.13	0.49
1:A:26:ALA:O	1:A:198:ALA:HA	2.13	0.49
2:O:334:GLY:HA2	2:O:434:PRO:HD3	1.94	0.49
2:B:245:ARG:HB3	2:B:430:LEU:CD1	2.43	0.49
2:B:262:ALA:HB2	2:B:268:GLU:HG2	1.94	0.49
1:A:281:ASP:OD1	9:I:33:UNK:HB1	2.13	0.49
2:B:102:ARG:HH22	2:B:161:GLU:HA	1.76	0.49
1:A:217:SER:O	1:A:218:GLY:C	2.51	0.49
2:B:257:VAL:O	2:B:323:GLY:HA3	2.13	0.49
1:N:178:THR:CG2	1:N:179:ARG:N	2.75	0.49
4:D:47:ALA:HA	4:D:90:TYR:HA	1.95	0.49
5:R:77:LYS:HA	5:R:191:ASP:O	2.13	0.49
3:C:78:TRP:CZ3	4:D:201:ARG:HG3	2.47	0.49
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.78	0.49
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.48	0.49
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.95	0.49
8:H:72:LYS:N	8:H:72:LYS:HD2	2.27	0.49
9:V:28:UNK:CA	9:V:72:ALA:HB2	2.43	0.48
1:A:106:MET:CE	1:A:110:VAL:HG21	2.43	0.48
2:B:389:SER:O	2:B:391:THR:N	2.46	0.48
7:G:36:ASN:O	7:G:40:ARG:HG3	2.13	0.48
2:B:335:GLU:HA	2:B:338:ARG:NH1	2.28	0.48
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.94	0.48
4:D:231:LYS:O	6:F:71:LYS:HE3	2.13	0.48
10:W:14:PHE:CD2	10:W:14:PHE:N	2.80	0.48
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.48	0.48
3:P:90:PHE:CZ	3:P:236:MET:HB3	2.48	0.48
1:A:275:ALA:HB3	1:A:357:ALA:HB1	1.94	0.48
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.48	0.48
5:R:101:ARG:HH22	5:R:127:VAL:CG1	2.19	0.48
1:N:49:ASN:HD22	1:N:51:LYS:N	2.05	0.48
3:C:41:CYS:HG	3:C:90:PHE:HD2	1.61	0.48
2:B:402:ILE:HG23	2:B:403:ASP:N	2.28	0.48
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.94	0.48
2:O:318:ASP:O	2:O:319:SER:HB2	2.13	0.48
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.95	0.48
2:B:60:THR:HG23	2:B:61:ALA:N	2.29	0.48
4:Q:144:ARG:HG2	4:Q:147:LEU:HD12	1.94	0.48
1:N:49:ASN:C	1:N:49:ASN:ND2	2.66	0.48
2:O:248:ASN:HD22	2:O:250:HIS:H	1.61	0.48
2:B:110:GLU:O	2:B:111:CYS:HB3	2.13	0.48
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.96	0.48
2:O:424:MET:HB2	2:O:436:LEU:HD13	1.94	0.48
4:D:68:VAL:HG11	4:D:92:PRO:HG3	1.94	0.48
2:O:46:ARG:HH21	2:O:376:GLN:HG3	1.78	0.48
1:A:75:PHE:HZ	1:A:86:PHE:HE2	1.61	0.48
1:N:240:GLU:HB3	1:N:422:LEU:HB3	1.96	0.48
3:C:54:MET:HG2	3:P:178:ARG:HA	1.95	0.48
2:O:152:PHE:HA	2:O:157:VAL:HG11	1.94	0.48
1:N:26:ALA:O	1:N:198:ALA:HA	2.14	0.48
2:B:422:LYS:O	2:B:436:LEU:HD21	2.14	0.48
2:O:78:LYS:HA	2:O:131:GLU:OE2	2.14	0.48
1:N:206:LYS:CA	1:N:209:VAL:HG12	2.43	0.48
2:O:76:THR:HG22	2:O:82:SER:N	2.20	0.48
5:E:134:ILE:HD11	5:E:193:VAL:HG21	1.96	0.48
5:E:82:PRO:HD2	5:E:85:LYS:HD3	1.95	0.48
3:P:2:ALA:CB	3:P:8:SER:HB3	2.40	0.48
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.26	0.48
1:A:351:GLU:O	1:A:354:VAL:HG22	2.13	0.48
8:H:32:LYS:O	8:H:36:ARG:HG3	2.14	0.48
1:A:282:ARG:HH21	9:I:35:UNK:HA	1.78	0.48
10:W:20:PHE:O	10:W:24:VAL:HG23	2.14	0.48
2:O:67:HIS:O	2:O:70:ARG:HB3	2.14	0.48
19:Q:3003:CDL:H511	7:T:26:ILE:HG21	1.96	0.48
15:P:3002:UQ:HM51	15:P:3002:UQ:C8	2.44	0.48
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.96	0.48
3:P:374:GLU:HG2	6:S:20:TYR:OH	2.14	0.48
3:P:71:CYS:SG	3:P:81:ARG:HD2	2.54	0.48
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.14	0.48
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.31	0.48
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.43	0.48
15:C:2002:UQ:HM51	15:C:2002:UQ:C8	2.44	0.48
7:G:40:ARG:HD2	19:G:2004:CDL:OA4	2.13	0.48
5:E:41:ALA:O	5:E:45:VAL:HG23	2.14	0.48
1:N:394:GLU:O	1:N:397:SER:HB3	2.13	0.48
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.94	0.48
3:C:323:GLN:OE1	7:G:47:LYS:HD3	2.14	0.48
3:P:34:PHE:HB2	21:P:381:HOH:O	2.13	0.48
6:S:98:ILE:O	6:S:102:LEU:HG	2.14	0.48
2:O:156:GLN:HE22	9:V:77:ARG:C	2.17	0.47
9:V:28:UNK:HA	9:V:72:ALA:HB2	1.94	0.47
1:N:87:ASN:OD1	2:O:286:LYS:HD2	2.13	0.47
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.44	0.47
4:Q:83:ARG:HB2	4:Q:84:PRO:HD2	1.95	0.47
2:B:248:ASN:ND2	2:B:248:ASN:C	2.67	0.47
1:N:21:ASN:CB	1:N:219:VAL:HA	2.44	0.47
5:R:165:TYR:HA	5:R:170:ARG:O	2.14	0.47
1:N:239:SER:HB2	7:T:17:SER:O	2.14	0.47
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.49	0.47
1:A:233:ARG:HH12	1:A:316:ASP:HB2	1.80	0.47
2:O:353:THR:CG2	2:O:354:GLU:N	2.77	0.47
2:B:76:THR:CG2	2:B:82:SER:HB2	2.45	0.47
2:O:341:MET:CE	2:O:341:MET:HA	2.44	0.47
5:R:147:ILE:HG22	5:R:148:ALA:H	1.78	0.47
1:N:53:ASN:N	1:N:173:ASN:ND2	2.62	0.47
2:B:60:THR:CG2	2:B:61:ALA:N	2.76	0.47
8:H:18:THR:O	8:H:22:GLU:HG3	2.14	0.47
1:A:136:GLN:O	1:A:140:GLU:HG3	2.13	0.47
1:N:77:LYS:HE3	2:O:359:LYS:HZ1	1.79	0.47
7:T:36:ASN:O	7:T:40:ARG:HG3	2.14	0.47
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.97	0.47
3:P:78:TRP:CD2	4:Q:197:GLU:HG3	2.49	0.47
4:D:144:ARG:HG2	4:D:147:LEU:HD12	1.97	0.47
2:O:295:LEU:O	2:O:299:VAL:HG23	2.14	0.47
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.44	0.47
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:9:HIS:CD2	3:P:11:LEU:HB2	2.49	0.47
2:O:338:ARG:NH1	2:O:338:ARG:HB2	2.28	0.47
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.97	0.47
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.96	0.47
1:A:394:GLU:O	1:A:397:SER:HB3	2.15	0.47
5:E:155:GLY:HA3	5:E:166:ASP:C	2.35	0.47
1:N:443:TRP:O	1:N:444:ILE:CB	2.63	0.47
2:O:76:THR:HG23	2:O:136:GLU:CD	2.35	0.47
5:R:78:LEU:HD13	5:R:132:TRP:CE2	2.50	0.47
1:A:387:GLY:O	1:A:388:ARG:HB3	2.13	0.47
5:E:102:THR:O	5:E:106:ILE:HG13	2.14	0.47
2:B:25:GLU:HB2	2:B:213:HIS:ND1	2.30	0.47
8:U:65:ARG:O	8:U:69:VAL:HG23	2.15	0.47
1:N:75:PHE:HZ	1:N:86:PHE:HE2	1.61	0.47
6:F:49:ARG:HD3	2:O:135:TRP:CE2	2.50	0.47
2:O:202:ALA:HB3	2:O:229:GLY:O	2.14	0.47
2:B:406:THR:OG1	2:B:408:ALA:HB3	2.15	0.47
4:D:70:VAL:HG21	4:D:83:ARG:NH1	2.28	0.47
6:F:78:GLU:CD	6:F:78:GLU:H	2.17	0.47
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.49	0.47
1:A:307:PHE:C	1:A:307:PHE:CD1	2.88	0.47
2:B:46:ARG:HG3	2:B:110:GLU:HG2	1.96	0.47
4:D:71:GLN:HG3	4:D:82:MET:HE2	1.97	0.47
1:A:269:VAL:HG22	1:A:406:MET:HE2	1.97	0.47
2:B:353:THR:CG2	2:B:354:GLU:N	2.78	0.47
2:B:341:MET:HA	2:B:341:MET:CE	2.45	0.47
1:A:350:THR:CG2	1:A:351:GLU:N	2.77	0.47
5:R:157:TYR:CE1	5:R:162:GLY:HA2	2.50	0.47
4:Q:167:GLU:CG	8:U:13:LEU:HD13	2.45	0.47
4:Q:43:MET:HE3	4:Q:189:PHE:CZ	2.50	0.47
3:C:156:TYR:N	3:C:156:TYR:CD2	2.81	0.47
3:C:269:ILE:HG22	3:C:269:ILE:O	2.14	0.47
13:P:502:HEM:HMC2	13:P:502:HEM:HBC2	1.97	0.47
2:B:312:PHE:CE2	2:B:314:VAL:HG23	2.50	0.47
5:R:113:ASP:OD2	5:R:116:LYS:HG3	2.14	0.47
10:J:49:GLY:N	10:J:54:HIS:ND1	2.63	0.47
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.50	0.47
5:E:95:PRO:HG3	3:P:263:LEU:HD23	1.97	0.47
9:V:64:LEU:HD12	9:V:77:ARG:C	2.36	0.46
2:B:26:ILE:O	2:B:26:ILE:HG12	2.16	0.46
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:152:SER:HB3	3:C:162:VAL:HG21	1.96	0.46
1:N:307:PHE:CD1	1:N:307:PHE:C	2.89	0.46
10:J:60:GLU:HA	10:J:60:GLU:OE2	2.15	0.46
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.97	0.46
1:A:21:ASN:HA	1:A:219:VAL:HG13	1.98	0.46
5:R:118:ARG:HB2	5:R:171:ILE:CG2	2.45	0.46
2:O:338:ARG:CB	2:O:338:ARG:HH11	2.28	0.46
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.50	0.46
8:H:65:ARG:O	8:H:68:CYS:HB3	2.16	0.46
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.95	0.46
1:A:240:GLU:HA	1:A:422:LEU:O	2.14	0.46
1:A:304:CYS:HB2	1:A:325:VAL:O	2.15	0.46
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.48	0.46
4:Q:200:GLN:NE2	17:Q:3091:BOG:H3	2.29	0.46
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.97	0.46
5:R:101:ARG:NH2	5:R:127:VAL:HG11	2.22	0.46
1:A:103:SER:HB3	1:A:202:GLY:O	2.15	0.46
2:O:393:THR:HG23	2:O:397:VAL:HB	1.97	0.46
2:O:76:THR:CG2	2:O:82:SER:HB2	2.43	0.46
2:O:27:THR:CG2	2:O:28:LYS:H	2.21	0.46
1:A:410:VAL:O	1:A:413:LYS:HB3	2.15	0.46
7:T:75:ALA:HA	7:T:78:GLU:HG3	1.97	0.46
6:S:78:GLU:CD	6:S:78:GLU:H	2.19	0.46
2:B:47:ILE:HD13	2:B:120:MET:HE2	1.95	0.46
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.97	0.46
2:O:424:MET:HG2	2:O:425:ALA:N	2.30	0.46
2:B:424:MET:HB2	2:B:436:LEU:HD13	1.97	0.46
2:O:19:PRO:HB3	2:O:41:PHE:CE2	2.50	0.46
8:U:72:LYS:N	8:U:72:LYS:HD2	2.29	0.46
1:A:178:THR:CG2	1:A:179:ARG:N	2.79	0.46
5:R:78:LEU:HB3	5:R:132:TRP:CH2	2.50	0.46
2:O:31:ASN:C	2:O:31:ASN:HD22	2.19	0.46
3:C:374:GLU:HG2	6:F:20:TYR:OH	2.15	0.46
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.97	0.46
3:C:268:HIS:HB3	21:C:1288:HOH:O	2.14	0.46
5:R:146:PRO:HB2	5:R:156:TYR:HB3	1.97	0.46
3:P:247:SER:N	3:P:248:PRO:HD3	2.31	0.46
1:N:19:LEU:C	1:N:21:ASN:H	2.19	0.46
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.16	0.46
8:H:54:CYS:HA	8:H:57:GLU:OE2	2.16	0.46
1:N:382:HIS:HB3	1:N:388:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.16	0.46
2:B:252:LEU:HD11	9:I:49:LEU:HB2	1.98	0.46
1:A:49:ASN:HD22	1:A:51:LYS:N	2.08	0.46
3:P:269:ILE:O	3:P:269:ILE:HG22	2.14	0.46
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.97	0.46
2:O:327:ILE:HG22	9:V:55:MET:CE	2.46	0.46
3:C:198:LEU:HD21	13:C:502:HEM:CMA	2.45	0.46
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.97	0.46
8:U:32:LYS:O	8:U:36:ARG:HG3	2.16	0.46
2:O:353:THR:HB	2:O:356:ASP:OD1	2.16	0.46
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.49	0.46
4:D:218:LEU:HD22	5:E:39:VAL:HG13	1.98	0.46
2:B:393:THR:HG23	2:B:397:VAL:HB	1.97	0.46
5:E:91:TRP:CE2	5:E:92:ARG:HG3	2.51	0.46
6:S:96:GLU:OE2	6:S:96:GLU:HA	2.16	0.46
1:N:7:THR:HG21	2:O:113:ARG:CD	2.44	0.45
1:A:106:MET:O	1:A:106:MET:HE2	2.16	0.45
1:N:351:GLU:O	1:N:354:VAL:HG22	2.16	0.45
9:V:31:UNK:O	9:V:73:PRO:HG2	2.16	0.45
5:R:126:ARG:NH2	5:R:170:ARG:HG3	2.30	0.45
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.30	0.45
4:Q:139:ALA:HB2	8:U:41:ASP:OD1	2.15	0.45
4:Q:43:MET:HE2	4:Q:91:PHE:CE2	2.50	0.45
4:D:195:GLU:HG3	4:D:198:HIS:HB2	1.97	0.45
1:N:269:VAL:HG22	1:N:406:MET:HE2	1.97	0.45
18:Q:501:HEC:HMC1	18:Q:501:HEC:HBC3	1.98	0.45
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.46	0.45
5:E:73:LYS:HB3	5:E:195:VAL:O	2.16	0.45
1:A:280:TYR:CG	1:A:281:ASP:N	2.84	0.45
2:O:402:ILE:HG23	2:O:403:ASP:H	1.81	0.45
4:D:97:ASN:OD1	4:D:99:GLU:HB2	2.16	0.45
3:P:17:ASN:HB2	17:P:2010:BOG:O3	2.15	0.45
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.16	0.45
1:N:106:MET:HG3	1:N:203:ILE:CG2	2.47	0.45
5:R:134:ILE:CD1	5:R:193:VAL:HG21	2.46	0.45
3:P:78:TRP:CZ3	4:Q:201:ARG:HG3	2.51	0.45
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.34	0.45
1:A:240:GLU:HB3	1:A:422:LEU:HB3	1.98	0.45
2:O:291:VAL:C	2:O:293:SER:H	2.19	0.45
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.52	0.45
2:B:76:THR:HG22	2:B:82:SER:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:TYR:CE2	1:A:396:ASP:OD2	2.69	0.45
1:N:23:LEU:HD23	1:N:24:ARG:N	2.31	0.45
1:N:294:LEU:HB2	1:N:341:GLU:HG3	1.99	0.45
2:O:399:ALA:CA	2:O:402:ILE:HG22	2.46	0.45
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.17	0.45
1:N:350:THR:HG22	1:N:352:SER:N	2.31	0.45
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.98	0.45
2:B:353:THR:HB	2:B:356:ASP:OD1	2.16	0.45
2:B:116:VAL:O	2:B:120:MET:HB2	2.16	0.45
1:A:49:ASN:ND2	1:A:49:ASN:C	2.69	0.45
2:O:248:ASN:C	2:O:248:ASN:ND2	2.67	0.45
5:R:166:ASP:OD2	5:R:170:ARG:HB2	2.16	0.45
5:R:71:LEU:HD13	5:R:92:ARG:HD3	1.98	0.45
2:B:218:GLN:O	2:B:222:GLN:HG3	2.16	0.45
2:B:357:VAL:O	2:B:361:LYS:HG3	2.16	0.45
2:B:338:ARG:HB2	2:B:338:ARG:NH1	2.31	0.45
2:B:325:TYR:CD1	9:I:60:ALA:CB	2.99	0.45
4:D:238:ARG:HD2	7:G:14:ILE:HD12	1.97	0.45
1:A:137:GLU:O	1:A:141:MET:HG3	2.17	0.45
2:B:195:VAL:O	2:B:199:PHE:HB2	2.16	0.45
1:A:223:TYR:OH	1:A:224:LYS:HE3	2.17	0.45
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.97	0.45
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.32	0.45
2:B:24:LEU:HD21	2:B:392:HIS:CD2	2.52	0.45
2:B:24:LEU:O	2:B:24:LEU:HG	2.17	0.45
2:O:397:VAL:O	2:O:401:LYS:HG2	2.16	0.45
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.99	0.45
8:H:10:GLU:HB2	8:H:11:GLU:OE2	2.16	0.45
2:B:152:PHE:HA	2:B:157:VAL:HG11	1.97	0.45
1:A:106:MET:HG3	1:A:203:ILE:CG2	2.47	0.45
2:B:46:ARG:HE	2:B:376:GLN:HA	1.82	0.45
1:N:136:GLN:O	1:N:140:GLU:HG3	2.17	0.45
1:A:370:ASP:O	2:B:374:THR:HG22	2.17	0.45
2:O:116:VAL:O	2:O:120:MET:HB2	2.17	0.45
5:R:147:ILE:CG2	5:R:148:ALA:N	2.80	0.45
1:N:161:THR:HG21	1:N:235:ARG:N	2.32	0.45
2:B:307:PHE:H	9:I:52:ARG:HG2	1.80	0.45
3:C:198:LEU:HD21	13:C:502:HEM:C3A	2.52	0.45
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.47	0.45
8:H:17:LEU:HD13	8:H:73:LEU:HD22	1.99	0.45
1:A:242:ARG:O	7:G:14:ILE:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:285:ILE:HD12	3:P:294:ALA:HB2	1.99	0.44
2:O:159:VAL:HG21	2:O:325:TYR:CE1	2.53	0.44
2:B:67:HIS:O	2:B:70:ARG:HB3	2.16	0.44
2:O:395:PRO:HA	2:O:398:VAL:CG1	2.47	0.44
2:B:389:SER:O	2:B:390:GLY:C	2.56	0.44
4:D:44:ASP:OD1	4:D:93:LYS:HE3	2.17	0.44
4:D:62:LYS:O	4:D:66:GLU:HG3	2.17	0.44
1:A:3:THR:OG1	1:A:6:GLN:HG3	2.17	0.44
5:E:10:PHE:O	5:E:14:ARG:HG3	2.17	0.44
2:O:62:ASN:O	2:O:65:THR:CG2	2.62	0.44
1:A:170:THR:CG2	1:A:171:THR:N	2.81	0.44
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.81	0.44
2:O:406:THR:OG1	2:O:408:ALA:HB3	2.17	0.44
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.53	0.44
3:P:358:SER:O	3:P:362:ILE:HG13	2.18	0.44
5:R:133:VAL:HG13	5:R:133:VAL:O	2.17	0.44
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.46	0.44
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.31	0.44
4:Q:161:ALA:O	4:Q:162:PRO:C	2.56	0.44
3:C:305:ILE:HB	3:C:306:PRO:HD3	2.00	0.44
7:G:24:ARG:HB2	7:G:27:PRO:HB3	2.00	0.44
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.37	0.44
2:B:248:ASN:HD22	2:B:250:HIS:H	1.65	0.44
1:N:350:THR:CG2	1:N:351:GLU:N	2.80	0.44
2:O:286:LYS:HE2	2:O:287:ARG:HH12	1.82	0.44
2:O:60:THR:CG2	2:O:61:ALA:N	2.80	0.44
2:O:110:GLU:O	2:O:111:CYS:HB3	2.17	0.44
1:N:106:MET:HE3	1:N:208:LEU:HA	1.98	0.44
2:B:312:PHE:CZ	2:B:314:VAL:CG2	3.01	0.44
1:A:23:LEU:C	1:A:23:LEU:HD23	2.38	0.44
5:E:75:GLU:HG2	5:E:194:VAL:HG22	1.98	0.44
1:A:281:ASP:C	1:A:281:ASP:OD1	2.55	0.44
5:R:109:GLU:HB3	5:R:123:ASP:HB2	2.00	0.44
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.52	0.44
1:A:53:ASN:H	1:A:173:ASN:ND2	2.16	0.44
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.99	0.44
2:B:19:PRO:HB2	2:B:41:PHE:CE1	2.52	0.44
1:N:191:LYS:CA	1:N:195:MET:HE2	2.48	0.44
2:O:71:LEU:CD2	9:V:68:ILE:HG13	2.48	0.44
5:R:177:PRO:HB2	5:R:178:TYR:CE1	2.53	0.44
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.53	0.44
8:H:11:GLU:H	8:H:11:GLU:CD	2.20	0.44
4:Q:95:TYR:HA	4:Q:96:PRO:HD3	1.85	0.44
7:G:80:ASP:O	7:G:81:GLN:OXT	2.36	0.44
1:A:112:LEU:O	1:A:116:VAL:HG23	2.18	0.44
4:D:168:ILE:HG12	4:D:168:ILE:O	2.18	0.44
5:R:124:LEU:HA	5:R:127:VAL:CG2	2.48	0.44
1:A:191:LYS:C	1:A:195:MET:HE2	2.37	0.44
7:T:40:ARG:HD2	19:T:3004:CDL:OA4	2.18	0.44
4:D:120:ARG:HH21	18:D:501:HEC:CGA	2.31	0.44
4:D:43:MET:HE3	4:D:189:PHE:CZ	2.53	0.44
5:R:163:SER:HA	5:R:174:GLY:HA3	2.00	0.44
1:N:143:ASN:ND2	9:V:48:PRO:HD2	2.27	0.43
2:O:276:GLN:HG2	2:O:281:ALA:HB2	2.00	0.43
2:B:218:GLN:HG2	2:B:222:GLN:OE1	2.18	0.43
4:Q:44:ASP:OD1	4:Q:93:LYS:HE3	2.17	0.43
2:O:24:LEU:HG	2:O:24:LEU:O	2.18	0.43
3:P:25:PRO:HB2	3:P:28:ILE:HG23	2.00	0.43
9:I:32:UNK:N	9:I:73:PRO:CG	2.74	0.43
3:P:101:ARG:NH2	13:P:502:HEM:HBD2	2.32	0.43
2:B:402:ILE:HG23	2:B:403:ASP:H	1.81	0.43
2:O:389:SER:O	2:O:391:THR:N	2.51	0.43
4:D:3:LEU:HD11	7:G:72:LYS:HE3	2.00	0.43
6:S:71:LYS:O	6:S:72:HIS:HB2	2.18	0.43
4:D:43:MET:HE2	4:D:91:PHE:CD2	2.53	0.43
5:R:146:PRO:CB	5:R:156:TYR:HB3	2.48	0.43
2:O:60:THR:HG23	2:O:61:ALA:N	2.33	0.43
2:B:291:VAL:C	2:B:293:SER:H	2.21	0.43
5:E:185:TYR:CB	5:E:195:VAL:HG22	2.47	0.43
5:R:193:VAL:HG13	5:R:193:VAL:O	2.18	0.43
1:A:272:VAL:O	1:A:275:ALA:HB3	2.18	0.43
7:G:75:ALA:HA	7:G:78:GLU:HG3	1.99	0.43
6:F:96:GLU:OE2	6:F:96:GLU:HA	2.18	0.43
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.48	0.43
5:E:74:ILE:HD11	5:E:96:LEU:CD2	2.48	0.43
3:C:178:ARG:HA	3:P:54:MET:HG2	1.99	0.43
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.89	0.43
4:D:138:PRO:HB3	8:H:58:LEU:HD22	2.00	0.43
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.51	0.43
2:O:152:PHE:HA	2:O:157:VAL:CG1	2.48	0.43
5:E:193:VAL:HG13	5:E:193:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:VAL:O	2:B:401:LYS:HG2	2.18	0.43
9:I:58:ARG:HA	9:I:58:ARG:HD3	1.90	0.43
3:C:9:HIS:CD2	3:C:11:LEU:HB2	2.54	0.43
1:N:26:ALA:CB	1:N:383:LEU:HD11	2.47	0.43
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.99	0.43
5:R:136:VAL:O	5:R:138:VAL:N	2.43	0.43
2:B:24:LEU:HD12	2:B:37:SER:O	2.19	0.43
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	2.00	0.43
5:R:109:GLU:C	5:R:111:GLU:N	2.72	0.43
10:J:20:PHE:O	10:J:24:VAL:HG23	2.19	0.43
2:B:168:TYR:HB2	2:B:173:ALA:HB2	2.01	0.43
2:B:366:ALA:O	2:B:370:MET:HG3	2.19	0.43
4:D:35:GLN:NE2	4:D:169:LEU:HD12	2.34	0.43
1:N:206:LYS:O	1:N:209:VAL:HG12	2.17	0.43
1:A:350:THR:HG22	1:A:352:SER:N	2.28	0.43
1:N:19:LEU:HB2	1:N:21:ASN:OD1	2.18	0.43
3:C:344:VAL:C	3:C:345:GLU:HG3	2.37	0.43
5:R:112:VAL:O	5:R:113:ASP:O	2.36	0.43
2:B:402:ILE:O	2:B:405:VAL:HG23	2.19	0.43
5:R:155:GLY:HA3	5:R:166:ASP:C	2.39	0.43
3:C:234:THR:HG21	4:D:219:LEU:HD12	2.01	0.43
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.99	0.43
8:U:17:LEU:HD13	8:U:73:LEU:HD22	2.00	0.43
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.18	0.43
3:C:105:TYR:O	3:C:315:THR:HG22	2.18	0.43
5:R:161:HIS:HB2	20:R:501:FES:S1	2.58	0.43
1:A:206:LYS:HA	1:A:209:VAL:CG1	2.49	0.43
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.54	0.43
3:C:117:GLY:O	13:C:502:HEM:HMC3	2.19	0.43
1:N:240:GLU:HA	1:N:422:LEU:O	2.19	0.43
1:A:240:GLU:CD	1:A:242:ARG:HE	2.21	0.43
3:C:325:LEU:HD22	3:C:370:ILE:HG13	2.00	0.43
3:P:305:ILE:HB	3:P:306:PRO:HD3	2.00	0.43
1:N:424:ALA:HB1	1:N:428:ILE:HG21	2.01	0.43
1:A:9:GLN:HG2	1:A:393:GLU:OE2	2.19	0.43
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.34	0.43
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.34	0.43
1:N:39:VAL:HA	1:N:196:VAL:O	2.19	0.43
5:R:71:LEU:HD13	5:R:92:ARG:NH1	2.34	0.43
2:O:402:ILE:O	2:O:405:VAL:HG23	2.19	0.42
5:E:161:HIS:HB2	20:E:501:FES:S1	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:VAL:O	5:E:59:ILE:HG12	2.19	0.42
1:A:62:LEU:HD11	1:A:127:ILE:HG12	2.00	0.42
5:E:97:PHE:CE2	5:E:137:GLY:HA3	2.54	0.42
5:R:85:LYS:O	5:R:99:ARG:HG3	2.20	0.42
2:O:47:ILE:HG22	2:O:48:GLY:N	2.34	0.42
2:O:312:PHE:CE2	2:O:314:VAL:HG23	2.54	0.42
2:O:399:ALA:C	2:O:402:ILE:HG22	2.39	0.42
3:C:247:SER:N	3:C:248:PRO:HD3	2.34	0.42
2:B:394:ALA:HB3	2:B:397:VAL:HG23	2.01	0.42
13:C:501:HEM:HMC1	13:C:501:HEM:HBC2	2.00	0.42
2:B:399:ALA:CA	2:B:402:ILE:HG22	2.50	0.42
7:G:77:TYR:O	8:H:47:ARG:NH1	2.52	0.42
2:O:168:TYR:HB2	2:O:173:ALA:HB2	2.01	0.42
9:V:28:UNK:CB	9:V:71:ASN:ND2	2.83	0.42
2:O:389:SER:O	2:O:390:GLY:C	2.58	0.42
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.76	0.42
6:F:77:LYS:HE2	6:F:77:LYS:HB3	1.82	0.42
1:A:328:PRO:HB3	1:A:427:PRO:HB2	2.02	0.42
5:E:126:ARG:HH11	5:E:126:ARG:HG2	1.85	0.42
10:J:14:PHE:CD2	10:J:14:PHE:N	2.85	0.42
2:B:28:LYS:HG2	2:B:28:LYS:O	2.18	0.42
5:E:134:ILE:CD1	5:E:193:VAL:HG21	2.50	0.42
1:A:398:ARG:HH11	1:A:398:ARG:CG	2.27	0.42
3:P:350:ILE:O	3:P:354:MET:HG2	2.19	0.42
9:I:65:VAL:HG12	9:I:66:ALA:N	2.34	0.42
7:T:24:ARG:HB2	7:T:27:PRO:HB3	2.01	0.42
2:O:245:ARG:HB3	2:O:430:LEU:CD1	2.49	0.42
8:U:18:THR:O	8:U:22:GLU:HG3	2.19	0.42
5:R:78:LEU:HD22	5:R:132:TRP:CE3	2.54	0.42
7:G:45:VAL:O	7:G:49:ALA:HB3	2.19	0.42
5:E:191:ASP:OD1	5:E:191:ASP:O	2.38	0.42
2:O:24:LEU:HD12	2:O:37:SER:O	2.18	0.42
1:N:137:GLU:O	1:N:141:MET:HG3	2.20	0.42
6:S:40:ASP:O	6:S:44:LYS:HG3	2.18	0.42
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.55	0.42
3:P:198:LEU:HD21	13:P:502:HEM:CMA	2.49	0.42
2:O:395:PRO:HA	2:O:398:VAL:HG12	2.00	0.42
2:O:129:ALA:N	2:O:130:PRO:CD	2.83	0.42
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.54	0.42
8:U:34:ARG:O	8:U:38:GLU:HG3	2.20	0.42
7:T:72:LYS:HE3	8:U:56:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:206:LYS:N	1:N:206:LYS:CD	2.64	0.42
3:C:269:ILE:CG2	14:C:2001:FNM:H23	2.48	0.42
2:O:357:VAL:O	2:O:361:LYS:HG3	2.20	0.42
2:B:84:ARG:HD2	6:S:107:TRP:HZ3	1.85	0.42
18:D:501:HEC:HMD1	18:D:501:HEC:HAD1	1.83	0.42
3:C:285:ILE:HA	3:C:286:PRO:HD2	1.92	0.42
5:E:189:GLY:O	5:E:192:LEU:N	2.52	0.42
10:W:52:TRP:O	10:W:56:LYS:HB2	2.19	0.42
7:T:72:LYS:CG	8:U:56:GLU:OE2	2.51	0.42
1:A:106:MET:HE3	1:A:208:LEU:HA	2.02	0.42
5:E:163:SER:HA	5:E:174:GLY:HA3	2.01	0.42
2:B:385:GLU:C	2:B:387:LEU:H	2.23	0.42
4:D:68:VAL:HG12	4:D:69:GLU:N	2.35	0.42
6:S:12:LEU:HB3	6:S:13:MET:CE	2.50	0.42
2:O:257:VAL:O	2:O:323:GLY:HA3	2.19	0.42
1:N:281:ASP:O	1:N:283:THR:N	2.53	0.42
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.54	0.42
1:A:432:LEU:HD23	1:A:432:LEU:HA	1.80	0.42
2:B:26:ILE:HA	2:B:35:ILE:O	2.19	0.42
9:I:38:UNK:O	9:I:40:UNK:N	2.52	0.42
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.55	0.42
6:F:71:LYS:O	6:F:72:HIS:HB2	2.20	0.42
6:S:77:LYS:O	6:S:77:LYS:HG2	2.19	0.42
1:A:161:THR:HG21	1:A:235:ARG:H	1.83	0.42
1:N:158:PHE:O	1:N:164:ALA:HB2	2.20	0.42
5:R:73:LYS:HB3	5:R:195:VAL:O	2.20	0.42
4:Q:79:GLU:HA	4:Q:79:GLU:OE2	2.20	0.42
1:N:170:THR:CG2	1:N:171:THR:N	2.83	0.41
3:P:223:PRO:HB2	3:P:227:PHE:HD2	1.84	0.41
5:E:189:GLY:O	5:E:190:ASP:C	2.59	0.41
1:N:123:GLU:OE1	1:N:123:GLU:HA	2.20	0.41
2:B:22:GLU:HG3	2:B:23:ASP:H	1.84	0.41
2:B:395:PRO:HA	2:B:398:VAL:HG12	2.02	0.41
2:O:63:LEU:HB2	2:O:182:ARG:HD3	2.02	0.41
4:Q:195:GLU:HG3	4:Q:195:GLU:O	2.20	0.41
10:W:48:GLU:HA	10:W:54:HIS:CE1	2.55	0.41
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.75	0.41
5:R:73:LYS:HG2	5:R:196:GLY:HA3	2.01	0.41
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.54	0.41
3:C:194:THR:O	3:C:197:HIS:HB3	2.21	0.41
1:A:228:VAL:O	1:A:228:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:284:PHE:CE2	9:V:71:ASN:O	2.73	0.41
2:O:312:PHE:CZ	2:O:314:VAL:CG2	3.03	0.41
1:N:105:ASP:O	1:N:106:MET:C	2.59	0.41
5:R:141:HIS:HB3	20:R:501:FES:S2	2.61	0.41
5:R:176:ALA:HA	5:R:177:PRO:HD2	1.95	0.41
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.82	0.41
2:B:295:LEU:O	2:B:299:VAL:HG23	2.20	0.41
2:B:395:PRO:HA	2:B:398:VAL:CG1	2.51	0.41
2:B:398:VAL:HG13	2:B:399:ALA:N	2.35	0.41
2:O:34:ILE:HD13	2:O:390:GLY:CA	2.51	0.41
1:A:90:THR:O	1:A:167:VAL:HG11	2.21	0.41
1:N:140:GLU:CG	9:V:50:LEU:HD12	2.49	0.41
1:N:62:LEU:C	1:N:64:PHE:H	2.23	0.41
1:A:233:ARG:NH1	1:A:316:ASP:HB2	2.34	0.41
6:F:13:MET:HE1	6:F:16:ILE:HD12	2.02	0.41
3:C:136:TRP:HH2	3:C:171:VAL:HG12	1.84	0.41
5:R:75:GLU:HG2	5:R:194:VAL:HG22	2.02	0.41
1:A:294:LEU:HB2	1:A:341:GLU:HG3	2.02	0.41
2:O:132:PHE:HB2	2:O:192:HIS:CE1	2.56	0.41
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.47	0.41
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.54	0.41
1:A:316:ASP:OD1	1:A:316:ASP:N	2.51	0.41
3:P:50:LEU:HD23	13:P:501:HEM:HBC1	2.03	0.41
4:D:142:VAL:O	4:D:142:VAL:HG23	2.21	0.41
4:D:38:SER:O	4:D:94:PRO:HG3	2.20	0.41
1:A:105:ASP:O	1:A:106:MET:C	2.59	0.41
2:O:359:LYS:O	2:O:362:ASN:HB2	2.21	0.41
2:O:178:CYS:SG	2:O:183:ILE:HD13	2.61	0.41
2:B:306:PRO:HA	9:I:52:ARG:HG2	2.02	0.41
10:W:60:GLU:CD	10:W:60:GLU:C	2.79	0.41
5:E:185:TYR:HB3	5:E:195:VAL:HG22	2.02	0.41
5:E:85:LYS:O	5:E:99:ARG:HG3	2.21	0.41
6:F:13:MET:CE	6:F:16:ILE:HD12	2.51	0.41
4:D:204:MET:HG2	17:D:2009:BOG:H5	2.02	0.41
2:B:35:ILE:HD13	2:B:217:LYS:HA	2.03	0.41
2:O:50:PHE:C	2:O:51:ILE:HG13	2.41	0.41
1:A:281:ASP:OD2	9:I:33:UNK:HB1	2.20	0.41
2:B:84:ARG:HD2	6:S:107:TRP:CZ3	2.56	0.41
1:A:191:LYS:CA	1:A:195:MET:HE2	2.51	0.41
2:O:222:GLN:O	2:O:223:PHE:HD2	2.04	0.41
2:O:57:TYR:N	2:O:57:TYR:CD1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:223:PRO:HB2	3:C:227:PHE:HD2	1.85	0.41
2:O:147:ASP:O	2:O:150:VAL:HG22	2.20	0.41
4:D:162:PRO:HA	4:D:163:PRO:HD2	2.01	0.41
1:N:14:THR:OG1	1:N:389:ARG:HG2	2.21	0.41
3:P:31:TRP:CH2	11:P:3007:PEE:H20	2.55	0.41
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.36	0.41
1:N:228:VAL:O	1:N:228:VAL:HG13	2.21	0.41
5:R:1:VAL:CG2	5:R:3:ASN:HD22	2.34	0.41
2:O:345:LYS:O	2:O:348:ALA:N	2.52	0.41
1:A:369:LEU:HD12	1:A:392:LEU:HD21	2.03	0.41
1:N:57:TYR:HA	1:N:90:THR:HG21	2.03	0.41
2:B:31:ASN:HD22	2:B:31:ASN:C	2.23	0.41
4:D:74:PRO:HA	4:D:79:GLU:O	2.20	0.41
5:E:71:LEU:HD13	5:E:92:ARG:HD3	2.02	0.41
1:N:18:THR:HG23	1:N:24:ARG:HG3	2.02	0.41
1:N:328:PRO:HB3	1:N:427:PRO:HB2	2.03	0.41
8:H:51:GLU:OE1	8:H:51:GLU:HA	2.20	0.41
10:W:26:LEU:O	10:W:30:LEU:HG	2.20	0.41
2:B:38:LEU:HD12	2:B:39:GLU:H	1.85	0.40
1:A:219:VAL:CG1	1:A:220:SER:N	2.84	0.40
10:W:56:LYS:HB3	10:W:56:LYS:HE2	1.86	0.40
4:D:239:PRO:HA	4:D:240:PRO:HD3	1.85	0.40
10:J:5:LEU:HD23	10:J:5:LEU:HA	1.95	0.40
6:S:79:GLN:HE21	6:S:79:GLN:HB3	1.68	0.40
2:B:109:VAL:HG21	2:B:119:VAL:HG12	2.02	0.40
3:C:350:ILE:O	3:C:354:MET:HG2	2.21	0.40
4:D:83:ARG:HB2	4:D:84:PRO:HD2	2.03	0.40
4:D:218:LEU:CD2	5:E:39:VAL:HG13	2.51	0.40
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	2.03	0.40
1:A:403:ASP:OD1	1:A:406:MET:HB2	2.21	0.40
5:E:84:GLY:N	5:E:100:HIS:O	2.47	0.40
2:O:256:ALA:HB2	2:O:325:TYR:CD1	2.57	0.40
2:O:267:ALA:C	2:O:269:ALA:H	2.24	0.40
5:E:153:PHE:CD2	5:E:172:ARG:NH1	2.89	0.40
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.57	0.40
2:O:31:ASN:ND2	2:O:31:ASN:C	2.74	0.40
4:Q:68:VAL:HG12	4:Q:69:GLU:N	2.36	0.40
1:A:369:LEU:CD1	1:A:392:LEU:HD21	2.51	0.40
3:C:266:PRO:HA	3:C:267:PRO:HD3	1.93	0.40
1:N:293:ARG:HB3	1:N:293:ARG:HE	1.71	0.40
2:O:21:ALA:O	2:O:22:GLU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:41:PHE:O	7:G:45:VAL:CG2	2.67	0.40
5:R:147:ILE:HG13	5:R:157:TYR:O	2.22	0.40
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.56	0.40
4:D:29:GLY:HA3	4:D:189:PHE:HB2	2.03	0.40
4:D:122:GLY:O	4:D:125:ASP:HB2	2.22	0.40
3:C:342:GLN:HB3	3:C:343:PRO:HD2	2.04	0.40
10:J:56:LYS:HE2	10:J:56:LYS:HB3	1.85	0.40
3:P:138:GLN:OE1	3:P:138:GLN:HA	2.22	0.40
1:A:69:LYS:HE3	1:A:70:ARG:HH21	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	441/446 (99%)	412 (93%)	23 (5%)	6 (1%)	14 42
1	N	440/446 (99%)	411 (93%)	22 (5%)	7 (2%)	12 38
2	B	419/441 (95%)	374 (89%)	35 (8%)	10 (2%)	7 25
2	O	420/441 (95%)	372 (89%)	41 (10%)	7 (2%)	11 36
3	C	378/380 (100%)	364 (96%)	14 (4%)	0	100 100
3	P	377/380 (99%)	360 (96%)	17 (4%)	0	100 100
4	D	239/241 (99%)	228 (95%)	11 (5%)	0	100 100
4	Q	239/241 (99%)	224 (94%)	15 (6%)	0	100 100
5	E	194/196 (99%)	170 (88%)	18 (9%)	6 (3%)	5 17
5	R	192/196 (98%)	156 (81%)	28 (15%)	8 (4%)	3 11
6	F	99/110 (90%)	93 (94%)	5 (5%)	1 (1%)	19 52
6	S	99/110 (90%)	91 (92%)	6 (6%)	2 (2%)	9 30
7	G	79/81 (98%)	69 (87%)	10 (13%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	T	76/81 (94%)	68 (90%)	8 (10%)	0	100 100
8	H	68/77 (88%)	62 (91%)	6 (9%)	0	100 100
8	U	65/77 (84%)	60 (92%)	4 (6%)	1 (2%)	13 40
9	I	29/47 (62%)	26 (90%)	2 (7%)	1 (3%)	5 16
9	V	29/47 (62%)	24 (83%)	5 (17%)	0	100 100
10	J	59/61 (97%)	55 (93%)	3 (5%)	1 (2%)	11 36
10	W	58/61 (95%)	54 (93%)	2 (3%)	2 (3%)	5 16
All	All	4000/4160 (96%)	3673 (92%)	275 (7%)	52 (1%)	15 44

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
2	B	26	ILE
2	B	226	ILE
2	B	227	ARG
2	B	389	SER
5	E	188	VAL
5	E	190	ASP
1	N	20	ASP
1	N	282	ARG
2	O	26	ILE
2	O	228	SER
2	O	389	SER
5	R	113	ASP
5	R	191	ASP
8	U	13	LEU
1	A	218	GLY
2	B	171	ALA
2	B	390	GLY
5	E	137	GLY
1	N	218	GLY
2	O	171	ALA
2	O	390	GLY
5	R	137	GLY
5	R	147	ILE
5	R	189	GLY
1	A	72	CYS
1	A	443	TRP
6	F	77	LYS

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Mol	Chain	Res	Type
1	N	72	CYS
1	N	262	TRP
1	N	443	TRP
5	R	149	ASN
1	A	262	TRP
5	R	110	ALA
6	S	77	LYS
10	W	56	LYS
2	B	29	LEU
5	E	141	HIS
10	J	56	LYS
6	S	11	ARG
10	W	61	ALA
2	B	220	ALA
2	B	231	GLY
2	O	29	LEU
5	E	189	GLY
1	A	71	PRO
2	B	265	GLY
5	E	120	PRO
2	O	231	GLY
9	I	48	PRO
1	N	71	PRO
5	R	188	VAL

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%)	355 (97%)	10 (3%)	52	85
1	N	365/368 (99%)	351 (96%)	14 (4%)	40	74
2	B	332/347 (96%)	327 (98%)	5 (2%)	72	93
2	O	333/347 (96%)	327 (98%)	6 (2%)	66	91
3	C	328/329 (100%)	323 (98%)	5 (2%)	72	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	P	328/329 (100%)	323 (98%)	5 (2%)	72 93
4	D	200/200 (100%)	197 (98%)	3 (2%)	72 93
4	Q	200/200 (100%)	197 (98%)	3 (2%)	72 93
5	E	166/166 (100%)	165 (99%)	1 (1%)	90 98
5	R	165/166 (99%)	159 (96%)	6 (4%)	42 76
6	F	93/96 (97%)	91 (98%)	2 (2%)	60 89
6	S	93/96 (97%)	90 (97%)	3 (3%)	46 80
7	G	71/71 (100%)	71 (100%)	0	100 100
7	T	69/71 (97%)	68 (99%)	1 (1%)	74 94
8	H	65/71 (92%)	64 (98%)	1 (2%)	72 93
8	U	63/71 (89%)	62 (98%)	1 (2%)	70 93
9	I	23/26 (88%)	22 (96%)	1 (4%)	35 70
9	V	23/26 (88%)	23 (100%)	0	100 100
10	J	49/49 (100%)	47 (96%)	2 (4%)	37 72
10	W	47/49 (96%)	46 (98%)	1 (2%)	61 90
All	All	3378/3446 (98%)	3308 (98%)	70 (2%)	61 90

All (70) 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	90	THR
1	A	106	MET
1	A	181	ASP
1	A	281	ASP
1	A	342	TRP
1	A	395	TRP
1	A	443	TRP
2	B	31	ASN
2	B	102	ARG
2	B	248	ASN
2	B	341	MET
2	B	402	ILE
3	C	5	ILE
3	C	91	PHE

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Mol	Chain	Res	Type
3	C	223	PRO
3	C	334	LEU
3	C	367	PHE
4	D	169	LEU
4	D	172	ASP
4	D	173	ASP
5	E	125	ASP
6	F	58	ARG
6	F	70	LEU
8	H	72	LYS
9	I	71	ASN
10	J	59	TYR
10	J	60	GLU
1	N	3	THR
1	N	18	THR
1	N	49	ASN
1	N	58	PHE
1	N	86	PHE
1	N	90	THR
1	N	106	MET
1	N	181	ASP
1	N	206	LYS
1	N	281	ASP
1	N	307	PHE
1	N	342	TRP
1	N	395	TRP
1	N	443	TRP
2	O	31	ASN
2	O	102	ARG
2	O	139	ASP
2	O	248	ASN
2	O	341	MET
2	O	402	ILE
3	P	5	ILE
3	P	91	PHE
3	P	223	PRO
3	P	334	LEU
3	P	367	PHE
4	Q	172	ASP
4	Q	173	ASP
4	Q	241	LYS
5	R	52	LYS

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Mol	Chain	Res	Type
5	R	113	ASP
5	R	125	ASP
5	R	126	ARG
5	R	187	PHE
5	R	191	ASP
6	S	14	ASP
6	S	58	ARG
6	S	70	LEU
7	T	2	ILE
8	U	72	LYS
10	W	59	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	118	GLN
1	A	126	GLN
1	A	147	ASN
1	A	173	ASN
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
1	A	339	GLN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	192	HIS
2	B	247	GLN
2	B	248	ASN
2	B	276	GLN
2	B	329	GLN
2	B	343	GLN
2	B	362	ASN
2	B	376	GLN
3	C	9	HIS
3	C	69	HIS
3	C	82	ASN
3	C	149	ASN
3	C	207	ASN
3	C	332	ASN
3	C	342	GLN

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Mol	Chain	Res	Type
4	D	35	GLN
4	D	50	ASN
4	D	71	GLN
4	D	148	HIS
4	D	200	GLN
5	E	3	ASN
5	E	57	GLN
5	E	164	HIS
5	E	186	GLN
6	F	79	GLN
7	G	23	GLN
7	G	44	GLN
7	G	79	ASN
8	H	71	HIS
8	H	75	ASN
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	85	HIS
1	N	118	GLN
1	N	126	GLN
1	N	143	ASN
1	N	147	ASN
1	N	173	ASN
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
1	N	339	GLN
2	O	31	ASN
2	O	156	GLN
2	O	192	HIS
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	329	GLN
2	O	343	GLN
2	O	362	ASN
2	O	376	GLN
3	P	9	HIS
3	P	69	HIS
3	P	82	ASN
3	P	207	ASN

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Mol	Chain	Res	Type
3	P	332	ASN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	71	GLN
4	Q	148	HIS
4	Q	200	GLN
5	R	3	ASN
5	R	57	GLN
5	R	164	HIS
6	S	79	GLN
7	T	44	GLN
7	T	79	ASN
8	U	71	HIS
8	U	75	ASN
10	W	8	GLN

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

Of 41 ligands modelled in this entry, 11 are unknown - leaving 30 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	PEE	A	2008	-	20,20,50	1.67	5 (25%)	21,25,55	0.64	0
14	FNM	C	2001	-	21,24,24	1.78	2 (9%)	21,34,34	1.93	2 (9%)
15	UQ	C	2002	-	19,19,63	2.46	11 (57%)	23,26,79	1.08	3 (13%)
11	PEE	C	2005	-	49,49,50	1.37	9 (18%)	50,54,55	0.90	5 (10%)
11	PEE	C	2007	-	47,47,50	1.18	6 (12%)	48,52,55	0.90	5 (10%)
16	AZI	C	2011	-	0,2,2	0.00	-	0,1,1	0.00	-
17	BOG	C	3010	-	10,11,20	0.84	1 (10%)	9,11,25	0.91	0
13	HEM	C	501	3	30,50,50	2.84	9 (30%)	24,82,82	2.27	7 (29%)
13	HEM	C	502	3	30,50,50	2.51	7 (23%)	24,82,82	2.25	6 (25%)
19	CDL	D	2003	-	41,41,99	1.12	1 (2%)	43,53,111	1.08	5 (11%)
17	BOG	D	2009	-	20,20,20	0.96	1 (5%)	25,25,25	0.95	2 (8%)
17	BOG	D	2091	-	20,20,20	1.10	2 (10%)	25,25,25	0.99	1 (4%)
18	HEC	D	501	4	24,50,50	1.63	3 (12%)	19,82,82	3.16	7 (36%)
20	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
19	CDL	G	2004	-	39,39,99	1.20	3 (7%)	41,51,111	1.12	4 (9%)
11	PEE	N	3008	-	4,4,50	3.66	4 (100%)	6,6,55	0.53	0
17	BOG	P	2010	-	18,18,20	1.16	3 (16%)	22,22,25	0.57	0
14	FNM	P	3001	-	21,24,24	1.79	3 (14%)	21,34,34	1.79	2 (9%)
15	UQ	P	3002	-	19,19,63	2.31	10 (52%)	23,26,79	1.06	3 (13%)
11	PEE	P	3005	-	49,49,50	1.36	9 (18%)	50,54,55	0.90	5 (10%)
11	PEE	P	3007	-	47,47,50	1.24	6 (12%)	48,52,55	0.86	4 (8%)
16	AZI	P	3011	-	0,2,2	0.00	-	0,1,1	0.00	-
13	HEM	P	501	3	30,50,50	2.82	9 (30%)	24,82,82	2.32	8 (33%)
13	HEM	P	502	3	30,50,50	2.61	9 (30%)	24,82,82	2.26	7 (29%)
19	CDL	Q	3003	-	41,41,99	1.17	2 (4%)	43,53,111	1.08	4 (9%)
17	BOG	Q	3009	-	20,20,20	0.93	1 (5%)	25,25,25	0.87	2 (8%)
17	BOG	Q	3091	-	20,20,20	1.12	2 (10%)	25,25,25	0.91	2 (8%)
18	HEC	Q	501	4	24,50,50	2.14	2 (8%)	19,82,82	3.06	6 (31%)
20	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
19	CDL	T	3004	-	39,39,99	1.20	3 (7%)	41,51,111	1.11	3 (7%)

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	2008	-	-	0/24/24/54	0/0/0/0
14	FNM	C	2001	-	-	0/12/31/31	0/3/3/3
15	UQ	C	2002	-	-	0/11/35/87	0/1/1/1
11	PEE	C	2005	-	-	0/53/53/54	0/0/0/0
11	PEE	C	2007	-	-	0/51/51/54	0/0/0/0
16	AZI	C	2011	-	-	0/0/0/0	0/0/0/0
17	BOG	C	3010	-	-	0/8/9/31	0/0/0/1
13	HEM	C	501	3	-	0/10/54/54	0/0/8/8
13	HEM	C	502	3	-	0/10/54/54	0/0/8/8
19	CDL	D	2003	-	-	0/51/51/110	0/0/0/0
17	BOG	D	2009	-	-	0/11/31/31	0/1/1/1
17	BOG	D	2091	-	-	0/11/31/31	0/1/1/1
18	HEC	D	501	4	-	0/6/54/54	0/0/8/8
20	FES	E	501	5	-	0/0/4/4	0/1/1/1
19	CDL	G	2004	-	-	0/49/49/110	0/0/0/0
11	PEE	N	3008	-	-	0/0/0/54	0/0/0/0
17	BOG	P	2010	-	-	0/6/26/31	0/1/1/1
14	FNM	P	3001	-	-	0/12/31/31	0/3/3/3
15	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	-	-	0/51/51/54	0/0/0/0
16	AZI	P	3011	-	-	0/0/0/0	0/0/0/0
13	HEM	P	501	3	-	0/10/54/54	0/0/8/8
13	HEM	P	502	3	-	0/10/54/54	0/0/8/8
19	CDL	Q	3003	-	-	0/51/51/110	0/0/0/0
17	BOG	Q	3009	-	-	0/11/31/31	0/1/1/1
17	BOG	Q	3091	-	-	0/11/31/31	0/1/1/1
18	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
20	FES	R	501	5	-	0/0/4/4	0/1/1/1
19	CDL	T	3004	-	-	0/49/49/110	0/0/0/0

All (123) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	501	HEM	C3B-CAB	-7.52	1.37	1.51
13	P	501	HEM	C3B-C4B	-7.25	1.45	1.51
13	C	501	HEM	C3B-C4B	-7.12	1.45	1.51
13	P	501	HEM	C3B-CAB	-6.98	1.38	1.51
18	Q	501	HEC	C3B-C2B	-6.87	1.33	1.40
13	P	502	HEM	C3B-C4B	-6.83	1.45	1.51
18	Q	501	HEC	C3C-C2C	-6.80	1.33	1.40
13	C	502	HEM	C2D-C3D	-6.48	1.35	1.54
13	C	502	HEM	C3B-CAB	-6.39	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	501	HEM	C2D-C3D	-5.86	1.36	1.54
13	P	501	HEM	C2D-C3D	-5.86	1.36	1.54
13	P	502	HEM	C3B-CAB	-5.80	1.40	1.51
13	P	502	HEM	C2D-C3D	-5.76	1.37	1.54
13	C	501	HEM	C3C-CAC	-5.64	1.40	1.51
13	C	502	HEM	C3C-CAC	-5.49	1.41	1.51
13	P	501	HEM	C3C-CAC	-5.22	1.41	1.51
13	P	502	HEM	C3C-CAC	-4.71	1.42	1.51
18	D	501	HEC	C3C-C2C	-4.69	1.35	1.40
18	D	501	HEC	C3B-C2B	-4.46	1.36	1.40
13	C	502	HEM	C2C-C1C	-4.46	1.44	1.52
13	C	501	HEM	C2C-C1C	-3.95	1.45	1.52
13	P	501	HEM	C2C-C1C	-3.76	1.45	1.52
13	C	501	HEM	C3D-C4D	-3.36	1.47	1.51
13	P	501	HEM	C3D-C4D	-3.34	1.47	1.51
13	P	502	HEM	C2C-C1C	-3.18	1.46	1.52
11	P	3007	PEE	C22-C21	-2.96	1.34	1.51
11	P	3005	PEE	C19-C18	-2.91	1.34	1.51
11	C	2005	PEE	C19-C18	-2.87	1.34	1.51
11	C	2007	PEE	C22-C21	-2.86	1.35	1.51
11	P	3007	PEE	C19-C18	-2.86	1.35	1.51
11	P	3005	PEE	C22-C21	-2.78	1.35	1.51
11	C	2005	PEE	C22-C21	-2.77	1.35	1.51
11	C	2007	PEE	C19-C18	-2.77	1.35	1.51
13	P	501	HEM	C2D-C1D	-2.58	1.43	1.51
13	C	501	HEM	C2D-C1D	-2.52	1.43	1.51
14	P	3001	FNM	C3-N2	-2.48	1.33	1.38
14	C	2001	FNM	C3-N2	-2.42	1.33	1.38
13	P	502	HEM	C2D-C1D	-2.21	1.44	1.51
13	P	502	HEM	C2B-C1B	-2.19	1.44	1.51
19	T	3004	CDL	OA8-CA6	-2.05	1.40	1.45
19	Q	3003	CDL	CA3-CA4	2.01	1.56	1.50
18	D	501	HEC	C4B-NB	2.01	1.39	1.36
11	P	3007	PEE	C3-C2	2.09	1.56	1.50
11	N	3008	PEE	P-O2P	2.09	1.62	1.54
11	A	2008	PEE	C1-C2	2.11	1.56	1.50
15	C	2002	UQ	C8-C9	2.12	1.37	1.33
19	Q	3003	CDL	O1-C1	2.13	1.49	1.43
19	D	2003	CDL	CA3-CA4	2.15	1.56	1.50
15	C	2002	UQ	C7-C8	2.16	1.54	1.50
11	C	2005	PEE	C11-C10	2.17	1.57	1.50
11	P	3005	PEE	C31-C30	2.18	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	P	3002	UQ	C5-C4	2.18	1.55	1.47
15	P	3002	UQ	O2-C2	2.18	1.42	1.37
17	Q	3009	BOG	O5-C1	2.19	1.47	1.41
19	G	2004	CDL	O1-C1	2.19	1.50	1.43
13	C	502	HEM	C1C-NC	2.21	1.38	1.36
15	P	3002	UQ	C3-C4	2.21	1.55	1.48
19	G	2004	CDL	CB3-CB4	2.24	1.57	1.50
17	P	2010	BOG	C4-C5	2.25	1.57	1.53
11	C	2007	PEE	C3-C2	2.25	1.57	1.50
11	P	3005	PEE	C11-C10	2.27	1.57	1.50
11	A	2008	PEE	C3-C2	2.27	1.57	1.50
17	D	2009	BOG	O5-C1	2.27	1.47	1.41
11	C	2005	PEE	C3-C2	2.29	1.57	1.50
11	P	3005	PEE	C1-C2	2.34	1.57	1.50
15	C	2002	UQ	C3-C4	2.34	1.55	1.48
11	C	2007	PEE	O2-C10	2.34	1.41	1.34
17	P	2010	BOG	C1-C2	2.35	1.57	1.52
11	C	2005	PEE	C1-C2	2.36	1.57	1.50
17	D	2091	BOG	C4-C5	2.38	1.58	1.53
11	C	2005	PEE	C31-C30	2.40	1.57	1.50
19	T	3004	CDL	O1-C1	2.40	1.50	1.43
15	C	2002	UQ	C5-C4	2.45	1.56	1.47
17	Q	3091	BOG	C4-C5	2.46	1.58	1.53
17	Q	3091	BOG	O5-C1	2.46	1.48	1.41
19	T	3004	CDL	CA3-CA4	2.47	1.57	1.50
11	P	3005	PEE	C3-C2	2.48	1.57	1.50
17	D	2091	BOG	O5-C1	2.49	1.48	1.41
17	C	3010	BOG	C2-C1	2.50	1.57	1.50
15	P	3002	UQ	C2-C1	2.51	1.56	1.48
11	N	3008	PEE	P-O3P	2.52	1.63	1.54
15	P	3002	UQ	C7-C8	2.53	1.54	1.50
15	P	3002	UQ	O3-C3	2.53	1.43	1.37
17	P	2010	BOG	O5-C1	2.55	1.47	1.43
14	P	3001	FNM	C26-C21	2.55	1.43	1.39
19	G	2004	CDL	CA3-CA4	2.57	1.58	1.50
11	C	2007	PEE	O3-C30	2.58	1.41	1.33
15	C	2002	UQ	O2-C2	2.60	1.43	1.37
11	P	3007	PEE	O2-C10	2.64	1.42	1.34
15	P	3002	UQ	CM5-C5	2.65	1.56	1.50
11	C	2007	PEE	P-O1P	2.69	1.61	1.51
11	P	3007	PEE	P-O1P	2.78	1.61	1.51
15	C	2002	UQ	O3-C3	2.80	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	3005	PEE	O3-C30	2.85	1.41	1.33
15	C	2002	UQ	C2-C1	2.85	1.57	1.48
11	A	2008	PEE	P-O1P	2.86	1.61	1.51
15	C	2002	UQ	CM5-C5	2.86	1.56	1.50
11	N	3008	PEE	P-O4P	2.92	1.65	1.54
11	P	3007	PEE	O3-C30	2.93	1.42	1.33
11	P	3005	PEE	P-O1P	2.94	1.61	1.51
11	A	2008	PEE	O2-C10	2.94	1.43	1.34
11	C	2005	PEE	P-O1P	2.99	1.62	1.51
11	P	3005	PEE	O2-C10	3.07	1.43	1.34
11	C	2005	PEE	O3-C30	3.07	1.42	1.33
11	C	2005	PEE	O2-C10	3.11	1.43	1.34
11	A	2008	PEE	O3-C30	3.16	1.42	1.33
13	C	502	HEM	CBC-CAC	3.39	1.48	1.29
13	C	501	HEM	CBC-CAC	3.43	1.49	1.29
15	P	3002	UQ	C6-C5	3.57	1.43	1.35
15	P	3002	UQ	C6-C1	3.61	1.56	1.46
13	C	501	HEM	CBB-CAB	3.64	1.50	1.29
13	P	501	HEM	CBC-CAC	3.81	1.51	1.29
15	C	2002	UQ	C6-C1	3.81	1.57	1.46
15	C	2002	UQ	C6-C5	3.85	1.44	1.35
13	P	502	HEM	CBC-CAC	3.88	1.51	1.29
13	P	501	HEM	CBB-CAB	4.03	1.52	1.29
13	C	502	HEM	CBB-CAB	4.07	1.52	1.29
13	P	502	HEM	CBB-CAB	4.60	1.55	1.29
15	P	3002	UQ	C7-C6	4.98	1.60	1.51
15	C	2002	UQ	C7-C6	5.12	1.60	1.51
11	N	3008	PEE	P-O1P	5.87	1.62	1.50
14	P	3001	FNM	C3-N4	6.31	1.33	1.28
14	C	2001	FNM	C3-N4	6.69	1.34	1.28

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Q	501	HEC	CBB-CAB-C3B	-7.55	110.58	127.35
18	D	501	HEC	CBB-CAB-C3B	-7.29	111.15	127.35
18	D	501	HEC	CBC-CAC-C3C	-6.07	113.87	127.35
18	Q	501	HEC	CBC-CAC-C3C	-5.64	114.81	127.35
13	C	501	HEM	CAA-C2A-C1A	-3.39	123.33	127.01
19	T	3004	CDL	CB4-OB6-CB5	-3.31	109.94	117.89
19	G	2004	CDL	CB4-OB6-CB5	-3.25	110.08	117.89
13	P	501	HEM	CAA-C2A-C1A	-3.18	123.55	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Q	501	HEC	CAA-C2A-C3A	-2.72	121.22	129.00
18	D	501	HEC	CAA-C2A-C3A	-2.68	121.35	129.00
19	D	2003	CDL	CB4-OB6-CB5	-2.65	111.54	117.89
19	Q	3003	CDL	CB4-OB6-CB5	-2.56	111.74	117.89
15	C	2002	UQ	C7-C6-C1	-2.46	115.66	118.56
19	D	2003	CDL	CA6-OA8-CA7	-2.33	111.24	117.14
15	P	3002	UQ	C7-C6-C1	-2.33	115.81	118.56
18	D	501	HEC	CAD-C3D-C2D	-2.33	122.36	129.00
19	Q	3003	CDL	CA4-OA6-CA5	-2.29	112.40	117.89
19	D	2003	CDL	CA6-CA4-CA3	-2.28	106.73	112.07
19	G	2004	CDL	CA4-OA6-CA5	-2.26	112.46	117.89
13	C	502	HEM	CMA-C3A-C4A	-2.25	124.63	128.36
19	Q	3003	CDL	CA6-OA8-CA7	-2.22	111.52	117.14
15	P	3002	UQ	C10-C9-C8	-2.20	119.17	123.50
19	Q	3003	CDL	CA6-CA4-CA3	-2.17	106.99	112.07
19	D	2003	CDL	CA4-OA6-CA5	-2.07	112.92	117.89
19	T	3004	CDL	CB6-CB4-CB3	-2.05	107.27	112.07
19	T	3004	CDL	CA4-OA6-CA5	-2.05	112.97	117.89
15	C	2002	UQ	C10-C9-C8	-2.05	119.48	123.50
19	G	2004	CDL	CB6-CB4-CB3	-2.03	107.32	112.07
19	D	2003	CDL	CB6-CB4-CB3	-2.02	107.36	112.07
11	C	2005	PEE	O3-C3-C2	2.03	114.14	108.69
19	G	2004	CDL	OB6-CB4-CB3	2.05	115.57	108.36
13	P	502	HEM	CBA-CAA-C2A	2.09	116.27	112.53
11	P	3005	PEE	O3-C3-C2	2.10	114.34	108.69
11	C	2007	PEE	O3-C3-C2	2.11	114.38	108.69
11	P	3007	PEE	C23-C22-C21	2.20	125.87	114.53
13	P	502	HEM	C3B-CAB-CBB	2.20	127.83	124.46
11	C	2007	PEE	C23-C22-C21	2.30	126.42	114.53
17	Q	3091	BOG	O1-C1-C2	2.35	111.00	108.04
11	P	3005	PEE	C23-C22-C21	2.36	126.71	114.53
13	P	501	HEM	C3C-CAC-CBC	2.37	128.09	124.46
17	Q	3009	BOG	O1-C1-C2	2.37	111.03	108.04
11	C	2005	PEE	C23-C22-C21	2.40	126.91	114.53
11	P	3007	PEE	C22-C21-C20	2.42	127.03	114.53
11	C	2005	PEE	C22-C21-C20	2.44	127.12	114.53
11	C	2007	PEE	C22-C21-C20	2.44	127.15	114.53
11	P	3005	PEE	C22-C21-C20	2.48	127.33	114.53
11	P	3007	PEE	C19-C18-C17	2.49	127.38	114.53
11	C	2005	PEE	C19-C18-C17	2.49	127.41	114.53
11	C	2007	PEE	C19-C18-C17	2.53	127.61	114.53
11	P	3005	PEE	C19-C18-C17	2.54	127.66	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	P	3005	PEE	C20-C19-C18	2.63	128.12	114.53
17	D	2009	BOG	O1-C1-C2	2.64	111.37	108.04
13	P	502	HEM	CMD-C2D-C3D	2.65	126.07	114.35
11	C	2005	PEE	C20-C19-C18	2.67	128.33	114.53
17	Q	3009	BOG	C1'-O1-C1	2.72	118.70	113.94
11	P	3007	PEE	C20-C19-C18	2.73	128.60	114.53
13	C	502	HEM	CMD-C2D-C3D	2.73	126.41	114.35
11	C	2007	PEE	C20-C19-C18	2.74	128.69	114.53
13	P	501	HEM	C2D-C3D-C4D	2.78	106.21	101.50
15	P	3002	UQ	C8-C7-C6	2.78	119.98	111.64
13	P	501	HEM	CMD-C2D-C3D	2.85	126.97	114.35
17	Q	3091	BOG	C1'-O1-C1	2.95	119.10	113.94
15	C	2002	UQ	C8-C7-C6	2.96	120.53	111.64
17	D	2009	BOG	C1'-O1-C1	3.17	119.48	113.94
13	C	501	HEM	CAD-C3D-C2D	3.21	122.45	113.22
13	C	501	HEM	CMD-C2D-C3D	3.25	128.72	114.35
13	C	501	HEM	C2D-C3D-C4D	3.34	107.16	101.50
13	C	502	HEM	CAD-C3D-C2D	3.34	122.83	113.22
13	P	502	HEM	CAD-C3D-C2D	3.39	122.95	113.22
14	C	2001	FNM	C21-N1-N2	3.40	123.27	116.01
14	P	3001	FNM	C21-N1-N2	3.47	123.42	116.01
17	D	2091	BOG	C1'-O1-C1	3.67	120.36	113.94
13	P	501	HEM	CAD-C3D-C2D	3.80	124.13	113.22
18	Q	501	HEC	CAD-C3D-C4D	3.88	131.22	127.01
13	C	501	HEM	CMC-C2C-C3C	3.95	126.38	116.53
13	P	501	HEM	CMC-C2C-C3C	4.41	127.54	116.53
13	P	502	HEM	CMC-C2C-C3C	4.43	127.60	116.53
13	C	501	HEM	CMB-C2B-C3B	4.64	128.12	116.53
18	D	501	HEC	CAA-C2A-C1A	4.69	132.10	127.01
13	C	502	HEM	CMB-C2B-C3B	4.69	128.25	116.53
13	P	501	HEM	CAD-C3D-C4D	4.84	129.54	112.47
13	C	502	HEM	CMC-C2C-C3C	5.03	129.08	116.53
13	C	501	HEM	CAD-C3D-C4D	5.03	130.21	112.47
13	P	501	HEM	CMB-C2B-C3B	5.13	129.33	116.53
18	Q	501	HEC	CBA-CAA-C2A	5.19	121.83	112.53
18	Q	501	HEC	CAA-C2A-C1A	5.22	132.67	127.01
18	D	501	HEC	CBA-CAA-C2A	5.22	121.89	112.53
13	P	502	HEM	CMB-C2B-C3B	5.42	130.06	116.53
13	P	502	HEM	CAD-C3D-C4D	5.61	132.25	112.47
18	D	501	HEC	CAD-C3D-C4D	5.83	133.34	127.01
13	C	502	HEM	CAD-C3D-C4D	6.17	134.23	112.47
14	P	3001	FNM	C27-S3-C3	7.03	109.64	100.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	C	2001	FNM	C27-S3-C3	7.81	110.67	100.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	2008	PEE	1	0
14	C	2001	FNM	2	0
15	C	2002	UQ	4	0
13	C	501	HEM	1	0
13	C	502	HEM	4	0
19	D	2003	CDL	2	0
17	D	2009	BOG	1	0
17	D	2091	BOG	1	0
18	D	501	HEC	3	0
20	E	501	FES	1	0
19	G	2004	CDL	1	0
17	P	2010	BOG	1	0
14	P	3001	FNM	1	0
15	P	3002	UQ	3	0
11	P	3007	PEE	1	0
13	P	501	HEM	1	0
13	P	502	HEM	4	0
19	Q	3003	CDL	3	0
17	Q	3091	BOG	1	0
18	Q	501	HEC	1	0
20	R	501	FES	2	0
19	T	3004	CDL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	443/446 (99%)	0.17	9 (2%) 68 58	29, 61, 87, 104	0
1	N	442/446 (99%)	0.34	21 (4%) 34 23	39, 69, 95, 104	0
2	B	421/441 (95%)	0.43	24 (5%) 27 17	50, 78, 116, 141	0
2	O	422/441 (95%)	0.30	17 (4%) 42 30	37, 74, 106, 120	0
3	C	380/380 (100%)	0.20	1 (0%) 94 92	21, 39, 73, 109	0
3	P	379/380 (99%)	0.23	5 (1%) 79 71	30, 62, 84, 96	0
4	D	241/241 (100%)	0.04	3 (1%) 81 73	30, 42, 78, 94	0
4	Q	241/241 (100%)	0.28	10 (4%) 41 29	50, 69, 99, 119	0
5	E	196/196 (100%)	1.18	56 (28%) 1 0	38, 88, 119, 125	0
5	R	196/196 (100%)	2.54	92 (46%) 0 0	42, 112, 159, 163	127 (64%)
6	F	101/110 (91%)	-0.11	0 100 100	29, 42, 60, 96	0
6	S	101/110 (91%)	0.29	4 (3%) 42 30	55, 68, 111, 135	0
7	G	81/81 (100%)	0.33	2 (2%) 61 48	32, 52, 93, 108	0
7	T	78/81 (96%)	0.82	10 (12%) 5 2	48, 82, 144, 161	0
8	H	70/77 (90%)	0.20	2 (2%) 55 43	39, 59, 84, 123	0
8	U	67/77 (87%)	1.14	13 (19%) 1 1	96, 115, 133, 140	0
9	I	31/47 (65%)	2.15	15 (48%) 0 0	81, 105, 125, 126	0
9	V	31/47 (65%)	2.10	13 (41%) 0 0	69, 109, 142, 145	0
10	J	61/61 (100%)	0.44	5 (8%) 14 7	44, 60, 92, 130	0
10	W	60/61 (98%)	1.06	5 (8%) 14 7	56, 77, 99, 111	0
All	All	4042/4160 (97%)	0.48	307 (7%) 17 9	21, 65, 116, 163	127 (3%)

All (307) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	R	193	VAL	14.2
5	R	195	VAL	13.9
5	R	133	VAL	13.8
10	W	62	SER	11.7
10	W	63	GLU	11.2
5	R	132	TRP	11.2
5	R	130	PRO	11.1
5	R	114	VAL	11.0
5	R	127	VAL	8.6
5	R	109	GLU	8.3
5	R	98	VAL	8.3
5	R	79	SER	7.8
5	R	115	SER	7.8
7	T	77	TYR	7.8
9	V	63	ASP	7.7
5	R	99	ARG	7.7
5	R	87	VAL	7.6
7	G	1	GLY	7.4
5	E	133	VAL	7.2
5	R	192	LEU	7.1
5	R	80	ASP	7.0
5	R	191	ASP	6.8
8	H	9	GLU	6.7
5	R	175	PRO	6.6
5	R	131	GLU	6.6
5	R	116	LYS	6.5
5	R	117	LEU	6.4
5	R	93	GLY	6.1
2	O	23	ASP	6.1
5	R	185	TYR	6.1
2	B	226	ILE	5.9
4	D	241	LYS	5.9
2	B	236	LYS	5.8
5	R	194	VAL	5.7
5	R	176	ALA	5.7
1	A	2	ALA	5.7
5	R	106	ILE	5.7
5	R	160	CYS	5.7
7	T	78	GLU	5.6
3	C	1	MET	5.5
5	R	100	HIS	5.5
5	R	174	GLY	5.5
5	R	112	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
5	R	162	GLY	5.4
5	R	81	ILE	5.3
5	R	177	PRO	5.2
1	N	218	GLY	5.2
5	R	86	ASN	5.1
5	R	119	ASP	5.1
5	R	172	ARG	5.1
5	R	163	SER	5.1
5	R	74	ILE	5.1
2	O	19	PRO	5.1
8	H	10	GLU	5.0
5	R	108	GLN	5.0
5	R	113	ASP	5.0
5	R	184	THR	4.9
5	R	78	LEU	4.9
5	E	195	VAL	4.8
9	V	77	ARG	4.8
5	R	183	PRO	4.8
5	E	74	ILE	4.8
5	R	164	HIS	4.7
5	E	132	TRP	4.6
5	R	120	PRO	4.6
5	R	76	ILE	4.6
5	R	89	PHE	4.5
5	E	188	VAL	4.5
9	I	47	ARG	4.4
10	J	64	GLU	4.4
5	R	128	LYS	4.4
10	J	63	GLU	4.3
5	R	153	PHE	4.2
2	B	402	ILE	4.2
9	I	51	CYS	4.2
4	Q	139	ALA	4.2
5	E	81	ILE	4.2
5	R	118	ARG	4.1
5	R	110	ALA	4.1
2	O	299	VAL	4.0
5	R	122	HIS	4.0
10	W	61	ALA	4.0
5	R	134	ILE	4.0
5	E	80	ASP	4.0
5	R	104	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
8	U	49	HIS	4.0
5	E	76	ILE	4.0
5	R	123	ASP	4.0
6	S	15	ARG	4.0
9	I	63	ASP	4.0
5	R	173	LYS	3.9
7	T	74	PRO	3.9
5	E	109	GLU	3.8
8	U	44	VAL	3.8
5	R	126	ARG	3.8
9	I	50	LEU	3.8
1	A	69	LYS	3.7
4	Q	143	VAL	3.7
5	E	122	HIS	3.7
5	R	94	LYS	3.7
5	R	105	GLU	3.7
2	O	24	LEU	3.6
5	R	189	GLY	3.6
5	E	110	ALA	3.6
5	E	114	VAL	3.6
5	E	101	ARG	3.6
9	V	76	VAL	3.6
4	Q	241	LYS	3.6
5	E	187	PHE	3.6
8	U	13	LEU	3.5
9	V	50	LEU	3.5
5	R	155	GLY	3.5
9	I	53	GLU	3.5
5	E	85	LYS	3.5
7	T	79	ASN	3.5
5	E	89	PHE	3.4
5	E	174	GLY	3.4
5	R	95	PRO	3.4
5	E	178	TYR	3.4
5	R	102	THR	3.4
5	R	136	VAL	3.4
5	E	98	VAL	3.4
9	V	70	LEU	3.4
5	R	159	PRO	3.4
1	N	122	LEU	3.4
5	E	186	GLN	3.3
8	U	54	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
5	E	106	ILE	3.3
5	R	178	TYR	3.3
9	V	59	SER	3.3
2	B	124	LEU	3.2
5	R	129	LYS	3.2
3	P	156	TYR	3.2
5	E	185	TYR	3.2
1	A	4	TYR	3.2
3	P	373	LEU	3.2
9	V	62	ARG	3.2
2	O	368	TYR	3.1
1	N	182	LEU	3.1
5	E	86	ASN	3.1
5	E	112	VAL	3.1
5	E	194	VAL	3.1
5	E	100	HIS	3.1
5	E	118	ARG	3.1
5	E	111	GLU	3.1
5	E	131	GLU	3.1
5	E	193	VAL	3.1
2	B	224	LEU	3.1
2	B	205	ALA	3.0
9	I	60	ALA	3.0
5	R	156	TYR	3.0
6	S	12	LEU	3.0
5	R	111	GLU	3.0
1	A	226	ASP	3.0
7	T	75	ALA	3.0
9	I	77	ARG	3.0
5	E	84	GLY	3.0
5	R	121	GLN	3.0
9	V	60	ALA	2.9
2	B	33	LEU	2.9
10	J	61	ALA	2.9
9	I	62	ARG	2.9
2	B	232	THR	2.9
5	R	182	VAL	2.9
5	E	72	SER	2.9
5	R	72	SER	2.9
6	S	11	ARG	2.9
2	O	402	ILE	2.9
2	O	207	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	O	383	GLY	2.8
1	N	75	PHE	2.8
2	B	439	LEU	2.8
5	E	99	ARG	2.8
5	E	192	LEU	2.8
6	S	90	LEU	2.8
5	E	156	TYR	2.8
5	E	149	ASN	2.8
5	R	84	GLY	2.8
4	Q	9	ALA	2.8
2	B	204	MET	2.8
5	R	171	ILE	2.8
5	E	75	GLU	2.7
5	E	83	GLU	2.7
2	B	400	GLN	2.7
1	N	127	ILE	2.7
4	D	143	VAL	2.7
8	U	26	GLN	2.7
1	N	124	GLU	2.7
7	T	24	ARG	2.7
2	O	22	GLU	2.7
2	B	223	PHE	2.7
7	T	26	ILE	2.7
9	V	57	GLY	2.7
5	E	130	PRO	2.7
5	R	187	PHE	2.7
5	R	140	THR	2.7
1	A	392	LEU	2.6
5	R	125	ASP	2.6
9	V	55	MET	2.6
4	Q	145	GLU	2.6
8	U	24	CYS	2.6
1	A	444	ILE	2.6
5	E	177	PRO	2.6
4	D	2	GLU	2.6
5	R	124	LEU	2.6
2	O	268	GLU	2.6
2	O	266	SER	2.6
2	B	417	PHE	2.6
1	A	21	ASN	2.5
5	E	102	THR	2.5
10	J	62	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	190	PHE	2.5
9	I	54	SER	2.5
9	I	70	LEU	2.5
8	U	61	PHE	2.5
5	E	78	LEU	2.5
5	R	161	HIS	2.5
5	E	126	ARG	2.5
1	N	216	PHE	2.5
4	Q	147	LEU	2.4
9	I	72	ALA	2.4
3	P	346	HIS	2.4
4	Q	171	TYR	2.4
5	E	180	LEU	2.4
5	R	88	ALA	2.4
5	E	124	LEU	2.4
9	I	52	ARG	2.4
5	E	163	SER	2.4
2	B	120	MET	2.4
1	N	223	TYR	2.4
1	N	174	ILE	2.4
4	Q	141	VAL	2.4
2	O	28	LYS	2.4
2	O	307	PHE	2.4
10	W	35	PHE	2.4
1	A	8	LEU	2.4
1	N	62	LEU	2.4
4	Q	138	PRO	2.4
5	E	153	PHE	2.4
1	N	57	TYR	2.4
5	R	85	LYS	2.4
2	B	419	SER	2.3
1	N	50	GLU	2.3
5	R	181	GLU	2.3
7	T	69	LEU	2.3
8	U	12	GLU	2.3
5	E	190	ASP	2.3
5	R	154	GLY	2.3
10	W	32	GLU	2.3
8	U	50	THR	2.3
5	E	137	GLY	2.3
5	E	136	VAL	2.3
5	E	73	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	N	178	THR	2.3
7	T	53	LEU	2.3
8	U	35	GLU	2.3
9	V	47	ARG	2.3
1	N	185	TYR	2.3
9	I	69	SER	2.2
5	R	103	GLN	2.2
1	N	354	VAL	2.2
5	E	90	LYS	2.2
2	B	350	GLY	2.2
5	R	97	PHE	2.2
1	A	405	ARG	2.2
10	J	60	GLU	2.2
4	Q	40	CYS	2.2
9	V	51	CYS	2.2
8	U	39	LEU	2.2
9	I	56	SER	2.2
2	O	303	THR	2.2
3	P	345	GLU	2.2
1	N	179	ARG	2.1
5	R	101	ARG	2.1
1	N	123	GLU	2.1
3	P	43	MET	2.1
1	N	52	ASN	2.1
2	O	250	HIS	2.1
5	R	152	ASP	2.1
2	B	369	LEU	2.1
5	E	172	ARG	2.1
7	T	38	TRP	2.1
9	V	53	GLU	2.1
2	B	397	VAL	2.1
2	B	398	VAL	2.1
7	G	30	PHE	2.1
5	R	144	CYS	2.1
2	B	200	THR	2.1
5	R	145	VAL	2.1
2	O	416	LYS	2.1
5	E	173	LYS	2.1
2	O	209	ILE	2.1
1	N	69	LYS	2.1
8	U	72	LYS	2.1
5	R	75	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	N	55	ALA	2.1
5	R	179	ASN	2.0
2	B	274	VAL	2.0
9	I	48	PRO	2.0
5	R	141	HIS	2.0
2	B	230	ALA	2.0
5	R	157	TYR	2.0
2	B	80	ALA	2.0
5	E	165	TYR	2.0
8	U	29	LYS	2.0
2	B	233	SER	2.0
5	E	191	ASP	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
12	UNL	P	3046	2/-	0.83	0.72	32.14	85,85,85,85	0
16	AZI	P	3011	3/3	0.91	0.50	19.13	74,74,76,77	0
12	UNL	C	2048	2/-	0.89	0.41	18.33	62,62,62,63	0
12	UNL	C	2046	2/-	0.76	0.51	14.42	87,87,87,91	0
17	BOG	D	2091	20/20	0.24	0.60	13.76	177,189,190,190	0
16	AZI	C	2011	3/3	0.83	0.50	11.18	68,68,69,71	0
17	BOG	P	2010	19/20	0.59	0.47	9.94	102,183,184,184	0
11	PEE	P	3007	48/51	0.90	0.36	7.50	76,90,105,106	0
15	UQ	C	2002	19/63	0.83	0.33	4.74	85,87,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
15	UQ	P	3002	19/63	0.84	0.39	4.70	138,141,143,143	0
11	PEE	C	2005	50/51	0.83	0.32	2.77	83,93,101,104	0
19	CDL	G	2004	40/100	0.91	0.22	2.59	60,70,85,86	0
11	PEE	C	2007	48/51	0.95	0.23	2.38	41,52,81,82	0
11	PEE	P	3005	50/51	0.83	0.31	2.17	74,100,105,105	0
12	UNL	A	3015	1/-	0.92	0.21	1.92	48,48,48,48	0
12	UNL	P	3048	2/-	0.61	0.25	1.83	92,92,92,95	0
19	CDL	Q	3003	42/100	0.84	0.26	1.62	119,124,137,138	0
11	PEE	A	2008	21/51	0.88	0.24	1.23	95,113,116,118	0
19	CDL	D	2003	42/100	0.87	0.21	0.97	81,93,97,98	0
14	FNM	P	3001	22/22	0.96	0.22	0.83	49,53,59,62	0
17	BOG	D	2009	20/20	0.90	0.20	0.77	56,63,65,67	0
17	BOG	C	3010	12/20	0.86	0.35	0.65	94,96,97,98	0
19	CDL	T	3004	40/100	0.87	0.21	0.63	94,97,106,107	0
18	HEC	D	501	43/43	0.98	0.18	0.17	23,30,35,37	0
17	BOG	Q	3009	20/20	0.90	0.19	0.14	71,79,81,82	0
13	HEM	P	501	43/43	0.98	0.21	0.02	40,43,54,58	0
13	HEM	C	502	43/43	0.99	0.19	-0.00	23,26,33,39	0
13	HEM	P	502	43/43	0.98	0.17	-0.11	34,40,55,62	0
13	HEM	C	501	43/43	0.99	0.22	-0.11	23,31,38,43	0
14	FNM	C	2001	22/22	0.98	0.18	-0.22	38,40,42,44	0
18	HEC	Q	501	43/43	0.96	0.18	-0.26	47,55,64,66	0
20	FES	R	501	4/4	0.96	0.17	-1.30	106,106,106,107	4
20	FES	E	501	4/4	0.98	0.11	-1.49	83,84,85,86	0
12	UNL	P	3013	1/-	0.92	0.30	-	56,56,56,56	0
12	UNL	D	2012	2/-	0.77	0.32	-	59,59,59,60	0
12	UNL	P	3014	1/-	0.85	0.31	-	55,55,55,55	0
17	BOG	Q	3091	20/20	0.28	0.64	-	178,186,187,187	0
12	UNL	C	2047	1/-	0.96	0.35	-	34,34,34,34	0
12	UNL	P	3047	1/-	0.76	0.28	-	47,47,47,47	0
12	UNL	R	3012	1/-	0.94	0.19	-	38,38,38,38	0
11	PEE	N	3008	5/51	0.95	0.15	-	88,88,89,89	0

6.5 Other polymers (i)

There are no such residues in this entry.