Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:15 AM GMT

PDB ID	:	3L74
Title	:	Cytochrome BC1 complex from chicken with famoxadone bound
Authors	:	Huang, L.; Berry, E.A.
Deposited on	:	2009-12-28
Resolution	:	2.76 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:

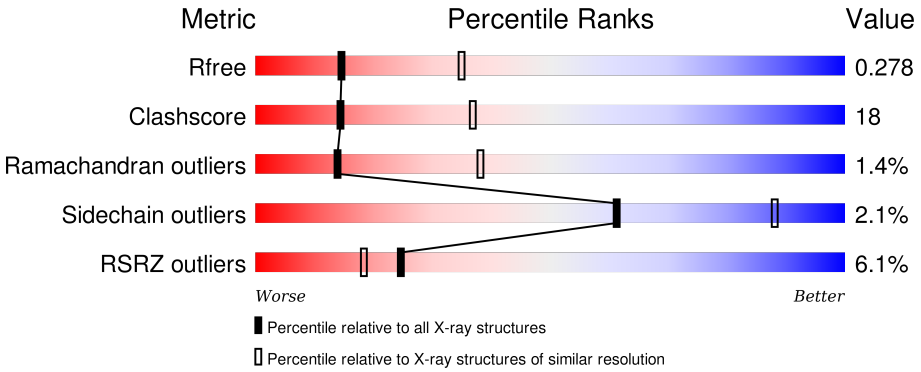
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.76 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	% 62% 35%
1	N	446	4% 60% 36%
2	B	441	6% 54% 39% 5%
2	O	441	3% 56% 38%
3	C	380	78% 22%

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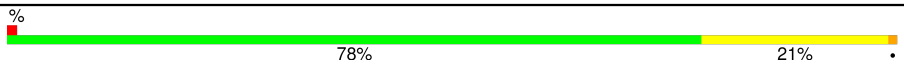
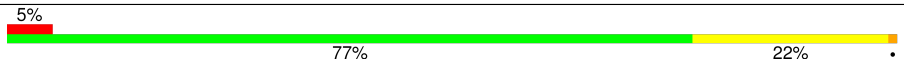
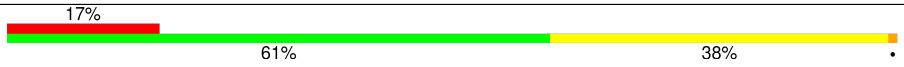
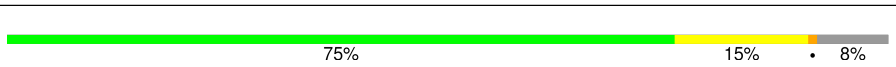
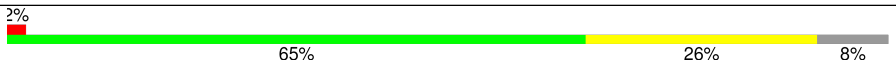
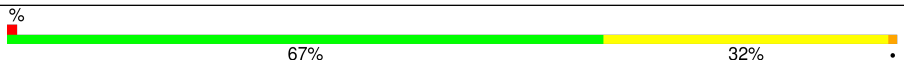
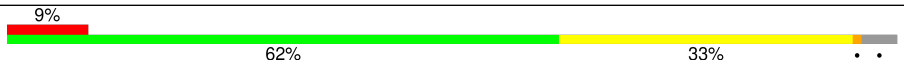
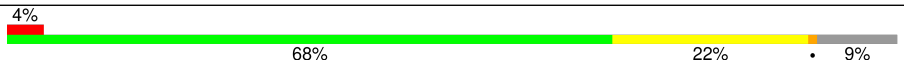
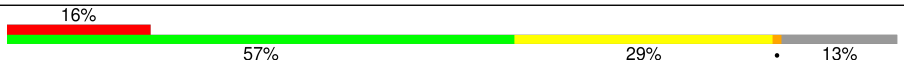
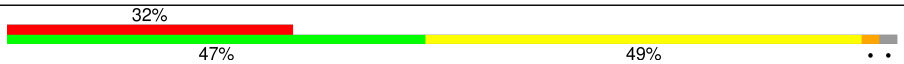
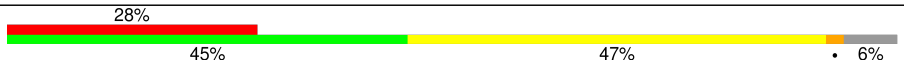
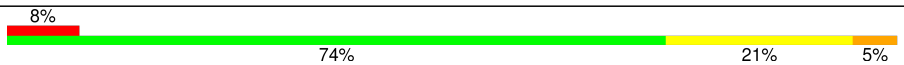
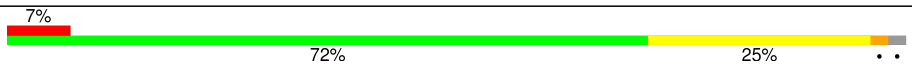
Mol	Chain	Length	Quality of chain
3	P	380	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	47	
9	V	47	
10	J	61	
10	W	61	

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	A	2005	-	-	-	X
11	PEE	C	2007	-	-	-	X
11	PEE	N	3005	-	-	-	X
11	PEE	N	3008	-	X	-	-
11	PEE	P	3007	-	-	-	X
12	UNL	A	3015	-	-	-	X
12	UNL	C	2046	-	-	-	X
12	UNL	C	2047	-	-	-	X
12	UNL	C	2048	-	-	-	X
12	UNL	P	3046	-	-	-	X
12	UNL	P	3048	-	-	-	X
15	UQ	C	2002	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	UQ	P	3002	-	-	-	X
16	AZI	C	2011	-	-	-	X
16	AZI	P	3011	-	-	-	X
17	BOG	D	2091	-	-	-	X
17	BOG	P	2010	-	-	-	X
19	CDL	G	2004	-	-	-	X

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32703 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			

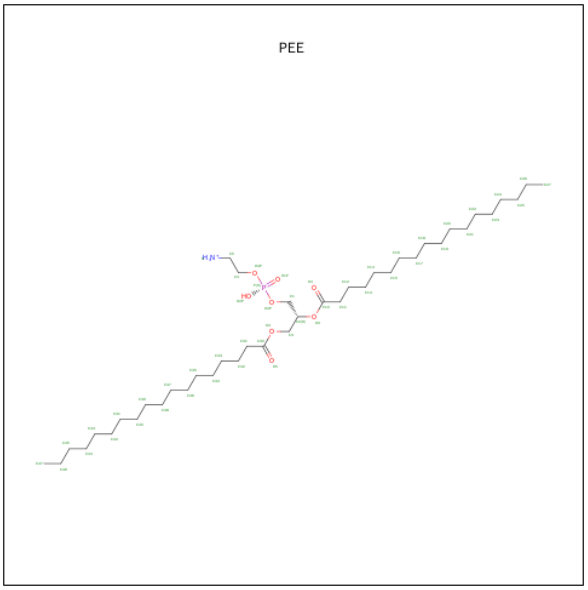
- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

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 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	C	1	Total C O P 21 12 8 1	0	0
11	N	1	Total C N O P 50 40 1 8 1	0	0
11	N	1	Total O P 5 4 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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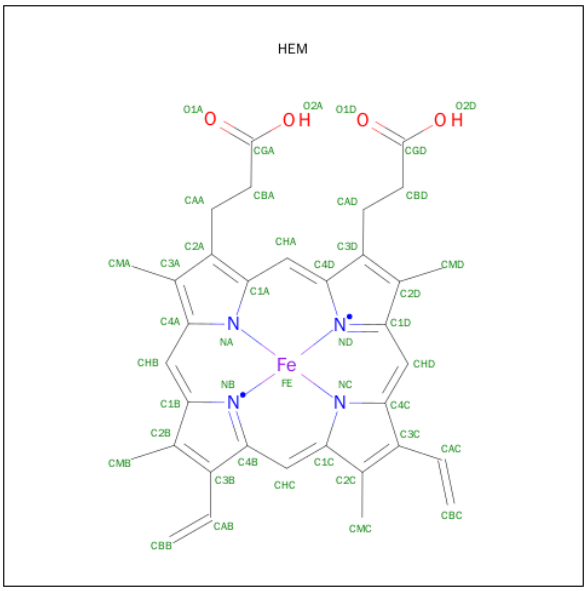
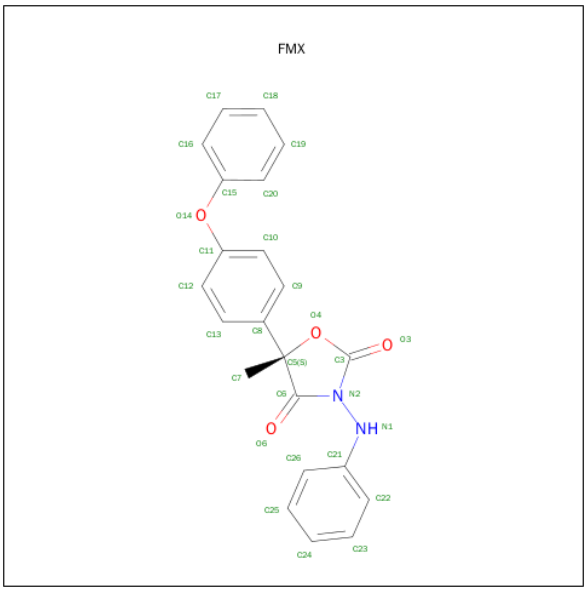
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	Q	1	Total O 1 1	0	0
12	A	1	Total O 1 1	0	0
12	C	3	Total O 5 5	0	0
12	E	1	Total O 2 2	0	0

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



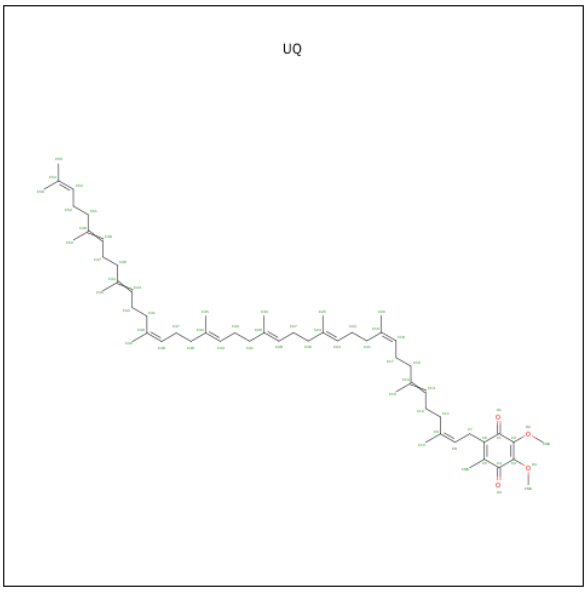
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C Fe N O 43 34 1 4 4	0	0
13	C	1	Total C Fe N O 43 34 1 4 4	0	0
13	P	1	Total C Fe N O 43 34 1 4 4	0	0
13	P	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 14 is FAMOXADONE (three-letter code: FMX) (formula: $C_{22}H_{18}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	N	O	0	0
			28	22	2	4		
14	P	1	Total	C	N	O	0	0
			28	22	2	4		

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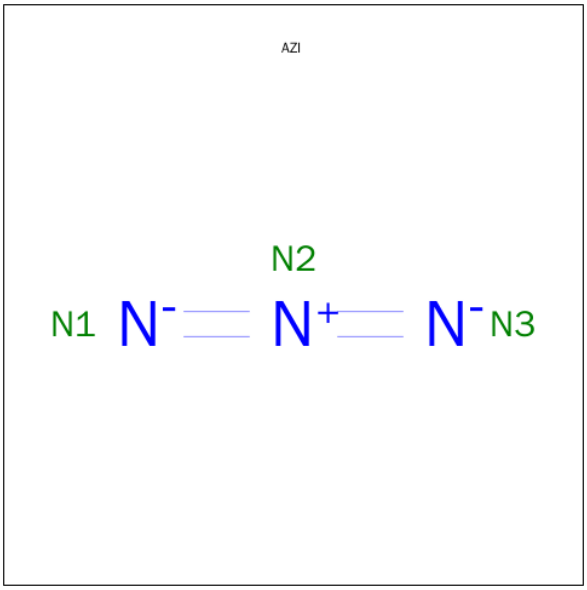
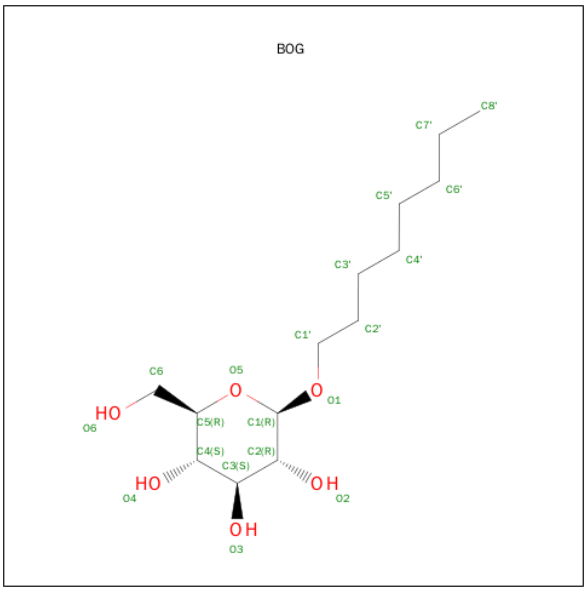
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	P	1	Total C O 19 15 4	0	0

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



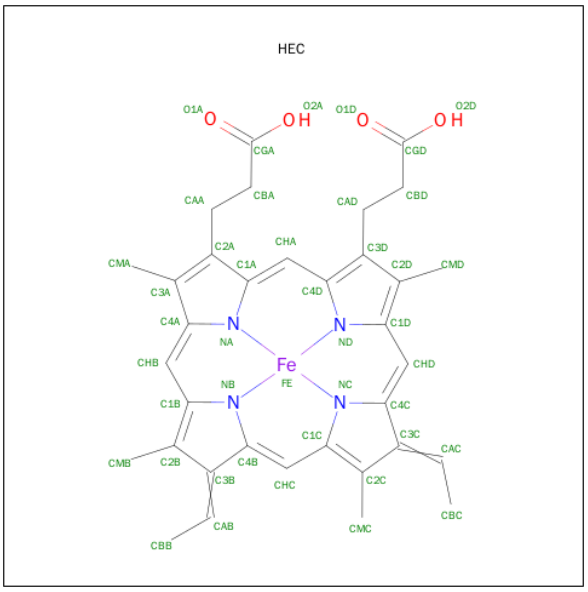
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total N 3 3	0	0
16	P	1	Total N 3 3	0	0

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



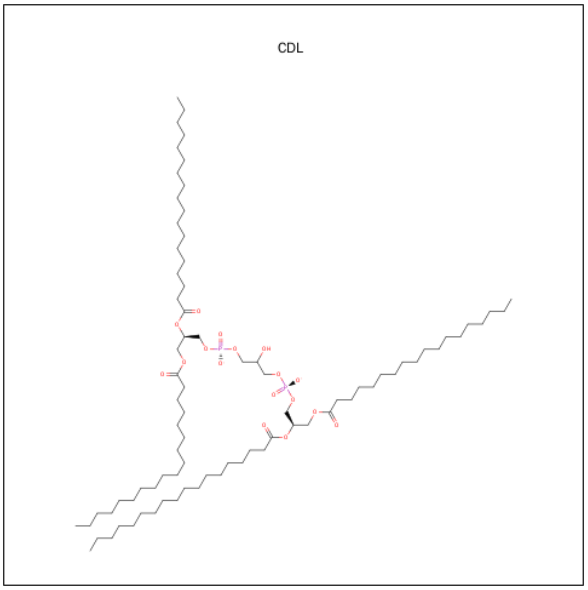
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	C	1	Total C O 12 10 2	0	0
17	D	1	Total C O 20 14 6	0	0
17	D	1	Total C O 20 14 6	0	0
17	P	1	Total C O 19 13 6	0	0
17	Q	1	Total C O 20 14 6	0	0
17	Q	1	Total C O 20 14 6	0	0

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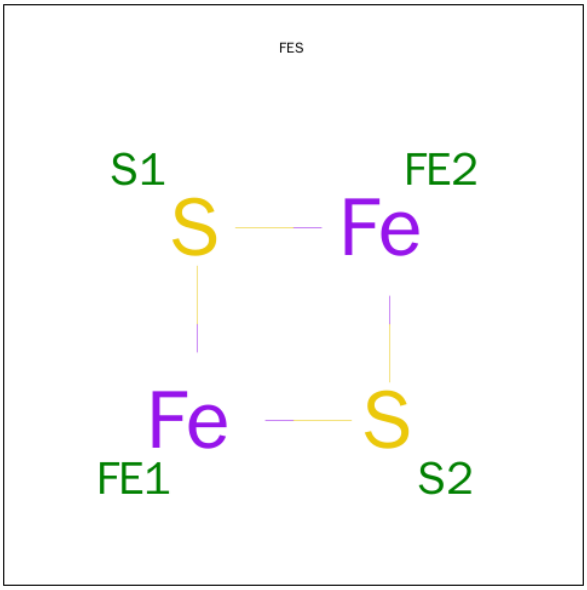
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	Q	1	Total C O P 42 23 17 2	0	0
19	T	1	Total C O P 40 21 17 2	0	0

- 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.

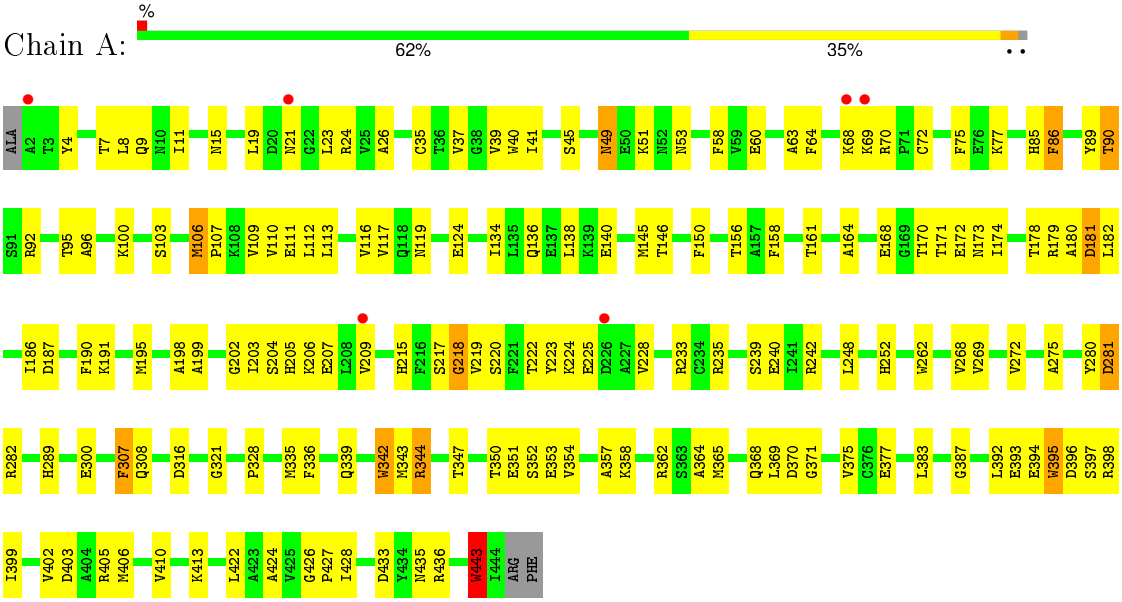
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	2	Total O 2 2	0	0
21	C	9	Total O 9 9	0	0
21	E	1	Total O 1 1	0	0
21	P	12	Total O 12 12	0	0
21	R	4	Total O 4 4	0	0

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.

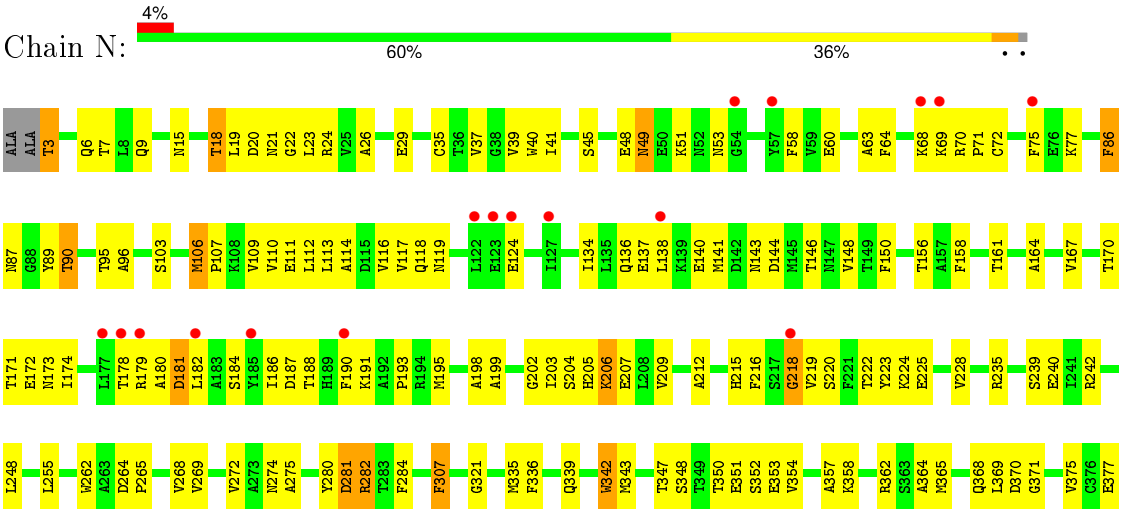
• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

Chain A:



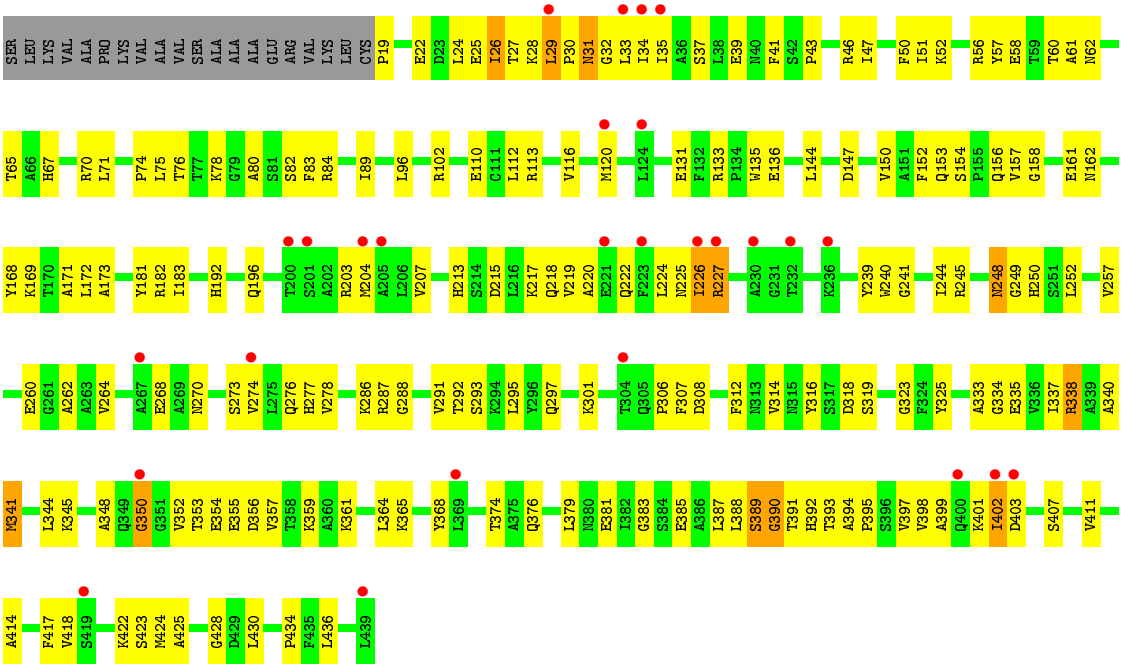
• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

Chain N:



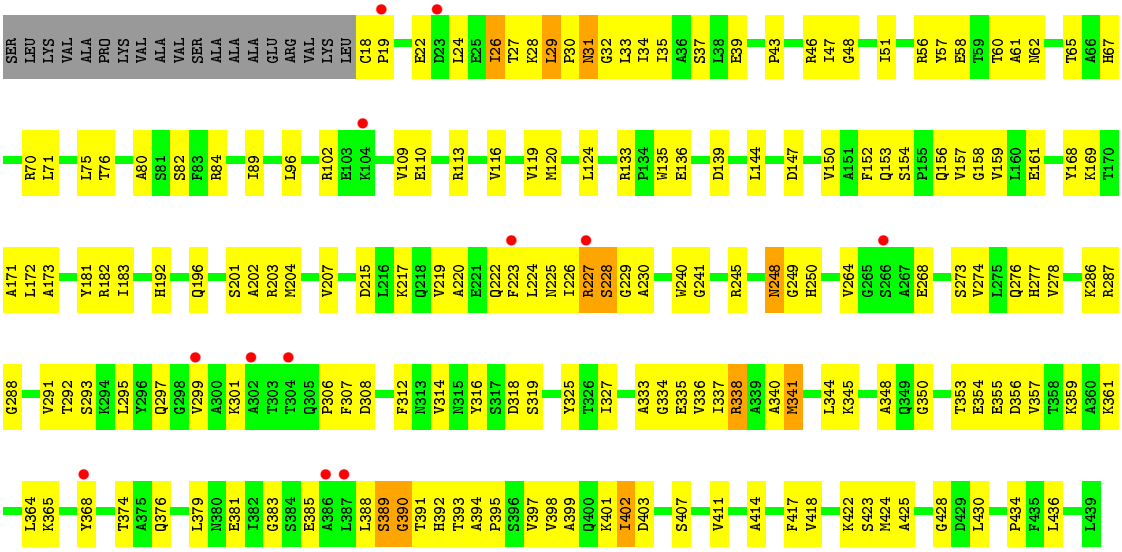
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

Chain B:



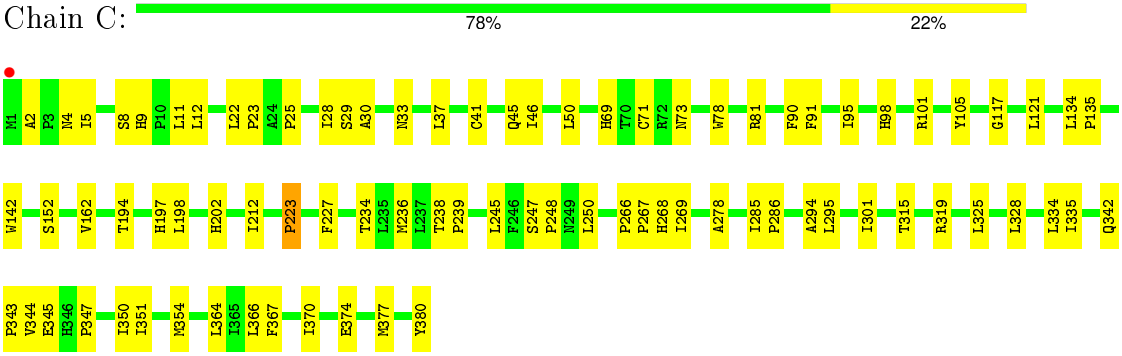
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

Chain O:



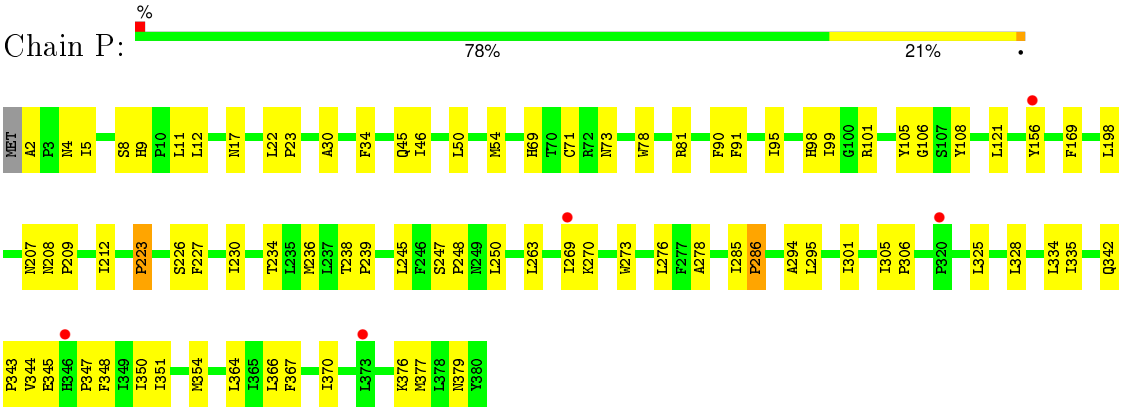
• Molecule 3: CYTOCHROME B

Chain C:



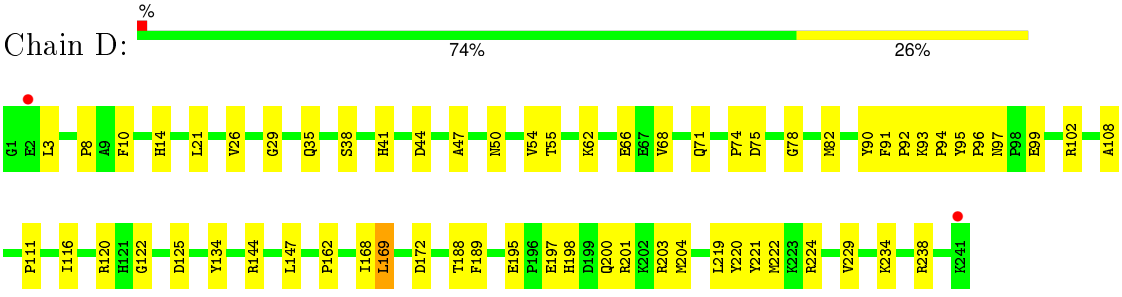
• Molecule 3: CYTOCHROME B

Chain P:



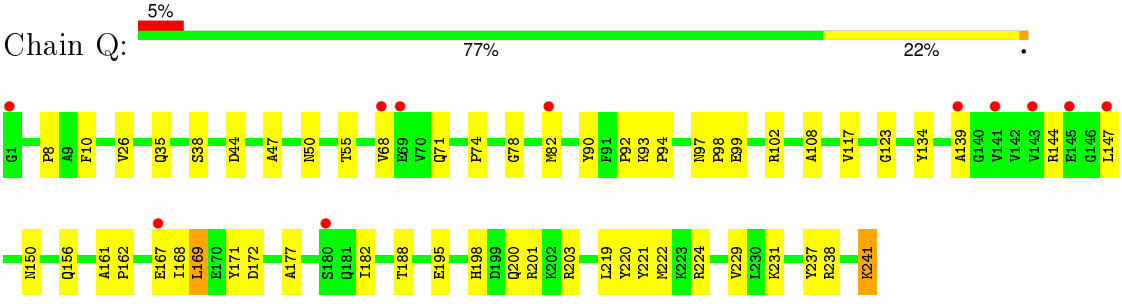
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain D:



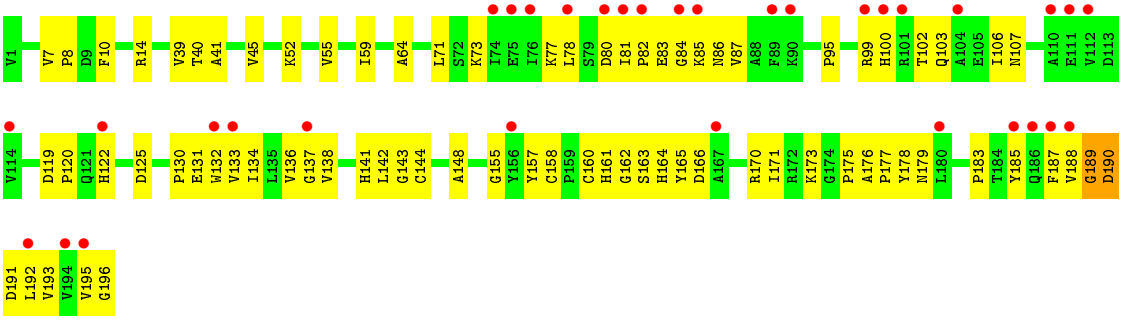
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain Q:

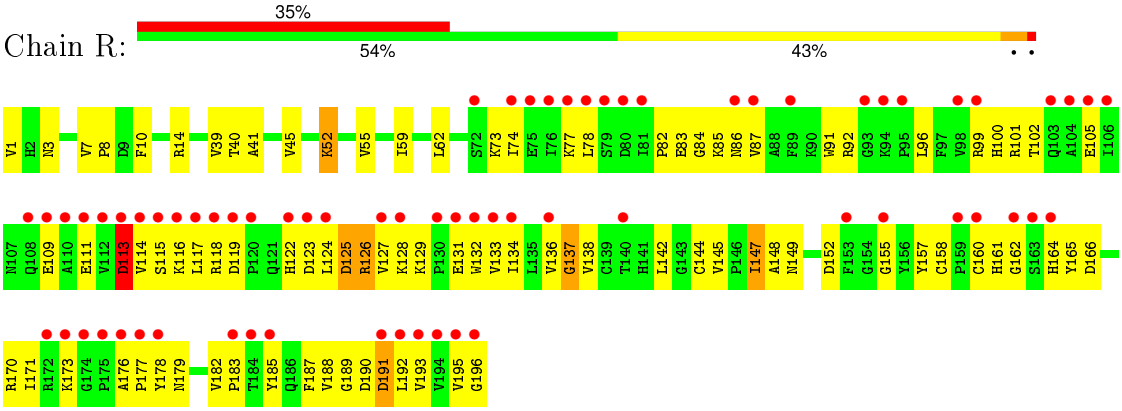


• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL

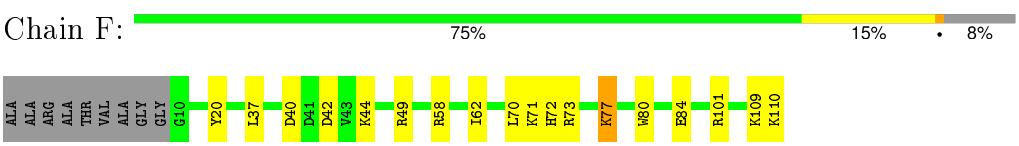
Chain E:



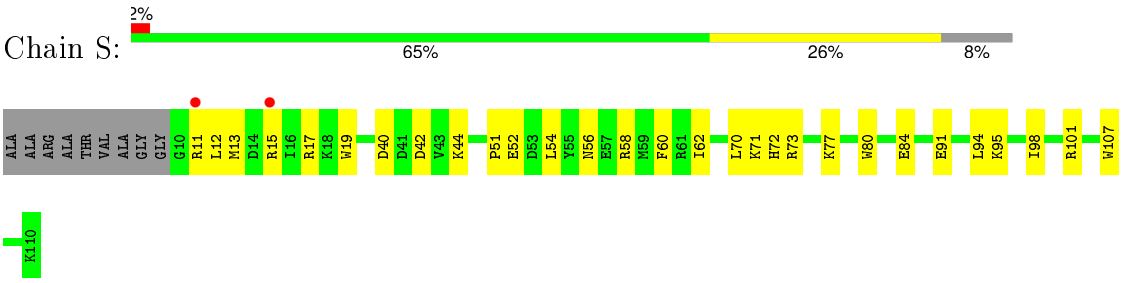
• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL



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

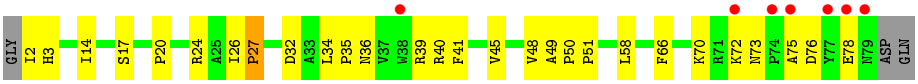


• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

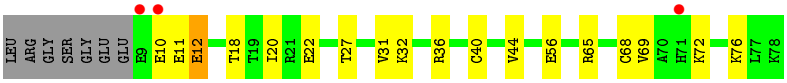


• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

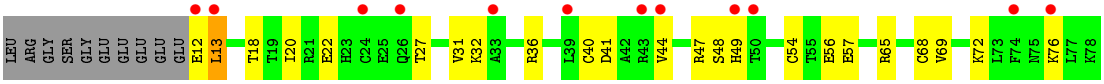
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C



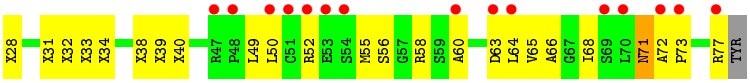
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII



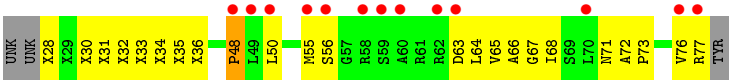
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII



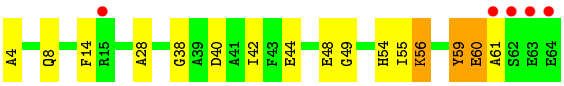
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL



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

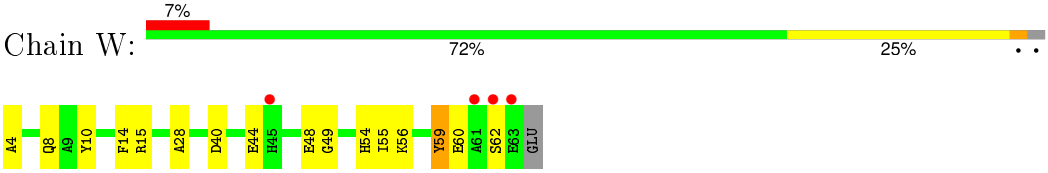


• Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN



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

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	171.89Å 181.69Å 240.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.66 – 2.76 58.66 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (58.66-2.76) 96.6 (58.66-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.286 0.253 , 0.278	Depositor DCC
R_{free} test set	3695 reflections (1.99%)	DCC
Wilson B-factor (Å^2)	57.5	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 199234 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	32703	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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, FMX, CDL, UQ, FES, HEC, PEE, 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	0.36	0/3196	0.59	0/4334
2	O	0.38	0/3202	0.62	1/4343 (0.0%)
3	C	0.51	0/3119	0.65	0/4270
3	P	0.45	0/3114	0.63	0/4263
4	D	0.46	0/1956	0.63	0/2658
4	Q	0.38	0/1956	0.60	0/2658
5	E	0.37	0/1547	0.60	1/2103 (0.0%)
5	R	0.35	0/1545	0.57	0/2098
6	F	0.53	0/911	0.66	0/1219
6	S	0.40	0/911	0.60	0/1219
7	G	0.49	0/698	0.67	0/946
7	T	0.44	0/676	0.64	0/918
8	H	0.44	0/582	0.60	0/779
8	U	0.31	0/561	0.54	0/751
9	I	0.35	0/218	0.62	0/293
9	V	0.35	0/218	0.59	0/293
10	J	0.42	0/508	0.59	0/682
10	W	0.43	0/490	0.56	0/660
All	All	0.42	0/32427	0.62	2/43997 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	227	ARG	N-CA-C	5.49	125.83	111.00
5	E	143	GLY	N-CA-C	5.23	126.18	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3353	141	0
1	N	3437	0	3349	154	0
2	B	3141	0	3142	195	0
2	O	3147	0	3146	180	0
3	C	3017	0	3063	78	0
3	P	3012	0	3058	77	0
4	D	1898	0	1846	50	0
4	Q	1898	0	1846	47	0
5	E	1513	0	1478	64	0
5	R	1512	0	1476	84	0
6	F	891	0	893	14	0
6	S	891	0	893	25	0
7	G	676	0	659	27	0
7	T	654	0	641	25	0
8	H	574	0	548	13	0
8	U	553	0	535	18	0
9	I	288	0	253	41	0
9	V	278	0	253	30	0
10	J	497	0	490	14	0
10	W	479	0	478	11	0
11	A	50	0	77	0	0
11	C	69	0	83	0	0
11	N	55	0	77	0	0
11	P	48	0	70	0	0
12	A	1	0	0	0	0
12	C	5	0	0	0	0
12	E	2	0	0	0	0
12	P	7	0	0	0	0
12	Q	1	0	0	0	0
13	C	86	0	60	8	0
13	P	86	0	60	7	0
14	C	28	0	18	2	0
14	P	28	0	18	2	0
15	C	19	0	17	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	P	19	0	17	3	0
16	C	3	0	0	0	0
16	P	3	0	0	0	0
17	C	12	0	18	0	0
17	D	40	0	56	3	0
17	P	19	0	24	1	0
17	Q	40	0	56	1	0
18	D	43	0	30	4	0
18	Q	43	0	30	2	0
19	D	42	0	28	2	0
19	G	40	0	24	2	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	1	0
21	A	2	0	0	0	0
21	C	9	0	0	2	0
21	E	1	0	0	0	0
21	P	12	0	0	2	0
21	R	4	0	0	0	0
All	All	32703	0	32215	1170	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 18.

All (1170) 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)
1:A:344:ARG:HB2	1:A:344:ARG:HH11	1.04	1.10
1:A:344:ARG:HB2	1:A:344:ARG:NH1	1.69	1.08
1:N:178:THR:HG22	1:N:180:ALA:H	1.18	1.08
2:B:76:THR:HG22	2:B:82:SER:H	1.13	1.07
1:A:178:THR:HG22	1:A:180:ALA:H	1.20	1.04
2:B:353:THR:HG22	2:B:355:GLU:H	1.20	1.01
7:T:72:LYS:HG2	8:U:56:GLU:OE2	1.59	1.00
2:O:353:THR:HG22	2:O:355:GLU:H	1.18	1.00
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.38	1.00
1:N:206:LYS:H	1:N:206:LYS:HD2	1.28	0.98
3:P:23:PRO:HG2	7:T:3:HIS:HB2	1.45	0.97
3:C:23:PRO:HG2	7:G:3:HIS:HB2	1.44	0.97
1:A:343:MET:O	1:A:347:THR:HG22	1.63	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:20:ILE:HD11	8:H:76:LYS:HD2	1.47	0.96
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.44	0.95
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.14	0.95
2:B:27:THR:HG22	2:B:28:LYS:H	1.29	0.95
8:U:20:ILE:HD11	8:U:76:LYS:HD2	1.46	0.94
1:N:343:MET:O	1:N:347:THR:HG22	1.64	0.94
4:D:47:ALA:H	4:D:50:ASN:HD22	1.18	0.92
1:N:206:LYS:H	1:N:206:LYS:CD	1.83	0.91
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.50	0.91
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.52	0.90
2:O:76:THR:HG22	2:O:82:SER:H	1.34	0.90
2:O:335:GLU:HA	2:O:338:ARG:HH12	1.35	0.89
9:I:64:LEU:HD12	9:I:77:ARG:O	1.73	0.88
2:O:376:GLN:HE22	9:V:77:ARG:NH2	1.72	0.88
2:O:27:THR:HG22	2:O:28:LYS:H	1.36	0.88
2:O:376:GLN:HE22	9:V:77:ARG:HH22	1.23	0.86
1:A:178:THR:HB	1:A:181:ASP:OD1	1.76	0.86
2:B:335:GLU:HA	2:B:338:ARG:HH12	1.39	0.85
2:B:22:GLU:HG2	2:B:39:GLU:HB3	1.57	0.85
5:E:134:ILE:HB	5:E:185:TYR:CE2	2.12	0.84
1:A:281:ASP:CG	9:I:33:UNK:HB1	1.98	0.83
2:O:338:ARG:HB2	2:O:338:ARG:HH11	1.44	0.82
1:N:49:ASN:HD22	1:N:51:LYS:H	1.26	0.82
1:A:178:THR:HG22	1:A:180:ALA:N	1.94	0.82
9:I:49:LEU:HD13	9:I:55:MET:HG2	1.60	0.82
5:R:85:LYS:HE2	5:R:87:VAL:HG22	1.62	0.82
1:N:178:THR:HB	1:N:181:ASP:OD1	1.81	0.81
5:R:101:ARG:HH22	5:R:127:VAL:HG11	1.44	0.80
2:B:27:THR:HG22	2:B:28:LYS:N	1.96	0.80
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.11	0.80
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.63	0.80
3:C:69:HIS:CD2	3:C:73:ASN:HD22	1.99	0.80
1:N:178:THR:HG22	1:N:180:ALA:N	1.95	0.79
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.80	0.79
1:N:350:THR:HG22	1:N:352:SER:H	1.49	0.78
5:E:85:LYS:HE2	5:E:87:VAL:HG22	1.65	0.78
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.23	0.78
2:B:338:ARG:HB2	2:B:338:ARG:HH11	1.48	0.78
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.01	0.78
2:O:31:ASN:ND2	2:O:33:LEU:H	1.80	0.78
9:I:71:ASN:HD22	9:I:71:ASN:H	1.27	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:GLN:HE22	9:I:34:UNK:CG	1.97	0.77
4:D:47:ALA:H	4:D:50:ASN:ND2	1.81	0.77
1:A:350:THR:HG22	1:A:352:SER:H	1.49	0.77
1:N:49:ASN:ND2	1:N:51:LYS:H	1.81	0.77
1:A:362:ARG:O	1:A:365:MET:HG2	1.84	0.77
2:B:31:ASN:ND2	2:B:33:LEU:H	1.81	0.77
1:N:22:GLY:O	1:N:193:PRO:HA	1.85	0.77
2:O:248:ASN:HD22	2:O:248:ASN:C	1.88	0.77
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.32	0.77
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.66	0.77
5:R:190:ASP:O	5:R:191:ASP:HB2	1.85	0.77
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.65	0.76
1:A:398:ARG:HH11	1:A:398:ARG:HG2	1.48	0.76
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.65	0.76
2:B:248:ASN:HD22	2:B:248:ASN:C	1.88	0.76
9:I:32:UNK:N	9:I:73:PRO:HG2	1.99	0.76
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.67	0.76
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.20	0.76
3:C:41:CYS:SG	3:C:90:PHE:HD2	2.08	0.76
2:B:153:GLN:HE22	9:I:34:UNK:HG2	1.48	0.76
2:O:192:HIS:O	2:O:196:GLN:HG3	1.84	0.76
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.67	0.76
1:N:362:ARG:O	1:N:365:MET:HG2	1.85	0.76
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.26	0.75
2:O:27:THR:HG22	2:O:28:LYS:N	2.01	0.75
1:A:49:ASN:HD22	1:A:51:LYS:H	1.34	0.75
1:N:19:LEU:O	1:N:21:ASN:N	2.19	0.75
10:W:55:ILE:HG22	10:W:59:TYR:HE1	1.50	0.75
1:A:344:ARG:HH11	1:A:344:ARG:CB	1.94	0.75
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.21	0.74
3:P:269:ILE:HG23	14:P:3001:FMX:H231	1.68	0.74
5:R:82:PRO:HD2	5:R:85:LYS:HD3	1.70	0.74
3:P:238:THR:HB	3:P:239:PRO:HD3	1.69	0.74
2:B:76:THR:HG22	2:B:82:SER:N	1.98	0.74
2:B:264:VAL:HG23	2:B:316:TYR:C	2.08	0.74
4:Q:222:MET:HE3	5:R:40:THR:HG23	1.70	0.74
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.70	0.73
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.69	0.73
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.70	0.73
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.70	0.73
2:O:353:THR:HG22	2:O:355:GLU:N	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:205:HIS:HB3	1:N:206:LYS:NZ	2.04	0.73
7:T:73:ASN:HB3	7:T:76:ASP:OD2	1.89	0.73
2:O:76:THR:HG23	2:O:136:GLU:OE1	1.88	0.73
3:C:328:LEU:HD23	7:G:51:PRO:HB3	1.70	0.73
3:P:101:ARG:C	3:P:101:ARG:HD2	2.10	0.73
9:I:71:ASN:N	9:I:71:ASN:HD22	1.87	0.72
2:B:153:GLN:NE2	9:I:34:UNK:CG	2.52	0.72
10:J:55:ILE:HG22	10:J:59:TYR:HE1	1.55	0.72
3:C:238:THR:HB	3:C:239:PRO:HD3	1.71	0.72
4:Q:241:LYS:HA	4:Q:241:LYS:HE3	1.71	0.72
2:B:47:ILE:HD13	2:B:120:MET:CE	2.19	0.72
2:B:227:ARG:NE	2:B:227:ARG:HA	2.05	0.72
2:O:47:ILE:HD13	2:O:120:MET:CE	2.20	0.72
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.72	0.72
1:N:206:LYS:HA	1:N:209:VAL:HG12	1.72	0.71
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.20	0.71
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.24	0.71
7:G:48:VAL:O	7:G:51:PRO:HD2	1.89	0.71
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.71	0.71
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.05	0.71
1:A:49:ASN:ND2	1:A:51:LYS:H	1.89	0.71
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.55	0.70
1:A:398:ARG:NH1	1:A:398:ARG:HG2	2.04	0.70
5:R:10:PHE:O	5:R:14:ARG:HG3	1.91	0.70
3:C:22:LEU:HD21	15:C:2002:UQ:HM32	1.73	0.70
2:O:335:GLU:HA	2:O:338:ARG:NH1	2.06	0.70
5:R:101:ARG:HG2	5:R:105:GLU:OE1	1.91	0.69
1:N:398:ARG:HG2	1:N:398:ARG:HH11	1.56	0.69
5:R:188:VAL:HG11	5:R:192:LEU:HD12	1.74	0.69
9:I:28:UNK:HA	9:I:72:ALA:HB2	1.75	0.69
2:B:153:GLN:NE2	9:I:34:UNK:HG2	2.06	0.69
1:N:282:ARG:HH21	9:V:36:UNK:CB	2.05	0.69
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.57	0.69
8:U:47:ARG:HG3	8:U:49:HIS:H	1.58	0.69
3:C:245:LEU:O	4:D:201:ARG:HD2	1.92	0.69
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.75	0.68
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.59	0.68
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.76	0.68
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.75	0.68
13:P:502:HEM:HMC2	13:P:502:HEM:HBC2	1.75	0.68
2:B:389:SER:O	2:B:391:THR:HG23	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:9:GLN:HG2	1:N:393:GLU:OE2	1.93	0.68
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.75	0.68
5:R:116:LYS:HA	5:R:116:LYS:HE2	1.76	0.68
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.75	0.68
3:C:269:ILE:HD12	5:R:160:CYS:SG	2.33	0.68
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.08	0.68
2:B:154:SER:O	2:B:157:VAL:HG12	1.93	0.68
2:B:113:ARG:O	2:B:116:VAL:HG23	1.93	0.68
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.29	0.68
1:A:103:SER:HB3	1:A:202:GLY:O	1.94	0.68
2:B:27:THR:HG21	2:B:217:LYS:HE3	1.76	0.67
3:P:328:LEU:HD23	7:T:51:PRO:HB3	1.76	0.67
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.60	0.67
2:O:297:GLN:O	2:O:301:LYS:HG3	1.93	0.67
1:N:178:THR:CG2	1:N:180:ALA:H	2.04	0.66
8:H:18:THR:O	8:H:22:GLU:HG3	1.96	0.66
1:A:222:THR:OG1	1:A:225:GLU:HG3	1.94	0.66
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.61	0.66
1:A:350:THR:HB	1:A:353:GLU:HG3	1.77	0.66
1:A:443:TRP:CE3	1:A:443:TRP:HA	2.29	0.66
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.59	0.66
2:B:297:GLN:O	2:B:301:LYS:HG3	1.95	0.66
4:D:222:MET:HE1	5:E:40:THR:HG23	1.77	0.66
7:T:48:VAL:O	7:T:51:PRO:HD2	1.95	0.66
4:D:204:MET:HG2	17:D:2009:BOG:H5	1.78	0.66
7:G:73:ASN:HB3	7:G:76:ASP:OD2	1.95	0.66
9:V:34:UNK:N	9:V:35:UNK:N	2.44	0.66
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.26	0.65
1:N:222:THR:OG1	1:N:225:GLU:HG3	1.96	0.65
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.78	0.65
3:C:41:CYS:SG	3:C:90:PHE:CD2	2.88	0.65
2:O:152:PHE:HA	2:O:157:VAL:HG11	1.78	0.65
1:A:178:THR:CG2	1:A:180:ALA:H	2.04	0.65
9:I:31:UNK:C	9:I:73:PRO:HG2	2.27	0.65
2:B:335:GLU:HA	2:B:338:ARG:NH1	2.10	0.65
2:B:27:THR:CG2	2:B:28:LYS:H	2.05	0.65
2:B:424:MET:HB2	2:B:436:LEU:HD13	1.79	0.65
5:R:82:PRO:HD2	5:R:85:LYS:CD	2.27	0.64
5:R:82:PRO:HG2	5:R:85:LYS:HB2	1.79	0.64
2:O:407:SER:O	2:O:411:VAL:HG23	1.97	0.64
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:LEU:HD23	9:I:68:ILE:HG13	1.78	0.64
2:O:43:PRO:O	2:O:113:ARG:HG3	1.97	0.64
1:A:443:TRP:HE3	1:A:443:TRP:HA	1.61	0.64
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.78	0.64
7:T:75:ALA:HA	7:T:78:GLU:HG3	1.80	0.64
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.32	0.64
1:N:398:ARG:HG2	1:N:398:ARG:NH1	2.10	0.64
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.78	0.64
7:G:75:ALA:HA	7:G:78:GLU:HG3	1.80	0.64
3:P:9:HIS:HD2	3:P:12:LEU:H	1.43	0.64
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.80	0.64
2:O:338:ARG:NH1	2:O:338:ARG:HB2	2.12	0.64
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.13	0.64
2:B:353:THR:HG22	2:B:355:GLU:N	2.03	0.64
2:O:424:MET:HB2	2:O:436:LEU:HD13	1.79	0.64
1:A:7:THR:HG21	2:B:113:ARG:CD	2.27	0.64
3:C:344:VAL:O	3:C:345:GLU:HG3	1.98	0.64
2:O:389:SER:O	2:O:391:THR:HG23	1.97	0.64
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.42	0.63
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.32	0.63
1:A:204:SER:HB3	1:A:207:GLU:HB2	1.79	0.63
3:C:101:ARG:C	3:C:101:ARG:HD2	2.18	0.63
1:N:350:THR:HB	1:N:353:GLU:HG3	1.79	0.63
1:A:170:THR:HG22	1:A:171:THR:N	2.12	0.63
5:R:122:HIS:O	5:R:125:ASP:HB2	1.99	0.63
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.34	0.63
2:B:43:PRO:O	2:B:113:ARG:HG3	1.98	0.63
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.61	0.63
1:A:9:GLN:HG2	1:A:393:GLU:OE2	1.97	0.63
3:P:247:SER:OG	3:P:250:LEU:HB2	1.99	0.63
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.64	0.63
3:P:350:ILE:O	3:P:354:MET:HG2	1.99	0.63
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.33	0.63
3:P:22:LEU:HD21	15:P:3002:UQ:HM32	1.81	0.63
10:J:40:ASP:O	10:J:44:GLU:HG3	1.99	0.63
2:B:152:PHE:HA	2:B:157:VAL:HG11	1.80	0.62
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.81	0.62
1:A:77:LYS:HE3	2:B:359:LYS:NZ	2.14	0.62
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.34	0.62
2:O:399:ALA:O	2:O:402:ILE:HG22	1.99	0.62
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:187:ASP:O	1:N:191:LYS:HE3	1.98	0.62
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.63	0.62
2:B:192:HIS:O	2:B:196:GLN:HG3	1.99	0.62
3:C:30:ALA:HB1	19:D:2003:CDL:H111	1.80	0.62
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.35	0.62
2:O:27:THR:CG2	2:O:28:LYS:H	2.11	0.62
1:N:170:THR:HG22	1:N:171:THR:N	2.15	0.62
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.14	0.62
2:O:338:ARG:CB	2:O:338:ARG:HH11	2.12	0.62
2:O:31:ASN:HD22	2:O:32:GLY:N	1.98	0.62
9:I:71:ASN:N	9:I:71:ASN:ND2	2.48	0.62
5:E:77:LYS:HE2	5:E:80:ASP:OD2	2.00	0.62
7:G:41:PHE:O	7:G:45:VAL:HG23	1.98	0.62
1:N:204:SER:HB3	1:N:207:GLU:HB2	1.80	0.62
1:N:269:VAL:HG22	1:N:406:MET:HE2	1.80	0.61
2:B:31:ASN:HD22	2:B:32:GLY:N	1.98	0.61
10:W:40:ASP:O	10:W:44:GLU:HG3	2.00	0.61
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.36	0.61
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.83	0.61
2:O:203:ARG:HD2	2:O:230:ALA:O	1.99	0.61
1:N:112:LEU:O	1:N:116:VAL:HG23	2.01	0.61
7:T:41:PHE:O	7:T:45:VAL:HG23	2.00	0.61
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.83	0.61
2:O:31:ASN:C	2:O:31:ASN:HD22	2.05	0.61
5:E:177:PRO:HB2	5:E:178:TYR:CD1	2.35	0.60
1:A:15:ASN:O	1:A:26:ALA:HA	2.01	0.60
8:U:27:THR:O	8:U:31:VAL:HG23	2.01	0.60
5:R:188:VAL:HB	5:R:192:LEU:HB2	1.83	0.60
3:C:269:ILE:HG23	14:C:2001:FMX:H231	1.82	0.60
2:B:381:GLU:OE1	2:B:381:GLU:HA	2.01	0.60
2:O:381:GLU:OE1	2:O:381:GLU:HA	2.01	0.60
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.83	0.60
4:Q:97:ASN:OD1	4:Q:99:GLU:HB2	2.02	0.60
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.35	0.60
4:Q:144:ARG:HG2	4:Q:147:LEU:HD12	1.83	0.60
2:O:46:ARG:HH11	2:O:110:GLU:HG3	1.65	0.60
2:B:306:PRO:HA	9:I:52:ARG:CG	2.31	0.60
2:B:46:ARG:HH11	2:B:110:GLU:HG3	1.65	0.60
4:D:144:ARG:HG2	4:D:147:LEU:HD12	1.83	0.60
2:O:33:LEU:CD2	2:O:224:LEU:HD12	2.32	0.60
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:55:ILE:CG2	10:W:59:TYR:HE1	2.15	0.60
2:B:292:THR:O	2:B:292:THR:HG22	2.01	0.60
2:B:153:GLN:NE2	9:I:34:UNK:HG1	2.17	0.60
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.37	0.60
2:B:31:ASN:HD22	2:B:31:ASN:C	2.04	0.59
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.84	0.59
1:N:103:SER:HB3	1:N:202:GLY:O	2.02	0.59
5:R:129:LYS:HB3	5:R:131:GLU:OE1	2.02	0.59
3:C:9:HIS:HD2	3:C:12:LEU:H	1.50	0.59
4:Q:47:ALA:HA	4:Q:90:TYR:HA	1.84	0.59
2:O:113:ARG:O	2:O:116:VAL:HG23	2.02	0.59
2:O:422:LYS:O	2:O:436:LEU:HD21	2.03	0.59
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.42	0.59
1:N:206:LYS:HA	1:N:209:VAL:CG1	2.33	0.59
1:N:410:VAL:O	1:N:413:LYS:HB3	2.02	0.59
1:A:49:ASN:HD22	1:A:51:LYS:N	2.01	0.59
5:R:147:ILE:HG22	5:R:148:ALA:N	2.18	0.59
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.85	0.59
1:N:15:ASN:O	1:N:26:ALA:HA	2.03	0.59
2:B:262:ALA:HB2	2:B:268:GLU:HG2	1.84	0.59
1:A:187:ASP:O	1:A:191:LYS:HE3	2.02	0.59
3:P:71:CYS:SG	3:P:81:ARG:HD2	2.43	0.59
5:R:101:ARG:HH22	5:R:127:VAL:CG1	2.16	0.59
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.84	0.59
3:C:71:CYS:SG	3:C:81:ARG:HD2	2.43	0.59
7:G:71:ARG:NH1	8:H:56:GLU:OE1	2.33	0.59
8:H:65:ARG:O	8:H:69:VAL:HG23	2.03	0.59
2:B:338:ARG:HB2	2:B:338:ARG:NH1	2.17	0.58
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.03	0.58
2:O:248:ASN:ND2	2:O:250:HIS:H	2.01	0.58
1:N:21:ASN:HB2	1:N:218:GLY:O	2.04	0.58
8:U:47:ARG:HD3	8:U:48:SER:H	1.68	0.58
2:B:226:ILE:O	2:B:226:ILE:HG23	2.03	0.58
2:O:292:THR:HG22	2:O:292:THR:O	2.03	0.58
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.33	0.58
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.04	0.58
2:O:150:VAL:O	2:O:153:GLN:HG3	2.04	0.58
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.86	0.58
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.86	0.58
1:A:350:THR:HG22	1:A:352:SER:N	2.18	0.58
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.39	0.58
1:N:114:ALA:HB2	1:N:216:PHE:CE1	2.38	0.58
3:C:285:ILE:HD12	3:C:294:ALA:HB2	1.86	0.57
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.86	0.57
1:A:272:VAL:O	1:A:275:ALA:HB3	2.04	0.57
5:E:82:PRO:HD2	5:E:85:LYS:HD3	1.84	0.57
2:B:248:ASN:ND2	2:B:250:HIS:H	2.03	0.57
5:E:78:LEU:HD11	5:E:187:PHE:HE1	1.70	0.57
2:B:341:MET:CE	2:B:417:PHE:HE2	2.17	0.57
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.85	0.57
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.18	0.57
1:N:77:LYS:HE3	2:O:359:LYS:NZ	2.18	0.57
2:B:150:VAL:O	2:B:153:GLN:HG3	2.05	0.57
2:O:361:LYS:O	2:O:365:LYS:HG3	2.03	0.57
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.86	0.57
2:O:56:ARG:HG3	2:O:56:ARG:NH1	2.19	0.57
2:B:422:LYS:O	2:B:436:LEU:HD21	2.05	0.57
4:D:200:GLN:NE2	17:D:2091:BOG:H5	2.19	0.57
2:O:308:ASP:OD2	9:V:55:MET:O	2.21	0.57
10:W:4:ALA:O	10:W:8:GLN:HG3	2.04	0.57
3:P:90:PHE:CZ	3:P:236:MET:HB3	2.39	0.57
2:O:273:SER:O	2:O:276:GLN:HB3	2.04	0.57
2:O:154:SER:O	2:O:157:VAL:HG12	2.04	0.57
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.86	0.57
2:B:52:LYS:HE2	2:B:388:LEU:HD23	1.86	0.57
2:O:357:VAL:O	2:O:361:LYS:HG3	2.05	0.57
10:J:55:ILE:CG2	10:J:59:TYR:HE1	2.17	0.57
2:O:76:THR:CG2	2:O:136:GLU:OE1	2.53	0.56
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.69	0.56
3:P:101:ARG:O	3:P:101:ARG:HD2	2.06	0.56
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.88	0.56
2:B:353:THR:HB	2:B:356:ASP:CG	2.25	0.56
2:B:338:ARG:CB	2:B:338:ARG:HH11	2.18	0.56
9:I:49:LEU:O	9:I:50:LEU:HD23	2.05	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	1.87	0.56
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.88	0.56
1:A:106:MET:HG3	1:A:203:ILE:HG21	1.87	0.56
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.20	0.56
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.71	0.56
1:N:49:ASN:C	1:N:49:ASN:HD22	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:383:LEU:O	1:N:387:GLY:HA2	2.05	0.56
2:O:308:ASP:OD2	9:V:56:SER:HA	2.06	0.56
2:O:376:GLN:NE2	9:V:77:ARG:NH2	2.47	0.56
7:G:40:ARG:HD2	19:G:2004:CDL:OA4	2.04	0.56
1:N:394:GLU:O	1:N:397:SER:HB3	2.06	0.56
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.87	0.56
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.86	0.56
5:E:83:GLU:HG2	5:E:102:THR:HA	1.88	0.56
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.87	0.56
2:B:273:SER:O	2:B:276:GLN:HB3	2.06	0.56
1:N:49:ASN:HD22	1:N:51:LYS:N	1.98	0.56
2:B:357:VAL:O	2:B:361:LYS:HG3	2.04	0.56
2:B:46:ARG:HH21	2:B:376:GLN:HG3	1.69	0.56
1:A:60:GLU:OE2	1:A:90:THR:HG22	2.06	0.56
2:O:306:PRO:HG2	9:V:50:LEU:O	2.06	0.56
3:P:285:ILE:HD12	3:P:294:ALA:HB2	1.87	0.56
4:D:47:ALA:N	4:D:50:ASN:HD22	1.98	0.55
2:O:341:MET:CE	2:O:417:PHE:HE2	2.18	0.55
5:R:115:SER:O	5:R:116:LYS:HG2	2.05	0.55
5:R:126:ARG:H	5:R:126:ARG:HD3	1.71	0.55
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.71	0.55
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.88	0.55
3:P:223:PRO:HB2	3:P:227:PHE:CD2	2.40	0.55
5:E:160:CYS:SG	3:P:269:ILE:HD12	2.47	0.55
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.89	0.55
3:C:344:VAL:O	3:C:344:VAL:HG23	2.07	0.55
7:T:40:ARG:HD2	19:T:3004:CDL:OA4	2.06	0.55
3:P:30:ALA:HB1	19:Q:3003:CDL:H111	1.89	0.55
8:H:40:CYS:O	8:H:44:VAL:HG23	2.06	0.55
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.45	0.55
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.21	0.55
1:N:60:GLU:OE2	1:N:90:THR:HG22	2.07	0.55
1:A:223:TYR:OH	1:A:224:LYS:HE3	2.07	0.55
2:O:402:ILE:HD13	2:O:402:ILE:C	2.26	0.55
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.88	0.55
3:C:78:TRP:CZ3	4:D:201:ARG:HG3	2.42	0.55
8:U:18:THR:O	8:U:22:GLU:HG3	2.05	0.55
2:B:156:GLN:HE22	9:I:77:ARG:C	2.09	0.55
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.37	0.55
2:B:56:ARG:NH1	2:B:56:ARG:HG3	2.18	0.55
4:D:47:ALA:HA	4:D:90:TYR:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:72:LYS:HG2	8:H:56:GLU:OE2	2.07	0.55
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.88	0.55
3:P:95:ILE:O	3:P:99:ILE:HG13	2.07	0.55
2:O:353:THR:HG22	2:O:354:GLU:N	2.22	0.54
2:B:248:ASN:ND2	2:B:248:ASN:C	2.60	0.54
5:R:78:LEU:HD13	5:R:132:TRP:CE2	2.42	0.54
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.35	0.54
3:P:198:LEU:HD21	13:P:502:HEM:HMA3	1.89	0.54
2:B:26:ILE:O	2:B:26:ILE:HG12	2.07	0.54
1:A:106:MET:O	1:A:106:MET:HE2	2.07	0.54
1:N:106:MET:HG3	1:N:203:ILE:HG21	1.90	0.54
2:O:202:ALA:HB3	2:O:229:GLY:O	2.07	0.54
5:E:73:LYS:HG2	5:E:196:GLY:HA3	1.89	0.54
5:E:10:PHE:O	5:E:14:ARG:HG3	2.07	0.54
1:N:205:HIS:HB3	1:N:206:LYS:HZ2	1.70	0.54
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.96	0.54
2:O:159:VAL:HG21	2:O:325:TYR:CE1	2.41	0.54
5:R:190:ASP:O	5:R:191:ASP:CB	2.55	0.54
2:B:60:THR:CG2	2:B:61:ALA:N	2.71	0.54
1:A:21:ASN:HB3	1:A:219:VAL:HG22	1.89	0.54
1:N:191:LYS:C	1:N:195:MET:HE2	2.28	0.54
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.41	0.54
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.42	0.54
3:C:223:PRO:HB2	3:C:227:PHE:CD2	2.43	0.54
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.90	0.54
1:A:383:LEU:O	1:A:387:GLY:HA2	2.08	0.54
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.42	0.54
1:A:269:VAL:HG22	1:A:406:MET:HE2	1.89	0.54
4:Q:241:LYS:HG3	4:Q:241:LYS:OXT	2.07	0.54
2:B:227:ARG:HE	2:B:227:ARG:HA	1.72	0.54
2:B:361:LYS:O	2:B:365:LYS:HG3	2.08	0.54
3:C:268:HIS:HB3	21:C:1288:HOH:O	2.07	0.54
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.89	0.54
5:E:171:ILE:HG12	5:E:176:ALA:O	2.08	0.54
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.88	0.54
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.41	0.54
3:P:286:PRO:HA	21:P:1285:HOH:O	2.08	0.54
2:B:353:THR:HG22	2:B:354:GLU:N	2.23	0.54
2:O:156:GLN:HE22	9:V:77:ARG:C	2.11	0.54
1:N:350:THR:HG22	1:N:352:SER:N	2.19	0.54
3:C:198:LEU:HD21	13:C:502:HEM:HMA3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.48	0.54
1:N:206:LYS:N	1:N:206:LYS:HD2	2.11	0.53
2:B:399:ALA:O	2:B:402:ILE:HG22	2.09	0.53
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.73	0.53
4:D:35:GLN:NE2	4:D:169:LEU:HD12	2.23	0.53
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.36	0.53
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.89	0.53
1:N:106:MET:HE2	1:N:106:MET:O	2.09	0.53
2:B:407:SER:O	2:B:411:VAL:HG23	2.09	0.53
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.44	0.53
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.41	0.53
1:A:145:MET:HB2	1:A:252:HIS:CE1	2.43	0.53
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.44	0.53
2:O:60:THR:CG2	2:O:61:ALA:N	2.71	0.53
2:O:26:ILE:O	2:O:26:ILE:HG12	2.07	0.53
3:C:28:ILE:CD1	15:C:2002:UQ:HM21	2.39	0.53
2:B:25:GLU:HB2	2:B:213:HIS:CG	2.43	0.53
2:O:248:ASN:C	2:O:248:ASN:ND2	2.60	0.53
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.44	0.53
4:Q:195:GLU:HG3	4:Q:198:HIS:HB2	1.90	0.53
9:V:31:UNK:C	9:V:73:PRO:HG2	2.38	0.53
3:P:9:HIS:CD2	3:P:11:LEU:H	2.27	0.53
2:O:388:LEU:O	2:O:389:SER:HB3	2.09	0.53
4:Q:203:ARG:HD3	10:W:40:ASP:OD1	2.09	0.53
2:O:385:GLU:OE1	2:O:392:HIS:HA	2.09	0.53
1:N:347:THR:HG21	1:N:444:ILE:C	2.27	0.53
2:B:31:ASN:ND2	2:B:31:ASN:C	2.63	0.53
1:A:49:ASN:C	1:A:49:ASN:HD22	2.11	0.53
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.09	0.53
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.44	0.53
1:A:394:GLU:O	1:A:397:SER:HB3	2.09	0.53
2:B:157:VAL:HG13	2:B:158:GLY:N	2.24	0.53
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.44	0.53
2:O:353:THR:HB	2:O:356:ASP:CG	2.28	0.52
3:P:245:LEU:O	4:Q:201:ARG:HD2	2.09	0.52
8:U:65:ARG:O	8:U:69:VAL:HG23	2.10	0.52
2:O:393:THR:HG23	2:O:397:VAL:HB	1.90	0.52
1:N:443:TRP:O	1:N:444:ILE:CB	2.56	0.52
2:O:33:LEU:HD22	2:O:224:LEU:HD12	1.92	0.52
1:N:21:ASN:CB	1:N:219:VAL:HA	2.39	0.52
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:HG12	1:A:220:SER:N	2.24	0.52
2:B:286:LYS:HE2	2:B:287:ARG:HH12	1.75	0.52
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.77	0.52
1:N:146:THR:O	1:N:150:PHE:HD1	1.92	0.52
2:B:393:THR:HG23	2:B:397:VAL:HB	1.90	0.52
3:P:34:PHE:HB2	21:P:381:HOH:O	2.09	0.52
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.44	0.52
1:N:205:HIS:HB3	1:N:206:LYS:HZ1	1.74	0.52
2:O:225:ASN:O	2:O:226:ILE:C	2.47	0.52
9:I:38:UNK:O	9:I:39:UNK:C	2.57	0.52
1:N:220:SER:HB2	1:N:225:GLU:HB2	1.90	0.52
3:P:78:TRP:CZ3	4:Q:201:ARG:HG3	2.44	0.52
2:B:274:VAL:O	2:B:278:VAL:HG23	2.10	0.52
1:A:106:MET:N	1:A:107:PRO:HD2	2.25	0.52
3:P:234:THR:HG21	4:Q:219:LEU:CD1	2.38	0.52
9:I:65:VAL:HG12	9:I:66:ALA:N	2.24	0.52
4:Q:38:SER:O	4:Q:94:PRO:HG3	2.09	0.52
2:B:388:LEU:O	2:B:389:SER:HB3	2.10	0.52
1:N:26:ALA:HB2	1:N:383:LEU:HD11	1.91	0.52
4:D:68:VAL:HG11	4:D:92:PRO:HG3	1.91	0.52
5:R:136:VAL:O	5:R:138:VAL:N	2.42	0.52
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.09	0.52
1:A:424:ALA:HB1	1:A:428:ILE:HG21	1.92	0.52
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.10	0.52
1:N:7:THR:HG21	2:O:113:ARG:CD	2.39	0.52
5:R:114:VAL:HG13	5:R:122:HIS:HD2	1.75	0.52
3:P:347:PRO:O	3:P:350:ILE:HG22	2.10	0.52
5:E:73:LYS:HB3	5:E:195:VAL:O	2.10	0.52
6:F:49:ARG:HD3	2:O:135:TRP:CE2	2.45	0.52
5:E:103:GLN:O	5:E:107:ASN:ND2	2.43	0.52
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.39	0.52
3:P:344:VAL:O	3:P:345:GLU:HG3	2.10	0.52
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.45	0.51
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.92	0.51
2:B:361:LYS:HD3	2:B:403:ASP:HA	1.92	0.51
3:C:269:ILE:CG2	14:C:2001:FMX:H231	2.40	0.51
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.91	0.51
1:A:170:THR:HG22	1:A:172:GLU:H	1.75	0.51
2:O:27:THR:HG21	2:O:217:LYS:HE3	1.93	0.51
5:R:77:LYS:HA	5:R:191:ASP:O	2.10	0.51
2:B:225:ASN:O	2:B:226:ILE:C	2.47	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LEU:HD11	1:A:174:ILE:HD12	1.92	0.51
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.45	0.51
2:B:248:ASN:HD22	2:B:249:GLY:N	2.07	0.51
1:A:206:LYS:HA	1:A:209:VAL:CG1	2.40	0.51
4:Q:68:VAL:HG11	4:Q:92:PRO:HG3	1.92	0.51
5:R:101:ARG:CZ	5:R:133:VAL:HB	2.41	0.51
4:D:71:GLN:HG3	4:D:82:MET:HE2	1.91	0.51
5:E:155:GLY:HA3	5:E:166:ASP:C	2.31	0.51
1:N:191:LYS:CA	1:N:195:MET:HE2	2.41	0.51
10:J:49:GLY:N	10:J:54:HIS:ND1	2.58	0.51
5:R:142:LEU:HD12	5:R:161:HIS:CE1	2.46	0.51
5:R:52:LYS:HD3	5:R:52:LYS:C	2.30	0.51
1:A:351:GLU:O	1:A:354:VAL:HG22	2.10	0.51
1:N:106:MET:N	1:N:107:PRO:HD2	2.25	0.51
2:B:312:PHE:CE2	2:B:314:VAL:HG23	2.45	0.51
1:A:307:PHE:C	1:A:307:PHE:CD1	2.83	0.51
1:A:146:THR:O	1:A:150:PHE:HD1	1.93	0.51
2:B:385:GLU:OE1	2:B:392:HIS:HA	2.11	0.51
1:N:268:VAL:O	1:N:272:VAL:HG23	2.10	0.51
8:H:27:THR:O	8:H:31:VAL:HG23	2.11	0.51
2:O:62:ASN:O	2:O:65:THR:HG22	2.10	0.51
3:P:269:ILE:O	3:P:269:ILE:HG22	2.09	0.51
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.41	0.51
4:D:203:ARG:HD3	10:J:40:ASP:OD1	2.11	0.51
3:P:376:LYS:O	6:S:17:ARG:NH1	2.44	0.51
1:A:220:SER:HB2	1:A:225:GLU:HB2	1.92	0.51
2:O:71:LEU:HD23	9:V:68:ILE:HG13	1.92	0.51
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.11	0.51
2:B:252:LEU:HD11	9:I:49:LEU:HB2	1.92	0.51
5:R:99:ARG:HB3	5:R:133:VAL:HG13	1.93	0.51
18:D:501:HEC:HMC1	18:D:501:HEC:HBC3	1.93	0.51
4:D:238:ARG:HD2	7:G:14:ILE:HD12	1.93	0.51
1:A:395:TRP:CE3	1:A:395:TRP:HA	2.45	0.51
2:O:152:PHE:HA	2:O:157:VAL:CG1	2.40	0.50
1:N:143:ASN:HD22	9:V:48:PRO:HD2	1.76	0.50
1:A:23:LEU:HD23	1:A:24:ARG:N	2.25	0.50
3:C:46:ILE:HA	13:C:501:HEM:HMC2	1.92	0.50
5:R:114:VAL:HG13	5:R:122:HIS:CD2	2.47	0.50
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.92	0.50
3:P:198:LEU:HD13	15:P:3002:UQ:HM53	1.93	0.50
2:B:24:LEU:HD12	2:B:37:SER:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.93	0.50
4:D:38:SER:O	4:D:94:PRO:HG3	2.12	0.50
3:C:105:TYR:O	3:C:315:THR:HG22	2.11	0.50
2:O:248:ASN:HD22	2:O:249:GLY:N	2.09	0.50
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.46	0.50
5:E:83:GLU:HA	5:E:100:HIS:CG	2.46	0.50
1:A:410:VAL:O	1:A:413:LYS:HB3	2.11	0.50
2:B:333:ALA:O	2:B:337:ILE:HG13	2.12	0.50
2:B:34:ILE:HD13	2:B:390:GLY:CA	2.42	0.50
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.94	0.50
4:D:41:HIS:HE1	4:D:111:PRO:HD2	1.76	0.50
5:E:99:ARG:HB3	5:E:133:VAL:HG13	1.94	0.50
4:D:71:GLN:HE21	4:D:82:MET:CE	2.25	0.50
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.93	0.50
3:C:377:MET:HE1	6:F:20:TYR:CD1	2.46	0.50
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.46	0.50
2:B:264:VAL:HG23	2:B:316:TYR:O	2.11	0.50
2:O:402:ILE:HG23	2:O:403:ASP:N	2.27	0.50
2:O:67:HIS:O	2:O:70:ARG:HB3	2.11	0.50
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.42	0.50
4:D:97:ASN:OD1	4:D:99:GLU:HB2	2.12	0.50
3:C:285:ILE:CD1	3:C:294:ALA:HB2	2.42	0.50
1:N:335:MET:HG3	1:N:339:GLN:HE21	1.76	0.50
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.44	0.50
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.94	0.50
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.47	0.50
5:E:163:SER:OG	5:E:175:PRO:HD2	2.12	0.50
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.47	0.49
5:E:165:TYR:HA	5:E:170:ARG:O	2.11	0.49
1:A:242:ARG:O	7:G:14:ILE:HA	2.11	0.49
6:S:11:ARG:O	6:S:15:ARG:HG3	2.12	0.49
2:B:308:ASP:OD2	9:I:56:SER:HA	2.11	0.49
1:A:53:ASN:HB3	1:A:173:ASN:ND2	2.27	0.49
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.41	0.49
2:O:286:LYS:HE2	2:O:287:ARG:HH12	1.77	0.49
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.11	0.49
1:N:138:LEU:HD11	1:N:174:ILE:HD12	1.95	0.49
3:C:350:ILE:O	3:C:354:MET:HG2	2.11	0.49
2:O:274:VAL:O	2:O:278:VAL:HG23	2.12	0.49
2:B:307:PHE:CD1	2:B:308:ASP:N	2.81	0.49
1:N:63:ALA:O	1:N:116:VAL:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:VAL:O	1:A:272:VAL:HG23	2.12	0.49
9:V:30:UNK:HG3	9:V:31:UNK:N	2.27	0.49
1:N:161:THR:HG21	1:N:235:ARG:H	1.77	0.49
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.47	0.49
7:T:72:LYS:HG2	8:U:56:GLU:CD	2.28	0.49
2:B:156:GLN:NE2	9:I:77:ARG:C	2.66	0.49
1:A:191:LYS:N	1:A:195:MET:HE2	2.28	0.49
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.94	0.49
2:B:19:PRO:HB2	2:B:41:PHE:CE1	2.47	0.49
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.47	0.49
9:V:65:VAL:HG12	9:V:66:ALA:N	2.27	0.49
1:A:134:ILE:HG22	1:A:174:ILE:HD13	1.95	0.49
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.47	0.49
1:A:358:LYS:HE3	1:A:399:ILE:O	2.13	0.49
8:U:12:GLU:O	8:U:13:LEU:HB2	2.12	0.49
1:N:307:PHE:CD1	1:N:307:PHE:C	2.86	0.49
1:A:281:ASP:OD1	9:I:33:UNK:HB1	2.11	0.49
2:O:33:LEU:HD21	2:O:224:LEU:HD12	1.95	0.49
1:N:170:THR:HG22	1:N:172:GLU:H	1.78	0.49
1:A:239:SER:HB2	7:G:17:SER:O	2.13	0.49
10:J:4:ALA:O	10:J:8:GLN:HG3	2.13	0.49
1:N:53:ASN:HB3	1:N:173:ASN:ND2	2.27	0.49
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.95	0.49
2:B:46:ARG:HD2	2:B:110:GLU:CD	2.33	0.49
15:P:3002:UQ:HM51	15:P:3002:UQ:C8	2.43	0.49
4:D:220:TYR:O	4:D:224:ARG:HG2	2.12	0.49
5:R:157:TYR:CE1	5:R:162:GLY:HA2	2.48	0.49
5:E:102:THR:O	5:E:106:ILE:HG13	2.13	0.49
2:B:25:GLU:HB2	2:B:213:HIS:ND1	2.28	0.49
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.95	0.48
19:D:2003:CDL:OB3	6:F:73:ARG:NH2	2.45	0.48
2:B:60:THR:HG23	2:B:61:ALA:N	2.28	0.48
13:C:502:HEM:HBD1	21:C:386:HOH:O	2.11	0.48
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.94	0.48
1:N:134:ILE:HG22	1:N:174:ILE:HD13	1.95	0.48
2:B:318:ASP:O	2:B:319:SER:HB2	2.11	0.48
3:P:46:ILE:HA	13:P:501:HEM:HMC2	1.93	0.48
2:O:395:PRO:HA	2:O:398:VAL:HG12	1.94	0.48
4:D:54:VAL:HG22	17:D:2091:BOG:H5'2	1.96	0.48
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.43	0.48
1:N:53:ASN:H	1:N:173:ASN:ND2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:312:PHE:CE2	2:O:314:VAL:HG23	2.47	0.48
3:C:9:HIS:CD2	3:C:11:LEU:H	2.31	0.48
1:A:112:LEU:O	1:A:116:VAL:HG23	2.13	0.48
5:R:155:GLY:HA3	5:R:166:ASP:C	2.33	0.48
1:N:206:LYS:CA	1:N:209:VAL:HG12	2.41	0.48
2:O:46:ARG:HH21	2:O:376:GLN:HG3	1.77	0.48
10:J:55:ILE:HG22	10:J:59:TYR:CE1	2.44	0.48
2:O:60:THR:HG23	2:O:61:ALA:N	2.28	0.48
5:R:161:HIS:HB2	20:R:501:FES:S1	2.53	0.48
2:B:157:VAL:CG2	9:I:64:LEU:HD21	2.27	0.48
3:P:269:ILE:CG2	14:P:3001:FMX:H231	2.42	0.48
1:A:275:ALA:HB3	1:A:357:ALA:HB1	1.96	0.48
8:U:65:ARG:O	8:U:68:CYS:HB3	2.13	0.48
6:S:12:LEU:HB3	6:S:13:MET:HE1	1.95	0.48
2:B:245:ARG:HB3	2:B:430:LEU:CD1	2.43	0.48
3:C:247:SER:OG	3:C:250:LEU:HB2	2.13	0.48
3:P:5:ILE:CG2	3:P:12:LEU:HD12	2.44	0.48
4:D:75:ASP:O	4:Q:99:GLU:HG2	2.13	0.48
1:A:370:ASP:O	2:B:374:THR:HG22	2.14	0.48
6:S:51:PRO:HD2	6:S:54:LEU:HD12	1.95	0.48
5:E:161:HIS:HB2	20:E:501:FES:S1	2.53	0.48
2:B:26:ILE:HA	2:B:35:ILE:O	2.13	0.48
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.29	0.48
2:B:424:MET:HG2	2:B:425:ALA:N	2.29	0.48
2:B:257:VAL:O	2:B:323:GLY:HA3	2.14	0.48
2:O:46:ARG:HD2	2:O:110:GLU:CD	2.34	0.48
1:A:280:TYR:CG	1:A:281:ASP:N	2.82	0.48
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.78	0.48
2:O:147:ASP:O	2:O:150:VAL:HG22	2.14	0.48
3:P:379:ASN:HA	6:S:17:ARG:HH12	1.77	0.48
4:Q:238:ARG:HD2	7:T:14:ILE:HD12	1.96	0.48
2:O:24:LEU:HD12	2:O:37:SER:O	2.13	0.48
1:N:219:VAL:HG12	1:N:220:SER:N	2.28	0.47
3:P:98:HIS:CD2	13:P:502:HEM:NC	2.82	0.47
2:O:307:PHE:CD1	2:O:308:ASP:N	2.82	0.47
3:C:45:GLN:HB3	13:C:501:HEM:HAB	1.95	0.47
2:B:218:GLN:HG2	2:B:222:GLN:OE1	2.14	0.47
4:Q:71:GLN:HG3	4:Q:82:MET:HE2	1.96	0.47
6:S:40:ASP:O	6:S:44:LYS:HG3	2.13	0.47
9:I:64:LEU:HA	9:I:77:ARG:O	2.14	0.47
5:E:86:ASN:ND2	5:E:148:ALA:HB2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:344:VAL:C	3:C:345:GLU:HG3	2.35	0.47
1:N:272:VAL:O	1:N:275:ALA:HB3	2.14	0.47
2:O:58:GLU:HG2	2:O:65:THR:HG22	1.95	0.47
5:E:133:VAL:HG13	5:E:133:VAL:O	2.14	0.47
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.49	0.47
1:A:228:VAL:O	1:A:228:VAL:HG13	2.15	0.47
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.29	0.47
13:C:501:HEM:HMC1	13:C:501:HEM:HBC2	1.96	0.47
2:B:402:ILE:HG23	2:B:403:ASP:N	2.29	0.47
1:A:191:LYS:CA	1:A:195:MET:HE2	2.44	0.47
3:C:325:LEU:HD22	3:C:370:ILE:HG13	1.94	0.47
1:N:209:VAL:O	1:N:212:ALA:HB3	2.15	0.47
1:N:21:ASN:HB2	1:N:219:VAL:HA	1.96	0.47
3:P:95:ILE:HD13	3:P:121:LEU:HD13	1.95	0.47
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.96	0.47
10:W:49:GLY:N	10:W:54:HIS:ND1	2.63	0.47
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.50	0.47
1:N:369:LEU:CD1	1:N:392:LEU:HD21	2.45	0.47
1:N:124:GLU:OE1	1:N:179:ARG:HG3	2.15	0.47
5:R:113:ASP:OD2	5:R:116:LYS:HG3	2.14	0.47
4:D:222:MET:CE	5:E:40:THR:HG23	2.43	0.47
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.44	0.47
1:N:23:LEU:HD23	1:N:24:ARG:N	2.29	0.47
1:A:371:GLY:O	1:A:375:VAL:HG23	2.14	0.47
2:O:57:TYR:N	2:O:57:TYR:CD1	2.83	0.47
3:C:5:ILE:CG2	3:C:12:LEU:HD12	2.45	0.47
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.97	0.47
6:S:12:LEU:HB3	6:S:13:MET:CE	2.45	0.47
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.95	0.47
3:C:319:ARG:HD2	3:C:374:GLU:OE2	2.15	0.47
6:F:109:LYS:O	6:F:110:LYS:HB2	2.14	0.47
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.50	0.47
1:N:228:VAL:O	1:N:228:VAL:HG13	2.15	0.47
1:N:255:LEU:HD13	1:N:422:LEU:HD13	1.96	0.47
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.96	0.47
2:O:31:ASN:ND2	2:O:31:ASN:C	2.65	0.47
1:N:87:ASN:OD1	2:O:286:LYS:HD2	2.15	0.47
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.14	0.47
3:C:350:ILE:HG23	3:C:351:ILE:N	2.29	0.47
2:B:345:LYS:O	2:B:348:ALA:N	2.48	0.47
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:159:VAL:HG21	2:O:325:TYR:HE1	1.80	0.47
5:R:124:LEU:HA	5:R:127:VAL:CG2	2.44	0.47
4:D:168:ILE:HG12	4:D:168:ILE:O	2.15	0.47
6:S:94:LEU:O	6:S:98:ILE:HG13	2.15	0.47
3:C:69:HIS:HD2	3:C:73:ASN:ND2	2.08	0.47
1:A:21:ASN:HA	1:A:219:VAL:HG13	1.97	0.47
3:P:247:SER:N	3:P:248:PRO:HD3	2.30	0.47
2:B:334:GLY:HA2	2:B:434:PRO:HD3	1.97	0.47
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.32	0.47
4:Q:35:GLN:NE2	4:Q:169:LEU:HD12	2.30	0.47
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.97	0.46
1:N:77:LYS:HE3	2:O:359:LYS:HZ1	1.80	0.46
1:N:136:GLN:OE1	9:V:50:LEU:HB3	2.14	0.46
1:A:37:VAL:HG22	1:A:109:VAL:HG11	1.97	0.46
2:B:325:TYR:CD1	9:I:60:ALA:CB	2.97	0.46
10:W:48:GLU:HA	10:W:54:HIS:CE1	2.51	0.46
5:E:190:ASP:CG	5:E:191:ASP:H	2.19	0.46
2:O:264:VAL:HG23	2:O:316:TYR:C	2.36	0.46
1:N:156:THR:HA	5:R:7:VAL:HG21	1.96	0.46
1:A:369:LEU:CD1	1:A:392:LEU:HD21	2.45	0.46
5:R:147:ILE:HG13	5:R:157:TYR:O	2.16	0.46
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.97	0.46
4:Q:139:ALA:HB2	8:U:41:ASP:OD1	2.15	0.46
3:C:98:HIS:CD2	13:C:502:HEM:NC	2.82	0.46
1:N:369:LEU:HD12	1:N:392:LEU:HD21	1.97	0.46
2:O:345:LYS:O	2:O:348:ALA:N	2.48	0.46
3:P:17:ASN:HB2	17:P:2010:BOG:O3	2.16	0.46
2:O:286:LYS:C	2:O:288:GLY:H	2.19	0.46
2:B:102:ARG:HH22	2:B:161:GLU:HA	1.80	0.46
9:V:28:UNK:CA	9:V:72:ALA:HB2	2.44	0.46
1:N:53:ASN:N	1:N:173:ASN:ND2	2.63	0.46
1:A:248:LEU:HD12	1:A:426:GLY:HA2	1.96	0.46
6:F:40:ASP:O	6:F:44:LYS:HG3	2.15	0.46
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.97	0.46
10:J:59:TYR:O	10:J:61:ALA:N	2.45	0.46
2:B:46:ARG:HD2	2:B:110:GLU:OE2	2.16	0.46
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.30	0.46
19:Q:3003:CDL:H511	7:T:26:ILE:HG21	1.97	0.46
1:A:63:ALA:O	1:A:116:VAL:HG13	2.16	0.46
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.51	0.46
2:B:67:HIS:O	2:B:70:ARG:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:353:THR:CG2	2:O:354:GLU:N	2.79	0.46
3:C:101:ARG:O	3:C:101:ARG:HD2	2.16	0.46
3:P:325:LEU:HD22	3:P:370:ILE:HG13	1.98	0.46
3:C:117:GLY:O	13:C:502:HEM:HMC3	2.15	0.46
1:N:49:ASN:ND2	1:N:51:LYS:N	2.58	0.46
5:E:189:GLY:O	5:E:192:LEU:N	2.48	0.46
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.46	0.46
2:B:414:ALA:O	2:B:418:VAL:HG23	2.15	0.46
1:A:45:SER:OG	1:A:92:ARG:HA	2.16	0.46
2:B:78:LYS:HA	2:B:131:GLU:OE2	2.16	0.46
1:N:178:THR:CG2	1:N:179:ARG:N	2.79	0.46
1:A:106:MET:HE3	1:A:110:VAL:HG21	1.98	0.46
1:N:424:ALA:HB1	1:N:428:ILE:HG21	1.98	0.46
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.98	0.46
2:B:62:ASN:O	2:B:65:THR:HG22	2.16	0.46
1:N:351:GLU:O	1:N:354:VAL:HG22	2.16	0.46
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.97	0.46
3:P:347:PRO:O	3:P:351:ILE:HG13	2.16	0.46
1:A:75:PHE:HZ	1:A:86:PHE:HE2	1.64	0.46
8:H:11:GLU:H	8:H:11:GLU:CD	2.19	0.46
1:N:184:SER:O	1:N:188:THR:OG1	2.28	0.46
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.51	0.46
2:O:402:ILE:HG23	2:O:403:ASP:H	1.81	0.46
4:D:3:LEU:HD11	7:G:72:LYS:CE	2.46	0.46
2:O:299:VAL:CG1	2:O:336:VAL:HG13	2.46	0.46
2:O:26:ILE:HA	2:O:35:ILE:O	2.16	0.45
1:A:124:GLU:OE1	1:A:179:ARG:HG3	2.16	0.45
2:O:76:THR:HG23	2:O:136:GLU:CD	2.36	0.45
2:O:31:ASN:HD22	2:O:33:LEU:H	1.61	0.45
1:N:106:MET:CE	1:N:110:VAL:HG21	2.47	0.45
5:R:113:ASP:HB3	5:R:116:LYS:HG3	1.99	0.45
19:Q:3003:CDL:OB3	6:S:73:ARG:NH2	2.49	0.45
2:B:19:PRO:O	2:B:41:PHE:HE1	1.98	0.45
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.52	0.45
5:R:91:TRP:CE2	5:R:92:ARG:HG3	2.51	0.45
1:N:350:THR:HG22	1:N:351:GLU:N	2.31	0.45
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.44	0.45
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.98	0.45
3:P:90:PHE:CE1	3:P:236:MET:HB3	2.51	0.45
3:P:45:GLN:HB3	13:P:501:HEM:HAB	1.99	0.45
2:O:395:PRO:HA	2:O:398:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:106:MET:C	1:N:106:MET:HE2	2.36	0.45
3:P:9:HIS:CD2	3:P:11:LEU:HB2	2.52	0.45
1:N:191:LYS:N	1:N:195:MET:HE2	2.31	0.45
1:N:70:ARG:HA	1:N:71:PRO:HD2	1.85	0.45
1:A:68:LYS:HD2	1:A:119:ASN:HB3	1.98	0.45
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.84	0.45
1:A:26:ALA:HB2	1:A:383:LEU:HD11	1.99	0.45
4:D:120:ARG:HH21	18:D:501:HEC:CGA	2.30	0.45
7:T:24:ARG:HB2	7:T:27:PRO:HB3	1.99	0.45
3:P:270:LYS:O	3:P:270:LYS:HG3	2.16	0.45
4:D:234:LYS:HD2	5:E:8:PRO:HB2	1.98	0.45
1:A:289:HIS:CD2	2:B:83:PHE:HD1	2.34	0.45
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.33	0.45
3:C:50:LEU:HD23	13:C:501:HEM:HBC1	1.98	0.45
2:B:239:TYR:CD1	2:B:260:GLU:HB2	2.52	0.45
5:R:73:LYS:HB3	5:R:195:VAL:O	2.16	0.45
2:O:156:GLN:NE2	9:V:77:ARG:C	2.69	0.45
5:R:99:ARG:NH2	5:R:149:ASN:OD1	2.49	0.45
3:P:69:HIS:HD2	3:P:73:ASN:ND2	2.11	0.45
1:N:106:MET:HG3	1:N:203:ILE:CG2	2.47	0.45
2:B:46:ARG:HE	2:B:376:GLN:HA	1.81	0.45
2:O:327:ILE:HG22	9:V:55:MET:CE	2.47	0.45
2:B:397:VAL:O	2:B:401:LYS:HG2	2.17	0.45
1:A:369:LEU:HD12	1:A:392:LEU:HD21	1.98	0.45
5:R:55:VAL:O	5:R:59:ILE:HG12	2.17	0.45
5:E:122:HIS:HB3	5:E:125:ASP:OD1	2.17	0.45
1:A:136:GLN:O	1:A:140:GLU:HG3	2.17	0.45
1:N:206:LYS:CE	1:N:206:LYS:H	2.27	0.45
1:A:106:MET:HG3	1:A:203:ILE:CG2	2.47	0.45
1:N:106:MET:HE3	1:N:110:VAL:HG21	1.98	0.45
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.98	0.45
1:A:205:HIS:O	1:A:209:VAL:HG12	2.16	0.45
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.82	0.45
2:O:222:GLN:HG2	2:O:222:GLN:O	2.17	0.45
2:O:215:ASP:O	2:O:219:VAL:HG23	2.17	0.45
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.47	0.45
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.17	0.45
2:O:157:VAL:HG13	2:O:158:GLY:N	2.31	0.45
2:O:399:ALA:CA	2:O:402:ILE:HG22	2.47	0.45
1:A:4:TYR:HE2	1:A:396:ASP:OD2	2.00	0.45
4:D:44:ASP:OD1	4:D:93:LYS:HE3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:334:LEU:HA	3:P:334:LEU:HD23	1.75	0.45
2:O:312:PHE:CZ	2:O:314:VAL:CG2	3.00	0.44
8:U:47:ARG:CD	8:U:48:SER:H	2.30	0.44
3:C:234:THR:HG21	4:D:219:LEU:CD1	2.47	0.44
5:E:84:GLY:N	5:E:100:HIS:O	2.45	0.44
4:Q:71:GLN:HE21	4:Q:82:MET:CE	2.30	0.44
2:O:222:GLN:O	2:O:223:PHE:HD2	2.00	0.44
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.99	0.44
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.18	0.44
2:B:308:ASP:OD2	9:I:55:MET:O	2.36	0.44
5:E:85:LYS:HG2	5:E:86:ASN:N	2.33	0.44
2:O:144:LEU:CB	2:O:183:ILE:HD12	2.47	0.44
2:B:215:ASP:O	2:B:219:VAL:HG23	2.16	0.44
1:A:158:PHE:O	1:A:164:ALA:HB2	2.17	0.44
1:N:158:PHE:O	1:N:164:ALA:HB2	2.16	0.44
10:W:60:GLU:CD	10:W:60:GLU:C	2.76	0.44
1:A:170:THR:CG2	1:A:171:THR:N	2.77	0.44
3:P:350:ILE:HG23	3:P:351:ILE:N	2.32	0.44
5:E:41:ALA:O	5:E:45:VAL:HG23	2.16	0.44
5:R:164:HIS:CD2	5:R:173:LYS:HD3	2.53	0.44
3:P:377:MET:HE1	6:S:19:TRP:HZ3	1.82	0.44
5:R:41:ALA:O	5:R:45:VAL:HG23	2.18	0.44
3:P:285:ILE:CD1	3:P:294:ALA:HB2	2.46	0.44
1:N:75:PHE:HZ	1:N:86:PHE:HE2	1.65	0.44
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.51	0.44
4:D:62:LYS:O	4:D:66:GLU:HG3	2.18	0.44
1:A:156:THR:HA	5:E:7:VAL:HG21	2.00	0.44
2:O:333:ALA:O	2:O:337:ILE:HG13	2.17	0.44
8:U:40:CYS:O	8:U:44:VAL:HG23	2.17	0.44
2:B:353:THR:CG2	2:B:354:GLU:N	2.81	0.44
2:B:157:VAL:CG1	2:B:158:GLY:N	2.80	0.44
9:V:65:VAL:O	9:V:76:VAL:HG23	2.16	0.44
1:A:350:THR:HG22	1:A:351:GLU:N	2.33	0.44
2:B:147:ASP:OD1	9:I:68:ILE:HD11	2.18	0.44
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.52	0.44
3:P:344:VAL:O	3:P:344:VAL:HG23	2.17	0.44
2:B:24:LEU:HD21	2:B:392:HIS:CD2	2.53	0.44
3:C:347:PRO:O	3:C:350:ILE:HG22	2.17	0.44
2:B:57:TYR:CD1	2:B:57:TYR:N	2.86	0.44
6:S:91:GLU:HG2	6:S:95:LYS:HE3	1.99	0.44
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:GLN:O	2:B:222:GLN:HG3	2.17	0.44
2:O:29:LEU:HB3	2:O:30:PRO:HD2	1.99	0.44
10:J:60:GLU:O	10:J:61:ALA:HB3	2.18	0.44
2:B:286:LYS:C	2:B:288:GLY:H	2.21	0.44
1:A:23:LEU:C	1:A:23:LEU:HD23	2.38	0.44
3:C:266:PRO:HA	3:C:267:PRO:HD3	1.86	0.44
5:E:52:LYS:C	5:E:52:LYS:HD3	2.38	0.44
5:R:85:LYS:HG2	5:R:86:ASN:N	2.33	0.44
10:J:48:GLU:HA	10:J:54:HIS:CE1	2.53	0.44
3:P:50:LEU:HD23	13:P:501:HEM:HBC1	2.00	0.44
2:O:18:CYS:HA	2:O:19:PRO:HD2	1.74	0.44
5:E:95:PRO:HG3	3:P:263:LEU:HD23	1.99	0.44
9:V:65:VAL:HB	9:V:77:ARG:HD3	1.99	0.44
9:V:28:UNK:HA	9:V:72:ALA:HB2	2.00	0.44
5:R:128:LYS:O	5:R:129:LYS:HG3	2.18	0.44
2:B:116:VAL:O	2:B:120:MET:HB2	2.18	0.44
3:C:202:HIS:NE2	15:C:2002:UQ:O4	2.42	0.44
5:R:117:LEU:O	5:R:118:ARG:C	2.56	0.44
5:E:119:ASP:OD2	5:E:179:ASN:ND2	2.51	0.44
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.53	0.44
1:N:95:THR:HG22	1:N:96:ALA:N	2.33	0.44
5:E:55:VAL:O	5:E:59:ILE:HG12	2.18	0.44
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.90	0.44
2:O:47:ILE:HG22	2:O:48:GLY:N	2.33	0.43
5:R:147:ILE:HG22	5:R:148:ALA:H	1.81	0.43
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.32	0.43
4:D:116:ILE:HG12	18:D:501:HEC:HMA3	1.99	0.43
1:N:223:TYR:OH	1:N:224:LYS:HE3	2.17	0.43
2:B:89:ILE:HD13	2:B:96:LEU:HB2	2.00	0.43
2:B:152:PHE:HA	2:B:157:VAL:CG1	2.46	0.43
2:O:76:THR:HG22	2:O:82:SER:N	2.17	0.43
2:B:71:LEU:O	2:B:74:PRO:HD2	2.18	0.43
5:E:136:VAL:O	5:E:138:VAL:N	2.47	0.43
7:T:36:ASN:O	7:T:40:ARG:HG3	2.18	0.43
2:O:334:GLY:HA2	2:O:434:PRO:HD3	1.98	0.43
1:N:416:TYR:OH	1:N:442:TYR:HB2	2.18	0.43
3:P:335:ILE:HD13	7:T:58:LEU:HD23	2.00	0.43
1:A:106:MET:CE	1:A:110:VAL:HG21	2.49	0.43
1:A:95:THR:HG22	1:A:96:ALA:N	2.33	0.43
5:R:177:PRO:HB2	5:R:178:TYR:CE1	2.54	0.43
5:R:109:GLU:C	5:R:111:GLU:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:TYR:HE1	2:B:381:GLU:OE2	2.02	0.43
1:A:85:HIS:HB2	1:A:100:LYS:HB2	2.00	0.43
9:I:64:LEU:HD12	9:I:77:ARG:C	2.37	0.43
5:R:133:VAL:HG13	5:R:133:VAL:O	2.18	0.43
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.48	0.43
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.47	0.43
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.48	0.43
2:B:385:GLU:C	2:B:387:LEU:H	2.22	0.43
3:C:247:SER:N	3:C:248:PRO:HD3	2.33	0.43
5:R:73:LYS:HG2	5:R:196:GLY:HA3	2.01	0.43
2:O:245:ARG:HB3	2:O:430:LEU:CD1	2.48	0.43
6:F:71:LYS:O	6:F:72:HIS:HB2	2.19	0.43
18:Q:501:HEC:HMC1	18:Q:501:HEC:HBC3	2.00	0.43
9:I:71:ASN:H	9:I:71:ASN:ND2	2.02	0.43
1:N:19:LEU:C	1:N:21:ASN:H	2.22	0.43
15:C:2002:UQ:HM51	15:C:2002:UQ:C8	2.48	0.43
1:A:240:GLU:HA	1:A:422:LEU:O	2.18	0.43
1:N:284:PHE:CE2	9:V:71:ASN:O	2.71	0.43
2:B:295:LEU:HD11	2:B:340:ALA:HB1	2.01	0.43
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.49	0.43
4:D:197:GLU:O	4:D:198:HIS:C	2.57	0.43
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	2.01	0.43
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.72	0.43
5:R:84:GLY:N	5:R:100:HIS:O	2.52	0.43
3:C:152:SER:HB3	3:C:162:VAL:HG21	2.00	0.43
2:B:312:PHE:CZ	2:B:314:VAL:CG2	3.02	0.43
3:C:142:TRP:CD1	3:C:266:PRO:HD3	2.54	0.43
1:N:248:LEU:HD12	1:N:426:GLY:HA2	2.01	0.43
8:H:32:LYS:O	8:H:36:ARG:HG3	2.19	0.43
3:C:25:PRO:HB2	3:C:28:ILE:HG23	2.00	0.43
3:C:78:TRP:CD2	4:D:197:GLU:HG3	2.54	0.43
2:O:397:VAL:O	2:O:401:LYS:HG2	2.18	0.43
1:N:37:VAL:HG22	1:N:109:VAL:HG11	2.01	0.43
5:E:191:ASP:OD1	5:E:191:ASP:O	2.37	0.43
18:Q:501:HEC:HMB1	18:Q:501:HEC:HBB3	2.01	0.43
4:Q:200:GLN:NE2	17:Q:3091:BOG:H3	2.33	0.43
4:Q:231:LYS:O	6:S:71:LYS:HE3	2.18	0.43
5:R:78:LEU:HD22	5:R:132:TRP:CZ3	2.54	0.43
9:I:38:UNK:C	9:I:40:UNK:N	2.80	0.43
1:N:137:GLU:O	1:N:141:MET:HG3	2.19	0.43
4:Q:117:VAL:O	4:Q:123:GLY:HA2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:74:ILE:HD11	5:R:96:LEU:HD23	2.01	0.43
5:R:137:GLY:O	5:R:145:VAL:HG22	2.19	0.43
1:N:49:ASN:C	1:N:49:ASN:ND2	2.72	0.42
5:R:124:LEU:HA	5:R:127:VAL:HG22	2.01	0.42
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.47	0.42
1:N:170:THR:CG2	1:N:171:THR:N	2.80	0.42
1:A:191:LYS:C	1:A:195:MET:HE2	2.39	0.42
2:B:58:GLU:HG2	2:B:65:THR:HG22	2.00	0.42
5:R:165:TYR:HA	5:R:170:ARG:O	2.18	0.42
1:A:182:LEU:O	1:A:186:ILE:HG13	2.19	0.42
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.54	0.42
2:O:156:GLN:O	2:O:159:VAL:HG22	2.19	0.42
2:O:31:ASN:HD21	2:O:33:LEU:H	1.61	0.42
5:R:171:ILE:O	5:R:171:ILE:HG23	2.18	0.42
5:R:122:HIS:HB3	5:R:125:ASP:OD1	2.19	0.42
5:E:77:LYS:CE	5:E:80:ASP:OD2	2.65	0.42
2:B:273:SER:HB3	2:B:364:LEU:HD21	2.02	0.42
9:V:67:GLY:O	9:V:68:ILE:HD13	2.20	0.42
1:A:64:PHE:CE2	1:A:86:PHE:CE1	3.07	0.42
1:A:161:THR:HG21	1:A:235:ARG:H	1.83	0.42
4:D:95:TYR:HA	4:D:96:PRO:HD3	1.85	0.42
1:A:178:THR:CG2	1:A:179:ARG:N	2.81	0.42
1:A:106:MET:C	1:A:106:MET:HE2	2.39	0.42
3:C:269:ILE:HG22	3:C:269:ILE:O	2.19	0.42
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.85	0.42
5:E:164:HIS:HB2	5:E:173:LYS:HB3	2.01	0.42
2:O:89:ILE:HD13	2:O:96:LEU:HB2	2.00	0.42
1:N:350:THR:CG2	1:N:351:GLU:N	2.83	0.42
1:N:398:ARG:HH11	1:N:398:ARG:CG	2.25	0.42
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.49	0.42
7:G:36:ASN:O	7:G:40:ARG:HG3	2.20	0.42
1:N:140:GLU:HG3	9:V:50:LEU:HD12	2.02	0.42
1:N:90:THR:O	1:N:167:VAL:HG11	2.19	0.42
2:B:270:ASN:O	2:B:274:VAL:HG23	2.19	0.42
2:O:291:VAL:C	2:O:293:SER:H	2.22	0.42
3:C:334:LEU:HA	3:C:334:LEU:HD23	1.86	0.42
6:F:84:GLU:CD	6:F:84:GLU:H	2.22	0.42
1:N:206:LYS:N	1:N:206:LYS:CD	2.63	0.42
2:B:402:ILE:HG23	2:B:403:ASP:H	1.83	0.42
2:B:395:PRO:HA	2:B:398:VAL:CG1	2.50	0.42
10:W:10:TYR:CE2	10:W:15:ARG:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:102:ARG:HA	4:D:108:ALA:O	2.19	0.42
3:C:95:ILE:HD13	3:C:121:LEU:HD13	2.01	0.42
4:D:122:GLY:O	4:D:125:ASP:HB2	2.18	0.42
2:O:34:ILE:HD13	2:O:390:GLY:CA	2.50	0.42
2:B:291:VAL:C	2:B:293:SER:H	2.22	0.42
2:O:31:ASN:HD21	2:O:33:LEU:CB	2.33	0.42
2:B:399:ALA:CA	2:B:402:ILE:HG22	2.50	0.42
2:O:424:MET:HG2	2:O:425:ALA:N	2.34	0.42
7:G:71:ARG:HD3	8:H:56:GLU:CD	2.39	0.42
5:R:164:HIS:HB2	5:R:173:LYS:HB3	2.02	0.42
1:N:239:SER:HB2	7:T:17:SER:O	2.20	0.42
3:P:305:ILE:HB	3:P:306:PRO:HD3	2.02	0.42
2:B:29:LEU:HB3	2:B:30:PRO:HD2	2.00	0.42
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.85	0.42
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.34	0.42
7:G:45:VAL:O	7:G:49:ALA:HB3	2.20	0.42
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	2.01	0.42
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.55	0.42
1:A:335:MET:HG3	1:A:339:GLN:HE21	1.85	0.42
3:C:194:THR:O	3:C:197:HIS:HB3	2.20	0.42
1:N:370:ASP:O	2:O:374:THR:HG22	2.20	0.42
2:O:295:LEU:HD11	2:O:340:ALA:HB1	2.01	0.42
2:O:157:VAL:CG1	2:O:158:GLY:N	2.82	0.42
5:R:131:GLU:CD	5:R:131:GLU:H	2.22	0.42
8:U:54:CYS:HA	8:U:57:GLU:OE2	2.20	0.42
1:N:240:GLU:HA	1:N:422:LEU:O	2.20	0.42
5:E:189:GLY:O	5:E:190:ASP:C	2.58	0.42
2:O:337:ILE:HD12	2:O:434:PRO:HD2	2.01	0.42
5:R:109:GLU:HB3	5:R:123:ASP:HB2	2.02	0.42
2:O:201:SER:OG	2:O:228:SER:HA	2.20	0.42
5:E:71:LEU:HD11	3:P:169:PHE:CE1	2.55	0.42
2:O:168:TYR:HB2	2:O:173:ALA:HB2	2.01	0.42
3:C:335:ILE:HD13	7:G:58:LEU:HD23	2.01	0.42
5:R:101:ARG:HB3	5:R:105:GLU:HB2	2.02	0.42
2:B:84:ARG:HD2	6:S:107:TRP:CZ3	2.55	0.42
2:B:71:LEU:HD12	2:B:144:LEU:HD23	2.02	0.42
1:N:170:THR:HG22	1:N:171:THR:H	1.84	0.42
4:D:54:VAL:HG12	4:D:55:THR:HG23	2.02	0.42
6:S:13:MET:HB3	6:S:17:ARG:HE	1.84	0.42
2:O:299:VAL:HG11	2:O:336:VAL:HG13	2.00	0.42
3:P:208:ASN:HB2	3:P:209:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:380:TYR:CZ	6:F:37:LEU:HD21	2.55	0.42
2:B:162:ASN:O	2:B:244:ILE:HD12	2.20	0.42
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.47	0.42
2:B:389:SER:O	2:B:390:GLY:C	2.58	0.42
1:N:26:ALA:CB	1:N:383:LEU:HD11	2.50	0.42
3:C:377:MET:HE1	6:F:20:TYR:HD1	1.85	0.42
2:O:318:ASP:O	2:O:319:SER:HB2	2.20	0.42
2:O:414:ALA:O	2:O:418:VAL:HG23	2.20	0.42
8:U:32:LYS:O	8:U:36:ARG:HG3	2.20	0.42
1:A:436:ARG:HD2	1:A:436:ARG:HA	1.76	0.42
1:A:281:ASP:C	1:A:281:ASP:OD1	2.58	0.41
2:O:31:ASN:HD21	2:O:33:LEU:HB3	1.85	0.41
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.48	0.41
4:D:195:GLU:HG3	4:D:198:HIS:HB2	2.02	0.41
1:A:26:ALA:O	1:A:198:ALA:HA	2.20	0.41
3:P:345:GLU:O	3:P:348:PHE:HB2	2.19	0.41
3:P:207:ASN:ND2	3:P:208:ASN:H	2.18	0.41
1:N:274:ASN:HA	1:N:274:ASN:HD22	1.65	0.41
2:B:24:LEU:HD23	2:B:392:HIS:CE1	2.55	0.41
6:F:77:LYS:HE2	6:F:77:LYS:HB3	1.82	0.41
4:Q:167:GLU:CG	8:U:13:LEU:HD13	2.50	0.41
1:A:233:ARG:HH12	1:A:316:ASP:HB2	1.85	0.41
6:S:52:GLU:HG3	6:S:56:ASN:ND2	2.34	0.41
2:B:31:ASN:HD21	2:B:33:LEU:H	1.60	0.41
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.29	0.41
18:D:501:HEC:HBB3	18:D:501:HEC:HMB1	2.01	0.41
1:N:242:ARG:O	7:T:14:ILE:HA	2.20	0.41
3:P:273:TRP:HA	3:P:276:LEU:CD1	2.49	0.41
10:J:14:PHE:CD2	10:J:14:PHE:N	2.87	0.41
7:T:66:PHE:CE2	7:T:70:LYS:HE3	2.56	0.41
2:O:102:ARG:HH22	2:O:161:GLU:HA	1.86	0.41
10:J:38:GLY:O	10:J:42:ILE:HG13	2.20	0.41
9:I:55:MET:O	9:I:58:ARG:HG2	2.20	0.41
1:A:170:THR:HG22	1:A:171:THR:H	1.83	0.41
5:E:132:TRP:CB	5:E:187:PHE:HZ	2.33	0.41
1:A:403:ASP:OD1	1:A:406:MET:HB2	2.20	0.41
4:Q:161:ALA:O	4:Q:162:PRO:C	2.59	0.41
8:H:11:GLU:O	8:H:12:GLU:HB2	2.20	0.41
4:Q:44:ASP:OD1	4:Q:93:LYS:HE3	2.21	0.41
1:A:217:SER:O	1:A:218:GLY:C	2.58	0.41
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:68:LYS:HD2	1:N:119:ASN:HB3	2.02	0.41
2:O:157:VAL:CG2	9:V:64:LEU:HD21	2.36	0.41
2:O:46:ARG:HD2	2:O:110:GLU:OE2	2.20	0.41
2:O:248:ASN:HD22	2:O:250:HIS:H	1.68	0.41
4:D:26:VAL:HG22	4:D:188:THR:HG22	2.01	0.41
1:A:37:VAL:HG23	1:A:113:LEU:HD11	2.01	0.41
2:O:225:ASN:O	2:O:227:ARG:N	2.53	0.41
2:B:337:ILE:HD12	2:B:434:PRO:HD2	2.01	0.41
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.19	0.41
5:R:1:VAL:CG2	5:R:3:ASN:HD22	2.34	0.41
2:B:389:SER:O	2:B:391:THR:N	2.54	0.41
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.50	0.41
3:C:101:ARG:CD	3:C:101:ARG:C	2.88	0.41
2:O:368:TYR:HE1	2:O:381:GLU:OE2	2.03	0.41
3:P:273:TRP:HA	3:P:276:LEU:HD12	2.02	0.41
6:S:84:GLU:H	6:S:84:GLU:CD	2.24	0.41
1:A:168:GLU:H	1:A:168:GLU:CD	2.23	0.41
3:P:156:TYR:CD2	3:P:156:TYR:N	2.88	0.41
2:B:307:PHE:H	9:I:52:ARG:HG2	1.86	0.41
1:A:362:ARG:HB2	2:B:112:LEU:HD11	2.03	0.41
2:B:224:LEU:HD23	2:B:224:LEU:HA	1.90	0.41
1:N:358:LYS:O	1:N:362:ARG:HG3	2.21	0.41
1:A:77:LYS:HE3	2:B:359:LYS:HZ1	1.85	0.41
5:E:77:LYS:HE2	5:E:80:ASP:CG	2.39	0.41
5:E:171:ILE:HG23	5:E:171:ILE:O	2.21	0.41
1:N:69:LYS:HE3	1:N:70:ARG:HH21	1.86	0.41
3:P:226:SER:O	3:P:230:ILE:HG13	2.20	0.41
1:A:106:MET:HE1	1:A:107:PRO:HA	2.03	0.41
2:B:314:VAL:HG11	2:B:316:TYR:CZ	2.56	0.41
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.47	0.41
7:G:73:ASN:HA	7:G:74:PRO:HD2	1.92	0.41
2:B:50:PHE:C	2:B:51:ILE:HG13	2.40	0.41
3:C:301:ILE:CD1	3:C:364:LEU:HD21	2.50	0.41
6:S:77:LYS:HE2	6:S:77:LYS:HB3	1.83	0.41
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.20	0.41
9:V:32:UNK:O	9:V:33:UNK:C	2.68	0.41
1:N:45:SER:HA	1:N:48:GLU:HG3	2.03	0.41
1:A:69:LYS:HE3	1:A:70:ARG:HH21	1.85	0.41
3:C:37:LEU:CD1	3:C:236:MET:HG3	2.51	0.41
10:J:56:LYS:O	10:J:60:GLU:HB2	2.20	0.41
3:C:28:ILE:HD11	15:C:2002:UQ:HM21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:118:ARG:HB2	5:R:171:ILE:CG2	2.50	0.41
3:P:223:PRO:HB2	3:P:227:PHE:HD2	1.86	0.41
6:S:77:LYS:O	6:S:77:LYS:HG2	2.21	0.41
6:S:71:LYS:O	6:S:72:HIS:HB2	2.20	0.41
3:C:342:GLN:HB3	3:C:343:PRO:HD2	2.03	0.41
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.56	0.41
3:P:54:MET:SD	5:R:62:LEU:HD21	2.61	0.41
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.55	0.41
4:D:14:HIS:HB3	4:D:21:LEU:HA	2.03	0.41
4:D:29:GLY:HA3	4:D:189:PHE:HB2	2.03	0.41
1:N:436:ARG:HA	1:N:436:ARG:HD2	1.80	0.41
5:E:106:ILE:HG21	5:E:130:PRO:HB3	2.02	0.41
1:A:402:VAL:HG22	1:A:406:MET:HE2	2.03	0.41
1:N:182:LEU:O	1:N:186:ILE:HG13	2.21	0.41
1:N:280:TYR:CG	1:N:281:ASP:N	2.89	0.41
5:E:193:VAL:HG13	5:E:193:VAL:O	2.21	0.41
1:A:106:MET:CE	1:A:107:PRO:HA	2.50	0.40
1:N:387:GLY:O	1:N:388:ARG:HB3	2.20	0.40
8:H:10:GLU:HB2	8:H:11:GLU:OE2	2.21	0.40
7:G:24:ARG:HB2	7:G:27:PRO:HB3	2.04	0.40
5:R:193:VAL:HG13	5:R:193:VAL:O	2.20	0.40
3:C:2:ALA:HB3	3:C:8:SER:HB3	2.02	0.40
1:A:49:ASN:ND2	1:A:49:ASN:C	2.73	0.40
2:B:46:ARG:HG3	2:B:110:GLU:HG2	2.04	0.40
3:C:30:ALA:O	3:C:33:ASN:HB2	2.20	0.40
3:C:347:PRO:O	3:C:351:ILE:HG13	2.20	0.40
8:U:12:GLU:HG2	8:U:13:LEU:N	2.36	0.40
2:B:350:GLY:C	2:B:352:VAL:H	2.23	0.40
1:N:371:GLY:O	1:N:375:VAL:HG23	2.21	0.40
2:O:268:GLU:HG2	2:O:268:GLU:O	2.21	0.40
1:N:26:ALA:O	1:N:198:ALA:HA	2.22	0.40
8:H:65:ARG:O	8:H:68:CYS:HB3	2.22	0.40
2:O:109:VAL:HG21	2:O:119:VAL:CG1	2.51	0.40
3:C:29:SER:HB2	19:G:2004:CDL:OB4	2.21	0.40
1:A:328:PRO:HB3	1:A:427:PRO:HB2	2.04	0.40
10:W:14:PHE:CD2	10:W:14:PHE:N	2.84	0.40
3:P:69:HIS:CD2	3:P:73:ASN:ND2	2.81	0.40
1:A:350:THR:CG2	1:A:351:GLU:N	2.84	0.40
2:O:399:ALA:HA	2:O:402:ILE:CG2	2.52	0.40
1:A:7:THR:O	1:A:11:ILE:HG13	2.22	0.40
3:P:98:HIS:HD2	13:P:502:HEM:C1C	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:116:LYS:O	5:R:117:LEU:HD23	2.21	0.40
5:E:170:ARG:HA	5:E:179:ASN:HB3	2.03	0.40
5:E:78:LEU:HD13	5:E:132:TRP:CE2	2.56	0.40
2:O:124:LEU:HD21	2:O:223:PHE:HB3	2.04	0.40
1:N:144:ASP:O	1:N:148:VAL:HG23	2.21	0.40
3:C:134:LEU:N	3:C:135:PRO:HD2	2.36	0.40
1:A:364:ALA:O	1:A:368:GLN:HG3	2.21	0.40
1:N:364:ALA:O	1:N:368:GLN:HG3	2.21	0.40
1:A:300:GLU:OE1	1:A:300:GLU:HA	2.21	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%)	415 (94%)	21 (5%)	5 (1%)	17 46
1	N	440/446 (99%)	413 (94%)	21 (5%)	6 (1%)	14 38
2	B	419/441 (95%)	370 (88%)	40 (10%)	9 (2%)	9 25
2	O	420/441 (95%)	374 (89%)	38 (9%)	8 (2%)	10 28
3	C	378/380 (100%)	363 (96%)	14 (4%)	1 (0%)	46 77
3	P	377/380 (99%)	361 (96%)	15 (4%)	1 (0%)	46 77
4	D	239/241 (99%)	227 (95%)	12 (5%)	0	100 100
4	Q	239/241 (99%)	223 (93%)	15 (6%)	1 (0%)	39 72
5	E	194/196 (99%)	174 (90%)	13 (7%)	7 (4%)	4 12
5	R	192/196 (98%)	163 (85%)	22 (12%)	7 (4%)	4 12
6	F	99/110 (90%)	94 (95%)	4 (4%)	1 (1%)	19 48
6	S	99/110 (90%)	92 (93%)	7 (7%)	0	100 100
7	G	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	15 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	T	76/81 (94%)	69 (91%)	7 (9%)	0	100 100
8	H	68/77 (88%)	61 (90%)	6 (9%)	1 (2%)	13 36
8	U	65/77 (84%)	60 (92%)	4 (6%)	1 (2%)	13 36
9	I	29/47 (62%)	25 (86%)	4 (14%)	0	100 100
9	V	29/47 (62%)	25 (86%)	3 (10%)	1 (3%)	5 14
10	J	59/61 (97%)	54 (92%)	3 (5%)	2 (3%)	5 14
10	W	58/61 (95%)	54 (93%)	2 (3%)	2 (3%)	5 14
All	All	4000/4160 (96%)	3688 (92%)	258 (6%)	54 (1%)	14 38

All (54) 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	171	ALA
2	O	228	SER
2	O	389	SER
5	R	113	ASP
5	R	191	ASP
1	A	218	GLY
2	B	171	ALA
2	B	390	GLY
5	E	137	GLY
1	N	218	GLY
5	R	137	GLY
5	R	189	GLY
8	U	13	LEU
1	A	72	CYS
1	N	72	CYS
1	N	262	TRP
9	V	48	PRO
1	A	262	TRP

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Mol	Chain	Res	Type
2	B	220	ALA
5	E	64	ALA
5	E	120	PRO
5	E	141	HIS
8	H	12	GLU
10	J	56	LYS
2	O	350	GLY
5	R	152	ASP
10	W	62	SER
1	A	443	TRP
7	G	33	ALA
10	J	60	GLU
1	N	443	TRP
2	O	220	ALA
2	O	390	GLY
4	Q	177	ALA
10	W	56	LYS
2	B	29	LEU
6	F	77	LYS
3	P	286	PRO
5	E	189	GLY
2	B	350	GLY
5	R	8	PRO
3	C	286	PRO
2	O	29	LEU
5	R	147	ILE

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%)	351 (96%)	14 (4%)	40 73
1	N	365/368 (99%)	348 (95%)	17 (5%)	32 64
2	B	332/347 (96%)	327 (98%)	5 (2%)	72 92
2	O	333/347 (96%)	327 (98%)	6 (2%)	66 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	328/329 (100%)	325 (99%)	3 (1%)	84 95
3	P	328/329 (100%)	325 (99%)	3 (1%)	84 95
4	D	200/200 (100%)	198 (99%)	2 (1%)	82 95
4	Q	200/200 (100%)	197 (98%)	3 (2%)	72 92
5	E	166/166 (100%)	166 (100%)	0	100 100
5	R	165/166 (99%)	160 (97%)	5 (3%)	48 80
6	F	93/96 (97%)	91 (98%)	2 (2%)	60 87
6	S	93/96 (97%)	91 (98%)	2 (2%)	60 87
7	G	71/71 (100%)	70 (99%)	1 (1%)	74 92
7	T	69/71 (97%)	67 (97%)	2 (3%)	50 81
8	H	65/71 (92%)	64 (98%)	1 (2%)	72 92
8	U	63/71 (89%)	62 (98%)	1 (2%)	70 91
9	I	23/26 (88%)	22 (96%)	1 (4%)	35 68
9	V	23/26 (88%)	23 (100%)	0	100 100
10	J	49/49 (100%)	48 (98%)	1 (2%)	63 89
10	W	47/49 (96%)	46 (98%)	1 (2%)	61 88
All	All	3378/3446 (98%)	3308 (98%)	70 (2%)	61 88

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	307	PHE
1	A	308	GLN
1	A	342	TRP
1	A	344	ARG
1	A	395	TRP
1	A	405	ARG
1	A	443	TRP
2	B	31	ASN

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Mol	Chain	Res	Type
2	B	248	ASN
2	B	338	ARG
2	B	341	MET
2	B	402	ILE
3	C	91	PHE
3	C	223	PRO
3	C	367	PHE
4	D	169	LEU
4	D	172	ASP
6	F	58	ARG
6	F	70	LEU
7	G	27	PRO
8	H	72	LYS
9	I	71	ASN
10	J	59	TYR
1	N	3	THR
1	N	18	THR
1	N	29	GLU
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	348	SER
1	N	395	TRP
1	N	405	ARG
1	N	443	TRP
2	O	31	ASN
2	O	139	ASP
2	O	248	ASN
2	O	338	ARG
2	O	341	MET
2	O	402	ILE
3	P	91	PHE
3	P	223	PRO
3	P	367	PHE
4	Q	169	LEU

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Mol	Chain	Res	Type
4	Q	172	ASP
4	Q	241	LYS
5	R	52	LYS
5	R	113	ASP
5	R	125	ASP
5	R	126	ARG
5	R	187	PHE
6	S	58	ARG
6	S	70	LEU
7	T	2	ILE
7	T	27	PRO
8	U	72	LYS
10	W	59	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	85	HIS
1	A	118	GLN
1	A	126	GLN
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	247	GLN
2	B	248	ASN
2	B	276	GLN
2	B	329	GLN
2	B	343	GLN
3	C	9	HIS
3	C	69	HIS
3	C	82	ASN
3	C	207	ASN
3	C	342	GLN
3	C	346	HIS
4	D	35	GLN
4	D	50	ASN

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Mol	Chain	Res	Type
4	D	71	GLN
4	D	148	HIS
4	D	200	GLN
5	E	3	ASN
5	E	57	GLN
5	E	86	ASN
5	E	103	GLN
5	E	107	ASN
6	F	79	GLN
7	G	23	GLN
7	G	44	GLN
7	G	79	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	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	305	GLN
2	O	329	GLN
2	O	343	GLN
2	O	376	GLN
3	P	9	HIS
3	P	69	HIS
3	P	82	ASN
3	P	86	ASN
3	P	207	ASN
3	P	313	GLN
3	P	342	GLN
4	Q	35	GLN

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Mol	Chain	Res	Type
4	Q	50	ASN
4	Q	71	GLN
4	Q	148	HIS
4	Q	200	GLN
5	R	3	ASN
5	R	57	GLN
6	S	56	ASN
6	S	79	GLN
7	T	23	GLN
7	T	44	GLN
7	T	79	ASN
8	U	71	HIS
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	2005	-	49,49,50	1.34	9 (18%)	50,54,55	0.90	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	FMX	C	2001	-	28,31,31	0.96	0	35,44,44	1.35	5 (14%)
15	UQ	C	2002	-	19,19,63	2.40	9 (47%)	23,26,79	0.99	2 (8%)
11	PEE	C	2007	-	47,47,50	1.19	6 (12%)	48,52,55	0.90	5 (10%)
11	PEE	C	2008	-	20,20,50	1.64	5 (25%)	21,25,55	0.67	0
16	AZI	C	2011	-	0,2,2	0.00	-	0,1,1	0.00	-
17	BOG	C	3010	-	10,11,20	0.83	1 (10%)	9,11,25	0.96	1 (11%)
13	HEM	C	501	3	30,50,50	2.98	9 (30%)	24,82,82	2.43	9 (37%)
13	HEM	C	502	3	30,50,50	2.62	7 (23%)	24,82,82	2.26	6 (25%)
19	CDL	D	2003	-	41,41,99	1.15	0	43,53,111	1.08	5 (11%)
17	BOG	D	2009	-	20,20,20	0.99	1 (5%)	25,25,25	0.93	2 (8%)
17	BOG	D	2091	-	20,20,20	1.10	2 (10%)	25,25,25	1.01	1 (4%)
18	HEC	D	501	4	24,50,50	1.93	2 (8%)	19,82,82	3.14	7 (36%)
20	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
19	CDL	G	2004	-	39,39,99	1.18	3 (7%)	41,51,111	1.08	3 (7%)
11	PEE	N	3005	-	49,49,50	1.33	9 (18%)	50,54,55	0.89	5 (10%)
11	PEE	N	3008	-	4,4,50	3.78	4 (100%)	6,6,55	0.49	0
17	BOG	P	2010	-	18,18,20	1.13	3 (16%)	22,22,25	0.57	0
14	FMX	P	3001	-	28,31,31	0.94	1 (3%)	35,44,44	1.28	4 (11%)
15	UQ	P	3002	-	19,19,63	2.27	10 (52%)	23,26,79	1.09	3 (13%)
11	PEE	P	3007	-	47,47,50	1.23	6 (12%)	48,52,55	0.87	4 (8%)
16	AZI	P	3011	-	0,2,2	0.00	-	0,1,1	0.00	-
13	HEM	P	501	3	30,50,50	2.91	10 (33%)	24,82,82	2.36	9 (37%)
13	HEM	P	502	3	30,50,50	2.64	9 (30%)	24,82,82	2.28	8 (33%)
19	CDL	Q	3003	-	41,41,99	1.16	1 (2%)	43,53,111	1.09	4 (9%)
17	BOG	Q	3009	-	20,20,20	0.94	1 (5%)	25,25,25	0.88	2 (8%)
17	BOG	Q	3091	-	20,20,20	1.09	2 (10%)	25,25,25	0.90	2 (8%)
18	HEC	Q	501	4	24,50,50	2.29	3 (12%)	19,82,82	3.11	7 (36%)
20	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
19	CDL	T	3004	-	39,39,99	1.17	3 (7%)	41,51,111	1.09	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	2005	-	-	0/53/53/54	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FMX	C	2001	-	-	0/14/33/33	0/4/4/4
15	UQ	C	2002	-	-	0/11/35/87	0/1/1/1
11	PEE	C	2007	-	-	0/51/51/54	0/0/0/0
11	PEE	C	2008	-	-	0/24/24/54	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	3005	-	-	0/53/53/54	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	FMX	P	3001	-	-	0/14/33/33	0/4/4/4
15	UQ	P	3002	-	-	0/11/35/87	0/1/1/1
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 (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	501	HEM	C3B-CAB	-7.90	1.36	1.51
13	P	501	HEM	C3B-C4B	-7.80	1.44	1.51
13	C	501	HEM	C3B-C4B	-7.65	1.45	1.51
18	Q	501	HEC	C3B-C2B	-7.53	1.32	1.40
13	C	502	HEM	C3B-CAB	-7.18	1.37	1.51
13	P	501	HEM	C3B-CAB	-6.92	1.38	1.51
13	P	502	HEM	C3B-C4B	-6.68	1.45	1.51
18	Q	501	HEC	C3C-C2C	-6.63	1.33	1.40
18	D	501	HEC	C3B-C2B	-6.57	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	501	HEM	C2D-C3D	-6.36	1.35	1.54
13	P	501	HEM	C2D-C3D	-6.23	1.35	1.54
13	C	502	HEM	C2D-C3D	-6.03	1.36	1.54
13	C	501	HEM	C3C-CAC	-5.95	1.40	1.51
13	P	502	HEM	C2D-C3D	-5.86	1.36	1.54
13	C	502	HEM	C3C-CAC	-5.81	1.40	1.51
13	P	502	HEM	C3B-CAB	-5.52	1.41	1.51
13	P	502	HEM	C3C-CAC	-4.93	1.42	1.51
13	P	501	HEM	C3C-CAC	-4.82	1.42	1.51
13	C	502	HEM	C2C-C1C	-4.64	1.43	1.52
18	D	501	HEC	C3C-C2C	-4.41	1.36	1.40
13	C	501	HEM	C2C-C1C	-4.23	1.44	1.52
13	P	501	HEM	C2C-C1C	-4.19	1.44	1.52
13	P	502	HEM	C2C-C1C	-3.89	1.45	1.52
13	P	501	HEM	C3D-C4D	-3.63	1.46	1.51
13	C	501	HEM	C3D-C4D	-3.00	1.47	1.51
11	P	3007	PEE	C22-C21	-2.92	1.34	1.51
11	N	3005	PEE	C19-C18	-2.91	1.34	1.51
11	A	2005	PEE	C19-C18	-2.91	1.34	1.51
11	P	3007	PEE	C19-C18	-2.90	1.34	1.51
11	C	2007	PEE	C19-C18	-2.87	1.34	1.51
11	N	3005	PEE	C22-C21	-2.85	1.35	1.51
11	C	2007	PEE	C22-C21	-2.81	1.35	1.51
11	A	2005	PEE	C22-C21	-2.75	1.35	1.51
13	C	502	HEM	C3B-C4B	-2.62	1.49	1.51
13	P	501	HEM	C2D-C1D	-2.56	1.43	1.51
13	P	501	HEM	C2B-C1B	-2.45	1.43	1.51
13	P	502	HEM	C2D-C1D	-2.45	1.43	1.51
19	T	3004	CDL	OA8-CA6	-2.12	1.40	1.45
13	C	501	HEM	C2D-C1D	-2.02	1.45	1.51
18	Q	501	HEC	C1C-CHC	-2.00	1.34	1.39
19	G	2004	CDL	CB3-CB4	2.00	1.56	1.50
11	N	3008	PEE	P-O2P	2.05	1.61	1.54
11	P	3007	PEE	C3-C2	2.05	1.56	1.50
19	Q	3003	CDL	O1-C1	2.09	1.49	1.43
17	Q	3009	BOG	O5-C1	2.12	1.47	1.41
11	N	3005	PEE	C31-C30	2.12	1.57	1.50
17	P	2010	BOG	C4-C5	2.14	1.57	1.53
19	G	2004	CDL	O1-C1	2.14	1.49	1.43
14	P	3001	FMX	C26-C21	2.15	1.42	1.39
15	P	3002	UQ	O2-C2	2.15	1.42	1.37
11	A	2005	PEE	C11-C10	2.17	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	N	3005	PEE	C11-C10	2.17	1.57	1.50
15	P	3002	UQ	C5-C4	2.19	1.55	1.47
17	P	2010	BOG	C1-C2	2.19	1.57	1.52
11	C	2007	PEE	O2-C10	2.21	1.40	1.34
19	G	2004	CDL	CA3-CA4	2.21	1.57	1.50
15	P	3002	UQ	C3-C4	2.24	1.55	1.48
15	P	3002	UQ	C7-C8	2.27	1.54	1.50
19	T	3004	CDL	O1-C1	2.29	1.50	1.43
11	C	2008	PEE	C1-C2	2.29	1.57	1.50
11	C	2008	PEE	C3-C2	2.29	1.57	1.50
11	C	2007	PEE	C3-C2	2.29	1.57	1.50
11	A	2005	PEE	C1-C2	2.31	1.57	1.50
15	C	2002	UQ	C5-C4	2.32	1.56	1.47
17	D	2091	BOG	C4-C5	2.33	1.58	1.53
17	D	2009	BOG	O5-C1	2.34	1.47	1.41
11	A	2005	PEE	C31-C30	2.36	1.57	1.50
15	C	2002	UQ	C3-C4	2.37	1.55	1.48
17	Q	3091	BOG	C4-C5	2.38	1.58	1.53
17	Q	3091	BOG	O5-C1	2.39	1.48	1.41
11	A	2005	PEE	C3-C2	2.42	1.57	1.50
17	C	3010	BOG	C2-C1	2.43	1.57	1.50
19	T	3004	CDL	CA3-CA4	2.43	1.57	1.50
11	N	3005	PEE	C3-C2	2.45	1.57	1.50
17	D	2091	BOG	O5-C1	2.47	1.48	1.41
11	N	3005	PEE	C1-C2	2.48	1.57	1.50
15	C	2002	UQ	O2-C2	2.49	1.43	1.37
15	P	3002	UQ	C2-C1	2.52	1.56	1.48
11	P	3007	PEE	O2-C10	2.53	1.41	1.34
13	P	502	HEM	C4C-NC	2.53	1.39	1.36
15	P	3002	UQ	O3-C3	2.55	1.43	1.37
11	C	2007	PEE	O3-C30	2.56	1.41	1.33
15	P	3002	UQ	CM5-C5	2.58	1.56	1.50
11	C	2008	PEE	P-O1P	2.59	1.60	1.51
17	P	2010	BOG	O5-C1	2.59	1.48	1.43
11	N	3005	PEE	O3-C30	2.61	1.41	1.33
11	N	3008	PEE	P-O3P	2.66	1.64	1.54
11	P	3007	PEE	P-O1P	2.75	1.61	1.51
11	C	2007	PEE	P-O1P	2.79	1.61	1.51
11	A	2005	PEE	O3-C30	2.80	1.41	1.33
11	C	2008	PEE	O2-C10	2.80	1.42	1.34
11	P	3007	PEE	O3-C30	2.87	1.42	1.33
11	N	3005	PEE	P-O1P	2.89	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	2002	UQ	O3-C3	2.91	1.44	1.37
11	A	2005	PEE	P-O1P	2.91	1.61	1.51
15	C	2002	UQ	C2-C1	2.92	1.57	1.48
15	C	2002	UQ	CM5-C5	2.94	1.57	1.50
11	N	3008	PEE	P-O4P	2.95	1.65	1.54
11	N	3005	PEE	O2-C10	2.97	1.43	1.34
11	A	2005	PEE	O2-C10	3.05	1.43	1.34
11	C	2008	PEE	O3-C30	3.18	1.42	1.33
13	C	501	HEM	CBB-CAB	3.32	1.48	1.29
15	P	3002	UQ	C6-C1	3.57	1.56	1.46
15	P	3002	UQ	C6-C5	3.65	1.43	1.35
13	P	501	HEM	CBB-CAB	3.68	1.50	1.29
13	P	501	HEM	CBC-CAC	3.68	1.50	1.29
15	C	2002	UQ	C6-C1	3.77	1.57	1.46
15	C	2002	UQ	C6-C5	3.84	1.44	1.35
13	C	502	HEM	CBC-CAC	3.94	1.52	1.29
13	C	501	HEM	CBC-CAC	4.04	1.52	1.29
13	P	502	HEM	CBC-CAC	4.07	1.52	1.29
13	C	502	HEM	CBB-CAB	4.36	1.54	1.29
15	C	2002	UQ	C7-C6	4.60	1.59	1.51
13	P	502	HEM	CBB-CAB	4.65	1.56	1.29
15	P	3002	UQ	C7-C6	4.87	1.60	1.51
11	N	3008	PEE	P-O1P	6.09	1.62	1.50

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	D	501	HEC	CBB-CAB-C3B	-8.14	109.25	127.35
18	Q	501	HEC	CBB-CAB-C3B	-8.00	109.58	127.35
18	D	501	HEC	CBC-CAC-C3C	-5.85	114.36	127.35
18	Q	501	HEC	CBC-CAC-C3C	-5.76	114.56	127.35
18	D	501	HEC	CAA-C2A-C3A	-3.60	118.72	129.00
18	Q	501	HEC	CAA-C2A-C3A	-3.45	119.15	129.00
13	C	501	HEM	CAA-C2A-C1A	-3.17	123.57	127.01
19	T	3004	CDL	CB4-OB6-CB5	-3.12	110.41	117.89
19	G	2004	CDL	CB4-OB6-CB5	-3.06	110.54	117.89
14	C	2001	FMX	O3-C3-N2	-2.74	124.64	128.60
19	D	2003	CDL	CB4-OB6-CB5	-2.62	111.60	117.89
14	P	3001	FMX	O3-C3-N2	-2.58	124.87	128.60
19	Q	3003	CDL	CB4-OB6-CB5	-2.56	111.75	117.89
15	P	3002	UQ	C7-C6-C1	-2.54	115.57	118.56
13	P	501	HEM	C3B-CAB-CBB	-2.46	120.69	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Q	3003	CDL	CA4-OA6-CA5	-2.36	112.23	117.89
15	P	3002	UQ	C10-C9-C8	-2.30	118.98	123.50
14	C	2001	FMX	C15-O14-C11	-2.28	113.15	118.81
15	C	2002	UQ	C7-C6-C1	-2.25	115.92	118.56
19	D	2003	CDL	CA6-OA8-CA7	-2.25	111.46	117.14
19	D	2003	CDL	CA6-CA4-CA3	-2.20	106.93	112.07
19	Q	3003	CDL	CA6-OA8-CA7	-2.20	111.59	117.14
19	G	2004	CDL	CB6-CB4-CB3	-2.17	107.00	112.07
19	G	2004	CDL	CA4-OA6-CA5	-2.17	112.69	117.89
19	D	2003	CDL	CA4-OA6-CA5	-2.14	112.75	117.89
19	T	3004	CDL	CB6-CB4-CB3	-2.14	107.06	112.07
19	Q	3003	CDL	CA6-CA4-CA3	-2.11	107.13	112.07
19	T	3004	CDL	CA4-OA6-CA5	-2.07	112.92	117.89
13	P	501	HEM	CAA-C2A-C1A	-2.03	124.80	127.01
14	P	3001	FMX	C15-O14-C11	-2.02	113.79	118.81
19	D	2003	CDL	CB6-CB4-CB3	-2.01	107.36	112.07
11	A	2005	PEE	O3-C3-C2	2.09	114.31	108.69
14	C	2001	FMX	O6-C6-C5	2.11	127.67	125.91
11	N	3005	PEE	O3-C3-C2	2.17	114.52	108.69
11	C	2007	PEE	O3-C3-C2	2.18	114.55	108.69
17	C	3010	BOG	C1'-O1-C1	2.18	119.40	114.15
11	P	3007	PEE	C23-C22-C21	2.24	126.09	114.53
18	Q	501	HEC	CBD-CAD-C3D	2.25	116.56	112.53
13	P	501	HEM	CMD-C2D-C3D	2.30	124.54	114.35
13	C	502	HEM	CBA-CAA-C2A	2.32	116.69	112.53
11	C	2007	PEE	C23-C22-C21	2.33	126.55	114.53
11	N	3005	PEE	C23-C22-C21	2.34	126.59	114.53
17	Q	3091	BOG	O1-C1-C2	2.35	111.01	108.04
11	A	2005	PEE	C23-C22-C21	2.39	126.87	114.53
13	C	501	HEM	CBD-CAD-C3D	2.41	120.55	113.55
11	P	3007	PEE	C22-C21-C20	2.42	127.03	114.53
17	Q	3009	BOG	O1-C1-C2	2.44	111.13	108.04
11	A	2005	PEE	C22-C21-C20	2.44	127.15	114.53
11	C	2007	PEE	C22-C21-C20	2.45	127.19	114.53
11	N	3005	PEE	C22-C21-C20	2.47	127.28	114.53
18	D	501	HEC	CBD-CAD-C3D	2.47	116.96	112.53
11	N	3005	PEE	C19-C18-C17	2.50	127.42	114.53
13	C	501	HEM	CAD-C3D-C2D	2.50	120.41	113.22
11	P	3007	PEE	C19-C18-C17	2.51	127.50	114.53
11	A	2005	PEE	C19-C18-C17	2.51	127.50	114.53
13	C	501	HEM	CMD-C2D-C3D	2.56	125.66	114.35
15	C	2002	UQ	C8-C7-C6	2.56	119.34	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	P	501	HEM	C2D-C3D-C4D	2.59	105.89	101.50
11	C	2007	PEE	C19-C18-C17	2.60	127.97	114.53
13	P	502	HEM	C2D-C3D-C4D	2.60	105.91	101.50
13	C	501	HEM	C2D-C3D-C4D	2.63	105.96	101.50
13	C	502	HEM	CMD-C2D-C3D	2.65	126.05	114.35
11	N	3005	PEE	C20-C19-C18	2.66	128.24	114.53
11	C	2007	PEE	C20-C19-C18	2.67	128.30	114.53
11	A	2005	PEE	C20-C19-C18	2.67	128.32	114.53
13	P	502	HEM	C3B-CAB-CBB	2.67	128.55	124.46
17	D	2009	BOG	C1'-O1-C1	2.74	118.73	113.94
11	P	3007	PEE	C20-C19-C18	2.74	128.68	114.53
17	Q	3009	BOG	C1'-O1-C1	2.75	118.76	113.94
15	P	3002	UQ	C8-C7-C6	2.82	120.10	111.64
17	Q	3091	BOG	C1'-O1-C1	2.85	118.92	113.94
13	P	502	HEM	CMD-C2D-C3D	2.89	127.12	114.35
17	D	2009	BOG	O1-C1-C2	2.89	111.69	108.04
13	P	502	HEM	CBA-CAA-C2A	2.91	117.74	112.53
18	Q	501	HEC	CAD-C3D-C4D	2.96	130.22	127.01
18	D	501	HEC	CBA-CAA-C2A	3.05	117.99	112.53
13	P	502	HEM	CAD-C3D-C2D	3.14	122.26	113.22
13	P	501	HEM	CAD-C3D-C2D	3.25	122.56	113.22
13	C	502	HEM	CAD-C3D-C2D	3.27	122.62	113.22
14	C	2001	FMX	C21-N1-N2	3.62	123.73	116.01
14	P	3001	FMX	C21-N1-N2	3.65	123.80	116.01
18	Q	501	HEC	CBA-CAA-C2A	3.72	119.20	112.53
17	D	2091	BOG	C1'-O1-C1	3.88	120.72	113.94
14	P	3001	FMX	O4-C3-N2	4.05	111.76	108.71
18	D	501	HEC	CAD-C3D-C4D	4.08	131.43	127.01
13	C	501	HEM	CMC-C2C-C3C	4.14	126.86	116.53
14	C	2001	FMX	O4-C3-N2	4.17	111.85	108.71
13	P	501	HEM	C3C-CAC-CBC	4.23	130.94	124.46
13	C	501	HEM	C3C-CAC-CBC	4.28	131.02	124.46
13	P	501	HEM	CMC-C2C-C3C	4.49	127.74	116.53
13	P	502	HEM	CMC-C2C-C3C	4.60	128.02	116.53
13	C	502	HEM	CMB-C2B-C3B	4.65	128.14	116.53
13	C	501	HEM	CMB-C2B-C3B	4.87	128.69	116.53
13	P	501	HEM	CMB-C2B-C3B	5.02	129.07	116.53
13	C	502	HEM	CMC-C2C-C3C	5.30	129.75	116.53
13	P	502	HEM	CMB-C2B-C3B	5.30	129.75	116.53
13	P	501	HEM	CAD-C3D-C4D	5.37	131.42	112.47
13	P	502	HEM	CAD-C3D-C4D	5.48	131.80	112.47
18	D	501	HEC	CAA-C2A-C1A	5.91	133.42	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	Q	501	HEC	CAA-C2A-C1A	5.98	133.50	127.01
13	C	501	HEM	CAD-C3D-C4D	6.00	133.63	112.47
13	C	502	HEM	CAD-C3D-C4D	6.15	134.16	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	2001	FMX	2	0
15	C	2002	UQ	5	0
13	C	501	HEM	4	0
13	C	502	HEM	4	0
19	D	2003	CDL	2	0
17	D	2009	BOG	1	0
17	D	2091	BOG	2	0
18	D	501	HEC	4	0
20	E	501	FES	1	0
19	G	2004	CDL	2	0
17	P	2010	BOG	1	0
14	P	3001	FMX	2	0
15	P	3002	UQ	3	0
13	P	501	HEM	3	0
13	P	502	HEM	4	0
19	Q	3003	CDL	3	0
17	Q	3091	BOG	1	0
18	Q	501	HEC	2	0
20	R	501	FES	1	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%)	0.06	6 (1%) 78 73	29, 57, 82, 98	0
1	N	442/446 (99%)	0.27	17 (3%) 44 37	33, 64, 89, 98	0
2	B	421/441 (95%)	0.40	27 (6%) 23 17	44, 74, 109, 137	0
2	O	422/441 (95%)	0.18	12 (2%) 56 50	32, 69, 100, 114	0
3	C	380/380 (100%)	0.05	1 (0%) 94 93	18, 33, 63, 102	0
3	P	379/380 (99%)	0.20	5 (1%) 79 75	26, 56, 76, 85	0
4	D	241/241 (100%)	-0.12	2 (0%) 87 83	25, 36, 70, 88	0
4	Q	241/241 (100%)	0.21	11 (4%) 36 29	39, 65, 91, 114	0
5	E	196/196 (100%)	0.82	33 (16%) 2 1	33, 80, 112, 120	0
5	R	196/196 (100%)	1.82	69 (35%) 0 0	32, 102, 153, 158	0
6	F	101/110 (91%)	-0.31	0 100 100	19, 35, 54, 85	0
6	S	101/110 (91%)	0.33	2 (1%) 68 63	52, 65, 106, 131	0
7	G	81/81 (100%)	0.05	1 (1%) 81 76	28, 46, 82, 97	0
7	T	78/81 (96%)	0.79	7 (8%) 12 8	43, 77, 139, 156	0
8	H	70/77 (90%)	0.05	3 (4%) 39 32	34, 51, 75, 115	0
8	U	67/77 (87%)	1.16	12 (17%) 2 1	87, 108, 130, 134	0
9	I	31/47 (65%)	2.22	15 (48%) 0 0	80, 102, 120, 121	0
9	V	31/47 (65%)	2.14	13 (41%) 0 0	65, 105, 136, 138	0
10	J	61/61 (100%)	0.33	5 (8%) 14 9	40, 53, 85, 124	0
10	W	60/61 (98%)	0.91	4 (6%) 21 15	52, 70, 96, 105	0
All	All	4042/4160 (97%)	0.34	245 (6%) 25 18	18, 61, 109, 158	0

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	W	63	GLU	12.4
5	R	195	VAL	9.3
10	W	62	SER	8.7
5	R	193	VAL	8.5
5	R	133	VAL	8.3
5	R	114	VAL	8.1
5	R	80	ASP	7.7
5	R	127	VAL	7.4
2	B	226	ILE	7.0
5	R	87	VAL	6.8
7	T	77	TYR	6.6
5	R	130	PRO	6.6
9	V	63	ASP	6.5
5	R	132	TRP	6.5
5	R	194	VAL	6.3
5	R	116	LYS	6.2
5	R	112	VAL	6.2
7	T	78	GLU	6.0
8	H	9	GLU	6.0
5	R	115	SER	5.9
5	R	176	ALA	5.8
3	C	1	MET	5.7
9	V	77	ARG	5.6
5	R	191	ASP	5.5
5	R	192	LEU	5.5
5	R	93	GLY	5.4
5	R	79	SER	5.3
10	W	61	ALA	5.2
5	R	184	THR	5.2
5	R	185	TYR	5.2
5	R	117	LEU	5.1
10	J	63	GLU	5.0
5	E	111	GLU	4.9
4	Q	139	ALA	4.9
5	R	113	ASP	4.9
5	R	104	ALA	4.9
5	R	118	ARG	4.8
7	T	75	ALA	4.8
5	R	109	GLU	4.7
5	R	175	PRO	4.6
5	R	98	VAL	4.6
10	J	61	ALA	4.6
8	U	49	HIS	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	402	ILE	4.5
9	I	51	CYS	4.4
9	I	63	ASP	4.4
1	A	69	LYS	4.3
6	S	11	ARG	4.3
5	R	136	VAL	4.3
2	B	33	LEU	4.2
5	E	112	VAL	4.2
5	R	172	ARG	4.1
10	J	64	GLU	4.1
8	H	10	GLU	4.1
5	R	120	PRO	4.0
5	E	133	VAL	4.0
5	R	174	GLY	4.0
2	O	19	PRO	4.0
7	T	79	ASN	4.0
1	N	182	LEU	4.0
9	I	77	ARG	4.0
8	U	44	VAL	3.9
5	R	119	ASP	3.9
5	R	94	LYS	3.9
5	R	183	PRO	3.9
5	R	99	ARG	3.9
5	E	89	PHE	3.8
9	I	47	ARG	3.8
10	J	62	SER	3.8
6	S	15	ARG	3.8
9	I	53	GLU	3.8
7	G	1	GLY	3.7
8	U	26	GLN	3.7
8	U	50	THR	3.7
9	V	55	MET	3.6
5	E	81	ILE	3.6
5	R	177	PRO	3.6
5	R	81	ILE	3.6
5	E	132	TRP	3.6
5	R	74	ILE	3.6
1	N	124	GLU	3.6
5	E	85	LYS	3.5
5	E	80	ASP	3.5
5	R	153	PHE	3.5
9	V	70	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
9	V	49	LEU	3.5
5	R	163	SER	3.5
5	R	164	HIS	3.4
5	E	114	VAL	3.4
1	A	2	ALA	3.4
2	B	236	LYS	3.4
9	I	50	LEU	3.3
5	R	173	LYS	3.3
2	O	299	VAL	3.3
7	T	74	PRO	3.3
9	I	52	ARG	3.3
2	B	29	LEU	3.3
5	E	186	GLN	3.3
5	E	195	VAL	3.3
2	O	304	THR	3.3
5	R	131	GLU	3.2
1	N	179	ARG	3.2
5	E	188	VAL	3.2
8	U	13	LEU	3.2
5	R	111	GLU	3.2
1	N	75	PHE	3.2
1	N	54	GLY	3.1
4	Q	145	GLU	3.1
9	I	70	LEU	3.1
5	R	103	GLN	3.1
5	R	162	GLY	3.1
5	R	122	HIS	3.1
4	Q	180	SER	3.1
5	R	89	PHE	3.1
5	R	160	CYS	3.1
5	E	122	HIS	3.1
5	R	108	GLN	3.1
9	V	62	ARG	3.1
4	Q	143	VAL	3.1
5	R	128	LYS	3.0
5	R	134	ILE	2.9
5	E	167	ALA	2.9
9	V	59	SER	2.9
5	R	178	TYR	2.9
9	V	76	VAL	2.9
3	P	346	HIS	2.9
5	R	72	SER	2.9

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Mol	Chain	Res	Type	RSRZ
5	E	76	ILE	2.8
5	E	101	ARG	2.8
2	B	369	LEU	2.8
5	R	155	GLY	2.8
2	B	350	GLY	2.8
5	E	100	HIS	2.8
5	R	76	ILE	2.7
5	R	124	LEU	2.7
2	B	223	PHE	2.7
2	B	230	ALA	2.7
5	E	82	PRO	2.7
9	I	60	ALA	2.7
9	V	50	LEU	2.7
5	E	185	TYR	2.7
5	R	123	ASP	2.7
5	R	105	GLU	2.7
5	R	95	PRO	2.7
5	E	78	LEU	2.7
5	R	140	THR	2.7
8	U	76	LYS	2.6
2	B	439	LEU	2.6
5	R	78	LEU	2.6
2	B	124	LEU	2.6
1	N	190	PHE	2.6
2	B	120	MET	2.6
4	Q	147	LEU	2.6
1	A	226	ASP	2.6
5	R	86	ASN	2.6
2	B	204	MET	2.5
8	H	71	HIS	2.5
9	I	64	LEU	2.5
1	A	68	LYS	2.5
4	D	241	LYS	2.5
5	E	194	VAL	2.5
2	B	200	THR	2.5
5	E	110	ALA	2.5
5	E	74	ILE	2.4
1	N	123	GLU	2.4
4	Q	141	VAL	2.4
1	N	218	GLY	2.4
5	E	137	GLY	2.4
2	O	23	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	209	VAL	2.4
2	B	205	ALA	2.4
5	R	196	GLY	2.4
1	N	178	THR	2.4
7	T	72	LYS	2.4
2	B	34	ILE	2.4
1	N	69	LYS	2.4
1	N	177	LEU	2.4
3	P	373	LEU	2.4
2	O	302	ALA	2.4
9	I	73	PRO	2.3
2	O	368	TYR	2.3
9	V	58	ARG	2.3
1	N	57	TYR	2.3
1	N	127	ILE	2.3
5	E	99	ARG	2.3
2	O	266	SER	2.3
9	I	72	ALA	2.3
5	R	159	PRO	2.3
9	V	56	SER	2.3
4	Q	69	GLU	2.2
2	B	201	SER	2.2
8	U	12	GLU	2.2
9	V	48	PRO	2.2
5	E	104	ALA	2.2
5	R	106	ILE	2.2
2	B	267	ALA	2.2
4	Q	68	VAL	2.2
1	N	122	LEU	2.2
2	B	400	GLN	2.2
5	E	75	GLU	2.2
1	N	68	LYS	2.2
2	B	274	VAL	2.2
5	E	192	LEU	2.2
8	U	39	LEU	2.1
2	O	223	PHE	2.1
9	V	60	ALA	2.1
2	B	304	THR	2.1
4	Q	82	MET	2.1
9	I	54	SER	2.1
5	E	84	GLY	2.1
3	P	320	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
10	J	15	ARG	2.1
5	E	156	TYR	2.1
5	R	77	LYS	2.1
8	U	43	ARG	2.1
2	B	221	GLU	2.1
5	R	75	GLU	2.1
1	N	138	LEU	2.1
9	I	69	SER	2.1
1	A	21	ASN	2.1
4	Q	167	GLU	2.1
10	W	45	HIS	2.1
4	Q	1	GLY	2.1
7	T	38	TRP	2.1
2	B	35	ILE	2.1
2	B	227	ARG	2.1
5	R	110	ALA	2.1
2	O	387	LEU	2.0
5	E	180	LEU	2.0
8	U	74	PHE	2.0
9	I	48	PRO	2.0
2	B	403	ASP	2.0
4	D	2	GLU	2.0
2	O	386	ALA	2.0
8	U	24	CYS	2.0
2	O	104	LYS	2.0
2	O	227	ARG	2.0
3	P	269	ILE	2.0
5	E	187	PHE	2.0
2	B	419	SER	2.0
3	P	156	TYR	2.0
8	U	33	ALA	2.0
5	E	90	LYS	2.0
1	N	185	TYR	2.0
2	B	232	THR	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
17	BOG	D	2091	20/20	0.23	0.71	24.77	171,182,183,184	0
12	UNL	P	3046	2/-	0.68	0.75	23.48	85,85,85,86	0
12	UNL	C	2046	2/-	0.78	0.47	21.53	78,78,78,80	0
16	AZI	P	3011	3/3	0.91	0.45	19.68	66,66,68,68	0
16	AZI	C	2011	3/3	0.81	0.48	15.87	62,62,63,64	0
17	BOG	P	2010	19/20	0.53	0.48	9.17	97,177,178,178	0
12	UNL	C	2048	2/-	0.93	0.24	7.31	41,41,41,45	0
12	UNL	C	2047	1/-	0.96	0.37	7.21	28,28,28,28	0
15	UQ	P	3002	19/63	0.75	0.40	6.20	132,136,138,138	0
15	UQ	C	2002	19/63	0.76	0.36	6.15	80,84,86,86	0
12	UNL	A	3015	1/-	0.84	0.29	3.75	45,45,45,45	0
11	PEE	P	3007	48/51	0.91	0.28	3.21	71,83,98,100	0
11	PEE	N	3005	50/51	0.83	0.30	2.84	64,92,98,98	0
19	CDL	G	2004	40/100	0.92	0.21	2.34	48,63,77,78	0
11	PEE	A	2005	50/51	0.83	0.30	2.28	74,85,89,90	0
11	PEE	C	2007	48/51	0.95	0.21	2.20	33,49,72,72	0
12	UNL	P	3048	2/-	0.41	0.28	2.07	93,93,93,95	0
19	CDL	Q	3003	42/100	0.83	0.26	1.86	114,118,123,124	0
11	PEE	C	2008	21/51	0.88	0.23	1.10	89,103,110,111	0
14	FMX	C	2001	28/28	0.93	0.21	1.09	31,49,61,62	0
17	BOG	C	3010	12/20	0.92	0.29	0.92	78,81,83,84	0
19	CDL	T	3004	40/100	0.84	0.23	0.87	85,89,100,101	0
17	BOG	Q	3009	20/20	0.87	0.22	0.81	69,80,83,84	0
19	CDL	D	2003	42/100	0.86	0.20	0.74	60,75,87,88	0
17	BOG	D	2009	20/20	0.93	0.19	0.61	47,57,61,61	0
14	FMX	P	3001	28/28	0.91	0.21	0.59	55,65,70,71	0
13	HEM	C	501	43/43	0.98	0.21	0.10	17,27,37,40	0
18	HEC	Q	501	43/43	0.96	0.18	-0.02	40,49,58,60	0
18	HEC	D	501	43/43	0.98	0.17	-0.06	14,25,29,32	0
13	HEM	C	502	43/43	0.99	0.17	-0.08	15,20,28,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	HEM	P	501	43/43	0.98	0.20	-0.14	37,41,52,56	0
13	HEM	P	502	43/43	0.98	0.16	-0.82	32,38,50,56	0
20	FES	E	501	4/4	0.98	0.11	-1.75	72,73,74,74	0
20	FES	R	501	4/4	0.98	0.10	-2.02	85,85,86,86	0
12	UNL	P	3014	1/-	0.79	0.43	-	55,55,55,55	0
11	PEE	N	3008	5/51	0.94	0.14	-	74,74,75,76	0
12	UNL	P	3047	1/-	0.84	0.30	-	45,45,45,45	0
17	BOG	Q	3091	20/20	0.32	0.80	-	172,179,180,180	0
12	UNL	E	2012	2/-	0.83	0.32	-	51,51,51,51	0
12	UNL	Q	3012	1/-	0.86	0.32	-	33,33,33,33	0
12	UNL	P	3013	1/-	0.62	0.48	-	72,72,72,72	0

6.5 Other polymers (i)

There are no such residues in this entry.