Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 10:14 AM GMT

PDB ID	:	3L73
Title	:	Cytochrome BC1 complex from chicken with triazolone inhibitor
Authors	:	Huang, L.; Berry, E.A.
Deposited on	:	2009-12-27
Resolution	:	3.04 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:

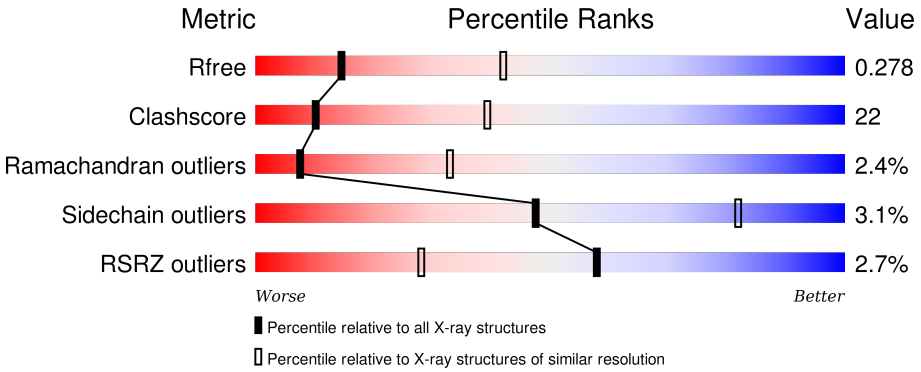
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.04 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	1995 (3.08-3.00)
Clashscore	102246	2351 (3.08-3.00)
Ramachandran outliers	100387	2272 (3.08-3.00)
Sidechain outliers	100360	2275 (3.08-3.00)
RSRZ outliers	91569	2013 (3.08-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	446	2% 62% 34% ·
1	N	446	58% 38% · ·
2	B	441	% 47% 42% 6% 5%
2	O	441	% 51% 40% · ·
3	C	380	2% 72% 27% ·

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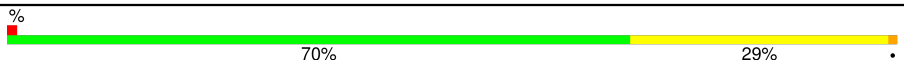
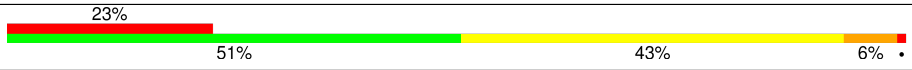
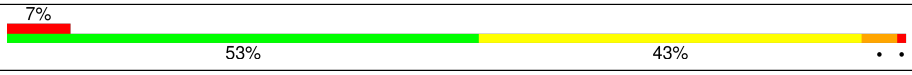
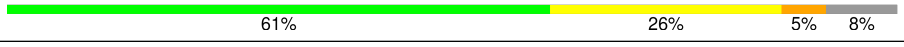
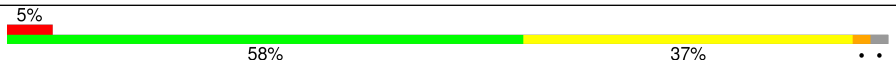
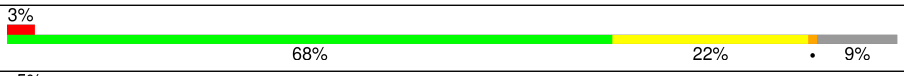
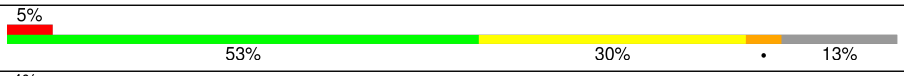
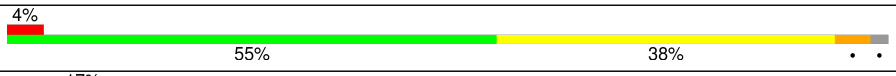
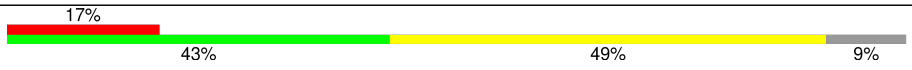
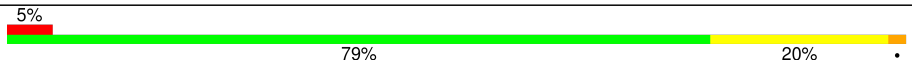
Mol	Chain	Length	Quality of chain
3	P	380	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	47	
9	V	47	
10	J	61	
10	W	61	

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	2008	-	-	-	X
11	PEE	C	2007	-	-	-	X
11	PEE	E	2005	-	-	-	X
11	PEE	R	3005	-	-	-	X
14	UQ	C	2002	-	-	-	X
14	UQ	P	3002	-	-	-	X
15	GOL	C	2011	-	-	-	X
15	GOL	P	3011	-	-	-	X
17	CDL	D	2003	-	-	-	X
17	CDL	G	2004	-	-	-	X
17	CDL	Q	3003	-	-	-	X
18	BOG	P	2010	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	FES	E	501	-	-	X	-
19	FES	R	501	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32645 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I.

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

- Molecule 2 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2.

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

- Molecule 3 is a protein called CYTOCHROME B.

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

- Molecule 4 is a protein called MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN.

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

- Molecule 5 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 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
			1509	950	263	290	6			

- Molecule 6 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN.

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

- Molecule 7 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C.

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

- Molecule 8 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII.

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

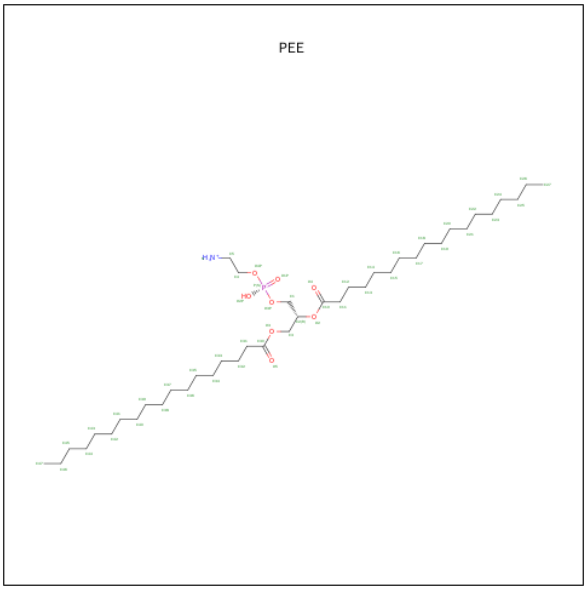
- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

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

- Molecule 10 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN.

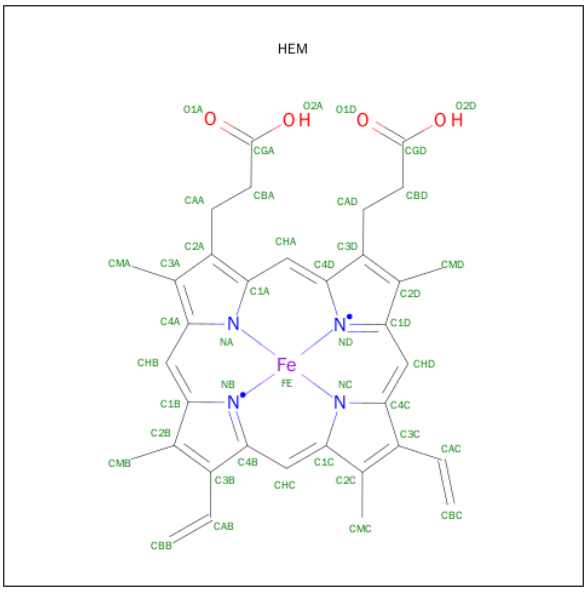
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	J	61	Total C N O 497 321 87 89	0	0	0
10	W	60	Total C N O 479 311 86 82	0	0	1

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



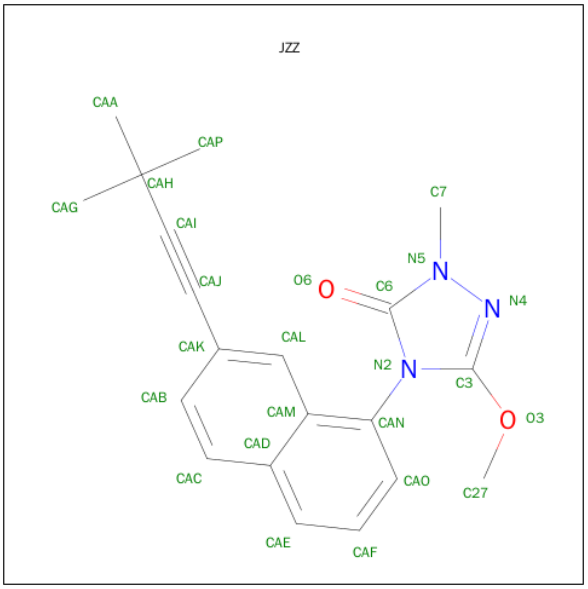
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C O P 21 12 8 1	0	0
11	C	1	Total C N O P 49 39 1 8 1	0	0
11	E	1	Total C N O P 50 40 1 8 1	0	0
11	P	1	Total C N O P 49 39 1 8 1	0	0
11	P	1	Total O P 5 4 1	0	0
11	R	1	Total C N O P 50 40 1 8 1	0	0

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



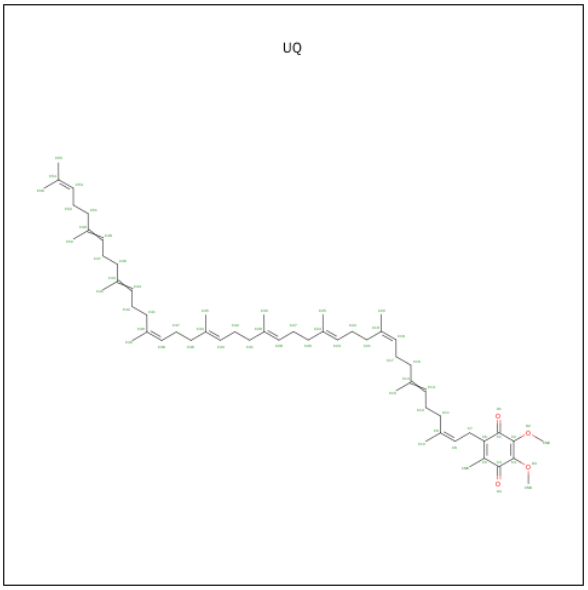
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is 4-[7-(3,3-DIMETHYLBUT-1-YN-1-YL)NAPHTHALEN-1-YL]-5-METHOXY-2-METHYL-2,4-DIHYDRO-3H-1,2,4-TRIAZOL-3-ONE (three-letter code: JZZ) (formula: $C_{20}H_{21}N_3O_2$).



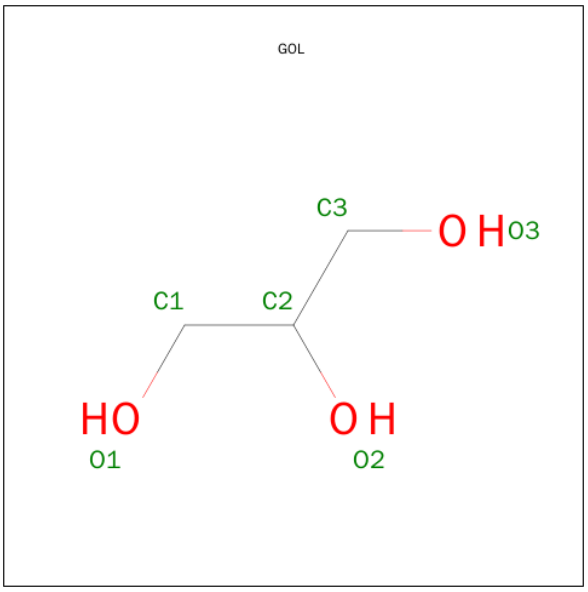
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	N	O	0	0
			25	20	3	2		
13	P	1	Total	C	N	O	0	0
			25	20	3	2		

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



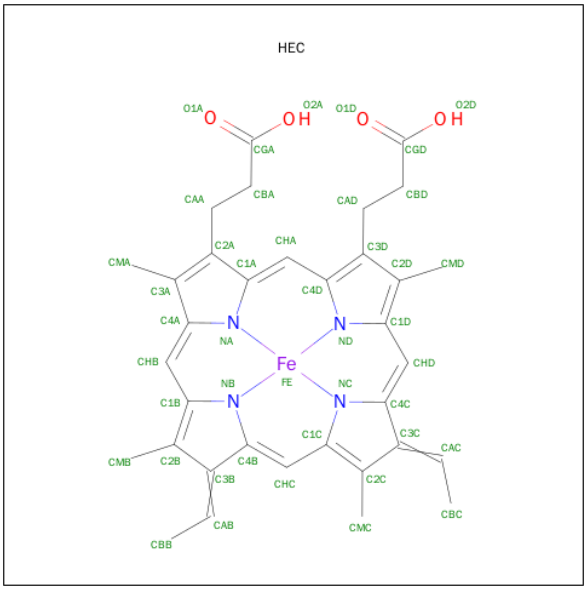
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			19	15	4		
14	P	1	Total	C	O	0	0
			19	15	4		

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



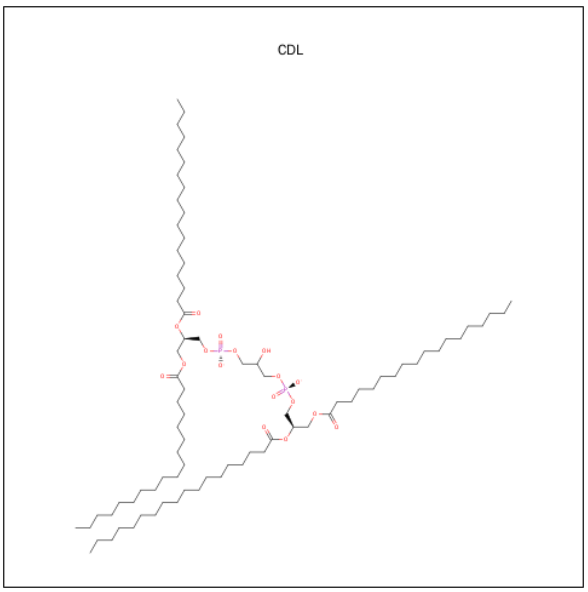
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	1	Total C O 6 3 3	0	0
15	P	1	Total C O 6 3 3	0	0

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



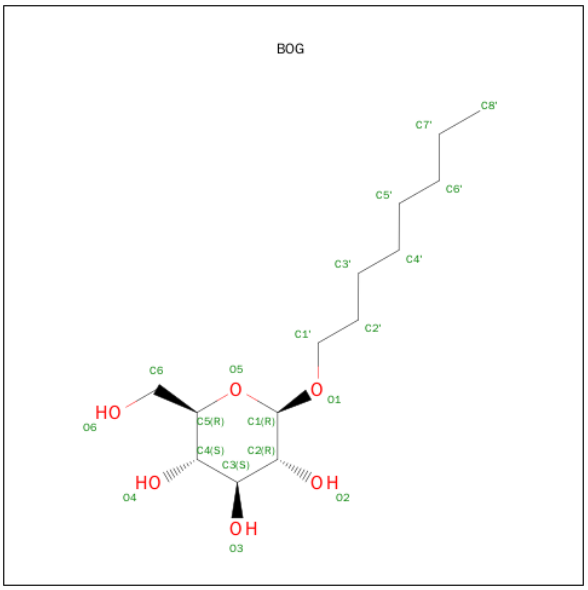
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	D	1	Total C Fe N O 43 34 1 4 4	0	0
16	Q	1	Total C Fe N O 43 34 1 4 4	0	0

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



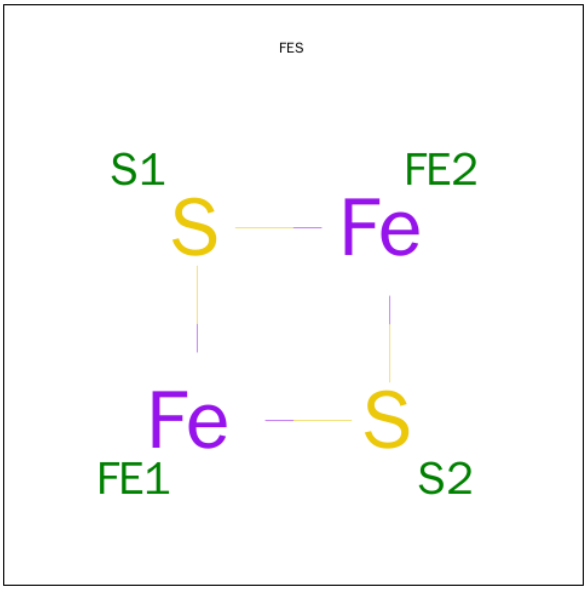
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	C	O	P	0	0
			42	23	17	2		
17	G	1	Total	C	O	P	0	0
			40	21	17	2		
17	Q	1	Total	C	O	P	0	0
			42	23	17	2		
17	T	1	Total	C	O	P	0	0
			40	21	17	2		

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



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

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



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

- Molecule 20 is water.

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

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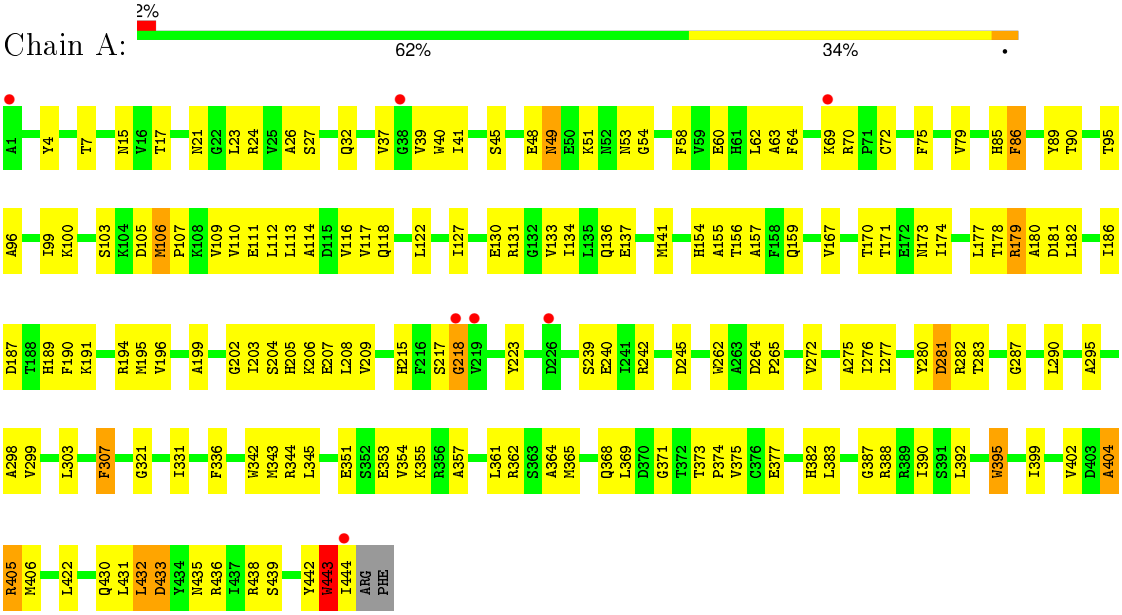
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	R	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

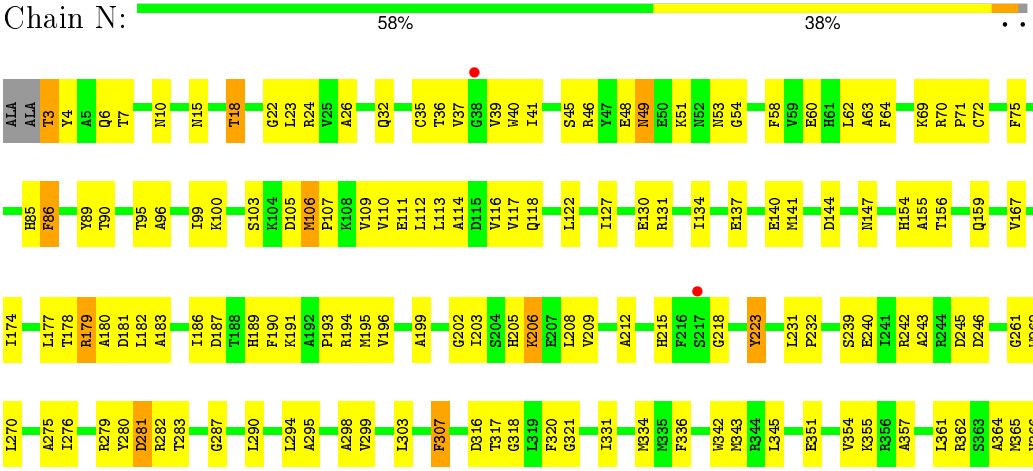
• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

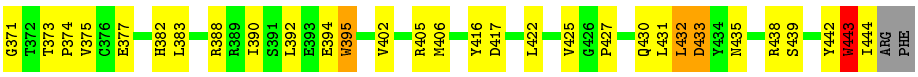
Chain A:



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

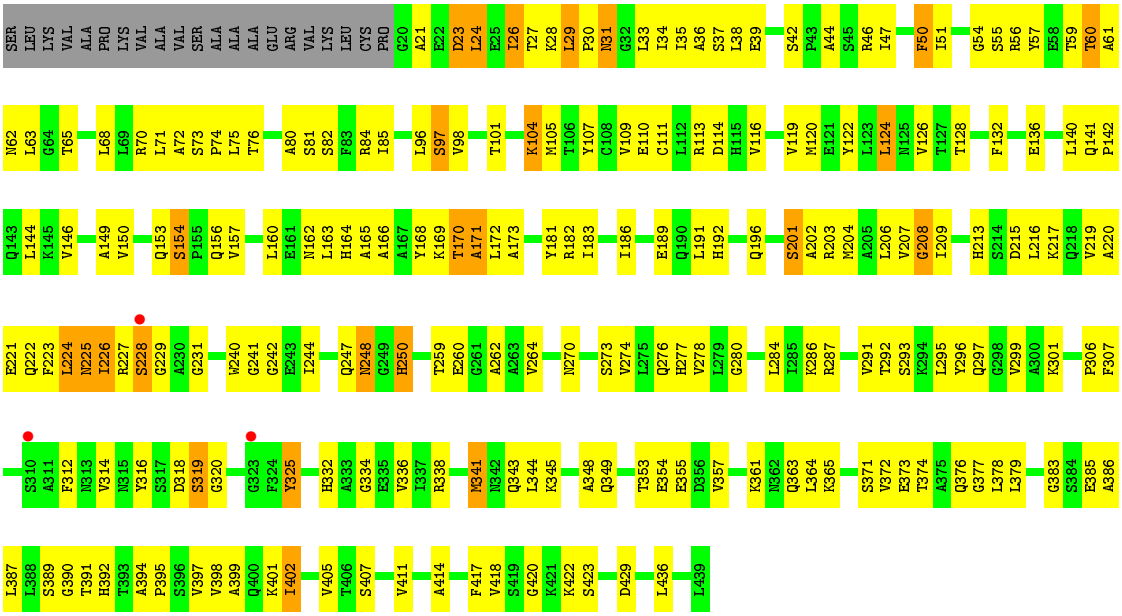
Chain N:





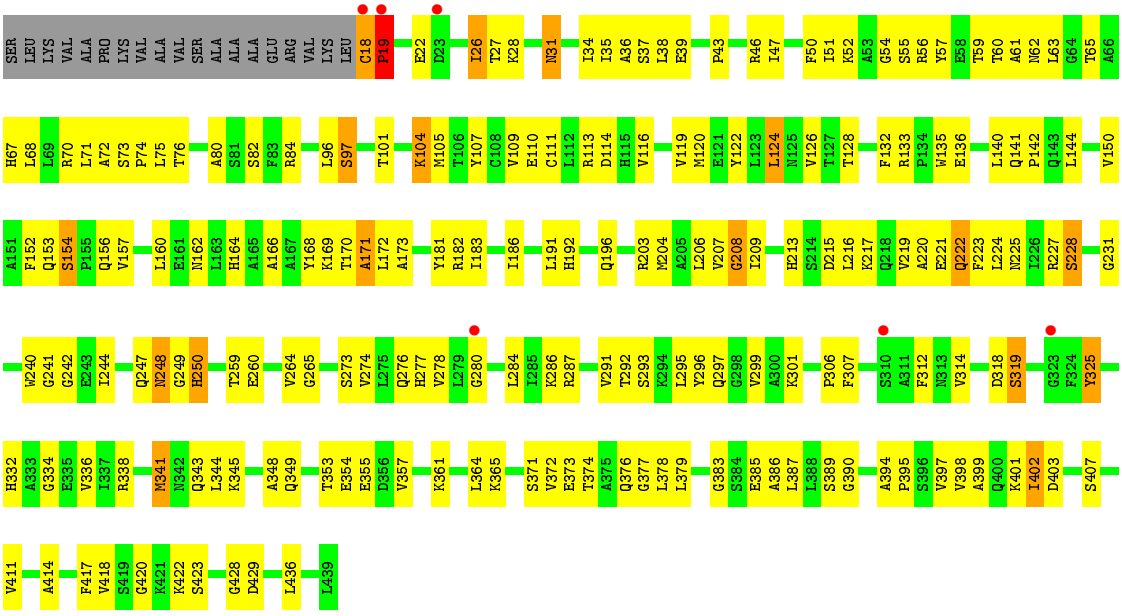
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

Chain B:



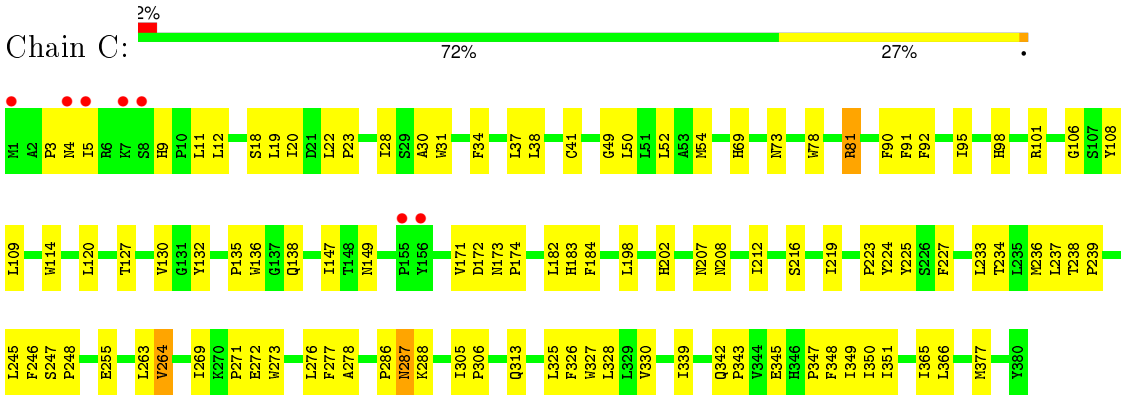
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

Chain O:



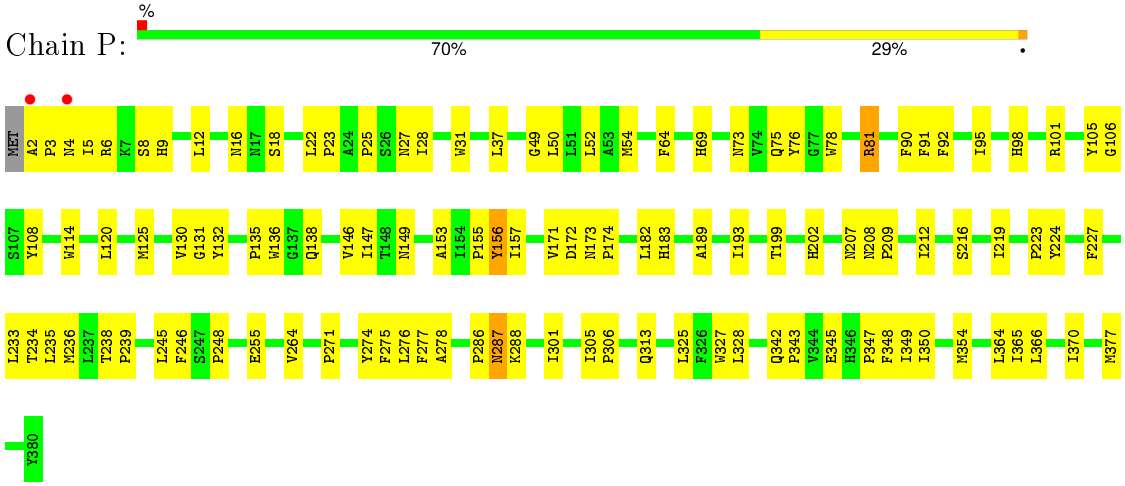
• Molecule 3: CYTOCHROME B

Chain C:



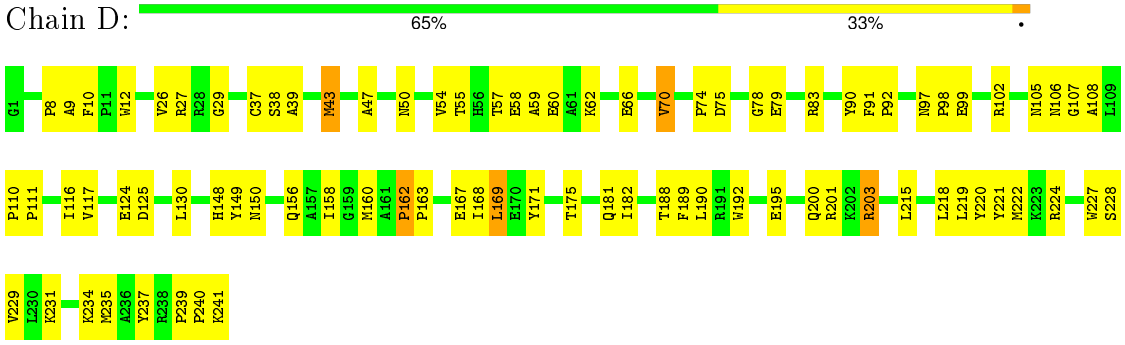
• Molecule 3: CYTOCHROME B

Chain P:



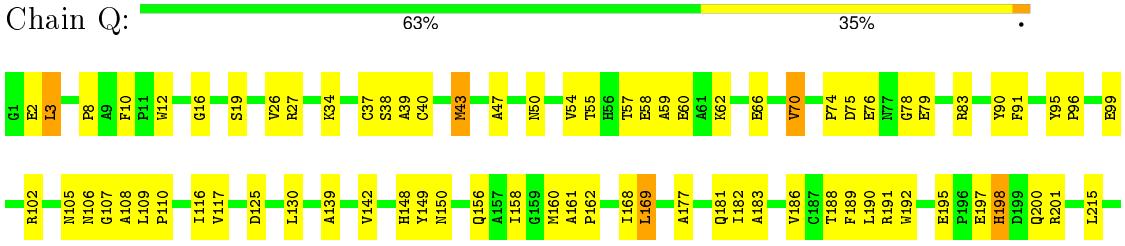
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain D:

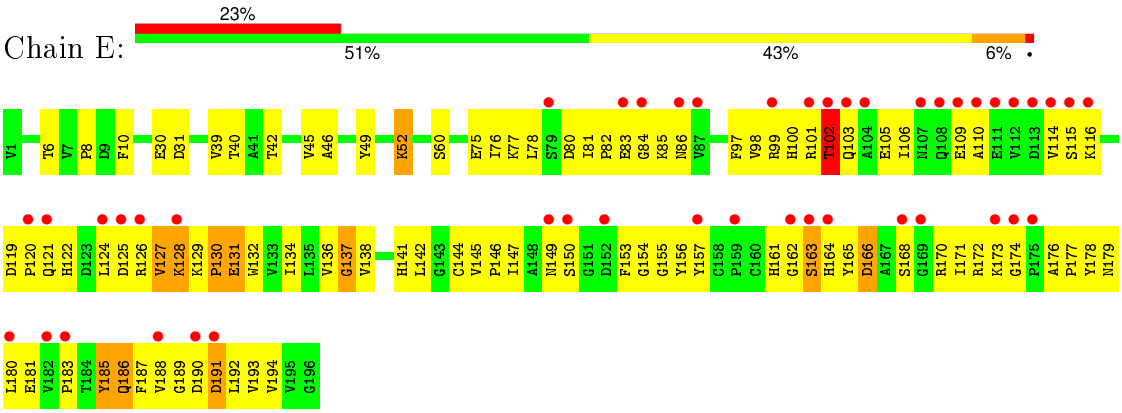


• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

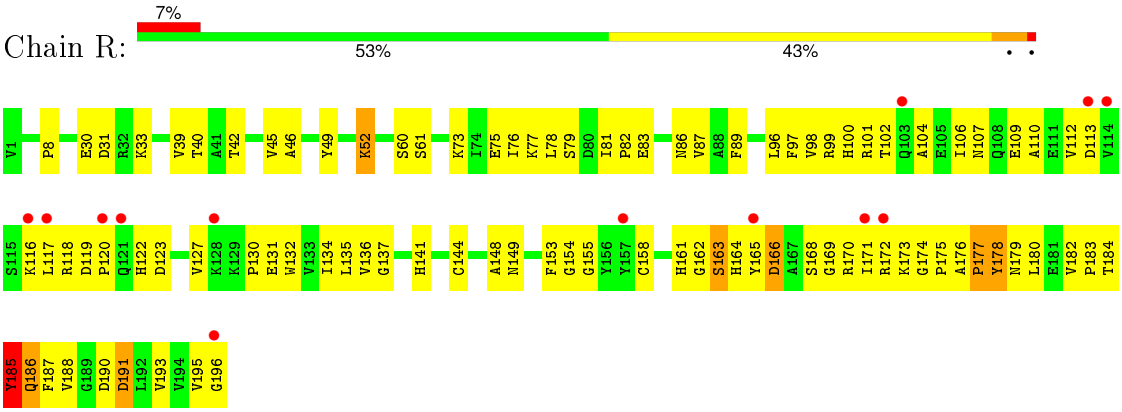
Chain Q:



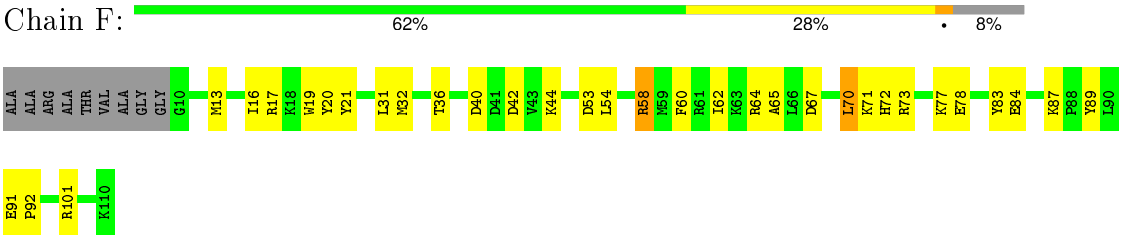
• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL



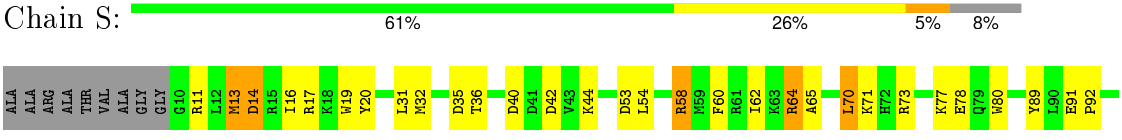
• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL



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



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

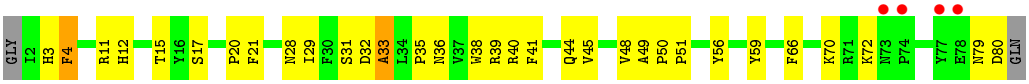


• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain G:

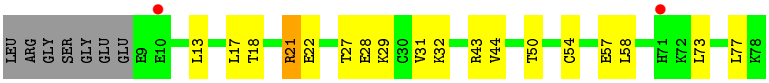
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain T:



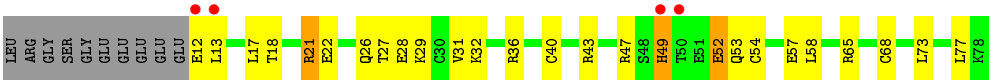
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain H:



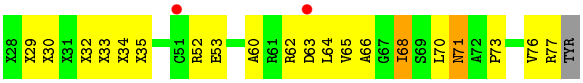
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain U:



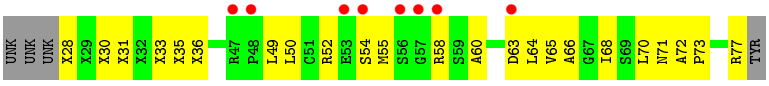
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain I:



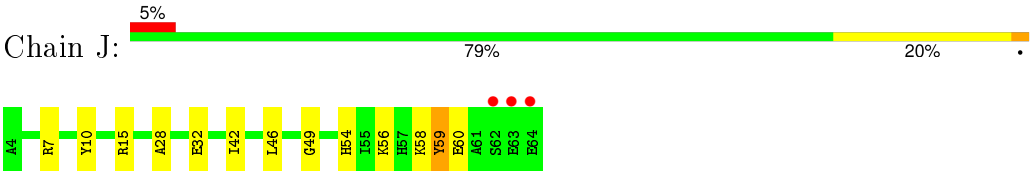
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain V:



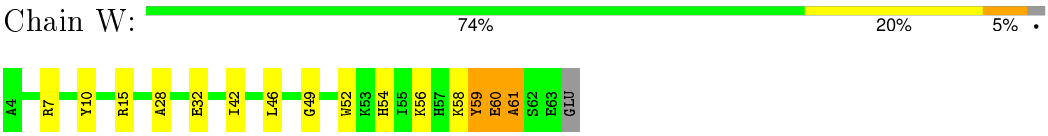
• Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN

Chain J:



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

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	171.50Å 182.93Å 241.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.97 – 3.04 24.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.97-3.04) 99.5 (24.97-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.293 0.246 , 0.278	Depositor DCC
R_{free} test set	2854 reflections (2.01%)	DCC
Wilson B-factor (Å^2)	75.9	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 51.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 166720 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	32645	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CDL, UQ, JZZ, HEC, PEE, BOG, HEM, FES

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	0.46	0/3518	0.68	0/4767
1	N	0.44	0/3508	0.66	0/4753
2	B	0.41	0/3187	0.65	0/4321
2	O	0.42	0/3202	0.66	0/4343
3	C	0.54	0/3119	0.70	0/4270
3	P	0.49	0/3114	0.66	0/4263
4	D	0.49	0/1956	0.67	0/2658
4	Q	0.41	0/1956	0.63	0/2658
5	E	0.39	0/1547	0.60	0/2103
5	R	0.40	0/1543	0.60	0/2098
6	F	0.55	0/911	0.68	0/1219
6	S	0.45	0/911	0.64	0/1219
7	G	0.52	0/694	0.69	0/941
7	T	0.46	0/684	0.66	0/929
8	H	0.44	0/582	0.64	0/779
8	U	0.35	0/561	0.61	0/751
9	I	0.44	0/218	0.59	0/293
9	V	0.39	0/218	0.60	0/293
10	J	0.44	0/508	0.63	0/682
10	W	0.41	0/490	0.61	0/660
All	All	0.46	0/32427	0.66	0/44000

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3447	0	3362	135	0
1	N	3437	0	3349	164	0
2	B	3133	0	3130	212	0
2	O	3147	0	3146	208	0
3	C	3017	0	3063	91	0
3	P	3012	0	3058	95	0
4	D	1898	0	1846	75	0
4	Q	1898	0	1846	76	0
5	E	1513	0	1478	108	0
5	R	1509	0	1474	103	0
6	F	891	0	893	24	0
6	S	891	0	893	29	0
7	G	672	0	653	32	0
7	T	662	0	645	33	0
8	H	574	0	548	19	0
8	U	553	0	535	26	0
9	I	287	0	249	28	0
9	V	277	0	250	32	0
10	J	497	0	490	16	0
10	W	479	0	478	21	0
11	A	21	0	13	0	0
11	C	49	0	72	4	0
11	E	50	0	77	1	0
11	P	54	0	72	4	0
11	R	50	0	77	1	0
12	C	86	0	60	6	0
12	P	86	0	60	5	0
13	C	25	0	21	2	0
13	P	25	0	21	6	0
14	C	19	0	17	4	0
14	P	19	0	17	5	0
15	C	6	0	8	1	0
15	P	6	0	8	1	0
16	D	43	0	30	1	0
16	Q	43	0	30	2	0
17	D	42	0	28	3	0
17	G	40	0	24	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	42	0	28	1	0
17	T	40	0	24	5	0
18	D	33	0	39	2	0
18	P	12	0	11	1	0
18	Q	33	0	39	1	0
19	E	4	0	0	2	0
19	R	4	0	0	2	0
20	C	8	0	0	1	0
20	E	1	0	0	0	0
20	P	9	0	0	0	0
20	R	1	0	0	0	0
All	All	32645	0	32162	1407	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 22.

All (1407) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.21	1.16
9:V:35:UNK:HG3	9:V:36:UNK:H	1.22	1.05
2:B:353:THR:HG22	2:B:355:GLU:H	1.19	1.04
2:O:76:THR:HG22	2:O:82:SER:H	1.22	1.04
2:O:353:THR:HG22	2:O:355:GLU:H	1.21	1.04
9:I:33:UNK:HG2	9:I:73:PRO:HB3	1.44	0.99
2:O:338:ARG:HH11	2:O:338:ARG:HG3	1.26	0.98
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.27	0.97
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.48	0.95
2:B:76:THR:HG22	2:B:82:SER:H	1.32	0.94
2:B:338:ARG:HG3	2:B:338:ARG:HH11	1.34	0.93
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.84	0.92
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.16	0.91
4:D:47:ALA:H	4:D:50:ASN:HD22	1.13	0.91
1:A:178:THR:HG22	1:A:180:ALA:H	1.36	0.91
1:N:178:THR:HG22	1:N:180:ALA:H	1.36	0.91
5:E:121:GLN:CG	5:E:170:ARG:HD3	2.01	0.91
2:O:18:CYS:HB2	2:O:19:PRO:HD3	1.52	0.89
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.54	0.87
9:I:32:UNK:N	9:I:73:PRO:HG2	1.90	0.87
7:T:41:PHE:O	7:T:45:VAL:HG23	1.74	0.87
1:N:10:ASN:ND2	2:O:19:PRO:HD2	1.89	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:127:VAL:HG12	5:E:128:LYS:H	1.39	0.86
2:O:154:SER:O	2:O:157:VAL:HG12	1.75	0.86
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.57	0.86
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.11	0.86
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.76	0.85
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.42	0.85
2:B:154:SER:O	2:B:157:VAL:HG12	1.77	0.85
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.59	0.85
3:P:9:HIS:HD2	3:P:12:LEU:H	1.25	0.85
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.12	0.84
7:G:41:PHE:O	7:G:45:VAL:HG23	1.79	0.83
2:B:341:MET:HE2	2:B:341:MET:HA	1.58	0.83
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.13	0.83
4:D:231:LYS:O	6:F:71:LYS:HE3	1.79	0.83
3:C:9:HIS:HD2	3:C:12:LEU:H	1.24	0.83
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.60	0.82
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.60	0.82
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.61	0.82
2:B:47:ILE:HD13	2:B:120:MET:CE	2.10	0.82
5:R:31:ASP:OD2	10:W:7:ARG:HG3	1.80	0.82
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.61	0.82
5:E:141:HIS:HB2	5:E:176:ALA:HB2	1.63	0.81
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.63	0.81
3:C:22:LEU:HD21	14:C:2002:UQ:HM32	1.62	0.80
1:N:170:THR:HG22	1:N:171:THR:H	1.47	0.80
6:S:91:GLU:HG2	6:S:95:LYS:HE3	1.62	0.80
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.17	0.79
2:O:27:THR:HG22	2:O:28:LYS:H	1.47	0.79
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.64	0.79
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.62	0.79
9:I:70:LEU:HD23	9:I:71:ASN:H	1.45	0.79
4:D:57:THR:HB	4:D:60:GLU:HG3	1.65	0.79
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.18	0.78
2:O:219:VAL:O	2:O:223:PHE:HB2	1.84	0.78
1:A:443:TRP:CE3	1:A:443:TRP:HA	2.19	0.78
2:B:29:LEU:HD12	2:B:33:LEU:HD23	1.66	0.78
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.66	0.77
1:N:187:ASP:O	1:N:191:LYS:HE3	1.85	0.77
2:O:27:THR:HG22	2:O:28:LYS:N	2.00	0.77
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.67	0.77
2:O:47:ILE:HD13	2:O:120:MET:CE	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.66	0.77
4:D:57:THR:HG22	4:D:59:ALA:H	1.49	0.77
1:N:112:LEU:O	1:N:116:VAL:HG23	1.84	0.77
5:E:31:ASP:OD2	10:J:7:ARG:HG3	1.85	0.77
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.66	0.77
2:O:422:LYS:O	2:O:436:LEU:HD21	1.82	0.77
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.48	0.76
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.66	0.76
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.50	0.76
1:A:295:ALA:O	1:A:299:VAL:HG23	1.86	0.76
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.65	0.76
1:A:103:SER:HB3	1:A:202:GLY:O	1.87	0.75
1:N:10:ASN:HD21	2:O:18:CYS:N	1.83	0.75
1:N:295:ALA:O	1:N:299:VAL:HG23	1.85	0.75
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.04	0.75
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.52	0.75
2:O:221:GLU:HG3	2:O:222:GLN:H	1.50	0.75
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.69	0.75
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.68	0.74
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.69	0.74
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.02	0.74
1:N:105:ASP:O	1:N:109:VAL:HG23	1.87	0.74
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.86	0.74
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.22	0.74
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.87	0.74
2:B:422:LYS:O	2:B:436:LEU:HD21	1.87	0.74
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.70	0.74
1:A:178:THR:HB	1:A:181:ASP:OD1	1.87	0.73
11:P:3007:PEE:H7	7:T:44:GLN:HE21	1.51	0.73
4:Q:62:LYS:O	4:Q:66:GLU:HG3	1.89	0.73
5:R:166:ASP:OD2	5:R:170:ARG:HB2	1.89	0.73
3:P:22:LEU:HD21	14:P:3002:UQ:HM32	1.70	0.73
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.07	0.73
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.71	0.72
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.71	0.72
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.71	0.72
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.54	0.72
2:O:338:ARG:NH1	2:O:338:ARG:HG3	1.98	0.72
2:O:18:CYS:HB2	2:O:19:PRO:CD	2.19	0.72
2:B:38:LEU:HD12	2:B:39:GLU:N	2.05	0.72
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:192:HIS:O	2:O:196:GLN:HG3	1.90	0.72
4:Q:57:THR:HB	4:Q:60:GLU:HG3	1.72	0.72
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.25	0.72
7:T:72:LYS:HE2	8:U:57:GLU:OE1	1.90	0.72
2:O:101:THR:HG23	2:O:104:LYS:HE3	1.70	0.72
2:B:122:TYR:O	2:B:126:VAL:HG23	1.90	0.72
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.71	0.71
1:N:170:THR:HG22	1:N:171:THR:N	2.05	0.71
2:B:31:ASN:N	2:B:31:ASN:HD22	1.88	0.71
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.20	0.71
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.71	0.71
1:A:443:TRP:HE3	1:A:443:TRP:HA	1.53	0.71
2:B:27:THR:HG22	2:B:28:LYS:N	2.06	0.71
10:W:60:GLU:HG2	10:W:60:GLU:O	1.89	0.71
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.71	0.71
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.72	0.70
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.19	0.70
2:O:361:LYS:O	2:O:365:LYS:HG3	1.92	0.70
2:B:338:ARG:HG3	2:B:338:ARG:NH1	2.04	0.70
2:B:341:MET:HE3	2:B:417:PHE:HE2	1.56	0.70
4:D:62:LYS:O	4:D:66:GLU:HG3	1.91	0.70
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.55	0.70
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.06	0.70
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.21	0.70
6:S:91:GLU:O	6:S:95:LYS:HG3	1.91	0.70
3:P:238:THR:HB	3:P:239:PRO:HD3	1.73	0.70
3:P:101:ARG:C	3:P:101:ARG:HD2	2.11	0.70
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.26	0.70
4:D:47:ALA:H	4:D:50:ASN:ND2	1.89	0.70
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.74	0.70
1:A:369:LEU:HD12	1:A:392:LEU:HD11	1.74	0.70
2:O:156:GLN:HE22	9:V:77:ARG:C	1.95	0.69
11:C:2007:PEE:H7	7:G:44:GLN:HE21	1.57	0.69
6:S:99:ARG:HB3	6:S:99:ARG:NH1	2.07	0.69
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.74	0.69
5:E:190:ASP:C	5:E:192:LEU:H	1.95	0.69
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.75	0.69
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.74	0.69
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.58	0.69
1:N:49:ASN:HD21	1:N:51:LYS:HE3	1.57	0.69
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:PRO:HA	9:I:52:ARG:CG	2.22	0.69
8:U:28:GLU:HG2	8:U:32:LYS:HE3	1.74	0.69
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.73	0.68
8:H:28:GLU:HG2	8:H:32:LYS:HE3	1.75	0.68
1:A:187:ASP:O	1:A:191:LYS:HE3	1.93	0.68
1:N:178:THR:HB	1:N:181:ASP:OD1	1.93	0.68
2:B:150:VAL:O	2:B:153:GLN:HG3	1.94	0.68
1:N:178:THR:HG22	1:N:179:ARG:N	2.09	0.68
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.28	0.68
2:B:164:HIS:O	2:B:173:ALA:HA	1.94	0.68
7:T:29:ILE:O	7:T:33:ALA:HB3	1.93	0.68
1:A:49:ASN:HD21	1:A:51:LYS:HE3	1.59	0.68
2:B:202:ALA:HB3	2:B:229:GLY:O	1.94	0.68
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.58	0.68
5:R:102:THR:O	5:R:106:ILE:HG13	1.94	0.68
1:N:402:VAL:HG22	1:N:406:MET:CE	2.23	0.68
2:O:160:LEU:HD12	9:V:64:LEU:HD13	1.74	0.68
5:E:127:VAL:HG12	5:E:128:LYS:N	2.08	0.68
2:O:399:ALA:O	2:O:402:ILE:HG22	1.94	0.68
2:B:101:THR:HG23	2:B:104:LYS:HE3	1.75	0.68
2:B:399:ALA:O	2:B:402:ILE:HG22	1.94	0.68
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.76	0.68
2:O:248:ASN:HD22	2:O:248:ASN:C	1.97	0.68
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.75	0.68
1:A:112:LEU:O	1:A:116:VAL:HG23	1.93	0.68
5:E:86:ASN:OD1	5:E:99:ARG:HB2	1.94	0.68
1:A:170:THR:HG22	1:A:171:THR:H	1.59	0.68
2:O:341:MET:CE	2:O:417:PHE:HE2	2.06	0.67
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.76	0.67
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.29	0.67
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.77	0.67
1:A:343:MET:HB3	1:A:444:ILE:HA	1.75	0.67
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.75	0.67
8:U:21:ARG:HG3	8:U:21:ARG:HH11	1.59	0.67
1:A:170:THR:HG22	1:A:171:THR:N	2.10	0.67
2:B:341:MET:CE	2:B:417:PHE:HE2	2.08	0.67
1:A:137:GLU:O	1:A:141:MET:HG3	1.95	0.67
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.41	0.67
9:I:33:UNK:CG	9:I:73:PRO:HB3	2.22	0.67
3:C:238:THR:HB	3:C:239:PRO:HD3	1.75	0.67
1:A:178:THR:HG22	1:A:179:ARG:N	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:70:LEU:HD23	9:I:71:ASN:N	2.10	0.66
1:N:371:GLY:O	1:N:375:VAL:HG23	1.96	0.66
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.35	0.66
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.61	0.66
2:O:122:TYR:O	2:O:126:VAL:HG23	1.94	0.66
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.78	0.66
2:B:318:ASP:O	2:B:319:SER:HB2	1.96	0.66
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.78	0.66
8:H:28:GLU:O	8:H:32:LYS:HG3	1.96	0.66
2:B:361:LYS:O	2:B:365:LYS:HG3	1.96	0.66
9:V:70:LEU:HD23	9:V:71:ASN:N	2.12	0.66
1:A:105:ASP:O	1:A:109:VAL:HG23	1.96	0.66
5:R:109:GLU:OE1	5:R:123:ASP:HB2	1.96	0.65
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.29	0.65
1:N:182:LEU:O	1:N:186:ILE:HG13	1.96	0.65
8:U:28:GLU:O	8:U:32:LYS:HG3	1.96	0.65
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.31	0.65
5:E:114:VAL:HG21	5:E:172:ARG:NH1	2.11	0.65
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.78	0.65
1:N:106:MET:O	1:N:110:VAL:HG23	1.96	0.65
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.31	0.65
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.76	0.65
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.32	0.65
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.32	0.65
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.12	0.65
5:R:86:ASN:OD1	5:R:99:ARG:HB2	1.97	0.65
5:E:109:GLU:OE2	5:E:153:PHE:HB3	1.95	0.65
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.12	0.65
9:V:64:LEU:HD12	9:V:77:ARG:O	1.97	0.65
8:U:18:THR:O	8:U:22:GLU:HG3	1.95	0.65
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.78	0.65
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.32	0.65
9:V:35:UNK:HG3	9:V:36:UNK:N	2.04	0.64
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.32	0.64
2:B:27:THR:HG22	2:B:28:LYS:H	1.61	0.64
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.77	0.64
2:O:318:ASP:O	2:O:319:SER:HB2	1.98	0.64
2:O:325:TYR:CD1	9:V:60:ALA:HB3	2.32	0.64
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.78	0.64
5:E:155:GLY:HA3	5:E:166:ASP:O	1.98	0.64
2:B:215:ASP:O	2:B:219:VAL:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:103:SER:HB3	1:N:202:GLY:O	1.97	0.64
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.79	0.64
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.78	0.64
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.32	0.64
7:T:79:ASN:O	7:T:80:ASP:HB2	1.98	0.64
5:R:169:GLY:O	5:R:179:ASN:HB3	1.97	0.64
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.33	0.64
7:G:29:ILE:O	7:G:33:ALA:HB3	1.98	0.64
3:P:147:ILE:HD11	13:P:3001:JZZ:CAB	2.27	0.64
16:Q:501:HEC:HMB1	16:Q:501:HEC:HBB3	1.80	0.64
10:J:10:TYR:CE2	10:J:15:ARG:HD2	2.33	0.64
2:O:38:LEU:HD12	2:O:39:GLU:N	2.13	0.63
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.33	0.63
5:E:163:SER:HA	5:E:174:GLY:HA3	1.80	0.63
5:E:122:HIS:HE1	5:E:124:LEU:HD12	1.63	0.63
5:R:83:GLU:HG3	5:R:100:HIS:CE1	2.33	0.63
1:A:106:MET:HE2	1:A:107:PRO:HA	1.80	0.63
2:B:299:VAL:CG1	2:B:336:VAL:HG13	2.29	0.63
3:C:81:ARG:HH22	15:C:2011:GOL:H11	1.63	0.63
3:P:202:HIS:NE2	14:P:3002:UQ:O4	2.27	0.63
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.14	0.63
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.79	0.63
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.32	0.63
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.81	0.63
2:O:273:SER:O	2:O:276:GLN:HB3	1.99	0.63
6:S:95:LYS:O	6:S:99:ARG:HG3	1.99	0.63
2:O:31:ASN:N	2:O:31:ASN:HD22	1.97	0.63
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.63	0.62
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.64	0.62
1:A:395:TRP:CE3	1:A:395:TRP:HA	2.34	0.62
2:B:341:MET:HE3	2:B:417:PHE:CE2	2.34	0.62
5:E:171:ILE:HG22	5:E:179:ASN:OD1	1.99	0.62
1:A:186:ILE:HG23	1:A:190:PHE:HD1	1.63	0.62
1:N:343:MET:HB3	1:N:444:ILE:HA	1.81	0.62
1:A:371:GLY:O	1:A:375:VAL:HG23	1.98	0.62
1:N:45:SER:HA	1:N:48:GLU:HG3	1.81	0.62
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.80	0.62
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.34	0.62
2:O:150:VAL:O	2:O:153:GLN:HG3	1.99	0.62
1:A:388:ARG:NH2	1:A:390:ILE:HG12	2.14	0.62
2:B:62:ASN:O	2:B:65:THR:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:382:HIS:HB3	1:N:388:ARG:O	1.99	0.62
1:N:178:THR:CG2	1:N:179:ARG:N	2.63	0.62
5:E:83:GLU:HB3	5:E:102:THR:CG2	2.30	0.62
3:P:22:LEU:HD21	14:P:3002:UQ:CM3	2.30	0.62
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.81	0.62
2:O:299:VAL:HG11	2:O:336:VAL:HG13	1.82	0.62
3:P:199:THR:HA	18:P:2010:BOG:O1	2.00	0.62
1:N:137:GLU:O	1:N:141:MET:HG3	1.99	0.61
5:R:135:LEU:HD23	5:R:182:VAL:HG22	1.82	0.61
2:B:248:ASN:HD22	2:B:248:ASN:C	2.03	0.61
9:I:34:UNK:HG3	9:I:35:UNK:N	2.14	0.61
10:W:10:TYR:CE2	10:W:15:ARG:HD2	2.36	0.61
2:B:37:SER:HB3	2:B:213:HIS:ND1	2.15	0.61
2:B:192:HIS:O	2:B:196:GLN:HG3	2.00	0.61
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.80	0.61
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.81	0.61
5:E:130:PRO:HG2	5:E:131:GLU:H	1.65	0.61
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.65	0.61
5:R:155:GLY:HA3	5:R:166:ASP:O	2.00	0.61
2:B:31:ASN:N	2:B:31:ASN:ND2	2.49	0.61
1:N:7:THR:HG21	2:O:113:ARG:CD	2.30	0.61
8:U:36:ARG:HB3	8:U:36:ARG:NH1	2.16	0.61
2:O:62:ASN:O	2:O:65:THR:HG22	2.00	0.61
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.82	0.61
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.35	0.61
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.82	0.61
4:Q:12:TRP:NE1	4:Q:125:ASP:OD2	2.27	0.61
1:A:178:THR:CG2	1:A:179:ARG:N	2.64	0.61
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.46	0.61
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.48	0.61
3:P:92:PHE:O	3:P:95:ILE:HG22	2.01	0.61
2:O:156:GLN:NE2	9:V:77:ARG:C	2.54	0.60
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.82	0.60
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.31	0.60
5:R:165:TYR:HA	5:R:170:ARG:O	2.01	0.60
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.82	0.60
2:B:292:THR:O	2:B:292:THR:HG22	2.01	0.60
2:O:72:ALA:HB1	2:O:75:LEU:HD12	1.83	0.60
2:O:215:ASP:O	2:O:219:VAL:HG23	2.00	0.60
2:B:31:ASN:ND2	2:B:31:ASN:H	1.99	0.60
5:E:106:ILE:O	5:E:110:ALA:HB3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:ILE:HD11	13:C:2001:JZZ:CAB	2.30	0.60
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.30	0.60
2:O:372:VAL:HG13	2:O:378:LEU:HA	1.83	0.60
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.17	0.60
2:O:299:VAL:CG1	2:O:336:VAL:HG13	2.32	0.60
1:N:4:TYR:HB3	2:O:114:ASP:OD2	2.01	0.60
2:B:372:VAL:O	2:B:372:VAL:HG12	2.01	0.60
2:B:201:SER:OG	2:B:228:SER:HA	2.02	0.60
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.84	0.60
3:P:52:LEU:HD13	12:P:501:HEM:HBD1	1.84	0.60
5:E:78:LEU:HD12	5:E:190:ASP:O	2.02	0.60
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.37	0.60
2:O:164:HIS:O	2:O:173:ALA:HA	2.02	0.60
4:D:222:MET:HE1	5:E:40:THR:HG23	1.84	0.60
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.84	0.60
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.67	0.60
2:O:76:THR:HG22	2:O:82:SER:N	2.05	0.60
2:B:372:VAL:HG13	2:B:378:LEU:HA	1.82	0.60
8:U:27:THR:O	8:U:31:VAL:HG23	2.02	0.60
9:I:33:UNK:HG2	9:I:73:PRO:CB	2.27	0.60
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.84	0.60
8:H:21:ARG:HG3	8:H:21:ARG:HH11	1.67	0.60
6:S:99:ARG:HB3	6:S:99:ARG:HH11	1.67	0.60
5:E:84:GLY:N	5:E:102:THR:HG23	2.17	0.60
2:O:357:VAL:O	2:O:361:LYS:HG3	2.02	0.60
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.66	0.60
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.01	0.60
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.36	0.59
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.02	0.59
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.84	0.59
8:H:18:THR:O	8:H:22:GLU:HG3	2.02	0.59
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.18	0.59
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.84	0.59
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.36	0.59
7:T:40:ARG:HB3	17:T:3004:CDL:HA32	1.84	0.59
1:N:388:ARG:NH2	1:N:390:ILE:HG12	2.17	0.59
2:O:170:THR:O	2:O:172:LEU:N	2.36	0.59
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.85	0.59
3:C:101:ARG:C	3:C:101:ARG:HD2	2.22	0.59
1:A:182:LEU:O	1:A:186:ILE:HG13	2.03	0.59
1:N:90:THR:O	1:N:167:VAL:HG11	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.84	0.59
1:A:106:MET:O	1:A:110:VAL:HG23	2.03	0.59
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.66	0.59
5:E:136:VAL:CG2	5:E:183:PRO:HD3	2.31	0.59
8:H:27:THR:O	8:H:31:VAL:HG23	2.03	0.59
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.85	0.59
5:R:186:GLN:HE21	5:R:188:VAL:HG13	1.68	0.59
5:E:116:LYS:HD2	5:E:116:LYS:N	2.18	0.59
9:I:29:UNK:O	9:I:30:UNK:HB2	2.02	0.59
2:B:46:ARG:HD2	2:B:110:GLU:HG2	1.84	0.59
9:V:70:LEU:HD23	9:V:71:ASN:H	1.67	0.59
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.84	0.59
2:O:372:VAL:O	2:O:372:VAL:HG12	2.03	0.58
2:O:325:TYR:HD1	9:V:60:ALA:HB3	1.68	0.58
2:O:27:THR:CG2	2:O:28:LYS:H	2.15	0.58
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.02	0.58
1:A:276:ILE:HG12	1:A:357:ALA:HB2	1.86	0.58
1:N:10:ASN:CG	2:O:19:PRO:HD2	2.23	0.58
1:N:331:ILE:HG21	1:N:431:LEU:HB2	1.85	0.58
3:C:9:HIS:CD2	3:C:12:LEU:H	2.15	0.58
9:V:49:LEU:HD22	9:V:54:SER:O	2.04	0.58
2:B:169:LYS:O	2:B:170:THR:HG23	2.02	0.58
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.38	0.58
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.84	0.58
1:N:361:LEU:O	1:N:364:ALA:HB3	2.03	0.58
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.85	0.58
5:E:187:PHE:C	5:E:189:GLY:H	2.06	0.58
5:E:84:GLY:N	5:E:100:HIS:O	2.36	0.58
2:B:357:VAL:O	2:B:361:LYS:HG3	2.03	0.58
1:A:331:ILE:HG21	1:A:431:LEU:HB2	1.86	0.58
2:O:292:THR:HG22	2:O:292:THR:O	2.03	0.58
2:O:248:ASN:HD21	2:O:250:HIS:HB2	1.68	0.58
1:A:7:THR:HG21	2:B:113:ARG:CD	2.33	0.58
5:E:165:TYR:HA	5:E:170:ARG:O	2.03	0.58
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.86	0.58
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.85	0.58
6:S:11:ARG:HA	6:S:14:ASP:HB2	1.85	0.58
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.69	0.58
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.69	0.58
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.86	0.57
2:O:417:PHE:O	2:O:422:LYS:HE3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.84	0.57
1:N:15:ASN:O	1:N:26:ALA:HA	2.05	0.57
8:U:17:LEU:HD13	8:U:73:LEU:HD22	1.86	0.57
2:B:26:ILE:O	2:B:26:ILE:HG12	2.02	0.57
4:D:57:THR:HG22	4:D:58:GLU:N	2.19	0.57
14:P:3002:UQ:HM51	14:P:3002:UQ:C8	2.35	0.57
5:E:99:ARG:HD3	5:E:105:GLU:OE2	2.05	0.57
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.84	0.57
10:W:7:ARG:HB3	10:W:7:ARG:NH1	2.19	0.57
5:R:81:ILE:HG12	5:R:87:VAL:HG21	1.86	0.57
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.37	0.57
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.38	0.57
2:B:72:ALA:HB1	2:B:75:LEU:HD12	1.86	0.57
5:E:189:GLY:O	5:E:192:LEU:N	2.38	0.57
2:O:52:LYS:O	2:O:203:ARG:NH2	2.23	0.57
2:B:28:LYS:O	2:B:29:LEU:O	2.22	0.57
5:R:49:TYR:CE1	10:W:32:GLU:HG3	2.39	0.57
2:O:47:ILE:HD13	2:O:120:MET:HE2	1.84	0.57
8:H:17:LEU:HD13	8:H:73:LEU:HD22	1.85	0.57
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.86	0.57
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.40	0.57
1:A:95:THR:HG22	1:A:96:ALA:N	2.20	0.57
2:O:76:THR:HG23	2:O:136:GLU:OE1	2.05	0.56
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.70	0.56
3:C:92:PHE:O	3:C:95:ILE:HG22	2.04	0.56
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.30	0.56
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.19	0.56
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.40	0.56
3:P:18:SER:HB2	3:P:202:HIS:HE1	1.71	0.56
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.40	0.56
8:U:43:ARG:HD2	8:U:47:ARG:NH2	2.19	0.56
3:P:236:MET:O	3:P:239:PRO:HD2	2.06	0.56
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.70	0.56
1:N:276:ILE:HG12	1:N:357:ALA:HB2	1.86	0.56
1:N:362:ARG:O	1:N:365:MET:HG2	2.05	0.56
2:B:189:GLU:N	2:B:189:GLU:OE1	2.39	0.56
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.86	0.56
5:E:106:ILE:C	5:E:110:ALA:HB3	2.26	0.56
12:P:502:HEM:HMB1	12:P:502:HEM:HBB2	1.88	0.56
5:R:106:ILE:O	5:R:109:GLU:HB3	2.06	0.56
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:ASP:OD1	2:B:24:LEU:N	2.39	0.56
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.41	0.56
2:O:27:THR:CG2	2:O:28:LYS:N	2.69	0.56
5:R:164:HIS:CD2	5:R:173:LYS:HB3	2.38	0.56
4:D:79:GLU:HA	4:D:79:GLU:OE2	2.05	0.56
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.36	0.56
5:R:185:TYR:HB3	5:R:195:VAL:HA	1.88	0.56
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.88	0.56
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.69	0.56
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.87	0.56
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.36	0.56
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.33	0.56
14:C:2002:UQ:HM51	14:C:2002:UQ:C8	2.36	0.56
5:R:185:TYR:O	5:R:186:GLN:HB3	2.06	0.56
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.41	0.56
2:B:312:PHE:HE1	9:I:62:ARG:O	1.89	0.56
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.36	0.56
14:P:3002:UQ:HM51	14:P:3002:UQ:H8	1.88	0.56
9:V:70:LEU:HD23	9:V:71:ASN:OD1	2.06	0.55
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.44	0.55
1:N:281:ASP:O	1:N:283:THR:N	2.39	0.55
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.71	0.55
2:O:150:VAL:HA	2:O:153:GLN:HG3	1.88	0.55
5:R:79:SER:OG	5:R:191:ASP:HB2	2.06	0.55
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.87	0.55
2:B:374:THR:HG22	2:B:376:GLN:H	1.71	0.55
2:O:46:ARG:HD2	2:O:110:GLU:HG2	1.88	0.55
10:J:7:ARG:NH1	10:J:7:ARG:HB3	2.20	0.55
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.41	0.55
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.07	0.55
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.41	0.55
2:O:374:THR:HG22	2:O:376:GLN:H	1.72	0.55
2:B:225:ASN:O	2:B:227:ARG:N	2.40	0.55
1:N:205:HIS:O	1:N:208:LEU:HB3	2.06	0.55
2:B:46:ARG:HD2	2:B:110:GLU:CG	2.37	0.55
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.89	0.55
1:A:4:TYR:HB3	2:B:114:ASP:OD2	2.07	0.55
4:D:37:CYS:C	4:D:39:ALA:H	2.10	0.55
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.41	0.55
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.22	0.55
1:N:69:LYS:HD2	1:N:70:ARG:NH2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:169:LYS:O	2:O:170:THR:HG23	2.07	0.55
1:A:191:LYS:CA	1:A:195:MET:HE2	2.37	0.55
8:U:21:ARG:HG3	8:U:21:ARG:NH1	2.22	0.55
2:O:345:LYS:O	2:O:349:GLN:HG3	2.07	0.55
1:A:15:ASN:O	1:A:26:ALA:HA	2.07	0.55
2:B:36:ALA:HB3	2:B:207:VAL:HG13	1.89	0.55
5:E:122:HIS:HB3	5:E:125:ASP:CG	2.27	0.55
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.14	0.55
2:O:56:ARG:HG3	2:O:171:ALA:HB1	1.88	0.55
2:O:264:VAL:HG12	2:O:265:GLY:N	2.22	0.55
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.37	0.54
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.89	0.54
2:B:417:PHE:O	2:B:422:LYS:HE3	2.07	0.54
4:D:47:ALA:HA	4:D:90:TYR:HA	1.88	0.54
5:E:77:LYS:HG3	5:E:191:ASP:O	2.06	0.54
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.74	0.54
2:B:170:THR:O	2:B:172:LEU:N	2.40	0.54
2:B:374:THR:HB	2:B:377:GLY:H	1.72	0.54
1:N:317:THR:HG23	1:N:318:GLY:N	2.23	0.54
2:B:47:ILE:HD13	2:B:120:MET:HE2	1.86	0.54
14:C:2002:UQ:HM51	14:C:2002:UQ:H8	1.89	0.54
1:A:60:GLU:OE2	1:A:90:THR:HG22	2.08	0.54
3:C:263:LEU:O	3:C:264:VAL:HG23	2.08	0.54
1:A:402:VAL:HG22	1:A:406:MET:CE	2.38	0.54
10:J:56:LYS:O	10:J:60:GLU:HB2	2.08	0.54
1:A:430:GLN:HG3	7:G:4:PHE:O	2.08	0.54
7:G:36:ASN:O	7:G:40:ARG:HG3	2.08	0.54
1:A:280:TYR:CG	1:A:281:ASP:N	2.76	0.54
5:R:83:GLU:HA	5:R:100:HIS:HB3	1.90	0.54
5:E:114:VAL:HG21	5:E:172:ARG:HH12	1.71	0.54
2:O:332:HIS:O	2:O:336:VAL:HG23	2.07	0.54
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.89	0.54
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.90	0.54
5:R:112:VAL:HG21	5:R:170:ARG:NH2	2.22	0.54
1:N:156:THR:HA	1:N:159:GLN:HB3	1.90	0.54
3:C:271:PRO:HG2	3:C:276:LEU:HD23	1.90	0.54
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.08	0.53
1:A:272:VAL:O	1:A:275:ALA:HB3	2.09	0.53
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.89	0.53
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.71	0.53
6:S:16:ILE:O	6:S:19:TRP:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:217:LYS:O	2:O:221:GLU:HG2	2.09	0.53
2:O:402:ILE:HD13	2:O:402:ILE:C	2.29	0.53
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.91	0.53
1:A:388:ARG:HH22	1:A:390:ILE:HG12	1.73	0.53
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.89	0.53
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.43	0.53
1:A:191:LYS:N	1:A:195:MET:HE2	2.22	0.53
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.73	0.53
1:N:209:VAL:O	1:N:212:ALA:HB3	2.08	0.53
5:R:52:LYS:HD3	5:R:52:LYS:C	2.29	0.53
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.91	0.53
2:O:132:PHE:CD1	2:O:191:LEU:HB3	2.43	0.53
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.09	0.53
4:Q:195:GLU:OE1	4:Q:201:ARG:NH2	2.41	0.53
5:R:135:LEU:HD13	5:R:180:LEU:HD12	1.90	0.53
1:N:430:GLN:HG3	7:T:4:PHE:O	2.08	0.53
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.44	0.53
2:B:225:ASN:O	2:B:226:ILE:C	2.47	0.53
5:R:170:ARG:HA	5:R:179:ASN:CB	2.38	0.53
7:G:40:ARG:HB3	17:G:2004:CDL:HA32	1.91	0.53
3:P:245:LEU:O	4:Q:201:ARG:HD2	2.09	0.53
1:N:22:GLY:O	1:N:193:PRO:HA	2.07	0.53
1:N:186:ILE:HG23	1:N:190:PHE:HD1	1.74	0.53
1:N:131:ARG:NH2	1:N:177:LEU:O	2.41	0.53
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.72	0.53
4:D:116:ILE:HG23	4:D:117:VAL:N	2.23	0.53
6:F:40:ASP:O	6:F:44:LYS:HG3	2.09	0.53
2:O:259:THR:HG22	2:O:260:GLU:N	2.24	0.53
5:E:52:LYS:C	5:E:52:LYS:HD3	2.29	0.53
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.44	0.53
1:A:90:THR:O	1:A:167:VAL:HG11	2.09	0.53
2:B:57:TYR:CD1	2:B:57:TYR:N	2.76	0.53
2:O:36:ALA:HB3	2:O:207:VAL:HG13	1.89	0.53
4:Q:2:GLU:O	4:Q:3:LEU:O	2.27	0.53
3:C:130:VAL:HG23	3:C:183:HIS:HB2	1.91	0.53
3:C:326:PHE:O	3:C:330:VAL:HG23	2.09	0.53
2:B:280:GLY:HA3	2:B:293:SER:OG	2.07	0.53
2:B:76:THR:HG22	2:B:82:SER:N	2.14	0.53
1:A:69:LYS:HD2	1:A:70:ARG:NH2	2.23	0.53
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.44	0.53
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:173:ASN:N	3:P:174:PRO:HD2	2.24	0.53
7:T:36:ASN:O	7:T:40:ARG:HG3	2.09	0.52
6:S:40:ASP:O	6:S:44:LYS:HG3	2.09	0.52
2:O:295:LEU:O	2:O:299:VAL:HG23	2.09	0.52
5:R:77:LYS:HA	5:R:191:ASP:O	2.10	0.52
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.26	0.52
5:E:187:PHE:C	5:E:189:GLY:N	2.63	0.52
11:P:3007:PEE:H50	17:T:3004:CDL:H712	1.91	0.52
3:C:236:MET:O	3:C:239:PRO:HD2	2.08	0.52
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.39	0.52
7:T:40:ARG:HD2	17:T:3004:CDL:OA4	2.10	0.52
4:D:116:ILE:HG21	4:D:190:LEU:HD13	1.90	0.52
2:B:156:GLN:HE22	9:I:77:ARG:C	2.13	0.52
2:B:96:LEU:HD12	2:B:97:SER:N	2.25	0.52
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.42	0.52
1:A:130:GLU:O	1:A:134:ILE:HG13	2.10	0.52
5:E:75:GLU:HA	5:E:193:VAL:O	2.09	0.52
2:O:225:ASN:O	2:O:227:ARG:HG3	2.09	0.52
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.25	0.52
1:N:354:VAL:HG23	1:N:355:LYS:N	2.25	0.52
2:O:338:ARG:NH1	2:O:338:ARG:CG	2.68	0.52
4:Q:116:ILE:HG21	4:Q:190:LEU:HD13	1.91	0.52
3:C:345:GLU:C	3:C:349:ILE:HG13	2.30	0.52
1:A:204:SER:HB3	1:A:207:GLU:HG3	1.92	0.52
2:B:50:PHE:CD1	2:B:50:PHE:N	2.77	0.52
1:N:106:MET:HE2	1:N:107:PRO:HA	1.91	0.52
10:W:49:GLY:N	10:W:54:HIS:ND1	2.58	0.52
2:B:297:GLN:O	2:B:301:LYS:HG3	2.09	0.52
5:E:136:VAL:O	5:E:138:VAL:N	2.41	0.52
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.91	0.52
3:P:138:GLN:HB2	3:P:255:GLU:O	2.10	0.52
6:S:91:GLU:CG	6:S:95:LYS:HE3	2.37	0.52
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.40	0.52
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.75	0.52
5:E:147:ILE:HG22	5:E:149:ASN:H	1.74	0.52
1:A:75:PHE:O	1:A:79:VAL:HG23	2.10	0.52
5:R:131:GLU:N	5:R:131:GLU:OE1	2.40	0.51
2:B:27:THR:CG2	2:B:28:LYS:N	2.73	0.51
2:B:325:TYR:HD1	9:I:60:ALA:HB3	1.76	0.51
2:O:397:VAL:O	2:O:401:LYS:HG2	2.10	0.51
5:E:141:HIS:HB2	5:E:176:ALA:CB	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:9:HIS:CD2	3:P:12:LEU:H	2.16	0.51
5:R:186:GLN:O	5:R:193:VAL:HG23	2.10	0.51
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.92	0.51
10:J:7:ARG:HH11	10:J:7:ARG:CB	2.23	0.51
2:B:207:VAL:HG12	2:B:208:GLY:H	1.76	0.51
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.92	0.51
6:F:32:MET:CE	6:F:87:LYS:HG2	2.40	0.51
5:R:141:HIS:HB3	19:R:501:FES:S2	2.50	0.51
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.92	0.51
2:B:28:LYS:HG3	2:B:34:ILE:HG12	1.91	0.51
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.92	0.51
2:O:345:LYS:HG2	2:O:418:VAL:CG1	2.40	0.51
2:O:221:GLU:C	2:O:223:PHE:H	2.13	0.51
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.25	0.51
3:P:132:TYR:O	3:P:135:PRO:HD2	2.11	0.51
3:C:245:LEU:O	4:D:201:ARG:HD2	2.10	0.51
4:Q:102:ARG:HG2	4:Q:102:ARG:HH11	1.75	0.51
2:B:345:LYS:O	2:B:349:GLN:HG3	2.09	0.51
5:R:76:ILE:O	5:R:193:VAL:HG12	2.10	0.51
5:E:190:ASP:C	5:E:192:LEU:N	2.63	0.51
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.92	0.51
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.11	0.51
3:C:207:ASN:ND2	3:C:208:ASN:H	2.08	0.51
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.46	0.51
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.26	0.51
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.10	0.51
2:B:307:PHE:H	9:I:52:ARG:HG2	1.74	0.51
5:E:185:TYR:O	5:E:186:GLN:HB3	2.09	0.51
4:D:167:GLU:HG3	8:H:13:LEU:CD2	2.41	0.51
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.45	0.51
1:N:140:GLU:HG3	9:V:50:LEU:HD12	1.93	0.51
2:B:105:MET:HE2	2:B:107:TYR:HE1	1.76	0.51
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.46	0.51
5:E:190:ASP:O	5:E:192:LEU:N	2.44	0.51
10:J:10:TYR:HE2	10:J:15:ARG:HD2	1.74	0.51
2:O:345:LYS:HG2	2:O:418:VAL:HG11	1.93	0.51
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.46	0.51
4:D:167:GLU:HG3	8:H:13:LEU:HD22	1.93	0.51
3:C:347:PRO:O	3:C:350:ILE:HG22	2.11	0.51
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.42	0.50
2:O:31:ASN:ND2	2:O:31:ASN:N	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:57:THR:HG22	4:Q:59:ALA:N	2.24	0.50
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.94	0.50
2:B:295:LEU:O	2:B:299:VAL:HG23	2.11	0.50
2:O:141:GLN:N	2:O:142:PRO:HD2	2.27	0.50
2:B:259:THR:HG22	2:B:260:GLU:N	2.26	0.50
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.40	0.50
17:D:2003:CDL:HB22	7:G:40:ARG:NH2	2.26	0.50
2:B:150:VAL:HA	2:B:153:GLN:HG3	1.92	0.50
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.42	0.50
2:B:68:LEU:HD23	2:B:186:ILE:HG21	1.94	0.50
10:W:7:ARG:HH11	10:W:7:ARG:CB	2.25	0.50
5:E:189:GLY:O	5:E:192:LEU:O	2.29	0.50
2:O:57:TYR:N	2:O:57:TYR:CD1	2.79	0.50
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.46	0.50
4:D:105:ASN:O	4:D:106:ASN:HB2	2.12	0.50
1:A:354:VAL:HG23	1:A:355:LYS:N	2.26	0.50
12:C:502:HEM:HMB1	12:C:502:HEM:HBB2	1.92	0.50
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.92	0.50
3:P:325:LEU:HD22	3:P:370:ILE:HG13	1.94	0.50
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.42	0.50
1:A:223:TYR:HD2	1:A:223:TYR:H	1.59	0.50
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.15	0.50
4:D:57:THR:HG22	4:D:59:ALA:N	2.23	0.50
5:R:163:SER:H	5:R:175:PRO:HD2	1.76	0.50
2:O:56:ARG:HG3	2:O:56:ARG:NH1	2.25	0.50
3:C:132:TYR:O	3:C:135:PRO:HD2	2.12	0.50
1:N:279:ARG:HH22	9:V:30:UNK:C	2.24	0.50
3:C:173:ASN:N	3:C:174:PRO:HD2	2.26	0.50
2:O:124:LEU:HD23	2:O:124:LEU:C	2.32	0.50
1:N:106:MET:CE	1:N:110:VAL:HG21	2.41	0.50
10:W:10:TYR:HE2	10:W:15:ARG:HD2	1.75	0.50
4:D:37:CYS:O	4:D:39:ALA:N	2.44	0.50
1:A:45:SER:HA	1:A:48:GLU:HG3	1.92	0.50
1:N:223:TYR:HD2	1:N:223:TYR:H	1.58	0.50
4:D:168:ILE:HG12	4:D:168:ILE:O	2.10	0.50
3:C:52:LEU:HD13	12:C:501:HEM:HBD1	1.94	0.50
1:N:4:TYR:CB	2:O:114:ASP:OD2	2.59	0.50
9:V:31:UNK:C	9:V:73:PRO:HG2	2.41	0.50
1:N:439:SER:HA	1:N:442:TYR:CE2	2.46	0.50
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.12	0.50
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:121:GLN:CB	5:E:170:ARG:HD3	2.40	0.50
3:C:377:MET:HE1	6:F:20:TYR:CD1	2.47	0.50
1:A:48:GLU:CD	1:A:54:GLY:H	2.15	0.50
6:F:91:GLU:HB3	6:F:92:PRO:HD3	1.94	0.50
2:B:141:GLN:N	2:B:142:PRO:HD2	2.27	0.50
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.47	0.49
1:A:89:TYR:O	1:A:95:THR:HG23	2.12	0.49
1:A:239:SER:HB2	7:G:17:SER:O	2.12	0.49
3:P:223:PRO:O	3:P:227:PHE:HD2	1.94	0.49
1:N:53:ASN:HB3	1:N:173:ASN:ND2	2.27	0.49
5:R:178:TYR:N	5:R:178:TYR:CD1	2.80	0.49
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.44	0.49
3:P:50:LEU:O	3:P:54:MET:HG3	2.12	0.49
3:C:286:PRO:O	3:C:287:ASN:CB	2.60	0.49
3:P:108:TYR:HB3	3:P:114:TRP:CE3	2.47	0.49
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.75	0.49
2:O:277:HIS:CD2	2:O:364:LEU:HD13	2.47	0.49
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.93	0.49
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.94	0.49
1:A:382:HIS:HB3	1:A:388:ARG:O	2.12	0.49
3:P:234:THR:HG21	4:Q:219:LEU:CD1	2.41	0.49
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.27	0.49
5:E:76:ILE:O	5:E:193:VAL:HG12	2.13	0.49
2:O:26:ILE:O	2:O:26:ILE:HG12	2.11	0.49
2:O:353:THR:HG22	2:O:354:GLU:N	2.28	0.49
2:O:222:GLN:HG2	2:O:222:GLN:O	2.12	0.49
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.42	0.49
1:N:63:ALA:O	1:N:116:VAL:HG13	2.12	0.49
3:P:49:GLY:C	12:P:501:HEM:HAC	2.33	0.49
2:O:280:GLY:HA3	2:O:293:SER:OG	2.12	0.49
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.28	0.49
2:O:71:LEU:HD12	2:O:144:LEU:HD23	1.93	0.49
1:N:191:LYS:C	1:N:195:MET:HE2	2.33	0.49
3:P:90:PHE:CE1	3:P:236:MET:HB3	2.47	0.49
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.43	0.49
2:B:338:ARG:CG	2:B:338:ARG:NH1	2.74	0.49
5:E:122:HIS:O	5:E:125:ASP:HB2	2.11	0.49
2:O:209:ILE:HD12	2:O:379:LEU:HB2	1.94	0.49
2:B:402:ILE:HD13	2:B:402:ILE:C	2.32	0.49
3:P:147:ILE:HD11	13:P:3001:JZZ:HAB	1.95	0.49
1:N:364:ALA:O	1:N:368:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.94	0.49
9:V:52:ARG:HG3	9:V:52:ARG:HH11	1.78	0.49
4:D:102:ARG:HA	4:D:108:ALA:O	2.12	0.49
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.47	0.49
8:U:27:THR:HG22	8:U:29:LYS:H	1.77	0.49
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.13	0.49
3:C:28:ILE:CD1	14:C:2002:UQ:HM21	2.43	0.49
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.53	0.49
1:A:387:GLY:O	1:A:388:ARG:HB3	2.13	0.49
5:E:147:ILE:O	5:E:156:TYR:HA	2.13	0.49
2:B:385:GLU:O	2:B:387:LEU:N	2.46	0.49
4:Q:148:HIS:CD2	4:Q:148:HIS:N	2.81	0.49
4:Q:47:ALA:HA	4:Q:90:TYR:HA	1.95	0.48
2:B:248:ASN:HA	2:O:181:TYR:CD2	2.47	0.48
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.94	0.48
1:A:23:LEU:HD23	1:A:24:ARG:N	2.28	0.48
1:N:270:LEU:HD13	1:N:320:PHE:CD1	2.48	0.48
3:P:347:PRO:O	3:P:350:ILE:HG22	2.13	0.48
6:S:70:LEU:HD12	6:S:70:LEU:C	2.33	0.48
2:O:96:LEU:HD12	2:O:97:SER:N	2.28	0.48
5:R:49:TYR:HE1	10:W:32:GLU:HG3	1.78	0.48
2:B:59:THR:O	2:B:61:ALA:N	2.45	0.48
3:P:155:PRO:O	3:P:156:TYR:HB2	2.13	0.48
2:B:248:ASN:HD21	2:B:250:HIS:HB2	1.77	0.48
2:O:248:ASN:C	2:O:248:ASN:ND2	2.67	0.48
6:F:67:ASP:CG	6:F:71:LYS:HZ3	2.17	0.48
2:B:56:ARG:HG3	2:B:171:ALA:HB1	1.95	0.48
1:N:134:ILE:HG21	1:N:174:ILE:HD13	1.96	0.48
1:N:281:ASP:HB2	9:V:33:UNK:HB2	1.95	0.48
5:R:161:HIS:HB2	19:R:501:FES:S1	2.53	0.48
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.96	0.48
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.28	0.48
4:D:148:HIS:CD2	4:D:148:HIS:N	2.82	0.48
5:R:82:PRO:O	5:R:100:HIS:HB3	2.13	0.48
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.78	0.48
1:A:217:SER:O	1:A:218:GLY:C	2.52	0.48
2:B:273:SER:O	2:B:276:GLN:HB3	2.13	0.48
2:B:27:THR:CG2	2:B:28:LYS:H	2.26	0.48
5:R:166:ASP:OD1	5:R:168:SER:N	2.45	0.48
4:Q:37:CYS:C	4:Q:39:ALA:H	2.17	0.48
3:P:27:ASN:HD22	3:P:209:PRO:HG2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:THR:HG23	1:A:205:HIS:NE2	2.28	0.48
3:P:136:TRP:HH2	3:P:171:VAL:HG12	1.79	0.48
2:O:221:GLU:O	2:O:223:PHE:N	2.46	0.48
17:Q:3003:CDL:HB22	7:T:40:ARG:NH2	2.29	0.48
1:A:133:VAL:O	1:A:136:GLN:HB2	2.14	0.48
2:O:414:ALA:O	2:O:418:VAL:HG23	2.14	0.48
1:N:351:GLU:O	1:N:354:VAL:HG22	2.12	0.48
4:D:220:TYR:O	4:D:224:ARG:HG2	2.13	0.48
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.47	0.48
5:R:104:ALA:HA	5:R:107:ASN:ND2	2.29	0.48
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.96	0.48
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.95	0.48
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	1.95	0.48
6:S:13:MET:O	6:S:17:ARG:HG3	2.14	0.48
4:Q:169:LEU:CD2	4:Q:182:ILE:HD11	2.44	0.48
1:A:131:ARG:NH2	1:A:177:LEU:O	2.47	0.48
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.14	0.48
5:R:75:GLU:HA	5:R:193:VAL:O	2.14	0.48
2:O:54:GLY:C	2:O:56:ARG:H	2.17	0.48
1:N:32:GLN:HE22	2:O:373:GLU:HA	1.79	0.48
5:E:97:PHE:O	5:E:134:ILE:HA	2.13	0.48
2:O:338:ARG:O	2:O:341:MET:HB2	2.14	0.48
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.14	0.48
5:R:186:GLN:NE2	5:R:188:VAL:HG13	2.28	0.48
3:P:31:TRP:CZ3	11:P:3007:PEE:H20	2.48	0.48
1:N:402:VAL:HA	1:N:406:MET:CE	2.44	0.48
1:N:45:SER:HA	1:N:48:GLU:CG	2.44	0.48
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.79	0.48
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.95	0.48
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.96	0.48
2:O:73:SER:N	2:O:74:PRO:HD2	2.29	0.48
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.13	0.48
1:N:240:GLU:HA	1:N:422:LEU:O	2.14	0.48
7:G:28:ASN:HB3	7:G:31:SER:OG	2.14	0.48
6:F:53:ASP:OD1	6:F:54:LEU:N	2.46	0.48
4:D:239:PRO:C	4:D:241:LYS:H	2.17	0.48
5:R:78:LEU:HD22	5:R:132:TRP:CE2	2.49	0.47
9:I:71:ASN:HD22	9:I:71:ASN:H	1.61	0.47
5:R:163:SER:HA	5:R:174:GLY:HA3	1.96	0.47
2:B:206:LEU:CD2	2:B:220:ALA:HB2	2.43	0.47
2:O:325:TYR:CD1	9:V:60:ALA:CB	2.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:21:ARG:HG3	8:H:21:ARG:NH1	2.28	0.47
2:B:96:LEU:HD13	2:B:109:VAL:HG12	1.95	0.47
3:C:49:GLY:C	12:C:501:HEM:HAC	2.34	0.47
2:B:162:ASN:O	2:B:244:ILE:HD12	2.14	0.47
3:P:313:GLN:NE2	6:S:36:THR:OG1	2.45	0.47
2:B:124:LEU:CD1	2:B:223:PHE:HB3	2.42	0.47
2:B:332:HIS:O	2:B:336:VAL:HG23	2.13	0.47
2:B:110:GLU:O	2:B:111:CYS:HB3	2.14	0.47
2:O:46:ARG:HD2	2:O:110:GLU:CG	2.44	0.47
2:O:110:GLU:O	2:O:111:CYS:HB3	2.13	0.47
10:J:49:GLY:N	10:J:54:HIS:ND1	2.61	0.47
2:B:262:ALA:O	2:B:320:GLY:HA3	2.14	0.47
1:A:362:ARG:O	1:A:365:MET:HG2	2.14	0.47
1:A:287:GLY:O	1:A:290:LEU:HG	2.14	0.47
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.14	0.47
3:C:50:LEU:O	3:C:54:MET:HG3	2.15	0.47
5:E:146:PRO:HG2	5:E:180:LEU:HD21	1.96	0.47
4:Q:57:THR:CG2	4:Q:58:GLU:N	2.77	0.47
1:N:53:ASN:N	1:N:173:ASN:ND2	2.62	0.47
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.40	0.47
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.43	0.47
5:E:101:ARG:HB2	5:E:131:GLU:HA	1.96	0.47
3:C:37:LEU:O	3:C:41:CYS:HB2	2.14	0.47
1:N:90:THR:O	1:N:90:THR:HG23	2.15	0.47
2:B:325:TYR:CD1	9:I:60:ALA:CB	2.97	0.47
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.95	0.47
1:A:205:HIS:O	1:A:208:LEU:HB3	2.15	0.47
1:N:36:THR:HG21	1:N:373:THR:HA	1.96	0.47
7:T:56:TYR:O	7:T:59:TYR:HB3	2.14	0.47
5:E:188:VAL:HG12	5:E:188:VAL:O	2.15	0.47
2:B:207:VAL:HG12	2:B:208:GLY:N	2.29	0.47
1:A:402:VAL:HA	1:A:406:MET:CE	2.44	0.47
1:A:344:ARG:HH22	1:A:353:GLU:CD	2.17	0.47
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.95	0.47
1:A:364:ALA:O	1:A:368:GLN:HG3	2.14	0.47
2:B:353:THR:HG22	2:B:354:GLU:N	2.29	0.47
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.43	0.47
5:E:101:ARG:HA	5:E:105:GLU:OE1	2.14	0.47
1:N:388:ARG:HH22	1:N:390:ILE:HG12	1.78	0.47
1:A:281:ASP:O	1:A:283:THR:N	2.47	0.47
1:N:154:HIS:O	1:N:156:THR:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:64:LEU:HD12	9:V:77:ARG:C	2.35	0.47
5:E:129:LYS:HG3	5:E:187:PHE:CE2	2.50	0.47
8:U:32:LYS:O	8:U:36:ARG:HG3	2.15	0.47
3:P:275:PHE:CG	13:P:3001:JZZ:HAGB	2.50	0.47
6:F:16:ILE:O	6:F:19:TRP:HB3	2.14	0.47
6:S:77:LYS:HE2	6:S:77:LYS:HB3	1.77	0.47
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.97	0.47
2:B:264:VAL:HG23	2:B:316:TYR:C	2.35	0.47
2:B:348:ALA:HA	2:B:414:ALA:HB3	1.97	0.47
8:U:28:GLU:CG	8:U:32:LYS:HE3	2.43	0.47
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.44	0.47
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.80	0.47
10:J:59:TYR:CD1	10:J:59:TYR:N	2.82	0.47
3:P:9:HIS:CD2	3:P:12:LEU:HG	2.50	0.47
4:D:57:THR:CG2	4:D:58:GLU:N	2.78	0.47
1:N:382:HIS:CE1	1:N:390:ILE:HB	2.50	0.47
2:B:345:LYS:HG2	2:B:418:VAL:CG1	2.45	0.47
3:P:365:ILE:HG22	3:P:366:LEU:HD23	1.96	0.47
1:N:231:LEU:HD23	1:N:232:PRO:HD2	1.95	0.47
8:H:50:THR:O	8:H:50:THR:HG23	2.14	0.47
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.50	0.47
10:J:56:LYS:HE2	10:J:56:LYS:HB3	1.72	0.47
1:N:75:PHE:O	1:N:79:VAL:HG23	2.15	0.47
2:B:338:ARG:O	2:B:341:MET:HB2	2.15	0.46
5:R:78:LEU:HD11	5:R:187:PHE:CD1	2.50	0.46
9:V:33:UNK:HA	9:V:73:PRO:HB3	1.97	0.46
3:P:172:ASP:HB3	3:P:174:PRO:HD2	1.97	0.46
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.30	0.46
1:N:144:ASP:OD2	1:N:147:ASN:ND2	2.47	0.46
3:C:327:TRP:CE2	7:G:48:VAL:HG22	2.50	0.46
6:S:53:ASP:OD1	6:S:54:LEU:N	2.48	0.46
3:C:120:LEU:HD23	3:C:120:LEU:HA	1.82	0.46
2:B:70:ARG:HG3	2:B:98:VAL:CG1	2.45	0.46
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.96	0.46
1:A:382:HIS:CE1	1:A:390:ILE:HB	2.50	0.46
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.45	0.46
12:P:502:HEM:HBB2	12:P:502:HEM:CMB	2.45	0.46
5:E:191:ASP:N	5:E:191:ASP:OD2	2.48	0.46
6:F:58:ARG:HD2	6:F:89:TYR:OH	2.14	0.46
8:U:22:GLU:O	8:U:26:GLN:HG2	2.16	0.46
2:B:42:SER:C	2:B:44:ALA:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:186:GLN:NE2	5:R:187:PHE:O	2.48	0.46
3:P:327:TRP:CE2	7:T:48:VAL:HG22	2.50	0.46
2:B:56:ARG:NH1	2:B:56:ARG:HG3	2.30	0.46
4:D:235:MET:HB3	7:G:15:THR:HG22	1.97	0.46
6:F:77:LYS:HE2	6:F:77:LYS:HB3	1.77	0.46
5:E:106:ILE:O	5:E:106:ILE:HG22	2.15	0.46
3:C:234:THR:HG21	4:D:219:LEU:CD1	2.45	0.46
1:A:351:GLU:O	1:A:354:VAL:HG22	2.16	0.46
3:C:286:PRO:O	3:C:287:ASN:HB2	2.15	0.46
4:Q:222:MET:HE1	5:R:40:THR:HG23	1.97	0.46
10:W:60:GLU:O	10:W:61:ALA:HB2	2.14	0.46
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.97	0.46
8:H:27:THR:HG22	8:H:29:LYS:H	1.81	0.46
1:A:331:ILE:CG2	1:A:431:LEU:HB2	2.45	0.46
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.50	0.46
5:E:161:HIS:HB2	19:E:501:FES:S1	2.56	0.46
3:P:208:ASN:HB2	3:P:209:PRO:HD2	1.98	0.46
4:Q:168:ILE:O	4:Q:168:ILE:HG12	2.15	0.46
10:W:56:LYS:O	10:W:60:GLU:HB3	2.15	0.46
5:E:115:SER:HB2	5:E:116:LYS:HD2	1.97	0.46
2:O:140:LEU:C	2:O:142:PRO:HD2	2.36	0.46
4:Q:79:GLU:HA	4:Q:79:GLU:OE2	2.16	0.46
7:G:65:GLU:O	7:G:69:LEU:HG	2.16	0.46
3:P:5:ILE:O	3:P:5:ILE:HG22	2.16	0.46
2:O:334:GLY:O	2:O:338:ARG:HG2	2.15	0.46
5:R:97:PHE:O	5:R:134:ILE:HA	2.16	0.46
5:R:118:ARG:NH1	5:R:174:GLY:O	2.48	0.46
2:B:54:GLY:C	2:B:56:ARG:H	2.18	0.46
1:N:331:ILE:CG2	1:N:431:LEU:HB2	2.46	0.46
3:C:245:LEU:O	4:D:201:ARG:CD	2.64	0.46
5:E:144:CYS:HB2	19:E:501:FES:S2	2.56	0.46
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.96	0.46
2:O:207:VAL:HG12	2:O:208:GLY:H	1.81	0.46
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.31	0.46
1:A:156:THR:HA	1:A:159:GLN:HB3	1.97	0.46
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.79	0.46
1:N:294:LEU:HD11	1:N:334:MET:CE	2.45	0.46
3:P:31:TRP:NE1	11:P:3007:PEE:O4	2.49	0.46
3:P:245:LEU:O	4:Q:201:ARG:CD	2.64	0.46
4:Q:43:MET:HE3	4:Q:91:PHE:CE2	2.51	0.46
10:W:59:TYR:N	10:W:59:TYR:CD1	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:VAL:O	2:B:278:VAL:HG23	2.16	0.46
1:A:114:ALA:O	1:A:118:GLN:HB2	2.16	0.46
3:C:269:ILE:HG22	3:C:269:ILE:O	2.16	0.46
5:R:185:TYR:HD2	5:R:185:TYR:N	2.14	0.46
5:R:177:PRO:HG2	5:R:178:TYR:HD1	1.81	0.46
2:O:385:GLU:O	2:O:387:LEU:N	2.48	0.46
3:C:5:ILE:O	3:C:5:ILE:HG22	2.16	0.46
2:O:31:ASN:H	2:O:31:ASN:ND2	2.13	0.45
2:O:348:ALA:HA	2:O:414:ALA:HB3	1.97	0.45
4:D:167:GLU:CG	8:H:13:LEU:HD22	2.46	0.45
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.51	0.45
4:D:227:TRP:O	4:D:228:SER:C	2.52	0.45
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.72	0.45
5:E:127:VAL:CG1	5:E:128:LYS:H	2.12	0.45
2:O:96:LEU:HD13	2:O:109:VAL:HG12	1.96	0.45
1:N:122:LEU:HD11	1:N:186:ILE:HD12	1.99	0.45
2:B:24:LEU:HD12	2:B:37:SER:O	2.16	0.45
2:B:140:LEU:C	2:B:142:PRO:HD2	2.36	0.45
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.97	0.45
16:D:501:HEC:HBB3	16:D:501:HEC:HMB1	1.97	0.45
1:N:180:ALA:O	1:N:183:ALA:HB3	2.16	0.45
2:B:397:VAL:O	2:B:401:LYS:HG2	2.16	0.45
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.51	0.45
7:T:66:PHE:CE2	7:T:70:LYS:HE3	2.52	0.45
1:A:106:MET:N	1:A:107:PRO:HD2	2.32	0.45
3:C:31:TRP:CH2	17:G:2004:CDL:H512	2.51	0.45
2:O:227:ARG:HB3	2:O:228:SER:H	1.47	0.45
2:B:81:SER:O	2:B:85:ILE:HG13	2.17	0.45
1:N:245:ASP:OD1	7:T:11:ARG:NE	2.41	0.45
5:R:117:LEU:HD21	5:R:172:ARG:NH1	2.31	0.45
8:H:58:LEU:O	8:H:58:LEU:HD12	2.15	0.45
5:R:134:ILE:HD12	5:R:185:TYR:HE1	1.80	0.45
3:P:101:ARG:O	3:P:101:ARG:HD2	2.16	0.45
1:A:53:ASN:HB3	1:A:173:ASN:ND2	2.32	0.45
2:B:395:PRO:O	2:B:398:VAL:HG12	2.17	0.45
2:O:162:ASN:O	2:O:244:ILE:HD12	2.17	0.45
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.79	0.45
3:P:286:PRO:O	3:P:287:ASN:CB	2.64	0.45
2:O:67:HIS:O	2:O:70:ARG:HB3	2.17	0.45
2:O:76:THR:CG2	2:O:82:SER:H	2.10	0.45
5:R:163:SER:OG	5:R:176:ALA:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:THR:CG2	1:A:171:THR:N	2.79	0.45
6:F:32:MET:HE1	6:F:87:LYS:HG2	1.98	0.45
3:C:342:GLN:HB3	3:C:343:PRO:HD2	1.99	0.45
5:R:107:ASN:C	5:R:109:GLU:N	2.70	0.45
7:T:40:ARG:CB	17:T:3004:CDL:HA32	2.45	0.45
1:N:70:ARG:HA	1:N:71:PRO:HD2	1.81	0.45
3:P:275:PHE:CD2	13:P:3001:JZZ:HAGB	2.52	0.45
1:N:48:GLU:CD	1:N:54:GLY:H	2.21	0.45
2:O:307:PHE:H	9:V:52:ARG:HG2	1.82	0.45
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.35	0.45
9:I:65:VAL:HG12	9:I:66:ALA:N	2.31	0.45
5:R:148:ALA:O	5:R:149:ASN:HB2	2.16	0.45
3:P:81:ARG:O	3:P:81:ARG:HD3	2.17	0.45
5:E:171:ILE:HG12	5:E:176:ALA:O	2.16	0.45
2:O:248:ASN:HD22	2:O:249:GLY:N	2.15	0.45
5:R:76:ILE:HD13	5:R:89:PHE:CE1	2.52	0.45
1:N:280:TYR:CG	1:N:281:ASP:N	2.85	0.45
3:P:350:ILE:O	3:P:354:MET:HG2	2.16	0.45
1:N:307:PHE:CD1	1:N:307:PHE:C	2.89	0.45
4:D:169:LEU:CD2	4:D:182:ILE:HD11	2.47	0.45
1:N:170:THR:CG2	1:N:171:THR:N	2.76	0.45
3:C:31:TRP:CZ3	11:C:2007:PEE:H20	2.51	0.45
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.46	0.45
1:N:86:PHE:CD1	1:N:99:ILE:HG12	2.52	0.45
4:D:234:LYS:HD2	5:E:8:PRO:HB2	1.99	0.45
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.97	0.45
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.52	0.45
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.98	0.45
1:A:307:PHE:C	1:A:307:PHE:CD1	2.90	0.45
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.57	0.45
5:R:185:TYR:CD2	5:R:185:TYR:N	2.85	0.45
1:N:433:ASP:CG	1:N:435:ASN:HB2	2.37	0.45
6:F:13:MET:O	6:F:17:ARG:HG3	2.17	0.45
3:C:9:HIS:CD2	3:C:12:LEU:HG	2.52	0.44
1:A:106:MET:CE	1:A:110:VAL:HG21	2.47	0.44
2:O:361:LYS:HA	2:O:402:ILE:HD11	1.99	0.44
3:C:41:CYS:SG	3:C:90:PHE:HD2	2.41	0.44
4:Q:40:CYS:SG	16:Q:501:HEC:HMC1	2.57	0.44
1:N:53:ASN:N	1:N:173:ASN:HD22	2.14	0.44
1:A:433:ASP:CG	1:A:435:ASN:HB2	2.37	0.44
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:246:PHE:C	3:P:248:PRO:HD3	2.37	0.44
2:B:38:LEU:HD12	2:B:38:LEU:C	2.36	0.44
8:H:28:GLU:CG	8:H:32:LYS:HE3	2.46	0.44
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	1.99	0.44
1:A:351:GLU:HA	1:A:354:VAL:HG22	1.99	0.44
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.53	0.44
3:P:75:GLN:HB2	5:R:61:SER:HA	1.98	0.44
4:D:200:GLN:HB2	18:D:2091:BOG:H3	1.99	0.44
1:N:62:LEU:HD11	1:N:127:ILE:HG12	2.00	0.44
2:O:76:THR:HG23	2:O:82:SER:HB2	1.99	0.44
5:E:136:VAL:HG23	5:E:181:GLU:O	2.17	0.44
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.43	0.44
10:J:7:ARG:NH1	10:J:7:ARG:CB	2.80	0.44
5:E:82:PRO:HG2	5:E:85:LYS:HB2	1.99	0.44
2:B:31:ASN:HD22	2:B:31:ASN:H	1.58	0.44
3:C:127:THR:O	3:C:130:VAL:HG22	2.18	0.44
4:Q:220:TYR:CZ	4:Q:224:ARG:HD3	2.52	0.44
1:N:294:LEU:HD11	1:N:334:MET:HE3	1.99	0.44
1:N:243:ALA:O	1:N:425:VAL:HA	2.17	0.44
3:P:271:PRO:HG2	3:P:276:LEU:HD23	2.00	0.44
2:O:206:LEU:HG	2:O:216:LEU:HD11	1.99	0.44
5:R:184:THR:O	5:R:185:TYR:HB3	2.17	0.44
5:R:76:ILE:HD12	5:R:98:VAL:HG21	2.00	0.44
5:R:76:ILE:HD13	5:R:89:PHE:CD1	2.52	0.44
2:B:209:ILE:HD12	2:B:379:LEU:HB2	2.00	0.44
1:N:191:LYS:CA	1:N:195:MET:HE2	2.47	0.44
3:C:147:ILE:HD11	13:C:2001:JZZ:HAB	1.98	0.44
2:O:297:GLN:O	2:O:301:LYS:HG3	2.17	0.44
1:N:239:SER:HB2	7:T:17:SER:O	2.17	0.44
5:R:110:ALA:HA	5:R:122:HIS:NE2	2.33	0.44
1:N:111:GLU:HG3	1:N:215:HIS:NE2	2.30	0.44
2:O:169:LYS:CG	2:O:240:TRP:HB2	2.47	0.44
2:O:374:THR:HB	2:O:377:GLY:H	1.81	0.44
1:A:53:ASN:N	1:A:173:ASN:ND2	2.65	0.44
5:E:150:SER:OG	5:E:157:TYR:HB3	2.18	0.44
4:Q:234:LYS:HD2	5:R:8:PRO:HB2	2.00	0.44
3:C:138:GLN:HB2	3:C:255:GLU:O	2.18	0.44
1:N:402:VAL:HG22	1:N:406:MET:HE1	2.00	0.44
1:N:85:HIS:HB2	1:N:100:LYS:HB2	2.00	0.44
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.47	0.44
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ASP:OD1	1:A:435:ASN:HB2	2.16	0.44
2:O:312:PHE:CZ	2:O:314:VAL:CG2	3.00	0.44
1:N:383:LEU:HD23	1:N:388:ARG:HA	1.98	0.44
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.48	0.44
2:B:24:LEU:O	2:B:24:LEU:HG	2.17	0.44
1:N:365:MET:HG3	1:N:366:VAL:N	2.33	0.44
5:E:76:ILE:HB	5:E:193:VAL:CG1	2.48	0.44
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.47	0.44
2:B:71:LEU:HD12	2:B:144:LEU:HD23	2.00	0.44
8:U:12:GLU:HG2	8:U:13:LEU:N	2.33	0.44
3:P:153:ALA:HB2	3:P:288:LYS:HG2	1.98	0.44
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.82	0.44
1:A:21:ASN:N	1:A:21:ASN:OD1	2.47	0.44
5:E:155:GLY:HA3	5:E:166:ASP:C	2.38	0.44
2:O:407:SER:O	2:O:411:VAL:HG23	2.17	0.44
1:A:111:GLU:HG3	1:A:215:HIS:NE2	2.33	0.44
2:O:247:GLN:NE2	2:O:429:ASP:HA	2.26	0.44
1:A:53:ASN:N	1:A:173:ASN:HD22	2.16	0.44
1:A:373:THR:HB	1:A:374:PRO:CD	2.47	0.44
5:E:178:TYR:H	5:E:178:TYR:HD1	1.66	0.44
3:C:28:ILE:HG12	3:C:225:TYR:OH	2.18	0.43
1:N:170:THR:CG2	1:N:171:THR:H	2.23	0.43
2:B:124:LEU:C	2:B:124:LEU:HD23	2.38	0.43
10:W:56:LYS:HB3	10:W:56:LYS:HE2	1.63	0.43
2:B:361:LYS:HA	2:B:402:ILE:HD11	1.99	0.43
4:D:54:VAL:HG11	4:D:192:TRP:NE1	2.33	0.43
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.53	0.43
3:C:34:PHE:HB2	20:C:381:HOH:O	2.18	0.43
5:R:112:VAL:HG11	5:R:170:ARG:NH2	2.34	0.43
1:A:122:LEU:HD11	1:A:186:ILE:HD12	2.00	0.43
5:E:130:PRO:HG2	5:E:131:GLU:OE1	2.18	0.43
3:C:263:LEU:O	3:C:264:VAL:CG2	2.66	0.43
3:C:246:PHE:C	3:C:248:PRO:HD3	2.37	0.43
8:U:58:LEU:HD12	8:U:58:LEU:O	2.18	0.43
2:O:59:THR:O	2:O:61:ALA:N	2.51	0.43
3:C:30:ALA:HB1	17:D:2003:CDL:H111	1.99	0.43
3:C:108:TYR:HB3	3:C:114:TRP:CE3	2.53	0.43
5:E:115:SER:CB	5:E:116:LYS:HD2	2.49	0.43
6:F:32:MET:HE3	6:F:87:LYS:HE2	2.00	0.43
3:P:207:ASN:ND2	3:P:208:ASN:H	2.16	0.43
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:SER:O	2:B:411:VAL:HG23	2.18	0.43
4:Q:109:LEU:HD12	4:Q:110:PRO:HD2	1.99	0.43
3:P:189:ALA:O	3:P:193:ILE:HG13	2.17	0.43
2:B:76:THR:CG2	2:B:82:SER:H	2.16	0.43
5:E:102:THR:C	5:E:103:GLN:HG3	2.39	0.43
5:E:187:PHE:O	5:E:189:GLY:N	2.50	0.43
2:B:402:ILE:O	2:B:405:VAL:HG23	2.19	0.43
4:D:27:ARG:NH1	4:D:55:THR:O	2.50	0.43
4:D:37:CYS:C	4:D:39:ALA:N	2.72	0.43
1:A:37:VAL:HG23	1:A:113:LEU:HD11	2.01	0.43
5:R:116:LYS:O	5:R:117:LEU:HD23	2.19	0.43
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.48	0.43
1:N:206:LYS:N	1:N:206:LYS:HD3	2.34	0.43
2:B:181:TYR:CD2	2:O:248:ASN:HA	2.54	0.43
5:R:112:VAL:HG11	5:R:170:ARG:CZ	2.48	0.43
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.49	0.43
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.82	0.43
4:Q:43:MET:HE3	4:Q:91:PHE:HE2	1.84	0.43
2:O:34:ILE:HD13	2:O:390:GLY:HA2	1.99	0.43
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.45	0.43
17:D:2003:CDL:HB22	7:G:40:ARG:HH21	1.84	0.43
2:B:104:LYS:C	2:B:104:LYS:HD2	2.39	0.43
2:O:54:GLY:O	2:O:56:ARG:N	2.51	0.43
4:D:239:PRO:HA	4:D:240:PRO:HD3	1.93	0.43
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.83	0.43
7:T:28:ASN:HB3	7:T:31:SER:OG	2.19	0.43
3:C:277:PHE:CG	3:C:278:ALA:N	2.86	0.43
5:E:171:ILE:HG23	5:E:171:ILE:O	2.18	0.43
1:N:106:MET:N	1:N:107:PRO:HD2	2.34	0.43
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.53	0.43
1:N:60:GLU:OE2	1:N:90:THR:HG22	2.18	0.43
4:D:29:GLY:HA3	4:D:189:PHE:HB2	2.01	0.43
2:O:259:THR:CG2	2:O:260:GLU:N	2.82	0.43
3:C:350:ILE:HG23	3:C:351:ILE:N	2.33	0.43
2:O:306:PRO:HA	9:V:52:ARG:CG	2.48	0.43
5:E:83:GLU:C	5:E:85:LYS:H	2.22	0.43
5:R:119:ASP:HB3	5:R:179:ASN:HD21	1.84	0.43
1:N:394:GLU:O	1:N:395:TRP:C	2.57	0.43
4:Q:169:LEU:HD22	4:Q:182:ILE:HD11	2.01	0.43
1:A:277:ILE:HD11	1:A:345:LEU:HD11	2.01	0.43
2:B:248:ASN:ND2	2:B:248:ASN:C	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:70:LEU:CD2	9:I:71:ASN:N	2.79	0.43
5:E:129:LYS:HB2	5:E:132:TRP:HB2	2.01	0.43
1:N:46:ARG:NH1	1:N:316:ASP:OD1	2.40	0.43
2:B:166:ALA:HB1	2:B:242:GLY:O	2.18	0.43
5:R:162:GLY:O	5:R:163:SER:C	2.56	0.43
3:P:101:ARG:CD	3:P:101:ARG:C	2.83	0.43
3:P:156:TYR:CD2	3:P:156:TYR:N	2.87	0.43
4:D:171:TYR:CD1	4:D:175:THR:HB	2.54	0.43
4:D:110:PRO:HA	4:D:111:PRO:HD2	1.83	0.43
1:A:436:ARG:HD2	1:A:436:ARG:HA	1.88	0.43
3:C:9:HIS:CD2	3:C:11:LEU:HB2	2.54	0.42
6:S:91:GLU:HB3	6:S:92:PRO:HD3	2.01	0.42
5:E:81:ILE:HG22	5:E:100:HIS:HB2	2.01	0.42
2:O:54:GLY:C	2:O:56:ARG:N	2.72	0.42
1:A:275:ALA:HB3	1:A:357:ALA:HB1	2.00	0.42
5:E:75:GLU:HB3	5:E:194:VAL:HG22	2.00	0.42
3:P:138:GLN:OE1	3:P:138:GLN:HA	2.19	0.42
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.37	0.42
4:D:162:PRO:HA	4:D:163:PRO:HD2	1.84	0.42
2:O:395:PRO:O	2:O:398:VAL:HG12	2.19	0.42
2:O:160:LEU:HB2	9:V:64:LEU:HD22	2.01	0.42
7:G:40:ARG:HD2	17:G:2004:CDL:OA4	2.19	0.42
1:N:402:VAL:HG13	1:N:406:MET:HE2	2.01	0.42
3:P:125:MET:CE	13:P:3001:JZZ:HAGA	2.49	0.42
1:A:382:HIS:HE1	1:A:390:ILE:HB	1.85	0.42
8:U:73:LEU:O	8:U:73:LEU:HD12	2.19	0.42
10:J:60:GLU:HA	10:J:60:GLU:OE2	2.19	0.42
5:E:52:LYS:CD	5:E:52:LYS:C	2.88	0.42
1:N:416:TYR:OH	1:N:442:TYR:HB2	2.19	0.42
3:P:130:VAL:HG23	3:P:183:HIS:HB2	2.01	0.42
3:C:272:GLU:O	3:C:273:TRP:C	2.56	0.42
3:C:109:LEU:HA	3:C:109:LEU:HD23	1.76	0.42
5:E:166:ASP:OD1	5:E:168:SER:N	2.45	0.42
11:C:2007:PEE:H50	17:G:2004:CDL:H712	2.01	0.42
6:S:60:PHE:O	6:S:64:ARG:HB2	2.19	0.42
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.19	0.42
2:B:395:PRO:HA	2:B:398:VAL:HG12	2.01	0.42
9:V:65:VAL:HG12	9:V:66:ALA:N	2.33	0.42
1:A:245:ASP:OD1	7:G:11:ARG:NE	2.47	0.42
2:O:50:PHE:CD1	2:O:50:PHE:N	2.88	0.42
1:A:178:THR:CG2	1:A:179:ARG:H	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:101:ARG:HH21	5:R:130:PRO:HA	1.84	0.42
1:N:106:MET:CG	1:N:203:ILE:HD13	2.46	0.42
1:N:351:GLU:HA	1:N:354:VAL:HG22	2.01	0.42
5:R:153:PHE:HE2	5:R:172:ARG:HH21	1.67	0.42
1:N:287:GLY:O	1:N:290:LEU:HG	2.19	0.42
5:E:49:TYR:CE1	10:J:32:GLU:HG3	2.54	0.42
8:H:43:ARG:NH1	8:H:43:ARG:HG2	2.34	0.42
2:O:68:LEU:HD23	2:O:186:ILE:HG21	2.00	0.42
1:N:10:ASN:HD21	2:O:19:PRO:HD2	1.80	0.42
5:R:155:GLY:HA3	5:R:166:ASP:C	2.39	0.42
1:N:369:LEU:HD11	1:N:392:LEU:HD21	2.00	0.42
1:A:369:LEU:HD11	1:A:392:LEU:HD21	2.02	0.42
1:N:95:THR:HG22	1:N:96:ALA:N	2.34	0.42
3:C:365:ILE:HG22	3:C:366:LEU:HD23	2.01	0.42
2:B:277:HIS:CD2	2:B:364:LEU:HD13	2.54	0.42
1:A:86:PHE:CD1	1:A:99:ILE:HG12	2.54	0.42
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.54	0.42
4:D:218:LEU:HD11	5:E:42:THR:HG22	2.01	0.42
10:J:42:ILE:HG22	10:J:46:LEU:HD12	2.02	0.42
2:B:334:GLY:O	2:B:338:ARG:HG2	2.20	0.42
5:E:127:VAL:O	5:E:128:LYS:HB2	2.20	0.42
5:R:100:HIS:HD2	5:R:131:GLU:O	2.02	0.42
5:R:81:ILE:HG12	5:R:87:VAL:CG2	2.49	0.42
1:N:382:HIS:HE1	1:N:390:ILE:HB	1.84	0.42
2:B:24:LEU:HD21	2:B:392:HIS:CD2	2.55	0.42
3:P:92:PHE:HA	3:P:95:ILE:HG22	2.02	0.42
1:N:89:TYR:O	1:N:95:THR:HG23	2.20	0.42
1:A:361:LEU:O	1:A:364:ALA:HB3	2.19	0.42
1:A:156:THR:HG23	1:A:157:ALA:N	2.35	0.42
2:B:270:ASN:O	2:B:274:VAL:HG23	2.19	0.42
3:P:131:GLY:HA3	3:P:183:HIS:CE1	2.54	0.42
1:A:62:LEU:HD11	1:A:127:ILE:HG12	2.01	0.42
3:P:345:GLU:C	3:P:349:ILE:HG13	2.38	0.42
3:C:182:LEU:HD23	3:C:182:LEU:HA	1.86	0.42
2:O:105:MET:HE2	2:O:107:TYR:HE1	1.84	0.42
7:T:72:LYS:NZ	8:U:57:GLU:OE1	2.53	0.42
2:B:35:ILE:HD13	2:B:217:LYS:HA	2.00	0.42
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.31	0.42
2:B:50:PHE:HD1	2:B:50:PHE:N	2.18	0.42
3:P:286:PRO:O	3:P:287:ASN:HB2	2.19	0.42
3:P:277:PHE:CG	3:P:278:ALA:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:48:VAL:O	7:T:51:PRO:HD2	2.19	0.42
10:W:60:GLU:CG	10:W:60:GLU:O	2.65	0.42
3:C:37:LEU:HD21	3:C:233:LEU:HA	2.01	0.42
2:O:96:LEU:HB3	9:V:70:LEU:HD22	2.01	0.42
9:V:70:LEU:CD2	9:V:71:ASN:OD1	2.68	0.42
5:E:149:ASN:HD22	5:E:149:ASN:N	2.17	0.42
9:V:52:ARG:HG3	9:V:52:ARG:NH1	2.33	0.42
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.54	0.42
4:D:70:VAL:HG21	4:D:83:ARG:NH2	2.34	0.42
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.81	0.42
1:N:417:ASP:O	1:N:438:ARG:NH2	2.53	0.42
4:D:98:PRO:HG2	4:D:99:GLU:OE1	2.20	0.42
7:G:80:ASP:O	7:G:81:GLN:C	2.58	0.42
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.54	0.42
2:B:76:THR:HG23	2:B:82:SER:HB2	2.02	0.42
2:O:222:GLN:O	2:O:223:PHE:CD2	2.73	0.42
5:R:83:GLU:CD	5:R:102:THR:HA	2.39	0.42
1:N:113:LEU:O	1:N:116:VAL:N	2.49	0.42
5:E:162:GLY:O	5:E:163:SER:C	2.58	0.42
2:O:291:VAL:C	2:O:293:SER:H	2.23	0.42
2:B:59:THR:C	2:B:61:ALA:N	2.71	0.42
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.84	0.42
6:S:58:ARG:HD2	6:S:89:TYR:OH	2.20	0.42
2:O:166:ALA:HB1	2:O:242:GLY:O	2.20	0.42
4:D:150:ASN:O	4:D:156:GLN:HA	2.20	0.42
4:D:102:ARG:NH1	4:D:102:ARG:HG2	2.35	0.42
3:C:198:LEU:HD21	12:C:502:HEM:CMA	2.49	0.42
3:C:98:HIS:CD2	12:C:502:HEM:NC	2.87	0.42
2:B:385:GLU:HB3	2:B:391:THR:O	2.20	0.42
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.82	0.42
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.60	0.42
5:R:76:ILE:HB	5:R:193:VAL:CG1	2.50	0.41
3:P:18:SER:CB	3:P:202:HIS:HE1	2.32	0.41
2:B:206:LEU:HG	2:B:206:LEU:O	2.20	0.41
3:P:132:TYR:HD2	13:P:3001:JZZ:H27A	1.85	0.41
1:A:383:LEU:HD23	1:A:388:ARG:HA	2.02	0.41
4:Q:27:ARG:NH1	4:Q:55:THR:O	2.49	0.41
1:A:154:HIS:O	1:A:156:THR:N	2.53	0.41
3:P:75:GLN:O	3:P:76:TYR:HB2	2.20	0.41
10:W:42:ILE:HG22	10:W:46:LEU:HD12	2.02	0.41
8:U:52:GLU:HG2	8:U:53:GLN:N	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:LEU:C	3:C:20:ILE:HG13	2.41	0.41
3:C:31:TRP:NE1	11:C:2007:PEE:O4	2.54	0.41
2:B:54:GLY:C	2:B:56:ARG:N	2.73	0.41
3:C:78:TRP:CZ3	4:D:201:ARG:HG3	2.56	0.41
1:N:261:GLY:HA2	1:N:317:THR:O	2.20	0.41
2:B:287:ARG:HB3	9:I:53:GLU:HG3	2.02	0.41
1:A:27:SER:HA	1:A:199:ALA:O	2.20	0.41
1:A:64:PHE:HE2	1:A:86:PHE:CE1	2.38	0.41
3:C:18:SER:HB2	3:C:202:HIS:HE1	1.85	0.41
7:G:56:TYR:O	7:G:59:TYR:HB3	2.20	0.41
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.54	0.41
3:P:235:LEU:HD23	3:P:235:LEU:HA	1.84	0.41
2:O:248:ASN:ND2	2:O:250:HIS:H	2.18	0.41
1:N:37:VAL:HG23	1:N:113:LEU:HD11	2.02	0.41
3:P:31:TRP:CH2	17:T:3004:CDL:H512	2.54	0.41
2:B:54:GLY:O	2:B:56:ARG:N	2.53	0.41
2:O:56:ARG:HA	2:O:171:ALA:O	2.20	0.41
2:B:345:LYS:HG2	2:B:418:VAL:HG11	2.01	0.41
4:Q:183:ALA:O	4:Q:186:VAL:HG12	2.20	0.41
2:B:163:LEU:C	2:B:165:ALA:N	2.74	0.41
7:T:35:PRO:O	7:T:38:TRP:HB3	2.19	0.41
3:P:25:PRO:HB2	3:P:28:ILE:HG23	2.03	0.41
2:O:206:LEU:O	2:O:206:LEU:HG	2.19	0.41
1:N:402:VAL:HG22	1:N:406:MET:HE2	2.00	0.41
3:C:233:LEU:O	3:C:237:LEU:HB2	2.20	0.41
4:Q:10:PHE:CD1	4:Q:10:PHE:N	2.89	0.41
1:N:79:VAL:O	1:N:82:MET:HG2	2.20	0.41
4:D:169:LEU:HD22	4:D:182:ILE:HD11	2.02	0.41
5:E:178:TYR:CD1	5:E:178:TYR:N	2.89	0.41
3:C:247:SER:N	3:C:248:PRO:HD3	2.34	0.41
8:H:43:ARG:HH11	8:H:43:ARG:HG2	1.86	0.41
5:R:73:LYS:HB3	5:R:196:GLY:O	2.20	0.41
3:C:339:ILE:HA	3:C:339:ILE:HD13	1.92	0.41
6:F:84:GLU:CD	6:F:84:GLU:H	2.23	0.41
8:U:65:ARG:O	8:U:68:CYS:HB3	2.20	0.41
5:R:171:ILE:N	5:R:179:ASN:OD1	2.46	0.41
2:B:153:GLN:NE2	9:I:34:UNK:HB1	2.35	0.41
1:N:402:VAL:HA	1:N:406:MET:HE1	2.02	0.41
3:P:146:VAL:HG12	3:P:147:ILE:N	2.35	0.41
1:N:130:GLU:O	1:N:134:ILE:HG13	2.19	0.41
2:B:59:THR:HG22	2:B:60:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:218:LEU:HD11	5:R:42:THR:HG22	2.01	0.41
4:Q:16:GLY:N	4:Q:19:SER:OG	2.54	0.41
1:N:114:ALA:O	1:N:118:GLN:HB2	2.20	0.41
2:B:33:LEU:CD2	2:B:224:LEU:HD12	2.49	0.41
2:B:128:THR:O	2:B:226:ILE:HD11	2.20	0.41
5:R:171:ILE:HB	5:R:178:TYR:O	2.20	0.41
1:N:106:MET:HE1	1:N:208:LEU:HA	2.02	0.41
2:B:153:GLN:HE22	9:I:34:UNK:HB1	1.85	0.41
3:C:101:ARG:CD	3:C:101:ARG:C	2.89	0.41
1:N:154:HIS:C	1:N:156:THR:N	2.74	0.41
3:P:78:TRP:CZ3	4:Q:201:ARG:HG3	2.56	0.41
3:P:172:ASP:OD1	3:P:173:ASN:N	2.51	0.41
1:N:373:THR:HB	1:N:374:PRO:CD	2.51	0.41
4:D:9:ALA:HA	4:D:125:ASP:OD1	2.20	0.41
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.54	0.41
2:O:152:PHE:HA	2:O:157:VAL:CG1	2.50	0.41
2:O:35:ILE:O	2:O:213:HIS:HE1	2.03	0.41
2:O:18:CYS:CB	2:O:19:PRO:CD	2.93	0.41
2:B:223:PHE:O	2:B:225:ASN:N	2.54	0.41
1:N:390:ILE:HG23	1:N:394:GLU:CD	2.41	0.41
1:A:133:VAL:O	1:A:137:GLU:HG3	2.20	0.41
3:C:172:ASP:HB3	3:C:174:PRO:HD2	2.02	0.41
4:D:239:PRO:HG2	4:D:241:LYS:HB2	2.02	0.41
4:D:169:LEU:HD23	4:D:169:LEU:O	2.20	0.41
2:B:146:VAL:O	2:B:149:ALA:N	2.53	0.41
6:S:32:MET:O	6:S:35:ASP:HB2	2.20	0.41
4:Q:70:VAL:HG21	4:Q:83:ARG:NH2	2.35	0.41
1:A:404:ALA:O	1:A:405:ARG:C	2.59	0.41
5:R:130:PRO:C	5:R:132:TRP:H	2.24	0.41
2:O:43:PRO:O	2:O:113:ARG:HG3	2.20	0.41
2:B:207:VAL:HG21	2:B:383:GLY:HA3	2.03	0.41
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.51	0.41
2:O:207:VAL:HG12	2:O:208:GLY:N	2.36	0.41
4:D:169:LEU:HD23	4:D:169:LEU:C	2.40	0.41
1:A:240:GLU:HA	1:A:422:LEU:O	2.21	0.41
6:F:31:LEU:HD21	6:F:65:ALA:HB2	2.03	0.41
4:D:158:ILE:HG12	4:D:160:MET:H	1.85	0.41
6:F:71:LYS:O	6:F:72:HIS:HB2	2.21	0.41
5:R:96:LEU:HD21	5:R:195:VAL:HG21	2.01	0.41
10:W:52:TRP:O	10:W:56:LYS:HB2	2.20	0.41
5:E:153:PHE:HE2	5:E:172:ARG:HH21	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:98:HIS:CD2	12:P:502:HEM:NC	2.89	0.41
3:C:287:ASN:O	3:C:288:LYS:C	2.58	0.41
4:Q:169:LEU:O	4:Q:169:LEU:HD23	2.20	0.41
4:D:239:PRO:C	4:D:241:LYS:N	2.74	0.41
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.20	0.41
2:O:59:THR:C	2:O:61:ALA:N	2.73	0.41
1:A:439:SER:HA	1:A:442:TYR:CE2	2.56	0.41
5:E:137:GLY:O	5:E:145:VAL:HG13	2.20	0.41
6:F:21:TYR:CG	6:F:83:TYR:HD1	2.39	0.41
4:Q:34:LYS:HG2	4:Q:34:LYS:O	2.20	0.41
6:F:70:LEU:HD12	6:F:70:LEU:C	2.40	0.41
3:C:136:TRP:HH2	3:C:171:VAL:HG12	1.86	0.41
7:G:34:LEU:HB2	7:G:35:PRO:HD3	2.03	0.41
1:A:32:GLN:HE22	2:B:373:GLU:HA	1.85	0.41
2:O:399:ALA:O	2:O:402:ILE:CG2	2.68	0.41
2:B:35:ILE:HD11	2:B:220:ALA:HB3	2.03	0.41
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.54	0.41
3:P:6:ARG:HD3	3:P:16:ASN:OD1	2.21	0.41
4:Q:161:ALA:O	4:Q:162:PRO:C	2.60	0.41
3:C:223:PRO:O	3:C:227:PHE:HD2	2.04	0.41
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.51	0.41
2:O:274:VAL:O	2:O:278:VAL:HG23	2.21	0.41
2:B:73:SER:N	2:B:74:PRO:HD2	2.36	0.41
2:O:341:MET:HE2	2:O:341:MET:HA	2.02	0.40
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.36	0.40
2:O:38:LEU:HD12	2:O:38:LEU:C	2.41	0.40
2:B:84:ARG:HG3	6:S:107:TRP:CZ3	2.56	0.40
2:B:292:THR:CG2	2:B:292:THR:O	2.68	0.40
4:Q:240:PRO:O	4:Q:241:LYS:C	2.59	0.40
1:A:134:ILE:HG21	1:A:174:ILE:HD13	2.02	0.40
5:R:33:LYS:HG2	7:T:21:PHE:CD1	2.56	0.40
4:Q:95:TYR:HA	4:Q:96:PRO:HD3	1.87	0.40
4:Q:99:GLU:H	4:Q:99:GLU:CD	2.24	0.40
5:R:171:ILE:HG12	5:R:176:ALA:O	2.21	0.40
2:B:259:THR:CG2	2:B:260:GLU:N	2.84	0.40
1:N:373:THR:N	1:N:374:PRO:HD2	2.36	0.40
1:N:64:PHE:HE2	1:N:86:PHE:CE1	2.38	0.40
4:Q:197:GLU:O	4:Q:198:HIS:C	2.59	0.40
4:Q:200:GLN:NE2	18:Q:3091:BOG:H5	2.36	0.40
11:E:2005:PEE:H13	11:E:2005:PEE:H8	2.03	0.40
11:R:3005:PEE:H13	11:R:3005:PEE:H8	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:37:SER:CB	2:O:213:HIS:ND1	2.69	0.40
1:A:395:TRP:O	1:A:399:ILE:HG13	2.20	0.40
2:O:207:VAL:HG21	2:O:383:GLY:HA3	2.03	0.40
4:D:97:ASN:HB2	4:D:98:PRO:HD2	2.03	0.40
3:P:64:PHE:CE1	15:P:3011:GOL:H12	2.56	0.40
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.57	0.40
3:P:120:LEU:HA	3:P:120:LEU:HD23	1.80	0.40
2:O:181:TYR:CD1	2:O:182:ARG:HG3	2.55	0.40
10:W:7:ARG:NH1	10:W:7:ARG:CB	2.83	0.40
5:R:106:ILE:HG21	5:R:130:PRO:HB3	2.04	0.40
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.50	0.40
5:R:171:ILE:O	5:R:171:ILE:HG23	2.22	0.40
2:O:104:LYS:HD2	2:O:104:LYS:C	2.42	0.40
7:G:40:ARG:CB	17:G:2004:CDL:HA32	2.52	0.40
4:D:102:ARG:HB3	4:D:107:GLY:HA2	2.02	0.40
2:B:325:TYR:CD2	2:B:325:TYR:C	2.95	0.40
3:C:98:HIS:CE1	12:C:502:HEM:NA	2.89	0.40
7:G:35:PRO:O	7:G:38:TRP:HB3	2.22	0.40
5:E:10:PHE:CB	7:G:18:LEU:HD11	2.51	0.40
1:N:246:ASP:HA	1:N:427:PRO:HB3	2.03	0.40
3:P:182:LEU:HA	3:P:182:LEU:HD23	1.85	0.40
5:E:125:ASP:C	5:E:126:ARG:HG3	2.42	0.40
5:E:126:ARG:O	5:E:127:VAL:CG2	2.69	0.40
1:A:63:ALA:O	1:A:116:VAL:HG13	2.21	0.40
1:N:342:TRP:O	1:N:345:LEU:HB2	2.21	0.40
2:B:292:THR:HG21	2:B:363:GLN:NE2	2.36	0.40
3:C:101:ARG:O	3:C:101:ARG:HD2	2.21	0.40
1:N:23:LEU:HD23	1:N:24:ARG:N	2.37	0.40
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.56	0.40
4:D:203:ARG:NH1	18:D:2091:BOG:O3	2.54	0.40
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.57	0.40
8:U:52:GLU:CG	8:U:53:GLN:N	2.84	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	442/446 (99%)	388 (88%)	46 (10%)	8 (2%)	11 42
1	N	440/446 (99%)	386 (88%)	45 (10%)	9 (2%)	9 38
2	B	418/441 (95%)	342 (82%)	56 (13%)	20 (5%)	3 15
2	O	420/441 (95%)	355 (84%)	51 (12%)	14 (3%)	5 24
3	C	378/380 (100%)	347 (92%)	28 (7%)	3 (1%)	24 64
3	P	377/380 (99%)	345 (92%)	26 (7%)	6 (2%)	12 45
4	D	239/241 (99%)	215 (90%)	22 (9%)	2 (1%)	24 64
4	Q	239/241 (99%)	213 (89%)	22 (9%)	4 (2%)	11 43
5	E	194/196 (99%)	150 (77%)	31 (16%)	13 (7%)	1 7
5	R	194/196 (99%)	156 (80%)	26 (13%)	12 (6%)	2 10
6	F	99/110 (90%)	94 (95%)	5 (5%)	0	100 100
6	S	99/110 (90%)	89 (90%)	10 (10%)	0	100 100
7	G	78/81 (96%)	68 (87%)	9 (12%)	1 (1%)	15 51
7	T	77/81 (95%)	66 (86%)	10 (13%)	1 (1%)	15 51
8	H	68/77 (88%)	65 (96%)	3 (4%)	0	100 100
8	U	65/77 (84%)	59 (91%)	4 (6%)	2 (3%)	5 26
9	I	29/47 (62%)	26 (90%)	2 (7%)	1 (3%)	5 23
9	V	29/47 (62%)	25 (86%)	4 (14%)	0	100 100
10	J	59/61 (97%)	58 (98%)	1 (2%)	0	100 100
10	W	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	11 43
All	All	4002/4160 (96%)	3500 (88%)	405 (10%)	97 (2%)	7 33

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
1	A	433	ASP
2	B	21	ALA
2	B	24	LEU
2	B	26	ILE
2	B	29	LEU
2	B	171	ALA

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Mol	Chain	Res	Type
2	B	226	ILE
2	B	228	SER
2	B	231	GLY
3	C	287	ASN
5	E	80	ASP
5	E	102	THR
5	E	127	VAL
5	E	128	LYS
1	N	282	ARG
1	N	433	ASP
2	O	26	ILE
2	O	171	ALA
2	O	228	SER
3	P	287	ASN
4	Q	3	LEU
8	U	49	HIS
10	W	61	ALA
1	A	72	CYS
1	A	218	GLY
2	B	224	LEU
2	B	371	SER
2	B	386	ALA
4	D	38	SER
5	E	130	PRO
5	E	163	SER
5	E	177	PRO
5	E	191	ASP
1	N	218	GLY
1	N	262	TRP
2	O	222	GLN
2	O	231	GLY
2	O	371	SER
2	O	386	ALA
5	R	137	GLY
5	R	154	GLY
5	R	163	SER
5	R	185	TYR
8	U	52	GLU
1	A	155	ALA
1	A	262	TRP
2	B	60	THR
2	B	221	GLU

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Mol	Chain	Res	Type
2	B	222	GLN
5	E	137	GLY
5	E	166	ASP
1	N	72	CYS
1	N	155	ALA
2	O	319	SER
4	Q	38	SER
4	Q	177	ALA
5	R	127	VAL
5	R	186	GLN
5	R	191	ASP
2	B	55	SER
2	B	389	SER
2	B	420	GLY
1	N	81	SER
1	N	443	TRP
2	O	19	PRO
2	O	55	SER
2	O	60	THR
3	P	156	TYR
3	P	274	TYR
4	Q	198	HIS
5	R	166	ASP
5	R	190	ASP
7	T	33	ALA
1	A	443	TRP
2	B	201	SER
5	E	120	PRO
5	E	154	GLY
5	E	186	GLN
7	G	33	ALA
1	N	206	LYS
2	O	389	SER
3	P	3	PRO
5	R	113	ASP
1	A	404	ALA
2	B	319	SER
3	C	3	PRO
5	R	120	PRO
3	C	264	VAL
3	P	157	ILE
2	B	208	GLY

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Mol	Chain	Res	Type
2	O	208	GLY
3	P	264	VAL
4	D	162	PRO
9	I	76	VAL
2	O	420	GLY
5	R	177	PRO

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%)	354 (97%)	11 (3%)	48 82
1	N	365/368 (99%)	351 (96%)	14 (4%)	40 77
2	B	331/347 (95%)	315 (95%)	16 (5%)	31 70
2	O	333/347 (96%)	319 (96%)	14 (4%)	36 74
3	C	328/329 (100%)	323 (98%)	5 (2%)	72 91
3	P	328/329 (100%)	324 (99%)	4 (1%)	78 93
4	D	200/200 (100%)	195 (98%)	5 (2%)	55 85
4	Q	200/200 (100%)	196 (98%)	4 (2%)	63 88
5	E	166/166 (100%)	160 (96%)	6 (4%)	42 78
5	R	165/166 (99%)	161 (98%)	4 (2%)	57 86
6	F	93/96 (97%)	89 (96%)	4 (4%)	35 73
6	S	93/96 (97%)	87 (94%)	6 (6%)	21 56
7	G	71/71 (100%)	70 (99%)	1 (1%)	74 92
7	T	70/71 (99%)	69 (99%)	1 (1%)	74 92
8	H	65/71 (92%)	64 (98%)	1 (2%)	72 91
8	U	63/71 (89%)	61 (97%)	2 (3%)	46 81
9	I	23/26 (88%)	21 (91%)	2 (9%)	13 41
9	V	23/26 (88%)	21 (91%)	2 (9%)	13 41
10	J	49/49 (100%)	48 (98%)	1 (2%)	63 88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	W	47/49 (96%)	45 (96%)	2 (4%)	35 73
All	All	3378/3446 (98%)	3273 (97%)	105 (3%)	47 82

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	58	PHE
1	A	86	PHE
1	A	106	MET
1	A	179	ARG
1	A	281	ASP
1	A	307	PHE
1	A	395	TRP
1	A	405	ARG
1	A	432	LEU
1	A	443	TRP
2	B	23	ASP
2	B	31	ASN
2	B	50	PHE
2	B	97	SER
2	B	104	LYS
2	B	124	LEU
2	B	154	SER
2	B	170	THR
2	B	225	ASN
2	B	248	ASN
2	B	250	HIS
2	B	296	TYR
2	B	325	TYR
2	B	341	MET
2	B	343	GLN
2	B	402	ILE
3	C	81	ARG
3	C	91	PHE
3	C	149	ASN
3	C	184	PHE
3	C	216	SER
4	D	43	MET
4	D	70	VAL
4	D	130	LEU
4	D	169	LEU

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Mol	Chain	Res	Type
4	D	203	ARG
5	E	6	THR
5	E	52	LYS
5	E	60	SER
5	E	102	THR
5	E	131	GLU
5	E	185	TYR
6	F	58	ARG
6	F	64	ARG
6	F	70	LEU
6	F	78	GLU
7	G	4	PHE
8	H	21	ARG
9	I	68	ILE
9	I	71	ASN
10	J	59	TYR
1	N	3	THR
1	N	18	THR
1	N	49	ASN
1	N	58	PHE
1	N	86	PHE
1	N	106	MET
1	N	179	ARG
1	N	223	TYR
1	N	281	ASP
1	N	307	PHE
1	N	395	TRP
1	N	405	ARG
1	N	432	LEU
1	N	443	TRP
2	O	18	CYS
2	O	19	PRO
2	O	31	ASN
2	O	97	SER
2	O	104	LYS
2	O	124	LEU
2	O	154	SER
2	O	248	ASN
2	O	250	HIS
2	O	296	TYR
2	O	325	TYR
2	O	341	MET

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Mol	Chain	Res	Type
2	O	343	GLN
2	O	402	ILE
3	P	81	ARG
3	P	91	PHE
3	P	149	ASN
3	P	216	SER
4	Q	43	MET
4	Q	70	VAL
4	Q	130	LEU
4	Q	169	LEU
5	R	52	LYS
5	R	60	SER
5	R	178	TYR
5	R	185	TYR
6	S	13	MET
6	S	14	ASP
6	S	58	ARG
6	S	64	ARG
6	S	70	LEU
6	S	78	GLU
7	T	4	PHE
8	U	21	ARG
8	U	49	HIS
9	V	58	ARG
9	V	68	ILE
10	W	59	TYR
10	W	60	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	85	HIS
1	A	173	ASN
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	247	GLN
2	B	248	ASN

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Mol	Chain	Res	Type
2	B	276	GLN
2	B	297	GLN
2	B	329	GLN
2	B	343	GLN
2	B	362	ASN
2	B	363	GLN
3	C	9	HIS
3	C	69	HIS
3	C	82	ASN
3	C	207	ASN
3	C	313	GLN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	148	HIS
5	E	57	GLN
5	E	122	HIS
5	E	149	ASN
5	E	164	HIS
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
9	I	71	ASN
1	N	32	GLN
1	N	118	GLN
1	N	143	ASN
1	N	173	ASN
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
2	O	31	ASN
2	O	153	GLN
2	O	156	GLN
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	297	GLN
2	O	329	GLN
2	O	343	GLN
2	O	362	ASN
2	O	363	GLN
3	P	9	HIS

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Mol	Chain	Res	Type
3	P	69	HIS
3	P	82	ASN
3	P	207	ASN
3	P	313	GLN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	148	HIS
4	Q	200	GLN
5	R	57	GLN
5	R	107	ASN
5	R	164	HIS
5	R	186	GLN
7	T	12	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN
8	U	71	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

29 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	PEE	A	2008	-	20,20,50	1.87	6 (30%)	21,25,55	0.68	0
13	JZZ	C	2001	-	22,27,27	3.68	5 (22%)	26,40,40	2.02	4 (15%)
14	UQ	C	2002	-	19,19,63	2.58	11 (57%)	23,26,79	1.33	3 (13%)
11	PEE	C	2007	-	48,48,50	1.33	8 (16%)	49,53,55	0.92	5 (10%)
15	GOL	C	2011	-	5,5,5	1.39	0	5,5,5	0.71	0
12	HEM	C	501	3	30,50,50	2.67	9 (30%)	24,82,82	2.40	9 (37%)
12	HEM	C	502	3	30,50,50	2.50	6 (20%)	24,82,82	2.18	7 (29%)
17	CDL	D	2003	-	41,41,99	1.20	3 (7%)	43,53,111	1.01	2 (4%)
18	BOG	D	2009	-	20,20,20	0.97	2 (10%)	25,25,25	0.92	2 (8%)
18	BOG	D	2091	-	13,13,20	1.34	2 (15%)	18,18,25	1.05	2 (11%)
16	HEC	D	501	4	24,50,50	2.90	4 (16%)	19,82,82	3.16	5 (26%)
11	PEE	E	2005	-	49,49,50	1.47	9 (18%)	50,54,55	0.99	5 (10%)
19	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
17	CDL	G	2004	-	39,39,99	1.20	2 (5%)	41,51,111	1.13	5 (12%)
18	BOG	P	2010	-	12,12,20	1.54	4 (33%)	17,17,25	0.71	0
13	JZZ	P	3001	-	22,27,27	3.82	5 (22%)	26,40,40	2.14	4 (15%)
14	UQ	P	3002	-	19,19,63	2.48	11 (57%)	23,26,79	1.32	3 (13%)
11	PEE	P	3007	-	48,48,50	1.29	7 (14%)	49,53,55	0.89	4 (8%)
11	PEE	P	3008	-	4,4,50	3.78	3 (75%)	6,6,55	0.54	0
15	GOL	P	3011	-	5,5,5	1.26	0	5,5,5	0.57	0
12	HEM	P	501	3	30,50,50	2.84	10 (33%)	24,82,82	2.13	7 (29%)
12	HEM	P	502	3	30,50,50	2.81	10 (33%)	24,82,82	2.16	6 (25%)
17	CDL	Q	3003	-	41,41,99	1.20	2 (4%)	43,53,111	1.05	3 (6%)
18	BOG	Q	3009	-	20,20,20	0.96	1 (5%)	25,25,25	0.92	2 (8%)
18	BOG	Q	3091	-	13,13,20	1.47	3 (23%)	18,18,25	1.12	2 (11%)
16	HEC	Q	501	4	24,50,50	2.43	2 (8%)	19,82,82	3.19	5 (26%)
11	PEE	R	3005	-	49,49,50	1.48	10 (20%)	50,54,55	0.98	5 (10%)
19	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
17	CDL	T	3004	-	39,39,99	1.20	2 (5%)	41,51,111	1.14	4 (9%)

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

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

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	3001	JZZ	N4-N5	-13.26	1.23	1.37
13	C	2001	JZZ	N4-N5	-12.72	1.24	1.37
13	P	3001	JZZ	CAN-N2	-10.49	1.33	1.45
13	C	2001	JZZ	CAN-N2	-10.17	1.33	1.45
16	D	501	HEC	C3B-C2B	-9.62	1.30	1.40
16	D	501	HEC	C3C-C2C	-9.28	1.31	1.40
16	Q	501	HEC	C3B-C2B	-8.30	1.32	1.40
12	C	502	HEM	C3C-CAC	-7.66	1.37	1.51
12	P	502	HEM	C3C-CAC	-7.33	1.37	1.51
16	Q	501	HEC	C3C-C2C	-7.31	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	P	501	HEM	C3B-CAB	-6.77	1.38	1.51
12	P	502	HEM	C3B-CAB	-6.75	1.38	1.51
12	C	502	HEM	C3B-CAB	-6.45	1.39	1.51
12	C	501	HEM	C3B-CAB	-6.34	1.39	1.51
12	P	502	HEM	C2D-C3D	-6.30	1.35	1.54
12	P	501	HEM	C3C-CAC	-6.23	1.39	1.51
12	C	501	HEM	C2D-C3D	-6.14	1.36	1.54
12	P	501	HEM	C2D-C3D	-5.80	1.37	1.54
12	C	502	HEM	C2D-C3D	-5.69	1.37	1.54
12	C	501	HEM	C3C-CAC	-5.35	1.41	1.51
12	P	501	HEM	C3B-C4B	-5.33	1.47	1.51
12	C	501	HEM	C2C-C1C	-4.37	1.44	1.52
12	P	502	HEM	C3B-C4B	-4.27	1.48	1.51
12	P	501	HEM	C2C-C1C	-3.91	1.45	1.52
12	P	502	HEM	C2C-C1C	-3.64	1.45	1.52
12	C	501	HEM	C3D-C4D	-3.63	1.46	1.51
12	C	501	HEM	C3B-C4B	-3.44	1.48	1.51
12	P	501	HEM	C3D-C4D	-3.12	1.47	1.51
11	E	2005	PEE	C19-C18	-2.95	1.34	1.51
11	P	3007	PEE	C22-C21	-2.92	1.34	1.51
11	R	3005	PEE	C19-C18	-2.83	1.35	1.51
13	P	3001	JZZ	CAN-CAM	-2.72	1.39	1.43
11	P	3007	PEE	C19-C18	-2.70	1.35	1.51
11	E	2005	PEE	C22-C21	-2.67	1.36	1.51
11	C	2007	PEE	C22-C21	-2.67	1.36	1.51
11	R	3005	PEE	C22-C21	-2.67	1.36	1.51
11	C	2007	PEE	C19-C18	-2.62	1.36	1.51
13	C	2001	JZZ	CAN-CAM	-2.52	1.39	1.43
16	D	501	HEC	C1D-CHD	-2.44	1.33	1.39
12	P	502	HEM	C3D-C4D	-2.42	1.48	1.51
12	P	502	HEM	C2D-C1D	-2.38	1.44	1.51
12	P	501	HEM	C2D-C1D	-2.17	1.44	1.51
13	P	3001	JZZ	O3-C3	2.01	1.36	1.33
11	C	2007	PEE	P-O2P	2.01	1.63	1.54
16	D	501	HEC	C1A-NA	2.02	1.39	1.36
18	P	2010	BOG	C4-C3	2.02	1.57	1.52
17	D	2003	CDL	OA6-CA5	2.03	1.40	1.34
17	G	2004	CDL	O1-C1	2.04	1.49	1.43
18	Q	3091	BOG	O5-C5	2.05	1.49	1.44
18	D	2009	BOG	C1-C2	2.10	1.58	1.52
11	P	3007	PEE	C31-C30	2.13	1.57	1.50
13	C	2001	JZZ	O3-C3	2.15	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	3007	PEE	C3-C2	2.18	1.56	1.50
17	D	2003	CDL	O1-C1	2.18	1.50	1.43
17	T	3004	CDL	O1-C1	2.19	1.50	1.43
17	D	2003	CDL	CA3-CA4	2.20	1.56	1.50
11	A	2008	PEE	C11-C10	2.22	1.57	1.50
11	C	2007	PEE	C31-C30	2.22	1.57	1.50
17	Q	3003	CDL	O1-C1	2.24	1.50	1.43
14	P	3002	UQ	O2-C2	2.25	1.42	1.37
11	R	3005	PEE	O2-C2	2.33	1.52	1.46
18	D	2009	BOG	O5-C1	2.36	1.47	1.41
14	P	3002	UQ	C8-C9	2.37	1.37	1.33
18	Q	3009	BOG	O5-C1	2.37	1.47	1.41
18	D	2091	BOG	O5-C1	2.37	1.47	1.41
11	R	3005	PEE	C31-C30	2.38	1.57	1.50
14	C	2002	UQ	C8-C9	2.38	1.37	1.33
17	Q	3003	CDL	CA3-CA4	2.40	1.57	1.50
17	T	3004	CDL	CB3-CB4	2.40	1.57	1.50
14	P	3002	UQ	C5-C4	2.40	1.56	1.47
11	E	2005	PEE	C11-C10	2.41	1.57	1.50
11	C	2007	PEE	C3-C2	2.43	1.57	1.50
11	E	2005	PEE	C1-C2	2.47	1.57	1.50
14	P	3002	UQ	CM5-C5	2.49	1.56	1.50
18	Q	3091	BOG	C4-C5	2.49	1.58	1.53
18	D	2091	BOG	C4-C5	2.49	1.58	1.53
17	G	2004	CDL	CB3-CB4	2.50	1.57	1.50
14	P	3002	UQ	C3-C4	2.51	1.56	1.48
14	C	2002	UQ	C3-C4	2.51	1.56	1.48
18	P	2010	BOG	O5-C1	2.54	1.47	1.43
18	P	2010	BOG	C4-C5	2.55	1.58	1.53
14	C	2002	UQ	C5-C4	2.55	1.57	1.47
11	E	2005	PEE	C31-C30	2.56	1.58	1.50
14	C	2002	UQ	O2-C2	2.58	1.43	1.37
18	P	2010	BOG	C1-C2	2.60	1.57	1.52
11	A	2008	PEE	C3-C2	2.64	1.58	1.50
11	P	3007	PEE	P-O1P	2.64	1.60	1.51
11	C	2007	PEE	O2-C10	2.66	1.42	1.34
14	C	2002	UQ	C7-C8	2.66	1.54	1.50
11	R	3005	PEE	C1-C2	2.67	1.58	1.50
12	C	502	HEM	C4C-NC	2.67	1.39	1.36
13	C	2001	JZZ	CAJ-CAI	2.68	1.22	1.19
11	R	3005	PEE	C3-C2	2.73	1.58	1.50
18	Q	3091	BOG	O5-C1	2.73	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	3002	UQ	C7-C8	2.74	1.55	1.50
14	P	3002	UQ	C2-C1	2.74	1.56	1.48
11	R	3005	PEE	C11-C10	2.74	1.58	1.50
11	P	3008	PEE	P-O3P	2.80	1.64	1.54
11	C	2007	PEE	P-O1P	2.81	1.61	1.51
12	C	501	HEM	C4C-NC	2.82	1.39	1.36
14	C	2002	UQ	CM5-C5	2.85	1.56	1.50
11	P	3007	PEE	O2-C10	2.88	1.42	1.34
11	E	2005	PEE	P-O1P	2.89	1.61	1.51
11	P	3008	PEE	P-O4P	2.89	1.65	1.54
11	E	2005	PEE	C3-C2	2.95	1.59	1.50
13	P	3001	JZZ	CAJ-CAI	2.96	1.23	1.19
12	C	502	HEM	CBC-CAC	2.96	1.46	1.29
11	A	2008	PEE	P-O1P	2.97	1.62	1.51
11	A	2008	PEE	C1-C2	2.99	1.59	1.50
11	R	3005	PEE	P-O1P	3.00	1.62	1.51
14	C	2002	UQ	O3-C3	3.01	1.44	1.37
14	C	2002	UQ	C2-C1	3.04	1.57	1.48
11	A	2008	PEE	O3-C30	3.12	1.42	1.33
11	A	2008	PEE	O2-C10	3.13	1.43	1.34
11	R	3005	PEE	O3-C30	3.20	1.42	1.33
14	P	3002	UQ	O3-C3	3.20	1.45	1.37
11	P	3007	PEE	O3-C30	3.26	1.43	1.33
11	E	2005	PEE	O2-C10	3.36	1.44	1.34
11	C	2007	PEE	O3-C30	3.40	1.43	1.33
11	E	2005	PEE	O3-C30	3.47	1.43	1.33
12	P	502	HEM	CBC-CAC	3.47	1.49	1.29
14	P	3002	UQ	C6-C5	3.66	1.43	1.35
12	C	501	HEM	CBB-CAB	3.66	1.50	1.29
14	P	3002	UQ	C6-C1	3.68	1.57	1.46
11	R	3005	PEE	O2-C10	3.70	1.45	1.34
14	C	2002	UQ	C6-C1	3.72	1.57	1.46
12	P	501	HEM	CBB-CAB	3.87	1.51	1.29
12	P	502	HEM	CBB-CAB	3.88	1.51	1.29
14	C	2002	UQ	C6-C5	4.01	1.44	1.35
12	P	502	HEM	C4C-NC	4.03	1.41	1.36
12	P	501	HEM	C4C-NC	4.11	1.41	1.36
12	C	502	HEM	CBB-CAB	4.17	1.53	1.29
12	P	501	HEM	CBC-CAC	4.19	1.53	1.29
12	C	501	HEM	CBC-CAC	4.76	1.56	1.29
14	P	3002	UQ	C7-C6	5.20	1.60	1.51
14	C	2002	UQ	C7-C6	5.26	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	3008	PEE	P-O1P	6.09	1.62	1.50

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	P	3001	JZZ	C27-O3-C3	-8.83	108.90	117.47
16	D	501	HEC	CBB-CAB-C3B	-8.50	108.47	127.35
16	Q	501	HEC	CBB-CAB-C3B	-8.28	108.94	127.35
13	C	2001	JZZ	C27-O3-C3	-8.07	109.64	117.47
16	D	501	HEC	CBC-CAC-C3C	-7.92	109.76	127.35
16	Q	501	HEC	CBC-CAC-C3C	-7.70	110.24	127.35
12	C	501	HEM	C3C-CAC-CBC	-4.19	118.02	124.46
12	C	501	HEM	CMA-C3A-C4A	-3.75	122.16	128.36
17	T	3004	CDL	CB4-OB6-CB5	-3.46	109.60	117.89
14	C	2002	UQ	C7-C6-C1	-3.34	114.63	118.56
17	G	2004	CDL	CB4-OB6-CB5	-3.21	110.18	117.89
16	Q	501	HEC	CAA-C2A-C3A	-3.15	120.00	129.00
14	P	3002	UQ	C7-C6-C1	-3.10	114.91	118.56
16	D	501	HEC	CAA-C2A-C3A	-3.00	120.44	129.00
12	P	501	HEM	C3C-CAC-CBC	-2.93	119.96	124.46
14	P	3002	UQ	C10-C9-C8	-2.69	118.22	123.50
17	G	2004	CDL	CA4-OA6-CA5	-2.66	111.51	117.89
14	C	2002	UQ	C10-C9-C8	-2.66	118.29	123.50
13	C	2001	JZZ	CAL-CAM-CAN	-2.58	119.23	124.50
17	T	3004	CDL	CA6-CA4-CA3	-2.53	106.14	112.07
17	T	3004	CDL	CA4-OA6-CA5	-2.52	111.85	117.89
13	P	3001	JZZ	CAL-CAM-CAN	-2.51	119.37	124.50
17	D	2003	CDL	CA6-CA4-CA3	-2.34	106.61	112.07
17	G	2004	CDL	CA6-CA4-CA3	-2.30	106.69	112.07
17	D	2003	CDL	CB4-OB6-CB5	-2.29	112.38	117.89
17	Q	3003	CDL	CA6-CA4-CA3	-2.29	106.71	112.07
17	Q	3003	CDL	CB4-OB6-CB5	-2.24	112.51	117.89
17	G	2004	CDL	CB6-CB4-CB3	-2.02	107.34	112.07
17	Q	3003	CDL	CB6-CB4-CB3	-2.02	107.35	112.07
13	C	2001	JZZ	CAO-CAN-N2	2.01	121.09	118.50
16	Q	501	HEC	CBA-CAA-C2A	2.04	116.18	112.53
12	P	502	HEM	C3B-C4B-CHC	2.07	126.08	123.16
17	G	2004	CDL	OB6-CB4-CB3	2.08	115.70	108.36
17	T	3004	CDL	OB6-CB4-CB3	2.20	116.12	108.36
16	D	501	HEC	CAD-C3D-C4D	2.23	129.43	127.01
11	C	2007	PEE	O3-C3-C2	2.24	114.72	108.69
12	C	502	HEM	C3B-CAB-CBB	2.29	127.97	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	P	3007	PEE	C22-C21-C20	2.32	126.50	114.53
11	P	3007	PEE	C23-C22-C21	2.35	126.66	114.53
12	P	502	HEM	CMD-C2D-C3D	2.38	124.86	114.35
12	C	501	HEM	CMD-C2D-C3D	2.39	124.92	114.35
11	R	3005	PEE	C23-C22-C21	2.39	126.89	114.53
18	Q	3009	BOG	O1-C1-C2	2.41	111.08	108.04
11	R	3005	PEE	O3-C3-C2	2.41	115.19	108.69
18	Q	3091	BOG	O1-C1-C2	2.41	111.06	108.21
11	E	2005	PEE	C23-C22-C21	2.42	127.02	114.53
18	D	2091	BOG	O1-C1-C2	2.43	111.07	108.21
11	P	3007	PEE	C19-C18-C17	2.46	127.22	114.53
11	C	2007	PEE	C23-C22-C21	2.48	127.32	114.53
11	C	2007	PEE	C22-C21-C20	2.48	127.35	114.53
13	P	3001	JZZ	CAN-CAM-CAD	2.50	120.60	118.50
11	E	2005	PEE	O3-C3-C2	2.52	115.46	108.69
12	C	502	HEM	C3C-CAC-CBC	2.53	128.33	124.46
11	C	2007	PEE	C19-C18-C17	2.55	127.68	114.53
11	E	2005	PEE	C22-C21-C20	2.57	127.81	114.53
11	E	2005	PEE	C19-C18-C17	2.58	127.85	114.53
11	R	3005	PEE	C22-C21-C20	2.59	127.92	114.53
11	E	2005	PEE	C20-C19-C18	2.60	127.97	114.53
11	R	3005	PEE	C19-C18-C17	2.62	128.04	114.53
11	R	3005	PEE	C20-C19-C18	2.63	128.10	114.53
18	D	2009	BOG	C1'-O1-C1	2.70	118.66	113.94
12	P	501	HEM	CMD-C2D-C3D	2.70	126.30	114.35
12	C	502	HEM	CMD-C2D-C3D	2.76	126.55	114.35
11	P	3007	PEE	C20-C19-C18	2.76	128.80	114.53
11	C	2007	PEE	C20-C19-C18	2.79	128.93	114.53
18	D	2009	BOG	O1-C1-C2	2.92	111.73	108.04
12	C	501	HEM	CMA-C3A-C2A	3.00	131.50	125.24
12	P	501	HEM	C2D-C3D-C4D	3.06	106.69	101.50
18	D	2091	BOG	C1'-O1-C1	3.10	118.37	113.29
12	C	501	HEM	C2D-C3D-C4D	3.15	106.83	101.50
18	Q	3009	BOG	C1'-O1-C1	3.20	119.53	113.94
12	C	501	HEM	CAD-C3D-C2D	3.30	122.69	113.22
12	P	501	HEM	CAD-C3D-C2D	3.32	122.77	113.22
12	C	502	HEM	CMC-C2C-C3C	3.53	125.34	116.53
18	Q	3091	BOG	C1'-O1-C1	3.57	119.14	113.29
14	C	2002	UQ	C8-C7-C6	3.64	122.58	111.64
14	P	3002	UQ	C8-C7-C6	3.64	122.58	111.64
12	P	502	HEM	CAD-C3D-C2D	3.65	123.71	113.22
12	C	502	HEM	CAD-C3D-C2D	3.90	124.42	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	2001	JZZ	C7-N5-N4	4.00	124.70	118.05
13	P	3001	JZZ	C7-N5-N4	4.13	124.92	118.05
12	C	501	HEM	CMC-C2C-C3C	4.16	126.92	116.53
12	P	501	HEM	CMC-C2C-C3C	4.22	127.06	116.53
12	P	501	HEM	CMB-C2B-C3B	4.24	127.12	116.53
12	P	502	HEM	CMC-C2C-C3C	4.41	127.54	116.53
12	C	501	HEM	CMB-C2B-C3B	4.55	127.89	116.53
12	P	502	HEM	CMB-C2B-C3B	4.96	128.92	116.53
12	C	501	HEM	CAD-C3D-C4D	5.02	130.19	112.47
12	P	501	HEM	CAD-C3D-C4D	5.05	130.28	112.47
12	C	502	HEM	CAD-C3D-C4D	5.18	130.75	112.47
12	C	502	HEM	CMB-C2B-C3B	5.29	129.74	116.53
12	P	502	HEM	CAD-C3D-C4D	5.37	131.42	112.47
16	D	501	HEC	CAA-C2A-C1A	5.90	133.41	127.01
16	Q	501	HEC	CAA-C2A-C1A	6.71	134.29	127.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

25 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	2001	JZZ	2	0
14	C	2002	UQ	4	0
11	C	2007	PEE	4	0
15	C	2011	GOL	1	0
12	C	501	HEM	2	0
12	C	502	HEM	4	0
17	D	2003	CDL	3	0
18	D	2091	BOG	2	0
16	D	501	HEC	1	0
11	E	2005	PEE	1	0
19	E	501	FES	2	0
17	G	2004	CDL	5	0
18	P	2010	BOG	1	0
13	P	3001	JZZ	6	0
14	P	3002	UQ	5	0
11	P	3007	PEE	4	0
15	P	3011	GOL	1	0
12	P	501	HEM	2	0
12	P	502	HEM	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Q	3003	CDL	1	0
18	Q	3091	BOG	1	0
16	Q	501	HEC	2	0
11	R	3005	PEE	1	0
19	R	501	FES	2	0
17	T	3004	CDL	5	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	444/446 (99%)	-0.42	7 (1%) 74 47	49, 78, 110, 121	0
1	N	442/446 (99%)	-0.31	2 (0%) 91 77	55, 88, 114, 124	0
2	B	420/441 (95%)	-0.27	3 (0%) 89 70	66, 97, 130, 152	0
2	O	422/441 (95%)	-0.24	6 (1%) 78 51	52, 92, 124, 143	0
3	C	380/380 (100%)	-0.60	7 (1%) 71 43	30, 51, 98, 137	0
3	P	379/380 (99%)	-0.55	2 (0%) 91 77	39, 75, 106, 134	0
4	D	241/241 (100%)	-0.56	0 100 100	42, 56, 102, 124	0
4	Q	241/241 (100%)	-0.25	0 100 100	64, 88, 119, 136	0
5	E	196/196 (100%)	0.85	45 (22%) 1 0	47, 154, 185, 192	124 (63%)
5	R	196/196 (100%)	0.07	13 (6%) 22 7	60, 109, 155, 165	0
6	F	101/110 (91%)	-0.74	0 100 100	41, 59, 76, 111	0
6	S	101/110 (91%)	-0.31	0 100 100	65, 84, 122, 139	0
7	G	80/81 (98%)	-0.41	0 100 100	46, 64, 114, 128	0
7	T	79/81 (97%)	0.05	4 (5%) 32 13	62, 96, 159, 169	0
8	H	70/77 (90%)	-0.46	2 (2%) 55 26	50, 77, 102, 138	0
8	U	67/77 (87%)	0.10	4 (5%) 25 9	101, 131, 147, 150	0
9	I	31/47 (65%)	0.65	2 (6%) 22 8	90, 127, 152, 153	0
9	V	31/47 (65%)	1.32	8 (25%) 1 0	93, 128, 156, 160	0
10	J	61/61 (100%)	-0.55	3 (4%) 33 13	59, 72, 116, 156	0
10	W	60/61 (98%)	-0.33	0 100 100	71, 85, 121, 131	0
All	All	4042/4160 (97%)	-0.28	108 (2%) 58 28	30, 83, 141, 192	124 (3%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	113	ASP	9.2
5	E	157	TYR	8.8
5	E	168	SER	8.3
9	V	63	ASP	7.0
5	E	112	VAL	6.3
5	E	107	ASN	6.3
5	E	173	LYS	5.8
5	E	114	VAL	5.6
9	V	54	SER	5.1
5	E	109	GLU	5.1
9	I	63	ASP	4.9
5	E	174	GLY	4.9
9	V	56	SER	4.9
5	E	103	GLN	4.9
5	E	102	THR	4.7
5	E	115	SER	4.6
5	E	111	GLU	4.6
3	C	4	ASN	4.5
5	E	169	GLY	4.5
10	J	64	GLU	4.2
3	C	155	PRO	4.2
9	V	47	ARG	4.2
5	E	163	SER	4.1
5	E	190	ASP	4.1
5	E	108	GLN	4.0
5	R	121	GLN	3.9
5	E	152	ASP	3.9
7	T	78	GLU	3.8
5	R	157	TYR	3.8
5	E	188	VAL	3.7
5	E	159	PRO	3.7
1	A	218	GLY	3.5
1	A	1	ALA	3.5
5	E	149	ASN	3.4
5	E	104	ALA	3.4
8	U	12	GLU	3.4
9	V	53	GLU	3.4
8	U	13	LEU	3.4
5	R	196	GLY	3.4
7	T	73	ASN	3.4
8	U	49	HIS	3.4
1	N	38	GLY	3.3
5	E	124	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
5	E	110	ALA	3.3
5	E	84	GLY	3.3
2	O	323	GLY	3.3
5	E	126	ARG	3.2
1	A	226	ASP	3.2
5	E	125	ASP	3.2
5	E	83	GLU	3.2
2	O	19	PRO	3.1
5	E	86	ASN	3.1
9	V	58	ARG	3.1
1	N	217	SER	3.1
9	V	57	GLY	3.1
5	E	121	GLN	3.1
5	E	120	PRO	3.1
2	O	310	SER	3.0
5	R	165	TYR	2.9
8	U	50	THR	2.9
5	E	175	PRO	2.9
9	V	48	PRO	2.9
2	B	228	SER	2.8
3	C	7	LYS	2.8
5	R	171	ILE	2.8
5	E	150	SER	2.7
5	E	116	LYS	2.7
7	T	77	TYR	2.6
9	I	51	CYS	2.6
1	A	219	VAL	2.6
2	B	310	SER	2.6
3	C	5	ILE	2.6
1	A	69	LYS	2.5
7	T	74	PRO	2.5
5	E	162	GLY	2.5
8	H	10	GLU	2.5
10	J	63	GLU	2.5
1	A	38	GLY	2.5
2	O	23	ASP	2.5
5	R	114	VAL	2.5
3	C	156	TYR	2.4
5	E	99	ARG	2.4
5	R	128	LYS	2.4
5	R	117	LEU	2.4
8	H	71	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
2	O	18	CYS	2.3
3	C	1	MET	2.3
3	C	8	SER	2.3
2	O	280	GLY	2.3
5	E	101	ARG	2.3
5	R	113	ASP	2.2
5	E	79	SER	2.2
5	E	182	VAL	2.2
5	E	191	ASP	2.1
2	B	323	GLY	2.1
5	R	116	LYS	2.1
5	E	128	LYS	2.1
5	E	180	LEU	2.1
5	E	164	HIS	2.1
5	R	103	GLN	2.1
5	E	183	PRO	2.1
5	E	87	VAL	2.1
5	R	172	ARG	2.1
3	P	4	ASN	2.0
10	J	62	SER	2.0
3	P	2	ALA	2.0
5	R	120	PRO	2.0
1	A	444	ILE	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
18	BOG	P	2010	12/20	0.54	0.55	9.18	149,151,153,154	0
14	UQ	P	3002	19/63	0.77	0.45	8.07	134,141,143,143	0
11	PEE	R	3005	50/51	0.68	0.45	7.78	94,113,121,122	0
11	PEE	E	2005	50/51	0.83	0.36	6.15	88,101,111,112	0
14	UQ	C	2002	19/63	0.88	0.30	4.65	95,99,101,102	0
11	PEE	C	2007	49/51	0.88	0.28	4.61	53,73,95,96	0
15	GOL	P	3011	6/6	0.86	0.32	3.52	90,91,93,95	0
15	GOL	C	2011	6/6	0.91	0.24	3.20	90,90,91,91	0
17	CDL	Q	3003	42/100	0.75	0.32	3.12	127,135,146,147	0
17	CDL	D	2003	42/100	0.84	0.25	2.95	94,105,109,110	0
11	PEE	A	2008	21/51	0.64	0.30	2.83	139,142,145,145	0
17	CDL	G	2004	40/100	0.89	0.26	2.65	72,83,101,103	0
11	PEE	P	3007	49/51	0.85	0.30	1.70	85,95,107,108	0
13	JZZ	P	3001	25/25	0.95	0.21	1.20	74,76,79,80	0
12	HEM	P	501	43/43	0.97	0.22	1.12	51,55,62,67	0
18	BOG	D	2009	20/20	0.94	0.17	0.73	58,73,76,76	0
18	BOG	Q	3009	20/20	0.93	0.23	0.67	86,92,94,95	0
12	HEM	C	501	43/43	0.97	0.21	0.67	30,42,53,55	0
12	HEM	C	502	43/43	0.98	0.19	0.66	31,37,47,52	0
17	CDL	T	3004	40/100	0.86	0.25	0.56	104,109,120,121	0
16	HEC	Q	501	43/43	0.96	0.20	0.47	71,75,83,84	0
12	HEM	P	502	43/43	0.98	0.19	0.33	42,52,65,70	0
16	HEC	D	501	43/43	0.98	0.16	0.07	39,45,50,56	0
13	JZZ	C	2001	25/25	0.96	0.16	-0.17	45,49,51,51	0
19	FES	E	501	4/4	0.95	0.13	-1.43	162,162,163,163	4
19	FES	R	501	4/4	0.98	0.06	-2.20	100,101,102,102	0
11	PEE	P	3008	5/51	0.88	0.17	-	108,109,110,110	0
18	BOG	D	2091	13/20	0.25	0.90	-	215,217,218,218	0
18	BOG	Q	3091	13/20	0.23	0.77	-	201,204,205,205	0

6.5 Other polymers (i)

There are no such residues in this entry.