



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:15 AM GMT

PDB ID : 3L70
Title : Cytochrome BC1 complex from chicken with trifloxystrobin bound
Authors : Huang, L.; Berry, E.A.
Deposited on : 2009-12-27
Resolution : 2.75 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

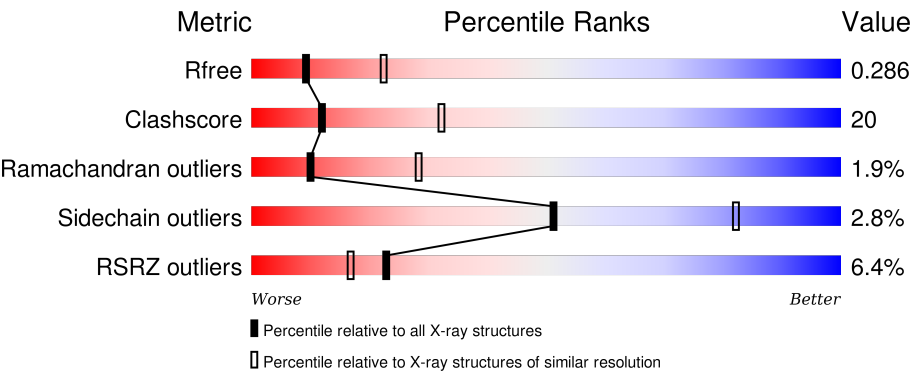
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div><div>2%</div><div>64%</div><div>33%</div><div>.</div></div>
1	N	446	<div><div>2%</div><div>61%</div><div>35%</div><div>..</div></div>
2	B	441	<div><div>4%</div><div>54%</div><div>38%</div><div>.</div><div>5%</div></div>
2	O	441	<div><div>4%</div><div>57%</div><div>35%</div><div>..</div></div>
3	C	380	<div><div>%</div><div>75%</div><div>24%</div><div>.</div></div>

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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	N	3008	-	X	-	-
11	PEE	P	3007	-	-	-	X
11	PEE	R	3005	-	-	-	X
13	JZV	C	2001	-	-	-	X
13	JZV	P	3001	-	-	-	X
14	UQ	C	2002	-	-	-	X
14	UQ	P	3002	-	-	-	X
15	CDL	C	2004	-	-	-	X
15	CDL	D	2003	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CDL	Q	3003	-	-	-	X
16	GOL	C	2011	-	-	-	X
16	GOL	P	3011	-	-	-	X
18	BOG	P	2010	-	-	-	X
19	FES	E	501	-	-	X	-
19	FES	R	501	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i.

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

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

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

- Molecule 3 is a protein called Cytochrome b.

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

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

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

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

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

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

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

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

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

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

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

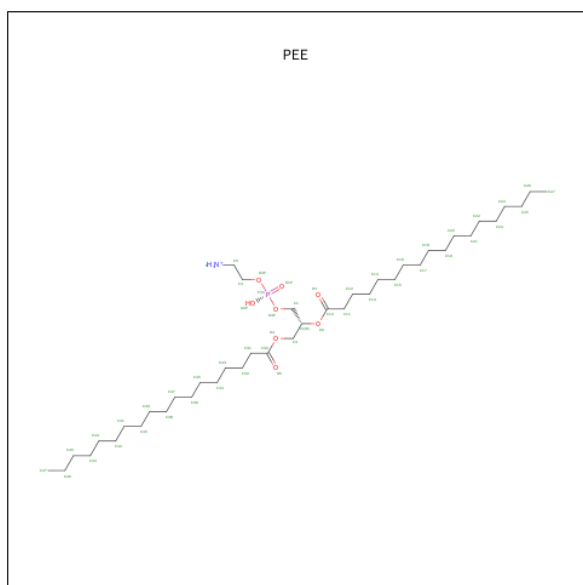
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

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

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

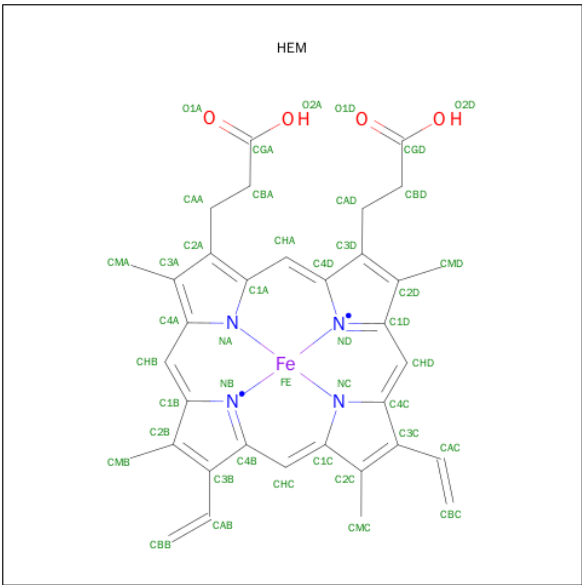
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	60	Total	C	N	O	0	0	1
			479	311	86	82			

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



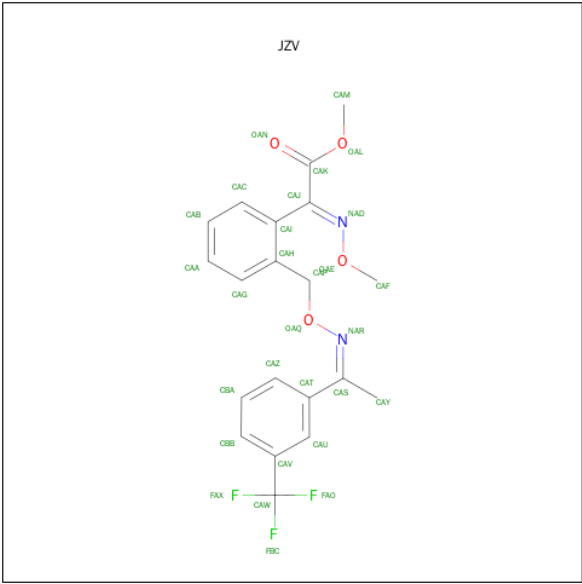
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	A	1	Total	C	O	P	0	0
			21	12	8	1		
11	C	1	Total	C	N	O	P	0
			49	39	1	8	1	
11	E	1	Total	C	N	O	P	0
			50	40	1	8	1	
11	N	1	Total	O	P		0	0
			5	4	1			
11	P	1	Total	C	N	O	P	0
			49	39	1	8	1	
11	R	1	Total	C	N	O	P	0
			50	40	1	8	1	

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



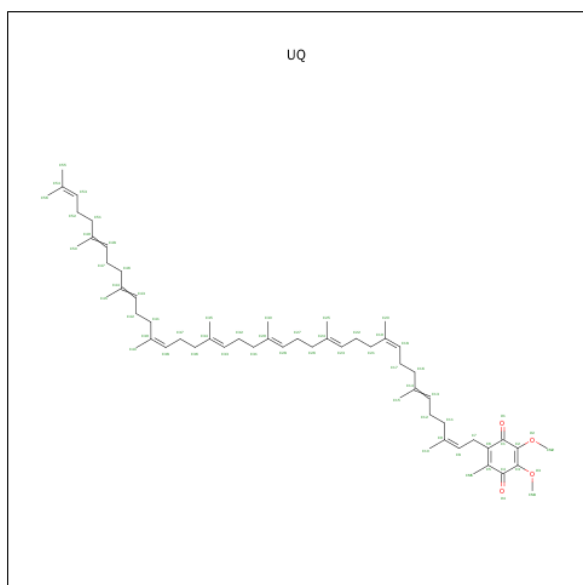
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 13 is METHYL (2E)-(METHOXYIMINO)(2-{[({(1Z)-1-[3-(TRIFLUOROMETHYL)PHENYL]ETHYLIDENE}AMINO)OXY]METHYL}PHENYL)ETHANOATE (three-letter code: JZV) (formula: C₂₀H₁₉F₃N₂O₄).



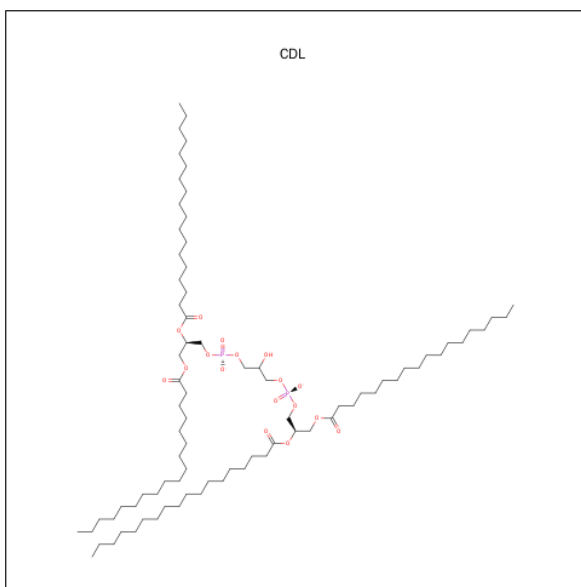
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	F	N	O	0	0
			29	20	3	2	4		
13	P	1	Total	C	F	N	O	0	0
			29	20	3	2	4		

- Molecule 14 is COENZYME Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-ISOMER (three-letter code: UQ) (formula: C₅₉H₉₀O₄).



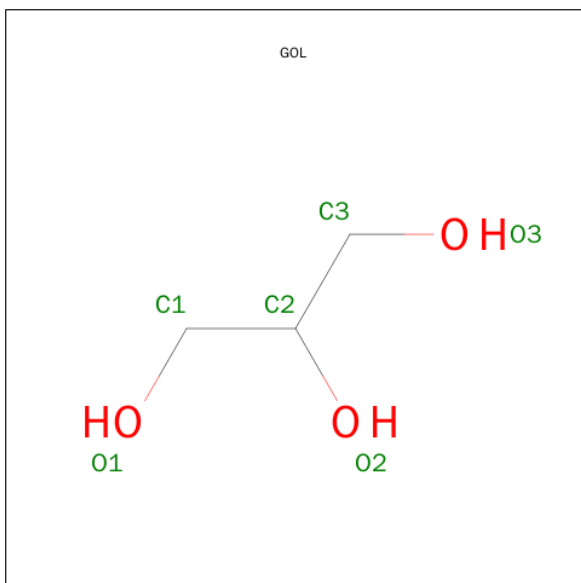
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			19	15	4		
14	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



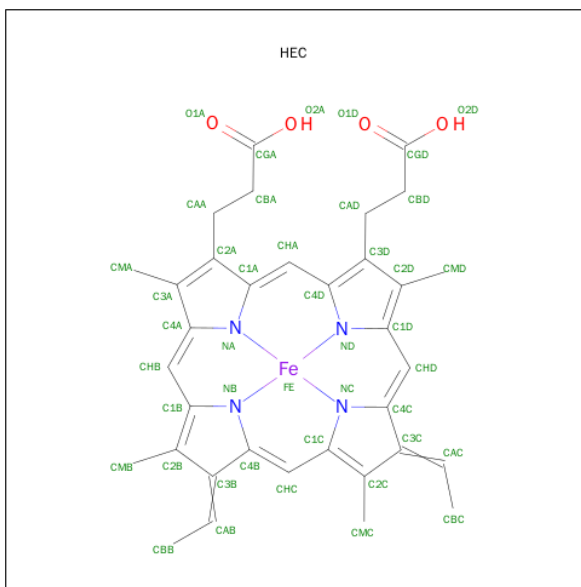
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	O	P	0	0
			40	21	17	2		
15	D	1	Total	C	O	P	0	0
			42	23	17	2		
15	P	1	Total	C	O	P	0	0
			40	21	17	2		
15	Q	1	Total	C	O	P	0	0
			42	23	17	2		

- Molecule 16 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



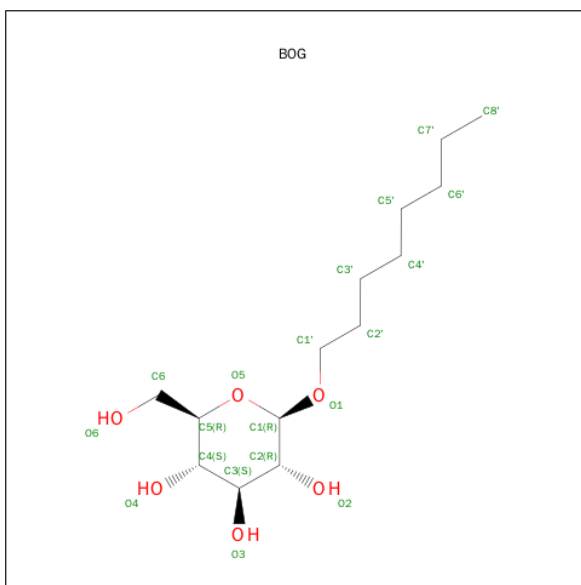
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total 6	C 3	O 3	0	0
16	P	1	Total 6	C 3	O 3	0	0

- Molecule 17 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



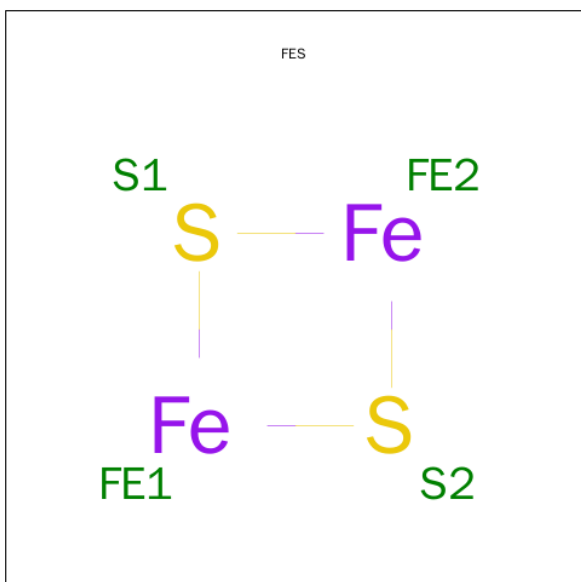
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
17	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 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	0	0
			20	14	6		
18	D	1	Total	C	O	0	0
			13	7	6		
18	P	1	Total	C	O	0	0
			12	6	6		
18	Q	1	Total	C	O	0	0
			20	14	6		
18	Q	1	Total	C	O	0	0
			13	7	6		

- 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	0	0
			4	2	2		
19	R	1	Total	Fe	S	0	0
			4	2	2		

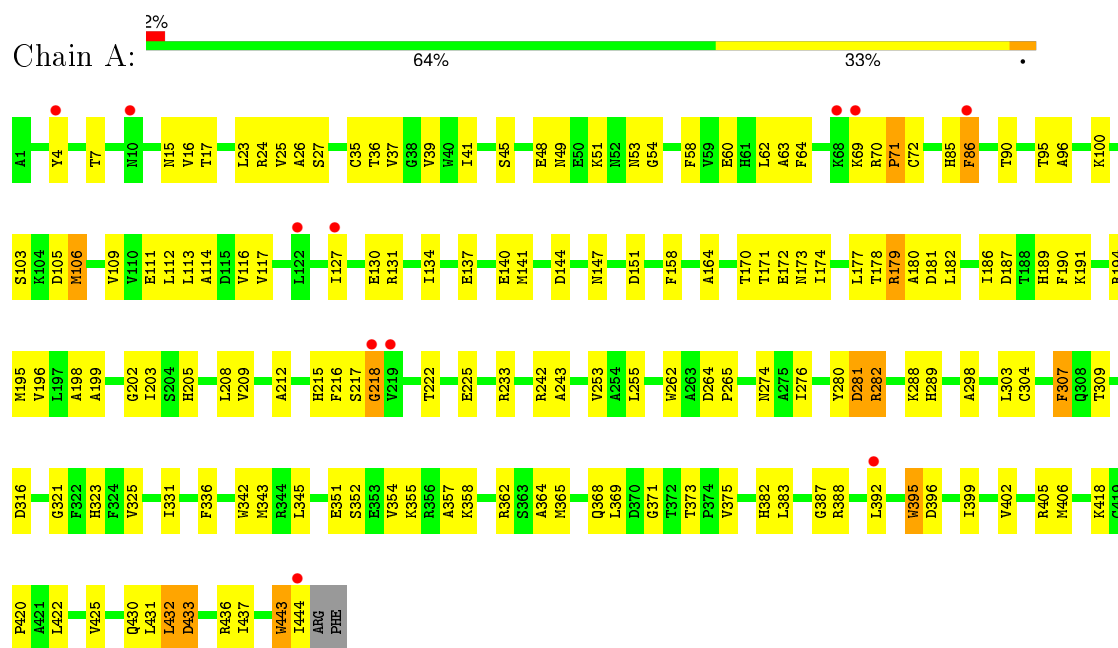
- Molecule 20 is water.

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

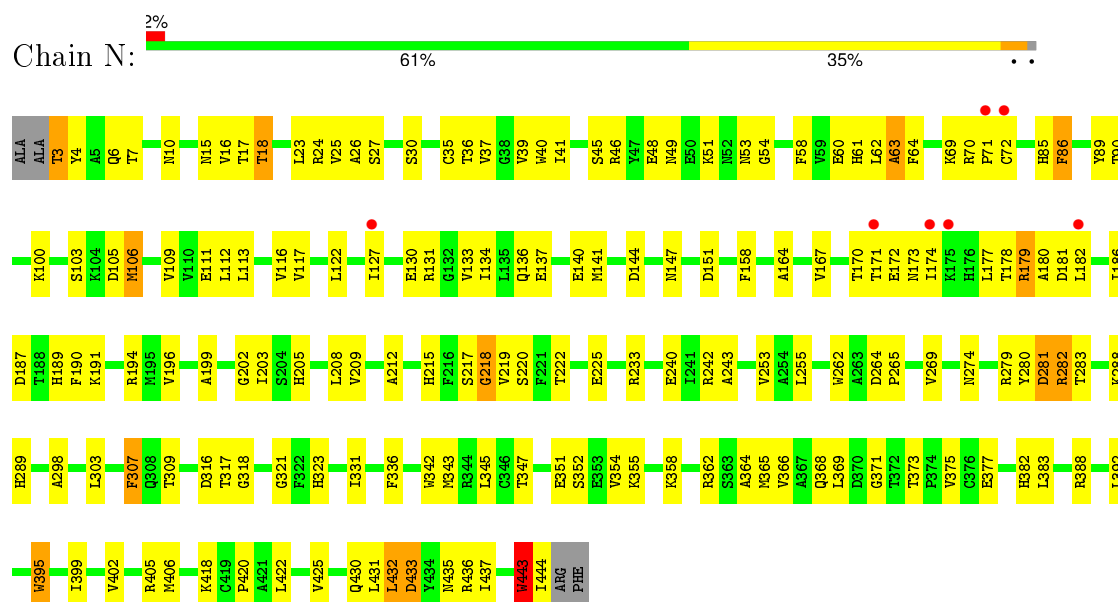
3 Residue-property plots

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.

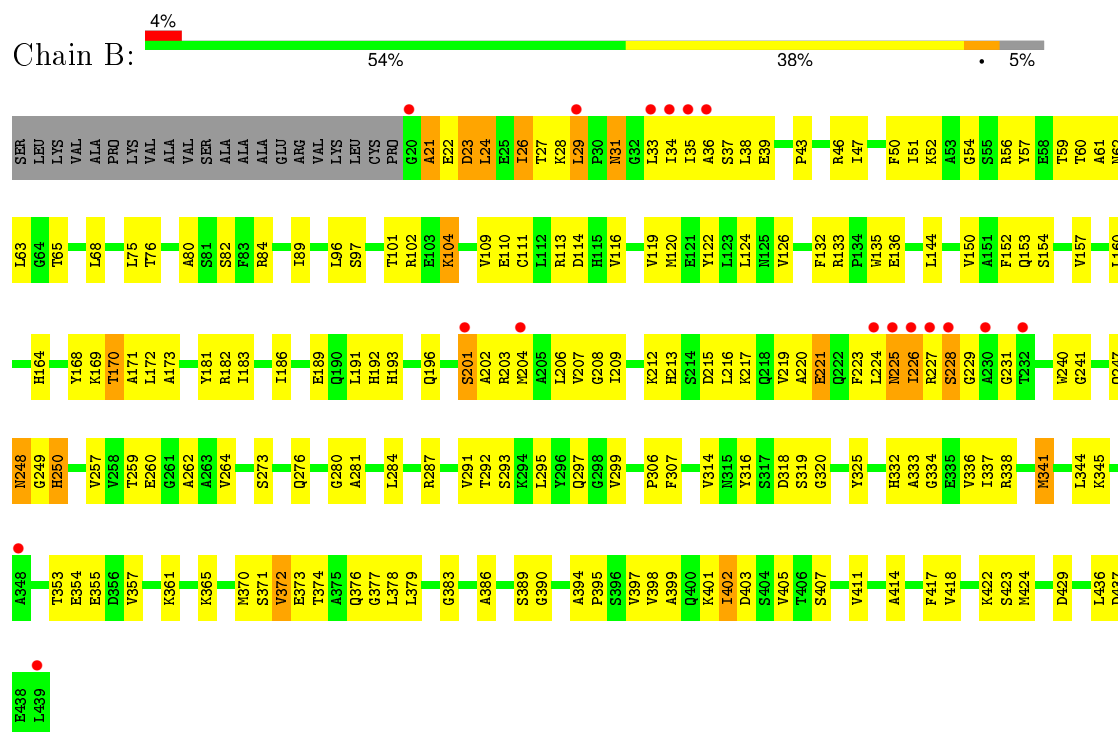
- Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i



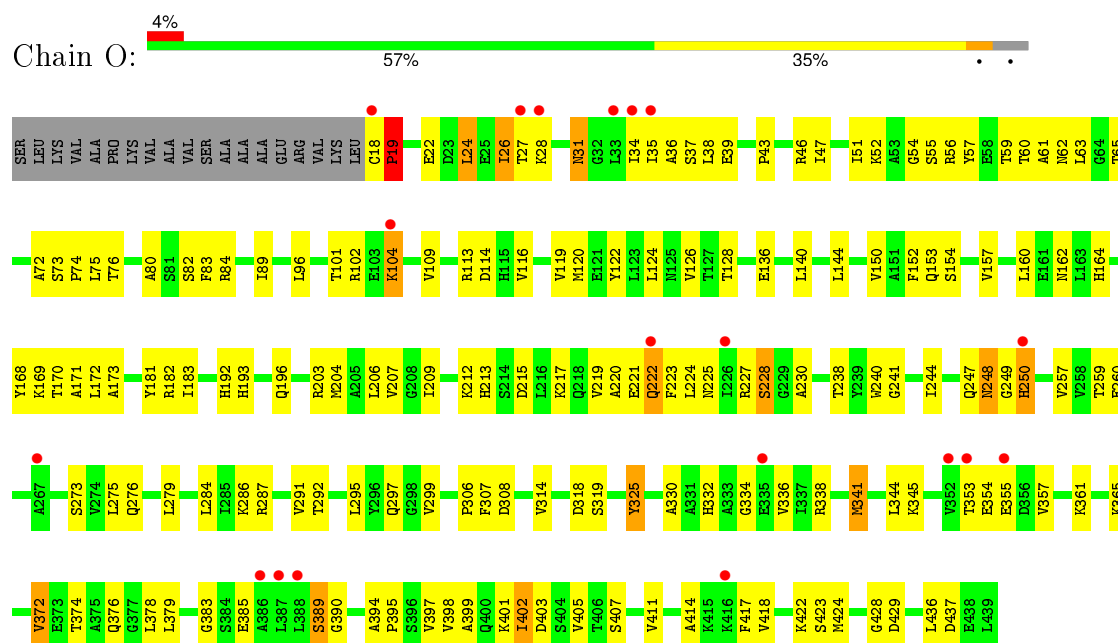
- Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i



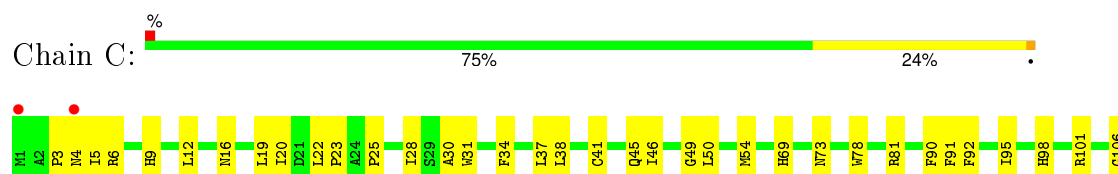
• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

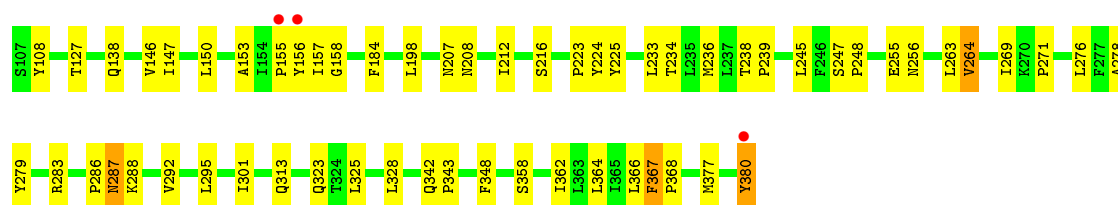


• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

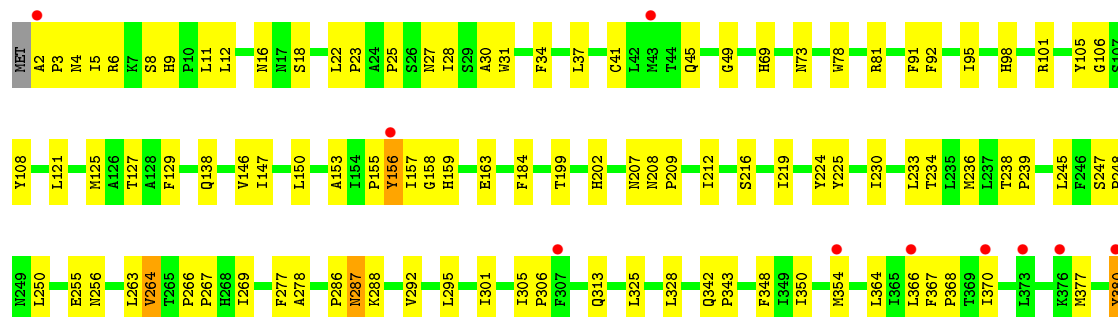


• Molecule 3: Cytochrome b

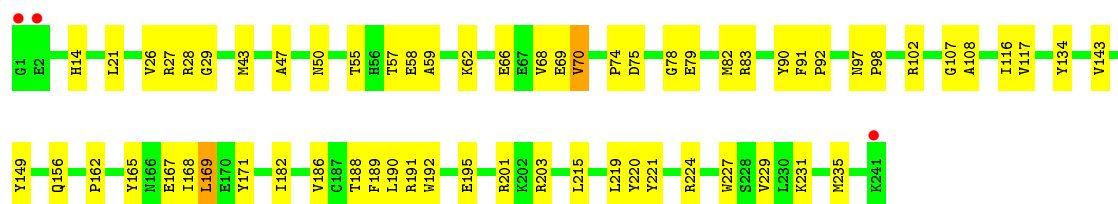
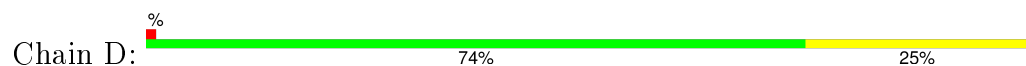




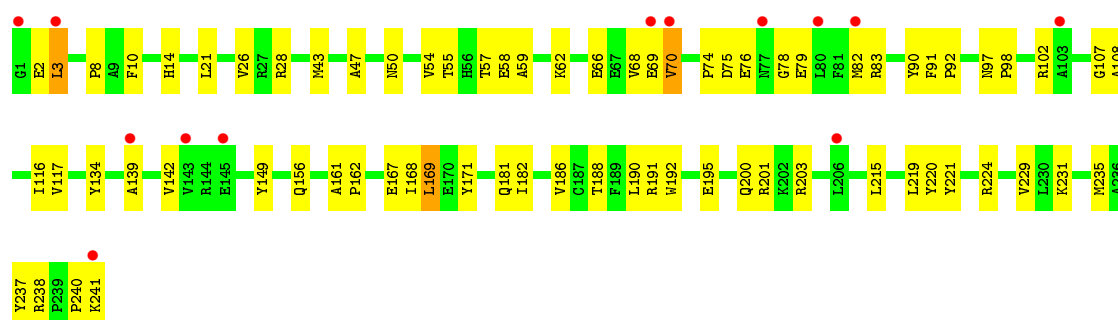
• Molecule 3: Cytochrome b



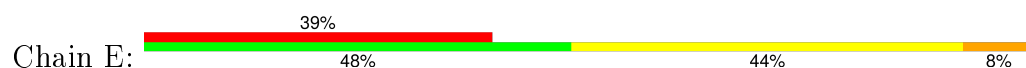
• Molecule 4: Mitochondrial cytochrome c1, heme protein

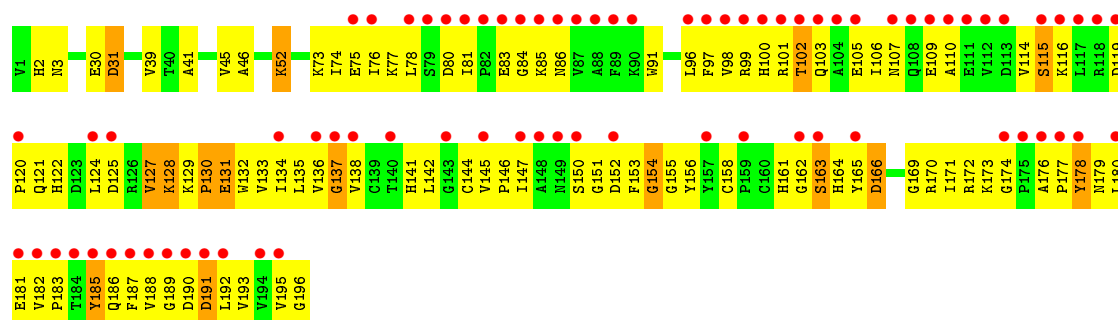


• Molecule 4: Mitochondrial cytochrome c1, heme protein

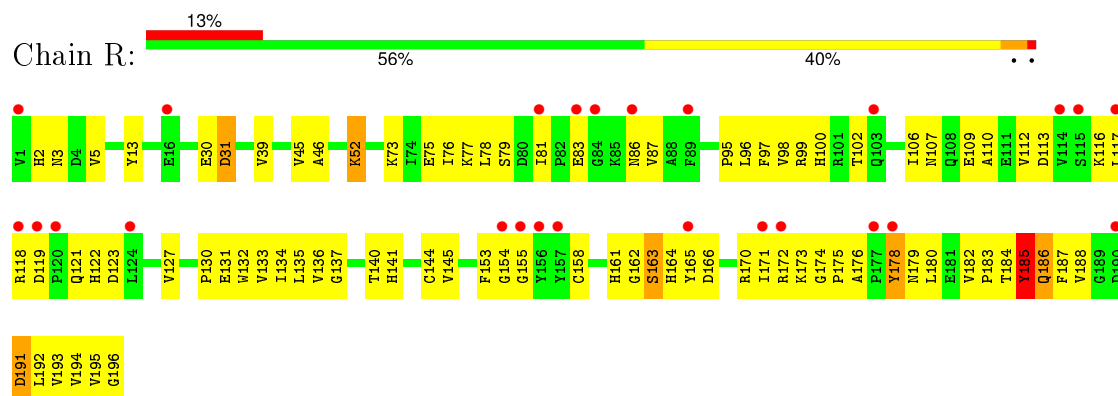


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

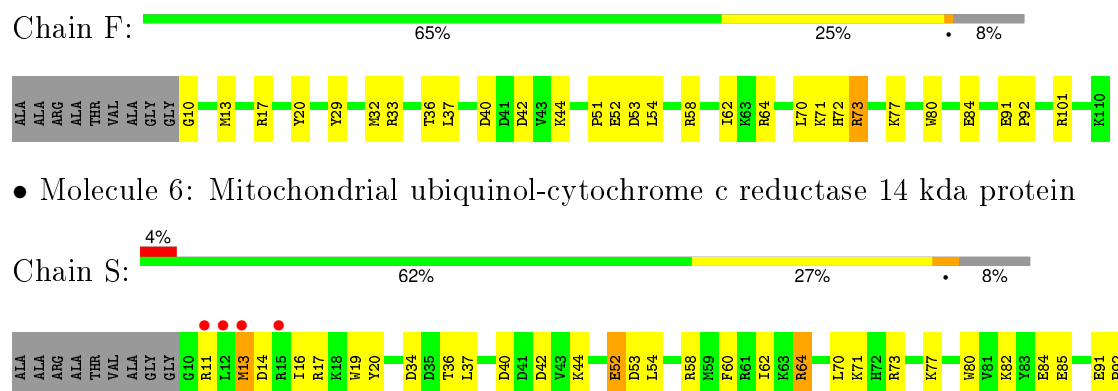




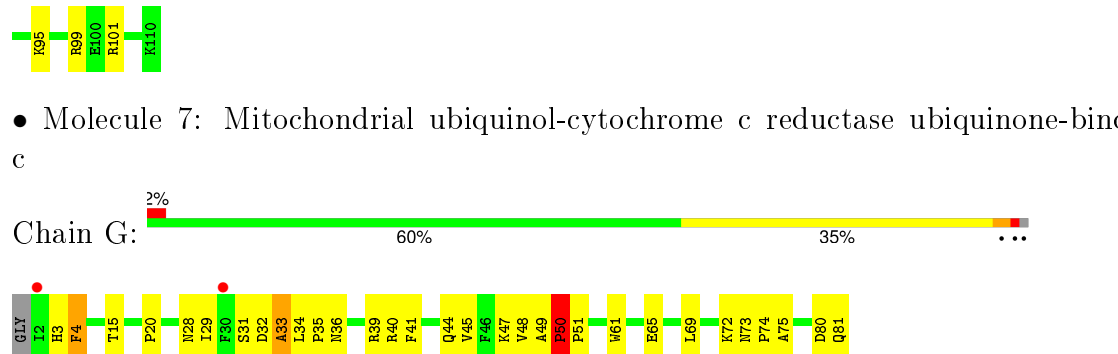
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



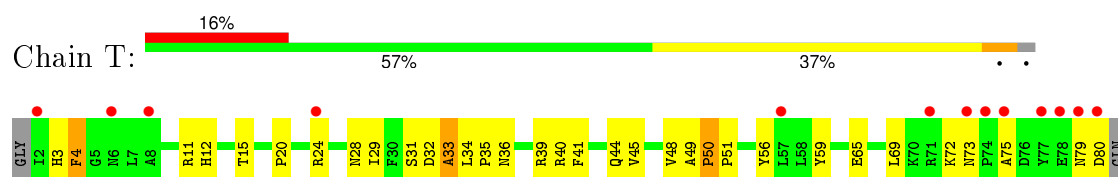
- Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein



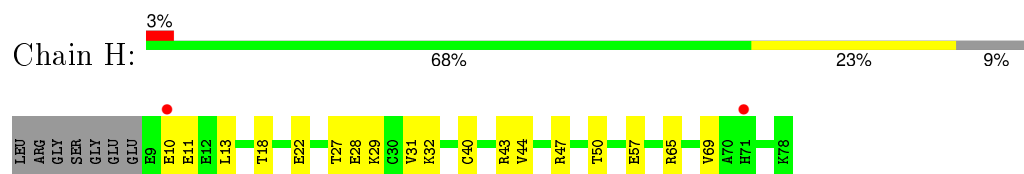
- Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein



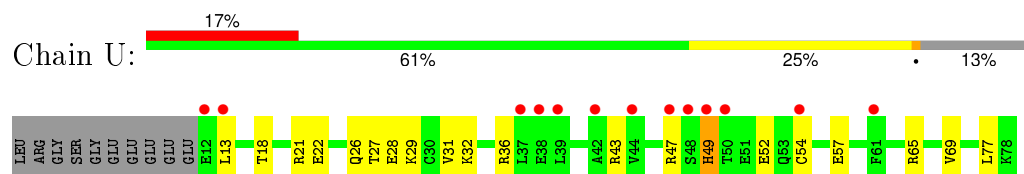
- Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c



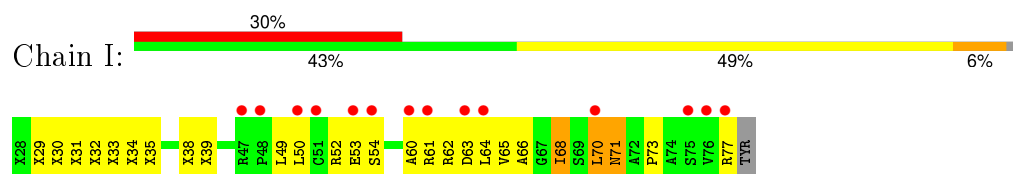
- Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii



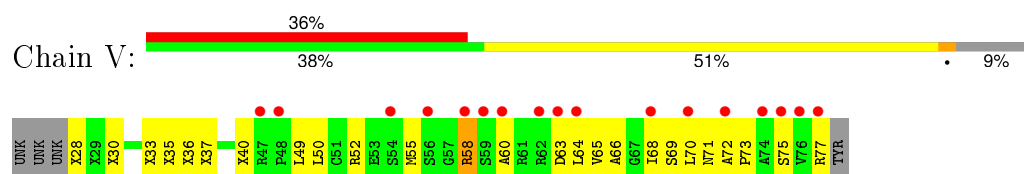
- Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii



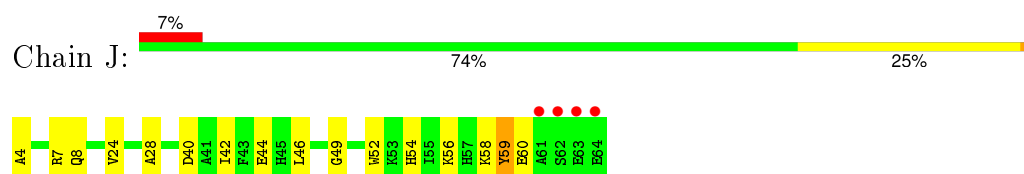
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



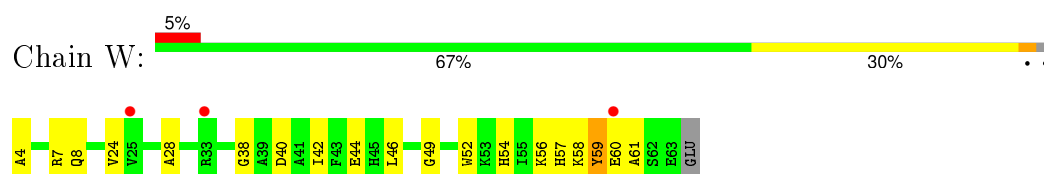
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	169.61Å 181.99Å 240.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.99 – 2.75 58.26 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.3 (24.99-2.75) 98.8 (58.26-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.267 , 0.297 0.259 , 0.286	Depositor DCC
R_{free} test set	9575 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.603	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	2 of 204662 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	32653	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, FES, HEC, HEM, PEE, JZV, BOG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/3518	0.65	0/4767
1	N	0.42	0/3508	0.64	0/4753
2	B	0.38	0/3187	0.63	0/4321
2	O	0.40	0/3202	0.63	0/4343
3	C	0.50	0/3119	0.66	0/4270
3	P	0.45	0/3114	0.64	0/4263
4	D	0.48	0/1956	0.64	0/2658
4	Q	0.39	0/1956	0.61	0/2658
5	E	0.37	0/1547	0.59	0/2103
5	R	0.37	0/1543	0.60	0/2098
6	F	0.54	1/911 (0.1%)	0.67	0/1219
6	S	0.43	0/911	0.61	0/1219
7	G	0.49	0/694	0.69	0/941
7	T	0.43	0/684	0.64	0/929
8	H	0.44	0/582	0.63	0/779
8	U	0.31	0/561	0.56	0/751
9	I	0.39	0/218	0.60	0/293
9	V	0.36	0/218	0.59	0/293
10	J	0.43	0/508	0.60	0/682
10	W	0.40	0/490	0.60	0/660
All	All	0.43	1/32427 (0.0%)	0.63	0/44000

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	10	GLY	N-CA	5.16	1.53	1.46

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	126	0
1	N	3437	0	3349	143	0
2	B	3133	0	3130	187	0
2	O	3147	0	3146	181	0
3	C	3017	0	3063	76	0
3	P	3012	0	3058	95	0
4	D	1898	0	1846	55	0
4	Q	1898	0	1846	67	0
5	E	1513	0	1478	122	0
5	R	1509	0	1474	94	0
6	F	891	0	893	20	0
6	S	891	0	893	33	0
7	G	672	0	653	32	0
7	T	662	0	645	35	0
8	H	574	0	548	16	0
8	U	553	0	535	22	0
9	I	287	0	250	37	0
9	V	277	0	251	32	0
10	J	497	0	490	16	0
10	W	479	0	478	16	0
11	A	21	0	13	0	0
11	C	49	0	72	4	0
11	E	50	0	77	1	0
11	N	5	0	0	0	0
11	P	49	0	72	3	0
11	R	50	0	77	2	0
12	C	86	0	60	9	0
12	P	86	0	60	7	0
13	C	29	0	19	4	0
13	P	29	0	19	4	0
14	C	19	0	17	4	0
14	P	19	0	17	5	0
15	C	40	0	24	4	0
15	D	42	0	28	4	0
15	P	40	0	24	4	0
15	Q	42	0	28	3	0
16	C	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	6	0	8	0	0
17	D	43	0	30	3	0
17	Q	43	0	30	1	0
18	D	33	0	39	0	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	1	0
20	R	1	0	0	0	0
All	All	32653	0	32160	1298	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1298) 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)
9:V:35:UNK:HG3	9:V:36:UNK:H	1.05	1.14
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.15	1.13
9:I:33:UNK:HG2	9:I:73:PRO:HB3	1.34	1.07
2:O:76:THR:HG22	2:O:82:SER:H	1.16	1.07
2:B:76:THR:HG22	2:B:82:SER:H	1.18	1.07
2:O:353:THR:HG22	2:O:355:GLU:H	1.18	1.05
2:B:353:THR:HG22	2:B:355:GLU:H	1.19	1.03
2:O:338:ARG:HH11	2:O:338:ARG:HG3	1.27	0.99
3:C:147:ILE:HG13	13:C:2001:JZV:HAP	1.44	0.99
2:B:338:ARG:HH11	2:B:338:ARG:HG3	1.28	0.99
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.27	0.99
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.78	0.99
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.42	0.98
1:N:178:THR:HG22	1:N:180:ALA:H	1.25	0.98
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.07	0.97
1:A:178:THR:HG22	1:A:180:ALA:H	1.25	0.96
3:P:9:HIS:HD2	3:P:12:LEU:H	1.09	0.95
3:C:9:HIS:HD2	3:C:12:LEU:H	1.11	0.93
4:D:47:ALA:H	4:D:50:ASN:HD22	1.12	0.91
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.50	0.91
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.51	0.90
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.54	0.90
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.36	0.89
3:P:147:ILE:HG13	13:P:3001:JZV:HAP	1.50	0.88
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.54	0.88
9:I:32:UNK:N	9:I:73:PRO:HG2	1.89	0.88
7:T:41:PHE:O	7:T:45:VAL:HG23	1.75	0.87
3:P:238:THR:HB	3:P:239:PRO:HD3	1.56	0.86
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.56	0.86
2:O:27:THR:HG22	2:O:28:LYS:H	1.40	0.86
7:G:41:PHE:O	7:G:45:VAL:HG23	1.76	0.85
1:A:178:THR:HB	1:A:181:ASP:OD1	1.75	0.85
9:V:35:UNK:HG3	9:V:36:UNK:N	1.89	0.85
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.57	0.85
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.42	0.85
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.58	0.85
2:O:18:CYS:HB2	2:O:19:PRO:HD3	1.58	0.84
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.60	0.84
9:V:64:LEU:HD12	9:V:77:ARG:O	1.78	0.84
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.60	0.84
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.59	0.83
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.61	0.83
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.04	0.83
11:P:3007:PEE:H7	7:T:44:GLN:HE21	1.45	0.82
5:E:127:VAL:HG12	5:E:128:LYS:H	1.43	0.82
1:N:10:ASN:ND2	2:O:19:PRO:HD2	1.95	0.81
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.62	0.81
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.45	0.81
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.62	0.81
2:O:192:HIS:O	2:O:196:GLN:HG3	1.81	0.81
12:C:502:HEM:HMC2	12:C:502:HEM:HBC2	1.63	0.81
2:O:248:ASN:HD22	2:O:248:ASN:C	1.83	0.81
9:I:34:UNK:HG3	9:I:35:UNK:N	1.96	0.80
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.45	0.80
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.44	0.80
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.64	0.80
3:C:238:THR:HB	3:C:239:PRO:HD3	1.64	0.79
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.80	0.79
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.65	0.79
3:C:22:LEU:HD21	14:C:2002:UQ:HM32	1.65	0.79
1:A:443:TRP:CE3	1:A:443:TRP:HA	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.65	0.79
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.01	0.78
2:B:47:ILE:HD13	2:B:120:MET:CE	2.14	0.78
1:A:343:MET:HB3	1:A:444:ILE:HA	1.64	0.78
1:N:178:THR:HB	1:N:181:ASP:OD1	1.82	0.78
2:B:248:ASN:HD22	2:B:248:ASN:C	1.87	0.78
2:O:221:GLU:HG3	2:O:222:GLN:H	1.49	0.77
2:O:154:SER:O	2:O:157:VAL:HG12	1.85	0.77
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.66	0.77
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.49	0.77
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.66	0.77
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.19	0.76
7:T:72:LYS:HE2	8:U:57:GLU:OE1	1.86	0.76
4:D:57:THR:HG22	4:D:59:ALA:H	1.49	0.76
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.66	0.76
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.21	0.76
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.34	0.75
5:E:141:HIS:HB2	5:E:176:ALA:HB2	1.68	0.75
2:B:192:HIS:O	2:B:196:GLN:HG3	1.87	0.75
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.22	0.75
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.51	0.75
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.66	0.75
11:C:2007:PEE:H7	7:G:44:GLN:HE21	1.49	0.75
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.17	0.75
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.68	0.75
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.51	0.74
5:E:121:GLN:CG	5:E:170:ARG:HD3	2.06	0.74
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.23	0.74
1:A:331:ILE:HG21	1:A:431:LEU:HB2	1.69	0.74
1:N:170:THR:HG22	1:N:171:THR:N	2.03	0.74
2:B:399:ALA:O	2:B:402:ILE:HG22	1.87	0.74
5:R:79:SER:OG	5:R:191:ASP:HB2	1.88	0.74
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.68	0.74
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.70	0.74
2:O:338:ARG:NH1	2:O:338:ARG:HG3	2.00	0.74
2:O:27:THR:HG22	2:O:28:LYS:N	2.03	0.73
2:B:154:SER:O	2:B:157:VAL:HG12	1.88	0.73
1:N:331:ILE:HG21	1:N:431:LEU:HB2	1.70	0.73
1:A:443:TRP:HE3	1:A:443:TRP:HA	1.52	0.73
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.35	0.73
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.24	0.73
2:B:31:ASN:N	2:B:31:ASN:HD22	1.86	0.73
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.52	0.72
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.71	0.72
2:B:27:THR:HG22	2:B:28:LYS:H	1.53	0.72
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.54	0.72
3:P:101:ARG:C	3:P:101:ARG:HD2	2.09	0.72
1:N:10:ASN:HD21	2:O:18:CYS:N	1.88	0.72
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.23	0.72
2:B:37:SER:HB3	2:B:213:HIS:ND1	2.05	0.72
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.70	0.72
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.88	0.72
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.25	0.72
5:E:84:GLY:N	5:E:102:THR:HG23	2.05	0.72
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.03	0.72
1:N:343:MET:HB3	1:N:444:ILE:HA	1.71	0.72
2:O:62:ASN:O	2:O:65:THR:HG22	1.90	0.72
3:C:9:HIS:CD2	3:C:12:LEU:H	2.03	0.72
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.26	0.71
2:B:47:ILE:HD13	2:B:120:MET:HE2	1.72	0.71
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.07	0.71
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.71	0.71
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.72	0.71
2:B:338:ARG:HG3	2:B:338:ARG:NH1	2.01	0.71
2:O:47:ILE:HD13	2:O:120:MET:CE	2.20	0.71
5:E:122:HIS:HB3	5:E:125:ASP:CG	2.11	0.71
3:C:245:LEU:O	4:D:201:ARG:HD2	1.91	0.71
3:P:9:HIS:CD2	3:P:12:LEU:H	2.01	0.71
2:O:399:ALA:O	2:O:402:ILE:HG22	1.90	0.70
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.06	0.70
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.72	0.70
2:O:225:ASN:O	2:O:227:ARG:HG3	1.90	0.70
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.71	0.70
2:B:202:ALA:HB3	2:B:229:GLY:O	1.91	0.70
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.71	0.70
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.22	0.70
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.55	0.70
2:O:76:THR:HG23	2:O:136:GLU:OE1	1.92	0.70
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.06	0.70
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.56	0.70
3:P:245:LEU:O	4:Q:201:ARG:HD2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.74	0.69
4:D:47:ALA:H	4:D:50:ASN:ND2	1.89	0.68
5:E:31:ASP:OD2	10:J:7:ARG:HG3	1.93	0.68
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.27	0.68
1:N:15:ASN:O	1:N:26:ALA:HA	1.93	0.68
2:B:76:THR:HG22	2:B:82:SER:N	2.02	0.68
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.26	0.68
2:O:407:SER:O	2:O:411:VAL:HG23	1.94	0.68
2:B:31:ASN:ND2	2:B:31:ASN:H	1.90	0.68
2:B:27:THR:HG22	2:B:28:LYS:N	2.07	0.68
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.94	0.68
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.76	0.68
1:N:105:ASP:O	1:N:109:VAL:HG23	1.92	0.68
2:O:101:THR:HG23	2:O:104:LYS:HE3	1.76	0.68
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.76	0.68
5:E:52:LYS:C	5:E:52:LYS:HD3	2.14	0.68
9:V:35:UNK:CG	9:V:36:UNK:H	1.89	0.67
5:R:166:ASP:OD2	5:R:170:ARG:HB2	1.95	0.67
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.75	0.67
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.59	0.67
1:A:369:LEU:HD12	1:A:392:LEU:HD11	1.75	0.67
4:D:57:THR:HG22	4:D:59:ALA:N	2.08	0.67
1:A:170:THR:HG22	1:A:171:THR:N	2.08	0.67
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.19	0.67
2:O:361:LYS:O	2:O:365:LYS:HG3	1.95	0.67
9:I:31:UNK:C	9:I:73:PRO:HG2	2.25	0.67
2:B:225:ASN:O	2:B:227:ARG:N	2.28	0.67
1:A:15:ASN:O	1:A:26:ALA:HA	1.95	0.67
10:W:7:ARG:HB3	10:W:7:ARG:NH1	2.10	0.67
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.30	0.67
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.75	0.66
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.11	0.66
4:D:62:LYS:O	4:D:66:GLU:HG3	1.95	0.66
9:I:70:LEU:HD23	9:I:71:ASN:N	2.10	0.66
5:R:186:GLN:HE21	5:R:188:VAL:HG13	1.59	0.66
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.31	0.66
3:P:153:ALA:HB2	3:P:288:LYS:HG2	1.78	0.66
1:A:281:ASP:CG	9:I:33:UNK:HB2	2.15	0.66
5:R:31:ASP:OD2	10:W:7:ARG:HG3	1.96	0.66
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.26	0.66
10:J:7:ARG:NH1	10:J:7:ARG:HB3	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:3004:CDL:HA32	7:T:40:ARG:HB3	1.77	0.66
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.77	0.66
9:I:64:LEU:HD12	9:I:77:ARG:O	1.95	0.66
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.77	0.66
2:B:62:ASN:O	2:B:65:THR:HG22	1.96	0.66
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.28	0.65
1:N:402:VAL:HG22	1:N:406:MET:CE	2.25	0.65
9:I:70:LEU:HD23	9:I:71:ASN:H	1.61	0.65
5:E:190:ASP:C	5:E:192:LEU:H	1.98	0.65
2:B:306:PRO:HA	9:I:52:ARG:CG	2.27	0.65
1:N:282:ARG:HH21	9:V:36:UNK:HA	1.61	0.65
5:E:127:VAL:HG12	5:E:128:LYS:N	2.11	0.65
4:Q:62:LYS:O	4:Q:66:GLU:HG3	1.96	0.65
3:C:45:GLN:HB3	12:C:501:HEM:HAB	1.78	0.65
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.78	0.65
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.77	0.65
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.78	0.65
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.31	0.64
2:O:219:VAL:O	2:O:223:PHE:HB2	1.97	0.64
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.26	0.64
2:O:59:THR:HG22	2:O:61:ALA:H	1.62	0.64
12:P:502:HEM:HMC2	12:P:502:HEM:HBC2	1.79	0.64
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.78	0.64
4:Q:57:THR:HG22	4:Q:59:ALA:N	2.12	0.64
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.12	0.64
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.80	0.64
2:O:18:CYS:HB2	2:O:19:PRO:CD	2.27	0.64
2:O:273:SER:O	2:O:276:GLN:HB3	1.97	0.64
5:R:52:LYS:HD3	5:R:52:LYS:C	2.17	0.64
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.79	0.64
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.80	0.64
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.33	0.64
3:C:101:ARG:C	3:C:101:ARG:HD2	2.17	0.64
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.13	0.64
3:P:342:GLN:NE2	3:P:343:PRO:HD2	2.13	0.64
1:N:170:THR:HG22	1:N:172:GLU:H	1.62	0.64
9:V:70:LEU:HD23	9:V:71:ASN:N	2.14	0.64
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.32	0.63
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.12	0.63
1:A:178:THR:HG22	1:A:180:ALA:N	2.07	0.63
2:B:31:ASN:N	2:B:31:ASN:ND2	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:THR:HG23	1:A:205:HIS:NE2	2.14	0.63
10:W:7:ARG:HH11	10:W:7:ARG:CB	2.11	0.63
2:O:160:LEU:HD12	9:V:64:LEU:HD13	1.79	0.63
5:E:78:LEU:HD12	5:E:190:ASP:O	1.98	0.63
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.79	0.63
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.81	0.63
10:J:7:ARG:HH11	10:J:7:ARG:CB	2.11	0.63
2:B:38:LEU:HD12	2:B:39:GLU:N	2.14	0.63
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.63	0.63
1:A:4:TYR:HB3	2:B:114:ASP:OD2	1.99	0.63
3:P:236:MET:O	3:P:239:PRO:HD2	1.99	0.62
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.81	0.62
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.28	0.62
2:O:248:ASN:HD21	2:O:250:HIS:HB2	1.64	0.62
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.82	0.62
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.80	0.62
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.34	0.62
1:A:60:GLU:OE2	1:A:90:THR:HG22	2.00	0.62
1:A:106:MET:HG3	1:A:203:ILE:CD1	2.29	0.62
2:O:217:LYS:O	2:O:221:GLU:HG2	1.99	0.62
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.29	0.62
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.00	0.62
2:O:353:THR:HG22	2:O:355:GLU:N	2.02	0.62
1:A:7:THR:HG21	2:B:113:ARG:CD	2.30	0.62
5:R:135:LEU:HD23	5:R:182:VAL:HG22	1.82	0.62
5:E:83:GLU:HB3	5:E:102:THR:CG2	2.29	0.62
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.80	0.62
8:U:28:GLU:O	8:U:32:LYS:HG3	1.99	0.62
3:P:25:PRO:HB2	3:P:28:ILE:HG23	1.82	0.62
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.00	0.61
7:T:79:ASN:O	7:T:80:ASP:HB2	2.00	0.61
1:A:69:LYS:HD2	1:A:70:ARG:NH2	2.10	0.61
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.81	0.61
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.81	0.61
2:B:407:SER:O	2:B:411:VAL:HG23	2.00	0.61
2:B:353:THR:HG22	2:B:355:GLU:N	2.04	0.61
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.82	0.61
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.80	0.61
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.30	0.61
2:B:338:ARG:HH11	2:B:338:ARG:CG	2.10	0.61
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.36	0.61
1:N:182:LEU:O	1:N:186:ILE:HG13	2.01	0.61
3:C:236:MET:O	3:C:239:PRO:HD2	1.99	0.61
2:B:292:THR:O	2:B:292:THR:HG22	2.00	0.61
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.83	0.61
8:H:18:THR:O	8:H:22:GLU:HG3	2.01	0.61
8:H:28:GLU:O	8:H:32:LYS:HG3	2.01	0.61
5:E:130:PRO:HG2	5:E:131:GLU:H	1.66	0.61
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.16	0.60
2:B:215:ASP:O	2:B:219:VAL:HG23	2.01	0.60
5:R:83:GLU:HG3	5:R:100:HIS:CE1	2.37	0.60
1:A:282:ARG:HH21	9:I:35:UNK:HA	1.67	0.60
1:N:136:GLN:OE1	9:V:50:LEU:HB3	2.01	0.60
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.83	0.60
2:B:96:LEU:H	9:I:70:LEU:HD22	1.66	0.60
5:R:96:LEU:HD21	5:R:195:VAL:HG21	1.81	0.60
1:N:371:GLY:O	1:N:375:VAL:HG23	2.01	0.60
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.83	0.60
1:A:23:LEU:HD23	1:A:24:ARG:N	2.17	0.60
2:O:27:THR:CG2	2:O:28:LYS:H	2.14	0.60
5:R:83:GLU:HA	5:R:100:HIS:HB3	1.83	0.60
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.69	0.60
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.34	0.60
1:N:219:VAL:HG12	1:N:220:SER:N	2.16	0.60
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.65	0.60
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.83	0.60
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.37	0.60
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.37	0.60
5:R:117:LEU:HD11	5:R:172:ARG:NH1	2.16	0.59
1:N:178:THR:HG22	1:N:180:ALA:N	2.08	0.59
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.37	0.59
3:P:22:LEU:HD21	14:P:3002:UQ:HM32	1.83	0.59
8:H:28:GLU:HG2	8:H:32:LYS:HE3	1.85	0.59
6:S:17:ARG:HG2	6:S:17:ARG:HH11	1.68	0.59
5:R:109:GLU:OE1	5:R:123:ASP:HB2	2.02	0.59
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.83	0.59
2:B:59:THR:HG22	2:B:61:ALA:H	1.66	0.59
5:R:81:ILE:HG12	5:R:87:VAL:HG21	1.84	0.59
5:E:122:HIS:HE1	5:E:124:LEU:HD12	1.68	0.59
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.02	0.59
5:E:116:LYS:HD2	5:E:116:LYS:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:27:THR:O	8:H:31:VAL:HG23	2.02	0.59
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.68	0.59
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.84	0.59
3:P:313:GLN:NE2	6:S:36:THR:OG1	2.36	0.59
15:C:2004:CDL:HA32	7:G:40:ARG:HB3	1.85	0.59
1:N:10:ASN:CG	2:O:19:PRO:HD2	2.21	0.59
1:N:69:LYS:HD2	1:N:70:ARG:NH2	2.15	0.59
5:R:171:ILE:HG12	5:R:176:ALA:O	2.02	0.59
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.84	0.59
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.85	0.59
8:U:27:THR:O	8:U:31:VAL:HG23	2.02	0.59
5:E:101:ARG:HA	5:E:105:GLU:OE1	2.03	0.59
2:B:361:LYS:O	2:B:365:LYS:HG3	2.02	0.59
5:R:76:ILE:O	5:R:193:VAL:HG12	2.03	0.59
5:E:163:SER:HA	5:E:174:GLY:HA3	1.85	0.59
1:A:170:THR:HG22	1:A:172:GLU:H	1.68	0.58
3:P:34:PHE:HB2	20:P:381:HOH:O	2.03	0.58
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.33	0.58
2:B:207:VAL:HG21	2:B:383:GLY:HA3	1.86	0.58
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.17	0.58
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.84	0.58
5:E:147:ILE:O	5:E:156:TYR:HA	2.04	0.58
2:B:341:MET:HA	2:B:341:MET:CE	2.34	0.58
1:A:430:GLN:HG3	7:G:4:PHE:O	2.03	0.58
1:N:63:ALA:O	1:N:116:VAL:HG13	2.03	0.58
1:N:282:ARG:NH2	9:V:37:UNK:N	2.51	0.58
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.39	0.58
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.67	0.58
8:U:27:THR:HG22	8:U:29:LYS:H	1.67	0.58
2:O:422:LYS:O	2:O:436:LEU:HD21	2.02	0.58
1:A:103:SER:HB3	1:A:202:GLY:O	2.04	0.58
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.51	0.58
1:N:112:LEU:O	1:N:116:VAL:HG23	2.03	0.58
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.85	0.58
2:O:248:ASN:C	2:O:248:ASN:ND2	2.56	0.58
5:E:187:PHE:C	5:E:189:GLY:H	2.06	0.58
1:N:60:GLU:OE2	1:N:90:THR:HG22	2.03	0.58
1:A:371:GLY:O	1:A:375:VAL:HG23	2.04	0.58
2:B:101:THR:HG23	2:B:104:LYS:HE3	1.86	0.58
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.86	0.58
5:E:106:ILE:C	5:E:110:ALA:HB3	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:414:ALA:O	2:O:418:VAL:HG23	2.04	0.58
1:A:402:VAL:HG22	1:A:406:MET:CE	2.34	0.58
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.84	0.58
5:E:76:ILE:O	5:E:193:VAL:HG12	2.04	0.58
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.34	0.58
3:P:313:GLN:HE21	6:S:36:THR:CB	2.17	0.58
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.34	0.58
2:O:341:MET:CE	2:O:417:PHE:HE2	2.15	0.57
5:E:99:ARG:HD3	5:E:105:GLU:OE2	2.03	0.57
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.34	0.57
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.86	0.57
2:O:332:HIS:O	2:O:336:VAL:HG23	2.03	0.57
2:O:215:ASP:O	2:O:219:VAL:HG23	2.04	0.57
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.38	0.57
3:C:153:ALA:HB2	3:C:288:LYS:HG2	1.85	0.57
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.39	0.57
5:R:102:THR:O	5:R:106:ILE:HG13	2.04	0.57
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.40	0.57
1:A:274:ASN:ND2	1:A:309:THR:HB	2.20	0.57
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.04	0.57
2:O:338:ARG:CG	2:O:338:ARG:HH11	2.09	0.57
3:C:147:ILE:CG1	13:C:2001:JZV:HAP	2.29	0.57
5:E:84:GLY:N	5:E:100:HIS:O	2.33	0.57
5:E:130:PRO:HG2	5:E:131:GLU:CD	2.25	0.57
1:A:178:THR:CG2	1:A:179:ARG:N	2.68	0.57
3:C:30:ALA:HB1	15:D:2003:CDL:H111	1.86	0.57
2:B:150:VAL:O	2:B:153:GLN:HG3	2.05	0.57
4:D:231:LYS:O	6:F:71:LYS:HE3	2.05	0.57
6:S:91:GLU:HG2	6:S:95:LYS:HE3	1.86	0.57
6:S:95:LYS:O	6:S:99:ARG:HG3	2.03	0.57
5:E:136:VAL:CG2	5:E:183:PRO:HD3	2.33	0.57
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.87	0.57
7:G:65:GLU:O	7:G:69:LEU:HG	2.04	0.57
5:R:86:ASN:OD1	5:R:99:ARG:HB2	2.05	0.57
2:O:292:THR:HG22	2:O:292:THR:O	2.02	0.57
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.20	0.57
1:A:364:ALA:O	1:A:368:GLN:HG3	2.05	0.57
4:Q:2:GLU:O	4:Q:3:LEU:O	2.22	0.57
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.86	0.56
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.87	0.56
2:B:357:VAL:O	2:B:361:LYS:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:364:ALA:O	1:N:368:GLN:HG3	2.05	0.56
2:O:341:MET:HE2	2:O:341:MET:HA	1.85	0.56
5:R:186:GLN:O	5:R:193:VAL:HG23	2.04	0.56
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.86	0.56
2:B:31:ASN:HD22	2:B:31:ASN:H	1.48	0.56
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.70	0.56
1:N:430:GLN:HG3	7:T:4:PHE:O	2.05	0.56
4:Q:169:LEU:HD22	4:Q:182:ILE:HD11	1.87	0.56
1:N:36:THR:HG21	1:N:373:THR:HA	1.86	0.56
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.45	0.56
2:O:299:VAL:HG11	2:O:336:VAL:HG13	1.86	0.56
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.87	0.56
7:G:28:ASN:HB3	7:G:31:SER:OG	2.06	0.56
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.35	0.56
9:V:70:LEU:HD23	9:V:71:ASN:OD1	2.06	0.56
2:B:332:HIS:O	2:B:336:VAL:HG23	2.06	0.56
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.45	0.56
1:N:178:THR:CG2	1:N:179:ARG:N	2.68	0.56
5:R:106:ILE:O	5:R:109:GLU:HB3	2.05	0.56
9:V:64:LEU:HD12	9:V:77:ARG:C	2.26	0.56
3:C:301:ILE:CD1	3:C:364:LEU:HD21	2.34	0.56
1:N:170:THR:CG2	1:N:171:THR:N	2.68	0.56
1:N:382:HIS:HB3	1:N:388:ARG:O	2.06	0.56
1:A:395:TRP:CE3	1:A:395:TRP:HA	2.41	0.56
2:B:414:ALA:O	2:B:418:VAL:HG23	2.06	0.56
5:E:109:GLU:OE2	5:E:153:PHE:HB3	2.06	0.56
1:N:279:ARG:HH22	9:V:30:UNK:C	2.19	0.56
2:B:28:LYS:O	2:B:29:LEU:O	2.24	0.56
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.88	0.56
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.70	0.56
1:N:187:ASP:O	1:N:191:LYS:HE3	2.06	0.56
6:S:53:ASP:OD1	6:S:54:LEU:N	2.39	0.56
2:O:38:LEU:HD12	2:O:39:GLU:N	2.21	0.55
2:O:402:ILE:HD13	2:O:402:ILE:C	2.27	0.55
5:R:186:GLN:NE2	5:R:188:VAL:HG13	2.20	0.55
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.41	0.55
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.89	0.55
15:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.07	0.55
2:B:23:ASP:OD1	2:B:24:LEU:N	2.38	0.55
5:R:117:LEU:HD21	5:R:172:ARG:NH1	2.21	0.55
2:B:201:SER:OG	2:B:228:SER:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:150:VAL:O	2:O:153:GLN:HG3	2.06	0.55
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.71	0.55
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.40	0.55
1:N:4:TYR:HB3	2:O:114:ASP:OD2	2.07	0.55
1:N:170:THR:HG22	1:N:171:THR:H	1.71	0.55
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.22	0.55
2:O:397:VAL:O	2:O:401:LYS:HG2	2.07	0.55
9:I:29:UNK:O	9:I:30:UNK:HB2	2.05	0.55
5:R:118:ARG:NH1	5:R:174:GLY:O	2.40	0.55
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.46	0.55
1:A:282:ARG:NH2	9:I:35:UNK:HA	2.22	0.55
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.87	0.55
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.06	0.55
17:Q:501:HEC:HMB1	17:Q:501:HEC:HBB3	1.89	0.55
2:B:248:ASN:HD21	2:B:250:HIS:HB2	1.71	0.55
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.41	0.55
5:E:106:ILE:O	5:E:110:ALA:HB3	2.07	0.55
1:A:187:ASP:O	1:A:191:LYS:HE3	2.07	0.55
3:C:301:ILE:HD11	3:C:364:LEU:CD2	2.34	0.55
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.89	0.55
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.72	0.55
2:O:341:MET:HA	2:O:341:MET:CE	2.37	0.55
2:B:422:LYS:O	2:B:436:LEU:HD21	2.06	0.55
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.71	0.55
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.39	0.55
2:B:338:ARG:CG	2:B:338:ARG:NH1	2.69	0.55
15:Q:3003:CDL:HB22	7:T:40:ARG:NH2	2.22	0.55
3:P:78:TRP:CZ3	4:Q:201:ARG:HG3	2.42	0.55
8:U:28:GLU:HG2	8:U:32:LYS:HE3	1.89	0.55
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.88	0.55
2:O:152:PHE:HA	2:O:157:VAL:HG11	1.88	0.55
2:O:338:ARG:NH1	2:O:338:ARG:CG	2.68	0.54
1:N:10:ASN:ND2	2:O:19:PRO:CD	2.70	0.54
3:C:286:PRO:O	3:C:287:ASN:HB2	2.08	0.54
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.22	0.54
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.07	0.54
2:O:152:PHE:HA	2:O:157:VAL:CG1	2.37	0.54
8:U:18:THR:O	8:U:22:GLU:HG3	2.07	0.54
2:O:31:ASN:N	2:O:31:ASN:HD22	2.05	0.54
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.88	0.54
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:233:ARG:HH21	1:N:316:ASP:HB2	1.73	0.54
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.71	0.54
5:E:146:PRO:HG2	5:E:180:LEU:HD21	1.89	0.54
2:O:357:VAL:O	2:O:361:LYS:HG3	2.07	0.54
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.88	0.54
5:E:135:LEU:HD11	5:E:169:GLY:HA3	1.88	0.54
5:E:188:VAL:HG12	5:E:188:VAL:O	2.08	0.54
2:B:76:THR:CG2	2:B:82:SER:H	2.06	0.54
5:R:184:THR:O	5:R:185:TYR:HB3	2.07	0.54
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.22	0.54
3:P:199:THR:HA	18:P:2010:BOG:O1	2.08	0.54
2:B:124:LEU:HD11	2:B:223:PHE:CB	2.33	0.54
4:Q:70:VAL:HG21	4:Q:83:ARG:CZ	2.38	0.54
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.89	0.54
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.10	0.54
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.37	0.54
2:O:374:THR:HG22	2:O:376:GLN:H	1.72	0.54
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.43	0.54
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.42	0.54
6:F:53:ASP:OD1	6:F:54:LEU:N	2.39	0.54
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.90	0.54
10:J:7:ARG:NH1	10:J:7:ARG:CB	2.70	0.54
3:P:30:ALA:HB1	15:Q:3003:CDL:H111	1.90	0.54
5:E:84:GLY:CA	5:E:102:THR:HG23	2.38	0.53
15:P:3004:CDL:H712	11:P:3007:PEE:H50	1.90	0.53
1:N:23:LEU:HD23	1:N:24:ARG:N	2.23	0.53
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.43	0.53
1:N:209:VAL:O	1:N:212:ALA:HB3	2.07	0.53
1:N:281:ASP:HB2	9:V:33:UNK:HB2	1.91	0.53
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.90	0.53
2:B:24:LEU:HD12	2:B:37:SER:O	2.07	0.53
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.74	0.53
10:J:56:LYS:O	10:J:60:GLU:HB2	2.08	0.53
1:A:151:ASP:OD2	5:E:2:HIS:NE2	2.28	0.53
3:C:263:LEU:O	3:C:264:VAL:HG23	2.08	0.53
11:R:3005:PEE:H58	10:W:24:VAL:HG11	1.90	0.53
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.88	0.53
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.73	0.53
1:A:36:THR:HG21	1:A:373:THR:HA	1.91	0.53
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.43	0.53
7:T:65:GLU:O	7:T:69:LEU:HG	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:2003:CDL:HB22	7:G:40:ARG:NH2	2.23	0.53
8:U:22:GLU:O	8:U:26:GLN:HG2	2.08	0.53
2:O:372:VAL:O	2:O:372:VAL:HG12	2.08	0.53
5:R:119:ASP:HB3	5:R:179:ASN:HD21	1.74	0.53
1:A:105:ASP:O	1:A:109:VAL:HG23	2.08	0.53
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.38	0.53
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.90	0.53
5:E:165:TYR:HA	5:E:170:ARG:O	2.09	0.53
4:D:70:VAL:HG21	4:D:83:ARG:CZ	2.39	0.53
3:C:45:GLN:CB	12:C:501:HEM:HAB	2.38	0.53
3:C:127:THR:HG21	12:C:501:HEM:HBB2	1.91	0.53
1:A:170:THR:CG2	1:A:171:THR:N	2.72	0.53
2:B:36:ALA:HB3	2:B:207:VAL:HG13	1.91	0.53
9:I:65:VAL:HG12	9:I:66:ALA:N	2.24	0.53
2:B:189:GLU:OE1	2:B:189:GLU:N	2.42	0.53
5:E:101:ARG:HB2	5:E:131:GLU:HA	1.90	0.53
2:B:152:PHE:HA	2:B:157:VAL:HG11	1.91	0.53
2:O:124:LEU:HD11	2:O:223:PHE:HB3	1.91	0.53
2:B:374:THR:HG22	2:B:376:GLN:H	1.74	0.53
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.90	0.53
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.90	0.53
1:A:358:LYS:HE3	1:A:399:ILE:O	2.08	0.53
5:R:131:GLU:N	5:R:131:GLU:OE1	2.40	0.53
1:N:7:THR:HG21	2:O:113:ARG:CD	2.38	0.52
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.91	0.52
2:O:299:VAL:CG1	2:O:336:VAL:HG13	2.39	0.52
10:W:52:TRP:O	10:W:56:LYS:HB2	2.09	0.52
6:F:84:GLU:CD	6:F:84:GLU:H	2.12	0.52
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.72	0.52
8:H:27:THR:HG22	8:H:29:LYS:H	1.74	0.52
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.73	0.52
2:B:152:PHE:HA	2:B:157:VAL:CG1	2.40	0.52
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.90	0.52
4:D:169:LEU:HD23	4:D:169:LEU:C	2.30	0.52
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.92	0.52
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.44	0.52
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.39	0.52
1:N:331:ILE:CG2	1:N:431:LEU:HB2	2.38	0.52
4:Q:43:MET:HE1	4:Q:91:PHE:HE2	1.75	0.52
5:R:164:HIS:CD2	5:R:173:LYS:HB3	2.45	0.52
1:A:280:TYR:CG	1:A:281:ASP:N	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.09	0.52
4:D:47:ALA:HA	4:D:90:TYR:HA	1.91	0.52
4:D:68:VAL:HG11	4:D:92:PRO:HG3	1.91	0.52
3:C:313:GLN:HE21	6:F:36:THR:CB	2.22	0.52
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.92	0.52
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.39	0.52
2:B:372:VAL:O	2:B:372:VAL:HG12	2.09	0.52
3:P:286:PRO:O	3:P:287:ASN:HB2	2.09	0.52
5:R:113:ASP:HB2	5:R:116:LYS:HB2	1.92	0.52
4:Q:167:GLU:CG	8:U:13:LEU:HD12	2.40	0.52
3:P:127:THR:HG21	12:P:501:HEM:HBB2	1.90	0.52
5:E:102:THR:O	5:E:103:GLN:HG3	2.10	0.52
5:E:78:LEU:HD11	5:E:187:PHE:CD2	2.45	0.52
2:B:59:THR:HG22	2:B:60:THR:N	2.25	0.52
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.44	0.52
1:N:317:THR:HG23	1:N:318:GLY:N	2.25	0.52
1:N:358:LYS:HE3	1:N:399:ILE:O	2.09	0.52
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.90	0.52
8:U:43:ARG:O	8:U:47:ARG:HG3	2.09	0.52
14:P:3002:UQ:HM51	14:P:3002:UQ:C8	2.40	0.52
9:V:65:VAL:HG12	9:V:66:ALA:N	2.25	0.52
5:E:114:VAL:HG21	5:E:172:ARG:NH1	2.24	0.52
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.45	0.52
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.92	0.52
2:O:222:GLN:HG2	2:O:222:GLN:O	2.10	0.52
7:T:48:VAL:O	7:T:51:PRO:HD2	2.10	0.52
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.10	0.52
8:H:10:GLU:O	8:H:11:GLU:HG3	2.10	0.52
1:N:173:ASN:O	1:N:177:LEU:HG	2.10	0.52
1:A:288:LYS:HE3	1:A:289:HIS:CE1	2.45	0.52
3:P:301:ILE:HD11	3:P:364:LEU:CD2	2.35	0.51
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.75	0.51
5:E:135:LEU:HD23	5:E:182:VAL:HG22	1.92	0.51
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.92	0.51
1:A:222:THR:OG1	1:A:225:GLU:HG3	2.09	0.51
3:C:31:TRP:NE1	11:C:2007:PEE:O4	2.43	0.51
2:B:402:ILE:HD13	2:B:402:ILE:C	2.31	0.51
6:S:91:GLU:O	6:S:95:LYS:HG3	2.09	0.51
5:R:163:SER:H	5:R:175:PRO:HD2	1.75	0.51
2:O:203:ARG:HD2	2:O:230:ALA:O	2.10	0.51
1:N:131:ARG:NH2	1:N:177:LEU:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:VAL:HG23	2:B:316:TYR:C	2.30	0.51
3:C:279:TYR:O	3:C:283:ARG:HG3	2.10	0.51
2:O:395:PRO:HA	2:O:398:VAL:HG12	1.91	0.51
1:N:140:GLU:HG3	9:V:50:LEU:HD12	1.92	0.51
4:Q:2:GLU:HB3	4:Q:3:LEU:HD12	1.91	0.51
4:D:169:LEU:HD22	4:D:182:ILE:HD11	1.92	0.51
1:N:45:SER:HA	1:N:48:GLU:HG3	1.92	0.51
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.93	0.51
10:W:40:ASP:O	10:W:44:GLU:HG3	2.09	0.51
4:D:102:ARG:HB3	4:D:107:GLY:HA2	1.92	0.51
2:O:248:ASN:ND2	2:O:250:HIS:H	2.09	0.51
3:C:78:TRP:CZ3	4:D:201:ARG:HG3	2.45	0.51
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.46	0.51
1:A:140:GLU:OE2	9:I:49:LEU:HA	2.10	0.51
4:Q:68:VAL:HG11	4:Q:92:PRO:HG3	1.93	0.51
3:P:9:HIS:CD2	3:P:12:LEU:HG	2.46	0.51
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.33	0.51
5:R:77:LYS:HA	5:R:191:ASP:O	2.10	0.51
5:R:78:LEU:HD11	5:R:187:PHE:CD1	2.46	0.51
5:E:190:ASP:O	5:E:192:LEU:N	2.43	0.51
2:O:207:VAL:HG21	2:O:383:GLY:HA3	1.93	0.51
2:B:57:TYR:CD1	2:B:57:TYR:N	2.78	0.51
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.45	0.51
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.11	0.51
2:O:57:TYR:N	2:O:57:TYR:CD1	2.78	0.51
2:O:26:ILE:O	2:O:26:ILE:HG12	2.09	0.51
2:B:248:ASN:ND2	2:B:248:ASN:C	2.59	0.51
2:B:402:ILE:HG23	2:B:403:ASP:N	2.26	0.51
6:S:11:ARG:HA	6:S:14:ASP:HB2	1.93	0.51
10:W:7:ARG:NH1	10:W:7:ARG:CB	2.72	0.50
2:O:222:GLN:O	2:O:223:PHE:CD2	2.64	0.50
9:I:71:ASN:HD22	9:I:71:ASN:H	1.59	0.50
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.46	0.50
2:B:299:VAL:CG1	2:B:336:VAL:HG13	2.40	0.50
2:O:43:PRO:O	2:O:113:ARG:HG3	2.11	0.50
6:S:13:MET:HA	6:S:16:ILE:HD12	1.93	0.50
9:I:49:LEU:HD22	9:I:54:SER:HB3	1.93	0.50
1:A:331:ILE:CG2	1:A:431:LEU:HB2	2.40	0.50
1:N:368:GLN:O	1:N:369:LEU:HD23	2.12	0.50
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.41	0.50
2:O:361:LYS:HA	2:O:402:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:10:ASN:HD21	2:O:19:PRO:HD2	1.75	0.50
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.41	0.50
5:R:165:TYR:HA	5:R:170:ARG:O	2.11	0.50
1:N:17:THR:HG23	1:N:205:HIS:NE2	2.27	0.50
3:C:207:ASN:ND2	3:C:208:ASN:H	2.10	0.50
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.30	0.50
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.94	0.50
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.46	0.50
3:P:147:ILE:CG1	13:P:3001:JZV:HAP	2.32	0.50
2:B:402:ILE:HG23	2:B:403:ASP:H	1.77	0.50
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.30	0.50
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.47	0.50
5:E:101:ARG:NH2	5:E:130:PRO:O	2.45	0.50
14:C:2002:UQ:HM51	14:C:2002:UQ:C8	2.41	0.50
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.41	0.50
3:P:45:GLN:HB3	12:P:501:HEM:HAB	1.94	0.50
1:A:62:LEU:HD11	1:A:127:ILE:HG12	1.94	0.50
5:R:185:TYR:HB3	5:R:195:VAL:HA	1.94	0.50
3:P:6:ARG:HG2	3:P:16:ASN:HB2	1.92	0.50
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.93	0.50
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.94	0.50
2:B:395:PRO:O	2:B:398:VAL:HG12	2.11	0.50
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.42	0.50
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.94	0.50
1:N:151:ASP:OD2	5:R:2:HIS:NE2	2.30	0.50
17:D:501:HEC:HBB3	17:D:501:HEC:HMB1	1.94	0.50
1:A:362:ARG:O	1:A:365:MET:HG2	2.11	0.50
2:B:259:THR:HG22	2:B:260:GLU:N	2.26	0.50
4:D:167:GLU:HG3	8:H:13:LEU:CD2	2.41	0.50
9:V:33:UNK:HA	9:V:73:PRO:HB3	1.94	0.49
9:I:38:UNK:O	9:I:39:UNK:C	2.59	0.49
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.94	0.49
1:N:158:PHE:O	1:N:164:ALA:HB2	2.12	0.49
5:R:178:TYR:N	5:R:178:TYR:CD1	2.80	0.49
2:O:76:THR:HG22	2:O:82:SER:N	2.02	0.49
2:O:334:GLY:O	2:O:338:ARG:HG2	2.12	0.49
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.94	0.49
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.93	0.49
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.41	0.49
2:B:33:LEU:CD2	2:B:224:LEU:HD12	2.37	0.49
2:O:52:LYS:O	2:O:203:ARG:NH2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.94	0.49
4:Q:21:LEU:HD21	4:Q:191:ARG:HG3	1.93	0.49
3:P:238:THR:HB	3:P:239:PRO:CD	2.37	0.49
3:P:138:GLN:HB2	3:P:255:GLU:O	2.12	0.49
2:B:287:ARG:HB3	9:I:53:GLU:HG3	1.94	0.49
2:B:26:ILE:O	2:B:26:ILE:HG12	2.12	0.49
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.52	0.49
3:P:301:ILE:CD1	3:P:364:LEU:HD21	2.36	0.49
2:B:402:ILE:O	2:B:405:VAL:HG23	2.13	0.49
7:T:28:ASN:HB3	7:T:31:SER:OG	2.13	0.49
1:N:362:ARG:O	1:N:365:MET:HG2	2.12	0.49
3:P:159:HIS:O	3:P:163:GLU:HG3	2.13	0.49
1:A:307:PHE:C	1:A:307:PHE:CD1	2.85	0.49
5:E:106:ILE:O	5:E:106:ILE:HG22	2.12	0.49
1:A:131:ARG:NH2	1:A:177:LEU:O	2.45	0.49
4:Q:200:GLN:NE2	18:Q:3091:BOG:H5	2.28	0.49
6:S:40:ASP:O	6:S:44:LYS:HG3	2.13	0.49
5:E:130:PRO:HG2	5:E:131:GLU:OE2	2.11	0.49
2:B:397:VAL:O	2:B:401:LYS:HG2	2.13	0.49
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.48	0.49
3:C:263:LEU:O	3:C:264:VAL:CG2	2.61	0.49
4:D:43:MET:HE1	4:D:91:PHE:HE2	1.78	0.49
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.31	0.49
3:C:34:PHE:HB2	20:C:381:HOH:O	2.12	0.49
5:R:95:PRO:HG2	5:R:145:VAL:HG11	1.94	0.49
5:E:127:VAL:O	5:E:128:LYS:HB2	2.13	0.49
5:E:122:HIS:HB3	5:E:125:ASP:OD1	2.13	0.49
4:D:21:LEU:HD21	4:D:191:ARG:HG3	1.94	0.49
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.76	0.49
3:C:138:GLN:HB2	3:C:255:GLU:O	2.13	0.49
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.95	0.49
7:G:36:ASN:O	7:G:40:ARG:HG3	2.13	0.49
1:A:205:HIS:O	1:A:208:LEU:HB3	2.13	0.49
1:A:173:ASN:O	1:A:177:LEU:HG	2.13	0.49
2:B:334:GLY:O	2:B:338:ARG:HG2	2.13	0.48
15:C:2004:CDL:OA4	7:G:40:ARG:HD2	2.13	0.48
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.94	0.48
1:N:64:PHE:HE2	1:N:86:PHE:CE1	2.31	0.48
2:O:325:TYR:CD1	9:V:60:ALA:HB3	2.48	0.48
1:N:402:VAL:HG22	1:N:406:MET:HE1	1.93	0.48
10:J:52:TRP:O	10:J:56:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:HG22	1:A:96:ALA:N	2.28	0.48
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.94	0.48
10:J:49:GLY:N	10:J:54:HIS:ND1	2.61	0.48
5:R:73:LYS:HB3	5:R:196:GLY:O	2.14	0.48
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.47	0.48
6:S:84:GLU:H	6:S:84:GLU:CD	2.15	0.48
5:E:178:TYR:HD1	5:E:178:TYR:H	1.61	0.48
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.53	0.48
5:E:131:GLU:H	5:E:131:GLU:CD	2.17	0.48
5:E:187:PHE:C	5:E:189:GLY:N	2.66	0.48
1:N:46:ARG:NH1	1:N:316:ASP:OD1	2.36	0.48
1:A:422:LEU:HD22	1:A:437:ILE:CD1	2.42	0.48
5:E:3:ASN:HD22	5:E:3:ASN:H	1.62	0.48
1:A:182:LEU:O	1:A:186:ILE:HG13	2.13	0.48
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.76	0.48
3:P:207:ASN:ND2	3:P:208:ASN:H	2.12	0.48
7:T:29:ILE:O	7:T:33:ALA:HB3	2.13	0.48
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.48	0.48
2:O:248:ASN:HD22	2:O:249:GLY:N	2.12	0.48
4:D:167:GLU:HG3	8:H:13:LEU:HD22	1.96	0.48
1:N:222:THR:OG1	1:N:225:GLU:HG3	2.13	0.48
1:N:49:ASN:ND2	1:N:51:LYS:H	2.12	0.48
2:B:89:ILE:HD13	2:B:96:LEU:HB2	1.96	0.48
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.48	0.48
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.96	0.48
6:F:40:ASP:O	6:F:44:LYS:HG3	2.14	0.48
6:S:16:ILE:O	6:S:19:TRP:HB3	2.14	0.48
6:F:13:MET:O	6:F:17:ARG:HG3	2.12	0.48
10:W:49:GLY:N	10:W:54:HIS:ND1	2.61	0.48
4:Q:195:GLU:OE1	4:Q:201:ARG:NH2	2.46	0.48
5:E:78:LEU:HD11	5:E:187:PHE:CE2	2.48	0.48
2:B:295:LEU:O	2:B:299:VAL:HG23	2.14	0.48
2:O:164:HIS:O	2:O:173:ALA:HA	2.14	0.48
5:E:185:TYR:O	5:E:186:GLN:HB3	2.14	0.48
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.49	0.48
1:N:269:VAL:HG22	1:N:406:MET:HE2	1.95	0.48
2:B:437:ASP:OD1	2:B:437:ASP:C	2.52	0.48
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.96	0.47
1:N:402:VAL:HG22	1:N:406:MET:HE2	1.93	0.47
5:E:190:ASP:C	5:E:192:LEU:N	2.67	0.47
7:T:80:ASP:HB3	8:U:47:ARG:HH11	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:70:VAL:HG21	4:Q:83:ARG:NH2	2.28	0.47
1:N:433:ASP:OD1	1:N:436:ARG:HG2	2.13	0.47
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.49	0.47
3:C:6:ARG:HG2	3:C:16:ASN:HB2	1.95	0.47
5:E:141:HIS:HB2	5:E:176:ALA:CB	2.42	0.47
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.95	0.47
1:A:37:VAL:HG22	1:A:109:VAL:HG11	1.96	0.47
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.14	0.47
1:N:48:GLU:CD	1:N:54:GLY:H	2.18	0.47
1:N:217:SER:O	1:N:218:GLY:C	2.52	0.47
5:E:141:HIS:HB3	19:E:501:FES:S2	2.54	0.47
1:A:178:THR:HG22	1:A:179:ARG:N	2.29	0.47
1:N:170:THR:CG2	1:N:171:THR:H	2.27	0.47
3:P:28:ILE:HG12	3:P:225:TYR:OH	2.15	0.47
5:E:116:LYS:HD2	5:E:116:LYS:H	1.78	0.47
4:D:220:TYR:O	4:D:224:ARG:HG2	2.14	0.47
4:D:186:VAL:O	4:D:190:LEU:HG	2.14	0.47
3:C:28:ILE:CD1	14:C:2002:UQ:HM21	2.44	0.47
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.44	0.47
1:N:53:ASN:HB3	1:N:173:ASN:ND2	2.29	0.47
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.14	0.47
1:N:137:GLU:O	1:N:141:MET:HG3	2.13	0.47
1:A:382:HIS:HB3	1:A:388:ARG:O	2.13	0.47
3:P:6:ARG:HD3	3:P:16:ASN:OD1	2.14	0.47
5:E:178:TYR:CD1	5:E:178:TYR:N	2.83	0.47
8:H:43:ARG:O	8:H:47:ARG:HG3	2.15	0.47
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.14	0.47
1:N:178:THR:HG22	1:N:179:ARG:N	2.29	0.47
9:I:34:UNK:CG	9:I:35:UNK:N	2.70	0.47
2:O:89:ILE:HD13	2:O:96:LEU:HB2	1.95	0.47
2:O:295:LEU:O	2:O:299:VAL:HG23	2.14	0.47
2:O:395:PRO:O	2:O:398:VAL:HG12	2.14	0.47
2:O:73:SER:N	2:O:74:PRO:HD2	2.29	0.47
5:E:77:LYS:HG3	5:E:191:ASP:O	2.13	0.47
5:E:155:GLY:HA3	5:E:166:ASP:O	2.15	0.47
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.47	0.47
2:O:221:GLU:C	2:O:223:PHE:H	2.17	0.47
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.45	0.47
2:B:361:LYS:HA	2:B:402:ILE:HD11	1.96	0.47
2:O:374:THR:HG22	2:O:376:GLN:N	2.29	0.47
2:O:402:ILE:HG23	2:O:403:ASP:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:161:ALA:O	4:Q:162:PRO:C	2.53	0.47
1:N:342:TRP:O	1:N:345:LEU:HB2	2.15	0.47
5:E:41:ALA:O	5:E:45:VAL:HG23	2.15	0.47
5:E:135:LEU:CD1	5:E:169:GLY:HA3	2.44	0.47
1:N:205:HIS:O	1:N:209:VAL:HG12	2.15	0.47
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.49	0.47
2:O:122:TYR:O	2:O:126:VAL:HG23	2.14	0.47
1:A:217:SER:O	1:A:218:GLY:C	2.52	0.47
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.95	0.47
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.50	0.47
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.77	0.47
1:N:307:PHE:CD1	1:N:307:PHE:C	2.86	0.47
3:P:31:TRP:NE1	11:P:3007:PEE:O4	2.48	0.47
5:R:112:VAL:HG21	5:R:170:ARG:NH2	2.29	0.47
8:H:28:GLU:CG	8:H:32:LYS:HE3	2.44	0.47
2:O:31:ASN:ND2	2:O:31:ASN:N	2.63	0.47
4:D:102:ARG:HA	4:D:108:ALA:O	2.14	0.47
1:A:144:ASP:OD2	1:A:147:ASN:ND2	2.47	0.47
1:A:158:PHE:O	1:A:164:ALA:HB2	2.15	0.47
1:N:354:VAL:HG23	1:N:355:LYS:N	2.30	0.47
3:P:350:ILE:O	3:P:354:MET:HG2	2.15	0.47
5:E:136:VAL:O	5:E:138:VAL:N	2.44	0.47
3:C:198:LEU:HD21	12:C:502:HEM:CMA	2.45	0.47
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.45	0.47
3:P:101:ARG:O	3:P:101:ARG:HD2	2.15	0.47
2:O:59:THR:HG22	2:O:60:THR:N	2.30	0.47
7:T:80:ASP:OD1	8:U:47:ARG:HD3	2.14	0.47
3:C:37:LEU:O	3:C:41:CYS:HB2	2.15	0.47
2:O:36:ALA:HB3	2:O:207:VAL:HG13	1.97	0.47
4:Q:3:LEU:N	4:Q:3:LEU:HD12	2.29	0.47
2:B:122:TYR:O	2:B:126:VAL:HG23	2.15	0.47
3:P:155:PRO:O	3:P:156:TYR:HB2	2.15	0.47
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.44	0.46
3:C:9:HIS:CD2	3:C:12:LEU:HG	2.50	0.46
10:J:7:ARG:HB2	10:J:7:ARG:HH11	1.80	0.46
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.96	0.46
1:N:219:VAL:CG1	1:N:220:SER:N	2.78	0.46
3:P:247:SER:OG	3:P:250:LEU:HB2	2.15	0.46
1:N:122:LEU:HD11	1:N:186:ILE:HD12	1.98	0.46
6:F:71:LYS:O	6:F:72:HIS:HB2	2.15	0.46
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:14:HIS:HB3	4:Q:21:LEU:HA	1.97	0.46
10:W:4:ALA:O	10:W:8:GLN:HG3	2.15	0.46
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.51	0.46
15:Q:3003:CDL:OB3	6:S:73:ARG:NH2	2.48	0.46
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.45	0.46
5:R:185:TYR:O	5:R:186:GLN:HB3	2.15	0.46
2:B:207:VAL:HG12	2:B:208:GLY:N	2.30	0.46
4:D:70:VAL:HG21	4:D:83:ARG:NH2	2.30	0.46
1:N:130:GLU:O	1:N:134:ILE:HG13	2.16	0.46
5:E:74:ILE:HG22	5:E:91:TRP:CD1	2.51	0.46
2:B:110:GLU:O	2:B:111:CYS:HB3	2.16	0.46
2:O:259:THR:HG22	2:O:260:GLU:N	2.29	0.46
6:S:17:ARG:NH1	6:S:17:ARG:HG2	2.29	0.46
8:U:21:ARG:HG3	8:U:21:ARG:HH11	1.80	0.46
2:B:27:THR:CG2	2:B:28:LYS:H	2.24	0.46
1:N:37:VAL:HG22	1:N:109:VAL:HG11	1.98	0.46
5:E:96:LEU:HD12	5:E:135:LEU:O	2.16	0.46
4:D:28:ARG:HD2	4:D:171:TYR:CD1	2.51	0.46
1:A:433:ASP:OD1	1:A:436:ARG:HG2	2.16	0.46
3:C:247:SER:N	3:C:248:PRO:HD3	2.30	0.46
2:O:437:ASP:OD1	2:O:437:ASP:C	2.54	0.46
2:B:21:ALA:O	2:B:22:GLU:HB3	2.15	0.46
12:P:502:HEM:HMB1	12:P:502:HEM:HBB2	1.97	0.46
3:P:202:HIS:NE2	14:P:3002:UQ:O4	2.43	0.46
1:A:64:PHE:HE2	1:A:86:PHE:CE1	2.34	0.46
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.51	0.46
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.46	0.46
2:O:259:THR:CG2	2:O:260:GLU:N	2.79	0.46
2:B:273:SER:O	2:B:276:GLN:HB3	2.16	0.46
2:B:212:LYS:HB3	2:B:215:ASP:OD2	2.16	0.46
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.80	0.46
2:O:307:PHE:H	9:V:52:ARG:HG2	1.81	0.46
1:N:288:LYS:HE3	1:N:289:HIS:CE1	2.51	0.46
1:A:49:ASN:ND2	1:A:51:LYS:H	2.14	0.46
2:O:24:LEU:HD12	2:O:37:SER:O	2.15	0.46
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.51	0.46
5:R:109:GLU:HG2	5:R:123:ASP:HB2	1.97	0.46
5:E:189:GLY:O	5:E:192:LEU:O	2.34	0.46
9:V:70:LEU:CD2	9:V:71:ASN:OD1	2.64	0.46
2:B:333:ALA:O	2:B:337:ILE:HG13	2.16	0.46
1:A:48:GLU:CD	1:A:54:GLY:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:PHE:CD1	2:B:50:PHE:N	2.83	0.46
5:E:133:VAL:HG13	5:E:133:VAL:O	2.16	0.46
2:B:248:ASN:HD22	2:B:249:GLY:N	2.14	0.46
1:A:368:GLN:O	1:A:369:LEU:HD23	2.16	0.46
2:B:259:THR:CG2	2:B:260:GLU:N	2.78	0.46
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.98	0.46
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.80	0.46
2:O:385:GLU:O	2:O:389:SER:HB3	2.15	0.46
5:R:141:HIS:HB3	19:R:501:FES:S2	2.56	0.46
10:J:40:ASP:O	10:J:44:GLU:HG3	2.15	0.46
3:P:153:ALA:CB	3:P:288:LYS:HG2	2.45	0.45
8:U:28:GLU:CG	8:U:32:LYS:HE3	2.46	0.45
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.46	0.45
9:I:39:UNK:HA	9:V:40:UNK:O	2.16	0.45
10:W:42:ILE:HG22	10:W:46:LEU:HD12	1.98	0.45
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.31	0.45
3:C:28:ILE:HG12	3:C:225:TYR:OH	2.17	0.45
2:B:307:PHE:H	9:I:52:ARG:HG2	1.81	0.45
1:A:205:HIS:O	1:A:209:VAL:HG12	2.16	0.45
5:R:162:GLY:O	5:R:163:SER:C	2.53	0.45
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.98	0.45
4:D:169:LEU:HD23	4:D:169:LEU:O	2.16	0.45
4:D:171:TYR:OH	4:D:182:ILE:HA	2.16	0.45
3:P:247:SER:N	3:P:248:PRO:HD3	2.31	0.45
1:A:137:GLU:O	1:A:141:MET:HG3	2.16	0.45
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	1.98	0.45
3:P:22:LEU:HD21	14:P:3002:UQ:CM3	2.47	0.45
2:O:31:ASN:H	2:O:31:ASN:ND2	2.13	0.45
4:Q:43:MET:HE1	4:Q:91:PHE:CE2	2.52	0.45
3:P:380:TYR:CZ	6:S:37:LEU:HD21	2.52	0.45
1:A:70:ARG:HA	1:A:71:PRO:HD2	1.81	0.45
2:B:372:VAL:HG13	2:B:378:LEU:HA	1.99	0.45
15:C:2004:CDL:H712	11:C:2007:PEE:H50	1.98	0.45
15:D:2003:CDL:OB3	6:F:73:ARG:NH2	2.49	0.45
5:R:163:SER:HA	5:R:174:GLY:HA3	1.99	0.45
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.44	0.45
1:A:418:LYS:O	1:A:420:PRO:HD3	2.16	0.45
4:Q:47:ALA:HA	4:Q:90:TYR:HA	1.99	0.45
7:T:36:ASN:O	7:T:40:ARG:HG3	2.17	0.45
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.97	0.45
2:B:225:ASN:O	2:B:226:ILE:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:170:THR:O	2:O:172:LEU:N	2.50	0.45
6:S:52:GLU:OE2	7:T:11:ARG:NH1	2.49	0.45
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.17	0.45
2:B:68:LEU:HD23	2:B:186:ILE:HG21	1.97	0.45
2:B:24:LEU:HD13	2:B:38:LEU:HB2	1.98	0.45
2:B:96:LEU:HD12	2:B:97:SER:N	2.32	0.45
5:E:189:GLY:O	5:E:192:LEU:N	2.50	0.45
5:E:144:CYS:CB	5:E:158:CYS:SG	3.05	0.45
1:A:255:LEU:O	1:A:321:GLY:HA3	2.16	0.45
6:F:91:GLU:HB3	6:F:92:PRO:HD3	1.99	0.45
15:D:2003:CDL:HA61	15:D:2003:CDL:H721	1.98	0.45
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.32	0.45
2:B:28:LYS:HG2	2:B:28:LYS:O	2.17	0.45
2:B:101:THR:OG1	2:B:104:LYS:HG3	2.17	0.45
1:A:45:SER:HA	1:A:48:GLU:HG3	1.98	0.45
10:W:38:GLY:O	10:W:42:ILE:HG13	2.16	0.45
2:O:75:LEU:HD11	2:O:140:LEU:HD22	1.97	0.45
3:C:328:LEU:HA	3:C:328:LEU:HD12	1.83	0.45
2:B:27:THR:CG2	2:B:28:LYS:N	2.77	0.45
5:R:140:THR:OG1	5:R:176:ALA:HB1	2.17	0.45
9:V:69:SER:HB2	9:V:72:ALA:H	1.81	0.45
2:B:207:VAL:HG12	2:B:208:GLY:H	1.82	0.45
2:B:318:ASP:O	2:B:319:SER:HB2	2.16	0.45
2:O:34:ILE:HD13	2:O:390:GLY:HA2	1.99	0.45
5:E:127:VAL:CG1	5:E:128:LYS:H	2.15	0.45
2:B:43:PRO:O	2:B:113:ARG:HG3	2.17	0.45
11:C:2007:PEE:H11	6:F:29:TYR:OH	2.17	0.45
4:D:167:GLU:CG	8:H:13:LEU:HD22	2.46	0.45
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.52	0.45
7:T:56:TYR:O	7:T:59:TYR:HB3	2.17	0.45
3:P:263:LEU:O	3:P:264:VAL:CG2	2.65	0.45
9:V:55:MET:HA	9:V:58:ARG:HG3	1.99	0.45
1:A:27:SER:HA	1:A:199:ALA:O	2.16	0.45
10:W:59:TYR:N	10:W:59:TYR:CD1	2.84	0.45
3:P:92:PHE:O	3:P:95:ILE:HG22	2.17	0.45
3:C:50:LEU:O	3:C:54:MET:HG3	2.17	0.45
15:P:3004:CDL:HA32	7:T:40:ARG:CB	2.46	0.44
3:P:106:GLY:HA2	3:P:108:TYR:CZ	2.52	0.44
2:B:395:PRO:O	2:B:398:VAL:CG1	2.65	0.44
7:G:80:ASP:O	7:G:81:GLN:C	2.55	0.44
3:C:19:LEU:C	3:C:20:ILE:HG13	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:255:LEU:O	1:N:321:GLY:HA3	2.17	0.44
2:B:164:HIS:O	2:B:173:ALA:HA	2.17	0.44
6:S:82:LYS:HD2	6:S:85:GLU:OE1	2.16	0.44
5:E:73:LYS:HB2	5:E:195:VAL:O	2.16	0.44
3:P:266:PRO:HA	3:P:267:PRO:HD3	1.85	0.44
4:D:57:THR:CG2	4:D:58:GLU:N	2.79	0.44
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.33	0.44
3:P:28:ILE:HD11	3:P:225:TYR:CE2	2.52	0.44
5:R:178:TYR:N	5:R:178:TYR:HD1	2.15	0.44
6:S:77:LYS:HE2	6:S:77:LYS:HB3	1.80	0.44
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.52	0.44
6:F:77:LYS:HE2	6:F:77:LYS:HB3	1.81	0.44
4:Q:168:ILE:O	4:Q:168:ILE:HG12	2.17	0.44
2:O:221:GLU:O	2:O:223:PHE:N	2.50	0.44
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.99	0.44
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.99	0.44
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.99	0.44
9:I:68:ILE:HD13	9:I:68:ILE:HA	1.84	0.44
8:U:65:ARG:O	8:U:69:VAL:HG23	2.17	0.44
2:B:353:THR:HG22	2:B:354:GLU:N	2.32	0.44
7:G:48:VAL:O	7:G:51:PRO:HD2	2.17	0.44
1:A:170:THR:HG22	1:A:171:THR:H	1.80	0.44
2:B:46:ARG:HD2	2:B:110:GLU:OE2	2.18	0.44
4:Q:134:TYR:CD2	4:Q:162:PRO:HG3	2.52	0.44
14:P:3002:UQ:HM51	14:P:3002:UQ:H8	1.99	0.44
4:Q:169:LEU:CD2	4:Q:182:ILE:HD11	2.48	0.44
5:E:3:ASN:H	5:E:3:ASN:ND2	2.15	0.44
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.47	0.44
3:C:358:SER:O	3:C:362:ILE:HG13	2.16	0.44
5:R:75:GLU:O	5:R:75:GLU:HG3	2.17	0.44
5:E:119:ASP:O	5:E:121:GLN:N	2.49	0.44
5:E:161:HIS:HB2	19:E:501:FES:S1	2.58	0.44
12:C:502:HEM:HMC2	12:C:502:HEM:CBC	2.41	0.44
2:O:345:LYS:HG2	2:O:418:VAL:CG1	2.47	0.44
5:R:133:VAL:HG13	5:R:133:VAL:O	2.17	0.44
4:Q:28:ARG:HD2	4:Q:171:TYR:CD1	2.53	0.44
3:C:380:TYR:CZ	6:F:37:LEU:HD21	2.53	0.44
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.99	0.44
3:C:323:GLN:OE1	7:G:47:LYS:HD3	2.18	0.44
3:P:150:LEU:HB3	3:P:292:VAL:HG22	1.99	0.44
5:E:171:ILE:HG23	5:E:171:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:361:LYS:HD3	2:O:403:ASP:HA	2.00	0.44
1:A:23:LEU:C	1:A:23:LEU:HD23	2.38	0.44
3:C:287:ASN:O	3:C:288:LYS:C	2.56	0.44
3:P:230:ILE:HG23	11:R:3005:PEE:H25	2.00	0.44
1:N:62:LEU:HD11	1:N:127:ILE:HG12	1.98	0.44
1:N:365:MET:HG3	1:N:366:VAL:N	2.33	0.44
1:N:243:ALA:O	1:N:425:VAL:HA	2.17	0.44
5:R:110:ALA:HA	5:R:122:HIS:NE2	2.32	0.44
1:A:63:ALA:O	1:A:116:VAL:HG13	2.18	0.44
1:A:112:LEU:O	1:A:116:VAL:HG23	2.18	0.44
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.39	0.44
14:C:2002:UQ:HM51	14:C:2002:UQ:H8	2.00	0.44
2:B:59:THR:CG2	2:B:60:THR:N	2.80	0.44
2:B:104:LYS:C	2:B:104:LYS:HD2	2.38	0.44
1:A:281:ASP:OD1	9:I:33:UNK:HB2	2.18	0.43
5:E:136:VAL:HG23	5:E:181:GLU:O	2.17	0.43
2:O:227:ARG:HB3	2:O:228:SER:H	1.48	0.43
4:Q:169:LEU:HD22	4:Q:182:ILE:CD1	2.48	0.43
2:B:56:ARG:HG3	2:B:56:ARG:HH11	1.83	0.43
4:D:143:VAL:HG21	4:D:149:TYR:HB2	1.99	0.43
5:E:73:LYS:HB3	5:E:196:GLY:O	2.17	0.43
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.99	0.43
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.55	0.43
5:E:97:PHE:O	5:E:134:ILE:HA	2.18	0.43
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.53	0.43
4:Q:238:ARG:CZ	5:R:5:VAL:HG22	2.48	0.43
2:B:341:MET:CE	2:B:417:PHE:HE2	2.14	0.43
3:C:98:HIS:CD2	12:C:502:HEM:NC	2.85	0.43
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.51	0.43
3:P:325:LEU:HD22	3:P:370:ILE:HG13	2.00	0.43
3:P:380:TYR:OH	6:S:34:ASP:OD1	2.32	0.43
3:P:121:LEU:O	3:P:125:MET:HG3	2.18	0.43
3:C:92:PHE:O	3:C:95:ILE:HG22	2.17	0.43
2:O:257:VAL:HG22	2:O:424:MET:HG3	2.00	0.43
4:D:235:MET:HB3	7:G:15:THR:HG22	2.01	0.43
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.98	0.43
7:G:50:PRO:HB2	7:G:51:PRO:HD3	2.01	0.43
9:I:71:ASN:N	9:I:71:ASN:HD22	2.16	0.43
3:C:46:ILE:HA	12:C:501:HEM:HMC2	2.00	0.43
8:U:36:ARG:HB3	8:U:36:ARG:NH1	2.33	0.43
4:Q:181:GLN:HA	8:U:77:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:69:GLU:OE1	4:Q:82:MET:HB3	2.18	0.43
2:O:76:THR:CG2	2:O:136:GLU:OE1	2.64	0.43
1:A:186:ILE:HG23	1:A:190:PHE:HD1	1.82	0.43
2:O:345:LYS:HG2	2:O:418:VAL:HG13	2.01	0.43
5:R:161:HIS:HB2	19:R:501:FES:S1	2.59	0.43
1:A:53:ASN:HB3	1:A:173:ASN:ND2	2.34	0.43
3:P:156:TYR:C	3:P:158:GLY:H	2.19	0.43
1:A:130:GLU:O	1:A:134:ILE:HG13	2.18	0.43
11:E:2005:PEE:H58	10:J:24:VAL:HG11	2.01	0.43
4:D:168:ILE:HG12	4:D:168:ILE:O	2.18	0.43
2:B:280:GLY:HA3	2:B:293:SER:OG	2.19	0.43
2:B:76:THR:HG23	2:B:82:SER:HB2	2.01	0.43
2:O:402:ILE:HG23	2:O:403:ASP:H	1.83	0.43
5:R:170:ARG:HA	5:R:179:ASN:CB	2.45	0.43
2:B:46:ARG:HD2	2:B:110:GLU:CG	2.48	0.43
1:N:280:TYR:CG	1:N:281:ASP:N	2.85	0.43
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.53	0.43
5:R:3:ASN:HD22	5:R:3:ASN:H	1.66	0.43
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.83	0.43
1:N:205:HIS:O	1:N:208:LEU:HB3	2.18	0.43
1:N:274:ASN:ND2	1:N:309:THR:HB	2.34	0.43
5:E:102:THR:C	5:E:103:GLN:HG3	2.39	0.43
2:O:39:GLU:OE2	2:O:113:ARG:NH2	2.50	0.43
5:R:96:LEU:HD12	5:R:135:LEU:O	2.19	0.43
2:B:170:THR:O	2:B:172:LEU:N	2.51	0.43
4:D:79:GLU:HA	4:D:79:GLU:OE2	2.19	0.43
1:N:351:GLU:HA	1:N:354:VAL:HG22	2.01	0.43
3:P:129:PHE:CE1	13:P:3001:JZV:HAFB	2.54	0.43
5:R:78:LEU:HD22	5:R:132:TRP:CE2	2.54	0.43
4:D:27:ARG:NH1	4:D:55:THR:O	2.52	0.43
5:E:52:LYS:O	5:E:52:LYS:HD3	2.19	0.43
8:U:32:LYS:O	8:U:36:ARG:HG3	2.19	0.43
3:P:367:PHE:N	3:P:368:PRO:HD2	2.34	0.43
2:O:162:ASN:O	2:O:244:ILE:HD12	2.18	0.43
3:C:146:VAL:HG21	3:C:269:ILE:HG21	2.00	0.43
5:E:83:GLU:C	5:E:85:LYS:H	2.22	0.43
5:E:127:VAL:CG1	5:E:128:LYS:N	2.78	0.43
2:O:221:GLU:HG3	2:O:222:GLN:N	2.26	0.43
1:A:140:GLU:OE2	9:I:50:LEU:N	2.41	0.43
3:P:277:PHE:CG	3:P:278:ALA:N	2.86	0.43
2:O:73:SER:N	2:O:74:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:224:TYR:HB3	4:D:227:TRP:CZ2	2.54	0.43
3:C:155:PRO:O	3:C:157:ILE:N	2.50	0.43
1:N:103:SER:HB3	1:N:202:GLY:O	2.19	0.43
10:J:42:ILE:HG22	10:J:46:LEU:HD12	2.00	0.43
9:I:31:UNK:O	9:I:32:UNK:O	2.37	0.42
5:R:155:GLY:HA3	5:R:166:ASP:O	2.19	0.42
1:N:269:VAL:HG22	1:N:406:MET:CE	2.49	0.42
1:A:191:LYS:N	1:A:195:MET:HE2	2.34	0.42
1:A:191:LYS:CA	1:A:195:MET:HE2	2.49	0.42
1:A:191:LYS:O	1:A:195:MET:HG3	2.18	0.42
2:B:56:ARG:HB2	2:B:102:ARG:O	2.19	0.42
1:N:281:ASP:O	1:N:283:THR:N	2.52	0.42
3:P:208:ASN:HB2	3:P:209:PRO:HD2	2.01	0.42
1:N:436:ARG:HA	1:N:436:ARG:HD2	1.82	0.42
3:P:219:ILE:HD12	3:P:224:TYR:CD1	2.53	0.42
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.54	0.42
5:E:137:GLY:O	5:E:145:VAL:HG13	2.19	0.42
5:R:153:PHE:CD1	5:R:153:PHE:N	2.86	0.42
5:E:122:HIS:CE1	5:E:124:LEU:HB2	2.55	0.42
3:C:286:PRO:O	3:C:287:ASN:CB	2.67	0.42
4:D:69:GLU:OE1	4:D:82:MET:HB3	2.18	0.42
3:C:49:GLY:C	12:C:501:HEM:HAC	2.40	0.42
2:O:96:LEU:H	9:V:70:LEU:HD22	1.84	0.42
9:V:70:LEU:HD23	9:V:71:ASN:H	1.83	0.42
3:P:18:SER:CB	3:P:202:HIS:HE1	2.32	0.42
1:N:90:THR:O	1:N:167:VAL:HG11	2.19	0.42
6:S:99:ARG:HB3	6:S:99:ARG:HH11	1.84	0.42
2:B:345:LYS:HG2	2:B:418:VAL:HG13	2.02	0.42
4:D:116:ILE:HG23	4:D:117:VAL:N	2.33	0.42
2:B:257:VAL:HG22	2:B:424:MET:HG3	2.01	0.42
1:N:27:SER:HA	1:N:199:ALA:O	2.19	0.42
2:B:374:THR:HG22	2:B:376:GLN:N	2.33	0.42
2:B:52:LYS:O	2:B:203:ARG:NH2	2.46	0.42
5:E:191:ASP:N	5:E:191:ASP:OD2	2.52	0.42
8:H:40:CYS:O	8:H:44:VAL:HG23	2.18	0.42
2:O:353:THR:HG22	2:O:354:GLU:N	2.35	0.42
1:A:111:GLU:HG3	1:A:215:HIS:NE2	2.35	0.42
2:O:227:ARG:O	2:O:228:SER:O	2.38	0.42
3:P:49:GLY:C	12:P:501:HEM:HAC	2.40	0.42
1:N:45:SER:HA	1:N:48:GLU:CG	2.49	0.42
1:N:144:ASP:OD2	1:N:147:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:418:LYS:O	1:N:420:PRO:HD3	2.19	0.42
1:A:16:VAL:HA	1:A:25:VAL:O	2.19	0.42
3:P:5:ILE:O	3:P:5:ILE:HG22	2.20	0.42
5:E:130:PRO:C	5:E:132:TRP:H	2.22	0.42
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.48	0.42
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.20	0.42
9:V:52:ARG:HG3	9:V:52:ARG:HH11	1.84	0.42
2:O:209:ILE:HD11	2:O:379:LEU:N	2.35	0.42
3:P:101:ARG:CD	3:P:101:ARG:C	2.83	0.42
2:B:22:GLU:O	2:B:23:ASP:OD2	2.38	0.42
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.64	0.42
4:Q:167:GLU:HG2	8:U:13:LEU:HD12	2.01	0.42
9:I:61:ARG:C	9:I:62:ARG:HG3	2.40	0.42
5:E:122:HIS:O	5:E:125:ASP:HB2	2.19	0.42
2:B:46:ARG:HD2	2:B:110:GLU:CD	2.40	0.42
2:B:287:ARG:HG3	2:B:287:ARG:NH1	2.34	0.42
2:O:287:ARG:NH1	2:O:287:ARG:HG3	2.35	0.42
3:P:263:LEU:O	3:P:264:VAL:HG23	2.20	0.42
10:J:4:ALA:O	10:J:8:GLN:HG3	2.20	0.42
2:B:144:LEU:HB2	2:B:183:ILE:HD12	2.01	0.42
2:B:341:MET:HA	2:B:341:MET:HE3	2.00	0.42
2:B:28:LYS:HG3	2:B:34:ILE:HG12	2.02	0.42
5:E:75:GLU:HA	5:E:193:VAL:O	2.20	0.42
4:D:26:VAL:HG22	4:D:188:THR:HG22	2.01	0.42
3:P:287:ASN:O	3:P:288:LYS:C	2.58	0.42
1:A:17:THR:CG2	1:A:205:HIS:NE2	2.83	0.42
2:B:292:THR:CG2	2:B:292:THR:O	2.66	0.42
5:E:162:GLY:O	5:E:163:SER:C	2.58	0.42
1:N:4:TYR:CB	2:O:114:ASP:OD2	2.67	0.42
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.55	0.42
1:A:253:VAL:O	1:A:323:HIS:HA	2.20	0.42
5:E:103:GLN:O	5:E:107:ASN:ND2	2.51	0.42
5:R:77:LYS:HE2	5:R:79:SER:CB	2.49	0.42
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.55	0.42
2:B:374:THR:HB	2:B:377:GLY:H	1.84	0.42
6:S:13:MET:O	6:S:17:ARG:HG3	2.19	0.42
3:P:150:LEU:HB3	3:P:292:VAL:CG2	2.50	0.42
10:W:57:HIS:HA	10:W:60:GLU:HB3	2.01	0.42
3:C:150:LEU:HB3	3:C:292:VAL:HG22	2.02	0.42
1:A:233:ARG:HH21	1:A:316:ASP:HB2	1.83	0.42
5:R:107:ASN:C	5:R:109:GLU:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:403:ASP:C	2:O:405:VAL:H	2.23	0.41
5:R:116:LYS:O	5:R:117:LEU:HD23	2.20	0.41
3:P:313:GLN:HE21	6:S:36:THR:HB	1.85	0.41
7:G:81:GLN:HG3	7:G:81:GLN:OXT	2.20	0.41
1:A:304:CYS:HB2	1:A:325:VAL:O	2.20	0.41
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.35	0.41
15:C:2004:CDL:HA32	7:G:40:ARG:CB	2.50	0.41
1:N:30:SER:O	1:N:202:GLY:HA2	2.19	0.41
1:N:240:GLU:HA	1:N:422:LEU:O	2.20	0.41
7:G:29:ILE:O	7:G:33:ALA:HB3	2.19	0.41
8:H:50:THR:O	8:H:50:THR:HG23	2.19	0.41
2:O:341:MET:HE2	2:O:341:MET:CA	2.49	0.41
5:E:52:LYS:CD	5:E:52:LYS:C	2.85	0.41
5:R:184:THR:HG22	5:R:185:TYR:N	2.35	0.41
5:E:152:ASP:OD2	5:E:153:PHE:CE1	2.73	0.41
3:P:219:ILE:HD12	3:P:224:TYR:CG	2.55	0.41
3:P:9:HIS:CD2	3:P:11:LEU:H	2.38	0.41
5:R:134:ILE:HD12	5:R:185:TYR:HD1	1.85	0.41
3:P:98:HIS:CD2	12:P:502:HEM:NC	2.88	0.41
1:A:209:VAL:O	1:A:212:ALA:HB3	2.20	0.41
8:U:27:THR:HG22	8:U:29:LYS:N	2.33	0.41
2:O:54:GLY:C	2:O:56:ARG:H	2.23	0.41
2:B:54:GLY:C	2:B:56:ARG:H	2.22	0.41
1:A:387:GLY:O	1:A:388:ARG:HB3	2.19	0.41
1:A:351:GLU:HA	1:A:354:VAL:HG22	2.02	0.41
2:O:275:LEU:HG	2:O:279:LEU:HD12	2.02	0.41
3:C:5:ILE:O	3:C:5:ILE:HG22	2.21	0.41
1:N:70:ARG:HA	1:N:71:PRO:HD2	1.80	0.41
5:R:97:PHE:O	5:R:134:ILE:HA	2.21	0.41
6:S:99:ARG:HB3	6:S:99:ARG:NH1	2.35	0.41
1:N:281:ASP:CB	9:V:33:UNK:HB1	2.50	0.41
10:J:56:LYS:HE2	10:J:56:LYS:HB3	1.77	0.41
4:Q:240:PRO:O	4:Q:241:LYS:C	2.59	0.41
4:D:116:ILE:HG12	17:D:501:HEC:HMA3	2.02	0.41
3:C:150:LEU:HB3	3:C:292:VAL:CG2	2.50	0.41
5:R:179:ASN:O	5:R:180:LEU:C	2.59	0.41
2:O:169:LYS:HD2	2:O:238:THR:HG21	2.02	0.41
6:S:91:GLU:HB3	6:S:92:PRO:HD3	2.03	0.41
1:N:23:LEU:HD23	1:N:23:LEU:C	2.41	0.41
6:F:51:PRO:HD2	6:F:54:LEU:HD12	2.01	0.41
2:O:395:PRO:O	2:O:398:VAL:CG1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:306:PRO:HA	9:V:52:ARG:CG	2.51	0.41
2:O:307:PHE:CD1	2:O:308:ASP:N	2.88	0.41
8:H:65:ARG:O	8:H:69:VAL:HG23	2.20	0.41
2:B:399:ALA:O	2:B:402:ILE:CG2	2.65	0.41
1:N:383:LEU:HD23	1:N:388:ARG:HA	2.02	0.41
4:Q:169:LEU:C	4:Q:169:LEU:HD23	2.41	0.41
8:H:10:GLU:C	8:H:11:GLU:HG3	2.41	0.41
1:N:289:HIS:CD2	2:O:83:PHE:HD1	2.39	0.41
1:N:16:VAL:HA	1:N:25:VAL:O	2.21	0.41
5:R:13:TYR:O	7:T:24:ARG:HG3	2.21	0.41
13:P:3001:JZV:HAY	13:P:3001:JZV:HAZ	1.81	0.41
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.50	0.41
1:A:26:ALA:O	1:A:198:ALA:HA	2.21	0.41
5:R:188:VAL:HG23	5:R:192:LEU:HB2	2.02	0.41
3:C:367:PHE:N	3:C:368:PRO:HD2	2.36	0.41
3:P:146:VAL:HG21	3:P:269:ILE:HG21	2.03	0.41
5:E:171:ILE:HG12	5:E:176:ALA:O	2.20	0.41
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.36	0.41
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.56	0.41
2:O:212:LYS:HB3	2:O:215:ASP:OD2	2.21	0.41
2:B:399:ALA:HA	2:B:402:ILE:HG22	2.02	0.41
2:B:403:ASP:C	2:B:405:VAL:H	2.24	0.41
3:P:286:PRO:O	3:P:287:ASN:CB	2.69	0.41
2:O:59:THR:CG2	2:O:60:THR:N	2.84	0.41
2:O:169:LYS:CG	2:O:240:TRP:HB2	2.49	0.41
4:Q:70:VAL:CG2	4:Q:83:ARG:CZ	2.98	0.41
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.83	0.41
3:P:45:GLN:CB	12:P:501:HEM:HAB	2.51	0.41
4:D:21:LEU:HD13	4:D:192:TRP:HB2	2.03	0.41
3:P:138:GLN:OE1	3:P:138:GLN:HA	2.21	0.41
1:A:342:TRP:O	1:A:345:LEU:HB2	2.20	0.41
1:N:133:VAL:O	1:N:137:GLU:HG3	2.20	0.41
3:P:156:TYR:CD2	3:P:156:TYR:N	2.89	0.41
4:D:165:TYR:CZ	4:D:168:ILE:HG13	2.55	0.41
1:N:422:LEU:HD22	1:N:437:ILE:CD1	2.51	0.41
2:O:318:ASP:O	2:O:319:SER:HB2	2.19	0.41
3:C:271:PRO:HG2	3:C:276:LEU:HD23	2.03	0.41
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.90	0.41
1:A:243:ALA:O	1:A:425:VAL:HA	2.20	0.41
2:B:262:ALA:O	2:B:320:GLY:HA3	2.20	0.41
6:F:32:MET:O	6:F:33:ARG:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:151:GLY:O	5:E:154:GLY:N	2.54	0.41
2:O:72:ALA:HB1	2:O:75:LEU:HD12	2.03	0.41
3:C:295:LEU:HD11	13:C:2001:JZV:HAZ	2.02	0.41
4:Q:57:THR:CG2	4:Q:58:GLU:N	2.83	0.41
3:P:37:LEU:O	3:P:41:CYS:HB2	2.20	0.41
5:R:95:PRO:HG2	5:R:145:VAL:CG1	2.51	0.41
1:A:45:SER:HA	1:A:48:GLU:CD	2.41	0.41
1:A:114:ALA:HB2	1:A:216:PHE:CE2	2.55	0.41
2:B:248:ASN:ND2	2:B:250:HIS:H	2.20	0.40
2:O:372:VAL:HG13	2:O:378:LEU:HA	2.03	0.40
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	2.02	0.40
5:E:75:GLU:O	5:E:75:GLU:HG3	2.21	0.40
5:R:134:ILE:HB	5:R:185:TYR:CE1	2.56	0.40
1:A:4:TYR:HE2	1:A:396:ASP:OD2	2.04	0.40
6:S:60:PHE:O	6:S:64:ARG:HB2	2.20	0.40
1:A:140:GLU:HG2	9:I:50:LEU:HG	2.02	0.40
17:D:501:HEC:HMD1	17:D:501:HEC:HAD1	1.92	0.40
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.55	0.40
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.56	0.40
1:A:276:ILE:HG12	1:A:357:ALA:HB2	2.02	0.40
7:G:73:ASN:HA	7:G:74:PRO:HD2	1.96	0.40
2:O:56:ARG:HB2	2:O:102:ARG:O	2.21	0.40
4:D:70:VAL:CG2	4:D:83:ARG:CZ	2.99	0.40
1:N:343:MET:O	1:N:347:THR:HG23	2.21	0.40
5:R:121:GLN:O	5:R:170:ARG:NH1	2.45	0.40
1:A:170:THR:CG2	1:A:171:THR:H	2.33	0.40
5:R:76:ILE:CD1	5:R:98:VAL:HG21	2.52	0.40
5:E:115:SER:CB	5:E:116:LYS:HD2	2.52	0.40
5:E:109:GLU:HA	5:E:109:GLU:OE1	2.21	0.40
1:N:62:LEU:O	1:N:64:PHE:N	2.55	0.40
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.21	0.40
1:A:354:VAL:HG23	1:A:355:LYS:N	2.35	0.40
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.36	0.40
1:N:253:VAL:O	1:N:323:HIS:HA	2.20	0.40
5:E:165:TYR:CE2	5:E:180:LEU:HG	2.57	0.40
13:C:2001:JZV:HAY	13:C:2001:JZV:HAZ	1.80	0.40
5:R:106:ILE:HG21	5:R:130:PRO:HB3	2.02	0.40
5:E:76:ILE:HB	5:E:193:VAL:CG1	2.51	0.40
4:Q:79:GLU:HA	4:Q:79:GLU:OE2	2.22	0.40
2:O:168:TYR:HB2	2:O:173:ALA:HB2	2.03	0.40
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:263:LEU:C	3:P:264:VAL:HG23	2.41	0.40
5:R:194:VAL:HG12	5:R:194:VAL:O	2.21	0.40
2:B:341:MET:HE2	2:B:341:MET:HA	2.02	0.40
2:B:217:LYS:HE2	2:B:221:GLU:OE2	2.21	0.40
2:B:276:GLN:HG2	2:B:281:ALA:HB2	2.03	0.40
2:B:370:MET:O	2:B:373:GLU:HG3	2.22	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%)	414 (94%)	22 (5%)	6 (1%)	14	38
1	N	440/446 (99%)	414 (94%)	19 (4%)	7 (2%)	12	34
2	B	418/441 (95%)	358 (86%)	46 (11%)	14 (3%)	5	14
2	O	420/441 (95%)	370 (88%)	40 (10%)	10 (2%)	7	22
3	C	378/380 (100%)	363 (96%)	10 (3%)	5 (1%)	15	40
3	P	377/380 (99%)	358 (95%)	14 (4%)	5 (1%)	15	40
4	D	239/241 (99%)	227 (95%)	12 (5%)	0	100	100
4	Q	239/241 (99%)	223 (93%)	15 (6%)	1 (0%)	39	72
5	E	194/196 (99%)	152 (78%)	28 (14%)	14 (7%)	1	2
5	R	194/196 (99%)	165 (85%)	22 (11%)	7 (4%)	4	12
6	F	99/110 (90%)	95 (96%)	4 (4%)	0	100	100
6	S	99/110 (90%)	91 (92%)	8 (8%)	0	100	100
7	G	78/81 (96%)	69 (88%)	6 (8%)	3 (4%)	4	11
7	T	77/81 (95%)	69 (90%)	6 (8%)	2 (3%)	7	19
8	H	68/77 (88%)	64 (94%)	4 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	U	65/77 (84%)	60 (92%)	3 (5%)	2 (3%)	5	15
9	I	29/47 (62%)	27 (93%)	2 (7%)	0	100	100
9	V	29/47 (62%)	28 (97%)	1 (3%)	0	100	100
10	J	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
10	W	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	11	32
All	All	4002/4160 (96%)	3659 (91%)	266 (7%)	77 (2%)	10	28

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	GLY
2	B	21	ALA
2	B	24	LEU
2	B	26	ILE
2	B	29	LEU
2	B	171	ALA
2	B	226	ILE
2	B	228	SER
3	C	287	ASN
5	E	127	VAL
5	E	128	LYS
5	E	130	PRO
5	E	163	SER
2	O	26	ILE
2	O	171	ALA
2	O	228	SER
3	P	287	ASN
4	Q	3	LEU
5	R	163	SER
8	U	52	GLU
10	W	61	ALA
1	A	282	ARG
2	B	231	GLY
5	E	80	ASP
5	E	102	THR
5	E	115	SER
5	E	177	PRO
5	E	191	ASP
1	N	218	GLY
1	N	282	ARG

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Mol	Chain	Res	Type
2	O	24	LEU
2	O	222	GLN
5	R	185	TYR
5	R	191	ASP
8	U	49	HIS
1	A	72	CYS
2	B	389	SER
5	E	137	GLY
1	N	63	ALA
1	N	72	CYS
1	N	262	TRP
1	N	433	ASP
2	O	372	VAL
2	O	389	SER
3	P	156	TYR
5	R	186	GLN
7	T	33	ALA
1	A	262	TRP
1	A	433	ASP
2	B	372	VAL
2	B	386	ALA
3	C	3	PRO
5	E	154	GLY
2	O	19	PRO
3	P	3	PRO
3	P	157	ILE
5	R	154	GLY
2	B	201	SER
2	B	221	GLU
2	B	371	SER
3	C	156	TYR
5	E	166	ASP
7	G	33	ALA
1	N	443	TRP
5	E	120	PRO
5	E	150	SER
7	G	61	TRP
2	O	55	SER
2	O	330	ALA
3	C	158	GLY
1	A	71	PRO
3	C	264	VAL

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Mol	Chain	Res	Type
5	R	137	GLY
3	P	264	VAL
5	R	127	VAL
7	T	50	PRO
7	G	50	PRO

5.3.2 Protein sidechains ⓘ

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	80
1	N	365/368 (99%)	352 (96%)	13 (4%)	42	75
2	B	331/347 (95%)	321 (97%)	10 (3%)	48	80
2	O	333/347 (96%)	324 (97%)	9 (3%)	52	83
3	C	328/329 (100%)	320 (98%)	8 (2%)	57	86
3	P	328/329 (100%)	322 (98%)	6 (2%)	66	90
4	D	200/200 (100%)	197 (98%)	3 (2%)	72	92
4	Q	200/200 (100%)	197 (98%)	3 (2%)	72	92
5	E	166/166 (100%)	161 (97%)	5 (3%)	48	80
5	R	165/166 (99%)	161 (98%)	4 (2%)	57	86
6	F	93/96 (97%)	88 (95%)	5 (5%)	27	58
6	S	93/96 (97%)	88 (95%)	5 (5%)	27	58
7	G	71/71 (100%)	69 (97%)	2 (3%)	51	82
7	T	70/71 (99%)	69 (99%)	1 (1%)	74	92
8	H	65/71 (92%)	65 (100%)	0	100	100
8	U	63/71 (89%)	62 (98%)	1 (2%)	70	91
9	I	23/26 (88%)	20 (87%)	3 (13%)	5	14
9	V	23/26 (88%)	20 (87%)	3 (13%)	5	14
10	J	49/49 (100%)	48 (98%)	1 (2%)	63	89
10	W	47/49 (96%)	46 (98%)	1 (2%)	61	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3378/3446 (98%)	3284 (97%)	94 (3%)	51 82

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	352	SER
1	A	395	TRP
1	A	405	ARG
1	A	432	LEU
1	A	443	TRP
2	B	23	ASP
2	B	31	ASN
2	B	104	LYS
2	B	170	THR
2	B	193	HIS
2	B	225	ASN
2	B	248	ASN
2	B	250	HIS
2	B	341	MET
2	B	402	ILE
3	C	81	ARG
3	C	91	PHE
3	C	184	PHE
3	C	216	SER
3	C	223	PRO
3	C	256	ASN
3	C	367	PHE
3	C	380	TYR
4	D	70	VAL
4	D	169	LEU
4	D	203	ARG
5	E	31	ASP
5	E	52	LYS
5	E	131	GLU
5	E	178	TYR
5	E	185	TYR

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Mol	Chain	Res	Type
6	F	52	GLU
6	F	58	ARG
6	F	64	ARG
6	F	70	LEU
6	F	73	ARG
7	G	4	PHE
7	G	50	PRO
9	I	68	ILE
9	I	70	LEU
9	I	71	ASN
10	J	59	TYR
1	N	3	THR
1	N	18	THR
1	N	58	PHE
1	N	86	PHE
1	N	106	MET
1	N	179	ARG
1	N	281	ASP
1	N	307	PHE
1	N	352	SER
1	N	395	TRP
1	N	405	ARG
1	N	432	LEU
1	N	443	TRP
2	O	19	PRO
2	O	31	ASN
2	O	104	LYS
2	O	193	HIS
2	O	248	ASN
2	O	250	HIS
2	O	325	TYR
2	O	341	MET
2	O	402	ILE
3	P	81	ARG
3	P	91	PHE
3	P	184	PHE
3	P	216	SER
3	P	256	ASN
3	P	380	TYR
4	Q	70	VAL
4	Q	169	LEU
4	Q	203	ARG

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Mol	Chain	Res	Type
5	R	31	ASP
5	R	52	LYS
5	R	178	TYR
5	R	185	TYR
6	S	13	MET
6	S	52	GLU
6	S	58	ARG
6	S	64	ARG
6	S	70	LEU
7	T	4	PHE
8	U	49	HIS
9	V	58	ARG
9	V	68	ILE
9	V	75	SER
10	W	59	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	85	HIS
1	A	267	ASN
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
1	A	311	ASN
1	A	339	GLN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	247	GLN
2	B	248	ASN
2	B	270	ASN
2	B	276	GLN
2	B	297	GLN
2	B	329	GLN
2	B	343	GLN
2	B	362	ASN
2	B	363	GLN
3	C	9	HIS
3	C	17	ASN
3	C	69	HIS

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Mol	Chain	Res	Type
3	C	82	ASN
3	C	207	ASN
3	C	313	GLN
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	148	HIS
5	E	3	ASN
5	E	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	85	HIS
1	N	118	GLN
1	N	143	ASN
1	N	173	ASN
1	N	267	ASN
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
1	N	311	ASN
1	N	339	GLN
2	O	31	ASN
2	O	153	GLN
2	O	156	GLN
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	297	GLN
2	O	329	GLN
2	O	343	GLN
2	O	362	ASN
2	O	363	GLN
3	P	9	HIS
3	P	17	ASN
3	P	69	HIS

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	1.84	6 (30%)	21,25,55	0.68	0
13	JZV	C	2001	-	30,30,30	1.90	6 (20%)	37,41,41	3.37	10 (27%)
14	UQ	C	2002	-	19,19,63	2.51	11 (57%)	23,26,79	1.30	3 (13%)
15	CDL	C	2004	-	39,39,99	1.18	2 (5%)	41,51,111	1.14	4 (9%)
11	PEE	C	2007	-	48,48,50	1.29	7 (14%)	49,53,55	0.95	4 (8%)
16	GOL	C	2011	-	5,5,5	1.24	0	5,5,5	0.65	0
12	HEM	C	501	3	30,50,50	3.15	9 (30%)	24,82,82	2.31	10 (41%)
12	HEM	C	502	3	30,50,50	2.57	7 (23%)	24,82,82	2.28	7 (29%)
15	CDL	D	2003	-	41,41,99	1.18	3 (7%)	43,53,111	1.07	2 (4%)
18	BOG	D	2009	-	20,20,20	0.92	1 (5%)	25,25,25	0.88	2 (8%)
18	BOG	D	2091	-	13,13,20	1.28	2 (15%)	18,18,25	1.05	2 (11%)
17	HEC	D	501	4	24,50,50	1.75	2 (8%)	19,82,82	3.20	6 (31%)
11	PEE	E	2005	-	49,49,50	1.46	9 (18%)	50,54,55	0.94	5 (10%)
19	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	PEE	N	3008	-	4,4,50	3.75	4 (100%)	6,6,55	0.58	0
18	BOG	P	2010	-	12,12,20	1.44	3 (25%)	17,17,25	0.61	0
13	JZV	P	3001	-	30,30,30	1.95	6 (20%)	37,41,41	3.50	11 (29%)
14	UQ	P	3002	-	19,19,63	2.49	11 (57%)	23,26,79	1.28	3 (13%)
15	CDL	P	3004	-	39,39,99	1.18	2 (5%)	41,51,111	1.16	5 (12%)
11	PEE	P	3007	-	48,48,50	1.27	7 (14%)	49,53,55	0.92	4 (8%)
16	GOL	P	3011	-	5,5,5	1.34	0	5,5,5	0.69	0
12	HEM	P	501	3	30,50,50	3.16	9 (30%)	24,82,82	2.13	7 (29%)
12	HEM	P	502	3	30,50,50	2.60	10 (33%)	24,82,82	2.30	7 (29%)
15	CDL	Q	3003	-	41,41,99	1.18	2 (4%)	43,53,111	1.08	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	1.37	2 (15%)	18,18,25	1.08	2 (11%)
17	HEC	Q	501	4	24,50,50	2.27	2 (8%)	19,82,82	3.33	6 (31%)
11	PEE	R	3005	-	49,49,50	1.44	10 (20%)	50,54,55	0.94	5 (10%)
19	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	JZV	C	2001	-	-	0/29/29/29	0/2/2/2
14	UQ	C	2002	-	-	0/11/35/87	0/1/1/1
15	CDL	C	2004	-	-	0/49/49/110	0/0/0/0
11	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
16	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
15	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
17	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
11	PEE	N	3008	-	-	0/0/0/54	0/0/0/0
18	BOG	P	2010	-	-	0/2/22/31	0/1/1/1
13	JZV	P	3001	-	-	0/29/29/29	0/2/2/2
14	UQ	P	3002	-	-	0/11/35/87	0/1/1/1
15	CDL	P	3004	-	-	0/49/49/110	0/0/0/0
11	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
16	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
15	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
17	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

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	P	501	HEM	C3B-C4B	-9.86	1.43	1.51
12	C	501	HEM	C3B-C4B	-8.71	1.44	1.51
17	Q	501	HEC	C3B-C2B	-7.38	1.33	1.40
17	Q	501	HEC	C3C-C2C	-7.29	1.33	1.40
12	P	501	HEM	C3B-CAB	-7.03	1.38	1.51
12	C	501	HEM	C3B-CAB	-6.97	1.38	1.51
12	C	502	HEM	C3B-CAB	-6.68	1.38	1.51
12	P	502	HEM	C3B-CAB	-6.55	1.39	1.51
12	C	501	HEM	C2D-C3D	-6.54	1.34	1.54
12	C	502	HEM	C2D-C3D	-6.42	1.35	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	D	501	HEC	C3C-C2C	-6.41	1.34	1.40
12	P	502	HEM	C3C-CAC	-6.32	1.39	1.51
12	P	502	HEM	C2D-C3D	-6.31	1.35	1.54
13	P	3001	JZV	CAT-CAS	-6.23	1.39	1.49
12	P	501	HEM	C2D-C3D	-6.10	1.36	1.54
13	C	2001	JZV	CAT-CAS	-6.01	1.39	1.49
12	C	501	HEM	C3C-CAC	-5.91	1.40	1.51
12	P	501	HEM	C3C-CAC	-5.85	1.40	1.51
12	C	502	HEM	C3C-CAC	-5.51	1.41	1.51
12	C	501	HEM	C3D-C4D	-5.19	1.44	1.51
12	C	502	HEM	C3B-C4B	-4.93	1.47	1.51
13	C	2001	JZV	CAI-CAJ	-4.68	1.39	1.48
13	P	3001	JZV	CAI-CAJ	-4.64	1.39	1.48
17	D	501	HEC	C3B-C2B	-4.62	1.35	1.40
12	C	501	HEM	C2C-C1C	-4.30	1.44	1.52
12	P	501	HEM	C2C-C1C	-4.21	1.44	1.52
12	P	502	HEM	C2C-C1C	-4.01	1.45	1.52
12	C	502	HEM	C2C-C1C	-3.90	1.45	1.52
12	P	501	HEM	C3D-C4D	-3.59	1.47	1.51
12	P	502	HEM	C3B-C4B	-3.40	1.48	1.51
12	P	502	HEM	C2D-C1D	-3.21	1.41	1.51
11	R	3005	PEE	C19-C18	-2.92	1.34	1.51
11	C	2007	PEE	C22-C21	-2.90	1.34	1.51
11	E	2005	PEE	C19-C18	-2.89	1.34	1.51
13	C	2001	JZV	OAQ-NAR	-2.89	1.36	1.42
11	P	3007	PEE	C22-C21	-2.88	1.34	1.51
13	P	3001	JZV	OAQ-NAR	-2.81	1.36	1.42
11	R	3005	PEE	C22-C21	-2.79	1.35	1.51
11	E	2005	PEE	C22-C21	-2.74	1.35	1.51
11	P	3007	PEE	C19-C18	-2.45	1.37	1.51
11	C	2007	PEE	C19-C18	-2.33	1.38	1.51
12	C	501	HEM	C2D-C1D	-2.28	1.44	1.51
12	P	502	HEM	C3D-C4D	-2.17	1.48	1.51
13	P	3001	JZV	OAE-NAD	-2.10	1.36	1.40
13	C	2001	JZV	OAE-NAD	-2.09	1.36	1.40
12	P	501	HEM	C2B-C1B	-2.02	1.45	1.51
15	D	2003	CDL	O1-C1	2.04	1.49	1.43
11	R	3005	PEE	O2-C2	2.08	1.51	1.46
18	D	2009	BOG	O5-C1	2.09	1.47	1.41
11	N	3008	PEE	P-O2P	2.09	1.62	1.54
15	Q	3003	CDL	O1-C1	2.10	1.49	1.43
15	P	3004	CDL	CB3-CB4	2.13	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	2003	CDL	OA6-CA5	2.15	1.40	1.34
15	Q	3003	CDL	CA3-CA4	2.16	1.56	1.50
11	A	2008	PEE	C11-C10	2.18	1.57	1.50
11	P	3007	PEE	C31-C30	2.21	1.57	1.50
15	C	2004	CDL	O1-C1	2.22	1.50	1.43
14	C	2002	UQ	C8-C9	2.25	1.37	1.33
18	Q	3009	BOG	O5-C1	2.25	1.47	1.41
15	P	3004	CDL	O1-C1	2.26	1.50	1.43
15	D	2003	CDL	CA3-CA4	2.26	1.57	1.50
12	P	502	HEM	C4C-NC	2.28	1.38	1.36
11	E	2005	PEE	C11-C10	2.29	1.57	1.50
11	P	3007	PEE	C3-C2	2.29	1.57	1.50
11	R	3005	PEE	C31-C30	2.30	1.57	1.50
14	P	3002	UQ	C8-C9	2.31	1.37	1.33
18	D	2091	BOG	O5-C1	2.31	1.47	1.41
14	P	3002	UQ	O2-C2	2.31	1.43	1.37
18	Q	3091	BOG	C4-C5	2.33	1.58	1.53
14	C	2002	UQ	C5-C4	2.33	1.56	1.47
11	C	2007	PEE	C31-C30	2.34	1.57	1.50
18	D	2091	BOG	C4-C5	2.35	1.58	1.53
18	P	2010	BOG	C1-C2	2.37	1.57	1.52
14	P	3002	UQ	C5-C4	2.38	1.56	1.47
11	C	2007	PEE	C3-C2	2.39	1.57	1.50
14	C	2002	UQ	C3-C4	2.40	1.55	1.48
11	R	3005	PEE	C11-C10	2.40	1.57	1.50
18	P	2010	BOG	C4-C5	2.42	1.58	1.53
15	C	2004	CDL	CB3-CB4	2.44	1.57	1.50
13	C	2001	JZV	CAJ-NAD	2.47	1.33	1.29
11	A	2008	PEE	C1-C2	2.49	1.57	1.50
18	Q	3091	BOG	O5-C1	2.49	1.48	1.41
18	P	2010	BOG	O5-C1	2.49	1.47	1.43
11	E	2005	PEE	C31-C30	2.50	1.58	1.50
14	C	2002	UQ	O2-C2	2.51	1.43	1.37
11	C	2007	PEE	O2-C10	2.55	1.41	1.34
14	P	3002	UQ	C3-C4	2.57	1.56	1.48
11	R	3005	PEE	C1-C2	2.57	1.58	1.50
11	P	3007	PEE	O2-C10	2.59	1.42	1.34
14	P	3002	UQ	CM5-C5	2.59	1.56	1.50
13	P	3001	JZV	CAJ-NAD	2.60	1.33	1.29
14	C	2002	UQ	C7-C8	2.61	1.54	1.50
11	R	3005	PEE	C3-C2	2.62	1.58	1.50
11	N	3008	PEE	P-O3P	2.65	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	2008	PEE	C3-C2	2.66	1.58	1.50
11	E	2005	PEE	C1-C2	2.68	1.58	1.50
14	P	3002	UQ	C2-C1	2.75	1.56	1.48
14	P	3002	UQ	C7-C8	2.75	1.55	1.50
11	P	3007	PEE	P-O1P	2.80	1.61	1.51
11	E	2005	PEE	C3-C2	2.81	1.58	1.50
14	C	2002	UQ	CM5-C5	2.85	1.56	1.50
11	N	3008	PEE	P-O4P	2.88	1.65	1.54
14	C	2002	UQ	O3-C3	2.88	1.44	1.37
14	P	3002	UQ	O3-C3	2.96	1.44	1.37
11	E	2005	PEE	P-O1P	2.97	1.62	1.51
11	R	3005	PEE	P-O1P	2.98	1.62	1.51
14	C	2002	UQ	C2-C1	3.00	1.57	1.48
11	A	2008	PEE	P-O1P	3.00	1.62	1.51
11	C	2007	PEE	P-O1P	3.06	1.62	1.51
11	R	3005	PEE	O3-C30	3.15	1.42	1.33
11	E	2005	PEE	O2-C10	3.15	1.43	1.34
11	A	2008	PEE	O2-C10	3.17	1.43	1.34
11	A	2008	PEE	O3-C30	3.18	1.42	1.33
11	C	2007	PEE	O3-C30	3.29	1.43	1.33
11	P	3007	PEE	O3-C30	3.34	1.43	1.33
12	C	501	HEM	CBB-CAB	3.35	1.48	1.29
12	P	502	HEM	CBB-CAB	3.36	1.48	1.29
11	R	3005	PEE	O2-C10	3.41	1.44	1.34
11	E	2005	PEE	O3-C30	3.45	1.43	1.33
12	C	502	HEM	CBC-CAC	3.45	1.49	1.29
12	P	502	HEM	CBC-CAC	3.53	1.49	1.29
14	P	3002	UQ	C6-C5	3.65	1.43	1.35
14	C	2002	UQ	C6-C1	3.69	1.57	1.46
12	C	502	HEM	CBB-CAB	3.70	1.50	1.29
14	P	3002	UQ	C6-C1	3.76	1.57	1.46
12	P	501	HEM	CBB-CAB	3.80	1.51	1.29
14	C	2002	UQ	C6-C5	3.91	1.44	1.35
12	P	501	HEM	CBC-CAC	4.04	1.52	1.29
12	C	501	HEM	CBC-CAC	4.26	1.53	1.29
13	C	2001	JZV	CAS-NAR	4.27	1.33	1.28
13	P	3001	JZV	CAS-NAR	4.61	1.33	1.28
14	C	2002	UQ	C7-C6	5.10	1.60	1.51
14	P	3002	UQ	C7-C6	5.24	1.60	1.51
11	N	3008	PEE	P-O1P	6.04	1.62	1.50

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	501	HEC	CBB-CAB-C3B	-8.52	108.43	127.35
17	D	501	HEC	CBB-CAB-C3B	-8.51	108.44	127.35
13	C	2001	JZV	CAY-CAS-NAR	-7.63	108.61	123.72
13	P	3001	JZV	CAY-CAS-NAR	-7.20	109.46	123.72
17	Q	501	HEC	CBC-CAC-C3C	-6.99	111.83	127.35
17	D	501	HEC	CBC-CAC-C3C	-6.46	113.00	127.35
17	Q	501	HEC	CAA-C2A-C3A	-3.40	119.28	129.00
15	P	3004	CDL	CB4-OB6-CB5	-3.29	109.98	117.89
14	C	2002	UQ	C7-C6-C1	-3.11	114.90	118.56
15	C	2004	CDL	CA4-OA6-CA5	-3.06	110.55	117.89
15	C	2004	CDL	CB4-OB6-CB5	-3.06	110.56	117.89
14	P	3002	UQ	C7-C6-C1	-2.94	115.10	118.56
17	D	501	HEC	CAA-C2A-C3A	-2.92	120.68	129.00
15	P	3004	CDL	CA4-OA6-CA5	-2.88	110.99	117.89
14	C	2002	UQ	C10-C9-C8	-2.78	118.05	123.50
14	P	3002	UQ	C10-C9-C8	-2.73	118.14	123.50
13	C	2001	JZV	OAN-CAK-CAJ	-2.66	119.51	123.58
12	C	501	HEM	C3B-CAB-CBB	-2.64	120.41	124.46
13	P	3001	JZV	CAP-CAH-CAG	-2.61	113.89	119.58
13	P	3001	JZV	CAM-OAL-CAK	-2.61	110.99	115.90
12	C	501	HEM	CBA-CAA-C2A	-2.57	107.91	112.53
15	D	2003	CDL	CA6-CA4-CA3	-2.57	106.06	112.07
15	P	3004	CDL	CA6-CA4-CA3	-2.53	106.16	112.07
15	D	2003	CDL	CB4-OB6-CB5	-2.51	111.87	117.89
15	Q	3003	CDL	CB4-OB6-CB5	-2.48	111.95	117.89
15	Q	3003	CDL	CA6-CA4-CA3	-2.48	106.28	112.07
13	C	2001	JZV	CAM-OAL-CAK	-2.37	111.44	115.90
15	C	2004	CDL	CA6-CA4-CA3	-2.37	106.53	112.07
13	P	3001	JZV	OAN-CAK-CAJ	-2.25	120.15	123.58
13	C	2001	JZV	CAP-CAH-CAG	-2.23	114.73	119.58
12	P	501	HEM	C3B-CAB-CBB	-2.19	121.09	124.46
15	P	3004	CDL	CB6-CB4-CB3	-2.11	107.15	112.07
15	Q	3003	CDL	CB6-CB4-CB3	-2.03	107.31	112.07
12	C	501	HEM	CAA-C2A-C1A	-2.02	124.81	127.01
13	P	3001	JZV	CAY-CAS-CAT	-2.01	116.79	119.66
15	C	2004	CDL	OB6-CB4-CB3	2.04	115.56	108.36
12	C	501	HEM	CBD-CAD-C3D	2.07	119.58	113.55
15	P	3004	CDL	OB6-CB4-CB3	2.09	115.73	108.36
12	P	502	HEM	C3B-CAB-CBB	2.21	127.85	124.46
13	C	2001	JZV	CAP-CAH-CAI	2.28	125.53	121.89
18	D	2009	BOG	C1'-O1-C1	2.29	117.94	113.94
11	R	3005	PEE	C23-C22-C21	2.33	126.55	114.53
12	P	502	HEM	CAA-C2A-C1A	2.36	129.57	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Q	3091	BOG	O1-C1-C2	2.38	111.02	108.21
11	R	3005	PEE	O3-C3-C2	2.38	115.11	108.69
11	E	2005	PEE	C23-C22-C21	2.40	126.90	114.53
18	D	2091	BOG	O1-C1-C2	2.40	111.04	108.21
11	E	2005	PEE	O3-C3-C2	2.40	115.16	108.69
11	P	3007	PEE	C22-C21-C20	2.41	126.98	114.53
11	C	2007	PEE	C22-C21-C20	2.47	127.27	114.53
11	P	3007	PEE	C23-C22-C21	2.48	127.32	114.53
11	R	3005	PEE	C22-C21-C20	2.48	127.34	114.53
11	R	3005	PEE	C19-C18-C17	2.49	127.37	114.53
11	E	2005	PEE	C22-C21-C20	2.50	127.44	114.53
11	E	2005	PEE	C19-C18-C17	2.51	127.52	114.53
17	Q	501	HEC	CAD-C3D-C4D	2.52	129.74	127.01
12	C	502	HEM	CAA-C2A-C1A	2.52	129.75	127.01
18	Q	3009	BOG	O1-C1-C2	2.55	111.26	108.04
11	C	2007	PEE	C23-C22-C21	2.59	127.92	114.53
12	C	502	HEM	C3B-CAB-CBB	2.62	128.47	124.46
11	C	2007	PEE	C19-C18-C17	2.63	128.09	114.53
11	P	3007	PEE	C19-C18-C17	2.64	128.18	114.53
11	E	2005	PEE	C20-C19-C18	2.64	128.19	114.53
11	R	3005	PEE	C20-C19-C18	2.69	128.42	114.53
12	P	501	HEM	CMD-C2D-C3D	2.70	126.28	114.35
12	C	501	HEM	CMD-C2D-C3D	2.70	126.31	114.35
13	P	3001	JZV	CAP-CAH-CAI	2.72	126.23	121.89
11	P	3007	PEE	C20-C19-C18	2.90	129.49	114.53
17	D	501	HEC	CBA-CAA-C2A	2.96	117.83	112.53
18	D	2009	BOG	O1-C1-C2	2.96	111.78	108.04
12	P	501	HEM	CAD-C3D-C2D	3.00	121.83	113.22
12	P	502	HEM	CMD-C2D-C3D	3.02	127.70	114.35
11	C	2007	PEE	C20-C19-C18	3.06	130.32	114.53
18	Q	3009	BOG	C1'-O1-C1	3.06	119.29	113.94
12	C	502	HEM	CMD-C2D-C3D	3.13	128.19	114.35
12	P	501	HEM	C2D-C3D-C4D	3.13	106.81	101.50
18	D	2091	BOG	C1'-O1-C1	3.14	118.43	113.29
12	C	501	HEM	CAD-C3D-C2D	3.15	122.27	113.22
12	C	502	HEM	CAD-C3D-C2D	3.20	122.42	113.22
18	Q	3091	BOG	C1'-O1-C1	3.39	118.83	113.29
14	C	2002	UQ	C8-C7-C6	3.47	122.06	111.64
12	C	501	HEM	C2D-C3D-C4D	3.48	107.40	101.50
12	P	502	HEM	CAD-C3D-C2D	3.49	123.25	113.22
14	P	3002	UQ	C8-C7-C6	3.53	122.23	111.64
17	D	501	HEC	CAD-C3D-C4D	3.67	130.99	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	502	HEM	CMC-C2C-C3C	3.89	126.25	116.53
12	P	501	HEM	CMB-C2B-C3B	3.96	126.41	116.53
17	Q	501	HEC	CBA-CAA-C2A	4.10	119.88	112.53
12	C	501	HEM	CMB-C2B-C3B	4.28	127.22	116.53
12	C	501	HEM	CMC-C2C-C3C	4.59	127.99	116.53
12	P	501	HEM	CMC-C2C-C3C	4.70	128.25	116.53
13	P	3001	JZV	CAP-OAQ-NAR	4.71	113.48	108.00
12	P	502	HEM	CMB-C2B-C3B	4.84	128.62	116.53
12	P	502	HEM	CMC-C2C-C3C	5.04	129.12	116.53
12	C	501	HEM	CAD-C3D-C4D	5.06	130.31	112.47
12	P	501	HEM	CAD-C3D-C4D	5.31	131.20	112.47
12	P	502	HEM	CAD-C3D-C4D	5.59	132.17	112.47
12	C	502	HEM	CMB-C2B-C3B	5.64	130.61	116.53
12	C	502	HEM	CAD-C3D-C4D	5.87	133.19	112.47
13	C	2001	JZV	CAP-OAQ-NAR	5.94	114.91	108.00
17	D	501	HEC	CAA-C2A-C1A	6.35	133.90	127.01
13	C	2001	JZV	CAT-CAS-NAR	6.73	133.53	115.70
13	P	3001	JZV	CAT-CAS-NAR	6.81	133.75	115.70
17	Q	501	HEC	CAA-C2A-C1A	6.87	134.46	127.01
13	C	2001	JZV	OAE-NAD-CAJ	7.06	119.53	111.11
13	P	3001	JZV	OAL-CAK-CAJ	7.38	119.21	111.73
13	P	3001	JZV	OAE-NAD-CAJ	7.42	119.95	111.11
13	C	2001	JZV	OAL-CAK-CAJ	7.47	119.30	111.73
13	C	2001	JZV	OAQ-NAR-CAS	11.65	131.00	112.14
13	P	3001	JZV	OAQ-NAR-CAS	13.34	133.72	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	2001	JZV	4	0
14	C	2002	UQ	4	0
15	C	2004	CDL	4	0
11	C	2007	PEE	4	0
12	C	501	HEM	5	0
12	C	502	HEM	4	0
15	D	2003	CDL	4	0
17	D	501	HEC	3	0
11	E	2005	PEE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	E	501	FES	2	0
18	P	2010	BOG	1	0
13	P	3001	JZV	4	0
14	P	3002	UQ	5	0
15	P	3004	CDL	4	0
11	P	3007	PEE	3	0
12	P	501	HEM	4	0
12	P	502	HEM	3	0
15	Q	3003	CDL	3	0
18	Q	3091	BOG	1	0
17	Q	501	HEC	1	0
11	R	3005	PEE	2	0
19	R	501	FES	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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%)	0.07	11 (2%) 61 54	32, 58, 86, 100	0
1	N	442/446 (99%)	0.17	7 (1%) 74 70	41, 68, 93, 100	0
2	B	420/441 (95%)	0.28	17 (4%) 42 35	48, 76, 111, 133	0
2	O	422/441 (95%)	0.38	19 (4%) 37 30	39, 74, 103, 122	0
3	C	380/380 (100%)	0.07	5 (1%) 79 75	21, 39, 83, 123	0
3	P	379/380 (99%)	0.22	10 (2%) 59 53	29, 58, 88, 125	0
4	D	241/241 (100%)	-0.06	3 (1%) 81 76	29, 41, 81, 103	0
4	Q	241/241 (100%)	0.21	13 (5%) 29 22	46, 67, 97, 120	0
5	E	196/196 (100%)	1.76	77 (39%) 0 0	34, 135, 167, 175	0
5	R	196/196 (100%)	0.62	25 (12%) 5 3	40, 86, 132, 147	0
6	F	101/110 (91%)	-0.30	0 100 100	26, 43, 61, 94	0
6	S	101/110 (91%)	0.04	4 (3%) 42 35	50, 65, 102, 121	0
7	G	80/81 (98%)	0.14	2 (2%) 61 54	33, 52, 97, 111	0
7	T	79/81 (97%)	0.97	13 (16%) 2 1	46, 78, 139, 149	0
8	H	70/77 (90%)	-0.01	2 (2%) 55 48	34, 58, 81, 119	0
8	U	67/77 (87%)	1.03	13 (19%) 1 1	82, 108, 128, 130	0
9	I	31/47 (65%)	2.21	14 (45%) 0 0	72, 107, 133, 134	0
9	V	31/47 (65%)	2.24	17 (54%) 0 0	66, 107, 132, 136	0
10	J	61/61 (100%)	0.26	4 (6%) 22 16	43, 54, 95, 139	0
10	W	60/61 (98%)	0.57	3 (5%) 32 25	55, 68, 99, 107	0
All	All	4042/4160 (97%)	0.33	259 (6%) 23 17	21, 64, 121, 175	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	V	63	ASP	11.4
5	E	98	VAL	10.2
5	E	188	VAL	8.6
7	T	2	ILE	7.3
5	E	84	GLY	7.1
5	E	87	VAL	7.0
7	T	77	TYR	6.7
5	E	157	TYR	6.6
5	E	102	THR	6.5
9	I	48	PRO	6.4
7	T	78	GLU	6.3
5	E	83	GLU	6.0
5	E	187	PHE	5.9
5	E	89	PHE	5.9
5	E	190	ASP	5.8
9	I	77	ARG	5.8
9	I	63	ASP	5.8
5	E	79	SER	5.7
5	E	104	ALA	5.6
5	E	148	ALA	5.6
5	E	107	ASN	5.5
5	R	81	ILE	5.5
5	E	86	ASN	5.4
3	P	2	ALA	5.4
5	E	183	PRO	5.3
10	J	63	GLU	5.3
5	E	85	LYS	5.2
5	R	178	TYR	5.1
5	E	116	LYS	5.1
9	V	77	ARG	5.1
7	T	74	PRO	4.9
5	E	192	LEU	4.9
5	E	76	ILE	4.9
2	B	226	ILE	4.8
5	E	81	ILE	4.8
2	O	386	ALA	4.7
5	E	143	GLY	4.7
2	B	33	LEU	4.6
5	E	145	VAL	4.6
9	I	50	LEU	4.6
6	S	13	MET	4.6
4	Q	145	GLU	4.5
5	E	82	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
5	E	163	SER	4.4
5	E	100	HIS	4.4
5	E	191	ASP	4.4
10	J	64	GLU	4.4
4	Q	241	LYS	4.4
5	E	88	ALA	4.4
5	E	149	ASN	4.4
5	E	138	VAL	4.3
5	E	103	GLN	4.3
8	U	44	VAL	4.3
7	T	6	ASN	4.3
5	R	171	ILE	4.2
8	U	49	HIS	4.2
7	T	80	ASP	4.1
5	E	90	LYS	4.1
5	E	108	GLN	4.1
10	J	62	SER	4.1
8	U	37	LEU	4.0
5	E	120	PRO	3.9
9	V	48	PRO	3.9
2	O	355	GLU	3.9
8	U	12	GLU	3.8
9	I	47	ARG	3.8
5	E	113	ASP	3.8
8	U	50	THR	3.8
5	R	155	GLY	3.7
1	A	444	ILE	3.7
3	C	155	PRO	3.7
7	T	73	ASN	3.6
10	J	61	ALA	3.6
1	A	10	ASN	3.6
5	E	78	LEU	3.6
9	V	47	ARG	3.6
5	E	176	ALA	3.5
5	E	111	GLU	3.5
5	E	137	GLY	3.5
5	R	177	PRO	3.5
2	O	222	GLN	3.4
9	I	61	ARG	3.4
5	E	115	SER	3.4
2	O	352	VAL	3.4
4	D	2	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
5	E	162	GLY	3.4
2	B	228	SER	3.4
5	R	157	TYR	3.3
5	E	175	PRO	3.3
2	B	232	THR	3.3
1	N	174	ILE	3.3
1	A	218	GLY	3.3
9	V	76	VAL	3.3
3	C	4	ASN	3.3
5	E	109	GLU	3.3
5	E	159	PRO	3.3
8	U	13	LEU	3.3
5	R	117	LEU	3.2
5	E	134	ILE	3.2
3	C	156	TYR	3.2
4	Q	143	VAL	3.2
5	E	140	THR	3.2
5	E	180	LEU	3.2
3	C	1	MET	3.2
5	E	185	TYR	3.1
4	Q	69	GLU	3.1
5	E	75	GLU	3.1
2	B	230	ALA	3.1
5	E	117	LEU	3.1
2	B	227	ARG	3.1
4	Q	3	LEU	3.1
5	R	165	TYR	3.1
10	W	33	ARG	3.1
9	V	60	ALA	3.1
5	E	177	PRO	3.1
8	H	71	HIS	3.1
5	E	195	VAL	3.1
5	E	124	LEU	3.1
2	O	226	ILE	3.1
2	B	29	LEU	3.0
9	V	59	SER	3.0
2	B	224	LEU	3.0
9	V	62	ARG	3.0
2	B	34	ILE	3.0
6	S	12	LEU	3.0
2	O	388	LEU	3.0
2	B	225	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
3	P	373	LEU	2.9
4	D	1	GLY	2.9
5	E	99	ARG	2.9
5	E	150	SER	2.9
5	R	154	GLY	2.9
2	B	35	ILE	2.9
2	O	18	CYS	2.9
1	A	86	PHE	2.9
2	O	387	LEU	2.9
7	T	57	LEU	2.9
8	U	42	ALA	2.9
5	E	178	TYR	2.8
3	C	380	TYR	2.8
2	B	204	MET	2.8
5	R	115	SER	2.8
1	A	69	LYS	2.8
5	R	120	PRO	2.8
9	V	58	ARG	2.7
5	R	119	ASP	2.7
5	E	181	GLU	2.7
5	R	84	GLY	2.7
1	N	71	PRO	2.7
1	A	127	ILE	2.7
5	R	114	VAL	2.7
1	N	171	THR	2.7
5	R	156	TYR	2.7
7	T	75	ALA	2.7
5	E	105	GLU	2.7
2	B	20	GLY	2.7
4	Q	80	LEU	2.7
9	I	51	CYS	2.7
8	U	54	CYS	2.6
2	O	34	ILE	2.6
5	R	83	GLU	2.6
7	T	79	ASN	2.6
5	E	184	THR	2.6
1	N	72	CYS	2.6
5	R	190	ASP	2.6
9	V	54	SER	2.5
1	A	219	VAL	2.5
4	Q	206	LEU	2.5
5	E	182	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
5	R	86	ASN	2.5
6	S	15	ARG	2.5
2	B	439	LEU	2.5
4	D	241	LYS	2.5
5	R	172	ARG	2.5
2	B	348	ALA	2.5
2	B	201	SER	2.5
1	N	175	LYS	2.4
7	T	8	ALA	2.4
7	T	71	ARG	2.4
5	E	189	GLY	2.4
5	E	119	ASP	2.4
3	P	370	ILE	2.4
4	Q	1	GLY	2.4
5	E	152	ASP	2.4
5	E	118	ARG	2.4
5	E	112	VAL	2.4
5	E	165	TYR	2.4
9	V	72	ALA	2.4
7	G	2	ILE	2.4
9	I	54	SER	2.4
9	I	60	ALA	2.4
9	I	75	SER	2.4
2	O	35	ILE	2.4
4	Q	70	VAL	2.4
1	A	4	TYR	2.3
2	B	36	ALA	2.3
5	E	110	ALA	2.3
5	R	118	ARG	2.3
3	P	376	LYS	2.3
5	E	97	PHE	2.3
2	O	104	LYS	2.3
4	Q	139	ALA	2.3
1	A	122	LEU	2.3
1	A	68	LYS	2.3
9	I	76	VAL	2.3
1	N	182	LEU	2.3
9	V	56	SER	2.3
10	W	60	GLU	2.3
4	Q	103	ALA	2.3
6	S	11	ARG	2.3
2	O	416	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
7	G	30	PHE	2.2
1	N	127	ILE	2.2
5	E	147	ILE	2.2
9	V	68	ILE	2.2
3	P	366	LEU	2.2
8	H	10	GLU	2.2
3	P	43	MET	2.2
4	Q	82	MET	2.2
5	E	136	VAL	2.2
8	U	47	ARG	2.2
5	E	125	ASP	2.2
5	R	1	VAL	2.2
4	Q	77	ASN	2.2
2	O	33	LEU	2.2
2	O	28	LYS	2.2
3	P	156	TYR	2.2
5	R	16	GLU	2.2
8	U	38	GLU	2.2
5	E	186	GLN	2.1
5	R	103	GLN	2.1
8	U	39	LEU	2.1
9	V	70	LEU	2.1
9	V	74	ALA	2.1
2	O	353	THR	2.1
5	E	194	VAL	2.1
8	U	61	PHE	2.1
2	O	250	HIS	2.1
8	U	48	SER	2.1
5	R	89	PHE	2.1
3	P	380	TYR	2.1
5	E	96	LEU	2.1
5	R	124	LEU	2.1
9	I	53	GLU	2.1
9	V	75	SER	2.1
3	P	307	PHE	2.1
5	E	101	ARG	2.1
2	O	335	GLU	2.1
9	I	64	LEU	2.0
9	V	64	LEU	2.0
5	E	80	ASP	2.0
1	A	392	LEU	2.0
10	W	25	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
7	T	24	ARG	2.0
3	P	354	MET	2.0
5	E	174	GLY	2.0
2	O	267	ALA	2.0
9	I	70	LEU	2.0
2	O	27	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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
16	GOL	P	3011	6/6	0.80	0.40	7.95	73,75,76,77	0
11	PEE	C	2007	49/51	0.85	0.30	7.15	43,58,70,73	0
14	UQ	P	3002	19/63	0.76	0.38	5.30	119,124,125,126	0
18	BOG	P	2010	12/20	0.46	0.35	5.20	135,137,138,138	0
16	GOL	C	2011	6/6	0.85	0.34	4.92	67,70,72,72	0
11	PEE	R	3005	50/51	0.71	0.42	4.41	80,98,108,110	0
11	PEE	E	2005	50/51	0.82	0.35	4.34	68,89,95,97	0
15	CDL	Q	3003	42/100	0.72	0.29	3.78	109,121,139,139	0
11	PEE	A	2008	21/51	0.54	0.39	3.58	129,133,134,135	0
14	UQ	C	2002	19/63	0.84	0.30	3.54	88,90,90,91	0
13	JZV	C	2001	29/29	0.93	0.23	2.82	38,46,86,87	0
11	PEE	P	3007	49/51	0.83	0.33	2.56	53,79,93,94	0
15	CDL	D	2003	42/100	0.81	0.29	2.49	82,92,106,108	0
13	JZV	P	3001	29/29	0.89	0.24	2.31	59,66,104,106	0
15	CDL	C	2004	40/100	0.91	0.22	2.26	66,80,91,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
18	BOG	Q	3009	20/20	0.89	0.23	1.03	62,75,77,78	0
12	HEM	P	501	43/43	0.97	0.22	1.02	33,40,48,54	0
12	HEM	C	501	43/43	0.98	0.21	0.51	23,30,37,42	0
15	CDL	P	3004	40/100	0.86	0.21	0.49	96,102,111,111	0
18	BOG	D	2009	20/20	0.93	0.17	0.40	53,59,62,64	0
17	HEC	D	501	43/43	0.98	0.17	0.24	21,29,34,35	0
12	HEM	P	502	43/43	0.98	0.17	0.16	29,41,54,59	0
17	HEC	Q	501	43/43	0.96	0.18	0.12	52,56,64,65	0
12	HEM	C	502	43/43	0.98	0.17	-0.19	24,27,35,41	0
19	FES	E	501	4/4	0.93	0.11	-1.98	144,144,145,145	0
19	FES	R	501	4/4	0.98	0.07	-2.76	74,76,77,78	0
18	BOG	D	2091	13/20	0.27	0.61	-	200,201,201,201	0
18	BOG	Q	3091	13/20	0.23	0.61	-	183,186,187,187	0
11	PEE	N	3008	5/51	0.83	0.20	-	110,111,112,112	0

6.5 Other polymers

There are no such residues in this entry.