



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 11, 2017 – 05:05 PM EST

PDB ID : 2A06
Title : Bovine cytochrome bc1 complex with stigmatellin bound
Authors : Huang, L.S.; Cobessi, D.; Tung, E.Y.; Berry, E.A.
Deposited on : unknown
Resolution : 2.10 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

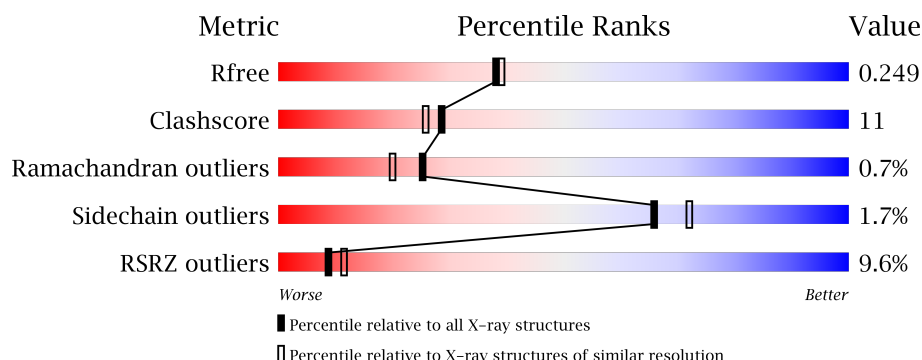
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



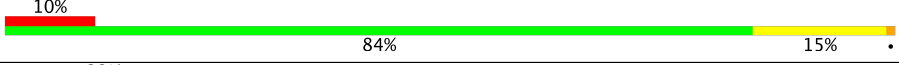

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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>3%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	N	446	<div> <div>7%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>
2	B	439	<div> <div>3%</div> <div>77%</div> <div>20%</div> <div>.</div> </div>
2	O	439	<div> <div>9%</div> <div>75%</div> <div>20%</div> <div>..</div> </div>
3	C	379	<div> <div>5%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	379	
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	78	
8	U	78	
9	I	78	
9	V	78	
10	J	62	
10	W	62	

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	JZR	C	2011	-	-	-	X
11	JZR	F	3012	-	-	-	X
11	JZR	P	3011	-	-	-	X
11	JZR	S	2012	-	-	-	X
12	PO4	A	2010	-	X	-	X
12	PO4	B	3009	-	X	-	-
12	PO4	D	4010	-	X	-	-
12	PO4	D	4011	-	X	-	X
12	PO4	I	4015	-	X	-	-
12	PO4	O	2009	-	X	-	-
12	PO4	P	3010	-	X	-	-
12	PO4	Q	4012	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	PO4	R	4013	-	X	-	X
12	PO4	R	4014	-	X	-	-
12	PO4	T	4016	-	X	-	-
13	AZI	A	4002	-	-	-	X
13	AZI	C	2005	-	-	-	X
13	AZI	P	3005	-	-	-	X
14	UNL	A	4032	-	-	-	X
14	UNL	B	4026	-	-	-	X
14	UNL	B	4034	-	-	-	X
14	UNL	B	4057	-	-	-	X
14	UNL	B	4079	-	-	-	X
14	UNL	B	4080	-	-	-	X
14	UNL	O	4037	-	-	-	X
14	UNL	O	4043	-	-	X	-
14	UNL	O	4084	-	-	-	X
14	UNL	P	4074	-	-	-	X
14	UNL	U	4049	-	-	-	X
14	UNL	U	4056	-	-	-	X
15	PEE	B	4017	-	-	-	X
15	PEE	D	2006	-	-	-	X
15	PEE	P	3007	-	-	-	X
15	PEE	Q	3006	-	-	-	X
20	GOL	C	2008	-	-	-	X
20	GOL	E	4006	-	-	-	X
20	GOL	O	4005	-	-	-	X
20	GOL	P	3008	-	-	-	X

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 33890 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 Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	10	0	1
			3398	2118	602	658	20			
1	N	443	Total	C	N	O	S	10	0	1
			3398	2118	602	658	20			

- Molecule 2 is a protein called Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	1
			3177	1996	562	612	7			
2	O	424	Total	C	N	O	S	0	0	0
			3180	1998	562	613	7			

- Molecule 3 is a protein called Cytochrome b, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	365	Total	C	N	O	S	0	0	0
			2897	1945	450	485	17			
3	P	370	Total	C	N	O	S	0	0	0
			2936	1973	455	490	18			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			
4	Q	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			

- Molecule 5 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			
5	R	196	Total	C	N	O	S	0	0	0
			1517	955	263	291	8			

- Molecule 6 is a protein called Ubiquinol-cytochrome c reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	99	Total	C	N	O	S	0	0	0
			861	545	155	159	2			
6	S	99	Total	C	N	O	S	0	0	0
			861	545	155	159	2			

- Molecule 7 is a protein called Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	75	Total	C	N	O	S	0	0	2
			621	406	117	97	1			
7	T	76	Total	C	N	O	S	0	0	2
			626	409	118	98	1			

- Molecule 8 is a protein called Ubiquinol-cytochrome c reductase complex 11 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	66	Total	C	N	O	S	0	0	0
			539	327	98	109	5			
8	U	66	Total	C	N	O	S	0	0	0
			539	327	98	109	5			

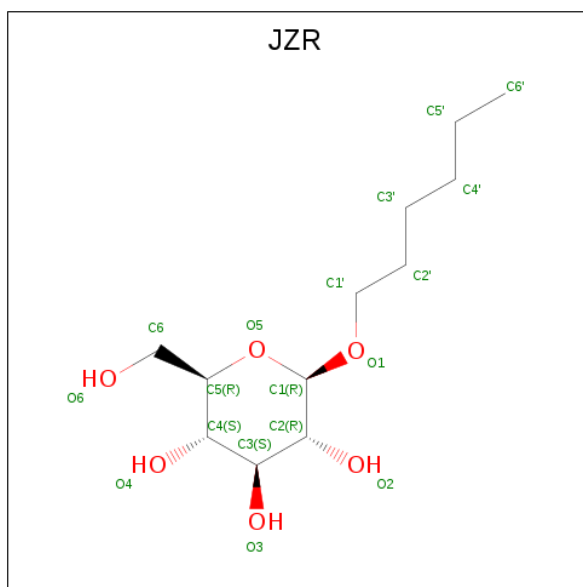
- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	42	Total	C	N	O	S	0	0	0
			285	174	55	55	1			
9	V	42	Total	C	N	O	S	0	0	0
			285	174	55	55	1			

- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

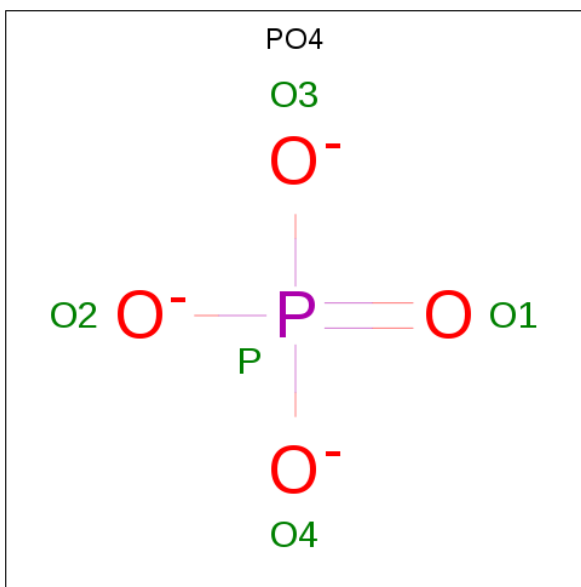
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	30	Total	C	N	O	0	0	1
			245	158	43	44			
10	W	62	Total	C	N	O	0	0	0
			507	333	88	86			

- Molecule 11 is hexyl beta-D-glucopyranoside (three-letter code: JZR) (formula: $C_{12}H_{24}O_6$).



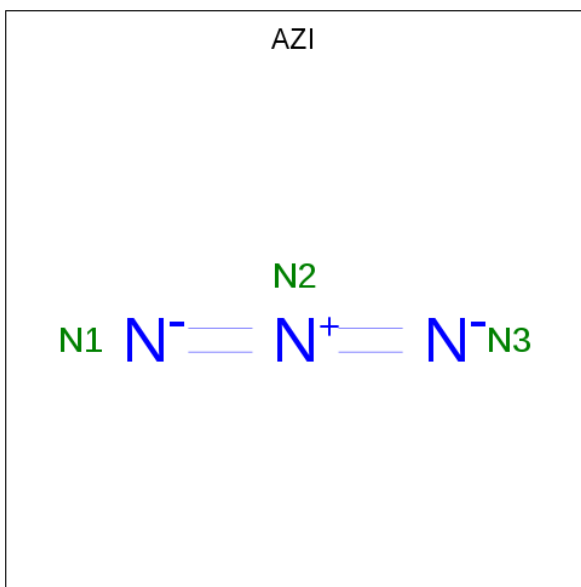
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			18	12	6		
11	C	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	P	1	Total	C	O	0	0
			18	12	6		
11	S	1	Total	C	O	0	0
			18	12	6		

- Molecule 12 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	O	P	0	0
			5	4	1		
12	B	1	Total	O	P	0	0
			5	4	1		
12	D	1	Total	O	P	0	0
			5	4	1		
12	D	1	Total	O	P	0	0
			5	4	1		
12	I	1	Total	O	P	0	0
			5	4	1		
12	O	1	Total	O	P	0	0
			5	4	1		
12	P	1	Total	O	P	0	0
			5	4	1		
12	Q	1	Total	O	P	0	0
			5	4	1		
12	R	1	Total	O	P	0	0
			5	4	1		
12	R	1	Total	O	P	0	0
			5	4	1		
12	T	1	Total	O	P	0	0
			5	4	1		

- Molecule 13 is AZIDE ION (three-letter code: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total N 3 3	0	0
13	C	1	Total N 3 3	0	0
13	G	1	Total N 3 3	0	0
13	P	1	Total N 3 3	0	0

- Molecule 14 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

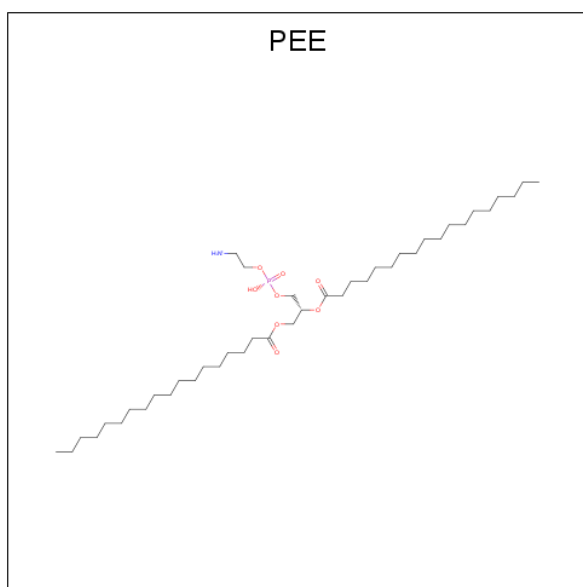
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	P	7	Total O 8 8	0	0
14	G	3	Total O 3 3	0	0
14	Q	1	Total O 1 1	0	0
14	D	7	Total O 7 7	0	0
14	E	2	Total O 2 2	0	0
14	B	11	Total O 11 11	0	0
14	I	2	Total O 2 2	0	0
14	C	6	Total O 7 7	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	V	4	Total	O	0	0
			4	4		
14	W	1	Total	O	0	0
			1	1		
14	A	10	Total	O	0	0
			10	10		
14	T	2	Total	O	0	0
			2	2		
14	N	4	Total	O	0	0
			5	5		
14	U	2	Total	O	0	0
			2	2		
14	O	8	Total	O	0	0
			9	9		
14	R	2	Total	O	0	0
			2	2		
14	S	1	Total	O	0	0
			1	1		
14	F	1	Total	O	0	0
			1	1		

- Molecule 15 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



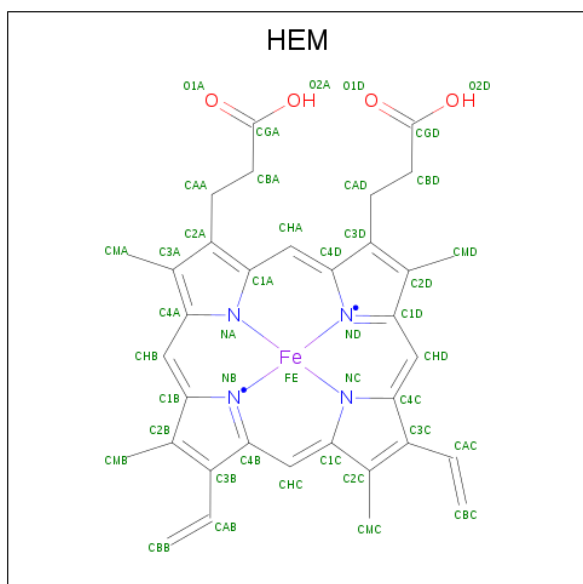
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	B	1	Total	C	O	0	0
			8	6	2		

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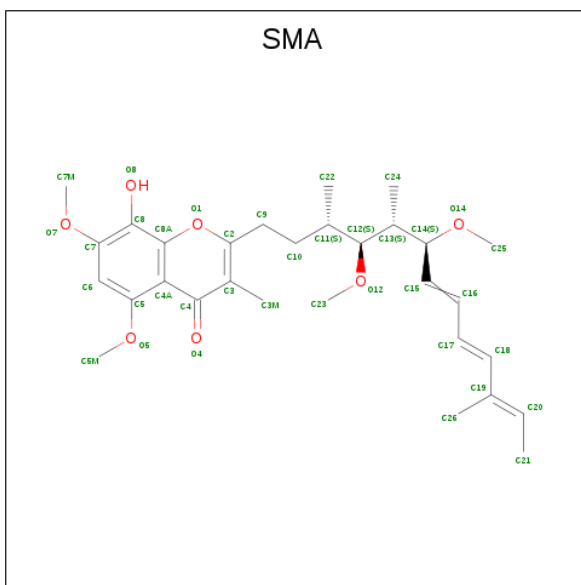
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total 49	C 39	N 1	O 8	P 1	0	0
15	D	1	Total 51	C 41	N 1	O 8	P 1	0	0
15	P	1	Total 49	C 39	N 1	O 8	P 1	0	0
15	Q	1	Total 51	C 41	N 1	O 8	P 1	0	0

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



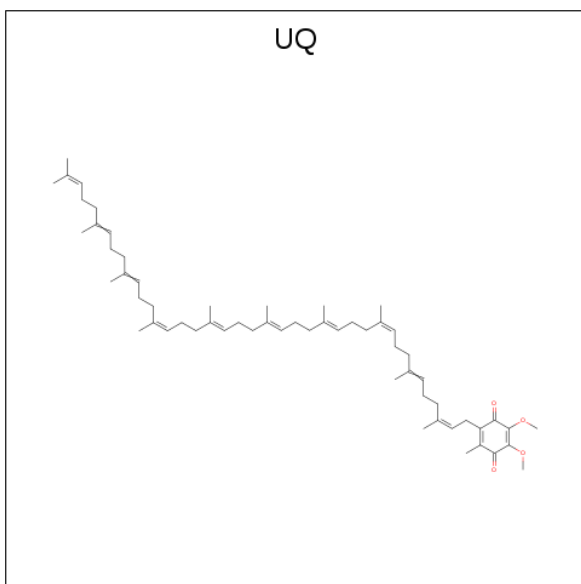
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 17 is STIGMATELLIN A (three-letter code: SMA) (formula: $\text{C}_{30}\text{H}_{42}\text{O}_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			37	30	7		
17	P	1	Total	C	O	0	0
			37	30	7		

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



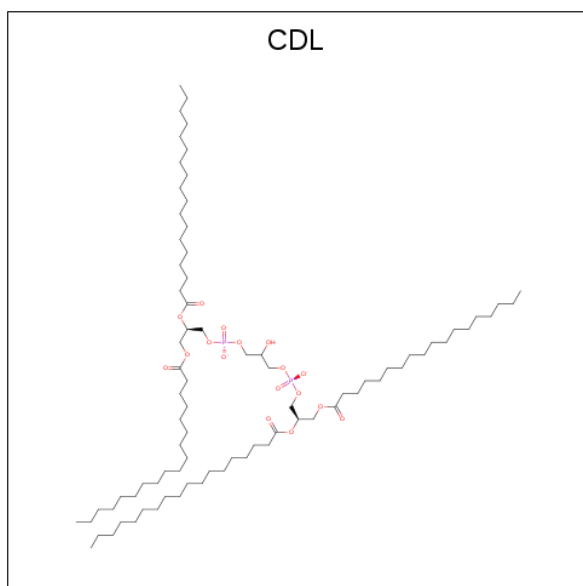
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total	C	O	0	0
			18	14	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	P	1	Total	C	O	0	0
			18	14	4		

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



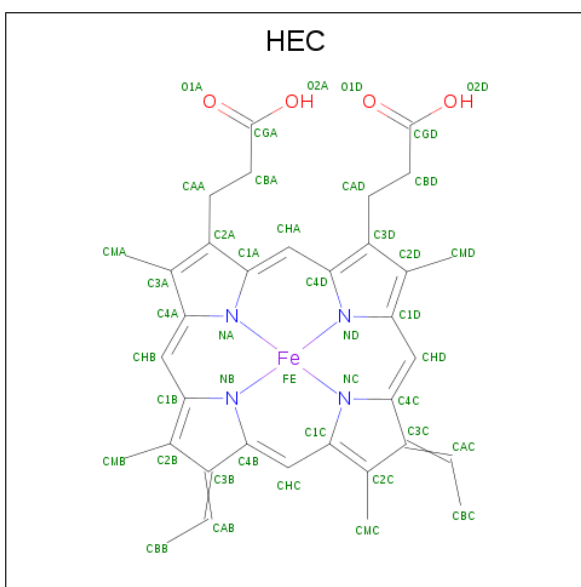
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	C	1	Total	C	O	P	0	0
			44	25	17	2		
19	D	1	Total	C	O	P	0	0
			39	24	13	2		
19	P	1	Total	C	O	P	0	0
			49	30	17	2		
19	Q	1	Total	C	O	P	0	0
			39	24	13	2		

- Molecule 20 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



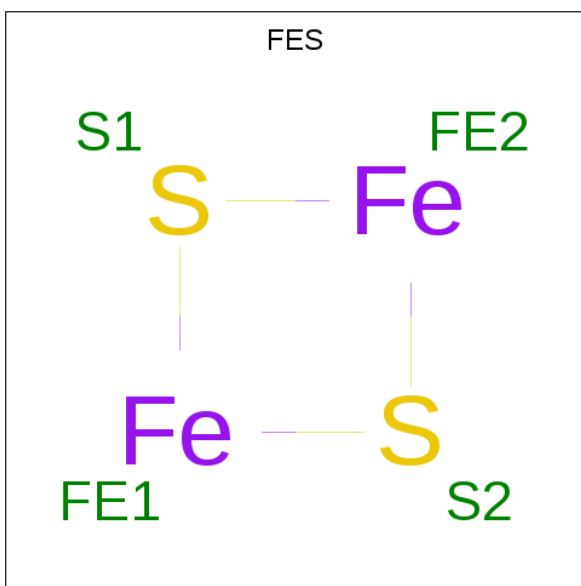
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	C	1	Total	C	O	0	0
			6	3	3		
20	C	1	Total	C	O	0	0
			6	3	3		
20	E	1	Total	C	O	0	0
			6	3	3		
20	E	1	Total	C	O	0	0
			5	3	2		
20	O	1	Total	C	O	0	0
			6	3	3		
20	P	1	Total	C	O	0	0
			6	3	3		
20	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 21 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 22 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

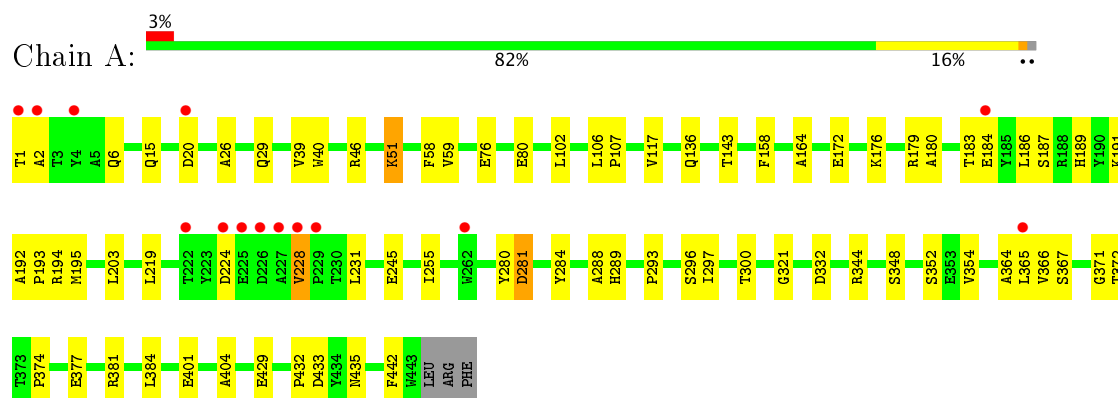
- Molecule 23 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	209	Total O 209 209	0	0
23	B	170	Total O 170 170	0	0
23	C	137	Total O 137 137	0	0
23	D	133	Total O 133 133	0	0
23	E	63	Total O 63 63	0	0
23	F	68	Total O 68 68	0	0
23	G	31	Total O 31 31	0	0
23	H	15	Total O 15 15	0	0
23	I	18	Total O 18 18	0	0
23	J	7	Total O 7 7	0	0
23	N	145	Total O 145 145	0	0
23	O	136	Total O 136 136	0	0
23	P	135	Total O 135 135	0	0
23	Q	126	Total O 126 126	0	0
23	R	77	Total O 77 77	0	0
23	S	81	Total O 81 81	0	0
23	T	17	Total O 17 17	0	0
23	U	16	Total O 16 16	0	0
23	V	16	Total O 16 16	0	0
23	W	12	Total O 12 12	0	0

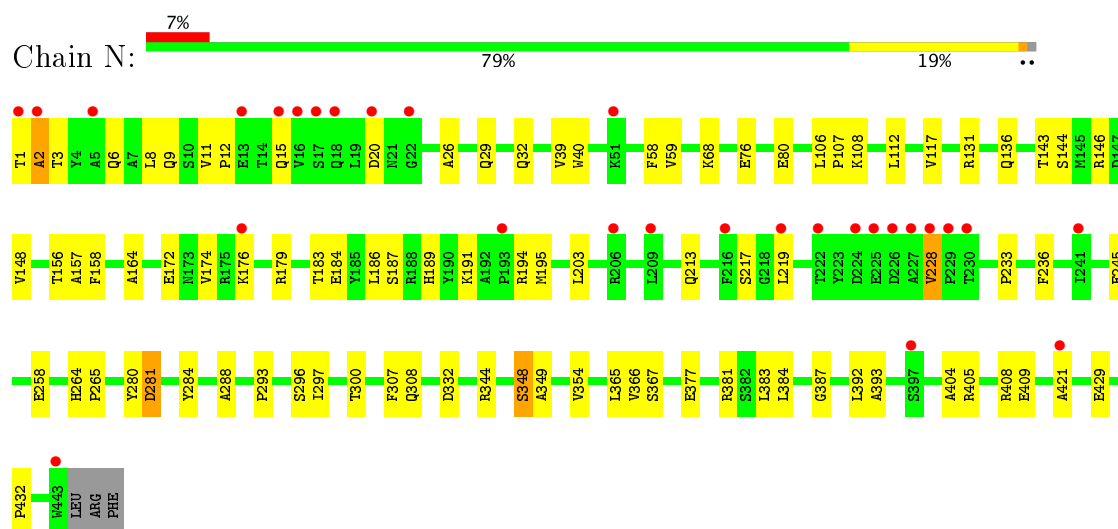
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

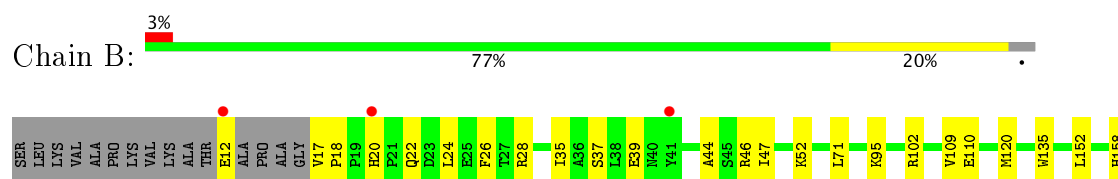
- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial

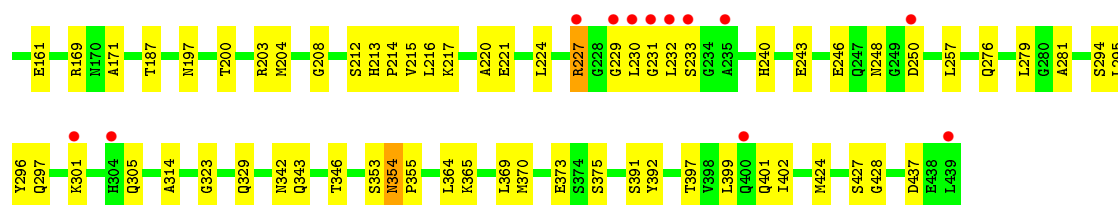


- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial

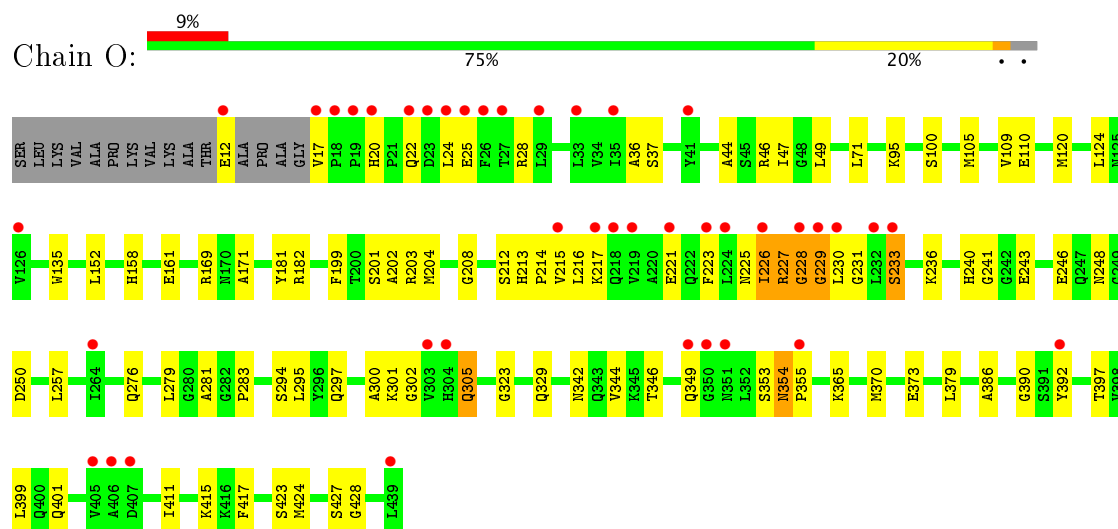


- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

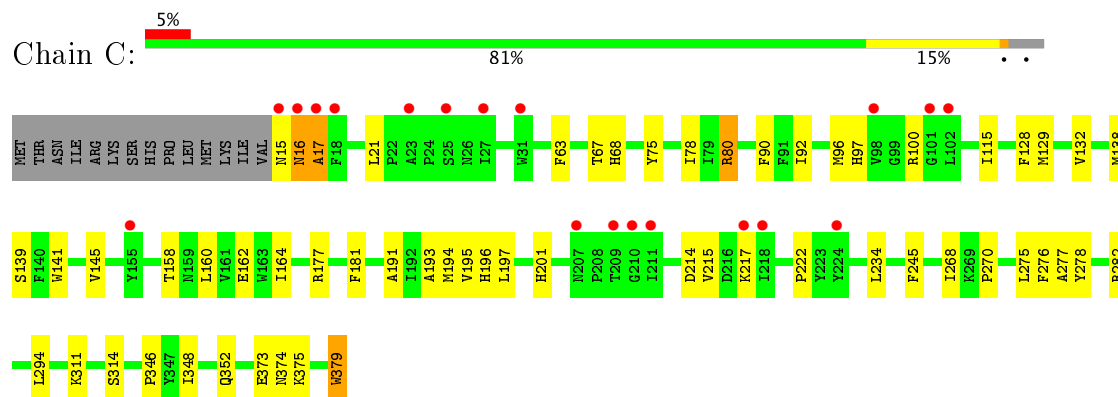




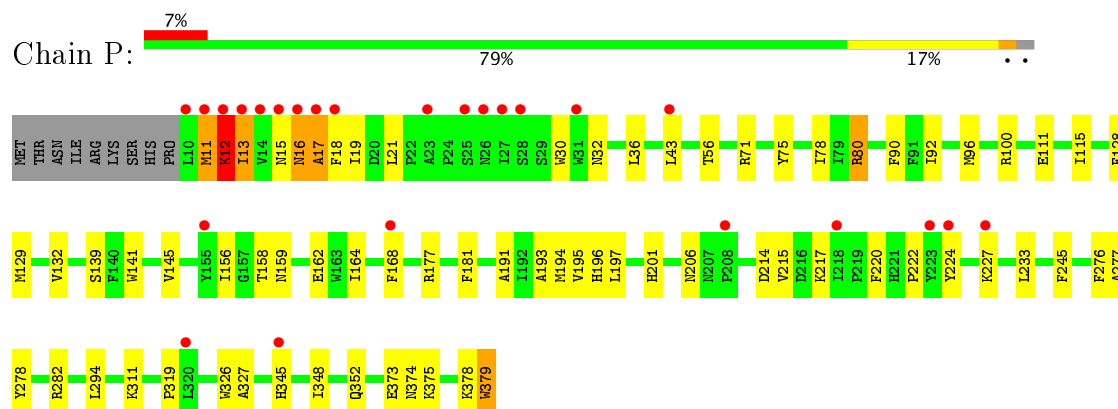
- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial



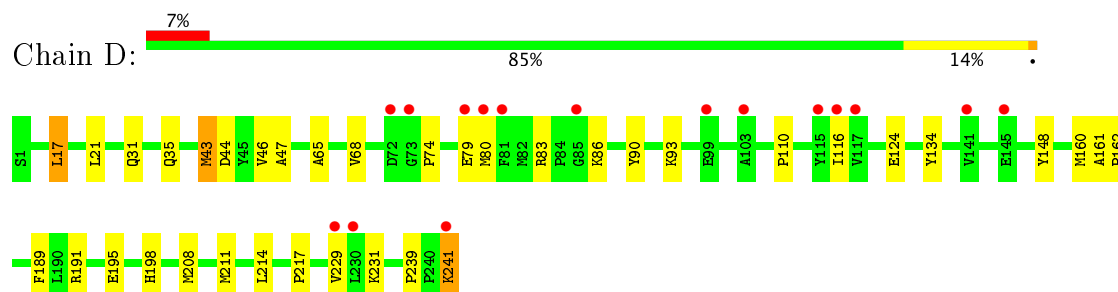
- Molecule 3: Cytochrome b, heme protein, mitochondrial



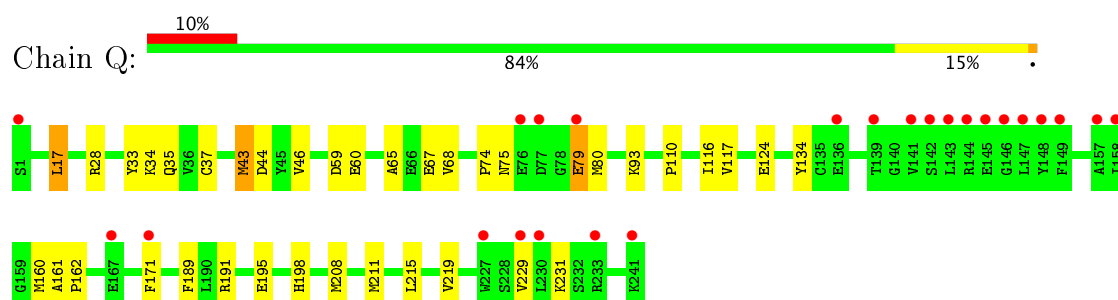
- Molecule 3: Cytochrome b, heme protein, mitochondrial



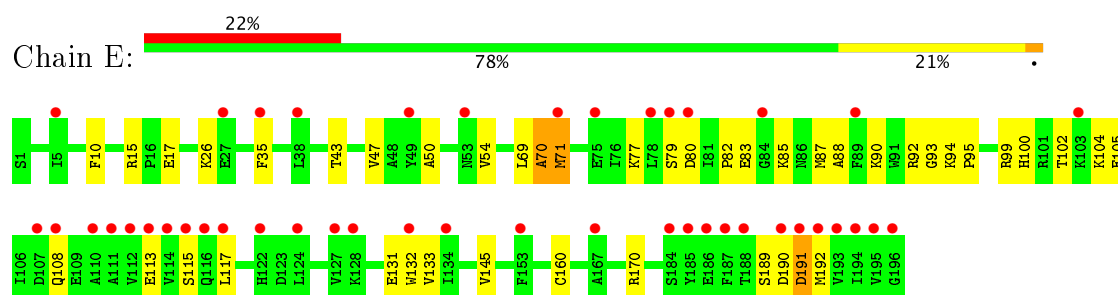
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



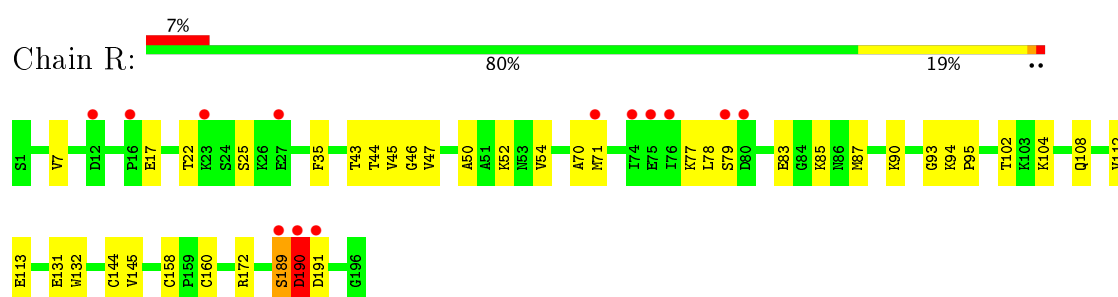
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



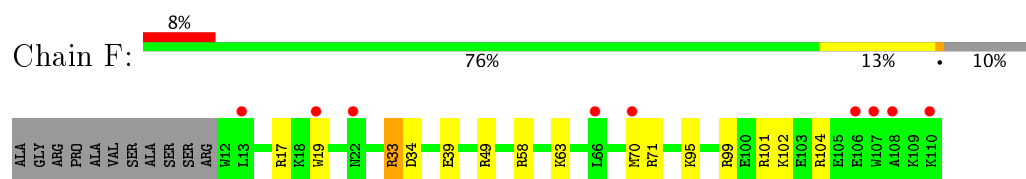
- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



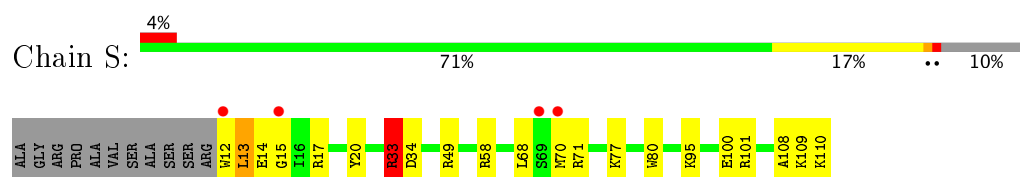
- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



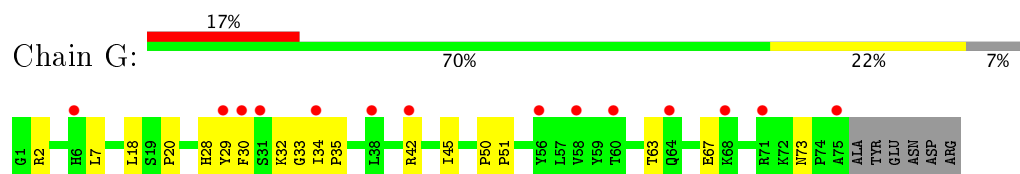
- Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein



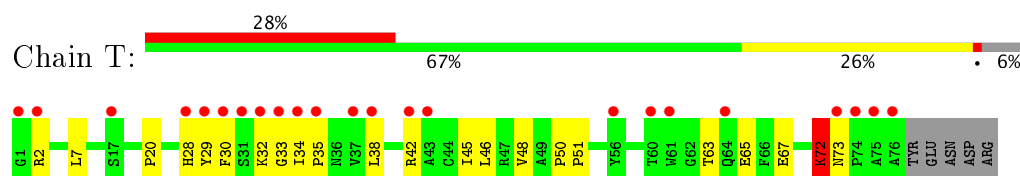
- Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein



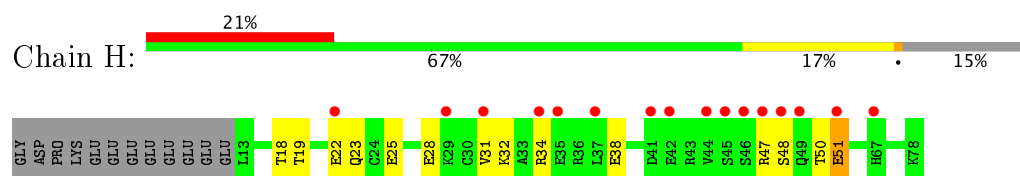
- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



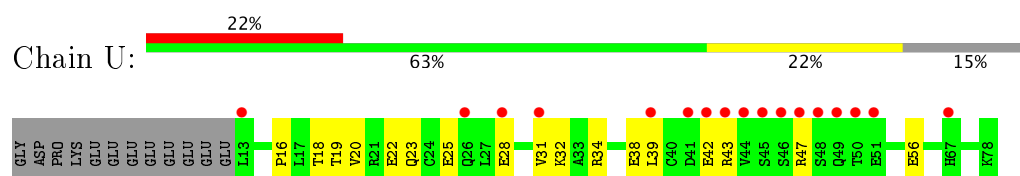
- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



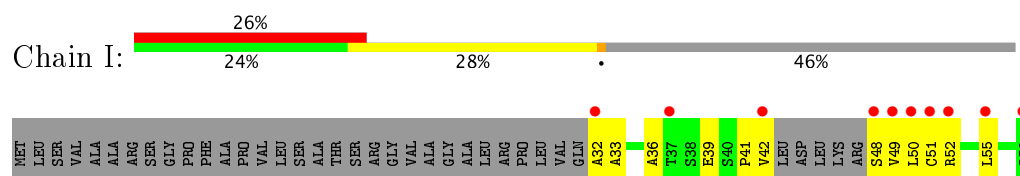
- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein



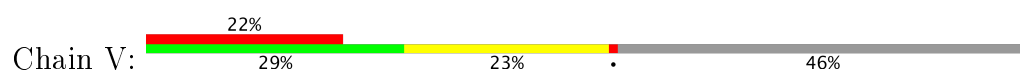
- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein

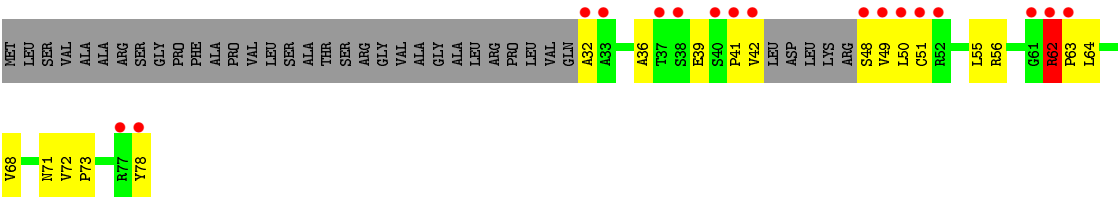


- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial

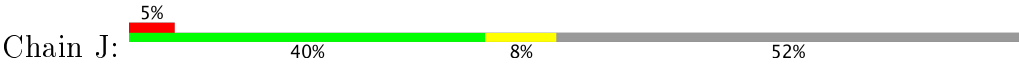


- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial

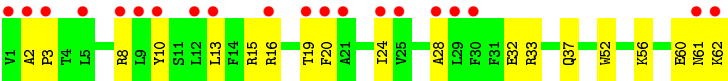




• Molecule 10: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



• Molecule 10: Ubiquinol-cytochrome c reductase complex 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	128.25Å 168.80Å 230.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.87 – 2.10 37.87 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (37.87-2.10) 91.8 (37.87-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.258 0.215 , 0.249	Depositor DCC
R_{free} test set	13752 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33890	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, GOL, CDL, UNL, PO4, UQ, FES, HEC, HEM, PEE, JZR, SMA

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	0/3467	0.67	0/4706
1	N	0.38	0/3467	0.64	0/4706
2	B	0.42	0/3235	0.65	0/4387
2	O	0.39	0/3239	0.65	1/4393 (0.0%)
3	C	0.48	0/2992	0.66	0/4097
3	P	0.44	0/3030	0.64	0/4145
4	D	0.44	0/1978	0.64	0/2684
4	Q	0.41	0/1978	0.62	0/2684
5	E	0.35	0/1553	0.70	3/2100 (0.1%)
5	R	0.41	0/1550	0.69	0/2094
6	F	0.45	0/878	0.66	0/1175
6	S	0.44	0/878	0.68	1/1175 (0.1%)
7	G	0.42	0/642	0.63	0/869
7	T	0.39	0/647	0.65	0/876
8	H	0.34	0/544	0.61	0/729
8	U	0.34	0/544	0.56	0/729
9	I	0.60	0/285	0.96	0/384
9	V	0.50	0/285	0.94	1/384 (0.3%)
10	J	0.38	0/252	0.56	0/333
10	W	0.36	0/520	0.59	0/699
All	All	0.42	0/31964	0.66	6/43349 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	70	ALA	C-N-CA	-6.85	104.57	121.70
2	O	228	GLY	N-CA-C	-6.31	97.33	113.10
5	E	71	MET	C-N-CA	-6.26	106.05	121.70
6	S	33	ARG	NE-CZ-NH2	-6.11	117.24	120.30
9	V	62	ARG	NE-CZ-NH2	5.70	123.15	120.30
5	E	69	LEU	C-N-CA	-5.27	108.53	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	70	ALA	Peptide

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	3398	0	3295	68	0
1	N	3398	0	3295	64	0
2	B	3177	0	3152	88	0
2	O	3180	0	3156	87	0
3	C	2897	0	2943	47	0
3	P	2936	0	2994	74	0
4	D	1919	0	1868	38	0
4	Q	1919	0	1868	36	0
5	E	1519	0	1503	34	0
5	R	1517	0	1498	38	0
6	F	861	0	854	20	0
6	S	861	0	854	26	0
7	G	621	0	626	14	0
7	T	626	0	631	18	0
8	H	539	0	524	17	0
8	U	539	0	524	18	0
9	I	285	0	288	41	0
9	V	285	0	288	32	0
10	J	245	0	229	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	W	507	0	513	22	0
11	A	18	0	24	1	0
11	C	18	0	24	0	0
11	F	36	0	48	4	0
11	P	18	0	24	0	0
11	S	18	0	24	6	0
12	A	5	0	0	0	0
12	B	5	0	0	0	0
12	D	10	0	0	0	0
12	I	5	0	0	1	0
12	O	5	0	0	0	0
12	P	5	0	0	0	0
12	Q	5	0	0	1	0
12	R	10	0	0	0	0
12	T	5	0	0	0	0
13	A	3	0	0	0	0
13	C	3	0	0	0	0
13	G	3	0	0	1	0
13	P	3	0	0	0	0
14	A	10	0	0	0	0
14	B	11	0	0	0	0
14	C	7	0	0	0	0
14	D	7	0	0	1	0
14	E	2	0	0	0	0
14	F	1	0	0	0	0
14	G	3	0	0	0	0
14	I	2	0	0	0	0
14	N	5	0	0	0	0
14	O	9	0	0	2	0
14	P	8	0	0	0	0
14	Q	1	0	0	0	0
14	R	2	0	0	0	0
14	S	1	0	0	0	0
14	T	2	0	0	0	0
14	U	2	0	0	0	0
14	V	4	0	0	0	0
14	W	1	0	0	0	0
15	B	8	0	8	1	0
15	C	49	0	72	0	0
15	D	51	0	82	2	0
15	P	49	0	72	3	0
15	Q	51	0	82	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	C	86	0	60	5	0
16	P	86	0	60	3	0
17	C	37	0	42	3	0
17	P	37	0	42	3	0
18	C	18	0	14	4	0
18	P	18	0	14	5	0
19	C	44	0	32	0	0
19	D	39	0	39	1	0
19	P	49	0	42	0	0
19	Q	39	0	39	0	0
20	C	12	0	16	0	0
20	E	11	0	13	0	0
20	O	6	0	8	0	0
20	P	12	0	16	2	0
21	D	43	0	30	4	0
21	Q	43	0	30	5	0
22	E	4	0	0	0	0
22	R	4	0	0	0	0
23	A	209	0	0	4	0
23	B	170	0	0	2	0
23	C	137	0	0	6	0
23	D	133	0	0	0	0
23	E	63	0	0	0	0
23	F	68	0	0	4	0
23	G	31	0	0	2	0
23	H	15	0	0	0	0
23	I	18	0	0	4	0
23	J	7	0	0	0	0
23	N	145	0	0	3	0
23	O	136	0	0	6	0
23	P	135	0	0	8	0
23	Q	126	0	0	0	0
23	R	77	0	0	1	0
23	S	81	0	0	2	0
23	T	17	0	0	0	0
23	U	16	0	0	0	0
23	V	16	0	0	0	0
23	W	12	0	0	0	0
All	All	33890	0	31860	708	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 11.

All (708) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:226:ILE:HG13	14:O:4043:UNL:O1	1.38	1.23
9:I:32:ALA:N	9:I:71:ASN:HB2	1.70	1.05
2:B:12:GLU:HG2	2:B:17:VAL:H	1.16	1.04
2:O:95:LYS:HB2	9:V:32:ALA:HB2	1.34	1.04
5:R:90:LYS:HE2	5:R:93:GLY:HA2	1.39	1.03
2:B:95:LYS:HD2	9:I:32:ALA:HB2	1.42	1.00
1:A:1:THR:HG21	2:B:212:SER:HB3	1.46	0.97
8:H:25:GLU:HB3	8:H:34:ARG:NH2	1.79	0.97
3:P:12:LYS:HE2	3:P:16:ASN:H	1.28	0.96
9:I:32:ALA:N	9:I:71:ASN:CB	2.31	0.92
2:B:12:GLU:HG2	2:B:17:VAL:N	1.86	0.90
8:U:25:GLU:HB3	8:U:34:ARG:NH2	1.87	0.89
2:B:95:LYS:HB2	9:I:32:ALA:HB2	1.55	0.86
4:Q:43:MET:HE3	4:Q:46:VAL:HG21	1.55	0.85
2:O:202:ALA:HB3	2:O:229:GLY:C	1.96	0.85
4:D:241:LYS:HA	4:D:241:LYS:NZ	1.92	0.85
2:B:397:THR:HG22	2:B:401:GLN:HE21	1.41	0.83
1:A:187:SER:O	1:A:191:LYS:HE2	1.79	0.82
10:W:16:ARG:HB2	10:W:19:THR:HG22	1.63	0.81
9:V:49:VAL:HG11	9:V:55:LEU:HD13	1.63	0.80
2:O:397:THR:HG22	2:O:401:GLN:HE21	1.46	0.80
3:P:21:LEU:HD21	18:P:3002:UQ:HM32	1.64	0.80
23:C:4219:HOH:O	3:P:56:THR:HG22	1.82	0.80
1:A:51:LYS:H	1:A:51:LYS:HE3	1.47	0.80
3:C:21:LEU:HD21	18:C:2002:UQ:HM32	1.64	0.80
1:A:29:GLN:HB3	2:B:12:GLU:O	1.81	0.79
23:A:4261:HOH:O	9:I:73:PRO:HG3	1.83	0.78
1:A:352:SER:HB3	6:S:110:LYS:HD2	1.65	0.78
2:B:95:LYS:HD2	9:I:32:ALA:CB	2.13	0.78
2:O:20:HIS:HB2	2:O:22:GLN:HG2	1.66	0.77
10:W:3:PRO:HB2	10:W:8:ARG:HD3	1.65	0.77
1:N:179:ARG:O	1:N:183:THR:HG23	1.85	0.77
4:D:116:ILE:HG12	21:D:501:HEC:HMA3	1.66	0.77
1:A:401:GLU:HG3	11:A:4004:JZR:H6'	1.67	0.77
2:B:397:THR:HG22	2:B:401:GLN:NE2	1.99	0.77
15:B:4017:PEE:C15	9:I:77:ARG:HH22	1.98	0.76
2:B:20:HIS:HB2	2:B:22:GLN:HG2	1.66	0.75
9:I:49:VAL:HG11	9:I:55:LEU:HD13	1.68	0.75
6:F:58:ARG:HD3	23:F:4062:HOH:O	1.86	0.75
9:V:36:ALA:HB2	9:V:73:PRO:HD2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:59:ASP:OD2	10:W:62:LYS:HB3	1.87	0.74
8:H:31:VAL:HA	8:H:34:ARG:NH1	2.02	0.74
9:I:62:ARG:O	9:I:78:TYR:HB3	1.87	0.74
2:O:161:GLU:OE1	9:V:64:LEU:HD12	1.88	0.74
2:O:95:LYS:HD2	2:O:110:GLU:OE2	1.88	0.74
3:P:129:MET:HE1	3:P:181:PHE:HD2	1.51	0.74
9:I:36:ALA:HB2	9:I:73:PRO:HD2	1.69	0.73
8:U:31:VAL:HA	8:U:34:ARG:NH1	2.03	0.73
4:D:241:LYS:HZ3	4:D:241:LYS:HA	1.50	0.73
3:P:43:LEU:HD21	15:Q:3006:PEE:H30	1.71	0.72
5:E:90:LYS:HE2	5:E:93:GLY:HA2	1.70	0.72
8:H:25:GLU:HB3	8:H:34:ARG:HH21	1.51	0.72
1:A:2:ALA:HB1	1:A:6:GLN:HB2	1.71	0.72
9:V:62:ARG:O	9:V:78:TYR:HB3	1.88	0.72
7:T:72:LYS:HG3	8:U:56:GLU:OE2	1.90	0.71
10:W:13:LEU:O	10:W:19:THR:HG23	1.91	0.71
8:U:25:GLU:HB3	8:U:34:ARG:HH21	1.55	0.71
10:W:33:ARG:O	10:W:37:GLN:HG3	1.91	0.70
7:G:63:THR:O	7:G:67:GLU:HG2	1.91	0.70
4:D:74:PRO:HD3	4:D:80:MET:HE1	1.73	0.70
2:O:397:THR:HG22	2:O:401:GLN:NE2	2.07	0.70
3:C:68:HIS:HD2	23:C:4195:HOH:O	1.74	0.69
4:D:43:MET:HE2	4:D:46:VAL:HG21	1.75	0.69
2:O:95:LYS:HE2	9:V:32:ALA:CB	2.22	0.69
5:R:44:THR:HG21	10:W:24:ILE:HD13	1.73	0.69
2:B:197:ASN:HB3	2:B:230:LEU:HG	1.74	0.69
5:R:70:ALA:N	5:R:71:MET:HE2	2.07	0.69
2:B:95:LYS:CD	9:I:32:ALA:HB2	2.21	0.68
4:D:110:PRO:HG3	21:D:501:HEC:HMD3	1.75	0.68
1:N:187:SER:O	1:N:191:LYS:HE2	1.93	0.68
4:Q:231:LYS:HD3	6:S:70:MET:HE3	1.75	0.68
7:T:63:THR:O	7:T:67:GLU:HG2	1.94	0.68
2:O:203:ARG:HH12	2:O:233:SER:HB3	1.58	0.68
2:O:49:LEU:HD11	2:O:204:MET:HE3	1.73	0.68
3:C:379:TRP:CZ3	6:F:33:ARG:HD3	2.28	0.67
10:J:33:ARG:O	10:J:37:GLN:HG3	1.94	0.67
8:U:28:GLU:HA	8:U:31:VAL:HG22	1.76	0.67
8:H:18:THR:O	8:H:22:GLU:HG3	1.94	0.67
4:Q:110:PRO:HG3	21:Q:501:HEC:HMD3	1.77	0.67
9:V:32:ALA:N	9:V:71:ASN:HB3	2.08	0.67
5:R:90:LYS:HE2	5:R:93:GLY:CA	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:12:LYS:HA	3:P:12:LYS:HE3	1.77	0.66
3:C:129:MET:HE1	3:C:181:PHE:HD2	1.60	0.66
9:I:36:ALA:HB3	9:I:73:PRO:HG2	1.76	0.66
2:B:95:LYS:CB	9:I:32:ALA:HB2	2.25	0.66
9:I:32:ALA:N	9:I:71:ASN:HB3	2.11	0.66
5:E:87:MET:CE	5:E:88:ALA:H	2.09	0.65
1:A:293:PRO:O	1:A:297:ILE:HG12	1.97	0.65
1:A:344:ARG:HG2	1:A:344:ARG:HH11	1.61	0.65
9:V:32:ALA:N	9:V:71:ASN:CB	2.59	0.65
3:P:12:LYS:HE2	3:P:16:ASN:N	2.06	0.65
2:O:95:LYS:HE2	9:V:32:ALA:HB3	1.78	0.65
2:B:20:HIS:HB2	2:B:22:GLN:CG	2.27	0.65
2:O:203:ARG:HH12	2:O:233:SER:CA	2.09	0.65
2:B:200:THR:HG21	2:B:229:GLY:CA	2.26	0.65
16:P:501:HEM:HMC1	16:P:501:HEM:HBC2	1.79	0.65
1:A:179:ARG:O	1:A:183:THR:HG23	1.97	0.65
4:D:231:LYS:HD3	6:F:70:MET:HE3	1.78	0.64
1:A:372:THR:HA	23:A:4296:HOH:O	1.96	0.64
3:C:92:ILE:O	3:C:96:MET:HG2	1.96	0.64
5:E:83:GLU:HG2	5:E:100:HIS:CE1	2.33	0.64
4:Q:44:ASP:OD1	4:Q:93:LYS:HE2	1.97	0.64
5:E:85:LYS:NZ	5:E:87:MET:SD	2.69	0.64
5:E:79:SER:HB3	5:E:191:ASP:OD2	1.98	0.64
2:B:203:ARG:HH11	2:B:232:LEU:HA	1.63	0.64
8:U:18:THR:O	8:U:22:GLU:HG3	1.97	0.64
8:H:28:GLU:HA	8:H:31:VAL:HG22	1.80	0.63
2:B:35:ILE:HD11	2:B:220:ALA:CB	2.28	0.63
3:P:12:LYS:NZ	3:P:16:ASN:HD22	1.95	0.63
4:Q:74:PRO:HD3	4:Q:80:MET:HE1	1.80	0.63
2:B:35:ILE:HD11	2:B:220:ALA:HB3	1.80	0.63
1:N:59:VAL:HG11	1:N:186:LEU:HD21	1.80	0.63
1:N:293:PRO:O	1:N:297:ILE:HG12	1.99	0.63
2:O:250:ASP:HB3	23:O:4203:HOH:O	1.99	0.63
3:P:129:MET:CE	3:P:181:PHE:HD2	2.12	0.63
2:B:12:GLU:CG	2:B:17:VAL:H	2.03	0.62
6:S:108:ALA:C	6:S:110:LYS:H	2.00	0.62
2:O:158:HIS:HB3	23:O:4207:HOH:O	1.98	0.62
2:O:202:ALA:HB3	2:O:229:GLY:O	1.99	0.62
6:S:14:GLU:HG2	23:S:4108:HOH:O	1.98	0.62
1:A:15:GLN:HE21	2:B:12:GLU:HB2	1.64	0.62
1:N:344:ARG:HG2	1:N:344:ARG:HH11	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:4237:HOH:O	5:E:26:LYS:HE2	1.99	0.62
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.82	0.62
2:O:95:LYS:CE	9:V:32:ALA:HB3	2.29	0.62
2:B:296:TYR:OH	9:I:52:ARG:HD3	2.00	0.62
8:H:25:GLU:HB3	8:H:34:ARG:HH22	1.63	0.62
1:A:136:GLN:NE2	9:I:51:CYS:HB2	2.15	0.62
2:B:354:ASN:N	2:B:355:PRO:HD2	2.15	0.61
2:B:24:LEU:HD13	2:B:392:TYR:CE2	2.35	0.61
1:A:143:THR:OG1	9:I:48:SER:HB3	2.00	0.61
5:E:160:CYS:HB3	17:P:3001:SMA:H4	1.82	0.61
2:B:200:THR:HG21	2:B:229:GLY:HA3	1.80	0.61
2:B:95:LYS:HB2	9:I:32:ALA:CB	2.29	0.61
2:B:95:LYS:HD3	2:B:110:GLU:OE2	2.01	0.61
1:A:117:VAL:HG11	1:A:195:MET:CE	2.30	0.61
1:A:366:VAL:HG21	2:B:44:ALA:HB2	1.82	0.61
1:N:366:VAL:HG21	2:O:44:ALA:HB2	1.82	0.61
5:R:17:GLU:OE2	5:R:17:GLU:N	2.28	0.61
2:B:37:SER:HB3	2:B:216:LEU:HD12	1.83	0.61
4:D:124:GLU:OE2	4:D:191:ARG:HD2	2.01	0.61
5:E:77:LYS:HD3	5:E:80:ASP:OD2	2.01	0.61
3:P:379:TRP:CZ3	6:S:33:ARG:HD3	2.36	0.61
2:O:28:ARG:HB2	2:O:28:ARG:NH1	2.16	0.61
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.82	0.60
3:P:92:ILE:O	3:P:96:MET:HG2	2.01	0.60
8:U:34:ARG:O	8:U:38:GLU:HG3	2.01	0.60
2:O:226:ILE:CG1	14:O:4043:UNL:O1	2.32	0.60
5:E:95:PRO:HG2	5:E:145:VAL:HG22	1.83	0.60
2:B:212:SER:OG	2:B:215:VAL:HG13	2.02	0.60
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.50	0.60
2:O:203:ARG:HH12	2:O:233:SER:CB	2.13	0.60
3:P:21:LEU:HD11	23:P:4171:HOH:O	2.01	0.60
4:D:44:ASP:OD1	4:D:93:LYS:HE2	2.01	0.60
2:O:24:LEU:HD23	2:O:392:TYR:CD2	2.37	0.60
10:W:10:TYR:OH	10:W:15:ARG:NH1	2.35	0.60
1:N:68:LYS:HA	1:N:68:LYS:HE3	1.83	0.60
2:O:226:ILE:HD11	23:O:4141:HOH:O	2.00	0.60
23:P:4186:HOH:O	6:S:20:TYR:HE1	1.84	0.60
9:V:36:ALA:CB	9:V:73:PRO:HD2	2.31	0.60
8:H:34:ARG:O	8:H:38:GLU:HG3	2.01	0.59
5:R:112:VAL:HG22	5:R:172:ARG:NH2	2.16	0.59
2:O:71:LEU:HD23	9:V:68:VAL:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:SER:O	1:A:300:THR:HG23	2.01	0.59
9:I:32:ALA:N	9:I:72:VAL:HG23	2.17	0.59
2:O:20:HIS:HB2	2:O:22:GLN:CG	2.32	0.59
2:O:279:LEU:HA	2:O:294:SER:HB3	1.84	0.59
2:B:161:GLU:OE1	9:I:64:LEU:HD12	2.02	0.59
1:N:195:MET:SD	1:N:219:LEU:HD21	2.43	0.59
9:V:32:ALA:N	9:V:72:VAL:HG23	2.18	0.59
5:R:112:VAL:CG2	5:R:172:ARG:NH2	2.66	0.59
2:B:169:ARG:HG3	2:B:240:HIS:HB2	1.83	0.59
2:O:28:ARG:HB2	2:O:28:ARG:HH11	1.67	0.59
8:U:28:GLU:O	8:U:31:VAL:HG22	2.03	0.59
1:A:288:ALA:HB2	1:A:300:THR:HG22	1.84	0.59
2:B:250:ASP:HB3	23:B:4230:HOH:O	2.02	0.59
5:E:71:MET:HE2	5:E:92:ARG:HD3	1.85	0.59
4:Q:60:GLU:HG3	10:W:62:LYS:NZ	2.18	0.58
4:Q:124:GLU:OE2	4:Q:191:ARG:HD2	2.03	0.58
8:H:28:GLU:O	8:H:31:VAL:HG22	2.03	0.58
5:E:145:VAL:HG23	3:P:141:TRP:CH2	2.38	0.58
5:R:79:SER:HB3	5:R:191:ASP:CG	2.23	0.58
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.49	0.58
3:C:141:TRP:CH2	5:R:145:VAL:HG23	2.39	0.58
5:E:17:GLU:N	5:E:17:GLU:OE2	2.28	0.58
1:N:1:THR:O	1:N:2:ALA:HB2	2.03	0.58
2:B:203:ARG:HH12	2:B:233:SER:H	1.50	0.58
2:O:365:LYS:HG2	2:O:399:LEU:HD22	1.85	0.58
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.85	0.58
3:P:100:ARG:C	3:P:100:ARG:HD2	2.24	0.58
3:C:129:MET:CE	3:C:181:PHE:HD2	2.16	0.57
1:N:29:GLN:HG3	1:N:203:LEU:O	2.05	0.57
2:O:276:GLN:HG2	2:O:281:ALA:HB2	1.86	0.57
8:U:31:VAL:HA	8:U:34:ARG:HH12	1.68	0.57
5:E:191:ASP:O	5:E:192:MET:HG2	2.04	0.57
9:I:70:LEU:O	9:I:71:ASN:HB2	2.02	0.57
2:B:208:GLY:HA3	2:B:216:LEU:HD11	1.84	0.57
3:P:43:LEU:HD21	15:Q:3006:PEE:C19	2.34	0.57
9:V:36:ALA:HB3	9:V:73:PRO:HG2	1.85	0.57
2:O:365:LYS:HG2	2:O:399:LEU:CD2	2.35	0.57
1:A:15:GLN:NE2	2:B:12:GLU:HB2	2.19	0.57
2:B:365:LYS:HG2	2:B:399:LEU:CD2	2.35	0.57
2:O:297:GLN:O	2:O:301:LYS:HG3	2.05	0.57
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:83:GLU:HG2	5:E:100:HIS:NE2	2.19	0.57
2:B:297:GLN:O	2:B:301:LYS:HG3	2.03	0.57
4:Q:75:ASN:HD21	4:Q:79:GLU:HG3	1.69	0.57
5:R:79:SER:HB3	5:R:191:ASP:OD2	2.05	0.57
1:A:117:VAL:HG11	1:A:195:MET:HE3	1.87	0.57
2:B:305:GLN:HB3	2:B:329:GLN:OE1	2.04	0.57
2:O:354:ASN:N	2:O:355:PRO:CD	2.68	0.57
2:O:427:SER:HB3	23:O:4207:HOH:O	2.04	0.57
1:A:172:GLU:OE2	1:A:176:LYS:HE3	2.05	0.56
2:O:236:LYS:H	2:O:236:LYS:HD2	1.70	0.56
6:S:49:ARG:HH22	11:S:2012:JZR:H4	1.70	0.56
1:N:189:HIS:HB3	1:N:194:ARG:HH21	1.71	0.56
2:B:365:LYS:HG2	2:B:399:LEU:HD22	1.87	0.56
2:O:212:SER:OG	2:O:215:VAL:HG13	2.05	0.56
5:E:94:LYS:HE3	3:P:168:PHE:O	2.05	0.56
6:S:100:GLU:HB3	11:S:2012:JZR:H6A	1.88	0.56
17:C:2001:SMA:H4	5:R:160:CYS:HB3	1.87	0.56
9:I:70:LEU:HB2	23:I:1826:HOH:O	2.04	0.56
1:N:76:GLU:HG2	1:N:80:GLU:OE2	2.05	0.56
2:O:227:ARG:HA	23:O:4150:HOH:O	2.06	0.56
3:P:277:ALA:HB1	3:P:294:LEU:CD1	2.35	0.56
7:G:42:ARG:HG3	7:G:42:ARG:HH11	1.71	0.56
2:O:169:ARG:HG3	2:O:240:HIS:HB2	1.88	0.56
1:A:106:LEU:HB3	1:A:107:PRO:HD3	1.87	0.56
16:C:501:HEM:HBC2	16:C:501:HEM:HMC1	1.88	0.56
3:C:373:GLU:HB2	23:C:4111:HOH:O	2.06	0.55
9:I:62:ARG:HD3	12:I:4015:PO4:O3	2.07	0.55
4:Q:116:ILE:HG12	21:Q:501:HEC:HMA3	1.89	0.55
6:F:95:LYS:HB2	6:F:95:LYS:NZ	2.20	0.55
1:A:289:HIS:HE1	11:S:2012:JZR:H1'A	1.71	0.55
1:N:189:HIS:CB	1:N:194:ARG:HH21	2.19	0.55
6:S:49:ARG:NH2	11:S:2012:JZR:H4	2.21	0.55
10:W:16:ARG:HB2	10:W:19:THR:CG2	2.36	0.55
6:F:101:ARG:HG2	6:F:101:ARG:HH11	1.71	0.55
8:H:47:ARG:HD3	8:H:50:THR:HB	1.89	0.55
6:S:13:LEU:O	6:S:17:ARG:N	2.40	0.55
3:P:96:MET:HE2	3:P:96:MET:HA	1.89	0.55
4:D:241:LYS:HZ2	4:D:241:LYS:HA	1.70	0.55
5:E:104:LYS:O	5:E:108:GLN:HG3	2.07	0.55
5:E:82:PRO:O	5:E:100:HIS:HB3	2.07	0.55
3:C:15:ASN:O	3:C:16:ASN:C	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:34:ILE:HB	7:T:35:PRO:HD3	1.89	0.55
9:I:62:ARG:HB3	9:I:63:PRO:HD2	1.89	0.54
2:O:353:SER:HB3	2:O:355:PRO:HD2	1.89	0.54
5:R:25:SER:HA	23:R:4077:HOH:O	2.06	0.54
8:H:31:VAL:HA	8:H:34:ARG:HH12	1.69	0.54
1:A:76:GLU:HG2	1:A:80:GLU:OE2	2.08	0.54
2:B:46:ARG:HD2	2:B:375:SER:OG	2.07	0.54
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.38	0.54
1:A:189:HIS:CB	1:A:194:ARG:HH21	2.19	0.54
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.42	0.54
4:D:43:MET:HE1	4:D:189:PHE:HZ	1.72	0.54
2:O:12:GLU:HG3	2:O:17:VAL:H	1.72	0.54
8:U:16:PRO:O	8:U:20:VAL:HG23	2.08	0.54
2:B:231:GLY:N	2:B:233:SER:OG	2.40	0.54
8:H:51:GLU:H	8:H:51:GLU:CD	2.10	0.54
4:Q:34:LYS:HE3	4:Q:67:GLU:OE1	2.07	0.54
1:A:189:HIS:HB3	1:A:194:ARG:HH21	1.72	0.54
1:N:296:SER:O	1:N:300:THR:HG23	2.07	0.54
3:P:156:ILE:HA	3:P:159:ASN:HD22	1.73	0.54
2:B:279:LEU:HB3	2:B:295:LEU:HG	1.90	0.54
5:E:87:MET:HE3	5:E:88:ALA:H	1.71	0.54
2:O:228:GLY:O	2:O:231:GLY:N	2.40	0.54
3:P:197:LEU:HD13	18:P:3002:UQ:HM53	1.89	0.54
5:E:50:ALA:O	5:E:54:VAL:HG23	2.08	0.54
1:N:381:ARG:HH11	1:N:381:ARG:HG2	1.73	0.53
2:O:225:ASN:HD21	2:O:227:ARG:NH2	2.06	0.53
1:A:39:VAL:HG11	1:A:195:MET:CE	2.37	0.53
7:G:34:ILE:HB	7:G:35:PRO:HD3	1.89	0.53
3:P:12:LYS:CA	3:P:12:LYS:HE3	2.39	0.53
1:N:354:VAL:HG21	1:N:404:ALA:HA	1.90	0.53
8:U:19:THR:O	8:U:23:GLN:HG3	2.07	0.53
1:A:51:LYS:N	1:A:51:LYS:HE3	2.21	0.53
2:B:203:ARG:NH1	2:B:233:SER:H	2.07	0.53
6:F:63:LYS:HE2	23:G:4088:HOH:O	2.08	0.53
2:O:225:ASN:HD21	2:O:227:ARG:CZ	2.22	0.53
5:R:104:LYS:O	5:R:108:GLN:HG3	2.09	0.53
6:S:12:TRP:O	6:S:15:GLY:N	2.41	0.53
3:P:145:VAL:HG21	17:P:3001:SMA:H6	1.91	0.53
3:C:375:LYS:O	6:F:17:ARG:NH1	2.42	0.53
2:B:279:LEU:HA	2:B:294:SER:HB3	1.91	0.53
3:P:201:HIS:NE2	18:P:3002:UQ:O4	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:29:TYR:O	7:T:33:GLY:HA3	2.09	0.53
1:A:429:GLU:OE2	7:G:7:LEU:HB2	2.09	0.52
1:N:106:LEU:HB3	1:N:107:PRO:HD3	1.92	0.52
2:O:279:LEU:HB3	2:O:295:LEU:HG	1.89	0.52
1:A:29:GLN:HG3	1:A:203:LEU:O	2.09	0.52
3:C:201:HIS:NE2	18:C:2002:UQ:O4	2.37	0.52
16:C:502:HEM:HMC2	16:C:502:HEM:HBC2	1.92	0.52
2:O:225:ASN:ND2	2:O:227:ARG:CZ	2.72	0.52
1:N:117:VAL:HG11	1:N:195:MET:CE	2.40	0.52
21:Q:501:HEC:HBC3	21:Q:501:HEC:HMC1	1.91	0.52
3:C:138:MET:SD	3:C:268:ILE:HG13	2.49	0.52
1:N:2:ALA:HA	1:N:6:GLN:OE1	2.10	0.52
2:O:217:LYS:O	2:O:221:GLU:HG3	2.10	0.52
4:Q:75:ASN:OD1	4:Q:79:GLU:HG2	2.10	0.52
1:A:136:GLN:HB3	9:I:51:CYS:HB3	1.91	0.52
9:I:36:ALA:CB	9:I:73:PRO:HD2	2.37	0.52
3:P:311:LYS:HG2	3:P:374:ASN:CG	2.30	0.52
6:S:95:LYS:HB2	6:S:95:LYS:NZ	2.25	0.52
1:N:288:ALA:HB2	1:N:300:THR:HG22	1.92	0.52
3:C:100:ARG:C	3:C:100:ARG:HD2	2.29	0.52
1:N:228:VAL:O	1:N:228:VAL:HG13	2.11	0.52
9:V:36:ALA:HB3	9:V:73:PRO:CG	2.40	0.52
5:E:87:MET:HE2	5:E:88:ALA:H	1.75	0.51
1:N:146:ARG:HH21	1:N:308:GLN:HE22	1.57	0.51
1:A:281:ASP:OD2	9:I:73:PRO:HB3	2.10	0.51
1:N:172:GLU:OE2	1:N:176:LYS:HE3	2.09	0.51
1:N:408:ARG:HD2	23:N:4206:HOH:O	2.09	0.51
1:N:405:ARG:O	1:N:409:GLU:HG3	2.10	0.51
1:A:381:ARG:HG2	1:A:381:ARG:HH11	1.75	0.51
4:Q:231:LYS:HD3	6:S:70:MET:CE	2.40	0.51
7:T:32:LYS:C	7:T:35:PRO:HD2	2.31	0.51
9:V:32:ALA:N	9:V:71:ASN:HB2	2.25	0.51
1:N:39:VAL:HG11	1:N:195:MET:CE	2.40	0.51
3:P:158:THR:HB	23:P:4121:HOH:O	2.11	0.51
2:O:236:LYS:N	2:O:236:LYS:HD2	2.26	0.51
2:B:24:LEU:HD13	2:B:392:TYR:CD2	2.45	0.50
21:D:501:HEC:HMC1	21:D:501:HEC:HBC3	1.92	0.50
7:G:29:TYR:O	7:G:33:GLY:HA3	2.09	0.50
2:B:227:ARG:HD3	2:B:227:ARG:N	2.26	0.50
5:E:102:THR:OG1	5:E:105:GLU:HG3	2.11	0.50
4:D:21:LEU:HD21	4:D:191:ARG:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:LEU:HD23	9:I:68:VAL:HG21	1.91	0.50
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.47	0.50
2:B:248:ASN:OD1	2:B:428:GLY:HA2	2.11	0.50
1:A:180:ALA:O	1:A:184:GLU:HG3	2.11	0.50
5:R:50:ALA:O	5:R:54:VAL:HG23	2.11	0.50
5:E:190:ASP:O	5:E:192:MET:HG2	2.12	0.50
9:I:64:LEU:HD23	9:I:77:ARG:O	2.12	0.50
4:Q:195:GLU:HG2	4:Q:198:HIS:HB2	1.94	0.50
1:N:429:GLU:OE2	7:T:7:LEU:HB2	2.12	0.50
1:N:136:GLN:NE2	9:V:51:CYS:HB2	2.27	0.50
3:C:245:PHE:CD1	4:D:17:LEU:HD13	2.47	0.50
10:J:56:LYS:HG2	10:J:60:GLU:CD	2.32	0.50
2:O:305:GLN:NE2	2:O:329:GLN:OE1	2.45	0.49
3:C:160:LEU:O	3:C:164:ILE:HG12	2.11	0.49
1:N:344:ARG:HG2	1:N:344:ARG:NH1	2.27	0.49
4:Q:208:MET:HA	15:Q:3006:PEE:H49	1.94	0.49
2:O:95:LYS:CE	9:V:32:ALA:CB	2.90	0.49
2:O:283:PRO:HB3	9:V:56:ARG:HG3	1.93	0.49
3:C:145:VAL:HG21	17:C:2001:SMA:H6	1.94	0.49
10:W:15:ARG:HG3	10:W:15:ARG:HH11	1.76	0.49
6:F:104:ARG:HH11	11:F:3012:JZR:H6	1.77	0.49
3:P:217:LYS:HG3	7:T:7:LEU:HD13	1.94	0.49
8:U:25:GLU:HB3	8:U:34:ARG:HH22	1.72	0.49
2:B:203:ARG:NH1	2:B:232:LEU:HA	2.28	0.49
3:C:197:LEU:HD13	18:C:2002:UQ:HM53	1.94	0.49
4:D:17:LEU:HD21	14:D:4083:UNL:O1	2.13	0.49
1:N:280:TYR:HA	1:N:284:TYR:CE2	2.47	0.49
1:N:383:LEU:O	1:N:387:GLY:HA2	2.12	0.49
2:O:95:LYS:O	2:O:109:VAL:HA	2.12	0.49
2:O:203:ARG:HH12	2:O:233:SER:HA	1.78	0.49
3:P:11:MET:HG2	3:P:12:LYS:N	2.27	0.49
7:G:32:LYS:C	7:G:35:PRO:HD2	2.33	0.49
3:P:164:ILE:O	3:P:177:ARG:HD2	2.13	0.49
2:O:47:ILE:HG21	2:O:120:MET:HE3	1.95	0.49
7:T:46:LEU:N	7:T:46:LEU:HD22	2.27	0.49
1:A:344:ARG:HG2	1:A:344:ARG:NH1	2.25	0.48
3:P:13:ILE:O	3:P:13:ILE:HG22	2.13	0.48
1:A:39:VAL:HG11	1:A:195:MET:HE2	1.93	0.48
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.95	0.48
2:B:243:GLU:HA	2:B:424:MET:O	2.13	0.48
2:B:246:GLU:O	2:B:427:SER:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:208:MET:HA	15:D:2006:PEE:H49	1.94	0.48
1:N:15:GLN:O	1:N:26:ALA:HA	2.13	0.48
8:U:39:LEU:O	8:U:42:GLU:HB3	2.13	0.48
2:O:95:LYS:HB2	9:V:32:ALA:CB	2.25	0.48
2:B:52:LYS:NZ	2:B:232:LEU:HD11	2.28	0.48
3:C:158:THR:O	3:C:162:GLU:HG3	2.13	0.48
3:C:68:HIS:CD2	23:C:4195:HOH:O	2.59	0.48
1:N:233:PRO:O	5:R:22:THR:HA	2.13	0.48
3:P:129:MET:HE1	3:P:181:PHE:CD2	2.40	0.48
3:P:311:LYS:HG2	3:P:374:ASN:OD1	2.14	0.48
5:R:77:LYS:HE3	5:R:79:SER:OG	2.13	0.48
23:A:4251:HOH:O	9:I:39:GLU:CG	2.62	0.48
1:N:308:GLN:HB3	23:N:4088:HOH:O	2.13	0.48
2:O:199:PHE:O	2:O:226:ILE:HD13	2.14	0.48
2:B:47:ILE:HG13	2:B:120:MET:HE1	1.96	0.48
2:B:217:LYS:HE2	2:B:221:GLU:OE2	2.14	0.48
2:B:354:ASN:N	2:B:355:PRO:CD	2.76	0.48
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.47	0.48
2:O:201:SER:H	2:O:226:ILE:HG23	1.78	0.48
2:O:246:GLU:O	2:O:427:SER:HA	2.14	0.48
4:D:160:MET:HB2	21:D:501:HEC:C1D	2.44	0.48
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.96	0.48
2:O:202:ALA:HB3	2:O:230:LEU:N	2.28	0.48
4:Q:43:MET:HE2	4:Q:189:PHE:CZ	2.49	0.48
2:B:232:LEU:O	2:B:233:SER:HB3	2.13	0.48
6:F:49:ARG:NH2	11:F:3012:JZR:H1	2.28	0.48
2:B:437:ASP:OD2	2:O:240:HIS:CD2	2.67	0.48
9:I:36:ALA:HB3	9:I:73:PRO:CG	2.42	0.47
10:W:56:LYS:O	10:W:60:GLU:HG3	2.13	0.47
2:B:397:THR:CG2	2:B:401:GLN:HE21	2.18	0.47
1:N:158:PHE:O	1:N:164:ALA:HB2	2.14	0.47
2:O:124:LEU:HD13	2:O:223:PHE:CB	2.44	0.47
3:P:115:ILE:HD13	3:P:195:VAL:HG12	1.95	0.47
3:P:319:PRO:HD2	23:P:4186:HOH:O	2.13	0.47
4:Q:43:MET:HE2	4:Q:189:PHE:HZ	1.80	0.47
4:D:74:PRO:CD	4:D:80:MET:HE1	2.41	0.47
2:O:397:THR:CG2	2:O:401:GLN:HE21	2.23	0.47
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.54	0.47
1:A:15:GLN:O	1:A:26:ALA:HA	2.14	0.47
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.50	0.47
5:E:77:LYS:HE3	5:E:79:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:34:ASP:O	6:F:58:ARG:NH2	2.47	0.47
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.97	0.47
6:F:104:ARG:HH11	11:F:3012:JZR:C6	2.27	0.47
4:D:231:LYS:HD3	6:F:70:MET:CE	2.44	0.47
9:I:71:ASN:ND2	23:I:1406:HOH:O	2.47	0.47
9:I:78:TYR:HA	23:I:1201:HOH:O	2.14	0.47
3:P:214:ASP:CG	7:T:2:ARG:HH22	2.18	0.47
3:C:191:ALA:HA	3:C:194:MET:CE	2.45	0.47
3:C:96:MET:HA	3:C:96:MET:HE2	1.97	0.47
3:P:327:ALA:HA	7:T:51:PRO:HB3	1.95	0.47
6:S:68:LEU:HD23	6:S:71:ARG:HH22	1.80	0.47
1:N:348:SER:O	1:N:349:ALA:C	2.54	0.47
10:W:2:ALA:HA	10:W:3:PRO:HD3	1.77	0.47
1:A:40:TRP:HB3	1:A:384:LEU:HD11	1.96	0.46
2:B:12:GLU:O	2:B:18:PRO:HD3	2.14	0.46
2:O:370:MET:O	2:O:373:GLU:HG2	2.15	0.46
5:R:189:SER:O	5:R:190:ASP:C	2.53	0.46
9:I:72:VAL:CG1	9:I:73:PRO:HD2	2.45	0.46
2:B:135:TRP:CE2	6:S:49:ARG:HD3	2.50	0.46
4:D:211:MET:HG3	15:D:2006:PEE:H48	1.97	0.46
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.50	0.46
10:W:20:PHE:CE1	10:W:24:ILE:HD11	2.49	0.46
4:D:47:ALA:HA	4:D:90:TYR:HA	1.96	0.46
8:H:19:THR:O	8:H:23:GLN:HG3	2.15	0.46
1:N:264:HIS:HA	1:N:265:PRO:HD3	1.83	0.46
1:N:3:THR:OG1	1:N:6:GLN:HG3	2.15	0.46
6:S:101:ARG:HG2	6:S:101:ARG:HH11	1.80	0.46
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.46	0.46
3:P:12:LYS:HA	3:P:12:LYS:CE	2.43	0.46
5:R:93:GLY:O	5:R:94:LYS:HG3	2.14	0.46
2:O:213:HIS:N	2:O:214:PRO:CD	2.79	0.46
2:O:344:VAL:HG11	2:O:417:PHE:CD2	2.50	0.46
4:Q:74:PRO:HB3	4:Q:80:MET:CE	2.45	0.46
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.98	0.46
2:B:102:ARG:HH22	2:B:161:GLU:CD	2.19	0.46
2:B:370:MET:O	2:B:373:GLU:HG2	2.16	0.46
3:C:215:VAL:HG13	23:C:4154:HOH:O	2.15	0.46
3:C:75:TYR:O	3:C:78:ILE:HG22	2.15	0.46
4:D:83:ARG:CZ	4:D:86:LYS:HE2	2.45	0.46
1:N:281:ASP:OD2	9:V:73:PRO:HB3	2.15	0.46
3:P:373:GLU:HB2	23:P:4170:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:13:LEU:HD22	23:S:4129:HOH:O	2.15	0.46
3:P:375:LYS:O	6:S:17:ARG:NH1	2.49	0.46
2:B:342:ASN:O	2:B:346:THR:HG23	2.15	0.46
2:B:354:ASN:H	2:B:355:PRO:HD2	1.81	0.46
6:S:108:ALA:C	6:S:110:LYS:N	2.68	0.46
10:W:3:PRO:CB	10:W:8:ARG:HD3	2.41	0.46
6:F:49:ARG:HD3	2:O:135:TRP:CE2	2.51	0.46
2:O:25:GLU:O	2:O:36:ALA:HA	2.15	0.46
8:U:28:GLU:CA	8:U:31:VAL:HG22	2.44	0.46
6:F:71:ARG:HD3	23:F:4076:HOH:O	2.15	0.46
3:C:214:ASP:CG	7:G:2:ARG:HH22	2.19	0.46
1:N:156:THR:HA	5:R:7:VAL:HG21	1.98	0.46
3:P:278:TYR:CZ	3:P:282:ARG:HD3	2.50	0.46
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.51	0.46
4:Q:74:PRO:CD	4:Q:80:MET:HE1	2.46	0.46
23:O:4201:HOH:O	9:V:32:ALA:HB1	2.16	0.46
9:V:50:LEU:O	9:V:51:CYS:HB3	2.16	0.46
3:C:115:ILE:HD13	3:C:195:VAL:HG12	1.98	0.45
16:C:502:HEM:HBA1	18:C:2002:UQ:O2	2.16	0.45
1:N:29:GLN:HB3	2:O:12:GLU:O	2.16	0.45
1:A:228:VAL:O	1:A:228:VAL:HG13	2.16	0.45
7:G:2:ARG:HA	23:G:4101:HOH:O	2.16	0.45
2:O:181:TYR:CE1	2:O:182:ARG:HG2	2.51	0.45
3:P:15:ASN:O	3:P:17:ALA:N	2.49	0.45
8:U:28:GLU:HA	8:U:31:VAL:CG2	2.44	0.45
10:W:3:PRO:HB2	10:W:8:ARG:CD	2.43	0.45
7:T:28:HIS:ND1	7:T:32:LYS:HD2	2.31	0.45
3:C:276:PHE:CG	3:C:277:ALA:N	2.84	0.45
6:S:109:LYS:O	6:S:110:LYS:HG2	2.16	0.45
4:D:148:TYR:CZ	4:D:161:ALA:HB2	2.52	0.45
2:O:386:ALA:O	2:O:390:GLY:HA2	2.17	0.45
5:R:190:ASP:HB2	5:R:191:ASP:H	1.42	0.45
3:P:158:THR:O	3:P:162:GLU:HG3	2.16	0.45
2:B:217:LYS:O	2:B:221:GLU:HG3	2.17	0.45
1:A:158:PHE:O	1:A:164:ALA:HB2	2.17	0.45
2:B:95:LYS:O	2:B:109:VAL:HA	2.17	0.45
3:C:80:ARG:C	3:C:80:ARG:HD3	2.37	0.45
3:C:164:ILE:O	3:C:177:ARG:HD2	2.16	0.45
1:A:39:VAL:CG1	1:A:195:MET:HE2	2.47	0.45
6:F:101:ARG:HG2	6:F:101:ARG:NH1	2.32	0.45
9:I:61:GLY:C	9:I:62:ARG:HG3	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:213:GLN:O	1:N:217:SER:OG	2.27	0.45
2:O:342:ASN:O	2:O:346:THR:HG23	2.16	0.45
5:R:44:THR:HG22	10:W:24:ILE:HG21	1.97	0.45
1:N:117:VAL:HG11	1:N:195:MET:HE1	1.99	0.44
2:O:100:SER:OG	2:O:105:MET:HG2	2.17	0.44
3:P:13:ILE:HA	3:P:17:ALA:HB2	1.99	0.44
1:A:288:ALA:CB	1:A:300:THR:HG22	2.46	0.44
2:O:227:ARG:HD2	2:O:227:ARG:N	2.32	0.44
3:P:348:ILE:O	3:P:352:GLN:HG3	2.17	0.44
3:P:75:TYR:O	3:P:78:ILE:HG22	2.17	0.44
8:U:42:GLU:HG2	8:U:43:ARG:N	2.32	0.44
4:D:74:PRO:HB3	4:D:80:MET:CE	2.47	0.44
3:P:129:MET:HE1	17:P:3001:SMA:H26	1.98	0.44
3:P:220:PHE:HE1	18:P:3002:UQ:HM23	1.82	0.44
4:Q:160:MET:HB2	21:Q:501:HEC:C1D	2.47	0.44
5:R:112:VAL:HG22	5:R:172:ARG:HH22	1.82	0.44
4:Q:60:GLU:HG3	10:W:62:LYS:HZ3	1.81	0.44
3:C:270:PRO:HG2	3:C:278:TYR:CG	2.52	0.44
1:A:102:LEU:CD2	2:B:369:LEU:HD12	2.47	0.44
3:C:348:ILE:O	3:C:352:GLN:HG3	2.17	0.44
4:D:195:GLU:HG2	4:D:198:HIS:HB2	2.00	0.44
10:J:56:LYS:O	10:J:60:GLU:HG3	2.17	0.44
2:O:248:ASN:OD1	2:O:428:GLY:HA2	2.17	0.44
3:P:11:MET:HE3	3:P:12:LYS:HB2	1.99	0.44
5:R:102:THR:OG1	5:R:104:LYS:HG2	2.18	0.44
10:W:52:TRP:O	10:W:56:LYS:HB2	2.17	0.44
4:D:74:PRO:HA	4:D:79:GLU:O	2.18	0.44
6:F:95:LYS:NZ	6:F:95:LYS:CB	2.80	0.44
1:N:39:VAL:HG11	1:N:195:MET:HE2	1.98	0.44
16:P:502:HEM:HBA1	18:P:3002:UQ:O2	2.18	0.44
1:A:371:GLY:O	1:A:374:PRO:HD2	2.18	0.44
3:C:191:ALA:HA	3:C:194:MET:HE3	2.00	0.44
4:D:214:LEU:O	4:D:217:PRO:HG2	2.17	0.44
9:V:32:ALA:N	9:V:72:VAL:CG2	2.80	0.44
2:B:46:ARG:O	2:B:47:ILE:HD13	2.17	0.44
3:C:132:VAL:HA	3:C:139:SER:HB3	1.98	0.44
2:O:217:LYS:HE2	2:O:221:GLU:OE2	2.18	0.44
5:R:112:VAL:HG21	5:R:172:ARG:NH2	2.32	0.44
5:R:43:THR:O	5:R:47:VAL:HG23	2.17	0.44
9:V:72:VAL:HG13	9:V:73:PRO:HD2	2.00	0.44
9:V:72:VAL:CG1	9:V:73:PRO:HD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:83:GLU:HG2	5:E:100:HIS:CD2	2.53	0.43
4:D:43:MET:CE	4:D:189:PHE:CZ	3.01	0.43
9:I:50:LEU:O	9:I:51:CYS:HB3	2.18	0.43
2:O:215:VAL:CG2	2:O:216:LEU:N	2.80	0.43
6:S:34:ASP:O	6:S:58:ARG:NH2	2.50	0.43
1:A:195:MET:SD	1:A:219:LEU:HD21	2.58	0.43
5:E:99:ARG:HB3	5:E:133:VAL:HG12	2.01	0.43
1:N:1:THR:O	1:N:2:ALA:CB	2.66	0.43
3:P:100:ARG:O	3:P:100:ARG:HD2	2.18	0.43
3:P:282:ARG:NH2	23:P:4173:HOH:O	2.51	0.43
3:P:43:LEU:HD21	15:Q:3006:PEE:H27	2.00	0.43
9:V:64:LEU:HD23	9:V:78:TYR:C	2.38	0.43
1:A:289:HIS:HE1	11:S:2012:JZR:C1'	2.32	0.43
2:B:28:ARG:CG	2:B:28:ARG:HH11	2.32	0.43
2:O:46:ARG:HG2	2:O:379:LEU:HD22	2.00	0.43
4:Q:195:GLU:O	4:Q:195:GLU:HG2	2.19	0.43
1:A:352:SER:OG	6:S:110:LYS:HB2	2.18	0.43
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.19	0.43
2:B:52:LYS:HZ3	2:B:232:LEU:HD11	1.82	0.43
3:C:197:LEU:HD23	3:C:197:LEU:HA	1.66	0.43
8:H:25:GLU:CB	8:H:34:ARG:NH2	2.67	0.43
3:P:378:LYS:HE3	6:S:17:ARG:NE	2.34	0.43
4:Q:211:MET:HG3	15:Q:3006:PEE:H48	2.00	0.43
2:B:46:ARG:HG2	2:B:110:GLU:HG2	2.00	0.43
1:A:364:ALA:HB2	9:I:33:ALA:HB1	2.01	0.43
2:O:46:ARG:O	2:O:47:ILE:HD13	2.19	0.43
3:P:227:LYS:HE3	20:P:4009:GOL:O1	2.18	0.43
3:P:80:ARG:C	3:P:80:ARG:HD3	2.39	0.43
2:B:187:THR:HB	23:B:4154:HOH:O	2.18	0.43
1:N:236:PHE:CG	1:N:258:GLU:HB2	2.54	0.43
7:T:30:PHE:O	7:T:34:ILE:HG12	2.18	0.43
4:D:124:GLU:OE2	4:D:191:ARG:CD	2.67	0.43
4:D:195:GLU:HG2	4:D:195:GLU:O	2.19	0.43
5:E:191:ASP:CG	5:E:191:ASP:O	2.56	0.43
3:P:191:ALA:HA	3:P:194:MET:CE	2.48	0.43
9:V:62:ARG:HB3	9:V:63:PRO:HD2	2.01	0.43
2:O:203:ARG:HD2	2:O:230:LEU:O	2.19	0.43
4:Q:229:VAL:CG2	7:T:20:PRO:HD3	2.48	0.43
3:C:100:ARG:CZ	16:C:502:HEM:HBD1	2.49	0.43
4:D:239:PRO:O	4:D:241:LYS:HE2	2.19	0.43
9:I:64:LEU:HD23	9:I:78:TYR:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:43:ARG:HD2	8:U:47:ARG:HH21	1.83	0.43
2:B:213:HIS:N	2:B:214:PRO:CD	2.81	0.42
5:E:113:GLU:HG3	5:E:115:SER:OG	2.19	0.42
5:R:17:GLU:H	5:R:17:GLU:CD	2.17	0.42
1:A:192:ALA:HB3	1:A:193:PRO:HD3	1.99	0.42
1:A:59:VAL:HG11	1:A:186:LEU:HD21	2.00	0.42
3:C:97:HIS:CD2	16:C:502:HEM:NC	2.86	0.42
7:G:30:PHE:O	7:G:34:ILE:HG12	2.19	0.42
4:Q:65:ALA:O	4:Q:68:VAL:HG22	2.18	0.42
3:C:193:ALA:O	3:C:196:HIS:HB3	2.19	0.42
3:C:270:PRO:HD2	3:C:275:LEU:HD23	2.01	0.42
4:D:31:GLN:O	4:D:35:GLN:HG2	2.19	0.42
6:F:39:GLU:HG3	23:F:4047:HOH:O	2.19	0.42
1:N:157:ALA:HB2	1:N:421:ALA:CB	2.49	0.42
1:N:40:TRP:HB3	1:N:384:LEU:HD11	2.00	0.42
1:N:8:LEU:HD22	1:N:392:LEU:HB3	2.01	0.42
3:P:193:ALA:O	3:P:196:HIS:HB3	2.19	0.42
1:A:352:SER:CB	6:S:110:LYS:HB2	2.50	0.42
3:P:378:LYS:HE3	6:S:17:ARG:CD	2.49	0.42
1:N:8:LEU:O	1:N:11:VAL:HG23	2.19	0.42
1:A:195:MET:HE2	1:A:195:MET:HB3	1.91	0.42
5:E:10:PHE:HB3	7:G:18:LEU:HD11	2.02	0.42
5:E:43:THR:O	5:E:47:VAL:HG23	2.20	0.42
3:P:276:PHE:CG	3:P:277:ALA:N	2.87	0.42
4:Q:43:MET:CE	4:Q:189:PHE:CZ	3.02	0.42
1:A:289:HIS:CE1	11:S:2012:JZR:H1'A	2.52	0.42
2:O:95:LYS:HE2	9:V:32:ALA:N	2.35	0.42
3:C:217:LYS:HG3	7:G:7:LEU:HD13	2.02	0.42
7:G:28:HIS:ND1	7:G:32:LYS:HD2	2.34	0.42
2:B:314:ALA:HA	9:I:63:PRO:HD3	2.02	0.42
5:R:112:VAL:HG21	5:R:172:ARG:HH21	1.84	0.42
5:E:117:LEU:HD13	5:E:170:ARG:HD2	2.01	0.42
5:E:15:ARG:NH2	13:G:4001:AZI:N1	2.68	0.42
5:R:85:LYS:NZ	5:R:87:MET:SD	2.72	0.42
1:N:284:TYR:HE1	9:V:73:PRO:HG3	1.84	0.42
10:W:16:ARG:O	10:W:19:THR:HG22	2.20	0.42
2:B:294:SER:OG	2:B:343:GLN:NE2	2.53	0.42
3:C:314:SER:O	23:C:4170:HOH:O	2.21	0.42
4:D:231:LYS:HA	4:D:231:LYS:HD3	1.89	0.42
1:N:131:ARG:NH1	1:N:174:VAL:O	2.51	0.42
2:O:241:GLY:HA2	2:O:423:SER:OG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:SER:HB3	2:B:355:PRO:HG2	2.01	0.42
4:D:116:ILE:HA	4:D:116:ILE:HD12	1.86	0.42
2:O:152:LEU:HD13	2:O:158:HIS:CE1	2.55	0.42
3:P:12:LYS:HE2	3:P:16:ASN:HB2	2.02	0.42
3:P:345:HIS:HE1	7:T:65:GLU:OE2	2.02	0.42
5:R:78:LEU:HB2	5:R:191:ASP:HB2	2.02	0.42
1:A:281:ASP:C	1:A:281:ASP:OD1	2.59	0.42
2:B:204:MET:HE1	2:B:224:LEU:HD22	2.01	0.42
3:C:234:LEU:HD12	19:D:2003:CDL:H712	2.01	0.42
3:C:311:LYS:HG2	3:C:374:ASN:CG	2.41	0.42
6:F:102:LYS:HD3	6:F:102:LYS:HA	1.83	0.42
8:H:28:GLU:CA	8:H:31:VAL:HG22	2.47	0.42
3:P:18:PHE:CD2	3:P:19:ILE:HD13	2.55	0.42
3:P:215:VAL:HG13	23:P:4193:HOH:O	2.18	0.42
3:P:233:LEU:HD11	4:Q:219:VAL:HG21	2.01	0.42
1:A:1:THR:CG2	2:B:212:SER:HB3	2.34	0.41
2:B:364:LEU:HG	2:B:402:ILE:HD13	2.00	0.41
3:P:224:TYR:HB3	20:P:4009:GOL:H31	2.02	0.41
3:P:326:TRP:NE1	7:T:48:VAL:HG22	2.35	0.41
1:N:143:THR:OG1	9:V:48:SER:HB3	2.20	0.41
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.55	0.41
1:A:117:VAL:HG11	1:A:195:MET:HE1	2.01	0.41
3:C:15:ASN:O	3:C:17:ALA:N	2.53	0.41
9:I:52:ARG:NH1	23:I:859:HOH:O	2.54	0.41
1:N:11:VAL:HA	1:N:12:PRO:HD3	1.92	0.41
1:N:146:ARG:NH2	1:N:308:GLN:HE22	2.17	0.41
2:O:257:LEU:O	2:O:323:GLY:HA3	2.21	0.41
1:A:280:TYR:HA	1:A:284:TYR:CE2	2.55	0.41
3:C:277:ALA:HB1	3:C:294:LEU:HD12	2.02	0.41
3:C:278:TYR:CZ	3:C:282:ARG:HD3	2.56	0.41
5:E:189:SER:C	5:E:190:ASP:OD1	2.59	0.41
6:F:99:ARG:NH2	23:F:4055:HOH:O	2.53	0.41
4:D:229:VAL:CG2	7:G:20:PRO:HD3	2.50	0.41
8:H:31:VAL:HA	8:H:34:ARG:HH11	1.84	0.41
1:N:39:VAL:CG1	1:N:195:MET:HE2	2.51	0.41
3:P:30:TRP:CZ3	15:P:3007:PEE:H21	2.55	0.41
3:P:96:MET:HE2	15:P:3007:PEE:H27	2.03	0.41
4:Q:215:LEU:HD21	5:R:46:GLY:HA3	2.02	0.41
5:R:70:ALA:C	5:R:71:MET:HE2	2.40	0.41
23:N:4088:HOH:O	9:V:39:GLU:CG	2.69	0.41
2:B:28:ARG:HG2	2:B:28:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:19:TRP:CD2	11:F:4003:JZR:H1'A	2.56	0.41
1:N:108:LYS:O	1:N:112:LEU:HG	2.21	0.41
2:O:411:ILE:O	2:O:415:LYS:HG3	2.20	0.41
5:R:95:PRO:HG2	5:R:145:VAL:HG22	2.02	0.41
5:R:44:THR:CG2	10:W:24:ILE:HG21	2.51	0.41
1:A:1:THR:HG22	2:B:39:GLU:OE1	2.20	0.41
2:B:46:ARG:HD2	2:B:375:SER:CB	2.50	0.41
3:C:129:MET:HE1	17:C:2001:SMA:H26	2.02	0.41
4:Q:28:ARG:HB3	4:Q:171:PHE:CE1	2.55	0.41
21:Q:501:HEC:HMB1	21:Q:501:HEC:HBB3	2.02	0.41
8:U:31:VAL:HG23	8:U:32:LYS:N	2.35	0.41
1:A:46:ARG:HG2	1:A:231:LEU:HD22	2.03	0.41
2:B:152:LEU:HD13	2:B:158:HIS:CE1	2.55	0.41
2:O:236:LYS:CD	2:O:236:LYS:H	2.32	0.41
5:R:52:LYS:NZ	10:W:32:GLU:OE2	2.48	0.41
2:B:257:LEU:O	2:B:323:GLY:HA3	2.21	0.41
2:B:26:PHE:CZ	2:B:391:SER:HA	2.56	0.41
1:N:332:ASP:OD1	1:N:432:PRO:HG3	2.21	0.41
4:Q:117:VAL:O	12:Q:4012:PO4:O2	2.38	0.41
1:A:332:ASP:OD1	1:A:432:PRO:HG3	2.21	0.41
3:P:206:ASN:HB3	16:P:502:HEM:O2D	2.20	0.41
1:A:366:VAL:HG23	1:A:367:SER:N	2.35	0.40
2:O:37:SER:HA	2:O:208:GLY:O	2.21	0.40
2:O:243:GLU:HA	2:O:424:MET:O	2.22	0.40
3:P:245:PHE:CD1	4:Q:17:LEU:HD13	2.56	0.40
4:D:74:PRO:CA	4:D:80:MET:HE2	2.51	0.40
3:P:326:TRP:CH2	15:P:3007:PEE:H51	2.57	0.40
3:P:32:ASN:O	3:P:36:LEU:HG	2.22	0.40
1:A:255:ILE:O	1:A:321:GLY:HA3	2.22	0.40
1:A:442:PHE:C	1:A:442:PHE:CD1	2.95	0.40
3:C:63:PHE:O	3:C:67:THR:HG23	2.22	0.40
4:D:65:ALA:O	4:D:68:VAL:HG22	2.21	0.40
9:I:72:VAL:HG13	9:I:73:PRO:HD2	2.03	0.40
1:N:9:GLN:HE22	1:N:393:ALA:HB1	1.87	0.40
3:P:197:LEU:HA	3:P:197:LEU:HD23	1.73	0.40
3:P:71:ARG:HD3	23:P:4196:HOH:O	2.22	0.40
7:T:50:PRO:HB2	7:T:51:PRO:HD3	2.02	0.40
7:T:72:LYS:HE2	7:T:72:LYS:HB2	1.97	0.40
1:A:2:ALA:HB1	1:A:6:GLN:CB	2.48	0.40
1:N:144:SER:O	1:N:148:VAL:HG23	2.20	0.40
1:N:307:PHE:CD1	1:N:307:PHE:C	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:366:VAL:HG23	1:N:367:SER:N	2.37	0.40
2:O:120:MET:HE2	2:O:120:MET:HB2	1.92	0.40
2:O:300:ALA:C	2:O:302:GLY:H	2.25	0.40
4:Q:33:TYR:CD1	4:Q:37:CYS:HB2	2.56	0.40
4:Q:79:GLU:HG2	4:Q:79:GLU:H	1.62	0.40
8:H:28:GLU:HA	8:H:31:VAL:CG2	2.48	0.40
8:H:31:VAL:HG23	8:H:32:LYS:N	2.36	0.40
3:P:111:GLU:CD	3:P:111:GLU:H	2.25	0.40
3:P:132:VAL:HA	3:P:139:SER:HB3	2.03	0.40
4:Q:116:ILE:HD12	4:Q:116:ILE:HA	1.90	0.40
4:Q:161:ALA:O	4:Q:162:PRO:C	2.60	0.40
7:T:38:LEU:O	7:T:42:ARG: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	441/446 (99%)	427 (97%)	12 (3%)	2 (0%)	32	28
1	N	441/446 (99%)	425 (96%)	14 (3%)	2 (0%)	32	28
2	B	418/439 (95%)	406 (97%)	11 (3%)	1 (0%)	51	52
2	O	420/439 (96%)	404 (96%)	11 (3%)	5 (1%)	15	9
3	C	363/379 (96%)	353 (97%)	8 (2%)	2 (1%)	28	24
3	P	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	13	7
4	D	239/241 (99%)	234 (98%)	5 (2%)	0	100	100
4	Q	239/241 (99%)	235 (98%)	4 (2%)	0	100	100
5	E	194/196 (99%)	179 (92%)	14 (7%)	1 (0%)	32	28
5	R	193/196 (98%)	183 (95%)	8 (4%)	2 (1%)	18	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	97/110 (88%)	97 (100%)	0	0	100	100
6	S	97/110 (88%)	95 (98%)	2 (2%)	0	100	100
7	G	73/81 (90%)	70 (96%)	3 (4%)	0	100	100
7	T	74/81 (91%)	71 (96%)	2 (3%)	1 (1%)	13	7
8	H	64/78 (82%)	63 (98%)	1 (2%)	0	100	100
8	U	64/78 (82%)	61 (95%)	3 (5%)	0	100	100
9	I	38/78 (49%)	35 (92%)	1 (3%)	2 (5%)	2	0
9	V	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	6	2
10	J	28/62 (45%)	26 (93%)	1 (4%)	1 (4%)	4	1
10	W	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11	5
All	All	3947/4220 (94%)	3811 (97%)	110 (3%)	26 (1%)	25	20

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	I	41	PRO
10	J	61	ASN
1	N	2	ALA
2	O	226	ILE
2	O	233	SER
3	P	11	MET
3	P	16	ASN
3	P	17	ALA
9	V	41	PRO
10	W	61	ASN
1	A	224	ASP
2	B	171	ALA
3	C	17	ALA
5	E	191	ASP
2	O	171	ALA
3	P	12	LYS
5	R	190	ASP
7	T	72	LYS
3	C	16	ASN
9	I	71	ASN
2	O	227	ARG
5	R	189	SER
2	O	229	GLY

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Mol	Chain	Res	Type
1	A	228	VAL
3	P	13	ILE
1	N	228	VAL

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	363/370 (98%)	356 (98%)	7 (2%)	62	68
1	N	363/370 (98%)	355 (98%)	8 (2%)	57	62
2	B	332/343 (97%)	330 (99%)	2 (1%)	89	92
2	O	332/343 (97%)	329 (99%)	3 (1%)	82	87
3	C	313/327 (96%)	307 (98%)	6 (2%)	62	68
3	P	317/327 (97%)	311 (98%)	6 (2%)	62	68
4	D	206/206 (100%)	203 (98%)	3 (2%)	70	76
4	Q	206/206 (100%)	202 (98%)	4 (2%)	62	68
5	E	168/168 (100%)	167 (99%)	1 (1%)	89	92
5	R	168/168 (100%)	165 (98%)	3 (2%)	64	70
6	F	90/98 (92%)	89 (99%)	1 (1%)	78	83
6	S	90/98 (92%)	88 (98%)	2 (2%)	57	62
7	G	66/71 (93%)	64 (97%)	2 (3%)	46	49
7	T	66/71 (93%)	63 (96%)	3 (4%)	32	30
8	H	63/74 (85%)	61 (97%)	2 (3%)	44	46
8	U	63/74 (85%)	63 (100%)	0	100	100
9	I	28/60 (47%)	27 (96%)	1 (4%)	40	41
9	V	28/60 (47%)	26 (93%)	2 (7%)	17	13
10	J	23/52 (44%)	23 (100%)	0	100	100
10	W	51/52 (98%)	51 (100%)	0	100	100
All	All	3336/3538 (94%)	3280 (98%)	56 (2%)	66	72

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASP
1	A	51	LYS
1	A	58	PHE
1	A	245	GLU
1	A	281	ASP
1	A	348	SER
1	A	365	LEU
2	B	227	ARG
2	B	354	ASN
3	C	80	ARG
3	C	90	PHE
3	C	128	PHE
3	C	222	PRO
3	C	346	PRO
3	C	379	TRP
4	D	17	LEU
4	D	43	MET
4	D	241	LYS
5	E	35	PHE
6	F	33	ARG
7	G	45	ILE
7	G	73	ASN
8	H	48	SER
8	H	51	GLU
9	I	42	VAL
1	N	20	ASP
1	N	32	GLN
1	N	58	PHE
1	N	184	GLU
1	N	245	GLU
1	N	281	ASP
1	N	348	SER
1	N	365	LEU
2	O	305	GLN
2	O	349	GLN
2	O	354	ASN
3	P	12	LYS
3	P	80	ARG
3	P	90	PHE
3	P	128	PHE
3	P	222	PRO
3	P	379	TRP

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Mol	Chain	Res	Type
4	Q	17	LEU
4	Q	35	GLN
4	Q	43	MET
4	Q	79	GLU
5	R	35	PHE
5	R	113	GLU
5	R	190	ASP
6	S	13	LEU
6	S	33	ARG
7	T	45	ILE
7	T	72	LYS
7	T	73	ASN
9	V	42	VAL
9	V	62	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	119	ASN
1	A	136	GLN
1	A	213	GLN
1	A	271	GLN
1	A	289	HIS
1	A	308	GLN
2	B	104	ASN
2	B	240	HIS
2	B	305	GLN
2	B	343	GLN
2	B	401	GLN
2	B	412	ASN
2	B	432	HIS
3	C	54	HIS
3	C	159	ASN
3	C	345	HIS
5	E	57	GLN
7	G	73	ASN
1	N	9	GLN
1	N	32	GLN
1	N	119	ASN
1	N	136	GLN
1	N	213	GLN

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Mol	Chain	Res	Type
1	N	271	GLN
1	N	301	ASN
1	N	308	GLN
2	O	104	ASN
2	O	154	ASN
2	O	240	HIS
2	O	305	GLN
2	O	401	GLN
2	O	412	ASN
2	O	432	HIS
3	P	16	ASN
3	P	159	ASN
3	P	345	HIS
4	Q	35	GLN
5	R	57	GLN
5	R	116	GLN
8	U	49	GLN

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](#)

Of 123 ligands modelled in this entry, 74 are unknown - leaving 49 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	PO4	A	2010	-	4,4,4	1.50	1 (25%)	6,6,6	5.02	5 (83%)
13	AZI	A	4002	-	0,2,2	0.00	-	0,1,1	0.00	-
11	JZR	A	4004	-	18,18,18	1.35	4 (22%)	23,23,23	0.60	0
12	PO4	B	3009	-	4,4,4	1.44	1 (25%)	6,6,6	5.03	5 (83%)
15	PEE	B	4017	-	4,7,50	0.49	0	3,7,55	0.40	0
17	SMA	C	2001	-	36,38,38	1.65	5 (13%)	44,52,52	1.79	5 (11%)
18	UQ	C	2002	-	18,18,63	2.37	9 (50%)	20,24,79	0.66	0
19	CDL	C	2004	-	43,43,99	1.13	2 (4%)	45,55,111	1.27	4 (8%)
13	AZI	C	2005	-	0,2,2	0.00	-	0,1,1	0.00	-
15	PEE	C	2007	-	48,48,50	1.07	5 (10%)	50,53,55	0.85	4 (8%)
20	GOL	C	2008	-	5,5,5	1.27	0	5,5,5	0.67	0
11	JZR	C	2011	-	18,18,18	1.83	5 (27%)	23,23,23	0.71	0
20	GOL	C	4008	-	5,5,5	1.22	0	5,5,5	0.56	0
16	HEM	C	501	3	28,50,50	1.96	8 (28%)	17,82,82	1.74	5 (29%)
16	HEM	C	502	3	28,50,50	1.73	7 (25%)	17,82,82	1.73	6 (35%)
19	CDL	D	2003	-	38,38,99	1.03	1 (2%)	41,47,111	1.12	3 (7%)
15	PEE	D	2006	-	50,50,50	1.23	6 (12%)	52,55,55	0.85	4 (7%)
12	PO4	D	4010	-	4,4,4	1.44	1 (25%)	6,6,6	5.03	5 (83%)
12	PO4	D	4011	-	4,4,4	1.41	1 (25%)	6,6,6	5.05	5 (83%)
21	HEC	D	501	4	28,50,50	1.93	4 (14%)	16,82,82	1.00	1 (6%)
20	GOL	E	4006	-	5,5,5	1.30	0	5,5,5	0.65	0
20	GOL	E	4007	-	4,4,5	1.48	1 (25%)	2,4,5	1.21	0
22	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	JZR	F	3012	-	18,18,18	1.88	5 (27%)	23,23,23	0.75	0
11	JZR	F	4003	-	18,18,18	1.84	5 (27%)	23,23,23	0.69	0
13	AZI	G	4001	-	0,2,2	0.00	-	0,1,1	0.00	-
12	PO4	I	4015	-	4,4,4	1.42	1 (25%)	6,6,6	5.04	5 (83%)
12	PO4	O	2009	-	4,4,4	1.42	1 (25%)	6,6,6	5.01	5 (83%)
20	GOL	O	4005	-	5,5,5	1.28	0	5,5,5	0.63	0
17	SMA	P	3001	-	36,38,38	1.65	5 (13%)	44,52,52	1.62	4 (9%)
18	UQ	P	3002	-	18,18,63	2.19	9 (50%)	20,24,79	0.59	0
19	CDL	P	3004	-	48,48,99	1.12	3 (6%)	50,60,111	1.15	4 (8%)
13	AZI	P	3005	-	0,2,2	0.00	-	0,1,1	0.00	-
15	PEE	P	3007	-	48,48,50	1.10	4 (8%)	50,53,55	0.85	4 (8%)
20	GOL	P	3008	-	5,5,5	1.22	0	5,5,5	0.54	0
12	PO4	P	3010	-	4,4,4	1.41	1 (25%)	6,6,6	5.02	5 (83%)
11	JZR	P	3011	-	18,18,18	1.82	5 (27%)	23,23,23	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	GOL	P	4009	-	5,5,5	1.06	0	5,5,5	0.54	0
16	HEM	P	501	3	28,50,50	1.88	8 (28%)	17,82,82	1.66	4 (23%)
16	HEM	P	502	3	28,50,50	1.89	9 (32%)	17,82,82	1.71	5 (29%)
19	CDL	Q	3003	-	38,38,99	1.06	2 (5%)	41,47,111	1.08	3 (7%)
15	PEE	Q	3006	-	50,50,50	1.21	7 (14%)	52,55,55	0.85	4 (7%)
12	PO4	Q	4012	-	4,4,4	1.53	1 (25%)	6,6,6	5.02	5 (83%)
21	HEC	Q	501	4	28,50,50	1.95	8 (28%)	16,82,82	1.01	1 (6%)
12	PO4	R	4013	-	4,4,4	1.47	1 (25%)	6,6,6	5.02	5 (83%)
12	PO4	R	4014	-	4,4,4	1.47	1 (25%)	6,6,6	5.03	5 (83%)
22	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	JZR	S	2012	-	18,18,18	1.87	6 (33%)	23,23,23	0.72	0
12	PO4	T	4016	-	4,4,4	1.48	1 (25%)	6,6,6	5.02	5 (83%)

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
12	PO4	A	2010	-	-	0/0/0/0	0/0/0/0
13	AZI	A	4002	-	-	0/0/0/0	0/0/0/0
11	JZR	A	4004	-	-	0/9/29/29	0/1/1/1
12	PO4	B	3009	-	-	0/0/0/0	0/0/0/0
15	PEE	B	4017	-	-	0/3/5/54	0/0/0/0
17	SMA	C	2001	-	-	0/33/34/34	0/2/2/2
18	UQ	C	2002	-	-	0/9/33/87	0/1/1/1
19	CDL	C	2004	-	-	0/52/52/110	0/0/0/0
13	AZI	C	2005	-	-	0/0/0/0	0/0/0/0
15	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
20	GOL	C	2008	-	-	0/4/4/4	0/0/0/0
11	JZR	C	2011	-	-	0/9/29/29	0/1/1/1
20	GOL	C	4008	-	-	0/4/4/4	0/0/0/0
16	HEM	C	501	3	-	0/6/54/54	0/0/8/8
16	HEM	C	502	3	-	0/6/54/54	0/0/8/8
19	CDL	D	2003	-	-	0/43/43/110	0/0/0/0
15	PEE	D	2006	-	-	0/54/54/54	0/0/0/0
12	PO4	D	4010	-	-	0/0/0/0	0/0/0/0
12	PO4	D	4011	-	-	0/0/0/0	0/0/0/0
21	HEC	D	501	4	-	0/6/54/54	0/0/8/8
20	GOL	E	4006	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	GOL	E	4007	-	-	0/2/2/4	0/0/0/0
22	FES	E	501	5	-	0/0/4/4	0/1/1/1
11	JZR	F	3012	-	-	0/9/29/29	0/1/1/1
11	JZR	F	4003	-	-	0/9/29/29	0/1/1/1
13	AZI	G	4001	-	-	0/0/0/0	0/0/0/0
12	PO4	I	4015	-	-	0/0/0/0	0/0/0/0
12	PO4	O	2009	-	-	0/0/0/0	0/0/0/0
20	GOL	O	4005	-	-	0/4/4/4	0/0/0/0
17	SMA	P	3001	-	-	0/33/34/34	0/2/2/2
18	UQ	P	3002	-	-	0/9/33/87	0/1/1/1
19	CDL	P	3004	-	-	0/57/57/110	0/0/0/0
13	AZI	P	3005	-	-	0/0/0/0	0/0/0/0
15	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
20	GOL	P	3008	-	-	0/4/4/4	0/0/0/0
12	PO4	P	3010	-	-	0/0/0/0	0/0/0/0
11	JZR	P	3011	-	-	0/9/29/29	0/1/1/1
20	GOL	P	4009	-	-	0/4/4/4	0/0/0/0
16	HEM	P	501	3	-	0/6/54/54	0/0/8/8
16	HEM	P	502	3	-	0/6/54/54	0/0/8/8
19	CDL	Q	3003	-	-	0/43/43/110	0/0/0/0
15	PEE	Q	3006	-	-	0/54/54/54	0/0/0/0
12	PO4	Q	4012	-	-	0/0/0/0	0/0/0/0
21	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
12	PO4	R	4013	-	-	0/0/0/0	0/0/0/0
12	PO4	R	4014	-	-	0/0/0/0	0/0/0/0
22	FES	R	501	5	-	0/0/4/4	0/1/1/1
11	JZR	S	2012	-	-	0/9/29/29	0/1/1/1
12	PO4	T	4016	-	-	0/0/0/0	0/0/0/0

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	501	HEC	C3B-C2B	-6.33	1.34	1.40
21	Q	501	HEC	C3B-C2B	-5.14	1.35	1.40
21	D	501	HEC	C3C-C2C	-4.93	1.35	1.40
16	P	501	HEM	C3C-CAC	-3.93	1.39	1.47
16	C	501	HEM	C3C-CAC	-3.90	1.40	1.47
21	Q	501	HEC	C3C-C2C	-3.62	1.36	1.40
16	C	501	HEM	C3C-C2C	-3.60	1.35	1.40
16	P	502	HEM	C3C-CAC	-3.30	1.41	1.47
16	P	501	HEM	C3C-C2C	-3.29	1.36	1.40
16	C	502	HEM	C3C-CAC	-3.19	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	502	HEM	C3C-C2C	-3.17	1.36	1.40
15	P	3007	PEE	C22-C21	-3.07	1.34	1.51
15	C	2007	PEE	C22-C21	-2.99	1.34	1.51
15	Q	3006	PEE	C19-C18	-2.98	1.34	1.51
15	C	2007	PEE	C19-C18	-2.96	1.34	1.51
15	D	2006	PEE	C19-C18	-2.95	1.34	1.51
16	P	501	HEM	C3B-CAB	-2.95	1.42	1.47
15	D	2006	PEE	C22-C21	-2.92	1.34	1.51
15	P	3007	PEE	C19-C18	-2.92	1.34	1.51
15	Q	3006	PEE	C22-C21	-2.89	1.35	1.51
16	P	502	HEM	C3B-CAB	-2.74	1.42	1.47
16	C	502	HEM	C3B-CAB	-2.46	1.43	1.47
19	C	2004	CDL	OA8-CA6	-2.33	1.40	1.45
19	P	3004	CDL	OA8-CA6	-2.27	1.40	1.45
19	Q	3003	CDL	OB8-CB6	-2.19	1.40	1.45
16	C	501	HEM	C3B-CAB	-2.19	1.43	1.47
19	P	3004	CDL	OB8-CB6	-2.04	1.40	1.45
19	C	2004	CDL	OB8-CB6	-2.02	1.40	1.45
11	S	2012	JZR	C4-C3	2.00	1.57	1.52
15	Q	3006	PEE	C31-C30	2.01	1.56	1.50
16	P	502	HEM	CMB-C2B	2.02	1.55	1.51
11	S	2012	JZR	C1-C2	2.03	1.58	1.52
11	P	3011	JZR	O5-C5	2.04	1.49	1.44
11	A	4004	JZR	C4-C3	2.04	1.57	1.52
17	C	2001	SMA	C6-C7	2.05	1.42	1.38
15	C	2007	PEE	O2-C10	2.05	1.40	1.34
15	D	2006	PEE	C3-C2	2.06	1.56	1.50
11	F	4003	JZR	C1-C2	2.06	1.58	1.52
17	C	2001	SMA	C7-C8	2.07	1.43	1.40
21	Q	501	HEC	C1B-NB	2.08	1.40	1.36
11	C	2011	JZR	O5-C5	2.13	1.49	1.44
16	C	501	HEM	C1C-NC	2.15	1.39	1.36
11	C	2011	JZR	C1-C2	2.15	1.58	1.52
11	F	4003	JZR	O5-C5	2.17	1.49	1.44
11	P	3011	JZR	C1-C2	2.19	1.58	1.52
18	P	3002	UQ	C5-C4	2.19	1.55	1.47
21	Q	501	HEC	C3C-C4C	2.20	1.47	1.43
18	C	2002	UQ	C3-C4	2.20	1.55	1.48
11	F	3012	JZR	C1-C2	2.21	1.58	1.52
11	F	3012	JZR	C4-C5	2.24	1.57	1.53
17	P	3001	SMA	C6-C7	2.25	1.42	1.38
19	P	3004	CDL	O1-C1	2.27	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Q	501	HEC	C3B-C4B	2.29	1.47	1.43
19	D	2003	CDL	O1-C1	2.29	1.50	1.43
15	Q	3006	PEE	C3-C2	2.29	1.57	1.50
19	Q	3003	CDL	O1-C1	2.30	1.50	1.43
11	S	2012	JZR	O5-C5	2.31	1.49	1.44
20	E	4007	GOL	C1-C2	2.31	1.56	1.50
16	C	502	HEM	C1D-ND	2.31	1.41	1.36
15	P	3007	PEE	P-O1P	2.32	1.59	1.50
12	O	2009	PO4	P-O1	2.36	1.55	1.50
18	P	3002	UQ	C3-C4	2.36	1.55	1.48
15	C	2007	PEE	O3-C30	2.37	1.40	1.33
18	C	2002	UQ	C5-C4	2.38	1.56	1.47
12	I	4015	PO4	P-O1	2.40	1.55	1.50
11	S	2012	JZR	C4-C5	2.41	1.58	1.53
11	F	3012	JZR	O5-C5	2.42	1.50	1.44
12	D	4011	PO4	P-O1	2.43	1.55	1.50
12	D	4010	PO4	P-O1	2.43	1.55	1.50
11	F	4003	JZR	C4-C5	2.44	1.58	1.53
12	P	3010	PO4	P-O1	2.45	1.55	1.50
11	P	3011	JZR	C4-C5	2.45	1.58	1.53
12	R	4013	PO4	P-O1	2.47	1.55	1.50
12	B	3009	PO4	P-O1	2.47	1.55	1.50
15	C	2007	PEE	P-O1P	2.49	1.60	1.50
12	Q	4012	PO4	P-O1	2.49	1.55	1.50
12	R	4014	PO4	P-O1	2.50	1.55	1.50
11	A	4004	JZR	O5-C1	2.51	1.48	1.41
16	P	502	HEM	C1D-ND	2.55	1.41	1.36
12	A	2010	PO4	P-O1	2.57	1.56	1.50
21	Q	501	HEC	C1C-NC	2.57	1.41	1.36
11	C	2011	JZR	C4-C5	2.59	1.58	1.53
12	T	4016	PO4	P-O1	2.60	1.56	1.50
15	Q	3006	PEE	P-O1P	2.61	1.60	1.50
21	D	501	HEC	C3B-C4B	2.61	1.47	1.43
18	C	2002	UQ	CM5-C5	2.64	1.56	1.50
15	Q	3006	PEE	O2-C10	2.65	1.42	1.34
16	C	502	HEM	CBC-CAC	2.67	1.47	1.28
18	P	3002	UQ	CM5-C5	2.71	1.56	1.50
16	C	501	HEM	CBC-CAC	2.72	1.48	1.28
18	P	3002	UQ	C6-C5	2.72	1.41	1.35
16	P	501	HEM	CBB-CAB	2.73	1.48	1.28
15	D	2006	PEE	O2-C10	2.74	1.42	1.34
21	D	501	HEC	C3C-C4C	2.78	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	4004	JZR	C4-C5	2.82	1.59	1.53
16	C	502	HEM	CBB-CAB	2.82	1.48	1.28
18	P	3002	UQ	O3-C3	2.82	1.43	1.36
15	D	2006	PEE	O3-C30	2.83	1.41	1.33
18	P	3002	UQ	C2-C1	2.84	1.57	1.48
11	A	4004	JZR	O1-C1	2.86	1.45	1.40
15	D	2006	PEE	P-O1P	2.88	1.61	1.50
17	P	3001	SMA	C7-C8	2.95	1.44	1.40
16	P	502	HEM	CBB-CAB	2.98	1.49	1.28
15	Q	3006	PEE	O3-C30	2.98	1.42	1.33
16	P	501	HEM	C4B-NB	2.99	1.42	1.36
18	C	2002	UQ	O3-C3	3.00	1.44	1.36
18	C	2002	UQ	C6-C5	3.03	1.41	1.35
15	P	3007	PEE	O3-C30	3.03	1.42	1.33
17	P	3001	SMA	C4-C3	3.11	1.50	1.41
11	P	3011	JZR	O5-C1	3.12	1.49	1.41
21	Q	501	HEC	C4C-NC	3.12	1.40	1.36
16	C	502	HEM	C1C-NC	3.15	1.40	1.36
18	P	3002	UQ	O2-C2	3.19	1.44	1.36
16	P	502	HEM	CBC-CAC	3.21	1.51	1.28
18	C	2002	UQ	C2-C1	3.22	1.58	1.48
16	C	501	HEM	CBB-CAB	3.27	1.51	1.28
16	P	501	HEM	C1B-NB	3.29	1.40	1.36
11	C	2011	JZR	O5-C1	3.30	1.50	1.41
16	P	501	HEM	C4D-ND	3.33	1.40	1.36
16	P	502	HEM	C1B-NB	3.36	1.40	1.36
16	P	501	HEM	CBC-CAC	3.36	1.52	1.28
18	C	2002	UQ	O2-C2	3.39	1.45	1.36
17	C	2001	SMA	O1-C2	3.40	1.39	1.35
16	C	501	HEM	CMA-C3A	3.41	1.58	1.51
11	F	4003	JZR	O5-C1	3.47	1.50	1.41
18	P	3002	UQ	C6-C1	3.56	1.56	1.46
18	C	2002	UQ	C6-C1	3.56	1.56	1.46
11	S	2012	JZR	O5-C1	3.59	1.50	1.41
11	F	3012	JZR	O5-C1	3.62	1.50	1.41
17	C	2001	SMA	C4-C3	3.65	1.51	1.41
16	P	502	HEM	C1C-NC	3.69	1.41	1.36
18	P	3002	UQ	C7-C6	3.74	1.57	1.51
16	C	502	HEM	C4C-NC	3.74	1.41	1.36
17	P	3001	SMA	O1-C2	3.88	1.40	1.35
16	C	501	HEM	C4C-NC	4.36	1.41	1.36
18	C	2002	UQ	C7-C6	4.44	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Q	501	HEC	C4A-NA	4.52	1.42	1.36
11	F	4003	JZR	O1-C1	4.58	1.48	1.40
11	C	2011	JZR	O1-C1	4.61	1.48	1.40
11	P	3011	JZR	O1-C1	4.66	1.48	1.40
11	F	3012	JZR	O1-C1	4.68	1.48	1.40
11	S	2012	JZR	O1-C1	4.69	1.48	1.40
17	P	3001	SMA	C4-C4A	6.10	1.50	1.41
17	C	2001	SMA	C4-C4A	6.69	1.50	1.41

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	O	2009	PO4	O4-P-O1	-7.04	80.98	110.97
12	R	4013	PO4	O4-P-O1	-7.03	81.06	110.97
12	I	4015	PO4	O4-P-O1	-7.00	81.16	110.97
12	D	4010	PO4	O4-P-O1	-7.00	81.18	110.97
12	T	4016	PO4	O4-P-O1	-6.98	81.25	110.97
12	A	2010	PO4	O4-P-O1	-6.98	81.27	110.97
12	Q	4012	PO4	O4-P-O1	-6.97	81.30	110.97
12	B	3009	PO4	O4-P-O1	-6.96	81.32	110.97
12	R	4014	PO4	O4-P-O1	-6.96	81.33	110.97
12	P	3010	PO4	O4-P-O1	-6.95	81.38	110.97
12	D	4011	PO4	O4-P-O1	-6.91	81.55	110.97
12	I	4015	PO4	O4-P-O2	-6.90	82.56	107.90
12	D	4011	PO4	O4-P-O2	-6.77	83.02	107.90
12	Q	4012	PO4	O4-P-O2	-6.75	83.11	107.90
12	R	4014	PO4	O4-P-O2	-6.74	83.15	107.90
12	P	3010	PO4	O4-P-O2	-6.73	83.16	107.90
12	D	4010	PO4	O4-P-O2	-6.71	83.25	107.90
12	A	2010	PO4	O4-P-O2	-6.70	83.28	107.90
12	B	3009	PO4	O4-P-O2	-6.69	83.33	107.90
12	R	4013	PO4	O4-P-O2	-6.65	83.47	107.90
12	T	4016	PO4	O4-P-O2	-6.63	83.54	107.90
12	O	2009	PO4	O4-P-O2	-6.54	83.89	107.90
12	D	4011	PO4	O4-P-O3	-6.19	85.16	107.90
12	T	4016	PO4	O4-P-O3	-6.17	85.22	107.90
12	B	3009	PO4	O4-P-O3	-6.13	85.37	107.90
12	O	2009	PO4	O4-P-O3	-6.13	85.38	107.90
12	Q	4012	PO4	O4-P-O3	-6.12	85.40	107.90
12	R	4013	PO4	O4-P-O3	-6.11	85.43	107.90
12	R	4014	PO4	O4-P-O3	-6.11	85.45	107.90
12	D	4010	PO4	O4-P-O3	-6.09	85.52	107.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	2010	PO4	O4-P-O3	-6.08	85.58	107.90
12	P	3010	PO4	O4-P-O3	-6.07	85.60	107.90
12	I	4015	PO4	O4-P-O3	-5.90	86.21	107.90
17	C	2001	SMA	C3-C4-C4A	-4.82	114.85	121.25
17	P	3001	SMA	C3-C4-C4A	-4.71	115.01	121.25
16	P	501	HEM	C4A-C3A-C2A	-4.26	104.03	107.00
17	P	3001	SMA	C9-C10-C11	-4.20	109.07	114.72
19	C	2004	CDL	CA4-OA6-CA5	-4.12	109.98	117.94
17	C	2001	SMA	C9-C10-C11	-3.99	109.35	114.72
17	C	2001	SMA	O1-C2-C9	-3.90	107.13	111.94
16	C	501	HEM	C4A-C3A-C2A	-3.65	104.46	107.00
16	C	501	HEM	C1D-C2D-C3D	-3.62	104.48	107.00
19	P	3004	CDL	CA4-OA6-CA5	-3.52	111.14	117.94
19	C	2004	CDL	CB4-OB6-CB5	-3.45	109.72	117.88
16	C	502	HEM	CBD-CAD-C3D	-3.37	106.04	112.47
16	P	502	HEM	CBD-CAD-C3D	-3.18	106.39	112.47
19	D	2003	CDL	CB6-CB4-CB3	-2.95	105.20	111.86
19	P	3004	CDL	CB4-OB6-CB5	-2.94	110.93	117.88
19	Q	3003	CDL	CB4-OB6-CB5	-2.86	111.12	117.88
19	P	3004	CDL	CA6-OA8-CA7	-2.82	109.98	117.17
21	Q	501	HEC	CBD-CAD-C3D	-2.75	107.23	112.48
19	Q	3003	CDL	CB6-CB4-CB3	-2.73	105.69	111.86
19	D	2003	CDL	CB4-OB6-CB5	-2.73	111.43	117.88
17	P	3001	SMA	O1-C2-C9	-2.70	108.62	111.94
19	C	2004	CDL	CA6-CA4-CA3	-2.59	106.01	111.86
16	C	502	HEM	CBA-CAA-C2A	-2.52	107.66	112.48
19	C	2004	CDL	CA6-OA8-CA7	-2.41	111.03	117.17
16	C	501	HEM	CBA-CAA-C2A	-2.40	107.90	112.48
16	C	502	HEM	CMD-C2D-C1D	-2.18	125.12	128.46
19	P	3004	CDL	CB6-CB4-CB3	-2.11	107.09	111.86
16	P	501	HEM	C4C-C3C-C2C	-2.06	105.46	106.90
21	D	501	HEC	CBD-CAD-C3D	-2.05	108.56	112.48
16	P	501	HEM	CMA-C3A-C4A	-2.05	125.32	128.46
19	Q	3003	CDL	OA4-PA1-OA2	2.01	112.07	106.73
17	C	2001	SMA	O8-C8-C8A	2.05	123.52	119.65
19	D	2003	CDL	OA4-PA1-OA2	2.10	112.33	106.73
16	P	502	HEM	CBA-CAA-C2A	2.16	116.61	112.48
16	C	502	HEM	C3B-C4B-NB	2.19	112.04	109.21
16	C	501	HEM	CMB-C2B-C3B	2.20	128.98	124.89
12	A	2010	PO4	O3-P-O2	2.22	116.05	107.90
12	O	2009	PO4	O3-P-O2	2.22	116.05	107.90
12	B	3009	PO4	O3-P-O2	2.22	116.07	107.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	T	4016	PO4	O3-P-O2	2.24	116.11	107.90
12	P	3010	PO4	O3-P-O2	2.24	116.13	107.90
12	R	4014	PO4	O3-P-O2	2.24	116.15	107.90
15	Q	3006	PEE	C23-C22-C21	2.24	126.02	114.45
15	D	2006	PEE	C23-C22-C21	2.25	126.06	114.45
16	P	502	HEM	C4C-C3C-C2C	2.25	108.47	106.90
12	I	4015	PO4	O3-P-O2	2.26	116.21	107.90
12	Q	4012	PO4	O3-P-O2	2.26	116.22	107.90
12	D	4010	PO4	O3-P-O2	2.28	116.28	107.90
12	R	4013	PO4	O3-P-O2	2.29	116.32	107.90
12	D	4011	PO4	O3-P-O2	2.33	116.46	107.90
15	P	3007	PEE	C23-C22-C21	2.33	126.47	114.45
16	C	502	HEM	CMC-C2C-C3C	2.37	129.29	124.89
15	C	2007	PEE	C23-C22-C21	2.37	126.68	114.45
15	P	3007	PEE	C22-C21-C20	2.38	126.72	114.45
15	C	2007	PEE	C22-C21-C20	2.38	126.74	114.45
16	P	502	HEM	CMC-C2C-C3C	2.39	129.32	124.89
16	P	502	HEM	C3B-C4B-NB	2.41	112.32	109.21
15	Q	3006	PEE	C19-C18-C17	2.44	127.05	114.45
15	D	2006	PEE	C22-C21-C20	2.46	127.12	114.45
15	Q	3006	PEE	C22-C21-C20	2.46	127.14	114.45
15	P	3007	PEE	C19-C18-C17	2.50	127.32	114.45
15	C	2007	PEE	C19-C18-C17	2.51	127.41	114.45
15	D	2006	PEE	C19-C18-C17	2.53	127.48	114.45
16	C	501	HEM	C3B-C4B-NB	2.54	112.50	109.21
16	C	502	HEM	CMB-C2B-C3B	2.57	129.67	124.89
15	D	2006	PEE	C20-C19-C18	2.74	128.60	114.45
15	Q	3006	PEE	C20-C19-C18	2.77	128.72	114.45
15	C	2007	PEE	C20-C19-C18	2.84	129.07	114.45
15	P	3007	PEE	C20-C19-C18	2.88	129.27	114.45
16	P	501	HEM	CMA-C3A-C2A	3.01	130.62	124.94
12	Q	4012	PO4	O2-P-O1	3.83	127.26	110.97
12	R	4013	PO4	O2-P-O1	3.90	127.58	110.97
12	D	4010	PO4	O2-P-O1	3.91	127.63	110.97
12	D	4011	PO4	O2-P-O1	3.92	127.67	110.97
12	T	4016	PO4	O2-P-O1	3.93	127.71	110.97
12	A	2010	PO4	O2-P-O1	3.94	127.73	110.97
12	O	2009	PO4	O2-P-O1	3.94	127.75	110.97
12	R	4014	PO4	O2-P-O1	3.95	127.78	110.97
12	P	3010	PO4	O2-P-O1	3.96	127.82	110.97
12	B	3009	PO4	O2-P-O1	3.98	127.91	110.97
12	I	4015	PO4	O2-P-O1	4.01	128.06	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
17	P	3001	SMA	C9-C2-C3	6.49	128.12	120.35
17	C	2001	SMA	C9-C2-C3	7.75	129.63	120.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	4004	JZR	1	0
15	B	4017	PEE	1	0
17	C	2001	SMA	3	0
18	C	2002	UQ	4	0
16	C	501	HEM	1	0
16	C	502	HEM	4	0
19	D	2003	CDL	1	0
15	D	2006	PEE	2	0
21	D	501	HEC	4	0
11	F	3012	JZR	3	0
11	F	4003	JZR	1	0
13	G	4001	AZI	1	0
12	I	4015	PO4	1	0
17	P	3001	SMA	3	0
18	P	3002	UQ	5	0
15	P	3007	PEE	3	0
20	P	4009	GOL	2	0
16	P	501	HEM	1	0
16	P	502	HEM	2	0
15	Q	3006	PEE	5	0
12	Q	4012	PO4	1	0
21	Q	501	HEC	5	0
11	S	2012	JZR	6	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	442/446 (99%)	0.08	14 (3%) 48 55	24, 37, 59, 111	1 (0%)
1	N	442/446 (99%)	0.48	29 (6%) 19 24	31, 50, 77, 132	1 (0%)
2	B	424/439 (96%)	0.19	15 (3%) 44 51	28, 41, 66, 102	0
2	O	424/439 (96%)	0.48	41 (9%) 8 11	31, 48, 87, 185	0
3	C	365/379 (96%)	0.35	19 (5%) 28 34	24, 34, 48, 108	0
3	P	370/379 (97%)	0.46	25 (6%) 18 23	28, 37, 52, 218	0
4	D	241/241 (100%)	0.42	16 (6%) 19 24	29, 39, 61, 78	0
4	Q	241/241 (100%)	0.58	24 (9%) 8 10	31, 45, 67, 87	0
5	E	196/196 (100%)	1.09	44 (22%) 1 1	32, 57, 105, 117	0
5	R	196/196 (100%)	0.30	13 (6%) 19 24	27, 46, 71, 99	0
6	F	99/110 (90%)	0.37	9 (9%) 10 13	24, 39, 71, 83	0
6	S	99/110 (90%)	0.26	4 (4%) 39 46	28, 40, 67, 88	0
7	G	75/81 (92%)	0.92	14 (18%) 1 2	26, 49, 77, 86	0
7	T	76/81 (93%)	1.51	23 (30%) 0 1	32, 55, 98, 114	0
8	H	66/78 (84%)	1.08	16 (24%) 1 1	40, 56, 73, 78	0
8	U	66/78 (84%)	1.17	17 (25%) 1 1	44, 63, 94, 104	0
9	I	42/78 (53%)	2.17	20 (47%) 0 0	33, 62, 90, 93	0
9	V	42/78 (53%)	2.03	17 (40%) 0 0	36, 78, 94, 100	0
10	J	30/62 (48%)	0.82	3 (10%) 8 10	40, 52, 80, 109	0
10	W	62/62 (100%)	2.06	20 (32%) 0 0	41, 64, 92, 123	0
All	All	3998/4220 (94%)	0.52	383 (9%) 9 11	24, 43, 80, 218	2 (0%)

All (383) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	13	ILE	21.8
10	W	1	VAL	21.0
10	W	62	LYS	12.6
2	O	12	GLU	10.6
10	W	2	ALA	10.5
7	T	76	ALA	10.2
9	I	50	LEU	10.1
7	T	1	GLY	9.4
3	P	18	PHE	9.2
3	P	11	MET	9.1
2	O	19	PRO	8.9
5	E	112	VAL	8.5
4	Q	241	LYS	8.5
1	A	2	ALA	8.2
1	N	222	THR	8.1
10	W	12	LEU	8.1
9	I	49	VAL	8.1
2	B	233	SER	7.9
9	V	50	LEU	7.8
3	C	17	ALA	7.6
1	N	1	THR	7.4
2	B	230	LEU	7.2
1	N	227	ALA	7.0
10	J	62	LYS	7.0
5	E	115	SER	6.8
3	P	12	LYS	6.7
2	B	231	GLY	6.7
2	O	228	GLY	6.6
1	A	222	THR	6.6
8	U	50	THR	6.5
1	A	225	GLU	6.4
2	B	232	LEU	6.1
2	B	20	HIS	6.1
1	A	1	THR	5.9
3	P	16	ASN	5.9
4	Q	1	SER	5.7
7	G	30	PHE	5.7
1	N	2	ALA	5.7
1	A	227	ALA	5.6
5	R	189	SER	5.5
7	T	34	ILE	5.4
8	U	47	ARG	5.4
7	T	32	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	226	ASP	5.4
2	O	218	GLN	5.3
5	E	114	VAL	5.3
9	I	78	TYR	5.3
9	V	38	SER	5.3
3	P	14	VAL	5.3
7	T	30	PHE	5.3
1	N	229	PRO	5.2
3	P	17	ALA	5.1
5	E	196	GLY	5.1
6	S	12	TRP	5.0
10	W	5	LEU	5.0
1	N	206	ARG	4.9
5	E	124	LEU	4.9
3	P	10	LEU	4.9
10	W	3	PRO	4.8
4	Q	76	GLU	4.8
5	E	194	ILE	4.8
1	N	228	VAL	4.8
8	H	34	ARG	4.8
5	E	117	LEU	4.7
3	C	18	PHE	4.7
4	D	241	LYS	4.7
3	C	16	ASN	4.7
7	T	31	SER	4.7
8	U	48	SER	4.7
7	T	73	ASN	4.7
5	R	191	ASP	4.6
4	D	81	PHE	4.6
9	I	51	CYS	4.5
2	O	232	LEU	4.5
5	E	116	GLN	4.5
2	B	12	GLU	4.4
1	N	230	THR	4.4
9	V	49	VAL	4.4
9	V	52	ARG	4.4
10	J	61	ASN	4.3
5	E	108	GLN	4.3
1	N	225	GLU	4.3
2	O	20	HIS	4.3
8	U	49	GLN	4.3
10	W	8	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
7	T	61	TRP	4.2
2	B	304	HIS	4.2
5	E	111	ALA	4.2
8	U	44	VAL	4.2
2	O	41	TYR	4.1
10	W	13	LEU	4.1
2	O	17	VAL	4.1
7	T	29	TYR	4.1
5	E	80	ASP	4.1
5	E	35	PHE	4.0
4	Q	158	ILE	4.0
5	E	188	THR	4.0
5	E	113	GLU	4.0
5	E	186	GLU	4.0
5	E	5	ILE	4.0
5	E	191	ASP	4.0
10	W	9	LEU	4.0
3	C	27	ILE	3.9
2	O	230	LEU	3.9
1	A	4	TYR	3.9
3	C	218	ILE	3.9
10	W	30	PHE	3.9
9	V	61	GLY	3.9
2	O	229	GLY	3.8
5	E	185	TYR	3.8
2	B	229	GLY	3.8
8	U	45	SER	3.8
7	G	29	TYR	3.8
4	Q	146	GLY	3.8
1	N	15	GLN	3.8
10	W	61	ASN	3.8
9	V	42	VAL	3.8
5	R	71	MET	3.8
8	H	46	SER	3.7
9	V	78	TYR	3.7
4	D	73	GLY	3.7
5	E	107	ASP	3.6
1	N	193	PRO	3.6
5	E	27	GLU	3.6
5	R	74	ILE	3.6
2	O	221	GLU	3.6
6	F	13	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
4	Q	139	THR	3.6
4	D	79	GLU	3.6
2	B	41	TYR	3.6
1	A	224	ASP	3.5
5	E	128	LYS	3.5
8	U	51	GLU	3.5
6	S	70	MET	3.5
5	E	127	VAL	3.5
1	N	226	ASP	3.5
9	I	42	VAL	3.5
4	Q	227	TRP	3.5
4	Q	77	ASP	3.4
9	I	62	ARG	3.4
5	E	187	PHE	3.4
5	R	76	ILE	3.4
7	G	42	ARG	3.4
2	O	215	VAL	3.4
4	Q	157	ALA	3.4
10	W	25	VAL	3.4
3	P	27	ILE	3.3
2	O	233	SER	3.3
8	H	44	VAL	3.3
5	E	190	ASP	3.3
4	Q	145	GLU	3.3
3	P	218	ILE	3.3
5	E	184	SER	3.3
5	R	190	ASP	3.3
5	R	23	LYS	3.3
8	H	42	GLU	3.3
7	G	34	ILE	3.3
8	U	39	LEU	3.3
2	O	18	PRO	3.3
3	P	223	TYR	3.2
1	N	209	LEU	3.2
4	D	230	LEU	3.2
6	F	110	LYS	3.2
3	C	23	ALA	3.2
4	Q	141	VAL	3.2
9	I	52	ARG	3.2
2	O	439	LEU	3.2
3	C	15	ASN	3.2
8	H	31	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
4	D	80	MET	3.1
9	I	48	SER	3.1
5	E	122	HIS	3.1
9	I	73	PRO	3.1
1	A	262	TRP	3.1
1	N	22	GLY	3.1
8	H	41	ASP	3.1
4	D	141	VAL	3.1
1	N	443	TRP	3.1
3	C	211	ILE	3.1
7	T	28	HIS	3.1
2	O	25	GLU	3.1
9	I	55	LEU	3.1
3	C	31	TRP	3.0
4	D	72	ASP	3.0
6	S	15	GLY	3.0
8	H	45	SER	3.0
4	D	145	GLU	3.0
3	C	25	SER	3.0
7	T	75	ALA	3.0
5	E	49	TYR	3.0
4	D	85	GLY	3.0
2	O	217	LYS	3.0
1	A	228	VAL	3.0
9	I	63	PRO	3.0
9	V	51	CYS	2.9
2	O	355	PRO	2.9
4	Q	148	TYR	2.9
3	C	209	THR	2.9
4	Q	79	GLU	2.9
5	E	110	ALA	2.9
9	V	32	ALA	2.9
5	R	75	GLU	2.9
1	N	224	ASP	2.8
3	P	26	ASN	2.8
1	N	51	LYS	2.8
5	E	103	LYS	2.8
4	Q	229	VAL	2.8
6	F	108	ALA	2.8
2	O	224	LEU	2.8
1	N	16	VAL	2.8
5	E	79	SER	2.8

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Mol	Chain	Res	Type	RSRZ
8	U	42	GLU	2.8
9	V	37	THR	2.8
10	W	19	THR	2.8
5	E	84	GLY	2.8
3	P	224	TYR	2.8
4	Q	147	LEU	2.8
4	Q	230	LEU	2.8
10	W	29	LEU	2.8
9	I	37	THR	2.8
9	I	58	GLN	2.8
3	C	155	TYR	2.8
7	T	42	ARG	2.7
5	E	53	ASN	2.7
4	D	229	VAL	2.7
4	Q	167	GLU	2.7
9	I	70	LEU	2.7
2	B	250	ASP	2.7
2	O	26	PHE	2.7
9	I	71	ASN	2.7
4	Q	144	ARG	2.7
8	U	13	LEU	2.7
1	N	13	GLU	2.7
5	E	89	PHE	2.7
1	N	176	LYS	2.6
10	W	20	PHE	2.6
4	Q	143	LEU	2.6
3	C	224	TYR	2.6
8	H	51	GLU	2.6
9	V	41	PRO	2.6
4	D	116	ILE	2.6
4	Q	149	PHE	2.6
9	V	40	SER	2.6
8	U	43	ARG	2.6
1	N	219	LEU	2.6
2	O	22	GLN	2.6
5	R	12	ASP	2.6
2	O	304	HIS	2.6
2	O	405	VAL	2.6
2	O	392	TYR	2.6
7	G	75	ALA	2.6
7	T	17	SER	2.6
2	B	235	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
9	V	48	SER	2.5
3	P	15	ASN	2.5
7	T	35	PRO	2.5
8	H	49	GLN	2.5
3	P	320	LEU	2.5
7	G	31	SER	2.5
10	W	21	ALA	2.5
7	G	56	TYR	2.5
8	U	46	SER	2.5
1	N	5	ALA	2.5
9	I	60	ALA	2.5
2	O	27	THR	2.5
7	T	2	ARG	2.5
3	P	31	TRP	2.5
5	E	134	ILE	2.5
1	A	20	ASP	2.5
5	R	80	ASP	2.5
4	D	103	ALA	2.5
3	P	227	LYS	2.5
7	G	60	THR	2.5
9	V	33	ALA	2.5
2	O	303	VAL	2.4
2	O	226	ILE	2.4
2	B	227	ARG	2.4
7	T	74	PRO	2.4
9	I	32	ALA	2.4
4	Q	142	SER	2.4
3	P	345	HIS	2.4
3	P	25	SER	2.4
7	G	58	VAL	2.4
7	T	64	GLN	2.4
4	D	117	VAL	2.3
7	G	64	GLN	2.3
6	S	69	SER	2.3
8	H	22	GLU	2.3
8	H	29	LYS	2.3
2	O	223	PHE	2.3
5	E	38	LEU	2.3
10	J	37	GLN	2.3
3	P	155	TYR	2.3
8	U	67	HIS	2.3
2	O	33	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
6	F	106	GLU	2.3
2	O	351	ASN	2.3
9	V	77	ARG	2.3
1	A	365	LEU	2.3
6	F	66	LEU	2.3
8	H	48	SER	2.3
1	A	184	GLU	2.3
1	N	17	SER	2.3
1	N	241	ILE	2.3
5	R	79	SER	2.3
7	T	38	LEU	2.3
3	C	207	ASN	2.3
10	W	24	ILE	2.3
2	O	29	LEU	2.2
9	I	64	LEU	2.2
3	P	168	PHE	2.2
2	O	126	VAL	2.2
8	U	31	VAL	2.2
8	H	67	HIS	2.2
6	F	107	TRP	2.2
7	T	43	ALA	2.2
8	U	26	GLN	2.2
1	N	397	SER	2.2
9	V	63	PRO	2.2
1	N	20	ASP	2.2
2	O	406	ALA	2.2
5	E	71	MET	2.2
10	W	28	ALA	2.2
3	P	43	LEU	2.2
8	H	37	LEU	2.2
1	N	18	GLN	2.2
2	B	439	LEU	2.2
7	T	33	GLY	2.2
2	O	264	ILE	2.2
4	Q	171	PHE	2.2
5	E	195	VAL	2.2
6	F	22	ASN	2.2
8	U	41	ASP	2.2
9	I	61	GLY	2.2
1	A	229	PRO	2.2
5	R	16	PRO	2.2
3	P	23	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
4	Q	233	ARG	2.1
7	T	60	THR	2.1
5	E	78	LEU	2.1
7	G	68	LYS	2.1
2	O	23	ASP	2.1
2	O	349	GLN	2.1
7	T	56	TYR	2.1
10	W	10	TYR	2.1
6	F	70	MET	2.1
4	D	99	GLU	2.1
5	E	167	ALA	2.1
5	R	27	GLU	2.1
3	C	210	GLY	2.1
5	E	193	VAL	2.1
4	Q	136	GLU	2.1
9	I	69	SER	2.1
2	O	219	VAL	2.1
3	C	98	VAL	2.1
1	N	421	ALA	2.1
7	G	71	ARG	2.1
8	U	28	GLU	2.1
3	C	101	GLY	2.1
3	P	28	SER	2.0
2	O	24	LEU	2.0
5	E	192	MET	2.0
1	N	216	PHE	2.0
8	H	35	GLU	2.0
6	F	19	TRP	2.0
9	V	62	ARG	2.0
3	C	102	LEU	2.0
5	E	75	GLU	2.0
7	T	37	VAL	2.0
5	E	153	PHE	2.0
8	H	47	ARG	2.0
10	W	16	ARG	2.0
2	B	400	GLN	2.0
4	D	115	TYR	2.0
3	P	208	PRO	2.0
5	E	132	TRP	2.0
7	G	6	HIS	2.0
2	O	35	ILE	2.0
7	G	38	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	301	LYS	2.0
2	O	350	GLY	2.0
2	O	407	ASP	2.0
3	C	217	LYS	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(\AA^2)	Q<0.9
14	UNL	B	4026	1/-	0.72	1.34	57.78	92,92,92,92	0
14	UNL	B	4080	1/-	0.61	0.68	33.08	67,67,67,67	0
14	UNL	U	4056	1/-	0.23	1.01	25.27	101,101,101,101	0
14	UNL	B	4057	1/-	0.77	0.85	22.35	57,57,57,57	0
14	UNL	O	4084	1/-	0.84	0.68	22.30	67,67,67,67	0
11	JZR	F	3012	18/18	0.17	0.72	20.36	159,162,164,164	0
14	UNL	A	4032	1/-	0.84	0.71	18.29	65,65,65,65	0
14	UNL	B	4079	1/-	0.80	0.43	16.21	66,66,66,66	0
11	JZR	S	2012	18/18	0.37	0.45	15.19	89,103,106,107	0
11	JZR	C	2011	18/18	0.60	0.48	13.93	106,118,123,125	0
20	GOL	O	4005	6/6	0.24	0.75	10.61	166,167,167,168	0
20	GOL	P	3008	6/6	0.89	0.50	10.49	83,84,85,88	0
13	AZI	P	3005	3/3	0.77	0.35	10.04	54,54,59,63	0
11	JZR	P	3011	18/18	0.56	0.41	8.46	99,107,109,109	0
13	AZI	A	4002	3/3	0.71	0.48	7.93	48,48,58,65	0
12	PO4	R	4013	5/5	0.78	0.25	7.24	114,114,116,116	0
13	AZI	C	2005	3/3	0.80	0.35	7.06	41,41,55,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
14	UNL	U	4049	1/-	0.64	0.69	5.67	77,77,77,77	0
20	GOL	C	2008	6/6	0.88	0.31	5.50	60,63,63,70	0
15	PEE	B	4017	8/51	0.67	0.42	5.10	85,88,91,92	0
14	UNL	P	4074	1/-	0.78	0.17	4.66	59,59,59,59	0
14	UNL	O	4037	1/-	0.73	0.82	4.57	62,62,62,62	0
14	UNL	B	4034	1/-	0.48	0.71	3.91	87,87,87,87	0
12	PO4	D	4011	5/5	0.79	0.31	3.58	130,130,130,131	0
15	PEE	D	2006	51/51	0.77	0.32	3.51	85,98,115,118	0
20	GOL	E	4006	6/6	0.83	0.24	2.88	67,71,72,75	0
12	PO4	A	2010	5/5	0.61	0.23	2.57	133,133,134,134	0
15	PEE	P	3007	49/51	0.92	0.23	2.13	35,58,75,76	0
15	PEE	Q	3006	51/51	0.90	0.20	2.09	53,65,110,110	0
12	PO4	Q	4012	5/5	0.87	0.18	1.90	108,109,110,110	0
15	PEE	C	2007	49/51	0.93	0.23	1.85	33,58,74,74	0
14	UNL	O	4043	1/-	0.84	0.29	1.56	80,80,80,80	0
18	UQ	C	2002	18/63	0.65	0.30	1.45	61,73,76,76	0
19	CDL	C	2004	44/100	0.91	0.21	1.33	54,83,104,106	0
19	CDL	P	3004	49/100	0.90	0.26	1.19	54,81,117,120	0
17	SMA	C	2001	37/37	0.96	0.16	1.14	25,33,44,46	0
12	PO4	I	4015	5/5	0.84	0.31	1.09	122,122,123,123	0
19	CDL	D	2003	39/100	0.86	0.20	0.84	64,84,106,107	0
17	SMA	P	3001	37/37	0.95	0.16	0.55	30,39,47,52	0
19	CDL	Q	3003	39/100	0.88	0.23	0.45	54,90,96,96	0
18	UQ	P	3002	18/63	0.77	0.24	0.37	60,82,85,86	0
11	JZR	A	4004	18/18	0.96	0.13	0.36	29,36,42,44	0
21	HEC	D	501	43/43	0.97	0.13	0.15	26,33,37,38	0
16	HEM	P	501	43/43	0.98	0.15	0.12	22,26,33,40	0
20	GOL	P	4009	6/6	0.95	0.23	0.12	67,70,71,72	0
13	AZI	G	4001	3/3	0.92	0.15	0.08	47,47,57,59	0
16	HEM	C	502	43/43	0.98	0.16	0.06	23,26,33,36	0
22	FES	E	501	4/4	0.99	0.13	0.03	38,39,40,40	0
20	GOL	C	4008	6/6	0.95	0.20	-0.03	53,55,60,60	0
16	HEM	C	501	43/43	0.98	0.12	-0.37	21,27,34,38	0
21	HEC	Q	501	43/43	0.98	0.11	-0.60	29,36,41,45	0
16	HEM	P	502	43/43	0.99	0.11	-0.72	23,27,37,39	0
22	FES	R	501	4/4	0.99	0.12	-0.87	27,29,30,30	0
12	PO4	D	4010	5/5	0.66	0.29	-	169,169,170,170	0
14	UNL	R	4055	1/-	0.73	0.14	-	73,73,73,73	0
14	UNL	B	4052	1/-	0.85	0.18	-	60,60,60,60	0
14	UNL	D	4059	1/-	0.75	0.90	-	57,57,57,57	0
14	UNL	V	4024	1/-	0.58	1.08	-	96,96,96,96	0
14	UNL	G	4064	1/-	0.88	0.52	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
12	PO4	P	3010	5/5	0.83	0.18	-	115,115,115,116	0
14	UNL	A	4076	1/-	0.69	0.44	-	68,68,68,68	0
14	UNL	D	4054	1/-	0.72	0.27	-	76,76,76,76	0
14	UNL	B	4030	1/-	0.82	0.45	-	70,70,70,70	0
12	PO4	T	4016	5/5	0.93	0.09	-	107,108,108,108	0
14	UNL	B	4051	1/-	0.85	0.23	-	78,78,78,78	0
14	UNL	W	4077	1/-	0.86	0.14	-	60,60,60,60	0
14	UNL	P	4040	1/-	0.58	0.30	-	73,73,73,73	0
14	UNL	A	4081	1/-	0.70	0.47	-	71,71,71,71	0
14	UNL	C	4018	2/-	0.91	0.35	-	74,74,74,76	0
14	UNL	A	4085	1/-	0.88	0.18	-	56,56,56,56	0
14	UNL	N	4029	1/-	0.71	1.40	-	94,94,94,94	0
14	UNL	T	4066	1/-	0.88	0.07	-	70,70,70,70	0
14	UNL	C	4063	1/-	0.96	1.03	-	74,74,74,74	0
14	UNL	P	4089	1/-	0.91	0.47	-	63,63,63,63	0
14	UNL	P	4060	1/-	0.32	0.34	-	88,88,88,88	0
14	UNL	Q	4044	1/-	0.65	1.64	-	88,88,88,88	0
14	UNL	C	4068	1/-	0.55	0.58	-	72,72,72,72	0
14	UNL	D	4027	1/-	0.74	0.29	-	87,87,87,87	0
14	UNL	S	4047	1/-	0.52	0.38	-	71,71,71,71	0
12	PO4	O	2009	5/5	0.97	0.10	-	76,79,81,81	0
14	UNL	D	4083	1/-	0.77	0.54	-	82,82,82,82	0
14	UNL	E	4050	1/-	0.89	0.38	-	65,65,65,65	0
14	UNL	O	4041	1/-	0.88	0.36	-	71,71,71,71	0
14	UNL	A	4038	1/-	0.72	0.60	-	85,85,85,85	0
20	GOL	E	4007	5/6	0.58	0.51	-	97,100,101,102	0
14	UNL	O	4020	2/-	0.61	0.23	-	96,96,96,97	0
14	UNL	O	4031	1/-	0.82	0.46	-	86,86,86,86	0
14	UNL	F	4028	1/-	0.84	0.58	-	82,82,82,82	0
12	PO4	R	4014	5/5	0.75	0.42	-	173,174,174,174	0
11	JZR	F	4003	18/18	0.38	0.66	-	176,180,181,181	0
14	UNL	P	4058	1/-	0.84	0.34	-	61,61,61,61	0
14	UNL	N	4073	1/-	0.79	0.17	-	69,69,69,69	0
14	UNL	A	4091	1/-	0.75	0.75	-	72,72,72,72	0
14	UNL	C	4045	1/-	0.79	0.41	-	71,71,71,71	0
14	UNL	P	4021	2/-	0.80	0.18	-	71,71,71,73	0
14	UNL	P	4046	1/-	0.91	0.48	-	65,65,65,65	0
14	UNL	A	4048	1/-	0.75	0.38	-	72,72,72,72	0
14	UNL	A	4035	1/-	0.80	0.99	-	69,69,69,69	0
14	UNL	I	4072	1/-	0.39	2.23	-	93,93,93,93	0
14	UNL	R	4069	1/-	0.94	0.41	-	62,62,62,62	0
14	UNL	N	4022	1/-	0.63	0.50	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
14	UNL	B	4025	1/-	0.64	1.81	-	93,93,93,93	0
14	UNL	G	4053	1/-	0.79	0.23	-	77,77,77,77	0
14	UNL	V	4090	1/-	0.92	0.98	-	74,74,74,74	0
14	UNL	D	4036	1/-	0.44	0.34	-	83,83,83,83	0
14	UNL	A	4087	1/-	0.86	0.33	-	60,60,60,60	0
14	UNL	V	4088	1/-	0.68	0.92	-	80,80,80,80	0
14	UNL	E	4061	1/-	0.60	0.19	-	79,79,79,79	0
14	UNL	D	4067	1/-	0.84	0.58	-	58,58,58,58	0
14	UNL	T	4065	1/-	0.84	0.73	-	66,66,66,66	0
14	UNL	I	4033	1/-	0.86	0.87	-	69,69,69,69	0
14	UNL	B	4042	1/-	0.79	0.42	-	81,81,81,81	0
12	PO4	B	3009	5/5	0.89	0.17	-	97,99,100,101	0
14	UNL	O	4082	1/-	0.82	0.14	-	73,73,73,73	0
14	UNL	C	4023	1/-	0.83	0.52	-	55,55,55,55	0
14	UNL	N	4019	2/-	0.77	0.30	-	76,76,76,76	0
14	UNL	G	4070	1/-	0.62	0.26	-	67,67,67,67	0
14	UNL	C	4086	1/-	0.93	0.25	-	50,50,50,50	0
14	UNL	O	4071	1/-	0.67	0.87	-	70,70,70,70	0
14	UNL	B	4039	1/-	0.87	0.31	-	73,73,73,73	0
14	UNL	V	4078	1/-	0.85	1.63	-	94,94,94,94	0
14	UNL	A	4075	1/-	0.94	0.89	-	64,64,64,64	0
14	UNL	D	4062	1/-	0.85	0.28	-	90,90,90,90	0

6.5 Other polymers

There are no such residues in this entry.