



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:25 AM GMT

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 : 2005-06-16
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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

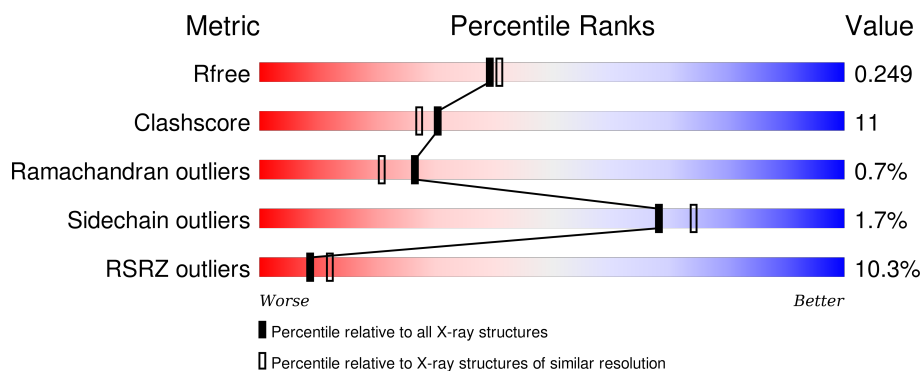
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

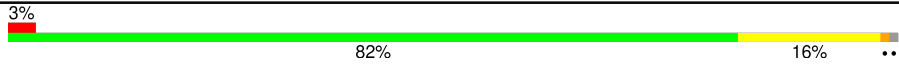


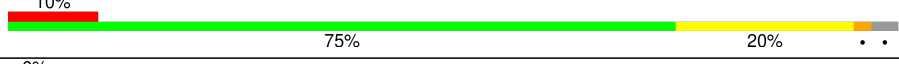
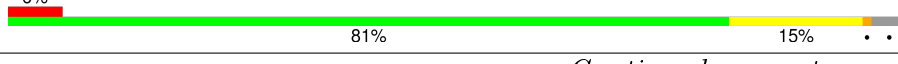
The reported resolution of this entry is 2.10 Å.

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.






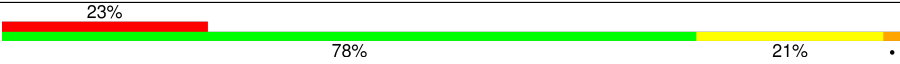
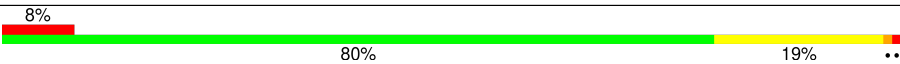

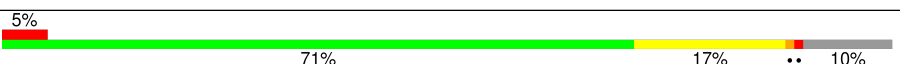
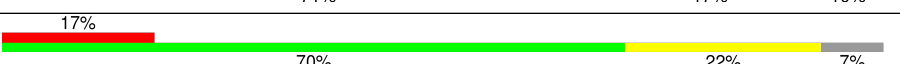

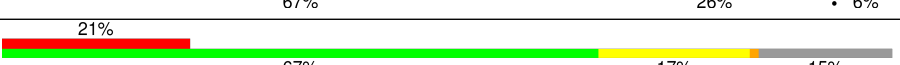
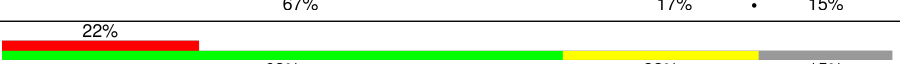




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	
1	N	446	
2	B	439	
2	O	439	
3	C	379	

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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	BHG	A	4004	X	-	-	-
11	BHG	C	2011	X	-	-	X
11	BHG	F	3012	X	-	-	X
11	BHG	F	4003	X	-	-	-
11	BHG	P	3011	X	-	-	X
11	BHG	S	2012	X	-	-	X
12	AZI	A	4002	-	-	-	X
12	AZI	C	2005	-	-	-	X
12	AZI	P	3005	-	-	-	X
13	PO4	A	2010	-	-	-	X
13	PO4	D	4011	-	-	-	X
13	PO4	R	4013	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	PEE	B	4017	-	-	-	X
20	PEE	D	2006	-	-	-	X
20	PEE	P	3007	-	-	-	X
20	PEE	Q	3006	-	-	-	X
21	UNL	A	4032	-	-	-	X
21	UNL	B	4026	-	-	-	X
21	UNL	B	4034	-	-	-	X
21	UNL	B	4057	-	-	-	X
21	UNL	B	4079	-	-	-	X
21	UNL	B	4080	-	-	-	X
21	UNL	O	4037	-	-	-	X
21	UNL	O	4043	-	-	X	-
21	UNL	O	4084	-	-	-	X
21	UNL	P	4074	-	-	-	X
21	UNL	U	4049	-	-	-	X
21	UNL	U	4056	-	-	-	X
22	GOL	C	2008	-	-	-	X
22	GOL	E	4006	-	-	-	X
22	GOL	O	4005	-	-	-	X
22	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			

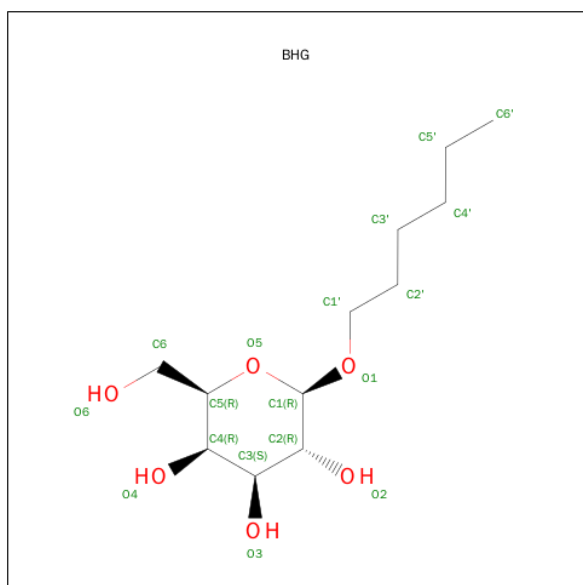
- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial.

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.

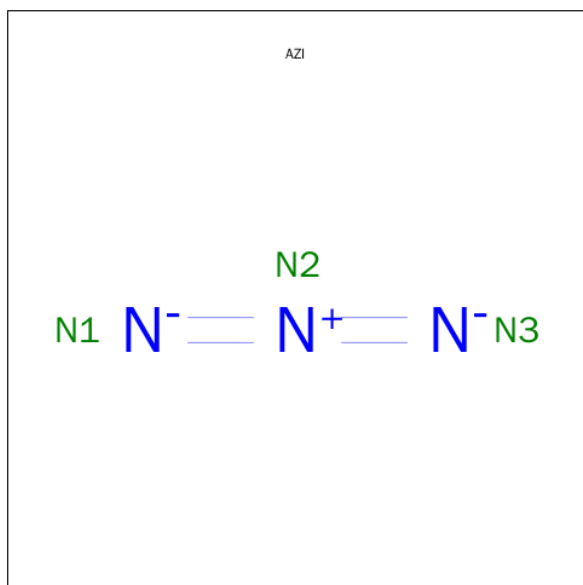
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	30	Total	C	N	O	0	0	1
			245	158	43	44			
10	W	62	Total	C	N	O	0	0	0
			507	333	88	86			

- Molecule 11 is SUGAR (2-HEXYLOXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-3,4,5-TRIOL) (three-letter code: BHG) (formula: $C_{12}H_{24}O_6$).



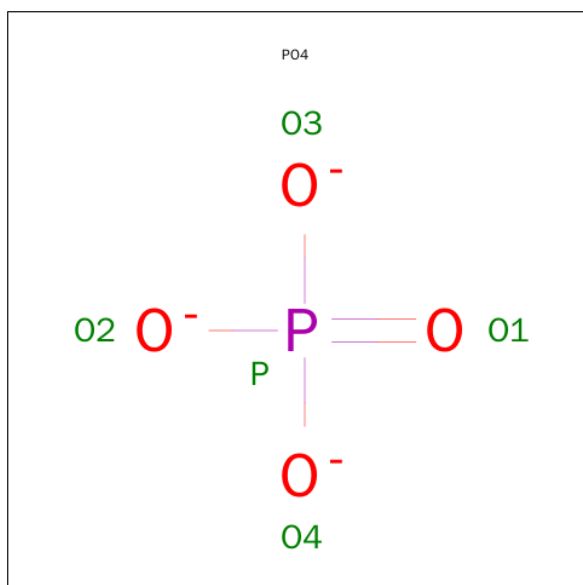
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			18	12	6		
11	S	1	Total	C	O	0	0
			18	12	6		
11	P	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	A	1	Total	C	O	0	0
			18	12	6		

- Molecule 12 is AZIDE ION (three-letter code: AZI) (formula: N_3).



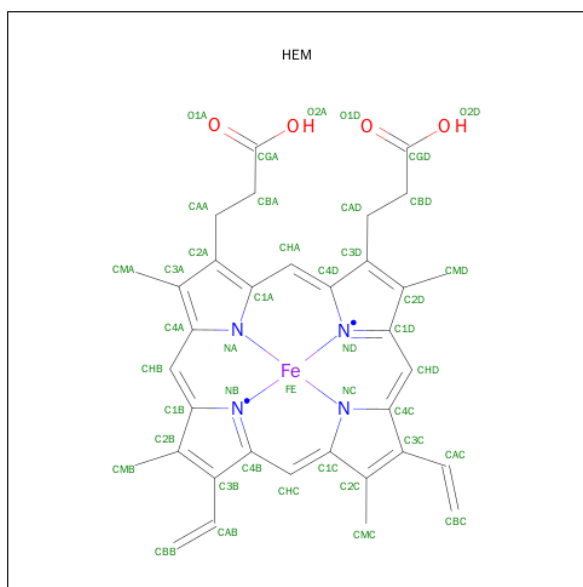
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total N 3 3	0	0
12	P	1	Total N 3 3	0	0
12	G	1	Total N 3 3	0	0
12	A	1	Total N 3 3	0	0

- Molecule 13 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



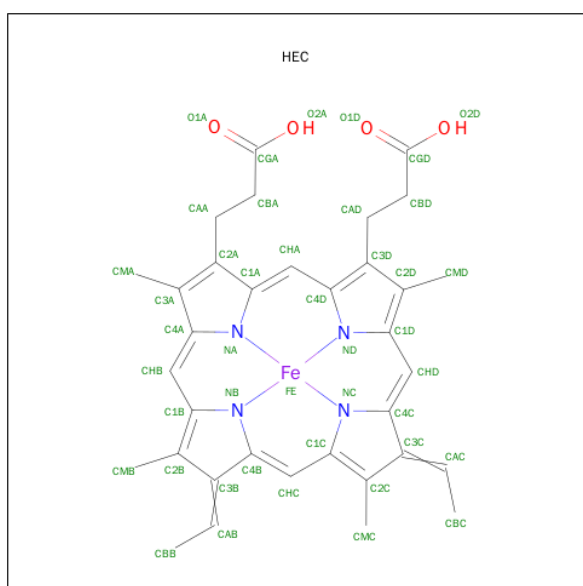
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	O	1	Total O P 5 4 1	0	0
13	A	1	Total O P 5 4 1	0	0
13	B	1	Total O P 5 4 1	0	0
13	P	1	Total O P 5 4 1	0	0
13	D	1	Total O P 5 4 1	0	0
13	D	1	Total O P 5 4 1	0	0
13	Q	1	Total O P 5 4 1	0	0
13	R	1	Total O P 5 4 1	0	0
13	R	1	Total O P 5 4 1	0	0
13	I	1	Total O P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

- Molecule 14 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



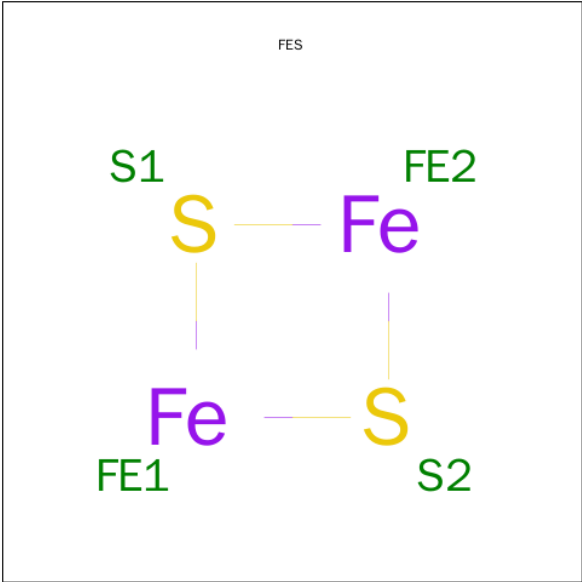
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 15 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



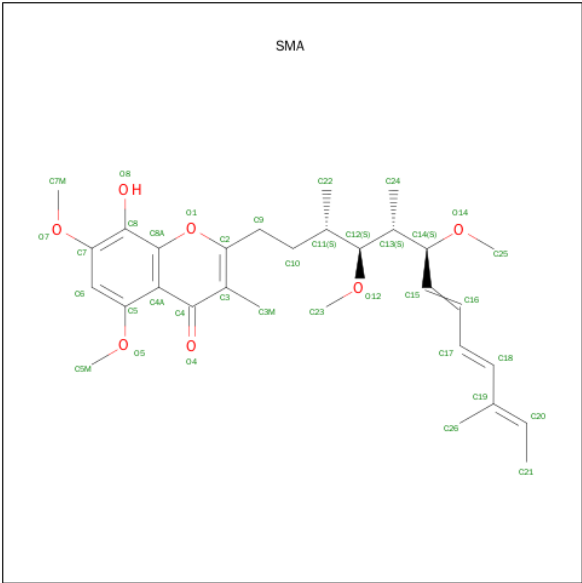
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
15	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



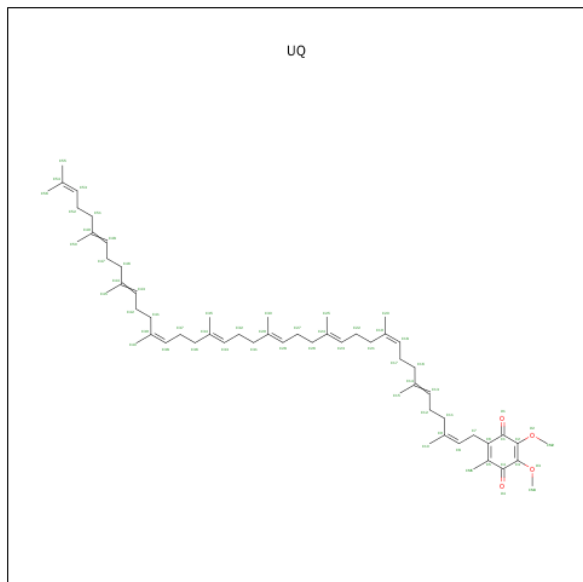
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	E	1	Total	Fe	S	0	0
			4	2	2		
16	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 17 is STIGMATELLIN A (three-letter code: SMA) (formula: C₃₀H₄₂O₇).



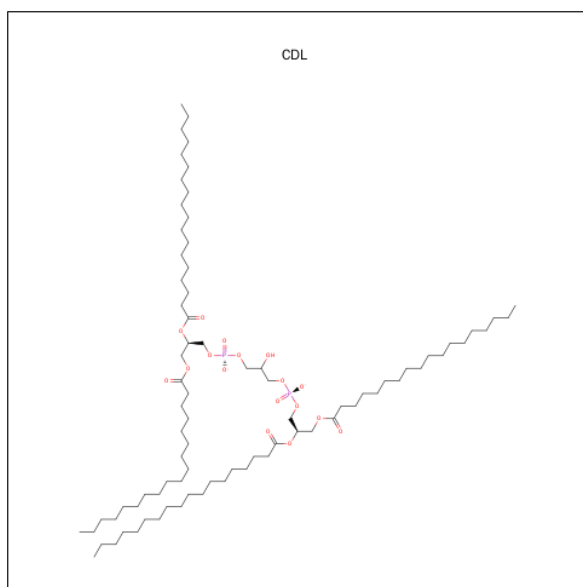
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			37	30	7		
17	P	1	Total	C	O	0	0
			37	30	7		

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



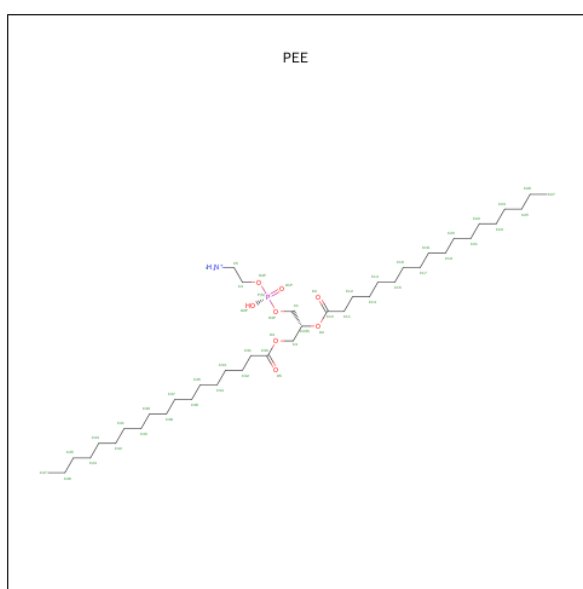
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total	C	O	0	0
			18	14	4		
18	P	1	Total	C	O	0	0
			18	14	4		

- Molecule 19 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 20 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).

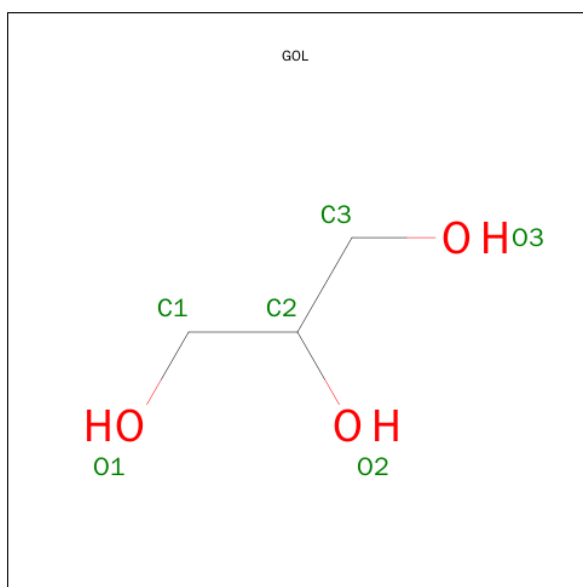


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
20	D	1	Total 51	C 41	N 1	O 8	P 1	0	0	
20	C	1	Total 49	C 39	N 1	O 8	P 1	0	0	
20	Q	1	Total 51	C 41	N 1	O 8	P 1	0	0	
20	P	1	Total 49	C 39	N 1	O 8	P 1	0	0	
20	B	1	Total 8	C 6	O 2				0	0

- Molecule 21 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	P	7	Total O 8 8	0	0
21	G	3	Total O 3 3	0	0
21	Q	1	Total O 1 1	0	0
21	D	7	Total O 7 7	0	0
21	E	2	Total O 2 2	0	0
21	B	11	Total O 11 11	0	0
21	I	2	Total O 2 2	0	0
21	C	6	Total O 7 7	0	0
21	V	4	Total O 4 4	0	0
21	W	1	Total O 1 1	0	0
21	A	10	Total O 10 10	0	0
21	T	2	Total O 2 2	0	0
21	N	4	Total O 5 5	0	0
21	U	2	Total O 2 2	0	0
21	O	8	Total O 9 9	0	0
21	R	2	Total O 2 2	0	0
21	S	1	Total O 1 1	0	0
21	F	1	Total O 1 1	0	0

- Molecule 22 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 23 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	209	Total	O	0	0
			209	209		
23	B	170	Total	O	0	0
			170	170		
23	C	137	Total	O	0	0
			137	137		
23	D	133	Total	O	0	0
			133	133		
23	E	63	Total	O	0	0
			63	63		

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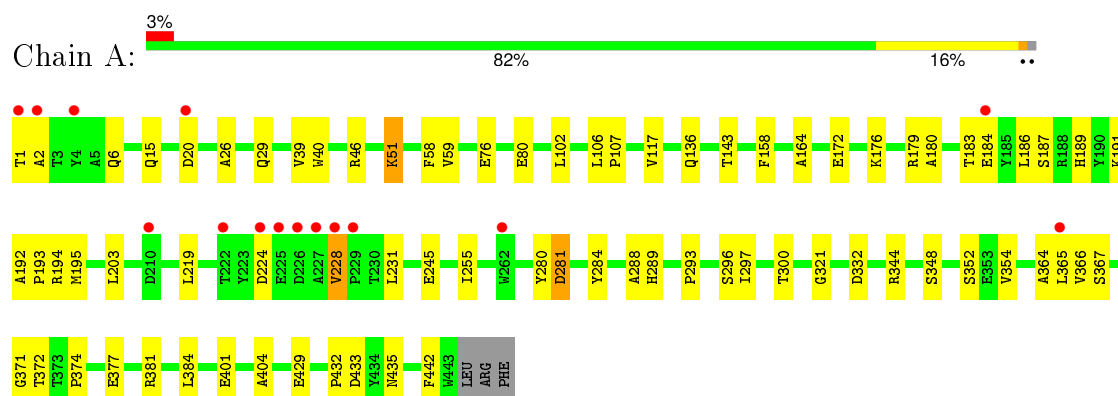
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	F	68	Total 68	O 68	0	0
23	G	31	Total 31	O 31	0	0
23	H	15	Total 15	O 15	0	0
23	I	18	Total 18	O 18	0	0
23	J	7	Total 7	O 7	0	0
23	N	145	Total 145	O 145	0	0
23	O	136	Total 136	O 136	0	0
23	P	135	Total 135	O 135	0	0
23	Q	126	Total 126	O 126	0	0
23	R	77	Total 77	O 77	0	0
23	S	81	Total 81	O 81	0	0
23	T	17	Total 17	O 17	0	0
23	U	16	Total 16	O 16	0	0
23	V	16	Total 16	O 16	0	0
23	W	12	Total 12	O 12	0	0

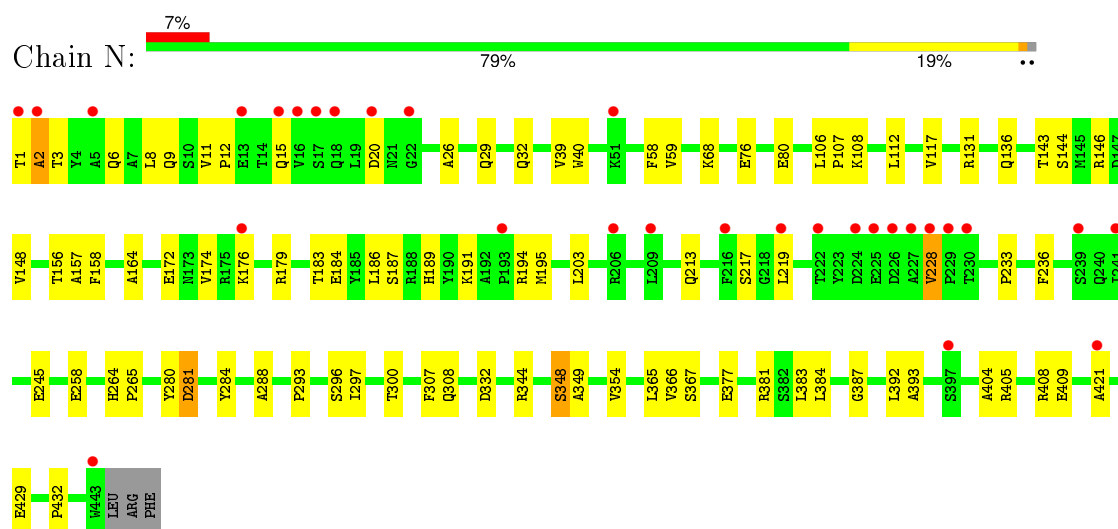
3 Residue-property plots [i](#)

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

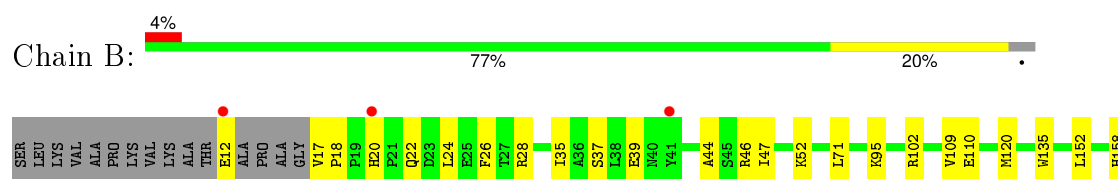
- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial

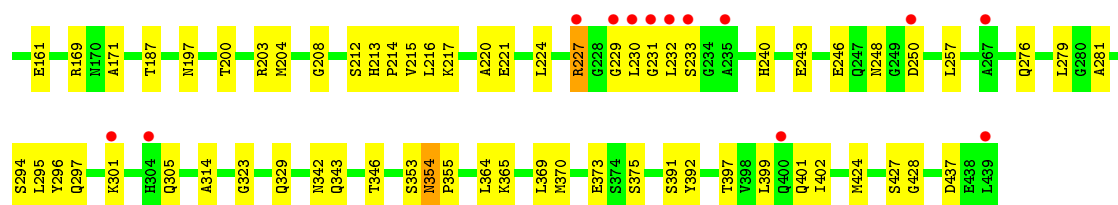


- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial

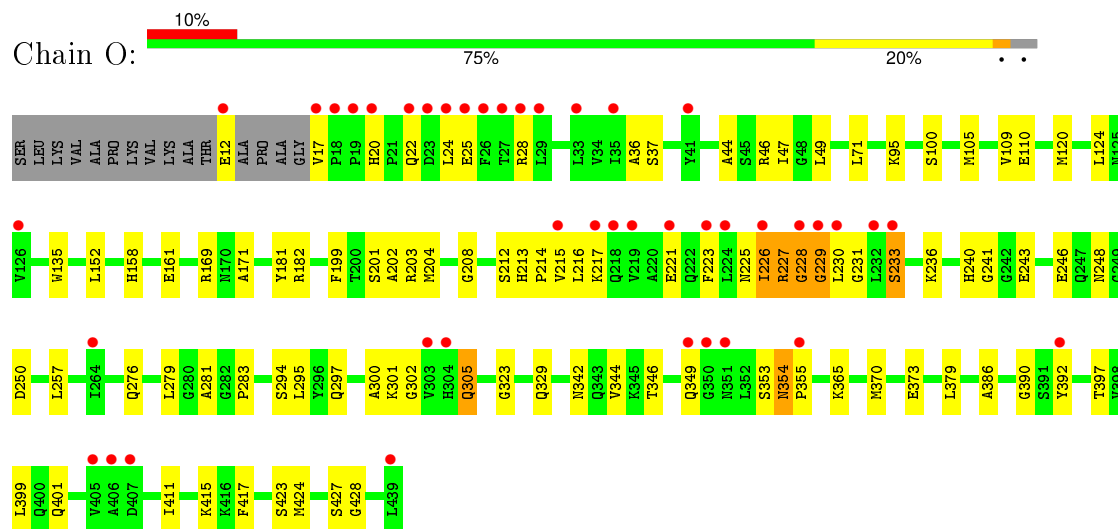


- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial

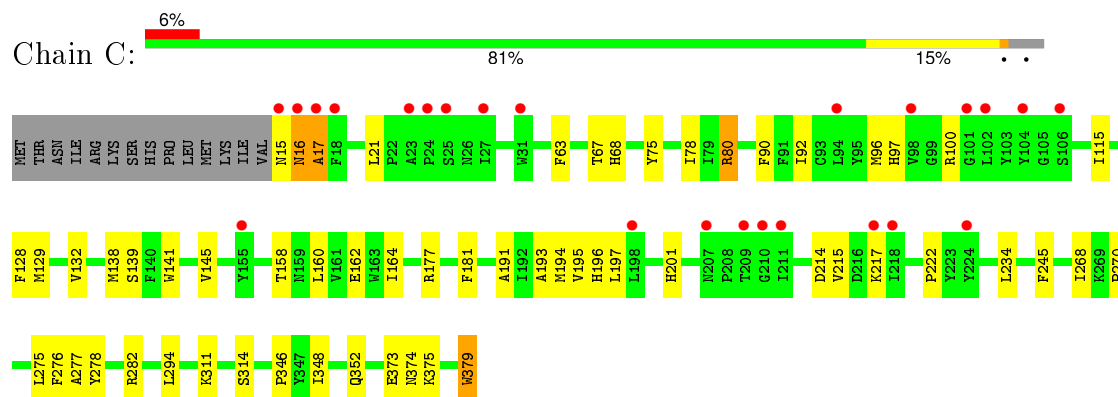




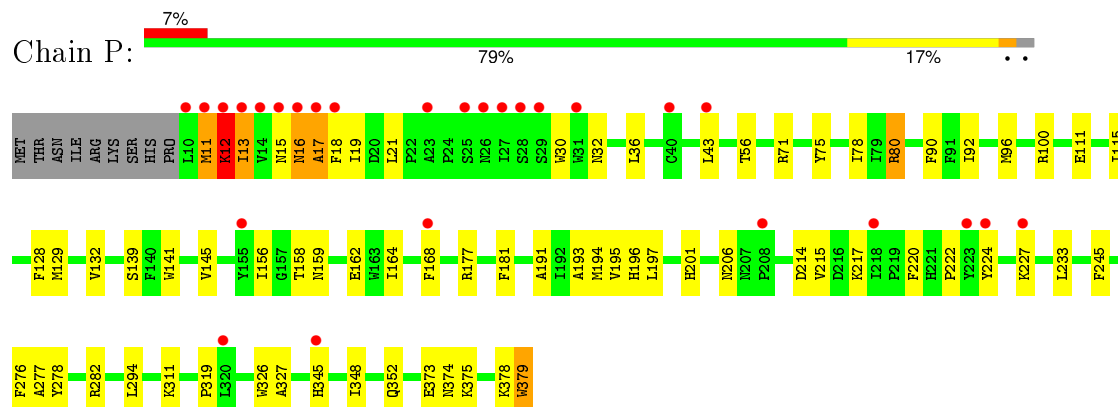
• Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial



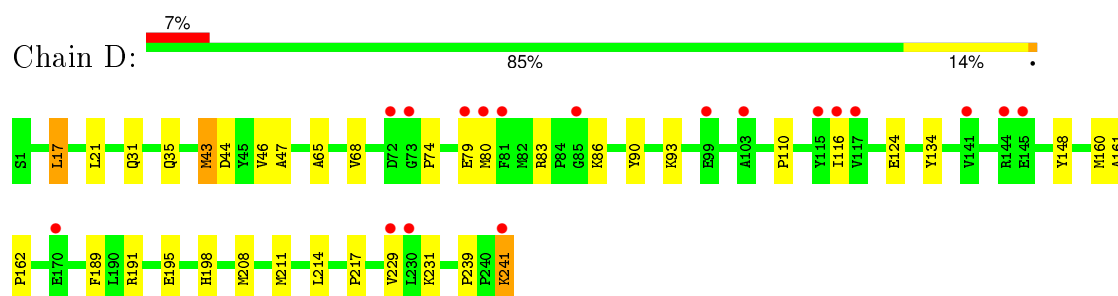
• Molecule 3: Cytochrome b, heme protein, mitochondrial



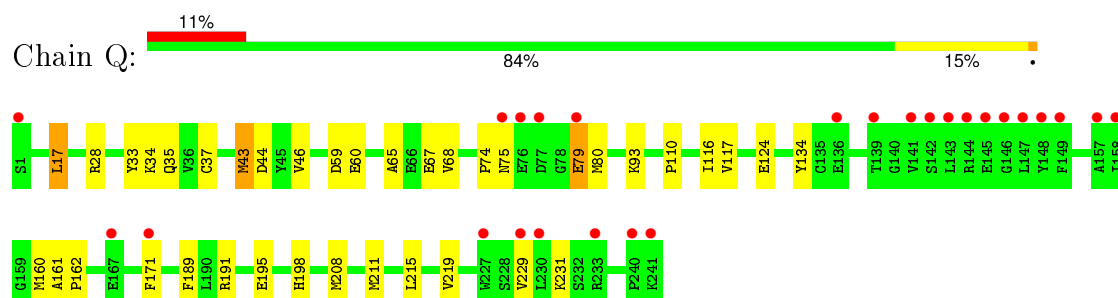
• Molecule 3: Cytochrome b, heme protein, mitochondrial



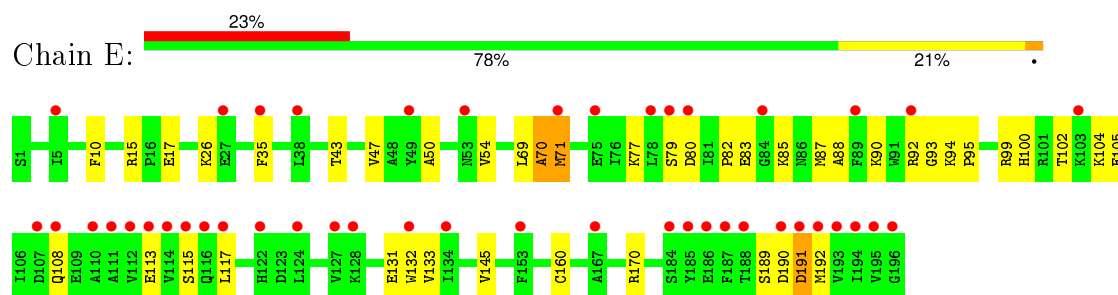
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



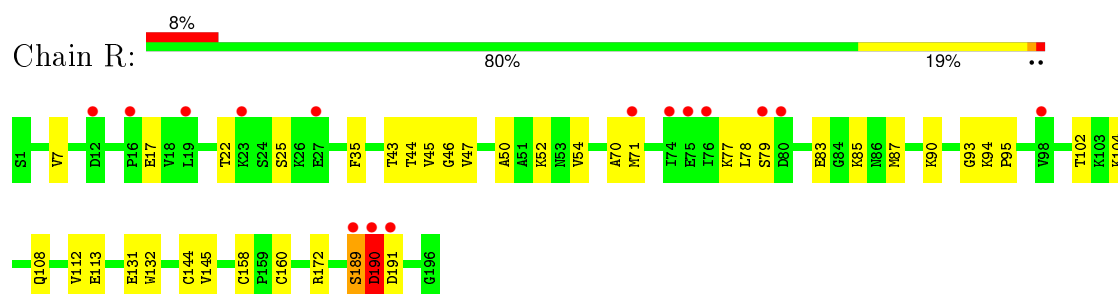
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



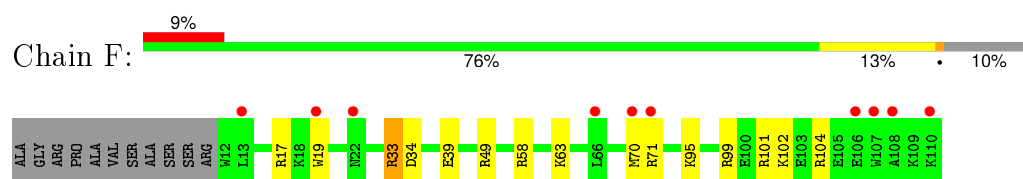
- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



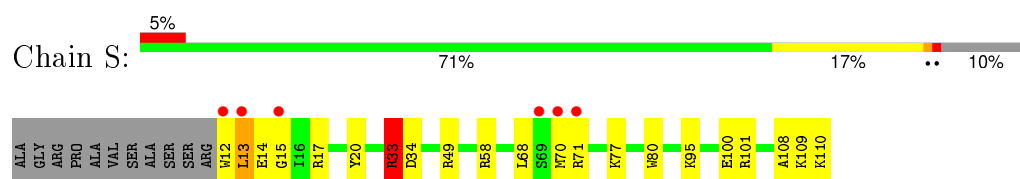
- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial



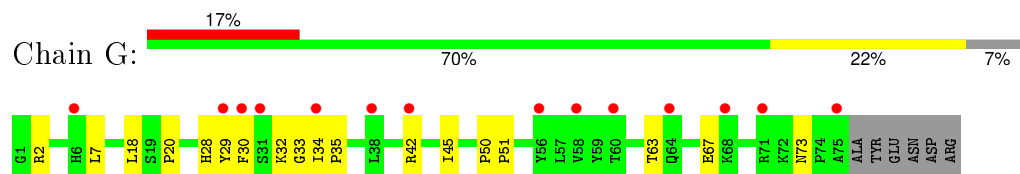
- Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein



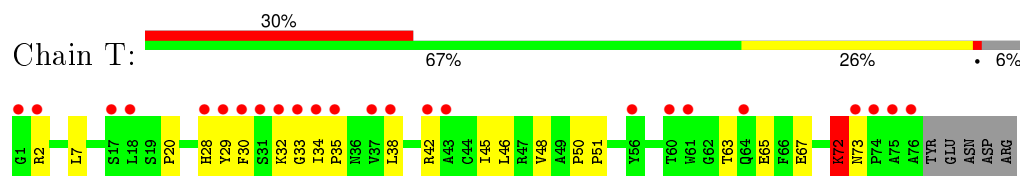
- Molecule 6: Ubiquinol-cytochrome c reductase complex 14 kDa protein



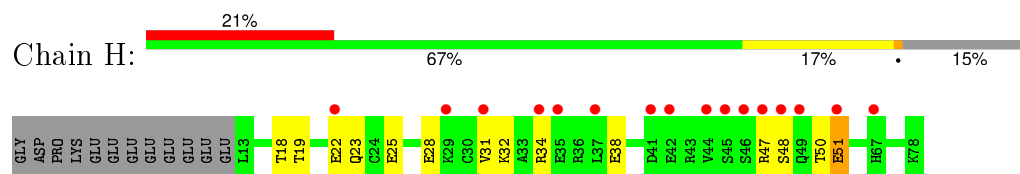
- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



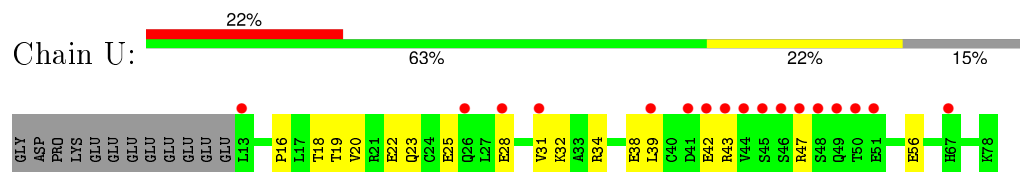
- Molecule 7: Ubiquinol-cytochrome c reductase complex ubiquinone-binding protein QP-C



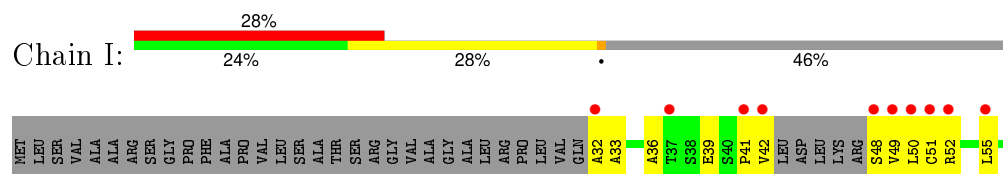
- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein



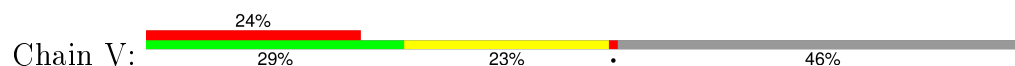
- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein

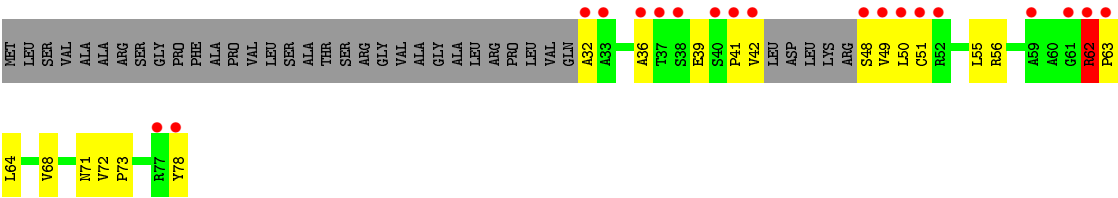


- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial

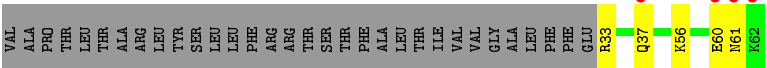
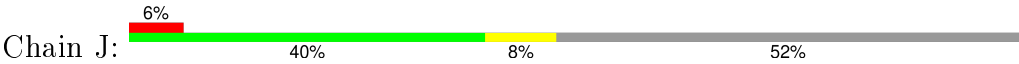


- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial

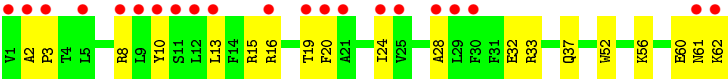




• Molecule 10: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



• 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 , 70.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 308092 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, GOL, CDL, UNL, PO4, UQ, BHG, FES, HEC, HEM, PEE, 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	3	0	0	0	0
12	C	3	0	0	0	0
12	G	3	0	0	1	0
12	P	3	0	0	0	0
13	A	5	0	0	0	0
13	B	5	0	0	0	0
13	D	10	0	0	0	0
13	I	5	0	0	1	0
13	O	5	0	0	0	0
13	P	5	0	0	0	0
13	Q	5	0	0	1	0
13	R	10	0	0	0	0
13	T	5	0	0	0	0
14	C	86	0	60	5	0
14	P	86	0	60	3	0
15	D	43	0	30	4	0
15	Q	43	0	30	5	0
16	E	4	0	0	0	0
16	R	4	0	0	0	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	B	8	0	8	1	0
20	C	49	0	72	0	0
20	D	51	0	82	2	0
20	P	49	0	72	3	0
20	Q	51	0	82	5	0
21	A	10	0	0	0	0
21	B	11	0	0	0	0
21	C	7	0	0	0	0
21	D	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	E	2	0	0	0	0
21	F	1	0	0	0	0
21	G	3	0	0	0	0
21	I	2	0	0	0	0
21	N	5	0	0	0	0
21	O	9	0	0	2	0
21	P	8	0	0	0	0
21	Q	1	0	0	0	0
21	R	2	0	0	0	0
21	S	1	0	0	0	0
21	T	2	0	0	0	0
21	U	2	0	0	0	0
21	V	4	0	0	0	0
21	W	1	0	0	0	0
22	C	12	0	16	0	0
22	E	11	0	13	0	0
22	O	6	0	8	0	0
22	P	12	0	16	2	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	21: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
3:C:21:LEU:HD21	18:C:2002:UQ:HM32	1.64	0.80
1:A:51:LYS:H	1:A:51:LYS:HE3	1.47	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
10:W:3:PRO:HB2	10:W:8:ARG:HD3	1.65	0.77
2:O:20:HIS:HB2	2:O:22:GLN:HG2	1.66	0.77
1:N:179:ARG:O	1:N:183:THR:HG23	1.85	0.77
4:D:116:ILE:HG12	15:D:501:HEC:HMA3	1.66	0.77
2:B:397:THR:HG22	2:B:401:GLN:NE2	1.99	0.77
1:A:401:GLU:HG3	11:A:4004:BHG:H6'1	1.67	0.77
20: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	20: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
9:V:62:ARG:O	9:V:78:TYR:HB3	1.88	0.72
1:A:2:ALA:HB1	1:A:6:GLN:HB2	1.71	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
4:D:43:MET:HE2	4:D:46:VAL:HG21	1.75	0.69
3:C:68:HIS:HD2	23:C:4195:HOH:O	1.74	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
5:R:70:ALA:N	5:R:71:MET:HE2	2.07	0.69
2:B:197:ASN:HB3	2:B:230:LEU:HG	1.74	0.69
2:B:95:LYS:CD	9:I:32:ALA:HB2	2.21	0.68
4:D:110:PRO:HG3	15: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
9:V:32:ALA:N	9:V:71:ASN:HB3	2.08	0.67
4:Q:110:PRO:HG3	15:Q:501:HEC:HMD3	1.77	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
9:V:32:ALA:N	9:V:71:ASN:CB	2.59	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
2:O:95:LYS:HE2	9:V:32:ALA:HB3	1.78	0.65
3:P:12:LYS:HE2	3:P:16:ASN:N	2.06	0.65
2:O:203:ARG:HH12	2:O:233:SER:CA	2.09	0.65
2:B:20:HIS:HB2	2:B:22:GLN:CG	2.27	0.65
2:B:200:THR:HG21	2:B:229:GLY:CA	2.26	0.65
14:P:501:HEM:HMC1	14: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
3:C:92:ILE:O	3:C:96:MET:HG2	1.96	0.64
1:A:372:THR:HA	23:A:4296:HOH:O	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
2:O:250:ASP:HB3	23:O:4203:HOH:O	1.99	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
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:202:ALA:HB3	2:O:229:GLY:O	1.99	0.62
2:O:158:HIS:HB3	23:O:4207:HOH:O	1.98	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
2:O:95:LYS:CE	9:V:32:ALA:HB3	2.29	0.62
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.82	0.62
8:H:25:GLU:HB3	8:H:34:ARG:HH22	1.63	0.62
2:B:296:TYR:OH	9:I:52:ARG:HD3	2.00	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
5:E:160:CYS:HB3	17:P:3001:SMA:H4	1.82	0.61
1:A:143:THR:OG1	9:I:48:SER:HB3	2.00	0.61
2:B:95:LYS:HB2	9:I:32:ALA:CB	2.29	0.61
2:B:200:THR:HG21	2:B:229:GLY:HA3	1.80	0.61
2:B:95:LYS:HD3	2:B:110:GLU:OE2	2.01	0.61
1:A:366:VAL:HG21	2:B:44:ALA:HB2	1.82	0.61
1:A:117:VAL:HG11	1:A:195:MET:CE	2.30	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
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
4:D:124:GLU:OE2	4:D:191:ARG:HD2	2.01	0.61
2:B:37:SER:HB3	2:B:216:LEU:HD12	1.83	0.61
2:O:28:ARG:NH1	2:O:28:ARG:HB2	2.16	0.61
8:U:34:ARG:O	8:U:38:GLU:HG3	2.01	0.60
3:P:92:ILE:O	3:P:96:MET:HG2	2.01	0.60
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.82	0.60
2:O:226:ILE:CG1	21: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
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
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.50	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
2:O:226:ILE:HD11	23:O:4141:HOH:O	2.00	0.60
9:V:36:ALA:CB	9:V:73:PRO:HD2	2.31	0.60
23:P:4186:HOH:O	6:S:20:TYR:HE1	1.84	0.60
1:N:68:LYS:HA	1:N:68:LYS:HE3	1.83	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
9:V:32:ALA:N	9:V:72:VAL:HG23	2.18	0.59
1:N:195:MET:SD	1:N:219:LEU:HD21	2.43	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
8:U:28:GLU:O	8:U:31:VAL:HG22	2.03	0.59
2:O:28:ARG:HB2	2:O:28:ARG:HH11	1.67	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
8:U:31:VAL:HA	8:U:34:ARG:HH12	1.68	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
9:I:70:LEU:O	9:I:71:ASN:HB2	2.02	0.57
5:E:191:ASP:O	5:E:192:MET:HG2	2.04	0.57
9:V:36:ALA:HB3	9:V:73:PRO:HG2	1.85	0.57
3:P:43:LEU:HD21	20:Q:3006:PEE:C19	2.34	0.57
2:B:208:GLY:HA3	2:B:216:LEU:HD11	1.84	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
5:R:79:SER:HB3	5:R:191:ASP:OD2	2.05	0.57
4:Q:75:ASN:HD21	4:Q:79:GLU:HG3	1.69	0.57
2:B:297:GLN:O	2:B:301:LYS:HG3	2.03	0.57
2:O:427:SER:HB3	23:O:4207:HOH:O	2.04	0.57
1:A:117:VAL:HG11	1:A:195:MET:HE3	1.87	0.57
2:O:354:ASN:N	2:O:355:PRO:CD	2.68	0.57
2:B:305:GLN:HB3	2:B:329:GLN:OE1	2.04	0.57
6:S:49:ARG:HH22	11:S:2012:BHG:H4	1.70	0.56
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
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:BHG:H62	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
2:O:227:ARG:HA	23:O:4150:HOH:O	2.06	0.56
1:N:76:GLU:HG2	1:N:80:GLU:OE2	2.05	0.56
3:P:277:ALA:HB1	3:P:294:LEU:CD1	2.35	0.56
2:O:169:ARG:HG3	2:O:240:HIS:HB2	1.88	0.56
7:G:42:ARG:HG3	7:G:42:ARG:HH11	1.71	0.56
1:A:106:LEU:HB3	1:A:107:PRO:HD3	1.87	0.56
14:C:501:HEM:HBC2	14:C:501:HEM:HMC1	1.88	0.56
9:I:62:ARG:HD3	13:I:4015:PO4:O3	2.07	0.55
4:Q:116:ILE:HG12	15:Q:501:HEC:HMA3	1.89	0.55
3:C:373:GLU:HB2	23:C:4111:HOH:O	2.06	0.55
1:A:289:HIS:HE1	11:S:2012:BHG:H1'2	1.71	0.55
6:F:95:LYS:HB2	6:F:95:LYS:NZ	2.20	0.55
1:N:189:HIS:CB	1:N:194:ARG:HH21	2.19	0.55
10:W:16:ARG:HB2	10:W:19:THR:CG2	2.36	0.55
6:S:49:ARG:NH2	11:S:2012:BHG:H4	2.21	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:82:PRO:O	5:E:100:HIS:HB3	2.07	0.55
5:E:104:LYS:O	5:E:108:GLN:HG3	2.07	0.55
7:T:34:ILE:HB	7:T:35:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:ASN:O	3:C:16:ASN:C	2.46	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
2:B:46:ARG:HD2	2:B:375:SER:OG	2.07	0.54
1:A:76:GLU:HG2	1:A:80:GLU:OE2	2.08	0.54
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.38	0.54
4:D:43:MET:HE1	4:D:189:PHE:HZ	1.72	0.54
1:A:189:HIS:CB	1:A:194:ARG:HH21	2.19	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
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.42	0.54
2:B:231:GLY:N	2:B:233:SER:OG	2.40	0.54
8:H:51:GLU:CD	8:H:51:GLU:H	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
3:P:156:ILE:HA	3:P:159:ASN:HD22	1.73	0.54
1:N:296:SER:O	1:N:300:THR:HG23	2.07	0.54
3:P:197:LEU:HD13	18:P:3002:UQ:HM53	1.89	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
2:B:279:LEU:HB3	2:B:295:LEU:HG	1.90	0.54
5:E:50:ALA:O	5:E:54:VAL:HG23	2.08	0.54
2:O:225:ASN:HD21	2:O:227:ARG:NH2	2.06	0.53
1:N:381:ARG:HH11	1:N:381:ARG:HG2	1.73	0.53
3:P:12:LYS:CA	3:P:12:LYS:HE3	2.39	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
8:U:19:THR:O	8:U:23:GLN:HG3	2.07	0.53
1:N:354:VAL:HG21	1:N:404:ALA:HA	1.90	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
3:P:201:HIS:NE2	18:P:3002:UQ:O4	2.31	0.53
2:B:279:LEU:HA	2:B:294:SER:HB3	1.91	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
2:O:279:LEU:HB3	2:O:295:LEU:HG	1.89	0.52
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
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
14:C:502:HEM:HMC2	14:C:502:HEM:HBC2	1.92	0.52
2:O:225:ASN:ND2	2:O:227:ARG:CZ	2.72	0.52
15:Q:501:HEC:HBC3	15:Q:501:HEC:HMC1	1.91	0.52
1:N:117:VAL:HG11	1:N:195:MET:CE	2.40	0.52
1:N:2:ALA:HA	1:N:6:GLN:OE1	2.10	0.52
4:Q:75:ASN:OD1	4:Q:79:GLU:HG2	2.10	0.52
3:C:138:MET:SD	3:C:268:ILE:HG13	2.49	0.52
2:O:217:LYS:O	2:O:221:GLU:HG3	2.10	0.52
9:I:36:ALA:CB	9:I:73:PRO:HD2	2.37	0.52
1:A:136:GLN:HB3	9:I:51:CYS:HB3	1.91	0.52
6:S:95:LYS:HB2	6:S:95:LYS:NZ	2.25	0.52
3:P:311:LYS:HG2	3:P:374:ASN:CG	2.30	0.52
1:N:288:ALA:HB2	1:N:300:THR:HG22	1.92	0.52
9:V:36:ALA:HB3	9:V:73:PRO:CG	2.40	0.52
3:C:100:ARG:C	3:C:100:ARG:HD2	2.29	0.52
1:N:228:VAL:HG13	1:N:228:VAL:O	2.11	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
4:Q:231:LYS:HD3	6:S:70:MET:CE	2.40	0.51
1:A:381:ARG:HG2	1:A:381:ARG:HH11	1.75	0.51
9:V:32:ALA:N	9:V:71:ASN:HB2	2.25	0.51
7:T:32:LYS:C	7:T:35:PRO:HD2	2.31	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
15:D:501:HEC:HMC1	15:D:501:HEC:HBC3	1.92	0.50
2:B:24:LEU:HD13	2:B:392:TYR:CD2	2.45	0.50
7:G:29:TYR:O	7:G:33:GLY:HA3	2.09	0.50
5:E:102:THR:OG1	5:E:105:GLU:HG3	2.11	0.50
2:B:227:ARG:HD3	2:B:227:ARG:N	2.26	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)
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.47	0.50
2:B:71:LEU:HD23	9:I:68:VAL:HG21	1.91	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
9:I:64:LEU:HD23	9:I:77:ARG:O	2.12	0.50
5:E:190:ASP:O	5:E:192:MET:HG2	2.12	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
4:Q:195:GLU:HG2	4:Q:198:HIS:HB2	1.94	0.50
10:J:56:LYS:HG2	10:J:60:GLU:CD	2.32	0.50
3:C:245:PHE:CD1	4:D:17:LEU:HD13	2.47	0.50
2:O:305:GLN:NE2	2:O:329:GLN:OE1	2.45	0.49
2:O:95:LYS:CE	9:V:32:ALA:CB	2.90	0.49
4:Q:208:MET:HA	20:Q:3006:PEE:H49	1.94	0.49
1:N:344:ARG:HG2	1:N:344:ARG:NH1	2.27	0.49
3:C:160:LEU:O	3:C:164:ILE:HG12	2.11	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:BHG:H61	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
1:N:280:TYR:HA	1:N:284:TYR:CE2	2.47	0.49
2:O:95:LYS:O	2:O:109:VAL:HA	2.12	0.49
3:P:11:MET:HG2	3:P:12:LYS:N	2.27	0.49
2:O:203:ARG:HH12	2:O:233:SER:HA	1.78	0.49
3:C:197:LEU:HD13	18:C:2002:UQ:HM53	1.94	0.49
2:B:203:ARG:NH1	2:B:232:LEU:HA	2.28	0.49
4:D:17:LEU:HD21	21:D:4083:UNL:O1	2.13	0.49
1:N:383:LEU:O	1:N:387:GLY:HA2	2.12	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
7:T:46:LEU:N	7:T:46:LEU:HD22	2.27	0.49
2:O:47:ILE:HG21	2:O:120:MET:HE3	1.95	0.49
1:A:344:ARG:NH1	1:A:344:ARG:HG2	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
4:D:208:MET:HA	20:D:2006:PEE:H49	1.94	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)
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.95	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
3:P:129:MET:HE1	3:P:181:PHE:CD2	2.40	0.48
3:C:68:HIS:CD2	23:C:4195:HOH:O	2.59	0.48
2:B:52:LYS:NZ	2:B:232:LEU:HD11	2.28	0.48
5:R:77:LYS:HE3	5:R:79:SER:OG	2.13	0.48
3:P:311:LYS:HG2	3:P:374:ASN:OD1	2.14	0.48
3:C:158:THR:O	3:C:162:GLU:HG3	2.13	0.48
1:N:233:PRO:O	5:R:22:THR:HA	2.13	0.48
2:O:199:PHE:O	2:O:226:ILE:HD13	2.14	0.48
1:N:308:GLN:HB3	23:N:4088:HOH:O	2.13	0.48
23:A:4251:HOH:O	9:I:39:GLU:CG	2.62	0.48
2:O:201:SER:H	2:O:226:ILE:HG23	1.78	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:O:246:GLU:O	2:O:427:SER:HA	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
4:Q:43:MET:HE2	4:Q:189:PHE:CZ	2.49	0.48
2:O:202:ALA:HB3	2:O:230:LEU:N	2.28	0.48
4:D:160:MET:HB2	15:D:501:HEC:C1D	2.44	0.48
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.96	0.48
2:B:232:LEU:O	2:B:233:SER:HB3	2.13	0.48
2:B:437:ASP:OD2	2:O:240:HIS:CD2	2.67	0.48
6:F:49:ARG:NH2	11:F:3012:BHG:H1	2.28	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
3:P:115:ILE:HD13	3:P:195:VAL:HG12	1.95	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
4:Q:43:MET:HE2	4:Q:189:PHE:HZ	1.80	0.47
3:P:319:PRO:HD2	23:P:4186:HOH:O	2.13	0.47
2:O:397:THR:CG2	2:O:401:GLN:HE21	2.23	0.47
4:D:74:PRO:CD	4:D:80:MET:HE1	2.41	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
6:F:34:ASP:O	6:F:58:ARG:NH2	2.47	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)
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.50	0.47
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.97	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
4:D:231:LYS:HD3	6:F:70:MET:CE	2.44	0.47
6:F:104:ARG:HH11	11:F:3012:BHG:C6	2.27	0.47
3:P:214:ASP:CG	7:T:2:ARG:HH22	2.18	0.47
3:C:96:MET:HA	3:C:96:MET:HE2	1.97	0.47
3:C:191:ALA:HA	3:C:194:MET:CE	2.45	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
10:W:2:ALA:HA	10:W:3:PRO:HD3	1.77	0.47
1:N:348:SER:O	1:N:349:ALA:C	2.54	0.47
2:B:12:GLU:O	2:B:18:PRO:HD3	2.14	0.46
5:R:189:SER:O	5:R:190:ASP:C	2.53	0.46
1:A:40:TRP:HB3	1:A:384:LEU:HD11	1.96	0.46
2:O:370:MET:O	2:O:373:GLU:HG2	2.15	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
10:W:20:PHE:CE1	10:W:24:ILE:HD11	2.49	0.46
4:D:211:MET:HG3	20:D:2006:PEE:H48	1.97	0.46
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.50	0.46
1:N:3:THR:OG1	1:N:6:GLN:HG3	2.15	0.46
1:N:264:HIS:HA	1:N:265:PRO:HD3	1.83	0.46
8:H:19:THR:O	8:H:23:GLN:HG3	2.15	0.46
4:D:47:ALA:HA	4:D:90:TYR:HA	1.96	0.46
6:S:101:ARG:HG2	6:S:101:ARG:HH11	1.80	0.46
5:R:93:GLY:O	5:R:94:LYS:HG3	2.14	0.46
3:P:12:LYS:HA	3:P:12:LYS:CE	2.43	0.46
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.46	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:O:344:VAL:HG11	2:O:417:PHE:CD2	2.50	0.46
2:O:213:HIS:N	2:O:214:PRO:CD	2.79	0.46
1:N:281:ASP:OD2	9:V:73:PRO:HB3	2.15	0.46
2:B:102:ARG:HH22	2:B:161:GLU:CD	2.19	0.46
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
3:C:215:VAL:HG13	23:C:4154:HOH:O	2.15	0.46
4:D:83:ARG:CZ	4:D:86:LYS:HE2	2.45	0.46
2:B:370:MET:O	2:B:373:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:373:GLU:HB2	23:P:4170:HOH:O	2.16	0.46
3:C:75:TYR:O	3:C:78:ILE:HG22	2.15	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
2:B:354:ASN:H	2:B:355:PRO:HD2	1.81	0.46
2:B:342:ASN:O	2:B:346:THR:HG23	2.15	0.46
8:U:28:GLU:CA	8:U:31:VAL:HG22	2.44	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
23:O:4201:HOH:O	9:V:32:ALA:HB1	2.16	0.46
4:Q:74:PRO:CD	4:Q:80:MET:HE1	2.46	0.46
9:V:50:LEU:O	9:V:51:CYS:HB3	2.16	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
3:C:214:ASP:CG	7:G:2:ARG:HH22	2.19	0.46
6:F:71:ARG:HD3	23:F:4076:HOH:O	2.15	0.46
14: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
3:C:115:ILE:HD13	3:C:195:VAL:HG12	1.98	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
3:P:15:ASN:O	3:P:17:ALA:N	2.49	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
1:A:228:VAL:O	1:A:228:VAL:HG13	2.16	0.45
7:T:28:HIS:ND1	7:T:32:LYS:HD2	2.31	0.45
6:S:109:LYS:O	6:S:110:LYS:HG2	2.16	0.45
3:C:276:PHE:CG	3:C:277:ALA:N	2.84	0.45
5:R:190:ASP:HB2	5:R:191:ASP:H	1.42	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
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
2:B:95:LYS:O	2:B:109:VAL:HA	2.17	0.45
1:A:158:PHE:O	1:A:164:ALA:HB2	2.17	0.45
3:C:80:ARG:HD3	3:C:80:ARG:C	2.37	0.45
3:C:164:ILE:O	3:C:177:ARG:HD2	2.16	0.45
9:I:61:GLY:C	9:I:62:ARG:HG3	2.37	0.45
5:R:44:THR:HG22	10:W:24:ILE:HG21	1.97	0.45
1:A:39:VAL:CG1	1:A:195:MET:HE2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:101:ARG:HG2	6:F:101:ARG:NH1	2.32	0.45
2:O:342:ASN:O	2:O:346:THR:HG23	2.16	0.45
1:N:213:GLN:O	1:N:217:SER:OG	2.27	0.45
1:N:117:VAL:HG11	1:N:195:MET:HE1	1.99	0.44
3:P:13:ILE:HA	3:P:17:ALA:HB2	1.99	0.44
2:O:100:SER:OG	2:O:105:MET:HG2	2.17	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
8:U:42:GLU:HG2	8:U:43:ARG:N	2.32	0.44
3:P:75:TYR:O	3:P:78:ILE:HG22	2.17	0.44
3:P:348:ILE:O	3:P:352:GLN:HG3	2.17	0.44
3:P:220:PHE:HE1	18:P:3002:UQ:HM23	1.82	0.44
4:Q:60:GLU:HG3	10:W:62:LYS:HZ3	1.81	0.44
3:P:129:MET:HE1	17:P:3001:SMA:H26	1.98	0.44
4:D:74:PRO:HB3	4:D:80:MET:CE	2.47	0.44
4:Q:160:MET:HB2	15:Q:501:HEC:C1D	2.47	0.44
5:R:112:VAL:HG22	5:R:172:ARG:HH22	1.82	0.44
3:C:270:PRO:HG2	3:C:278:TYR:CG	2.52	0.44
10:J:56:LYS:O	10:J:60:GLU:HG3	2.17	0.44
3:C:348:ILE:O	3:C:352:GLN:HG3	2.17	0.44
1:A:102:LEU:CD2	2:B:369:LEU:HD12	2.47	0.44
4:D:195:GLU:HG2	4:D:198:HIS:HB2	2.00	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
2:O:248:ASN:OD1	2:O:428:GLY:HA2	2.17	0.44
14:P:502:HEM:HBA1	18:P:3002:UQ:O2	2.18	0.44
4:D:74:PRO:HA	4:D:79:GLU:O	2.18	0.44
1:N:39:VAL:HG11	1:N:195:MET:HE2	1.98	0.44
6:F:95:LYS:NZ	6:F:95:LYS:CB	2.80	0.44
9:V:32:ALA:N	9:V:72:VAL:CG2	2.80	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
1:A:371:GLY:O	1:A:374:PRO:HD2	2.18	0.44
2:B:46:ARG:O	2:B:47:ILE:HD13	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
5:R:112:VAL:HG21	5:R:172:ARG:NH2	2.32	0.44
2:O:217:LYS:HE2	2:O:221:GLU:OE2	2.18	0.44
3:C:132:VAL:HA	3:C:139:SER:HB3	1.98	0.44
5:R:43:THR:O	5:R:47:VAL:HG23	2.17	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
9:V:64:LEU:HD23	9:V:78:TYR:C	2.38	0.43
3:P:43:LEU:HD21	20:Q:3006:PEE:H27	2.00	0.43
1:A:195:MET:SD	1:A:219:LEU:HD21	2.58	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
5:E:99:ARG:HB3	5:E:133:VAL:HG12	2.01	0.43
3:P:282:ARG:NH2	23:P:4173:HOH:O	2.51	0.43
1:A:289:HIS:HE1	11:S:2012:BHG:C1'	2.32	0.43
4:Q:195:GLU:O	4:Q:195:GLU:HG2	2.19	0.43
2:O:46:ARG:HG2	2:O:379:LEU:HD22	2.00	0.43
2:B:28:ARG:CG	2:B:28:ARG:HH11	2.32	0.43
8:H:25:GLU:CB	8:H:34:ARG:NH2	2.67	0.43
3:C:197:LEU:HA	3:C:197:LEU:HD23	1.66	0.43
1:A:352:SER:OG	6:S:110:LYS:HB2	2.18	0.43
4:Q:211:MET:HG3	20:Q:3006:PEE:H48	2.00	0.43
2:B:52:LYS:HZ3	2:B:232:LEU:HD11	1.82	0.43
3:P:378:LYS:HE3	6:S:17:ARG:NE	2.34	0.43
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.19	0.43
2:B:46:ARG:HG2	2:B:110:GLU:HG2	2.00	0.43
2:O:46:ARG:O	2:O:47:ILE:HD13	2.19	0.43
3:P:227:LYS:HE3	22:P:4009:GOL:O1	2.18	0.43
1:A:364:ALA:HB2	9:I:33:ALA:HB1	2.01	0.43
3:P:80:ARG:C	3:P:80:ARG:HD3	2.39	0.43
7:T:30:PHE:O	7:T:34:ILE:HG12	2.18	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
9:V:62:ARG:HB3	9:V:63:PRO:HD2	2.01	0.43
5:E:191:ASP:CG	5:E:191:ASP:O	2.56	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
3:P:191:ALA:HA	3:P:194:MET:CE	2.48	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
4:D:239:PRO:O	4:D:241:LYS:HE2	2.19	0.43
3:C:100:ARG:CZ	14:C:502:HEM:HBD1	2.49	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
5:R:17:GLU:H	5:R:17:GLU:CD	2.17	0.42
5:E:113:GLU:HG3	5:E:115:SER:OG	2.19	0.42
2:B:213:HIS:N	2:B:214:PRO:CD	2.81	0.42
3:C:97:HIS:CD2	14: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
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
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:40:TRP:HB3	1:N:384:LEU:HD11	2.00	0.42
3:C:270:PRO:HD2	3:C:275:LEU:HD23	2.01	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
3:C:193:ALA:O	3:C:196:HIS:HB3	2.19	0.42
1:N:8:LEU:HD22	1:N:392:LEU:HB3	2.01	0.42
4:D:31:GLN:O	4:D:35:GLN:HG2	2.19	0.42
3:P:193:ALA:O	3:P:196:HIS:HB3	2.19	0.42
1:N:8:LEU:O	1:N:11:VAL:HG23	2.19	0.42
2:O:95:LYS:HE2	9:V:32:ALA:N	2.35	0.42
4:Q:43:MET:CE	4:Q:189:PHE:CZ	3.02	0.42
1:A:195:MET:HE2	1:A:195:MET:HB3	1.91	0.42
1:A:289:HIS:CE1	11:S:2012:BHG:H1'2	2.52	0.42
3:P:276:PHE:CG	3:P:277:ALA:N	2.87	0.42
5:E:43:THR:O	5:E:47:VAL:HG23	2.20	0.42
5:E:10:PHE:HB3	7:G:18:LEU:HD11	2.02	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
7:G:28:HIS:ND1	7:G:32:LYS:HD2	2.34	0.42
3:C:217:LYS:HG3	7:G:7:LEU:HD13	2.02	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
5:E:15:ARG:NH2	12:G:4001:AZI:N1	2.68	0.42
5:R:85:LYS:NZ	5:R:87:MET:SD	2.72	0.42
5:E:117:LEU:HD13	5:E:170:ARG:HD2	2.01	0.42
4:D:231:LYS:HA	4:D:231:LYS:HD3	1.89	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
2:O:241:GLY:HA2	2:O:423:SER:OG	2.20	0.42
1:N:131:ARG:NH1	1:N:174:VAL:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:12:LYS:HE2	3:P:16:ASN:HB2	2.02	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
2:B:353:SER:HB3	2:B:355:PRO:HG2	2.01	0.42
5:R:78:LEU:HB2	5:R:191:ASP:HB2	2.02	0.42
3:P:345:HIS:HE1	7:T:65:GLU:OE2	2.02	0.42
1:A:281:ASP:C	1:A:281:ASP:OD1	2.59	0.42
8:H:28:GLU:CA	8:H:31:VAL:HG22	2.47	0.42
3:C:311:LYS:HG2	3:C:374:ASN:CG	2.41	0.42
3:P:215:VAL:HG13	23:P:4193:HOH:O	2.18	0.42
3:C:234:LEU:HD12	19:D:2003:CDL:H712	2.01	0.42
3:P:233:LEU:HD11	4:Q:219:VAL:HG21	2.01	0.42
3:P:18:PHE:CD2	3:P:19:ILE:HD13	2.55	0.42
6:F:102:LYS:HD3	6:F:102:LYS:HA	1.83	0.42
2:B:204:MET:HE1	2:B:224:LEU:HD22	2.01	0.42
1:A:1:THR:CG2	2:B:212:SER:HB3	2.34	0.41
3:P:326:TRP:NE1	7:T:48:VAL:HG22	2.35	0.41
3:P:224:TYR:HB3	22:P:4009:GOL:H31	2.02	0.41
2:B:364:LEU:HG	2:B:402:ILE:HD13	2.00	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
9:I:52:ARG:NH1	23:I:859:HOH:O	2.54	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
1:N:146:ARG:NH2	1:N:308:GLN:HE22	2.17	0.41
1:N:11:VAL:HA	1:N:12:PRO:HD3	1.92	0.41
2:O:257:LEU:O	2:O:323:GLY:HA3	2.21	0.41
8:H:31:VAL:HA	8:H:34:ARG:HH11	1.84	0.41
5:R:70:ALA:C	5:R:71:MET:HE2	2.40	0.41
5:E:189:SER:C	5:E:190:ASP:OD1	2.59	0.41
3:P:30:TRP:CZ3	20:P:3007:PEE:H21	2.55	0.41
3:P:96:MET:HE2	20:P:3007:PEE:H27	2.03	0.41
1:N:39:VAL:CG1	1:N:195:MET:HE2	2.51	0.41
3:C:277:ALA:HB1	3:C:294:LEU:HD12	2.02	0.41
23:N:4088:HOH:O	9:V:39:GLU:CG	2.69	0.41
3:C:278:TYR:CZ	3:C:282:ARG:HD3	2.56	0.41
4:Q:215:LEU:HD21	5:R:46:GLY:HA3	2.02	0.41
4:D:229:VAL:CG2	7:G:20:PRO:HD3	2.50	0.41
1:A:280:TYR:HA	1:A:284:TYR:CE2	2.55	0.41
6:F:99:ARG:NH2	23:F:4055:HOH:O	2.53	0.41
5:R:44:THR:CG2	10:W:24:ILE:HG21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:95:PRO:HG2	5:R:145:VAL:HG22	2.02	0.41
2:B:28:ARG:HG2	2:B:28:ARG:HH11	1.86	0.41
2:O:411:ILE:O	2:O:415:LYS:HG3	2.20	0.41
6:F:19:TRP:CD2	11:F:4003:BHG:H1'2	2.56	0.41
1:N:108:LYS:O	1:N:112:LEU:HG	2.21	0.41
2:B:46:ARG:HD2	2:B:375:SER:CB	2.50	0.41
1:A:1:THR:HG22	2:B:39:GLU:OE1	2.20	0.41
8:U:31:VAL:HG23	8:U:32:LYS:N	2.35	0.41
15:Q:501:HEC:HMB1	15:Q:501:HEC:HBB3	2.02	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
2:O:236:LYS:CD	2:O:236:LYS:H	2.32	0.41
2:B:152:LEU:HD13	2:B:158:HIS:CE1	2.55	0.41
1:A:46:ARG:HG2	1:A:231:LEU:HD22	2.03	0.41
5:R:52:LYS:NZ	10:W:32:GLU:OE2	2.48	0.41
1:N:332:ASP:OD1	1:N:432:PRO:HG3	2.21	0.41
4:Q:117:VAL:O	13:Q:4012:PO4:O2	2.38	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
3:P:206:ASN:HB3	14:P:502:HEM:O2D	2.20	0.41
1:A:332:ASP:OD1	1:A:432:PRO:HG3	2.21	0.41
1:A:366:VAL:HG23	1:A:367:SER:N	2.35	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
2:O:37:SER:HA	2:O:208:GLY:O	2.21	0.40
4:D:74:PRO:CA	4:D:80:MET:HE2	2.51	0.40
3:P:326:TRP:CH2	20:P:3007:PEE:H51	2.57	0.40
3:P:32:ASN:O	3:P:36:LEU:HG	2.22	0.40
9:I:72:VAL:HG13	9:I:73:PRO:HD2	2.03	0.40
3:P:197:LEU:HD23	3:P:197:LEU:HA	1.73	0.40
7:T:72:LYS:HE2	7:T:72:LYS:HB2	1.97	0.40
7:T:50:PRO:HB2	7:T:51:PRO:HD3	2.02	0.40
4:D:65:ALA:O	4:D:68:VAL:HG22	2.21	0.40
1:A:255:ILE:O	1:A:321:GLY:HA3	2.22	0.40
3:P:71:ARG:HD3	23:P:4196:HOH:O	2.22	0.40
1:N:9:GLN:HE22	1:N:393:ALA:HB1	1.87	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
1:A:2:ALA:HB1	1:A:6:GLN:CB	2.48	0.40
1:N:366:VAL:HG23	1:N:367:SER:N	2.37	0.40
4:Q:79:GLU:HG2	4:Q:79:GLU:H	1.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:120:MET:HE2	2:O:120:MET:HB2	1.92	0.40
1:N:307:PHE:CD1	1:N:307:PHE:C	2.94	0.40
4:Q:33:TYR:CD1	4:Q:37:CYS:HB2	2.56	0.40
2:O:300:ALA:C	2:O:302:GLY:H	2.25	0.40
1:N:144:SER:O	1:N:148:VAL:HG23	2.20	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
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
3:P:132:VAL:HA	3:P:139:SER:HB3	2.03	0.40
7:T:38:LEU:O	7:T:42:ARG:HG3	2.22	0.40
3:P:111:GLU:CD	3:P:111:GLU:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	34	30
1	N	441/446 (99%)	425 (96%)	14 (3%)	2 (0%)	34	30
2	B	418/439 (95%)	406 (97%)	11 (3%)	1 (0%)	52	53
2	O	420/439 (96%)	404 (96%)	11 (3%)	5 (1%)	16	10
3	C	363/379 (96%)	353 (97%)	8 (2%)	2 (1%)	30	24
3	P	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	14	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%)	34	30
5	R	193/196 (98%)	183 (95%)	8 (4%)	2 (1%)	19	13

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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%)	14	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%)	7	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%)	26	21

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%)	65	70
1	N	363/370 (98%)	355 (98%)	8 (2%)	60	64
2	B	332/343 (97%)	330 (99%)	2 (1%)	90	94
2	O	332/343 (97%)	329 (99%)	3 (1%)	84	89
3	C	313/327 (96%)	307 (98%)	6 (2%)	65	70
3	P	317/327 (97%)	311 (98%)	6 (2%)	65	70
4	D	206/206 (100%)	203 (98%)	3 (2%)	72	78
4	Q	206/206 (100%)	202 (98%)	4 (2%)	65	70
5	E	168/168 (100%)	167 (99%)	1 (1%)	90	94
5	R	168/168 (100%)	165 (98%)	3 (2%)	66	72
6	F	90/98 (92%)	89 (99%)	1 (1%)	80	85
6	S	90/98 (92%)	88 (98%)	2 (2%)	60	64
7	G	66/71 (93%)	64 (97%)	2 (3%)	48	51
7	T	66/71 (93%)	63 (96%)	3 (4%)	34	32
8	H	63/74 (85%)	61 (97%)	2 (3%)	46	48
8	U	63/74 (85%)	63 (100%)	0	100	100
9	I	28/60 (47%)	27 (96%)	1 (4%)	42	43
9	V	28/60 (47%)	26 (93%)	2 (7%)	18	14
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%)	68	74

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
13	PO4	A	2010	-	4,4,4	0.86	0	6,6,6	0.89	0
12	AZI	A	4002	-	0,2,2	0.00	-	0,1,1	0.00	-
11	BHG	A	4004	-	18,18,18	1.32	3 (16%)	23,23,23	0.63	0
13	PO4	B	3009	-	4,4,4	0.84	0	6,6,6	0.89	0
20	PEE	B	4017	-	4,7,50	0.49	0	4,7,55	0.39	0
17	SMA	C	2001	-	35,38,38	1.71	5 (14%)	40,52,52	1.67	4 (10%)
18	UQ	C	2002	-	18,18,63	2.31	10 (55%)	20,24,79	0.59	0
19	CDL	C	2004	-	43,43,99	1.12	1 (2%)	45,55,111	1.27	4 (8%)
12	AZI	C	2005	-	0,2,2	0.00	-	0,1,1	0.00	-
20	PEE	C	2007	-	48,48,50	1.06	4 (8%)	49,53,55	0.83	4 (8%)
22	GOL	C	2008	-	5,5,5	1.24	0	5,5,5	0.71	0
11	BHG	C	2011	-	18,18,18	1.78	5 (27%)	23,23,23	0.73	0
22	GOL	C	4008	-	5,5,5	1.19	0	5,5,5	0.59	0
14	HEM	C	501	3	30,50,50	2.97	13 (43%)	24,82,82	2.30	9 (37%)
14	HEM	C	502	3	30,50,50	2.82	13 (43%)	24,82,82	2.45	10 (41%)
19	CDL	D	2003	-	38,38,99	1.01	1 (2%)	41,47,111	1.04	2 (4%)
20	PEE	D	2006	-	50,50,50	1.22	6 (12%)	51,55,55	0.83	4 (7%)
13	PO4	D	4010	-	4,4,4	0.85	0	6,6,6	0.89	0
13	PO4	D	4011	-	4,4,4	0.81	0	6,6,6	0.89	0
15	HEC	D	501	4	24,50,50	1.96	4 (16%)	19,82,82	2.60	3 (15%)
22	GOL	E	4006	-	5,5,5	1.27	0	5,5,5	0.68	0
22	GOL	E	4007	-	4,4,5	1.45	1 (25%)	2,4,5	1.13	0
16	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	BHG	F	3012	-	18,18,18	1.82	5 (27%)	23,23,23	0.75	0
11	BHG	F	4003	-	18,18,18	1.79	4 (22%)	23,23,23	0.73	0
12	AZI	G	4001	-	0,2,2	0.00	-	0,1,1	0.00	-
13	PO4	I	4015	-	4,4,4	0.84	0	6,6,6	0.89	0
13	PO4	O	2009	-	4,4,4	0.86	0	6,6,6	0.89	0
22	GOL	O	4005	-	5,5,5	1.25	0	5,5,5	0.67	0
17	SMA	P	3001	-	35,38,38	1.71	5 (14%)	40,52,52	1.58	3 (7%)
18	UQ	P	3002	-	18,18,63	2.14	9 (50%)	20,24,79	0.52	0
19	CDL	P	3004	-	48,48,99	1.11	4 (8%)	50,60,111	1.15	4 (8%)
12	AZI	P	3005	-	0,2,2	0.00	-	0,1,1	0.00	-
20	PEE	P	3007	-	48,48,50	1.09	4 (8%)	49,53,55	0.84	4 (8%)
22	GOL	P	3008	-	5,5,5	1.19	0	5,5,5	0.57	0
13	PO4	P	3010	-	4,4,4	0.81	0	6,6,6	0.89	0
11	BHG	P	3011	-	18,18,18	1.77	4 (22%)	23,23,23	0.77	1 (4%)
22	GOL	P	4009	-	5,5,5	1.03	0	5,5,5	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEM	P	501	3	30,50,50	2.82	10 (33%)	24,82,82	2.22	9 (37%)
14	HEM	P	502	3	30,50,50	2.82	12 (40%)	24,82,82	2.38	8 (33%)
19	CDL	Q	3003	-	38,38,99	1.04	2 (5%)	41,47,111	1.01	2 (4%)
20	PEE	Q	3006	-	50,50,50	1.20	6 (12%)	51,55,55	0.83	4 (7%)
13	PO4	Q	4012	-	4,4,4	0.95	0	6,6,6	0.89	0
15	HEC	Q	501	4	24,50,50	1.88	4 (16%)	19,82,82	2.63	3 (15%)
13	PO4	R	4013	-	4,4,4	0.90	0	6,6,6	0.89	0
13	PO4	R	4014	-	4,4,4	0.87	0	6,6,6	0.89	0
16	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	BHG	S	2012	-	18,18,18	1.82	4 (22%)	23,23,23	0.72	0
13	PO4	T	4016	-	4,4,4	0.81	0	6,6,6	0.89	0

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
13	PO4	A	2010	-	-	0/0/0/0	0/0/0/0
12	AZI	A	4002	-	-	0/0/0/0	0/0/0/0
11	BHG	A	4004	-	1/1/5/5	0/9/29/29	0/1/1/1
13	PO4	B	3009	-	-	0/0/0/0	0/0/0/0
20	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
12	AZI	C	2005	-	-	0/0/0/0	0/0/0/0
20	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
22	GOL	C	2008	-	-	0/4/4/4	0/0/0/0
11	BHG	C	2011	-	1/1/5/5	0/9/29/29	0/1/1/1
22	GOL	C	4008	-	-	0/4/4/4	0/0/0/0
14	HEM	C	501	3	-	0/10/54/54	0/0/8/8
14	HEM	C	502	3	-	0/10/54/54	0/0/8/8
19	CDL	D	2003	-	-	0/43/43/110	0/0/0/0
20	PEE	D	2006	-	-	0/54/54/54	0/0/0/0
13	PO4	D	4010	-	-	0/0/0/0	0/0/0/0
13	PO4	D	4011	-	-	0/0/0/0	0/0/0/0
15	HEC	D	501	4	-	0/6/54/54	0/0/8/8
22	GOL	E	4006	-	-	0/4/4/4	0/0/0/0
22	GOL	E	4007	-	-	0/2/2/4	0/0/0/0
16	FES	E	501	5	-	0/0/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BHG	F	3012	-	1/1/5/5	0/9/29/29	0/1/1/1
11	BHG	F	4003	-	1/1/5/5	0/9/29/29	0/1/1/1
12	AZI	G	4001	-	-	0/0/0/0	0/0/0/0
13	PO4	I	4015	-	-	0/0/0/0	0/0/0/0
13	PO4	O	2009	-	-	0/0/0/0	0/0/0/0
22	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
12	AZI	P	3005	-	-	0/0/0/0	0/0/0/0
20	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
22	GOL	P	3008	-	-	0/4/4/4	0/0/0/0
13	PO4	P	3010	-	-	0/0/0/0	0/0/0/0
11	BHG	P	3011	-	1/1/5/5	0/9/29/29	0/1/1/1
22	GOL	P	4009	-	-	0/4/4/4	0/0/0/0
14	HEM	P	501	3	-	0/10/54/54	0/0/8/8
14	HEM	P	502	3	-	0/10/54/54	0/0/8/8
19	CDL	Q	3003	-	-	0/43/43/110	0/0/0/0
20	PEE	Q	3006	-	-	0/54/54/54	0/0/0/0
13	PO4	Q	4012	-	-	0/0/0/0	0/0/0/0
15	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
13	PO4	R	4013	-	-	0/0/0/0	0/0/0/0
13	PO4	R	4014	-	-	0/0/0/0	0/0/0/0
16	FES	R	501	5	-	0/0/4/4	0/1/1/1
11	BHG	S	2012	-	1/1/5/5	0/9/29/29	0/1/1/1
13	PO4	T	4016	-	-	0/0/0/0	0/0/0/0

All (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	502	HEM	C3B-C4B	-8.11	1.44	1.51
14	C	501	HEM	C3B-C4B	-7.49	1.45	1.51
14	P	501	HEM	C3B-C4B	-7.44	1.45	1.51
14	C	501	HEM	C2D-C3D	-6.71	1.34	1.54
15	D	501	HEC	C3B-C2B	-6.39	1.34	1.40
14	C	502	HEM	C3B-C4B	-6.28	1.46	1.51
14	C	502	HEM	C2D-C3D	-6.20	1.35	1.54
14	P	501	HEM	C3C-CAC	-6.08	1.39	1.51
14	C	501	HEM	C3C-CAC	-6.06	1.40	1.51
14	P	501	HEM	C3D-C4D	-5.77	1.44	1.51
14	P	501	HEM	C2D-C3D	-5.45	1.38	1.54
14	P	502	HEM	C3C-CAC	-5.41	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	502	HEM	C3C-CAC	-5.30	1.41	1.51
15	Q	501	HEC	C3B-C2B	-5.19	1.35	1.40
15	D	501	HEC	C3C-C2C	-4.98	1.35	1.40
14	P	501	HEM	C3B-CAB	-4.96	1.42	1.51
14	P	502	HEM	C3B-CAB	-4.74	1.42	1.51
14	P	502	HEM	C3D-C4D	-4.52	1.45	1.51
14	C	502	HEM	C3D-C4D	-4.50	1.45	1.51
14	C	502	HEM	C3B-CAB	-4.44	1.43	1.51
14	C	501	HEM	C3B-CAB	-4.16	1.43	1.51
14	P	502	HEM	C2D-C3D	-4.14	1.42	1.54
14	C	501	HEM	C2C-C1C	-3.97	1.45	1.52
14	P	502	HEM	C2C-C1C	-3.74	1.45	1.52
15	Q	501	HEC	C3C-C2C	-3.64	1.36	1.40
14	C	502	HEM	C2C-C1C	-3.22	1.46	1.52
14	P	501	HEM	C2D-C1D	-3.18	1.41	1.51
20	P	3007	PEE	C22-C21	-3.02	1.34	1.51
14	P	501	HEM	C2C-C1C	-3.00	1.46	1.52
20	C	2007	PEE	C22-C21	-2.94	1.34	1.51
20	Q	3006	PEE	C19-C18	-2.94	1.34	1.51
20	C	2007	PEE	C19-C18	-2.91	1.34	1.51
20	D	2006	PEE	C19-C18	-2.90	1.34	1.51
20	D	2006	PEE	C22-C21	-2.87	1.34	1.51
14	C	501	HEM	C3D-C4D	-2.87	1.47	1.51
20	P	3007	PEE	C19-C18	-2.87	1.34	1.51
20	Q	3006	PEE	C22-C21	-2.84	1.35	1.51
14	P	502	HEM	C2D-C1D	-2.80	1.42	1.51
14	C	502	HEM	C2D-C1D	-2.62	1.43	1.51
14	C	502	HEM	C2B-C1B	-2.54	1.43	1.51
19	C	2004	CDL	OA8-CA6	-2.30	1.40	1.45
14	P	502	HEM	C2B-C1B	-2.27	1.44	1.51
19	P	3004	CDL	OA8-CA6	-2.25	1.40	1.45
14	P	501	HEM	C2B-C1B	-2.21	1.44	1.51
19	Q	3003	CDL	OB8-CB6	-2.17	1.40	1.45
14	C	501	HEM	C2B-C1B	-2.03	1.45	1.51
19	P	3004	CDL	OB8-CB6	-2.01	1.40	1.45
14	C	501	HEM	CAD-C3D	-2.01	1.50	1.54
19	P	3004	CDL	CA3-CA4	2.01	1.56	1.50
17	C	2001	SMA	C6-C7	2.05	1.42	1.38
17	C	2001	SMA	C7-C8	2.06	1.43	1.40
20	D	2006	PEE	C3-C2	2.06	1.56	1.50
11	C	2011	BHG	C1-C2	2.06	1.58	1.52
11	C	2011	BHG	O5-C5	2.06	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	2002	UQ	C7-C8	2.08	1.54	1.49
11	P	3011	BHG	C1-C2	2.10	1.58	1.52
11	F	4003	BHG	O5-C5	2.10	1.49	1.44
11	F	3012	BHG	C1-C2	2.12	1.58	1.52
18	P	3002	UQ	C5-C4	2.16	1.55	1.47
22	E	4007	GOL	C1-C2	2.21	1.56	1.50
19	P	3004	CDL	O1-C1	2.22	1.50	1.43
11	F	3012	BHG	C4-C5	2.22	1.57	1.53
18	C	2002	UQ	C3-C4	2.22	1.55	1.48
15	D	501	HEC	C3B-C4B	2.23	1.47	1.42
11	S	2012	BHG	O5-C5	2.24	1.49	1.44
19	D	2003	CDL	O1-C1	2.24	1.50	1.43
14	P	502	HEM	CHD-C4C	2.24	1.41	1.36
17	P	3001	SMA	C6-C7	2.25	1.42	1.38
19	Q	3003	CDL	O1-C1	2.25	1.50	1.43
20	Q	3006	PEE	C3-C2	2.30	1.57	1.50
20	P	3007	PEE	P-O1P	2.31	1.59	1.51
20	C	2007	PEE	O3-C30	2.32	1.40	1.33
18	C	2002	UQ	C5-C4	2.34	1.56	1.47
11	F	3012	BHG	O5-C5	2.35	1.50	1.44
15	D	501	HEC	C3C-C4C	2.38	1.48	1.42
18	P	3002	UQ	C3-C4	2.38	1.55	1.48
14	C	502	HEM	CHC-C1C	2.39	1.42	1.36
11	S	2012	BHG	C4-C5	2.40	1.58	1.53
11	F	4003	BHG	C4-C5	2.42	1.58	1.53
11	A	4004	BHG	O5-C1	2.43	1.48	1.41
11	P	3011	BHG	C4-C5	2.44	1.58	1.53
20	C	2007	PEE	P-O1P	2.48	1.60	1.51
18	P	3002	UQ	C6-C5	2.54	1.41	1.35
20	Q	3006	PEE	O2-C10	2.57	1.42	1.34
11	C	2011	BHG	C4-C5	2.58	1.58	1.53
20	Q	3006	PEE	P-O1P	2.61	1.60	1.51
18	P	3002	UQ	O3-C3	2.62	1.43	1.37
20	D	2006	PEE	O2-C10	2.65	1.42	1.34
14	C	501	HEM	C1C-NC	2.68	1.39	1.36
18	C	2002	UQ	CM5-C5	2.73	1.56	1.50
20	D	2006	PEE	O3-C30	2.77	1.41	1.33
18	C	2002	UQ	O3-C3	2.79	1.44	1.37
15	Q	501	HEC	C4C-NC	2.80	1.40	1.36
11	A	4004	BHG	O1-C1	2.80	1.45	1.40
11	A	4004	BHG	C4-C5	2.80	1.59	1.53
18	P	3002	UQ	CM5-C5	2.81	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	2002	UQ	C6-C5	2.82	1.41	1.35
18	P	3002	UQ	C2-C1	2.86	1.57	1.48
20	D	2006	PEE	P-O1P	2.89	1.61	1.51
20	Q	3006	PEE	O3-C30	2.91	1.42	1.33
17	P	3001	SMA	C7-C8	2.92	1.44	1.40
20	P	3007	PEE	O3-C30	2.96	1.42	1.33
18	P	3002	UQ	O2-C2	2.97	1.44	1.37
11	P	3011	BHG	O5-C1	3.02	1.49	1.41
17	P	3001	SMA	C4-C3	3.11	1.50	1.41
18	C	2002	UQ	O2-C2	3.16	1.45	1.37
14	C	502	HEM	CBC-CAC	3.17	1.47	1.29
11	C	2011	BHG	O5-C1	3.19	1.50	1.41
14	C	501	HEM	CBC-CAC	3.24	1.48	1.29
18	C	2002	UQ	C2-C1	3.24	1.58	1.48
14	P	501	HEM	CBB-CAB	3.25	1.48	1.29
11	F	4003	BHG	O5-C1	3.36	1.50	1.41
14	C	502	HEM	CBB-CAB	3.36	1.48	1.29
14	C	501	HEM	CMA-C3A	3.37	1.58	1.51
11	S	2012	BHG	O5-C1	3.48	1.50	1.41
11	F	3012	BHG	O5-C1	3.50	1.50	1.41
18	P	3002	UQ	C6-C1	3.54	1.56	1.46
18	P	3002	UQ	C7-C6	3.54	1.57	1.51
18	C	2002	UQ	C6-C1	3.54	1.56	1.46
14	P	502	HEM	CBB-CAB	3.55	1.49	1.29
14	C	502	HEM	C1C-NC	3.63	1.40	1.36
17	C	2001	SMA	C4-C3	3.65	1.51	1.41
17	C	2001	SMA	O1-C2	3.76	1.39	1.35
14	P	502	HEM	CBC-CAC	3.84	1.51	1.29
14	C	501	HEM	CBB-CAB	3.92	1.51	1.29
14	P	501	HEM	CBC-CAC	4.02	1.52	1.29
15	Q	501	HEC	C4A-NA	4.02	1.42	1.36
14	P	502	HEM	C1C-NC	4.15	1.41	1.36
14	C	502	HEM	C4C-NC	4.19	1.41	1.36
18	C	2002	UQ	C7-C6	4.19	1.59	1.51
17	P	3001	SMA	O1-C2	4.27	1.40	1.35
11	F	4003	BHG	O1-C1	4.47	1.48	1.40
11	C	2011	BHG	O1-C1	4.50	1.48	1.40
11	P	3011	BHG	O1-C1	4.55	1.48	1.40
11	F	3012	BHG	O1-C1	4.56	1.48	1.40
11	S	2012	BHG	O1-C1	4.58	1.48	1.40
14	C	501	HEM	C4C-NC	4.78	1.41	1.36
17	P	3001	SMA	C4-C4A	6.29	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	2001	SMA	C4-C4A	6.90	1.50	1.41

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	501	HEC	CBB-CAB-C3B	-8.02	109.52	127.35
15	D	501	HEC	CBC-CAC-C3C	-7.92	109.75	127.35
15	D	501	HEC	CBB-CAB-C3B	-7.03	111.72	127.35
15	Q	501	HEC	CBC-CAC-C3C	-6.92	111.97	127.35
17	P	3001	SMA	C9-C10-C11	-4.82	109.07	114.75
17	C	2001	SMA	C3-C4-C4A	-4.69	114.85	121.35
17	C	2001	SMA	C9-C10-C11	-4.59	109.35	114.75
17	P	3001	SMA	C3-C4-C4A	-4.58	115.01	121.35
19	C	2004	CDL	CA4-OA6-CA5	-4.21	109.98	117.92
19	P	3004	CDL	CA4-OA6-CA5	-3.60	111.14	117.92
19	C	2004	CDL	CB4-OB6-CB5	-3.40	109.72	117.89
15	Q	501	HEC	CBD-CAD-C3D	-2.95	107.23	112.53
19	D	2003	CDL	CB6-CB4-CB3	-2.94	105.20	112.07
19	P	3004	CDL	CB4-OB6-CB5	-2.90	110.93	117.89
19	P	3004	CDL	CA6-OA8-CA7	-2.83	109.98	117.14
19	Q	3003	CDL	CB4-OB6-CB5	-2.82	111.12	117.89
19	Q	3003	CDL	CB6-CB4-CB3	-2.73	105.69	112.07
14	C	502	HEM	CBA-CAA-C2A	-2.72	107.66	112.53
19	D	2003	CDL	CB4-OB6-CB5	-2.69	111.43	117.89
14	P	501	HEM	CAA-C2A-C1A	-2.60	124.18	127.01
19	C	2004	CDL	CA6-CA4-CA3	-2.59	106.01	112.07
14	C	501	HEM	CBA-CAA-C2A	-2.58	107.90	112.53
14	C	502	HEM	CBD-CAD-C3D	-2.58	106.04	113.55
14	C	502	HEM	CAA-C2A-C1A	-2.51	124.28	127.01
14	C	501	HEM	CAA-C2A-C1A	-2.49	124.31	127.01
14	P	502	HEM	CBD-CAD-C3D	-2.46	106.39	113.55
19	C	2004	CDL	CA6-OA8-CA7	-2.42	111.03	117.14
15	D	501	HEC	CBD-CAD-C3D	-2.21	108.56	112.53
19	P	3004	CDL	CB6-CB4-CB3	-2.13	107.09	112.07
17	C	2001	SMA	O8-C8-C8A	2.09	123.52	119.78
14	P	501	HEM	CMD-C2D-C3D	2.17	123.93	114.35
14	C	502	HEM	C3B-CAB-CBB	2.20	127.83	124.46
20	Q	3006	PEE	C23-C22-C21	2.22	126.02	114.53
20	D	2006	PEE	C23-C22-C21	2.23	126.06	114.53
14	P	502	HEM	CBA-CAA-C2A	2.28	116.61	112.53
11	P	3011	BHG	O1-C1-C2	2.28	110.92	108.04
20	P	3007	PEE	C23-C22-C21	2.31	126.47	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	501	HEM	C3C-CAC-CBC	2.33	128.03	124.46
20	C	2007	PEE	C23-C22-C21	2.35	126.68	114.53
20	P	3007	PEE	C22-C21-C20	2.36	126.72	114.53
20	C	2007	PEE	C22-C21-C20	2.37	126.74	114.53
20	Q	3006	PEE	C19-C18-C17	2.42	127.05	114.53
20	D	2006	PEE	C22-C21-C20	2.44	127.12	114.53
20	Q	3006	PEE	C22-C21-C20	2.44	127.14	114.53
20	P	3007	PEE	C19-C18-C17	2.48	127.32	114.53
20	C	2007	PEE	C19-C18-C17	2.49	127.41	114.53
20	D	2006	PEE	C19-C18-C17	2.51	127.48	114.53
14	P	501	HEM	CMA-C3A-C2A	2.58	130.62	125.24
14	P	501	HEM	C2D-C3D-C4D	2.64	105.98	101.50
20	D	2006	PEE	C20-C19-C18	2.72	128.60	114.53
20	Q	3006	PEE	C20-C19-C18	2.75	128.72	114.53
14	P	502	HEM	C2D-C3D-C4D	2.81	106.26	101.50
20	C	2007	PEE	C20-C19-C18	2.82	129.07	114.53
20	P	3007	PEE	C20-C19-C18	2.85	129.27	114.53
14	C	501	HEM	CMD-C2D-C3D	3.03	127.73	114.35
14	C	501	HEM	C3C-CAC-CBC	3.05	129.13	124.46
14	C	502	HEM	CMD-C2D-C3D	3.07	127.93	114.35
14	C	502	HEM	C2D-C3D-C4D	3.20	106.93	101.50
14	P	502	HEM	CMD-C2D-C3D	3.23	128.66	114.35
14	C	502	HEM	CAD-C3D-C4D	3.49	124.78	112.47
14	P	502	HEM	CAD-C3D-C4D	3.54	124.96	112.47
14	C	501	HEM	CMC-C2C-C3C	3.84	126.12	116.53
14	C	501	HEM	C2D-C3D-C4D	3.90	108.11	101.50
14	P	501	HEM	CMC-C2C-C3C	4.02	126.57	116.53
14	C	501	HEM	CAD-C3D-C4D	4.09	126.90	112.47
14	C	501	HEM	CAD-C3D-C2D	4.09	124.98	113.22
14	P	501	HEM	CAD-C3D-C2D	4.30	125.57	113.22
14	P	501	HEM	CAD-C3D-C4D	4.50	128.36	112.47
14	P	501	HEM	CMB-C2B-C3B	4.61	128.04	116.53
14	P	502	HEM	CMB-C2B-C3B	4.80	128.52	116.53
14	C	501	HEM	CMB-C2B-C3B	4.99	128.98	116.53
14	C	502	HEM	CAD-C3D-C2D	5.09	127.85	113.22
14	C	502	HEM	CMC-C2C-C3C	5.11	129.29	116.53
14	P	502	HEM	CMC-C2C-C3C	5.12	129.32	116.53
14	C	502	HEM	CMB-C2B-C3B	5.26	129.67	116.53
14	P	502	HEM	CAD-C3D-C2D	5.38	128.67	113.22
17	P	3001	SMA	C9-C2-C3	5.73	128.12	120.56
17	C	2001	SMA	C9-C2-C3	6.88	129.63	120.56

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	C	2011	BHG	C4
11	P	3011	BHG	C4
11	F	3012	BHG	C4
11	S	2012	BHG	C4
11	F	4003	BHG	C4
11	A	4004	BHG	C4

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	BHG	1	0
20	B	4017	PEE	1	0
17	C	2001	SMA	3	0
18	C	2002	UQ	4	0
14	C	501	HEM	1	0
14	C	502	HEM	4	0
19	D	2003	CDL	1	0
20	D	2006	PEE	2	0
15	D	501	HEC	4	0
11	F	3012	BHG	3	0
11	F	4003	BHG	1	0
12	G	4001	AZI	1	0
13	I	4015	PO4	1	0
17	P	3001	SMA	3	0
18	P	3002	UQ	5	0
20	P	3007	PEE	3	0
22	P	4009	GOL	2	0
14	P	501	HEM	1	0
14	P	502	HEM	2	0
20	Q	3006	PEE	5	0
13	Q	4012	PO4	1	0
15	Q	501	HEC	5	0
11	S	2012	BHG	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.14	15 (3%) 49 58	24, 37, 59, 111	1 (0%)
1	N	442/446 (99%)	0.55	30 (6%) 20 28	31, 50, 77, 132	1 (0%)
2	B	424/439 (96%)	0.26	16 (3%) 44 53	28, 41, 66, 102	0
2	O	424/439 (96%)	0.55	42 (9%) 9 13	31, 48, 87, 185	0
3	C	365/379 (96%)	0.41	24 (6%) 22 29	24, 34, 48, 108	0
3	P	370/379 (97%)	0.53	27 (7%) 18 24	28, 37, 52, 218	0
4	D	241/241 (100%)	0.48	18 (7%) 17 23	29, 39, 61, 78	0
4	Q	241/241 (100%)	0.65	26 (10%) 8 10	31, 45, 67, 87	0
5	E	196/196 (100%)	1.18	45 (22%) 1 1	32, 57, 105, 117	0
5	R	196/196 (100%)	0.36	15 (7%) 16 22	27, 46, 71, 99	0
6	F	99/110 (90%)	0.43	10 (10%) 9 12	24, 39, 71, 83	0
6	S	99/110 (90%)	0.32	6 (6%) 25 33	28, 40, 67, 88	0
7	G	75/81 (92%)	1.00	14 (18%) 2 2	26, 49, 77, 86	0
7	T	76/81 (93%)	1.61	24 (31%) 1 1	32, 55, 98, 114	0
8	H	66/78 (84%)	1.16	16 (24%) 1 1	40, 56, 73, 78	0
8	U	66/78 (84%)	1.25	17 (25%) 1 1	44, 63, 94, 104	0
9	I	42/78 (53%)	2.30	22 (52%) 0 0	33, 62, 90, 93	0
9	V	42/78 (53%)	2.17	19 (45%) 0 0	36, 78, 94, 100	0
10	J	30/62 (48%)	0.88	4 (13%) 4 6	40, 52, 80, 109	0
10	W	62/62 (100%)	2.19	21 (33%) 0 1	41, 64, 92, 123	0
All	All	3998/4220 (94%)	0.59	411 (10%) 9 12	24, 43, 80, 218	2 (0%)

All (411) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	13	ILE	22.9
10	W	1	VAL	22.3
10	W	62	LYS	13.0
10	W	2	ALA	11.1
2	O	12	GLU	10.9
7	T	76	ALA	10.8
9	I	50	LEU	10.6
7	T	1	GLY	9.8
3	P	18	PHE	9.7
3	P	11	MET	9.4
2	O	19	PRO	9.2
5	E	112	VAL	9.0
4	Q	241	LYS	8.6
1	A	2	ALA	8.6
9	I	49	VAL	8.6
1	N	222	THR	8.5
10	W	12	LEU	8.4
2	B	233	SER	8.3
9	V	50	LEU	8.2
3	C	17	ALA	8.0
1	N	1	THR	7.7
2	B	230	LEU	7.6
1	N	227	ALA	7.4
10	J	62	LYS	7.2
5	E	115	SER	7.1
2	B	231	GLY	7.0
3	P	12	LYS	7.0
2	O	228	GLY	6.9
1	A	222	THR	6.9
8	U	50	THR	6.8
1	A	225	GLU	6.6
2	B	232	LEU	6.4
2	B	20	HIS	6.3
1	A	1	THR	6.2
3	P	16	ASN	6.1
7	G	30	PHE	6.0
1	N	2	ALA	6.0
4	Q	1	SER	5.9
1	A	227	ALA	5.9
7	T	34	ILE	5.7
5	R	189	SER	5.7
3	P	14	VAL	5.7
5	E	114	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	226	ASP	5.6
8	U	47	ARG	5.6
9	V	38	SER	5.6
2	O	218	GLN	5.5
7	T	30	PHE	5.5
7	T	32	LYS	5.5
9	I	78	TYR	5.5
3	P	17	ALA	5.4
1	N	229	PRO	5.3
5	E	196	GLY	5.3
10	W	5	LEU	5.3
6	S	12	TRP	5.2
3	P	10	LEU	5.2
5	E	124	LEU	5.2
5	E	194	ILE	5.1
1	N	206	ARG	5.1
1	N	228	VAL	5.1
10	W	3	PRO	5.0
3	C	18	PHE	5.0
5	E	117	LEU	5.0
4	Q	76	GLU	4.9
8	H	34	ARG	4.9
7	T	31	SER	4.9
8	U	48	SER	4.9
4	D	81	PHE	4.8
4	D	241	LYS	4.8
3	C	16	ASN	4.8
7	T	73	ASN	4.8
5	R	191	ASP	4.8
9	V	49	VAL	4.7
9	I	51	CYS	4.7
2	O	232	LEU	4.7
5	E	116	GLN	4.6
2	B	12	GLU	4.6
1	N	230	THR	4.6
9	V	52	ARG	4.6
10	J	61	ASN	4.5
2	O	17	VAL	4.4
1	N	225	GLU	4.4
5	E	111	ALA	4.4
2	O	20	HIS	4.4
5	E	108	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
8	U	44	VAL	4.4
7	T	61	TRP	4.4
8	U	49	GLN	4.4
10	W	8	ARG	4.4
2	B	304	HIS	4.3
4	Q	158	ILE	4.3
5	E	80	ASP	4.3
10	W	13	LEU	4.3
2	O	41	TYR	4.3
5	E	35	PHE	4.2
5	E	5	ILE	4.2
5	E	188	THR	4.2
7	T	29	TYR	4.2
3	C	27	ILE	4.2
10	W	9	LEU	4.2
3	C	218	ILE	4.2
5	E	191	ASP	4.2
5	E	186	GLU	4.1
2	O	230	LEU	4.1
5	E	113	GLU	4.1
10	W	30	PHE	4.1
1	A	4	TYR	4.1
9	V	61	GLY	4.1
2	O	229	GLY	4.0
9	V	42	VAL	4.0
2	B	229	GLY	4.0
4	Q	146	GLY	3.9
5	E	185	TYR	3.9
8	U	45	SER	3.9
7	G	29	TYR	3.9
10	W	61	ASN	3.9
1	N	15	GLN	3.9
8	H	46	SER	3.9
9	V	78	TYR	3.9
5	R	74	ILE	3.9
4	D	73	GLY	3.9
5	R	71	MET	3.9
6	F	13	LEU	3.8
5	E	107	ASP	3.8
1	N	193	PRO	3.8
5	E	27	GLU	3.8
4	Q	139	THR	3.7

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Mol	Chain	Res	Type	RSRZ
5	E	127	VAL	3.7
2	O	221	GLU	3.7
2	B	41	TYR	3.7
9	I	42	VAL	3.7
4	D	79	GLU	3.7
1	A	224	ASP	3.7
2	O	215	VAL	3.7
8	U	51	GLU	3.6
1	N	226	ASP	3.6
4	Q	227	TRP	3.6
5	E	128	LYS	3.6
5	E	187	PHE	3.6
5	R	76	ILE	3.6
6	S	70	MET	3.6
4	Q	157	ALA	3.6
4	Q	77	ASP	3.6
10	W	25	VAL	3.6
3	P	27	ILE	3.6
9	I	62	ARG	3.6
3	P	218	ILE	3.5
8	H	44	VAL	3.5
7	G	42	ARG	3.5
5	E	190	ASP	3.5
4	Q	141	VAL	3.5
7	G	34	ILE	3.5
3	C	23	ALA	3.5
8	U	39	LEU	3.4
2	O	18	PRO	3.4
2	O	233	SER	3.4
2	O	439	LEU	3.4
5	R	190	ASP	3.4
1	N	209	LEU	3.4
4	D	230	LEU	3.4
3	P	223	TYR	3.4
5	E	184	SER	3.4
4	Q	145	GLU	3.4
8	H	31	VAL	3.4
6	F	110	LYS	3.4
5	R	23	LYS	3.4
9	I	52	ARG	3.4
8	H	42	GLU	3.4
4	D	141	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	15	ASN	3.3
9	I	48	SER	3.3
1	A	262	TRP	3.3
3	C	211	ILE	3.3
1	N	443	TRP	3.3
1	N	22	GLY	3.2
5	E	122	HIS	3.2
8	H	41	ASP	3.2
4	D	80	MET	3.2
1	A	228	VAL	3.2
9	I	73	PRO	3.2
9	I	55	LEU	3.2
6	S	15	GLY	3.2
3	C	31	TRP	3.2
7	T	75	ALA	3.2
7	T	28	HIS	3.2
2	O	25	GLU	3.1
4	D	72	ASP	3.1
9	V	51	CYS	3.1
3	C	25	SER	3.1
8	H	45	SER	3.1
5	E	49	TYR	3.1
4	D	85	GLY	3.1
9	I	63	PRO	3.1
4	D	145	GLU	3.1
2	O	217	LYS	3.1
9	V	32	ALA	3.1
5	E	110	ALA	3.1
2	O	355	PRO	3.1
3	C	209	THR	3.0
4	Q	148	TYR	3.0
4	Q	229	VAL	3.0
6	F	108	ALA	3.0
9	V	37	THR	3.0
1	N	224	ASP	3.0
4	Q	79	GLU	3.0
1	N	16	VAL	3.0
2	O	224	LEU	3.0
5	R	75	GLU	3.0
9	I	37	THR	2.9
1	N	51	LYS	2.9
4	D	229	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
4	Q	230	LEU	2.9
10	W	29	LEU	2.9
5	E	84	GLY	2.9
4	Q	147	LEU	2.9
3	P	26	ASN	2.9
5	E	79	SER	2.9
5	E	103	LYS	2.9
3	P	224	TYR	2.9
10	W	19	THR	2.9
8	U	42	GLU	2.9
8	U	13	LEU	2.9
9	I	70	LEU	2.9
3	C	155	TYR	2.9
2	O	26	PHE	2.8
5	E	89	PHE	2.8
7	T	42	ARG	2.8
5	E	53	ASN	2.8
9	I	58	GLN	2.8
4	Q	167	GLU	2.8
2	B	250	ASP	2.8
9	I	71	ASN	2.8
4	D	116	ILE	2.8
2	O	405	VAL	2.8
4	Q	143	LEU	2.8
1	N	13	GLU	2.8
4	Q	144	ARG	2.8
4	Q	149	PHE	2.8
1	N	219	LEU	2.8
9	V	41	PRO	2.7
3	C	224	TYR	2.7
10	W	20	PHE	2.7
9	V	40	SER	2.7
2	B	235	ALA	2.7
5	R	12	ASP	2.7
1	N	176	LYS	2.7
7	G	75	ALA	2.7
8	U	43	ARG	2.7
3	P	320	LEU	2.7
8	H	51	GLU	2.7
1	N	5	ALA	2.7
2	O	22	GLN	2.7
9	I	60	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
10	W	21	ALA	2.7
7	T	17	SER	2.7
9	V	48	SER	2.7
2	O	304	HIS	2.7
3	P	15	ASN	2.7
2	O	392	TYR	2.7
5	E	134	ILE	2.6
2	O	303	VAL	2.6
3	P	31	TRP	2.6
7	G	31	SER	2.6
7	G	56	TYR	2.6
2	O	226	ILE	2.6
2	O	27	THR	2.6
4	D	103	ALA	2.6
9	V	33	ALA	2.6
7	T	35	PRO	2.6
8	H	49	GLN	2.6
8	U	46	SER	2.6
7	G	60	THR	2.6
7	T	2	ARG	2.6
1	A	20	ASP	2.6
5	R	80	ASP	2.6
9	I	32	ALA	2.6
3	P	227	LYS	2.6
7	T	74	PRO	2.6
7	G	58	VAL	2.6
4	D	117	VAL	2.5
4	Q	142	SER	2.5
2	B	227	ARG	2.5
3	P	25	SER	2.5
2	O	223	PHE	2.5
3	P	345	HIS	2.5
6	S	69	SER	2.5
1	A	365	LEU	2.5
2	O	33	LEU	2.5
5	E	38	LEU	2.5
7	T	64	GLN	2.5
6	F	66	LEU	2.4
7	G	64	GLN	2.4
1	N	241	ILE	2.4
3	P	155	TYR	2.4
2	O	351	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	O	126	VAL	2.4
7	T	43	ALA	2.4
8	H	22	GLU	2.4
8	H	29	LYS	2.4
9	V	77	ARG	2.4
8	U	67	HIS	2.4
2	O	29	LEU	2.4
3	P	168	PHE	2.4
7	T	38	LEU	2.4
8	H	48	SER	2.4
8	U	31	VAL	2.4
2	O	406	ALA	2.4
10	W	24	ILE	2.4
6	F	106	GLU	2.4
9	I	64	LEU	2.4
10	J	37	GLN	2.4
1	N	17	SER	2.4
5	R	79	SER	2.4
1	A	184	GLU	2.4
3	P	43	LEU	2.4
6	F	107	TRP	2.4
8	H	37	LEU	2.4
3	C	207	ASN	2.4
2	O	264	ILE	2.3
2	B	439	LEU	2.3
8	H	67	HIS	2.3
1	N	20	ASP	2.3
9	V	63	PRO	2.3
10	W	28	ALA	2.3
5	E	195	VAL	2.3
1	N	397	SER	2.3
5	E	71	MET	2.3
4	Q	171	PHE	2.3
7	T	33	GLY	2.3
9	I	61	GLY	2.3
2	O	219	VAL	2.3
5	E	193	VAL	2.3
1	A	229	PRO	2.3
3	P	23	ALA	2.3
1	N	18	GLN	2.3
8	U	41	ASP	2.3
5	R	16	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
7	T	60	THR	2.3
5	E	167	ALA	2.3
5	E	78	LEU	2.3
3	C	98	VAL	2.2
2	O	349	GLN	2.2
8	U	26	GLN	2.2
2	O	23	ASP	2.2
6	F	22	ASN	2.2
4	Q	233	ARG	2.2
7	T	56	TYR	2.2
3	C	210	GLY	2.2
1	N	421	ALA	2.2
4	D	99	GLU	2.2
5	R	27	GLU	2.2
2	O	24	LEU	2.2
6	F	70	MET	2.2
9	I	69	SER	2.2
1	N	216	PHE	2.2
5	E	153	PHE	2.2
7	G	68	LYS	2.2
10	W	10	TYR	2.2
3	C	101	GLY	2.2
7	T	37	VAL	2.2
2	O	35	ILE	2.2
9	V	36	ALA	2.2
4	Q	136	GLU	2.2
3	C	102	LEU	2.2
6	F	19	TRP	2.2
3	P	28	SER	2.2
5	E	192	MET	2.1
3	C	198	LEU	2.1
7	G	38	LEU	2.1
2	O	350	GLY	2.1
7	G	71	ARG	2.1
5	E	75	GLU	2.1
8	U	28	GLU	2.1
9	V	62	ARG	2.1
2	O	407	ASP	2.1
3	C	106	SER	2.1
2	B	400	GLN	2.1
3	C	24	PRO	2.1
3	P	208	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	104	TYR	2.1
4	D	115	TYR	2.1
7	G	6	HIS	2.1
5	E	132	TRP	2.1
8	H	35	GLU	2.1
2	B	301	LYS	2.1
3	C	217	LYS	2.1
3	C	94	LEU	2.1
8	H	47	ARG	2.1
10	W	16	ARG	2.1
6	S	13	LEU	2.1
4	Q	240	PRO	2.1
9	I	41	PRO	2.1
4	Q	75	ASN	2.1
5	E	92	ARG	2.0
5	R	19	LEU	2.0
3	P	29	SER	2.0
5	R	98	VAL	2.0
2	O	28	ARG	2.0
3	P	40	CYS	2.0
6	F	71	ARG	2.0
7	T	18	LEU	2.0
10	W	11	SER	2.0
2	B	267	ALA	2.0
9	V	59	ALA	2.0
4	D	144	ARG	2.0
6	S	71	ARG	2.0
9	I	77	ARG	2.0
4	D	170	GLU	2.0
10	J	60	GLU	2.0
1	A	210	ASP	2.0
1	N	239	SER	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
21	UNL	B	4026	1/-	0.72	1.34	58.28	92,92,92,92	0
21	UNL	B	4080	1/-	0.61	0.68	33.08	67,67,67,67	0
21	UNL	U	4056	1/-	0.23	1.01	25.14	101,101,101,101	0
21	UNL	B	4057	1/-	0.77	0.85	22.33	57,57,57,57	0
21	UNL	O	4084	1/-	0.84	0.68	22.30	67,67,67,67	0
11	BHG	F	3012	18/18	0.17	0.72	20.32	159,162,164,164	0
21	UNL	A	4032	1/-	0.84	0.72	18.56	65,65,65,65	0
21	UNL	B	4079	1/-	0.80	0.43	16.03	66,66,66,66	0
11	BHG	S	2012	18/18	0.37	0.45	15.23	89,103,106,107	0
11	BHG	C	2011	18/18	0.60	0.48	13.89	106,118,123,125	0
22	GOL	O	4005	6/6	0.24	0.75	10.63	166,167,167,168	0
22	GOL	P	3008	6/6	0.89	0.50	10.45	83,84,85,88	0
12	AZI	P	3005	3/3	0.77	0.35	10.09	54,54,59,63	0
11	BHG	P	3011	18/18	0.56	0.41	8.49	99,107,109,109	0
12	AZI	A	4002	3/3	0.71	0.48	7.95	48,48,58,65	0
13	PO4	R	4013	5/5	0.78	0.25	7.24	114,114,116,116	0
12	AZI	C	2005	3/3	0.80	0.35	7.12	41,41,55,60	0
21	UNL	U	4049	1/-	0.64	0.69	5.77	77,77,77,77	0
22	GOL	C	2008	6/6	0.88	0.31	5.51	60,63,63,70	0
20	PEE	B	4017	8/51	0.67	0.42	5.12	85,88,91,92	0
21	UNL	P	4074	1/-	0.78	0.17	4.69	59,59,59,59	0
21	UNL	O	4037	1/-	0.73	0.82	4.58	62,62,62,62	0
21	UNL	B	4034	1/-	0.48	0.70	3.91	87,87,87,87	0
13	PO4	D	4011	5/5	0.79	0.31	3.58	130,130,130,131	0
20	PEE	D	2006	51/51	0.77	0.32	3.53	85,98,115,118	0
22	GOL	E	4006	6/6	0.83	0.24	2.86	67,71,72,75	0
13	PO4	A	2010	5/5	0.61	0.23	2.58	133,133,134,134	0
20	PEE	P	3007	49/51	0.92	0.23	2.12	35,58,75,76	0
20	PEE	Q	3006	51/51	0.91	0.20	2.10	53,65,110,110	0
13	PO4	Q	4012	5/5	0.87	0.18	1.92	108,109,110,110	0
20	PEE	C	2007	49/51	0.93	0.23	1.86	33,58,74,74	0
21	UNL	O	4043	1/-	0.84	0.29	1.55	80,80,80,80	0
18	UQ	C	2002	18/63	0.65	0.30	1.43	61,73,76,76	0
19	CDL	C	2004	44/100	0.91	0.21	1.31	54,83,104,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
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	1.11	25,33,44,46	0
13	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	BHG	A	4004	18/18	0.96	0.13	0.37	29,36,42,44	0
12	AZI	G	4001	3/3	0.92	0.15	0.13	47,47,57,59	0
14	HEM	P	501	43/43	0.98	0.15	0.13	22,26,33,40	0
22	GOL	P	4009	6/6	0.95	0.23	0.13	67,70,71,72	0
15	HEC	D	501	43/43	0.97	0.13	0.13	26,33,37,38	0
14	HEM	C	502	43/43	0.98	0.16	0.08	23,26,33,36	0
16	FES	E	501	4/4	0.99	0.13	0.04	38,39,40,40	0
22	GOL	C	4008	6/6	0.95	0.20	-0.01	53,55,60,60	0
14	HEM	C	501	43/43	0.98	0.12	-0.37	21,27,34,38	0
15	HEC	Q	501	43/43	0.98	0.11	-0.60	29,36,41,45	0
14	HEM	P	502	43/43	0.99	0.11	-0.72	23,27,37,39	0
16	FES	R	501	4/4	0.99	0.12	-0.87	27,29,30,30	0
21	UNL	D	4062	1/-	0.85	0.27	-	90,90,90,90	0
13	PO4	D	4010	5/5	0.66	0.29	-	169,169,170,170	0
21	UNL	A	4087	1/-	0.86	0.33	-	60,60,60,60	0
21	UNL	B	4052	1/-	0.85	0.18	-	60,60,60,60	0
21	UNL	D	4054	1/-	0.72	0.27	-	76,76,76,76	0
21	UNL	V	4024	1/-	0.58	1.07	-	96,96,96,96	0
21	UNL	G	4064	1/-	0.88	0.52	-	56,56,56,56	0
13	PO4	T	4016	5/5	0.93	0.09	-	107,108,108,108	0
21	UNL	A	4076	1/-	0.69	0.44	-	68,68,68,68	0
13	PO4	P	3010	5/5	0.83	0.18	-	115,115,115,116	0
21	UNL	B	4030	1/-	0.82	0.45	-	70,70,70,70	0
21	UNL	C	4018	2/-	0.91	0.35	-	74,74,74,76	0
21	UNL	B	4051	1/-	0.85	0.23	-	78,78,78,78	0
21	UNL	W	4077	1/-	0.86	0.14	-	60,60,60,60	0
21	UNL	P	4040	1/-	0.58	0.30	-	73,73,73,73	0
21	UNL	A	4081	1/-	0.70	0.47	-	71,71,71,71	0
21	UNL	Q	4044	1/-	0.65	1.64	-	88,88,88,88	0
21	UNL	A	4048	1/-	0.75	0.38	-	72,72,72,72	0
21	UNL	N	4029	1/-	0.72	1.40	-	94,94,94,94	0
21	UNL	T	4066	1/-	0.88	0.07	-	70,70,70,70	0
21	UNL	C	4063	1/-	0.96	1.03	-	74,74,74,74	0
21	UNL	S	4047	1/-	0.52	0.38	-	71,71,71,71	0
21	UNL	P	4060	1/-	0.32	0.34	-	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	UNL	C	4068	1/-	0.55	0.58	-	72,72,72,72	0
21	UNL	A	4085	1/-	0.88	0.18	-	56,56,56,56	0
21	UNL	P	4089	1/-	0.91	0.47	-	63,63,63,63	0
21	UNL	O	4020	2/-	0.61	0.23	-	96,96,96,97	0
13	PO4	O	2009	5/5	0.97	0.10	-	76,79,81,81	0
21	UNL	O	4031	1/-	0.82	0.46	-	86,86,86,86	0
21	UNL	P	4058	1/-	0.84	0.34	-	61,61,61,61	0
21	UNL	O	4041	1/-	0.88	0.36	-	71,71,71,71	0
21	UNL	A	4038	1/-	0.72	0.60	-	85,85,85,85	0
22	GOL	E	4007	5/6	0.58	0.51	-	97,100,101,102	0
21	UNL	N	4073	1/-	0.79	0.17	-	69,69,69,69	0
21	UNL	A	4091	1/-	0.75	0.75	-	72,72,72,72	0
21	UNL	F	4028	1/-	0.84	0.58	-	82,82,82,82	0
21	UNL	R	4055	1/-	0.73	0.14	-	73,73,73,73	0
21	UNL	C	4045	1/-	0.79	0.41	-	71,71,71,71	0
21	UNL	E	4050	1/-	0.89	0.38	-	65,65,65,65	0
21	UNL	P	4046	1/-	0.91	0.48	-	65,65,65,65	0
13	PO4	R	4014	5/5	0.75	0.43	-	173,174,174,174	0
21	UNL	D	4067	1/-	0.84	0.58	-	58,58,58,58	0
21	UNL	G	4053	1/-	0.79	0.23	-	77,77,77,77	0
21	UNL	D	4027	1/-	0.74	0.29	-	87,87,87,87	0
21	UNL	A	4035	1/-	0.80	0.99	-	69,69,69,69	0
21	UNL	I	4072	1/-	0.39	2.22	-	93,93,93,93	0
21	UNL	R	4069	1/-	0.94	0.41	-	62,62,62,62	0
21	UNL	N	4022	1/-	0.63	0.50	-	81,81,81,81	0
21	UNL	D	4083	1/-	0.77	0.54	-	82,82,82,82	0
21	UNL	P	4021	2/-	0.80	0.18	-	71,71,71,73	0
11	BHG	F	4003	18/18	0.38	0.66	-	176,180,181,181	0
21	UNL	V	4090	1/-	0.92	0.98	-	74,74,74,74	0
21	UNL	D	4036	1/-	0.44	0.34	-	83,83,83,83	0
21	UNL	V	4088	1/-	0.68	0.92	-	80,80,80,80	0
21	UNL	B	4025	1/-	0.64	1.82	-	93,93,93,93	0
21	UNL	E	4061	1/-	0.60	0.19	-	79,79,79,79	0
21	UNL	T	4065	1/-	0.84	0.73	-	66,66,66,66	0
21	UNL	B	4042	1/-	0.80	0.42	-	81,81,81,81	0
21	UNL	I	4033	1/-	0.86	0.87	-	69,69,69,69	0
21	UNL	D	4059	1/-	0.75	0.90	-	57,57,57,57	0
13	PO4	B	3009	5/5	0.89	0.17	-	97,99,100,101	0
21	UNL	O	4082	1/-	0.82	0.14	-	73,73,73,73	0
21	UNL	C	4023	1/-	0.83	0.52	-	55,55,55,55	0
21	UNL	G	4070	1/-	0.62	0.26	-	67,67,67,67	0
21	UNL	C	4086	1/-	0.93	0.25	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	UNL	O	4071	1/-	0.67	0.87	-	70,70,70,70	0
21	UNL	B	4039	1/-	0.87	0.31	-	73,73,73,73	0
21	UNL	N	4019	2/-	0.77	0.30	-	76,76,76,76	0
21	UNL	A	4075	1/-	0.94	0.89	-	64,64,64,64	0
21	UNL	V	4078	1/-	0.85	1.63	-	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.