



Full wwPDB X-ray Structure Validation Report

Oct 21, 2014 – 08:06 PM EDT

PDB ID : 1PP9
Title : Bovine cytochrome bc1 complex with stigmatellin bound
Authors : Huang, L.S.; Cobessi, D.; Tung, E.Y.; Berry, E.A.
Deposited on : 2003-06-16
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

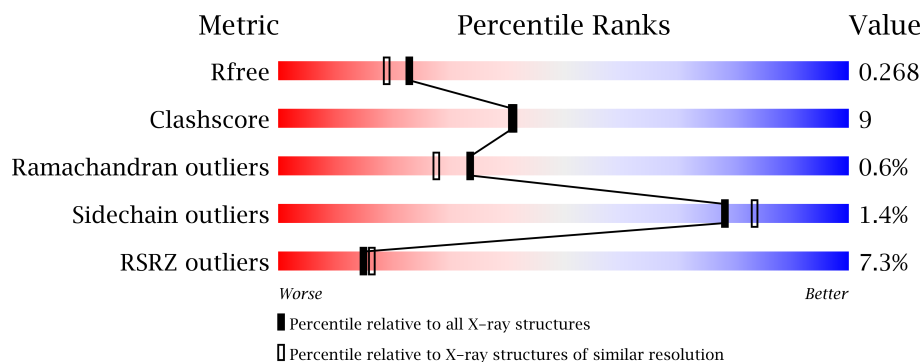
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance

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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	446	
1	N	446	
2	B	439	
2	O	439	
3	C	379	
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	

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Mol	Chain	Length	Quality of chain
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 that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
11	BHG	A	4002	-	X
11	BHG	C	2008	-	X
11	BHG	F	3011	-	X
11	BHG	F	4001	-	X
11	BHG	P	3008	-	X
11	BHG	S	2011	-	X
12	PO4	B	3010	-	X
13	AZI	A	4005	-	X
13	AZI	C	2014	-	X
13	AZI	D	4004	-	X
13	AZI	P	3014	X	X
18	UQ	P	3002	-	X
19	CDL	G	2003	-	X
19	CDL	G	2004	-	X
20	PEE	A	4003	-	X
20	PEE	C	2007	-	X
20	PEE	C	2012	-	X
20	PEE	D	2006	-	X
20	PEE	G	2005	-	X
20	PEE	Q	3006	-	X
20	PEE	T	3005	-	X
21	GOL	B	2013	-	X
21	GOL	C	2009	-	X
21	GOL	O	3013	-	X
21	GOL	P	3009	-	X

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 33959 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			3403	2121	602	660	20			
1	N	443	Total	C	N	O	S	10	0	1
			3403	2121	602	660	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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	365	Total	C	N	O	S	0	0	0
			2892	1940	450	485	17			
3	P	370	Total	C	N	O	S	0	0	0
			2931	1968	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
			1519	957	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			

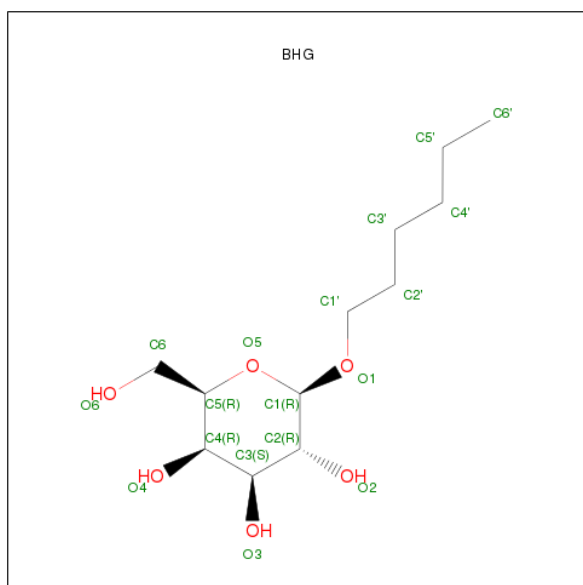
- Molecule 9 is a protein called Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial.

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.

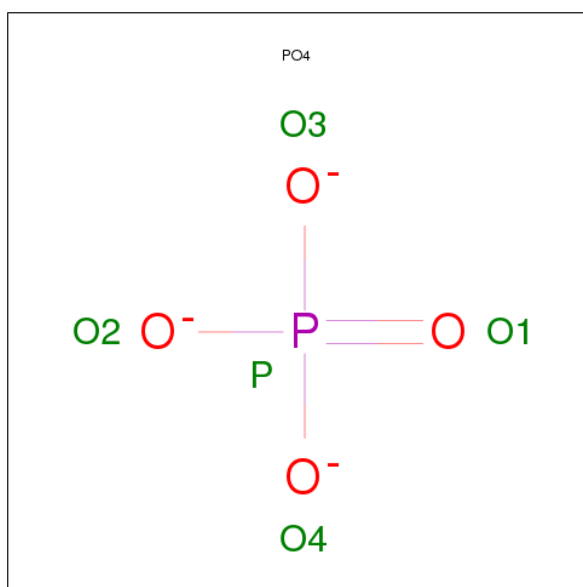
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	62	Total	C	N	O	0	0	0
			507	333	88	86			
10	W	62	Total	C	N	O	0	0	0
			507	333	88	86			

- Molecule 11 is SUGAR (2-HEXYLOXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-3,4,5-TRIOL) (three-letter code: BHG) (formula: C₁₂H₂₄O₆).



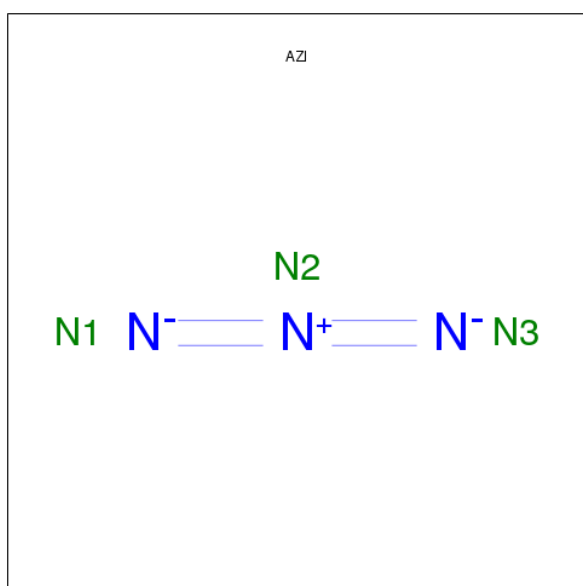
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			18	12	6		
11	S	1	Total	C	O	0	0
			18	12	6		
11	P	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	F	1	Total	C	O	0	0
			18	12	6		
11	A	1	Total	C	O	0	0
			18	12	6		

- Molecule 12 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	O	1	Total	O	P	0	0
			5	4	1		
12	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 13 is AZIDE ION (three-letter code: AZI) (formula: N_3).



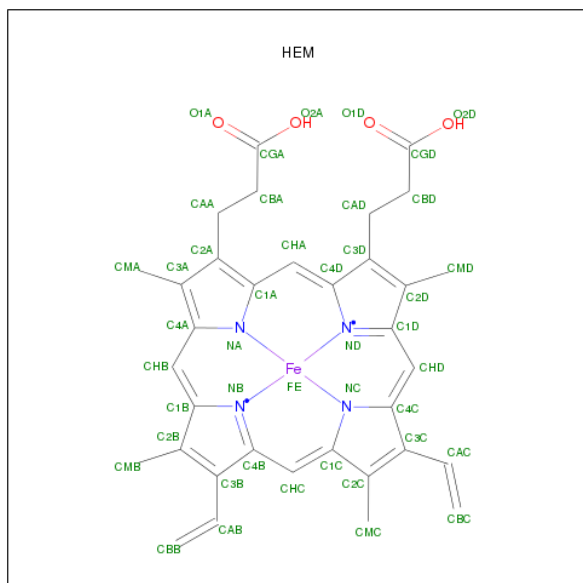
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total	N	0	0
			3	3		
13	P	1	Total	N	0	0
			3	3		

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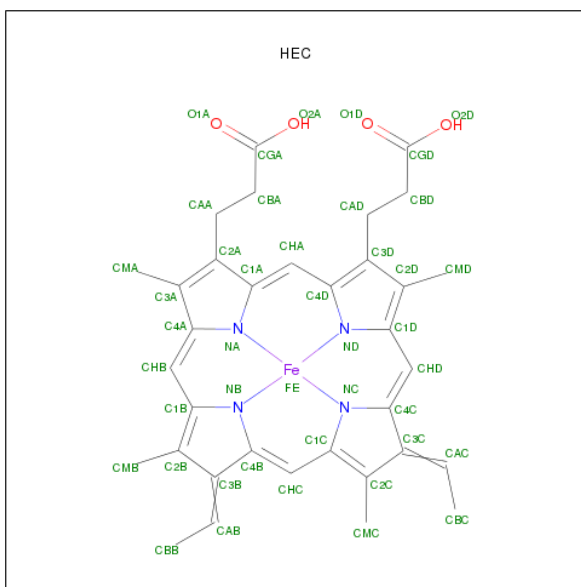
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	D	1	Total N 3 3	0	0
13	A	1	Total N 3 3	0	0

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



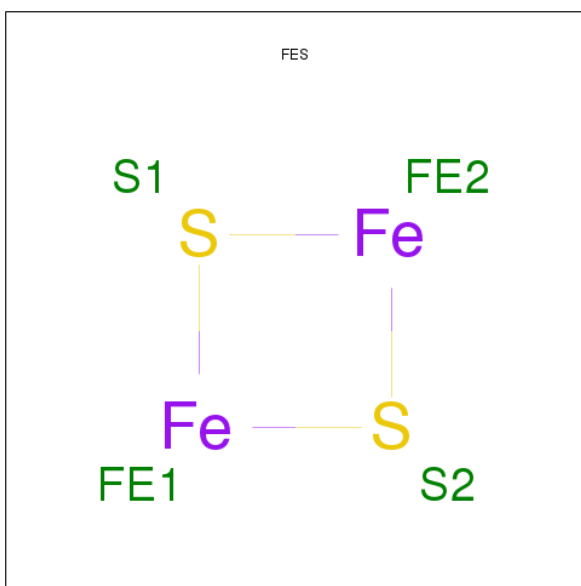
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
14	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



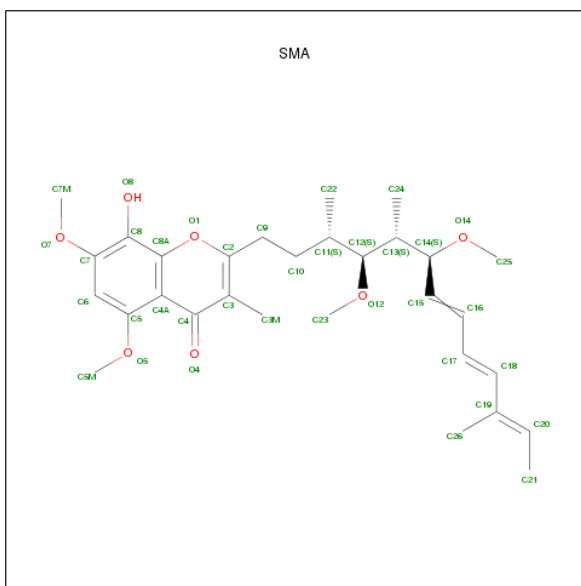
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



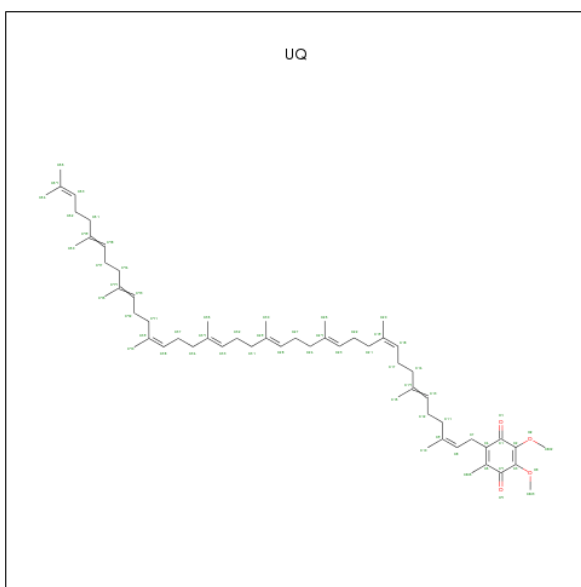
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	E	1	Total	Fe	S	0	0
			4	2	2		
16	R	1	Total	Fe	S	0	0
			4	2	2		

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



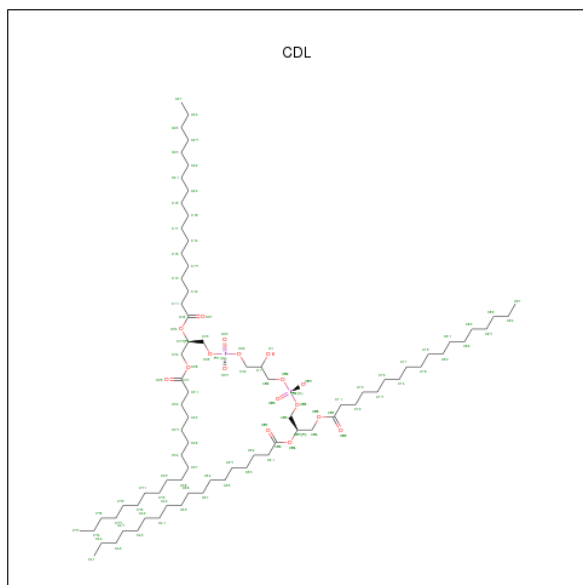
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total	C	O	0	0
			37	30	7		
17	P	1	Total	C	O	0	0
			37	30	7		

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



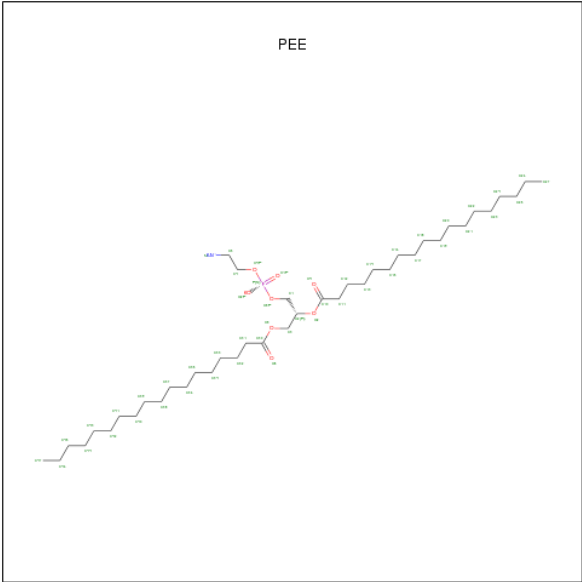
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	C	1	Total	C	O	0	0
			14	10	4		
18	P	1	Total	C	O	0	0
			14	10	4		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	G	1	Total	C	O	P	0	0
			50	31	17	2		
19	G	1	Total	C	O	P	0	0
			44	25	17	2		
19	Q	1	Total	C	O	P	0	0
			50	31	17	2		
19	T	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	G	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
20	D	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
20	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
20	C	1	Total	O	P			0	0
			5	4	1				
20	T	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
20	Q	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
20	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
20	N	1	Total	O	P			0	0
			5	4	1				
20	A	1	Total	C	O			0	0
			6	3	3				

- Molecule 21 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 22 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	187	Total	O	0	0
			187	187		
22	B	149	Total	O	0	0
			149	149		
22	C	125	Total	O	0	0
			125	125		
22	D	118	Total	O	0	0
			118	118		
22	E	54	Total	O	0	0
			54	54		
22	F	57	Total	O	0	0
			57	57		
22	G	24	Total	O	0	0
			24	24		
22	H	14	Total	O	0	0
			14	14		

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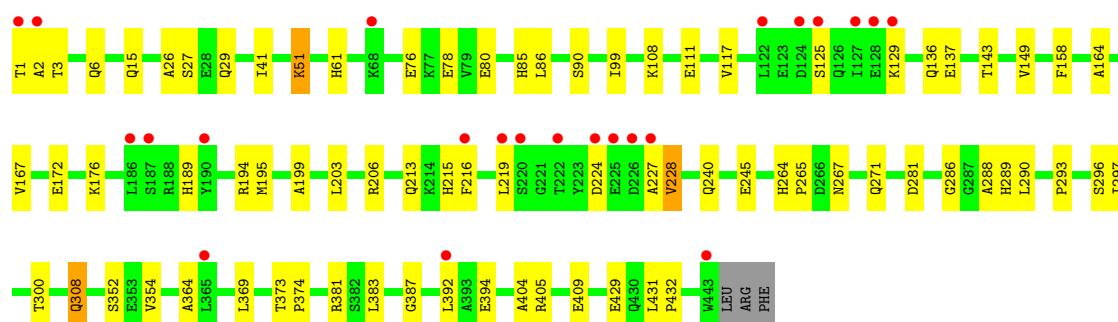
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	I	16	Total 16	O 16	0	0
22	J	5	Total 5	O 5	0	0
22	N	134	Total 134	O 134	0	0
22	O	130	Total 130	O 130	0	0
22	P	122	Total 122	O 122	0	0
22	Q	109	Total 109	O 109	0	0
22	R	64	Total 64	O 64	0	0
22	S	73	Total 73	O 73	0	0
22	T	21	Total 21	O 21	0	0
22	U	16	Total 16	O 16	0	0
22	V	10	Total 10	O 10	0	0
22	W	9	Total 9	O 9	0	0

3 Residue-property plots

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

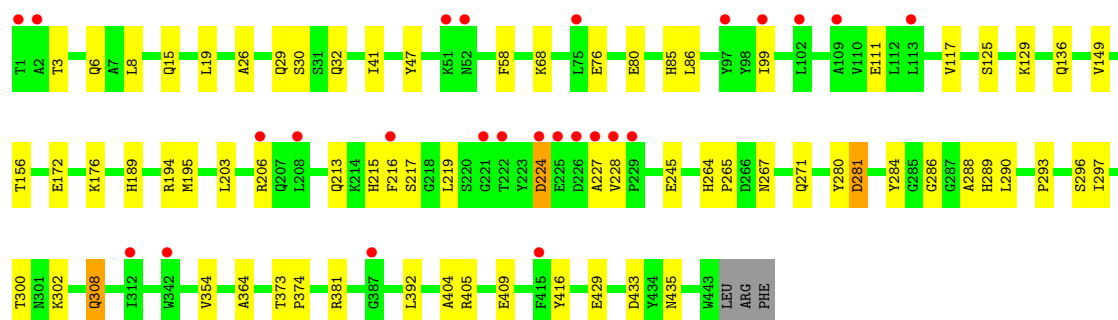
- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

Chain A: 



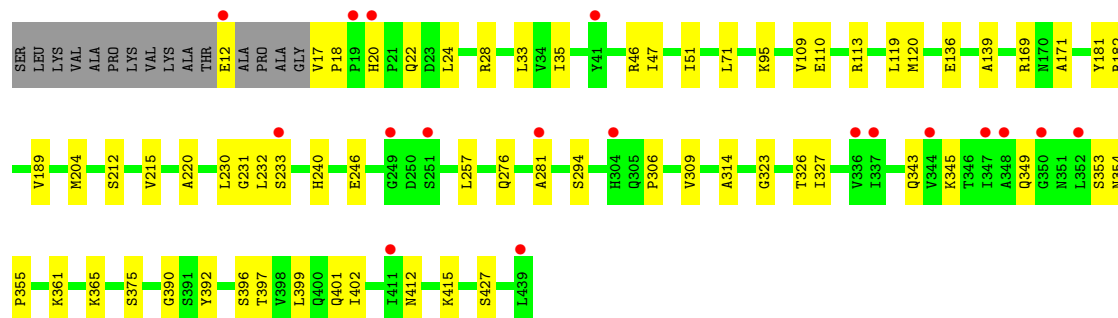
- Molecule 1: Ubiquinol-cytochrome C reductase complex core protein I, mitochondrial

Chain N: 



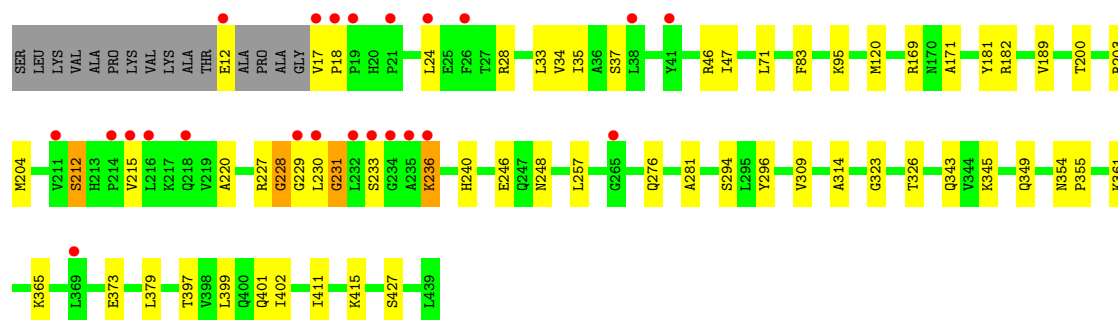
- Molecule 2: Ubiquinol-cytochrome C reductase complex core protein 2, mitochondrial

Chain B: 



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

Chain O:



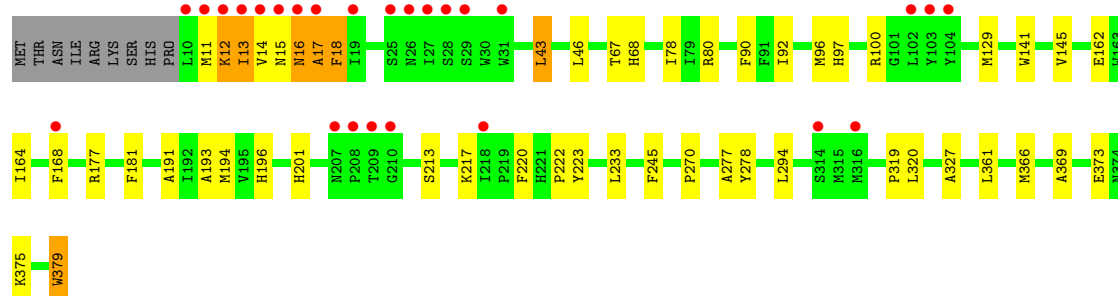
- Molecule 3: Cytochrome b

Chain C:



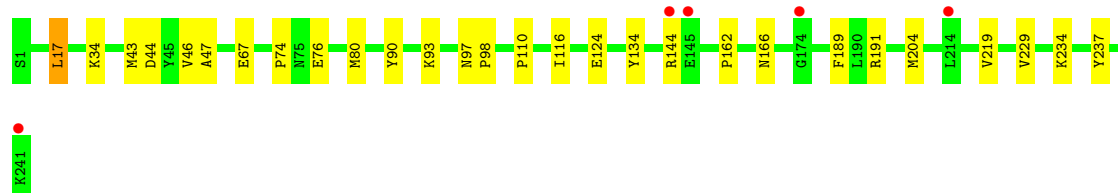
- Molecule 3: Cytochrome b

Chain P:



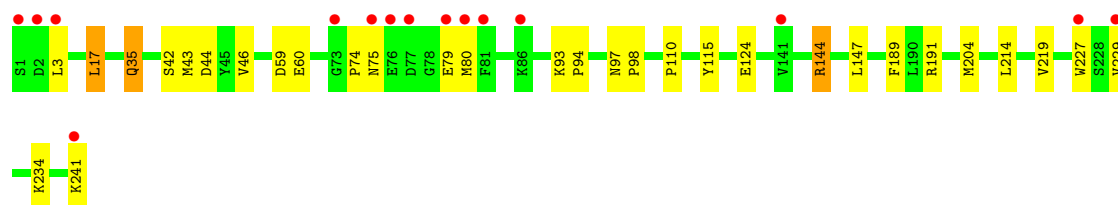
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



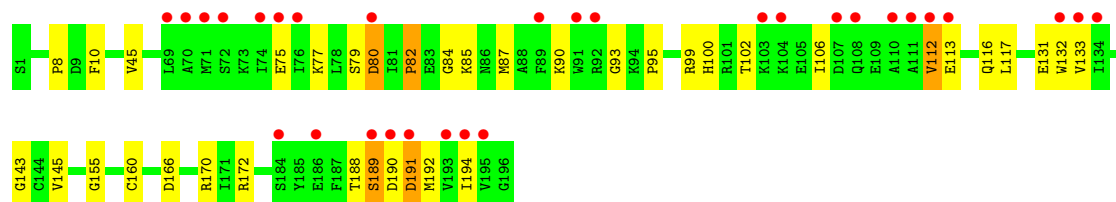
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain Q:



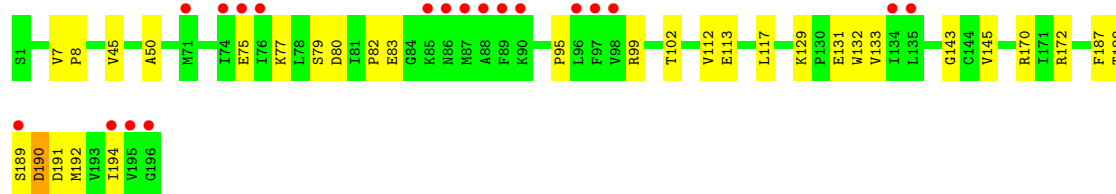
- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

Chain E:



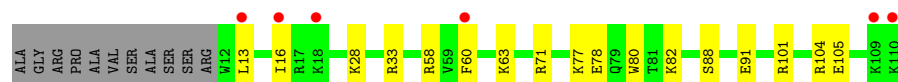
- Molecule 5: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

Chain R:



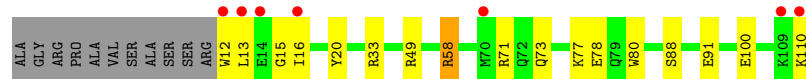
- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain F:



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

Chain S:



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

Chain G:



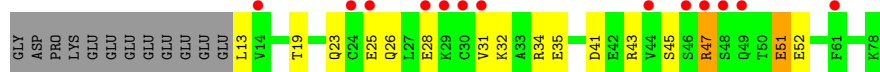
- Molecule 7: Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C

Chain T:



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

Chain H:



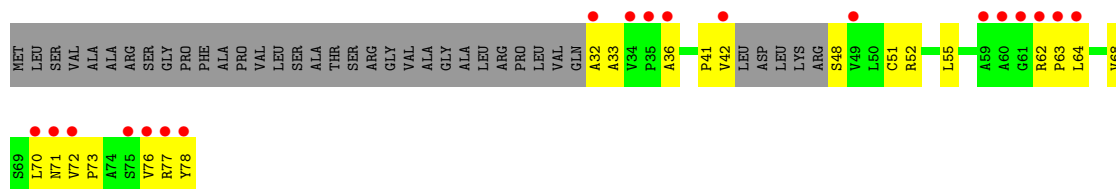
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain U:



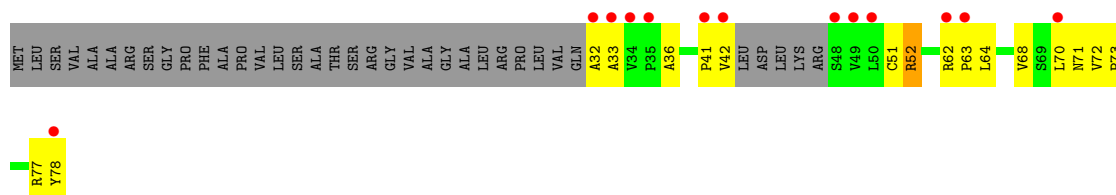
- Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

Chain I:



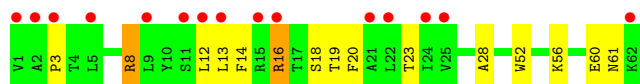
- Molecule 9: Ubiquinol-cytochrome C reductase iron-sulfur subunit, mitochondrial

Chain V:



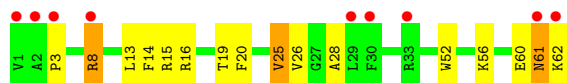
- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain J:



- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain W:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.12Å 171.06Å 227.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.98 – 2.10 40.02 – 2.08	Depositor EDS
% Data completeness (in resolution range)	97.3 (24.98-2.10) 96.1 (40.02-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.287 0.249 , 0.268	Depositor DCC
R_{free} test set	15323 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	2 of 308206 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33959	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, 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	0.32	0/3472	0.66	0/4714
1	N	0.33	0/3472	0.67	0/4714
2	B	0.32	0/3235	0.65	0/4387
2	O	0.31	0/3239	0.65	1/4393 (0.0%)
3	C	0.36	0/2986	0.65	1/4089 (0.0%)
3	P	0.35	0/3024	0.64	0/4137
4	D	0.34	0/1978	0.65	0/2684
4	Q	0.34	0/1978	0.65	0/2684
5	E	0.31	0/1553	0.67	1/2100 (0.0%)
5	R	0.35	0/1553	0.69	1/2100 (0.0%)
6	F	0.32	0/878	0.64	0/1175
6	S	0.32	0/878	0.65	0/1175
7	G	0.32	0/642	0.65	0/869
7	T	0.34	0/647	0.68	0/876
8	H	0.30	0/544	0.60	0/729
8	U	0.31	0/544	0.56	0/729
9	I	0.32	0/285	0.66	0/384
9	V	0.32	0/285	0.69	0/384
10	J	0.36	0/520	0.65	0/699
10	W	0.36	0/520	0.65	0/699
All	All	0.33	0/32233	0.65	4/43721 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	228	GLY	N-CA-C	-6.96	95.71	113.10
5	R	143	GLY	N-CA-C	5.70	127.36	113.10
5	E	143	GLY	N-CA-C	5.38	126.54	113.10
3	C	109	PHE	N-CA-C	-5.22	96.91	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3403	0	3302	63	0
1	N	3403	0	3302	53	0
2	B	3177	0	3152	64	0
2	O	3180	0	3156	56	0
3	C	2892	0	2938	39	0
3	P	2931	0	2989	59	0
4	D	1919	0	1868	25	0
4	Q	1919	0	1868	36	0
5	E	1519	0	1503	30	0
5	R	1519	0	1503	25	0
6	F	861	0	854	14	0
6	S	861	0	854	20	0
7	G	621	0	626	17	0
7	T	626	0	631	23	0
8	H	539	0	524	14	0
8	U	539	0	524	10	0
9	I	285	0	288	37	0
9	V	285	0	288	31	0
10	J	507	0	513	24	0
10	W	507	0	513	27	0
11	A	18	0	24	1	0
11	C	18	0	24	0	0
11	F	36	0	48	3	0
11	P	18	0	24	0	0
11	S	18	0	24	8	0
12	B	5	0	0	0	0
12	O	5	0	0	0	0
13	A	3	0	0	0	0
13	C	3	0	0	0	0
13	D	3	0	0	0	0
13	P	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	C	86	0	60	5	0
14	P	86	0	60	3	0
15	D	43	0	30	3	0
15	Q	43	0	30	2	0
16	E	4	0	0	0	0
16	R	4	0	0	0	0
17	C	37	0	42	1	0
17	P	37	0	42	2	0
18	C	14	0	9	3	0
18	P	14	0	9	5	0
19	G	94	0	76	5	0
19	Q	50	0	44	0	0
19	T	49	0	42	0	0
20	A	6	0	5	0	0
20	C	54	0	72	2	0
20	D	51	0	82	1	0
20	G	49	0	72	0	0
20	N	5	0	0	0	0
20	P	49	0	72	2	0
20	Q	51	0	82	9	0
20	T	49	0	72	1	0
21	B	6	0	8	0	0
21	C	6	0	8	0	0
21	O	6	0	8	0	0
21	P	6	0	8	0	0
22	A	187	0	0	8	0
22	B	149	0	0	2	0
22	C	125	0	0	4	0
22	D	118	0	0	2	0
22	E	54	0	0	2	0
22	F	57	0	0	3	0
22	G	24	0	0	1	0
22	H	14	0	0	0	0
22	I	16	0	0	1	0
22	J	5	0	0	0	0
22	N	134	0	0	1	0
22	O	130	0	0	1	0
22	P	122	0	0	6	0
22	Q	109	0	0	1	0
22	R	64	0	0	0	0
22	S	73	0	0	2	0
22	T	21	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	U	16	0	0	0	0
22	V	10	0	0	1	0
22	W	9	0	0	0	0
All	All	33959	0	32273	593	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (593) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:95:LYS:HB2	9:V:32:ALA:HB2	1.20	1.12
2:B:12:GLU:HG2	2:B:17:VAL:H	1.15	1.09
7:T:45:ILE:HG22	7:T:46:LEU:HD22	1.31	1.04
2:O:200:THR:HB	2:O:229:GLY:HA2	1.36	1.04
3:P:43:LEU:HD21	20:Q:3006:PEE:H192	1.40	1.01
5:E:166:ASP:HA	22:E:541:HOH:O	1.59	1.01
1:A:136:GLN:HE21	9:I:51:CYS:HB3	1.34	0.91
4:Q:59:ASP:OD2	10:W:62:LYS:HB3	1.71	0.91
6:S:13:LEU:HD12	6:S:16:ILE:HD11	1.52	0.91
6:F:104:ARG:HH11	11:F:3011:BHG:H61	1.36	0.91
1:A:293:PRO:O	1:A:297:ILE:HG12	1.71	0.90
1:N:136:GLN:HE21	9:V:51:CYS:HB3	1.37	0.89
2:O:229:GLY:C	2:O:231:GLY:H	1.76	0.89
9:V:64:LEU:HD12	9:V:77:ARG:O	1.73	0.88
9:I:32:ALA:N	9:I:72:VAL:HG23	1.88	0.88
10:W:16:ARG:HB2	10:W:19:THR:HG22	1.56	0.87
1:A:1:THR:HG21	2:B:212:SER:HB3	1.55	0.86
9:V:52:ARG:HH11	9:V:52:ARG:HB3	1.40	0.86
3:C:129:MET:HE1	3:C:181:PHE:HD2	1.41	0.85
2:B:12:GLU:HG2	2:B:17:VAL:N	1.90	0.85
2:O:236:LYS:H	2:O:236:LYS:HD2	1.42	0.84
2:O:95:LYS:CB	9:V:32:ALA:HB2	2.06	0.84
1:N:293:PRO:O	1:N:297:ILE:HG12	1.78	0.83
4:D:74:PRO:HG3	4:D:80:MET:HE1	1.59	0.83
2:B:95:LYS:HB2	9:I:32:ALA:HB2	1.57	0.83
9:I:36:ALA:HB2	9:I:73:PRO:HD2	1.61	0.83
3:P:12:LYS:HE2	3:P:16:ASN:H	1.42	0.82
9:V:52:ARG:HB3	9:V:52:ARG:NH1	1.94	0.82
10:J:16:ARG:HB2	10:J:19:THR:HG22	1.58	0.82
9:I:64:LEU:HD12	9:I:77:ARG:O	1.78	0.81
1:N:29:GLN:HB3	2:O:12:GLU:O	1.80	0.80
7:T:72:LYS:HG3	8:U:56:GLU:OE2	1.81	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:P:12:LYS:HA	3:P:12:LYS:HE3	1.62	0.80
2:O:200:THR:CB	2:O:229:GLY:HA2	2.11	0.79
1:A:1:THR:HG21	2:B:212:SER:CB	2.13	0.78
10:J:16:ARG:NH1	10:J:19:THR:HG21	1.99	0.78
9:I:32:ALA:N	9:I:71:ASN:HB3	1.99	0.77
4:Q:110:PRO:HG3	15:Q:501:HEC:HMD3	1.66	0.77
10:W:13:LEU:O	10:W:19:THR:HG23	1.84	0.76
1:A:2:ALA:HB1	1:A:6:GLN:HB2	1.65	0.76
10:W:3:PRO:HB2	10:W:8:ARG:NH1	2.01	0.76
3:P:43:LEU:HD21	20:Q:3006:PEE:C19	2.17	0.75
4:Q:74:PRO:HG3	4:Q:80:MET:HE1	1.69	0.74
3:P:379:TRP:CZ3	6:S:33:ARG:HD3	2.22	0.74
3:P:129:MET:HE1	3:P:181:PHE:HD2	1.52	0.74
9:I:32:ALA:N	9:I:71:ASN:CB	2.51	0.74
2:O:71:LEU:HD23	9:V:68:VAL:HG21	1.69	0.74
10:W:16:ARG:HH11	10:W:19:THR:HG21	1.54	0.73
1:A:3:THR:OG1	1:A:6:GLN:HG3	1.88	0.73
8:U:28:GLU:O	8:U:31:VAL:HG22	1.89	0.73
1:A:352:SER:HB3	6:S:110:LYS:HD2	1.71	0.72
8:H:43:ARG:O	8:H:47:ARG:HD2	1.89	0.72
6:F:13:LEU:O	6:F:16:ILE:HG12	1.89	0.72
2:B:71:LEU:HD23	9:I:68:VAL:HG21	1.70	0.72
10:J:16:ARG:HB2	10:J:16:ARG:HH11	1.55	0.72
3:C:129:MET:CE	3:C:181:PHE:HD2	2.02	0.71
5:E:113:GLU:HB3	5:E:116:GLN:NE2	2.05	0.71
5:E:113:GLU:HB3	5:E:116:GLN:HE21	1.55	0.71
10:J:13:LEU:O	10:J:19:THR:HG23	1.90	0.71
4:Q:35:GLN:HG3	22:Q:3086:HOH:O	1.91	0.71
1:A:51:LYS:H	1:A:51:LYS:HZ1	1.39	0.70
4:Q:74:PRO:HG3	4:Q:80:MET:CE	2.22	0.70
3:P:96:MET:HE2	20:P:3007:PEE:H181	1.74	0.70
3:C:129:MET:HE1	3:C:181:PHE:CD2	2.26	0.70
2:B:47:ILE:HG21	2:B:120:MET:HE3	1.73	0.69
8:H:28:GLU:O	8:H:31:VAL:HG22	1.92	0.69
2:B:231:GLY:N	2:B:233:SER:H	1.90	0.69
3:P:68:HIS:HD2	22:P:3131:HOH:O	1.75	0.69
1:A:352:SER:HB3	6:S:110:LYS:CD	2.23	0.69
3:C:379:TRP:CZ3	6:F:33:ARG:HD3	2.28	0.69
4:Q:75:ASN:HD21	4:Q:79:GLU:HG2	1.58	0.69
1:A:136:GLN:HE21	9:I:51:CYS:CB	2.04	0.68
22:A:4185:HOH:O	9:I:73:PRO:HG3	1.94	0.68
1:N:29:GLN:HG3	1:N:203:LEU:O	1.94	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:353:SER:HB3	2:B:355:PRO:HD2	1.76	0.68
9:I:36:ALA:CB	9:I:73:PRO:HD2	2.23	0.68
5:R:79:SER:HB3	5:R:191:ASP:OD1	1.93	0.68
2:B:95:LYS:HD3	2:B:110:GLU:OE2	1.94	0.68
1:A:86:LEU:HD13	1:A:99:ILE:HG12	1.76	0.67
2:O:169:ARG:HG3	2:O:240:HIS:HB2	1.76	0.67
6:S:100:GLU:HB3	11:S:2011:BHG:H62	1.76	0.67
10:W:16:ARG:NH1	10:W:19:THR:HG21	2.10	0.67
1:N:32:GLN:OE1	2:O:373:GLU:HB2	1.94	0.67
3:P:129:MET:CE	3:P:181:PHE:HD2	2.08	0.66
1:A:2:ALA:O	2:B:113:ARG:NE	2.28	0.66
10:W:8:ARG:HG2	10:W:8:ARG:HH11	1.60	0.65
5:R:190:ASP:HB2	5:R:192:MET:HG2	1.79	0.65
7:G:60:THR:O	7:G:64:GLN:HG3	1.95	0.65
10:J:16:ARG:HB2	10:J:19:THR:CG2	2.26	0.65
2:O:365:LYS:HG2	2:O:399:LEU:HD22	1.78	0.65
6:S:13:LEU:HA	6:S:16:ILE:HG12	1.78	0.65
4:D:74:PRO:HG3	4:D:80:MET:CE	2.27	0.64
3:P:96:MET:CE	20:P:3007:PEE:H181	2.27	0.64
2:B:95:LYS:HD2	9:I:32:ALA:HB2	1.79	0.64
3:P:129:MET:HE1	3:P:181:PHE:CD2	2.32	0.64
9:I:36:ALA:HB3	9:I:73:PRO:HG2	1.78	0.64
1:N:136:GLN:NE2	9:V:51:CYS:HB3	2.11	0.64
2:B:231:GLY:N	2:B:232:LEU:N	2.46	0.64
7:T:60:THR:O	7:T:64:GLN:HG3	1.98	0.64
10:J:16:ARG:HH11	10:J:16:ARG:CB	2.10	0.64
8:H:25:GLU:HG2	8:H:34:ARG:HH22	1.62	0.64
2:O:236:LYS:H	2:O:236:LYS:CD	2.07	0.63
2:O:95:LYS:HB2	9:V:32:ALA:CB	2.12	0.63
2:B:95:LYS:CB	9:I:32:ALA:HB2	2.26	0.63
2:O:47:ILE:HG21	2:O:120:MET:HE3	1.81	0.63
6:F:28:LYS:HE3	22:F:4052:HOH:O	1.98	0.63
4:Q:75:ASN:ND2	4:Q:79:GLU:HG2	2.13	0.63
7:T:71:ARG:HH11	7:T:72:LYS:HZ2	1.45	0.63
5:E:113:GLU:CB	5:E:116:GLN:HE21	2.12	0.62
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.80	0.62
10:J:14:PHE:HA	10:J:20:PHE:HD2	1.64	0.62
10:J:16:ARG:CG	10:J:16:ARG:HH11	2.12	0.62
9:V:32:ALA:N	9:V:71:ASN:CB	2.63	0.62
2:B:397:THR:O	2:B:401:GLN:HG3	2.00	0.62
2:O:296:TYR:OH	9:V:52:ARG:NE	2.33	0.62
3:C:29:SER:HB2	19:G:2004:CDL:HA31	1.82	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:47:ILE:HG21	2:B:120:MET:CE	2.30	0.61
3:C:96:MET:HE2	20:C:2007:PEE:H181	1.80	0.61
2:B:412:ASN:HA	2:B:415:LYS:HD2	1.80	0.61
10:J:3:PRO:HD2	10:J:8:ARG:CZ	2.30	0.61
1:N:41:ILE:HG12	1:N:195:MET:HG2	1.83	0.61
2:O:397:THR:O	2:O:401:GLN:HG3	2.01	0.61
2:O:227:ARG:C	2:O:229:GLY:N	2.50	0.61
4:Q:60:GLU:HG3	10:W:62:LYS:NZ	2.15	0.61
1:A:29:GLN:HG3	1:A:203:LEU:O	2.00	0.61
9:V:32:ALA:N	9:V:71:ASN:HB2	2.15	0.61
2:O:35:ILE:N	2:O:35:ILE:HD12	2.16	0.60
1:N:172:GLU:OE2	1:N:176:LYS:HE3	2.01	0.60
2:O:203:ARG:HH12	2:O:233:SER:HA	1.65	0.60
4:D:116:ILE:HG12	15:D:501:HEC:HMA3	1.83	0.60
3:P:145:VAL:HG21	17:P:3001:SMA:H6	1.84	0.60
4:Q:43:MET:HE2	4:Q:46:VAL:HG21	1.84	0.60
9:I:36:ALA:HB3	9:I:73:PRO:CG	2.31	0.60
1:N:308:GLN:HG2	22:N:3026:HOH:O	2.01	0.60
3:P:14:VAL:O	3:P:18:PHE:HB3	2.01	0.60
7:T:71:ARG:HH11	7:T:72:LYS:NZ	1.99	0.60
2:O:47:ILE:HG21	2:O:120:MET:CE	2.32	0.60
1:N:86:LEU:HD13	1:N:99:ILE:HG12	1.82	0.60
5:E:85:LYS:NZ	5:E:87:MET:SD	2.75	0.60
1:N:216:PHE:HD2	1:N:219:LEU:HD22	1.67	0.59
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.33	0.59
2:B:412:ASN:HD22	2:B:415:LYS:HD2	1.67	0.59
3:P:43:LEU:HD21	20:Q:3006:PEE:C20	2.33	0.59
9:V:36:ALA:HB2	9:V:73:PRO:HD2	1.84	0.59
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.37	0.59
2:O:227:ARG:C	2:O:229:GLY:H	2.02	0.59
1:A:296:SER:O	1:A:300:THR:HG23	2.02	0.59
7:G:40:ARG:HB3	19:G:2004:CDL:HB32	1.85	0.59
7:G:45:ILE:HG22	7:G:46:LEU:HD12	1.85	0.59
10:J:3:PRO:HD2	10:J:8:ARG:NH2	2.18	0.59
2:B:354:ASN:N	2:B:355:PRO:CD	2.66	0.59
2:B:169:ARG:HG3	2:B:240:HIS:HB2	1.84	0.59
7:T:66:PHE:CZ	7:T:70:LYS:HD2	2.38	0.58
3:C:96:MET:CE	20:C:2007:PEE:H181	2.34	0.58
2:B:189:VAL:HG23	22:B:3089:HOH:O	2.03	0.58
5:E:77:LYS:HE3	5:E:79:SER:OG	2.03	0.58
2:B:309:VAL:HG23	2:B:326:THR:HG22	1.85	0.58
1:N:8:LEU:HD22	1:N:392:LEU:HB3	1.84	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:289:HIS:HE1	11:S:2011:BHG:H1'2	1.69	0.58
2:B:20:HIS:HB2	2:B:22:GLN:HG3	1.84	0.58
10:J:12:LEU:O	10:J:13:LEU:HD23	2.04	0.58
9:V:32:ALA:N	9:V:72:VAL:HG23	2.18	0.58
2:B:365:LYS:HG2	2:B:399:LEU:HD22	1.86	0.58
1:N:286:GLY:HA3	1:N:290:LEU:HD21	1.85	0.58
1:N:30:SER:HA	2:O:18:PRO:HG3	1.85	0.58
2:O:229:GLY:C	2:O:231:GLY:N	2.47	0.57
2:B:139:ALA:HB3	11:S:2011:BHG:H5'1	1.86	0.57
10:W:8:ARG:HH11	10:W:8:ARG:CG	2.18	0.57
1:A:136:GLN:NE2	9:I:51:CYS:CB	2.67	0.57
7:T:71:ARG:HD3	7:T:72:LYS:HZ3	1.70	0.57
3:C:145:VAL:HG21	17:C:2001:SMA:H6	1.84	0.57
6:F:82:LYS:HE3	22:F:4032:HOH:O	2.04	0.57
1:N:373:THR:HB	1:N:374:PRO:HD3	1.86	0.57
9:V:62:ARG:O	9:V:78:TYR:HB3	2.05	0.57
3:P:129:MET:HE2	3:P:181:PHE:HB2	1.87	0.56
10:J:3:PRO:HB2	10:J:8:ARG:HD3	1.86	0.56
10:W:25:VAL:HG12	10:W:26:VAL:N	2.20	0.56
2:B:95:LYS:CG	9:I:32:ALA:HB2	2.35	0.56
2:B:20:HIS:HB2	2:B:22:GLN:CG	2.36	0.56
4:D:43:MET:HE1	4:D:189:PHE:HZ	1.69	0.56
9:I:32:ALA:N	9:I:71:ASN:HB2	2.19	0.56
8:H:25:GLU:CG	8:H:34:ARG:HH22	2.19	0.56
5:E:190:ASP:O	5:E:192:MET:HG2	2.05	0.56
7:T:30:PHE:O	7:T:34:ILE:HG12	2.06	0.56
8:U:25:GLU:HG2	8:U:34:ARG:HH22	1.71	0.56
3:P:319:PRO:HD2	22:P:3113:HOH:O	2.05	0.55
7:G:63:THR:O	7:G:67:GLU:HG2	2.06	0.55
5:E:90:LYS:HE2	5:E:93:GLY:HA2	1.87	0.55
7:G:30:PHE:O	7:G:34:ILE:HG12	2.06	0.55
3:C:217:LYS:HG3	7:G:7:LEU:HD13	1.89	0.55
11:F:3011:BHG:H62	2:O:83:PHE:HB2	1.89	0.55
3:P:201:HIS:NE2	18:P:3002:UQ:O4	2.28	0.55
7:T:34:ILE:HB	7:T:35:PRO:HD3	1.89	0.55
4:Q:241:LYS:OXT	4:Q:241:LYS:HD3	2.06	0.55
1:A:51:LYS:NZ	1:A:51:LYS:H	2.03	0.55
9:I:62:ARG:O	9:I:78:TYR:HB3	2.07	0.55
2:B:12:GLU:CG	2:B:17:VAL:H	2.04	0.55
1:N:136:GLN:HE21	9:V:51:CYS:CB	2.15	0.55
2:B:95:LYS:HD2	9:I:32:ALA:CB	2.37	0.55
1:N:364:ALA:HB2	9:V:33:ALA:HB1	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:341:GLN:NE2	22:C:2099:HOH:O	2.39	0.54
3:C:245:PHE:CD1	4:D:17:LEU:HD13	2.41	0.54
5:R:77:LYS:HE3	5:R:79:SER:OG	2.07	0.54
6:F:63:LYS:HE2	22:G:1280:HOH:O	2.06	0.54
7:T:63:THR:O	7:T:67:GLU:HG2	2.07	0.54
9:V:36:ALA:HB3	9:V:73:PRO:HG2	1.89	0.54
3:P:12:LYS:HA	3:P:12:LYS:CE	2.37	0.54
1:A:216:PHE:HD2	1:A:219:LEU:HD22	1.71	0.54
1:A:172:GLU:OE2	1:A:176:LYS:HE3	2.06	0.54
7:T:45:ILE:HG22	7:T:46:LEU:CD2	2.22	0.54
1:A:76:GLU:HG2	1:A:80:GLU:OE2	2.07	0.54
2:B:12:GLU:O	2:B:18:PRO:HD3	2.08	0.54
2:O:411:ILE:O	2:O:415:LYS:HG3	2.08	0.54
5:R:191:ASP:N	5:R:191:ASP:OD2	2.40	0.54
10:W:56:LYS:HG2	10:W:60:GLU:CD	2.28	0.54
1:A:41:ILE:HG12	1:A:195:MET:HG2	1.89	0.53
3:P:100:ARG:C	3:P:100:ARG:HD2	2.28	0.53
2:B:306:PRO:HA	9:I:52:ARG:HE	1.74	0.53
3:P:43:LEU:HD21	20:Q:3006:PEE:H201	1.89	0.53
4:Q:59:ASP:OD2	10:W:62:LYS:CB	2.52	0.53
5:R:188:THR:HG21	5:R:194:ILE:CD1	2.37	0.53
4:Q:60:GLU:HG3	10:W:62:LYS:HZ3	1.74	0.53
2:B:294:SER:OG	2:B:343:GLN:NE2	2.42	0.53
4:D:166:ASN:HB3	8:H:13:LEU:HD23	1.91	0.53
2:O:229:GLY:O	2:O:230:LEU:HB2	2.07	0.53
3:P:220:PHE:HE1	18:P:3002:UQ:CM2	2.22	0.53
10:W:56:LYS:O	10:W:60:GLU:HG3	2.09	0.53
9:V:32:ALA:N	9:V:71:ASN:HB3	2.24	0.53
2:B:353:SER:CB	2:B:355:PRO:HD2	2.38	0.52
4:D:34:LYS:NZ	4:D:67:GLU:OE1	2.31	0.52
5:E:90:LYS:CE	5:E:93:GLY:HA2	2.40	0.52
5:E:99:ARG:HB3	5:E:133:VAL:HG12	1.91	0.52
9:I:72:VAL:HG13	9:I:73:PRO:HD2	1.92	0.52
2:O:95:LYS:HG3	9:V:32:ALA:N	2.24	0.52
4:Q:229:VAL:CG2	7:T:20:PRO:HD3	2.40	0.52
8:H:41:ASP:O	8:H:45:SER:HB2	2.09	0.52
4:D:234:LYS:HD3	5:E:8:PRO:HB2	1.91	0.52
2:B:314:ALA:HA	9:I:63:PRO:HD3	1.90	0.52
10:J:13:LEU:HB3	10:J:23:THR:OG1	2.10	0.52
1:N:76:GLU:HG2	1:N:80:GLU:OE2	2.09	0.52
2:O:276:GLN:HG2	2:O:281:ALA:HB2	1.91	0.52
2:O:189:VAL:HG23	22:O:3052:HOH:O	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.92	0.52
1:N:30:SER:CA	2:O:18:PRO:HG3	2.39	0.52
1:A:289:HIS:HE1	11:S:2011:BHG:C1'	2.23	0.52
2:O:181:TYR:CE1	2:O:182:ARG:HG2	2.44	0.52
4:D:34:LYS:HE3	22:D:4097:HOH:O	2.09	0.52
9:V:72:VAL:HG13	9:V:73:PRO:HD2	1.91	0.52
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.91	0.52
5:E:102:THR:O	5:E:106:ILE:HG13	2.09	0.52
3:P:12:LYS:CE	3:P:15:ASN:HB3	2.39	0.52
3:P:220:PHE:HE1	18:P:3002:UQ:HM22	1.74	0.52
3:C:129:MET:HE2	3:C:181:PHE:HB2	1.91	0.51
3:P:162:GLU:OE2	3:P:168:PHE:HD1	1.93	0.51
6:S:88:SER:OG	6:S:91:GLU:HB2	2.09	0.51
3:P:379:TRP:CE3	6:S:33:ARG:HD3	2.44	0.51
6:S:71:ARG:O	6:S:73:GLN:HG3	2.10	0.51
3:P:12:LYS:CA	3:P:12:LYS:HE3	2.36	0.51
10:W:52:TRP:O	10:W:56:LYS:HB2	2.11	0.51
1:N:206:ARG:HH11	1:N:206:ARG:HG3	1.75	0.51
5:R:77:LYS:HD3	5:R:80:ASP:OD2	2.10	0.51
1:A:227:ALA:O	1:A:228:VAL:C	2.49	0.51
2:B:33:LEU:CD2	2:B:220:ALA:HB1	2.41	0.51
14:C:502:HEM:HBA1	18:C:2002:UQ:O2	2.11	0.51
4:D:234:LYS:HE2	5:E:10:PHE:CE1	2.46	0.51
2:O:309:VAL:HG23	2:O:326:THR:HG22	1.93	0.51
2:O:294:SER:OG	2:O:343:GLN:NE2	2.44	0.51
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.59	0.51
1:A:206:ARG:HG3	1:A:206:ARG:HH11	1.76	0.51
7:G:40:ARG:CB	19:G:2004:CDL:HB32	2.41	0.51
1:N:68:LYS:HA	1:N:68:LYS:HE3	1.93	0.51
6:S:12:TRP:O	6:S:16:ILE:N	2.36	0.51
10:W:16:ARG:HB2	10:W:19:THR:CG2	2.33	0.51
1:N:381:ARG:HH11	1:N:381:ARG:HG2	1.75	0.51
8:U:25:GLU:CG	8:U:34:ARG:HH22	2.24	0.51
3:C:369:ALA:O	3:C:373:GLU:HG3	2.11	0.50
5:E:189:SER:C	5:E:190:ASP:OD1	2.49	0.50
5:R:188:THR:HG21	5:R:194:ILE:HD12	1.91	0.50
1:A:308:GLN:HG2	22:A:4140:HOH:O	2.10	0.50
7:T:71:ARG:HB2	7:T:72:LYS:HD3	1.93	0.50
3:C:68:HIS:HD2	22:C:2126:HOH:O	1.95	0.50
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.42	0.50
1:N:136:GLN:NE2	9:V:51:CYS:CB	2.72	0.50
2:B:35:ILE:HD12	2:B:35:ILE:N	2.27	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:P:245:PHE:CG	4:Q:17:LEU:HD13	2.47	0.50
5:R:129:LYS:HG3	5:R:187:PHE:CE1	2.47	0.50
6:F:88:SER:OG	6:F:91:GLU:HB2	2.12	0.50
11:F:3011:BHG:H4	1:N:289:HIS:CE1	2.47	0.50
1:A:373:THR:HB	1:A:374:PRO:HD3	1.92	0.50
2:O:229:GLY:O	2:O:231:GLY:N	2.44	0.50
3:P:15:ASN:O	3:P:17:ALA:N	2.44	0.50
4:Q:124:GLU:OE2	4:Q:191:ARG:CD	2.60	0.50
1:A:90:SER:HB3	22:A:4116:HOH:O	2.11	0.50
2:B:95:LYS:CD	9:I:32:ALA:HB2	2.42	0.50
2:O:200:THR:O	2:O:204:MET:HG3	2.12	0.50
5:R:80:ASP:O	5:R:82:PRO:HD3	2.12	0.50
1:A:289:HIS:CE1	11:S:2011:BHG:H1'2	2.47	0.50
3:C:191:ALA:HA	3:C:194:MET:HE2	1.94	0.50
7:G:66:PHE:CZ	7:G:70:LYS:HD2	2.47	0.50
1:N:125:SER:O	1:N:129:LYS:HG3	2.11	0.50
1:A:125:SER:O	1:A:129:LYS:HG3	2.12	0.49
2:O:354:ASN:N	2:O:355:PRO:CD	2.75	0.49
3:P:164:ILE:O	3:P:177:ARG:HD2	2.12	0.49
20:Q:3006:PEE:H351	5:R:50:ALA:CB	2.42	0.49
9:V:32:ALA:HA	9:V:71:ASN:HD22	1.77	0.49
3:C:96:MET:HA	3:C:96:MET:HE2	1.93	0.49
15:D:501:HEC:HMC1	15:D:501:HEC:HBC3	1.94	0.49
10:W:3:PRO:HB2	10:W:8:ARG:HH11	1.74	0.49
5:E:82:PRO:O	5:E:100:HIS:HB3	2.12	0.49
1:A:364:ALA:HB2	9:I:33:ALA:HB1	1.95	0.49
5:R:99:ARG:HB3	5:R:133:VAL:HG12	1.94	0.49
1:N:405:ARG:O	1:N:409:GLU:HG3	2.13	0.49
1:A:172:GLU:HG3	1:A:176:LYS:HE3	1.95	0.49
8:H:28:GLU:O	8:H:32:LYS:HG2	2.13	0.49
1:N:227:ALA:O	1:N:228:VAL:HB	2.13	0.49
3:C:15:ASN:O	3:C:16:ASN:C	2.50	0.49
1:N:264:HIS:ND1	1:N:265:PRO:HD2	2.28	0.49
6:S:78:GLU:CD	6:S:78:GLU:H	2.16	0.48
3:C:191:ALA:HA	3:C:194:MET:CE	2.43	0.48
3:P:191:ALA:HA	3:P:194:MET:CE	2.43	0.48
6:S:100:GLU:OE1	11:S:2011:BHG:H4	2.13	0.48
2:B:109:VAL:HB	2:B:119:LEU:HD12	1.94	0.48
3:C:21:LEU:HD21	18:C:2002:UQ:HM32	1.95	0.48
3:C:251:GLY:HA3	22:C:2091:HOH:O	2.13	0.48
3:C:371:THR:O	3:C:375:LYS:HG2	2.13	0.48
10:J:16:ARG:CG	10:J:16:ARG:NH1	2.75	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:R:79:SER:CB	5:R:191:ASP:OD1	2.61	0.48
6:S:13:LEU:HB3	22:S:2070:HOH:O	2.13	0.48
3:C:97:HIS:CD2	14:C:502:HEM:NC	2.81	0.48
4:D:110:PRO:HG3	15:D:501:HEC:HMD3	1.95	0.48
1:A:143:THR:OG1	9:I:48:SER:HB3	2.13	0.48
3:P:245:PHE:CD1	4:Q:17:LEU:HD13	2.48	0.48
1:A:15:GLN:NE2	2:B:12:GLU:HB2	2.29	0.48
1:A:431:LEU:HD12	1:A:432:PRO:HD2	1.96	0.48
2:B:24:LEU:HD13	2:B:392:TYR:CD2	2.49	0.48
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.96	0.48
3:C:379:TRP:CE3	6:F:33:ARG:HD3	2.47	0.48
2:O:365:LYS:HG2	2:O:399:LEU:CD2	2.42	0.48
1:A:117:VAL:HG11	1:A:195:MET:HE1	1.96	0.48
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.49	0.48
4:D:124:GLU:OE2	4:D:191:ARG:HD2	2.14	0.48
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.49	0.48
3:C:141:TRP:CH2	5:R:145:VAL:HG23	2.49	0.48
4:Q:43:MET:HE1	4:Q:189:PHE:HZ	1.79	0.48
4:Q:3:LEU:HD12	8:U:55:THR:HG22	1.96	0.48
10:W:61:ASN:C	10:W:62:LYS:HG3	2.35	0.48
5:E:155:GLY:N	22:E:541:HOH:O	2.46	0.47
6:F:78:GLU:H	6:F:78:GLU:CD	2.16	0.47
2:O:354:ASN:HB3	2:O:355:PRO:HD3	1.96	0.47
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.95	0.47
10:J:16:ARG:O	10:J:19:THR:HG22	2.14	0.47
10:J:16:ARG:CB	10:J:19:THR:HG22	2.38	0.47
10:W:8:ARG:CG	10:W:8:ARG:NH1	2.75	0.47
1:A:213:GLN:HG2	22:A:4055:HOH:O	2.15	0.47
2:B:212:SER:OG	2:B:215:VAL:HG23	2.15	0.47
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.44	0.47
3:P:14:VAL:O	3:P:15:ASN:O	2.32	0.47
1:A:429:GLU:OE2	7:G:7:LEU:HB2	2.14	0.47
10:J:52:TRP:O	10:J:56:LYS:HB2	2.13	0.47
1:N:296:SER:O	1:N:300:THR:HG23	2.14	0.47
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.96	0.47
3:C:100:ARG:C	3:C:100:ARG:HD2	2.35	0.47
2:O:361:LYS:HE2	2:O:402:ILE:O	2.14	0.47
3:P:14:VAL:C	3:P:15:ASN:CA	2.83	0.47
1:A:167:VAL:HG13	22:A:4111:HOH:O	2.15	0.47
2:B:345:LYS:O	2:B:349:GLN:HG3	2.14	0.47
2:B:246:GLU:O	2:B:427:SER:HA	2.15	0.47
3:P:193:ALA:O	3:P:196:HIS:HB3	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:396:SER:HB3	22:B:3031:HOH:O	2.14	0.47
1:N:111:GLU:HG3	1:N:215:HIS:CE1	2.50	0.47
8:U:28:GLU:O	8:U:32:LYS:HG2	2.15	0.47
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.50	0.47
7:T:46:LEU:HD23	22:T:3018:HOH:O	2.13	0.47
1:A:394:GLU:HA	11:A:4002:BHG:H2	1.96	0.47
3:C:162:GLU:OE2	3:C:168:PHE:HD1	1.98	0.47
2:O:17:VAL:HG13	2:O:18:PRO:HD2	1.96	0.47
4:Q:234:LYS:HD3	5:R:8:PRO:HB2	1.95	0.47
2:B:257:LEU:O	2:B:323:GLY:HA3	2.15	0.47
2:B:95:LYS:HE3	9:I:72:VAL:HG21	1.97	0.47
5:E:79:SER:HB3	5:E:191:ASP:OD2	2.15	0.47
1:N:172:GLU:HG3	1:N:176:LYS:HE3	1.96	0.47
3:P:97:HIS:CD2	14:P:502:HEM:NC	2.83	0.47
7:T:46:LEU:HD22	7:T:46:LEU:N	2.30	0.47
1:A:286:GLY:HA3	1:A:290:LEU:HD21	1.95	0.47
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.97	0.47
4:D:124:GLU:OE2	4:D:191:ARG:CD	2.63	0.46
3:P:361:LEU:O	3:P:366:MET:HG3	2.15	0.46
14:P:502:HEM:HBA1	18:P:3002:UQ:O2	2.15	0.46
3:C:104:TYR:CD1	3:C:208:PRO:HA	2.51	0.46
4:D:44:ASP:OD1	4:D:93:LYS:HE2	2.15	0.46
5:E:85:LYS:HZ3	5:E:87:MET:HA	1.80	0.46
2:O:33:LEU:CD2	2:O:220:ALA:HB1	2.45	0.46
3:P:375:LYS:HD2	3:P:375:LYS:N	2.29	0.46
1:A:15:GLN:HE21	2:B:12:GLU:HB2	1.81	0.46
2:B:46:ARG:HD2	2:B:375:SER:OG	2.14	0.46
3:C:245:PHE:CG	4:D:17:LEU:HD13	2.50	0.46
3:P:92:ILE:O	3:P:96:MET:HG2	2.16	0.46
7:G:34:ILE:HB	7:G:35:PRO:HD3	1.95	0.46
8:H:31:VAL:HG23	8:H:32:LYS:N	2.30	0.46
10:J:16:ARG:HH12	10:J:19:THR:HG21	1.76	0.46
1:A:369:LEU:HD12	1:A:392:LEU:HD21	1.98	0.46
1:N:47:TYR:HB3	1:N:189:HIS:CE1	2.51	0.46
3:P:277:ALA:HB1	3:P:294:LEU:CD1	2.45	0.46
22:P:3113:HOH:O	6:S:20:TYR:HE1	1.99	0.46
2:O:24:LEU:HD12	2:O:37:SER:O	2.15	0.46
15:Q:501:HEC:HBC3	15:Q:501:HEC:HMC1	1.98	0.46
22:A:4072:HOH:O	6:S:110:LYS:HD2	2.15	0.46
3:C:233:LEU:HD11	4:D:219:VAL:HG21	1.98	0.46
1:N:354:VAL:HG21	1:N:404:ALA:HA	1.96	0.46
3:P:129:MET:CE	3:P:181:PHE:CD2	2.94	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:Q:3006:PEE:H351	5:R:50:ALA:HB1	1.98	0.46
10:W:56:LYS:HG2	10:W:60:GLU:CG	2.46	0.46
1:A:29:GLN:HB3	2:B:12:GLU:O	2.16	0.46
9:I:70:LEU:HB3	22:I:1016:HOH:O	2.16	0.46
4:Q:124:GLU:OE2	4:Q:191:ARG:HD2	2.16	0.46
1:A:15:GLN:O	1:A:26:ALA:HA	2.16	0.46
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.51	0.46
9:I:36:ALA:CB	9:I:73:PRO:HB2	2.46	0.46
2:B:365:LYS:HG2	2:B:399:LEU:CD2	2.45	0.45
3:C:193:ALA:O	3:C:196:HIS:HB3	2.16	0.45
3:P:327:ALA:HA	7:T:51:PRO:HB3	1.98	0.45
8:U:31:VAL:HG23	8:U:32:LYS:N	2.30	0.45
9:V:36:ALA:CB	9:V:73:PRO:HB2	2.46	0.45
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.82	0.45
7:G:40:ARG:NH2	19:G:2004:CDL:HB31	2.32	0.45
3:P:43:LEU:CD2	20:Q:3006:PEE:H192	2.29	0.45
8:U:41:ASP:O	8:U:45:SER:HB2	2.15	0.45
2:O:71:LEU:CD2	9:V:68:VAL:HG21	2.43	0.45
5:E:95:PRO:HG2	5:E:145:VAL:HG22	1.98	0.45
9:V:62:ARG:HB3	9:V:63:PRO:HD2	1.99	0.45
10:W:16:ARG:O	10:W:19:THR:HG22	2.17	0.45
1:N:117:VAL:HG11	1:N:195:MET:HE1	1.99	0.45
5:E:145:VAL:HG23	3:P:141:TRP:CH2	2.52	0.45
3:P:96:MET:HE2	3:P:96:MET:HA	1.99	0.45
1:A:85:HIS:O	1:A:99:ILE:HA	2.16	0.45
1:N:195:MET:HE1	1:N:219:LEU:HD21	1.99	0.45
3:P:217:LYS:HG3	7:T:7:LEU:HD13	1.99	0.45
10:J:16:ARG:HG3	10:J:16:ARG:NH1	2.32	0.45
9:V:36:ALA:HB3	9:V:73:PRO:CG	2.46	0.45
3:C:92:ILE:O	3:C:96:MET:HG2	2.17	0.44
1:N:19:LEU:HD22	1:N:213:GLN:HG3	1.99	0.44
3:P:13:ILE:O	3:P:13:ILE:HG22	2.17	0.44
3:P:12:LYS:HE2	3:P:16:ASN:HB2	1.99	0.44
3:P:213:SER:OG	3:P:217:LYS:NZ	2.42	0.44
5:R:112:VAL:CG2	5:R:172:ARG:NH2	2.80	0.44
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.98	0.44
2:B:28:ARG:HH21	2:B:390:GLY:HA3	1.81	0.44
3:C:304:ILE:HB	3:C:305:PRO:HD3	1.99	0.44
7:G:38:LEU:HB3	7:G:42:ARG:NH1	2.32	0.44
8:H:51:GLU:HG3	8:H:52:GLU:N	2.32	0.44
9:V:36:ALA:CB	9:V:73:PRO:HD2	2.47	0.44
8:H:31:VAL:O	8:H:35:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:76:VAL:O	9:I:76:VAL:HG13	2.16	0.44
1:N:213:GLN:O	1:N:217:SER:OG	2.25	0.44
4:Q:144:ARG:HG3	4:Q:147:LEU:HD12	1.98	0.44
4:Q:44:ASP:OD1	4:Q:93:LYS:HE2	2.18	0.44
7:T:71:ARG:NH1	7:T:72:LYS:HD2	2.31	0.44
6:S:110:LYS:O	6:S:110:LYS:HG3	2.17	0.44
2:B:327:ILE:HG21	9:I:55:LEU:HD11	1.98	0.44
3:P:270:PRO:HG2	3:P:278:TYR:CG	2.53	0.44
7:G:40:ARG:CZ	19:G:2004:CDL:HB31	2.47	0.44
5:R:75:GLU:HG2	5:R:194:ILE:HG12	2.00	0.44
2:B:230:LEU:HB3	2:B:233:SER:OG	2.18	0.44
3:C:197:LEU:HD21	14:C:502:HEM:HMA1	2.00	0.44
18:P:3002:UQ:HM31	22:P:3116:HOH:O	2.17	0.44
6:S:58:ARG:HD3	22:S:2031:HOH:O	2.18	0.44
14:C:501:HEM:HBC2	14:C:501:HEM:HMC1	2.00	0.43
4:Q:42:SER:HB3	4:Q:94:PRO:HD2	2.00	0.43
5:R:117:LEU:HD13	5:R:170:ARG:HD2	2.00	0.43
6:S:49:ARG:HH22	11:S:2011:BHG:H4	1.83	0.43
1:A:86:LEU:HD13	1:A:99:ILE:CG1	2.45	0.43
2:B:361:LYS:HE2	2:B:402:ILE:O	2.18	0.43
10:J:56:LYS:HG2	10:J:60:GLU:CD	2.39	0.43
2:O:314:ALA:HA	9:V:63:PRO:HD3	2.00	0.43
5:R:112:VAL:HG22	5:R:172:ARG:NH2	2.33	0.43
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.54	0.43
3:C:129:MET:CE	3:C:181:PHE:CD2	2.90	0.43
4:D:204:MET:HE3	20:D:2006:PEE:O4	2.18	0.43
8:H:19:THR:O	8:H:23:GLN:HG3	2.19	0.43
1:N:288:ALA:HB2	1:N:300:THR:HG22	2.01	0.43
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.17	0.43
1:A:27:SER:HA	1:A:199:ALA:O	2.18	0.43
1:N:15:GLN:O	1:N:26:ALA:HA	2.18	0.43
3:P:369:ALA:O	3:P:373:GLU:HG3	2.19	0.43
3:P:78:ILE:HD12	4:Q:204:MET:CE	2.49	0.43
3:C:68:HIS:HE1	22:C:2049:HOH:O	2.01	0.43
7:G:50:PRO:HB2	7:G:51:PRO:HD3	2.01	0.43
2:B:181:TYR:CD2	2:O:248:ASN:HA	2.54	0.43
5:E:112:VAL:HG22	5:E:172:ARG:NH2	2.34	0.43
22:D:4077:HOH:O	6:F:71:ARG:HD3	2.18	0.43
2:O:228:GLY:O	2:O:231:GLY:HA2	2.18	0.43
2:B:136:GLU:HG2	11:S:2011:BHG:H2'1	2.00	0.43
14:C:501:HEM:O2D	14:C:501:HEM:O2A	2.37	0.43
4:D:47:ALA:HA	4:D:90:TYR:HA	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:36:ALA:HB2	9:I:73:PRO:CD	2.40	0.43
7:T:72:LYS:CG	8:U:56:GLU:OE2	2.62	0.43
1:A:383:LEU:O	1:A:387:GLY:HA2	2.18	0.43
1:A:61:HIS:CE1	1:A:137:GLU:OE1	2.72	0.43
1:N:224:ASP:OD1	1:N:227:ALA:HB2	2.18	0.43
2:O:345:LYS:O	2:O:349:GLN:HG3	2.19	0.43
4:Q:204:MET:HB3	4:Q:204:MET:HE3	1.83	0.43
4:Q:74:PRO:HG3	4:Q:80:MET:HE2	1.99	0.43
5:E:75:GLU:HG2	5:E:194:ILE:HG12	2.00	0.43
7:G:32:LYS:C	7:G:35:PRO:HD2	2.39	0.43
1:N:416:TYR:HB3	10:W:15:ARG:NH2	2.33	0.43
1:A:381:ARG:HG2	22:A:4120:HOH:O	2.19	0.42
2:B:181:TYR:CE1	2:B:182:ARG:HG2	2.54	0.42
7:G:48:VAL:O	7:G:51:PRO:HD2	2.19	0.42
1:N:3:THR:OG1	1:N:6:GLN:HG3	2.19	0.42
1:A:111:GLU:HG3	1:A:215:HIS:CE1	2.54	0.42
3:C:269:LYS:HA	3:C:270:PRO:HD3	1.81	0.42
9:I:77:ARG:O	9:I:78:TYR:HB2	2.19	0.42
1:N:280:TYR:HA	1:N:284:TYR:CE2	2.54	0.42
1:A:117:VAL:HG11	1:A:195:MET:CE	2.49	0.42
1:A:240:GLN:NE2	22:A:4184:HOH:O	2.51	0.42
3:P:67:THR:HB	4:Q:115:TYR:OH	2.20	0.42
3:P:68:HIS:HE1	22:P:3053:HOH:O	2.03	0.42
1:A:381:ARG:HG2	1:A:381:ARG:HH11	1.84	0.42
2:O:28:ARG:HB2	2:O:28:ARG:NH1	2.35	0.42
8:U:23:GLN:O	8:U:26:GLN:HG2	2.20	0.42
1:A:158:PHE:O	1:A:164:ALA:HB2	2.20	0.42
1:A:78:GLU:OE2	1:A:108:LYS:HD2	2.20	0.42
3:C:270:PRO:HG2	3:C:278:TYR:CG	2.54	0.42
4:D:43:MET:CE	4:D:46:VAL:HG21	2.50	0.42
1:N:286:GLY:HA3	1:N:290:LEU:CD2	2.47	0.42
4:D:97:ASN:HB2	4:D:98:PRO:HD2	2.01	0.42
1:A:267:ASN:O	1:A:271:GLN:HG2	2.20	0.42
3:P:320:LEU:HG	22:P:3113:HOH:O	2.19	0.42
7:T:71:ARG:HB2	7:T:72:LYS:H	1.66	0.42
3:P:46:LEU:HD11	20:Q:3006:PEE:H472	2.01	0.42
4:Q:43:MET:HE2	4:Q:46:VAL:CG2	2.48	0.42
4:Q:75:ASN:HD21	4:Q:79:GLU:CG	2.30	0.42
5:R:95:PRO:HG2	5:R:145:VAL:HG22	2.02	0.42
1:N:267:ASN:O	1:N:271:GLN:HG2	2.19	0.42
1:N:281:ASP:OD1	1:N:281:ASP:C	2.58	0.42
2:O:17:VAL:HA	2:O:18:PRO:HD3	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:O:257:LEU:O	2:O:323:GLY:HA3	2.19	0.42
7:T:32:LYS:C	7:T:35:PRO:HD2	2.40	0.42
10:W:14:PHE:HA	10:W:20:PHE:HD2	1.85	0.41
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.56	0.41
4:D:229:VAL:CG2	7:G:20:PRO:HD3	2.49	0.41
1:N:156:THR:HA	5:R:7:VAL:HG21	2.01	0.41
2:O:203:ARG:HH12	2:O:233:SER:CA	2.32	0.41
2:O:212:SER:OG	2:O:215:VAL:HG23	2.20	0.41
5:E:117:LEU:HD13	5:E:170:ARG:HD2	2.03	0.41
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.55	0.41
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.68	0.41
2:O:246:GLU:O	2:O:427:SER:HA	2.19	0.41
2:B:46:ARG:O	2:B:47:ILE:HD13	2.21	0.41
9:I:36:ALA:HB3	9:I:73:PRO:HB2	2.02	0.41
1:N:302:LYS:HD3	1:N:302:LYS:HA	1.93	0.41
2:B:412:ASN:HD22	2:B:412:ASN:HA	1.67	0.41
8:H:31:VAL:CG2	8:H:32:LYS:N	2.83	0.41
1:N:429:GLU:OE2	7:T:7:LEU:HB2	2.21	0.41
5:E:84:GLY:N	5:E:100:HIS:O	2.54	0.41
5:E:160:CYS:HB3	17:P:3001:SMA:H4	2.03	0.41
7:T:50:PRO:HB2	7:T:51:PRO:HD3	2.03	0.41
1:A:264:HIS:ND1	1:A:265:PRO:HD2	2.36	0.41
6:F:63:LYS:HG3	22:F:4045:HOH:O	2.20	0.41
8:H:51:GLU:HG3	8:H:52:GLU:H	1.86	0.41
4:Q:124:GLU:OE2	4:Q:191:ARG:HD3	2.21	0.41
6:S:12:TRP:O	6:S:15:GLY:N	2.53	0.41
10:W:16:ARG:HG3	10:W:16:ARG:NH1	2.36	0.41
6:F:101:ARG:O	6:F:105:GLU:HG3	2.21	0.41
8:H:23:GLN:O	8:H:26:GLN:HG2	2.20	0.41
1:N:85:HIS:O	1:N:99:ILE:HA	2.20	0.41
2:B:71:LEU:CD2	9:I:68:VAL:HG21	2.44	0.41
2:O:34:VAL:C	2:O:35:ILE:HD12	2.41	0.41
10:J:14:PHE:CD1	10:J:14:PHE:N	2.87	0.41
2:O:47:ILE:HG13	2:O:120:MET:CE	2.51	0.41
1:A:288:ALA:HB2	1:A:300:THR:HG22	2.02	0.41
1:A:405:ARG:O	1:A:409:GLU:HG3	2.20	0.41
9:I:62:ARG:HB3	9:I:63:PRO:HD2	2.02	0.41
3:P:162:GLU:OE2	3:P:168:PHE:CD1	2.73	0.41
2:B:95:LYS:HB2	9:I:32:ALA:CB	2.41	0.40
5:E:80:ASP:O	5:E:82:PRO:HD3	2.21	0.40
1:N:19:LEU:CD2	1:N:213:GLN:HG3	2.51	0.40
4:D:43:MET:HE2	4:D:46:VAL:HG21	2.01	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:56:LYS:HB3	10:J:56:LYS:HE2	1.76	0.40
4:Q:204:MET:HE3	20:Q:3006:PEE:O4	2.21	0.40
10:J:18:SER:OG	10:J:19:THR:N	2.55	0.40
3:P:223:TYR:HB3	4:Q:227:TRP:CZ2	2.56	0.40
4:Q:214:LEU:HA	20:T:3005:PEE:H361	2.03	0.40
9:V:62:ARG:HB2	9:V:78:TYR:CG	2.56	0.40
2:B:47:ILE:HG13	2:B:120:MET:CE	2.52	0.40
3:P:191:ALA:HA	3:P:194:MET:HE2	2.03	0.40
3:P:233:LEU:HD11	4:Q:219:VAL:HG21	2.03	0.40
9:V:70:LEU:HB3	22:V:1017:HOH:O	2.22	0.40
10:W:56:LYS:HE2	10:W:56:LYS:HB3	1.75	0.40
3:C:21:LEU:HD21	18:C:2002:UQ:CM3	2.52	0.40
5:E:188:THR:C	5:E:189:SER:O	2.60	0.40
14:P:501:HEM:HMC1	14:P:501:HEM:HBC2	2.02	0.40
10:W:14:PHE:N	10:W:14:PHE:CD1	2.89	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%)	425 (96%)	14 (3%)	2 (0%)	38	33
1	N	441/446 (99%)	425 (96%)	15 (3%)	1 (0%)	56	57
2	B	418/439 (95%)	409 (98%)	8 (2%)	1 (0%)	56	57
2	O	420/439 (96%)	406 (97%)	12 (3%)	2 (0%)	38	33
3	C	363/379 (96%)	354 (98%)	6 (2%)	3 (1%)	27	20
3	P	366/379 (97%)	353 (96%)	8 (2%)	5 (1%)	16	9
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%)	183 (94%)	7 (4%)	4 (2%)	11	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	R	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	38	33
6	F	97/110 (88%)	96 (99%)	1 (1%)	0	100	100
6	S	97/110 (88%)	96 (99%)	1 (1%)	0	100	100
7	G	73/81 (90%)	72 (99%)	1 (1%)	0	100	100
7	T	74/81 (91%)	69 (93%)	4 (5%)	1 (1%)	16	9
8	H	64/78 (82%)	61 (95%)	3 (5%)	0	100	100
8	U	64/78 (82%)	62 (97%)	1 (2%)	1 (2%)	14	7
9	I	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	8	2
9	V	38/78 (49%)	36 (95%)	1 (3%)	1 (3%)	8	2
10	J	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	14	6
10	W	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	14	6
All	All	3980/4220 (94%)	3851 (97%)	104 (3%)	25 (1%)	33	28

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	ASP
3	C	16	ASN
3	C	17	ALA
9	I	41	PRO
10	J	61	ASN
1	N	224	ASP
3	P	17	ALA
7	T	72	LYS
9	V	41	PRO
10	W	61	ASN
2	B	171	ALA
5	E	112	VAL
2	O	171	ALA
2	O	231	GLY
3	P	16	ASN
8	U	48	SER
5	R	189	SER
1	A	228	VAL
3	C	18	PHE
5	E	189	SER
5	E	191	ASP
3	P	11	MET

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Mol	Chain	Res	Type
3	P	18	PHE
5	E	82	PRO
3	P	13	ILE

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	364/370 (98%)	359 (99%)	5 (1%)	78	83
1	N	364/370 (98%)	359 (99%)	5 (1%)	78	83
2	B	332/343 (97%)	332 (100%)	0	100	100
2	O	332/343 (97%)	330 (99%)	2 (1%)	92	95
3	C	312/327 (95%)	307 (98%)	5 (2%)	75	79
3	P	316/327 (97%)	310 (98%)	6 (2%)	69	73
4	D	206/206 (100%)	203 (98%)	3 (2%)	76	81
4	Q	206/206 (100%)	203 (98%)	3 (2%)	76	81
5	E	168/168 (100%)	167 (99%)	1 (1%)	92	95
5	R	168/168 (100%)	166 (99%)	2 (1%)	82	87
6	F	90/98 (92%)	89 (99%)	1 (1%)	84	88
6	S	90/98 (92%)	89 (99%)	1 (1%)	84	88
7	G	66/71 (93%)	65 (98%)	1 (2%)	76	81
7	T	66/71 (93%)	64 (97%)	2 (3%)	53	55
8	H	63/74 (85%)	61 (97%)	2 (3%)	51	52
8	U	63/74 (85%)	62 (98%)	1 (2%)	75	79
9	I	28/60 (47%)	27 (96%)	1 (4%)	47	46
9	V	28/60 (47%)	26 (93%)	2 (7%)	21	16
10	J	51/52 (98%)	49 (96%)	2 (4%)	43	43
10	W	51/52 (98%)	49 (96%)	2 (4%)	43	43
All	All	3364/3538 (95%)	3317 (99%)	47 (1%)	78	83

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	149	VAL
1	A	245	GLU
1	A	281	ASP
1	A	308	GLN
3	C	80	ARG
3	C	90	PHE
3	C	128	PHE
3	C	222	PRO
3	C	379	TRP
4	D	17	LEU
4	D	76	GLU
4	D	144	ARG
5	E	80	ASP
6	F	58	ARG
7	G	45	ILE
8	H	47	ARG
8	H	51	GLU
9	I	42	VAL
10	J	8	ARG
10	J	16	ARG
1	N	58	PHE
1	N	149	VAL
1	N	245	GLU
1	N	281	ASP
1	N	308	GLN
2	O	212	SER
2	O	236	LYS
3	P	12	LYS
3	P	43	LEU
3	P	80	ARG
3	P	90	PHE
3	P	222	PRO
3	P	379	TRP
4	Q	17	LEU
4	Q	35	GLN
4	Q	144	ARG
5	R	113	GLU
5	R	190	ASP
6	S	58	ARG
7	T	45	ILE
7	T	73	ASN
8	U	46	SER

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Mol	Chain	Res	Type
9	V	42	VAL
9	V	52	ARG
10	W	8	ARG
10	W	25	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	61	HIS
1	A	136	GLN
1	A	213	GLN
1	A	271	GLN
1	A	289	HIS
2	B	22	GLN
2	B	104	ASN
2	B	343	GLN
2	B	412	ASN
3	C	68	HIS
3	C	159	ASN
4	D	106	ASN
5	E	57	GLN
5	E	116	GLN
7	G	73	ASN
1	N	15	GLN
1	N	61	HIS
1	N	136	GLN
1	N	165	GLN
1	N	213	GLN
1	N	271	GLN
2	O	104	ASN
2	O	240	HIS
2	O	343	GLN
2	O	412	ASN
3	P	68	HIS
3	P	159	ASN
4	Q	106	ASN
4	Q	121	HIS
5	R	57	GLN
6	S	73	GLN
7	T	28	HIS
9	V	71	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

41 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
11	BHG	A	4002	-	18,18,18	1.83	4 (22%)	23,23,23	0.77	1 (4%)
20	PEE	A	4003	-	5,5,50	1.53	1 (20%)	5,5,55	14.35	2 (40%)
13	AZI	A	4005	-	2,2,2	1.79	0	0,1,1	0.00	-
21	GOL	B	2013	-	5,5,5	1.20	0	5,5,5	0.71	0
12	PO4	B	3010	-	4,4,4	0.74	0	6,6,6	0.83	0
17	SMA	C	2001	-	38,38,38	1.83	7 (18%)	50,52,52	1.94	7 (14%)
18	UQ	C	2002	-	14,14,63	2.64	8 (57%)	18,20,79	0.71	0
20	PEE	C	2007	-	48,48,50	1.17	5 (10%)	53,53,55	0.87	5 (9%)
11	BHG	C	2008	-	18,18,18	1.75	5 (27%)	23,23,23	0.71	0
21	GOL	C	2009	-	5,5,5	1.24	0	5,5,5	0.69	0
20	PEE	C	2012	-	4,4,50	1.91	2 (50%)	6,6,55	0.79	0
13	AZI	C	2014	-	2,2,2	2.11	1 (50%)	0,1,1	0.00	-
14	HEM	C	501	3	42,50,50	2.99	18 (42%)	27,82,82	2.09	6 (22%)
14	HEM	C	502	3	42,50,50	2.74	19 (45%)	27,82,82	1.75	7 (25%)
20	PEE	D	2006	-	50,50,50	1.22	7 (14%)	55,55,55	0.94	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	AZI	D	4004	-	2,2,2	1.75	0	0,1,1	0.00	-
15	HEC	D	501	4	50,50,50	3.01	12 (24%)	56,82,82	2.19	12 (21%)
16	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	BHG	F	3011	-	18,18,18	1.83	4 (22%)	23,23,23	0.74	0
11	BHG	F	4001	-	18,18,18	1.73	5 (27%)	23,23,23	0.70	0
19	CDL	G	2003	-	47,49,99	1.15	2 (4%)	57,61,111	1.36	6 (10%)
19	CDL	G	2004	-	41,43,99	1.17	2 (4%)	50,55,111	1.53	7 (14%)
20	PEE	G	2005	-	48,48,50	1.27	7 (14%)	53,53,55	0.98	6 (11%)
20	PEE	N	3012	-	4,4,50	1.83	2 (50%)	6,6,55	0.75	0
12	PO4	O	2010	-	4,4,4	0.78	0	6,6,6	0.82	0
21	GOL	O	3013	-	5,5,5	1.20	0	5,5,5	0.77	0
17	SMA	P	3001	-	38,38,38	2.08	10 (26%)	50,52,52	1.99	7 (14%)
18	UQ	P	3002	-	14,14,63	2.52	8 (57%)	18,20,79	0.55	0
20	PEE	P	3007	-	48,48,50	1.22	5 (10%)	53,53,55	0.86	4 (7%)
11	BHG	P	3008	-	18,18,18	1.76	5 (27%)	23,23,23	0.70	0
21	GOL	P	3009	-	5,5,5	1.26	0	5,5,5	0.68	0
13	AZI	P	3014	-	2,2,2	2.48	2 (100%)	0,1,1	0.00	-
14	HEM	P	501	3	42,50,50	2.79	15 (35%)	27,82,82	1.84	6 (22%)
14	HEM	P	502	3	42,50,50	2.89	16 (38%)	27,82,82	2.12	8 (29%)
19	CDL	Q	3003	-	47,49,99	1.13	4 (8%)	57,61,111	1.42	6 (10%)
20	PEE	Q	3006	-	50,50,50	1.21	6 (12%)	55,55,55	0.91	4 (7%)
15	HEC	Q	501	4	50,50,50	3.08	8 (16%)	56,82,82	1.99	8 (14%)
16	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
11	BHG	S	2011	-	18,18,18	1.77	3 (16%)	23,23,23	0.78	0
19	CDL	T	3004	-	46,48,99	1.19	4 (8%)	56,60,111	1.39	5 (8%)
20	PEE	T	3005	-	48,48,50	1.29	8 (16%)	53,53,55	0.95	6 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BHG	A	4002	-	1/1/5/5	0/9/29/29	0/1/1/1
20	PEE	A	4003	-	-	0/4/4/54	0/0/0/0
13	AZI	A	4005	-	-	0/0/0/0	0/0/0/0
21	GOL	B	2013	-	-	0/4/4/4	0/0/0/0
12	PO4	B	3010	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SMA	C	2001	-	-	0/33/34/34	0/2/2/2
18	UQ	C	2002	-	-	0/4/28/87	0/1/1/1
20	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
11	BHG	C	2008	-	1/1/5/5	0/9/29/29	0/1/1/1
21	GOL	C	2009	-	-	0/4/4/4	0/0/0/0
20	PEE	C	2012	-	-	0/0/0/54	0/0/0/0
13	AZI	C	2014	-	-	0/0/0/0	0/0/0/0
14	HEM	C	501	3	-	0/14/114/114	0/0/8/8
14	HEM	C	502	3	-	0/14/114/114	0/0/8/8
20	PEE	D	2006	-	-	0/54/54/54	0/0/0/0
13	AZI	D	4004	-	-	0/0/0/0	0/0/0/0
15	HEC	D	501	4	-	0/10/54/54	0/0/8/8
16	FES	E	501	5	-	0/0/4/4	0/1/1/1
11	BHG	F	3011	-	1/1/5/5	0/9/29/29	0/1/1/1
11	BHG	F	4001	-	1/1/5/5	0/9/29/29	0/1/1/1
19	CDL	G	2003	-	1/1/9/9	0/58/58/110	0/0/0/0
19	CDL	G	2004	-	1/1/9/9	0/52/52/110	0/0/0/0
20	PEE	G	2005	-	-	0/52/52/54	0/0/0/0
20	PEE	N	3012	-	-	0/0/0/54	0/0/0/0
12	PO4	O	2010	-	-	0/0/0/0	0/0/0/0
21	GOL	O	3013	-	-	0/4/4/4	0/0/0/0
17	SMA	P	3001	-	-	0/33/34/34	0/2/2/2
18	UQ	P	3002	-	-	0/4/28/87	0/1/1/1
20	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
11	BHG	P	3008	-	1/1/5/5	0/9/29/29	0/1/1/1
21	GOL	P	3009	-	-	0/4/4/4	0/0/0/0
13	AZI	P	3014	-	-	0/0/0/0	0/0/0/0
14	HEM	P	501	3	-	0/14/114/114	0/0/8/8
14	HEM	P	502	3	-	0/14/114/114	0/0/8/8
19	CDL	Q	3003	-	1/1/9/9	0/58/58/110	0/0/0/0
20	PEE	Q	3006	-	-	0/54/54/54	0/0/0/0
15	HEC	Q	501	4	-	0/10/54/54	0/0/8/8
16	FES	R	501	5	-	0/0/4/4	0/1/1/1
11	BHG	S	2011	-	1/1/5/5	0/9/29/29	0/1/1/1
19	CDL	T	3004	-	1/1/9/9	0/57/57/110	0/0/0/0
20	PEE	T	3005	-	-	0/52/52/54	0/0/0/0

All (205) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Q	501	HEC	C3B-CAB	13.99	1.53	1.34
15	Q	501	HEC	C3C-CAC	12.42	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	501	HEC	C3B-CAB	12.39	1.51	1.34
15	D	501	HEC	C3C-CAC	12.26	1.51	1.34
14	C	501	HEM	C3C-C2C	-9.63	1.37	1.45
14	P	501	HEM	C3B-C2B	-9.13	1.36	1.45
14	C	502	HEM	C3C-C2C	-8.79	1.38	1.45
14	P	502	HEM	C3B-C2B	-8.77	1.37	1.45
14	P	501	HEM	C3C-C2C	-8.34	1.38	1.45
14	C	501	HEM	C3B-C2B	-8.13	1.37	1.45
17	P	3001	SMA	C4-C4A	7.65	1.52	1.41
14	P	502	HEM	CMC-C2C	6.95	1.56	1.45
17	C	2001	SMA	C4-C4A	6.77	1.50	1.41
14	C	502	HEM	C3B-C2B	-6.43	1.39	1.45
15	Q	501	HEC	C3C-C2C	-6.25	1.34	1.40
18	P	3002	UQ	C6-C1	6.20	1.56	1.43
15	D	501	HEC	C3B-C2B	-6.15	1.34	1.40
18	C	2002	UQ	C6-C1	5.99	1.55	1.43
14	P	502	HEM	C1B-C2B	5.39	1.49	1.45
14	C	501	HEM	CMB-C2B	5.10	1.53	1.45
14	C	502	HEM	CMB-C2B	5.04	1.53	1.45
15	D	501	HEC	C3C-C2C	-5.03	1.35	1.40
14	P	502	HEM	CBB-CAB	4.91	1.57	1.29
14	P	501	HEM	CMC-C2C	4.89	1.53	1.45
14	P	501	HEM	CBB-CAB	4.85	1.56	1.29
11	F	3011	BHG	O1-C1	4.76	1.48	1.40
11	S	2011	BHG	O1-C1	4.66	1.48	1.40
11	A	4002	BHG	O1-C1	4.64	1.48	1.40
14	P	502	HEM	CMD-C2D	4.53	1.52	1.45
14	C	502	HEM	CMD-C2D	4.53	1.52	1.45
14	C	501	HEM	CBB-CAB	4.47	1.54	1.29
14	C	501	HEM	CBC-CAC	4.39	1.54	1.29
11	P	3008	BHG	O1-C1	4.38	1.48	1.40
14	C	502	HEM	CBB-CAB	4.36	1.53	1.29
11	C	2008	BHG	O1-C1	4.36	1.48	1.40
11	F	4001	BHG	O1-C1	4.31	1.48	1.40
14	C	502	HEM	CBC-CAC	4.28	1.53	1.29
17	P	3001	SMA	O1-C2	4.26	1.40	1.35
17	P	3001	SMA	C20-C19	4.23	1.35	1.33
14	P	502	HEM	C3C-C2C	-4.20	1.42	1.45
14	C	501	HEM	CMD-C2D	4.19	1.52	1.45
14	P	502	HEM	CBC-CAC	4.12	1.52	1.29
14	P	501	HEM	CBC-CAC	4.04	1.52	1.29
14	C	501	HEM	C1B-C2B	3.96	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	502	HEM	C1A-NA	3.82	1.42	1.36
14	P	501	HEM	CMB-C2B	3.77	1.51	1.45
15	Q	501	HEC	C3B-C4B	3.74	1.51	1.42
14	C	501	HEM	CHC-C4B	-3.74	1.35	1.39
14	C	501	HEM	CMC-C2C	3.72	1.51	1.45
14	C	501	HEM	C1A-C2A	3.68	1.49	1.43
11	S	2011	BHG	O5-C1	3.67	1.51	1.41
14	P	501	HEM	C3D-C2D	-3.63	1.34	1.43
14	P	502	HEM	C4C-NC	3.58	1.42	1.33
15	Q	501	HEC	C3B-C2B	-3.58	1.37	1.40
18	P	3002	UQ	C7-C6	3.54	1.57	1.40
18	C	2002	UQ	C7-C6	3.53	1.57	1.40
11	F	3011	BHG	O5-C1	3.51	1.50	1.41
14	P	502	HEM	C1A-C2A	3.51	1.49	1.43
17	C	2001	SMA	C4-C3	3.49	1.51	1.41
17	C	2001	SMA	C20-C19	3.46	1.35	1.33
14	P	502	HEM	C1C-NC	3.45	1.42	1.33
17	P	3001	SMA	C4-C3	3.43	1.51	1.41
14	P	501	HEM	C4C-NC	3.38	1.42	1.33
14	C	502	HEM	C4D-ND	3.35	1.42	1.33
17	C	2001	SMA	O1-C2	3.33	1.39	1.35
11	A	4002	BHG	O5-C1	3.32	1.50	1.41
14	P	502	HEM	C4A-C3A	3.30	1.48	1.43
20	D	2006	PEE	O3-C30	3.22	1.43	1.33
11	F	4001	BHG	O5-C1	3.21	1.50	1.41
14	P	501	HEM	C4A-C3A	3.19	1.48	1.43
14	C	502	HEM	CMC-C2C	3.18	1.50	1.45
11	C	2008	BHG	O5-C1	3.17	1.49	1.41
14	C	502	HEM	C1C-NC	3.17	1.41	1.33
11	P	3008	BHG	O5-C1	3.16	1.49	1.41
14	P	502	HEM	C3D-C2D	-3.16	1.35	1.43
14	P	501	HEM	C4A-NA	3.16	1.41	1.36
14	C	502	HEM	CHC-C4B	-3.16	1.36	1.39
20	P	3007	PEE	O3-C30	3.07	1.42	1.33
17	P	3001	SMA	C4A-C8A	3.06	1.45	1.41
17	P	3001	SMA	C6-C7	3.05	1.44	1.38
18	C	2002	UQ	C3-C4	3.02	1.57	1.48
18	C	2002	UQ	C2-C1	3.01	1.57	1.48
14	C	501	HEM	C3D-C2D	-2.99	1.35	1.43
20	C	2007	PEE	O3-C30	2.96	1.42	1.33
20	P	3007	PEE	P-O1P	2.95	1.62	1.51
20	Q	3006	PEE	C19-C18	-2.95	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Q	3006	PEE	O3-C30	2.91	1.42	1.33
17	C	2001	SMA	C6-C7	2.90	1.44	1.38
18	C	2002	UQ	O3-C3	2.88	1.44	1.37
15	Q	501	HEC	C4D-ND	2.86	1.41	1.36
20	G	2005	PEE	C22-C21	-2.85	1.34	1.51
17	C	2001	SMA	C7-C8	2.85	1.44	1.40
15	D	501	HEC	C4D-C3D	2.84	1.48	1.43
20	T	3005	PEE	C22-C21	-2.84	1.34	1.51
20	Q	3006	PEE	C22-C21	-2.83	1.34	1.51
20	D	2006	PEE	C19-C18	-2.83	1.34	1.51
20	T	3005	PEE	O3-C30	2.82	1.41	1.33
20	C	2007	PEE	C19-C18	-2.81	1.34	1.51
20	Q	3006	PEE	P-O1P	2.81	1.61	1.51
14	P	502	HEM	CMB-C2B	2.81	1.50	1.45
14	C	501	HEM	C1D-ND	2.80	1.40	1.33
20	G	2005	PEE	C19-C18	-2.80	1.34	1.51
20	D	2006	PEE	P-O1P	2.80	1.61	1.51
20	T	3005	PEE	P-O1P	2.79	1.61	1.51
14	C	501	HEM	C4D-C3D	2.78	1.50	1.43
15	Q	501	HEC	C1C-C2C	2.78	1.48	1.43
20	D	2006	PEE	C22-C21	-2.77	1.34	1.51
20	P	3007	PEE	C19-C18	-2.76	1.34	1.51
14	P	502	HEM	C3C-C4C	-2.76	1.43	1.45
20	P	3007	PEE	C22-C21	-2.76	1.34	1.51
18	C	2002	UQ	CM5-C5	2.74	1.56	1.50
20	T	3005	PEE	C19-C18	-2.72	1.35	1.51
20	G	2005	PEE	P-O1P	2.71	1.61	1.51
15	D	501	HEC	C3C-C4C	2.70	1.49	1.42
20	C	2007	PEE	C22-C21	-2.69	1.35	1.51
18	P	3002	UQ	CM5-C5	2.68	1.56	1.50
14	C	502	HEM	C1D-ND	2.68	1.40	1.33
13	P	3014	AZI	N1-N2	-2.66	1.11	1.21
17	P	3001	SMA	C7-C8	2.66	1.44	1.40
20	G	2005	PEE	O3-C30	2.64	1.41	1.33
20	G	2005	PEE	O2-C10	2.64	1.42	1.34
14	C	501	HEM	C3C-C4C	-2.63	1.43	1.45
20	C	2007	PEE	P-O1P	2.63	1.61	1.51
20	D	2006	PEE	O2-C10	2.62	1.42	1.34
20	Q	3006	PEE	O2-C10	2.61	1.42	1.34
20	T	3005	PEE	O2-C10	2.60	1.42	1.34
18	P	3002	UQ	C2-C1	2.59	1.56	1.48
18	C	2002	UQ	O2-C2	2.59	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	501	HEC	C4D-ND	2.58	1.40	1.36
15	D	501	HEC	C1D-C2D	2.56	1.47	1.43
11	P	3008	BHG	C4-C5	2.56	1.58	1.53
20	P	3007	PEE	O2-C10	2.55	1.42	1.34
19	T	3004	CDL	CB3-CB4	2.54	1.57	1.50
17	P	3001	SMA	C8-C8A	2.54	1.43	1.41
20	C	2007	PEE	O2-C10	2.52	1.41	1.34
11	A	4002	BHG	C4-C5	2.49	1.58	1.53
15	D	501	HEC	C1A-C2A	2.48	1.48	1.42
14	C	501	HEM	C4A-C3A	2.48	1.47	1.43
14	C	502	HEM	C3D-C2D	-2.46	1.37	1.43
19	G	2004	CDL	O1-C1	2.45	1.51	1.43
17	C	2001	SMA	C4A-C8A	2.44	1.44	1.41
11	C	2008	BHG	C4-C5	2.43	1.58	1.53
11	S	2011	BHG	O5-C5	2.43	1.50	1.44
19	T	3004	CDL	OB8-CB6	-2.40	1.39	1.45
13	C	2014	AZI	N1-N2	-2.40	1.12	1.21
15	Q	501	HEC	C3C-C4C	2.36	1.48	1.42
18	P	3002	UQ	C3-C4	2.36	1.55	1.48
14	P	501	HEM	C1C-NC	2.36	1.39	1.33
20	C	2012	PEE	P-O4P	2.35	1.63	1.52
14	P	501	HEM	C4D-C3D	2.33	1.49	1.43
19	T	3004	CDL	OA8-CA6	-2.32	1.39	1.45
11	F	4001	BHG	C4-C5	2.32	1.58	1.53
15	D	501	HEC	C1B-NB	2.32	1.40	1.36
19	T	3004	CDL	O1-C1	2.31	1.50	1.43
14	C	502	HEM	FE-NB	2.31	2.03	1.95
20	G	2005	PEE	C3-C2	2.31	1.57	1.50
14	P	501	HEM	CMD-C2D	2.29	1.49	1.45
13	P	3014	AZI	N3-N2	-2.29	1.13	1.21
11	A	4002	BHG	O5-C5	2.29	1.50	1.44
18	P	3002	UQ	O2-C2	2.29	1.43	1.37
14	C	501	HEM	C1C-C2C	2.28	1.49	1.43
20	T	3005	PEE	C3-C2	2.27	1.57	1.50
14	P	501	HEM	C1A-C2A	2.28	1.47	1.43
20	G	2005	PEE	C1-C2	2.27	1.57	1.50
18	P	3002	UQ	O3-C3	2.27	1.43	1.37
20	N	3012	PEE	P-O4P	2.26	1.63	1.52
19	G	2003	CDL	CA3-CA4	2.26	1.57	1.50
11	F	3011	BHG	C4-C5	2.26	1.58	1.53
14	C	502	HEM	C1A-C2A	2.24	1.47	1.43
11	F	3011	BHG	O5-C5	2.23	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	502	HEM	C1D-C2D	2.23	1.49	1.43
20	Q	3006	PEE	C3-C2	2.23	1.57	1.50
20	C	2012	PEE	P-O3P	2.23	1.63	1.52
19	Q	3003	CDL	CA3-CA4	2.20	1.56	1.50
20	D	2006	PEE	C3-C2	2.19	1.56	1.50
20	N	3012	PEE	P-O3P	2.19	1.63	1.52
18	P	3002	UQ	C5-C4	2.18	1.55	1.46
19	Q	3003	CDL	O1-C1	2.18	1.50	1.43
20	T	3005	PEE	C1-C2	2.17	1.56	1.50
18	C	2002	UQ	C5-C4	2.15	1.55	1.46
17	P	3001	SMA	C6-C5	2.14	1.45	1.37
20	A	4003	PEE	O2-C2	2.13	1.48	1.43
15	D	501	HEC	C3B-C4B	2.11	1.47	1.42
14	C	502	HEM	C1A-NA	2.11	1.39	1.36
19	G	2003	CDL	O1-C1	2.10	1.50	1.43
14	P	502	HEM	C1D-C2D	2.09	1.49	1.43
17	P	3001	SMA	C9-C2	-2.08	1.48	1.50
14	C	502	HEM	C4D-C3D	2.08	1.49	1.43
14	C	501	HEM	C1A-NA	2.07	1.39	1.36
14	C	502	HEM	C1B-C2B	2.06	1.46	1.45
11	C	2008	BHG	O5-C5	2.06	1.49	1.44
20	D	2006	PEE	C31-C30	2.06	1.56	1.50
11	P	3008	BHG	O5-C5	2.05	1.49	1.44
14	C	501	HEM	C1C-NC	2.04	1.38	1.33
19	Q	3003	CDL	OA8-CA6	-2.04	1.40	1.45
11	F	4001	BHG	O5-C5	2.04	1.49	1.44
15	D	501	HEC	C4C-NC	2.04	1.39	1.36
11	F	4001	BHG	C1-C2	2.04	1.58	1.52
19	G	2004	CDL	OA8-CA6	-2.02	1.40	1.45
19	Q	3003	CDL	OB8-CB6	-2.02	1.40	1.45
14	P	501	HEM	C1A-NA	2.01	1.39	1.36
14	C	502	HEM	C4C-NC	2.01	1.38	1.33
11	P	3008	BHG	C1-C2	2.01	1.58	1.52
20	T	3005	PEE	C31-C30	2.01	1.56	1.50
11	C	2008	BHG	C1-C2	2.00	1.58	1.52

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	4003	PEE	O2-C2-C1	-24.49	110.39	119.54
20	A	4003	PEE	O2-C2-C3	-20.68	111.82	119.54
15	D	501	HEC	CBB-CAB-C3B	-8.92	107.87	127.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	501	HEC	CBB-CAB-C3B	-8.78	108.16	127.36
15	D	501	HEC	CBC-CAC-C3C	-8.03	109.80	127.36
17	P	3001	SMA	C9-C2-C3	8.02	130.10	120.42
17	C	2001	SMA	C9-C2-C3	8.01	130.09	120.42
14	C	501	HEM	C3A-C4A-NA	6.26	113.68	109.50
17	P	3001	SMA	C9-C10-C11	-6.03	105.94	114.60
14	C	501	HEM	C4A-C3A-C2A	-5.84	102.93	107.00
15	Q	501	HEC	CBC-CAC-C3C	-5.72	114.85	127.36
17	C	2001	SMA	C9-C10-C11	-5.47	106.74	114.60
14	P	501	HEM	C3A-C4A-NA	5.05	112.87	109.50
17	P	3001	SMA	C3-C4-C4A	-5.00	114.62	121.30
17	C	2001	SMA	C3-C4-C4A	-4.81	114.88	121.30
14	C	502	HEM	CBD-CAD-C3D	-4.72	104.27	114.51
14	P	502	HEM	C4A-NA-C1A	-4.64	102.16	107.93
14	P	502	HEM	CMA-C3A-C4A	-4.55	121.48	128.46
19	T	3004	CDL	OA4-PA1-OA3	-4.51	105.23	118.70
14	P	502	HEM	C3A-C4A-NA	4.51	112.51	109.50
19	Q	3003	CDL	OA4-PA1-OA3	-4.49	105.28	118.70
15	Q	501	HEC	C4D-ND-C1D	-4.46	102.83	107.12
17	P	3001	SMA	O1-C2-C9	-4.43	105.83	112.08
19	G	2003	CDL	OB4-PB2-OB3	-4.41	105.53	118.70
19	Q	3003	CDL	OB4-PB2-OB3	-4.41	105.55	118.70
19	G	2004	CDL	OB4-PB2-OB3	-4.39	105.61	118.70
19	G	2003	CDL	OA4-PA1-OA3	-4.36	105.69	118.70
19	G	2004	CDL	OA4-PA1-OA3	-4.35	105.72	118.70
19	T	3004	CDL	OB4-PB2-OB3	-4.27	105.96	118.70
19	G	2004	CDL	CB4-OB6-CB5	-4.26	109.83	117.68
15	D	501	HEC	C2B-C1B-NB	4.25	112.34	109.50
14	C	502	HEM	C3A-C4A-NA	4.18	112.29	109.50
14	P	501	HEM	C4A-NA-C1A	-4.18	102.73	107.93
17	C	2001	SMA	O1-C2-C9	-4.16	106.22	112.08
15	Q	501	HEC	C2B-C1B-NB	3.99	112.16	109.50
19	Q	3003	CDL	CA4-OA6-CA5	-3.71	110.83	117.68
19	T	3004	CDL	CB4-OB6-CB5	-3.71	110.84	117.68
14	P	501	HEM	C4A-C3A-C2A	-3.61	104.48	107.00
19	G	2003	CDL	CA4-OA6-CA5	-3.47	111.28	117.68
15	D	501	HEC	CMD-C2D-C1D	-3.37	123.28	128.46
15	Q	501	HEC	C2D-C1D-ND	3.31	111.71	109.50
14	C	501	HEM	CBA-CAA-C2A	-3.30	107.13	112.63
14	C	501	HEM	C1A-C2A-C3A	3.25	110.29	106.92
17	P	3001	SMA	O1-C2-C3	3.21	124.05	120.32
19	T	3004	CDL	CA4-OA6-CA5	-3.17	110.42	117.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D	501	HEC	C2C-C1C-NC	3.14	111.60	109.50
15	D	501	HEC	C4D-ND-C1D	-3.14	104.10	107.12
15	D	501	HEC	C3A-C4A-NA	3.09	113.63	109.32
14	P	502	HEM	CMC-C2C-C3C	3.09	131.57	124.26
14	P	502	HEM	C1A-C2A-C3A	-3.08	103.73	106.92
19	Q	3003	CDL	CB6-CB4-CB3	-3.05	104.86	111.86
20	G	2005	PEE	O4P-C4-C5	3.05	114.29	109.37
14	P	502	HEM	CMA-C3A-C2A	2.98	130.56	124.94
17	C	2001	SMA	O1-C2-C3	2.87	123.66	120.32
19	G	2003	CDL	CB4-OB6-CB5	-2.85	111.16	117.86
19	Q	3003	CDL	CA6-OA8-CA7	-2.84	111.59	116.47
19	G	2004	CDL	CA6-CA4-CA3	-2.83	105.37	111.86
19	Q	3003	CDL	CB4-OB6-CB5	-2.74	111.41	117.86
14	P	502	HEM	C2A-C1A-NA	2.74	113.54	109.73
14	C	502	HEM	CMA-C3A-C2A	2.73	130.09	124.94
19	G	2003	CDL	CA6-OA8-CA7	-2.69	111.85	116.47
14	C	502	HEM	CMA-C3A-C4A	-2.67	124.35	128.46
19	G	2004	CDL	OA6-CA5-C11	2.66	113.82	110.46
20	P	3007	PEE	C20-C19-C18	2.66	128.70	114.56
20	T	3005	PEE	C20-C19-C18	2.65	128.66	114.56
14	C	502	HEM	CMC-C2C-C3C	2.64	130.50	124.26
20	C	2007	PEE	C20-C19-C18	2.64	128.58	114.56
17	C	2001	SMA	C10-C9-C2	2.64	119.95	113.35
20	T	3005	PEE	O4P-C4-C5	2.62	113.61	109.37
17	P	3001	SMA	C10-C9-C2	2.62	119.92	113.35
20	G	2005	PEE	C20-C19-C18	2.60	128.39	114.56
14	C	502	HEM	C4A-NA-C1A	-2.60	104.70	107.93
15	D	501	HEC	CMA-C3A-C2A	2.59	129.83	124.94
20	P	3007	PEE	C19-C18-C17	2.56	128.15	114.56
20	D	2006	PEE	O4P-C4-C5	2.55	113.49	109.37
14	P	501	HEM	CMC-C2C-C3C	2.53	130.25	124.26
20	D	2006	PEE	C20-C19-C18	2.53	128.00	114.56
20	T	3005	PEE	C19-C18-C17	2.53	128.00	114.56
15	D	501	HEC	C2D-C1D-ND	2.53	111.19	109.50
20	Q	3006	PEE	C19-C18-C17	2.51	127.91	114.56
20	Q	3006	PEE	C20-C19-C18	2.47	127.67	114.56
20	C	2007	PEE	C19-C18-C17	2.46	127.63	114.56
19	G	2003	CDL	CB6-CB4-CB3	-2.45	106.23	111.86
14	C	501	HEM	C4A-NA-C1A	-2.44	104.90	107.93
20	G	2005	PEE	C19-C18-C17	2.44	127.50	114.56
17	C	2001	SMA	C3M-C3-C4	-2.42	117.00	121.04
20	D	2006	PEE	C19-C18-C17	2.40	127.32	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	Q	501	HEC	CMC-C2C-C1C	-2.40	124.77	128.46
19	T	3004	CDL	CB6-OB8-CB7	-2.39	112.36	116.47
14	P	501	HEM	CMA-C3A-C2A	2.38	129.43	124.94
20	D	2006	PEE	C22-C21-C20	2.37	127.13	114.56
17	P	3001	SMA	C3M-C3-C4	-2.35	117.11	121.04
15	D	501	HEC	C4B-C3B-C2B	2.34	108.88	106.35
20	P	3007	PEE	C22-C21-C20	2.34	126.99	114.56
20	C	2007	PEE	C22-C21-C20	2.33	126.95	114.56
20	C	2007	PEE	C23-C22-C21	2.32	126.88	114.56
19	G	2004	CDL	CA4-OA6-CA5	-2.31	112.42	117.86
20	P	3007	PEE	C23-C22-C21	2.30	126.80	114.56
20	G	2005	PEE	C22-C21-C20	2.30	126.78	114.56
20	T	3005	PEE	C22-C21-C20	2.30	126.77	114.56
15	D	501	HEC	CMD-C2D-C3D	2.29	129.26	124.94
14	C	501	HEM	CAA-C2A-C3A	-2.28	122.48	129.00
14	P	502	HEM	CBD-CAD-C3D	-2.25	109.63	114.51
20	G	2005	PEE	O4P-P-O3P	2.24	111.05	104.68
20	Q	3006	PEE	C22-C21-C20	2.22	126.36	114.56
20	G	2005	PEE	C23-C22-C21	2.18	126.14	114.56
19	G	2004	CDL	CB6-CB4-CB3	-2.17	106.88	111.86
20	T	3005	PEE	O3-C3-C2	2.16	114.49	108.80
20	T	3005	PEE	C23-C22-C21	2.15	126.00	114.56
20	C	2007	PEE	O4P-C4-C5	2.13	112.80	109.37
15	Q	501	HEC	C1D-C2D-C3D	2.12	108.47	107.00
14	P	501	HEM	CAD-C3D-C4D	2.12	128.59	125.60
15	D	501	HEC	C3B-C2B-C1B	-2.11	104.88	107.11
15	Q	501	HEC	CBA-CAA-C2A	-2.11	109.12	112.63
20	D	2006	PEE	C23-C22-C21	2.08	125.63	114.56
14	C	502	HEM	C4A-C3A-C2A	-2.08	105.55	107.00
20	Q	3006	PEE	C23-C22-C21	2.08	125.58	114.56
11	A	4002	BHG	C1'-O1-C1	2.04	117.51	113.91

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	F	3011	BHG	C4
19	Q	3003	CDL	CA4
11	S	2011	BHG	C4
11	P	3008	BHG	C4
11	C	2008	BHG	C4
19	G	2004	CDL	CA4
11	F	4001	BHG	C4

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Mol	Chain	Res	Type	Atom
11	A	4002	BHG	C4
19	T	3004	CDL	CA4
19	G	2003	CDL	CA4

There are no torsion outliers.

There are no ring outliers.

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%)	0.24	23 (5%)	26 29	27, 43, 65, 115	1 (0%)
1	N	442/446 (99%)	0.38	25 (5%)	23 25	28, 43, 63, 128	1 (0%)
2	B	424/439 (96%)	0.25	18 (4%)	35 39	29, 45, 67, 132	0
2	O	424/439 (96%)	0.25	23 (5%)	25 27	33, 47, 73, 162	0
3	C	365/379 (96%)	0.29	5 (1%)	72 76	25, 34, 47, 106	0
3	P	370/379 (97%)	0.41	26 (7%)	16 18	26, 34, 52, 165	0
4	D	241/241 (100%)	0.07	5 (2%)	60 65	28, 39, 59, 80	0
4	Q	241/241 (100%)	0.14	15 (6%)	20 22	28, 38, 59, 81	0
5	E	196/196 (100%)	0.72	30 (15%)	3 3	29, 54, 96, 117	0
5	R	196/196 (100%)	0.42	19 (9%)	8 9	29, 43, 61, 85	0
6	F	99/110 (90%)	0.35	6 (6%)	21 23	29, 44, 70, 80	0
6	S	99/110 (90%)	0.42	7 (7%)	16 17	28, 39, 79, 109	0
7	G	75/81 (92%)	0.39	4 (5%)	25 28	31, 50, 72, 80	0
7	T	76/81 (93%)	0.98	10 (13%)	4 5	30, 50, 97, 117	0
8	H	66/78 (84%)	1.04	13 (19%)	2 1	40, 55, 87, 101	0
8	U	66/78 (84%)	0.49	8 (12%)	5 6	40, 54, 79, 89	0
9	I	42/78 (53%)	2.18	19 (45%)	1 1	40, 75, 88, 93	0
9	V	42/78 (53%)	1.80	13 (30%)	1 1	45, 72, 92, 97	0
10	J	62/62 (100%)	1.14	15 (24%)	1 1	35, 60, 85, 116	0
10	W	62/62 (100%)	0.71	9 (14%)	3 3	34, 51, 80, 111	0
All	All	4030/4220 (95%)	0.39	293 (7%)	15 16	25, 42, 76, 165	2 (0%)

All (293) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	76	ALA	28.3
10	J	1	VAL	17.7
1	N	1	THR	11.7
3	P	13	ILE	11.3
1	A	222	THR	10.7
10	W	2	ALA	8.9
1	N	229	PRO	8.1
2	O	233	SER	7.7
7	T	73	ASN	7.4
3	P	16	ASN	7.2
5	E	194	ILE	7.1
10	W	1	VAL	7.1
5	R	89	PHE	7.1
6	S	12	TRP	6.6
5	E	71	MET	6.4
3	P	14	VAL	6.3
10	J	2	ALA	6.3
2	O	232	LEU	6.1
9	I	78	TYR	6.1
7	T	75	ALA	6.0
1	A	1	THR	5.7
3	C	17	ALA	5.7
9	I	63	PRO	5.6
2	O	19	PRO	5.6
5	E	76	ILE	5.6
1	N	222	THR	5.4
3	P	11	MET	5.3
9	I	59	ALA	5.2
2	B	41	TYR	5.2
9	V	42	VAL	5.2
3	P	10	LEU	5.1
9	I	62	ARG	5.1
1	N	2	ALA	5.1
2	O	234	GLY	4.9
9	V	78	TYR	4.8
5	R	74	ILE	4.8
6	F	13	LEU	4.8
10	J	62	LYS	4.7
9	V	32	ALA	4.6
1	A	219	LEU	4.6
8	H	49	GLN	4.5
9	I	60	ALA	4.4
10	J	3	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
5	R	96	LEU	4.4
4	Q	241	LYS	4.4
1	N	227	ALA	4.3
10	W	62	LYS	4.3
1	A	226	ASP	4.3
10	J	16	ARG	4.2
1	A	122	LEU	4.1
10	W	61	ASN	4.1
2	B	233	SER	4.1
1	A	186	LEU	4.1
5	E	112	VAL	4.1
6	F	109	LYS	4.1
9	I	61	GLY	4.0
1	A	2	ALA	3.9
6	S	110	LYS	3.9
8	H	47	ARG	3.9
4	Q	73	GLY	3.9
8	U	45	SER	3.9
10	J	5	LEU	3.8
2	B	304	HIS	3.8
10	J	22	LEU	3.8
5	E	103	LYS	3.8
1	N	99	ILE	3.8
9	I	77	ARG	3.8
5	E	70	ALA	3.8
2	O	17	VAL	3.7
1	N	113	LEU	3.7
1	A	190	TYR	3.7
2	O	229	GLY	3.7
5	E	75	GLU	3.7
5	R	88	ALA	3.7
7	T	74	PRO	3.6
5	E	80	ASP	3.6
5	E	110	ALA	3.6
5	R	196	GLY	3.6
2	B	344	VAL	3.6
8	H	61	PHE	3.5
5	E	108	GLN	3.5
1	A	187	SER	3.5
2	B	336	VAL	3.5
9	I	76	VAL	3.5
5	R	87	MET	3.4

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Mol	Chain	Res	Type	RSRZ
5	R	98	VAL	3.4
9	V	34	VAL	3.4
7	T	34	ILE	3.4
3	P	168	PHE	3.3
6	S	13	LEU	3.3
10	J	12	LEU	3.3
8	U	48	SER	3.3
2	O	230	LEU	3.3
5	R	76	ILE	3.3
5	E	195	VAL	3.3
9	V	63	PRO	3.3
5	E	92	ARG	3.3
9	I	70	LEU	3.2
1	N	75	LEU	3.2
9	V	33	ALA	3.2
9	I	35	PRO	3.2
1	N	342	TRP	3.2
1	A	443	TRP	3.2
2	B	19	PRO	3.2
2	O	41	TYR	3.2
5	E	74	ILE	3.1
1	A	125	SER	3.1
4	Q	1	SER	3.1
1	A	127	ILE	3.1
1	A	225	GLU	3.1
6	F	110	LYS	3.1
3	P	19	ILE	3.1
9	I	49	VAL	3.1
4	Q	76	GLU	3.1
9	I	32	ALA	3.1
5	E	191	ASP	3.0
2	O	235	ALA	3.0
9	V	62	ARG	3.0
10	W	30	PHE	3.0
5	E	186	GLU	3.0
5	R	194	ILE	3.0
1	N	216	PHE	3.0
5	R	85	LYS	3.0
1	A	224	ASP	3.0
9	V	48	SER	3.0
5	R	75	GLU	2.9
3	P	208	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	20	HIS	2.9
4	Q	141	VAL	2.9
5	R	97	PHE	2.9
4	D	241	LYS	2.9
2	O	215	VAL	2.9
10	J	21	ALA	2.9
8	U	51	GLU	2.9
9	V	70	LEU	2.9
8	U	47	ARG	2.9
3	P	31	TRP	2.9
3	P	12	LYS	2.9
3	P	104	TYR	2.9
4	Q	79	GLU	2.9
5	R	195	VAL	2.9
1	A	128	GLU	2.9
5	R	90	LYS	2.9
2	O	12	GLU	2.8
5	R	134	ILE	2.8
1	N	51	LYS	2.8
8	H	29	LYS	2.8
1	A	227	ALA	2.8
3	P	26	ASN	2.8
2	O	18	PRO	2.8
3	P	29	SER	2.8
4	Q	2	ASP	2.8
1	N	102	LEU	2.8
1	A	124	ASP	2.8
3	P	25	SER	2.8
3	P	314	SER	2.8
1	N	228	VAL	2.8
9	V	49	VAL	2.8
2	O	24	LEU	2.8
6	S	14	GLU	2.8
6	S	70	MET	2.8
3	P	17	ALA	2.7
1	N	226	ASP	2.7
5	E	132	TRP	2.7
8	H	46	SER	2.7
2	O	369	LEU	2.7
3	P	27	ILE	2.7
3	C	18	PHE	2.7
7	T	30	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	350	GLY	2.7
2	O	236	LYS	2.7
1	N	206	ARG	2.7
8	U	50	THR	2.7
5	E	190	ASP	2.7
4	D	144	ARG	2.7
7	T	42	ARG	2.6
4	Q	81	PHE	2.6
4	Q	3	LEU	2.6
7	T	70	LYS	2.6
8	H	28	GLU	2.6
1	N	224	ASP	2.6
7	G	74	PRO	2.6
5	E	111	ALA	2.6
3	P	218	ILE	2.6
7	T	72	LYS	2.6
3	P	15	ASN	2.6
6	F	16	ILE	2.6
4	Q	227	TRP	2.6
5	E	104	LYS	2.6
1	N	225	GLU	2.6
1	A	392	LEU	2.6
1	N	387	GLY	2.6
4	Q	75	ASN	2.6
9	V	35	PRO	2.6
4	Q	229	VAL	2.6
2	O	21	PRO	2.5
1	A	220	SER	2.5
1	N	221	GLY	2.5
1	N	415	PHE	2.5
10	W	3	PRO	2.5
3	P	207	ASN	2.5
1	N	109	ALA	2.5
7	G	56	TYR	2.5
1	N	312	ILE	2.5
2	B	337	ILE	2.5
5	E	91	TRP	2.5
1	N	52	ASN	2.5
10	J	24	ILE	2.5
5	E	72	SER	2.4
4	D	145	GLU	2.4
5	E	133	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
8	H	48	SER	2.4
6	S	16	ILE	2.4
6	S	109	LYS	2.4
9	V	41	PRO	2.4
4	Q	77	ASP	2.4
1	A	216	PHE	2.4
3	C	102	LEU	2.4
1	N	97	TYR	2.4
1	A	129	LYS	2.4
3	P	316	MET	2.4
5	E	89	PHE	2.4
1	N	208	LEU	2.4
8	U	49	GLN	2.4
2	O	211	VAL	2.4
5	E	193	VAL	2.4
9	I	75	SER	2.4
5	R	71	MET	2.4
3	P	28	SER	2.3
10	J	11	SER	2.3
8	H	31	VAL	2.3
4	Q	86	LYS	2.3
8	U	71	HIS	2.3
2	B	411	ILE	2.3
9	I	72	VAL	2.3
8	H	25	GLU	2.3
2	O	265	GLY	2.3
2	B	347	ILE	2.3
2	B	439	LEU	2.3
3	P	102	LEU	2.3
5	R	135	LEU	2.3
8	U	27	LEU	2.3
10	J	13	LEU	2.3
2	B	249	GLY	2.3
5	E	107	ASP	2.3
2	B	348	ALA	2.3
5	E	184	SER	2.3
5	R	189	SER	2.3
2	O	26	PHE	2.2
2	B	12	GLU	2.2
10	W	8	ARG	2.2
8	H	14	VAL	2.2
5	E	113	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	O	214	PRO	2.2
2	B	281	ALA	2.2
10	J	15	ARG	2.2
3	P	209	THR	2.2
1	A	68	LYS	2.2
5	R	86	ASN	2.2
3	C	130	GLY	2.2
2	B	352	LEU	2.2
3	C	31	TRP	2.2
2	B	251	SER	2.2
3	P	210	GLY	2.1
8	H	30	CYS	2.1
1	A	365	LEU	2.1
10	J	9	LEU	2.1
2	O	218	GLN	2.1
3	P	103	TYR	2.1
2	O	38	LEU	2.1
8	H	24	CYS	2.1
10	W	29	LEU	2.1
4	D	174	GLY	2.1
4	D	214	LEU	2.1
5	E	189	SER	2.1
7	T	38	LEU	2.1
9	I	64	LEU	2.1
9	I	34	VAL	2.1
9	V	50	LEU	2.1
10	W	33	ARG	2.1
9	I	71	ASN	2.1
8	H	44	VAL	2.1
7	G	30	PHE	2.1
2	O	216	LEU	2.0
5	E	69	LEU	2.0
6	F	18	LYS	2.0
7	G	53	VAL	2.0
4	Q	80	MET	2.0
6	F	60	PHE	2.0
9	I	42	VAL	2.0
10	J	25	VAL	2.0
9	I	36	ALA	2.0
5	E	134	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
11	BHG	A	4002	18/18	0.82	18.66	130,143,145,145	0
11	BHG	F	3011	18/18	0.45	17.32	114,118,122,122	0
11	BHG	S	2011	18/18	0.40	11.57	73,86,91,91	0
13	AZI	C	2014	3/3	0.38	9.99	53,53,57,59	0
20	PEE	T	3005	49/51	0.49	9.91	96,121,136,136	0
21	GOL	P	3009	6/6	0.32	9.43	59,65,67,68	0
11	BHG	P	3008	18/18	0.39	9.29	100,102,107,109	0
20	PEE	G	2005	49/51	0.52	9.14	105,123,129,129	0
21	GOL	C	2009	6/6	0.40	8.84	56,59,63,67	0
21	GOL	B	2013	6/6	0.94	7.18	145,148,148,149	0
11	BHG	C	2008	18/18	0.39	6.95	109,112,116,116	0
13	AZI	P	3014	3/3	0.38	6.43	54,54,55,61	0
11	BHG	F	4001	18/18	0.48	5.03	168,171,173,173	0
20	PEE	D	2006	51/51	0.24	4.84	52,66,94,95	0
21	GOL	O	3013	6/6	0.45	4.54	112,115,116,116	0
13	AZI	D	4004	3/3	0.29	3.83	69,69,72,73	0
20	PEE	C	2012	5/51	0.24	3.64	116,116,116,116	0
20	PEE	C	2007	49/51	0.30	3.63	39,53,68,69	0
12	PO4	B	3010	5/5	0.23	3.31	99,100,100,100	0
19	CDL	G	2003	50/100	0.27	3.27	62,96,113,113	0
19	CDL	G	2004	44/100	0.26	3.26	62,79,105,107	0
20	PEE	Q	3006	51/51	0.21	2.54	45,59,83,83	0
13	AZI	A	4005	3/3	0.38	2.51	72,72,73,74	0
18	UQ	P	3002	14/63	0.31	2.42	90,93,97,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
20	PEE	A	4003	6/51	0.19	2.18	110,111,112,113	0
19	CDL	T	3004	49/100	0.30	1.98	54,69,98,101	0
20	PEE	P	3007	49/51	0.26	1.60	35,54,62,63	0
18	UQ	C	2002	14/63	0.30	1.51	74,78,80,82	0
17	SMA	P	3001	37/37	0.17	0.94	24,32,37,37	0
19	CDL	Q	3003	50/100	0.22	0.72	55,78,90,92	0
20	PEE	N	3012	5/51	0.20	0.57	94,94,94,96	0
14	HEM	P	501	43/43	0.16	0.51	25,29,37,42	0
14	HEM	C	502	43/43	0.15	0.44	22,26,31,33	0
14	HEM	C	501	43/43	0.15	0.17	21,26,33,37	0
14	HEM	P	502	43/43	0.14	0.06	24,27,32,37	0
15	HEC	D	501	43/43	0.11	-0.08	29,33,36,38	0
16	FES	E	501	4/4	0.13	-0.10	34,35,37,37	0
17	SMA	C	2001	37/37	0.13	-0.25	25,30,32,38	0
16	FES	R	501	4/4	0.12	-0.38	31,31,33,33	0
15	HEC	Q	501	43/43	0.10	-0.44	32,35,36,37	0
12	PO4	O	2010	5/5	0.11	-0.48	106,106,107,108	0

6.5 Other polymers ⓘ

There are no such residues in this entry.