



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:46 AM GMT

PDB ID : 1KB9
Title : YEAST CYTOCHROME BC1 COMPLEX
Authors : Lange, C.; Nett, J.H.; Trumpower, B.L.; Hunte, C.
Deposited on : 2001-11-05
Resolution : 2.30 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>

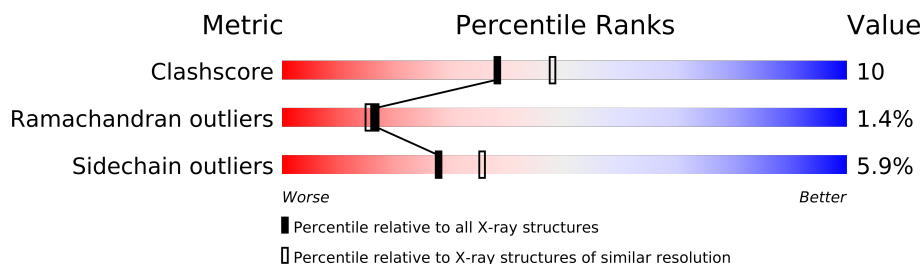
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	431	
2	B	352	
3	C	385	
4	D	246	
5	E	185	
6	F	74	
7	G	125	
8	H	93	
9	I	55	
10	J	127	
11	K	107	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 18040 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3343	2109	576	652	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLU	CONFLICT	UNP P07256

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	352	Total	C	N	O	S	0	0	0
			2734	1747	453	533	1			

- Molecule 3 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	385	Total	C	N	O	S	0	0	0
			3088	2080	484	503	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	270	VAL	ASP	CONFLICT	UNP P00163

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	246	Total	C	N	O	S	0	0	0
			1940	1237	334	360	9			

- Molecule 5 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	185	Total	C	N	O	S	0	0	0
			1410	893	242	265	10			

- Molecule 6 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	74	Total	C	N	O	S	0	0	0
			623	391	108	122	2			

- Molecule 7 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	125	Total	C	N	O	S	0	0	0
			1011	648	172	189	2			

- Molecule 8 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	93	Total	C	N	O	S	98	0	0
			772	510	131	129	2			

- Molecule 9 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	55	Total	C	N	O	0	0	0
			449	298	75	76			

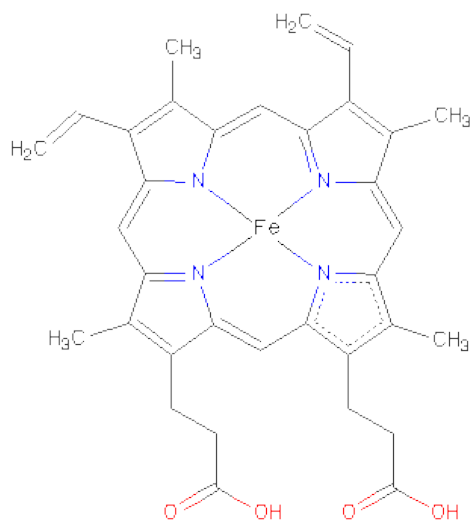
- Molecule 10 is a protein called HEAVY CHAIN (VH) OF FV-FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			

- Molecule 11 is a protein called LIGHT CHAIN (VL) OF FV-FRAGMENT.

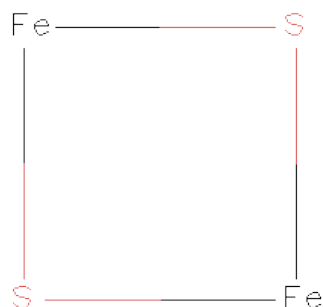
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

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



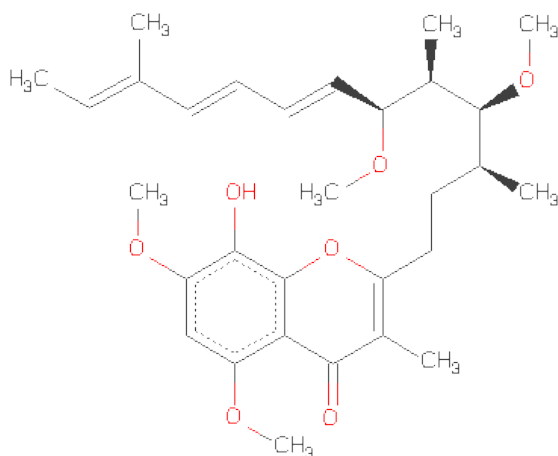
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



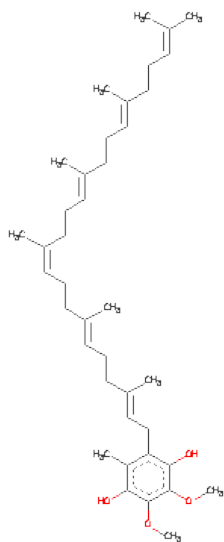
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 14 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



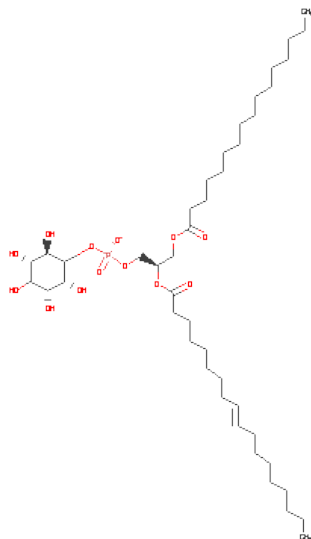
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			37	30	7		

- Molecule 15 is 5-(3,7,11,15,19,23-HEXAMETHYL-TETRACOSA-2,6,10,14,18,22-HEX AENYL)-2,3-DIMETHOXY-6-METHYL-BENZENE-1,4-DIOL (three-letter code: UQ6) (formula: $C_{39}H_{60}O_4$).



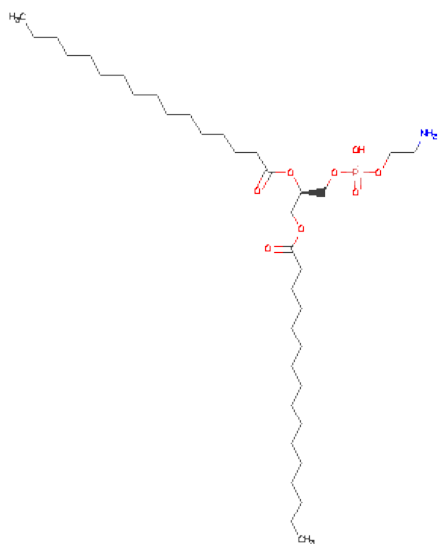
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			43	39	4		

- Molecule 16 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOINOSITOL (three-letter code: PIE) (formula: $C_{43}H_{80}O_{13}P$).



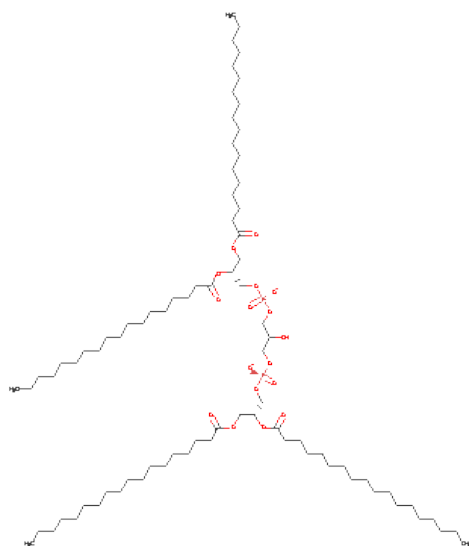
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	C	1	Total	C	O	P	0	0
			49	35	13	1		

- Molecule 17 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
17	C	1	Total	C	N	O	P	0	0
			38	28	1	8	1		

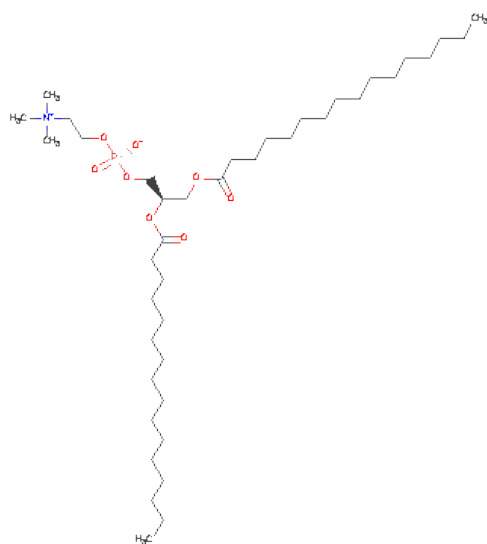
- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	C	1	Total	C	O	P	0	0
			76	57	17	2		

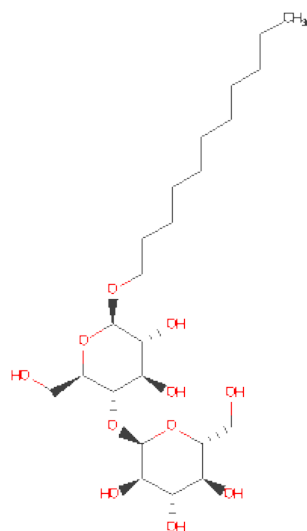
- Molecule 19 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (three-letter code: PCF)

(formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
19	A	1	37	27	1	8	1	0	0

- Molecule 20 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
20	A	1	34	23	11	0	0

- Molecule 21 is water.

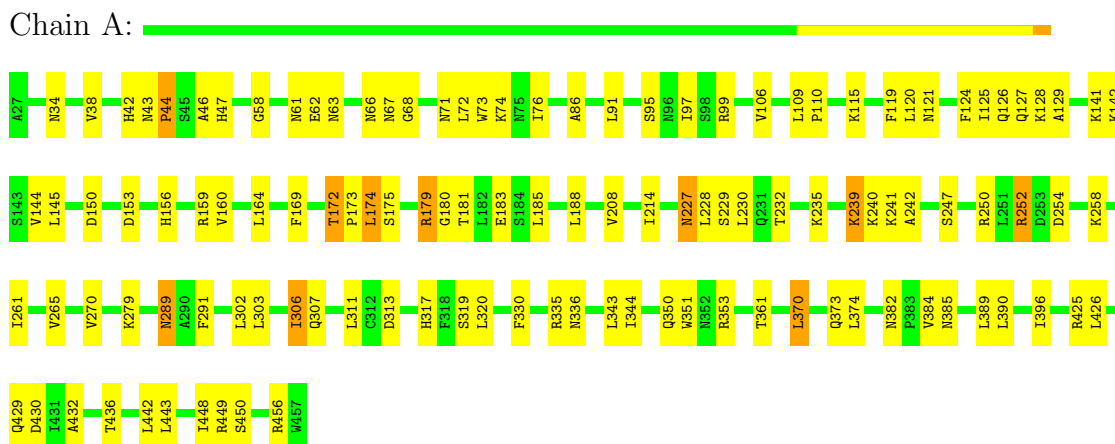
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	45	Total 45	O 45	0	0
21	B	9	Total 9	O 9	0	0
21	C	106	Total 106	O 106	0	0
21	D	67	Total 67	O 67	0	0
21	E	28	Total 28	O 28	0	0
21	F	7	Total 7	O 7	0	0
21	G	36	Total 36	O 36	0	0
21	H	14	Total 14	O 14	0	0
21	I	2	Total 2	O 2	0	0
21	J	5	Total 5	O 5	0	0
21	K	2	Total 2	O 2	0	0

3 Residue-property plots

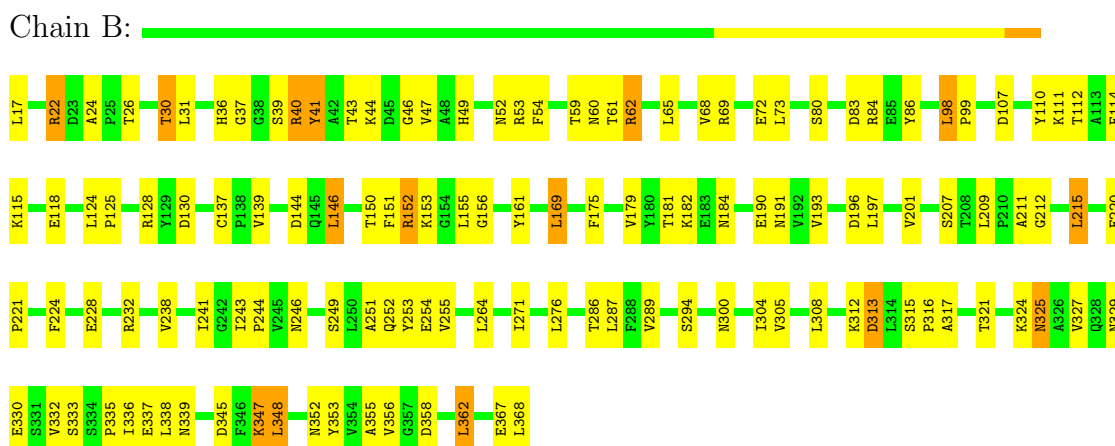
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

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

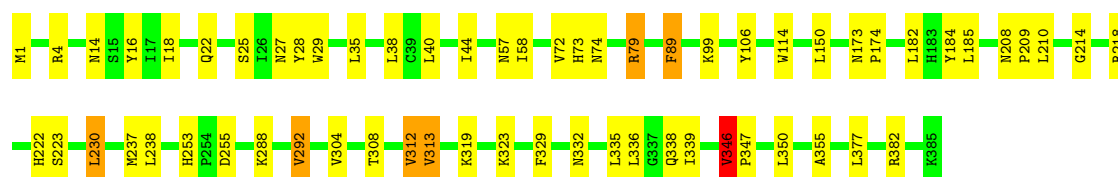


- Molecule 2: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX CORE PROTEIN 2



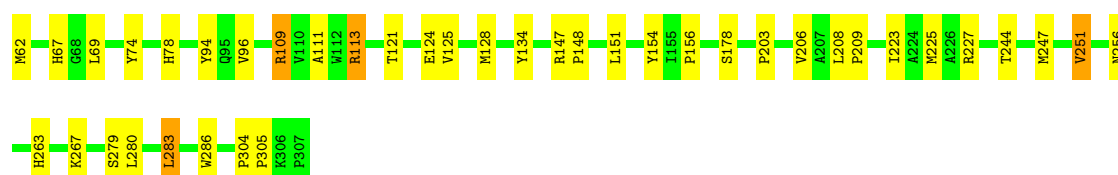
- Molecule 3: CYTOCHROME B





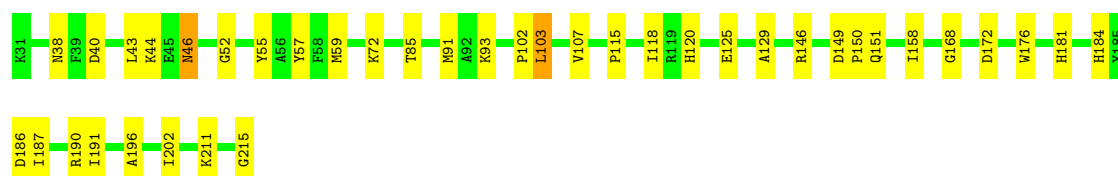
• Molecule 4: CYTOCHROME C1, HEME PROTEIN

Chain D:



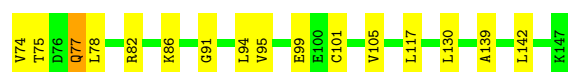
• Molecule 5: UBIQUINOL-CYTOCHROME C REDUCTASE IRON-SULFUR SUBUNIT

Chain E:



• Molecule 6: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 17 KD PROTEIN

Chain F:



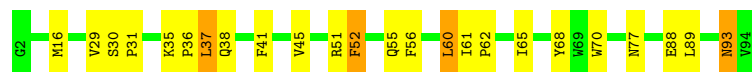
• Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KD PROTEIN

Chain G:



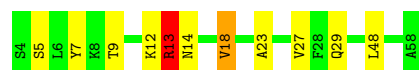
• Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C

Chain H:



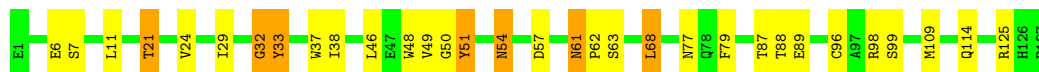
• Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN

Chain I:



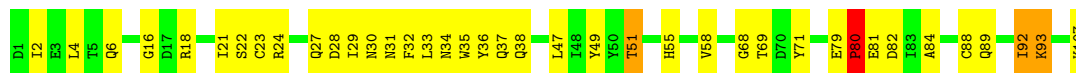
- Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

Chain J: 



- Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT

Chain K: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.47Å 163.92Å 147.28Å 90.00° 117.50° 90.00°	Depositor
Resolution (Å)	14.96 – 2.30	Depositor
% Data completeness (in resolution range)	84.7 (14.96-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.218 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18040	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: UMQ, CDL, PIE, FES, HEM, PEF, PCF, SMA, UQ6

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	0.34	0/3404	0.58	0/4614
2	B	0.31	0/2780	0.57	0/3764
3	C	0.45	0/3190	0.65	2/4353 (0.0%)
4	D	0.35	0/2001	0.60	0/2726
5	E	0.34	0/1443	0.61	0/1957
6	F	0.33	0/637	0.51	0/858
7	G	0.35	0/1031	0.62	1/1397 (0.1%)
8	H	0.39	0/803	0.52	0/1088
9	I	0.40	0/462	0.48	0/622
10	J	0.33	0/1043	0.61	1/1422 (0.1%)
11	K	0.31	0/863	0.53	0/1172
All	All	0.36	0/17657	0.59	4/23973 (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
4	D	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	32	GLY	N-CA-C	5.55	126.98	113.10
3	C	79	ARG	NE-CZ-NH1	-5.46	117.57	120.30
7	G	71	ARG	NE-CZ-NH1	-5.33	117.63	120.30
3	C	346	VAL	N-CA-C	5.12	124.83	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	94	TYR	Sidechain

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	3343	0	3321	72	0
2	B	2734	0	2774	80	0
3	C	3088	0	3125	40	0
4	D	1940	0	1862	22	0
5	E	1410	0	1386	30	0
6	F	623	0	581	11	0
7	G	1011	0	1026	14	0
8	H	772	0	736	16	0
9	I	449	0	445	9	0
10	J	1015	0	959	25	0
11	K	842	0	820	24	0
12	C	86	0	60	4	0
12	D	43	0	30	0	0
13	E	4	0	0	1	0
14	C	37	0	40	4	0
15	C	43	0	58	11	0
16	C	49	0	58	2	0
17	C	83	0	118	3	0
18	C	76	0	99	5	0
19	A	37	0	48	9	0
20	A	34	0	44	4	0
21	A	45	0	0	0	0
21	B	9	0	0	0	0
21	C	106	0	0	1	0
21	D	67	0	0	1	0
21	E	28	0	0	0	0
21	F	7	0	0	0	0
21	G	36	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	H	14	0	0	0	0
21	I	2	0	0	0	0
21	J	5	0	0	0	0
21	K	2	0	0	0	0
All	All	18040	0	17590	348	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 10.

All (348) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:77:GLN:H	6:F:77:GLN:HE21	1.03	1.01
11:K:31:ASN:HD22	11:K:51:THR:HG21	1.31	0.95
15:C:506:UQ6:H103	15:C:506:UQ6:H1M1	1.51	0.92
2:B:347:LYS:HD3	2:B:347:LYS:H	1.37	0.88
1:A:317:HIS:HE1	1:A:351:TRP:HE1	1.25	0.85
3:C:253:HIS:HD2	3:C:255:ASP:H	1.26	0.83
1:A:99:ARG:HD3	1:A:174:LEU:HD12	1.59	0.83
7:G:31:GLN:HA	7:G:31:GLN:HE21	1.44	0.82
19:A:514:PCF:H141	20:A:521:UMQ:H62	1.63	0.80
6:F:77:GLN:H	6:F:77:GLN:NE2	1.77	0.79
3:C:22:GLN:HE22	15:C:506:UQ6:H3M3	1.49	0.78
6:F:78:LEU:HD13	6:F:142:LEU:HD22	1.68	0.76
7:G:77:ARG:HD3	7:G:88:LEU:HD11	1.67	0.75
17:C:510:PEF:H181	17:C:510:PEF:H372	1.71	0.73
2:B:182:LYS:HB2	2:B:211:ALA:HB2	1.71	0.72
5:E:115:PRO:HD2	5:E:158:ILE:HD11	1.69	0.72
1:A:63:ASN:HB2	1:A:66:ASN:ND2	2.05	0.71
2:B:336:ILE:HG21	2:B:339:ASN:HB2	1.73	0.71
2:B:30:THR:HG23	2:B:190:GLU:HB3	1.72	0.71
15:C:506:UQ6:H103	15:C:506:UQ6:C1M	2.20	0.71
18:C:511:CDL:HB22	7:G:85:HIS:NE2	2.05	0.71
1:A:74:LYS:HG3	1:A:95:SER:HB3	1.71	0.71
5:E:72:LYS:HZ3	9:I:29:GLN:HE22	1.38	0.70
2:B:181:THR:HB	2:B:212:GLY:H	1.56	0.70
3:C:58:ILE:H	3:C:173:ASN:HD22	1.38	0.70
2:B:336:ILE:HD12	2:B:336:ILE:H	1.57	0.69
5:E:72:LYS:NZ	9:I:29:GLN:HE22	1.89	0.69
3:C:44:ILE:HD12	15:C:506:UQ6:H202	1.75	0.69
7:G:77:ARG:HD2	21:G:155:HOH:O	1.93	0.67
11:K:32:PHE:HD2	11:K:92:ILE:HG22	1.59	0.67
2:B:300:ASN:O	2:B:304:ILE:HG12	1.94	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:29:ILE:H	10:J:77:ASN:HD21	1.41	0.67
4:D:62:MET:HB3	4:D:67:HIS:NE2	2.09	0.67
1:A:258:LYS:HG2	1:A:335:ARG:HG3	1.77	0.66
17:C:510:PEF:H42	8:H:51:ARG:HD2	1.78	0.65
10:J:61:ASN:HD22	10:J:63:SER:H	1.44	0.65
11:K:31:ASN:ND2	11:K:51:THR:HG21	2.09	0.65
2:B:49:HIS:HD2	2:B:161:TYR:H	1.45	0.65
2:B:65:LEU:O	2:B:69:ARG:HG2	1.97	0.65
4:D:113:ARG:HG2	4:D:151:LEU:O	1.96	0.65
2:B:287:LEU:HD21	2:B:304:ILE:HG21	1.77	0.64
11:K:6:GLN:HG2	11:K:23:CYS:SG	2.37	0.64
15:C:506:UQ6:H1M1	15:C:506:UQ6:C10	2.25	0.64
3:C:214:GLY:O	3:C:218:ARG:HD2	1.97	0.64
5:E:172:ASP:H	5:E:184:HIS:HD2	1.47	0.63
6:F:91:GLY:O	6:F:95:VAL:HG13	1.99	0.62
19:A:514:PCF:H152	19:A:514:PCF:O13	1.99	0.62
1:A:156:HIS:HD2	1:A:159:ARG:HH21	1.47	0.62
11:K:37:GLN:HB2	11:K:47:LEU:HD11	1.82	0.61
1:A:73:TRP:CE3	1:A:76:ILE:HD11	2.35	0.61
10:J:54:ASN:H	10:J:54:ASN:HD22	1.46	0.61
6:F:77:GLN:HE21	6:F:77:GLN:N	1.86	0.61
1:A:109:LEU:HG	1:A:110:PRO:HD2	1.82	0.60
1:A:42:HIS:CD2	1:A:42:HIS:H	2.19	0.60
11:K:27:GLN:HG2	11:K:28:ASP:H	1.67	0.60
5:E:44:LYS:NZ	5:E:52:GLY:H	2.00	0.60
3:C:44:ILE:HD12	15:C:506:UQ6:C20	2.31	0.59
11:K:29:ILE:HG22	11:K:92:ILE:HD12	1.85	0.59
2:B:241:ILE:HG12	2:B:287:LEU:HB3	1.83	0.59
5:E:172:ASP:H	5:E:184:HIS:CD2	2.20	0.59
2:B:336:ILE:CG2	2:B:339:ASN:HB2	2.33	0.59
2:B:115:LYS:HB2	2:B:118:GLU:HG3	1.85	0.58
2:B:24:ALA:HB3	2:B:191:ASN:ND2	2.18	0.58
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.85	0.58
3:C:58:ILE:H	3:C:173:ASN:ND2	2.02	0.58
2:B:150:THR:HG22	2:B:352:ASN:ND2	2.19	0.58
1:A:68:GLY:HA3	1:A:185:LEU:HD11	1.86	0.57
1:A:252:ARG:HD3	1:A:254:ASP:OD1	2.04	0.57
3:C:25:SER:OG	7:G:79:HIS:HD2	1.87	0.57
3:C:1:MET:N	21:C:587:HOH:O	2.37	0.57
2:B:49:HIS:CD2	2:B:161:TYR:H	2.22	0.57
3:C:208:ASN:HD22	3:C:210:LEU:H	1.52	0.57
7:G:53:ASN:ND2	7:G:56:MET:H	2.03	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:44:LYS:HB2	2:B:47:VAL:HG21	1.87	0.56
1:A:229:SER:HB3	1:A:232:THR:HB	1.86	0.56
5:E:43:LEU:HD21	8:H:29:VAL:HG11	1.88	0.56
3:C:323:LYS:HE3	8:H:55:GLN:HE22	1.70	0.56
7:G:43:LEU:HD13	7:G:48:LEU:HD11	1.87	0.56
5:E:107:VAL:CG1	5:E:118:ILE:HB	2.36	0.56
4:D:109:ARG:HG3	4:D:178:SER:CB	2.36	0.56
1:A:313:ASP:OD1	1:A:335:ARG:HD3	2.05	0.55
6:F:74:VAL:HG12	6:F:75:THR:H	1.71	0.55
1:A:58:GLY:H	1:A:61:ASN:HD22	1.54	0.55
1:A:270:VAL:HG21	1:A:396:ILE:HD13	1.88	0.55
2:B:347:LYS:HG2	2:B:348:LEU:N	2.22	0.55
10:J:61:ASN:ND2	10:J:63:SER:H	2.05	0.55
5:E:168:GLY:HA2	5:E:176:TRP:CD1	2.42	0.55
5:E:72:LYS:NZ	9:I:29:GLN:NE2	2.54	0.55
10:J:29:ILE:HG12	10:J:77:ASN:ND2	2.21	0.55
1:A:289:ASN:HD22	1:A:289:ASN:C	2.10	0.55
2:B:252:GLN:O	2:B:255:VAL:HG22	2.07	0.55
1:A:67:ASN:HD22	1:A:181:THR:HG23	1.73	0.54
4:D:247:MET:O	4:D:251:VAL:HG22	2.08	0.54
1:A:317:HIS:CE1	1:A:351:TRP:HE1	2.15	0.54
20:A:521:UMQ:O2'	9:I:18:VAL:HG22	2.06	0.54
1:A:169:PHE:O	1:A:172:THR:HB	2.08	0.54
1:A:63:ASN:HB2	1:A:66:ASN:HD22	1.71	0.54
5:E:55:TYR:O	5:E:59:MET:HG2	2.08	0.54
7:G:31:GLN:HA	7:G:31:GLN:NE2	2.20	0.54
1:A:124:PHE:HA	1:A:128:LYS:HD3	1.90	0.54
2:B:238:VAL:HG13	2:B:356:VAL:HB	1.89	0.53
3:C:253:HIS:CD2	3:C:255:ASP:H	2.16	0.53
2:B:68:VAL:O	2:B:72:GLU:HG3	2.08	0.53
12:C:502:HEM:HMC2	12:C:502:HEM:HBC2	1.91	0.53
1:A:302:LEU:HB2	1:A:350:GLN:HG3	1.90	0.53
5:E:107:VAL:HG12	5:E:118:ILE:HB	1.91	0.53
1:A:350:GLN:HE22	1:A:353:ARG:HH21	1.56	0.53
10:J:87:THR:HG22	10:J:88:THR:N	2.24	0.53
1:A:265:VAL:HG21	1:A:426:LEU:HD12	1.91	0.52
1:A:344:ILE:HG21	1:A:448:ILE:HD12	1.91	0.52
14:C:505:SMA:H21	14:C:505:SMA:H39	1.91	0.52
10:J:38:ILE:HA	10:J:49:VAL:HG23	1.89	0.52
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.91	0.52
19:A:514:PCF:H151	20:A:521:UMQ:H6'1	1.92	0.52
1:A:306:ILE:HA	1:A:311:LEU:HD22	1.90	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:56:PHE:O	8:H:60:LEU:HB2	2.09	0.52
3:C:57:ASN:HA	3:C:173:ASN:HD21	1.75	0.52
1:A:172:THR:HG23	1:A:173:PRO:HD2	1.91	0.52
7:G:15:ILE:HG23	7:G:21:LEU:HB3	1.92	0.52
5:E:129:ALA:HB2	5:E:187:ILE:HG23	1.91	0.52
3:C:347:PRO:HG3	8:H:77:ASN:HB2	1.91	0.52
11:K:34:ASN:HD22	11:K:49:TYR:HA	1.75	0.52
3:C:22:GLN:NE2	15:C:506:UQ6:H3M3	2.23	0.52
2:B:246:ASN:HB2	2:B:249:SER:HB3	1.92	0.52
2:B:329:ASN:O	2:B:332:VAL:HG23	2.10	0.51
1:A:142:LYS:NZ	1:A:142:LYS:HB2	2.25	0.51
1:A:303:LEU:O	1:A:307:GLN:HG3	2.10	0.51
12:C:501:HEM:HBC2	12:C:501:HEM:HHD	1.93	0.51
11:K:47:LEU:HA	11:K:58:VAL:HG11	1.93	0.51
11:K:4:LEU:HD23	11:K:88:CYS:SG	2.51	0.51
2:B:315:SER:N	2:B:316:PRO:HD3	2.26	0.51
5:E:103:LEU:O	5:E:120:HIS:HB3	2.10	0.51
11:K:32:PHE:CD2	11:K:92:ILE:HG22	2.43	0.51
4:D:74:TYR:CE1	6:F:139:ALA:HA	2.46	0.51
10:J:99:SER:HB3	10:J:109:MET:HG2	1.91	0.51
6:F:82:ARG:O	6:F:86:LYS:HG3	2.10	0.51
2:B:110:TYR:HD1	2:B:209:LEU:HD23	1.76	0.51
2:B:264:LEU:HD12	2:B:317:ALA:HB2	1.92	0.51
4:D:286:TRP:CE3	5:E:59:MET:HG3	2.46	0.51
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.92	0.50
1:A:71:ASN:HA	1:A:97:ILE:HG13	1.94	0.50
8:H:89:LEU:O	8:H:93:ASN:HB2	2.11	0.50
11:K:2:ILE:H	11:K:2:ILE:HD12	1.76	0.50
5:E:125:GLU:HB3	5:E:187:ILE:HG12	1.92	0.50
9:I:5:SER:O	9:I:9:THR:HG23	2.12	0.50
1:A:68:GLY:HA3	1:A:185:LEU:CD1	2.41	0.50
1:A:289:ASN:ND2	1:A:291:PHE:H	2.10	0.50
1:A:235:LYS:HB2	1:A:235:LYS:NZ	2.26	0.50
19:A:514:PCF:H402	16:C:508:PIE:H382	1.93	0.49
3:C:27:ASN:HB2	18:C:511:CDL:OB3	2.11	0.49
1:A:373:GLN:HG3	1:A:374:LEU:N	2.26	0.49
2:B:69:ARG:O	2:B:73:LEU:HD23	2.12	0.49
11:K:55:HIS:O	11:K:58:VAL:HG22	2.11	0.49
1:A:350:GLN:NE2	1:A:353:ARG:HD3	2.27	0.49
2:B:137:CYS:SG	2:B:139:VAL:HG22	2.51	0.49
2:B:324:LYS:O	2:B:327:VAL:HG22	2.13	0.49
1:A:289:ASN:HD22	1:A:291:PHE:H	1.59	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:127:GLN:C	1:A:129:ALA:H	2.16	0.49
10:J:38:ILE:HD12	10:J:46:LEU:HD22	1.94	0.49
2:B:41:TYR:HB3	2:B:215:LEU:HD13	1.94	0.49
1:A:121:ASN:HD21	1:A:125:ILE:HD12	1.77	0.48
8:H:61:ILE:HB	8:H:62:PRO:HD3	1.95	0.48
3:C:329:PHE:HE2	17:C:510:PEF:H432	1.78	0.48
2:B:313:ASP:O	2:B:316:PRO:HD3	2.13	0.48
10:J:11:LEU:HD13	10:J:125:ARG:HD2	1.96	0.48
19:A:514:PCF:H153	19:A:514:PCF:H11	1.94	0.48
4:D:227:ARG:HH11	4:D:244:THR:HG21	1.78	0.48
2:B:52:ASN:ND2	2:B:80:SER:OG	2.46	0.48
10:J:24:VAL:HG21	10:J:29:ILE:HD11	1.95	0.48
1:A:67:ASN:ND2	1:A:180:GLY:HA2	2.28	0.48
4:D:286:TRP:CD2	8:H:37:LEU:HD12	2.49	0.48
2:B:294:SER:HB3	2:B:358:ASP:HB3	1.95	0.48
3:C:40:LEU:HD23	15:C:506:UQ6:H18	1.94	0.48
1:A:429:GLN:HE22	9:I:13:ARG:NH2	2.09	0.48
3:C:335:LEU:HD13	3:C:339:ILE:HG12	1.96	0.47
19:A:514:PCF:O13	19:A:514:PCF:C15	2.62	0.47
2:B:232:ARG:HB3	2:B:232:ARG:NH2	2.29	0.47
11:K:2:ILE:HD12	11:K:2:ILE:N	2.29	0.47
7:G:71:ARG:NH1	21:G:148:HOH:O	2.41	0.47
1:A:430:ASP:OD2	1:A:449:ARG:NH2	2.48	0.47
10:J:87:THR:HG22	10:J:88:THR:H	1.80	0.47
2:B:40:ARG:HB2	2:B:84:ARG:O	2.14	0.47
1:A:450:SER:HB3	19:A:514:PCF:H112	1.95	0.47
5:E:72:LYS:HZ2	9:I:29:GLN:NE2	2.12	0.47
2:B:44:LYS:HB2	2:B:47:VAL:CG2	2.44	0.47
10:J:49:VAL:CG1	10:J:68:LEU:HD23	2.45	0.47
11:K:4:LEU:CD2	11:K:88:CYS:SG	3.02	0.47
6:F:101:CYS:O	6:F:105:VAL:HG23	2.14	0.47
1:A:46:ALA:O	1:A:47:HIS:HB2	2.15	0.47
2:B:26:THR:OG1	2:B:191:ASN:ND2	2.48	0.47
1:A:121:ASN:ND2	1:A:125:ILE:HD12	2.29	0.46
2:B:151:PHE:O	2:B:156:GLY:HA3	2.14	0.46
2:B:252:GLN:HG3	2:B:253:TYR:N	2.31	0.46
2:B:39:SER:OG	2:B:84:ARG:HD3	2.16	0.46
2:B:355:ALA:HB1	2:B:362:LEU:HD23	1.98	0.46
2:B:197:LEU:O	2:B:201:VAL:HG23	2.15	0.46
10:J:51:TYR:CD2	10:J:51:TYR:C	2.89	0.46
2:B:182:LYS:HB2	2:B:211:ALA:CB	2.43	0.46
1:A:72:LEU:HD13	1:A:144:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:255:VAL:HG12	2:B:321:THR:HG21	1.96	0.46
4:D:134:TYR:OH	4:D:156:PRO:HD3	2.16	0.46
5:E:146:ARG:CZ	5:E:202:ILE:HD11	2.45	0.46
3:C:28:TYR:CE2	18:C:511:CDL:HA32	2.50	0.46
1:A:179:ARG:HG2	1:A:179:ARG:HH21	1.81	0.46
10:J:29:ILE:H	10:J:77:ASN:ND2	2.11	0.46
1:A:67:ASN:ND2	1:A:181:THR:HG23	2.31	0.46
4:D:121:THR:OG1	4:D:124:GLU:HG3	2.16	0.46
4:D:111:ALA:HA	4:D:154:TYR:HA	1.97	0.46
11:K:33:LEU:HD22	11:K:71:TYR:CG	2.51	0.46
5:E:120:HIS:CD2	5:E:151:GLN:HG2	2.51	0.46
2:B:317:ALA:O	2:B:321:THR:HG22	2.16	0.46
3:C:89:PHE:HE2	12:C:501:HEM:HBB2	1.81	0.46
2:B:308:LEU:HB2	2:B:348:LEU:HD22	1.98	0.45
2:B:232:ARG:HB3	2:B:232:ARG:HH21	1.80	0.45
10:J:98:ARG:O	10:J:109:MET:HA	2.16	0.45
3:C:4:ARG:HE	3:C:14:ASN:ND2	2.14	0.45
1:A:58:GLY:H	1:A:61:ASN:ND2	2.13	0.45
11:K:51:THR:HG1	11:K:71:TYR:HD2	1.62	0.45
10:J:37:TRP:CZ3	10:J:96:CYS:HB3	2.52	0.45
2:B:321:THR:O	2:B:325:ASN:HB2	2.17	0.45
5:E:120:HIS:HD2	5:E:151:GLN:HG2	1.80	0.45
1:A:279:LYS:HG3	1:A:319:SER:HB3	1.98	0.45
4:D:304:PRO:HA	4:D:305:PRO:HD3	1.81	0.45
2:B:37:GLY:HA3	2:B:179:VAL:HG11	1.99	0.45
2:B:155:LEU:HD12	2:B:155:LEU:N	2.31	0.45
5:E:93:LYS:HD3	5:E:215:GLY:HA3	1.98	0.45
10:J:48:TRP:CZ2	10:J:50:GLY:HA2	2.51	0.45
3:C:16:TYR:O	15:C:506:UQ6:H1M2	2.17	0.45
18:C:511:CDL:HA4	18:C:511:CDL:H112	1.49	0.45
2:B:46:GLY:O	2:B:49:HIS:HB3	2.16	0.45
4:D:147:ARG:HG2	4:D:148:PRO:O	2.16	0.45
10:J:61:ASN:HD22	10:J:61:ASN:C	2.20	0.45
2:B:228:GLU:HA	2:B:353:TYR:O	2.17	0.45
1:A:160:VAL:CG2	1:A:436:THR:HG22	2.47	0.45
11:K:33:LEU:HD23	11:K:35:TRP:HE1	1.82	0.44
3:C:27:ASN:OD1	3:C:29:TRP:HB2	2.17	0.44
19:A:514:PCF:C14	20:A:521:UMQ:H62	2.41	0.44
1:A:172:THR:HG23	1:A:242:ALA:HA	1.99	0.44
10:J:6:GLU:H	10:J:114:GLN:HE21	1.66	0.44
19:A:514:PCF:C15	19:A:514:PCF:H11	2.48	0.44
3:C:218:ARG:HG3	8:H:16:MET:CE	2.48	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:254:GLU:HG2	2:B:276:LEU:HD23	1.98	0.44
5:E:44:LYS:HB3	8:H:35:LYS:HA	2.00	0.44
3:C:346:VAL:HG12	3:C:347:PRO:N	2.33	0.44
4:D:223:ILE:HG12	4:D:225:MET:H	1.82	0.44
4:D:125:VAL:HA	4:D:128:MET:HE3	1.99	0.44
1:A:385:ASN:O	1:A:389:LEU:HG	2.17	0.43
1:A:239:LYS:HB2	1:A:240:LYS:H	1.70	0.43
2:B:61:THR:HG23	2:B:111:LYS:NZ	2.32	0.43
4:D:263:HIS:NE2	4:D:267:LYS:HE3	2.34	0.43
5:E:191:ILE:HD13	5:E:196:ALA:HB3	2.00	0.43
10:J:61:ASN:HD22	10:J:62:PRO:N	2.15	0.43
4:D:78:HIS:HD2	21:D:517:HOH:O	2.01	0.43
2:B:43:THR:HG22	2:B:175:PHE:HD1	1.82	0.43
2:B:24:ALA:HB3	2:B:191:ASN:HD21	1.84	0.43
3:C:18:ILE:HA	3:C:222:HIS:HB2	2.00	0.43
2:B:305:VAL:HG11	2:B:368:LEU:HB3	2.00	0.43
1:A:317:HIS:HE1	1:A:351:TRP:NE1	2.05	0.43
1:A:156:HIS:HD2	1:A:159:ARG:NH2	2.13	0.43
7:G:77:ARG:HD3	7:G:88:LEU:CD1	2.44	0.43
1:A:73:TRP:CZ3	1:A:76:ILE:HD11	2.53	0.43
4:D:227:ARG:NH1	4:D:244:THR:HG21	2.33	0.43
2:B:62:ARG:HH21	2:B:62:ARG:HB2	1.83	0.43
2:B:60:ASN:HB2	2:B:111:LYS:NZ	2.33	0.43
2:B:251:ALA:O	2:B:255:VAL:HG13	2.18	0.43
14:C:505:SMA:H14	14:C:505:SMA:H36	2.01	0.43
2:B:36:HIS:HB2	2:B:184:ASN:OD1	2.19	0.43
3:C:332:ASN:HD21	3:C:355:ALA:HA	1.84	0.43
1:A:91:LEU:HD23	1:A:106:VAL:HG11	2.00	0.43
1:A:74:LYS:HG3	1:A:95:SER:CB	2.44	0.43
1:A:62:GLU:OE1	1:A:67:ASN:HA	2.19	0.43
1:A:169:PHE:O	1:A:175:SER:HB3	2.18	0.43
3:C:73:HIS:O	3:C:74:ASN:HB2	2.18	0.43
7:G:120:LEU:O	7:G:123:ILE:HG12	2.19	0.43
11:K:24:ARG:HA	11:K:69:THR:O	2.19	0.43
2:B:220:GLU:HA	2:B:221:PRO:HD3	1.91	0.43
1:A:247:SER:O	1:A:432:ALA:HA	2.19	0.42
5:E:44:LYS:HZ2	5:E:52:GLY:H	1.66	0.42
2:B:146:LEU:HD23	2:B:286:THR:HG22	2.01	0.42
3:C:313:VAL:HG22	3:C:319:LYS:HE3	2.01	0.42
2:B:83:ASP:HB2	2:B:86:TYR:H	1.84	0.42
3:C:304:VAL:HG13	3:C:308:THR:HG23	2.00	0.42
1:A:74:LYS:HB2	1:A:97:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:74:VAL:HG12	6:F:75:THR:N	2.34	0.42
10:J:49:VAL:HG12	10:J:68:LEU:HD23	2.00	0.42
2:B:22:ARG:HH12	2:B:332:VAL:HB	1.84	0.42
5:E:149:ASP:HA	5:E:150:PRO:HD2	1.90	0.42
3:C:106:TYR:HB3	3:C:114:TRP:CD2	2.55	0.42
7:G:53:ASN:HD21	7:G:56:MET:H	1.68	0.42
14:C:505:SMA:C10	14:C:505:SMA:H36	2.49	0.42
3:C:230:LEU:HA	3:C:230:LEU:HD12	1.89	0.42
1:A:456:ARG:HH21	1:A:456:ARG:HG3	1.84	0.42
3:C:312:VAL:HG21	7:G:5:PHE:CE1	2.54	0.42
3:C:237:MET:CE	16:C:508:PIE:H291	2.49	0.42
11:K:79:GLU:HA	11:K:80:PRO:HA	1.80	0.42
10:J:7:SER:OG	10:J:21:THR:HG23	2.20	0.42
15:C:506:UQ6:H121	15:C:506:UQ6:H101	1.55	0.42
1:A:382:ASN:OD1	1:A:384:VAL:HG22	2.20	0.42
6:F:95:VAL:O	6:F:99:GLU:HB2	2.20	0.42
4:D:279:SER:O	4:D:283:LEU:HB2	2.20	0.42
5:E:186:ASP:OD2	5:E:190:ARG:HD2	2.20	0.42
2:B:347:LYS:N	2:B:347:LYS:HD3	2.15	0.41
14:C:505:SMA:C16	14:C:505:SMA:H39	2.49	0.41
3:C:288:LYS:O	3:C:292:VAL:HG13	2.20	0.41
2:B:182:LYS:HD3	2:B:207:SER:HA	2.01	0.41
1:A:350:GLN:NE2	1:A:353:ARG:HH21	2.19	0.41
11:K:93:LYS:HB3	11:K:93:LYS:NZ	2.35	0.41
8:H:35:LYS:HA	8:H:36:PRO:HD2	1.89	0.41
2:B:347:LYS:HG2	2:B:348:LEU:H	1.84	0.41
12:C:501:HEM:HHD	12:C:501:HEM:CBC	2.49	0.41
1:A:38:VAL:HA	1:A:208:VAL:HG13	2.01	0.41
2:B:59:THR:HA	2:B:112:THR:HA	2.02	0.41
1:A:43:ASN:HA	1:A:44:PRO:HD2	1.81	0.41
2:B:193:VAL:HG23	2:B:196:ASP:HB2	2.03	0.41
2:B:124:LEU:HB2	2:B:125:PRO:HD3	2.02	0.41
5:E:38:ASN:HD21	5:E:40:ASP:CG	2.23	0.41
18:C:511:CDL:H771	18:C:511:CDL:H802	1.85	0.41
1:A:370:LEU:O	1:A:374:LEU:HB2	2.21	0.41
5:E:181:HIS:HB2	13:E:504:FES:S1	2.61	0.41
1:A:250:ARG:NH1	1:A:442:LEU:O	2.54	0.41
2:B:98:LEU:N	2:B:99:PRO:HD2	2.35	0.41
3:C:173:ASN:HB3	3:C:174:PRO:HD3	2.03	0.41
1:A:214:ILE:O	1:A:214:ILE:HD12	2.21	0.41
3:C:338:GLN:HG3	8:H:70:TRP:CH2	2.55	0.41
11:K:21:ILE:HG22	11:K:22:SER:N	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:52:PHE:O	8:H:56:PHE:HB3	2.20	0.41
2:B:152:ARG:HD3	2:B:224:PHE:CD1	2.56	0.41
11:K:36:TYR:HE2	11:K:89:GLN:HG2	1.86	0.41
2:B:241:ILE:HA	2:B:352:ASN:O	2.21	0.41
2:B:238:VAL:HA	2:B:289:VAL:O	2.21	0.41
2:B:238:VAL:CG1	2:B:356:VAL:HB	2.51	0.41
9:I:23:ALA:O	9:I:27:VAL:HG23	2.21	0.41
1:A:86:ALA:HB2	1:A:119:PHE:CZ	2.56	0.41
15:C:506:UQ6:H171	15:C:506:UQ6:H151	1.92	0.40
2:B:271:ILE:HG21	2:B:287:LEU:HD11	2.03	0.40
8:H:61:ILE:O	8:H:65:ILE:HG13	2.22	0.40
4:D:208:LEU:HA	4:D:209:PRO:HD3	1.94	0.40
10:J:33:TYR:HB3	10:J:99:SER:O	2.20	0.40
10:J:51:TYR:HD2	10:J:51:TYR:C	2.25	0.40
5:E:57:TYR:HB3	9:I:7:TYR:OH	2.21	0.40
1:A:141:LYS:NZ	1:A:188:LEU:O	2.54	0.40
2:B:243:ILE:HA	2:B:244:PRO:HD3	1.87	0.40
2:B:49:HIS:HE1	2:B:130:ASP:OD1	2.05	0.40
8:H:51:ARG:HA	8:H:51:ARG:HD3	1.80	0.40
2:B:114:PHE:O	2:B:169:LEU:HD11	2.21	0.40
8:H:30:SER:HA	8:H:31:PRO:HD3	1.95	0.40
11:K:38:GLN:O	11:K:84:ALA:HB1	2.22	0.40
3:C:72:VAL:HA	5:E:85:THR:HG22	2.03	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	429/431 (100%)	397 (92%)	28 (6%)	4 (1%)	25	26
2	B	350/352 (99%)	311 (89%)	31 (9%)	8 (2%)	10	7
3	C	383/385 (100%)	369 (96%)	12 (3%)	2 (0%)	38	45
4	D	244/246 (99%)	237 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	183/185 (99%)	171 (93%)	9 (5%)	3 (2%)	14	12
6	F	72/74 (97%)	69 (96%)	3 (4%)	0	100	100
7	G	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
8	H	91/93 (98%)	79 (87%)	7 (8%)	5 (6%)	3	1
9	I	53/55 (96%)	50 (94%)	1 (2%)	2 (4%)	5	2
10	J	125/127 (98%)	111 (89%)	12 (10%)	2 (2%)	14	12
11	K	105/107 (98%)	89 (85%)	11 (10%)	5 (5%)	4	1
All	All	2158/2180 (99%)	2004 (93%)	123 (6%)	31 (1%)	16	15

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	335	PRO
3	C	223	SER
5	E	103	LEU
8	H	93	ASN
2	B	153	LYS
2	B	333	SER
5	E	46	ASN
8	H	37	LEU
9	I	13	ARG
10	J	33	TYR
11	K	30	ASN
11	K	51	THR
1	A	44	PRO
1	A	227	ASN
8	H	38	GLN
11	K	68	GLY
1	A	228	LEU
2	B	22	ARG
2	B	367	GLU
9	I	12	LYS
11	K	80	PRO
1	A	230	LEU
2	B	152	ARG
2	B	348	LEU
3	C	346	VAL
11	K	16	GLY
2	B	313	ASP
5	E	102	PRO

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Mol	Chain	Res	Type
8	H	52	PHE
10	J	32	GLY
8	H	45	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	370/370 (100%)	342 (92%)	28 (8%)	19	22
2	B	301/301 (100%)	278 (92%)	23 (8%)	19	22
3	C	338/338 (100%)	320 (95%)	18 (5%)	32	41
4	D	204/204 (100%)	197 (97%)	7 (3%)	49	64
5	E	151/151 (100%)	148 (98%)	3 (2%)	68	84
6	F	67/67 (100%)	63 (94%)	4 (6%)	27	35
7	G	109/109 (100%)	104 (95%)	5 (5%)	37	48
8	H	77/77 (100%)	73 (95%)	4 (5%)	32	42
9	I	45/45 (100%)	41 (91%)	4 (9%)	14	16
10	J	112/112 (100%)	104 (93%)	8 (7%)	21	26
11	K	93/93 (100%)	86 (92%)	7 (8%)	19	23
All	All	1867/1867 (100%)	1756 (94%)	111 (6%)	28	35

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	115	LYS
1	A	120	LEU
1	A	126	GLN
1	A	145	LEU
1	A	150	ASP
1	A	153	ASP
1	A	164	LEU
1	A	172	THR
1	A	174	LEU

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Mol	Chain	Res	Type
1	A	179	ARG
1	A	183	GLU
1	A	227	ASN
1	A	239	LYS
1	A	241	LYS
1	A	252	ARG
1	A	261	ILE
1	A	289	ASN
1	A	306	ILE
1	A	320	LEU
1	A	330	PHE
1	A	336	ASN
1	A	343	LEU
1	A	361	THR
1	A	370	LEU
1	A	390	LEU
1	A	425	ARG
1	A	443	LEU
2	B	17	LEU
2	B	30	THR
2	B	31	LEU
2	B	40	ARG
2	B	41	TYR
2	B	53	ARG
2	B	54	PHE
2	B	62	ARG
2	B	98	LEU
2	B	107	ASP
2	B	128	ARG
2	B	144	ASP
2	B	146	LEU
2	B	169	LEU
2	B	215	LEU
2	B	312	LYS
2	B	325	ASN
2	B	330	GLU
2	B	337	GLU
2	B	338	LEU
2	B	345	ASP
2	B	347	LYS
2	B	362	LEU
3	C	35	LEU

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Mol	Chain	Res	Type
3	C	38	LEU
3	C	79	ARG
3	C	89	PHE
3	C	99	LYS
3	C	150	LEU
3	C	182	LEU
3	C	184	TYR
3	C	185	LEU
3	C	230	LEU
3	C	238	LEU
3	C	292	VAL
3	C	312	VAL
3	C	313	VAL
3	C	336	LEU
3	C	350	LEU
3	C	377	LEU
3	C	382	ARG
4	D	69	LEU
4	D	109	ARG
4	D	113	ARG
4	D	251	VAL
4	D	256	ASN
4	D	280	LEU
4	D	283	LEU
5	E	46	ASN
5	E	91	MET
5	E	211	LYS
6	F	77	GLN
6	F	94	LEU
6	F	117	LEU
6	F	130	LEU
7	G	16	LEU
7	G	31	GLN
7	G	48	LEU
7	G	86	HIS
7	G	127	LYS
8	H	41	PHE
8	H	60	LEU
8	H	68	TYR
8	H	88	GLU
9	I	13	ARG
9	I	14	ASN

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Mol	Chain	Res	Type
9	I	18	VAL
9	I	48	LEU
10	J	21	THR
10	J	51	TYR
10	J	54	ASN
10	J	57	ASP
10	J	61	ASN
10	J	68	LEU
10	J	79	PHE
10	J	89	GLU
11	K	18	ARG
11	K	80	PRO
11	K	81	GLU
11	K	82	ASP
11	K	92	ILE
11	K	93	LYS
11	K	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS
1	A	61	ASN
1	A	63	ASN
1	A	66	ASN
1	A	67	ASN
1	A	121	ASN
1	A	126	GLN
1	A	156	HIS
1	A	171	ASN
1	A	199	ASN
1	A	200	HIS
1	A	289	ASN
1	A	298	GLN
1	A	317	HIS
1	A	336	ASN
1	A	350	GLN
1	A	385	ASN
1	A	388	ASN
1	A	429	GLN
2	B	49	HIS
2	B	52	ASN

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Mol	Chain	Res	Type
2	B	55	ASN
2	B	191	ASN
2	B	252	GLN
2	B	258	ASN
2	B	325	ASN
2	B	328	GLN
2	B	329	ASN
3	C	14	ASN
3	C	22	GLN
3	C	43	GLN
3	C	173	ASN
3	C	208	ASN
3	C	253	HIS
3	C	332	ASN
4	D	78	HIS
4	D	79	ASN
4	D	127	ASN
4	D	256	ASN
5	E	38	ASN
5	E	106	ASN
5	E	184	HIS
6	F	77	GLN
7	G	31	GLN
7	G	53	ASN
7	G	57	GLN
7	G	79	HIS
9	I	14	ASN
9	I	29	GLN
10	J	54	ASN
10	J	59	ASN
10	J	61	ASN
10	J	77	ASN
10	J	78	GLN
10	J	114	GLN
11	K	31	ASN
11	K	34	ASN
11	K	89	GLN
11	K	90	HIS
11	K	91	HIS

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 ⓘ

12 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$
19	PCF	A	514	-	36,36,49	1.76	3 (8%)	44,44,57	1.55	5 (11%)
20	UMQ	A	521	-	35,35,35	0.92	1 (2%)	46,46,46	1.47	6 (13%)
12	HEM	C	501	3	49,50,50	1.84	10 (20%)	46,82,82	1.42	5 (10%)
12	HEM	C	502	3	49,50,50	1.76	14 (28%)	46,82,82	1.28	3 (6%)
14	SMA	C	505	-	38,38,38	1.86	8 (21%)	50,52,52	2.24	13 (26%)
15	UQ6	C	506	-	43,43,43	2.41	13 (30%)	55,55,55	2.08	18 (32%)
16	PIE	C	508	-	49,49,57	2.12	10 (20%)	61,61,69	2.30	15 (24%)
17	PEF	C	510	-	44,44,46	0.74	0	49,49,51	1.09	3 (6%)
18	CDL	C	511	-	75,75,99	1.06	4 (5%)	87,87,111	1.45	13 (14%)
17	PEF	C	513	-	37,37,46	1.03	1 (2%)	42,42,51	1.02	2 (4%)
12	HEM	D	503	4	49,50,50	1.97	10 (20%)	46,82,82	1.29	3 (6%)
13	FES	E	504	5	0,4,4	0.00	-	0,4,4	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PCF	A	514	-	-	0/40/40/53	0/0/0/0
20	UMQ	A	521	-	-	0/20/60/60	0/2/2/2
12	HEM	C	501	3	-	0/14/114/114	0/0/8/8
12	HEM	C	502	3	-	0/14/114/114	0/0/8/8
14	SMA	C	505	-	2/2/5/10	0/33/34/34	0/0/2/2
15	UQ6	C	506	-	-	0/39/39/39	0/1/1/1
16	PIE	C	508	-	-	0/44/68/76	0/1/1/1
17	PEF	C	510	-	-	0/48/48/50	0/0/0/0
18	CDL	C	511	-	1/1/9/9	2/86/86/110	0/0/0/0
17	PEF	C	513	-	-	0/41/41/50	0/0/0/0
12	HEM	D	503	4	-	0/14/114/114	0/0/8/8
13	FES	E	504	5	-	0/0/4/4	0/0/1/1

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	508	PIE	P-O14	-9.97	1.31	1.59
19	A	514	PCF	O13-C11	-8.03	1.09	1.44
15	C	506	UQ6	C7-C6	6.08	1.59	1.51
14	C	505	SMA	C4-C4A	5.92	1.49	1.40
14	C	505	SMA	C4A-C8A	5.60	1.48	1.41
15	C	506	UQ6	O5-C5	-5.42	1.23	1.37
15	C	506	UQ6	O2-C2	-5.21	1.24	1.37
12	D	503	HEM	C3B-C2B	-4.99	1.35	1.43
12	C	501	HEM	C3C-C2C	-4.76	1.35	1.43
12	D	503	HEM	C3C-C2C	-4.76	1.35	1.43
12	C	501	HEM	C3D-C2D	-4.73	1.35	1.43
15	C	506	UQ6	C2-C3	4.60	1.47	1.39
17	C	513	PEF	C36-C35	-4.53	1.53	1.55
12	D	503	HEM	C3D-C2D	-4.42	1.36	1.43
16	C	508	PIE	C47-C29	4.36	1.55	1.31
19	A	514	PCF	C43-C42	-4.35	1.53	1.55
12	C	501	HEM	C2B-C1B	-4.31	1.43	1.44
15	C	506	UQ6	C5-C4	4.31	1.46	1.39
12	C	502	HEM	C3C-C2C	-4.31	1.36	1.43
12	C	501	HEM	C3B-C2B	-4.30	1.36	1.43
12	D	503	HEM	CBB-CAB	4.22	1.53	1.28
12	C	502	HEM	C3D-C2D	-4.21	1.36	1.43
12	D	503	HEM	CBC-CAC	4.09	1.52	1.28
12	C	502	HEM	C3B-C2B	-4.07	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	508	PIE	C6'-C5'	3.99	1.63	1.52
12	C	502	HEM	C4A-C3A	3.96	1.45	1.40
12	D	503	HEM	C3B-CAB	3.79	1.52	1.40
12	D	503	HEM	C3C-CAC	3.74	1.52	1.40
12	C	501	HEM	CMC-C2C	3.62	1.58	1.47
14	C	505	SMA	C13-C12	3.59	1.62	1.54
15	C	506	UQ6	C5-C6	3.50	1.46	1.40
16	C	508	PIE	P-O12	3.49	1.57	1.48
20	A	521	UMQ	C3-C2	-3.44	1.43	1.52
15	C	506	UQ6	C23-C24	3.42	1.39	1.32
15	C	506	UQ6	C28-C29	3.37	1.39	1.32
12	D	503	HEM	C4A-C3A	3.33	1.44	1.40
12	C	501	HEM	C4A-C3A	3.27	1.44	1.40
15	C	506	UQ6	C18-C19	3.23	1.39	1.32
16	C	508	PIE	C4'-C5'	3.14	1.61	1.52
15	C	506	UQ6	C8-C9	3.12	1.39	1.32
12	C	502	HEM	CHB-C1B	3.11	1.40	1.35
15	C	506	UQ6	C13-C14	3.06	1.39	1.32
18	C	511	CDL	OB2-CB2	-3.04	1.32	1.44
16	C	508	PIE	C6'-C1'	3.03	1.60	1.52
18	C	511	CDL	OA8-CA6	-2.99	1.38	1.45
16	C	508	PIE	C42-C41	-2.88	1.54	1.55
12	C	502	HEM	FE-NA	2.79	2.04	1.92
12	D	503	HEM	CHA-C4D	2.73	1.39	1.35
12	C	502	HEM	CHA-C4D	2.69	1.39	1.35
18	C	511	CDL	OA6-CA4	-2.68	1.39	1.46
12	D	503	HEM	FE-NA	2.67	2.03	1.92
12	C	501	HEM	CMB-C2B	2.66	1.55	1.47
15	C	506	UQ6	C2-C1	2.53	1.46	1.40
12	C	502	HEM	CMB-C2B	2.53	1.55	1.47
16	C	508	PIE	O31-C3	-2.52	1.39	1.45
15	C	506	UQ6	C33-C34	2.51	1.40	1.32
14	C	505	SMA	O12-C12	-2.37	1.36	1.42
12	C	502	HEM	CBC-CAC	2.36	1.42	1.28
16	C	508	PIE	C1-C2	2.30	1.57	1.50
14	C	505	SMA	C6-C7	2.30	1.43	1.38
12	C	501	HEM	CBC-CAC	2.28	1.42	1.28
12	C	502	HEM	CBB-CAB	2.26	1.41	1.28
19	A	514	PCF	P-O14	2.17	1.53	1.48
14	C	505	SMA	O7-C7	2.17	1.40	1.37
14	C	505	SMA	C5-C4A	2.17	1.46	1.42
12	C	501	HEM	CHA-C4D	2.11	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	508	PIE	O22-C21	-2.11	1.16	1.22
12	C	502	HEM	CHC-C1C	2.08	1.40	1.36
12	C	502	HEM	C2D-C1D	-2.08	1.44	1.44
18	C	511	CDL	O1-C1	2.06	1.50	1.43
12	C	502	HEM	FE-NB	2.04	2.05	1.97
12	C	501	HEM	C2D-C1D	-2.03	1.44	1.44
14	C	505	SMA	C20-C19	2.01	1.36	1.33
12	C	502	HEM	CMC-C2C	2.00	1.53	1.47

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	508	PIE	O11-P-O14	9.54	132.25	103.05
16	C	508	PIE	P-O14-C5'	8.68	146.45	120.21
14	C	505	SMA	O1-C2-C9	6.89	114.42	110.58
15	C	506	UQ6	C3M-O3-C3	6.79	133.47	114.90
12	D	503	HEM	C3B-C4B-NB	-6.28	109.51	114.00
14	C	505	SMA	C26-C19-C18	-6.07	108.28	118.09
12	C	501	HEM	C3B-C4B-NB	-5.94	109.75	114.00
19	A	514	PCF	C3-C2-C1	-5.87	98.47	111.86
12	C	502	HEM	C3B-C4B-NB	-5.63	109.97	114.00
16	C	508	PIE	O13-P-O12	-5.42	102.36	118.72
15	C	506	UQ6	C17-C18-C19	5.38	139.41	127.80
20	A	521	UMQ	CA-O1'-C1'	-5.16	104.66	113.96
14	C	505	SMA	O14-C14-C15	4.85	129.90	110.74
18	C	511	CDL	CB4-OB6-CB5	-4.84	105.98	117.92
15	C	506	UQ6	C4M-O4-C4	4.52	127.26	114.90
18	C	511	CDL	OA4-PA1-OA3	-4.51	105.11	118.72
18	C	511	CDL	OB4-PB2-OB3	-4.35	105.59	118.72
16	C	508	PIE	C6'-C5'-C4'	-4.22	104.67	110.68
17	C	510	PEF	C2-O2-C10	-4.10	107.80	117.92
14	C	505	SMA	C3-C4-C4A	-3.91	115.55	121.65
14	C	505	SMA	O12-C12-C13	3.85	113.88	107.80
17	C	513	PEF	C2-O2-C10	-3.84	108.45	117.92
14	C	505	SMA	O14-C14-C13	3.74	117.80	108.36
19	A	514	PCF	O14-P-O12	-3.68	107.62	118.72
16	C	508	PIE	C3-C2-C1	-3.68	103.48	111.86
19	A	514	PCF	P-O13-C11	3.65	132.57	118.53
18	C	511	CDL	PA1-OA2-CA2	3.61	132.72	120.24
14	C	505	SMA	O1-C8A-C8	3.61	120.54	115.90
14	C	505	SMA	O7-C7-C8	3.43	118.05	114.50
18	C	511	CDL	CA6-CA4-CA3	-3.41	104.08	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	506	UQ6	C11-C12-C13	3.41	121.35	111.62
16	C	508	PIE	C38-C37-C36	-3.41	96.18	114.61
14	C	505	SMA	C4-C3-C2	3.22	121.57	116.97
20	A	521	UMQ	O1'-C1'-C2'	3.19	112.24	108.18
15	C	506	UQ6	C21-C19-C18	3.18	127.20	121.08
16	C	508	PIE	C48-C47-C29	-3.08	107.99	125.43
18	C	511	CDL	CB6-CB4-CB3	-3.07	104.87	111.86
15	C	506	UQ6	C22-C23-C24	2.98	134.23	127.80
20	A	521	UMQ	C3'-C4'-C5'	-2.93	104.26	110.85
15	C	506	UQ6	C27-C28-C29	2.91	134.07	127.80
12	C	501	HEM	C4A-CHB-C1B	-2.89	123.66	127.47
12	C	502	HEM	C2D-C1D-ND	-2.88	109.53	112.93
16	C	508	PIE	C48-C49-C50	-2.84	107.92	113.25
18	C	511	CDL	CA4-OA6-CA5	-2.84	110.92	117.92
18	C	511	CDL	C20-C19-C18	-2.80	108.16	114.46
15	C	506	UQ6	C30-C29-C31	-2.78	111.16	115.39
18	C	511	CDL	OB2-CB2-C1	-2.71	100.11	108.62
20	A	521	UMQ	O1-C1-O5	-2.68	104.02	110.69
15	C	506	UQ6	C20-C19-C18	-2.68	118.22	123.52
15	C	506	UQ6	C25-C24-C26	-2.62	111.41	115.39
12	D	503	HEM	C2D-C1D-ND	-2.62	109.84	112.93
18	C	511	CDL	CB6-OB8-CB7	-2.56	109.64	117.13
12	C	502	HEM	CBD-CAD-C3D	-2.51	108.89	114.37
20	A	521	UMQ	C1'-C2'-C3'	-2.44	105.24	110.00
18	C	511	CDL	PA1-OA5-CA3	-2.44	111.81	120.24
15	C	506	UQ6	C11-C9-C8	2.44	125.77	121.08
15	C	506	UQ6	C1M-C1-C2	-2.43	115.49	120.35
16	C	508	PIE	P-O11-C1	2.40	128.53	120.24
12	C	501	HEM	C2D-C1D-ND	-2.39	110.10	112.93
15	C	506	UQ6	C7-C6-C5	-2.36	117.93	120.96
14	C	505	SMA	C3M-C3-C4	-2.36	117.18	120.37
15	C	506	UQ6	C15-C14-C16	-2.36	111.80	115.39
15	C	506	UQ6	C1M-C1-C6	2.31	123.66	120.42
15	C	506	UQ6	C16-C14-C13	2.31	125.52	121.08
17	C	513	PEF	O4P-P-O3P	2.31	111.25	104.68
14	C	505	SMA	O7-C7-C6	-2.30	120.22	124.23
14	C	505	SMA	C18-C19-C20	2.29	126.23	118.91
16	C	508	PIE	C39-C38-C37	2.27	126.88	114.61
16	C	508	PIE	C2-O21-C21	-2.27	112.33	117.92
17	C	510	PEF	C3-C2-C1	2.25	117.00	111.86
18	C	511	CDL	C58-C57-C56	-2.21	109.48	114.46
14	C	505	SMA	O1-C8A-C4A	-2.20	119.03	121.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	510	PEF	O3-C3-C2	-2.17	103.14	108.83
12	C	501	HEM	CMD-C2D-C3D	2.17	130.51	125.60
19	A	514	PCF	C43-C42-C41	-2.14	109.66	114.46
20	A	521	UMQ	C6'-C5'-C4'	-2.13	107.25	113.25
15	C	506	UQ6	C17-C16-C14	2.12	119.75	112.74
16	C	508	PIE	O31-C31-O32	2.07	129.07	123.43
16	C	508	PIE	O13-P-O14	-2.06	103.04	109.44
12	D	503	HEM	CMA-C3A-C4A	-2.04	125.48	128.62
15	C	506	UQ6	C6-C7-C8	2.03	115.63	112.25
16	C	508	PIE	O14-C5'-C6'	2.02	112.57	108.44
18	C	511	CDL	CA6-OA8-CA7	-2.02	111.21	117.13
19	A	514	PCF	C3-O31-C31	-2.02	111.22	117.13
12	C	501	HEM	CMC-C2C-C3C	-2.02	121.41	126.16
16	C	508	PIE	C28-C29-C47	-2.01	114.03	125.43

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	C	511	CDL	CA4
14	C	505	SMA	C12
14	C	505	SMA	C14

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	C	511	CDL	CA4-OA6-CA5-C11
18	C	511	CDL	CA4-OA6-CA5-OA7

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.