



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:15 PM GMT

PDB ID : 1SQP
Title : Crystal Structure Analysis of Bovine Bcl with Myxothiazol
Authors : Esser, L.; Quinn, B.; Li, Y.F.; Zhang, M.; Elberry, M.; Yu, L.; Yu, C.A.; Xia, D.
Deposited on : 2004-03-19
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

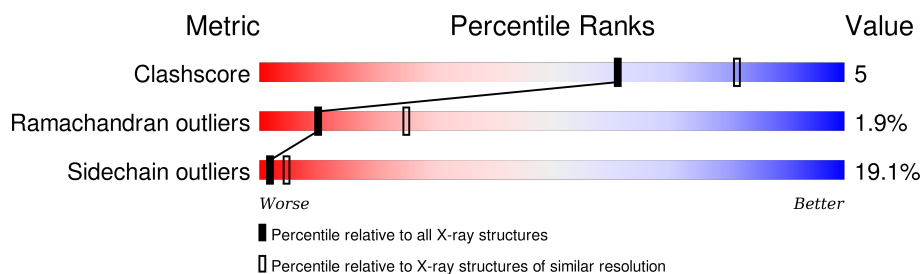
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	480	
2	B	453	
3	C	379	
4	D	241	
5	E	196	
6	F	110	
7	G	81	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	78	
9	I	78	
10	J	62	
11	K	56	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CDL	A	447	X	-	-	-
13	CDL	D	242	X	-	-	-
13	CDL	G	82	X	-	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 17274 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3458	2161	609	668	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3172	1993	562	610	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	378	Total	C	N	O	S	0	0	0
			3003	2013	471	501	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			

- Molecule 5 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)].

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

- Molecule 6 is a protein called sub6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	105	Total	C	N	O	S	0	0	0
			911	576	165	168	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	0
			628	410	118	99	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	67	Total	C	N	O	S	0	0	0
			548	332	99	112	5			

- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	57	Total	C	N	O	S	0	0	0
			406	253	77	74	2			

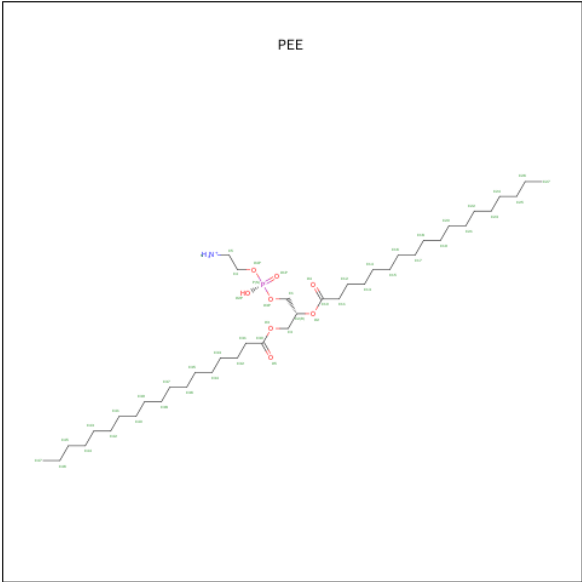
- Molecule 10 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			502	329	87	86			

- Molecule 11 is a protein called Ubiquinol-cytochrome c reductase complex 6.4 kDa protein.

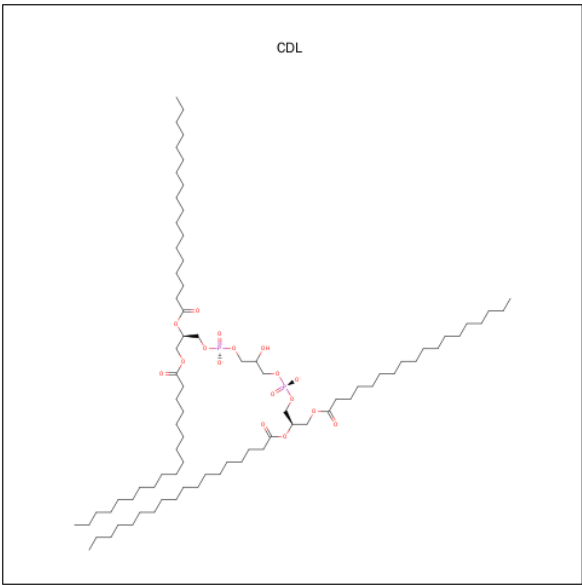
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	53	Total	C	N	O	S	0	0	0
			436	292	78	65	1			

- Molecule 12 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: PEE) (formula: C₄₁H₈₃NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	E	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
12	A	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
12	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 13 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



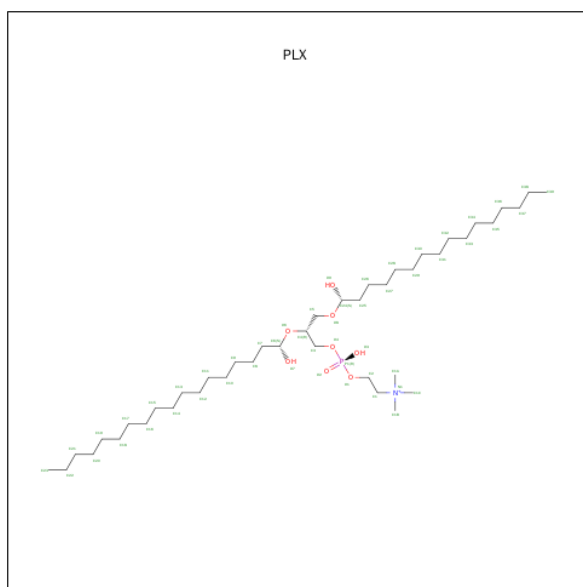
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	O	P	0	0
			64	45	17	2		

Continued on next page...

Continued from previous page...

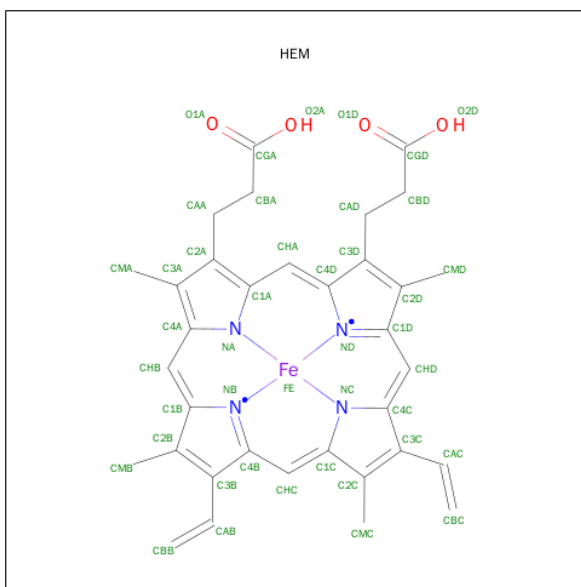
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	D	1	Total	C	O	P	0	0
			64	45	17	2		
13	G	1	Total	C	O	P	0	0
			64	45	17	2		

- Molecule 14 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (three-letter code: PLX) (formula: $C_{42}H_{89}NO_8P$).



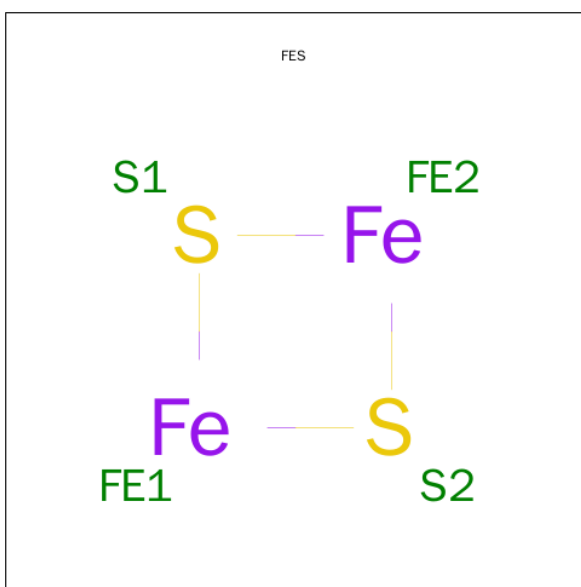
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	J	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



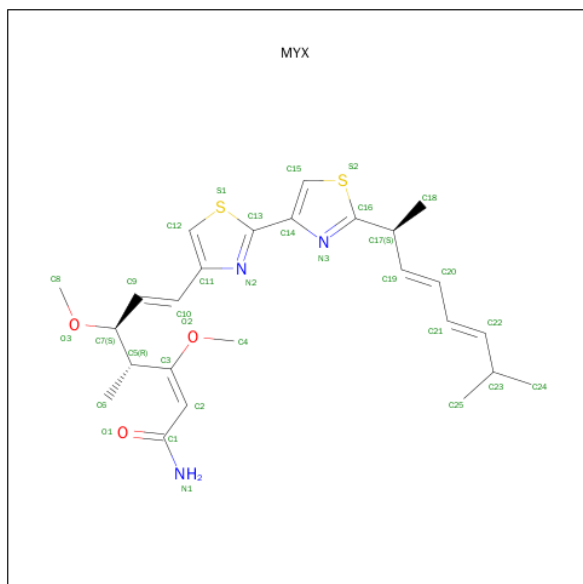
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
15	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
15	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

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



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

- Molecule 17 is (2Z,6E)-7-{2'-[(2E,4E)-1,6-DIMETHYLHEPTA-2,4-DIENYL]-2,4'-BI-1,3-THIAZOL-4-YL}-3,5-DIMETHOXY-4-METHYLHEPTA-2,6-DIENAMIDE (three-letter code: MYX) (formula: C₂₅H₃₃N₃O₃S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	N	O	S	0	0
			33	25	3	3	2		

- Molecule 18 is water.

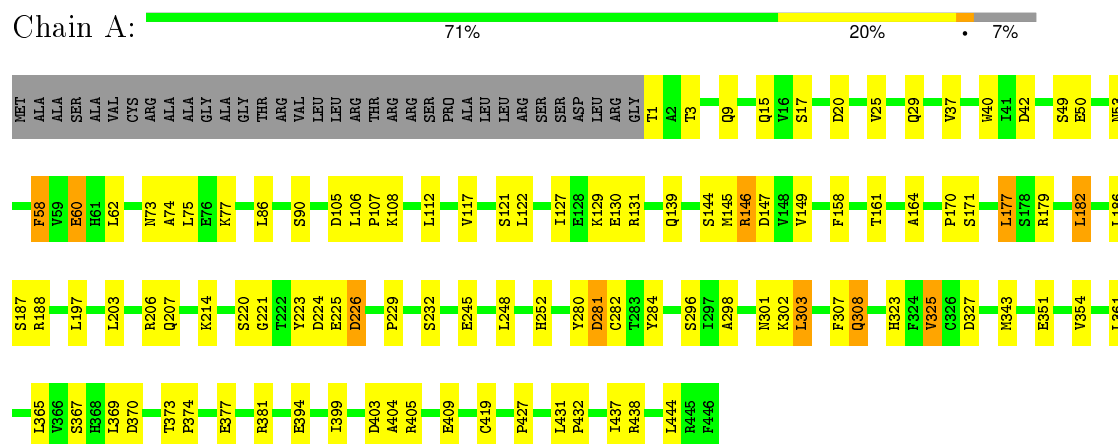
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	51	Total	O	0	0
			51	51		
18	B	84	Total	O	0	0
			84	84		
18	C	36	Total	O	0	0
			36	36		
18	D	11	Total	O	0	0
			11	11		
18	E	2	Total	O	0	0
			2	2		
18	F	15	Total	O	0	0
			15	15		
18	G	11	Total	O	0	0
			11	11		
18	I	2	Total	O	0	0
			2	2		
18	K	3	Total	O	0	0
			3	3		

3 Residue-property plots

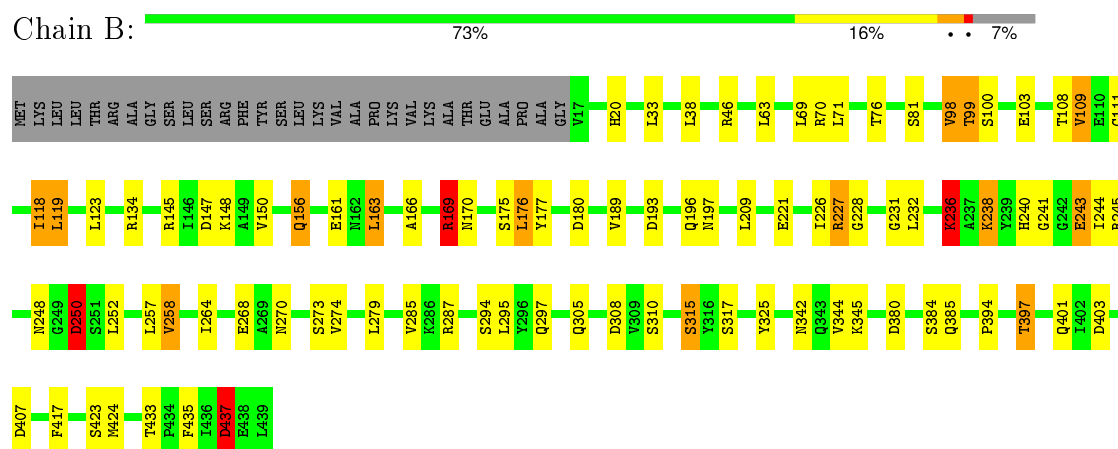
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



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

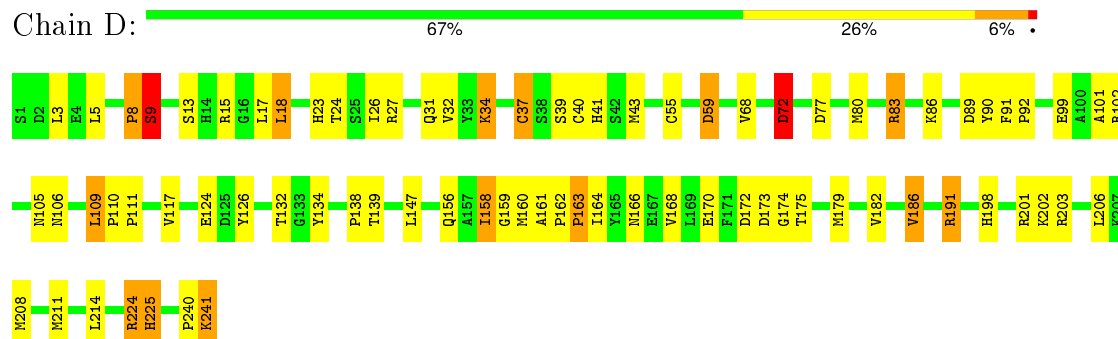


- Molecule 3: Cytochrome b

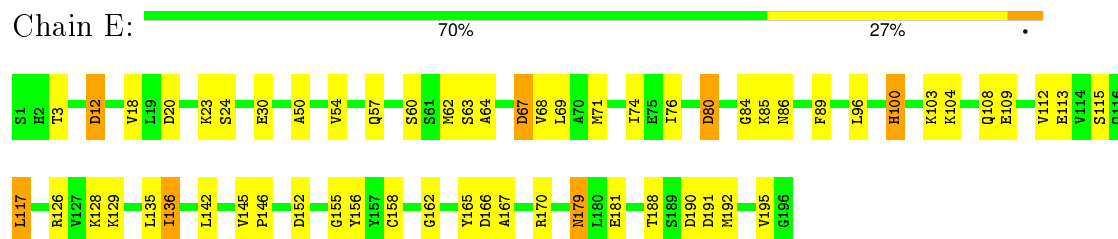




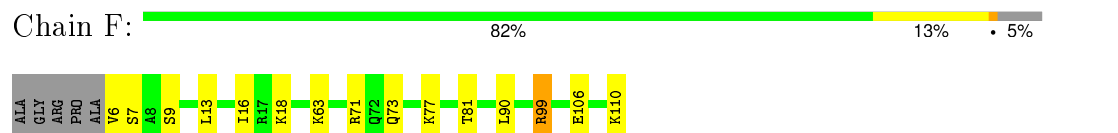
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



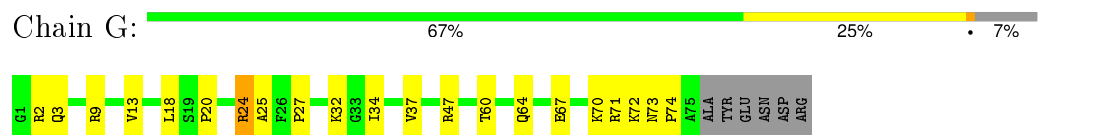
- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)]



- Molecule 6: sub6



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

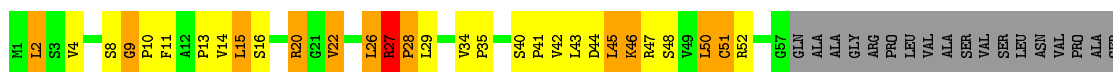
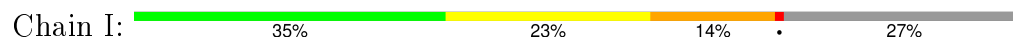


- Molecule 8: Ubiquinol-cytochrome c reductase complex 11 kDa protein





- Molecule 9: Ubiquinol-cytochrome c reductase iron-sulfur subunit, mitochondrial precursor (EC 1.10.2.2) (Rieske iron-sulfur protein) (RISP) [Contains: Ubiquinol-cytochrome c reductase 8 kDa protein (Complex III subunit IX)]



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



- Molecule 11: Ubiquinol-cytochrome c reductase complex 6.4 kDa protein



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	153.70Å 153.70Å 596.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70	Depositor
% Data completeness (in resolution range)	94.1 (40.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.263 , 0.314	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17274	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MYX, CDL, PLX, FES, HEM, PEE

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	0.90	0/3531	0.84	5/4792 (0.1%)
2	B	0.99	0/3232	0.88	8/4386 (0.2%)
3	C	1.01	0/3100	0.82	3/4242 (0.1%)
4	D	0.97	0/1978	0.86	5/2684 (0.2%)
5	E	1.01	0/1553	0.82	6/2100 (0.3%)
6	F	0.99	0/930	0.88	0/1246
7	G	1.15	0/649	0.78	0/878
8	H	0.90	0/553	0.88	0/741
9	I	1.31	0/411	1.15	2/558 (0.4%)
10	J	1.06	0/515	0.85	0/696
11	K	1.13	0/452	0.82	0/618
All	All	0.99	0/16904	0.86	29/22941 (0.1%)

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
1	A	0	1
2	B	0	1
6	F	0	1
All	All	0	3

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	172	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	327	ASP	CB-CG-OD2	6.56	124.20	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	308	ASP	CB-CG-OD2	6.40	124.06	118.30
2	B	147	ASP	CB-CG-OD2	6.28	123.95	118.30
3	C	320	LEU	CA-CB-CG	5.78	128.59	115.30
3	C	239	LEU	CA-CB-CG	5.71	128.43	115.30
9	I	44	ASP	CB-CG-OD2	5.51	123.26	118.30
2	B	193	ASP	CB-CG-OD2	5.51	123.25	118.30
4	D	109	LEU	CA-CB-CG	5.50	127.95	115.30
2	B	403	ASP	CB-CG-OD2	5.42	123.18	118.30
3	C	252	ASP	CB-CG-OD2	5.36	123.12	118.30
5	E	152	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	224	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	226	ASP	CB-CG-OD2	5.30	123.07	118.30
9	I	45	LEU	CA-CB-CG	5.29	127.47	115.30
2	B	163	LEU	CA-CB-CG	5.28	127.44	115.30
5	E	166	ASP	CB-CG-OD2	5.28	123.05	118.30
2	B	180	ASP	CB-CG-OD2	5.27	123.05	118.30
5	E	190	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	20	ASP	CB-CG-OD2	5.25	123.03	118.30
5	E	80	ASP	CB-CG-OD2	5.16	122.95	118.30
4	D	89	ASP	CB-CG-OD2	5.15	122.93	118.30
4	D	72	ASP	CB-CG-OD2	5.13	122.92	118.30
2	B	380	ASP	CB-CG-OD2	5.12	122.91	118.30
5	E	67	ASP	CB-CG-OD2	5.10	122.89	118.30
5	E	191	ASP	CB-CG-OD2	5.10	122.89	118.30
4	D	59	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	105	ASP	CB-CG-OD2	5.04	122.83	118.30
2	B	437	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	LEU	Peptide
2	B	169	ARG	Mainchain
6	F	99	ARG	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3356	32	0
2	B	3172	0	3152	44	0
3	C	3003	0	3065	33	0
4	D	1919	0	1869	35	0
5	E	1519	0	1504	12	0
6	F	911	0	902	3	0
7	G	628	0	636	8	0
8	H	548	0	530	3	0
9	I	406	0	437	27	0
10	J	502	0	505	3	0
11	K	436	0	445	11	0
12	A	49	0	75	1	0
12	C	49	0	75	0	0
12	E	49	0	75	3	0
13	A	64	0	72	1	0
13	D	64	0	72	0	0
13	G	64	0	72	2	0
14	J	52	0	88	4	0
15	C	86	0	60	4	0
15	D	43	0	30	11	0
16	E	4	0	0	0	0
17	C	33	0	33	1	0
18	A	51	0	0	0	0
18	B	84	0	0	2	0
18	C	36	0	0	0	0
18	D	11	0	0	0	0
18	E	2	0	0	1	0
18	F	15	0	0	0	0
18	G	11	0	0	1	0
18	I	2	0	0	0	0
18	K	3	0	0	0	0
All	All	17274	0	17053	186	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (186) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:CYS:SG	15:D:243:HEM:HAC	1.33	1.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:11:MET:CE	3:C:11:MET:SD	2.02	1.48
11:K:38:TRP:HE3	11:K:41:ILE:CD1	1.25	1.48
11:K:38:TRP:CE3	11:K:41:ILE:CD1	2.04	1.41
4:D:37:CYS:SG	15:D:243:HEM:HAB	1.62	1.35
4:D:40:CYS:SG	15:D:243:HEM:CAC	2.18	1.30
11:K:38:TRP:CE3	11:K:41:ILE:HD11	1.72	1.19
11:K:38:TRP:HE3	11:K:41:ILE:HD13	1.05	1.14
4:D:40:CYS:HG	15:D:243:HEM:HAC	1.20	0.97
4:D:40:CYS:HG	15:D:243:HEM:CAC	1.74	0.94
11:K:38:TRP:CZ3	11:K:41:ILE:HD11	2.15	0.81
11:K:38:TRP:CE3	11:K:41:ILE:HD12	2.16	0.78
11:K:38:TRP:CE3	11:K:41:ILE:HD13	1.97	0.78
9:I:4:VAL:HB	9:I:10:PRO:HG2	1.68	0.73
2:B:325:TYR:HB3	9:I:28:PRO:HD2	1.70	0.73
4:D:37:CYS:SG	15:D:243:HEM:C3B	2.82	0.72
1:A:149:VAL:HG21	1:A:252:HIS:HB3	1.73	0.70
4:D:126:TYR:HE2	15:D:243:HEM:O2A	1.77	0.67
2:B:310:SER:HB3	9:I:28:PRO:HD3	1.75	0.66
4:D:117:VAL:HG21	4:D:191:ARG:HA	1.76	0.66
3:C:109:PHE:HB3	3:C:112:THR:HG23	1.78	0.65
9:I:9:GLY:HA2	9:I:26:LEU:O	2.01	0.61
2:B:248:ASN:HB3	2:B:250:ASP:HB2	1.83	0.60
3:C:126:THR:HG21	15:C:382:HEM:HBB2	1.83	0.60
4:D:159:GLY:HA3	15:D:243:HEM:HBD2	1.84	0.59
4:D:72:ASP:HB2	4:D:83:ARG:HG2	1.85	0.59
4:D:224:ARG:HD3	7:G:25:ALA:O	2.02	0.59
2:B:385:GLN:HG2	9:I:2:LEU:HD12	1.83	0.59
1:A:58:PHE:HB3	1:A:182:LEU:HD21	1.85	0.59
12:A:448:PEE:H14	14:J:63:PLX:H72	1.84	0.58
2:B:264:ILE:HD12	2:B:315:SER:HB3	1.84	0.58
9:I:34:VAL:HB	9:I:35:PRO:HD3	1.85	0.58
2:B:169:ARG:HD3	2:B:238:LYS:HB3	1.85	0.58
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.84	0.58
3:C:119:LEU:HD22	15:C:381:HEM:HBB2	1.86	0.57
7:G:34:ILE:HA	7:G:37:VAL:HG22	1.85	0.57
4:D:23:HIS:HA	4:D:26:ILE:HD12	1.87	0.56
4:D:147:LEU:HB3	4:D:158:ILE:HA	1.87	0.56
5:E:170:ARG:HA	5:E:179:ASN:HB3	1.86	0.56
3:C:51:LEU:HD11	3:C:80:ARG:HA	1.88	0.56
2:B:170:ASN:ND2	2:B:236:LYS:O	2.38	0.56
5:E:20:ASP:HB3	5:E:23:LYS:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:142:GLY:HA2	17:C:383:MYX:H82	1.87	0.56
1:A:145:MET:O	1:A:149:VAL:HG23	2.06	0.55
2:B:394:PRO:HG2	2:B:397:THR:HG23	1.89	0.55
3:C:8:HIS:HD2	3:C:11:MET:HG3	1.70	0.55
2:B:99:THR:HG22	9:I:14:VAL:HG13	1.90	0.54
5:E:117:LEU:HD21	5:E:170:ARG:HB3	1.90	0.54
2:B:245:ARG:NH2	2:B:433:THR:O	2.40	0.54
9:I:46:LYS:HG2	9:I:47:ARG:N	2.23	0.54
3:C:309:THR:HG21	3:C:367:PRO:O	2.08	0.54
2:B:176:LEU:HD11	9:I:11:PHE:HB3	1.90	0.54
4:D:37:CYS:O	4:D:41:HIS:HB2	2.08	0.53
10:J:10:TYR:HA	10:J:14:PHE:HB2	1.91	0.53
3:C:369:ALA:O	3:C:373:GLU:HG3	2.08	0.53
12:E:197:PEE:H62	14:J:63:PLX:H171	1.89	0.53
1:A:351:GLU:H	11:K:12:GLN:NE2	2.07	0.53
2:B:279:LEU:HB3	2:B:295:LEU:HG	1.90	0.53
2:B:150:VAL:HG11	9:I:47:ARG:HD3	1.91	0.52
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.91	0.52
1:A:86:LEU:HD23	2:B:285:VAL:HG13	1.90	0.52
5:E:50:ALA:O	5:E:54:VAL:HG23	2.10	0.52
3:C:357:LEU:O	3:C:361:LEU:HB2	2.10	0.52
7:G:9:ARG:HD3	18:G:693:HOH:O	2.08	0.52
9:I:20:ARG:HE	9:I:51:CYS:HA	1.74	0.52
3:C:75:TYR:CD1	5:E:57:GLN:HG2	2.44	0.51
5:E:12:ASP:HB2	18:E:674:HOH:O	2.11	0.51
2:B:264:ILE:HG12	9:I:2:LEU:HD23	1.92	0.51
2:B:227:ARG:HH22	2:B:231:GLY:HA2	1.76	0.51
2:B:384:SER:HB2	9:I:2:LEU:O	2.12	0.50
6:F:63:LYS:HD3	7:G:13:VAL:HG11	1.93	0.50
2:B:71:LEU:HD23	9:I:15:LEU:HG	1.93	0.50
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.47	0.50
3:C:343:VAL:HG22	3:C:348:ILE:HG23	1.94	0.50
2:B:161:GLU:HG2	2:B:175:SER:OG	2.11	0.50
3:C:267:HIS:HD2	3:C:269:LYS:HB2	1.76	0.50
1:A:158:PHE:O	1:A:164:ALA:HB2	2.12	0.49
4:D:40:CYS:SG	15:D:243:HEM:C3C	3.00	0.49
1:A:432:PRO:HB2	1:A:437:ILE:HG13	1.94	0.49
1:A:146:ARG:HH12	1:A:308:GLN:HE22	1.60	0.49
1:A:131:ARG:NH2	1:A:177:LEU:O	2.45	0.49
1:A:373:THR:HB	1:A:374:PRO:HD3	1.94	0.48
4:D:134:TYR:CE2	4:D:162:PRO:HB3	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:24:ARG:HD2	7:G:27:PRO:HA	1.95	0.48
4:D:161:ALA:O	4:D:163:PRO:HD3	2.13	0.48
2:B:156:GLN:HG2	9:I:27:ARG:HG3	1.95	0.48
2:B:150:VAL:CG1	9:I:47:ARG:HD3	2.44	0.48
4:D:138:PRO:HB3	8:H:58:LEU:HD13	1.96	0.48
1:A:62:LEU:HD13	1:A:122:LEU:HD23	1.95	0.48
1:A:431:LEU:HD12	1:A:432:PRO:HD2	1.96	0.48
2:B:76:THR:HG23	2:B:81:SER:HA	1.94	0.48
4:D:208:MET:HA	12:E:197:PEE:H48	1.96	0.48
10:J:37:GLN:HA	10:J:40:ASP:HB2	1.96	0.48
2:B:243:GLU:HA	2:B:424:MET:O	2.14	0.48
2:B:134:ARG:NH1	18:B:580:HOH:O	2.46	0.48
2:B:70:ARG:HG3	2:B:98:VAL:HG22	1.96	0.48
1:A:280:TYR:HB3	1:A:307:PHE:CE2	2.49	0.47
6:F:9:SER:O	6:F:13:LEU:HG	2.13	0.47
2:B:100:SER:O	9:I:13:PRO:HD2	2.13	0.47
1:A:75:LEU:HD12	1:A:112:LEU:HD22	1.97	0.47
1:A:354:VAL:HG21	1:A:404:ALA:HA	1.96	0.47
3:C:28:SER:HB3	3:C:30:TRP:H	1.79	0.47
3:C:309:THR:HG23	3:C:370:GLY:HA3	1.96	0.47
3:C:361:LEU:HA	3:C:365:LEU:HB2	1.95	0.47
10:J:8:ARG:O	10:J:12:LEU:HB2	2.14	0.46
2:B:342:ASN:HD22	2:B:345:LYS:HD2	1.80	0.46
2:B:108:THR:HG21	18:B:556:HOH:O	2.16	0.46
1:A:361:LEU:HD23	1:A:399:ILE:HG12	1.98	0.46
4:D:225:HIS:O	7:G:20:PRO:HB3	2.16	0.46
3:C:116:GLY:HA2	3:C:119:LEU:HD12	1.97	0.46
1:A:325:VAL:HG21	9:I:43:LEU:HD12	1.97	0.46
1:A:301:ASN:HB2	1:A:303:LEU:HG	1.98	0.46
3:C:113:TRP:O	15:C:381:HEM:HBC2	2.15	0.46
5:E:84:GLY:H	5:E:100:HIS:HB3	1.81	0.46
4:D:101:ALA:HB1	4:D:110:PRO:HD2	1.98	0.46
13:G:82:CDL:HA61	13:G:82:CDL:H512	1.98	0.45
3:C:77:TRP:CZ3	4:D:201:ARG:HB3	2.51	0.45
1:A:419:CYS:SG	1:A:438:ARG:NH1	2.89	0.45
4:D:32:VAL:O	4:D:37:CYS:SG	2.74	0.45
9:I:14:VAL:HB	9:I:22:VAL:HG23	1.99	0.45
4:D:240:PRO:HB2	4:D:241:LYS:HD3	1.99	0.45
2:B:344:VAL:HG11	2:B:417:PHE:CD2	2.52	0.45
2:B:325:TYR:HB3	9:I:28:PRO:CD	2.42	0.45
6:F:13:LEU:HA	6:F:16:ILE:HD12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:447:CDL:HB61	13:A:447:CDL:H111	1.99	0.45
4:D:32:VAL:HB	4:D:186:VAL:HG13	1.97	0.45
3:C:324:LEU:HD12	3:C:369:ALA:HB2	1.99	0.45
2:B:111:CYS:HB3	2:B:119:LEU:HD13	1.99	0.45
1:A:252:HIS:NE2	9:I:43:LEU:HG	2.32	0.44
9:I:43:LEU:HA	9:I:46:LYS:HB3	1.98	0.44
11:K:39:ARG:HD3	11:K:39:ARG:H	1.82	0.44
2:B:394:PRO:HG2	2:B:397:THR:CG2	2.47	0.44
1:A:298:ALA:HA	1:A:303:LEU:HB2	2.00	0.44
4:D:110:PRO:HA	4:D:111:PRO:HD3	1.84	0.44
1:A:248:LEU:O	1:A:427:PRO:HG3	2.17	0.44
3:C:51:LEU:HD23	3:C:69:ILE:HD13	1.99	0.44
3:C:246:ALA:HB1	3:C:249:LEU:HB2	2.00	0.44
9:I:27:ARG:HA	9:I:28:PRO:HD2	1.98	0.43
1:A:53:ASN:HB3	1:A:170:PRO:HD2	2.01	0.43
4:D:166:ASN:HB3	8:H:13:LEU:HD22	2.01	0.43
4:D:166:ASN:HD22	8:H:13:LEU:HD22	1.84	0.43
3:C:319:PRO:HB3	7:G:47:ARG:HH11	1.83	0.43
3:C:47:THR:HG21	3:C:82:MET:HB3	2.01	0.43
3:C:250:LEU:HD22	3:C:250:LEU:H	1.84	0.43
2:B:118:ILE:H	2:B:118:ILE:HG13	1.72	0.43
1:A:144:SER:HA	9:I:42:VAL:HG11	2.01	0.43
3:C:284:ILE:HA	3:C:285:PRO:HD3	1.93	0.43
3:C:98:VAL:HG22	15:C:381:HEM:HAC	2.01	0.42
13:G:82:CDL:H121	13:G:82:CDL:H311	2.00	0.42
3:C:11:MET:CG	3:C:11:MET:CE	2.93	0.42
2:B:103:GLU:OE1	2:B:317:SER:N	2.52	0.42
4:D:225:HIS:CD2	7:G:20:PRO:HB2	2.53	0.42
2:B:325:TYR:CB	9:I:28:PRO:HD2	2.44	0.42
3:C:239:LEU:HD13	3:C:240:MET:HG2	2.01	0.42
2:B:99:THR:HB	9:I:14:VAL:HG22	2.02	0.42
3:C:280:ILE:HG13	3:C:335:LEU:HD22	2.01	0.42
5:E:136:ILE:HG13	5:E:136:ILE:H	1.73	0.42
9:I:20:ARG:HD2	9:I:48:SER:HB2	2.02	0.42
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.95	0.42
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.55	0.42
1:A:25:VAL:HG13	1:A:197:LEU:HD23	2.00	0.42
1:A:106:LEU:N	1:A:107:PRO:HD2	2.34	0.42
5:E:109:GLU:HG3	5:E:167:ALA:HB3	2.01	0.42
1:A:60:GLU:OE1	2:B:287:ARG:NH2	2.49	0.41
2:B:258:VAL:HG12	2:B:423:SER:HB2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:136:ILE:HD12	5:E:181:GLU:HB3	2.01	0.41
4:D:8:PRO:HB2	4:D:9:SER:H	1.69	0.41
3:C:301:LEU:HA	3:C:304:ILE:HD12	2.02	0.41
14:J:63:PLX:H1C2	14:J:63:PLX:H21	1.73	0.41
1:A:158:PHE:HB3	1:A:161:THR:HG1	1.85	0.41
2:B:241:GLY:HA2	2:B:423:SER:OG	2.20	0.41
4:D:31:GLN:HA	4:D:34:LYS:HB3	2.01	0.41
11:K:38:TRP:C	11:K:40:LEU:N	2.74	0.41
1:A:158:PHE:HB3	1:A:161:THR:OG1	2.21	0.41
4:D:147:LEU:HD13	4:D:158:ILE:HG13	2.01	0.41
3:C:140:PHE:CE1	3:C:170:VAL:O	2.74	0.41
11:K:45:VAL:HA	11:K:46:PRO:HD3	1.88	0.41
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.97	0.41
2:B:148:LYS:HG3	2:B:177:TYR:HB3	2.03	0.41
2:B:270:ASN:O	2:B:274:VAL:HG23	2.22	0.40
3:C:240:MET:SD	12:E:197:PEE:H17	2.61	0.40
4:D:160:MET:SD	15:D:243:HEM:C1A	3.14	0.40
4:D:163:PRO:HG2	15:D:243:HEM:HMC2	2.02	0.40
2:B:156:GLN:H	2:B:156:GLN:NE2	2.20	0.40
1:A:444:LEU:HD22	14:J:63:PLX:H52	2.04	0.40
2:B:109:VAL:HG22	2:B:119:LEU:HD23	2.04	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	444/480 (92%)	418 (94%)	20 (4%)	6 (1%)	14	35
2	B	421/453 (93%)	390 (93%)	27 (6%)	4 (1%)	19	45
3	C	376/379 (99%)	353 (94%)	19 (5%)	4 (1%)	17	42
4	D	239/241 (99%)	211 (88%)	21 (9%)	7 (3%)	6	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	194/196 (99%)	162 (84%)	29 (15%)	3 (2%)	13	32
6	F	103/110 (94%)	98 (95%)	5 (5%)	0	100	100
7	G	73/81 (90%)	66 (90%)	5 (7%)	2 (3%)	6	16
8	H	65/78 (83%)	58 (89%)	5 (8%)	2 (3%)	5	12
9	I	55/78 (70%)	31 (56%)	16 (29%)	8 (14%)	0	0
10	J	59/62 (95%)	50 (85%)	7 (12%)	2 (3%)	5	10
11	K	51/56 (91%)	43 (84%)	7 (14%)	1 (2%)	9	24
All	All	2080/2214 (94%)	1880 (90%)	161 (8%)	39 (2%)	10	25

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	250	ASP
3	C	154	PRO
4	D	8	PRO
7	G	73	ASN
9	I	29	LEU
10	J	56	LYS
11	K	52	PHE
1	A	50	GLU
1	A	220	SER
2	B	437	ASP
3	C	157	GLY
4	D	18	LEU
5	E	155	GLY
8	H	48	SER
9	I	8	SER
9	I	50	LEU
2	B	236	LYS
4	D	158	ILE
4	D	198	HIS
5	E	64	ALA
9	I	9	GLY
10	J	4	THR
1	A	74	ALA
1	A	282	CYS
3	C	9	PRO
8	H	13	LEU
9	I	27	ARG
9	I	51	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	229	PRO
3	C	343	VAL
4	D	9	SER
4	D	163	PRO
9	I	41	PRO
4	D	174	GLY
2	B	228	GLY
9	I	40	SER
1	A	221	GLY
5	E	162	GLY
7	G	74	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/394 (94%)	315 (85%)	55 (15%)	4	9
2	B	332/355 (94%)	288 (87%)	44 (13%)	5	11
3	C	326/327 (100%)	262 (80%)	64 (20%)	1	4
4	D	206/206 (100%)	158 (77%)	48 (23%)	1	2
5	E	168/168 (100%)	130 (77%)	38 (23%)	1	3
6	F	96/99 (97%)	85 (88%)	11 (12%)	7	16
7	G	66/71 (93%)	55 (83%)	11 (17%)	3	7
8	H	64/74 (86%)	42 (66%)	22 (34%)	0	0
9	I	44/60 (73%)	32 (73%)	12 (27%)	0	1
10	J	51/52 (98%)	32 (63%)	19 (37%)	0	0
11	K	42/45 (93%)	29 (69%)	13 (31%)	0	0
All	All	1765/1851 (95%)	1428 (81%)	337 (19%)	2	4

All (337) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	3	THR
1	A	9	GLN
1	A	15	GLN
1	A	17	SER
1	A	29	GLN
1	A	37	VAL
1	A	42	ASP
1	A	49	SER
1	A	58	PHE
1	A	60	GLU
1	A	73	ASN
1	A	77	LYS
1	A	90	SER
1	A	108	LYS
1	A	117	VAL
1	A	121	SER
1	A	127	ILE
1	A	129	LYS
1	A	130	GLU
1	A	139	GLN
1	A	146	ARG
1	A	147	ASP
1	A	171	SER
1	A	177	LEU
1	A	179	ARG
1	A	182	LEU
1	A	186	LEU
1	A	187	SER
1	A	188	ARG
1	A	203	LEU
1	A	206	ARG
1	A	207	GLN
1	A	214	LYS
1	A	223	TYR
1	A	225	GLU
1	A	226	ASP
1	A	232	SER
1	A	245	GLU
1	A	281	ASP
1	A	296	SER
1	A	302	LYS
1	A	308	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	323	HIS
1	A	325	VAL
1	A	343	MET
1	A	365	LEU
1	A	367	SER
1	A	369	LEU
1	A	370	ASP
1	A	381	ARG
1	A	394	GLU
1	A	403	ASP
1	A	405	ARG
1	A	409	GLU
2	B	20	HIS
2	B	33	LEU
2	B	38	LEU
2	B	46	ARG
2	B	63	LEU
2	B	69	LEU
2	B	98	VAL
2	B	99	THR
2	B	109	VAL
2	B	118	ILE
2	B	119	LEU
2	B	123	LEU
2	B	145	ARG
2	B	156	GLN
2	B	163	LEU
2	B	169	ARG
2	B	176	LEU
2	B	189	VAL
2	B	196	GLN
2	B	197	ASN
2	B	209	LEU
2	B	221	GLU
2	B	226	ILE
2	B	227	ARG
2	B	232	LEU
2	B	236	LYS
2	B	238	LYS
2	B	240	HIS
2	B	243	GLU
2	B	250	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	252	LEU
2	B	257	LEU
2	B	258	VAL
2	B	268	GLU
2	B	273	SER
2	B	294	SER
2	B	297	GLN
2	B	305	GLN
2	B	315	SER
2	B	397	THR
2	B	401	GLN
2	B	407	ASP
2	B	435	PHE
2	B	437	ASP
3	C	3	ASN
3	C	12	LYS
3	C	13	ILE
3	C	28	SER
3	C	39	ILE
3	C	42	ILE
3	C	45	ILE
3	C	51	LEU
3	C	56	THR
3	C	57	SER
3	C	60	THR
3	C	61	THR
3	C	64	SER
3	C	74	ASN
3	C	78	ILE
3	C	80	ARG
3	C	82	MET
3	C	90	PHE
3	C	92	ILE
3	C	112	THR
3	C	120	LEU
3	C	124	MET
3	C	138	MET
3	C	151	SER
3	C	156	ILE
3	C	158	THR
3	C	160	LEU
3	C	161	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	171	ASP
3	C	174	THR
3	C	175	LEU
3	C	177	ARG
3	C	194	MET
3	C	198	LEU
3	C	212	SER
3	C	226	ILE
3	C	227	LYS
3	C	233	LEU
3	C	237	LEU
3	C	239	LEU
3	C	241	LEU
3	C	242	LEU
3	C	250	LEU
3	C	254	ASP
3	C	262	LEU
3	C	264	THR
3	C	268	ILE
3	C	281	LEU
3	C	282	ARG
3	C	284	ILE
3	C	287	LYS
3	C	288	LEU
3	C	292	LEU
3	C	296	PHE
3	C	300	ILE
3	C	311	LYS
3	C	316	MET
3	C	334	THR
3	C	343	VAL
3	C	344	GLU
3	C	348	ILE
3	C	350	ILE
3	C	360	LEU
3	C	379	TRP
4	D	3	LEU
4	D	5	LEU
4	D	9	SER
4	D	13	SER
4	D	15	ARG
4	D	17	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	18	LEU
4	D	24	THR
4	D	27	ARG
4	D	34	LYS
4	D	37	CYS
4	D	39	SER
4	D	43	MET
4	D	55	CYS
4	D	59	ASP
4	D	68	VAL
4	D	72	ASP
4	D	77	ASP
4	D	80	MET
4	D	83	ARG
4	D	86	LYS
4	D	90	TYR
4	D	99	GLU
4	D	102	ARG
4	D	105	ASN
4	D	106	ASN
4	D	109	LEU
4	D	124	GLU
4	D	132	THR
4	D	139	THR
4	D	156	GLN
4	D	164	ILE
4	D	168	VAL
4	D	170	GLU
4	D	173	ASP
4	D	175	THR
4	D	179	MET
4	D	182	VAL
4	D	186	VAL
4	D	191	ARG
4	D	202	LYS
4	D	203	ARG
4	D	206	LEU
4	D	211	MET
4	D	214	LEU
4	D	224	ARG
4	D	225	HIS
4	D	241	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	3	THR
5	E	12	ASP
5	E	18	VAL
5	E	24	SER
5	E	30	GLU
5	E	60	SER
5	E	62	MET
5	E	63	SER
5	E	67	ASP
5	E	68	VAL
5	E	69	LEU
5	E	71	MET
5	E	74	ILE
5	E	76	ILE
5	E	80	ASP
5	E	85	LYS
5	E	86	ASN
5	E	89	PHE
5	E	96	LEU
5	E	100	HIS
5	E	103	LYS
5	E	104	LYS
5	E	108	GLN
5	E	112	VAL
5	E	113	GLU
5	E	115	SER
5	E	117	LEU
5	E	126	ARG
5	E	128	LYS
5	E	129	LYS
5	E	135	LEU
5	E	136	ILE
5	E	142	LEU
5	E	158	CYS
5	E	179	ASN
5	E	188	THR
5	E	192	MET
5	E	195	VAL
6	F	6	VAL
6	F	7	SER
6	F	18	LYS
6	F	71	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	73	GLN
6	F	77	LYS
6	F	81	THR
6	F	90	LEU
6	F	99	ARG
6	F	106	GLU
6	F	110	LYS
7	G	2	ARG
7	G	3	GLN
7	G	18	LEU
7	G	24	ARG
7	G	32	LYS
7	G	60	THR
7	G	64	GLN
7	G	67	GLU
7	G	70	LYS
7	G	71	ARG
7	G	72	LYS
8	H	13	LEU
8	H	18	THR
8	H	21	ARG
8	H	22	GLU
8	H	27	LEU
8	H	28	GLU
8	H	30	CYS
8	H	32	LYS
8	H	34	ARG
8	H	36	ARG
8	H	38	GLU
8	H	42	GLU
8	H	43	ARG
8	H	50	THR
8	H	55	THR
8	H	56	GLU
8	H	65	ARG
8	H	68	CYS
8	H	71	HIS
8	H	72	LYS
8	H	77	LEU
8	H	78	LYS
9	I	2	LEU
9	I	15	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	16	SER
9	I	20	ARG
9	I	22	VAL
9	I	26	LEU
9	I	27	ARG
9	I	28	PRO
9	I	45	LEU
9	I	46	LYS
9	I	50	LEU
9	I	52	ARG
10	J	4	THR
10	J	8	ARG
10	J	9	LEU
10	J	12	LEU
10	J	15	ARG
10	J	16	ARG
10	J	25	VAL
10	J	30	PHE
10	J	36	ASP
10	J	37	GLN
10	J	42	ILE
10	J	44	GLU
10	J	45	HIS
10	J	48	GLU
10	J	53	LYS
10	J	56	LYS
10	J	58	LYS
10	J	59	TYR
10	J	60	GLU
11	K	1	MET
11	K	2	LEU
11	K	6	LEU
11	K	13	LEU
11	K	16	ASN
11	K	20	THR
11	K	38	TRP
11	K	39	ARG
11	K	40	LEU
11	K	43	ASP
11	K	44	TRP
11	K	51	LYS
11	K	53	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	73	ASN
1	A	119	ASN
2	B	162	ASN
2	B	170	ASN
2	B	197	ASN
2	B	248	ASN
2	B	276	GLN
2	B	277	HIS
2	B	342	ASN
3	C	8	HIS
3	C	114	ASN
3	C	267	HIS
3	C	286	ASN
4	D	35	GLN
5	E	57	GLN
5	E	161	HIS
6	F	73	GLN
7	G	3	GLN
9	I	31	GLN
11	K	12	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
13	CDL	A	447	-	63,63,99	1.66	8 (12%)	65,75,111	1.59	8 (12%)
12	PEE	A	448	-	48,48,50	1.37	4 (8%)	49,53,55	1.41	6 (12%)
12	PEE	C	380	-	48,48,50	1.30	4 (8%)	49,53,55	1.35	7 (14%)
15	HEM	C	381	3	30,50,50	2.56	10 (33%)	24,82,82	3.27	10 (41%)
15	HEM	C	382	3	30,50,50	2.65	11 (36%)	24,82,82	3.25	11 (45%)
17	MYX	C	383	-	30,34,34	2.57	6 (20%)	20,45,45	1.52	3 (15%)
13	CDL	D	242	-	63,63,99	1.68	9 (14%)	65,75,111	1.57	7 (10%)
15	HEM	D	243	4	30,50,50	2.75	11 (36%)	24,82,82	2.94	12 (50%)
12	PEE	E	197	-	48,48,50	1.32	4 (8%)	49,53,55	1.28	4 (8%)
16	FES	E	198	5	0,4,4	0.00	-	0,4,4	0.00	-
13	CDL	G	82	-	63,63,99	1.73	8 (12%)	65,75,111	1.69	10 (15%)
14	PLX	J	63	-	51,51,51	0.80	3 (5%)	49,59,59	0.65	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CDL	A	447	-	1/1/9/9	0/74/74/110	0/0/0/0
12	PEE	A	448	-	-	0/52/52/54	0/0/0/0
12	PEE	C	380	-	-	0/52/52/54	0/0/0/0
15	HEM	C	381	3	-	0/10/54/54	0/0/8/8
15	HEM	C	382	3	-	0/10/54/54	0/0/8/8
17	MYX	C	383	-	-	0/24/36/36	0/2/2/2
13	CDL	D	242	-	1/1/9/9	0/74/74/110	0/0/0/0
15	HEM	D	243	4	-	0/10/54/54	0/0/8/8
12	PEE	E	197	-	-	0/52/52/54	0/0/0/0
16	FES	E	198	5	-	0/0/4/4	0/1/1/1
13	CDL	G	82	-	1/1/9/9	0/74/74/110	0/0/0/0
14	PLX	J	63	-	-	0/53/55/55	0/0/0/0

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	D	243	HEM	C3D-C4D	-7.51	1.41	1.51
15	C	381	HEM	C3D-C4D	-6.77	1.42	1.51
15	C	382	HEM	C3D-C4D	-6.70	1.43	1.51
15	D	243	HEM	C2D-C3D	-6.49	1.35	1.54
15	C	382	HEM	C2D-C3D	-6.02	1.36	1.54
15	C	381	HEM	C2D-C3D	-5.70	1.37	1.54
15	C	381	HEM	C3B-C4B	-4.90	1.47	1.51
15	C	382	HEM	C3B-C4B	-4.59	1.47	1.51
15	C	381	HEM	C2C-C1C	-4.56	1.43	1.52
15	D	243	HEM	C3B-C4B	-3.70	1.48	1.51
15	D	243	HEM	C2C-C1C	-2.94	1.47	1.52
15	C	382	HEM	C2C-C1C	-2.86	1.47	1.52
15	C	381	HEM	C2D-C1D	-2.37	1.44	1.51
15	D	243	HEM	C2B-C1B	-2.17	1.44	1.51
17	C	383	MYX	C13-S1	-2.14	1.70	1.73
15	C	381	HEM	C2B-C1B	-2.01	1.45	1.51
13	D	242	CDL	C11-CA5	2.06	1.56	1.50
15	C	382	HEM	CAA-C2A	2.06	1.55	1.52
15	C	381	HEM	C1C-NC	2.10	1.38	1.36
14	J	63	PLX	C7-C6	2.11	1.55	1.50
14	J	63	PLX	O7-C6	2.13	1.44	1.39
15	C	382	HEM	CHC-C1C	2.16	1.41	1.36
15	D	243	HEM	CHC-C1C	2.17	1.41	1.36
15	D	243	HEM	C4C-NC	2.37	1.38	1.36
15	C	382	HEM	C4C-NC	2.67	1.39	1.36
14	J	63	PLX	O8-C24	2.72	1.45	1.40
17	C	383	MYX	C21-C20	2.84	1.52	1.44
17	C	383	MYX	C2-C1	2.94	1.53	1.47
12	C	380	PEE	P-O2P	3.11	1.68	1.54
15	D	243	HEM	C1C-NC	3.18	1.39	1.36
13	A	447	CDL	PB2-OB4	3.28	1.68	1.54
12	A	448	PEE	P-O2P	3.34	1.69	1.54
15	C	381	HEM	CHD-C4C	3.46	1.44	1.36
12	E	197	PEE	P-O2P	3.49	1.69	1.54
15	C	382	HEM	C1C-NC	3.54	1.40	1.36
13	A	447	CDL	OB6-CB5	3.55	1.44	1.34
13	G	82	CDL	OB8-CB7	3.56	1.44	1.33
13	D	242	CDL	PA1-OA4	3.57	1.70	1.54
13	D	242	CDL	PB2-OB4	3.57	1.70	1.54
13	G	82	CDL	PB2-OB4	3.69	1.70	1.54
13	G	82	CDL	PA1-OA4	3.82	1.71	1.54
13	A	447	CDL	PA1-OA4	3.85	1.71	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	E	197	PEE	O2-C10	3.90	1.46	1.34
12	A	448	PEE	O2-C10	3.90	1.46	1.34
15	C	382	HEM	CHD-C4C	3.91	1.45	1.36
15	C	381	HEM	CBC-CAC	3.91	1.51	1.29
13	D	242	CDL	OB6-CB5	3.91	1.46	1.34
13	D	242	CDL	OB8-CB7	3.94	1.45	1.33
12	E	197	PEE	O3-C30	4.03	1.45	1.33
12	C	380	PEE	O3-C30	4.05	1.45	1.33
13	A	447	CDL	OB8-CB7	4.06	1.45	1.33
15	D	243	HEM	CHD-C4C	4.06	1.45	1.36
13	A	447	CDL	OA8-CA7	4.25	1.46	1.33
15	C	382	HEM	CBC-CAC	4.26	1.53	1.29
12	C	380	PEE	O2-C10	4.27	1.47	1.34
12	A	448	PEE	O3-C30	4.39	1.46	1.33
13	A	447	CDL	OA6-CA5	4.43	1.47	1.34
15	C	382	HEM	CBB-CAB	4.49	1.55	1.29
15	C	381	HEM	CBB-CAB	4.52	1.55	1.29
13	G	82	CDL	OB6-CB5	4.64	1.48	1.34
13	G	82	CDL	OA6-CA5	4.66	1.48	1.34
15	D	243	HEM	CBC-CAC	4.70	1.56	1.29
13	D	242	CDL	OA8-CA7	4.71	1.47	1.33
13	D	242	CDL	OA6-CA5	4.73	1.48	1.34
15	D	243	HEM	CBB-CAB	4.74	1.56	1.29
12	C	380	PEE	P-O1P	4.74	1.68	1.51
13	D	242	CDL	PA1-OA3	4.80	1.68	1.51
13	G	82	CDL	PA1-OA3	4.87	1.68	1.51
12	E	197	PEE	P-O1P	4.88	1.69	1.51
13	G	82	CDL	OA8-CA7	4.89	1.48	1.33
13	A	447	CDL	PA1-OA3	5.00	1.69	1.51
12	A	448	PEE	P-O1P	5.17	1.70	1.51
13	A	447	CDL	PB2-OB3	5.20	1.70	1.51
13	D	242	CDL	PB2-OB3	5.29	1.70	1.51
13	G	82	CDL	PB2-OB3	5.46	1.71	1.51
17	C	383	MYX	O2-C3	5.87	1.47	1.35
17	C	383	MYX	C2-C3	6.57	1.39	1.33
17	C	383	MYX	C13-N2	9.04	1.44	1.31

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	381	HEM	C3B-CAB-CBB	-8.24	111.82	124.46
15	C	382	HEM	C3C-CAC-CBC	-7.40	113.10	124.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D	243	HEM	C3C-CAC-CBC	-7.05	113.64	124.46
15	C	382	HEM	C3B-CAB-CBB	-6.95	113.79	124.46
13	G	82	CDL	OB8-CB7-OB9	-6.29	107.25	123.49
13	A	447	CDL	OB6-CB5-OB7	-5.97	107.64	123.67
15	C	381	HEM	C3C-CAC-CBC	-5.75	115.64	124.46
13	D	242	CDL	OB8-CB7-OB9	-5.54	109.20	123.49
15	C	381	HEM	C1D-CHD-C4C	-5.48	116.66	125.82
13	A	447	CDL	OA8-CA7-OA9	-5.32	109.76	123.49
13	G	82	CDL	OA6-CA5-OA7	-5.30	109.44	123.67
13	D	242	CDL	OB6-CB5-OB7	-5.24	109.60	123.67
13	A	447	CDL	OB8-CB7-OB9	-5.16	110.17	123.49
12	C	380	PEE	O3-C30-O5	-5.10	110.32	123.49
12	E	197	PEE	O3-C30-O5	-5.02	110.52	123.49
15	C	382	HEM	C4B-CHC-C1C	-4.98	117.50	125.82
12	A	448	PEE	O3-C30-O5	-4.93	110.78	123.49
12	A	448	PEE	O2-C10-O4	-4.80	110.80	123.67
12	E	197	PEE	O2-C10-O4	-4.56	111.43	123.67
13	G	82	CDL	OA7-CA5-C11	-4.53	105.58	123.72
15	D	243	HEM	C3B-CAB-CBB	-4.47	117.60	124.46
15	C	382	HEM	C1D-CHD-C4C	-4.16	118.88	125.82
13	D	242	CDL	OB7-CB5-C51	-4.09	107.36	123.72
13	D	242	CDL	OA8-CA7-OA9	-3.94	113.33	123.49
12	A	448	PEE	O4-C10-C11	-3.90	108.12	123.72
13	G	82	CDL	OB9-CB7-C71	-3.86	108.29	123.72
12	C	380	PEE	O4-C10-C11	-3.84	108.34	123.72
15	D	243	HEM	C4B-CHC-C1C	-3.84	119.41	125.82
13	G	82	CDL	OB6-CB5-OB7	-3.81	113.45	123.67
13	G	82	CDL	OA8-CA7-OA9	-3.81	113.67	123.49
15	C	381	HEM	C4B-CHC-C1C	-3.77	119.52	125.82
13	D	242	CDL	OA9-CA7-C31	-3.75	108.70	123.72
13	A	447	CDL	OA9-CA7-C31	-3.69	108.95	123.72
12	E	197	PEE	O4-C10-C11	-3.65	109.13	123.72
12	A	448	PEE	O5-C30-C31	-3.50	109.72	123.72
13	A	447	CDL	OB9-CB7-C71	-3.48	109.78	123.72
13	G	82	CDL	OB7-CB5-C51	-3.44	109.97	123.72
13	D	242	CDL	OB9-CB7-C71	-3.43	110.01	123.72
15	D	243	HEM	C1D-CHD-C4C	-3.32	120.27	125.82
13	A	447	CDL	OB7-CB5-C51	-3.31	110.49	123.72
13	G	82	CDL	OA9-CA7-C31	-3.26	110.66	123.72
13	D	242	CDL	OA6-CA5-OA7	-3.21	115.05	123.67
15	C	382	HEM	CBA-CAA-C2A	-3.07	107.02	112.53
12	E	197	PEE	O5-C30-C31	-3.07	111.44	123.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	447	CDL	OA7-CA5-C11	-2.93	111.98	123.72
12	C	380	PEE	O5-C30-C31	-2.75	112.70	123.72
15	D	243	HEM	CAA-C2A-C1A	-2.72	124.05	127.01
15	D	243	HEM	CAA-CBA-CGA	-2.65	107.89	112.75
12	C	380	PEE	O2-C10-O4	-2.62	116.64	123.67
17	C	383	MYX	C23-C22-C21	-2.58	120.29	126.11
13	A	447	CDL	OA6-CA5-OA7	-2.48	117.02	123.67
12	A	448	PEE	C3-C2-C1	-2.03	107.31	112.07
12	C	380	PEE	O2-C2-C3	2.02	115.48	108.36
13	G	82	CDL	OA6-CA5-C11	2.14	116.18	111.53
13	G	82	CDL	OA6-CA4-CA3	2.29	116.43	108.36
12	A	448	PEE	O3-C3-C2	2.47	115.33	108.69
15	D	243	HEM	CMD-C2D-C3D	2.47	125.27	114.35
12	C	380	PEE	C2-O2-C10	2.51	123.91	117.89
15	C	382	HEM	CMD-C2D-C3D	2.54	125.57	114.35
17	C	383	MYX	O3-C7-C5	2.93	114.71	107.86
12	C	380	PEE	O2-C2-C1	2.95	118.75	108.36
15	C	381	HEM	CMD-C2D-C3D	3.04	127.79	114.35
15	D	243	HEM	C2D-C3D-C4D	3.20	106.92	101.50
15	C	382	HEM	C2D-C3D-C4D	3.67	107.72	101.50
15	C	382	HEM	CMC-C2C-C3C	3.71	125.79	116.53
15	D	243	HEM	CMC-C2C-C3C	3.73	125.84	116.53
15	C	381	HEM	C2D-C3D-C4D	3.85	108.03	101.50
15	C	381	HEM	CAD-C3D-C2D	3.92	124.48	113.22
15	D	243	HEM	CAD-C3D-C2D	3.97	124.64	113.22
15	C	382	HEM	CAD-C3D-C2D	4.03	124.80	113.22
15	C	381	HEM	CMB-C2B-C3B	4.07	126.68	116.53
15	C	382	HEM	CAD-C3D-C4D	4.18	127.22	112.47
15	C	381	HEM	CMC-C2C-C3C	4.26	127.15	116.53
15	C	381	HEM	CAD-C3D-C4D	4.26	127.49	112.47
15	C	382	HEM	CMB-C2B-C3B	4.35	127.38	116.53
15	D	243	HEM	CAD-C3D-C4D	4.38	127.92	112.47
15	D	243	HEM	CMB-C2B-C3B	4.62	128.06	116.53
17	C	383	MYX	C4-O2-C3	4.63	124.33	116.28

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	D	242	CDL	CA4
13	G	82	CDL	CA4
13	A	447	CDL	CA4

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	447	CDL	1	0
12	A	448	PEE	1	0
15	C	381	HEM	3	0
15	C	382	HEM	1	0
17	C	383	MYX	1	0
15	D	243	HEM	11	0
12	E	197	PEE	3	0
13	G	82	CDL	2	0
14	J	63	PLX	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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.