



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:15 PM GMT

PDB ID : 1EZV
Title : STRUCTURE OF THE YEAST CYTOCHROME BC1 COMPLEX CO-CRYSTALLIZED WITH AN ANTIBODY FV-FRAGMENT
Authors : Hunte, C.; Koepke, J.; Lange, C.; Rossmanith, T.; Michel, H.
Deposited on : 2000-05-12
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>

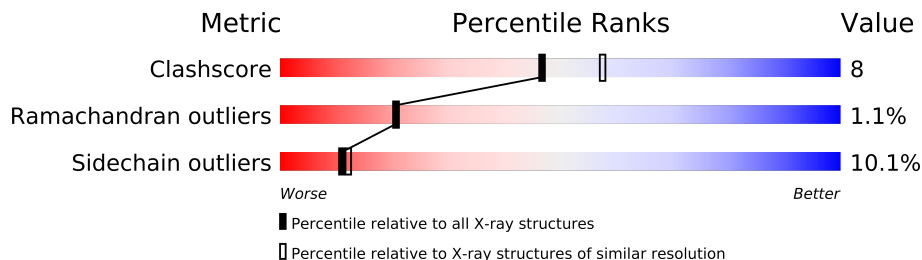
The following versions of software and data (see [references](#)) were used in the production of this report:

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	430	
2	B	352	
3	C	385	
4	D	245	
5	E	185	
6	H	74	
7	F	125	
8	G	93	
9	I	55	
10	X	127	
11	Y	107	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 17781 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	430	Total	C	N	O	S	0	0	0
			3338	2106	575	651	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	DELETION	UNP P07256
A	152	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
			2735	1747	453	534	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
			3089	2080	484	504	21			

- Molecule 4 is a protein called CYTOCHROME C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	245	Total	C	N	O	S	0	0	0
			1934	1232	333	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
			1411	893	242	266	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	74	Total	C	N	O	S	0	0	0
			624	391	108	123	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	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	G	93	Total	C	N	O	S	98	0	0
			773	510	131	130	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			

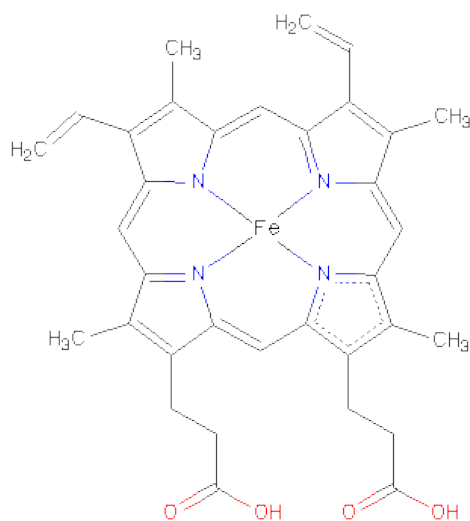
- Molecule 10 is a protein called HEAVY CHAIN (VH) OF FV-FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	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.

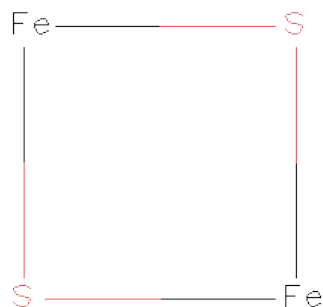
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	Y	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

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



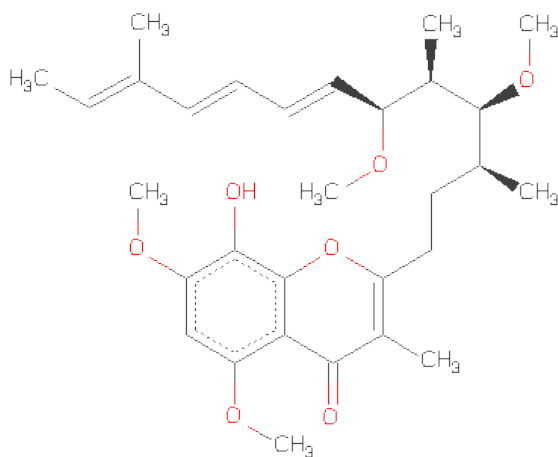
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



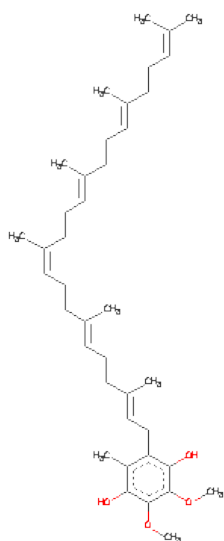
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	E	1	Total	Fe	S	0	0
			4	2	2		

- 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-HEXAENYL)-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 water.

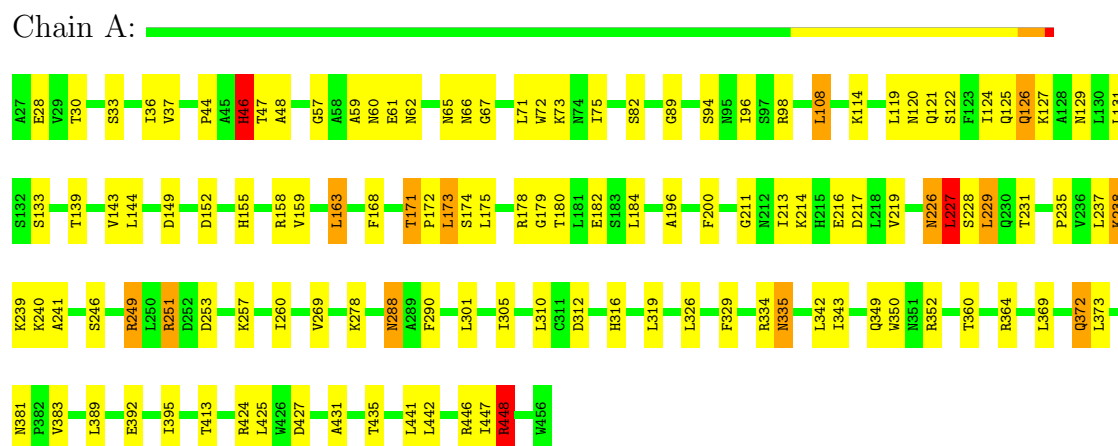
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	47	Total	O	0	0
			47	47		
16	B	11	Total	O	0	0
			11	11		
16	C	114	Total	O	0	0
			114	114		
16	D	71	Total	O	0	0
			71	71		
16	E	33	Total	O	0	0
			33	33		
16	F	36	Total	O	0	0
			36	36		
16	G	20	Total	O	0	0
			20	20		
16	H	6	Total	O	0	0
			6	6		
16	I	1	Total	O	0	0
			1	1		
16	X	5	Total	O	0	0
			5	5		
16	Y	2	Total	O	0	0
			2	2		

3 Residue-property plots

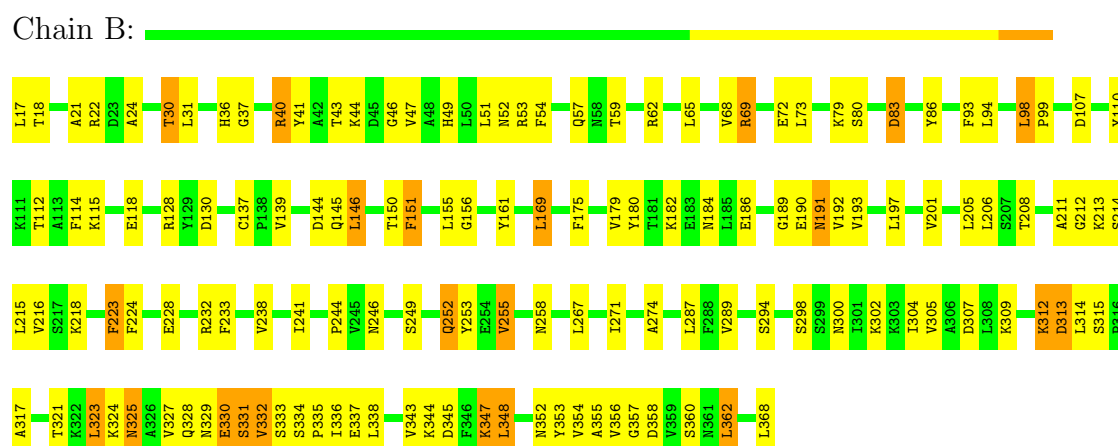
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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





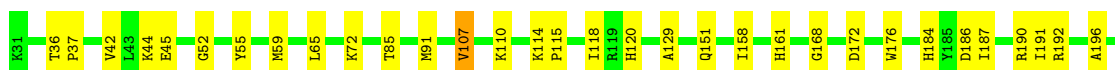
• Molecule 4: CYTOCHROME C1

Chain D:



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

Chain E:



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

Chain H:



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

Chain F:



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

Chain G:



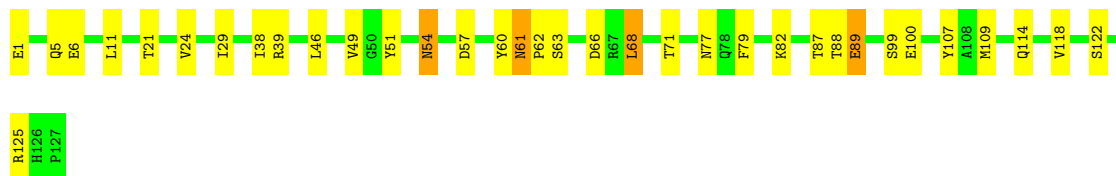
• Molecule 9: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.3 KD PROTEIN

Chain I:



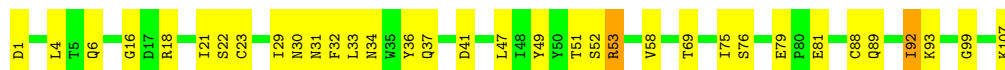
- Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

Chain X: 



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

Chain Y: 



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 147.27Å 90.00° 117.50° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	84.7 (15.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17781	wwPDB-VP
Average B, all atoms (Å ²)	70.0	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: HEM, FES, 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	0/3399	0.49	0/4606
2	B	0.31	0/2781	0.47	0/3764
3	C	0.44	0/3191	0.53	0/4353
4	D	0.34	0/1994	0.48	0/2714
5	E	0.35	0/1444	0.52	0/1957
6	H	0.33	0/638	0.42	0/858
7	F	0.34	0/1032	0.52	1/1397 (0.1%)
8	G	0.38	0/804	0.43	0/1088
9	I	0.40	0/462	0.43	0/622
10	X	0.32	0/1043	0.47	0/1422
11	Y	0.31	0/863	0.43	0/1172
All	All	0.36	0/17651	0.49	1/23953 (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
1	A	0	4
2	B	0	2
3	C	0	5
4	D	0	4
5	E	0	1
6	H	0	1
7	F	0	1
8	G	0	1
10	X	0	1
11	Y	0	1
All	All	0	21

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	71	ARG	NE-CZ-NH1	-5.33	117.63	120.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	LEU	Peptide
1	A	249	ARG	Sidechain
1	A	446	ARG	Sidechain
1	A	448	ARG	Sidechain
2	B	332	VAL	Peptide
2	B	69	ARG	Sidechain
3	C	218	ARG	Sidechain
3	C	222	HIS	Mainchain
3	C	279	TYR	Sidechain
3	C	314	ARG	Sidechain
3	C	79	ARG	Sidechain
4	D	109	ARG	Sidechain
4	D	154	TYR	Sidechain
4	D	94	TYR	Sidechain
4	D	97	TYR	Sidechain
5	E	192	ARG	Sidechain
7	F	71	ARG	Sidechain
8	G	40	ILE	Peptide
6	H	98	TYR	Sidechain
10	X	60	TYR	Sidechain
11	Y	79	GLU	Peptide

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	3338	0	3316	66	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2735	0	2774	79	0
3	C	3089	0	3125	27	0
4	D	1934	0	1855	18	0
5	E	1411	0	1386	22	0
6	H	624	0	581	9	0
7	F	1012	0	1026	14	0
8	G	773	0	736	6	0
9	I	449	0	445	7	0
10	X	1015	0	959	20	0
11	Y	842	0	820	16	0
12	C	86	0	60	3	0
12	D	43	0	30	0	0
13	E	4	0	0	0	0
14	C	37	0	40	5	0
15	C	43	0	58	12	0
16	A	47	0	0	1	0
16	B	11	0	0	0	0
16	C	114	0	0	1	0
16	D	71	0	0	0	0
16	E	33	0	0	0	0
16	F	36	0	0	2	0
16	G	20	0	0	1	0
16	H	6	0	0	0	0
16	I	1	0	0	0	0
16	X	5	0	0	1	0
16	Y	2	0	0	0	0
All	All	17781	0	17211	279	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 8.

All (279) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:C:506:UQ6:H103	15:C:506:UQ6:H1M1	1.11	1.09
15:C:506:UQ6:H103	15:C:506:UQ6:C1M	1.93	0.98
15:C:506:UQ6:H1M1	15:C:506:UQ6:C10	1.97	0.92
6:H:77:GLN:H	6:H:77:GLN:HE21	1.11	0.91
2:B:347:LYS:HD3	2:B:347:LYS:H	1.43	0.82
1:A:316:HIS:HE1	1:A:350:TRP:HE1	1.29	0.81
2:B:182:LYS:HB2	2:B:211:ALA:HB2	1.64	0.80
3:C:7:ASN:HD22	3:C:10:LEU:H	1.31	0.77
3:C:40:LEU:HD23	15:C:506:UQ6:H18	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:253:HIS:HD2	3:C:255:ASP:H	1.34	0.76
1:A:108:LEU:HB2	2:B:323:LEU:HD22	1.68	0.76
7:F:31:GLN:HE21	7:F:31:GLN:HA	1.51	0.74
5:E:107:VAL:HG12	5:E:118:ILE:HB	1.68	0.74
10:X:6:GLU:H	10:X:114:GLN:HE21	1.38	0.71
3:C:58:ILE:H	3:C:173:ASN:HD22	1.38	0.70
6:H:78:LEU:HD13	6:H:142:LEU:HD22	1.71	0.70
7:F:77:ARG:HD3	7:F:88:LEU:HD11	1.74	0.70
5:E:115:PRO:HD2	5:E:158:ILE:HD11	1.73	0.69
7:F:77:ARG:HD2	16:F:155:HOH:O	1.93	0.69
5:E:72:LYS:NZ	9:I:29:GLN:HE22	1.90	0.69
5:E:44:LYS:NZ	5:E:52:GLY:H	1.91	0.69
10:X:38:ILE:HD12	10:X:46:LEU:HD22	1.75	0.68
1:A:349:GLN:HE22	1:A:352:ARG:HH21	1.41	0.68
1:A:73:LYS:HG3	1:A:94:SER:HB3	1.76	0.68
2:B:325:ASN:HD22	2:B:328:GLN:HE22	1.43	0.67
6:H:77:GLN:HE21	6:H:77:GLN:N	1.91	0.67
2:B:49:HIS:HD2	2:B:161:TYR:H	1.43	0.67
6:H:91:GLY:O	6:H:95:VAL:HG13	1.95	0.66
1:A:155:HIS:HD2	1:A:158:ARG:HH21	1.44	0.66
1:A:257:LYS:HG2	1:A:334:ARG:HG3	1.78	0.66
2:B:258:ASN:HD21	2:B:324:LYS:HG2	1.61	0.66
1:A:120:ASN:HD21	1:A:124:ILE:HD12	1.60	0.65
1:A:98:ARG:HD3	1:A:173:LEU:HD12	1.76	0.65
3:C:22:GLN:HE22	15:C:506:UQ6:H3M3	1.60	0.65
1:A:66:ASN:HD22	1:A:180:THR:HG23	1.62	0.65
5:E:72:LYS:HZ3	9:I:29:GLN:HE22	1.45	0.64
3:C:346:VAL:HG23	16:G:103:HOH:O	1.97	0.64
2:B:65:LEU:O	2:B:69:ARG:HG2	1.97	0.63
1:A:216:GLU:HA	1:A:219:VAL:HG12	1.80	0.63
2:B:313:ASP:HB3	2:B:344:LYS:O	1.98	0.63
5:E:44:LYS:HB3	8:G:35:LYS:HA	1.81	0.62
4:D:147:ARG:HG2	4:D:148:PRO:O	1.99	0.62
1:A:62:ASN:HB2	1:A:65:ASN:ND2	2.15	0.62
11:Y:4:LEU:HD22	11:Y:88:CYS:SG	2.40	0.61
2:B:49:HIS:CD2	2:B:161:TYR:H	2.18	0.61
11:Y:29:ILE:HG22	11:Y:92:ILE:HD12	1.81	0.61
4:D:62:MET:HB3	4:D:67:HIS:NE2	2.16	0.60
2:B:255:VAL:HB	2:B:321:THR:HG21	1.84	0.59
1:A:72:TRP:CE3	1:A:75:ILE:HD11	2.37	0.59
2:B:150:THR:HG22	2:B:352:ASN:ND2	2.18	0.59
10:X:54:ASN:HD22	10:X:54:ASN:H	1.50	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:168:GLY:HA2	5:E:176:TRP:CD1	2.38	0.59
8:G:52:PHE:O	8:G:56:PHE:HB3	2.02	0.59
1:A:305:ILE:HA	1:A:310:LEU:HD22	1.84	0.59
4:D:113:ARG:HG2	4:D:151:LEU:O	2.03	0.58
10:X:29:ILE:H	10:X:77:ASN:HD21	1.49	0.58
3:C:58:ILE:H	3:C:173:ASN:ND2	2.03	0.57
2:B:315:SER:HB3	2:B:344:LYS:HB2	1.87	0.57
3:C:157:VAL:O	3:C:161:ILE:HG12	2.05	0.57
2:B:246:ASN:HB2	2:B:249:SER:HB3	1.86	0.57
2:B:155:LEU:HD12	2:B:155:LEU:H	1.70	0.57
5:E:72:LYS:HZ2	9:I:29:GLN:NE2	2.03	0.57
11:Y:34:ASN:HD22	11:Y:49:TYR:HA	1.69	0.57
5:E:72:LYS:NZ	9:I:29:GLN:NE2	2.52	0.56
2:B:317:ALA:O	2:B:321:THR:HG22	2.05	0.56
8:G:56:PHE:O	8:G:60:LEU:HB2	2.05	0.56
10:X:38:ILE:HA	10:X:49:VAL:HG23	1.87	0.56
1:A:62:ASN:HB2	1:A:65:ASN:HD22	1.68	0.56
7:F:43:LEU:HD13	7:F:48:LEU:HD11	1.88	0.56
5:E:172:ASP:H	5:E:184:HIS:HD2	1.53	0.56
5:E:44:LYS:HZ3	5:E:52:GLY:H	1.53	0.56
11:Y:32:PHE:HB2	11:Y:92:ILE:HG22	1.87	0.56
1:A:66:ASN:ND2	1:A:179:GLY:HA2	2.21	0.56
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.88	0.56
2:B:238:VAL:HG13	2:B:356:VAL:HB	1.88	0.55
3:C:57:ASN:HA	3:C:173:ASN:HD21	1.71	0.55
1:A:301:LEU:HB2	1:A:349:GLN:HG3	1.89	0.55
11:Y:36:TYR:HE2	11:Y:89:GLN:HG2	1.72	0.55
2:B:325:ASN:HA	2:B:328:GLN:NE2	2.22	0.55
2:B:228:GLU:HA	2:B:353:TYR:O	2.06	0.55
7:F:15:ILE:HG23	7:F:21:LEU:HB3	1.89	0.54
5:E:172:ASP:H	5:E:184:HIS:CD2	2.25	0.54
2:B:24:ALA:HB3	2:B:191:ASN:ND2	2.23	0.54
4:D:121:THR:OG1	4:D:124:GLU:HG3	2.08	0.54
2:B:300:ASN:O	2:B:304:ILE:HG12	2.08	0.54
1:A:288:ASN:HD22	1:A:288:ASN:C	2.11	0.53
2:B:305:VAL:O	2:B:309:LYS:HB2	2.08	0.53
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.91	0.53
4:D:247:MET:O	4:D:251:VAL:HG22	2.08	0.53
4:D:297:THR:HG21	5:E:42:VAL:HG11	1.89	0.53
11:Y:6:GLN:HG2	11:Y:23:CYS:SG	2.49	0.53
5:E:55:TYR:O	5:E:59:MET:HG2	2.08	0.53
11:Y:31:ASN:HD22	11:Y:51:THR:CG2	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:214:LYS:HB2	1:A:217:ASP:HB2	1.92	0.52
3:C:44:ILE:HD12	15:C:506:UQ6:C20	2.39	0.52
1:A:47:THR:HG21	2:B:327:VAL:HG12	1.92	0.52
1:A:71:LEU:HD13	1:A:143:VAL:HG21	1.90	0.52
4:D:125:VAL:HA	4:D:128:MET:HE3	1.92	0.51
10:X:24:VAL:HG21	10:X:29:ILE:HD11	1.92	0.51
1:A:67:GLY:HA3	1:A:184:LEU:CD1	2.40	0.51
10:X:61:ASN:HD22	10:X:63:SER:H	1.56	0.51
2:B:294:SER:HB3	2:B:358:ASP:HB3	1.93	0.51
2:B:252:GLN:HG3	2:B:253:TYR:N	2.25	0.51
2:B:347:LYS:HG2	2:B:348:LEU:N	2.26	0.51
2:B:68:VAL:O	2:B:72:GLU:HG3	2.10	0.51
7:F:53:ASN:ND2	7:F:56:MET:H	2.09	0.51
3:C:25:SER:OG	7:F:79:HIS:HD2	1.94	0.51
2:B:115:LYS:HB2	2:B:118:GLU:HG3	1.93	0.51
2:B:305:VAL:HG11	2:B:368:LEU:HB3	1.93	0.50
1:A:413:THR:HB	16:A:480:HOH:O	2.11	0.50
10:X:6:GLU:H	10:X:114:GLN:NE2	2.05	0.50
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.93	0.50
1:A:269:VAL:HG21	1:A:395:ILE:HD13	1.93	0.50
1:A:316:HIS:CE1	1:A:350:TRP:HE1	2.19	0.50
2:B:44:LYS:HB2	2:B:47:VAL:HG21	1.93	0.49
3:C:208:ASN:HD22	3:C:210:LEU:H	1.59	0.49
15:C:506:UQ6:H4M3	15:C:506:UQ6:O5	2.11	0.49
11:Y:37:GLN:HB2	11:Y:47:LEU:HD11	1.95	0.49
7:F:71:ARG:NH1	16:F:148:HOH:O	2.43	0.49
1:A:171:THR:HG23	1:A:241:ALA:HA	1.93	0.49
2:B:241:ILE:HG12	2:B:287:LEU:HB3	1.94	0.49
1:A:57:GLY:H	1:A:60:ASN:HD22	1.61	0.49
4:D:74:TYR:CE1	6:H:139:ALA:HA	2.47	0.49
16:X:130:HOH:O	11:Y:49:TYR:HB2	2.12	0.49
10:X:61:ASN:ND2	10:X:63:SER:H	2.11	0.49
3:C:198:LEU:HD11	15:C:506:UQ6:H153	1.95	0.49
2:B:312:LYS:O	2:B:313:ASP:HB2	2.13	0.49
10:X:61:ASN:HD22	10:X:62:PRO:N	2.11	0.48
1:A:121:GLN:O	1:A:126:GLN:HB2	2.12	0.48
1:A:122:SER:O	1:A:127:LYS:HD3	2.13	0.48
3:C:18:ILE:HA	3:C:222:HIS:HB2	1.95	0.48
14:C:505:SMA:H21	14:C:505:SMA:H39	1.94	0.48
2:B:83:ASP:HB2	2:B:86:TYR:H	1.78	0.48
2:B:46:GLY:O	2:B:49:HIS:HB3	2.13	0.48
1:A:372:GLN:HG3	1:A:373:LEU:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:H:74:VAL:HG12	6:H:75:THR:H	1.77	0.48
10:X:87:THR:HB	10:X:89:GLU:HB2	1.96	0.47
1:A:73:LYS:HB2	1:A:96:ILE:HD11	1.96	0.47
1:A:66:ASN:ND2	1:A:180:THR:HG23	2.27	0.47
2:B:325:ASN:HD22	2:B:328:GLN:NE2	2.08	0.47
1:A:155:HIS:HD2	1:A:158:ARG:NH2	2.10	0.47
2:B:51:LEU:HD21	2:B:180:TYR:CE1	2.49	0.47
1:A:343:ILE:HG21	1:A:447:ILE:HD12	1.96	0.47
1:A:72:TRP:CZ3	1:A:75:ILE:HD11	2.50	0.47
1:A:59:ALA:O	1:A:172:PRO:HB3	2.15	0.47
11:Y:49:TYR:O	11:Y:53:ARG:HB2	2.15	0.47
5:E:120:HIS:CD2	5:E:151:GLN:HG2	2.50	0.46
12:C:401:HEM:HH2	12:C:401:HEM:HBC2	1.97	0.46
2:B:146:LEU:HD13	2:B:354:VAL:HG22	1.97	0.46
3:C:253:HIS:CD2	3:C:255:ASP:H	2.22	0.46
5:E:129:ALA:HB2	5:E:187:ILE:HG23	1.97	0.46
1:A:48:ALA:HA	1:A:211:GLY:HA3	1.97	0.46
4:D:304:PRO:HA	4:D:305:PRO:HD3	1.74	0.46
2:B:197:LEU:O	2:B:201:VAL:HG23	2.15	0.46
1:A:288:ASN:HD22	1:A:290:PHE:H	1.61	0.46
6:H:77:GLN:H	6:H:77:GLN:NE2	1.94	0.46
2:B:98:LEU:N	2:B:99:PRO:HD2	2.30	0.46
2:B:182:LYS:HB2	2:B:211:ALA:CB	2.41	0.46
10:X:68:LEU:HA	10:X:82:LYS:O	2.16	0.46
3:C:52:MET:CE	15:C:506:UQ6:H352	2.46	0.46
8:G:61:ILE:HB	8:G:62:PRO:HD3	1.98	0.46
1:A:349:GLN:NE2	1:A:352:ARG:HH21	2.12	0.45
2:B:274:ALA:HB2	2:B:287:LEU:HD12	1.97	0.45
2:B:287:LEU:HD21	2:B:304:ILE:HG21	1.97	0.45
1:A:381:ASN:OD1	1:A:383:VAL:HG22	2.16	0.45
7:F:18:SER:HA	7:F:19:PRO:HD3	1.82	0.45
2:B:223:PHE:CD2	2:B:244:PRO:HB3	2.51	0.45
2:B:40:ARG:HD3	2:B:155:LEU:HG	1.98	0.45
1:A:238:LYS:HB2	1:A:239:LYS:H	1.62	0.45
3:C:7:ASN:ND2	3:C:10:LEU:H	2.05	0.45
2:B:52:ASN:ND2	2:B:80:SER:OG	2.50	0.45
4:D:111:ALA:HA	4:D:154:TYR:HA	1.98	0.45
14:C:505:SMA:C16	14:C:505:SMA:H39	2.47	0.45
2:B:175:PHE:CZ	2:B:179:VAL:HG21	2.52	0.45
3:C:323:LYS:HE3	8:G:55:GLN:HE22	1.81	0.45
1:A:312:ASP:OD1	1:A:334:ARG:HD3	2.16	0.45
1:A:75:ILE:HG23	1:A:139:THR:HG21	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:271:ILE:HG21	2:B:287:LEU:HD11	1.99	0.45
1:A:288:ASN:ND2	1:A:290:PHE:H	2.15	0.45
1:A:251:ARG:HD3	1:A:253:ASP:OD1	2.16	0.45
11:Y:21:ILE:HG22	11:Y:22:SER:N	2.31	0.45
2:B:321:THR:O	2:B:325:ASN:HB2	2.18	0.44
2:B:224:PHE:CD1	2:B:224:PHE:N	2.85	0.44
10:X:68:LEU:HD12	10:X:68:LEU:H	1.83	0.44
2:B:59:THR:HA	2:B:112:THR:HA	1.99	0.44
11:Y:6:GLN:HG3	11:Y:99:GLY:HA3	1.99	0.44
5:E:120:HIS:HD2	5:E:151:GLN:HG2	1.82	0.44
7:F:45:PHE:O	7:F:48:LEU:HB2	2.17	0.44
3:C:1:MET:N	16:C:585:HOH:O	2.42	0.44
2:B:214:SER:OG	2:B:216:VAL:HG23	2.18	0.44
2:B:252:GLN:HE21	2:B:252:GLN:HB2	1.66	0.44
11:Y:47:LEU:HA	11:Y:58:VAL:HG11	1.99	0.44
10:X:99:SER:HB3	10:X:109:MET:HG2	1.99	0.44
1:A:168:PHE:O	1:A:171:THR:HB	2.18	0.44
2:B:37:GLY:HA3	2:B:179:VAL:HG11	2.00	0.44
1:A:73:LYS:HG3	1:A:94:SER:CB	2.48	0.43
2:B:325:ASN:ND2	2:B:328:GLN:HE22	2.11	0.43
2:B:49:HIS:HE1	2:B:130:ASP:OD1	2.01	0.43
8:G:35:LYS:HA	8:G:36:PRO:HD2	1.76	0.43
10:X:49:VAL:HG12	10:X:68:LEU:HD23	1.99	0.43
2:B:24:ALA:HB3	2:B:191:ASN:HD21	1.81	0.43
2:B:110:TYR:CD2	2:B:205:LEU:HD23	2.53	0.43
1:A:226:ASN:HB3	1:A:227:LEU:H	1.57	0.43
4:D:286:TRP:CE3	5:E:59:MET:HG3	2.53	0.43
1:A:89:GLY:O	2:B:323:LEU:HD23	2.18	0.43
2:B:36:HIS:HB2	2:B:184:ASN:OD1	2.19	0.43
4:D:230:PHE:O	4:D:247:MET:HE1	2.19	0.43
1:A:246:SER:O	1:A:431:ALA:HA	2.18	0.43
1:A:349:GLN:NE2	1:A:352:ARG:HD3	2.34	0.43
2:B:145:GLN:HB3	2:B:354:VAL:HG11	2.01	0.43
14:C:505:SMA:H14	14:C:505:SMA:H36	2.00	0.43
3:C:27:ASN:OD1	3:C:29:TRP:HB2	2.19	0.43
9:I:14:ASN:HA	9:I:14:ASN:HD22	1.56	0.43
3:C:4:ARG:HE	3:C:14:ASN:ND2	2.17	0.43
4:D:263:HIS:NE2	4:D:267:LYS:HE3	2.33	0.43
2:B:325:ASN:HA	2:B:328:GLN:HE21	1.82	0.42
2:B:334:SER:HA	2:B:335:PRO:HD3	1.90	0.42
2:B:151:PHE:O	2:B:156:GLY:HA3	2.18	0.42
7:F:120:LEU:O	7:F:123:ILE:HG12	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:233:PHE:HB3	2:B:357:GLY:HA2	2.01	0.42
1:A:127:LYS:HD2	1:A:127:LYS:HA	1.88	0.42
10:X:87:THR:HG22	10:X:88:THR:H	1.85	0.42
11:Y:37:GLN:HB2	11:Y:47:LEU:CD1	2.49	0.42
2:B:330:GLU:HG3	2:B:331:SER:N	2.33	0.42
9:I:5:SER:O	9:I:9:THR:HG23	2.20	0.42
1:A:159:VAL:CG2	1:A:435:THR:HG22	2.49	0.42
1:A:163:LEU:HD13	1:A:326:LEU:HD13	2.02	0.42
3:C:72:VAL:HA	5:E:85:THR:HG22	2.01	0.42
3:C:332:ASN:HD21	3:C:355:ALA:HA	1.85	0.42
1:A:196:ALA:O	1:A:200:PHE:HB2	2.20	0.42
4:D:302:PHE:HB2	7:F:73:TYR:CD1	2.54	0.42
1:A:168:PHE:O	1:A:174:SER:HB3	2.19	0.42
6:H:117:LEU:O	6:H:118:GLU:HG3	2.20	0.42
5:E:186:ASP:OD2	5:E:190:ARG:HD2	2.19	0.42
10:X:49:VAL:HG12	10:X:68:LEU:CD2	2.50	0.41
15:C:506:UQ6:H301	15:C:506:UQ6:H322	1.72	0.41
12:C:401:HEM:HHD	12:C:401:HEM:CBC	2.50	0.41
2:B:21:ALA:HA	2:B:189:GLY:O	2.20	0.41
4:D:65:ALA:HB2	6:H:124:VAL:HG11	2.02	0.41
1:A:427:ASP:OD1	1:A:448:ARG:NH1	2.52	0.41
1:A:47:THR:HG21	2:B:327:VAL:CG1	2.50	0.41
7:F:115:LYS:HA	7:F:115:LYS:HD3	1.92	0.41
2:B:298:SER:O	2:B:302:LYS:HB2	2.20	0.41
5:E:36:THR:HA	5:E:37:PRO:HD2	1.92	0.41
10:X:29:ILE:HG12	10:X:77:ASN:ND2	2.35	0.41
11:Y:75:ILE:HG22	11:Y:76:SER:N	2.36	0.41
2:B:114:PHE:O	2:B:169:LEU:HD11	2.20	0.41
15:C:506:UQ6:C4M	15:C:506:UQ6:O5	2.69	0.41
2:B:98:LEU:HD11	2:B:192:VAL:HG22	2.02	0.41
2:B:30:THR:HG23	2:B:190:GLU:HB3	2.02	0.41
9:I:23:ALA:O	9:I:27:VAL:HG23	2.21	0.41
1:A:335:ASN:HD22	1:A:335:ASN:C	2.24	0.41
1:A:67:GLY:HA3	1:A:184:LEU:HD11	2.02	0.41
2:B:146:LEU:HA	2:B:146:LEU:HD12	1.94	0.41
3:C:222:HIS:ND1	3:C:223:SER:N	2.66	0.41
3:C:173:ASN:HB3	3:C:174:PRO:HD3	2.02	0.41
2:B:151:PHE:CD2	2:B:155:LEU:HB2	2.56	0.41
1:A:364:ARG:HD2	2:B:72:GLU:OE1	2.20	0.41
4:D:208:LEU:HA	4:D:208:LEU:HD12	1.95	0.41
2:B:355:ALA:HB1	2:B:362:LEU:HD23	2.03	0.41
15:C:506:UQ6:H121	15:C:506:UQ6:H101	1.58	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:61:GLU:OE1	1:A:66:ASN:HA	2.21	0.41
14:C:505:SMA:C10	14:C:505:SMA:H36	2.49	0.41
7:F:19:PRO:HA	7:F:22:SER:HB3	2.03	0.41
1:A:213:ILE:HG13	1:A:213:ILE:H	1.63	0.41
2:B:137:CYS:SG	2:B:139:VAL:HG22	2.61	0.41
5:E:191:ILE:HD13	5:E:196:ALA:HB3	2.04	0.40
3:C:117:GLY:O	12:C:402:HEM:HMC3	2.20	0.40
2:B:93:PHE:HD1	2:B:94:LEU:O	2.03	0.40
1:A:46:HIS:CE1	2:B:332:VAL:HG21	2.55	0.40
10:X:6:GLU:N	10:X:114:GLN:HE21	2.14	0.40
11:Y:34:ASN:ND2	11:Y:49:TYR:HA	2.36	0.40
10:X:100:GLU:O	10:X:107:TYR:HA	2.21	0.40
2:B:238:VAL:HA	2:B:289:VAL:O	2.22	0.40
1:A:171:THR:HG23	1:A:172:PRO:HD2	2.04	0.40
14:C:505:SMA:C16	14:C:505:SMA:C25	3.00	0.40
2:B:325:ASN:HD22	2:B:325:ASN:HA	1.64	0.40
1:A:228:SER:HB3	1:A:231:THR:HB	2.04	0.40
1:A:249:ARG:NH1	1:A:441:LEU:O	2.55	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	428/430 (100%)	396 (92%)	27 (6%)	5 (1%)	19	19
2	B	350/352 (99%)	311 (89%)	31 (9%)	8 (2%)	10	7
3	C	383/385 (100%)	369 (96%)	13 (3%)	1 (0%)	50	60
4	D	243/245 (99%)	238 (98%)	5 (2%)	0	100	100
5	E	183/185 (99%)	174 (95%)	7 (4%)	2 (1%)	21	21
6	H	72/74 (97%)	68 (94%)	4 (6%)	0	100	100
7	F	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
8	G	91/93 (98%)	76 (84%)	10 (11%)	5 (6%)	3	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
10	X	125/127 (98%)	116 (93%)	9 (7%)	0	100	100
11	Y	105/107 (98%)	91 (87%)	11 (10%)	3 (3%)	7	4
All	All	2156/2178 (99%)	2009 (93%)	123 (6%)	24 (1%)	21	21

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	336	ILE
8	G	52	PHE
8	G	93	ASN
2	B	313	ASP
2	B	329	ASN
2	B	333	SER
3	C	156	PHE
5	E	45	GLU
11	Y	16	GLY
11	Y	30	ASN
11	Y	52	SER
1	A	227	LEU
2	B	57	GLN
8	G	4	PRO
8	G	41	PHE
1	A	229	LEU
2	B	22	ARG
5	E	161	HIS
1	A	44	PRO
1	A	235	PRO
1	A	46	HIS
2	B	79	LYS
2	B	212	GLY
8	G	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	369/369 (100%)	323 (88%)	46 (12%)	7	7
2	B	301/301 (100%)	254 (84%)	47 (16%)	4	3
3	C	338/338 (100%)	312 (92%)	26 (8%)	18	22
4	D	203/203 (100%)	195 (96%)	8 (4%)	43	57
5	E	151/151 (100%)	145 (96%)	6 (4%)	42	56
6	H	67/67 (100%)	59 (88%)	8 (12%)	8	8
7	F	109/109 (100%)	100 (92%)	9 (8%)	16	19
8	G	77/77 (100%)	69 (90%)	8 (10%)	10	11
9	I	45/45 (100%)	41 (91%)	4 (9%)	14	16
10	X	112/112 (100%)	95 (85%)	17 (15%)	4	4
11	Y	93/93 (100%)	83 (89%)	10 (11%)	9	10
All	All	1865/1865 (100%)	1676 (90%)	189 (10%)	11	12

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	30	THR
1	A	33	SER
1	A	36	ILE
1	A	37	VAL
1	A	46	HIS
1	A	82	SER
1	A	114	LYS
1	A	119	LEU
1	A	125	GLN
1	A	126	GLN
1	A	129	ASN
1	A	131	LEU
1	A	133	SER
1	A	144	LEU
1	A	149	ASP
1	A	152	ASP
1	A	163	LEU
1	A	171	THR
1	A	173	LEU
1	A	175	LEU
1	A	178	ARG
1	A	182	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	226	ASN
1	A	227	LEU
1	A	229	LEU
1	A	237	LEU
1	A	238	LYS
1	A	240	LYS
1	A	251	ARG
1	A	260	ILE
1	A	278	LYS
1	A	288	ASN
1	A	319	LEU
1	A	329	PHE
1	A	335	ASN
1	A	342	LEU
1	A	360	THR
1	A	369	LEU
1	A	372	GLN
1	A	389	LEU
1	A	392	GLU
1	A	424	ARG
1	A	425	LEU
1	A	442	LEU
1	A	448	ARG
2	B	17	LEU
2	B	18	THR
2	B	30	THR
2	B	31	LEU
2	B	40	ARG
2	B	41	TYR
2	B	43	THR
2	B	53	ARG
2	B	54	PHE
2	B	62	ARG
2	B	73	LEU
2	B	83	ASP
2	B	98	LEU
2	B	107	ASP
2	B	128	ARG
2	B	144	ASP
2	B	146	LEU
2	B	151	PHE
2	B	169	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	186	GLU
2	B	191	ASN
2	B	193	VAL
2	B	206	LEU
2	B	208	THR
2	B	213	LYS
2	B	215	LEU
2	B	218	LYS
2	B	223	PHE
2	B	232	ARG
2	B	252	GLN
2	B	255	VAL
2	B	267	LEU
2	B	307	ASP
2	B	312	LYS
2	B	314	LEU
2	B	323	LEU
2	B	325	ASN
2	B	330	GLU
2	B	331	SER
2	B	337	GLU
2	B	338	LEU
2	B	343	VAL
2	B	345	ASP
2	B	347	LYS
2	B	348	LEU
2	B	360	SER
2	B	362	LEU
3	C	5	LYS
3	C	12	LEU
3	C	35	LEU
3	C	38	LEU
3	C	79	ARG
3	C	89	PHE
3	C	99	LYS
3	C	101	LEU
3	C	150	LEU
3	C	156	PHE
3	C	182	LEU
3	C	184	TYR
3	C	185	LEU
3	C	223	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	230	LEU
3	C	238	LEU
3	C	247	SER
3	C	304	VAL
3	C	312	VAL
3	C	313	VAL
3	C	321	LEU
3	C	336	LEU
3	C	350	LEU
3	C	377	LEU
3	C	382	ARG
3	C	385	LYS
4	D	69	LEU
4	D	113	ARG
4	D	140	GLU
4	D	251	VAL
4	D	256	ASN
4	D	268	ARG
4	D	280	LEU
4	D	283	LEU
5	E	65	LEU
5	E	91	MET
5	E	107	VAL
5	E	110	LYS
5	E	114	LYS
5	E	211	LYS
6	H	74	VAL
6	H	77	GLN
6	H	79	GLU
6	H	89	GLU
6	H	94	LEU
6	H	117	LEU
6	H	118	GLU
6	H	130	LEU
7	F	16	LEU
7	F	21	LEU
7	F	30	ASN
7	F	31	GLN
7	F	41	LEU
7	F	48	LEU
7	F	86	HIS
7	F	115	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	F	127	LYS
8	G	38	GLN
8	G	48	SER
8	G	49	PHE
8	G	52	PHE
8	G	60	LEU
8	G	68	TYR
8	G	71	LYS
8	G	88	GLU
9	I	13	ARG
9	I	14	ASN
9	I	18	VAL
9	I	48	LEU
10	X	1	GLU
10	X	5	GLN
10	X	11	LEU
10	X	21	THR
10	X	39	ARG
10	X	51	TYR
10	X	54	ASN
10	X	57	ASP
10	X	61	ASN
10	X	66	ASP
10	X	68	LEU
10	X	71	THR
10	X	79	PHE
10	X	89	GLU
10	X	118	VAL
10	X	122	SER
10	X	125	ARG
11	Y	1	ASP
11	Y	18	ARG
11	Y	33	LEU
11	Y	41	ASP
11	Y	53	ARG
11	Y	69	THR
11	Y	81	GLU
11	Y	92	ILE
11	Y	93	LYS
11	Y	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	60	ASN
1	A	62	ASN
1	A	65	ASN
1	A	66	ASN
1	A	120	ASN
1	A	155	HIS
1	A	170	ASN
1	A	198	ASN
1	A	199	HIS
1	A	273	ASN
1	A	288	ASN
1	A	297	GLN
1	A	316	HIS
1	A	335	ASN
1	A	349	GLN
1	A	384	ASN
1	A	387	ASN
1	A	428	GLN
2	B	49	HIS
2	B	52	ASN
2	B	55	ASN
2	B	191	ASN
2	B	252	GLN
2	B	258	ASN
2	B	325	ASN
2	B	328	GLN
3	C	7	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	H	77	GLN
7	F	31	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	F	53	ASN
7	F	57	GLN
7	F	79	HIS
7	F	91	ASN
7	F	97	GLN
9	I	14	ASN
9	I	29	GLN
10	X	54	ASN
10	X	59	ASN
10	X	61	ASN
10	X	77	ASN
10	X	78	GLN
10	X	114	GLN
11	Y	31	ASN
11	Y	34	ASN
11	Y	89	GLN
11	Y	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 ⓘ

6 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
12	HEM	C	401	3	49,50,50	1.93	11 (22%)	46,82,82	1.43	5 (10%)
12	HEM	C	402	3	49,50,50	1.77	13 (26%)	46,82,82	1.28	2 (4%)
14	SMA	C	505	-	38,38,38	1.87	8 (21%)	50,52,52	2.26	15 (30%)
15	UQ6	C	506	-	43,43,43	2.47	16 (37%)	55,55,55	2.18	17 (30%)
12	HEM	D	3	4	49,50,50	1.99	10 (20%)	46,82,82	1.34	3 (6%)
13	FES	E	4	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
12	HEM	C	401	3	-	0/14/114/114	0/0/8/8
12	HEM	C	402	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
12	HEM	D	3	4	-	0/14/114/114	0/0/8/8
13	FES	E	4	5	-	0/0/4/4	0/0/1/1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	506	UQ6	O5-C5	-6.72	1.20	1.37
14	C	505	SMA	C4-C4A	5.88	1.49	1.40
14	C	505	SMA	C4A-C8A	5.77	1.48	1.41
15	C	506	UQ6	O2-C2	-5.62	1.23	1.37
15	C	506	UQ6	C2-C3	5.60	1.48	1.39
15	C	506	UQ6	C7-C6	5.29	1.58	1.51
12	C	401	HEM	C2B-C1B	-5.06	1.43	1.44
12	D	3	HEM	C3B-C2B	-5.02	1.35	1.43
12	C	401	HEM	C3C-C2C	-4.86	1.35	1.43
12	D	3	HEM	C3C-C2C	-4.78	1.35	1.43
12	C	401	HEM	C3D-C2D	-4.69	1.35	1.43
15	C	506	UQ6	C13-C14	4.46	1.41	1.32
12	C	402	HEM	C3D-C2D	-4.37	1.36	1.43
12	D	3	HEM	C3D-C2D	-4.35	1.36	1.43
12	C	401	HEM	C3B-C2B	-4.31	1.36	1.43
12	C	402	HEM	C3C-C2C	-4.25	1.36	1.43
12	D	3	HEM	CBC-CAC	4.18	1.53	1.28
12	D	3	HEM	CBB-CAB	4.17	1.53	1.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	402	HEM	C3B-C2B	-4.14	1.36	1.43
12	D	3	HEM	C3B-CAB	3.89	1.52	1.40
12	C	402	HEM	C4A-C3A	3.87	1.45	1.40
14	C	505	SMA	C13-C12	3.59	1.62	1.54
12	D	3	HEM	C3C-CAC	3.55	1.51	1.40
12	D	3	HEM	C4A-C3A	3.50	1.44	1.40
12	C	401	HEM	CMC-C2C	3.45	1.58	1.47
12	C	401	HEM	C4A-C3A	3.32	1.44	1.40
15	C	506	UQ6	C11-C9	3.27	1.59	1.51
15	C	506	UQ6	C18-C19	3.26	1.39	1.32
12	D	3	HEM	CHA-C4D	3.07	1.40	1.35
12	C	402	HEM	CHB-C1B	3.05	1.40	1.35
12	D	3	HEM	FE-NA	2.98	2.05	1.92
12	C	401	HEM	CMB-C2B	2.93	1.56	1.47
15	C	506	UQ6	C16-C14	2.83	1.58	1.51
12	C	402	HEM	CHA-C4D	2.81	1.39	1.35
15	C	506	UQ6	C5-C4	2.74	1.44	1.39
12	C	402	HEM	FE-NA	2.70	2.04	1.92
12	C	402	HEM	CBC-CAC	2.57	1.43	1.28
14	C	505	SMA	C5-C4A	2.52	1.47	1.42
15	C	506	UQ6	C23-C24	2.51	1.38	1.32
12	C	401	HEM	CHA-C4D	2.41	1.39	1.35
15	C	506	UQ6	C33-C34	2.41	1.40	1.32
15	C	506	UQ6	C4-C3	-2.41	1.35	1.39
12	C	401	HEM	C2D-C1D	-2.38	1.44	1.44
12	C	402	HEM	CMB-C2B	2.37	1.54	1.47
15	C	506	UQ6	C7-C8	2.36	1.55	1.50
14	C	505	SMA	O12-C12	-2.35	1.36	1.42
12	C	402	HEM	FE-NB	2.30	2.06	1.97
12	C	401	HEM	CBC-CAC	2.27	1.42	1.28
15	C	506	UQ6	C2-C1	2.24	1.46	1.40
15	C	506	UQ6	C28-C29	2.22	1.37	1.32
12	C	402	HEM	CBB-CAB	2.15	1.41	1.28
15	C	506	UQ6	C6-C1	-2.13	1.37	1.40
14	C	505	SMA	O7-C7	2.12	1.40	1.37
14	C	505	SMA	C6-C7	2.11	1.42	1.38
14	C	505	SMA	C20-C19	2.09	1.36	1.33
12	C	401	HEM	CBB-CAB	2.05	1.40	1.28
12	C	402	HEM	CMC-C2C	2.00	1.53	1.47
12	C	402	HEM	CMD-C2D	2.00	1.53	1.47

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	506	UQ6	C3M-O3-C3	7.15	134.43	114.90
12	D	3	HEM	C3B-C4B-NB	-6.41	109.42	114.00
14	C	505	SMA	O1-C2-C9	6.37	114.13	110.58
12	C	401	HEM	C3B-C4B-NB	-6.24	109.54	114.00
14	C	505	SMA	C26-C19-C18	-6.12	108.19	118.09
12	C	402	HEM	C3B-C4B-NB	-5.78	109.86	114.00
14	C	505	SMA	O14-C14-C15	4.80	129.71	110.74
15	C	506	UQ6	C17-C18-C19	4.71	137.96	127.80
15	C	506	UQ6	C11-C12-C13	4.58	124.69	111.62
15	C	506	UQ6	C4M-O4-C4	4.55	127.35	114.90
15	C	506	UQ6	C17-C16-C14	4.01	126.00	112.74
14	C	505	SMA	O14-C14-C13	4.00	118.45	108.36
14	C	505	SMA	O7-C7-C8	3.95	118.59	114.50
14	C	505	SMA	C3-C4-C4A	-3.94	115.51	121.65
14	C	505	SMA	O12-C12-C13	3.91	113.98	107.80
15	C	506	UQ6	C22-C23-C24	3.47	135.29	127.80
15	C	506	UQ6	C7-C6-C5	-3.46	116.52	120.96
15	C	506	UQ6	C11-C9-C8	3.45	127.72	121.08
14	C	505	SMA	O1-C8A-C8	3.34	120.20	115.90
14	C	505	SMA	C4-C3-C2	3.18	121.51	116.97
15	C	506	UQ6	C10-C9-C11	-2.99	110.84	115.39
12	C	402	HEM	C2D-C1D-ND	-2.98	109.41	112.93
12	D	3	HEM	C2D-C1D-ND	-2.88	109.53	112.93
15	C	506	UQ6	C1M-C1-C2	-2.76	114.83	120.35
15	C	506	UQ6	C1M-C1-C6	2.72	124.23	120.42
12	C	401	HEM	C4A-CHB-C1B	-2.67	123.96	127.47
14	C	505	SMA	O7-C7-C6	-2.58	119.73	124.23
15	C	506	UQ6	C25-C24-C26	-2.39	111.76	115.39
12	C	401	HEM	C2D-C1D-ND	-2.37	110.13	112.93
14	C	505	SMA	C5M-O5-C5	-2.35	114.63	117.78
14	C	505	SMA	C18-C19-C20	2.32	126.32	118.91
14	C	505	SMA	C3M-C3-C4	-2.30	117.26	120.37
12	C	401	HEM	CMD-C2D-C3D	2.23	130.66	125.60
15	C	506	UQ6	C21-C19-C18	2.23	125.37	121.08
15	C	506	UQ6	C15-C14-C16	-2.20	112.05	115.39
12	C	401	HEM	CBD-CAD-C3D	-2.16	109.66	114.37
15	C	506	UQ6	C30-C29-C31	-2.15	112.11	115.39
14	C	505	SMA	O12-C12-C11	2.13	111.11	107.79
12	D	3	HEM	CMA-C3A-C4A	-2.12	125.37	128.62
14	C	505	SMA	O5-C5-C6	-2.11	120.41	123.59
15	C	506	UQ6	C20-C19-C18	-2.09	119.39	123.52
15	C	506	UQ6	C31-C29-C28	2.01	124.95	121.08

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	C	505	SMA	C12
14	C	505	SMA	C14

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 ⓘ

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.