



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:15 PM GMT

PDB ID : 1SQX
Title : Crystal Structure Analysis of Bovine Bcl with Stigmatellin A
Authors : Esser, L.; Quinn, B.; Li, Y.F.; Zhang, M.; Elberry, M.; Yu, L.; Yu, C.A.; Xia, D.
Deposited on : 2004-03-21
Resolution : 2.60 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

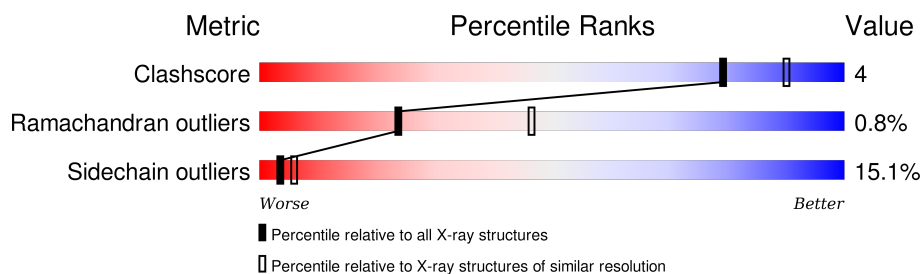
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)





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	446	 82% 15% •
2	B	439	 80% 14% • •
3	C	379	 78% 18% •
4	E	196	 82% 17% •
5	D	241	 77% 18% 5%
6	G	81	 74% 16% • 7%
7	I	78	 36% 24% 9% • 27%

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Mol	Chain	Length	Quality of chain
8	F	110	 79% 14% • 5%
9	K	56	 70% 25% 5%
10	H	78	 59% 26% • 14%
11	J	62	 77% 18% • •

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 16978 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	E	196	Total	C	N	O	S	0	0	0
			1519	957	263	291	8			

- 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	D	241	Total	C	N	O	S	0	0	0
			1919	1225	330	349	15			

- Molecule 6 is a protein called Ubiquinol-cytochrome C reductase complex 14 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	75	Total	C	N	O	S	0	0	0
			628	410	118	99	1			

- Molecule 7 is a protein called Ubiquinol-cytochrome C reductase complex ubiquinone-binding protein QP-C.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	105	Total	C	N	O	S	0	0	0
			911	576	165	168	2			

- 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	K	53	Total	C	N	O	S	0	0	0
			438	293	78	66	1			

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

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

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

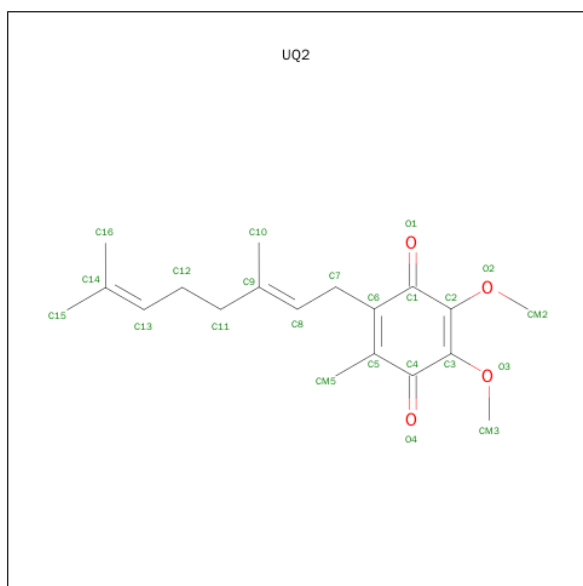
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	J	60	Total	C	N	O	0	0	0
			495	324	86	85			

- Molecule 12 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



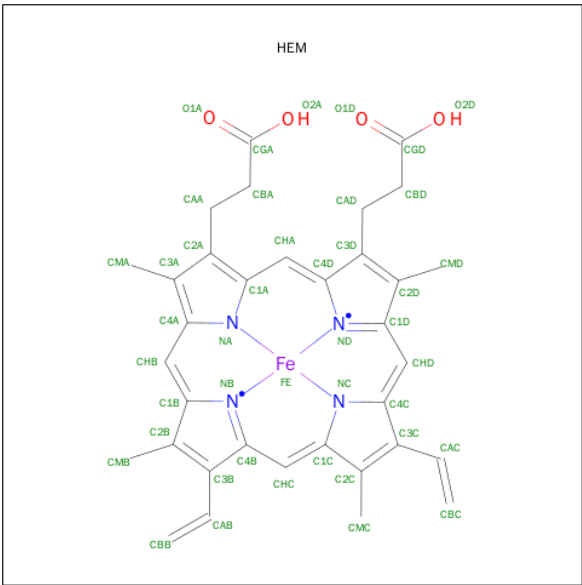
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 13 is UBIQUINONE-2 (three-letter code: UQ2) (formula: $C_{19}H_{26}O_4$).



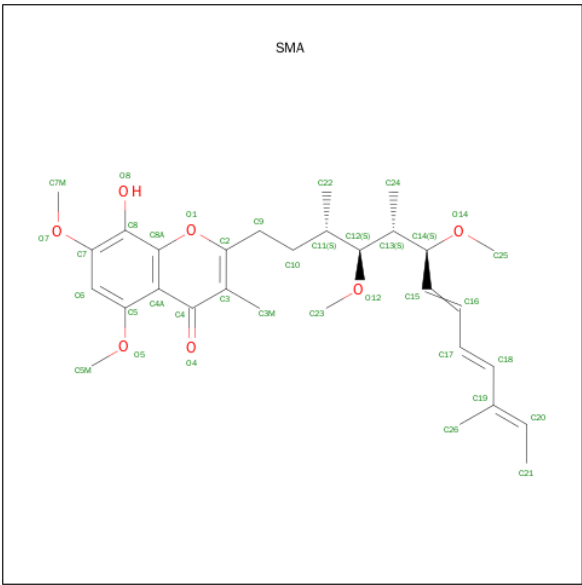
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			23	19	4		

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



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

- Molecule 15 is STIGMATELLIN A (three-letter code: SMA) (formula: C₃₀H₄₂O₇).



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

- Molecule 16 is water.

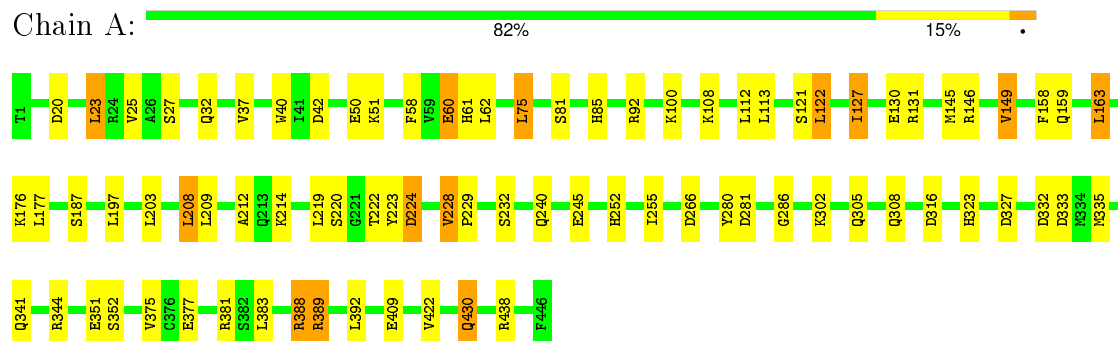
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	65	Total 65	O 65	0	0
16	B	99	Total 99	O 99	0	0
16	C	36	Total 36	O 36	0	0
16	D	19	Total 19	O 19	0	0
16	E	8	Total 8	O 8	0	0
16	F	32	Total 32	O 32	0	0
16	G	19	Total 19	O 19	0	0
16	H	6	Total 6	O 6	0	0
16	I	2	Total 2	O 2	0	0
16	K	2	Total 2	O 2	0	0

3 Residue-property plots

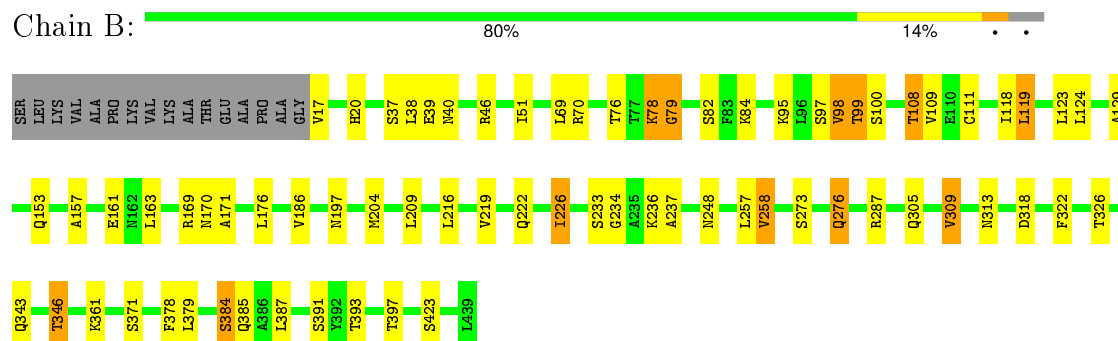
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

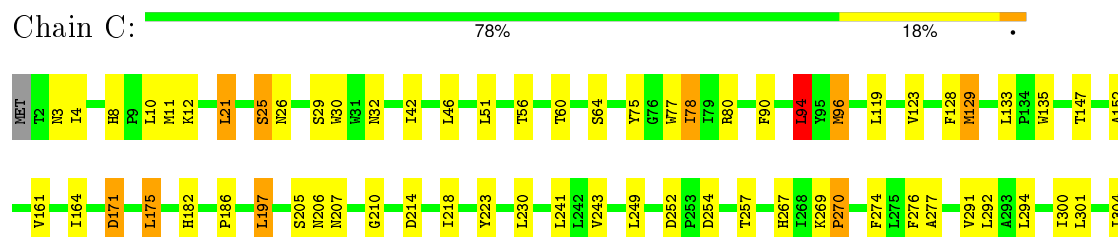
- Molecule 1: Ubiquinol-cytochrome-c reductase complex core protein I, mitochondrial precursor

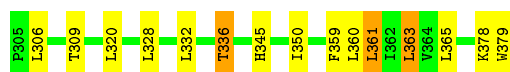


- Molecule 2: Ubiquinol-cytochrome-c reductase complex core protein 2, mitochondrial precursor



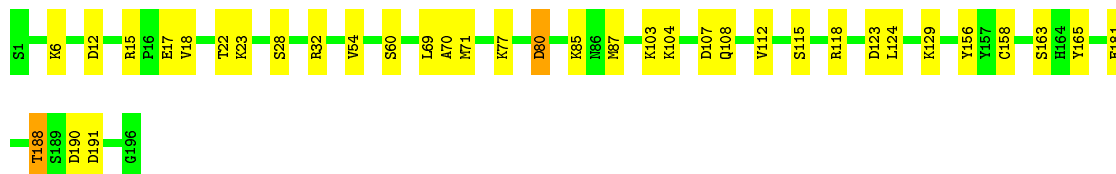
- Molecule 3: Cytochrome b





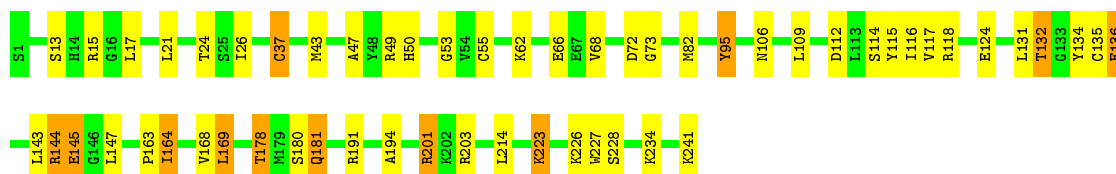
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain E: 82% 17% .



- 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)]

Chain D: 77% 18% 5%



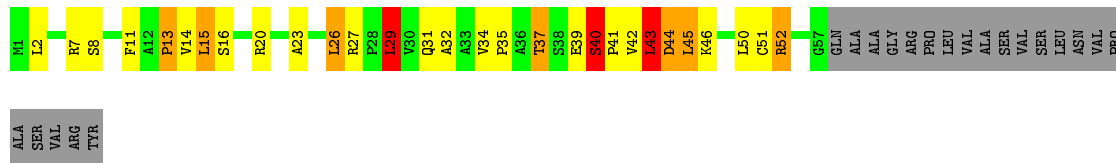
- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein

Chain G: 74% 16% 7%



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

Chain I: 36% 24% 9% 27%



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

Chain F: 79% 14% 5%



- 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)]

protein (Complex III subunit IX)]

Chain K:

70%

25%

5%



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

Chain H:

59%

26%

14%



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

Chain J:

77%

18%



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	154.38Å 154.38Å 590.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	94.2 (40.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.233 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16978	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: HEM, UQ2, FES, SMA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.84	1/3531 (0.0%)	0.81	8/4792 (0.2%)
2	B	0.85	0/3232	0.80	1/4386 (0.0%)
3	C	0.97	0/3100	0.80	5/4242 (0.1%)
4	E	0.89	0/1553	0.78	4/2100 (0.2%)
5	D	0.90	0/1978	0.79	1/2684 (0.0%)
6	G	1.07	0/649	0.75	0/878
7	I	1.03	0/411	0.95	1/558 (0.2%)
8	F	0.95	0/930	0.84	0/1246
9	K	1.01	0/454	0.76	0/621
10	H	0.77	0/553	0.85	1/741 (0.1%)
11	J	1.00	0/508	0.78	0/686
All	All	0.91	1/16899 (0.0%)	0.80	21/22934 (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	4
2	B	0	7
3	C	0	2
4	E	0	1
5	D	0	5
7	I	0	8
11	J	0	1
All	All	0	28

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	ILE	CA-CB	5.14	1.66	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	ASP	CB-CG-OD1	7.48	125.03	118.30
3	C	94	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	224	ASP	CB-CG-OD1	5.98	123.69	118.30
7	I	44	ASP	CB-CG-OD2	5.65	123.38	118.30
4	E	123	ASP	CB-CG-OD2	5.63	123.37	118.30
3	C	252	ASP	CB-CG-OD2	5.63	123.36	118.30
5	D	72	ASP	CB-CG-OD1	5.45	123.20	118.30
4	E	80	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	327	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	23	LEU	CA-CB-CG	5.30	127.48	115.30
10	H	60	ASP	CB-CG-OD1	5.27	123.04	118.30
2	B	318	ASP	CB-CG-OD2	5.24	123.01	118.30
3	C	214	ASP	CB-CG-OD2	5.21	122.99	118.30
4	E	191	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	333	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	316	ASP	CB-CG-OD2	5.08	122.88	118.30
3	C	171	ASP	CB-CG-OD2	5.08	122.87	118.30
4	E	190	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	332	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	20	ASP	CB-CG-OD2	5.03	122.82	118.30
3	C	361	LEU	CA-CB-CG	5.02	126.86	115.30

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	PHE	Peptide
1	A	228	VAL	Peptide
1	A	280	TYR	Peptide
1	A	388	ARG	Peptide
2	B	169	ARG	Peptide
2	B	226	ILE	Peptide
2	B	233	SER	Peptide
2	B	234	GLY	Peptide
2	B	248	ASN	Peptide
2	B	39	GLU	Peptide
2	B	79	GLY	Peptide

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Mol	Chain	Res	Type	Group
3	C	25	SER	Peptide
3	C	270	PRO	Peptide
5	D	115	TYR	Peptide
5	D	144	ARG	Peptide
5	D	145	GLU	Peptide
5	D	53	GLY	Peptide
5	D	73	GLY	Peptide
4	E	188	THR	Peptide
7	I	23	ALA	Peptide
7	I	26	LEU	Peptide
7	I	34	VAL	Peptide
7	I	35	PRO	Peptide
7	I	37	THR	Peptide
7	I	42	VAL	Mainchain,Peptide
7	I	52	ARG	Peptide
11	J	59	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3458	0	3356	23	0
2	B	3172	0	3152	25	0
3	C	3003	0	3065	31	0
4	E	1519	0	1503	4	0
5	D	1919	0	1870	15	0
6	G	628	0	636	2	0
7	I	406	0	437	11	0
8	F	911	0	904	4	0
9	K	438	0	447	6	0
10	H	548	0	530	2	0
11	J	495	0	493	3	0
12	E	4	0	0	0	0
13	C	23	0	26	4	0
14	C	86	0	60	4	0
14	D	43	0	30	2	0
15	C	37	0	41	3	0
16	A	65	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	B	99	0	0	2	0
16	C	36	0	0	0	0
16	D	19	0	0	1	0
16	E	8	0	0	0	0
16	F	32	0	0	0	0
16	G	19	0	0	0	0
16	H	6	0	0	0	0
16	I	2	0	0	0	0
16	K	2	0	0	0	0
All	All	16978	0	16550	116	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 4.

All (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:GLN:HE22	2:B:393:THR:H	1.11	0.93
5:D:37:CYS:SG	14:D:242:HEM:HAB	2.19	0.82
13:C:380:UQ2:H2M3	14:C:381:HEM:HBA2	1.64	0.78
9:K:38:TRP:CE3	9:K:41:ILE:HD13	2.22	0.74
3:C:94:LEU:HD21	3:C:123:VAL:HG11	1.72	0.72
2:B:100:SER:O	7:I:13:PRO:HD2	1.90	0.72
3:C:21:LEU:HD21	13:C:380:UQ2:H3M3	1.71	0.71
2:B:385:GLN:NE2	2:B:393:THR:H	1.86	0.70
14:C:381:HEM:HMC2	14:C:381:HEM:HBC2	1.77	0.67
2:B:99:THR:HB	7:I:14:VAL:HG22	1.77	0.66
9:K:38:TRP:CE3	9:K:41:ILE:CD1	2.79	0.66
7:I:43:LEU:HA	7:I:46:LYS:HD3	1.77	0.65
3:C:75:TYR:HB3	3:C:78:ILE:HD11	1.78	0.65
2:B:76:THR:HG22	2:B:82:SER:H	1.62	0.65
8:F:28:LYS:HB3	8:F:74:ILE:HG12	1.81	0.61
5:D:47:ALA:H	5:D:50:HIS:CD2	2.21	0.58
3:C:29:SER:HA	3:C:32:ASN:HD22	1.68	0.57
3:C:30:TRP:HZ3	3:C:96:MET:HG3	1.71	0.56
1:A:341:GLN:HE22	1:A:344:ARG:HE	1.54	0.55
2:B:258:VAL:HG12	2:B:423:SER:HB2	1.89	0.55
2:B:70:ARG:HG3	2:B:98:VAL:HG22	1.88	0.55
5:D:178:THR:HG23	5:D:181:GLN:HB2	1.89	0.54
4:E:156:TYR:HB2	4:E:165:TYR:HB2	1.89	0.54
2:B:153:GLN:HE22	7:I:46:LYS:HG3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HD12	1:A:112:LEU:HD22	1.89	0.53
7:I:29:LEU:HA	7:I:32:ALA:HB3	1.91	0.52
3:C:119:LEU:HD22	14:C:381:HEM:HBB2	1.92	0.52
3:C:206:ASN:HD21	3:C:210:GLY:HA2	1.75	0.52
5:D:136:GLU:H	5:D:136:GLU:CD	2.12	0.52
3:C:94:LEU:HD21	3:C:123:VAL:CG1	2.39	0.52
5:D:21:LEU:HB3	5:D:26:ILE:HD11	1.93	0.50
2:B:111:CYS:HB3	2:B:119:LEU:HD13	1.94	0.50
1:A:375:VAL:HG13	1:A:389:ARG:HH22	1.76	0.50
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.47	0.50
1:A:25:VAL:HG12	1:A:197:LEU:HB3	1.93	0.50
6:G:73:ASN:HB3	6:G:74:PRO:HD3	1.93	0.49
3:C:301:LEU:HA	3:C:304:ILE:HD12	1.93	0.49
1:A:430:GLN:HG3	1:A:430:GLN:O	2.12	0.49
9:K:19:PRO:O	9:K:22:SER:OG	2.29	0.49
9:K:48:ILE:HA	11:J:33:ARG:HD3	1.95	0.48
1:A:255:ILE:HG21	1:A:335:MET:HE1	1.96	0.48
11:J:10:TYR:HA	11:J:14:PHE:HB2	1.95	0.48
3:C:147:THR:HG22	3:C:161:VAL:HG13	1.94	0.48
4:E:17:GLU:HG3	4:E:28:SER:HB2	1.94	0.47
1:A:131:ARG:NH2	1:A:177:LEU:O	2.47	0.47
7:I:40:SER:HA	7:I:41:PRO:HD3	1.86	0.47
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.97	0.47
1:A:145:MET:O	1:A:149:VAL:HG22	2.14	0.47
4:E:158:CYS:HB3	4:E:163:SER:HB2	1.96	0.47
3:C:206:ASN:ND2	3:C:207:ASN:H	2.13	0.46
3:C:276:PHE:HB3	3:C:336:THR:HG22	1.97	0.46
2:B:37:SER:HB3	2:B:216:LEU:HD12	1.97	0.46
1:A:240:GLN:HG3	1:A:422:VAL:HB	1.98	0.46
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.97	0.46
3:C:277:ALA:HB1	3:C:294:LEU:HD12	1.98	0.46
1:A:252:HIS:CD2	1:A:323:HIS:HE1	2.33	0.46
3:C:270:PRO:HA	15:C:383:SMA:H10	1.96	0.46
3:C:230:LEU:HD22	5:D:223:LYS:HG2	1.98	0.46
3:C:133:LEU:HA	3:C:175:LEU:HD21	1.98	0.46
3:C:197:LEU:HG	13:C:380:UQ2:H5M3	1.97	0.46
3:C:152:ALA:CB	3:C:291:VAL:HG11	2.45	0.46
3:C:300:ILE:HD11	3:C:363:LEU:HD13	1.97	0.45
4:E:15:ARG:HD2	4:E:32:ARG:HG2	1.98	0.45
9:K:33:VAL:HG22	9:K:38:TRP:HE3	1.81	0.45
3:C:135:TRP:CE3	3:C:175:LEU:HG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:LEU:HD11	2:B:219:VAL:HG13	1.99	0.45
1:A:308:GLN:HE21	1:A:323:HIS:CD2	2.34	0.45
3:C:77:TRP:CZ3	5:D:201:ARG:HB3	2.52	0.45
9:K:38:TRP:CD2	9:K:41:ILE:CD1	3.00	0.45
5:D:131:LEU:HD11	14:D:242:HEM:HMB1	2.00	0.44
1:A:62:LEU:HD13	1:A:122:LEU:HD23	2.00	0.44
2:B:276:GLN:HE21	2:B:276:GLN:HB3	1.67	0.44
1:A:252:HIS:HE1	7:I:43:LEU:HB3	1.82	0.44
3:C:359:PHE:O	3:C:363:LEU:HB2	2.16	0.44
2:B:309:VAL:HG13	2:B:326:THR:HG22	2.00	0.44
2:B:343:GLN:O	2:B:346:THR:HG22	2.18	0.43
2:B:170:ASN:HD22	2:B:237:ALA:HA	1.83	0.43
1:A:108:LYS:HD3	1:A:108:LYS:HA	1.84	0.43
2:B:78:LYS:HD3	2:B:129:ALA:HB1	2.01	0.43
8:F:53:ASN:H	8:F:53:ASN:HD22	1.65	0.43
6:G:26:PHE:HB3	6:G:29:TYR:HB2	2.00	0.42
2:B:108:THR:HG23	16:B:593:HOH:O	2.18	0.42
2:B:76:THR:HG21	16:B:589:HOH:O	2.18	0.42
8:F:50:LEU:HD21	8:F:90:LEU:HD23	2.02	0.42
1:A:60:GLU:OE1	2:B:287:ARG:NH2	2.52	0.42
16:D:720:HOH:O	11:J:51:LEU:HB3	2.18	0.42
3:C:129:MET:HB3	3:C:182:HIS:HB2	2.01	0.42
3:C:332:LEU:O	3:C:336:THR:HG23	2.19	0.42
3:C:26:ASN:HD21	8:F:69:SER:CB	2.33	0.42
2:B:209:LEU:HD11	2:B:378:PHE:CD2	2.54	0.42
3:C:223:TYR:HB3	5:D:227:TRP:CZ2	2.55	0.42
7:I:15:LEU:HA	7:I:15:LEU:HD22	1.86	0.42
13:C:380:UQ2:C8	13:C:380:UQ2:H5M1	2.50	0.42
1:A:220:SER:HA	1:A:223:TYR:HB2	2.01	0.42
2:B:313:ASN:HD22	2:B:322:PHE:HD1	1.67	0.42
1:A:92:ARG:HD3	1:A:163:LEU:HD12	2.02	0.42
5:D:47:ALA:H	5:D:50:HIS:HD2	1.66	0.42
1:A:61:HIS:HB3	1:A:130:GLU:HG3	2.02	0.42
2:B:384:SER:HB2	7:I:2:LEU:O	2.20	0.41
5:D:181:GLN:HG2	10:H:77:LEU:HB3	2.01	0.41
1:A:25:VAL:HG11	1:A:212:ALA:CB	2.51	0.41
5:D:117:VAL:HG11	5:D:191:ARG:HD2	2.01	0.41
1:A:255:ILE:HD13	1:A:335:MET:CE	2.49	0.41
3:C:186:PRO:HG2	14:C:382:HEM:HMC1	2.03	0.41
2:B:157:ALA:O	2:B:161:GLU:HG2	2.21	0.41
5:D:163:PRO:HD2	5:D:164:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:118:ARG:HG3	5:D:194:ALA:HB1	2.03	0.41
7:I:43:LEU:HD22	7:I:46:LYS:HE2	2.02	0.40
3:C:270:PRO:HB3	3:C:274:PHE:HB2	2.03	0.40
3:C:270:PRO:HG3	15:C:383:SMA:C8A	2.52	0.40
15:C:383:SMA:H36	15:C:383:SMA:H15	1.94	0.40
3:C:8:HIS:HD2	3:C:11:MET:H	1.70	0.40
2:B:100:SER:O	7:I:13:PRO:CD	2.66	0.40
3:C:25:SER:HA	3:C:218:ILE:HG12	2.03	0.40
5:D:132:THR:HG22	10:H:17:LEU:HD22	2.04	0.40
1:A:27:SER:HB3	1:A:208:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	444/446 (100%)	425 (96%)	15 (3%)	4 (1%)	21	42
2	B	421/439 (96%)	403 (96%)	16 (4%)	2 (0%)	34	60
3	C	376/379 (99%)	361 (96%)	15 (4%)	0	100	100
4	E	194/196 (99%)	184 (95%)	9 (5%)	1 (0%)	34	60
5	D	239/241 (99%)	223 (93%)	14 (6%)	2 (1%)	24	46
6	G	73/81 (90%)	66 (90%)	5 (7%)	2 (3%)	6	10
7	I	55/78 (70%)	35 (64%)	14 (26%)	6 (11%)	0	0
8	F	103/110 (94%)	102 (99%)	1 (1%)	0	100	100
9	K	51/56 (91%)	47 (92%)	4 (8%)	0	100	100
10	H	65/78 (83%)	63 (97%)	2 (3%)	0	100	100
11	J	58/62 (94%)	53 (91%)	5 (9%)	0	100	100
All	All	2079/2166 (96%)	1962 (94%)	100 (5%)	17 (1%)	24	46

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	A	229	PRO
7	I	40	SER
7	I	43	LEU
1	A	286	GLY
2	B	171	ALA
7	I	45	LEU
5	D	95	TYR
6	G	73	ASN
6	G	74	PRO
1	A	232	SER
4	E	70	ALA
5	D	169	LEU
7	I	29	LEU
7	I	51	CYS
7	I	13	PRO
2	B	79	GLY

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%)	329 (89%)	41 (11%)	8	13
2	B	332/343 (97%)	294 (89%)	38 (11%)	7	12
3	C	326/327 (100%)	282 (86%)	44 (14%)	5	8
4	E	168/168 (100%)	144 (86%)	24 (14%)	4	7
5	D	206/206 (100%)	165 (80%)	41 (20%)	1	2
6	G	66/71 (93%)	55 (83%)	11 (17%)	3	4
7	I	44/60 (73%)	26 (59%)	18 (41%)	0	0
8	F	96/98 (98%)	81 (84%)	15 (16%)	3	5
9	K	43/46 (94%)	35 (81%)	8 (19%)	2	3
10	H	64/74 (86%)	45 (70%)	19 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	J	50/52 (96%)	42 (84%)	8 (16%)	3	5
All	All	1765/1815 (97%)	1498 (85%)	267 (15%)	3	6

All (267) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	32	GLN
1	A	37	VAL
1	A	42	ASP
1	A	50	GLU
1	A	51	LYS
1	A	58	PHE
1	A	60	GLU
1	A	75	LEU
1	A	81	SER
1	A	113	LEU
1	A	121	SER
1	A	122	LEU
1	A	127	ILE
1	A	146	ARG
1	A	149	VAL
1	A	163	LEU
1	A	176	LYS
1	A	187	SER
1	A	203	LEU
1	A	208	LEU
1	A	209	LEU
1	A	214	LYS
1	A	219	LEU
1	A	222	THR
1	A	224	ASP
1	A	228	VAL
1	A	245	GLU
1	A	281	ASP
1	A	302	LYS
1	A	305	GLN
1	A	351	GLU
1	A	352	SER
1	A	381	ARG
1	A	383	LEU
1	A	388	ARG

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Mol	Chain	Res	Type
1	A	389	ARG
1	A	392	LEU
1	A	409	GLU
1	A	430	GLN
1	A	438	ARG
2	B	17	VAL
2	B	20	HIS
2	B	38	LEU
2	B	40	ASN
2	B	46	ARG
2	B	69	LEU
2	B	78	LYS
2	B	84	LYS
2	B	95	LYS
2	B	97	SER
2	B	98	VAL
2	B	99	THR
2	B	108	THR
2	B	109	VAL
2	B	118	ILE
2	B	119	LEU
2	B	123	LEU
2	B	163	LEU
2	B	176	LEU
2	B	186	VAL
2	B	197	ASN
2	B	222	GLN
2	B	226	ILE
2	B	236	LYS
2	B	257	LEU
2	B	258	VAL
2	B	273	SER
2	B	276	GLN
2	B	305	GLN
2	B	309	VAL
2	B	346	THR
2	B	361	LYS
2	B	371	SER
2	B	379	LEU
2	B	384	SER
2	B	387	LEU
2	B	391	SER

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Mol	Chain	Res	Type
2	B	397	THR
3	C	3	ASN
3	C	4	ILE
3	C	10	LEU
3	C	12	LYS
3	C	21	LEU
3	C	42	ILE
3	C	46	LEU
3	C	51	LEU
3	C	56	THR
3	C	60	THR
3	C	64	SER
3	C	78	ILE
3	C	80	ARG
3	C	90	PHE
3	C	94	LEU
3	C	96	MET
3	C	128	PHE
3	C	129	MET
3	C	164	ILE
3	C	171	ASP
3	C	175	LEU
3	C	197	LEU
3	C	205	SER
3	C	241	LEU
3	C	243	VAL
3	C	249	LEU
3	C	254	ASP
3	C	257	THR
3	C	267	HIS
3	C	269	LYS
3	C	292	LEU
3	C	306	LEU
3	C	309	THR
3	C	320	LEU
3	C	328	LEU
3	C	336	THR
3	C	345	HIS
3	C	350	ILE
3	C	360	LEU
3	C	361	LEU
3	C	363	LEU

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Mol	Chain	Res	Type
3	C	365	LEU
3	C	378	LYS
3	C	379	TRP
4	E	6	LYS
4	E	12	ASP
4	E	18	VAL
4	E	22	THR
4	E	23	LYS
4	E	54	VAL
4	E	60	SER
4	E	69	LEU
4	E	71	MET
4	E	77	LYS
4	E	80	ASP
4	E	85	LYS
4	E	87	MET
4	E	103	LYS
4	E	104	LYS
4	E	107	ASP
4	E	108	GLN
4	E	112	VAL
4	E	115	SER
4	E	118	ARG
4	E	124	LEU
4	E	129	LYS
4	E	181	GLU
4	E	188	THR
5	D	13	SER
5	D	15	ARG
5	D	17	LEU
5	D	24	THR
5	D	37	CYS
5	D	43	MET
5	D	49	ARG
5	D	55	CYS
5	D	62	LYS
5	D	66	GLU
5	D	68	VAL
5	D	82	MET
5	D	95	TYR
5	D	106	ASN
5	D	109	LEU

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Mol	Chain	Res	Type
5	D	112	ASP
5	D	114	SER
5	D	116	ILE
5	D	124	GLU
5	D	132	THR
5	D	134	TYR
5	D	135	CYS
5	D	136	GLU
5	D	143	LEU
5	D	144	ARG
5	D	145	GLU
5	D	147	LEU
5	D	164	ILE
5	D	168	VAL
5	D	169	LEU
5	D	178	THR
5	D	180	SER
5	D	181	GLN
5	D	201	ARG
5	D	203	ARG
5	D	214	LEU
5	D	223	LYS
5	D	226	LYS
5	D	228	SER
5	D	234	LYS
5	D	241	LYS
6	G	2	ARG
6	G	3	GLN
6	G	18	LEU
6	G	24	ARG
6	G	31	SER
6	G	37	VAL
6	G	45	ILE
6	G	53	VAL
6	G	69	SER
6	G	70	LYS
6	G	72	LYS
7	I	7	ARG
7	I	8	SER
7	I	11	PHE
7	I	15	LEU
7	I	16	SER

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Mol	Chain	Res	Type
7	I	20	ARG
7	I	26	LEU
7	I	27	ARG
7	I	29	LEU
7	I	31	GLN
7	I	37	THR
7	I	39	GLU
7	I	40	SER
7	I	43	LEU
7	I	44	ASP
7	I	45	LEU
7	I	50	LEU
7	I	52	ARG
8	F	6	VAL
8	F	9	SER
8	F	44	LYS
8	F	53	ASN
8	F	72	GLN
8	F	73	GLN
8	F	74	ILE
8	F	77	LYS
8	F	85	GLU
8	F	90	LEU
8	F	94	LEU
8	F	95	LYS
8	F	99	ARG
8	F	106	GLU
8	F	110	LYS
9	K	1	MET
9	K	2	LEU
9	K	4	ARG
9	K	6	LEU
9	K	13	LEU
9	K	39	ARG
9	K	51	LYS
9	K	53	LYS
10	H	13	LEU
10	H	18	THR
10	H	23	GLN
10	H	26	GLN
10	H	27	LEU
10	H	28	GLU

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Mol	Chain	Res	Type
10	H	32	LYS
10	H	36	ARG
10	H	37	LEU
10	H	39	LEU
10	H	47	ARG
10	H	49	GLN
10	H	51	GLU
10	H	56	GLU
10	H	60	ASP
10	H	65	ARG
10	H	68	CYS
10	H	72	LYS
10	H	78	LYS
11	J	5	LEU
11	J	8	ARG
11	J	51	LEU
11	J	53	LYS
11	J	55	ILE
11	J	56	LYS
11	J	58	LYS
11	J	60	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	ASN
1	A	215	HIS
1	A	240	GLN
1	A	252	HIS
1	A	274	ASN
1	A	308	GLN
1	A	323	HIS
1	A	341	GLN
1	A	359	ASN
1	A	418	GLN
2	B	104	ASN
2	B	153	GLN
2	B	162	ASN
2	B	170	ASN
2	B	174	ASN
2	B	197	ASN
2	B	222	GLN

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Mol	Chain	Res	Type
2	B	248	ASN
2	B	270	ASN
2	B	276	GLN
2	B	277	HIS
2	B	284	HIS
2	B	313	ASN
2	B	342	ASN
2	B	362	ASN
2	B	385	GLN
3	C	8	HIS
3	C	32	ASN
3	C	114	ASN
3	C	206	ASN
3	C	322	GLN
3	C	345	HIS
3	C	352	GLN
5	D	50	HIS
7	I	31	GLN
8	F	53	ASN
9	K	12	GLN
9	K	16	ASN

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](#)

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	$\# Z > 2$
13	UQ2	C	380	-	23,23,23	2.38	6 (26%)	28,31,31	1.13	2 (7%)
14	HEM	C	381	3	30,50,50	2.68	12 (40%)	24,82,82	3.28	13 (54%)
14	HEM	C	382	3	30,50,50	2.67	9 (30%)	24,82,82	3.00	11 (45%)
15	SMA	C	383	-	35,38,38	1.14	2 (5%)	40,52,52	2.05	11 (27%)
14	HEM	D	242	5	30,50,50	2.77	11 (36%)	24,82,82	3.54	10 (41%)
12	FES	E	200	4	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
13	UQ2	C	380	-	-	0/15/39/39	0/1/1/1
14	HEM	C	381	3	-	0/10/54/54	0/0/8/8
14	HEM	C	382	3	-	0/10/54/54	0/0/8/8
15	SMA	C	383	-	-	0/33/34/34	0/2/2/2
14	HEM	D	242	5	-	0/10/54/54	0/0/8/8
12	FES	E	200	4	-	0/0/4/4	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	242	HEM	C3D-C4D	-7.69	1.41	1.51
14	C	381	HEM	C3D-C4D	-6.70	1.43	1.51
14	C	382	HEM	C3D-C4D	-6.68	1.43	1.51
14	C	382	HEM	C2D-C3D	-6.24	1.35	1.54
14	D	242	HEM	C2D-C3D	-6.16	1.36	1.54
14	C	381	HEM	C2D-C3D	-5.79	1.37	1.54
14	D	242	HEM	C3B-C4B	-5.40	1.47	1.51
14	C	382	HEM	C3B-C4B	-5.01	1.47	1.51
14	C	381	HEM	C3B-C4B	-4.87	1.47	1.51
14	D	242	HEM	C2C-C1C	-3.75	1.45	1.52
14	C	381	HEM	C2C-C1C	-3.25	1.46	1.52
14	C	382	HEM	C2C-C1C	-2.55	1.47	1.52
14	C	381	HEM	C2B-C1B	-2.26	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	D	242	HEM	C2D-C1D	-2.14	1.44	1.51
14	D	242	HEM	C2B-C1B	-2.14	1.44	1.51
14	C	381	HEM	C2D-C1D	-2.11	1.45	1.51
14	D	242	HEM	C4C-NC	2.04	1.38	1.36
14	C	381	HEM	CHC-C1C	2.15	1.41	1.36
15	C	383	SMA	C9-C2	2.29	1.54	1.50
14	C	381	HEM	C4C-NC	2.39	1.38	1.36
13	C	380	UQ2	C7-C6	2.57	1.56	1.51
14	C	382	HEM	C4C-NC	2.90	1.39	1.36
13	C	380	UQ2	C7-C8	3.00	1.55	1.50
14	D	242	HEM	C1C-NC	3.11	1.39	1.36
13	C	380	UQ2	C13-C14	3.14	1.41	1.32
14	C	382	HEM	C1C-NC	3.32	1.40	1.36
15	C	383	SMA	C3-C2	3.42	1.43	1.39
13	C	380	UQ2	C3-C2	3.57	1.51	1.35
14	D	242	HEM	CHD-C4C	3.58	1.44	1.36
14	C	381	HEM	C1C-NC	3.63	1.40	1.36
14	C	382	HEM	CHD-C4C	3.84	1.45	1.36
14	C	381	HEM	CHD-C4C	4.06	1.45	1.36
14	D	242	HEM	CBB-CAB	4.52	1.55	1.29
14	C	381	HEM	CBC-CAC	4.54	1.55	1.29
14	C	381	HEM	CBB-CAB	4.57	1.55	1.29
14	C	382	HEM	CBC-CAC	4.57	1.55	1.29
13	C	380	UQ2	C8-C9	4.59	1.42	1.33
14	D	242	HEM	CBC-CAC	4.60	1.55	1.29
14	C	382	HEM	CBB-CAB	4.62	1.56	1.29
13	C	380	UQ2	C6-C5	7.27	1.52	1.35

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	D	242	HEM	C3C-CAC-CBC	-9.64	109.67	124.46
14	D	242	HEM	C3B-CAB-CBB	-8.46	111.48	124.46
14	C	381	HEM	C3B-CAB-CBB	-8.45	111.49	124.46
14	C	382	HEM	C3B-CAB-CBB	-7.09	113.58	124.46
14	C	381	HEM	C1D-CHD-C4C	-4.89	117.64	125.82
14	C	382	HEM	C3C-CAC-CBC	-4.56	117.46	124.46
14	C	382	HEM	C4B-CHC-C1C	-4.29	118.65	125.82
14	C	382	HEM	C1D-CHD-C4C	-4.21	118.78	125.82
14	D	242	HEM	C1D-CHD-C4C	-4.12	118.93	125.82
14	C	381	HEM	C3C-CAC-CBC	-4.09	118.19	124.46
14	D	242	HEM	C4B-CHC-C1C	-3.98	119.17	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	381	HEM	C4B-CHC-C1C	-3.53	119.92	125.82
15	C	383	SMA	C17-C18-C19	-2.96	117.61	126.32
15	C	383	SMA	O5-C5-C6	-2.89	119.02	123.60
15	C	383	SMA	O7-C7-C6	-2.87	119.31	124.21
14	C	382	HEM	CBA-CAA-C2A	-2.70	107.69	112.53
14	C	381	HEM	CAA-C2A-C3A	-2.48	121.93	129.00
13	C	380	UQ2	C5-C6-C1	-2.42	117.36	120.12
15	C	383	SMA	C6-C7-C8	-2.12	118.44	120.56
13	C	380	UQ2	C10-C9-C11	2.29	118.91	115.41
14	C	381	HEM	CBA-CAA-C2A	2.45	116.92	112.53
15	C	383	SMA	O12-C12-C13	2.51	112.08	107.94
14	C	382	HEM	CMD-C2D-C3D	2.53	125.55	114.35
14	D	242	HEM	CMD-C2D-C3D	2.70	126.28	114.35
14	C	381	HEM	CMD-C2D-C3D	2.89	127.13	114.35
14	C	381	HEM	CAA-C2A-C1A	2.98	130.24	127.01
15	C	383	SMA	C9-C2-C3	3.00	124.51	120.56
15	C	383	SMA	C25-O14-C14	3.11	119.66	113.20
15	C	383	SMA	O14-C14-C13	3.19	115.80	108.09
15	C	383	SMA	O5-C5-C4A	3.45	121.34	115.89
14	C	381	HEM	C2D-C3D-C4D	3.57	107.54	101.50
14	C	382	HEM	C2D-C3D-C4D	3.63	107.65	101.50
14	D	242	HEM	C2D-C3D-C4D	3.66	107.71	101.50
15	C	383	SMA	C22-C11-C10	3.70	116.52	110.35
14	C	382	HEM	CAD-C3D-C2D	3.85	124.29	113.22
14	D	242	HEM	CMC-C2C-C3C	3.89	126.25	116.53
14	C	381	HEM	CAD-C3D-C2D	4.05	124.85	113.22
14	D	242	HEM	CAD-C3D-C4D	4.08	126.86	112.47
14	C	382	HEM	CMB-C2B-C3B	4.22	127.07	116.53
14	D	242	HEM	CAD-C3D-C2D	4.25	125.42	113.22
14	D	242	HEM	CMB-C2B-C3B	4.25	127.15	116.53
14	C	382	HEM	CMC-C2C-C3C	4.27	127.19	116.53
14	C	381	HEM	CAD-C3D-C4D	4.29	127.60	112.47
14	C	382	HEM	CAD-C3D-C4D	4.38	127.92	112.47
14	C	381	HEM	CMB-C2B-C3B	4.46	127.65	116.53
14	C	381	HEM	CMC-C2C-C3C	4.90	128.77	116.53
15	C	383	SMA	O7-C7-C8	6.85	121.36	114.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	380	UQ2	4	0
14	C	381	HEM	3	0
14	C	382	HEM	1	0
15	C	383	SMA	3	0
14	D	242	HEM	2	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.