



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:15 PM GMT

PDB ID : 1SQV
Title : Crystal Structure Analysis of Bovine Bcl with UHDBT
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 : 2.85 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

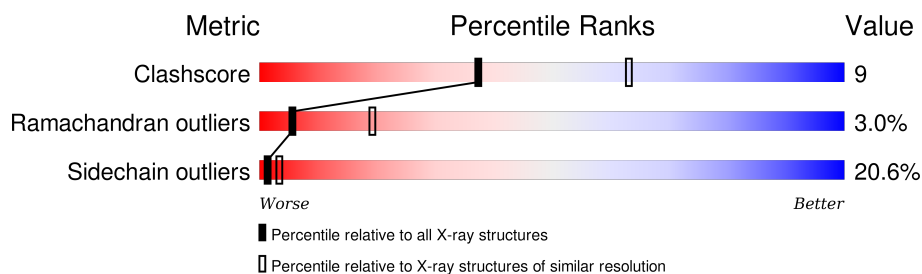
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)

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	
2	B	439	
3	C	379	
4	D	241	
5	E	196	
6	F	110	
7	G	81	

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Mol	Chain	Length	Quality of chain
8	H	78	<div><div></div><div>58%</div><div>21%</div><div>8%</div><div>14%</div></div>
9	I	78	<div><div></div><div>18%</div><div>36%</div><div>12%</div><div>8%</div><div>27%</div></div>
10	J	62	<div><div></div><div>52%</div><div>44%</div><div></div><div></div></div>
11	K	56	<div><div></div><div>59%</div><div>25%</div><div>5%</div><div></div><div>9%</div></div>

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 16953 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.

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.

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
			1918	1225	330	348	15			

- Molecule 5 is a protein called Ubiquinol-cytochrome c reductase iron-sulfur subunit.

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 Ubiquinol-cytochrome C reductase complex 14 kDa protein.

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 complex 8 kDa protein.

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

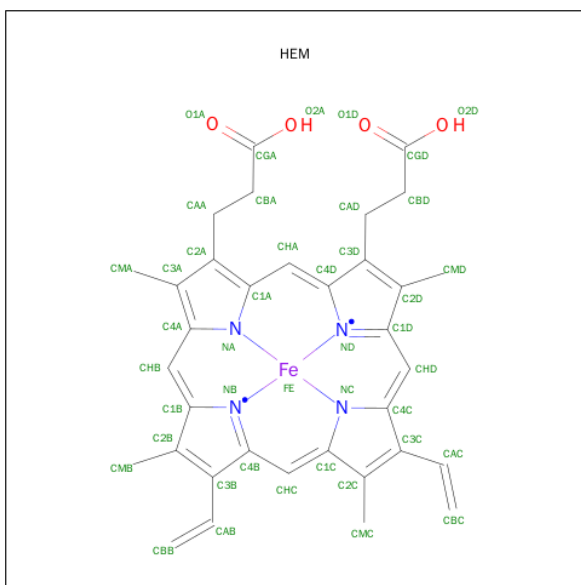
- Molecule 10 is a protein called Ubiquinol-cytochrome C reductase complex 7.2 kDa protein.

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

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

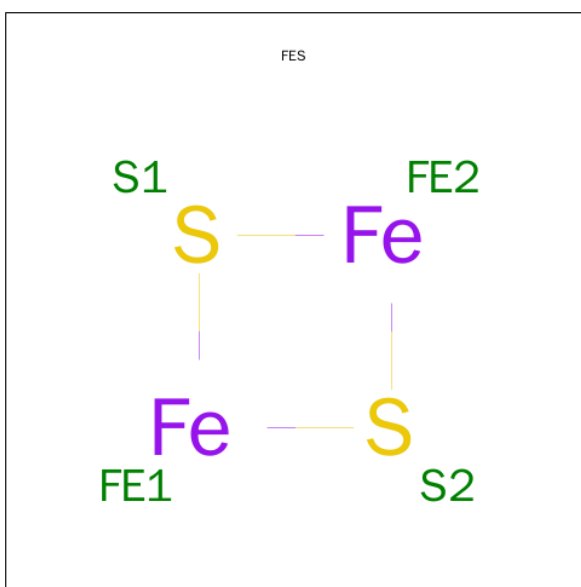
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	51	Total	C	N	O	S	0	0	0
			418	278	75	64	1			

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



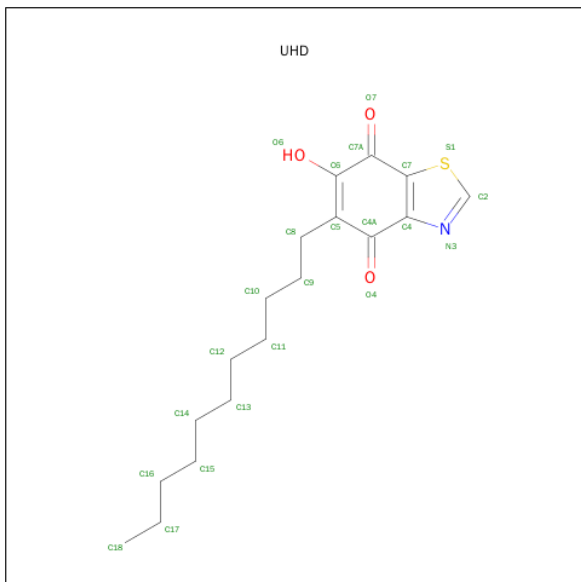
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



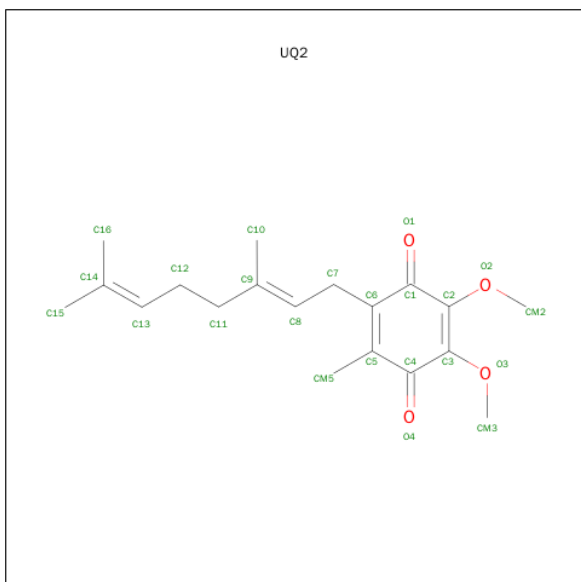
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 14 is 6-HYDROXY-5-UNDECYL-1,3-BENZOTHIAZOLE-4,7-DIONE (three-letter code: UHD) (formula: $C_{18}H_{25}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	N	O	S	0	0
			23	18	1	3	1		

- Molecule 15 is UBIQUINONE-2 (three-letter code: UQ2) (formula: $C_{19}H_{26}O_4$).



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

- Molecule 16 is water.

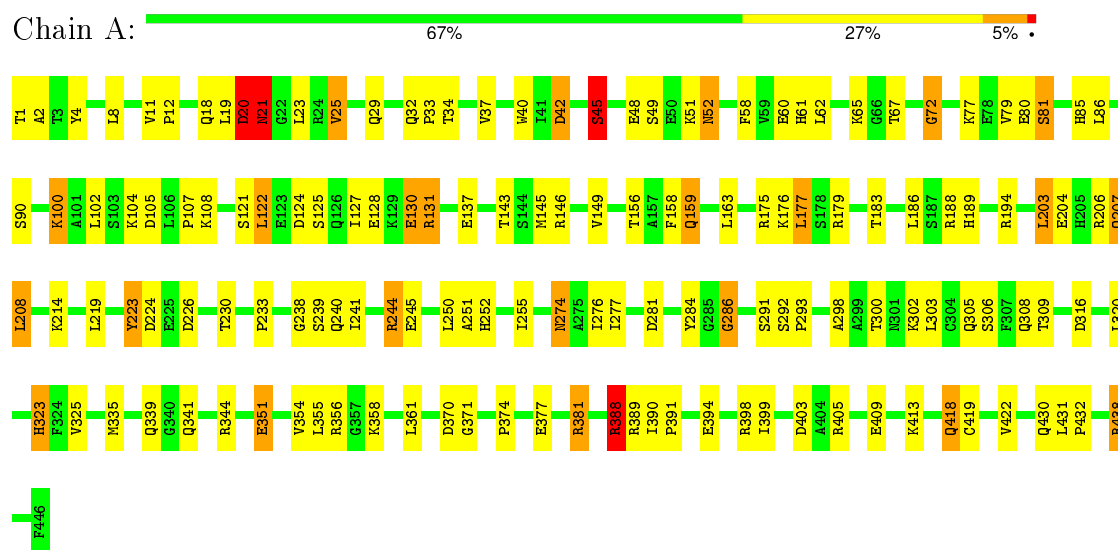
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	70	Total 70	O 70	0	0
16	B	103	Total 103	O 103	0	0
16	C	26	Total 26	O 26	0	0
16	D	21	Total 21	O 21	0	0
16	E	8	Total 8	O 8	0	0
16	F	31	Total 31	O 31	0	0
16	G	16	Total 16	O 16	0	0
16	I	10	Total 10	O 10	0	0
16	K	6	Total 6	O 6	0	0

3 Residue-property plots

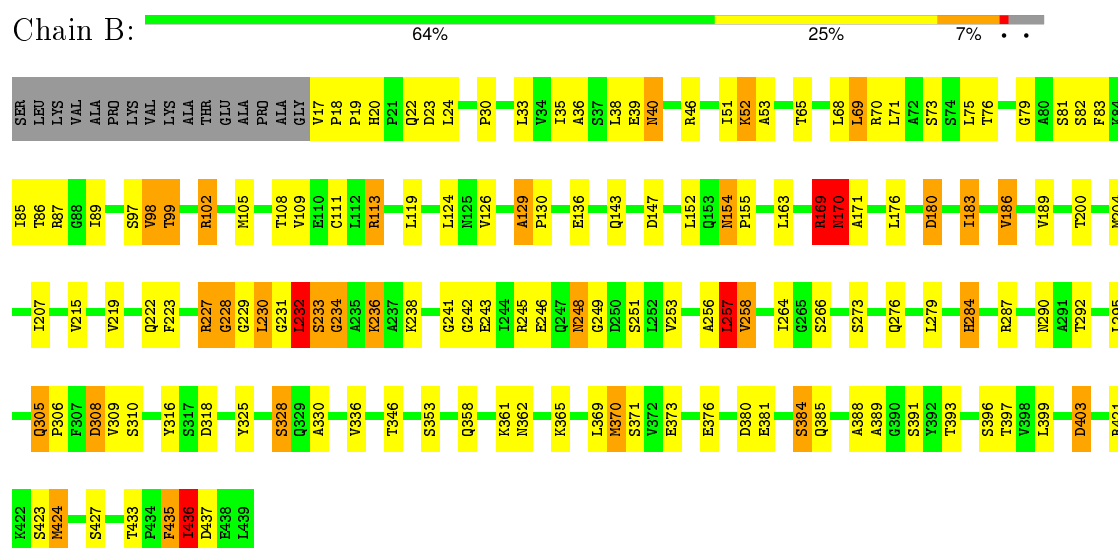
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

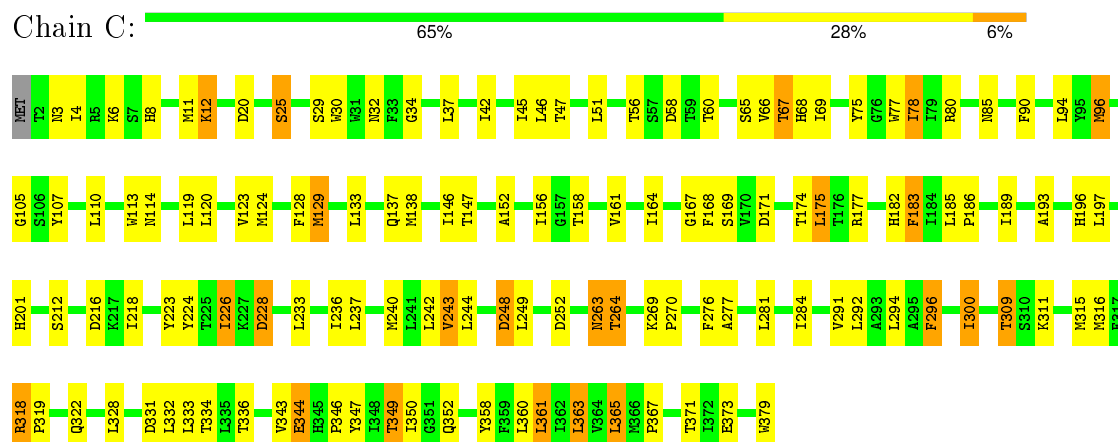
- Molecule 1: Ubiquinol-cytochrome c reductase complex core protein I, mitochondrial



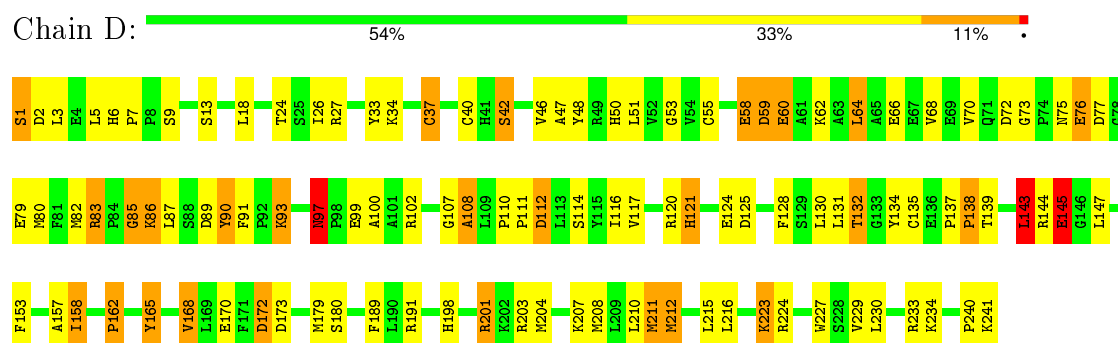
- Molecule 2: Ubiquinol-cytochrome c reductase complex core protein 2, mitochondrial



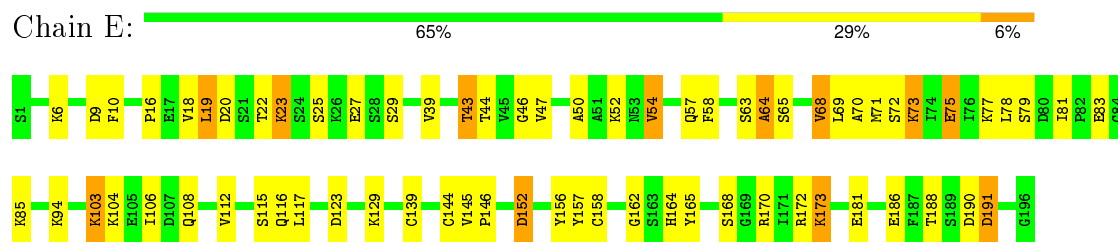
- Molecule 3: Cytochrome b



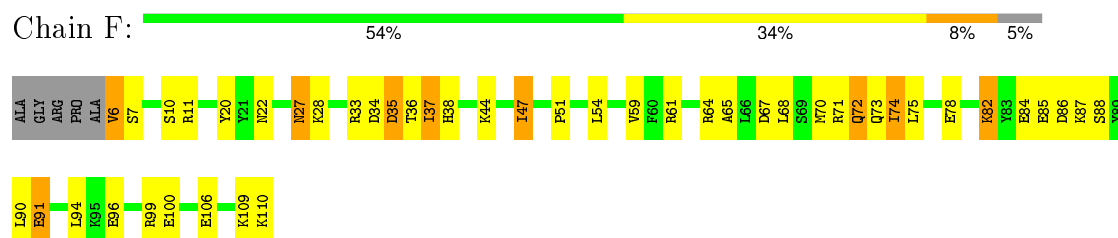
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



- Molecule 5: Ubiquinol-cytochrome c reductase iron-sulfur subunit

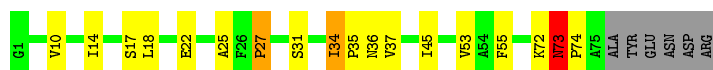


- Molecule 6: Ubiquinol-cytochrome C reductase complex 14 kDa protein



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

Chain G:  70% 19% 7%

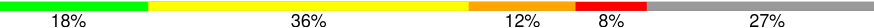


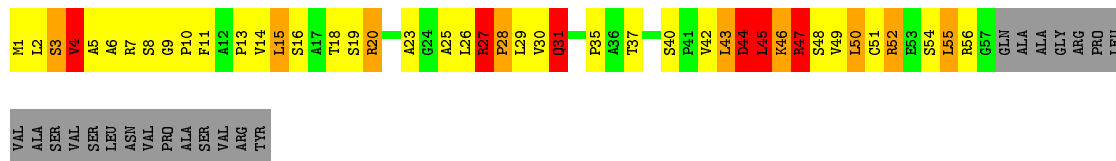
- Molecule 8: Ubiquinol-cytochrome C reductase complex 11 kDa protein

Chain H:  58% 21% 8% 14%



- Molecule 9: Ubiquinol-cytochrome C reductase complex 8 kDa protein

Chain I:  18% 36% 12% 8% 27%



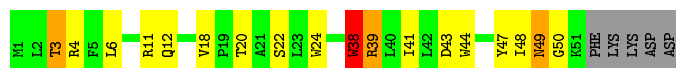
- Molecule 10: Ubiquinol-cytochrome C reductase complex 7.2 kDa protein

Chain J:  52% 44% 2%



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

Chain K:  59% 25% 5% 9%



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	153.67Å 153.67Å 589.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.85	Depositor
% Data completeness (in resolution range)	85.5 (40.00-2.85)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16953	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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, UHD, UQ2, FES

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	0.47	0/3531	0.89	5/4792 (0.1%)
2	B	0.52	0/3232	0.92	8/4386 (0.2%)
3	C	0.51	0/3100	0.88	3/4242 (0.1%)
4	D	0.46	0/1977	0.89	4/2684 (0.1%)
5	E	0.46	0/1553	0.86	4/2100 (0.2%)
6	F	0.52	0/930	0.94	3/1246 (0.2%)
7	G	0.57	0/649	0.87	0/878
8	H	0.50	1/553 (0.2%)	0.96	2/741 (0.3%)
9	I	0.62	0/411	1.22	2/558 (0.4%)
10	J	0.52	0/515	0.83	0/696
11	K	0.49	0/433	0.91	1/594 (0.2%)
All	All	0.50	1/16884 (0.0%)	0.90	32/22917 (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	8
2	B	0	12
3	C	0	3
4	D	0	21
5	E	0	5
6	F	0	1
8	H	0	5
9	I	0	16
10	J	0	1
11	K	0	3
All	All	0	75

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	57	GLU	CD-OE2	5.20	1.31	1.25

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	203	LEU	CA-CB-CG	6.19	129.53	115.30
9	I	45	LEU	CA-CB-CG	6.17	129.48	115.30
2	B	180	ASP	CB-CG-OD2	6.16	123.84	118.30
2	B	147	ASP	CB-CG-OD2	6.00	123.70	118.30
4	D	172	ASP	CB-CG-OD1	5.96	123.67	118.30
5	E	123	ASP	CB-CG-OD1	5.94	123.65	118.30
3	C	248	ASP	CB-CG-OD1	5.87	123.58	118.30
6	F	35	ASP	CB-CG-OD2	5.84	123.55	118.30
3	C	58	ASP	CB-CG-OD1	5.82	123.54	118.30
2	B	318	ASP	CB-CG-OD2	5.77	123.49	118.30
5	E	191	ASP	CB-CG-OD1	5.56	123.30	118.30
6	F	34	ASP	CB-CG-OD2	5.54	123.29	118.30
2	B	403	ASP	CB-CG-OD2	5.47	123.23	118.30
2	B	257	LEU	CB-CG-CD2	5.38	120.15	111.00
1	A	20	ASP	CB-CG-OD1	5.38	123.14	118.30
2	B	232	LEU	CA-CB-CG	5.38	127.67	115.30
4	D	89	ASP	CB-CG-OD2	5.38	123.14	118.30
4	D	59	ASP	CB-CG-OD1	5.37	123.14	118.30
9	I	44	ASP	CB-CG-OD2	5.37	123.14	118.30
5	E	190	ASP	CB-CG-OD1	5.35	123.12	118.30
11	K	43	ASP	CB-CG-OD2	5.35	123.11	118.30
2	B	308	ASP	CB-CG-OD2	5.26	123.04	118.30
8	H	37	LEU	CA-CB-CG	5.24	127.36	115.30
8	H	60	ASP	CB-CG-OD2	5.23	123.01	118.30
2	B	23	ASP	CB-CG-OD2	5.23	123.01	118.30
4	D	125	ASP	CB-CG-OD2	5.21	122.99	118.30
6	F	86	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	403	ASP	CB-CG-OD1	5.04	122.83	118.30
3	C	20	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	316	ASP	CB-CG-OD2	5.03	122.83	118.30
5	E	152	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (75) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	ASP	Peptide
1	A	137	GLU	Mainchain
1	A	158	PHE	Peptide
1	A	20	ASP	Peptide
1	A	238	GLY	Peptide
1	A	388	ARG	Peptide
1	A	45	SER	Peptide
1	A	52	ASN	Peptide
2	B	108	THR	Mainchain
2	B	169	ARG	Peptide
2	B	19	PRO	Peptide
2	B	228	GLY	Peptide
2	B	231	GLY	Peptide
2	B	233	SER	Peptide
2	B	234	GLY	Peptide
2	B	248	ASN	Peptide
2	B	30	PRO	Mainchain
2	B	39	GLU	Peptide
2	B	436	ILE	Peptide
2	B	79	GLY	Peptide
3	C	167	GLY	Peptide
3	C	25	SER	Peptide
3	C	344	GLU	Peptide
4	D	1	SER	Peptide
4	D	107	GLY	Peptide
4	D	121	HIS	Peptide
4	D	137	PRO	Peptide
4	D	143	LEU	Peptide
4	D	144	ARG	Peptide
4	D	145	GLU	Peptide
4	D	157	ALA	Peptide
4	D	158	ILE	Peptide
4	D	162	PRO	Peptide
4	D	165	TYR	Peptide
4	D	168	VAL	Peptide
4	D	172	ASP	Peptide
4	D	240	PRO	Peptide
4	D	53	GLY	Peptide
4	D	73	GLY	Peptide
4	D	85	GLY	Peptide
4	D	86	LYS	Peptide
4	D	90	TYR	Peptide
4	D	93	LYS	Peptide

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Mol	Chain	Res	Type	Group
4	D	97	ASN	Peptide
5	E	63	SER	Peptide
5	E	64	ALA	Peptide
5	E	68	VAL	Peptide
5	E	70	ALA	Peptide
5	E	94	LYS	Peptide
6	F	6	VAL	Peptide
8	H	26	GLN	Peptide
8	H	27	LEU	Peptide
8	H	43	ARG	Peptide
8	H	48	SER	Peptide
8	H	52	GLU	Peptide
9	I	23	ALA	Peptide
9	I	25	ALA	Peptide
9	I	26	LEU	Peptide
9	I	28	PRO	Peptide
9	I	29	LEU	Peptide
9	I	3	SER	Peptide
9	I	31	GLN	Peptide
9	I	35	PRO	Peptide
9	I	37	THR	Peptide
9	I	4	VAL	Peptide
9	I	44	ASP	Peptide
9	I	45	LEU	Peptide
9	I	46	LYS	Peptide
9	I	52	ARG	Peptide
9	I	55	LEU	Peptide
9	I	6	ALA	Peptide
10	J	59	TYR	Peptide
11	K	3	THR	Peptide
11	K	38	TRP	Peptide
11	K	50	GLY	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	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3172	0	3152	86	0
3	C	3003	0	3065	65	0
4	D	1918	0	1870	36	0
5	E	1519	0	1503	19	0
6	F	911	0	904	18	0
7	G	628	0	636	7	0
8	H	548	0	530	4	0
9	I	406	0	437	36	0
10	J	502	0	505	8	0
11	K	418	0	425	4	0
12	C	86	0	60	10	0
12	D	43	0	30	5	0
13	E	4	0	0	0	0
14	C	23	0	24	3	0
15	C	23	0	26	4	0
16	A	70	0	0	3	0
16	B	103	0	0	5	0
16	C	26	0	0	1	0
16	D	21	0	0	0	0
16	E	8	0	0	0	0
16	F	31	0	0	2	0
16	G	16	0	0	0	0
16	I	10	0	0	2	0
16	K	6	0	0	0	0
All	All	16953	0	16523	308	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 9.

All (308) 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)
16:B:623:HOH:O	9:I:11:PHE:HB2	1.70	0.92
2:B:310:SER:HB3	9:I:28:PRO:HD3	1.52	0.90
16:B:627:HOH:O	9:I:4:VAL:HG21	1.75	0.85
2:B:385:GLN:HA	9:I:2:LEU:HD12	1.60	0.81
2:B:388:ALA:HB3	9:I:2:LEU:HD13	1.64	0.80
2:B:76:THR:HG22	2:B:82:SER:H	1.46	0.80
2:B:215:VAL:O	2:B:219:VAL:HG23	1.84	0.77
12:C:382:HEM:HBC2	12:C:382:HEM:HMC2	1.66	0.75
2:B:99:THR:HB	9:I:14:VAL:HG22	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:309:THR:HG21	3:C:367:PRO:O	1.88	0.73
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.70	0.73
2:B:46:ARG:HH11	2:B:46:ARG:HG3	1.54	0.72
5:E:20:ASP:HB3	5:E:23:LYS:HB2	1.72	0.72
2:B:264:ILE:HD11	9:I:2:LEU:HA	1.71	0.71
1:A:145:MET:O	1:A:149:VAL:HG23	1.90	0.70
2:B:170:ASN:HD22	2:B:238:LYS:H	1.38	0.69
2:B:169:ARG:HD2	2:B:238:LYS:HE2	1.74	0.68
1:A:61:HIS:HB3	1:A:130:GLU:HG3	1.76	0.68
6:F:96:GLU:O	6:F:100:GLU:HG3	1.94	0.67
6:F:38:HIS:HB3	16:F:750:HOH:O	1.95	0.66
3:C:75:TYR:HB3	3:C:78:ILE:HD11	1.78	0.65
3:C:197:LEU:HD21	15:C:384:UQ2:H5M3	1.77	0.65
1:A:156:THR:O	1:A:159:GLN:HB2	1.96	0.65
1:A:240:GLN:HG3	1:A:422:VAL:HB	1.79	0.64
1:A:244:ARG:NH2	16:A:514:HOH:O	2.10	0.64
3:C:30:TRP:HZ3	3:C:96:MET:HG3	1.63	0.64
1:A:335:MET:HE3	1:A:339:GLN:HG3	1.80	0.64
16:A:530:HOH:O	9:I:42:VAL:HG12	1.97	0.63
1:A:308:GLN:HE21	1:A:323:HIS:CD2	2.17	0.63
2:B:385:GLN:NE2	2:B:393:THR:H	1.97	0.62
1:A:308:GLN:HE21	1:A:323:HIS:HD2	1.45	0.62
2:B:126:VAL:O	2:B:130:PRO:HG3	1.99	0.62
7:G:73:ASN:HB3	7:G:74:PRO:HD3	1.82	0.62
1:A:149:VAL:HG21	1:A:252:HIS:HB3	1.82	0.62
6:F:65:ALA:HA	6:F:68:LEU:HD12	1.81	0.61
2:B:176:LEU:HD13	9:I:13:PRO:CD	2.31	0.61
1:A:281:ASP:OD1	9:I:47:ARG:HA	2.01	0.61
2:B:76:THR:CG2	2:B:82:SER:H	2.14	0.61
3:C:237:LEU:HD13	4:D:212:MET:HG2	1.83	0.60
2:B:385:GLN:HE22	2:B:393:THR:H	1.49	0.60
1:A:29:GLN:HG2	2:B:18:PRO:HD3	1.83	0.60
3:C:47:THR:HG22	5:E:58:PHE:HZ	1.67	0.60
3:C:233:LEU:CD2	4:D:216:LEU:HG	2.31	0.60
2:B:258:VAL:HG12	2:B:423:SER:HB2	1.84	0.59
3:C:119:LEU:HD13	12:C:382:HEM:HBB2	1.84	0.59
3:C:77:TRP:CZ3	4:D:201:ARG:HB3	2.37	0.59
2:B:245:ARG:NH2	2:B:433:THR:O	2.35	0.59
4:D:70:VAL:HB	4:D:83:ARG:HB3	1.85	0.59
10:J:10:TYR:HA	10:J:14:PHE:HB2	1.83	0.59
3:C:25:SER:HA	3:C:218:ILE:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ARG:NE	16:A:514:HOH:O	2.33	0.58
9:I:20:ARG:HG3	9:I:51:CYS:SG	2.42	0.58
8:H:62:LEU:HD23	8:H:65:ARG:HH12	1.67	0.58
2:B:264:ILE:HG12	9:I:2:LEU:HD22	1.85	0.58
3:C:224:TYR:O	3:C:228:ASP:HB2	2.03	0.58
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.44	0.58
3:C:3:ASN:HB3	3:C:6:LYS:HG3	1.85	0.58
2:B:76:THR:HG22	2:B:82:SER:N	2.18	0.57
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.86	0.57
4:D:60:GLU:O	4:D:64:LEU:HG	2.05	0.56
2:B:129:ALA:N	2:B:130:PRO:HD3	2.21	0.56
1:A:351:GLU:H	11:K:12:GLN:HE21	1.54	0.56
3:C:197:LEU:CD2	15:C:384:UQ2:H5M3	2.35	0.56
4:D:211:MET:CE	10:J:31:PHE:HE2	2.19	0.55
11:K:38:TRP:HD1	11:K:41:ILE:CD1	2.19	0.55
9:I:28:PRO:HA	9:I:30:VAL:HG22	1.88	0.55
1:A:45:SER:HA	1:A:48:GLU:HG2	1.88	0.55
3:C:361:LEU:HA	3:C:365:LEU:HB2	1.89	0.55
4:D:211:MET:HE1	10:J:31:PHE:HE2	1.73	0.54
1:A:371:GLY:O	1:A:374:PRO:HD2	2.08	0.54
2:B:76:THR:HG22	2:B:81:SER:HA	1.89	0.54
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.43	0.54
4:D:131:LEU:HD11	12:D:242:HEM:HMB3	1.88	0.54
5:E:168:SER:HB3	5:E:170:ARG:HG3	1.88	0.54
11:K:38:TRP:CE3	11:K:38:TRP:HA	2.41	0.53
3:C:216:ASP:OD2	4:D:233:ARG:NH2	2.40	0.53
2:B:111:CYS:SG	2:B:119:LEU:HD12	2.49	0.53
1:A:419:CYS:SG	1:A:438:ARG:NH1	2.81	0.53
3:C:34:GLY:HA3	12:C:382:HEM:HBA2	1.91	0.53
15:C:384:UQ2:H8	15:C:384:UQ2:H5M1	1.89	0.53
1:A:281:ASP:HB3	1:A:284:TYR:CD1	2.44	0.53
2:B:40:ASN:HD22	2:B:40:ASN:C	2.12	0.53
1:A:2:ALA:O	2:B:113:ARG:HD3	2.08	0.53
3:C:45:ILE:HA	12:C:381:HEM:HAB	1.90	0.52
3:C:137:GLN:HE22	3:C:263:ASN:HB3	1.75	0.52
2:B:111:CYS:HB3	2:B:119:LEU:HD12	1.91	0.52
3:C:296:PHE:O	3:C:300:ILE:HB	2.09	0.52
2:B:52:LYS:HD3	2:B:233:SER:OG	2.09	0.52
6:F:106:GLU:HA	6:F:109:LYS:HD2	1.91	0.52
3:C:147:THR:HG22	3:C:161:VAL:HG13	1.92	0.52
2:B:279:LEU:HB3	2:B:295:LEU:HG	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:SER:HB3	2:B:336:VAL:HG21	1.92	0.52
4:D:97:ASN:HB3	4:D:100:ALA:H	1.75	0.52
3:C:29:SER:HA	3:C:32:ASN:HD22	1.75	0.52
9:I:43:LEU:HA	9:I:46:LYS:HD3	1.91	0.51
1:A:49:SER:H	1:A:52:ASN:HB2	1.75	0.51
4:D:108:ALA:HB1	12:D:242:HEM:HMD1	1.91	0.51
1:A:25:VAL:HG23	1:A:208:LEU:HD13	1.91	0.51
2:B:53:ALA:O	2:B:105:MET:HE2	2.10	0.51
1:A:65:LYS:O	1:A:72:GLY:HA2	2.11	0.51
3:C:300:ILE:HD11	3:C:363:LEU:HD13	1.92	0.51
1:A:80:GLU:HG2	2:B:284:HIS:HB2	1.93	0.51
5:E:50:ALA:O	5:E:54:VAL:HG23	2.11	0.51
2:B:246:GLU:O	2:B:427:SER:HA	2.11	0.50
4:D:99:GLU:HA	4:D:102:ARG:HB2	1.94	0.50
12:C:382:HEM:HBC2	12:C:382:HEM:CMC	2.40	0.50
6:F:51:PRO:HD2	6:F:54:LEU:HD12	1.94	0.50
1:A:21:ASN:HB3	1:A:23:LEU:H	1.76	0.50
2:B:85:ILE:O	2:B:89:ILE:HG13	2.12	0.50
5:E:18:VAL:HG11	7:G:22:GLU:OE1	2.10	0.50
4:D:42:SER:HB2	4:D:112:ASP:HB3	1.94	0.50
2:B:170:ASN:ND2	2:B:238:LYS:H	2.07	0.50
1:A:255:ILE:HD13	1:A:335:MET:CE	2.41	0.50
2:B:176:LEU:HD13	9:I:13:PRO:HD3	1.93	0.50
6:F:67:ASP:O	6:F:71:ARG:HG2	2.12	0.50
4:D:128:PHE:O	4:D:132:THR:HB	2.12	0.50
6:F:82:LYS:HB2	6:F:85:GLU:HB2	1.93	0.50
4:D:47:ALA:N	4:D:50:HIS:HD2	2.09	0.50
1:A:48:GLU:HB2	1:A:52:ASN:HB3	1.94	0.49
1:A:291:SER:HB3	1:A:356:ARG:CZ	2.42	0.49
2:B:68:LEU:HD23	2:B:186:VAL:HG22	1.94	0.49
1:A:19:LEU:HB3	1:A:21:ASN:HB2	1.93	0.49
1:A:240:GLN:HB3	7:G:17:SER:HB2	1.93	0.49
2:B:33:LEU:HD23	2:B:35:ILE:HD11	1.95	0.49
2:B:102:ARG:HD2	16:B:641:HOH:O	2.11	0.49
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.48	0.49
1:A:277:ILE:HB	1:A:309:THR:HG21	1.94	0.49
3:C:319:PRO:HA	3:C:322:GLN:HB2	1.95	0.49
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.94	0.49
2:B:169:ARG:HG3	2:B:238:LYS:HB2	1.93	0.49
6:F:28:LYS:HB3	6:F:74:ILE:HG13	1.94	0.49
2:B:242:GLY:O	2:B:423:SER:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:GLN:HA	1:A:418:GLN:HE21	1.78	0.49
4:D:215:LEU:HD21	5:E:46:GLY:HA3	1.95	0.48
2:B:424:MET:HB2	2:B:436:ILE:HD11	1.95	0.48
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.47	0.48
3:C:349:THR:HA	3:C:352:GLN:HE21	1.78	0.48
10:J:33:ARG:HD3	11:K:48:ILE:HA	1.95	0.48
1:A:284:TYR:HE1	9:I:20:ARG:HG2	1.78	0.48
2:B:89:ILE:HG12	2:B:119:LEU:HD21	1.95	0.48
1:A:189:HIS:O	1:A:194:ARG:NH1	2.46	0.48
5:E:164:HIS:HB2	5:E:173:LYS:HB2	1.95	0.48
3:C:128:PHE:CD1	3:C:146:ILE:HD12	2.48	0.48
3:C:270:PRO:HB3	14:C:383:UHD:O4	2.13	0.48
1:A:79:VAL:HG11	1:A:86:LEU:HB2	1.94	0.48
2:B:369:LEU:HD11	2:B:399:LEU:HD11	1.96	0.48
2:B:97:SER:HB2	9:I:15:LEU:O	2.14	0.48
4:D:138:PRO:HB3	8:H:58:LEU:HD13	1.96	0.48
4:D:26:ILE:HG23	4:D:189:PHE:HA	1.95	0.48
2:B:70:ARG:HG3	2:B:98:VAL:HG22	1.95	0.48
1:A:341:GLN:HE22	1:A:344:ARG:HH21	1.62	0.48
6:F:28:LYS:HB3	6:F:74:ILE:CG1	2.43	0.47
1:A:431:LEU:HD12	1:A:432:PRO:HD2	1.96	0.47
2:B:385:GLN:NE2	2:B:393:THR:N	2.62	0.47
7:G:34:ILE:HG13	7:G:35:PRO:HD3	1.95	0.47
4:D:48:TYR:HA	4:D:51:LEU:HD12	1.96	0.47
1:A:252:HIS:CE1	9:I:43:LEU:HB2	2.49	0.47
1:A:77:LYS:O	1:A:81:SER:HB2	2.15	0.47
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.95	0.47
3:C:113:TRP:HA	12:C:382:HEM:HHD	1.97	0.47
2:B:389:ALA:HB2	9:I:2:LEU:HD11	1.96	0.47
1:A:149:VAL:HG21	1:A:252:HIS:CB	2.42	0.47
2:B:365:LYS:NZ	2:B:403:ASP:OD1	2.30	0.47
3:C:186:PRO:HA	3:C:189:ILE:HD12	1.97	0.47
9:I:1:MET:SD	16:I:671:HOH:O	2.60	0.47
2:B:99:THR:HB	9:I:14:VAL:CG2	2.43	0.47
2:B:253:VAL:HG23	2:B:330:ALA:HA	1.96	0.47
1:A:131:ARG:NH2	1:A:177:LEU:O	2.44	0.46
9:I:16:SER:HB3	9:I:19:SER:O	2.15	0.46
15:C:384:UQ2:C8	15:C:384:UQ2:H5M1	2.45	0.46
3:C:65:SER:O	3:C:68:HIS:HB3	2.16	0.46
3:C:8:HIS:HD2	3:C:11:MET:H	1.62	0.46
2:B:305:GLN:HB2	2:B:306:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:315:MET:HA	3:C:318:ARG:HG3	1.98	0.46
3:C:244:LEU:HD22	4:D:204:MET:HB2	1.98	0.46
6:F:35:ASP:OD2	6:F:61:ARG:HD2	2.16	0.46
1:A:62:LEU:HD13	1:A:122:LEU:HD23	1.96	0.46
1:A:122:LEU:HB2	1:A:179:ARG:HE	1.81	0.46
2:B:36:ALA:O	2:B:207:ILE:HA	2.15	0.46
3:C:67:THR:HG23	16:C:685:HOH:O	2.15	0.46
1:A:388:ARG:NH2	1:A:394:GLU:OE1	2.49	0.45
4:D:33:TYR:HA	4:D:37:CYS:SG	2.55	0.45
4:D:110:PRO:HA	4:D:111:PRO:HD3	1.82	0.45
2:B:180:ASP:HA	2:B:183:ILE:HG13	1.97	0.45
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.97	0.45
3:C:146:ILE:HG12	14:C:383:UHD:H82	1.97	0.45
9:I:11:PHE:HZ	9:I:27:ARG:CZ	2.30	0.45
4:D:75:ASN:O	4:D:77:ASP:N	2.48	0.45
2:B:435:PHE:O	2:B:436:ILE:HB	2.17	0.45
1:A:355:LEU:HA	1:A:358:LYS:HE3	1.99	0.45
2:B:325:TYR:HB3	9:I:28:PRO:HD2	1.98	0.45
2:B:316:TYR:OH	9:I:10:PRO:HB3	2.17	0.44
9:I:4:VAL:HG12	9:I:10:PRO:HG3	1.99	0.44
3:C:373:GLU:HB3	6:F:20:TYR:OH	2.18	0.44
4:D:108:ALA:HB1	12:D:242:HEM:HAD1	2.00	0.44
3:C:332:LEU:HD21	3:C:358:TYR:CE1	2.52	0.44
3:C:47:THR:HG22	5:E:58:PHE:CZ	2.50	0.44
1:A:361:LEU:HD23	1:A:399:ILE:HG12	1.98	0.44
8:H:65:ARG:HH11	8:H:65:ARG:HB3	1.83	0.44
2:B:65:THR:O	2:B:69:LEU:HB2	2.18	0.44
12:D:242:HEM:CMB	12:D:242:HEM:HBB2	2.48	0.44
7:G:25:ALA:O	7:G:27:PRO:HD3	2.18	0.44
1:A:11:VAL:HA	1:A:12:PRO:HD3	1.86	0.44
6:F:68:LEU:HD21	6:F:75:LEU:HD23	2.00	0.44
2:B:176:LEU:HD13	9:I:13:PRO:HD2	1.98	0.44
9:I:51:CYS:SG	9:I:52:ARG:N	2.91	0.44
3:C:51:LEU:HD13	12:C:381:HEM:HBA1	2.00	0.44
3:C:270:PRO:HB3	14:C:383:UHD:C4A	2.48	0.44
2:B:154:ASN:HA	2:B:155:PRO:HD2	1.85	0.44
3:C:75:TYR:HB3	3:C:78:ILE:CD1	2.47	0.43
2:B:33:LEU:HD23	2:B:35:ILE:CD1	2.48	0.43
3:C:331:ASP:O	3:C:334:THR:HB	2.17	0.43
9:I:43:LEU:HD23	9:I:46:LYS:HZ3	1.83	0.43
3:C:240:MET:HB3	4:D:208:MET:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:LEU:O	3:C:123:VAL:HG12	2.18	0.43
2:B:256:ALA:HB2	2:B:325:TYR:CD2	2.54	0.43
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.86	0.43
2:B:143:GLN:O	2:B:143:GLN:HG3	2.19	0.43
3:C:233:LEU:HD22	4:D:216:LEU:HG	1.99	0.43
3:C:85:ASN:HD22	3:C:243:VAL:HG12	1.84	0.43
4:D:117:VAL:HG11	4:D:191:ARG:HD2	2.01	0.43
2:B:380:ASP:O	2:B:384:SER:OG	2.36	0.43
2:B:99:THR:CB	9:I:14:VAL:HG22	2.44	0.43
3:C:233:LEU:HA	3:C:236:ILE:HD12	2.00	0.43
2:B:241:GLY:HA2	2:B:423:SER:OG	2.18	0.43
4:D:211:MET:HE1	10:J:31:PHE:CE2	2.54	0.43
1:A:286:GLY:HA3	16:B:659:HOH:O	2.18	0.43
2:B:119:LEU:HA	2:B:119:LEU:HD23	1.60	0.43
3:C:129:MET:HB3	3:C:182:HIS:HB2	2.00	0.43
6:F:72:GLN:HA	6:F:72:GLN:HE21	1.84	0.43
2:B:257:LEU:HD23	2:B:424:MET:HG3	2.00	0.43
3:C:223:TYR:CE1	4:D:230:LEU:HD12	2.54	0.43
5:E:75:GLU:H	5:E:75:GLU:HG2	1.65	0.42
2:B:325:TYR:CD1	9:I:28:PRO:HD2	2.54	0.42
2:B:370:MET:O	2:B:373:GLU:HB2	2.19	0.42
3:C:105:GLY:HA2	3:C:107:TYR:CE2	2.55	0.42
2:B:124:LEU:HD11	2:B:219:VAL:CG1	2.50	0.42
9:I:1:MET:HB3	16:I:671:HOH:O	2.20	0.42
3:C:75:TYR:CE1	5:E:57:GLN:HG2	2.55	0.42
2:B:73:SER:HB3	2:B:98:VAL:HG11	2.01	0.42
1:A:292:SER:HA	1:A:293:PRO:HD3	1.84	0.42
1:A:430:GLN:HG2	1:A:430:GLN:O	2.20	0.42
4:D:120:ARG:HA	4:D:120:ARG:HD3	1.79	0.42
3:C:193:ALA:O	3:C:196:HIS:HB3	2.19	0.42
1:A:281:ASP:HB2	9:I:20:ARG:NE	2.35	0.42
4:D:124:GLU:CD	4:D:191:ARG:HD3	2.39	0.42
1:A:390:ILE:HA	1:A:391:PRO:HD3	1.87	0.42
2:B:381:GLU:HA	2:B:381:GLU:OE1	2.20	0.42
1:A:233:PRO:HB2	5:E:22:THR:O	2.19	0.42
2:B:200:THR:HG21	2:B:229:GLY:H	1.85	0.42
3:C:311:LYS:HE3	6:F:37:ILE:HD11	2.02	0.42
3:C:197:LEU:HD22	3:C:201:HIS:CE1	2.54	0.42
1:A:255:ILE:HD13	1:A:335:MET:HE1	2.01	0.42
10:J:47:ASN:HB3	10:J:50:LYS:HB2	2.00	0.42
2:B:83:PHE:CZ	2:B:87:ARG:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:VAL:HG21	1:A:86:LEU:HD22	2.02	0.42
6:F:47:ILE:H	6:F:47:ILE:HG12	1.58	0.42
6:F:64:ARG:HB3	16:F:749:HOH:O	2.20	0.42
3:C:37:LEU:HD22	12:C:382:HEM:HAB	2.02	0.41
1:A:156:THR:HG21	1:A:241:ILE:HG22	2.02	0.41
2:B:243:GLU:HA	2:B:424:MET:O	2.20	0.41
5:E:39:VAL:O	5:E:43:THR:OG1	2.38	0.41
12:D:242:HEM:HBB2	12:D:242:HEM:HMB2	2.01	0.41
2:B:365:LYS:HG2	2:B:399:LEU:HD22	2.01	0.41
2:B:227:ARG:NH2	2:B:230:LEU:O	2.45	0.41
3:C:277:ALA:HB1	3:C:294:LEU:HD11	2.02	0.41
1:A:381:ARG:HH22	9:I:56:ARG:HD2	1.86	0.41
1:A:255:ILE:HD13	1:A:335:MET:HE2	2.01	0.41
4:D:223:LYS:HD2	4:D:227:TRP:CD1	2.55	0.41
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.54	0.41
1:A:67:THR:HA	1:A:121:SER:H	1.85	0.41
12:C:382:HEM:CBC	12:C:382:HEM:HMC2	2.44	0.41
1:A:42:ASP:O	1:A:194:ARG:NH2	2.53	0.41
3:C:226:ILE:HG23	4:D:223:LYS:HB2	2.02	0.41
1:A:274:ASN:HA	1:A:274:ASN:HD22	1.54	0.41
10:J:38:GLY:O	10:J:42:ILE:HG12	2.21	0.41
3:C:66:VAL:HA	3:C:69:ILE:HD12	2.03	0.41
3:C:182:HIS:HE1	12:C:381:HEM:C4C	2.39	0.41
3:C:133:LEU:HA	3:C:175:LEU:HD21	2.01	0.41
2:B:305:GLN:CB	2:B:306:PRO:HD2	2.50	0.41
1:A:207:GLN:H	1:A:207:GLN:HG3	1.73	0.41
1:A:255:ILE:HD12	1:A:422:VAL:HG22	2.02	0.41
6:F:59:VAL:HG21	7:G:10:VAL:HG13	2.03	0.41
3:C:152:ALA:CB	3:C:291:VAL:HG11	2.50	0.41
4:D:143:LEU:HB2	4:D:145:GLU:H	1.85	0.41
1:A:251:ALA:O	1:A:325:VAL:HA	2.21	0.41
2:B:222:GLN:HB3	2:B:223:PHE:CD2	2.56	0.41
6:F:33:ARG:O	6:F:36:THR:OG1	2.35	0.41
1:A:341:GLN:NE2	1:A:344:ARG:HH21	2.19	0.41
3:C:8:HIS:CD2	3:C:11:MET:H	2.39	0.41
5:E:16:PRO:HA	5:E:19:LEU:HD12	2.02	0.41
2:B:308:ASP:OD1	9:I:31:GLN:HB2	2.20	0.41
2:B:126:VAL:HG22	16:B:626:HOH:O	2.21	0.41
4:D:83:ARG:HD2	4:D:85:GLY:H	1.85	0.41
2:B:200:THR:HB	2:B:227:ARG:HA	2.03	0.41
1:A:60:GLU:OE2	2:B:287:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:6:HIS:HA	4:D:7:PRO:HD3	1.96	0.41
3:C:183:PHE:O	3:C:186:PRO:HD2	2.21	0.40
3:C:334:THR:OG1	7:G:55:PHE:HD1	2.04	0.40
10:J:51:LEU:HB2	10:J:54:HIS:CE1	2.57	0.40
3:C:94:LEU:HD22	3:C:120:LEU:HD12	2.03	0.40
2:B:71:LEU:CD2	9:I:15:LEU:HG	2.51	0.40
5:E:43:THR:O	5:E:47:VAL:HG23	2.21	0.40
5:E:103:LYS:HA	5:E:106:ILE:HD12	2.02	0.40
8:H:66:ASP:HA	8:H:69:VAL:HB	2.03	0.40
1:A:388:ARG:HH22	1:A:394:GLU:CD	2.24	0.40
3:C:105:GLY:HA2	3:C:107:TYR:CZ	2.56	0.40
1:A:276:ILE:HD11	1:A:354:VAL:HA	2.02	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	444/446 (100%)	397 (89%)	37 (8%)	10 (2%)	8	26
2	B	421/439 (96%)	383 (91%)	26 (6%)	12 (3%)	6	20
3	C	376/379 (99%)	332 (88%)	39 (10%)	5 (1%)	15	42
4	D	239/241 (99%)	199 (83%)	30 (13%)	10 (4%)	3	11
5	E	194/196 (99%)	168 (87%)	21 (11%)	5 (3%)	7	23
6	F	103/110 (94%)	98 (95%)	3 (3%)	2 (2%)	10	32
7	G	73/81 (90%)	66 (90%)	5 (7%)	2 (3%)	6	22
8	H	65/78 (83%)	57 (88%)	7 (11%)	1 (2%)	13	38
9	I	55/78 (70%)	28 (51%)	17 (31%)	10 (18%)	0	0
10	J	59/62 (95%)	48 (81%)	8 (14%)	3 (5%)	2	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	49/56 (88%)	42 (86%)	4 (8%)	3 (6%)	2	5
All	All	2078/2166 (96%)	1818 (88%)	197 (10%)	63 (3%)	5	19

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
2	B	52	LYS
2	B	232	LEU
2	B	437	ASP
3	C	347	TYR
4	D	76	GLU
4	D	93	LYS
4	D	108	ALA
5	E	65	SER
8	H	26	GLN
9	I	4	VAL
9	I	5	ALA
9	I	27	ARG
9	I	45	LEU
9	I	47	ARG
11	K	4	ARG
11	K	39	ARG
1	A	21	ASN
1	A	72	GLY
1	A	125	SER
1	A	239	SER
1	A	286	GLY
2	B	249	GLY
4	D	58	GLU
4	D	87	LEU
4	D	90	TYR
5	E	68	VAL
9	I	43	LEU
10	J	56	LYS
1	A	224	ASP
3	C	177	ARG
4	D	80	MET
4	D	138	PRO
7	G	73	ASN
10	J	3	PRO
1	A	223	TYR

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Mol	Chain	Res	Type
2	B	171	ALA
2	B	236	LYS
2	B	436	ILE
3	C	12	LYS
4	D	198	HIS
5	E	73	LYS
6	F	27	ASN
7	G	27	PRO
10	J	49	GLY
1	A	107	PRO
5	E	64	ALA
5	E	83	GLU
6	F	91	GLU
9	I	31	GLN
1	A	33	PRO
2	B	170	ASN
2	B	266	SER
9	I	9	GLY
9	I	50	LEU
11	K	49	ASN
2	B	228	GLY
9	I	40	SER
2	B	129	ALA
3	C	264	THR
3	C	346	PRO
2	B	234	GLY
4	D	229	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/370 (100%)	307 (83%)	63 (17%)	2	6
2	B	332/343 (97%)	280 (84%)	52 (16%)	3	8
3	C	326/327 (100%)	267 (82%)	59 (18%)	2	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	206/206 (100%)	145 (70%)	61 (30%)	0	1
5	E	168/168 (100%)	130 (77%)	38 (23%)	1	2
6	F	96/98 (98%)	73 (76%)	23 (24%)	1	2
7	G	66/71 (93%)	56 (85%)	10 (15%)	3	9
8	H	64/74 (86%)	50 (78%)	14 (22%)	1	3
9	I	44/60 (73%)	29 (66%)	15 (34%)	0	0
10	J	51/52 (98%)	34 (67%)	17 (33%)	0	0
11	K	41/46 (89%)	29 (71%)	12 (29%)	0	1
All	All	1764/1815 (97%)	1400 (79%)	364 (21%)	1	3

All (364) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	18	GLN
1	A	20	ASP
1	A	21	ASN
1	A	25	VAL
1	A	32	GLN
1	A	34	THR
1	A	37	VAL
1	A	42	ASP
1	A	45	SER
1	A	51	LYS
1	A	58	PHE
1	A	81	SER
1	A	90	SER
1	A	100	LYS
1	A	102	LEU
1	A	104	LYS
1	A	108	LYS
1	A	122	LEU
1	A	127	ILE
1	A	128	GLU
1	A	130	GLU
1	A	131	ARG
1	A	143	THR
1	A	146	ARG
1	A	163	LEU

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Mol	Chain	Res	Type
1	A	175	ARG
1	A	176	LYS
1	A	177	LEU
1	A	183	THR
1	A	186	LEU
1	A	188	ARG
1	A	203	LEU
1	A	204	GLU
1	A	206	ARG
1	A	207	GLN
1	A	208	LEU
1	A	214	LYS
1	A	219	LEU
1	A	223	TYR
1	A	226	ASP
1	A	230	THR
1	A	244	ARG
1	A	245	GLU
1	A	250	LEU
1	A	274	ASN
1	A	300	THR
1	A	302	LYS
1	A	305	GLN
1	A	306	SER
1	A	320	LEU
1	A	323	HIS
1	A	351	GLU
1	A	370	ASP
1	A	381	ARG
1	A	388	ARG
1	A	389	ARG
1	A	398	ARG
1	A	405	ARG
1	A	409	GLU
1	A	413	LYS
1	A	418	GLN
1	A	438	ARG
2	B	17	VAL
2	B	20	HIS
2	B	22	GLN
2	B	24	LEU
2	B	38	LEU

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Mol	Chain	Res	Type
2	B	40	ASN
2	B	69	LEU
2	B	86	THR
2	B	98	VAL
2	B	99	THR
2	B	102	ARG
2	B	109	VAL
2	B	113	ARG
2	B	152	LEU
2	B	154	ASN
2	B	163	LEU
2	B	169	ARG
2	B	170	ASN
2	B	183	ILE
2	B	186	VAL
2	B	189	VAL
2	B	227	ARG
2	B	230	LEU
2	B	232	LEU
2	B	236	LYS
2	B	248	ASN
2	B	251	SER
2	B	257	LEU
2	B	258	VAL
2	B	273	SER
2	B	276	GLN
2	B	284	HIS
2	B	290	ASN
2	B	292	THR
2	B	305	GLN
2	B	309	VAL
2	B	328	SER
2	B	346	THR
2	B	353	SER
2	B	358	GLN
2	B	361	LYS
2	B	362	ASN
2	B	370	MET
2	B	371	SER
2	B	376	GLU
2	B	384	SER
2	B	391	SER

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Mol	Chain	Res	Type
2	B	396	SER
2	B	397	THR
2	B	421	ARG
2	B	424	MET
2	B	435	PHE
3	C	4	ILE
3	C	12	LYS
3	C	42	ILE
3	C	46	LEU
3	C	56	THR
3	C	60	THR
3	C	67	THR
3	C	78	ILE
3	C	80	ARG
3	C	90	PHE
3	C	96	MET
3	C	110	LEU
3	C	114	ASN
3	C	124	MET
3	C	129	MET
3	C	138	MET
3	C	156	ILE
3	C	158	THR
3	C	164	ILE
3	C	168	PHE
3	C	169	SER
3	C	171	ASP
3	C	174	THR
3	C	175	LEU
3	C	183	PHE
3	C	185	LEU
3	C	212	SER
3	C	226	ILE
3	C	228	ASP
3	C	242	LEU
3	C	243	VAL
3	C	248	ASP
3	C	249	LEU
3	C	252	ASP
3	C	263	ASN
3	C	264	THR
3	C	269	LYS

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Mol	Chain	Res	Type
3	C	276	PHE
3	C	281	LEU
3	C	284	ILE
3	C	292	LEU
3	C	296	PHE
3	C	300	ILE
3	C	309	THR
3	C	316	MET
3	C	318	ARG
3	C	328	LEU
3	C	333	LEU
3	C	336	THR
3	C	343	VAL
3	C	344	GLU
3	C	349	THR
3	C	350	ILE
3	C	360	LEU
3	C	361	LEU
3	C	363	LEU
3	C	365	LEU
3	C	371	THR
3	C	379	TRP
4	D	1	SER
4	D	2	ASP
4	D	3	LEU
4	D	5	LEU
4	D	9	SER
4	D	13	SER
4	D	18	LEU
4	D	24	THR
4	D	27	ARG
4	D	34	LYS
4	D	37	CYS
4	D	40	CYS
4	D	42	SER
4	D	46	VAL
4	D	55	CYS
4	D	58	GLU
4	D	59	ASP
4	D	60	GLU
4	D	62	LYS
4	D	64	LEU

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Mol	Chain	Res	Type
4	D	66	GLU
4	D	68	VAL
4	D	72	ASP
4	D	76	GLU
4	D	79	GLU
4	D	82	MET
4	D	83	ARG
4	D	86	LYS
4	D	91	PHE
4	D	97	ASN
4	D	112	ASP
4	D	114	SER
4	D	116	ILE
4	D	121	HIS
4	D	130	LEU
4	D	132	THR
4	D	134	TYR
4	D	135	CYS
4	D	139	THR
4	D	143	LEU
4	D	145	GLU
4	D	147	LEU
4	D	153	PHE
4	D	158	ILE
4	D	162	PRO
4	D	165	TYR
4	D	168	VAL
4	D	170	GLU
4	D	173	ASP
4	D	179	MET
4	D	180	SER
4	D	201	ARG
4	D	203	ARG
4	D	207	LYS
4	D	210	LEU
4	D	211	MET
4	D	212	MET
4	D	223	LYS
4	D	224	ARG
4	D	234	LYS
4	D	241	LYS
5	E	6	LYS

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Mol	Chain	Res	Type
5	E	9	ASP
5	E	10	PHE
5	E	19	LEU
5	E	23	LYS
5	E	25	SER
5	E	27	GLU
5	E	29	SER
5	E	43	THR
5	E	44	THR
5	E	52	LYS
5	E	54	VAL
5	E	69	LEU
5	E	71	MET
5	E	72	SER
5	E	73	LYS
5	E	75	GLU
5	E	77	LYS
5	E	78	LEU
5	E	79	SER
5	E	81	ILE
5	E	85	LYS
5	E	103	LYS
5	E	104	LYS
5	E	108	GLN
5	E	112	VAL
5	E	115	SER
5	E	116	GLN
5	E	117	LEU
5	E	129	LYS
5	E	139	CYS
5	E	152	ASP
5	E	172	ARG
5	E	173	LYS
5	E	181	GLU
5	E	186	GLU
5	E	188	THR
5	E	191	ASP
6	F	6	VAL
6	F	7	SER
6	F	10	SER
6	F	11	ARG
6	F	22	ASN

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Mol	Chain	Res	Type
6	F	27	ASN
6	F	37	ILE
6	F	44	LYS
6	F	47	ILE
6	F	70	MET
6	F	72	GLN
6	F	73	GLN
6	F	74	ILE
6	F	78	GLU
6	F	82	LYS
6	F	84	GLU
6	F	87	LYS
6	F	88	SER
6	F	90	LEU
6	F	91	GLU
6	F	94	LEU
6	F	99	ARG
6	F	110	LYS
7	G	14	ILE
7	G	18	LEU
7	G	31	SER
7	G	34	ILE
7	G	36	ASN
7	G	37	VAL
7	G	45	ILE
7	G	53	VAL
7	G	72	LYS
7	G	73	ASN
8	H	18	THR
8	H	27	LEU
8	H	29	LYS
8	H	30	CYS
8	H	37	LEU
8	H	39	LEU
8	H	47	ARG
8	H	49	GLN
8	H	52	GLU
8	H	60	ASP
8	H	65	ARG
8	H	68	CYS
8	H	72	LYS
8	H	77	LEU

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Mol	Chain	Res	Type
9	I	3	SER
9	I	7	ARG
9	I	8	SER
9	I	15	LEU
9	I	18	THR
9	I	20	ARG
9	I	27	ARG
9	I	44	ASP
9	I	45	LEU
9	I	47	ARG
9	I	48	SER
9	I	49	VAL
9	I	50	LEU
9	I	54	SER
9	I	55	LEU
10	J	1	VAL
10	J	5	LEU
10	J	6	THR
10	J	8	ARG
10	J	12	LEU
10	J	15	ARG
10	J	16	ARG
10	J	18	SER
10	J	24	ILE
10	J	40	ASP
10	J	44	GLU
10	J	46	ILE
10	J	53	LYS
10	J	56	LYS
10	J	58	LYS
10	J	59	TYR
10	J	60	GLU
11	K	3	THR
11	K	6	LEU
11	K	11	ARG
11	K	18	VAL
11	K	20	THR
11	K	22	SER
11	K	24	TRP
11	K	38	TRP
11	K	39	ARG
11	K	44	TRP

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Mol	Chain	Res	Type
11	K	47	TYR
11	K	49	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	141	ASN
1	A	173	ASN
1	A	189	HIS
1	A	215	HIS
1	A	274	ASN
1	A	323	HIS
1	A	341	GLN
1	A	359	ASN
1	A	418	GLN
1	A	435	ASN
2	B	104	ASN
2	B	143	GLN
2	B	162	ASN
2	B	170	ASN
2	B	276	GLN
2	B	305	GLN
2	B	342	ASN
2	B	385	GLN
3	C	8	HIS
3	C	32	ASN
3	C	85	ASN
3	C	114	ASN
3	C	206	ASN
3	C	207	ASN
3	C	352	GLN
4	D	50	HIS
4	D	166	ASN
5	E	53	ASN
5	E	57	GLN
5	E	116	GLN
6	F	53	ASN
6	F	72	GLN
7	G	23	GLN
11	K	12	GLN
11	K	16	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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	381	3	30,50,50	2.97	10 (33%)	24,82,82	3.99	10 (41%)
12	HEM	C	382	3	30,50,50	2.84	9 (30%)	24,82,82	3.34	12 (50%)
14	UHD	C	383	-	20,24,24	2.48	7 (35%)	16,31,31	1.46	1 (6%)
15	UQ2	C	384	-	23,23,23	2.04	5 (21%)	28,31,31	1.40	4 (14%)
12	HEM	D	242	4	30,50,50	2.92	10 (33%)	24,82,82	3.06	11 (45%)
13	FES	E	197	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	381	3	-	0/10/54/54	0/0/8/8
12	HEM	C	382	3	-	0/10/54/54	0/0/8/8
14	UHD	C	383	-	-	0/11/31/31	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	UQ2	C	384	-	-	0/15/39/39	0/1/1/1
12	HEM	D	242	4	-	0/10/54/54	0/0/8/8
13	FES	E	197	5	-	0/0/4/4	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	381	HEM	C3D-C4D	-9.02	1.40	1.51
12	D	242	HEM	C3D-C4D	-8.68	1.40	1.51
12	C	382	HEM	C3D-C4D	-8.21	1.41	1.51
14	C	383	UHD	C4-C4A	-7.80	1.40	1.49
12	C	382	HEM	C3B-C4B	-6.73	1.45	1.51
12	C	381	HEM	C3B-C4B	-6.53	1.46	1.51
12	C	381	HEM	C2D-C3D	-6.39	1.35	1.54
12	D	242	HEM	C3B-C4B	-6.25	1.46	1.51
12	D	242	HEM	C2D-C3D	-6.25	1.35	1.54
12	C	382	HEM	C2D-C3D	-5.73	1.37	1.54
14	C	383	UHD	C7-C7A	-4.34	1.39	1.50
12	C	381	HEM	C2C-C1C	-4.07	1.44	1.52
12	D	242	HEM	C2C-C1C	-4.07	1.44	1.52
12	C	382	HEM	C2C-C1C	-3.75	1.45	1.52
14	C	383	UHD	O6-C6	-3.24	1.22	1.33
12	C	382	HEM	C2D-C1D	-2.59	1.43	1.51
12	D	242	HEM	C2D-C1D	-2.38	1.44	1.51
12	C	382	HEM	C2B-C1B	-2.22	1.44	1.51
14	C	383	UHD	C5-C4A	-2.20	1.41	1.47
12	D	242	HEM	C2B-C1B	-2.16	1.44	1.51
14	C	383	UHD	C6-C7A	-2.16	1.41	1.46
12	C	381	HEM	C2D-C1D	-2.14	1.44	1.51
12	C	381	HEM	C2B-C1B	-2.00	1.45	1.51
15	C	384	UQ2	C7-C8	2.26	1.54	1.50
12	D	242	HEM	C1C-NC	2.44	1.39	1.36
12	C	381	HEM	C1C-NC	2.60	1.39	1.36
15	C	384	UQ2	C13-C14	2.79	1.40	1.32
14	C	383	UHD	C6-C5	3.00	1.41	1.36
15	C	384	UQ2	C3-C2	3.27	1.49	1.35
14	C	383	UHD	C2-S1	3.38	1.79	1.68
12	D	242	HEM	CHD-C4C	3.48	1.44	1.36
12	C	382	HEM	CHD-C4C	3.60	1.44	1.36
12	C	381	HEM	CHD-C4C	3.62	1.44	1.36
15	C	384	UQ2	C8-C9	4.22	1.41	1.33
12	C	381	HEM	CBB-CAB	4.40	1.54	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	381	HEM	CBC-CAC	4.48	1.55	1.29
12	C	382	HEM	CBB-CAB	4.50	1.55	1.29
12	C	382	HEM	CBC-CAC	4.52	1.55	1.29
12	D	242	HEM	CBB-CAB	4.59	1.55	1.29
12	D	242	HEM	CBC-CAC	4.60	1.55	1.29
15	C	384	UQ2	C6-C5	6.63	1.50	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	381	HEM	C3B-CAB-CBB	-12.21	105.73	124.46
12	C	382	HEM	C3B-CAB-CBB	-9.21	110.32	124.46
12	C	381	HEM	C3C-CAC-CBC	-9.10	110.50	124.46
12	D	242	HEM	C3C-CAC-CBC	-8.20	111.88	124.46
12	C	382	HEM	C1D-CHD-C4C	-6.41	115.10	125.82
14	C	383	UHD	O4-C4A-C4	-4.77	116.80	122.10
12	C	381	HEM	C1D-CHD-C4C	-4.76	117.87	125.82
12	C	381	HEM	C4B-CHC-C1C	-4.60	118.13	125.82
12	D	242	HEM	C1D-CHD-C4C	-4.40	118.47	125.82
12	D	242	HEM	C3B-CAB-CBB	-3.96	118.38	124.46
12	C	382	HEM	C3C-CAC-CBC	-3.95	118.40	124.46
15	C	384	UQ2	C5-C6-C1	-3.63	115.98	120.12
12	C	382	HEM	C4B-CHC-C1C	-3.42	120.10	125.82
12	D	242	HEM	C4B-CHC-C1C	-3.25	120.38	125.82
15	C	384	UQ2	C11-C9-C8	-2.39	116.52	121.05
12	C	382	HEM	C3B-C4B-NB	-2.27	107.29	111.63
12	D	242	HEM	CMA-C3A-C4A	-2.15	124.81	128.36
12	C	382	HEM	CBA-CAA-C2A	-2.06	108.84	112.53
15	C	384	UQ2	C8-C7-C6	2.41	118.88	111.64
12	C	381	HEM	CMD-C2D-C3D	2.61	125.91	114.35
12	D	242	HEM	CMD-C2D-C3D	2.91	127.20	114.35
12	C	382	HEM	C2D-C3D-C4D	2.97	106.54	101.50
15	C	384	UQ2	C10-C9-C11	3.20	120.29	115.41
12	C	381	HEM	CMC-C2C-C3C	3.41	125.05	116.53
12	C	382	HEM	CMD-C2D-C3D	3.42	129.49	114.35
12	D	242	HEM	C2D-C3D-C4D	3.47	107.39	101.50
12	C	381	HEM	CAD-C3D-C4D	3.82	125.94	112.47
12	D	242	HEM	CMC-C2C-C3C	3.97	126.43	116.53
12	C	382	HEM	CMB-C2B-C3B	3.99	126.48	116.53
12	C	381	HEM	C2D-C3D-C4D	4.00	108.28	101.50
12	C	382	HEM	CAD-C3D-C2D	4.12	125.05	113.22
12	D	242	HEM	CAD-C3D-C2D	4.13	125.08	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	242	HEM	CAD-C3D-C4D	4.23	127.37	112.47
12	C	381	HEM	CMB-C2B-C3B	4.31	127.30	116.53
12	C	381	HEM	CAD-C3D-C2D	4.32	125.65	113.22
12	C	382	HEM	CAD-C3D-C4D	4.34	127.76	112.47
12	C	382	HEM	CMC-C2C-C3C	4.62	128.07	116.53
12	D	242	HEM	CMB-C2B-C3B	4.95	128.88	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	381	HEM	3	0
12	C	382	HEM	7	0
14	C	383	UHD	3	0
15	C	384	UQ2	4	0
12	D	242	HEM	5	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.