



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:42 PM GMT

PDB ID : 4GD3
Title : Structure of E. coli hydrogenase-1 in complex with cytochrome b
Authors : Volbeda, A.; Fontecilla-Camps, J.C.; Darnault, C.
Deposited on : 2012-07-31
Resolution : 3.30 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>

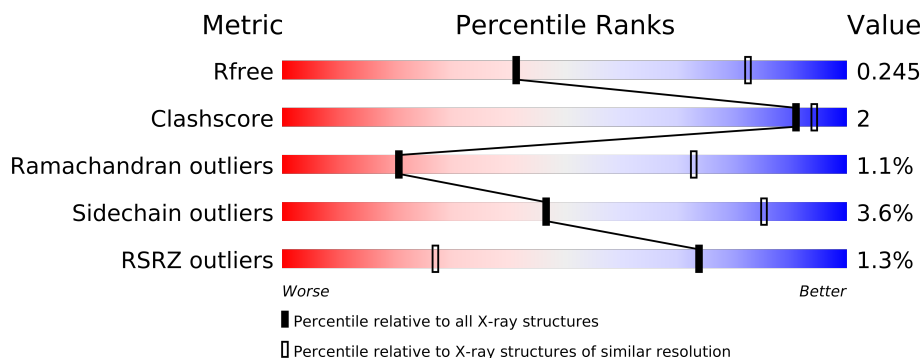
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 3.30 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))
R_{free}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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.

Mol	Chain	Length	Quality of chain
1	Q	335	
1	R	335	
1	S	335	
1	T	335	
2	J	582	
2	K	582	
2	L	582	
2	M	582	
3	A	235	
3	B	235	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	LMT	A	302	-	X
10	LMT	T	404	-	X
6	CL	J	604	-	X
6	CL	K	605	-	X
6	CL	L	604	-	X
6	CL	M	601	-	X
6	CL	M	605	-	X
6	CL	Q	405	-	X
6	CL	S	405	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 31252 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 Hydrogenase-1 small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	304	Total	C	N	O	S	0	7	0
			2329	1477	400	430	22			
1	T	300	Total	C	N	O	S	0	4	0
			2283	1445	393	423	22			
1	Q	304	Total	C	N	O	S	0	7	0
			2329	1477	400	430	22			
1	R	300	Total	C	N	O	S	0	4	0
			2283	1445	393	423	22			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	242	CYS	PRO	ENGINEERED MUTATION	UNP P69739
S	328	ARG	-	EXPRESSION TAG	UNP P69739
S	329	SER	-	EXPRESSION TAG	UNP P69739
S	330	HIS	-	EXPRESSION TAG	UNP P69739
S	331	HIS	-	EXPRESSION TAG	UNP P69739
S	332	HIS	-	EXPRESSION TAG	UNP P69739
S	333	HIS	-	EXPRESSION TAG	UNP P69739
S	334	HIS	-	EXPRESSION TAG	UNP P69739
S	335	HIS	-	EXPRESSION TAG	UNP P69739
T	242	CYS	PRO	ENGINEERED MUTATION	UNP P69739
T	328	ARG	-	EXPRESSION TAG	UNP P69739
T	329	SER	-	EXPRESSION TAG	UNP P69739
T	330	HIS	-	EXPRESSION TAG	UNP P69739
T	331	HIS	-	EXPRESSION TAG	UNP P69739
T	332	HIS	-	EXPRESSION TAG	UNP P69739
T	333	HIS	-	EXPRESSION TAG	UNP P69739
T	334	HIS	-	EXPRESSION TAG	UNP P69739
T	335	HIS	-	EXPRESSION TAG	UNP P69739
Q	242	CYS	PRO	ENGINEERED MUTATION	UNP P69739
Q	328	ARG	-	EXPRESSION TAG	UNP P69739
Q	329	SER	-	EXPRESSION TAG	UNP P69739

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	330	HIS	-	EXPRESSION TAG	UNP P69739
Q	331	HIS	-	EXPRESSION TAG	UNP P69739
Q	332	HIS	-	EXPRESSION TAG	UNP P69739
Q	333	HIS	-	EXPRESSION TAG	UNP P69739
Q	334	HIS	-	EXPRESSION TAG	UNP P69739
Q	335	HIS	-	EXPRESSION TAG	UNP P69739
R	242	CYS	PRO	ENGINEERED MUTATION	UNP P69739
R	328	ARG	-	EXPRESSION TAG	UNP P69739
R	329	SER	-	EXPRESSION TAG	UNP P69739
R	330	HIS	-	EXPRESSION TAG	UNP P69739
R	331	HIS	-	EXPRESSION TAG	UNP P69739
R	332	HIS	-	EXPRESSION TAG	UNP P69739
R	333	HIS	-	EXPRESSION TAG	UNP P69739
R	334	HIS	-	EXPRESSION TAG	UNP P69739
R	335	HIS	-	EXPRESSION TAG	UNP P69739

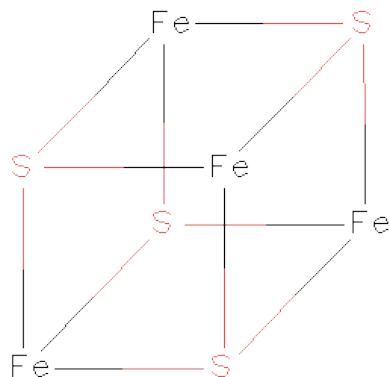
- Molecule 2 is a protein called Hydrogenase-1 large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	581	Total	C	N	O	S	0	33	0
			4733	3011	822	871	29			
2	M	581	Total	C	N	O	S	0	35	0
			4743	3020	825	869	29			
2	J	581	Total	C	N	O	S	0	33	0
			4733	3011	822	871	29			
2	K	581	Total	C	N	O	S	0	35	0
			4743	3020	825	869	29			

- Molecule 3 is a protein called Ni/Fe-hydrogenase 1 B-type cytochrome subunit.

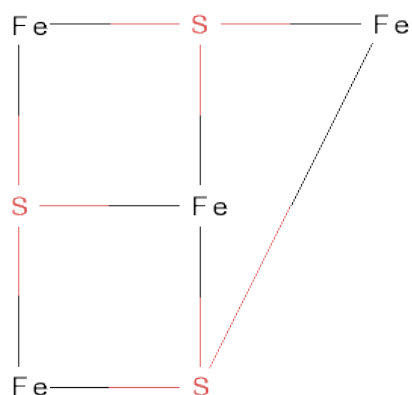
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	179	Total	C	N	O	S	0	0	0
			1360	916	215	218	11			
3	B	179	Total	C	N	O	S	0	0	0
			1360	916	215	218	11			

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	S	1	Total	Fe	S	0	0
			8	4	4		
4	S	1	Total	Fe	S	0	0
			8	4	4		
4	T	1	Total	Fe	S	0	0
			8	4	4		
4	T	1	Total	Fe	S	0	0
			8	4	4		
4	Q	1	Total	Fe	S	0	0
			8	4	4		
4	Q	1	Total	Fe	S	0	0
			8	4	4		
4	R	1	Total	Fe	S	0	0
			8	4	4		
4	R	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is FE4-S3 CLUSTER (three-letter code: F4S) (formula: Fe₄S₃).

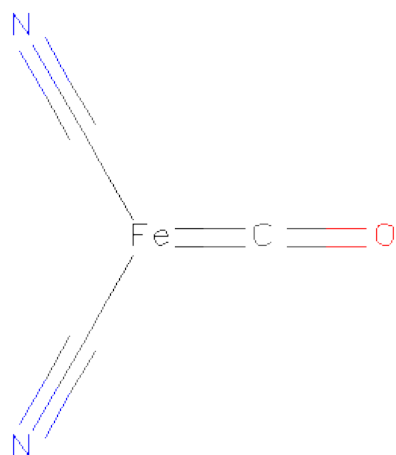


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	S	1	Total	Fe	S	0	0
			7	4	3		
5	T	1	Total	Fe	S	0	0
			7	4	3		
5	Q	1	Total	Fe	S	0	0
			7	4	3		
5	R	1	Total	Fe	S	0	0
			7	4	3		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Cl	0	0
			1	1		
6	Q	2	Total	Cl	0	0
			2	2		
6	K	2	Total	Cl	0	0
			2	2		
6	L	1	Total	Cl	0	0
			1	1		
6	S	2	Total	Cl	0	0
			2	2		
6	M	2	Total	Cl	0	0
			2	2		

- Molecule 7 is CARBONMONOXIDE-(DICYANO)IRON (three-letter code: FCO) (formula: C₃FeN₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	M	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	J	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		
7	K	1	Total	C	Fe	N	O	0	0
			7	3	1	2	1		

- Molecule 8 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	1	Total	Ni	0	0
			1	1		
8	L	1	Total	Ni	0	0
			1	1		
8	K	1	Total	Ni	0	0
			1	1		
8	M	1	Total	Ni	0	0
			1	1		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

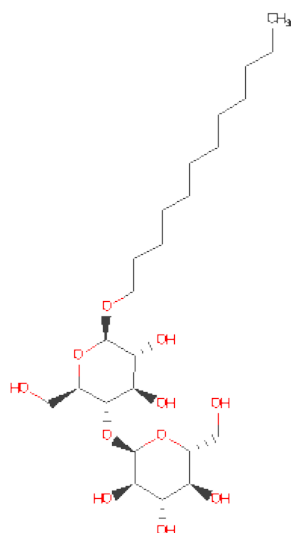
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	J	1	Total	Mg	0	0
			1	1		

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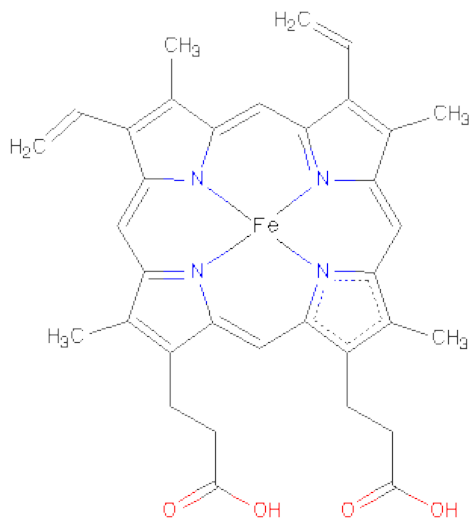
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	1	Total	Mg	0	0
			1	1		
9	K	1	Total	Mg	0	0
			1	1		
9	M	1	Total	Mg	0	0
			1	1		

- Molecule 10 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	T	1	Total	C	O	0	0
			23	12	11		
10	R	1	Total	C	O	0	0
			23	12	11		
10	A	1	Total	C	O	0	0
			23	12	11		
10	B	1	Total	C	O	0	0
			23	12	11		

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
11	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	T	3	Total	O	0	0
			3	3		
12	Q	5	Total	O	0	0
			5	5		
12	S	5	Total	O	0	0
			5	5		
12	L	4	Total	O	0	0
			4	4		
12	R	2	Total	O	0	0
			2	2		
12	M	8	Total	O	0	0
			8	8		
12	J	4	Total	O	0	0
			4	4		
12	K	9	Total	O	0	0
			9	9		



Age Group	Percentage
18-24	95%
25-34	90%
35-44	85%
45-54	80%
55-64	75%
65-74	70%
75-84	65%
85+	60%



Government	Percentage
Current government	95%
Previous government	5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	126.00Å 165.30Å 212.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.30 49.12 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.00-3.30) 99.2 (49.12-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.200 , 0.236 0.214 , 0.245	Depositor DCC
R_{free} test set	3633 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	89.2	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 53.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 73321 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31252	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, MG, CL, SF4, LMT, F4S, HEM, FCO

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	Q	0.55	1/2407 (0.0%)	0.65	0/3275
1	R	0.51	0/2352	0.59	0/3200
1	S	0.50	0/2407	0.62	0/3275
1	T	0.51	0/2352	0.60	0/3200
2	J	0.46	0/4940	0.56	0/6715
2	K	0.45	0/4956	0.55	0/6736
2	L	0.43	0/4940	0.55	0/6715
2	M	0.45	0/4956	0.56	0/6736
3	A	0.55	2/1406 (0.1%)	0.63	1/1916 (0.1%)
3	B	0.56	1/1406 (0.1%)	0.63	1/1916 (0.1%)
All	All	0.48	4/32122 (0.0%)	0.58	2/43684 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	200	TYR	CA-C	-5.87	1.37	1.52
3	A	201	MET	C-N	-5.61	1.21	1.34
3	A	200	TYR	CA-C	-5.42	1.38	1.52
1	Q	115	CYS	CB-SG	-5.26	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	MET	C-N-CA	5.47	135.36	121.70
3	B	201	MET	C-N-CA	5.29	134.93	121.70

There are no chirality outliers.

There are no planarity outliers.

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	Q	2329	0	0	4	0
1	R	2283	0	0	5	0
1	S	2329	0	0	5	0
1	T	2283	0	0	11	0
2	J	4733	0	0	7	0
2	K	4743	0	0	10	0
2	L	4733	0	0	8	0
2	M	4743	0	0	9	0
3	A	1360	0	0	5	0
3	B	1360	0	0	4	0
4	Q	16	0	0	0	0
4	R	16	0	0	0	0
4	S	16	0	0	0	0
4	T	16	0	0	0	0
5	Q	7	0	0	0	0
5	R	7	0	0	0	0
5	S	7	0	0	0	0
5	T	7	0	0	0	0
6	J	1	0	0	0	0
6	K	2	0	0	4	0
6	L	1	0	0	0	0
6	M	2	0	0	4	0
6	Q	2	0	0	0	0
6	S	2	0	0	0	0
7	J	7	0	0	0	0
7	K	7	0	0	0	0
7	L	7	0	0	1	0
7	M	7	0	0	0	0
8	J	1	0	0	0	0
8	K	1	0	0	0	0
8	L	1	0	0	0	0
8	M	1	0	0	0	0
9	J	1	0	0	0	0
9	K	1	0	0	0	0
9	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	M	1	0	0	0	0
10	A	23	0	0	0	0
10	B	23	0	0	0	0
10	R	23	0	0	0	0
10	T	23	0	0	0	0
11	A	43	0	0	0	0
11	B	43	0	0	0	0
12	J	4	0	0	0	0
12	K	9	0	0	0	0
12	L	4	0	0	0	0
12	M	8	0	0	0	0
12	Q	5	0	0	0	0
12	R	2	0	0	0	0
12	S	5	0	0	0	0
12	T	3	0	0	0	0
All	All	31252	0	0	63	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 2.

All (63) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:S:101[B]:ARG:NH1	1:S:101[B]:ARG:CG	2.37	0.87
1:Q:101[B]:ARG:CG	1:Q:101[B]:ARG:NH1	2.39	0.84
1:T:26:ARG:NH2	6:M:601:CL:CL	2.66	0.65
2:M:254[B]:MET:CE	2:M:254[B]:MET:CA	2.82	0.57
2:K:379[A]:VAL:O	2:K:380[A]:LYS:C	2.46	0.54
2:M:379[A]:VAL:O	2:M:380[A]:LYS:C	2.46	0.54
2:L:379[A]:VAL:O	2:L:380[A]:LYS:C	2.46	0.54
2:M:54:ARG:NH2	2:M:75:ILE:O	2.41	0.53
2:J:379[A]:VAL:O	2:J:380[A]:LYS:C	2.47	0.53
2:L:254[B]:MET:CA	2:L:254[B]:MET:CE	2.87	0.53
1:T:115:CYS:SG	1:T:122:GLN:NE2	2.82	0.52
2:K:254[B]:MET:CA	2:K:254[B]:MET:CE	2.88	0.52
2:M:39:ASP:OD1	2:M:39:ASP:N	2.42	0.52
1:T:254:GLU:OE2	3:A:171:TYR:OH	2.28	0.52
1:T:22:GLU:OE1	1:T:26:ARG:NH1	2.43	0.52
2:J:220:HIS:O	2:J:224:GLY:N	2.44	0.51
3:B:54:PHE:CE1	3:B:57:GLY:CA	2.94	0.50
1:R:17:CYS:O	2:K:77:GLY:N	2.44	0.50
2:M:92:GLU:OE2	2:M:107:ARG:NH2	2.45	0.50
1:S:34:ASP:OD1	2:L:169[B]:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:13:VAL:O	3:B:14:PHE:CB	2.61	0.49
3:A:13:VAL:O	3:A:14:PHE:CB	2.61	0.49
1:T:34:ASP:OD1	2:M:169[B]:ARG:NH2	2.45	0.49
2:J:54:ARG:NH2	2:J:75:ILE:O	2.45	0.49
2:K:92:GLU:OE2	2:K:107:ARG:NH2	2.45	0.49
1:Q:34:ASP:OD1	2:J:169[B]:ARG:NH2	2.46	0.48
2:L:54:ARG:NH2	2:L:75:ILE:O	2.46	0.48
2:K:78:VAL:O	6:K:601:CL:CL	2.68	0.48
2:J:254[B]:MET:CE	2:J:254[B]:MET:CA	2.91	0.48
2:M:117:HIS:CE1	6:M:601:CL:CL	3.04	0.47
2:K:54:ARG:NH2	2:K:75:ILE:O	2.48	0.47
1:Q:185:ARG:NH2	1:Q:227:TYR:OH	2.48	0.47
1:S:241:PHE:O	1:S:242:CYS:C	2.52	0.47
2:M:253:ASN:CB	6:M:605:CL:CL	3.00	0.47
3:B:153:GLU:C	3:B:155:SER:N	2.68	0.47
3:A:54:PHE:CE1	3:A:57:GLY:CA	2.98	0.47
3:A:153:GLU:C	3:A:155:SER:N	2.67	0.46
1:T:221:CYS:O	1:T:266:ARG:NH2	2.50	0.45
2:K:243:ILE:O	6:K:605:CL:CL	2.72	0.45
1:T:171:ASP:O	1:T:179:LEU:N	2.49	0.45
2:K:39:ASP:N	2:K:39:ASP:OD1	2.50	0.45
1:Q:222:LYS:O	1:Q:226:THR:OG1	2.35	0.45
1:S:17:CYS:O	2:L:77:GLY:N	2.50	0.44
2:L:39:ASP:OD1	2:L:39:ASP:N	2.49	0.43
1:S:185:ARG:NH2	1:S:227:TYR:OH	2.52	0.43
2:J:39:ASP:N	2:J:39:ASP:OD1	2.51	0.43
1:R:26:ARG:NH2	6:K:601:CL:CL	2.89	0.42
1:R:171:ASP:O	1:R:179:LEU:N	2.52	0.42
1:T:241:PHE:O	1:T:242:CYS:C	2.58	0.42
2:M:558:ALA:N	2:M:565:GLU:OE1	2.52	0.42
2:K:220:HIS:O	2:K:224:GLY:N	2.52	0.42
2:L:220:HIS:O	2:L:224:GLY:N	2.53	0.41
1:R:173:ASP:O	1:R:175:MET:N	2.53	0.41
1:R:221:CYS:O	1:R:266:ARG:NH2	2.53	0.41
2:J:540:ASP:CB	2:J:541:PRO:CD	2.98	0.41
2:K:232:TRP:N	2:K:232:TRP:CD1	2.88	0.41
1:T:276:HIS:O	1:T:277:SER:C	2.60	0.40
1:T:260:ARG:NH1	3:A:179:ASP:OD1	2.54	0.40
1:T:173:ASP:O	1:T:175:MET:N	2.54	0.40
2:L:79:CYS:CB	7:L:601:FCO:C2	3.00	0.40
3:B:54:PHE:CD1	3:B:54:PHE:O	2.75	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	Q	309/335 (92%)	282 (91%)	20 (6%)	7 (2%)	10	54
1	R	302/335 (90%)	282 (93%)	14 (5%)	6 (2%)	11	58
1	S	309/335 (92%)	283 (92%)	19 (6%)	7 (2%)	10	54
1	T	302/335 (90%)	279 (92%)	17 (6%)	6 (2%)	11	58
2	J	612/582 (105%)	571 (93%)	39 (6%)	2 (0%)	50	92
2	K	614/582 (106%)	578 (94%)	35 (6%)	1 (0%)	56	94
2	L	612/582 (105%)	567 (93%)	44 (7%)	1 (0%)	56	94
2	M	614/582 (106%)	572 (93%)	42 (7%)	0	100	100
3	A	173/235 (74%)	147 (85%)	19 (11%)	7 (4%)	5	36
3	B	173/235 (74%)	147 (85%)	20 (12%)	6 (4%)	6	41
All	All	4020/4138 (97%)	3708 (92%)	269 (7%)	43 (1%)	21	73

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	267	VAL
1	S	296	VAL
1	S	297	HIS
1	S	303	VAL
1	T	277	SER
1	Q	267	VAL
1	Q	296	VAL
1	Q	297	HIS
1	Q	303	VAL
3	A	158	ALA
3	B	158	ALA
1	S	266	ARG
1	T	275	THR
1	Q	242	CYS
1	Q	266	ARG
1	R	275	THR

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Mol	Chain	Res	Type
1	R	277	SER
3	A	14	PHE
3	A	155	SER
3	B	14	PHE
3	B	155	SER
1	Q	42	LEU
1	R	42	LEU
1	R	242	CYS
3	B	12	TYR
1	S	42	LEU
1	S	242	CYS
1	T	42	LEU
1	T	174	ARG
1	T	242	CYS
2	J	98	LYS
1	R	174	ARG
3	A	12	TYR
3	A	88	SER
3	B	88	SER
2	L	98	LYS
3	A	154	HIS
3	A	157	TYR
1	T	267	VAL
1	R	267	VAL
3	B	157	TYR
2	J	538	PRO
2	K	538	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	247/274 (90%)	233 (94%)	14 (6%)	29	74
1	R	241/274 (88%)	234 (97%)	7 (3%)	55	89
1	S	247/274 (90%)	236 (96%)	11 (4%)	38	81
1	T	241/274 (88%)	233 (97%)	8 (3%)	50	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	512/481 (106%)	501 (98%)	11 (2%)	66	92
2	K	513/481 (107%)	507 (99%)	6 (1%)	82	95
2	L	512/481 (106%)	501 (98%)	11 (2%)	66	92
2	M	513/481 (107%)	506 (99%)	7 (1%)	78	95
3	A	123/203 (61%)	102 (83%)	21 (17%)	3	15
3	B	123/203 (61%)	102 (83%)	21 (17%)	3	15
All	All	3272/3426 (96%)	3155 (96%)	117 (4%)	47	85

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	90	SER
1	S	125	ARG
1	S	175	MET
1	S	260	ARG
1	S	265	SER
1	S	266	ARG
1	S	268	VAL
1	S	272	GLN
1	S	273	MET
1	S	285	THR
1	S	297	HIS
2	L	6	GLU
2	L	39	ASP
2	L	97	ILE
2	L	245[A]	GLU
2	L	245[B]	GLU
2	L	265	THR
2	L	317	LYS
2	L	482	LEU
2	L	561[A]	GLU
2	L	561[B]	GLU
2	L	579	CYS
1	T	17	CYS
1	T	90	SER
1	T	171	ASP
1	T	175	MET
1	T	260	ARG
1	T	266	ARG
1	T	269	ASP

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Mol	Chain	Res	Type
1	T	297	HIS
2	M	6	GLU
2	M	39	ASP
2	M	317	LYS
2	M	482	LEU
2	M	561[A]	GLU
2	M	561[B]	GLU
2	M	579	CYS
1	Q	17	CYS
1	Q	90	SER
1	Q	125	ARG
1	Q	175	MET
1	Q	193	ARG
1	Q	224	PRO
1	Q	260	ARG
1	Q	265	SER
1	Q	266	ARG
1	Q	268	VAL
1	Q	272	GLN
1	Q	273	MET
1	Q	285	THR
1	Q	297	HIS
2	J	6	GLU
2	J	39	ASP
2	J	97	ILE
2	J	245[A]	GLU
2	J	245[B]	GLU
2	J	265	THR
2	J	317	LYS
2	J	475	THR
2	J	561[A]	GLU
2	J	561[B]	GLU
2	J	579	CYS
1	R	17	CYS
1	R	90	SER
1	R	175	MET
1	R	260	ARG
1	R	266	ARG
1	R	269	ASP
1	R	297	HIS
2	K	6	GLU
2	K	39	ASP

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Mol	Chain	Res	Type
2	K	317	LYS
2	K	561[A]	GLU
2	K	561[B]	GLU
2	K	579	CYS
3	A	12	TYR
3	A	14	PHE
3	A	24	LEU
3	A	29	MET
3	A	54	PHE
3	A	56	MET
3	A	60	ARG
3	A	65	SER
3	A	68	MET
3	A	73	VAL
3	A	74	LEU
3	A	76	MET
3	A	77	ARG
3	A	82	PHE
3	A	134	PHE
3	A	140	SER
3	A	188	MET
3	A	191	ILE
3	A	204	ARG
3	A	208	MET
3	A	209	SER
3	B	12	TYR
3	B	14	PHE
3	B	24	LEU
3	B	29	MET
3	B	54	PHE
3	B	56	MET
3	B	60	ARG
3	B	68	MET
3	B	73	VAL
3	B	74	LEU
3	B	75	LEU
3	B	76	MET
3	B	77	ARG
3	B	82	PHE
3	B	134	PHE
3	B	140	SER
3	B	188	MET

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Mol	Chain	Res	Type
3	B	191	ILE
3	B	204	ARG
3	B	208	MET
3	B	209	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

Of 40 ligands modelled in this entry, 18 are monoatomic - leaving 22 for Mogul analysis.

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	$\# Z > 2$
11	HEM	A	301	3	49,50,50	2.37	13 (26%)	46,82,82	1.76	5 (10%)
10	LMT	A	302	-	24,24,36	0.77	1 (4%)	34,35,47	0.82	1 (2%)
11	HEM	B	301	3	49,50,50	2.28	14 (28%)	46,82,82	1.76	6 (13%)
10	LMT	B	302	-	24,24,36	0.68	1 (4%)	34,35,47	0.82	2 (5%)
7	FCO	J	601	2	2,6,6	0.24	0	0,6,6	0.00	-
7	FCO	K	602	2	2,6,6	0.04	0	0,6,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FCO	L	601	2	2,6,6	0.08	0	0,6,6	0.00	-
7	FCO	M	602	2	2,6,6	0.06	0	0,6,6	0.00	-
4	SF4	Q	401	1	12,12,12	5.01	10 (83%)	0,24,24	0.00	-
4	SF4	Q	402	1	12,12,12	4.22	10 (83%)	0,24,24	0.00	-
5	F4S	Q	403	1	3,9,9	8.09	3 (100%)	0,15,15	0.00	-
4	SF4	R	401	1	12,12,12	6.86	11 (91%)	0,24,24	0.00	-
4	SF4	R	402	1	12,12,12	4.27	10 (83%)	0,24,24	0.00	-
5	F4S	R	403	1	3,9,9	8.20	3 (100%)	0,15,15	0.00	-
10	LMT	R	404	-	24,24,36	0.80	1 (4%)	34,35,47	1.16	3 (8%)
4	SF4	S	401	1	12,12,12	6.53	10 (83%)	0,24,24	0.00	-
4	SF4	S	402	1	12,12,12	4.99	11 (91%)	0,24,24	0.00	-
5	F4S	S	403	1	3,9,9	16.94	3 (100%)	0,15,15	0.00	-
4	SF4	T	401	1	12,12,12	6.21	12 (100%)	0,24,24	0.00	-
4	SF4	T	402	1	12,12,12	5.69	11 (91%)	0,24,24	0.00	-
5	F4S	T	403	1	3,9,9	17.54	3 (100%)	0,15,15	0.00	-
10	LMT	T	404	-	24,24,36	0.76	1 (4%)	34,35,47	1.24	3 (8%)

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
11	HEM	A	301	3	-	0/14/114/114	0/0/8/8
10	LMT	A	302	-	-	0/8/48/61	0/2/2/2
11	HEM	B	301	3	-	0/14/114/114	0/0/8/8
10	LMT	B	302	-	-	0/8/48/61	0/2/2/2
7	FCO	J	601	2	-	0/0/6/6	0/0/0/0
7	FCO	K	602	2	-	0/0/6/6	0/0/0/0
7	FCO	L	601	2	-	0/0/6/6	0/0/0/0
7	FCO	M	602	2	-	0/0/6/6	0/0/0/0
4	SF4	Q	401	1	-	0/0/48/48	0/0/5/5
4	SF4	Q	402	1	-	0/0/48/48	0/0/5/5
5	F4S	Q	403	1	-	0/0/24/24	0/0/3/3
4	SF4	R	401	1	-	0/0/48/48	0/0/5/5
4	SF4	R	402	1	-	0/0/48/48	0/0/5/5
5	F4S	R	403	1	-	0/0/24/24	0/0/3/3
10	LMT	R	404	-	-	0/8/48/61	0/2/2/2
4	SF4	S	401	1	-	0/0/48/48	0/0/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	S	402	1	-	0/0/48/48	0/0/5/5
5	F4S	S	403	1	-	0/0/24/24	0/0/3/3
4	SF4	T	401	1	-	0/0/48/48	0/0/5/5
4	SF4	T	402	1	-	0/0/48/48	0/0/5/5
5	F4S	T	403	1	-	0/0/24/24	0/0/3/3
10	LMT	T	404	-	-	0/8/48/61	0/2/2/2

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	403	F4S	S2-FE2	-24.55	2.16	2.33
5	S	403	F4S	S3-FE2	-24.37	2.16	2.33
5	S	403	F4S	S1-FE2	-13.68	2.24	2.33
5	T	403	F4S	S3-FE2	-13.11	2.24	2.33
5	T	403	F4S	S1-FE2	-12.17	2.25	2.33
4	R	401	SF4	S1-FE2	-11.15	2.25	2.33
5	Q	403	F4S	S1-FE2	-10.49	2.26	2.33
5	R	403	F4S	S3-FE2	-10.18	2.26	2.33
4	T	402	SF4	S4-FE1	-10.17	2.26	2.33
4	S	401	SF4	S4-FE3	-10.05	2.26	2.33
4	T	401	SF4	S3-FE2	-9.88	2.26	2.33
4	S	402	SF4	S1-FE4	-9.72	2.26	2.33
4	S	401	SF4	S3-FE2	-9.59	2.26	2.33
4	S	401	SF4	S1-FE2	-9.54	2.26	2.33
4	R	401	SF4	S2-FE4	-9.38	2.26	2.33
4	R	401	SF4	S4-FE3	-9.01	2.27	2.33
5	S	403	F4S	S2-FE2	-8.91	2.27	2.33
4	T	401	SF4	S2-FE3	-8.64	2.27	2.33
4	T	401	SF4	S1-FE2	-8.60	2.27	2.33
5	R	403	F4S	S2-FE2	-8.52	2.27	2.33
4	T	402	SF4	S2-FE3	-8.35	2.27	2.33
5	Q	403	F4S	S3-FE2	-8.16	2.27	2.33
4	R	401	SF4	S3-FE4	-8.13	2.27	2.33
4	S	401	SF4	S3-FE4	-7.97	2.27	2.33
4	R	402	SF4	S1-FE2	-7.96	2.27	2.33
4	R	401	SF4	S1-FE3	-7.79	2.28	2.33
4	R	401	SF4	S2-FE1	-7.76	2.28	2.33
4	S	402	SF4	S4-FE3	-7.57	2.28	2.33
4	S	401	SF4	S2-FE1	-7.54	2.28	2.33
4	Q	401	SF4	S1-FE2	-7.28	2.28	2.33
4	Q	401	SF4	S3-FE4	-7.26	2.28	2.33
4	Q	402	SF4	S4-FE2	-7.17	2.28	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	402	SF4	S2-FE4	-7.07	2.28	2.33
4	Q	402	SF4	S2-FE4	-6.92	2.28	2.33
4	Q	401	SF4	S4-FE3	-6.79	2.28	2.33
4	T	402	SF4	S3-FE2	-6.61	2.28	2.33
4	S	402	SF4	S1-FE2	-6.54	2.28	2.33
4	T	401	SF4	S3-FE4	-6.52	2.28	2.33
4	T	401	SF4	S2-FE1	-6.20	2.29	2.33
4	T	402	SF4	S1-FE2	-6.07	2.29	2.33
11	A	301	HEM	C3D-C2D	6.01	1.54	1.43
4	T	402	SF4	S3-FE4	-6.00	2.29	2.33
11	B	301	HEM	C3B-C2B	-5.93	1.33	1.43
4	S	402	SF4	S4-FE1	-5.78	2.29	2.33
4	Q	401	SF4	S4-FE2	-5.72	2.29	2.33
11	A	301	HEM	C2D-C1D	5.67	1.46	1.44
4	T	401	SF4	S4-FE3	-5.66	2.29	2.33
4	Q	401	SF4	S2-FE1	-5.64	2.29	2.33
4	T	402	SF4	S4-FE3	-5.55	2.29	2.33
4	Q	401	SF4	S2-FE4	-5.51	2.29	2.33
4	S	401	SF4	S1-FE4	-5.49	2.29	2.33
4	T	401	SF4	S4-FE1	-5.43	2.29	2.33
11	A	301	HEM	C3B-C2B	-5.39	1.34	1.43
4	R	401	SF4	S3-FE1	-5.38	2.29	2.33
4	T	402	SF4	S1-FE4	-5.34	2.29	2.33
11	B	301	HEM	C3C-C2C	-5.32	1.34	1.43
4	S	401	SF4	S2-FE3	-5.28	2.29	2.33
11	B	301	HEM	C3D-C2D	5.24	1.52	1.43
5	R	403	F4S	S1-FE2	5.04	2.36	2.33
4	Q	402	SF4	S1-FE3	-4.96	2.29	2.33
11	A	301	HEM	C3C-CAC	4.95	1.56	1.40
4	T	401	SF4	S1-FE4	-4.88	2.30	2.33
11	A	301	HEM	C3C-C2C	-4.87	1.35	1.43
4	Q	402	SF4	S3-FE4	-4.79	2.30	2.33
11	A	301	HEM	C3B-CAB	4.78	1.55	1.40
11	B	301	HEM	C3C-CAC	4.77	1.55	1.40
11	B	301	HEM	C2D-C1D	4.72	1.45	1.44
11	B	301	HEM	C3B-CAB	4.63	1.55	1.40
4	S	401	SF4	S4-FE1	-4.61	2.30	2.33
4	S	401	SF4	S1-FE3	-4.58	2.30	2.33
4	Q	401	SF4	S3-FE1	-4.53	2.30	2.33
4	R	402	SF4	S4-FE3	-4.53	2.30	2.33
4	S	402	SF4	S2-FE4	-4.53	2.30	2.33
5	Q	403	F4S	S2-FE2	-4.45	2.30	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	301	HEM	C3D-C4D	4.37	1.45	1.44
4	T	401	SF4	S3-FE1	-4.33	2.30	2.33
4	R	401	SF4	S4-FE2	-4.13	2.30	2.33
4	T	402	SF4	S2-FE1	-4.04	2.30	2.33
4	R	402	SF4	S4-FE1	-4.00	2.30	2.33
11	B	301	HEM	C3D-C4D	3.93	1.45	1.44
4	R	402	SF4	S1-FE4	-3.93	2.30	2.33
4	T	401	SF4	S4-FE2	-3.89	2.30	2.33
11	A	301	HEM	C4A-C3A	3.81	1.44	1.40
4	R	402	SF4	S2-FE1	-3.80	2.30	2.33
11	B	301	HEM	C4A-C3A	3.77	1.44	1.40
4	Q	401	SF4	S1-FE4	-3.76	2.30	2.33
4	R	401	SF4	S4-FE1	-3.76	2.30	2.33
4	Q	402	SF4	S4-FE3	-3.69	2.30	2.33
11	A	301	HEM	FE-NA	3.65	2.08	1.92
4	S	402	SF4	S3-FE1	-3.64	2.30	2.33
4	R	402	SF4	S3-FE2	-3.59	2.30	2.33
4	Q	402	SF4	S1-FE4	-3.54	2.30	2.33
4	Q	401	SF4	S2-FE3	-3.54	2.30	2.33
4	R	401	SF4	S3-FE2	-3.53	2.30	2.33
4	Q	402	SF4	S2-FE1	-3.50	2.30	2.33
4	S	402	SF4	S2-FE1	-3.43	2.30	2.33
4	Q	402	SF4	S3-FE1	-3.42	2.30	2.33
11	B	301	HEM	FE-NA	3.37	2.06	1.92
4	R	402	SF4	S3-FE4	-3.29	2.31	2.33
4	R	401	SF4	S2-FE3	-3.28	2.31	2.33
11	A	301	HEM	FE-ND	3.23	2.09	1.97
4	T	402	SF4	S2-FE4	-3.08	2.31	2.33
4	T	401	SF4	S1-FE3	-3.01	2.31	2.33
4	T	402	SF4	S3-FE1	2.96	2.35	2.33
10	A	302	LMT	O1'-C1'	2.84	1.43	1.25
10	R	404	LMT	O1'-C1'	2.81	1.43	1.25
10	T	404	LMT	O1'-C1'	2.81	1.43	1.25
4	S	402	SF4	S4-FE2	-2.81	2.31	2.33
10	B	302	LMT	O1'-C1'	2.76	1.43	1.25
4	T	401	SF4	S2-FE4	-2.74	2.31	2.33
11	A	301	HEM	CMC-C2C	2.67	1.55	1.47
4	Q	402	SF4	S3-FE2	-2.65	2.31	2.33
11	B	301	HEM	CMC-C2C	2.47	1.55	1.47
11	A	301	HEM	CMB-C2B	2.39	1.54	1.47
11	A	301	HEM	CMD-C2D	2.38	1.54	1.47
4	Q	402	SF4	S1-FE2	-2.36	2.31	2.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	402	SF4	S3-FE1	-2.33	2.31	2.33
11	B	301	HEM	CMB-C2B	2.30	1.54	1.47
11	B	301	HEM	FE-ND	2.30	2.06	1.97
4	R	402	SF4	S2-FE3	-2.28	2.31	2.33
11	B	301	HEM	CMD-C2D	2.27	1.54	1.47
4	S	402	SF4	S2-FE3	-2.24	2.31	2.33
4	Q	401	SF4	S4-FE1	-2.19	2.31	2.33
4	S	402	SF4	S1-FE3	-2.17	2.31	2.33
11	B	301	HEM	FE-NB	2.10	2.05	1.97
4	T	402	SF4	S4-FE2	2.06	2.34	2.33
4	S	402	SF4	S3-FE2	-2.06	2.31	2.33
4	S	401	SF4	S2-FE4	-2.01	2.31	2.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	301	HEM	C3B-C4B-NB	-7.23	108.83	114.00
11	A	301	HEM	C3B-C4B-NB	-6.89	109.07	114.00
11	A	301	HEM	C4D-ND-C1D	5.76	111.06	105.16
11	B	301	HEM	C4D-ND-C1D	5.38	110.67	105.16
11	A	301	HEM	C2D-C1D-ND	-3.46	108.84	112.93
11	B	301	HEM	C2D-C1D-ND	-3.32	109.01	112.93
10	T	404	LMT	C3B-C4B-C5B	-2.80	105.21	110.20
11	B	301	HEM	CAD-C3D-C4D	2.65	129.29	124.53
10	R	404	LMT	C3B-C4B-C5B	-2.62	105.52	110.20
10	T	404	LMT	C2'-C3'-C4'	2.54	115.12	109.61
11	A	301	HEM	CAA-CBA-CGA	-2.50	105.45	113.47
11	B	301	HEM	CAA-CBA-CGA	-2.42	105.69	113.47
10	A	302	LMT	O5'-C1'-C2'	-2.36	104.51	110.85
11	B	301	HEM	C1B-NB-C4B	2.26	107.48	105.16
10	R	404	LMT	C2'-C3'-C4'	2.22	114.44	109.61
10	B	302	LMT	O5'-C5'-C6'	2.14	111.61	106.34
10	B	302	LMT	O5'-C1'-C2'	-2.14	105.10	110.85
11	A	301	HEM	CAD-C3D-C4D	2.13	128.36	124.53
10	R	404	LMT	O5'-C5'-C6'	2.11	111.53	106.34
10	T	404	LMT	O5'-C5'-C6'	2.03	111.34	106.34

There are no chirality outliers.

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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Q	304/335 (90%)	-0.19	0 100 100	59, 83, 151, 200	1 (0%)
1	R	300/335 (89%)	0.11	4 (1%) 74 27	69, 100, 138, 204	1 (0%)
1	S	304/335 (90%)	-0.11	1 (0%) 91 63	63, 87, 134, 185	1 (0%)
1	T	300/335 (89%)	-0.01	2 (0%) 84 42	60, 103, 161, 227	1 (0%)
2	J	581/582 (99%)	0.02	2 (0%) 91 63	67, 101, 128, 142	4 (0%)
2	K	581/582 (99%)	0.07	11 (1%) 64 20	67, 103, 136, 164	5 (0%)
2	L	581/582 (99%)	-0.00	9 (1%) 70 24	73, 109, 140, 164	4 (0%)
2	M	581/582 (99%)	0.01	6 (1%) 79 33	56, 103, 155, 188	5 (0%)
3	A	179/235 (76%)	0.16	7 (3%) 37 8	74, 126, 212, 223	0
3	B	179/235 (76%)	0.16	5 (2%) 50 12	78, 126, 227, 249	0
All	All	3890/4138 (94%)	0.01	47 (1%) 74 29	56, 101, 160, 249	22 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	115	LEU	5.4
3	B	210	ASP	4.2
2	L	284	GLN	3.7
2	J	355	ARG	3.5
2	K	193	LYS	3.3
2	K	46	ALA	3.1
3	A	129	ALA	2.9
2	L	15	ALA	2.7
2	K	29	GLY	2.7
2	L	285	PHE	2.7
2	K	369	ILE	2.6
2	L	16	GLY	2.6
2	K	285	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	K	194	LEU	2.5
2	K	356	TYR	2.5
2	L	357	PRO	2.3
1	R	66	GLN	2.3
3	A	206	ASP	2.3
2	L	355	ARG	2.3
1	S	266	ARG	2.3
2	K	281	ALA	2.2
3	A	205	GLU	2.2
1	R	71	TYR	2.2
2	J	317	LYS	2.2
2	L	438	LEU	2.2
2	M	17[A]	ARG	2.2
2	M	41	ASN	2.2
2	M	521	GLY	2.2
2	K	192	TYR	2.2
2	M	197[A]	GLU	2.2
1	R	4	LYS	2.2
3	B	111	TRP	2.2
1	R	70	LYS	2.1
3	A	128	ILE	2.1
1	T	302	ALA	2.1
2	L	358	ASN	2.1
2	K	282	ILE	2.1
3	B	128	ILE	2.1
2	M	139[A]	LYS	2.1
1	T	149	CYS	2.1
2	L	17[A]	ARG	2.0
2	M	229	HIS	2.0
3	A	209	SER	2.0
3	A	130	GLN	2.0
3	B	14	PHE	2.0
3	A	131	ALA	2.0
2	K	131	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	CL	L	604	1/1	0.66	51.56	100,100,100,100	0
6	CL	M	605	1/1	0.89	30.22	91,91,91,91	0
6	CL	J	604	1/1	0.31	12.83	96,96,96,96	0
6	CL	K	605	1/1	0.61	8.04	102,102,102,102	0
6	CL	Q	405	1/1	0.29	4.49	92,92,92,92	0
6	CL	S	405	1/1	0.37	2.98	92,92,92,92	0
10	LMT	A	302	23/35	0.30	2.30	114,132,152,153	0
10	LMT	T	404	23/35	0.23	2.05	135,143,147,149	0
6	CL	M	601	1/1	0.59	1.69	92,92,92,92	0
11	HEM	A	301	43/43	0.19	0.90	77,87,97,101	0
10	LMT	R	404	23/35	0.31	0.87	145,151,157,158	0
7	FCO	J	601	7/7	0.30	0.79	80,81,89,89	0
6	CL	K	601	1/1	0.30	0.75	103,103,103,103	0
10	LMT	B	302	23/35	0.24	0.60	119,140,162,163	0
11	HEM	B	301	43/43	0.22	0.13	78,88,97,102	0
6	CL	Q	404	1/1	0.20	-0.07	82,82,82,82	0
7	FCO	L	601	7/7	0.19	-0.49	88,90,98,99	0
4	SF4	T	401	8/8	0.18	-0.57	57,61,64,66	0
4	SF4	T	402	8/8	0.20	-0.64	68,71,73,73	0
5	F4S	Q	403	7/7	0.17	-0.67	64,68,73,77	0
4	SF4	R	402	8/8	0.21	-0.80	73,77,79,80	0
5	F4S	S	403	7/7	0.14	-0.81	76,78,84,86	0
4	SF4	R	401	8/8	0.17	-0.87	63,67,70,71	0
6	CL	S	404	1/1	0.17	-0.92	90,90,90,90	0
7	FCO	M	602	7/7	0.17	-0.93	81,83,90,93	0
4	SF4	Q	402	8/8	0.11	-1.11	66,67,69,70	0
4	SF4	S	401	8/8	0.11	-1.14	63,64,67,70	0
4	SF4	Q	401	8/8	0.12	-1.15	61,62,67,68	0
4	SF4	S	402	8/8	0.11	-1.20	70,72,73,73	0
8	NI	M	603	1/1	0.15	-1.26	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	NI	L	602	1/1	0.16	-1.29	91,91,91,91	0
5	F4S	T	403	7/7	0.24	-1.30	82,85,92,97	0
5	F4S	R	403	7/7	0.24	-1.38	83,86,92,97	0
7	FCO	K	602	7/7	0.13	-1.40	89,91,95,97	0
9	MG	M	604	1/1	0.10	-1.48	95,95,95,95	0
8	NI	K	603	1/1	0.12	-1.60	92,92,92,92	0
9	MG	K	604	1/1	0.13	-1.76	97,97,97,97	0
8	NI	J	602	1/1	0.17	-1.77	81,81,81,81	0
9	MG	L	603	1/1	0.16	-1.89	99,99,99,99	0
9	MG	J	603	1/1	0.05	-2.21	87,87,87,87	0

6.5 Other polymers ⓘ

There are no such residues in this entry.