



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:32 PM GMT

PDB ID : 1KQF  
Title : FORMATE DEHYDROGENASE N FROM E. COLI  
Authors : Jormakka, M.; Tornroth, S.; Byrne, B.; Iwata, S.  
Deposited on : 2002-01-05  
Resolution : 1.60 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](mailto: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.

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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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

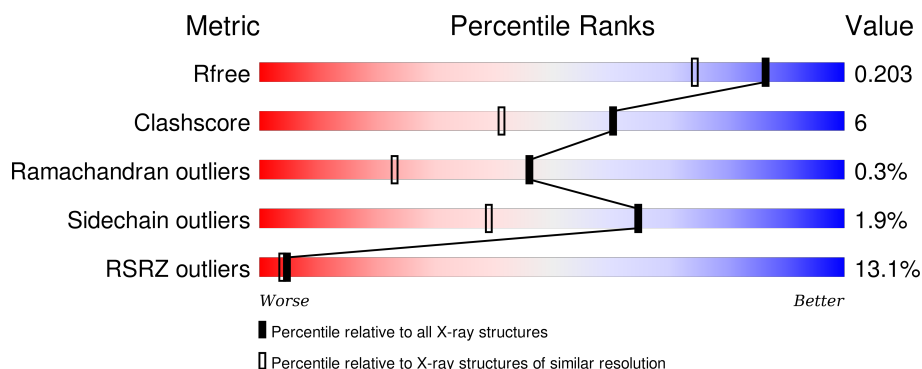
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	1015	<div> <div>11%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
2	B	294	<div> <div>11%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
3	C	217	<div> <div>70%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13989 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 FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, MAJOR SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	982	Total	C	N	O	S	Se	0	0	0
			7719	4872	1352	1457	37	1			

- Molecule 2 is a protein called FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, IRON-SULFUR SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	289	Total	C	N	O	S	0	0	0
			2207	1383	381	421	22			

- Molecule 3 is a protein called FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, CYTOCHROME B556(FDN) SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	216	Total	C	N	O	S	0	0	0
			1783	1192	301	276	14			

- Molecule 4 is MOLYBDENUM(VI) ION (three-letter code: 6MO) (formula: Mo).

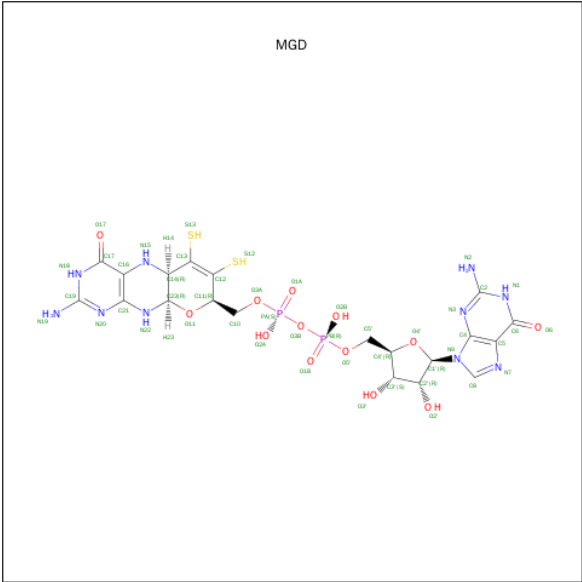
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mo	0	0
			1	1		

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



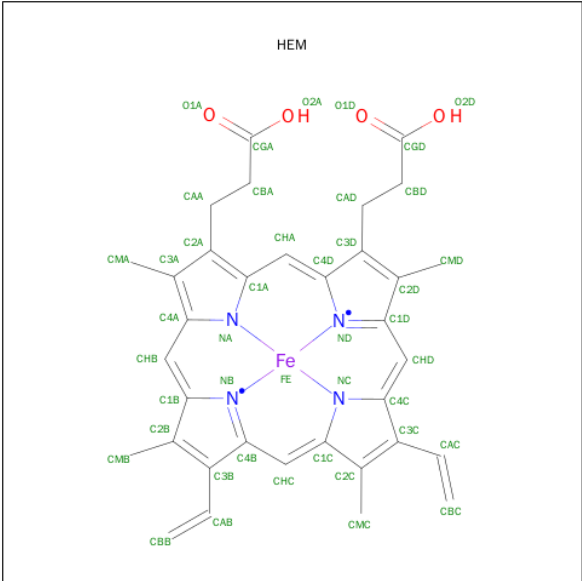
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		
5	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 6 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
6	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



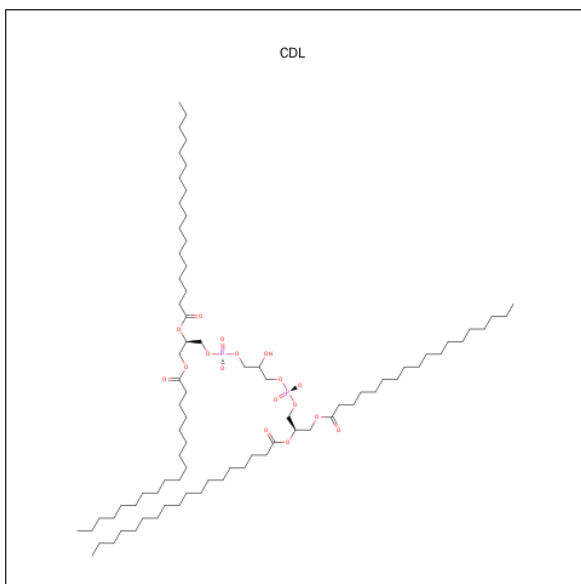
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 8 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	O	P	0	0
			70	51	17	2		

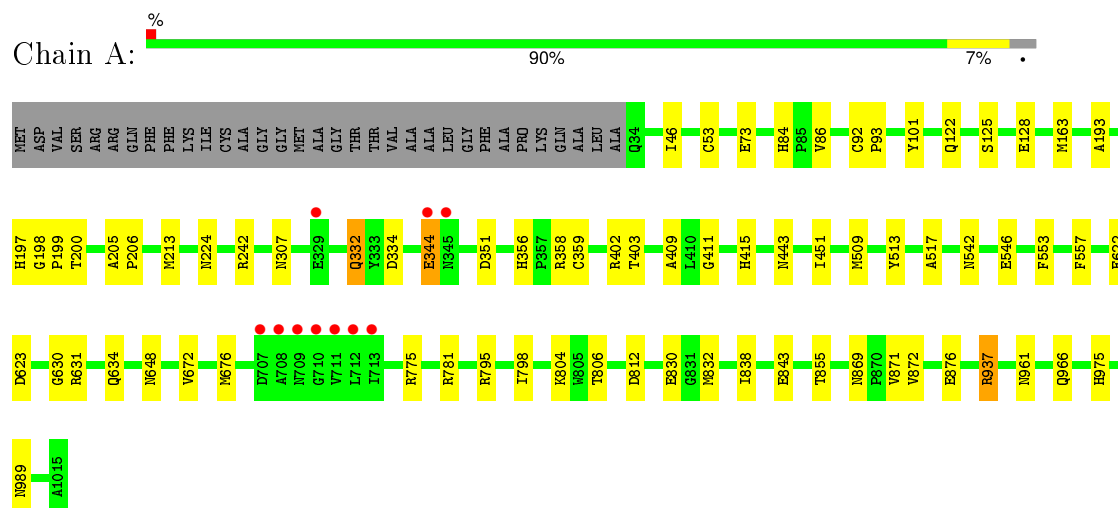
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1497	Total	O	0	0
			1497	1497		
9	B	399	Total	O	0	0
			399	399		
9	C	93	Total	O	0	0
			93	93		

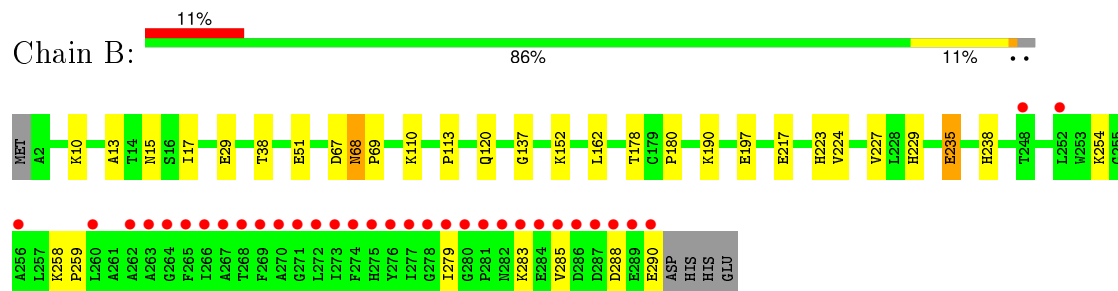
### 3 Residue-property plots

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.

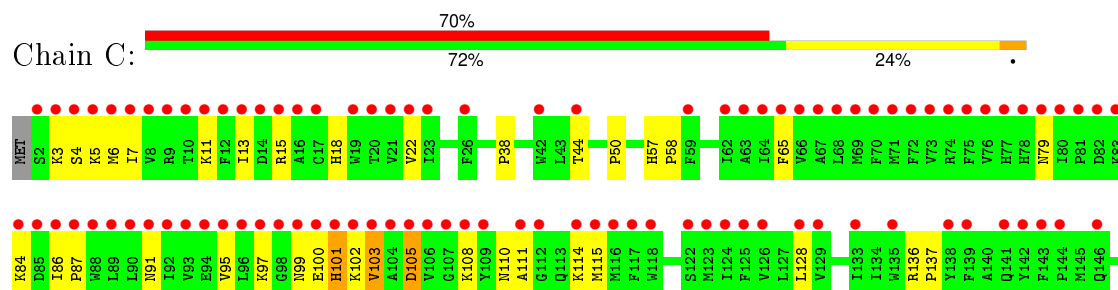
#### • Molecule 1: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, MAJOR SUBUNIT

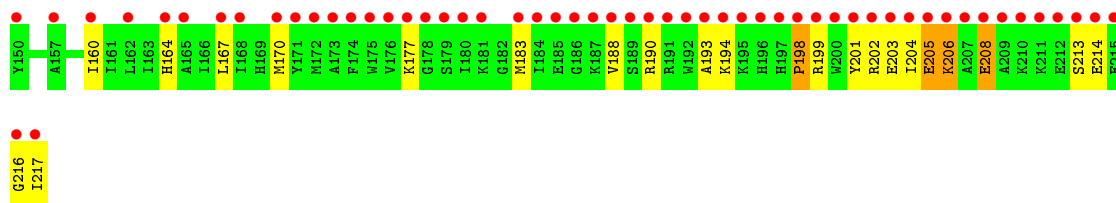


#### • Molecule 2: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, IRON-SULFUR SUBUNIT



#### • Molecule 3: FORMATE DEHYDROGENASE, NITRATE-INDUCIBLE, CYTOCHROME B556(FDN) SUBUNIT







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.00Å 203.00Å 203.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.60 39.81 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.9 (40.00-1.60) 94.1 (39.81-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 1.60Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.177 , 0.195 0.187 , 0.203	Depositor DCC
$R_{free}$ test set	3446 reflections (1.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.9	EDS
Estimated twinning fraction	0.013 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 341515 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13989	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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: 6MO, MGD, CDL, SF4, SEC, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.34	0/7910	0.69	2/10749 (0.0%)
2	B	0.32	0/2255	0.68	2/3056 (0.1%)
3	C	0.33	0/1840	0.62	0/2483
All	All	0.33	0/12005	0.68	4/16288 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	334	ASP	N-CA-C	-6.00	94.79	111.00
2	B	227	VAL	N-CA-C	-5.85	95.21	111.00
1	A	975	HIS	N-CA-C	5.28	125.26	111.00
2	B	224	VAL	N-CA-C	-5.07	97.31	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	7719	0	7457	60	0
2	B	2207	0	2140	21	0
3	C	1783	0	1836	57	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	8	0	0	0	0
5	B	32	0	0	0	0
6	A	94	0	44	1	0
7	C	86	0	60	2	0
8	C	70	0	83	0	0
9	A	1497	0	0	16	2
9	B	399	0	0	6	0
9	C	93	0	0	10	0
All	All	13989	0	11620	132	2

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 6.

All (132) 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)
1:A:359:CYS:HB3	9:A:1672:HOH:O	1.66	0.95
1:A:356:HIS:HD2	1:A:358:ARG:H	1.15	0.93
1:A:869:ASN:HB3	1:A:872:VAL:HG23	1.52	0.91
1:A:224:ASN:HD22	1:A:403:THR:H	1.16	0.88
1:A:622:GLU:OE1	1:A:648:ASN:HB2	1.73	0.86
3:C:15:ARG:HG2	3:C:183:MET:HE3	1.64	0.80
3:C:202:ARG:O	3:C:206:LYS:HD2	1.83	0.78
1:A:830:GLU:HG3	1:A:832:MET:CE	2.16	0.76
3:C:101:HIS:HD2	3:C:102:LYS:H	1.33	0.76
1:A:832:MET:SD	9:A:1601:HOH:O	2.47	0.73
2:B:152:LYS:HB3	9:B:1187:HOH:O	1.89	0.71
3:C:193:ALA:HB1	3:C:201:TYR:HB2	1.73	0.71
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.73	0.70
2:B:279:ILE:HD13	3:C:97:LYS:HA	1.74	0.70
1:A:197:HIS:HD2	1:A:200:THR:OG1	1.76	0.69
1:A:307:ASN:HB3	1:A:832:MET:HE1	1.75	0.69
1:A:205:ALA:HB3	1:A:206:PRO:HD3	1.74	0.68
1:A:830:GLU:HG3	1:A:832:MET:HE2	1.74	0.68
1:A:509:MET:SD	9:A:2296:HOH:O	2.52	0.68
2:B:197:GLU:HG3	9:B:1185:HOH:O	1.94	0.67
1:A:781:ARG:HA	1:A:798:ILE:HD11	1.76	0.66
3:C:84:LYS:HB3	9:C:1932:HOH:O	1.95	0.66
3:C:5:LYS:HG2	3:C:6:MET:SD	2.36	0.66
1:A:307:ASN:CB	1:A:832:MET:HE1	2.27	0.65
1:A:937:ARG:NH2	9:A:1412:HOH:O	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:101:HIS:CD2	3:C:102:LYS:HG3	2.32	0.64
1:A:351:ASP:HB3	9:A:1672:HOH:O	1.97	0.64
2:B:285:VAL:HG12	2:B:288:ASP:H	1.62	0.64
3:C:7:ILE:HG13	3:C:188:VAL:HG23	1.78	0.64
3:C:101:HIS:CD2	3:C:102:LYS:H	2.16	0.62
3:C:15:ARG:HA	3:C:183:MET:CE	2.30	0.62
1:A:871:VAL:HG12	1:A:871:VAL:O	1.99	0.61
3:C:213:SER:HA	9:C:1896:HOH:O	2.00	0.61
1:A:622:GLU:CD	1:A:648:ASN:HB2	2.21	0.60
3:C:198:PRO:HA	9:C:1844:HOH:O	2.00	0.59
3:C:86:ILE:HB	3:C:87:PRO:HD3	1.84	0.59
3:C:190:ARG:O	3:C:194:LYS:HG3	2.02	0.59
1:A:332:GLN:HG3	9:A:2386:HOH:O	2.02	0.59
1:A:869:ASN:HB3	1:A:872:VAL:CG2	2.31	0.59
3:C:204:ILE:O	3:C:208:GLU:HB2	2.02	0.58
3:C:201:TYR:HB3	9:C:1844:HOH:O	2.03	0.58
2:B:137:GLY:HA3	3:C:136:ARG:HD2	1.84	0.58
1:A:122:GLN:HG2	9:A:2086:HOH:O	2.05	0.56
3:C:202:ARG:HA	3:C:205:GLU:OE1	2.06	0.56
3:C:15:ARG:HA	3:C:183:MET:HE2	1.88	0.55
3:C:199:ARG:O	3:C:203:GLU:HG2	2.06	0.55
1:A:830:GLU:HG3	1:A:832:MET:HE3	1.88	0.55
1:A:224:ASN:HD21	1:A:795:ARG:HH22	1.54	0.55
3:C:216:GLY:O	3:C:217:ILE:C	2.45	0.55
3:C:190:ARG:NH1	3:C:201:TYR:OH	2.36	0.54
1:A:307:ASN:HB3	1:A:832:MET:CE	2.37	0.54
1:A:84:HIS:HE1	1:A:634:GLN:OE1	1.90	0.54
3:C:194:LYS:O	3:C:198:PRO:HG3	2.08	0.53
3:C:101:HIS:HD2	3:C:102:LYS:N	2.04	0.53
1:A:876:GLU:HG3	9:A:1903:HOH:O	2.08	0.53
1:A:224:ASN:HD22	1:A:403:THR:N	1.97	0.52
1:A:415:HIS:HD2	9:A:1099:HOH:O	1.92	0.52
3:C:11:LYS:HG2	3:C:13:ILE:H	1.75	0.52
3:C:217:ILE:HD12	9:C:1896:HOH:O	2.09	0.52
2:B:238:HIS:HE1	9:B:932:HOH:O	1.93	0.52
1:A:332:GLN:CG	9:A:2386:HOH:O	2.57	0.51
1:A:84:HIS:CD2	1:A:86:VAL:H	2.28	0.51
1:A:411:GLY:O	1:A:415:HIS:HE1	1.92	0.51
3:C:190:ARG:HD3	3:C:201:TYR:OH	2.11	0.51
1:A:961:ASN:OD1	1:A:966:GLN:OE1	2.28	0.51
2:B:29:GLU:OE1	2:B:223:HIS:HE1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:MET:HG3	1:A:443:ASN:HA	1.92	0.51
3:C:101:HIS:CD2	3:C:102:LYS:N	2.79	0.50
1:A:73:GLU:HG3	9:A:1433:HOH:O	2.10	0.50
2:B:283:LYS:HD3	3:C:177:LYS:HB2	1.94	0.50
1:A:193:ALA:HA	1:A:451:ILE:HD11	1.94	0.50
1:A:125:SER:OG	1:A:128:GLU:HG3	2.12	0.50
1:A:92:CYS:CB	1:A:93:PRO:HD2	2.42	0.50
1:A:989:ASN:ND2	6:A:1018:MGD:H192	2.10	0.49
2:B:68:ASN:HA	2:B:69:PRO:C	2.32	0.49
1:A:630:GLY:O	1:A:631:ARG:HB2	2.13	0.49
2:B:10:LYS:HB2	2:B:120:GLN:HB3	1.95	0.49
1:A:344:GLU:H	1:A:344:GLU:CD	2.16	0.49
2:B:283:LYS:HD3	3:C:177:LYS:CB	2.43	0.48
3:C:44:THR:HB	3:C:50:PRO:HG3	1.95	0.48
3:C:170:MET:HG2	7:C:810:HEM:CAB	2.44	0.48
3:C:101:HIS:HD2	3:C:102:LYS:HG3	1.77	0.48
3:C:4:SER:OG	3:C:190:ARG:NH2	2.47	0.47
3:C:170:MET:HG2	7:C:810:HEM:HAB	1.95	0.47
1:A:542:ASN:O	1:A:546:GLU:HG3	2.14	0.47
3:C:108:LYS:HB3	9:C:1740:HOH:O	2.13	0.47
1:A:46:ILE:HD11	9:A:1544:HOH:O	2.14	0.47
1:A:832:MET:HE3	1:A:832:MET:HB2	1.55	0.47
1:A:163:MET:HG2	1:A:553:PHE:HB2	1.96	0.46
1:A:356:HIS:CD2	1:A:358:ARG:H	2.08	0.46
1:A:871:VAL:O	1:A:871:VAL:CG1	2.61	0.46
3:C:194:LYS:HA	9:C:1844:HOH:O	2.16	0.46
1:A:224:ASN:HD21	1:A:795:ARG:NH2	2.14	0.45
3:C:214:GLU:HA	3:C:214:GLU:OE1	2.16	0.45
3:C:167:LEU:HA	3:C:170:MET:HE2	1.99	0.45
1:A:198:GLY:N	1:A:199:PRO:CD	2.80	0.45
3:C:99:ASN:O	3:C:103:VAL:HG22	2.17	0.44
3:C:100:GLU:HB3	9:C:1107:HOH:O	2.16	0.44
3:C:11:LYS:HE2	3:C:13:ILE:HB	1.98	0.44
1:A:513:TYR:HB2	1:A:517:ALA:HB2	1.99	0.44
3:C:18:HIS:O	3:C:22:VAL:HG23	2.17	0.44
3:C:91:ASN:O	3:C:95:VAL:HG23	2.18	0.44
3:C:57:HIS:HB3	3:C:58:PRO:CD	2.48	0.44
1:A:623:ASP:HB3	9:A:1891:HOH:O	2.18	0.43
3:C:3:LYS:HD3	3:C:3:LYS:HA	1.83	0.43
1:A:634:GLN:HB3	9:A:1246:HOH:O	2.18	0.43
3:C:65:PHE:CZ	3:C:128:LEU:HD22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:LYS:HD3	9:B:1161:HOH:O	2.18	0.43
3:C:99:ASN:HB3	3:C:102:LYS:HD2	2.00	0.43
3:C:160:ILE:O	3:C:164:HIS:HD2	2.01	0.43
2:B:13:ALA:HB1	3:C:38:PRO:CB	2.48	0.43
1:A:359:CYS:CB	9:A:1672:HOH:O	2.43	0.43
2:B:217:GLU:HG2	9:B:1069:HOH:O	2.17	0.43
2:B:38:THR:HG22	2:B:38:THR:O	2.17	0.43
2:B:258:LYS:HB2	2:B:259:PRO:CD	2.48	0.43
1:A:830:GLU:CG	1:A:832:MET:HE2	2.46	0.43
3:C:110:ASN:O	3:C:114:LYS:HG3	2.19	0.43
1:A:242:ARG:HB2	2:B:180:PRO:O	2.18	0.42
2:B:235:GLU:HG3	9:B:1027:HOH:O	2.18	0.42
1:A:775:ARG:HD3	1:A:812:ASP:HA	2.01	0.42
1:A:672:VAL:O	1:A:676:MET:HG2	2.19	0.42
1:A:224:ASN:ND2	1:A:402:ARG:HA	2.34	0.42
3:C:111:ALA:O	3:C:115:MET:HG3	2.19	0.42
2:B:15:ASN:OD1	2:B:17:ILE:HG12	2.20	0.42
3:C:105:ASP:HB3	9:C:1932:HOH:O	2.19	0.41
3:C:79:ASN:HD22	3:C:114:LYS:HA	1.85	0.41
2:B:235:GLU:H	2:B:235:GLU:CD	2.24	0.41
3:C:11:LYS:HG2	3:C:13:ILE:HG22	2.03	0.41
1:A:804:LYS:HE3	1:A:806:THR:CG2	2.51	0.41
3:C:105:ASP:HB2	9:C:1672:HOH:O	2.20	0.41
1:A:623:ASP:CB	9:A:1891:HOH:O	2.69	0.40
2:B:110:LYS:O	2:B:254:LYS:HE2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2324:HOH:O	9:A:2324:HOH:O[6_456]	1.12	1.08
9:A:1746:HOH:O	9:A:1746:HOH:O[6_456]	1.25	0.95

## 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	979/1015 (96%)	951 (97%)	26 (3%)	2 (0%)	52	28
2	B	287/294 (98%)	278 (97%)	9 (3%)	0	100	100
3	C	214/217 (99%)	206 (96%)	6 (3%)	2 (1%)	21	5
All	All	1480/1526 (97%)	1435 (97%)	41 (3%)	4 (0%)	46	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	208	GLU
1	A	409	ALA
1	A	838	ILE
3	C	198	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	815/837 (97%)	807 (99%)	8 (1%)	82	67
2	B	238/243 (98%)	229 (96%)	9 (4%)	40	13
3	C	188/189 (100%)	182 (97%)	6 (3%)	46	18
All	All	1241/1269 (98%)	1218 (98%)	23 (2%)	65	39

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	CYS
1	A	101	TYR
1	A	332	GLN
1	A	344	GLU
1	A	557	PHE
1	A	843	GLU

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Mol	Chain	Res	Type
1	A	855	THR
1	A	937	ARG
2	B	51	GLU
2	B	67	ASP
2	B	68	ASN
2	B	113	PRO
2	B	162	LEU
2	B	178	THR
2	B	229	HIS
2	B	235	GLU
2	B	290	GLU
3	C	101	HIS
3	C	103	VAL
3	C	105	ASP
3	C	137	PRO
3	C	205	GLU
3	C	206	LYS

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

Mol	Chain	Res	Type
1	A	84	HIS
1	A	191	ASN
1	A	197	HIS
1	A	224	ASN
1	A	332	GLN
1	A	341	GLN
1	A	356	HIS
1	A	362	ASN
1	A	415	HIS
1	A	479	GLN
1	A	689	GLN
1	A	865	ASN
1	A	966	GLN
1	A	989	ASN
2	B	185	HIS
2	B	223	HIS
2	B	238	HIS
3	C	79	ASN
3	C	101	HIS
3	C	164	HIS
3	C	196	HIS



### 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 ⓘ

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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$
5	SF4	A	1017	1	0,12,12	0.00	-	0,24,24	0.00	-
6	MGD	A	1018	4	38,52,52	2.22	9 (23%)	43,81,81	3.04	21 (48%)
6	MGD	A	1019	4	38,52,52	2.65	11 (28%)	43,81,81	2.79	18 (41%)
5	SF4	B	805	2	0,12,12	0.00	-	0,24,24	0.00	-
5	SF4	B	806	2	0,12,12	0.00	-	0,24,24	0.00	-
5	SF4	B	807	2	0,12,12	0.00	-	0,24,24	0.00	-
5	SF4	B	808	2	0,12,12	0.00	-	0,24,24	0.00	-
7	HEM	C	809	3	30,50,50	2.40	10 (33%)	24,82,82	2.87	10 (41%)
7	HEM	C	810	3	30,50,50	2.35	10 (33%)	24,82,82	2.80	11 (45%)
8	CDL	C	812	-	69,69,99	2.88	21 (30%)	71,81,111	2.75	14 (19%)

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
5	SF4	A	1017	1	-	0/0/48/48	0/6/5/5
6	MGD	A	1018	4	-	0/18/66/66	0/6/6/6
6	MGD	A	1019	4	-	0/18/66/66	0/6/6/6
5	SF4	B	805	2	-	0/0/48/48	0/6/5/5
5	SF4	B	806	2	-	0/0/48/48	0/6/5/5
5	SF4	B	807	2	-	0/0/48/48	0/6/5/5
5	SF4	B	808	2	-	0/0/48/48	0/6/5/5
7	HEM	C	809	3	-	0/10/54/54	0/0/8/8
7	HEM	C	810	3	-	0/10/54/54	0/0/8/8
8	CDL	C	812	-	-	0/80/80/110	0/0/0/0

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	812	CDL	OB8-CB6	-14.78	1.12	1.45
6	A	1018	MGD	O3A-C10	-9.35	1.06	1.44
6	A	1019	MGD	O3A-C10	-9.16	1.07	1.44
7	C	810	HEM	C2D-C3D	-6.76	1.34	1.54
7	C	809	HEM	C2D-C3D	-6.08	1.36	1.54
7	C	809	HEM	C3B-C4B	-5.76	1.46	1.51
6	A	1019	MGD	C23-C14	-5.63	1.49	1.53
7	C	810	HEM	C3B-C4B	-5.14	1.47	1.51
6	A	1019	MGD	O11-C23	-4.76	1.36	1.43
7	C	809	HEM	C3D-C4D	-3.99	1.46	1.51
7	C	810	HEM	C3D-C4D	-3.52	1.47	1.51
7	C	809	HEM	C2C-C1C	-3.46	1.46	1.52
8	C	812	CDL	OB8-CB7	-3.39	1.23	1.33
6	A	1019	MGD	O11-C11	-3.18	1.39	1.43
7	C	810	HEM	C2C-C1C	-3.18	1.46	1.52
6	A	1019	MGD	O5'-C5'	-3.13	1.32	1.44
8	C	812	CDL	C39-C38	-2.60	1.36	1.51
8	C	812	CDL	C42-C41	-2.35	1.37	1.51
6	A	1018	MGD	O5'-C5'	-2.30	1.35	1.44
6	A	1018	MGD	PB-O1B	-2.30	1.42	1.51
8	C	812	CDL	CA3-CA4	-2.19	1.44	1.50
8	C	812	CDL	C19-C18	-2.17	1.35	1.51
8	C	812	CDL	OB2-CB2	-2.10	1.36	1.44
6	A	1019	MGD	PA-O2A	-2.04	1.46	1.54
6	A	1018	MGD	PA-O2A	-2.02	1.46	1.54
6	A	1019	MGD	C16-C21	2.06	1.45	1.41
7	C	810	HEM	FE-NC	2.10	2.04	1.95
6	A	1018	MGD	O2'-C2'	2.13	1.48	1.43
7	C	809	HEM	C3C-CAC	2.19	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	810	HEM	CMA-C3A	2.20	1.56	1.51
8	C	812	CDL	PA1-OA5	2.20	1.69	1.59
6	A	1018	MGD	C23-N22	2.27	1.49	1.44
6	A	1019	MGD	C2-N1	2.27	1.39	1.35
7	C	809	HEM	FE-NC	2.31	2.04	1.95
8	C	812	CDL	OB9-CB7	2.34	1.29	1.22
6	A	1018	MGD	C2-N1	2.36	1.39	1.35
7	C	809	HEM	C1C-NC	2.44	1.39	1.36
8	C	812	CDL	C52-C51	2.45	1.61	1.52
8	C	812	CDL	C79-C78	2.55	1.71	1.49
8	C	812	CDL	PB2-OB3	2.60	1.60	1.51
8	C	812	CDL	C12-C11	2.62	1.62	1.52
7	C	810	HEM	C3B-CAB	2.62	1.56	1.51
7	C	809	HEM	CAA-C2A	2.65	1.56	1.52
7	C	810	HEM	C1C-NC	2.90	1.39	1.36
8	C	812	CDL	CB3-CB4	2.97	1.59	1.50
7	C	810	HEM	C4C-NC	2.99	1.39	1.36
8	C	812	CDL	PB2-OB4	3.22	1.68	1.54
7	C	809	HEM	C4C-NC	3.34	1.40	1.36
7	C	810	HEM	C3C-CAC	3.42	1.57	1.51
6	A	1019	MGD	O4'-C1'	3.52	1.45	1.41
8	C	812	CDL	OA8-CA7	3.60	1.44	1.33
8	C	812	CDL	C11-CA5	3.68	1.61	1.50
7	C	809	HEM	C3B-CAB	3.69	1.58	1.51
8	C	812	CDL	PA1-OA3	4.26	1.66	1.51
6	A	1019	MGD	C6-N1	4.74	1.41	1.33
6	A	1018	MGD	C6-N1	4.79	1.42	1.33
6	A	1018	MGD	C17-N18	4.86	1.42	1.33
6	A	1019	MGD	C17-N18	5.09	1.42	1.33
8	C	812	CDL	C51-CB5	5.76	1.67	1.50
8	C	812	CDL	OB6-CB5	7.19	1.55	1.34
8	C	812	CDL	OA6-CA5	9.14	1.61	1.34

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	812	CDL	CB6-OB8-CB7	-9.65	89.86	116.85
8	C	812	CDL	CA6-CA4-CA3	-7.33	94.93	112.07
6	A	1019	MGD	C21-N22-C23	-6.38	111.17	123.67
6	A	1018	MGD	C4'-O4'-C1'	-6.05	103.07	109.72
8	C	812	CDL	C52-C51-CB5	-5.91	90.36	113.59
8	C	812	CDL	OB7-CB5-C51	-5.61	101.26	123.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1019	MGD	C5-C6-N1	-5.37	116.24	123.59
6	A	1018	MGD	C5-C6-N1	-5.00	116.75	123.59
7	C	810	HEM	CAA-C2A-C1A	-4.85	121.74	127.01
6	A	1019	MGD	N3-C2-N1	-4.67	120.33	127.44
6	A	1018	MGD	N3-C2-N1	-4.64	120.38	127.44
7	C	809	HEM	C3C-CAC-CBC	-4.64	117.34	124.46
8	C	812	CDL	OA6-CA5-OA7	-4.54	111.48	123.67
6	A	1019	MGD	O4'-C1'-N9	-4.44	98.80	108.10
6	A	1018	MGD	N18-C19-N20	-4.44	118.25	125.53
6	A	1018	MGD	C21-N22-C23	-4.03	115.78	123.67
6	A	1019	MGD	N18-C19-N20	-3.96	119.04	125.53
6	A	1018	MGD	C6-C5-C4	-3.77	116.39	120.90
6	A	1019	MGD	C6-C5-C4	-3.73	116.44	120.90
8	C	812	CDL	CB6-CB4-CB3	-3.65	103.53	112.07
7	C	810	HEM	CMA-C3A-C4A	-3.49	122.59	128.36
7	C	809	HEM	CMA-C3A-C4A	-3.29	122.91	128.36
8	C	812	CDL	CA6-OA8-CA7	-2.83	108.93	116.85
8	C	812	CDL	OA4-PA1-OA3	-2.80	97.33	112.53
8	C	812	CDL	O1-C1-CA2	-2.77	98.79	109.35
6	A	1019	MGD	C4'-O4'-C1'	-2.58	106.88	109.72
8	C	812	CDL	OA7-CA5-C11	-2.50	113.73	123.72
7	C	810	HEM	C3C-CAC-CBC	-2.42	120.74	124.46
8	C	812	CDL	OB6-CB5-OB7	-2.37	117.32	123.67
7	C	809	HEM	CAA-C2A-C1A	-2.36	124.44	127.01
6	A	1019	MGD	C1'-N9-C4	-2.28	123.50	126.94
6	A	1018	MGD	O4'-C1'-N9	-2.26	103.38	108.10
8	C	812	CDL	CA4-OA6-CA5	-2.11	112.83	117.89
6	A	1018	MGD	N2-C2-N1	-2.05	113.81	117.20
6	A	1018	MGD	C21-C16-N15	2.02	121.39	118.85
7	C	810	HEM	C3B-C4B-CHC	2.08	126.09	123.16
8	C	812	CDL	OA6-CA4-CA3	2.10	115.77	108.36
6	A	1018	MGD	C4-C5-N7	2.21	111.51	109.48
6	A	1018	MGD	C2'-C1'-N9	2.34	117.86	114.29
7	C	809	HEM	CMA-C3A-C2A	2.40	130.25	125.24
6	A	1019	MGD	C17-C16-C21	2.49	116.82	114.56
6	A	1019	MGD	O3B-PB-O5'	2.53	109.66	102.94
6	A	1019	MGD	PA-O3B-PB	2.56	139.93	132.73
6	A	1018	MGD	O5'-C5'-C4'	2.70	119.06	109.12
6	A	1019	MGD	O5'-C5'-C4'	2.72	119.16	109.12
7	C	810	HEM	CMA-C3A-C2A	2.89	131.28	125.24
6	A	1018	MGD	N19-C19-N20	2.93	122.05	117.20
7	C	810	HEM	CMD-C2D-C3D	2.97	127.47	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	810	HEM	CAD-C3D-C4D	3.25	123.92	112.47
7	C	809	HEM	CMD-C2D-C3D	3.30	128.96	114.35
6	A	1018	MGD	C17-C16-C21	3.41	117.65	114.56
7	C	809	HEM	CAA-CBA-CGA	3.46	119.09	112.75
6	A	1018	MGD	O4'-C4'-C5'	3.75	122.74	109.32
7	C	809	HEM	C2D-C3D-C4D	3.81	107.96	101.50
7	C	810	HEM	C2D-C3D-C4D	3.81	107.96	101.50
6	A	1019	MGD	N2-C2-N3	3.85	125.19	117.80
6	A	1019	MGD	C16-C21-N22	3.96	122.49	118.34
6	A	1018	MGD	C16-C21-N22	4.06	122.59	118.34
6	A	1018	MGD	N2-C2-N3	4.17	125.80	117.80
6	A	1019	MGD	O11-C23-C14	4.18	111.82	108.96
6	A	1019	MGD	C17-N18-C19	4.21	121.79	115.94
6	A	1018	MGD	C19-N20-C21	4.26	124.11	114.54
6	A	1019	MGD	C19-N20-C21	4.26	124.12	114.54
6	A	1018	MGD	C17-N18-C19	4.59	122.31	115.94
7	C	809	HEM	CMC-C2C-C3C	4.93	128.83	116.53
7	C	810	HEM	CAD-C3D-C2D	5.18	128.11	113.22
6	A	1018	MGD	C6-N1-C2	5.22	123.19	115.94
7	C	810	HEM	CMC-C2C-C3C	5.45	130.14	116.53
7	C	809	HEM	CMB-C2B-C3B	5.46	130.15	116.53
7	C	810	HEM	CMB-C2B-C3B	5.60	130.50	116.53
6	A	1019	MGD	C6-N1-C2	5.68	123.83	115.94
7	C	809	HEM	CAD-C3D-C2D	6.85	132.91	113.22
6	A	1018	MGD	O11-C23-C14	8.78	114.96	108.96
8	C	812	CDL	OB6-CB5-C51	13.73	141.36	111.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1018	MGD	1	0
7	C	810	HEM	2	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	981/1015 (96%)	-0.18	10 (1%) 84 84	11, 18, 30, 56	0
2	B	289/294 (98%)	0.49	33 (11%) 7 5	11, 18, 52, 67	0
3	C	216/217 (99%)	4.00	151 (69%) 0 0	30, 49, 63, 65	0
All	All	1486/1526 (97%)	0.56	194 (13%) 5 4	11, 19, 54, 67	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	217	ILE	18.5
3	C	207	ALA	14.6
2	B	285	VAL	13.5
3	C	209	ALA	12.3
3	C	216	GLY	12.2
2	B	287	ASP	12.0
3	C	2	SER	11.9
2	B	288	ASP	11.1
3	C	204	ILE	11.1
2	B	289	GLU	11.0
2	B	286	ASP	11.0
3	C	192	TRP	11.0
3	C	212	GLU	10.5
3	C	211	LYS	10.4
3	C	90	LEU	10.3
3	C	105	ASP	10.3
3	C	201	TYR	10.1
3	C	213	SER	10.1
3	C	210	LYS	10.1
3	C	86	ILE	10.0
2	B	290	GLU	10.0
3	C	80	ILE	9.9
3	C	89	LEU	9.7

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Mol	Chain	Res	Type	RSRZ
3	C	214	GLU	9.5
3	C	92	ILE	9.2
3	C	93	VAL	9.0
3	C	103	VAL	8.8
3	C	101	HIS	8.7
3	C	3	LYS	8.6
3	C	5	LYS	8.5
3	C	7	ILE	8.4
3	C	215	GLU	8.2
3	C	88	TRP	7.9
3	C	73	VAL	7.9
3	C	96	LEU	7.8
3	C	6	MET	7.8
3	C	206	LYS	7.8
3	C	4	SER	7.8
3	C	106	VAL	7.4
3	C	188	VAL	7.4
3	C	200	TRP	7.4
3	C	142	TYR	7.2
3	C	81	PRO	7.0
3	C	70	PHE	6.9
3	C	83	LYS	6.9
3	C	77	HIS	6.8
3	C	91	ASN	6.7
3	C	118	TRP	6.6
3	C	13	ILE	6.6
3	C	75	PHE	6.5
3	C	175	TRP	6.3
3	C	205	GLU	6.2
3	C	208	GLU	6.2
3	C	97	LYS	6.1
3	C	104	ALA	6.1
2	B	269	PHE	6.1
3	C	102	LYS	6.1
2	B	260	LEU	6.1
3	C	191	ARG	6.0
2	B	274	PHE	6.0
1	A	709	ASN	5.9
1	A	708	ALA	5.9
3	C	194	LYS	5.6
2	B	284	GLU	5.5
3	C	193	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
3	C	202	ARG	5.5
2	B	279	ILE	5.5
3	C	171	TYR	5.4
3	C	109	TYR	5.4
3	C	87	PRO	5.2
2	B	267	ALA	5.2
3	C	94	GLU	5.2
3	C	8	VAL	5.1
3	C	12	PHE	5.1
2	B	278	GLY	5.1
2	B	283	LYS	5.0
3	C	196	HIS	5.0
3	C	99	ASN	4.9
3	C	78	HIS	4.9
3	C	76	VAL	4.8
3	C	19	TRP	4.8
3	C	197	HIS	4.8
3	C	98	GLY	4.7
3	C	150	TYR	4.7
3	C	176	VAL	4.7
3	C	186	GLY	4.7
3	C	85	ASP	4.7
3	C	72	PHE	4.6
3	C	189	SER	4.6
3	C	174	PHE	4.6
3	C	74	ARG	4.6
3	C	203	GLU	4.5
3	C	190	ARG	4.5
3	C	198	PRO	4.5
2	B	252	LEU	4.5
1	A	711	VAL	4.4
3	C	100	GLU	4.4
3	C	82	ASP	4.4
3	C	180	ILE	4.4
3	C	95	VAL	4.3
2	B	271	GLY	4.2
2	B	281	PRO	4.1
3	C	26	PHE	4.0
3	C	69	MET	4.0
3	C	199	ARG	4.0
3	C	181	LYS	3.9
3	C	115	MET	3.9

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Mol	Chain	Res	Type	RSRZ
3	C	143	PHE	3.8
3	C	66	VAL	3.8
3	C	138	TYR	3.7
3	C	112	GLY	3.7
3	C	117	PHE	3.6
3	C	14	ASP	3.6
3	C	65	PHE	3.6
3	C	84	LYS	3.6
3	C	139	PHE	3.6
3	C	178	GLY	3.6
3	C	42	TRP	3.6
3	C	111	ALA	3.6
1	A	344	GLU	3.5
2	B	282	ASN	3.5
3	C	11	LYS	3.5
2	B	266	ILE	3.5
2	B	256	ALA	3.5
3	C	107	GLY	3.5
3	C	17	CYS	3.4
2	B	276	TYR	3.4
2	B	277	ILE	3.3
3	C	172	MET	3.3
1	A	329	GLU	3.2
3	C	10	THR	3.2
3	C	125	PHE	3.2
3	C	141	GLN	3.2
3	C	179	SER	3.1
2	B	265	PHE	3.1
3	C	16	ALA	3.1
3	C	184	ILE	3.1
3	C	173	ALA	3.1
3	C	170	MET	3.1
3	C	71	MET	3.0
3	C	185	GLU	3.0
3	C	68	LEU	3.0
3	C	187	LYS	3.0
3	C	23	ILE	2.9
1	A	710	GLY	2.9
2	B	273	ILE	2.9
2	B	280	GLY	2.9
3	C	64	ILE	2.9
3	C	122	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	272	LEU	2.9
3	C	135	TRP	2.8
3	C	146	GLN	2.8
3	C	22	VAL	2.8
3	C	195	LYS	2.8
3	C	108	LYS	2.8
3	C	144	PRO	2.8
3	C	157	ALA	2.7
3	C	62	ILE	2.7
3	C	67	ALA	2.7
1	A	713	ILE	2.7
3	C	114	LYS	2.7
2	B	270	ALA	2.7
3	C	183	MET	2.6
1	A	712	LEU	2.6
2	B	275	HIS	2.6
3	C	177	LYS	2.6
3	C	133	ILE	2.6
3	C	126	VAL	2.5
3	C	165	ALA	2.5
2	B	262	ALA	2.5
3	C	15	ARG	2.5
2	B	268	THR	2.5
3	C	167	LEU	2.5
1	A	345	ASN	2.4
3	C	162	LEU	2.4
1	A	707	ASP	2.4
3	C	9	ARG	2.4
2	B	248	THR	2.4
3	C	20	THR	2.4
3	C	124	ILE	2.3
3	C	160	ILE	2.3
3	C	59	PHE	2.3
2	B	263	ALA	2.3
3	C	129	VAL	2.3
3	C	79	ASN	2.2
3	C	123	MET	2.2
2	B	264	GLY	2.2
3	C	63	ALA	2.1
3	C	168	ILE	2.1
3	C	21	VAL	2.1
3	C	44	THR	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	116	MET	2.0
3	C	164	HIS	2.0
3	C	128	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	CDL	C	812	70/100	0.76	0.26	1.77	44,56,61,61	0
6	MGD	A	1019	47/47	0.96	0.12	0.45	11,14,16,18	0
7	HEM	C	809	43/43	0.92	0.15	0.42	29,33,35,37	0
7	HEM	C	810	43/43	0.87	0.25	0.25	44,45,48,49	0
6	MGD	A	1018	47/47	0.96	0.11	0.11	11,13,14,15	0
5	SF4	B	806	8/8	0.99	0.09	-0.72	12,13,13,13	0
5	SF4	B	807	8/8	0.98	0.08	-0.82	14,15,16,16	0
5	SF4	A	1017	8/8	0.99	0.10	-0.83	11,12,12,12	0
5	SF4	B	805	8/8	0.99	0.09	-1.07	12,13,13,14	0
5	SF4	B	808	8/8	0.98	0.07	-1.40	16,18,19,19	0
4	6MO	A	1016	1/1	0.99	0.09	-5.81	16,16,16,16	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.