



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:36 AM GMT

PDB ID : 2BC5
Title : Crystal structure of E. coli cytochrome b562 with engineered c-type heme linkages
Authors : Faraone-Mennella, J.; Tezcan, F.A.; Gray, H.B.; Winkler, J.R.
Deposited on : 2005-10-18
Resolution : 2.25 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>

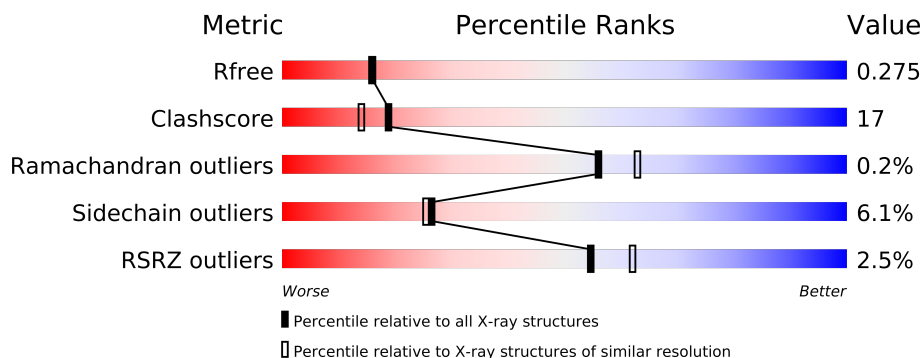
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.25 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	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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	A	106	
1	B	106	
1	C	106	
1	D	106	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	C	500	-	X
2	SO4	C	508	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3629 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 Soluble cytochrome b562.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	106	Total	C	N	O	S	10	0	0
			820	504	144	167	5			
1	B	106	Total	C	N	O	S	9	0	0
			820	504	144	167	5			
1	C	106	Total	C	N	O	S	8	0	0
			820	504	144	167	5			
1	D	106	Total	C	N	O	S	6	0	0
			820	504	144	167	5			

There are 12 discrepancies between the modelled and reference sequences:

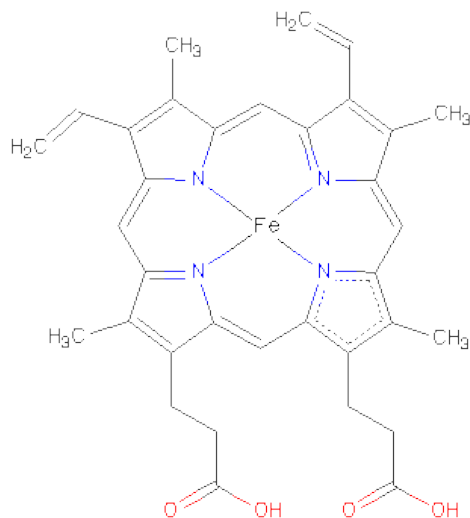
Chain	Residue	Modelled	Actual	Comment	Reference
A	59	TRP	LYS	ENGINEERED	UNP P0ABE7
A	98	CYS	ARG	ENGINEERED	UNP P0ABE7
A	101	CYS	TYR	ENGINEERED	UNP P0ABE7
B	59	TRP	LYS	ENGINEERED	UNP P0ABE7
B	98	CYS	ARG	ENGINEERED	UNP P0ABE7
B	101	CYS	TYR	ENGINEERED	UNP P0ABE7
C	59	TRP	LYS	ENGINEERED	UNP P0ABE7
C	98	CYS	ARG	ENGINEERED	UNP P0ABE7
C	101	CYS	TYR	ENGINEERED	UNP P0ABE7
D	59	TRP	LYS	ENGINEERED	UNP P0ABE7
D	98	CYS	ARG	ENGINEERED	UNP P0ABE7
D	101	CYS	TYR	ENGINEERED	UNP P0ABE7

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

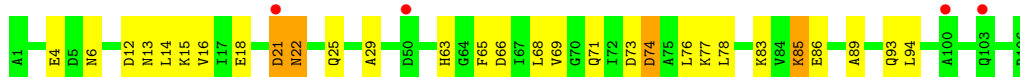
- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	B	31	Total	O	0	0
			31	31		
4	C	46	Total	O	0	0
			46	46		
4	D	26	Total	O	0	0
			26	26		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.86Å 68.16Å 90.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.40 – 2.25 24.36 – 2.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (24.40-2.25) 98.7 (24.36-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 2.26Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.277 0.233 , 0.275	Depositor DCC
R_{free} test set	1313 reflections (7.39%)	DCC
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 20.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 19081 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3629	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.34% 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: HEM, SO4

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	0.45	0/830	0.58	0/1117
1	B	0.36	0/830	0.58	0/1117
1	C	0.37	0/830	0.56	0/1117
1	D	0.37	0/830	0.56	0/1117
All	All	0.39	0/3320	0.57	0/4468

There are no bond length outliers.

There are no bond angle outliers.

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	A	820	0	809	31	0
1	B	820	0	809	30	0
1	C	820	0	809	31	0
1	D	820	0	809	35	0
2	A	5	0	0	2	0
2	B	15	0	0	2	0
2	C	20	0	0	1	0
2	D	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	43	0	30	0	0
3	B	43	0	30	2	0
3	C	43	0	30	0	0
3	D	43	0	30	2	0
4	A	29	0	0	2	0
4	B	31	0	0	2	0
4	C	46	0	0	2	0
4	D	26	0	0	2	0
All	All	3629	0	3356	113	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 17.

All (113) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:91:ALA:HA	1:C:94:LEU:HD12	1.48	0.94
1:D:22:ASN:C	1:D:22:ASN:HD22	1.79	0.83
1:C:22:ASN:N	1:C:25:GLN:HE21	1.78	0.81
1:D:22:ASN:ND2	1:D:25:GLN:H	1.79	0.80
1:D:22:ASN:H	1:D:25:GLN:HE21	1.30	0.78
1:C:21:ASP:H	1:C:25:GLN:NE2	1.82	0.77
1:D:22:ASN:HD21	1:D:25:GLN:H	1.31	0.77
1:D:83:LYS:HD3	1:D:86:GLU:OE1	1.85	0.77
1:A:27:LYS:HD3	1:A:80:ASN:ND2	1.99	0.77
1:D:22:ASN:HD21	1:D:25:GLN:HG3	1.51	0.76
1:D:22:ASN:ND2	1:D:25:GLN:HG3	2.01	0.74
1:A:39:ASP:HA	1:A:42:LYS:HE3	1.68	0.74
1:C:22:ASN:H	1:C:25:GLN:HE21	1.34	0.73
1:D:21:ASP:H	1:D:25:GLN:NE2	1.88	0.71
1:A:39:ASP:O	1:A:42:LYS:HG2	1.90	0.71
1:C:12:ASP:O	1:C:15:LYS:HG3	1.93	0.68
1:D:13:ASN:HD22	1:D:29:ALA:HA	1.59	0.68
1:A:12:ASP:O	1:A:15:LYS:HE3	1.94	0.67
1:D:22:ASN:N	1:D:25:GLN:HE21	1.92	0.67
1:D:74:ASP:CG	4:D:525:HOH:O	2.33	0.67
1:D:22:ASN:H	1:D:25:GLN:NE2	1.94	0.66
1:B:85:LYS:HB3	1:D:89:ALA:HB2	1.78	0.66
1:B:85:LYS:HZ3	1:D:85:LYS:HB2	1.62	0.65
1:B:92:GLU:OE1	1:D:78:LEU:HD21	1.97	0.64
1:C:15:LYS:O	1:C:19:LYS:HG3	1.98	0.63
1:C:22:ASN:H	1:C:25:GLN:NE2	1.96	0.62
1:D:85:LYS:HD2	2:D:502:SO4:O1	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:85:LYS:HB2	2:A:503:SO4:O3	1.99	0.62
1:B:4:GLU:OE2	3:B:150:HEM:O2A	2.16	0.62
1:C:22:ASN:N	1:C:25:GLN:NE2	2.46	0.62
1:C:22:ASN:OD1	1:C:25:GLN:HG3	1.99	0.61
1:D:22:ASN:C	1:D:22:ASN:ND2	2.52	0.61
1:B:13:ASN:HD22	1:B:29:ALA:HA	1.65	0.61
1:A:17:ILE:O	1:A:20:ALA:HB2	2.00	0.60
1:A:46:PRO:HA	1:A:49:GLU:HG3	1.83	0.60
1:D:4:GLU:OE2	3:D:150:HEM:O1A	2.21	0.59
1:A:71:GLN:HB3	1:A:94:LEU:HD23	1.85	0.58
1:B:71:GLN:HB3	1:B:94:LEU:HD23	1.86	0.58
1:C:21:ASP:N	1:C:25:GLN:NE2	2.52	0.58
1:D:65:PHE:O	1:D:69:VAL:HG23	2.03	0.58
1:C:84:VAL:O	1:C:88:GLN:HG3	2.04	0.57
1:A:80:ASN:OD1	1:B:54:ASP:O	2.22	0.56
1:A:66:ASP:OD2	1:B:73:ASP:OD2	2.23	0.56
1:B:85:LYS:NZ	1:D:85:LYS:HB2	2.21	0.56
1:A:12:ASP:O	1:A:15:LYS:HG3	2.06	0.56
1:D:22:ASN:N	1:D:25:GLN:NE2	2.52	0.56
1:B:12:ASP:O	1:B:16:VAL:HG23	2.06	0.56
1:C:86:GLU:HG3	4:C:518:HOH:O	2.05	0.56
1:A:93:GLN:HG2	1:C:86:GLU:OE2	2.06	0.55
1:A:77:LYS:HD3	1:B:60:ASP:HB2	1.89	0.54
1:A:13:ASN:HD22	1:A:29:ALA:HA	1.72	0.54
1:C:60:ASP:HB2	1:D:77:LYS:HD2	1.89	0.54
1:A:84:VAL:HG12	1:A:88:GLN:HE21	1.72	0.54
1:D:21:ASP:H	1:D:25:GLN:HE22	1.53	0.53
1:B:46:PRO:HD2	4:B:526:HOH:O	2.07	0.53
1:A:84:VAL:HG12	1:A:88:GLN:NE2	2.24	0.53
1:B:85:LYS:HB3	1:D:89:ALA:CB	2.39	0.52
1:B:13:ASN:HD21	1:B:32:LYS:HD2	1.75	0.51
3:D:150:HEM:HMC2	3:D:150:HEM:HBC2	1.92	0.51
1:A:23:ALA:CB	4:A:504:HOH:O	2.58	0.51
1:B:21:ASP:N	1:B:25:GLN:OE1	2.36	0.51
1:D:71:GLN:HB3	1:D:94:LEU:HD23	1.92	0.51
1:A:89:ALA:HB2	1:C:85:LYS:HB3	1.94	0.50
1:C:85:LYS:HD2	1:C:88:GLN:HE21	1.77	0.50
1:B:8:GLU:OE2	3:B:150:HEM:O1A	2.29	0.50
1:C:21:ASP:CB	1:C:25:GLN:HE22	2.25	0.49
1:D:13:ASN:ND2	1:D:29:ALA:HA	2.26	0.49
1:C:85:LYS:HD2	1:C:88:GLN:NE2	2.27	0.49
1:C:84:VAL:N	2:C:508:SO4:O4	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:90:ALA:HA	1:B:93:GLN:OE1	2.13	0.49
1:A:15:LYS:HA	1:A:18:GLU:OE1	2.13	0.49
1:C:21:ASP:HB2	1:C:25:GLN:HE22	1.78	0.48
1:D:14:LEU:O	1:D:18:GLU:HG3	2.14	0.48
1:D:22:ASN:HD21	1:D:25:GLN:N	2.08	0.48
1:A:19:LYS:O	1:A:20:ALA:C	2.51	0.48
1:A:71:GLN:HB3	1:A:94:LEU:CD2	2.45	0.47
1:C:66:ASP:OD2	1:D:73:ASP:OD2	2.32	0.47
1:A:27:LYS:HD3	1:A:80:ASN:HD22	1.78	0.47
1:B:45:PRO:HD3	1:B:61:PHE:CE2	2.50	0.47
1:C:91:ALA:CA	1:C:94:LEU:HD12	2.33	0.47
1:C:91:ALA:HA	1:C:94:LEU:CD1	2.34	0.46
1:D:12:ASP:O	1:D:16:VAL:HG23	2.15	0.46
1:B:85:LYS:NZ	1:D:85:LYS:CB	2.78	0.46
1:B:92:GLU:OE2	1:B:93:GLN:HG3	2.15	0.46
1:C:46:PRO:HD2	4:C:510:HOH:O	2.16	0.46
1:A:13:ASN:ND2	1:A:29:ALA:HA	2.31	0.45
1:A:23:ALA:HB1	4:A:504:HOH:O	2.16	0.45
1:A:15:LYS:HD2	1:A:16:VAL:N	2.31	0.45
1:B:106:ARG:OXT	1:B:106:ARG:HG2	2.16	0.45
1:B:85:LYS:HA	1:B:85:LYS:HD2	1.79	0.44
1:A:85:LYS:HD3	1:C:85:LYS:NZ	2.32	0.44
1:A:89:ALA:CB	1:C:85:LYS:HB3	2.47	0.44
1:B:22:ASN:OD1	1:B:25:GLN:HG3	2.17	0.44
1:D:68:LEU:HD12	1:D:94:LEU:HD22	2.00	0.44
1:C:65:PHE:O	1:C:69:VAL:HG23	2.18	0.44
1:C:22:ASN:CG	1:C:25:GLN:HG3	2.38	0.44
1:B:2:ASP:HB2	4:B:529:HOH:O	2.18	0.43
1:B:46:PRO:HA	1:B:49:GLU:HG3	1.99	0.43
1:B:57:GLU:HG3	2:B:504:SO4:O3	2.19	0.43
1:A:76:LEU:HD13	1:A:76:LEU:HA	1.88	0.43
1:D:6:ASN:HA	4:D:516:HOH:O	2.17	0.43
1:C:63:HIS:HA	1:C:66:ASP:OD2	2.19	0.42
1:B:22:ASN:N	1:B:25:GLN:OE1	2.52	0.42
1:D:15:LYS:HA	1:D:18:GLU:OE1	2.20	0.42
1:B:102:HIS:O	1:B:106:ARG:HB3	2.19	0.42
1:A:71:GLN:CB	1:A:94:LEU:HD23	2.48	0.41
1:D:63:HIS:HA	1:D:66:ASP:OD2	2.20	0.41
1:B:71:GLN:CB	1:B:94:LEU:HD23	2.49	0.41
1:B:57:GLU:HG3	2:B:504:SO4:S	2.61	0.41
1:C:102:HIS:HA	1:C:106:ARG:HB2	2.02	0.41
1:C:68:LEU:O	1:C:72:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:85:LYS:HB2	2:A:503:SO4:S	2.62	0.40
1:A:84:VAL:O	1:A:88:GLN:HG3	2.20	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	104/106 (98%)	102 (98%)	1 (1%)	1 (1%)	22	17
1	B	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
1	C	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
1	D	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
All	All	416/424 (98%)	408 (98%)	7 (2%)	1 (0%)	56	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ALA

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	86/86 (100%)	82 (95%)	4 (5%)	36	40
1	B	86/86 (100%)	82 (95%)	4 (5%)	36	40
1	C	86/86 (100%)	79 (92%)	7 (8%)	17	14
1	D	86/86 (100%)	80 (93%)	6 (7%)	21	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	344/344 (100%)	323 (94%)	21 (6%)	26	25

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	15	LYS
1	A	76	LEU
1	A	80	ASN
1	B	21	ASP
1	B	76	LEU
1	B	85	LYS
1	B	92	GLU
1	C	15	LYS
1	C	18	GLU
1	C	21	ASP
1	C	74	ASP
1	C	76	LEU
1	C	85	LYS
1	C	92	GLU
1	D	21	ASP
1	D	22	ASN
1	D	74	ASP
1	D	76	LEU
1	D	85	LYS
1	D	93	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	13	ASN
1	A	80	ASN
1	A	88	GLN
1	A	99	ASN
1	B	13	ASN
1	B	80	ASN
1	B	99	ASN
1	C	25	GLN
1	C	41	GLN
1	C	63	HIS

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Mol	Chain	Res	Type
1	C	71	GLN
1	C	88	GLN
1	C	99	ASN
1	D	13	ASN
1	D	22	ASN
1	D	25	GLN
1	D	71	GLN
1	D	80	ASN
1	D	93	GLN
1	D	99	ASN
1	D	103	GLN

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 ⓘ

13 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	$\# Z > 2$
3	HEM	A	150	1	49,50,50	2.86	14 (28%)	46,82,82	1.43	7 (15%)
2	SO4	A	503	-	4,4,4	2.10	3 (75%)	6,6,6	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	B	150	1	49,50,50	2.33	15 (30%)	46,82,82	1.36	4 (8%)
2	SO4	B	501	-	4,4,4	1.64	1 (25%)	6,6,6	0.90	0
2	SO4	B	504	-	4,4,4	1.54	0	6,6,6	0.91	0
2	SO4	B	505	-	4,4,4	1.55	0	6,6,6	0.88	0
3	HEM	C	150	1	49,50,50	2.27	16 (32%)	46,82,82	1.42	6 (13%)
2	SO4	C	500	-	4,4,4	1.66	1 (25%)	6,6,6	0.99	0
2	SO4	C	506	-	4,4,4	2.02	2 (50%)	6,6,6	0.96	0
2	SO4	C	507	-	4,4,4	1.80	2 (50%)	6,6,6	0.90	0
2	SO4	C	508	-	4,4,4	1.84	3 (75%)	6,6,6	0.93	0
3	HEM	D	150	1	49,50,50	2.05	12 (24%)	46,82,82	1.67	5 (10%)
2	SO4	D	502	-	4,4,4	1.85	2 (50%)	6,6,6	0.86	0

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
3	HEM	A	150	1	-	0/14/114/114	0/0/8/8
2	SO4	A	503	-	-	0/0/0/0	0/0/0/0
3	HEM	B	150	1	-	0/14/114/114	0/0/8/8
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	504	-	-	0/0/0/0	0/0/0/0
2	SO4	B	505	-	-	0/0/0/0	0/0/0/0
3	HEM	C	150	1	-	0/14/114/114	0/0/8/8
2	SO4	C	500	-	-	0/0/0/0	0/0/0/0
2	SO4	C	506	-	-	0/0/0/0	0/0/0/0
2	SO4	C	507	-	-	0/0/0/0	0/0/0/0
2	SO4	C	508	-	-	0/0/0/0	0/0/0/0
3	HEM	D	150	1	-	0/14/114/114	0/0/8/8
2	SO4	D	502	-	-	0/0/0/0	0/0/0/0

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	150	HEM	C2B-C1B	11.40	1.47	1.44
3	A	150	HEM	C3D-C4D	9.06	1.46	1.44
3	B	150	HEM	C3D-C4D	7.71	1.46	1.44
3	D	150	HEM	C3D-C4D	7.12	1.46	1.44
3	C	150	HEM	C2D-C1D	6.05	1.46	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	150	HEM	C3D-C2D	-5.66	1.33	1.43
3	C	150	HEM	C2B-C1B	5.51	1.45	1.44
3	C	150	HEM	C3D-C2D	-5.22	1.34	1.43
3	A	150	HEM	FE-NA	5.05	2.14	1.92
3	B	150	HEM	C3D-C2D	-4.76	1.35	1.43
3	B	150	HEM	C4A-C3A	4.70	1.46	1.40
3	B	150	HEM	C2D-C1D	4.66	1.45	1.44
3	B	150	HEM	C3C-C2C	-4.60	1.35	1.43
3	D	150	HEM	C3D-C2D	-4.59	1.35	1.43
3	C	150	HEM	FE-NA	4.57	2.12	1.92
3	D	150	HEM	C4A-C3A	4.56	1.45	1.40
3	A	150	HEM	C3B-C4B	4.36	1.49	1.44
3	B	150	HEM	C3B-C2B	-4.31	1.36	1.43
3	C	150	HEM	C3C-C2C	-4.30	1.36	1.43
3	A	150	HEM	C3C-C2C	-4.19	1.36	1.43
3	C	150	HEM	C3B-C4B	4.10	1.49	1.44
3	A	150	HEM	C4A-C3A	3.96	1.45	1.40
3	D	150	HEM	C3C-C2C	-3.85	1.37	1.43
3	D	150	HEM	C3B-C2B	-3.81	1.37	1.43
3	C	150	HEM	C3D-C4D	3.79	1.45	1.44
3	C	150	HEM	C4A-C3A	3.75	1.44	1.40
3	B	150	HEM	CHA-C4D	3.71	1.41	1.35
3	D	150	HEM	C2D-C1D	-3.47	1.43	1.44
3	B	150	HEM	FE-NA	3.27	2.06	1.92
3	B	150	HEM	C1A-C2A	3.21	1.49	1.43
3	D	150	HEM	C2B-C1B	3.13	1.45	1.44
3	C	150	HEM	CHA-C4D	3.08	1.40	1.35
3	A	150	HEM	CHA-C4D	2.98	1.40	1.35
3	C	150	HEM	C3B-C2B	-2.93	1.38	1.43
3	D	150	HEM	CBC-CAC	2.78	1.45	1.28
3	A	150	HEM	CBB-CAB	2.75	1.44	1.28
3	A	150	HEM	CHD-C4C	2.67	1.41	1.36
3	A	150	HEM	C3B-C2B	-2.65	1.39	1.43
2	C	506	SO4	O1-S	-2.65	1.38	1.47
2	A	503	SO4	O1-S	-2.62	1.38	1.47
2	A	503	SO4	O4-S	-2.60	1.38	1.47
2	D	502	SO4	O1-S	-2.46	1.39	1.47
2	C	506	SO4	O3-S	-2.46	1.38	1.47
3	A	150	HEM	C2D-C1D	2.42	1.45	1.44
3	C	150	HEM	CMD-C2D	2.41	1.54	1.47
3	B	150	HEM	CHB-C1B	2.41	1.39	1.35
3	A	150	HEM	CHB-C1B	2.39	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	150	HEM	CHD-C4C	2.37	1.40	1.36
3	D	150	HEM	C3B-C4B	2.27	1.47	1.44
3	B	150	HEM	FE-NC	2.26	2.06	1.97
3	D	150	HEM	FE-NC	2.25	2.06	1.97
2	C	507	SO4	O1-S	-2.24	1.39	1.47
3	B	150	HEM	CBC-CAC	2.23	1.41	1.28
3	D	150	HEM	CHD-C4C	2.23	1.40	1.36
2	C	508	SO4	O1-S	-2.20	1.39	1.47
3	A	150	HEM	CBC-CAC	2.19	1.41	1.28
2	C	500	SO4	O1-S	-2.17	1.40	1.47
3	B	150	HEM	CBB-CAB	2.15	1.41	1.28
3	B	150	HEM	CHC-C1C	2.15	1.40	1.36
3	C	150	HEM	FE-NC	2.15	2.05	1.97
2	C	507	SO4	O3-S	-2.14	1.40	1.47
3	C	150	HEM	CBB-CAB	2.12	1.41	1.28
3	B	150	HEM	C3B-C4B	2.12	1.47	1.44
2	D	502	SO4	O3-S	-2.11	1.40	1.47
2	C	508	SO4	O4-S	-2.11	1.40	1.47
3	C	150	HEM	CBC-CAC	2.10	1.41	1.28
3	C	150	HEM	CMB-C2B	2.08	1.53	1.47
2	C	508	SO4	O3-S	-2.08	1.40	1.47
2	B	501	SO4	O1-S	-2.04	1.40	1.47
3	D	150	HEM	CHB-C1B	2.02	1.38	1.35
2	A	503	SO4	O3-S	-2.02	1.40	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	150	HEM	CBA-CAA-C2A	6.70	124.50	112.69
3	B	150	HEM	C3B-C4B-NB	-5.42	110.12	114.00
3	D	150	HEM	C3B-C4B-NB	-5.38	110.15	114.00
3	C	150	HEM	C3B-C4B-NB	-4.84	110.53	114.00
3	C	150	HEM	CBD-CAD-C3D	-3.87	105.92	114.37
3	A	150	HEM	CBD-CAD-C3D	-3.85	105.97	114.37
3	A	150	HEM	CBA-CAA-C2A	3.68	119.17	112.69
3	A	150	HEM	C3B-C4B-NB	-3.51	111.48	114.00
3	D	150	HEM	CBD-CAD-C3D	-3.37	107.02	114.37
3	B	150	HEM	C3A-C4A-NA	3.34	111.93	109.41
3	C	150	HEM	CHD-C4C-NC	-3.17	121.97	124.73
3	A	150	HEM	CAD-C3D-C4D	3.09	130.09	124.53
3	C	150	HEM	C3A-C4A-NA	3.05	111.72	109.41
3	D	150	HEM	CHD-C4C-NC	-2.96	122.16	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	150	HEM	CHD-C4C-NC	-2.93	122.19	124.73
3	B	150	HEM	CBA-CAA-C2A	2.75	117.54	112.69
3	C	150	HEM	CBA-CAA-C2A	2.47	117.04	112.69
3	A	150	HEM	CHD-C4C-NC	-2.36	122.68	124.73
3	A	150	HEM	C3A-C4A-NA	2.17	111.05	109.41
3	C	150	HEM	C4A-C3A-C2A	-2.06	105.56	107.00
3	A	150	HEM	CAD-C3D-C2D	-2.03	122.72	127.25
3	D	150	HEM	C4A-CHB-C1B	-2.02	124.81	127.47

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	A	106/106 (100%)	0.06	3 (2%) 50 57	14, 28, 46, 56	4 (3%)
1	B	106/106 (100%)	-0.08	1 (0%) 81 86	16, 27, 40, 48	3 (2%)
1	C	106/106 (100%)	-0.03	2 (1%) 64 70	16, 27, 39, 53	3 (2%)
1	D	106/106 (100%)	0.13	4 (3%) 38 44	18, 33, 46, 53	2 (1%)
All	All	424/424 (100%)	0.02	10 (2%) 54 63	14, 29, 45, 56	12 (2%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	21	ASP	3.4
1	A	21	ASP	3.1
1	A	56	PRO	3.0
1	B	21	ASP	2.8
1	A	22	ASN	2.5
1	D	103	GLN	2.3
1	D	21	ASP	2.3
1	D	100	ALA	2.2
1	D	50	ASP	2.1
1	C	82	GLY	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
2	SO4	C	508	5/5	0.41	4.34	78,79,81,81	0
2	SO4	C	500	5/5	0.19	3.47	76,77,79,80	0
2	SO4	A	503	5/5	0.22	1.92	84,84,86,87	0
2	SO4	C	507	5/5	0.25	1.83	71,72,74,75	0
2	SO4	B	505	5/5	0.19	0.62	58,59,60,61	0
2	SO4	D	502	5/5	0.17	0.17	75,76,76,78	0
2	SO4	B	501	5/5	0.16	0.14	80,81,81,81	0
3	HEM	B	150	43/43	0.13	0.03	9,20,47,61	0
3	HEM	A	150	43/43	0.12	-0.13	16,23,50,55	0
3	HEM	D	150	43/43	0.13	-0.17	18,29,53,65	0
3	HEM	C	150	43/43	0.11	-0.29	11,18,48,62	0
2	SO4	B	504	5/5	0.13	-0.83	66,67,69,69	0
2	SO4	C	506	5/5	0.11	-1.58	89,90,91,91	0

6.5 Other polymers ⓘ

There are no such residues in this entry.