W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:25 pm GMT

PDB ID	:	2QD3
Title	:	Wild type human ferrochelatase crystallized with ammonium sulfate
Authors	:	Medlock, A.E.; Dailey, T.A.; Ross, T.A.; Dailey, H.A.; Lanzilotta, W.N.
Deposited on	:	2007-06-20
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.
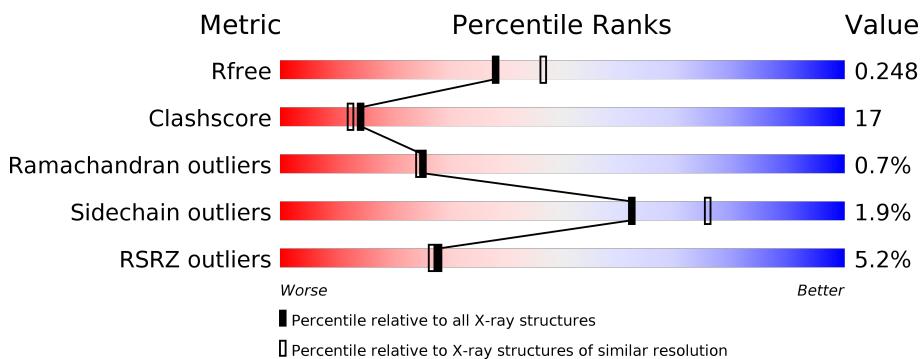
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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. 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 <=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	359	5% / 69% / 29% / •
1	B	359	5% / 66% / 33% / •
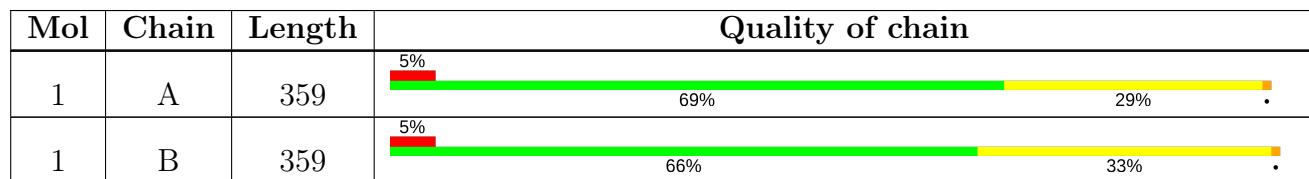
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HEM	B	925	-	-	-	X
4	CHD	A	501	-	-	-	X
4	CHD	A	502	-	-	-	X
5	GOL	B	506	-	-	X	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 6524 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 Ferrochelatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	7	0
			2949	1873	517	539	20			
1	B	359	Total	C	N	O	S	0	7	0
			2946	1872	514	540	20			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).
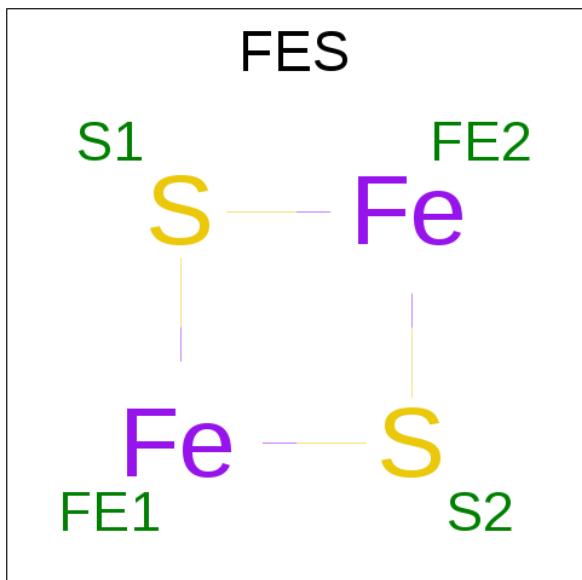
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
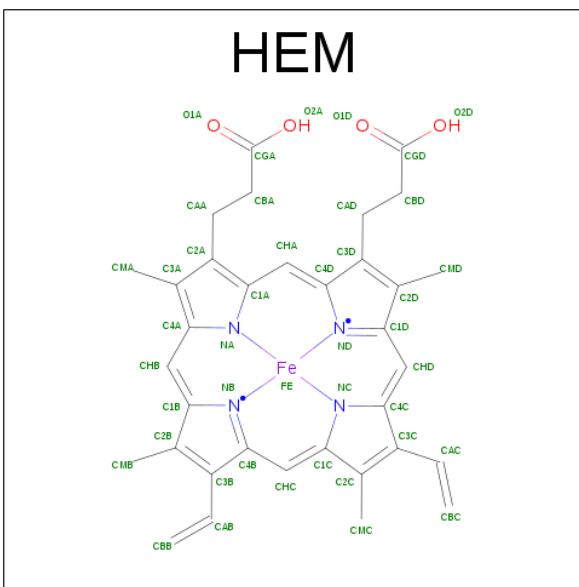
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0

- Molecule 4 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).
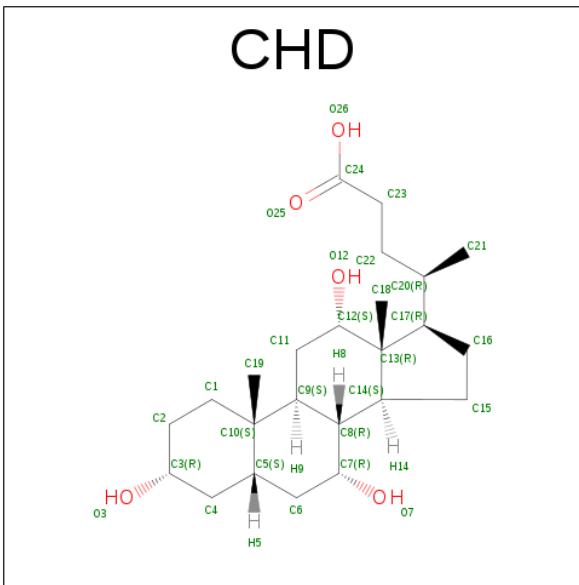
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	29	24	5	0	0
4	A	1	29	24	5	0	0
4	A	1	29	24	5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 29	C 24	O 5	0	0
4	B	1	Total 29	C 24	O 5	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
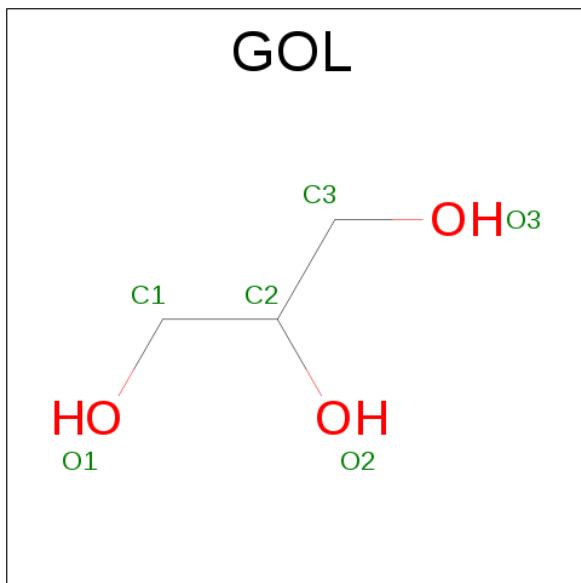
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 6	C 3	O 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	224	Total 224	O 224	0	0
6	B	203	Total 203	O 203	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Ferrochelatase
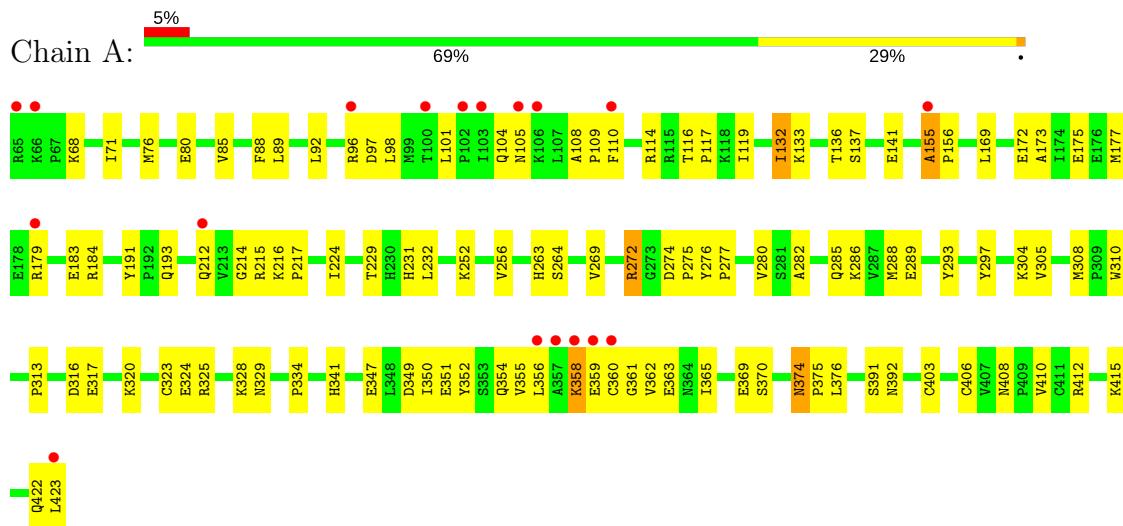
- Molecule 1: Ferrochelatase
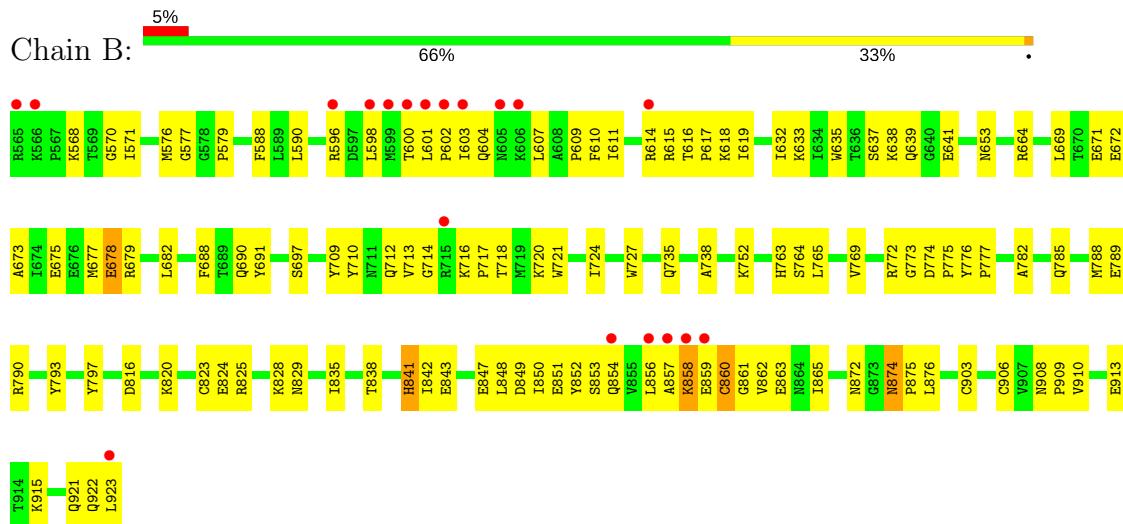
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.07Å 93.09Å 111.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.80 – 2.20 47.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.80-2.20) 100.0 (47.80-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.242 0.214 , 0.248	Depositor DCC
R_{free} test set	2367 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6524	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.38 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.2515e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CHD, FES, 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	0.33	0/3019	0.59	1/4086 (0.0%)
1	B	0.33	0/3016	0.58	1/4084 (0.0%)
All	All	0.33	0/6035	0.59	2/8170 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	724	ILE	N-CA-C	-5.35	96.56	111.00
1	A	224	ILE	N-CA-C	-5.10	97.23	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2949	0	2952	109	0
1	B	2946	0	2945	105	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	B	43	0	30	9	0
4	A	87	0	117	6	0
4	B	58	0	78	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	6	0	8	4	0
6	A	224	0	0	11	0
6	B	203	0	0	8	0
All	All	6524	0	6130	213	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (213) 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:B:716:LYS:HD2	1:B:717:PRO:HD2	1.51	0.92
1:A:155:ALA:HB1	1:A:156:PRO:CD	2.01	0.89
1:B:823[A]:CYS:SG	1:B:862:VAL:HG12	2.12	0.89
1:B:615:ARG:HD2	4:B:504:CHD:H232	1.55	0.89
1:A:305:VAL:HG21	4:A:501:CHD:H161	1.55	0.88
1:A:155:ALA:HB1	1:A:156:PRO:HD3	1.56	0.85
1:B:765:LEU:HD22	3:B:925:HEM:CBB	2.13	0.78
1:A:323[A]:CYS:SG	1:A:362:VAL:HG12	2.24	0.77
1:B:785:GLN:O	1:B:789:GLU:HG3	1.83	0.77
1:B:637:SER:O	1:B:641:GLU:HG3	1.86	0.75
1:A:285:GLN:O	1:A:289:GLU:HG3	1.86	0.74
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.70	0.73
1:A:422:GLN:HG2	1:A:423:LEU:HD22	1.69	0.72
1:A:215:ARG:HD3	6:A:823:HOH:O	1.88	0.72
1:B:922:GLN:HG2	1:B:923:LEU:HD22	1.70	0.72
1:A:269:VAL:O	1:A:272[B]:ARG:HG2	1.90	0.71
1:B:858:LYS:HA	1:B:858:LYS:HE3	1.72	0.71
1:A:374:ASN:HD22	1:A:374:ASN:C	1.94	0.71
1:B:816:ASP:HB3	1:B:852:TYR:CE1	2.26	0.71
1:B:679[B]:ARG:HG2	1:B:679[B]:ARG:HH11	1.57	0.70
1:A:422:GLN:HG2	1:A:423:LEU:CD2	2.21	0.70
1:A:374:ASN:HD22	1:A:375:PRO:N	1.90	0.70
1:A:101:LEU:HB2	1:A:104:GLN:HG3	1.73	0.69
1:A:320:LYS:O	1:A:324:GLU:HG3	1.93	0.69
1:B:908:ASN:OD1	1:B:910:VAL:HG12	1.94	0.67
1:B:610:PHE:CZ	1:B:614:ARG:HD2	2.30	0.67
1:A:374:ASN:ND2	1:A:376:LEU:H	1.93	0.66
1:A:252:LYS:HD3	1:A:329:ASN:HD21	1.59	0.66
1:B:716:LYS:HD2	1:B:717:PRO:CD	2.23	0.66
1:A:408:ASN:OD1	1:A:410:VAL:HG12	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412[A]:ARG:NH2	1:B:825:ARG:HB3	2.11	0.66
1:A:229:THR:HB	1:A:286:LYS:HD3	1.79	0.65
1:B:675:GLU:O	1:B:679[B]:ARG:HG3	1.96	0.64
1:B:820:LYS:O	1:B:824:GLU:HG3	1.98	0.64
1:A:277:PRO:HB3	5:B:506:GOL:H2	1.79	0.63
1:B:577:GLY:HA2	1:B:632:ILE:HD13	1.79	0.63
1:B:765:LEU:HD22	3:B:925:HEM:HBB2	1.81	0.63
1:A:68:LYS:CB	1:A:155:ALA:HB3	2.28	0.63
1:B:671:GLU:O	1:B:675:GLU:HG3	2.00	0.62
1:A:347:GLU:HA	1:A:351:GLU:HG2	1.83	0.61
1:A:68:LYS:HB3	1:A:155:ALA:HB3	1.82	0.60
1:B:849:ASP:O	1:B:854:GLN:HG3	2.00	0.60
1:A:320:LYS:HD2	1:A:359:GLU:OE2	2.01	0.60
1:A:76:MET:HG2	1:A:191:TYR:OH	2.01	0.60
1:B:843:GLU:OE2	3:B:925:HEM:HBC2	2.02	0.60
1:A:184:ARG:NH2	6:A:668:HOH:O	2.35	0.59
1:A:155:ALA:CB	1:A:156:PRO:CD	2.78	0.59
1:B:922:GLN:HG2	1:B:923:LEU:CD2	2.33	0.59
1:A:85:VAL:HG13	6:A:722:HOH:O	2.03	0.58
1:A:412[A]:ARG:HD2	1:A:415:LYS:HE3	1.84	0.58
1:A:229:THR:HB	1:A:286:LYS:CD	2.34	0.58
1:A:110:PHE:CZ	1:A:114:ARG:HD2	2.39	0.57
1:A:350:ILE:O	1:A:354:GLN:HB2	2.04	0.57
1:B:616:THR:HB	1:B:617:PRO:HD3	1.86	0.57
1:B:769:VAL:O	1:B:772:ARG:HG2	2.05	0.57
1:A:285:GLN:HG2	1:B:782:ALA:HB1	1.87	0.56
1:A:349:ASP:O	1:A:354:GLN:HG3	2.06	0.56
1:B:607:LEU:O	1:B:611:ILE:HG13	2.04	0.56
1:B:874:ASN:HD22	1:B:875:PRO:N	2.04	0.56
1:A:132:ILE:HD13	1:A:136:THR:HG1	1.71	0.56
1:B:874:ASN:HD22	1:B:874:ASN:C	2.07	0.56
1:A:359:GLU:HG3	1:A:360[B]:CYS:N	2.21	0.55
1:A:173:ALA:O	1:A:177:MET:HG3	2.06	0.55
1:A:423:LEU:HD23	6:A:825:HOH:O	2.07	0.55
3:B:925:HEM:HHC	3:B:925:HEM:HBB2	1.88	0.54
1:A:71:ILE:HD12	1:A:71:ILE:N	2.22	0.54
1:B:598[B]:LEU:HD21	1:B:697[B]:SER:HA	1.89	0.54
1:B:776:TYR:HB3	1:B:777:PRO:HD3	1.89	0.54
1:B:752:LYS:HE3	1:B:863:GLU:OE1	2.08	0.54
1:A:355:VAL:O	1:A:358:LYS:HB2	2.08	0.54
1:B:576:MET:HG2	1:B:691:TYR:OH	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ILE:HD13	1:A:136:THR:OG1	2.08	0.53
1:B:874:ASN:ND2	1:B:876:LEU:H	2.06	0.53
1:B:675:GLU:O	1:B:679[A]:ARG:HG3	2.08	0.53
1:B:615:ARG:NH2	1:B:618:LYS:HZ3	2.06	0.53
1:A:98:LEU:HB2	6:A:733:HOH:O	2.09	0.52
1:B:602:PRO:HG2	1:B:607:LEU:HD11	1.90	0.52
1:B:675:GLU:HG2	1:B:709:TYR:OH	2.09	0.52
1:B:847:GLU:O	1:B:851:GLU:HB2	2.09	0.52
1:A:359:GLU:HG3	1:A:360[A]:CYS:N	2.23	0.52
1:A:305:VAL:HG23	4:A:502:CHD:H7	1.92	0.52
1:A:132:ILE:O	1:A:132:ILE:HD13	2.10	0.52
1:A:276:TYR:HB3	1:A:277:PRO:HD3	1.91	0.52
1:A:263:HIS:HD2	1:A:264:SER:O	1.92	0.52
1:A:328:LYS:CB	1:A:363:GLU:HG3	2.41	0.51
1:B:615:ARG:NH2	1:B:618:LYS:NZ	2.59	0.51
1:A:137:SER:O	1:A:141:GLU:HG3	2.11	0.51
1:A:252:LYS:HD3	1:A:329:ASN:ND2	2.24	0.51
1:B:848:LEU:HD23	1:B:852:TYR:CD2	2.46	0.51
1:B:909:PRO:O	1:B:913[B]:GLU:HG3	2.11	0.51
1:A:175:GLU:O	1:A:179:ARG:HG3	2.11	0.50
1:B:679[B]:ARG:HG2	1:B:679[B]:ARG:NH1	2.24	0.50
3:B:925:HEM:HBD2	3:B:925:HEM:HHA	1.94	0.50
1:A:288:MET:HG3	1:A:297:TYR:CE2	2.46	0.50
1:A:374:ASN:ND2	1:A:374:ASN:C	2.63	0.50
1:B:777:PRO:CB	5:B:506:GOL:H31	2.42	0.50
1:B:908:ASN:CG	1:B:910:VAL:HG12	2.32	0.49
1:A:68:LYS:HE3	1:A:183:GLU:OE1	2.12	0.49
1:A:328:LYS:HB2	1:A:363:GLU:HG3	1.94	0.49
1:A:252:LYS:HE2	1:A:363:GLU:OE1	2.12	0.49
1:B:824:GLU:HG2	1:B:860[B]:CYS:SG	2.52	0.49
1:B:789:GLU:HG2	1:B:793:TYR:OH	2.13	0.49
1:B:841:HIS:CE1	1:B:843:GLU:HB2	2.46	0.49
1:B:774:ASP:HA	1:B:775:PRO:HD3	1.67	0.48
1:A:412[A]:ARG:HG2	1:A:412[A]:ARG:HH11	1.78	0.48
1:A:354:GLN:O	1:A:358:LYS:HG2	2.13	0.48
1:B:828:LYS:CB	1:B:863:GLU:HG3	2.44	0.48
1:A:277:PRO:CB	5:B:506:GOL:H2	2.43	0.48
1:A:116:THR:HB	1:A:117:PRO:HD3	1.94	0.48
1:B:600:THR:O	1:B:601:LEU:HD23	2.14	0.47
1:A:96:ARG:NH2	1:A:105:ASN:OD1	2.45	0.47
1:A:316:ASP:HB3	1:A:352:TYR:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:848:LEU:HD23	1:B:852:TYR:HD2	1.79	0.47
1:B:571:ILE:HD12	1:B:571:ILE:N	2.30	0.47
1:A:412[A]:ARG:HG2	6:A:660:HOH:O	2.13	0.47
1:A:212:GLN:C	1:A:214:GLY:H	2.16	0.47
1:B:598[B]:LEU:CD2	1:B:697[B]:SER:HA	2.45	0.47
1:A:352:TYR:O	1:A:356:LEU:HB3	2.15	0.47
1:A:217:PRO:HB2	6:A:790:HOH:O	2.15	0.46
1:B:763:HIS:HD2	1:B:764:SER:O	1.98	0.46
1:A:85:VAL:O	1:A:88:PHE:HB3	2.16	0.46
1:A:80[A]:GLU:H	1:A:80[A]:GLU:CD	2.19	0.46
1:B:639:GLN:HG2	6:B:980:HOH:O	2.15	0.46
1:A:422:GLN:HG2	1:A:423:LEU:HD23	1.98	0.46
1:A:80[A]:GLU:N	1:A:80[A]:GLU:CD	2.69	0.46
1:A:369:GLU:HG2	1:A:370:SER:O	2.16	0.46
1:A:231:HIS:CE1	1:A:232:LEU:HG	2.51	0.45
1:A:89:LEU:HD11	1:A:119:ILE:HD12	1.98	0.45
1:A:68:LYS:CD	1:A:155:ALA:HB3	2.46	0.45
1:A:316:ASP:HB2	1:A:356:LEU:HD22	1.97	0.45
1:B:602:PRO:O	1:B:603:ILE:C	2.53	0.45
1:B:614:ARG:HD3	6:B:1101:HOH:O	2.16	0.45
1:B:710:TYR:HA	1:B:713:VAL:HG12	1.98	0.45
1:B:735:GLN:HG3	1:B:790:ARG:NH2	2.30	0.45
1:A:68:LYS:HD3	1:A:155:ALA:HB3	1.99	0.45
1:A:412[A]:ARG:HH22	1:B:825:ARG:HD3	1.82	0.45
1:A:88:PHE:HD2	6:A:722:HOH:O	2.00	0.45
1:A:274:ASP:HA	1:A:275:PRO:HD3	1.72	0.44
1:A:289:GLU:HG2	1:A:293:TYR:OH	2.16	0.44
1:A:324:GLU:HG2	1:A:360[A]:CYS:SG	2.56	0.44
1:B:842:ILE:HG21	3:B:925:HEM:HBD1	1.99	0.44
1:B:735:GLN:HG3	1:B:790:ARG:CZ	2.46	0.44
1:B:825:ARG:HH11	1:B:825:ARG:HG3	1.83	0.44
1:A:216:LYS:HE3	1:A:217:PRO:HD2	1.99	0.44
1:B:638:LYS:NZ	6:B:1097:HOH:O	2.49	0.44
1:A:272[B]:ARG:O	1:A:403:CYS:HB3	2.17	0.44
1:B:673:ALA:O	1:B:677:MET:HG3	2.17	0.44
1:A:92:LEU:HD13	4:A:501:CHD:H183	1.99	0.44
1:B:738:ALA:CB	1:B:790:ARG:HD3	2.48	0.44
1:A:316:ASP:OD2	1:A:317:GLU:N	2.50	0.44
1:B:601:LEU:O	1:B:604:GLN:HB2	2.18	0.44
1:B:669:LEU:HB2	1:B:672:GLU:HG3	1.98	0.44
1:B:579:PRO:HD3	1:B:588:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:ILE:HD11	3:B:925:HEM:O1A	2.18	0.43
1:A:119:ILE:HG21	6:A:722:HOH:O	2.17	0.43
1:B:828:LYS:HB2	1:B:863:GLU:HG3	1.99	0.43
1:B:777:PRO:HB2	5:B:506:GOL:H31	2.01	0.43
1:B:678:GLU:HG3	1:B:718:THR:OG1	2.17	0.43
1:B:838:THR:HG21	6:B:1015:HOH:O	2.18	0.43
1:A:119:ILE:HD11	4:A:501:CHD:H211	2.01	0.43
1:B:568:LYS:NZ	1:B:653:ASN:O	2.39	0.43
1:A:193:GLN:HG2	1:A:280:VAL:HA	2.00	0.43
1:B:853:SER:O	1:B:857:ALA:HB3	2.19	0.43
1:A:132:ILE:HG23	1:A:133:LYS:N	2.34	0.43
1:B:841:HIS:HE1	6:B:1023:HOH:O	2.02	0.43
1:A:282:ALA:HB1	1:B:785:GLN:HG2	2.01	0.42
1:B:857:ALA:C	1:B:859:GLU:H	2.22	0.42
1:B:598[A]:LEU:C	1:B:598[A]:LEU:HD23	2.39	0.42
1:B:915:LYS:HE2	1:B:915:LYS:HB3	1.85	0.42
1:B:721:TRP:H	1:B:921:GLN:NE2	2.17	0.42
1:B:570:GLY:HA3	1:B:682:LEU:HD13	2.01	0.42
3:B:925:HEM:HBC1	6:B:1000:HOH:O	2.18	0.42
1:A:184:ARG:HG3	6:A:610:HOH:O	2.17	0.42
1:B:632:ILE:HG23	1:B:633:LYS:N	2.34	0.42
1:A:169:LEU:HB2	1:A:172:GLU:HG3	2.02	0.42
1:A:212:GLN:C	1:A:214:GLY:N	2.73	0.42
1:B:598[A]:LEU:HD23	1:B:598[A]:LEU:O	2.20	0.42
1:B:590:LEU:HD13	1:B:609:PRO:HA	2.01	0.42
1:B:635:TRP:CE3	1:B:872:ASN:HB3	2.55	0.42
1:A:391:SER:O	1:A:392:ASN:HB2	2.20	0.42
1:A:408:ASN:CG	1:A:410:VAL:HG12	2.39	0.42
1:B:690:GLN:HG3	6:B:1019:HOH:O	2.19	0.42
1:A:374:ASN:HD22	1:A:375:PRO:CD	2.33	0.41
1:A:313:PRO:CG	1:B:773:GLY:HA2	2.50	0.41
1:B:752:LYS:HD3	1:B:829:ASN:HD21	1.85	0.41
1:A:304[A]:LYS:NZ	1:A:308:MET:O	2.52	0.41
1:A:119:ILE:CD1	4:A:501:CHD:H211	2.50	0.41
1:A:334:PRO:HD2	6:A:700:HOH:O	2.20	0.41
1:B:712:GLN:C	1:B:714:GLY:H	2.23	0.41
1:B:788:MET:HG3	1:B:797:TYR:CE2	2.55	0.41
1:A:304[A]:LYS:HD2	1:A:310:TRP:HB2	2.03	0.41
1:A:325:ARG:HG3	1:A:325:ARG:HH11	1.86	0.41
3:B:925:HEM:CMB	4:B:504:CHD:H193	2.51	0.41
1:B:847:GLU:HG2	1:B:851:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ILE:O	1:A:365:ILE:HG23	2.21	0.41
1:B:852:TYR:O	1:B:856:LEU:HB3	2.21	0.41
1:B:865:ILE:O	1:B:865:ILE:HG23	2.21	0.41
1:B:903:CYS:HB2	1:B:906:CYS:HB2	2.03	0.41
1:B:601:LEU:HD22	4:B:505:CHD:H152	2.02	0.41
1:A:76:MET:HG3	4:A:501:CHD:H11	2.02	0.41
1:B:610:PHE:CE2	1:B:614:ARG:HD2	2.56	0.41
1:A:252:LYS:O	1:A:256:VAL:HG23	2.21	0.40
1:A:403:CYS:HB2	1:A:406:CYS:HB2	2.02	0.40
1:A:132:ILE:CG2	1:A:133:LYS:N	2.84	0.40
1:A:216:LYS:HE2	1:A:217:PRO:O	2.21	0.40
1:B:860[B]:CYS:O	1:B:860[B]:CYS:SG	2.79	0.40
1:A:97:ASP:CG	1:A:408:ASN:HD21	2.25	0.40
1:B:610:PHE:O	1:B:614:ARG:HG3	2.22	0.40
1:B:664:ARG:NH2	6:B:1091:HOH:O	2.50	0.40
1:B:835:ILE:HG13	1:B:835:ILE:O	2.22	0.40
1:B:850:ILE:O	1:B:854:GLN:HB2	2.21	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	364/359 (101%)	344 (94%)	18 (5%)	2 (0%)	32	34
1	B	364/359 (101%)	339 (93%)	21 (6%)	4 (1%)	17	13
All	All	728/718 (101%)	683 (94%)	39 (5%)	6 (1%)	25	21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ALA

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Mol	Chain	Res	Type
1	A	361	GLY
1	B	861	GLY
1	B	596	ARG
1	B	860[A]	CYS
1	B	860[B]	CYS

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	331/324 (102%)	325 (98%)	6 (2%)	64	77
1	B	331/324 (102%)	324 (98%)	7 (2%)	59	72
All	All	662/648 (102%)	649 (98%)	13 (2%)	62	74

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	ILE
1	A	272[A]	ARG
1	A	272[B]	ARG
1	A	341	HIS
1	A	358	LYS
1	A	374	ASN
1	B	678	GLU
1	B	688	PHE
1	B	720	LYS
1	B	727	TRP
1	B	841	HIS
1	B	858	LYS
1	B	874	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	GLN
1	A	231	HIS
1	A	263	HIS
1	A	329	ASN
1	A	354	GLN
1	A	364	ASN
1	A	374	ASN
1	A	421	GLN
1	B	622	GLN
1	B	712	GLN
1	B	731	HIS
1	B	829	ASN
1	B	841	HIS
1	B	854	GLN
1	B	864	ASN
1	B	874	ASN
1	B	921	GLN

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 ⓘ

9 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
4	CHD	A	501	-	29,32,32	1.94	10 (34%)	47,51,51	1.72	14 (29%)
4	CHD	A	502	-	29,32,32	1.90	10 (34%)	47,51,51	1.69	15 (31%)
4	CHD	A	503	-	29,32,32	1.99	11 (37%)	47,51,51	1.76	15 (31%)
2	FES	A	601	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CHD	B	504	-	29,32,32	1.98	12 (41%)	47,51,51	1.78	15 (31%)
4	CHD	B	505	-	29,32,32	1.99	12 (41%)	47,51,51	1.74	14 (29%)
5	GOL	B	506	-	5,5,5	0.03	0	5,5,5	0.12	0
2	FES	B	924	-	0,4,4	0.00	-	0,4,4	0.00	-
3	HEM	B	925	-	28,50,50	1.76	4 (14%)	17,82,82	1.11	1 (5%)

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
4	CHD	A	501	-	-	0/7/74/74	0/4/4/4
4	CHD	A	502	-	-	0/7/74/74	0/4/4/4
4	CHD	A	503	-	-	0/7/74/74	0/4/4/4
2	FES	A	601	-	-	0/0/4/4	0/1/1/1
4	CHD	B	504	-	-	0/7/74/74	0/4/4/4
4	CHD	B	505	-	-	0/7/74/74	0/4/4/4
5	GOL	B	506	-	-	0/4/4/4	0/0/0/0
2	FES	B	924	-	-	0/0/4/4	0/1/1/1
3	HEM	B	925	-	-	0/6/54/54	0/0/8/8

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	925	HEM	C3B-C2B	-6.44	1.31	1.40
3	B	925	HEM	C4A-CHB	-3.20	1.31	1.40
3	B	925	HEM	C1A-CHA	-2.85	1.32	1.40
3	B	925	HEM	C3C-C2C	-2.22	1.37	1.40
4	B	504	CHD	O7-C7	2.00	1.47	1.43
4	B	505	CHD	C20-C17	2.03	1.58	1.54
4	B	504	CHD	C8-C9	2.04	1.57	1.53
4	A	503	CHD	C20-C17	2.06	1.58	1.54
4	B	504	CHD	C18-C13	2.06	1.57	1.54
4	A	502	CHD	C19-C10	2.09	1.58	1.54
4	B	504	CHD	C4-C3	2.09	1.55	1.51
4	B	505	CHD	O7-C7	2.09	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	CHD	C19-C10	2.16	1.58	1.54
4	A	502	CHD	C8-C14	2.17	1.58	1.53
4	A	501	CHD	C8-C14	2.19	1.58	1.53
4	B	505	CHD	C8-C14	2.21	1.58	1.53
4	A	501	CHD	C19-C10	2.24	1.58	1.54
4	A	501	CHD	C13-C12	2.26	1.58	1.54
4	B	505	CHD	C19-C10	2.27	1.58	1.54
4	B	504	CHD	C8-C14	2.30	1.58	1.53
4	A	503	CHD	C13-C12	2.36	1.58	1.54
4	A	502	CHD	C8-C7	2.37	1.57	1.53
4	B	504	CHD	C13-C12	2.46	1.58	1.54
4	B	504	CHD	C8-C7	2.50	1.57	1.53
4	A	503	CHD	C18-C13	2.51	1.58	1.54
4	A	501	CHD	C8-C7	2.55	1.57	1.53
4	A	503	CHD	C8-C14	2.56	1.58	1.53
4	A	503	CHD	C8-C7	2.57	1.57	1.53
4	A	502	CHD	C18-C13	2.58	1.58	1.54
4	A	501	CHD	C18-C13	2.58	1.58	1.54
4	B	505	CHD	C13-C12	2.61	1.58	1.54
4	B	505	CHD	C10-C9	2.61	1.61	1.56
4	A	502	CHD	C13-C12	2.62	1.58	1.54
4	A	501	CHD	O12-C12	2.63	1.48	1.43
4	B	505	CHD	C18-C13	2.67	1.58	1.54
4	B	505	CHD	C8-C7	2.70	1.58	1.53
4	A	502	CHD	C6-C5	2.73	1.58	1.53
4	A	502	CHD	C10-C9	2.77	1.61	1.56
4	A	503	CHD	O12-C12	2.80	1.48	1.43
4	B	504	CHD	C10-C9	2.80	1.61	1.56
4	A	501	CHD	C10-C9	2.80	1.61	1.56
4	A	503	CHD	C10-C9	2.82	1.61	1.56
4	B	504	CHD	O12-C12	2.83	1.48	1.43
4	A	502	CHD	O12-C12	2.83	1.48	1.43
4	B	505	CHD	O12-C12	2.87	1.48	1.43
4	B	505	CHD	C6-C5	2.93	1.58	1.53
4	A	503	CHD	C6-C5	3.05	1.58	1.53
4	A	501	CHD	C6-C5	3.15	1.59	1.53
4	B	504	CHD	C6-C5	3.16	1.59	1.53
4	A	501	CHD	C16-C17	3.26	1.61	1.54
4	A	503	CHD	C16-C17	3.49	1.61	1.54
4	A	502	CHD	C16-C17	3.51	1.61	1.54
4	B	505	CHD	C16-C17	3.60	1.62	1.54
4	B	504	CHD	C16-C17	3.62	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	502	CHD	C11-C9	3.66	1.59	1.53
4	B	505	CHD	C11-C9	3.93	1.60	1.53
4	A	501	CHD	C11-C9	4.02	1.60	1.53
4	A	503	CHD	C11-C9	4.03	1.60	1.53
4	B	504	CHD	C11-C9	4.30	1.60	1.53

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	505	CHD	C18-C13-C12	-3.89	105.12	109.08
4	A	503	CHD	C18-C13-C12	-3.84	105.17	109.08
4	A	502	CHD	C18-C13-C12	-3.80	105.21	109.08
4	A	501	CHD	C18-C13-C12	-3.77	105.25	109.08
4	B	504	CHD	C18-C13-C12	-3.69	105.32	109.08
4	A	502	CHD	C19-C10-C1	-3.58	102.37	108.24
4	A	501	CHD	C19-C10-C1	-3.41	102.64	108.24
4	B	505	CHD	C19-C10-C1	-3.40	102.65	108.24
4	A	503	CHD	C19-C10-C1	-3.29	102.83	108.24
4	B	504	CHD	O12-C12-C13	-3.29	105.63	111.12
4	A	503	CHD	O12-C12-C13	-3.27	105.66	111.12
4	A	501	CHD	O12-C12-C13	-3.21	105.76	111.12
4	B	505	CHD	O12-C12-C13	-3.13	105.90	111.12
4	A	502	CHD	O12-C12-C13	-3.11	105.93	111.12
4	B	504	CHD	C19-C10-C1	-3.05	103.24	108.24
4	B	504	CHD	C6-C5-C10	-2.83	109.57	112.66
3	B	925	HEM	CBA-CAA-C2A	-2.78	107.17	112.48
4	B	504	CHD	C9-C11-C12	-2.78	110.66	114.32
4	A	503	CHD	C9-C8-C7	-2.69	108.76	111.92
4	A	503	CHD	C6-C5-C10	-2.68	109.73	112.66
4	A	501	CHD	C16-C17-C13	-2.64	100.93	103.57
4	A	501	CHD	C9-C11-C12	-2.53	110.99	114.32
4	A	501	CHD	C6-C5-C10	-2.52	109.90	112.66
4	B	505	CHD	C6-C5-C10	-2.48	109.95	112.66
4	A	502	CHD	C9-C8-C7	-2.46	109.04	111.92
4	B	504	CHD	C16-C17-C13	-2.45	101.12	103.57
4	A	502	CHD	C11-C9-C10	-2.39	111.21	113.74
4	A	502	CHD	C6-C5-C10	-2.36	110.08	112.66
4	B	505	CHD	C9-C11-C12	-2.33	111.26	114.32
4	B	505	CHD	C11-C9-C10	-2.32	111.29	113.74
4	B	504	CHD	C9-C8-C7	-2.32	109.20	111.92
4	A	502	CHD	C9-C11-C12	-2.30	111.29	114.32
4	B	504	CHD	C19-C10-C5	-2.28	106.38	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	CHD	C9-C11-C12	-2.25	111.36	114.32
4	A	503	CHD	C16-C17-C13	-2.24	101.33	103.57
4	A	501	CHD	C11-C9-C10	-2.24	111.38	113.74
4	B	505	CHD	C16-C17-C13	-2.24	101.34	103.57
4	A	503	CHD	C11-C9-C10	-2.19	111.42	113.74
4	B	505	CHD	C9-C8-C7	-2.17	109.38	111.92
4	A	502	CHD	C5-C4-C3	-2.12	109.77	112.87
4	A	501	CHD	C9-C8-C7	-2.10	109.46	111.92
4	A	502	CHD	C16-C17-C13	-2.03	101.55	103.57
4	A	503	CHD	C21-C20-C22	-2.01	107.18	110.35
4	A	502	CHD	C19-C10-C9	2.01	114.04	111.16
4	A	502	CHD	C6-C5-C4	2.01	113.42	111.13
4	A	501	CHD	C19-C10-C9	2.04	114.09	111.16
4	A	501	CHD	C1-C10-C5	2.09	111.04	107.79
4	B	505	CHD	C19-C10-C9	2.12	114.20	111.16
4	B	505	CHD	C6-C5-C4	2.15	113.57	111.13
4	B	505	CHD	C1-C10-C5	2.20	111.20	107.79
4	B	504	CHD	C19-C10-C9	2.22	114.34	111.16
4	A	503	CHD	C1-C10-C5	2.23	111.25	107.79
4	A	501	CHD	C6-C5-C4	2.25	113.69	111.13
4	B	504	CHD	C1-C10-C5	2.27	111.31	107.79
4	A	503	CHD	C6-C5-C4	2.28	113.72	111.13
4	A	502	CHD	C11-C12-C13	2.28	113.59	111.22
4	A	503	CHD	C19-C10-C9	2.34	114.51	111.16
4	A	502	CHD	C1-C10-C5	2.35	111.43	107.79
4	B	505	CHD	C11-C12-C13	2.37	113.68	111.22
4	B	504	CHD	C13-C17-C20	2.51	122.54	119.49
4	A	501	CHD	C11-C12-C13	2.52	113.83	111.22
4	B	504	CHD	C11-C12-C13	2.59	113.90	111.22
4	A	503	CHD	C11-C12-C13	2.60	113.92	111.22
4	B	504	CHD	C17-C13-C14	2.74	102.87	100.08
4	A	501	CHD	C17-C13-C12	2.91	120.35	117.67
4	A	503	CHD	C17-C13-C12	2.94	120.38	117.67
4	A	501	CHD	C17-C13-C14	2.94	103.08	100.08
4	A	502	CHD	C17-C13-C12	2.99	120.42	117.67
4	A	502	CHD	C17-C13-C14	3.03	103.17	100.08
4	B	504	CHD	C6-C5-C4	3.17	114.72	111.13
4	B	504	CHD	C17-C13-C12	3.17	120.59	117.67
4	B	505	CHD	C17-C13-C12	3.21	120.63	117.67
4	B	505	CHD	C17-C13-C14	3.27	103.42	100.08
4	A	503	CHD	C17-C13-C14	3.52	103.66	100.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	CHD	5	0
4	A	502	CHD	1	0
4	B	504	CHD	2	0
4	B	505	CHD	1	0
5	B	506	GOL	4	0
3	B	925	HEM	9	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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(Å²)	Q<0.9
1	A	359/359 (100%)	0.13	18 (5%)	30	28	13, 27, 44, 52	0
1	B	359/359 (100%)	0.16	19 (5%)	27	26	13, 28, 50, 57	0
All	All	718/718 (100%)	0.15	37 (5%)	28	27	13, 27, 46, 57	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	923	LEU	6.4
1	A	423	LEU	4.6
1	B	857	ALA	4.6
1	B	603	ILE	3.6
1	A	357	ALA	3.5
1	A	356	LEU	3.5
1	B	596	ARG	3.3
1	A	103	ILE	3.3
1	A	155	ALA	3.1
1	B	605	ASN	3.0
1	B	600	THR	3.0
1	B	565	ARG	2.9
1	B	602	PRO	2.9
1	A	106	LYS	2.9
1	A	65	ARG	2.9
1	B	598[A]	LEU	2.7
1	A	360[A]	CYS	2.6
1	A	105	ASN	2.6
1	B	859	GLU	2.6
1	B	854	GLN	2.6
1	B	856	LEU	2.6
1	B	599	MET	2.6
1	A	359	GLU	2.6
1	B	606	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	100	THR	2.5
1	A	66	LYS	2.5
1	B	614	ARG	2.4
1	A	102	PRO	2.3
1	A	358	LYS	2.3
1	A	96	ARG	2.3
1	B	715	ARG	2.2
1	B	601	LEU	2.1
1	B	566	LYS	2.1
1	A	179	ARG	2.1
1	B	858	LYS	2.1
1	A	212	GLN	2.0
1	A	110	PHE	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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	HEM	B	925	43/43	0.61	0.48	5.71	30,30,31,31	43
5	GOL	B	506	6/6	0.88	0.28	5.62	37,37,37,37	0
4	CHD	A	501	29/29	0.73	0.28	3.18	55,55,56,56	0
4	CHD	A	502	29/29	0.79	0.27	2.32	63,63,63,63	0
4	CHD	A	503	29/29	0.79	0.33	1.32	73,73,74,74	0
4	CHD	B	504	29/29	0.68	0.28	0.98	63,63,64,64	0
4	CHD	B	505	29/29	0.74	0.33	0.73	65,65,66,66	0
2	FES	B	924	4/4	0.99	0.07	-1.89	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	FES	A	601	4/4	0.98	0.07	-2.52	22,23,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.