



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:35 AM GMT

PDB ID : 2HRC
Title : 1.7 angstrom structure of human ferrochelatase variant R115L
Authors : Medlock, A.; Swartz, L.; Dailey, T.A.; Dailey, H.A.; Lanzilotta, W.N.
Deposited on : 2006-07-20
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 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

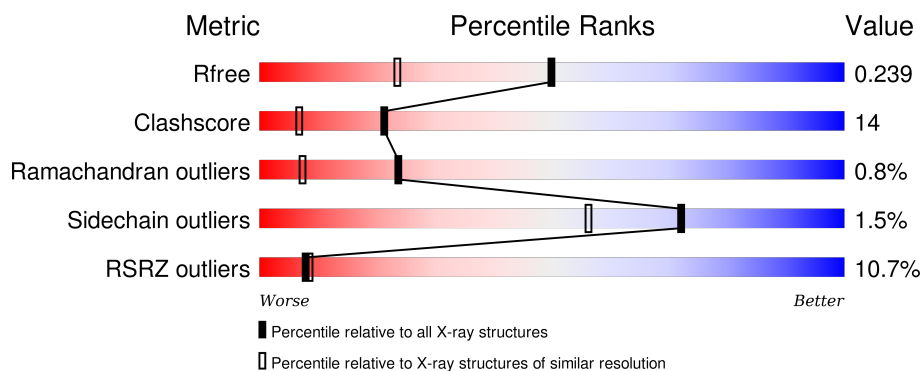
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	359	<div> <div>11%</div> <div>72%</div> <div>27%</div> <div>.</div> </div>
1	B	359	<div> <div>11%</div> <div>74%</div> <div>24%</div> <div>.</div> </div>

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
4	IMD	A	1601	-	-	-	X
4	IMD	B	1602	-	-	-	X
6	GOL	A	707	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6923 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	21	0
			3057	1935	533	569	20			
1	B	359	Total	C	N	O	S	0	20	0
			3062	1939	537	567	19			

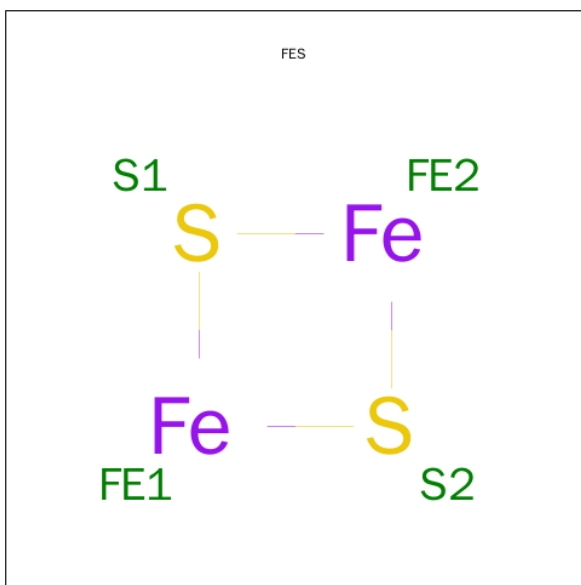
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	LEU	ARG	ENGINEERED	UNP P22830
B	615	LEU	ARG	ENGINEERED	UNP P22830

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

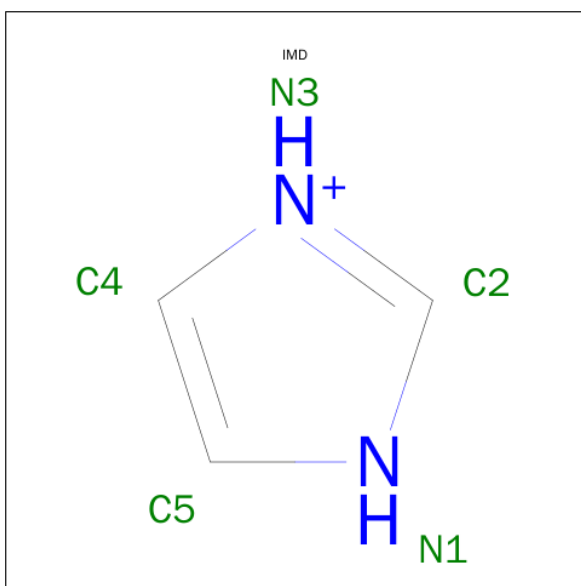
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



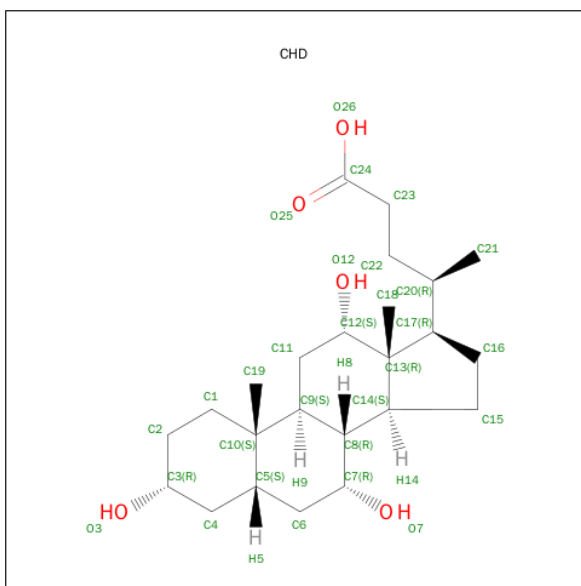
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

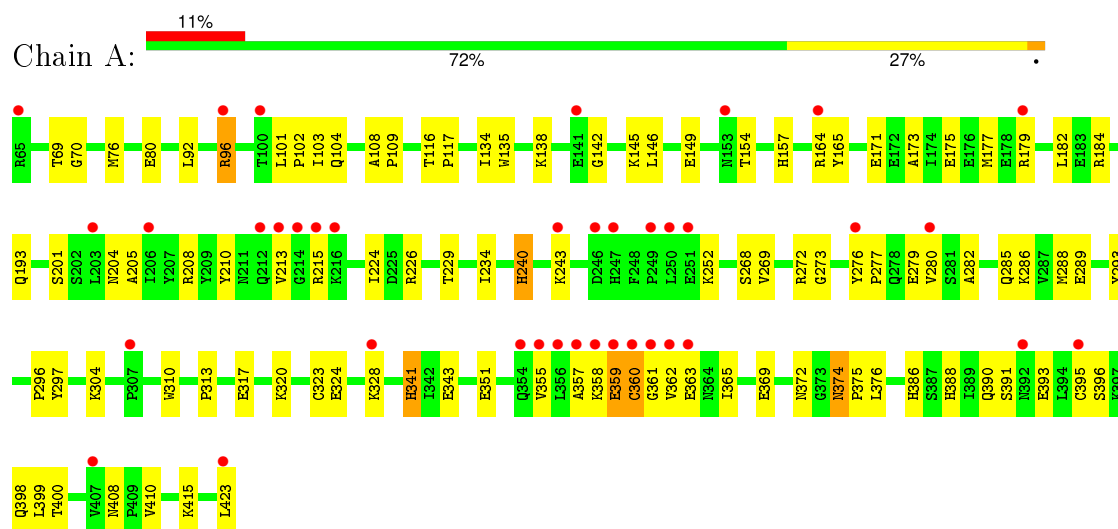
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	306	Total	O	0	0
			306	306		
7	B	298	Total	O	0	0
			298	298		

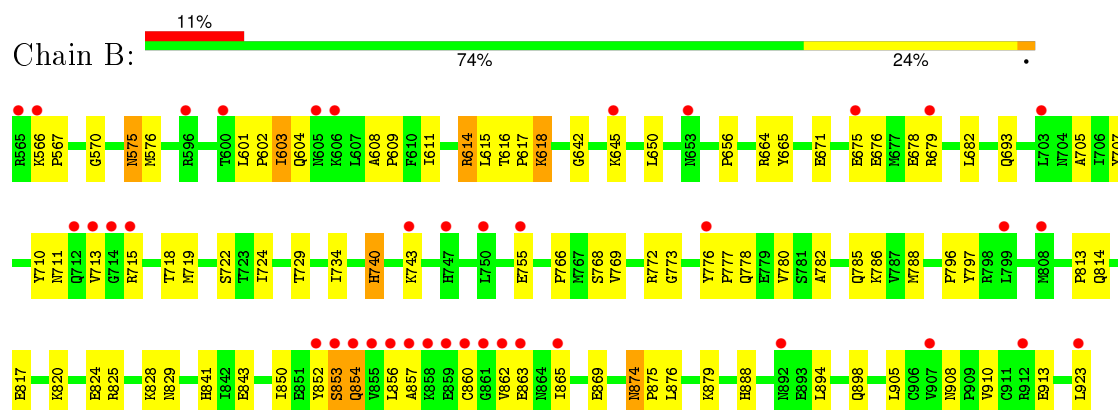
3 Residue-property plots

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: 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	88.53Å 92.98Å 110.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.84 – 1.70 41.84 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.84-1.70) 99.7 (41.84-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 1.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.221 , 0.242 0.221 , 0.239	Depositor DCC
R_{free} test set	4998 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 54.7	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 145522 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6923	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 54.37 % 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 3.6882e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: GOL, CHD, IMD, FES, CL

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	0.28	0/3127	0.56	1/4230 (0.0%)
1	B	0.28	0/3132	0.57	1/4234 (0.0%)
All	All	0.28	0/6259	0.56	2/8464 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	724	ILE	N-CA-C	-5.66	95.72	111.00
1	A	224	ILE	N-CA-C	-5.52	96.11	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	3057	0	3025	87	0
1	B	3062	0	3047	105	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	5	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	5	1	0
5	A	87	0	117	1	0
5	B	87	0	117	3	0
6	A	6	0	8	3	0
7	A	306	0	0	5	0
7	B	298	0	0	9	0
All	All	6923	0	6324	181	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 14.

All (181) 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:664[A]:ARG:NH1	1:B:705:ALA:HB2	1.68	1.07
1:B:664[A]:ARG:HH11	1:B:705:ALA:HB2	1.26	1.00
1:A:164[A]:ARG:NH1	1:A:205:ALA:HB2	1.76	0.99
1:A:164[A]:ARG:HH11	1:A:205:ALA:HB2	1.29	0.96
1:A:398:GLN:HE22	1:B:797:TYR:H	1.17	0.93
1:A:297:TYR:H	1:B:898:GLN:HE22	1.15	0.89
1:A:323[B]:CYS:SG	1:A:362:VAL:HG12	2.18	0.84
1:B:814:GLN:HB2	1:B:817[B]:GLU:HG2	1.61	0.82
1:A:285[B]:GLN:HE21	1:B:778:GLN:HE22	1.27	0.80
1:B:650:LEU:HD11	1:B:879[B]:LYS:NZ	1.98	0.79
1:B:853:SER:O	1:B:854:GLN:HG3	1.83	0.77
1:A:324:GLU:HG2	1:A:360:CYS:SG	2.26	0.76
1:A:229:THR:HB	1:A:286:LYS:HE2	1.70	0.73
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.73	0.71
1:B:650:LEU:HD11	1:B:879[B]:LYS:HZ1	1.57	0.70
1:A:277:PRO:HB3	6:A:707:GOL:H2	1.75	0.69
1:B:664[A]:ARG:HG3	1:B:665:TYR:CE2	2.28	0.68
1:B:862:VAL:HG21	1:B:865:ILE:HG13	1.76	0.68
1:B:862:VAL:HG21	1:B:865:ILE:CG1	2.24	0.68
1:B:608:ALA:HB3	1:B:609:PRO:HD3	1.77	0.65
1:A:269:VAL:O	1:A:272[A]:ARG:HG2	1.96	0.65
1:A:175[A]:GLU:O	1:A:179[A]:ARG:HG3	1.96	0.65
1:A:285[B]:GLN:NE2	1:B:778:GLN:HE22	1.94	0.65
1:B:769:VAL:O	1:B:772[A]:ARG:HG2	1.97	0.64
1:A:297:TYR:N	1:B:898:GLN:HE22	1.94	0.64
1:A:285[A]:GLN:HG3	1:B:782:ALA:HB1	1.79	0.64
1:B:602:PRO:C	1:B:603:ILE:HD13	2.18	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:SER:OG	1:A:393[B]:GLU:HG2	1.97	0.63
1:A:268:SER:O	1:A:272[B]:ARG:HG3	2.00	0.62
1:A:142:GLY:O	1:A:145[B]:LYS:HG3	1.98	0.62
1:A:234:ILE:HG13	1:A:286:LYS:HE3	1.81	0.62
1:A:395[B]:CYS:SG	1:A:399:LEU:HD22	2.40	0.62
1:B:710:TYR:HA	1:B:713:VAL:HG12	1.82	0.61
1:A:240:HIS:HD2	1:A:369:GLU:O	1.82	0.61
1:B:734:ILE:HG13	1:B:786[B]:LYS:HE3	1.82	0.61
1:B:820:LYS:O	1:B:824:GLU:HG3	2.00	0.61
1:B:722:SER:OG	1:B:888:HIS:HE1	1.85	0.60
1:B:853:SER:HB3	7:B:1858:HOH:O	2.02	0.59
1:A:351:GLU:O	1:A:355:VAL:HG23	2.02	0.59
1:B:874:ASN:HD22	1:B:875:PRO:N	2.00	0.59
1:B:611:ILE:HA	1:B:614:ARG:HG2	1.83	0.59
1:A:320:LYS:O	1:A:324:GLU:HG3	2.01	0.59
1:A:395[B]:CYS:SG	1:A:396:SER:N	2.75	0.59
1:A:395[B]:CYS:SG	1:A:399:LEU:CD2	2.91	0.58
1:B:740:HIS:HD2	1:B:869:GLU:O	1.86	0.58
1:B:768:SER:O	1:B:772[B]:ARG:HG3	2.04	0.58
1:A:398:GLN:HE22	1:B:797:TYR:N	1.95	0.58
1:A:164[A]:ARG:HG3	1:A:165:TYR:CE2	2.39	0.58
1:A:313:PRO:HG2	1:B:773:GLY:HA2	1.85	0.58
1:B:707:TYR:CE1	1:B:711[A]:ASN:ND2	2.72	0.58
1:A:285[A]:GLN:OE1	1:B:786[A]:LYS:NZ	2.37	0.57
1:A:374:ASN:HD22	1:A:375:PRO:N	2.02	0.57
1:A:76:MET:HB2	1:A:164[B]:ARG:NH2	2.19	0.57
1:A:374:ASN:ND2	1:A:376:LEU:H	2.03	0.57
1:B:664[A]:ARG:HH12	1:B:705:ALA:HB2	1.66	0.56
1:A:273:GLY:HA2	1:B:813:PRO:HG2	1.87	0.56
1:A:374:ASN:C	1:A:374:ASN:HD22	2.09	0.56
1:B:618:LYS:NZ	1:B:618:LYS:HB2	2.21	0.56
1:B:857:ALA:HA	7:B:1765:HOH:O	2.05	0.55
1:B:566:LYS:HD2	1:B:567:PRO:HD2	1.89	0.55
1:B:841:HIS:CE1	1:B:843:GLU:HB2	2.42	0.55
1:B:862:VAL:HG21	1:B:865:ILE:HD11	1.89	0.55
1:B:879[B]:LYS:HE3	1:B:879[B]:LYS:O	2.07	0.54
1:A:276:TYR:HB3	1:A:277:PRO:HD3	1.89	0.54
1:B:874:ASN:HD22	1:B:874:ASN:C	2.10	0.54
1:A:101:LEU:HB2	1:A:104:GLN:HG3	1.90	0.53
1:A:388:HIS:ND1	1:A:393[B]:GLU:HG3	2.23	0.53
1:B:862:VAL:HG21	1:B:865:ILE:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:874:ASN:ND2	1:B:876:LEU:H	2.05	0.53
1:A:175[B]:GLU:HG2	1:A:179[B]:ARG:HH11	1.74	0.53
1:B:860:CYS:HB2	7:B:1765:HOH:O	2.09	0.52
1:B:575:ASN:HD22	1:B:576:MET:H	1.56	0.52
1:A:96:ARG:HG2	1:A:96:ARG:HH11	1.75	0.52
1:B:729:THR:HB	1:B:786[B]:LYS:HE2	1.90	0.52
1:B:601:LEU:HB2	1:B:604:GLN:HG3	1.90	0.52
1:B:676:GLU:HA	1:B:679[A]:ARG:HE	1.74	0.52
1:A:282:ALA:HB1	1:B:785:GLN:HG2	1.91	0.52
1:B:566:LYS:CD	1:B:567:PRO:HD2	2.40	0.52
1:B:828:LYS:HB3	1:B:863:GLU:H	1.74	0.52
1:B:888:HIS:HD2	7:B:1818:HOH:O	1.92	0.51
1:B:642:GLY:HA2	1:B:645[B]:LYS:HD3	1.91	0.51
1:A:395[B]:CYS:SG	1:A:399:LEU:CB	2.98	0.51
1:B:776:TYR:HB3	1:B:777:PRO:HD3	1.92	0.51
1:A:145[B]:LYS:HD2	1:A:146:LEU:HG	1.93	0.51
1:B:713:VAL:HG21	1:B:715[B]:ARG:HH21	1.77	0.50
1:B:675[B]:GLU:O	1:B:679[B]:ARG:HG3	2.11	0.50
1:B:825:ARG:HG3	1:B:825:ARG:HH11	1.76	0.50
1:A:213:VAL:HG13	1:A:215:ARG:HG2	1.94	0.50
1:A:395[B]:CYS:SG	1:A:399:LEU:HB3	2.51	0.50
1:B:615:LEU:HD22	1:B:618:LYS:HD2	1.94	0.50
1:B:841:HIS:HD2	7:B:1773:HOH:O	1.95	0.50
1:B:894:LEU:HD11	1:B:923:LEU:HD11	1.93	0.50
1:A:204:ASN:O	1:A:208:ARG:HG3	2.12	0.50
1:B:852:TYR:O	1:B:854:GLN:N	2.42	0.49
1:A:175[B]:GLU:O	1:A:179[B]:ARG:HG3	2.12	0.49
1:B:879[B]:LYS:HA	1:B:879[B]:LYS:HE3	1.94	0.49
1:B:678:GLU:OE1	1:B:719:MET:HG3	2.13	0.49
1:B:602:PRO:O	1:B:603:ILE:C	2.50	0.48
1:A:408:ASN:OD1	1:A:410:VAL:HG12	2.13	0.48
1:B:570:GLY:HA3	1:B:682:LEU:HD13	1.95	0.48
1:A:171:GLU:O	1:A:175[A]:GLU:HG3	2.13	0.48
1:B:576:MET:HB2	1:B:664[B]:ARG:NH2	2.29	0.48
1:B:788:MET:HG3	1:B:797:TYR:CE2	2.49	0.48
1:A:386:HIS:O	1:A:390:GLN:HG3	2.14	0.48
1:B:675[A]:GLU:O	1:B:679[A]:ARG:HG3	2.13	0.48
1:A:210:TYR:HA	1:A:213:VAL:HG12	1.96	0.47
1:A:252:LYS:HE3	7:A:1751:HOH:O	2.14	0.47
1:B:772[B]:ARG:HG2	7:B:1897:HOH:O	2.14	0.47
1:B:841:HIS:HE1	7:B:1844:HOH:O	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175[B]:GLU:HG2	1:A:179[B]:ARG:NH1	2.30	0.47
1:A:135:TRP:CZ3	1:A:372:ASN:HB3	2.50	0.47
1:A:286:LYS:HD3	7:B:1734:HOH:O	2.15	0.47
1:A:243:LYS:HG3	7:A:1680:HOH:O	2.14	0.47
1:B:734:ILE:HG13	1:B:786[B]:LYS:CE	2.45	0.47
1:A:149:GLU:HG2	7:A:1903:HOH:O	2.13	0.47
1:A:359:GLU:O	1:A:361:GLY:N	2.48	0.46
1:A:328:LYS:HB3	1:A:363:GLU:H	1.80	0.46
1:B:908:ASN:OD1	1:B:910:VAL:HG12	2.15	0.46
1:A:365:ILE:HD13	7:A:1822:HOH:O	2.16	0.46
1:A:365:ILE:HG23	1:A:365:ILE:O	2.15	0.46
1:A:277:PRO:CB	6:A:707:GOL:H2	2.44	0.46
1:B:615:LEU:HD21	5:B:1603:CHD:H232	1.98	0.46
1:B:567:PRO:HA	1:B:656:PRO:HG2	1.97	0.46
1:A:134:ILE:CG2	1:A:138[B]:LYS:HE3	2.46	0.46
1:B:755:GLU:OE2	1:B:829:ASN:HB2	2.16	0.46
1:A:116:THR:HB	1:A:117:PRO:HD3	1.97	0.46
5:B:1605:CHD:H212	5:B:1605:CHD:H12	1.98	0.46
1:A:80[B]:GLU:HG3	7:A:1642:HOH:O	2.15	0.45
1:A:102:PRO:O	1:A:103:ILE:C	2.53	0.45
1:A:142:GLY:O	1:A:145[B]:LYS:HE3	2.17	0.45
1:B:862:VAL:HG11	1:B:865:ILE:HD12	1.99	0.45
1:A:317[B]:GLU:OE2	1:B:905:LEU:HD13	2.16	0.44
1:A:70:GLY:HA3	1:A:182:LEU:HD13	1.99	0.44
1:B:879[B]:LYS:HE3	1:B:879[B]:LYS:CA	2.47	0.44
1:B:850:ILE:HG23	1:B:854:GLN:NE2	2.33	0.44
1:B:566:LYS:CG	1:B:567:PRO:HD2	2.47	0.44
1:B:566:LYS:HG3	1:B:567:PRO:HD2	1.99	0.44
1:B:616:THR:HB	1:B:617:PRO:HD3	1.99	0.44
1:A:288:MET:HG3	1:A:297:TYR:CD2	2.53	0.43
1:B:740:HIS:HA	1:B:743:LYS:HG2	2.00	0.43
1:A:193:GLN:HG2	1:A:280:VAL:HA	2.00	0.43
1:A:296:PRO:HA	1:B:898:GLN:NE2	2.34	0.43
1:A:289[B]:GLU:HG2	1:A:293:TYR:OH	2.18	0.43
1:A:135:TRP:CE3	1:A:372:ASN:HB3	2.54	0.43
1:A:341:HIS:NE2	1:A:343:GLU:HB2	2.33	0.43
1:A:226:ARG:HD3	1:A:279:GLU:OE1	2.18	0.43
1:B:615:LEU:CD2	1:B:618:LYS:HD2	2.49	0.43
4:B:1602:IMD:H2	7:B:1670:HOH:O	2.19	0.43
1:B:862:VAL:CG2	1:B:865:ILE:HG13	2.47	0.42
1:B:908:ASN:CG	1:B:910:VAL:HG12	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD23	1:A:92:LEU:C	2.39	0.42
1:A:398:GLN:NE2	1:B:796:PRO:HA	2.35	0.42
1:B:602:PRO:HB2	1:B:603:ILE:HD13	2.01	0.42
1:A:96:ARG:NH1	1:A:96:ARG:HG2	2.33	0.42
1:A:388:HIS:CE1	1:A:393[B]:GLU:HG3	2.54	0.42
1:B:679[B]:ARG:HB3	1:B:679[B]:ARG:CZ	2.49	0.42
1:B:825:ARG:NH1	1:B:825:ARG:HG3	2.34	0.42
1:B:820:LYS:HB2	1:B:856:LEU:HD11	2.02	0.42
1:A:69:THR:HG23	1:A:184:ARG:HD2	2.02	0.42
6:A:707:GOL:H31	1:B:777:PRO:HB3	2.02	0.41
1:B:618:LYS:NZ	1:B:618:LYS:CB	2.82	0.41
1:B:671:GLU:O	1:B:675[B]:GLU:HG3	2.20	0.41
1:B:713:VAL:HG21	1:B:715[B]:ARG:NH2	2.35	0.41
1:B:828:LYS:O	1:B:862:VAL:HG22	2.21	0.41
1:A:400:THR:HA	1:A:415:LYS:HD2	2.02	0.41
1:B:603:ILE:N	1:B:603:ILE:HD13	2.36	0.41
1:A:164[A]:ARG:NH1	1:A:201:SER:O	2.54	0.41
1:B:678:GLU:OE1	1:B:718:THR:OG1	2.33	0.41
1:A:173:ALA:O	1:A:177:MET:HG3	2.21	0.41
1:B:650:LEU:HD11	1:B:879[B]:LYS:HZ3	1.79	0.41
1:A:304:LYS:HG3	1:A:310:TRP:CG	2.55	0.41
1:B:602:PRO:CB	1:B:603:ILE:HD13	2.51	0.41
1:B:766:PRO:HG2	5:B:1603:CHD:H11	2.03	0.41
1:A:208:ARG:HG2	1:A:208:ARG:NH1	2.35	0.41
1:A:154:THR:OG1	1:A:157:HIS:CE1	2.74	0.41
1:B:713:VAL:O	1:B:715[B]:ARG:HG3	2.21	0.40
1:B:693:GLN:HG2	1:B:780:VAL:HA	2.02	0.40
1:B:707:TYR:CZ	1:B:913[B]:GLU:HB3	2.56	0.40
1:A:423:LEU:HD22	1:A:423:LEU:N	2.36	0.40
5:A:701:CHD:H212	5:A:701:CHD:H12	2.02	0.40
1:B:879[B]:LYS:CE	1:B:879[B]:LYS:O	2.69	0.40

There are no symmetry-related clashes.

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	378/359 (105%)	365 (97%)	9 (2%)	4 (1%)	17	4
1	B	377/359 (105%)	365 (97%)	10 (3%)	2 (0%)	34	15
All	All	755/718 (105%)	730 (97%)	19 (2%)	6 (1%)	24	7

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	853	SER
1	B	854	GLN
1	A	357	ALA
1	A	358	LYS
1	A	360	CYS
1	A	359	GLU

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	343/324 (106%)	339 (99%)	4 (1%)	78	65
1	B	344/324 (106%)	338 (98%)	6 (2%)	68	51
All	All	687/648 (106%)	677 (98%)	10 (2%)	72	56

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	A	240	HIS
1	A	341	HIS
1	A	374	ASN
1	B	575	ASN
1	B	603	ILE
1	B	614	ARG

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Mol	Chain	Res	Type
1	B	618	LYS
1	B	740	HIS
1	B	874	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	HIS
1	A	240	HIS
1	A	374	ASN
1	A	390	GLN
1	A	398	GLN
1	A	421	GLN
1	B	575	ASN
1	B	740	HIS
1	B	814	GLN
1	B	829	ASN
1	B	841	HIS
1	B	854	GLN
1	B	864	ASN
1	B	874	ASN
1	B	888	HIS
1	B	898	GLN
1	B	921	GLN
1	B	922	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

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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$
3	FES	A	1501	1	0,4,4	0.00	-	0,4,4	0.00	-
4	IMD	A	1601	-	3,5,5	0.35	0	4,5,5	0.58	0
5	CHD	A	701	-	29,32,32	1.96	11 (37%)	48,51,51	1.74	13 (27%)
5	CHD	A	702	-	29,32,32	1.92	9 (31%)	48,51,51	1.66	13 (27%)
5	CHD	A	703	-	29,32,32	1.94	11 (37%)	48,51,51	1.72	15 (31%)
6	GOL	A	707	-	5,5,5	0.14	0	5,5,5	0.21	0
3	FES	B	1502	1	0,4,4	0.00	-	0,4,4	0.00	-
4	IMD	B	1602	-	3,5,5	0.35	0	4,5,5	0.58	0
5	CHD	B	1603	-	29,32,32	1.90	10 (34%)	48,51,51	1.69	14 (29%)
5	CHD	B	1604	-	29,32,32	1.96	11 (37%)	48,51,51	1.72	14 (29%)
5	CHD	B	1605	-	29,32,32	1.95	13 (44%)	48,51,51	1.78	14 (29%)

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	FES	A	1501	1	-	0/0/4/4	0/1/1/1
4	IMD	A	1601	-	-	0/0/0/0	0/1/1/1
5	CHD	A	701	-	-	0/7/74/74	0/4/4/4
5	CHD	A	702	-	-	0/7/74/74	0/4/4/4
5	CHD	A	703	-	-	0/7/74/74	0/4/4/4
6	GOL	A	707	-	-	0/4/4/4	0/0/0/0
3	FES	B	1502	1	-	0/0/4/4	0/1/1/1
4	IMD	B	1602	-	-	0/0/0/0	0/1/1/1
5	CHD	B	1603	-	-	0/7/74/74	0/4/4/4
5	CHD	B	1604	-	-	0/7/74/74	0/4/4/4
5	CHD	B	1605	-	-	0/7/74/74	0/4/4/4

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	703	CHD	C8-C9	2.01	1.57	1.53
5	B	1605	CHD	C20-C17	2.01	1.58	1.54
5	B	1603	CHD	O7-C7	2.02	1.47	1.43
5	B	1605	CHD	O7-C7	2.02	1.47	1.43
5	B	1605	CHD	C4-C3	2.03	1.55	1.51
5	B	1604	CHD	O7-C7	2.04	1.48	1.43
5	A	701	CHD	C4-C3	2.15	1.55	1.51
5	B	1603	CHD	C8-C14	2.15	1.58	1.53
5	A	701	CHD	C19-C10	2.24	1.58	1.54
5	B	1604	CHD	C19-C10	2.24	1.58	1.54
5	A	703	CHD	C19-C10	2.25	1.58	1.54
5	B	1605	CHD	C19-C10	2.26	1.58	1.54
5	A	703	CHD	C8-C14	2.26	1.58	1.53
5	B	1603	CHD	C13-C12	2.27	1.58	1.54
5	A	701	CHD	C13-C12	2.29	1.58	1.54
5	B	1604	CHD	C8-C14	2.29	1.58	1.53
5	A	702	CHD	C8-C14	2.30	1.58	1.53
5	A	702	CHD	C8-C7	2.37	1.57	1.53
5	B	1605	CHD	C13-C12	2.48	1.58	1.54
5	A	702	CHD	C13-C12	2.50	1.58	1.54
5	B	1604	CHD	C13-C12	2.51	1.58	1.54
5	B	1603	CHD	C8-C7	2.54	1.57	1.53
5	A	703	CHD	C13-C12	2.55	1.58	1.54
5	A	701	CHD	C8-C14	2.55	1.58	1.53
5	A	703	CHD	C8-C7	2.56	1.57	1.53
5	B	1605	CHD	C8-C7	2.59	1.57	1.53
5	A	703	CHD	C18-C13	2.60	1.58	1.54
5	B	1605	CHD	C8-C14	2.63	1.59	1.53
5	B	1604	CHD	C10-C9	2.64	1.61	1.56
5	B	1603	CHD	O12-C12	2.64	1.48	1.43
5	B	1604	CHD	C18-C13	2.64	1.58	1.54
5	A	702	CHD	C18-C13	2.64	1.58	1.54
5	B	1603	CHD	C18-C13	2.67	1.58	1.54
5	A	701	CHD	O12-C12	2.67	1.48	1.43
5	B	1603	CHD	C10-C9	2.69	1.61	1.56
5	A	703	CHD	C10-C9	2.69	1.61	1.56
5	A	702	CHD	C10-C9	2.73	1.61	1.56
5	B	1604	CHD	O12-C12	2.74	1.48	1.43
5	A	701	CHD	C8-C7	2.76	1.58	1.53
5	B	1605	CHD	C10-C9	2.76	1.61	1.56
5	A	703	CHD	O12-C12	2.77	1.48	1.43
5	B	1605	CHD	C18-C13	2.77	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1605	CHD	O12-C12	2.80	1.48	1.43
5	B	1604	CHD	C8-C7	2.81	1.58	1.53
5	A	701	CHD	C10-C9	2.82	1.61	1.56
5	A	701	CHD	C18-C13	2.83	1.59	1.54
5	A	702	CHD	C6-C5	2.83	1.58	1.53
5	A	702	CHD	O12-C12	2.84	1.48	1.43
5	A	701	CHD	C6-C5	2.92	1.58	1.53
5	B	1603	CHD	C6-C5	2.93	1.58	1.53
5	A	701	CHD	C16-C17	2.97	1.61	1.54
5	B	1605	CHD	C6-C5	3.00	1.59	1.53
5	B	1605	CHD	C16-C17	3.01	1.61	1.54
5	A	703	CHD	C6-C5	3.02	1.59	1.53
5	B	1604	CHD	C6-C5	3.05	1.59	1.53
5	B	1605	CHD	C11-C9	3.26	1.59	1.53
5	B	1603	CHD	C16-C17	3.26	1.61	1.54
5	A	702	CHD	C16-C17	3.30	1.62	1.54
5	B	1604	CHD	C16-C17	3.31	1.62	1.54
5	A	703	CHD	C16-C17	3.32	1.62	1.54
5	A	701	CHD	C11-C9	3.67	1.59	1.53
5	A	703	CHD	C11-C9	3.80	1.60	1.53
5	A	702	CHD	C11-C9	3.82	1.60	1.53
5	B	1603	CHD	C11-C9	3.95	1.60	1.53
5	B	1604	CHD	C11-C9	3.95	1.60	1.53

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1605	CHD	C18-C13-C12	-4.47	104.73	109.09
5	A	701	CHD	C18-C13-C12	-4.47	104.73	109.09
5	A	703	CHD	C18-C13-C12	-4.05	105.14	109.09
5	B	1604	CHD	C18-C13-C12	-4.01	105.18	109.09
5	A	702	CHD	C18-C13-C12	-3.85	105.33	109.09
5	B	1603	CHD	C18-C13-C12	-3.79	105.39	109.09
5	B	1605	CHD	C16-C17-C13	-3.64	99.98	103.60
5	A	701	CHD	C16-C17-C13	-3.46	100.16	103.60
5	A	701	CHD	C19-C10-C1	-3.42	102.45	108.20
5	B	1603	CHD	O12-C12-C13	-3.42	105.57	111.11
5	A	701	CHD	O12-C12-C13	-3.39	105.62	111.11
5	B	1604	CHD	C19-C10-C1	-3.39	102.51	108.20
5	B	1605	CHD	C19-C10-C1	-3.31	102.64	108.20
5	A	703	CHD	O12-C12-C13	-3.30	105.77	111.11
5	A	703	CHD	C19-C10-C1	-3.27	102.69	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1604	CHD	O12-C12-C13	-3.21	105.92	111.11
5	B	1605	CHD	O12-C12-C13	-3.17	105.97	111.11
5	A	702	CHD	C19-C10-C1	-3.17	102.87	108.20
5	A	702	CHD	O12-C12-C13	-3.16	105.98	111.11
5	B	1603	CHD	C19-C10-C1	-2.98	103.19	108.20
5	B	1605	CHD	C11-C9-C10	-2.81	110.86	113.79
5	B	1603	CHD	C9-C11-C12	-2.73	110.91	114.36
5	A	702	CHD	C6-C5-C10	-2.56	109.83	112.66
5	B	1603	CHD	C6-C5-C10	-2.54	109.86	112.66
5	A	702	CHD	C11-C9-C10	-2.52	111.17	113.79
5	A	703	CHD	C9-C11-C12	-2.52	111.18	114.36
5	A	701	CHD	C11-C9-C10	-2.51	111.18	113.79
5	B	1604	CHD	C9-C11-C12	-2.51	111.19	114.36
5	A	702	CHD	C9-C8-C7	-2.51	108.95	111.92
5	B	1604	CHD	C6-C5-C10	-2.47	109.93	112.66
5	B	1604	CHD	C11-C9-C10	-2.47	111.23	113.79
5	A	703	CHD	C6-C5-C10	-2.43	109.98	112.66
5	B	1603	CHD	C16-C17-C13	-2.43	101.19	103.60
5	A	703	CHD	C11-C9-C10	-2.39	111.30	113.79
5	B	1603	CHD	C11-C9-C10	-2.39	111.31	113.79
5	A	703	CHD	C16-C17-C13	-2.32	101.29	103.60
5	B	1603	CHD	C9-C8-C7	-2.31	109.19	111.92
5	A	702	CHD	C9-C11-C12	-2.27	111.49	114.36
5	A	703	CHD	C9-C8-C7	-2.27	109.24	111.92
5	B	1604	CHD	C16-C17-C13	-2.26	101.35	103.60
5	B	1605	CHD	C9-C8-C7	-2.25	109.26	111.92
5	B	1605	CHD	C21-C20-C22	-2.25	106.60	110.35
5	B	1605	CHD	C9-C11-C12	-2.24	111.53	114.36
5	A	701	CHD	C9-C11-C12	-2.22	111.55	114.36
5	B	1604	CHD	C9-C8-C7	-2.21	109.31	111.92
5	A	701	CHD	C9-C8-C7	-2.16	109.36	111.92
5	A	701	CHD	C6-C5-C10	-2.11	110.33	112.66
5	B	1605	CHD	C6-C5-C10	-2.10	110.34	112.66
5	A	702	CHD	C16-C17-C13	-2.03	101.58	103.60
5	A	703	CHD	C23-C22-C20	-2.02	112.37	114.75
5	B	1603	CHD	C13-C17-C20	2.01	121.95	119.50
5	A	703	CHD	C19-C10-C9	2.02	114.21	111.18
5	B	1604	CHD	C19-C10-C9	2.02	114.21	111.18
5	A	703	CHD	C1-C10-C5	2.03	111.14	107.81
5	B	1604	CHD	C1-C10-C5	2.07	111.21	107.81
5	B	1603	CHD	C1-C10-C5	2.14	111.33	107.81
5	A	701	CHD	C1-C10-C5	2.14	111.33	107.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	702	CHD	C1-C10-C5	2.16	111.36	107.81
5	A	701	CHD	C11-C12-C13	2.19	113.43	111.20
5	B	1605	CHD	C11-C12-C13	2.20	113.43	111.20
5	B	1605	CHD	C1-C10-C5	2.22	111.46	107.81
5	A	702	CHD	C11-C12-C13	2.30	113.53	111.20
5	A	703	CHD	C6-C5-C4	2.36	113.68	111.05
5	A	701	CHD	C6-C5-C4	2.40	113.72	111.05
5	A	703	CHD	C11-C12-C13	2.47	113.71	111.20
5	B	1603	CHD	C11-C12-C13	2.48	113.72	111.20
5	B	1604	CHD	C11-C12-C13	2.48	113.72	111.20
5	B	1604	CHD	C6-C5-C4	2.49	113.83	111.05
5	B	1605	CHD	C6-C5-C4	2.51	113.85	111.05
5	B	1603	CHD	C6-C5-C4	2.56	113.91	111.05
5	A	701	CHD	C17-C13-C14	2.62	102.70	100.05
5	A	702	CHD	C6-C5-C4	2.69	114.06	111.05
5	B	1605	CHD	C17-C13-C14	2.72	102.80	100.05
5	B	1603	CHD	C17-C13-C14	2.80	102.88	100.05
5	B	1603	CHD	C17-C13-C12	2.86	120.22	117.68
5	A	703	CHD	C17-C13-C12	3.09	120.42	117.68
5	B	1604	CHD	C17-C13-C12	3.10	120.43	117.68
5	A	702	CHD	C17-C13-C12	3.16	120.48	117.68
5	A	702	CHD	C17-C13-C14	3.18	103.27	100.05
5	B	1604	CHD	C17-C13-C14	3.21	103.30	100.05
5	A	703	CHD	C17-C13-C14	3.30	103.39	100.05
5	A	701	CHD	C17-C13-C12	4.02	121.24	117.68
5	B	1605	CHD	C17-C13-C12	4.07	121.28	117.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	CHD	1	0
6	A	707	GOL	3	0
4	B	1602	IMD	1	0
5	B	1603	CHD	2	0
5	B	1605	CHD	1	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(Å ²)	Q<0.9
1	A	359/359 (100%)	0.84	38 (10%) 8 9	10, 19, 33, 44	1 (0%)
1	B	359/359 (100%)	0.81	39 (10%) 7 8	10, 19, 34, 43	0
All	All	718/718 (100%)	0.82	77 (10%) 8 8	10, 19, 34, 44	1 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	CYS	16.6
1	A	359	GLU	10.9
1	B	857	ALA	10.7
1	B	860	CYS	9.5
1	B	854	GLN	8.8
1	A	355	VAL	8.7
1	A	358	LYS	8.4
1	B	862	VAL	8.3
1	A	362	VAL	8.2
1	A	356	LEU	8.1
1	B	858	LYS	7.8
1	B	853	SER	7.6
1	B	861	GLY	6.6
1	A	395[A]	CYS	6.6
1	B	855	VAL	6.3
1	B	565	ARG	6.0
1	B	923	LEU	5.9
1	B	713	VAL	5.6
1	B	856	LEU	5.5
1	A	212	GLN	5.3
1	A	250	LEU	5.0
1	A	96	ARG	4.7
1	A	423	LEU	4.7
1	A	246	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	354	GLN	4.5
1	A	213	VAL	4.4
1	B	566	LYS	4.3
1	B	715[A]	ARG	4.0
1	A	357	ALA	4.0
1	B	859	GLU	3.8
1	A	363	GLU	3.6
1	B	596	ARG	3.6
1	B	712	GLN	3.6
1	A	214	GLY	3.6
1	B	912	ARG	3.4
1	B	852	TYR	3.4
1	B	755	GLU	3.4
1	A	249	PRO	3.3
1	B	714	GLY	3.3
1	A	179[A]	ARG	3.2
1	A	216	LYS	3.1
1	A	65	ARG	3.1
1	A	153	ASN	3.1
1	A	407	VAL	3.0
1	A	392	ASN	2.9
1	A	361	GLY	2.8
1	B	600	THR	2.8
1	B	750	LEU	2.8
1	A	203	LEU	2.7
1	A	276	TYR	2.7
1	A	215	ARG	2.6
1	A	251	GLU	2.6
1	B	799	LEU	2.6
1	B	907	VAL	2.5
1	B	808	MET	2.5
1	B	679[A]	ARG	2.5
1	B	743	LYS	2.5
1	B	863	GLU	2.5
1	B	865	ILE	2.4
1	A	243	LYS	2.4
1	A	100	THR	2.4
1	B	653	ASN	2.3
1	A	247	HIS	2.3
1	B	645[A]	LYS	2.3
1	B	747	HIS	2.3
1	B	606	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	164[A]	ARG	2.1
1	B	605	ASN	2.1
1	A	206	ILE	2.1
1	B	892	ASN	2.1
1	A	280	VAL	2.1
1	A	307	PRO	2.0
1	B	776	TYR	2.0
1	A	141[A]	GLU	2.0
1	A	328	LYS	2.0
1	B	675[A]	GLU	2.0
1	B	703	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, 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
6	GOL	A	707	6/6	0.81	0.25	6.61	29,29,29,29	0
4	IMD	A	1601	5/5	0.52	0.27	4.57	37,37,37,37	0
4	IMD	B	1602	5/5	0.62	0.23	4.35	36,36,36,36	0
5	CHD	A	701	29/29	0.89	0.14	1.39	20,21,24,25	0
5	CHD	B	1605	29/29	0.89	0.14	1.18	20,21,25,26	0
5	CHD	B	1603	29/29	0.56	0.17	1.05	33,33,36,36	0
5	CHD	A	703	29/29	0.68	0.18	0.82	35,35,36,37	0
5	CHD	B	1604	29/29	0.71	0.17	0.52	41,41,43,43	0
5	CHD	A	702	29/29	0.77	0.13	0.42	31,31,33,33	0
2	CL	A	802	1/1	0.99	0.09	-0.96	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	FES	A	1501	4/4	0.99	0.06	-1.63	15,16,16,17	0
3	FES	B	1502	4/4	0.99	0.05	-1.96	16,16,16,17	0
2	CL	B	924	1/1	0.99	0.07	-2.56	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.