



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:39 pm GMT

PDB ID : 2QD4
Title : Wild type human ferrochelatase crystallized with MnCl₂
Authors : Medlock, A.E.; Dailey, T.A.; Ross, T.A.; Dailey, H.A.; Lanzilotta, W.N.
Deposited on : 2007-06-20
Resolution : 2.00 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

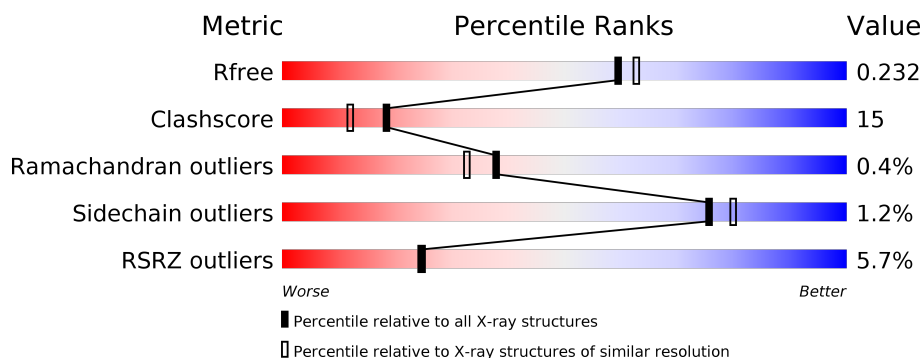
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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>6%</div> <div> <div></div> <div>71%</div> <div>28%</div> </div> <div></div> </div>
1	B	359	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>30%</div> </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	CHD	A	801	-	-	-	X
4	CHD	B	928	-	-	-	X
5	GOL	A	601	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6580 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.

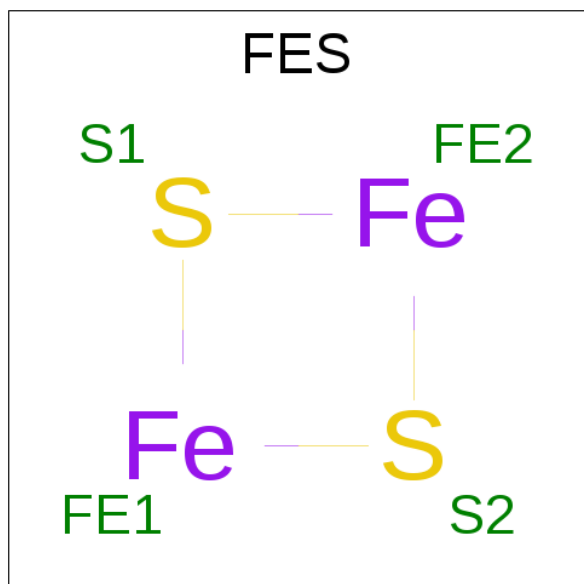
- Molecule 1 is a protein called Ferrochelatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	8	0
			2949	1872	515	541	21			
1	B	359	Total	C	N	O	S	0	6	0
			2937	1867	510	539	21			

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

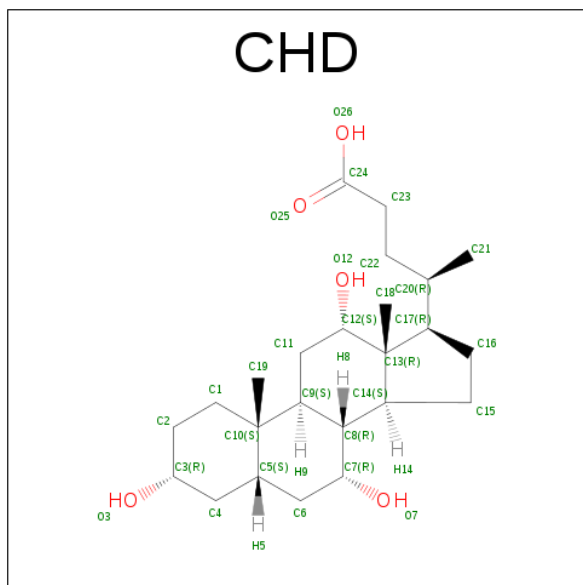
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cl	0	0
			2	2		
2	A	4	Total	Cl	0	0
			4	4		

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



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

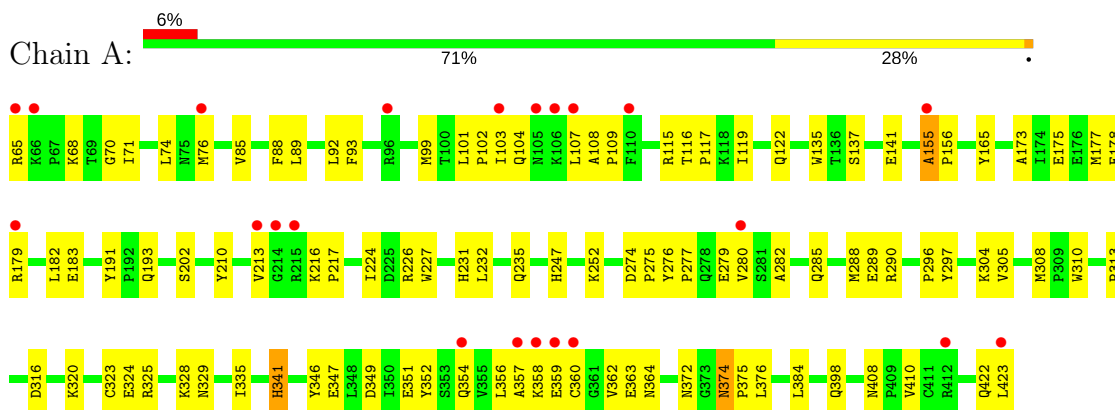
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	253	Total	O	0	0
			253	253		
6	B	247	Total	O	0	0
			247	247		

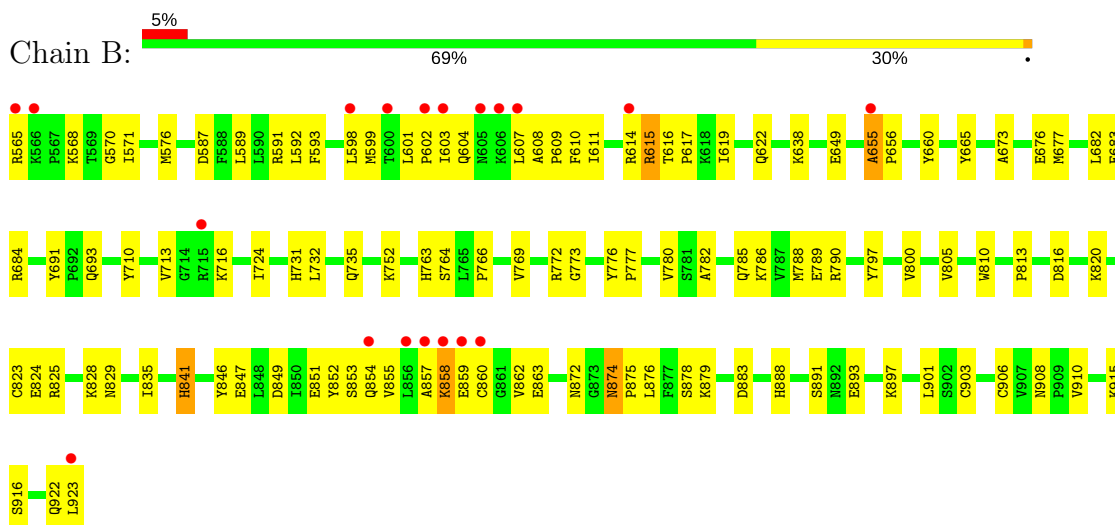
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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	87.59Å 93.06Å 109.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.85 – 2.00 42.85 – 1.99	Depositor EDS
% Data completeness (in resolution range)	93.3 (42.85-2.00) 96.1 (42.85-1.99)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 1.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.230 0.211 , 0.232	Depositor DCC
R_{free} test set	2928 reflections (5.18%)	DCC
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6580	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 46.63 % 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 1.1134e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, 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	0.30	0/3019	0.59	1/4087 (0.0%)
1	B	0.31	0/3007	0.58	1/4072 (0.0%)
All	All	0.31	0/6026	0.58	2/8159 (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	A	224	ILE	N-CA-C	-5.78	95.38	111.00
1	B	724	ILE	N-CA-C	-5.67	95.68	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	2949	0	2946	92	0
1	B	2937	0	2936	94	0
2	A	4	0	0	2	0
2	B	2	0	0	2	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	87	0	117	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	87	0	117	11	0
5	A	6	0	8	3	0
6	A	253	0	0	3	0
6	B	247	0	0	6	0
All	All	6580	0	6124	182	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 15.

All (182) 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:422:GLN:HG2	1:A:423:LEU:HD22	1.42	0.99
1:B:823[B]:CYS:SG	1:B:862:VAL:HG12	2.09	0.91
1:A:155:ALA:HB1	1:A:156:PRO:CD	2.00	0.90
1:B:655:ALA:HB1	1:B:656:PRO:CD	2.01	0.89
1:A:323[B]:CYS:SG	1:A:362:VAL:HG12	2.14	0.87
1:B:922:GLN:O	1:B:923:LEU:HB2	1.79	0.80
1:A:155:ALA:HB1	1:A:156:PRO:HD3	1.62	0.80
1:B:800:VAL:HG12	1:B:813:PRO:HG2	1.64	0.79
1:B:568:LYS:HE3	1:B:683:GLU:OE1	1.84	0.77
1:B:855:VAL:O	1:B:859:GLU:HG2	1.85	0.77
1:A:277:PRO:HB3	5:A:601:GOL:H2	1.69	0.73
1:B:908:ASN:OD1	1:B:910:VAL:HG12	1.88	0.73
1:A:285:GLN:O	1:A:289:GLU:HG3	1.89	0.72
1:B:598:LEU:HD11	4:B:928:CHD:H162	1.71	0.72
1:B:710:TYR:HA	1:B:713:VAL:HG12	1.72	0.71
1:B:601:LEU:HB2	1:B:604:GLN:HG3	1.74	0.70
1:A:374:ASN:ND2	1:A:376:LEU:H	1.90	0.70
1:A:76[B]:MET:HG2	1:A:191:TYR:OH	1.92	0.69
1:B:772:ARG:HD2	6:B:1052:HOH:O	1.91	0.69
1:B:565:ARG:HG3	1:B:656:PRO:HG2	1.76	0.68
1:B:874:ASN:ND2	1:B:876:LEU:H	1.91	0.68
1:A:374:ASN:HD22	1:A:374:ASN:C	1.98	0.67
1:B:655:ALA:HB1	1:B:656:PRO:HD3	1.75	0.67
1:A:422:GLN:O	1:A:423:LEU:HB2	1.94	0.67
1:A:374:ASN:HD22	1:A:375:PRO:N	1.93	0.67
1:B:874:ASN:HD22	1:B:874:ASN:C	1.99	0.66
1:B:615:ARG:HH12	4:B:928:CHD:H11	1.60	0.66
1:A:175:GLU:O	1:A:179[B]:ARG:HG2	1.94	0.65
1:A:408:ASN:OD1	1:A:410:VAL:HG12	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:874:ASN:HD22	1:B:875:PRO:N	1.95	0.65
1:B:785:GLN:O	1:B:789:GLU:HG3	1.97	0.64
1:B:610:PHE:CE2	1:B:614:ARG:HD2	2.34	0.63
1:B:776:TYR:HB3	1:B:777:PRO:HD3	1.79	0.63
1:A:357:ALA:HA	1:A:360[A]:CYS:SG	2.39	0.62
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.79	0.62
1:A:68:LYS:CB	1:A:155:ALA:HB3	2.30	0.62
1:B:601:LEU:HD21	4:B:926:CHD:H7	1.81	0.62
1:B:649:GLU:HB3	6:B:1092:HOH:O	1.98	0.62
1:B:608:ALA:HB3	1:B:609:PRO:HD3	1.81	0.62
1:A:276:TYR:HB3	1:A:277:PRO:HD3	1.81	0.61
1:A:320:LYS:O	1:A:324:GLU:HG3	2.01	0.61
1:B:820:LYS:O	1:B:824:GLU:HG3	2.00	0.61
1:B:857:ALA:O	1:B:862:VAL:HG13	2.00	0.60
1:B:568:LYS:CB	1:B:655:ALA:HB3	2.33	0.59
1:B:610:PHE:CZ	1:B:614:ARG:HD2	2.38	0.58
1:A:68:LYS:HB3	1:A:155:ALA:HB3	1.85	0.58
1:B:769:VAL:O	1:B:772:ARG:HG2	2.03	0.58
1:B:589:LEU:HD21	1:B:619:ILE:HD12	1.83	0.58
1:A:313:PRO:HG2	1:B:773:GLY:HA2	1.86	0.58
1:B:576[B]:MET:HG2	1:B:691:TYR:OH	2.04	0.57
1:A:347:GLU:HA	1:A:351:GLU:HG2	1.87	0.56
1:B:805:VAL:HG21	4:B:928:CHD:H112	1.87	0.56
1:B:849:ASP:O	1:B:854:GLN:HG3	2.06	0.56
1:B:655:ALA:HB1	1:B:656:PRO:HD2	1.84	0.56
1:A:76[A]:MET:HG3	1:A:165:TYR:CD1	2.41	0.55
1:B:847:GLU:HG3	1:B:851:GLU:OE1	2.07	0.55
1:B:854:GLN:O	1:B:858:LYS:HG2	2.06	0.55
1:B:763:HIS:HD2	1:B:764:SER:O	1.89	0.54
1:A:155:ALA:CB	1:A:156:PRO:CD	2.79	0.54
1:B:616:THR:HB	1:B:617:PRO:HD3	1.89	0.54
1:B:576[A]:MET:HG3	1:B:665:TYR:CD1	2.43	0.54
5:A:601:GOL:H31	1:B:777:PRO:CB	2.38	0.54
1:B:888:HIS:ND1	1:B:893[A]:GLU:HG3	2.23	0.54
1:A:341:HIS:HB2	2:A:701:CL:CL	2.45	0.54
1:B:655:ALA:CB	1:B:656:PRO:CD	2.81	0.54
1:B:816:ASP:HB3	1:B:852:TYR:CE1	2.43	0.54
1:A:252:LYS:HE2	1:A:363:GLU:OE1	2.08	0.53
1:B:915:LYS:HG3	1:B:916:SER:N	2.23	0.53
1:A:247:HIS:HE1	6:A:929:HOH:O	1.91	0.53
1:B:788:MET:HG3	1:B:797:TYR:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:GLY:HA3	1:B:682:LEU:HD13	1.90	0.53
1:B:810:TRP:CH2	4:B:928:CHD:H213	2.45	0.52
1:B:589:LEU:HD21	1:B:619:ILE:CD1	2.40	0.52
5:A:601:GOL:H31	1:B:777:PRO:HB3	1.91	0.52
1:B:891:SER:OG	1:B:893[A]:GLU:HG2	2.10	0.52
1:B:752:LYS:HE2	1:B:863:GLU:OE1	2.10	0.52
1:A:349:ASP:O	1:A:354:GLN:HG3	2.10	0.51
1:A:89:LEU:HD21	1:A:119:ILE:CD1	2.41	0.51
1:A:89:LEU:HD21	1:A:119:ILE:HD12	1.91	0.51
1:B:568:LYS:HB3	1:B:655:ALA:HB3	1.92	0.51
1:B:874:ASN:HD22	1:B:876:LEU:H	1.57	0.51
1:B:766:PRO:HG2	4:B:926:CHD:H11	1.92	0.51
1:A:71:ILE:N	1:A:71:ILE:HD12	2.26	0.51
1:A:226:ARG:HD3	1:A:279:GLU:OE2	2.10	0.51
1:B:607:LEU:O	1:B:611:ILE:HG13	2.11	0.51
1:A:285:GLN:HG2	1:B:782:ALA:HB1	1.93	0.50
1:B:825:ARG:HH11	1:B:825:ARG:HG3	1.76	0.50
1:B:752:LYS:HD3	1:B:829:ASN:HD21	1.76	0.50
1:A:325:ARG:HH11	1:A:325:ARG:HG3	1.75	0.50
1:A:328:LYS:CB	1:A:363:GLU:HG3	2.41	0.50
1:A:316:ASP:HB3	1:A:352:TYR:CE1	2.47	0.50
1:B:788:MET:HG3	1:B:797:TYR:CD2	2.47	0.50
1:A:347:GLU:HA	1:A:351:GLU:CG	2.42	0.50
1:A:93:PHE:HD2	1:A:99:MET:HE1	1.77	0.50
1:A:115:ARG:NH1	6:A:870:HOH:O	2.44	0.50
1:A:231:HIS:CE1	1:A:232:LEU:HG	2.46	0.49
1:A:193:GLN:HG2	1:A:280:VAL:HA	1.94	0.49
1:A:354:GLN:O	1:A:358:LYS:HB2	2.13	0.49
1:A:102:PRO:O	1:A:107:LEU:HD12	2.11	0.49
1:B:841:HIS:HB2	2:B:924:CL:CL	2.50	0.49
1:A:356:LEU:O	1:A:359:GLU:HG3	2.13	0.48
1:A:235:GLN:HG3	1:A:290:ARG:NH2	2.28	0.48
1:B:576[A]:MET:HG3	1:B:665:TYR:CE1	2.48	0.48
1:A:305:VAL:HG21	4:A:801:CHD:H112	1.95	0.48
1:A:374:ASN:HD22	1:A:376:LEU:H	1.60	0.48
1:A:323[B]:CYS:HB2	1:A:360[B]:CYS:SG	2.53	0.48
1:B:735:GLN:HG3	1:B:790:ARG:NH2	2.28	0.47
1:B:602:PRO:O	1:B:603:ILE:C	2.52	0.47
1:B:782:ALA:O	1:B:786:LYS:HG2	2.14	0.47
1:A:329:ASN:HD22	1:A:364:ASN:HB2	1.79	0.47
1:A:70:GLY:HA3	1:A:182:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:THR:HB	1:A:117:PRO:HD3	1.96	0.47
1:A:92:LEU:HD13	4:A:801:CHD:H62	1.97	0.47
1:A:313:PRO:CG	1:B:773:GLY:HA2	2.44	0.47
4:B:926:CHD:H61	6:B:1118:HOH:O	2.15	0.47
1:A:122:GLN:HG2	1:A:346:TYR:CE2	2.50	0.46
1:B:853:SER:O	1:B:857:ALA:HB3	2.14	0.46
1:A:175:GLU:O	1:A:179[A]:ARG:HG3	2.15	0.46
1:A:210:TYR:HA	1:A:213:VAL:HG12	1.98	0.46
1:A:99:MET:HG2	4:A:802:CHD:H62	1.98	0.46
1:A:89:LEU:HD11	1:A:119:ILE:HD12	1.97	0.46
1:A:76[A]:MET:HG3	1:A:165:TYR:HD1	1.80	0.46
1:A:216:LYS:HE2	1:A:217:PRO:O	2.16	0.46
1:B:587:ASP:O	1:B:591:ARG:HG3	2.16	0.46
1:A:65:ARG:HG3	1:A:156:PRO:HG2	1.97	0.46
1:A:74:LEU:HD13	1:A:202:SER:HB3	1.97	0.46
1:B:693:GLN:HG2	1:B:780:VAL:HA	1.97	0.46
1:B:824:GLU:HG2	1:B:860[B]:CYS:SG	2.56	0.45
1:A:310:TRP:CH2	4:A:801:CHD:H213	2.51	0.45
1:A:101:LEU:HB2	1:A:104:GLN:HG3	1.97	0.45
1:B:660:TYR:HE2	1:B:676:GLU:HG2	1.81	0.45
1:B:888:HIS:CE1	1:B:893[A]:GLU:HG3	2.51	0.45
1:B:571:ILE:HD12	1:B:571:ILE:N	2.32	0.45
1:A:135:TRP:CE3	1:A:372:ASN:HB3	2.51	0.45
1:A:288:MET:HG3	1:A:297:TYR:CD2	2.52	0.45
1:A:115:ARG:HH12	4:A:802:CHD:H211	1.81	0.44
1:A:115:ARG:NH1	4:A:802:CHD:H211	2.32	0.44
1:A:102:PRO:O	1:A:103:ILE:C	2.55	0.44
1:A:374:ASN:ND2	1:A:374:ASN:C	2.70	0.44
1:B:684:ARG:NH2	6:B:932:HOH:O	2.31	0.44
1:B:915:LYS:HE2	6:B:1048:HOH:O	2.16	0.44
1:A:282:ALA:HB1	1:B:785:GLN:HG2	1.98	0.44
1:A:360[A]:CYS:SG	1:A:362:VAL:HG13	2.57	0.44
1:A:137:SER:O	1:A:141:GLU:HG3	2.18	0.43
1:B:599:MET:HB2	4:B:926:CHD:H62	2.01	0.43
1:B:622:GLN:HG2	1:B:846:TYR:CE2	2.54	0.43
1:B:638:LYS:NZ	6:B:1011:HOH:O	2.50	0.43
1:B:673:ALA:O	1:B:677:MET:HG3	2.19	0.42
1:A:329:ASN:ND2	1:A:364:ASN:HB2	2.33	0.42
1:B:593:PHE:CE1	1:B:611:ILE:HG22	2.54	0.42
1:B:903:CYS:HB2	1:B:906:CYS:HB2	2.02	0.42
1:B:598:LEU:HD12	4:B:928:CHD:O25	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LYS:HB2	1:A:216:LYS:HE3	1.81	0.42
1:A:335:ILE:O	1:A:335:ILE:HG13	2.20	0.42
1:A:135:TRP:CZ3	1:A:372:ASN:HB3	2.55	0.42
1:B:841:HIS:CD2	1:B:841:HIS:N	2.87	0.42
1:A:173:ALA:O	1:A:177:MET:HG3	2.20	0.41
1:B:716[B]:LYS:HB2	1:B:716[B]:LYS:HE3	1.90	0.41
1:A:398:GLN:HG2	2:A:703:CL:CL	2.58	0.41
1:A:296:PRO:HB2	1:B:901:LEU:HB2	2.02	0.41
1:A:304:LYS:NZ	1:A:308:MET:O	2.53	0.41
1:A:305:VAL:HG11	4:A:801:CHD:H21	2.03	0.41
1:A:325:ARG:HG3	1:A:325:ARG:NH1	2.35	0.41
1:A:85:VAL:O	1:A:88:PHE:HB3	2.20	0.41
1:B:879:LYS:HG2	1:B:883[A]:ASP:OD2	2.20	0.41
1:A:103:ILE:HG13	1:A:107:LEU:HG	2.02	0.41
1:A:155:ALA:HB1	1:A:156:PRO:HD2	1.95	0.41
1:A:252:LYS:HD3	1:A:329:ASN:HD21	1.85	0.41
1:A:328:LYS:HB2	1:A:363:GLU:HG3	2.02	0.41
1:A:328:LYS:HB3	1:A:363:GLU:HG3	2.01	0.41
1:A:217:PRO:HB2	6:A:964:HOH:O	2.19	0.41
1:A:68:LYS:HE2	1:A:183:GLU:OE2	2.21	0.41
1:B:731:HIS:CE1	1:B:732:LEU:HG	2.56	0.41
1:A:274:ASP:HA	1:A:275:PRO:HD3	1.80	0.41
1:A:227:TRP:CE3	1:A:384:LEU:HD11	2.56	0.40
1:B:710:TYR:HA	1:B:713:VAL:CG1	2.48	0.40
1:B:828:LYS:CB	1:B:863:GLU:HG3	2.51	0.40
1:B:835:ILE:O	1:B:835:ILE:HG13	2.22	0.40
1:B:897:LYS:HB3	2:B:925:CL:CL	2.58	0.40
1:B:592:LEU:HD11	4:B:928:CHD:H7	2.03	0.40
1:B:922:GLN:HG2	1:B:923:LEU:CD2	2.52	0.40
1:B:615:ARG:NH2	4:B:926:CHD:H211	2.37	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	365/359 (102%)	352 (96%)	12 (3%)	1 (0%)	44	40
1	B	363/359 (101%)	351 (97%)	10 (3%)	2 (1%)	28	21
All	All	728/718 (101%)	703 (97%)	22 (3%)	3 (0%)	38	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ALA
1	B	655	ALA
1	B	872	ASN

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	332/324 (102%)	329 (99%)	3 (1%)	82	87
1	B	330/324 (102%)	325 (98%)	5 (2%)	70	74
All	All	662/648 (102%)	654 (99%)	8 (1%)	75	80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	178	GLU
1	A	341	HIS
1	A	374	ASN
1	B	615	ARG
1	B	841	HIS
1	B	858	LYS
1	B	874	ASN
1	B	878	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	HIS
1	A	314	GLN
1	A	329	ASN
1	A	354	GLN
1	A	364	ASN
1	A	374	ASN
1	A	421	GLN
1	B	712	GLN
1	B	731	HIS
1	B	763	HIS
1	B	829	ASN
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 ⓘ

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	501	-	0,4,4	0.00	-	0,4,4	0.00	-
5	GOL	A	601	-	5,5,5	0.10	0	5,5,5	0.15	0
4	CHD	A	801	-	29,32,32	2.06	13 (44%)	47,51,51	1.73	14 (29%)
4	CHD	A	802	-	29,32,32	1.99	11 (37%)	47,51,51	1.67	13 (27%)
4	CHD	A	803	-	29,32,32	2.07	13 (44%)	47,51,51	1.73	13 (27%)
3	FES	B	502	-	0,4,4	0.00	-	0,4,4	0.00	-
4	CHD	B	926	-	29,32,32	1.98	12 (41%)	47,51,51	1.73	13 (27%)
4	CHD	B	927	-	29,32,32	2.01	12 (41%)	47,51,51	1.76	15 (31%)
4	CHD	B	928	-	29,32,32	2.08	13 (44%)	47,51,51	1.72	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	501	-	-	0/0/4/4	0/1/1/1
5	GOL	A	601	-	-	0/4/4/4	0/0/0/0
4	CHD	A	801	-	-	0/7/74/74	0/4/4/4
4	CHD	A	802	-	-	0/7/74/74	0/4/4/4
4	CHD	A	803	-	-	0/7/74/74	0/4/4/4
3	FES	B	502	-	-	0/0/4/4	0/1/1/1
4	CHD	B	926	-	-	0/7/74/74	0/4/4/4
4	CHD	B	927	-	-	0/7/74/74	0/4/4/4
4	CHD	B	928	-	-	0/7/74/74	0/4/4/4

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	CHD	C20-C17	2.01	1.58	1.54
4	B	926	CHD	O7-C7	2.04	1.47	1.43
4	B	928	CHD	C4-C3	2.06	1.55	1.51
4	B	927	CHD	C20-C17	2.06	1.58	1.54
4	A	801	CHD	C20-C17	2.07	1.58	1.54
4	B	927	CHD	O7-C7	2.08	1.47	1.43
4	A	803	CHD	C4-C3	2.09	1.55	1.51
4	A	802	CHD	C19-C10	2.09	1.58	1.54
4	A	801	CHD	C8-C9	2.10	1.58	1.53
4	B	928	CHD	C19-C10	2.11	1.58	1.54
4	A	803	CHD	C8-C9	2.14	1.58	1.53
4	B	926	CHD	C4-C3	2.14	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	CHD	C19-C10	2.16	1.58	1.54
4	B	928	CHD	C20-C17	2.16	1.58	1.54
4	B	926	CHD	C19-C10	2.17	1.58	1.54
4	B	928	CHD	C8-C9	2.17	1.58	1.53
4	A	801	CHD	C4-C3	2.18	1.55	1.51
4	A	802	CHD	O7-C7	2.19	1.48	1.43
4	B	927	CHD	C8-C14	2.31	1.58	1.53
4	B	927	CHD	C19-C10	2.33	1.58	1.54
4	A	803	CHD	C19-C10	2.34	1.58	1.54
4	B	926	CHD	C8-C14	2.37	1.58	1.53
4	A	802	CHD	C8-C14	2.39	1.58	1.53
4	B	926	CHD	C13-C12	2.41	1.58	1.54
4	A	801	CHD	C8-C7	2.46	1.57	1.53
4	B	928	CHD	C8-C14	2.47	1.58	1.53
4	B	926	CHD	C8-C7	2.50	1.57	1.53
4	A	803	CHD	C8-C14	2.50	1.58	1.53
4	B	927	CHD	C13-C12	2.51	1.58	1.54
4	A	802	CHD	C13-C12	2.53	1.58	1.54
4	B	928	CHD	C8-C7	2.53	1.57	1.53
4	B	926	CHD	C18-C13	2.55	1.58	1.54
4	A	801	CHD	C13-C12	2.55	1.58	1.54
4	A	802	CHD	C8-C7	2.55	1.57	1.53
4	B	927	CHD	C10-C9	2.60	1.61	1.56
4	B	927	CHD	C18-C13	2.61	1.58	1.54
4	A	802	CHD	C18-C13	2.63	1.58	1.54
4	A	803	CHD	C13-C12	2.63	1.58	1.54
4	B	928	CHD	C13-C12	2.65	1.58	1.54
4	A	801	CHD	C8-C14	2.66	1.59	1.53
4	A	803	CHD	C18-C13	2.68	1.58	1.54
4	B	926	CHD	C10-C9	2.72	1.61	1.56
4	A	801	CHD	C18-C13	2.74	1.58	1.54
4	B	927	CHD	C8-C7	2.76	1.58	1.53
4	A	803	CHD	O12-C12	2.77	1.48	1.43
4	B	928	CHD	C18-C13	2.77	1.58	1.54
4	A	802	CHD	O12-C12	2.81	1.48	1.43
4	B	927	CHD	O12-C12	2.84	1.48	1.43
4	A	803	CHD	C8-C7	2.86	1.58	1.53
4	A	802	CHD	C6-C5	2.90	1.58	1.53
4	A	802	CHD	C10-C9	2.90	1.61	1.56
4	A	801	CHD	O12-C12	2.95	1.48	1.43
4	B	926	CHD	C6-C5	2.97	1.58	1.53
4	B	927	CHD	C6-C5	2.99	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	CHD	C10-C9	3.01	1.61	1.56
4	B	928	CHD	C10-C9	3.06	1.62	1.56
4	B	926	CHD	O12-C12	3.10	1.48	1.43
4	B	928	CHD	C6-C5	3.16	1.59	1.53
4	A	803	CHD	C6-C5	3.16	1.59	1.53
4	A	801	CHD	C6-C5	3.18	1.59	1.53
4	B	928	CHD	O12-C12	3.22	1.49	1.43
4	A	801	CHD	C10-C9	3.23	1.62	1.56
4	A	802	CHD	C16-C17	3.37	1.61	1.54
4	A	803	CHD	C16-C17	3.48	1.61	1.54
4	B	928	CHD	C16-C17	3.51	1.61	1.54
4	A	801	CHD	C16-C17	3.51	1.61	1.54
4	B	927	CHD	C16-C17	3.52	1.61	1.54
4	A	801	CHD	C11-C9	3.54	1.59	1.53
4	B	926	CHD	C16-C17	3.65	1.62	1.54
4	B	928	CHD	C11-C9	3.72	1.59	1.53
4	A	802	CHD	C11-C9	3.91	1.60	1.53
4	B	926	CHD	C11-C9	3.94	1.60	1.53
4	B	927	CHD	C11-C9	4.10	1.60	1.53
4	A	803	CHD	C11-C9	4.11	1.60	1.53

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	CHD	C18-C13-C12	-4.23	104.78	109.08
4	B	928	CHD	C18-C13-C12	-4.14	104.87	109.08
4	A	803	CHD	C18-C13-C12	-3.95	105.06	109.08
4	B	927	CHD	C18-C13-C12	-3.92	105.09	109.08
4	A	802	CHD	C18-C13-C12	-3.84	105.17	109.08
4	B	926	CHD	C18-C13-C12	-3.65	105.36	109.08
4	B	928	CHD	C19-C10-C1	-3.59	102.34	108.24
4	A	801	CHD	C19-C10-C1	-3.55	102.41	108.24
4	B	927	CHD	C19-C10-C1	-3.52	102.45	108.24
4	A	803	CHD	C19-C10-C1	-3.49	102.50	108.24
4	B	926	CHD	O12-C12-C13	-3.27	105.66	111.12
4	A	801	CHD	O12-C12-C13	-3.26	105.68	111.12
4	B	928	CHD	O12-C12-C13	-3.25	105.70	111.12
4	A	802	CHD	O12-C12-C13	-3.20	105.78	111.12
4	B	927	CHD	O12-C12-C13	-3.19	105.79	111.12
4	A	802	CHD	C19-C10-C1	-3.14	103.09	108.24
4	A	803	CHD	O12-C12-C13	-3.12	105.92	111.12
4	B	926	CHD	C19-C10-C1	-3.11	103.14	108.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	926	CHD	C6-C5-C10	-2.82	109.58	112.66
4	B	926	CHD	C9-C11-C12	-2.66	110.81	114.32
4	B	926	CHD	C9-C8-C7	-2.61	108.86	111.92
4	B	927	CHD	C6-C5-C10	-2.58	109.84	112.66
4	A	801	CHD	C16-C17-C13	-2.58	101.00	103.57
4	B	928	CHD	C9-C11-C12	-2.55	110.97	114.32
4	B	926	CHD	C16-C17-C13	-2.51	101.07	103.57
4	A	802	CHD	C6-C5-C10	-2.50	109.93	112.66
4	A	802	CHD	C9-C8-C7	-2.48	109.01	111.92
4	A	803	CHD	C9-C11-C12	-2.46	111.08	114.32
4	A	803	CHD	C6-C5-C10	-2.41	110.02	112.66
4	B	927	CHD	C11-C9-C10	-2.40	111.20	113.74
4	A	802	CHD	C9-C11-C12	-2.36	111.21	114.32
4	B	928	CHD	C6-C5-C10	-2.36	110.08	112.66
4	A	801	CHD	C9-C11-C12	-2.33	111.26	114.32
4	B	928	CHD	C16-C17-C13	-2.33	101.25	103.57
4	A	801	CHD	C6-C5-C10	-2.29	110.16	112.66
4	B	927	CHD	C9-C8-C7	-2.27	109.26	111.92
4	B	927	CHD	C16-C17-C13	-2.25	101.33	103.57
4	A	803	CHD	C16-C17-C13	-2.24	101.34	103.57
4	B	927	CHD	C9-C11-C12	-2.19	111.44	114.32
4	B	928	CHD	C9-C8-C7	-2.19	109.36	111.92
4	B	928	CHD	C11-C9-C10	-2.18	111.43	113.74
4	B	926	CHD	C11-C9-C10	-2.17	111.44	113.74
4	A	801	CHD	C11-C9-C10	-2.16	111.46	113.74
4	A	801	CHD	C9-C8-C7	-2.15	109.39	111.92
4	A	802	CHD	C11-C9-C10	-2.15	111.47	113.74
4	A	803	CHD	C9-C8-C7	-2.04	109.53	111.92
4	B	927	CHD	C16-C15-C14	-2.02	101.08	105.12
4	A	802	CHD	C16-C17-C13	-2.01	101.57	103.57
4	B	928	CHD	C19-C10-C9	2.05	114.09	111.16
4	A	801	CHD	C6-C5-C4	2.06	113.47	111.13
4	B	927	CHD	C19-C10-C9	2.09	114.15	111.16
4	A	801	CHD	C1-C10-C5	2.11	111.07	107.79
4	B	926	CHD	C1-C10-C5	2.12	111.08	107.79
4	A	803	CHD	C6-C5-C4	2.13	113.54	111.13
4	A	803	CHD	C1-C10-C5	2.13	111.09	107.79
4	B	928	CHD	C1-C10-C5	2.16	111.13	107.79
4	B	928	CHD	C6-C5-C4	2.18	113.61	111.13
4	A	802	CHD	C1-C10-C5	2.23	111.25	107.79
4	A	802	CHD	C11-C12-C13	2.24	113.54	111.22
4	A	801	CHD	C19-C10-C9	2.26	114.39	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	802	CHD	C6-C5-C4	2.27	113.71	111.13
4	B	927	CHD	C1-C10-C5	2.32	111.39	107.79
4	B	927	CHD	C11-C12-C13	2.34	113.65	111.22
4	A	803	CHD	C19-C10-C9	2.37	114.55	111.16
4	B	927	CHD	C6-C5-C4	2.41	113.87	111.13
4	B	926	CHD	C11-C12-C13	2.42	113.73	111.22
4	B	928	CHD	C11-C12-C13	2.45	113.76	111.22
4	A	801	CHD	C11-C12-C13	2.46	113.77	111.22
4	A	803	CHD	C11-C12-C13	2.52	113.83	111.22
4	B	926	CHD	C6-C5-C4	2.85	114.36	111.13
4	A	802	CHD	C17-C13-C14	2.85	102.99	100.08
4	B	926	CHD	C17-C13-C14	2.88	103.02	100.08
4	B	926	CHD	C17-C13-C12	2.88	120.32	117.67
4	B	928	CHD	C17-C13-C14	2.95	103.09	100.08
4	B	927	CHD	C17-C13-C12	2.99	120.42	117.67
4	A	801	CHD	C17-C13-C14	3.07	103.21	100.08
4	A	803	CHD	C17-C13-C14	3.09	103.23	100.08
4	B	927	CHD	C17-C13-C14	3.37	103.52	100.08
4	A	803	CHD	C17-C13-C12	3.48	120.87	117.67
4	A	802	CHD	C17-C13-C12	3.54	120.92	117.67
4	B	928	CHD	C17-C13-C12	3.65	121.03	117.67
4	A	801	CHD	C17-C13-C12	3.72	121.09	117.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	GOL	3	0
4	A	801	CHD	4	0
4	A	802	CHD	3	0
4	B	926	CHD	5	0
4	B	928	CHD	6	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, 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%)	0.21	22 (6%)	22 22	12, 23, 42, 47	0
1	B	359/359 (100%)	0.20	19 (5%)	27 27	13, 23, 45, 56	0
All	All	718/718 (100%)	0.21	41 (5%)	24 25	12, 23, 43, 56	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	423	LEU	4.4
1	B	923	LEU	4.3
1	A	357	ALA	4.3
1	A	103	ILE	4.2
1	A	358	LYS	4.1
1	B	858	LYS	3.9
1	B	859	GLU	3.7
1	B	857	ALA	3.6
1	A	360[A]	CYS	3.6
1	A	65	ARG	3.6
1	B	655	ALA	3.6
1	B	715	ARG	3.5
1	B	860[A]	CYS	3.4
1	A	179[A]	ARG	3.2
1	A	155	ALA	3.1
1	A	110	PHE	3.0
1	B	606	LYS	3.0
1	A	215	ARG	2.9
1	A	106	LYS	2.9
1	B	600	THR	2.9
1	A	76[A]	MET	2.7
1	B	565	ARG	2.7
1	A	412	ARG	2.7
1	B	614	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	105	ASN	2.7
1	B	603	ILE	2.6
1	A	280	VAL	2.5
1	B	566	LYS	2.4
1	A	213	VAL	2.4
1	A	214	GLY	2.4
1	A	359	GLU	2.4
1	A	96	ARG	2.4
1	B	602	PRO	2.3
1	B	607	LEU	2.3
1	A	107	LEU	2.3
1	B	598	LEU	2.3
1	B	854	GLN	2.2
1	B	856	LEU	2.2
1	B	605	ASN	2.1
1	A	354	GLN	2.1
1	A	66	LYS	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
5	GOL	A	601	6/6	0.84	0.30	5.66	35,35,35,35	0
4	CHD	A	801	29/29	0.75	0.29	2.80	48,49,51,51	0
4	CHD	B	928	29/29	0.76	0.27	2.24	49,49,51,51	0
4	CHD	A	802	29/29	0.74	0.26	1.91	54,54,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CHD	A	803	29/29	0.79	0.35	1.80	60,60,62,62	0
4	CHD	B	927	29/29	0.70	0.35	1.36	61,61,62,62	0
4	CHD	B	926	29/29	0.72	0.24	0.90	56,57,58,58	0
3	FES	A	501	4/4	0.99	0.10	-0.79	19,19,20,20	0
3	FES	B	502	4/4	0.99	0.10	-1.09	20,20,20,21	0
2	CL	A	701	1/1	0.98	0.09	-1.55	33,33,33,33	0
2	CL	B	924	1/1	0.98	0.05	-2.45	32,32,32,32	0
2	CL	A	706	1/1	0.97	0.07	-	46,46,46,46	0
2	CL	A	703	1/1	0.98	0.08	-	39,39,39,39	0
2	CL	B	925	1/1	0.98	0.09	-	42,42,42,42	0
2	CL	A	705	1/1	0.96	0.10	-	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.