



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:09 AM GMT

PDB ID : 3HCR
Title : Human Ferrochelatase with deuteroporphyrin and Ni Bound
Authors : Medlock, A.E.; Dailey, H.A.; Lanzilotta, W.N.
Deposited on : 2009-05-06
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 (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

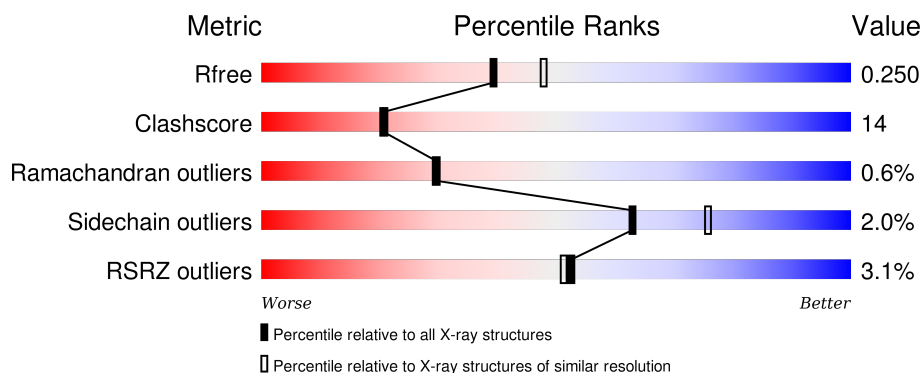
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 $\leq 5\%$. 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>4%</div> <div>76%</div> <div>23%</div> <div>.</div> </div>
1	B	359	<div> <div>2%</div> <div>74%</div> <div>25%</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
3	IMD	A	2	-	X	-	-
5	OXY	A	425	-	-	-	X
5	OXY	B	926	-	-	-	X
9	GOL	B	925	-	-	-	X

2 Entry composition [i](#)

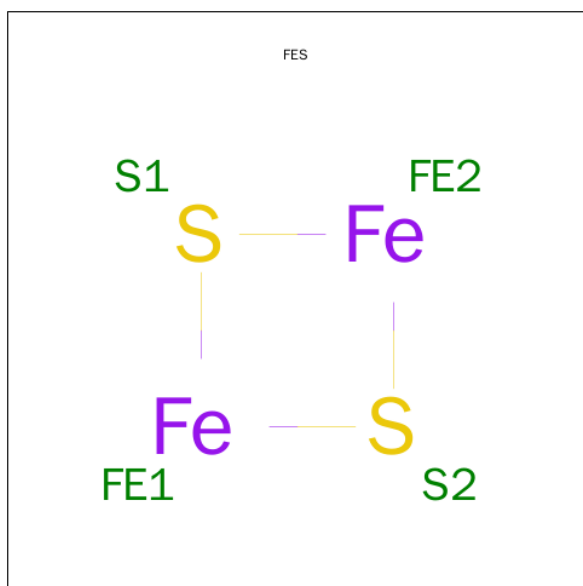
There are 10 unique types of molecules in this entry. The entry contains 6360 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, mitochondrial.

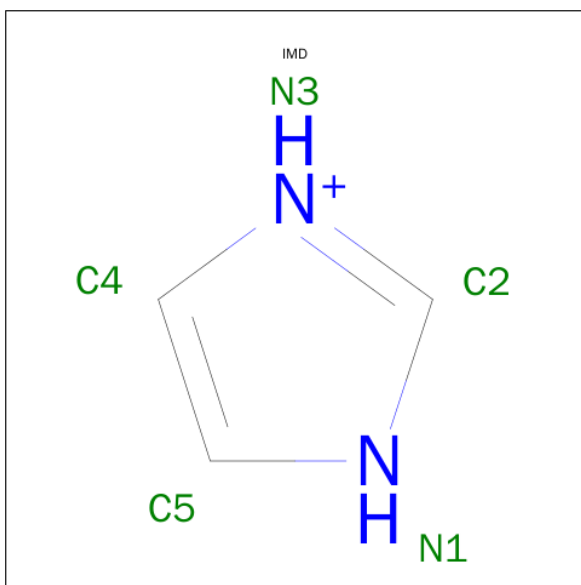
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2891	1841	503	529	18			
1	B	359	Total	C	N	O	S	0	1	0
			2900	1846	504	532	18			

- Molecule 2 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



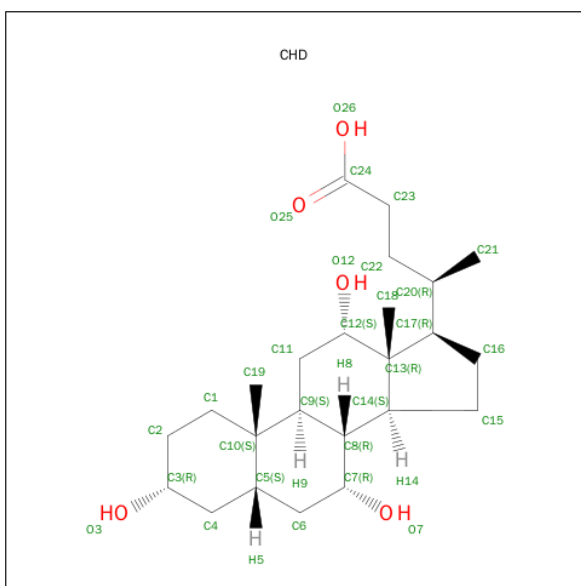
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			4	2	2		
2	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



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

- Molecule 4 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



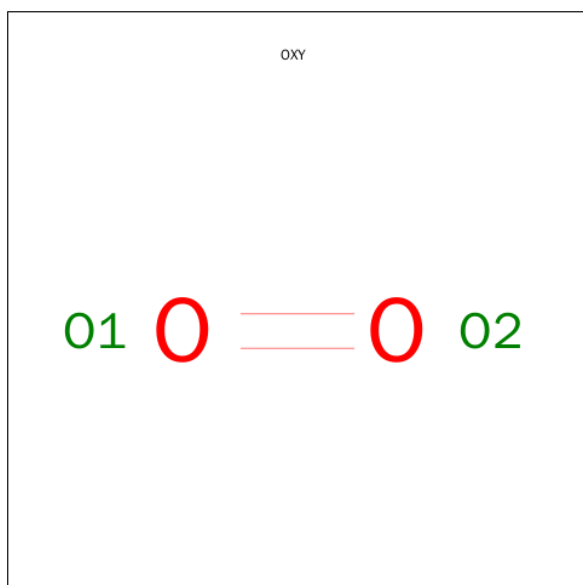
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			29	24	5		
4	A	1	Total	C	O	0	0
			29	24	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).

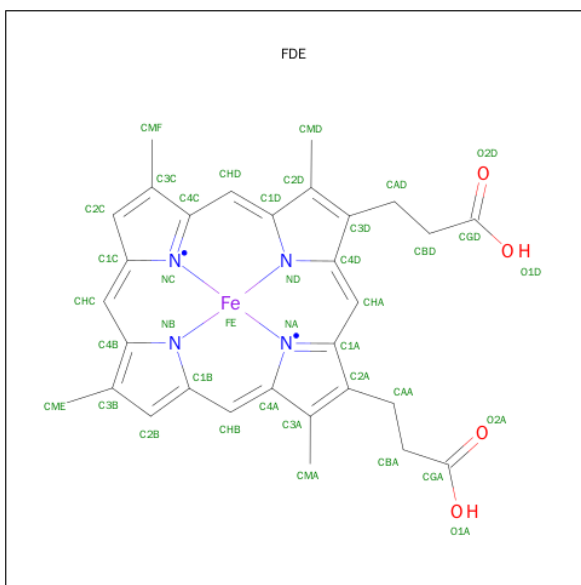


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			2	2		
5	B	1	Total	O	0	0
			2	2		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is FE(III) DEUTEROPORPHYRIN IX (three-letter code: FDE) (formula: C₃₀H₂₈FeN₄O₄).



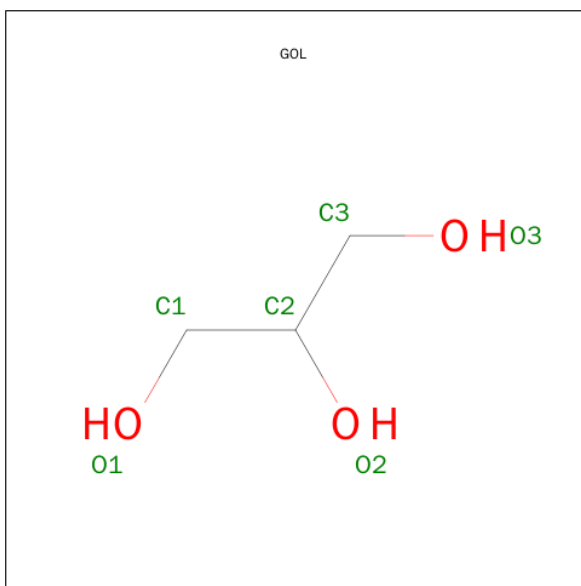
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	Fe	N	O	0	0
			39	30	1	4	4		
7	B	1	Total	C	Fe	N	O	0	0
			39	30	1	4	4		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

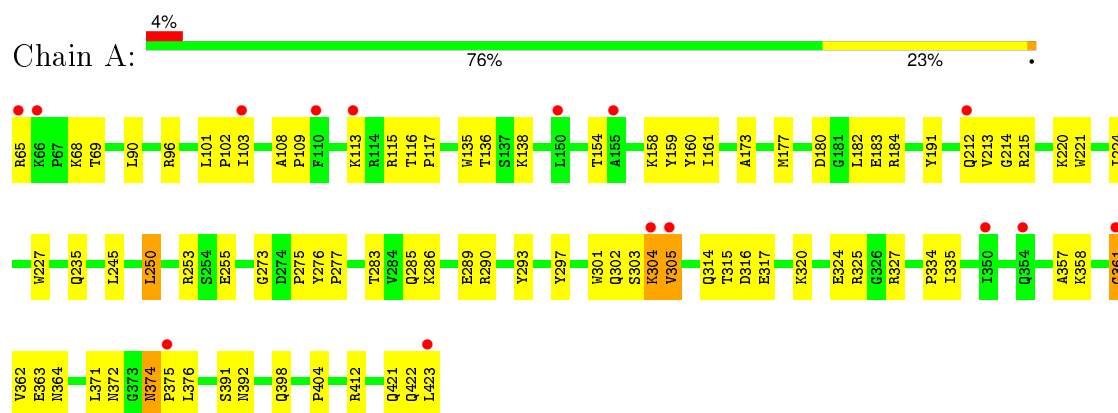
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	172	Total	O	0	0
			172	172		
10	B	164	Total	O	0	0
			164	164		

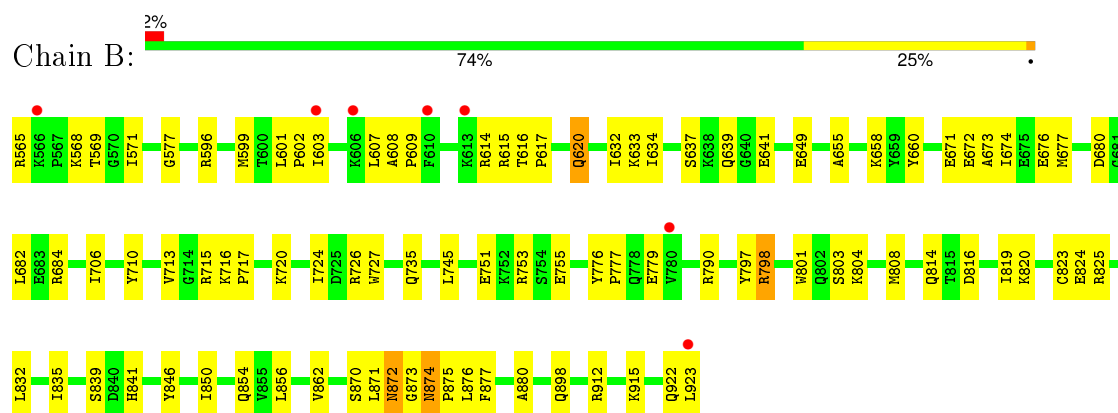
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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, mitochondrial



• Molecule 1: Ferrochelatase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.42Å 92.94Å 109.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.32 – 2.20 47.32 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.0 (47.32-2.20) 96.3 (47.32-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.20Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.215 , 0.250 0.220 , 0.250	Depositor DCC
R_{free} test set	2230 reflections (5.62%)	DCC
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.889	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 84955 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6360	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 43.94 % 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 1.6398e-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, 0.375 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, FDE, OXY, CL, SO4, IMD, CHD, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/2961	0.58	1/4011 (0.0%)
1	B	0.32	0/2970	0.58	1/4023 (0.0%)
All	All	0.33	0/5931	0.58	2/8034 (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	-5.47	96.23	111.00
1	B	724	ILE	N-CA-C	-5.14	97.12	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	2891	0	2899	90	0
1	B	2900	0	2904	88	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	5	0	4	2	0
3	B	5	0	4	1	0
4	A	58	0	78	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	58	0	78	5	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	1	0
7	A	39	0	22	0	0
7	B	39	0	22	0	0
8	A	5	0	0	0	0
8	B	5	0	0	0	0
9	B	6	0	8	3	0
10	A	172	0	0	14	0
10	B	164	0	0	14	0
All	All	6360	0	6019	174	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 (174) 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:304:LYS:H	1:A:304:LYS:HD3	1.16	1.04
1:A:297:TYR:H	1:B:898:GLN:HE22	1.03	0.94
1:A:250:LEU:HD23	1:A:250:LEU:H	1.38	0.87
1:B:682:LEU:HG	10:B:296:HOH:O	1.75	0.87
1:A:398:GLN:HE22	1:B:797:TYR:H	1.15	0.86
1:B:720:LYS:HE3	1:B:923:LEU:HD22	1.59	0.83
1:B:634:ILE:HG13	10:B:193:HOH:O	1.80	0.82
1:A:304:LYS:CD	1:A:304:LYS:H	1.94	0.80
1:B:615:ARG:HD2	4:B:924:CHD:H231	1.64	0.79
1:B:735:GLN:HG3	1:B:790:ARG:HH12	1.47	0.79
1:A:68:LYS:HE3	1:A:183:GLU:OE1	1.85	0.77
1:B:672:GLU:O	1:B:676[A]:GLU:HG2	1.85	0.76
1:B:808:MET:HB2	10:B:245:HOH:O	1.85	0.75
1:A:297:TYR:N	1:B:898:GLN:HE22	1.84	0.74
1:A:250:LEU:HB2	10:A:514:HOH:O	1.85	0.74
1:B:637:SER:O	1:B:641:GLU:HG3	1.88	0.73
1:B:912:ARG:NH2	1:B:912:ARG:HB2	2.04	0.72
1:A:115:ARG:HD2	4:A:424:CHD:H231	1.72	0.72
1:A:357:ALA:O	1:A:361:GLY:HA2	1.90	0.71
1:A:177:MET:O	1:A:182:LEU:HD13	1.90	0.71
1:A:235:GLN:HG3	1:A:290:ARG:NH2	2.05	0.70
1:B:639:GLN:HE21	1:B:873:GLY:HA2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ASN:HD22	1:A:375:PRO:CD	2.08	0.66
1:B:720:LYS:CE	1:B:923:LEU:HD22	2.26	0.65
1:B:755:GLU:HB3	10:B:243:HOH:O	1.97	0.65
1:A:108:ALA:HB3	1:A:109:PRO:HD3	1.78	0.65
1:B:912:ARG:HB3	10:B:100:HOH:O	1.96	0.65
1:B:922:GLN:HG2	1:B:923:LEU:CD1	2.27	0.65
1:B:565:ARG:HH11	1:B:565:ARG:HB2	1.62	0.65
1:A:398:GLN:HE22	1:B:797:TYR:N	1.92	0.64
1:B:614:ARG:HH11	1:B:614:ARG:HG2	1.62	0.64
1:A:374:ASN:HD22	1:A:375:PRO:HD2	1.61	0.64
1:A:422:GLN:HG2	1:A:423:LEU:HD12	1.80	0.64
1:A:314:GLN:HG2	10:A:456:HOH:O	1.97	0.64
1:B:850:ILE:O	1:B:854:GLN:HG2	1.97	0.64
1:A:235:GLN:HG3	1:A:290:ARG:HH21	1.63	0.64
1:B:856:LEU:HG	1:B:862:VAL:HG21	1.79	0.63
1:A:314:GLN:HB2	1:A:317:GLU:HG2	1.80	0.62
1:B:680:ASP:HB2	10:B:296:HOH:O	2.01	0.61
1:A:101:LEU:HD21	4:A:424:CHD:H7	1.82	0.61
1:A:173:ALA:O	1:A:177:MET:HG3	2.02	0.60
1:A:357:ALA:HA	1:A:362:VAL:HG12	1.84	0.60
1:B:874:ASN:HD22	1:B:875:PRO:CD	2.14	0.59
1:B:568:LYS:HD2	1:B:655:ALA:O	2.01	0.59
1:A:297:TYR:H	1:B:898:GLN:NE2	1.87	0.59
1:A:422:GLN:HG2	1:A:423:LEU:CD1	2.32	0.59
1:B:874:ASN:HD22	1:B:875:PRO:HD2	1.67	0.59
1:A:285:GLN:O	1:A:289:GLU:HG3	2.03	0.59
1:B:922:GLN:HG2	1:B:923:LEU:HD13	1.84	0.58
1:B:616:THR:O	1:B:620:GLN:HB2	2.04	0.57
1:A:358:LYS:HA	10:A:562:HOH:O	2.04	0.57
1:A:215:ARG:HB3	1:A:215:ARG:HH11	1.70	0.56
1:A:212:GLN:HA	1:A:212:GLN:OE1	2.05	0.56
1:B:816:ASP:HB2	10:B:227:HOH:O	2.04	0.56
1:A:69:THR:OG1	1:A:154:THR:HB	2.06	0.56
1:B:776:TYR:HB3	1:B:777:PRO:HD3	1.88	0.56
1:B:713:VAL:HG12	1:B:715:ARG:HG2	1.88	0.56
1:A:213:VAL:HG23	1:A:215:ARG:HG2	1.88	0.55
1:B:716:LYS:N	1:B:716:LYS:HD2	2.21	0.55
1:A:304:LYS:N	1:A:304:LYS:HD3	2.01	0.55
1:B:745:LEU:HB3	1:B:753:ARG:NH1	2.21	0.55
1:B:671:GLU:N	1:B:671:GLU:OE1	2.27	0.55
1:B:777:PRO:HB3	9:B:925:GOL:H2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ASN:HD22	1:A:375:PRO:N	2.04	0.55
1:A:277:PRO:CB	9:B:925:GOL:H12	2.37	0.54
1:A:277:PRO:HB2	9:B:925:GOL:H12	1.88	0.54
1:A:316:ASP:HB2	10:A:516:HOH:O	2.07	0.53
1:B:565:ARG:HH11	1:B:565:ARG:CB	2.21	0.53
1:A:304:LYS:O	1:A:305:VAL:HG22	2.08	0.53
1:B:820:LYS:HE2	1:B:824:GLU:OE1	2.09	0.53
1:A:215:ARG:HD3	10:A:547:HOH:O	2.07	0.53
1:A:212:GLN:C	1:A:214:GLY:H	2.12	0.53
1:A:325:ARG:HG3	1:A:325:ARG:HH11	1.74	0.52
1:B:616:THR:HB	1:B:617:PRO:HD3	1.91	0.52
1:B:870:SER:C	1:B:872:ASN:H	2.12	0.52
1:B:823:CYS:SG	1:B:862:VAL:HG22	2.50	0.52
1:B:673:ALA:O	1:B:677:MET:HG3	2.10	0.52
1:A:335:ILE:HG13	1:A:335:ILE:O	2.09	0.51
1:A:221:TRP:H	1:A:421:GLN:NE2	2.09	0.51
1:B:608:ALA:N	1:B:609:PRO:HD2	2.25	0.51
1:A:220:LYS:HZ2	1:A:423:LEU:HD22	1.77	0.50
1:B:790:ARG:HH11	1:B:790:ARG:HG2	1.77	0.50
1:A:374:ASN:ND2	1:A:376:LEU:H	2.09	0.50
1:B:726:ARG:HD3	1:B:779:GLU:OE2	2.11	0.50
1:B:804:LYS:HD3	1:B:814:GLN:NE2	2.27	0.50
1:B:874:ASN:HD22	1:B:875:PRO:N	2.08	0.50
1:A:327:ARG:HD3	6:A:1:CL:CL	2.49	0.49
1:B:874:ASN:ND2	1:B:876:LEU:H	2.10	0.49
1:A:304:LYS:N	1:A:304:LYS:CD	2.71	0.49
1:A:304:LYS:HB2	10:A:550:HOH:O	2.11	0.49
1:B:839:SER:O	1:B:841:HIS:HD2	1.96	0.49
1:A:220:LYS:NZ	1:A:423:LEU:HD22	2.28	0.48
1:A:245:LEU:HB3	1:A:253:ARG:NH1	2.29	0.48
1:B:912:ARG:HH21	1:B:912:ARG:HB2	1.75	0.48
1:A:334:PRO:HG2	10:A:567:HOH:O	2.12	0.48
1:A:184:ARG:HG3	1:A:184:ARG:HH11	1.79	0.48
1:A:286:LYS:NZ	10:A:511:HOH:O	2.46	0.48
4:B:924:CHD:H161	4:B:3:CHD:H151	1.96	0.48
1:B:856:LEU:HG	1:B:862:VAL:CG2	2.41	0.48
1:A:102:PRO:O	1:A:103:ILE:C	2.52	0.48
1:B:649:GLU:HA	1:B:649:GLU:OE2	2.14	0.48
1:B:565:ARG:CB	1:B:565:ARG:NH1	2.77	0.47
1:B:674:ILE:HD11	1:B:706:ILE:HG12	1.96	0.47
1:B:835:ILE:O	1:B:835:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:LYS:HB3	10:B:193:HOH:O	2.15	0.47
1:B:603:ILE:HG13	1:B:607:LEU:HG	1.96	0.47
1:A:136:THR:CG2	1:A:161:ILE:HD12	2.45	0.47
1:B:803:SER:O	3:B:1:IMD:H4	2.15	0.47
1:B:854:GLN:HA	1:B:854:GLN:NE2	2.30	0.47
1:A:276:TYR:HB3	1:A:277:PRO:HD3	1.95	0.47
1:B:922:GLN:HG2	1:B:923:LEU:HD12	1.95	0.47
1:B:577:GLY:HA2	1:B:632:ILE:HD13	1.96	0.47
1:A:273:GLY:HA3	1:A:404:PRO:HD2	1.97	0.46
1:B:658:LYS:HD3	1:B:660:TYR:OH	2.15	0.46
1:B:571:ILE:HD12	1:B:571:ILE:N	2.30	0.46
1:B:596:ARG:HA	1:B:599:MET:O	2.16	0.46
1:A:135:TRP:CE2	1:A:372:ASN:HB3	2.51	0.46
1:B:912:ARG:HD2	10:B:100:HOH:O	2.15	0.46
1:A:180:ASP:HB2	1:A:182:LEU:CD1	2.45	0.46
1:A:374:ASN:HD22	1:A:374:ASN:C	2.17	0.46
1:A:289:GLU:HG2	1:A:293:TYR:OH	2.15	0.46
1:A:305:VAL:HG23	1:A:305:VAL:O	2.16	0.46
1:A:136:THR:HG22	1:A:161:ILE:HD12	1.97	0.46
1:B:602:PRO:O	1:B:603:ILE:C	2.54	0.45
1:B:720:LYS:HE2	10:B:140:HOH:O	2.16	0.45
1:A:158:LYS:HD3	1:A:160:TYR:OH	2.17	0.45
1:B:846:TYR:CD2	1:B:856:LEU:HD22	2.52	0.45
1:B:715:ARG:NH2	10:B:295:HOH:O	2.47	0.45
1:B:684:ARG:HG3	10:B:182:HOH:O	2.16	0.45
1:B:569:THR:HG23	1:B:684:ARG:HD2	1.99	0.44
1:A:302:GLN:HB3	1:A:315:THR:OG1	2.18	0.44
1:A:304:LYS:HD3	10:A:34:HOH:O	2.17	0.44
1:A:325:ARG:HG3	1:A:325:ARG:NH1	2.32	0.44
1:A:371:LEU:C	10:A:537:HOH:O	2.56	0.44
10:A:543:HOH:O	1:B:825:ARG:HD3	2.17	0.44
1:B:874:ASN:HD22	1:B:874:ASN:C	2.21	0.43
1:A:320:LYS:O	1:A:324:GLU:HG3	2.18	0.43
1:A:250:LEU:CD2	1:A:250:LEU:H	2.17	0.43
1:A:301:TRP:O	1:A:314:GLN:HA	2.18	0.43
1:A:283:THR:HG22	1:A:335:ILE:HD11	2.00	0.43
1:A:103:ILE:O	1:A:103:ILE:HG13	2.17	0.43
1:A:372:ASN:HA	10:A:509:HOH:O	2.18	0.43
1:A:304:LYS:O	1:A:305:VAL:CG2	2.66	0.43
1:A:158:LYS:HD3	1:A:160:TYR:CZ	2.53	0.43
1:B:710:TYR:CE2	1:B:717:PRO:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:GLU:C	1:A:364:ASN:HD22	2.21	0.43
1:B:915:LYS:HD3	10:B:197:HOH:O	2.19	0.43
1:B:601:LEU:HD21	4:B:924:CHD:H151	2.01	0.43
1:A:215:ARG:CB	1:A:215:ARG:HH11	2.31	0.43
1:A:65:ARG:HB3	10:A:517:HOH:O	2.17	0.43
1:B:825:ARG:HH11	1:B:825:ARG:HG3	1.83	0.43
1:B:751:GLU:CD	1:B:751:GLU:H	2.22	0.43
1:B:912:ARG:HH21	1:B:912:ARG:CB	2.33	0.42
1:B:639:GLN:NE2	1:B:873:GLY:HA2	2.27	0.42
1:B:601:LEU:HD21	4:B:924:CHD:H7	2.01	0.42
1:A:303:SER:HB2	3:A:2:IMD:HN3	1.83	0.42
4:B:924:CHD:H112	10:B:245:HOH:O	2.19	0.42
1:A:212:GLN:C	1:A:214:GLY:N	2.73	0.42
1:A:391:SER:O	1:A:392:ASN:HB2	2.19	0.42
1:A:90:LEU:HD13	1:A:90:LEU:C	2.40	0.42
1:A:191:TYR:HE1	10:A:533:HOH:O	2.02	0.42
1:B:819:ILE:HD11	1:B:832:LEU:HD21	2.00	0.42
1:A:158:LYS:NZ	1:A:180:ASP:OD2	2.43	0.41
1:A:374:ASN:ND2	1:A:375:PRO:HD2	2.31	0.41
1:B:877:PHE:O	1:B:880:ALA:HB3	2.20	0.41
1:A:116:THR:HB	1:A:117:PRO:HD3	2.02	0.41
1:B:614:ARG:NH1	1:B:614:ARG:HG2	2.33	0.41
1:A:275:PRO:HD3	1:B:798:ARG:NH2	2.36	0.41
1:A:303:SER:CB	3:A:2:IMD:HN3	2.33	0.41
1:B:922:GLN:O	1:B:923:LEU:HB2	2.21	0.41
1:A:215:ARG:CB	1:A:215:ARG:NH1	2.84	0.41
1:A:159:TYR:C	1:A:159:TYR:CD1	2.94	0.41
1:B:801:TRP:O	1:B:814:GLN:HA	2.21	0.40
1:B:912:ARG:HB2	1:B:912:ARG:CZ	2.51	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	357/359 (99%)	335 (94%)	20 (6%)	2 (1%)	30	29
1	B	358/359 (100%)	339 (95%)	17 (5%)	2 (1%)	30	29
All	All	715/718 (100%)	674 (94%)	37 (5%)	4 (1%)	30	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	872	ASN
1	A	361	GLY
1	A	305	VAL
1	B	871	LEU

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	324/324 (100%)	315 (97%)	9 (3%)	51	63
1	B	325/324 (100%)	321 (99%)	4 (1%)	78	88
All	All	649/648 (100%)	636 (98%)	13 (2%)	63	76

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

Mol	Chain	Res	Type
1	A	96	ARG
1	A	113	LYS
1	A	138	LYS
1	A	227	TRP
1	A	250	LEU
1	A	255	GLU
1	A	304	LYS
1	A	374	ASN
1	A	412	ARG
1	B	620	GLN
1	B	727	TRP
1	B	798	ARG

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Mol	Chain	Res	Type
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	231	HIS
1	A	235	GLN
1	A	329	ASN
1	A	364	ASN
1	A	374	ASN
1	A	390	GLN
1	A	398	GLN
1	A	421	GLN
1	B	653	ASN
1	B	735	GLN
1	B	814	GLN
1	B	841	HIS
1	B	854	GLN
1	B	874	ASN
1	B	898	GLN
1	B	921	GLN
1	B	922	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	IMD	A	2	7	3,5,5	2.20	2 (66%)	4,5,5	2.94	3 (75%)
4	CHD	A	4	-	29,32,32	1.50	5 (17%)	48,51,51	1.46	10 (20%)
4	CHD	A	424	-	29,32,32	1.44	5 (17%)	48,51,51	1.40	8 (16%)
5	OXY	A	425	-	1,1,1	0.08	0	0,0,0	0.00	-
7	FDE	A	426	3	20,46,46	2.27	8 (40%)	20,76,76	4.89	9 (45%)
8	SO4	A	427	-	4,4,4	0.23	0	6,6,6	0.08	0
2	FES	A	501	1	0,4,4	0.00	-	0,4,4	0.00	-
3	IMD	B	1	7	3,5,5	0.46	0	4,5,5	0.62	0
8	SO4	B	2	-	4,4,4	0.22	0	6,6,6	0.08	0
4	CHD	B	3	-	29,32,32	1.46	6 (20%)	48,51,51	1.42	9 (18%)
2	FES	B	502	1	0,4,4	0.00	-	0,4,4	0.00	-
4	CHD	B	924	-	29,32,32	1.51	8 (27%)	48,51,51	1.37	6 (12%)
9	GOL	B	925	-	5,5,5	0.22	0	5,5,5	0.31	0
5	OXY	B	926	-	1,1,1	0.19	0	0,0,0	0.00	-
7	FDE	B	927	3	20,46,46	2.38	10 (50%)	20,76,76	4.27	13 (65%)

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	IMD	A	2	7	-	0/0/0/0	0/1/1/1
4	CHD	A	4	-	-	0/7/74/74	0/4/4/4
4	CHD	A	424	-	-	0/7/74/74	0/4/4/4
5	OXY	A	425	-	-	0/0/0/0	0/0/0/0
7	FDE	A	426	3	-	0/6/50/50	0/0/8/8
8	SO4	A	427	-	-	0/0/0/0	0/0/0/0
2	FES	A	501	1	-	0/0/4/4	0/1/1/1
3	IMD	B	1	7	-	0/0/0/0	0/1/1/1
8	SO4	B	2	-	-	0/0/0/0	0/0/0/0
4	CHD	B	3	-	-	0/7/74/74	0/4/4/4
2	FES	B	502	1	-	0/0/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CHD	B	924	-	-	0/7/74/74	0/4/4/4
9	GOL	B	925	-	-	0/4/4/4	0/0/0/0
5	OXY	B	926	-	-	0/0/0/0	0/0/0/0
7	FDE	B	927	3	-	0/6/50/50	0/0/8/8

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	927	FDE	C4A-CHB	-4.17	1.28	1.39
7	A	426	FDE	C4A-CHB	-3.27	1.30	1.39
7	A	426	FDE	C4B-NB	-2.89	1.32	1.36
7	B	927	FDE	C1B-NB	-2.84	1.32	1.36
7	B	927	FDE	C4B-NB	-2.71	1.33	1.36
7	B	927	FDE	C1D-CHD	-2.02	1.34	1.39
4	B	924	CHD	C4-C5	2.00	1.57	1.53
4	A	424	CHD	C4-C3	2.01	1.55	1.51
7	A	426	FDE	C4D-CHA	2.01	1.45	1.39
7	B	927	FDE	C4D-CHA	2.04	1.45	1.39
4	A	4	CHD	C8-C9	2.05	1.57	1.53
4	B	3	CHD	C8-C9	2.07	1.57	1.53
4	B	3	CHD	C6-C5	2.08	1.57	1.53
4	B	924	CHD	C4-C3	2.11	1.55	1.51
4	B	924	CHD	C8-C9	2.12	1.58	1.53
3	A	2	IMD	C5-C4	2.16	1.44	1.36
4	B	924	CHD	C8-C7	2.17	1.57	1.53
7	B	927	FDE	CMA-C3A	2.17	1.56	1.51
4	A	424	CHD	C20-C17	2.19	1.58	1.54
4	B	3	CHD	C20-C17	2.25	1.58	1.54
4	B	3	CHD	C6-C7	2.26	1.56	1.52
4	B	924	CHD	C6-C5	2.27	1.57	1.53
4	A	4	CHD	C20-C17	2.28	1.58	1.54
4	B	3	CHD	C11-C9	2.33	1.57	1.53
4	A	424	CHD	C11-C9	2.35	1.57	1.53
7	A	426	FDE	CMA-C3A	2.38	1.56	1.51
4	B	924	CHD	C18-C13	2.39	1.58	1.54
4	A	424	CHD	C6-C7	2.39	1.56	1.52
4	A	4	CHD	C6-C7	2.40	1.56	1.52
4	A	4	CHD	C11-C9	2.42	1.57	1.53
4	A	424	CHD	C18-C13	2.46	1.58	1.54
4	B	3	CHD	C18-C13	2.55	1.58	1.54
4	B	924	CHD	C6-C7	2.56	1.56	1.52
4	A	4	CHD	C18-C13	2.58	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	924	CHD	C11-C9	2.63	1.58	1.53
7	B	927	FDE	CAA-C2A	2.69	1.57	1.52
7	A	426	FDE	C1C-CHC	2.72	1.49	1.43
3	A	2	IMD	C5-N1	2.92	1.50	1.37
7	A	426	FDE	CAA-C2A	3.74	1.59	1.52
7	A	426	FDE	C3D-C2D	3.81	1.49	1.37
7	B	927	FDE	C1C-CHC	3.87	1.51	1.43
7	B	927	FDE	C2A-C3A	4.26	1.50	1.37
7	B	927	FDE	C3D-C2D	4.58	1.51	1.37
7	A	426	FDE	C2A-C3A	5.34	1.53	1.37

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	426	FDE	CAA-C2A-C1A	-8.99	117.25	127.01
7	A	426	FDE	CBA-CAA-C2A	-8.50	97.29	112.53
7	A	426	FDE	CMA-C3A-C4A	-8.30	114.62	128.36
7	B	927	FDE	CBA-CAA-C2A	-7.95	98.27	112.53
7	B	927	FDE	CAA-C2A-C1A	-7.66	118.69	127.01
7	B	927	FDE	CMA-C3A-C4A	-4.63	120.70	128.36
4	B	924	CHD	C9-C11-C12	-4.18	109.09	114.36
4	A	424	CHD	C9-C11-C12	-3.95	109.37	114.36
7	B	927	FDE	CAD-C3D-C4D	-3.91	122.77	127.01
7	A	426	FDE	CAD-CBD-CGD	-3.89	105.61	112.75
7	A	426	FDE	CMF-C3C-C2C	-3.70	117.84	124.84
4	B	3	CHD	C9-C11-C12	-3.69	109.70	114.36
4	A	4	CHD	C9-C11-C12	-3.66	109.74	114.36
7	B	927	FDE	CMF-C3C-C2C	-3.64	117.96	124.84
7	B	927	FDE	CAD-CBD-CGD	-3.42	106.48	112.75
7	B	927	FDE	CBD-CAD-C3D	-3.29	106.63	112.53
7	A	426	FDE	CAD-C3D-C4D	-3.23	123.50	127.01
3	A	2	IMD	C5-C4-N3	-2.96	102.42	107.74
4	B	924	CHD	C16-C15-C14	-2.77	99.55	105.12
4	A	4	CHD	C11-C9-C10	-2.67	111.02	113.79
7	B	927	FDE	CMA-C3A-C2A	-2.64	119.73	125.24
4	A	424	CHD	C16-C15-C14	-2.63	99.83	105.12
4	B	3	CHD	C11-C9-C10	-2.62	111.07	113.79
4	A	4	CHD	C13-C14-C8	-2.58	111.43	114.75
4	A	424	CHD	C11-C9-C10	-2.57	111.12	113.79
4	A	4	CHD	C13-C17-C20	-2.50	116.46	119.50
4	B	3	CHD	C13-C14-C8	-2.48	111.55	114.75
4	B	3	CHD	C16-C15-C14	-2.46	100.17	105.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4	CHD	C23-C22-C20	-2.45	111.87	114.75
4	A	4	CHD	C16-C15-C14	-2.43	100.22	105.12
4	A	424	CHD	C13-C14-C8	-2.37	111.69	114.75
7	B	927	FDE	C2C-C3C-C4C	-2.37	104.46	107.34
4	B	924	CHD	C10-C9-C8	-2.33	109.33	111.88
4	B	924	CHD	C6-C5-C10	-2.31	110.11	112.66
4	B	3	CHD	C13-C17-C20	-2.25	116.76	119.50
4	B	3	CHD	C18-C13-C14	-2.25	107.67	111.22
4	A	4	CHD	C6-C5-C10	-2.24	110.19	112.66
4	A	4	CHD	C18-C13-C14	-2.23	107.69	111.22
4	A	424	CHD	C10-C9-C8	-2.20	109.47	111.88
4	A	424	CHD	C6-C5-C10	-2.17	110.27	112.66
4	B	924	CHD	C11-C9-C10	-2.14	111.56	113.79
4	B	3	CHD	C6-C5-C10	-2.14	110.30	112.66
4	B	3	CHD	C10-C9-C8	-2.14	109.54	111.88
4	B	924	CHD	C18-C13-C14	-2.10	107.91	111.22
4	A	4	CHD	C10-C9-C8	-2.04	109.64	111.88
4	A	424	CHD	C18-C13-C14	-2.03	108.02	111.22
7	A	426	FDE	CAD-C3D-C2D	2.00	134.72	129.00
7	B	927	FDE	CAD-C3D-C2D	2.21	135.31	129.00
4	A	424	CHD	C17-C13-C12	2.34	119.75	117.68
3	A	2	IMD	C4-N3-C2	2.54	113.57	105.76
4	B	3	CHD	C17-C13-C12	2.86	120.21	117.68
7	B	927	FDE	CMD-C2D-C3D	2.90	131.30	125.24
4	A	4	CHD	C17-C13-C12	3.07	120.40	117.68
3	A	2	IMD	C4-C5-N1	4.07	115.05	107.74
7	A	426	FDE	C2B-C1B-NB	4.80	115.00	108.64
7	B	927	FDE	C2B-C1B-NB	6.46	117.21	108.64
7	B	927	FDE	CAA-CBA-CGA	9.84	130.78	112.75
7	A	426	FDE	CAA-CBA-CGA	13.12	136.80	112.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2	IMD	2	0
4	A	424	CHD	2	0
3	B	1	IMD	1	0
4	B	3	CHD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	924	CHD	5	0
9	B	925	GOL	3	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%)	0.21	15 (4%)	40 39	8, 33, 58, 72	3 (0%)
1	B	359/359 (100%)	0.24	7 (1%)	70 68	9, 35, 59, 68	2 (0%)
All	All	718/718 (100%)	0.22	22 (3%)	52 51	8, 34, 58, 72	5 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	423	LEU	6.0
1	B	923	LEU	4.6
1	B	610	PHE	3.9
1	B	603	ILE	3.3
1	A	65	ARG	3.3
1	B	606	LYS	3.0
1	A	375	PRO	2.7
1	A	305	VAL	2.6
1	A	361	GLY	2.5
1	B	613	LYS	2.5
1	A	155	ALA	2.4
1	A	304	LYS	2.4
1	A	110	PHE	2.3
1	A	354	GLN	2.3
1	B	780	VAL	2.3
1	A	150	LEU	2.2
1	A	66	LYS	2.2
1	B	566	LYS	2.2
1	A	103	ILE	2.2
1	A	113	LYS	2.2
1	A	212	GLN	2.1
1	A	350	ILE	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	OXY	A	425	2/2	0.92	0.28	7.40	44,44,44,46	0
9	GOL	B	925	6/6	0.81	0.31	6.74	35,36,38,39	0
5	OXY	B	926	2/2	0.92	0.29	6.69	44,44,44,44	0
4	CHD	B	3	29/29	0.87	0.31	1.94	73,74,83,85	0
4	CHD	A	424	29/29	0.70	0.26	1.71	76,78,87,88	0
4	CHD	A	4	29/29	0.71	0.37	1.58	117,118,120,120	0
4	CHD	B	924	29/29	0.75	0.22	1.37	53,58,71,72	0
6	CL	A	1	1/1	0.92	0.14	0.19	59,59,59,59	0
3	IMD	A	2	5/5	0.90	0.17	-0.12	26,27,28,28	0
3	IMD	B	1	5/5	0.93	0.14	-0.17	28,29,30,31	0
7	FDE	B	927	39/39	0.96	0.12	-0.30	17,26,37,41	0
7	FDE	A	426	39/39	0.96	0.12	-0.47	21,26,36,39	0
2	FES	A	501	4/4	0.95	0.06	-2.12	26,27,28,29	0
2	FES	B	502	4/4	0.95	0.06	-2.15	26,27,28,28	0
8	SO4	B	2	5/5	0.94	0.16	-	85,85,86,86	0
8	SO4	A	427	5/5	0.94	0.16	-	92,92,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.