Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 03:33 AM EDT

PDB ID	:	7JRD
Title	:	The crystal structure of lactoferrin binding protein B (LbpB) from Neisseria meningitidis in complex with human lactoferrin
Authors	:	Yadav, R.; Noinaj, N.
Deposited on	:	2020-08-12
Resolution	:	2.85 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

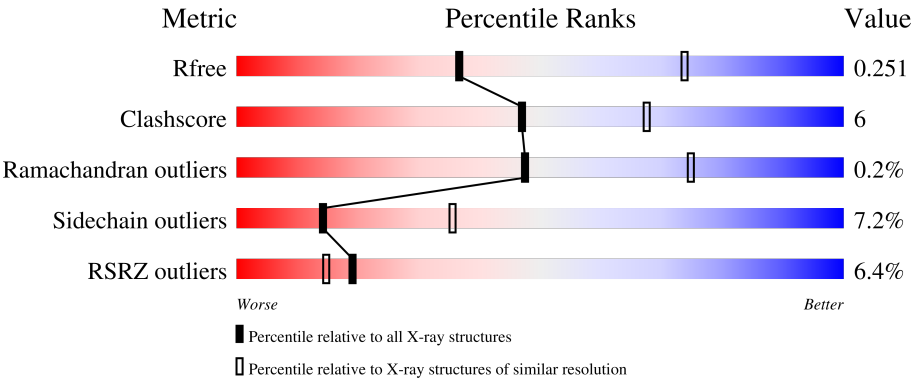
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	722	9% 62% 15% 22%
2	B	692	2% 83% 15%

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	SO4	B	714	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9547 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 Lactoferrin-binding protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	566	Total	C	N	O	S	0	1	0
			4234	2657	741	830	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q9JYK4
A	-2	ALA	-	expression tag	UNP Q9JYK4
A	-1	MET	-	expression tag	UNP Q9JYK4
A	0	GLY	-	expression tag	UNP Q9JYK4

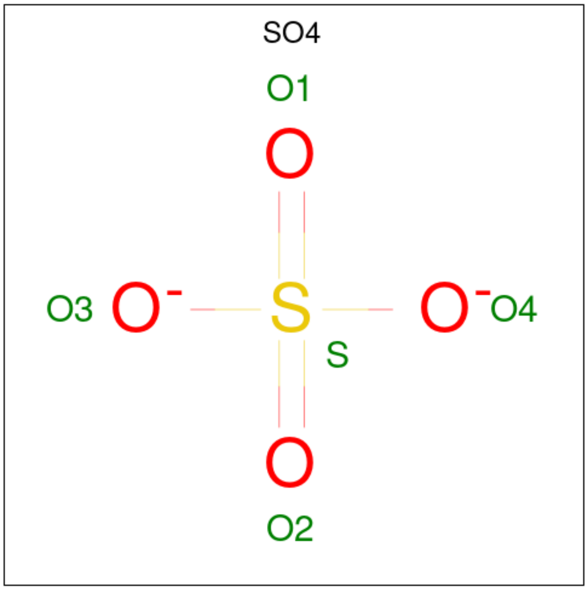
- Molecule 2 is a protein called Lactotransferrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	688	Total	C	N	O	S	0	0	0
			5225	3272	926	990	37			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	ALA	THR	conflict	UNP W8QEY1

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

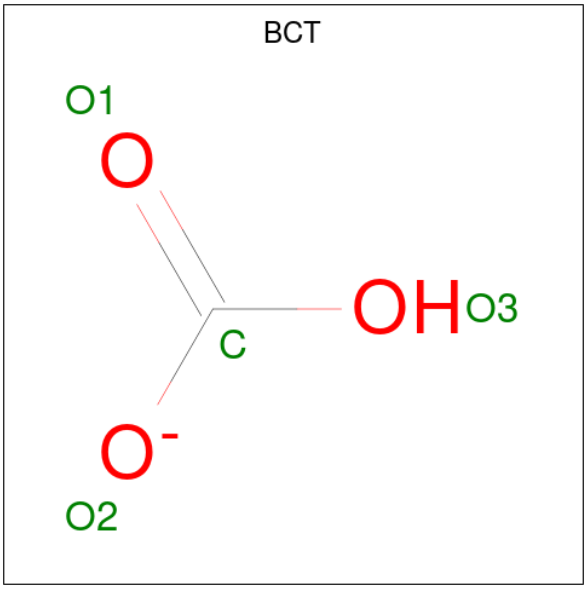


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0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

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 5 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 4 1 3	0	0
5	B	1	Total C O 4 1 3	0	0

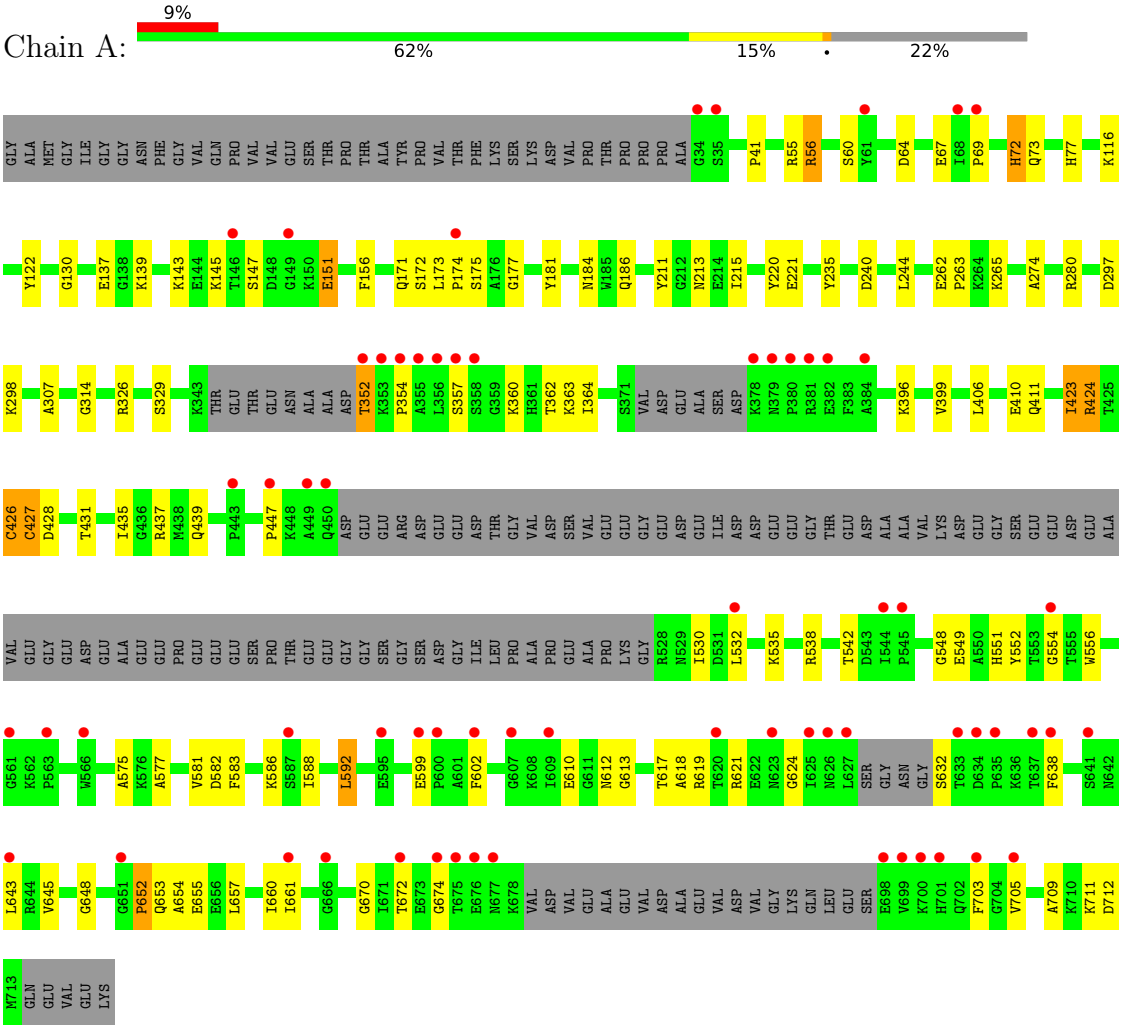
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	10	Total O 10 10	0	0
6	B	3	Total O 3 3	0	0

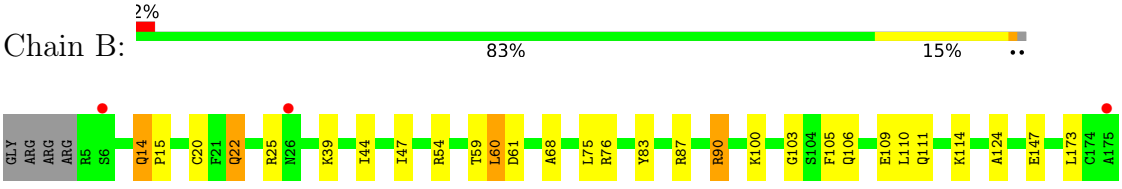
3 Residue-property plots (i)

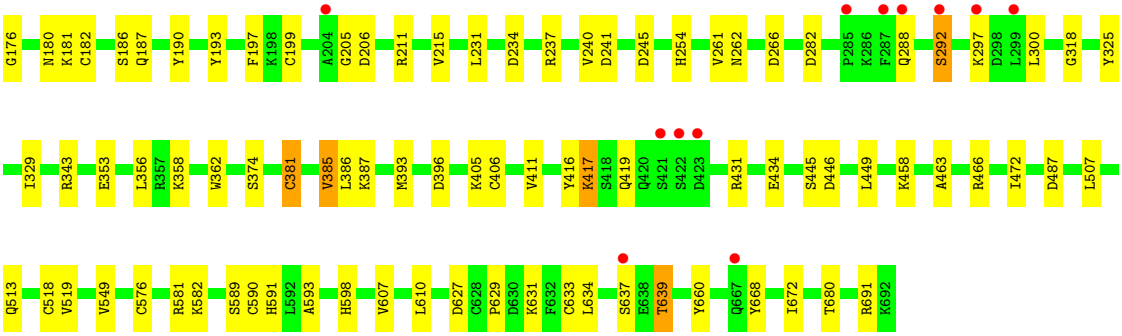
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Lactoferrin-binding protein B



• Molecule 2: Lactotransferrin




G176 N180 K181 C182 S186 Q187 Y190 Y193 F197 K198 C199 A204 G205 D206 R211 V215 L231 D234 R237 V240 D241 D245 H254 V261 N262 D266 D282 P285 K286 F287 Q288 S292 K297 D298 L299 L300 G318 Y325
I329 R343 E353 L356 R357 K358 W362 S374 C381 V385 L386 K387 M393 D396 K405 C406 V411 Y416 K417 S418 Q419 Q420 S421 S422 D423 R431 E434 S445 D446 L449 K458 A463 R466 I472 D487 L507
Q513 C518 V519 V549 C576 R581 K582 S589 C590 H591 L592 A593 H598 V607 L610 D627 Q628 P629 D630 K631 F632 C633 L634 S637 E638 T639 Y660 Q667 Y668 I672 T680 R691 K692

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	120.39Å 120.39Å 207.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.78 – 2.85 47.78 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.78-2.85) 99.9 (47.78-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.201 , 0.251 0.201 , 0.251	Depositor DCC
R_{free} test set	2000 reflections (5.53%)	wwPDB-VP
Wilson B-factor (Å^2)	77.5	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9547	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, BCT, FE

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	0.26	0/4316	0.48	0/5839
2	B	0.25	0/5339	0.44	0/7241
All	All	0.25	0/9655	0.45	0/13080

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	426	CYS	Peptide
2	B	292	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4234	0	3904	62	0
2	B	5225	0	5000	54	0
3	A	15	0	0	1	0
3	B	50	0	0	6	0
4	B	2	0	0	0	0
5	B	8	0	0	1	0
6	A	10	0	0	1	0
6	B	3	0	0	0	0
All	All	9547	0	8904	115	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 6.

All (115) 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:426:CYS:SG	1:A:427:CYS:N	2.43	0.90
2:B:14:GLN:HG2	2:B:15:PRO:HD3	1.56	0.85
1:A:181:TYR:HB2	1:A:235:TYR:HB2	1.67	0.76
1:A:56:ARG:NH1	1:A:73:GLN:OE1	2.18	0.76
1:A:396:LYS:O	1:A:535:LYS:NZ	2.18	0.75
2:B:61:ASP:OD1	2:B:254:HIS:NE2	2.21	0.74
2:B:358:LYS:HD2	2:B:639:THR:HG21	1.70	0.74
1:A:406:LEU:HA	1:A:411:GLN:HE22	1.54	0.72
1:A:67:GLU:HG3	1:A:69:PRO:HG2	1.74	0.68
1:A:265:LYS:NZ	3:A:803:SO4:O3	2.26	0.68
1:A:41:PRO:O	1:A:326:ARG:NH2	2.27	0.67
2:B:691:ARG:NH2	3:B:714:SO4:S	2.67	0.67
2:B:83:TYR:HB2	2:B:90:ARG:HD2	1.77	0.66
1:A:143:LYS:NZ	1:A:151:GLU:OE1	2.29	0.66
1:A:588:ILE:HD11	1:A:657:LEU:HD11	1.77	0.66
1:A:262:GLU:HG3	1:A:263:PRO:HD2	1.78	0.65
2:B:633:CYS:HB2	2:B:637:SER:HB2	1.80	0.63
1:A:410:GLU:OE2	1:A:424[B]:ARG:NH1	2.34	0.60
2:B:691:ARG:NH2	3:B:714:SO4:O4	2.34	0.60
1:A:69:PRO:HB2	1:A:72:HIS:HB2	1.82	0.59
2:B:22:GLN:HG2	2:B:25:ARG:HH21	1.68	0.58
1:A:599:GLU:HA	1:A:621:ARG:HG3	1.84	0.58
1:A:439:GLN:HB3	1:A:530:ILE:HG12	1.85	0.57
2:B:356:LEU:HD13	2:B:374:SER:HB2	1.88	0.56
1:A:175:SER:HB3	1:A:362:THR:HG23	1.88	0.56
1:A:177:GLY:N	1:A:240:ASP:OD1	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ARG:HB3	1:A:532:LEU:HD23	1.87	0.56
1:A:582:ASP:O	1:A:586:LYS:N	2.34	0.56
1:A:56:ARG:NH2	1:A:213:ASN:O	2.31	0.55
1:A:145:LYS:HA	1:A:151:GLU:HA	1.87	0.55
2:B:124:ALA:N	5:B:704:BCT:O1	2.37	0.55
1:A:652:PRO:O	1:A:654:ALA:N	2.23	0.55
2:B:416:TYR:O	2:B:431:ARG:NH1	2.40	0.55
2:B:176:GLY:HA3	2:B:181:LYS:HA	1.90	0.54
2:B:691:ARG:NH2	3:B:714:SO4:O3	2.37	0.54
1:A:592:LEU:HD21	1:A:602:PHE:HB2	1.89	0.53
1:A:426:CYS:N	1:A:435:ILE:O	2.41	0.53
2:B:114:LYS:HB2	2:B:205:GLY:HA2	1.91	0.52
2:B:68:ALA:HB1	2:B:75:LEU:HB2	1.92	0.52
1:A:618:ALA:HB3	1:A:643:LEU:HB2	1.91	0.51
1:A:577:ALA:HA	1:A:592:LEU:HA	1.91	0.51
2:B:105:PHE:O	2:B:237:ARG:NH1	2.40	0.51
2:B:215:VAL:HG21	2:B:240:VAL:HG11	1.93	0.51
2:B:411:VAL:HG21	2:B:610:LEU:HD23	1.93	0.51
2:B:419:GLN:N	2:B:434:GLU:OE1	2.44	0.51
2:B:106:GLN:H	2:B:109:GLU:HG3	1.76	0.50
2:B:591:HIS:NE2	3:B:709:SO4:O2	2.44	0.50
2:B:180:ASN:ND2	2:B:187:GLN:OE1	2.44	0.50
1:A:280:ARG:HA	1:A:314:GLY:HA2	1.93	0.49
2:B:44:ILE:H	2:B:44:ILE:HD12	1.77	0.49
2:B:193:TYR:OH	2:B:254:HIS:NE2	2.46	0.49
1:A:173:LEU:HG	1:A:364:ILE:HG13	1.95	0.49
1:A:613:GLY:HA2	1:A:648:GLY:HA2	1.94	0.49
2:B:627:ASP:HB3	2:B:631:LYS:HB2	1.95	0.49
2:B:197:PHE:CZ	2:B:215:VAL:HG12	2.48	0.48
2:B:668:TYR:CZ	2:B:672:ILE:HD11	2.49	0.48
1:A:556:TRP:CD1	1:A:575:ALA:HB1	2.47	0.48
2:B:47:ILE:HD11	2:B:60:LEU:HD21	1.96	0.48
2:B:582:LYS:NZ	2:B:589:SER:OG	2.45	0.48
2:B:458:LYS:HB3	2:B:507:LEU:HD11	1.96	0.47
1:A:171:GLN:HB3	1:A:363:LYS:HE2	1.95	0.47
1:A:220:TYR:O	2:B:513:GLN:NE2	2.48	0.47
1:A:624:GLY:H	1:A:638:PHE:H	1.63	0.46
2:B:76:ARG:NH2	3:B:710:SO4:O4	2.41	0.46
1:A:548:GLY:O	1:A:583:PHE:N	2.48	0.46
1:A:56:ARG:HD3	1:A:213:ASN:O	2.15	0.46
1:A:122:TYR:CZ	1:A:184:ASN:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:TYR:CD2	1:A:711:LYS:HB3	2.50	0.46
1:A:556:TRP:CE2	1:A:592:LEU:HB2	2.50	0.46
2:B:114:LYS:HB3	2:B:173:LEU:HD21	1.98	0.46
1:A:175:SER:OG	1:A:357:SER:HA	2.16	0.45
2:B:417:LYS:HD3	2:B:417:LYS:HA	1.74	0.45
1:A:244:LEU:HB3	1:A:274:ALA:HB3	1.97	0.45
1:A:411:GLN:HE21	1:A:423:ILE:HD11	1.82	0.45
1:A:174:PRO:HA	1:A:360:LYS:O	2.16	0.45
2:B:318:GLY:HA3	2:B:387:LYS:HD2	1.98	0.45
2:B:396:ASP:HA	2:B:598:HIS:CD2	2.52	0.44
2:B:411:VAL:HG13	2:B:607:VAL:HG13	2.00	0.44
2:B:446:ASP:N	2:B:446:ASP:OD1	2.51	0.44
2:B:103:GLY:HA2	2:B:237:ARG:NE	2.33	0.44
2:B:14:GLN:H	2:B:14:GLN:CD	2.22	0.43
1:A:352:THR:OG1	1:A:354:PRO:HD3	2.18	0.43
1:A:55:ARG:HD2	1:A:156:PHE:O	2.18	0.43
1:A:211:TYR:CZ	1:A:221:GLU:HG3	2.54	0.43
2:B:463:ALA:HB3	2:B:466:ARG:HD3	2.00	0.43
2:B:362:TRP:CE2	2:B:634:LEU:HD21	2.53	0.42
2:B:381:CYS:HB3	2:B:393:MET:SD	2.59	0.42
2:B:629:PRO:HA	2:B:633:CYS:SG	2.59	0.42
1:A:307:ALA:HB2	1:A:329:SER:HA	2.01	0.42
1:A:554:GLY:HA3	1:A:709:ALA:HA	2.02	0.42
2:B:472:ILE:HD13	2:B:593:ALA:HB3	2.01	0.42
1:A:130:GLY:HA2	1:A:186:GLN:HE21	1.84	0.42
1:A:549:GLU:HA	1:A:582:ASP:HA	2.00	0.42
2:B:20:CYS:HB2	2:B:300:LEU:HD11	2.02	0.42
1:A:60:SER:O	1:A:67:GLU:HB2	2.20	0.42
1:A:172:SER:HB3	1:A:363:LYS:HA	2.02	0.42
2:B:386:LEU:HD11	2:B:406:CYS:HB3	2.01	0.42
2:B:660:TYR:OH	3:B:714:SO4:O2	2.26	0.41
2:B:100:LYS:O	2:B:237:ARG:NH2	2.54	0.41
2:B:381:CYS:O	2:B:385:VAL:HG12	2.21	0.41
1:A:137:GLU:CD	1:A:137:GLU:H	2.24	0.41
1:A:139:LYS:HD3	1:A:139:LYS:HA	1.90	0.41
1:A:538:ARG:HH22	1:A:670:GLY:HA2	1.86	0.41
1:A:672:THR:O	1:A:674:GLY:N	2.54	0.41
1:A:621:ARG:HD3	1:A:621:ARG:HA	1.90	0.41
1:A:645:VAL:HG22	1:A:661:ILE:HG23	2.03	0.41
2:B:190:TYR:CG	2:B:199:CYS:HB2	2.56	0.41
1:A:298:LYS:NZ	6:A:901:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:VAL:HB	1:A:588:ILE:HG13	2.02	0.41
2:B:147:GLU:OE1	2:B:147:GLU:N	2.48	0.41
1:A:151:GLU:O	1:A:151:GLU:HG2	2.22	0.40
1:A:552:TYR:HA	1:A:711:LYS:HA	2.03	0.40
1:A:643:LEU:HD13	1:A:703:PHE:CZ	2.56	0.40
2:B:325:TYR:CZ	2:B:329:ILE:HD11	2.56	0.40
2:B:582:LYS:HD3	2:B:590:CYS:HB2	2.03	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	555/722 (77%)	503 (91%)	49 (9%)	3 (0%)	29 57
2	B	686/692 (99%)	646 (94%)	40 (6%)	0	100 100
All	All	1241/1414 (88%)	1149 (93%)	89 (7%)	3 (0%)	47 75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	653	GLN
1	A	447	PRO
1	A	652	PRO

5.3.2 Protein sidechains (i)

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	408/599 (68%)	379 (93%)	29 (7%)	14 36
2	B	548/575 (95%)	507 (92%)	41 (8%)	13 34
All	All	956/1174 (81%)	886 (93%)	70 (7%)	14 35

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ARG
1	A	64	ASP
1	A	72	HIS
1	A	77	HIS
1	A	116	LYS
1	A	147	SER
1	A	151	GLU
1	A	215	ILE
1	A	297	ASP
1	A	352	THR
1	A	399	VAL
1	A	423	ILE
1	A	424[A]	ARG
1	A	424[B]	ARG
1	A	427	CYS
1	A	428	ASP
1	A	431	THR
1	A	542	THR
1	A	551	HIS
1	A	592	LEU
1	A	610	GLU
1	A	612	ASN
1	A	617	THR
1	A	619	ARG
1	A	632	SER
1	A	655	GLU
1	A	660	ILE
1	A	705	VAL
1	A	712	ASP
2	B	14	GLN
2	B	22	GLN
2	B	39	LYS
2	B	54	ARG
2	B	59	THR

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Mol	Chain	Res	Type
2	B	60	LEU
2	B	87	ARG
2	B	90	ARG
2	B	110	LEU
2	B	111	GLN
2	B	182	CYS
2	B	186	SER
2	B	206	ASP
2	B	211	ARG
2	B	231	LEU
2	B	234	ASP
2	B	241	ASP
2	B	245	ASP
2	B	261	VAL
2	B	262	ASN
2	B	266	ASP
2	B	282	ASP
2	B	288	GLN
2	B	292	SER
2	B	297	LYS
2	B	343	ARG
2	B	353	GLU
2	B	381	CYS
2	B	385	VAL
2	B	405	LYS
2	B	417	LYS
2	B	445	SER
2	B	449	LEU
2	B	487	ASP
2	B	518	CYS
2	B	519	VAL
2	B	549	VAL
2	B	576	CYS
2	B	581	ARG
2	B	639	THR
2	B	680	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	GLN
1	A	411	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 2 are 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	SO4	B	705	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	714	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	709	-	4,4,4	0.13	0	6,6,6	0.05	0
5	BCT	B	704	4	2,3,3	0.38	0	2,3,3	0.31	0
3	SO4	A	801	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	710	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	706	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	707	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	713	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	803	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	B	711	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	712	-	4,4,4	0.14	0	6,6,6	0.05	0
5	BCT	B	703	4	2,3,3	0.41	0	2,3,3	0.08	0
3	SO4	A	802	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	B	708	-	4,4,4	0.14	0	6,6,6	0.05	0

There are no bond length outliers.

There are no bond angle outliers.

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
3	B	714	SO4	4	0
3	B	709	SO4	1	0
5	B	704	BCT	1	0
3	B	710	SO4	1	0
3	A	803	SO4	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, 95^{th} 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	566/722 (78%)	0.49	65 (11%)	4	3	49, 91, 184, 248	0
2	B	688/692 (99%)	0.08	15 (2%)	62	59	48, 73, 121, 225	0
All	All	1254/1414 (88%)	0.27	80 (6%)	19	15	48, 78, 160, 248	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	ALA	11.4
1	A	356	LEU	10.8
1	A	354	PRO	8.3
1	A	357	SER	7.8
1	A	358	SER	7.6
1	A	600	PRO	5.8
1	A	633	THR	5.4
1	A	701	HIS	4.8
1	A	450	GLN	4.5
1	A	643	LEU	4.3
1	A	353	LYS	4.2
1	A	634	ASP	3.9
1	A	674	GLY	3.9
1	A	676	GLU	3.8
1	A	699	VAL	3.8
1	A	638	PHE	3.8
2	B	285	PRO	3.8
1	A	698	GLU	3.7
1	A	602	PHE	3.6
1	A	382	GLU	3.5
1	A	675	THR	3.4
2	B	26	ASN	3.4
1	A	449	ALA	3.4
1	A	703	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	609	ILE	3.4
1	A	68	ILE	3.4
1	A	623	ASN	3.4
1	A	700	LYS	3.3
1	A	69	PRO	3.3
1	A	61	TYR	3.3
1	A	627	LEU	3.3
1	A	381	ARG	3.3
1	A	379	ASN	3.2
1	A	587	SER	3.2
2	B	287	PHE	3.2
1	A	599	GLU	3.2
1	A	626	ASN	3.2
1	A	635	PRO	3.1
1	A	443	PRO	3.0
2	B	297	LYS	3.0
1	A	620	THR	2.9
1	A	661	ILE	2.9
2	B	288	GLN	2.9
2	B	292	SER	2.9
1	A	34	GLY	2.8
1	A	595	GLU	2.8
1	A	651	GLY	2.8
2	B	667	GLN	2.8
1	A	532	LEU	2.6
1	A	380	PRO	2.6
1	A	566	TRP	2.6
1	A	705	VAL	2.6
1	A	666	GLY	2.6
1	A	563	PRO	2.6
1	A	544	ILE	2.5
1	A	352	THR	2.5
2	B	6	SER	2.5
1	A	607	GLY	2.5
1	A	545	PRO	2.5
2	B	204	ALA	2.4
1	A	677	ASN	2.4
1	A	384	ALA	2.3
2	B	175	ALA	2.3
1	A	625	ILE	2.3
1	A	378	LYS	2.3
1	A	561	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	423	ASP	2.2
2	B	421	SER	2.2
1	A	447	PRO	2.2
1	A	149	GLY	2.2
1	A	35	SER	2.2
1	A	641	SER	2.2
1	A	637	THR	2.2
2	B	422	SER	2.1
1	A	174	PRO	2.1
1	A	672	THR	2.1
2	B	299	LEU	2.1
1	A	554	GLY	2.0
1	A	146	THR	2.0
2	B	637	SER	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
3	SO4	B	714	5/5	0.60	0.22	153,153,171,262	0
3	SO4	B	711	5/5	0.80	0.26	125,134,147,161	0
3	SO4	B	706	5/5	0.82	0.24	120,129,145,160	0
3	SO4	B	712	5/5	0.83	0.32	126,126,129,154	0
3	SO4	A	801	5/5	0.85	0.17	164,165,171,176	0
3	SO4	A	802	5/5	0.86	0.18	119,126,153,230	0
3	SO4	A	803	5/5	0.86	0.34	203,204,227,309	0
3	SO4	B	709	5/5	0.89	0.38	111,112,143,149	0
3	SO4	B	705	5/5	0.90	0.53	122,138,148,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	BCT	B	704	4/4	0.90	0.17	65,65,73,76	0
3	SO4	B	713	5/5	0.91	0.40	120,121,124,139	0
3	SO4	B	707	5/5	0.93	0.17	98,101,119,121	0
3	SO4	B	710	5/5	0.95	0.12	88,106,117,129	0
3	SO4	B	708	5/5	0.95	0.10	90,100,113,116	0
4	FE	B	701	1/1	0.97	0.17	68,68,68,68	0
4	FE	B	702	1/1	0.98	0.22	72,72,72,72	0
5	BCT	B	703	4/4	0.99	0.15	43,59,60,66	0

6.5 Other polymers (i)

There are no such residues in this entry.