



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:29 PM GMT

PDB ID : 4F7K
Title : Crystal structure of Lac15 from a marine microbial metagenome
Authors : Ge, H.; Xiao, Y.
Deposited on : 2012-05-16
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

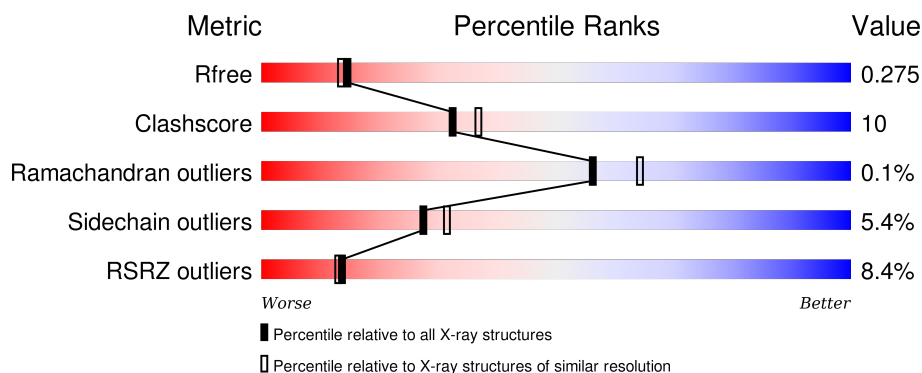
1 Overall quality at a glance

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	425	<div> <div>5%</div> <div>75%</div> <div>11%</div> <div>•</div> <div>11%</div> </div>
1	B	425	<div> <div>9%</div> <div>64%</div> <div>21%</div> <div>•</div> <div>12%</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
2	GOL	A	501	-	-	-	X
2	GOL	A	502	-	-	X	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6042 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 Laccase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	25	3	0
			2900	1835	515	541	9			
1	B	373	Total	C	N	O	S	35	0	0
			2863	1812	506	536	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	440	LEU	-	EXPRESSION TAG	UNP E1ACR6
A	441	GLU	-	EXPRESSION TAG	UNP E1ACR6
A	442	HIS	-	EXPRESSION TAG	UNP E1ACR6
A	443	HIS	-	EXPRESSION TAG	UNP E1ACR6
A	444	HIS	-	EXPRESSION TAG	UNP E1ACR6
A	445	HIS	-	EXPRESSION TAG	UNP E1ACR6
A	446	HIS	-	EXPRESSION TAG	UNP E1ACR6
A	447	HIS	-	EXPRESSION TAG	UNP E1ACR6
B	440	LEU	-	EXPRESSION TAG	UNP E1ACR6
B	441	GLU	-	EXPRESSION TAG	UNP E1ACR6
B	442	HIS	-	EXPRESSION TAG	UNP E1ACR6
B	443	HIS	-	EXPRESSION TAG	UNP E1ACR6
B	444	HIS	-	EXPRESSION TAG	UNP E1ACR6
B	445	HIS	-	EXPRESSION TAG	UNP E1ACR6
B	446	HIS	-	EXPRESSION TAG	UNP E1ACR6
B	447	HIS	-	EXPRESSION TAG	UNP E1ACR6

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	153	Total	O	0	0
			153	153		
3	B	96	Total	O	0	0
			96	96		

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.

Chain A: 5% 75% 11% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.41Å 91.36Å 86.15Å 90.00° 112.10° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 39.65 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-2.20) 98.3 (39.65-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.214 , 0.265 0.228 , 0.275	Depositor DCC
R_{free} test set	2234 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 44251 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6042	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	0.67	1/2982 (0.0%)	0.87	5/4072 (0.1%)
1	B	0.71	4/2936 (0.1%)	1.11	9/4010 (0.2%)
All	All	0.69	5/5918 (0.1%)	0.99	14/8082 (0.2%)

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	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	264	ASP	CG-OD1	-16.26	0.88	1.25
1	B	264	ASP	CG-OD2	11.99	1.52	1.25
1	B	163	ARG	NE-CZ	7.84	1.43	1.33
1	B	296	GLU	CB-CG	-7.14	1.38	1.52
1	A	295	SER	CB-OG	5.69	1.49	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	ARG	NE-CZ-NH2	-30.16	105.22	120.30
1	B	163	ARG	NE-CZ-NH1	28.39	134.50	120.30
1	B	264	ASP	CB-CG-OD2	-28.33	92.80	118.30
1	A	62	ARG	NE-CZ-NH1	-20.15	110.22	120.30
1	A	62	ARG	NE-CZ-NH2	17.16	128.88	120.30
1	B	264	ASP	CB-CG-OD1	15.53	132.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	62	ARG	CD-NE-CZ	6.15	132.21	123.60
1	B	163	ARG	CD-NE-CZ	-5.69	115.64	123.60
1	B	163	ARG	CG-CD-NE	-5.69	99.86	111.80
1	B	186	LEU	CA-CB-CG	5.60	128.17	115.30
1	B	164	ILE	CB-CA-C	-5.51	100.57	111.60
1	A	191	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	B	217	ARG	NE-CZ-NH1	-5.09	117.75	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	289	ASN	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	2900	0	2810	43	0
1	B	2863	0	2778	74	0
2	A	18	0	24	5	0
2	B	12	0	16	2	0
3	A	153	0	0	6	0
3	B	96	0	0	3	0
All	All	6042	0	5628	118	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 10.

All (118) 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:62:ARG:HG2	1:B:62:ARG:HH11	1.31	0.95
1:A:60:ARG:HH11	1:A:60:ARG:HG2	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ASP:CG	1:A:310:MET:H	1.82	0.83
1:A:166:GLU:H	1:A:166:GLU:CD	1.85	0.81
1:B:188:ASN:HD22	1:B:188:ASN:H	1.31	0.79
1:B:370:ARG:NH2	3:B:682:HOH:O	2.16	0.77
1:A:195:GLU:HG2	2:A:502:GOL:H2	1.67	0.76
1:B:279:LEU:O	2:B:502:GOL:H11	1.85	0.76
1:B:204:ASP:OD1	1:B:290:THR:OG1	2.05	0.74
1:B:416:GLY:H	1:B:438:VAL:HG22	1.54	0.71
1:B:349:ASP:N	1:B:435:TRP:CH2	2.58	0.71
1:A:99:THR:HG23	3:A:608:HOH:O	1.90	0.71
1:B:118:ALA:H	1:B:303:ASN:HD21	1.39	0.69
1:B:186:LEU:N	3:B:665:HOH:O	2.25	0.69
1:A:309:ASP:CG	1:A:310:MET:N	2.48	0.68
1:B:352:LEU:HB2	1:B:434:THR:HG21	1.78	0.65
1:A:31:GLN:HE21	1:A:52:GLY:H	1.42	0.65
1:A:263:THR:HG23	1:A:265:ALA:H	1.62	0.64
1:A:60:ARG:HG2	1:A:60:ARG:NH1	2.10	0.64
1:B:348:THR:O	1:B:349:ASP:HB2	1.97	0.64
1:B:200:VAL:CG1	1:B:261:VAL:HG21	2.29	0.62
1:B:62:ARG:HG2	1:B:62:ARG:NH1	2.08	0.62
1:A:289:ASN:HD22	1:A:290:THR:N	1.97	0.62
1:A:309:ASP:OD1	1:A:310:MET:N	2.30	0.61
1:B:31:GLN:HE21	1:B:52:GLY:H	1.49	0.61
1:B:164:ILE:H	1:B:188:ASN:HD21	1.48	0.60
1:B:311:GLY:HA3	1:B:360:THR:O	2.03	0.59
1:B:203:GLY:HA3	1:B:290:THR:H	1.66	0.59
1:A:86:LEU:HB3	1:A:88:ILE:HG23	1.85	0.58
1:B:227:GLU:HG3	1:B:262:ILE:HD13	1.85	0.58
1:B:87:ARG:HD2	1:B:117:ASP:OD2	2.03	0.57
1:B:415:PRO:HA	1:B:438:VAL:HG13	1.86	0.56
1:B:155:LEU:HD22	1:B:196:PRO:HD2	1.87	0.56
1:A:130:TRP:HB2	1:A:429:ALA:O	2.05	0.56
1:B:164:ILE:HD11	1:B:189:PHE:CB	2.37	0.55
1:B:280:LEU:O	2:B:502:GOL:H12	2.06	0.54
1:A:31:GLN:HE21	1:A:52:GLY:N	2.05	0.54
2:A:501:GOL:H12	1:B:370:ARG:CZ	2.37	0.53
1:A:250:ALA:HB1	1:A:251:PRO:HD2	1.89	0.53
1:A:162:TRP:HZ3	1:A:191:ARG:HB2	1.73	0.53
1:A:151:VAL:HG12	1:A:205:ARG:HG2	1.90	0.53
1:B:200:VAL:HG11	1:B:261:VAL:HG21	1.89	0.53
1:A:289:ASN:HD22	1:A:289:ASN:C	2.10	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:LEU:HD22	1:B:373:HIS:CD2	2.43	0.53
1:A:195:GLU:CG	2:A:502:GOL:H2	2.39	0.53
1:B:429:ALA:O	1:B:430:ALA:HB3	2.09	0.52
1:B:54:THR:HA	1:B:55:PRO:C	2.30	0.52
1:B:164:ILE:HG23	1:B:170:LEU:HD23	1.91	0.52
1:A:318:LEU:HD13	1:A:373:HIS:CG	2.45	0.52
1:B:188:ASN:ND2	1:B:188:ASN:H	2.06	0.51
1:A:87:ARG:HD3	1:A:117:ASP:OD2	2.11	0.51
1:B:161:ASP:OD2	1:B:217:ARG:NH1	2.44	0.51
1:B:349:ASP:HA	1:B:435:TRP:CH2	2.46	0.51
1:B:152:ASP:OD2	1:B:292:ARG:NH1	2.45	0.50
1:B:48:LEU:O	1:B:136:GLY:HA3	2.12	0.50
1:A:99:THR:CG2	3:A:608:HOH:O	2.54	0.50
1:B:317:THR:HG22	1:B:366:VAL:HB	1.94	0.50
1:A:375:ILE:HD13	1:A:422:CYS:SG	2.52	0.49
1:A:417:ASN:HD21	1:A:437:GLU:HG3	1.78	0.49
1:B:349:ASP:CA	1:B:435:TRP:CH2	2.95	0.49
1:A:234:ASP:OD2	1:A:395:ARG:HD3	2.12	0.49
1:B:93:ASP:HB3	1:B:99:THR:HG21	1.94	0.49
1:B:352:LEU:HB2	1:B:434:THR:CG2	2.42	0.48
1:A:133:VAL:HG22	3:A:724:HOH:O	2.13	0.48
1:A:95:VAL:H	1:A:99:THR:CG2	2.26	0.48
1:A:232:ALA:HB3	1:A:256:ASP:HB2	1.96	0.48
1:A:95:VAL:H	1:A:99:THR:HG22	1.78	0.47
1:A:54:THR:HA	1:A:55:PRO:C	2.34	0.47
1:B:201:ARG:HH21	1:B:290:THR:HA	1.80	0.46
1:B:229:LYS:HG2	1:B:297:ILE:HG13	1.96	0.46
1:B:98:MET:HE2	1:B:435:TRP:CE3	2.50	0.46
1:B:355:PHE:CE1	1:B:361:ALA:HB2	2.51	0.46
1:B:309:ASP:OD1	1:B:309:ASP:N	2.48	0.46
1:B:188:ASN:N	1:B:188:ASN:HD22	2.01	0.46
1:B:232:ALA:HB3	1:B:256:ASP:HB2	1.98	0.46
1:B:416:GLY:O	1:B:438:VAL:N	2.49	0.46
1:B:429:ALA:HB1	1:B:433:LYS:NZ	2.32	0.45
1:A:60:ARG:CG	1:A:60:ARG:NH1	2.79	0.45
1:B:349:ASP:HA	1:B:435:TRP:HH2	1.81	0.45
2:A:502:GOL:H12	3:A:616:HOH:O	2.17	0.45
1:A:86:LEU:HB3	1:A:88:ILE:CG2	2.47	0.45
1:B:429:ALA:O	1:B:430:ALA:CB	2.65	0.44
1:B:290:THR:HG22	1:B:291:THR:N	2.32	0.44
1:B:348:THR:O	1:B:349:ASP:CB	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:HIS:HE1	1:B:397:THR:OG1	2.00	0.44
1:B:220:PRO:HD2	1:B:271:PHE:HE2	1.81	0.44
1:A:308:PRO:HG2	1:A:391:LEU:HD21	1.99	0.44
1:B:186:LEU:N	1:B:186:LEU:HD23	2.33	0.44
1:A:162:TRP:CZ3	1:A:191:ARG:HB2	2.53	0.43
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.84	0.43
1:B:290:THR:HG22	1:B:292:ARG:H	1.82	0.43
1:B:90:ASN:HA	1:B:418:TRP:CH2	2.54	0.43
1:A:211:ILE:HG12	1:A:254:ARG:HG3	2.00	0.43
1:B:164:ILE:HD11	1:B:189:PHE:HB3	2.01	0.42
1:B:371:PHE:CD2	1:B:424:MET:CE	3.03	0.42
1:B:293:GLN:HB2	1:B:294:PRO:HD2	2.01	0.42
1:B:155:LEU:HD12	1:B:283:ILE:HD13	2.01	0.42
1:B:86:LEU:CD2	1:B:113:PHE:CE1	3.02	0.42
1:B:29:VAL:HG13	1:B:72:GLN:HB2	2.02	0.42
1:A:110:GLU:HG2	3:A:732:HOH:O	2.19	0.42
1:B:170:LEU:HA	1:B:170:LEU:HD23	1.82	0.42
1:B:118:ALA:H	1:B:303:ASN:ND2	2.12	0.42
1:A:289:ASN:ND2	1:A:292:ARG:H	2.18	0.42
1:B:98:MET:CE	1:B:435:TRP:CE3	3.03	0.41
1:B:195:GLU:HA	1:B:196:PRO:HA	1.92	0.41
1:B:380:HIS:HE1	1:B:418:TRP:CD1	2.38	0.41
1:A:371:PHE:HB2	1:A:424:MET:CE	2.50	0.41
1:A:225:GLY:HA2	3:A:707:HOH:O	2.19	0.41
1:B:201:ARG:HH11	1:B:201:ARG:HG3	1.85	0.41
1:A:55:PRO:HB2	2:A:502:GOL:C1	2.51	0.41
1:B:267:ILE:O	1:B:282:GLU:HA	2.21	0.41
1:B:86:LEU:HA	3:B:647:HOH:O	2.21	0.41
1:B:266:PRO:HA	1:B:285:VAL:HG23	2.03	0.41
1:B:358:GLY:N	1:B:412:PHE:O	2.46	0.40
1:B:84:HIS:HD2	1:B:124:HIS:NE2	2.18	0.40
1:A:98:MET:HE1	1:A:347:LEU:HD22	2.03	0.40
1:A:420:LEU:O	1:A:434:THR:HG23	2.20	0.40
1:B:62:ARG:CG	1:B:62:ARG:NH1	2.79	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	372/425 (88%)	366 (98%)	6 (2%)	0	100	100
1	B	365/425 (86%)	355 (97%)	9 (2%)	1 (0%)	46	50
All	All	737/850 (87%)	721 (98%)	15 (2%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	202	ARG

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	306/344 (89%)	291 (95%)	15 (5%)	31	36
1	B	304/344 (88%)	286 (94%)	18 (6%)	24	27
All	All	610/688 (89%)	577 (95%)	33 (5%)	27	31

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	99	THR
1	A	110	GLU
1	A	133	VAL
1	A	166	GLU

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Mol	Chain	Res	Type
1	A	198	THR
1	A	254	ARG
1	A	271	PHE
1	A	289	ASN
1	A	305	VAL
1	A	308	PRO
1	A	310	MET
1	A	317	THR
1	A	391	LEU
1	A	401	ASP
1	B	62	ARG
1	B	68	ASP
1	B	110	GLU
1	B	164	ILE
1	B	186	LEU
1	B	188	ASN
1	B	197	VAL
1	B	242	GLN
1	B	254	ARG
1	B	289	ASN
1	B	304	GLU
1	B	318	LEU
1	B	348	THR
1	B	350	THR
1	B	356	GLU
1	B	357	ARG
1	B	364	ARG
1	B	434	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	90	ASN
1	A	242	GLN
1	A	289	ASN
1	A	303	ASN
1	A	417	ASN
1	B	31	GLN
1	B	84	HIS
1	B	90	ASN
1	B	188	ASN

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Mol	Chain	Res	Type
1	B	303	ASN
1	B	373	HIS
1	B	417	ASN

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](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	501	-	5,5,5	0.40	0	5,5,5	0.51	0
2	GOL	A	502	-	5,5,5	0.48	0	5,5,5	0.55	0
2	GOL	A	503	-	5,5,5	0.43	0	5,5,5	0.44	0
2	GOL	B	501	-	5,5,5	0.37	0	5,5,5	0.13	0
2	GOL	B	502	-	5,5,5	0.29	0	5,5,5	0.60	0

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
2	GOL	A	501	-	-	0/4/4/4	0/0/0/0
2	GOL	A	502	-	-	0/4/4/4	0/0/0/0
2	GOL	A	503	-	-	0/4/4/4	0/0/0/0
2	GOL	B	501	-	-	0/4/4/4	0/0/0/0
2	GOL	B	502	-	-	0/4/4/4	0/0/0/0

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.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GOL	1	0
2	A	502	GOL	4	0
2	B	502	GOL	2	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	377/425 (88%)	0.45	23 (6%) 25 24	23, 46, 80, 106	15 (3%)
1	B	373/425 (87%)	0.58	40 (10%) 8 7	30, 55, 103, 128	16 (4%)
All	All	750/850 (88%)	0.52	63 (8%) 14 13	23, 50, 92, 128	31 (4%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	ALA	7.0
1	B	348	THR	5.9
1	B	429	ALA	5.1
1	B	430	ALA	4.8
1	B	387	ALA	4.6
1	B	435	TRP	4.5
1	A	310	MET	4.3
1	B	263	THR	4.2
1	B	347	LEU	4.1
1	B	405	THR	4.1
1	B	297	ILE	4.0
1	A	262	ILE	3.7
1	B	388	ASP	3.6
1	B	350	THR	3.5
1	A	86	LEU	3.5
1	A	397	THR	3.3
1	A	252	ALA	3.1
1	B	111	TYR	2.9
1	B	71	PHE	2.9
1	B	104	GLU	2.8
1	B	436	VAL	2.8
1	A	84	HIS	2.8
1	B	25	PRO	2.8
1	B	29	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	348	THR	2.8
1	B	70	ARG	2.8
1	B	69	ILE	2.7
1	B	251	PRO	2.7
1	A	250	ALA	2.7
1	A	349	ASP	2.7
1	A	355	PHE	2.6
1	B	106	GLY	2.6
1	B	102	VAL	2.6
1	B	287	GLY	2.6
1	A	430	ALA	2.5
1	B	290	THR	2.5
1	B	252	ALA	2.5
1	A	350	THR	2.5
1	A	41	GLY	2.5
1	A	398	THR	2.4
1	A	88	ILE	2.4
1	B	390	ASN	2.4
1	A	312	SER	2.4
1	A	122	TRP	2.4
1	A	85	GLY	2.3
1	B	346	GLY	2.3
1	A	251	PRO	2.3
1	B	26	VAL	2.3
1	B	310	MET	2.3
1	B	109	PHE	2.3
1	A	265	ALA	2.2
1	A	263	THR	2.2
1	B	250	ALA	2.2
1	B	79	SER	2.2
1	B	389	GLY	2.2
1	A	211	ILE	2.2
1	B	27	GLU	2.2
1	B	78	GLY	2.1
1	B	62	ARG	2.1
1	A	218	ILE	2.1
1	B	75	ILE	2.1
1	B	285	VAL	2.1
1	B	41	GLY	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
2	GOL	A	501	6/6	0.60	0.24	7.88	77,79,79,79	0
2	GOL	A	502	6/6	0.85	0.32	6.06	35,37,40,42	6
2	GOL	B	502	6/6	0.81	0.15	1.19	58,62,63,65	0
2	GOL	A	503	6/6	0.66	0.13	-	66,70,71,73	0
2	GOL	B	501	6/6	0.69	0.16	-	93,94,94,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.