



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:58 PM GMT

PDB ID : 3VMT
Title : Crystal structure of Staphylococcus aureus membrane-bound transglycosylase in complex with a Lipid II analog
Authors : Huang, C.Y.; Shih, H.W.; Lin, L.Y.; Tien, Y.W.; Cheng, T.J.R.; Cheng, W.C.; Wong, C.H.; Ma, C.
Deposited on : 2011-12-15
Resolution : 2.30 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

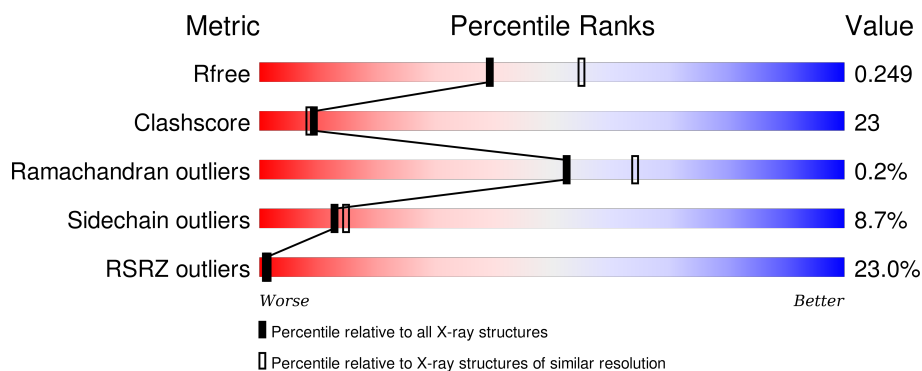
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	263	<div> <div>17%</div> <div>51%</div> <div>30%</div> <div>•</div> <div>16%</div> </div>
1	B	263	<div> <div>21%</div> <div>49%</div> <div>29%</div> <div>5%</div> <div>17%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3695 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 Monofunctional glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1813	1151	311	344	7			
1	B	218	Total	C	N	O	S	0	0	0
			1785	1133	307	338	7			

There are 42 discrepancies between the modelled and reference sequences:

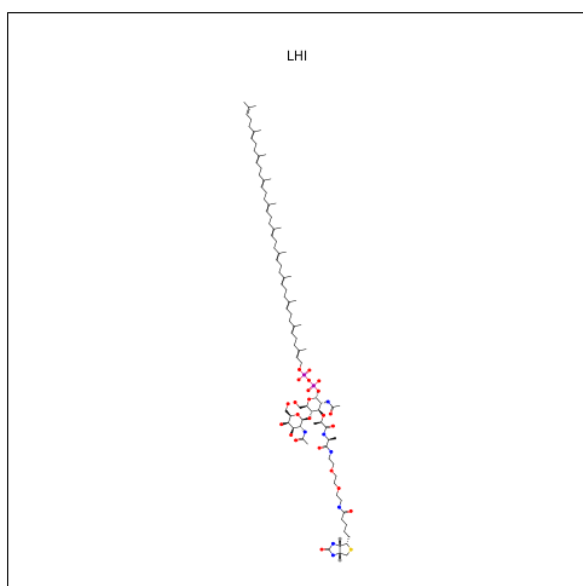
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	EXPRESSION TAG	UNP Q99T05
A	8	GLY	-	EXPRESSION TAG	UNP Q99T05
A	9	SER	-	EXPRESSION TAG	UNP Q99T05
A	10	SER	-	EXPRESSION TAG	UNP Q99T05
A	11	HIS	-	EXPRESSION TAG	UNP Q99T05
A	12	HIS	-	EXPRESSION TAG	UNP Q99T05
A	13	HIS	-	EXPRESSION TAG	UNP Q99T05
A	14	HIS	-	EXPRESSION TAG	UNP Q99T05
A	15	HIS	-	EXPRESSION TAG	UNP Q99T05
A	16	HIS	-	EXPRESSION TAG	UNP Q99T05
A	17	SER	-	EXPRESSION TAG	UNP Q99T05
A	18	SER	-	EXPRESSION TAG	UNP Q99T05
A	19	GLY	-	EXPRESSION TAG	UNP Q99T05
A	20	LEU	-	EXPRESSION TAG	UNP Q99T05
A	21	VAL	-	EXPRESSION TAG	UNP Q99T05
A	22	PRO	-	EXPRESSION TAG	UNP Q99T05
A	23	ARG	-	EXPRESSION TAG	UNP Q99T05
A	24	GLY	-	EXPRESSION TAG	UNP Q99T05
A	25	SER	-	EXPRESSION TAG	UNP Q99T05
A	26	HIS	-	EXPRESSION TAG	UNP Q99T05
A	27	MET	-	EXPRESSION TAG	UNP Q99T05
B	7	MET	-	EXPRESSION TAG	UNP Q99T05
B	8	GLY	-	EXPRESSION TAG	UNP Q99T05
B	9	SER	-	EXPRESSION TAG	UNP Q99T05
B	10	SER	-	EXPRESSION TAG	UNP Q99T05

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	HIS	-	EXPRESSION TAG	UNP Q99T05
B	12	HIS	-	EXPRESSION TAG	UNP Q99T05
B	13	HIS	-	EXPRESSION TAG	UNP Q99T05
B	14	HIS	-	EXPRESSION TAG	UNP Q99T05
B	15	HIS	-	EXPRESSION TAG	UNP Q99T05
B	16	HIS	-	EXPRESSION TAG	UNP Q99T05
B	17	SER	-	EXPRESSION TAG	UNP Q99T05
B	18	SER	-	EXPRESSION TAG	UNP Q99T05
B	19	GLY	-	EXPRESSION TAG	UNP Q99T05
B	20	LEU	-	EXPRESSION TAG	UNP Q99T05
B	21	VAL	-	EXPRESSION TAG	UNP Q99T05
B	22	PRO	-	EXPRESSION TAG	UNP Q99T05
B	23	ARG	-	EXPRESSION TAG	UNP Q99T05
B	24	GLY	-	EXPRESSION TAG	UNP Q99T05
B	25	SER	-	EXPRESSION TAG	UNP Q99T05
B	26	HIS	-	EXPRESSION TAG	UNP Q99T05
B	27	MET	-	EXPRESSION TAG	UNP Q99T05

- Molecule 2 is [(2R,3R,4R,5S,6R)-4-[(2R)-1-[(2S)-1-[2-[2-[2-[5-[(3AS,4S,6AR)-2-OXIDANYLIDENE-1,3,3A,4,6,6A-HEXAHYDROTHIENO[3,4-D]IMIDAZOL-4-YL]PENTANOYLAMINO]ETHOXY]ETHOXY]ETHYLAMINO]-1-OXIDANYLIDENE-PROPAN-2-YL]AMINO]-1-OXIDANYLIDENE-PROPAN-2-YL]OXY-3-ACETAMIDO-5-[(2S,3R,4R,5R,6R)-3-ACETAMIDO-6-(HYDROXYMETHYL)-4,5-BIS(OXIDANYL)OXAN-2-YL]OXY-6-(HYDROXYMETHYL)OXAN-2-YL] [OXIDANYL(3,7,11,15,19,23,27,31,35,39,43-UNDECAMETHYLTETRATETRACONTA-2,6,10,14,18,22,26,30,34,38,42-UNDECAENOXY)PHOSPHORYL] HYDROGEN PHOSPHATE (three-letter code: LHI) (formula: C₉₃H₁₅₅N₇O₂₃P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			43	20	3	18	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total	O	0	0
			41	41		
4	B	11	Total	O	0	0
			11	11		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.49 Å 67.43 Å 152.19 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.08 – 2.30 29.26 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.4 (28.08-2.30) 98.0 (29.26-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.197 , 0.242 0.206 , 0.249	Depositor DCC
R_{free} test set	1547 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.967	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 72.2	EDS
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 30693 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3695	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 4.50% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, LHI

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	0.33	0/1845	0.50	0/2487
1	B	0.28	0/1816	0.45	0/2448
All	All	0.30	0/3661	0.47	0/4935

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1813	0	1791	83	0
1	B	1785	0	1767	81	0
2	A	43	0	33	9	0
3	A	2	0	0	0	0
4	A	41	0	0	0	0
4	B	11	0	0	0	0
All	All	3695	0	3591	165	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 23.

All (165) 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:41:ARG:HD2	1:B:44:LEU:HD11	1.50	0.93
1:B:66:THR:HA	1:B:67:ARG:HG3	1.53	0.89
1:B:202:ASN:HD22	1:B:204:ASN:H	1.19	0.87
1:B:67:ARG:HH22	1:B:70:VAL:HG22	1.42	0.84
1:B:266:GLN:O	1:B:269:ARG:HB2	1.84	0.77
1:A:130:GLY:HA2	2:A:301:LHI:H20	1.66	0.77
1:B:67:ARG:HH21	1:B:162:ARG:HD2	1.52	0.74
1:B:67:ARG:HH21	1:B:162:ARG:CD	2.02	0.73
1:A:42:ILE:HG23	1:A:43:LEU:HD12	1.72	0.72
1:A:114:GLY:HA2	1:A:117:ARG:NH2	2.04	0.72
1:B:151:THR:HG22	1:B:155:LYS:HE3	1.71	0.72
1:A:109:GLY:O	1:A:133:THR:HG21	1.90	0.71
1:B:44:LEU:HD12	1:B:45:LYS:HG2	1.72	0.70
1:B:141:ASN:ND2	1:B:180:ILE:HG22	2.07	0.70
1:B:202:ASN:ND2	1:B:204:ASN:H	1.89	0.69
1:A:67:ARG:HB3	1:A:68:ASP:C	2.13	0.69
1:A:66:THR:HG23	1:A:67:ARG:HG3	1.75	0.68
1:A:66:THR:HA	1:A:67:ARG:HG2	1.75	0.68
1:B:54:ILE:O	1:B:58:ILE:HG12	1.93	0.68
1:B:168:ASN:H	1:B:168:ASN:HD22	1.42	0.68
1:B:67:ARG:HG2	1:B:68:ASP:O	1.94	0.68
1:A:130:GLY:N	2:A:301:LHI:HOA6	1.92	0.67
1:A:107:HIS:NE2	1:A:133:THR:OG1	2.29	0.66
1:A:202:ASN:HD21	1:A:204:ASN:HB2	1.60	0.65
1:B:181:TYR:CZ	1:B:183:GLY:HA2	2.32	0.65
1:B:150:PHE:O	1:B:154:VAL:HG23	1.98	0.64
1:A:155:LYS:O	1:A:159:VAL:HG23	1.98	0.64
1:B:67:ARG:NH2	1:B:70:VAL:HG22	2.12	0.63
1:B:159:VAL:O	1:B:163:VAL:HG23	1.98	0.63
1:A:56:LEU:O	1:A:60:ILE:HG13	1.99	0.63
1:A:225:ALA:HB1	1:A:229:TYR:CD2	2.34	0.62
1:B:152:ARG:HA	1:B:155:LYS:HD3	1.80	0.62
1:A:65:SER:HB3	1:A:155:LYS:HB2	1.81	0.61
1:B:113:LYS:O	1:B:117:ARG:HD2	2.01	0.61
1:A:112:LEU:O	1:A:116:THR:HG23	2.01	0.60
1:A:130:GLY:CA	2:A:301:LHI:H20	2.31	0.60
1:B:52:ILE:HG13	1:B:53:ILE:N	2.17	0.60
1:B:212:THR:H	1:B:215:GLN:NE2	1.99	0.60
1:A:106:ASN:N	1:A:106:ASN:HD22	2.00	0.59
1:A:133:THR:HG22	1:A:136:GLN:HG3	1.85	0.59
1:A:230:ASN:ND2	1:A:232:ASN:H	2.00	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ARG:HG2	1:B:69:ASN:HA	1.85	0.58
1:A:118:ALA:HB2	1:A:131:GLY:HA3	1.86	0.58
1:B:110:PHE:CG	1:B:111:ASP:N	2.72	0.57
1:A:46:ILE:HA	1:A:49:THR:HG22	1.84	0.57
1:A:180:ILE:HG13	1:A:182:PHE:CE2	2.40	0.57
1:B:226:PRO:HB2	1:B:228:VAL:HG22	1.85	0.57
1:A:98:SER:HA	1:A:252:GLN:HE22	1.68	0.57
1:A:45:LYS:HD3	1:A:46:ILE:HG23	1.85	0.57
1:B:45:LYS:HZ2	1:B:48:LEU:HB2	1.70	0.56
1:A:65:SER:O	1:A:68:ASP:HB2	2.05	0.56
1:A:66:THR:HA	1:A:67:ARG:CG	2.34	0.56
1:B:66:THR:HB	1:B:67:ARG:HD2	1.87	0.56
1:A:211:ILE:HG13	1:A:215:GLN:HE21	1.70	0.56
1:A:61:MET:HA	1:A:61:MET:CE	2.35	0.55
1:A:220:ALA:HB3	1:A:245:ASN:HD21	1.72	0.55
1:A:149:SER:HB3	1:A:152:ARG:HG2	1.89	0.54
1:A:110:PHE:CE1	1:A:115:THR:HG21	2.42	0.54
1:B:41:ARG:CD	1:B:44:LEU:HD11	2.32	0.54
1:B:135:THR:HG21	1:B:164:GLU:HG2	1.88	0.54
1:B:60:ILE:O	1:B:64:LEU:HD23	2.07	0.54
1:B:62:TYR:O	1:B:66:THR:HG23	2.08	0.54
1:A:148:ARG:HA	1:A:148:ARG:HE	1.72	0.54
1:B:225:ALA:HB1	1:B:229:TYR:CD2	2.43	0.53
1:B:47:LEU:O	1:B:51:LEU:HD13	2.08	0.53
1:A:114:GLY:HA3	2:A:301:LHI:HA1B	1.90	0.53
1:A:144:TYR:C	1:A:146:ASN:H	2.11	0.53
1:A:50:ILE:O	1:A:54:ILE:HG23	2.09	0.53
1:A:230:ASN:HD22	1:A:231:ILE:N	2.07	0.53
1:B:67:ARG:NH2	1:B:162:ARG:HD2	2.23	0.52
1:A:202:ASN:C	1:A:202:ASN:HD22	2.13	0.51
1:A:133:THR:CG2	1:A:136:GLN:H	2.23	0.51
1:A:110:PHE:HE2	1:A:112:LEU:HD23	1.75	0.51
1:B:67:ARG:NH1	1:B:69:ASN:OD1	2.44	0.51
1:A:180:ILE:HD12	1:A:223:VAL:HG21	1.93	0.50
1:B:66:THR:HA	1:B:67:ARG:CG	2.35	0.50
1:B:53:ILE:O	1:B:57:PHE:N	2.42	0.50
1:A:190:GLU:OE1	1:A:201:VAL:HG22	2.11	0.50
1:A:131:GLY:HA2	2:A:301:LHI:HN7	1.77	0.49
1:A:168:ASN:OD1	1:A:171:GLU:HG3	2.12	0.49
1:B:67:ARG:HH22	1:B:70:VAL:CG2	2.21	0.49
1:A:50:ILE:O	1:A:53:ILE:HG22	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:O	1:A:51:LEU:HB2	2.12	0.49
1:B:99:MET:CE	1:B:248:LYS:HD2	2.42	0.49
1:A:130:GLY:N	2:A:301:LHI:H20	2.28	0.49
1:A:235:SER:O	1:A:239:THR:HG23	2.13	0.48
1:A:250:LYS:HD2	1:A:257:GLU:OE1	2.13	0.48
1:B:202:ASN:C	1:B:202:ASN:HD22	2.17	0.48
1:B:48:LEU:HD23	1:B:48:LEU:C	2.34	0.48
1:A:133:THR:HG22	1:A:136:GLN:CG	2.43	0.48
1:B:190:GLU:OE1	1:B:201:VAL:HG22	2.14	0.48
1:B:141:ASN:HD21	1:B:180:ILE:HG22	1.79	0.47
1:B:189:LEU:HG	1:B:201:VAL:HG11	1.96	0.47
1:A:114:GLY:O	1:A:118:ALA:HB2	2.14	0.47
1:A:152:ARG:HA	1:A:155:LYS:HE2	1.96	0.47
1:A:86:ASP:N	1:A:170:ASN:HD21	2.13	0.47
1:A:100:GLU:OE1	2:A:301:LHI:H17	2.15	0.47
1:B:180:ILE:HD12	1:B:223:VAL:HG21	1.96	0.47
1:A:131:GLY:O	2:A:301:LHI:HA1A	2.15	0.47
1:B:246:LEU:HD23	1:B:249:MET:HE3	1.97	0.46
1:B:50:ILE:O	1:B:54:ILE:HD13	2.15	0.46
1:A:230:ASN:HD22	1:A:230:ASN:C	2.18	0.46
1:B:202:ASN:HD21	1:B:204:ASN:HB2	1.79	0.46
1:B:63:PHE:O	1:B:66:THR:O	2.33	0.46
1:B:67:ARG:HG2	1:B:68:ASP:C	2.35	0.46
1:A:61:MET:HA	1:A:61:MET:HE2	1.96	0.46
1:A:54:ILE:HG13	1:A:55:ALA:N	2.31	0.46
1:A:79:LYS:NZ	1:A:179:ASN:HD22	2.14	0.46
1:B:199:THR:HA	1:B:209:SER:O	2.15	0.46
1:A:202:ASN:ND2	1:A:204:ASN:HB2	2.29	0.46
1:A:49:THR:HA	1:A:52:ILE:HG22	1.97	0.46
1:B:235:SER:O	1:B:239:THR:HG23	2.17	0.45
1:B:146:ASN:HD22	1:B:146:ASN:N	2.14	0.45
1:B:66:THR:CA	1:B:67:ARG:HG3	2.37	0.45
1:A:42:ILE:HG23	1:A:43:LEU:CD1	2.45	0.45
1:B:197:PHE:CD2	1:B:215:GLN:HG2	2.51	0.45
1:B:66:THR:HB	1:B:67:ARG:CD	2.47	0.45
1:A:133:THR:HG23	1:A:136:GLN:H	1.82	0.45
1:B:151:THR:O	1:B:155:LYS:HD2	2.17	0.45
1:A:181:TYR:CZ	1:A:183:GLY:HA2	2.51	0.44
1:B:245:ASN:O	1:B:249:MET:HE2	2.17	0.44
1:A:150:PHE:O	1:A:154:VAL:HG23	2.16	0.44
1:B:140:LYS:HA	1:B:144:TYR:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASN:ND2	1:A:106:ASN:N	2.64	0.44
1:B:104:PHE:CD1	1:B:134:ILE:HB	2.51	0.44
1:A:60:ILE:O	1:A:64:LEU:HD22	2.17	0.44
1:B:99:MET:HE3	1:B:248:LYS:HD2	1.99	0.44
1:A:41:ARG:NH1	1:A:41:ARG:HB2	2.33	0.44
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.82	0.44
1:A:202:ASN:HD22	1:A:204:ASN:N	2.15	0.44
1:A:250:LYS:HD3	1:A:260:TYR:CG	2.53	0.44
1:A:203:LYS:O	1:A:210:HIS:HE1	2.01	0.44
1:B:245:ASN:C	1:B:249:MET:HE2	2.38	0.43
1:B:146:ASN:N	1:B:146:ASN:ND2	2.65	0.43
1:A:130:GLY:HA2	1:A:131:GLY:HA2	1.54	0.43
1:A:44:LEU:HD12	1:A:44:LEU:C	2.39	0.43
1:B:96:PHE:CE2	1:B:220:ALA:HA	2.53	0.43
1:B:168:ASN:HD21	1:B:171:GLU:HG3	1.84	0.43
1:A:266:GLN:HA	1:A:269:ARG:HD3	1.99	0.43
1:B:70:VAL:O	1:B:73:LEU:HB2	2.19	0.43
1:B:180:ILE:O	1:B:187:TYR:HA	2.18	0.43
1:A:149:SER:HB3	1:A:152:ARG:CG	2.47	0.43
1:A:45:LYS:HD3	1:A:46:ILE:N	2.34	0.43
1:B:165:LYS:HD3	1:B:165:LYS:O	2.19	0.43
2:A:301:LHI:H19	2:A:301:LHI:H13	2.01	0.42
1:B:144:TYR:HB3	1:B:145:ASP:H	1.55	0.42
1:B:99:MET:HG3	1:B:99:MET:O	2.19	0.42
1:B:229:TYR:OH	1:B:237:ASN:HB3	2.19	0.42
1:A:202:ASN:HD22	1:A:204:ASN:H	1.66	0.42
1:B:53:ILE:H	1:B:53:ILE:HG13	1.59	0.42
1:B:217:ALA:HB2	1:B:249:MET:HE3	2.01	0.42
1:B:152:ARG:HD3	1:B:155:LYS:HD3	2.01	0.41
1:A:65:SER:O	1:A:67:ARG:HA	2.21	0.41
1:B:168:ASN:HD21	1:B:171:GLU:CG	2.34	0.41
1:A:60:ILE:HG22	1:A:64:LEU:CD2	2.50	0.41
1:B:45:LYS:NZ	1:B:45:LYS:HA	2.36	0.41
1:B:110:PHE:CD2	1:B:111:ASP:N	2.88	0.41
1:B:67:ARG:NH1	1:B:69:ASN:HA	2.36	0.41
1:A:133:THR:HG23	1:A:135:THR:N	2.35	0.41
1:B:223:VAL:HG12	1:B:224:ASN:ND2	2.36	0.41
1:A:202:ASN:ND2	1:A:204:ASN:H	2.18	0.41
1:B:117:ARG:N	1:B:117:ARG:HE	2.18	0.41
1:A:67:ARG:HA	1:A:68:ASP:HB2	2.02	0.40
1:A:144:TYR:C	1:A:146:ASN:N	2.74	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:THR:O	1:B:53:ILE:HG13	2.21	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	218/263 (83%)	205 (94%)	13 (6%)	0	100	100
1	B	214/263 (81%)	206 (96%)	7 (3%)	1 (0%)	34	41
All	All	432/526 (82%)	411 (95%)	20 (5%)	1 (0%)	52	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	145	ASP

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	202/239 (84%)	188 (93%)	14 (7%)	19	24
1	B	199/239 (83%)	178 (89%)	21 (11%)	8	9
All	All	401/478 (84%)	366 (91%)	35 (9%)	13	15

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ARG
1	A	45	LYS
1	A	51	LEU
1	A	52	ILE
1	A	61	MET
1	A	69	ASN
1	A	73	LEU
1	A	74	ARG
1	A	148	ARG
1	A	177	LEU
1	A	180	ILE
1	A	202	ASN
1	A	230	ASN
1	A	238	PHE
1	B	41	ARG
1	B	43	LEU
1	B	46	ILE
1	B	52	ILE
1	B	53	ILE
1	B	56	LEU
1	B	57	PHE
1	B	64	LEU
1	B	66	THR
1	B	73	LEU
1	B	99	MET
1	B	107	HIS
1	B	117	ARG
1	B	147	ASP
1	B	148	ARG
1	B	153	LYS
1	B	155	LYS
1	B	168	ASN
1	B	170	ASN
1	B	202	ASN
1	B	205	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	78	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	87	ASN
1	A	106	ASN
1	A	166	GLN
1	A	170	ASN
1	A	179	ASN
1	A	202	ASN
1	A	204	ASN
1	A	210	HIS
1	A	215	GLN
1	A	230	ASN
1	A	232	ASN
1	A	233	ASN
1	A	245	ASN
1	A	252	GLN
1	A	262	GLN
1	A	266	GLN
1	A	268	ASN
1	B	78	ASN
1	B	106	ASN
1	B	146	ASN
1	B	166	GLN
1	B	168	ASN
1	B	202	ASN
1	B	215	GLN
1	B	224	ASN
1	B	251	GLN
1	B	268	ASN

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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$
2	LHI	A	301	3	41,44,129	4.50	17 (41%)	58,65,170	2.53	28 (48%)

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	LHI	A	301	3	-	0/36/77/191	0/2/2/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	LHI	C16-C20	2.38	1.58	1.53
2	A	301	LHI	C39-C14	3.19	1.61	1.51
2	A	301	LHI	CA1-C99	3.63	1.57	1.50
2	A	301	LHI	C14-C15	3.69	1.63	1.52
2	A	301	LHI	C11-C10	4.02	1.60	1.53
2	A	301	LHI	C19-C20	4.27	1.60	1.53
2	A	301	LHI	OB3-C14	4.40	1.54	1.44
2	A	301	LHI	C99-N7	4.77	1.52	1.34
2	A	301	LHI	C9-C10	5.13	1.61	1.53
2	A	301	LHI	C98-C97	5.82	1.62	1.50
2	A	301	LHI	C97-N6	5.92	1.57	1.34
2	A	301	LHI	C10-N6	6.18	1.56	1.45
2	A	301	LHI	C20-N7	6.62	1.56	1.45
2	A	301	LHI	OC4-C99	10.03	1.46	1.23
2	A	301	LHI	OA4-C15	10.37	1.43	1.23
2	A	301	LHI	C15-N2	12.26	1.50	1.33
2	A	301	LHI	OC3-C97	12.41	1.52	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	LHI	OA4-C15-N2	-5.02	114.19	123.09
2	A	301	LHI	C11-OA2-C12	-4.58	104.86	113.75
2	A	301	LHI	OA2-C11-OA3	-3.16	107.20	111.36
2	A	301	LHI	OC4-C99-CA1	-2.90	116.74	122.06
2	A	301	LHI	OC3-C97-C98	-2.68	117.14	122.06
2	A	301	LHI	PC5-OB6-PC6	-2.67	123.71	132.67
2	A	301	LHI	C10-N6-C97	-2.46	116.78	123.10
2	A	301	LHI	OC3-C97-N6	-2.22	117.33	121.86
2	A	301	LHI	C19-OB2-C8	-2.02	112.72	118.01
2	A	301	LHI	CA1-C99-N7	2.01	119.96	116.11
2	A	301	LHI	C39-C14-C15	2.03	116.41	111.05
2	A	301	LHI	OA2-C12-C8	2.10	114.18	109.75
2	A	301	LHI	OB2-C8-C9	2.20	113.23	107.49
2	A	301	LHI	C8-C9-C10	2.50	115.21	110.30
2	A	301	LHI	OA5-C18-C21	2.71	113.22	106.36
2	A	301	LHI	OA7-C16-C20	2.89	115.54	109.66
2	A	301	LHI	C9-C8-C12	2.96	116.97	110.55
2	A	301	LHI	C17-C16-C20	2.97	114.54	110.43
2	A	301	LHI	OB3-C9-C8	3.21	115.86	107.49
2	A	301	LHI	C19-OA5-C18	3.48	120.49	113.75
2	A	301	LHI	OB3-C14-C39	3.49	117.67	107.50
2	A	301	LHI	OA3-C11-C10	3.55	114.95	108.42
2	A	301	LHI	C11-C10-N6	3.78	118.12	111.01
2	A	301	LHI	C19-C20-N7	4.10	118.73	111.01
2	A	301	LHI	C16-C20-N7	4.39	119.76	110.66
2	A	301	LHI	C9-C10-N6	4.67	119.22	111.07
2	A	301	LHI	C16-C17-C18	5.48	119.75	110.20
2	A	301	LHI	OA5-C18-C17	6.39	121.67	109.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	LHI	9	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	222/263 (84%)	1.10	46 (20%) 1 2	40, 60, 153, 206	0
1	B	218/263 (82%)	1.44	55 (25%) 1 1	49, 91, 170, 209	0
All	All	440/526 (83%)	1.27	101 (22%) 1 1	40, 74, 161, 209	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	ILE	14.8
1	A	42	ILE	14.2
1	B	63	PHE	10.9
1	B	43	LEU	10.3
1	B	44	LEU	10.0
1	B	41	ARG	9.3
1	B	119	LEU	9.3
1	B	46	ILE	8.8
1	A	43	LEU	8.0
1	A	120	PHE	6.8
1	B	228	VAL	6.4
1	A	44	LEU	6.4
1	A	48	LEU	6.3
1	A	122	THR	6.2
1	A	46	ILE	6.1
1	B	118	ALA	6.0
1	B	148	ARG	5.9
1	A	41	ARG	5.9
1	A	45	LYS	5.8
1	B	112	LEU	5.5
1	A	47	LEU	5.5
1	B	47	LEU	5.3
1	A	118	ALA	5.2
1	B	117	ARG	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	150	PHE	4.9
1	B	49	THR	4.9
1	B	152	ARG	4.7
1	B	114	GLY	4.3
1	A	63	PHE	4.3
1	B	226	PRO	4.3
1	A	97	ILE	4.1
1	B	67	ARG	4.1
1	B	64	LEU	4.0
1	A	152	ARG	3.9
1	B	147	ASP	3.8
1	B	165	LYS	3.7
1	A	134	ILE	3.5
1	B	176	TYR	3.5
1	B	62	TYR	3.4
1	A	130	GLY	3.3
1	A	148	ARG	3.3
1	A	60	ILE	3.3
1	B	144	TYR	3.2
1	B	66	THR	3.2
1	B	161	HIS	3.2
1	A	96	PHE	3.1
1	A	98	SER	3.1
1	A	173	LEU	3.1
1	B	45	LYS	3.1
1	B	61	MET	3.0
1	A	172	ILE	3.0
1	B	110	PHE	2.9
1	A	54	ILE	2.9
1	B	60	ILE	2.9
1	A	95	ALA	2.9
1	A	121	SER	2.9
1	B	113	LYS	2.9
1	B	153	LYS	2.9
1	B	229	TYR	2.9
1	B	158	PHE	2.8
1	B	51	LEU	2.8
1	A	219	LEU	2.7
1	A	207	THR	2.6
1	A	176	TYR	2.6
1	B	146	ASN	2.6
1	B	56	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	116	THR	2.5
1	B	177	LEU	2.5
1	B	149	SER	2.5
1	A	177	LEU	2.5
1	B	233	ASN	2.5
1	B	151	THR	2.4
1	A	208	MET	2.4
1	A	254	TYR	2.4
1	B	156	GLU	2.4
1	A	51	LEU	2.4
1	B	90	GLU	2.3
1	B	48	LEU	2.3
1	B	173	LEU	2.3
1	A	145	ASP	2.3
1	B	166	GLN	2.3
1	A	53	ILE	2.3
1	A	269	ARG	2.3
1	A	56	LEU	2.2
1	A	99	MET	2.2
1	A	66	THR	2.2
1	B	133	THR	2.2
1	A	223	VAL	2.2
1	B	141	ASN	2.2
1	B	138	VAL	2.2
1	A	49	THR	2.2
1	B	52	ILE	2.2
1	B	231	ILE	2.2
1	A	92	VAL	2.2
1	A	149	SER	2.2
1	B	135	THR	2.2
1	A	135	THR	2.1
1	A	220	ALA	2.1
1	B	145	ASP	2.0
1	A	174	SER	2.0
1	A	206	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(\AA^2)	Q<0.9
3	MG	A	303	1/1	0.78	0.26	1.93	88,88,88,88	0
2	LHI	A	301	43/126	0.84	0.20	-0.24	59,98,136,226	0
3	MG	A	302	1/1	0.90	0.16	-1.89	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.