Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:57 PM GMT

PDB ID	:	3VMS
Title	:	Crystal structure of Staphylococcus aureus membrane-bound transglycosylase in complex with NBD-Lipid II
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	:	3.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

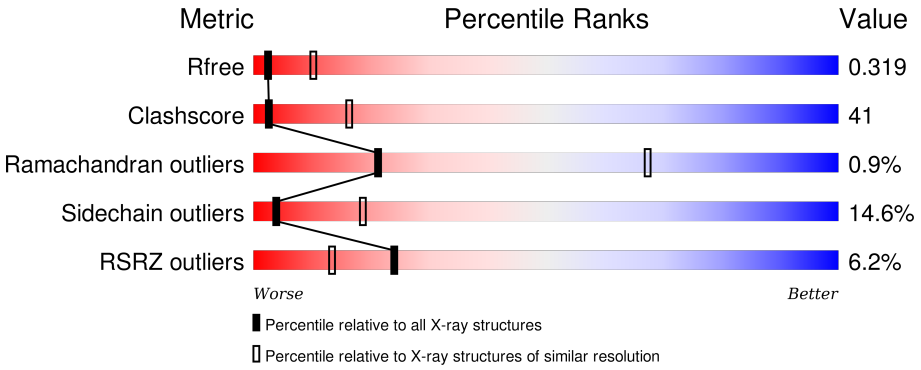
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 <=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	4% 33% 42% 8% 16%
1	B	263	6% 32% 42% 9% 17%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3565 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	220	Total	C	N	O	S	0	0	0
			1794	1139	306	342	7			
1	B	217	Total	C	N	O	S	0	0	0
			1771	1123	303	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

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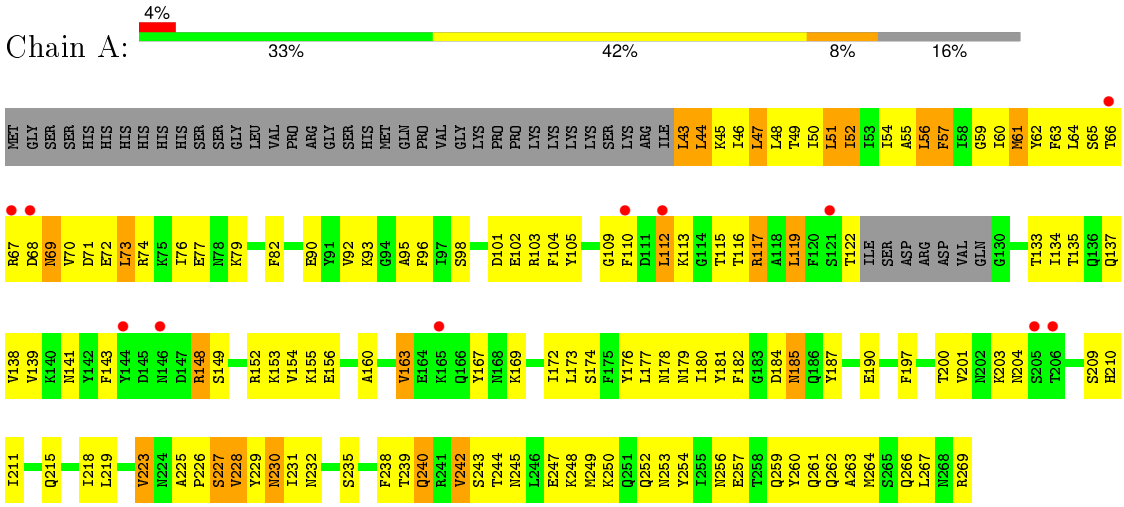
Chain	Residue	Modelled	Actual	Comment	Reference
B	11	HIS	-	EXPRESSION TAG	UNP Q99T05
B	12	HIS	-	EXPRESSION TAG	UNP Q99T05
B	13	HIS	-	EXPRESSION TAG	UNP Q99T05
B	14	HIS	-	EXPRESSION TAG	UNP Q99T05
B	15	HIS	-	EXPRESSION TAG	UNP Q99T05
B	16	HIS	-	EXPRESSION TAG	UNP Q99T05
B	17	SER	-	EXPRESSION TAG	UNP Q99T05
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

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 (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.

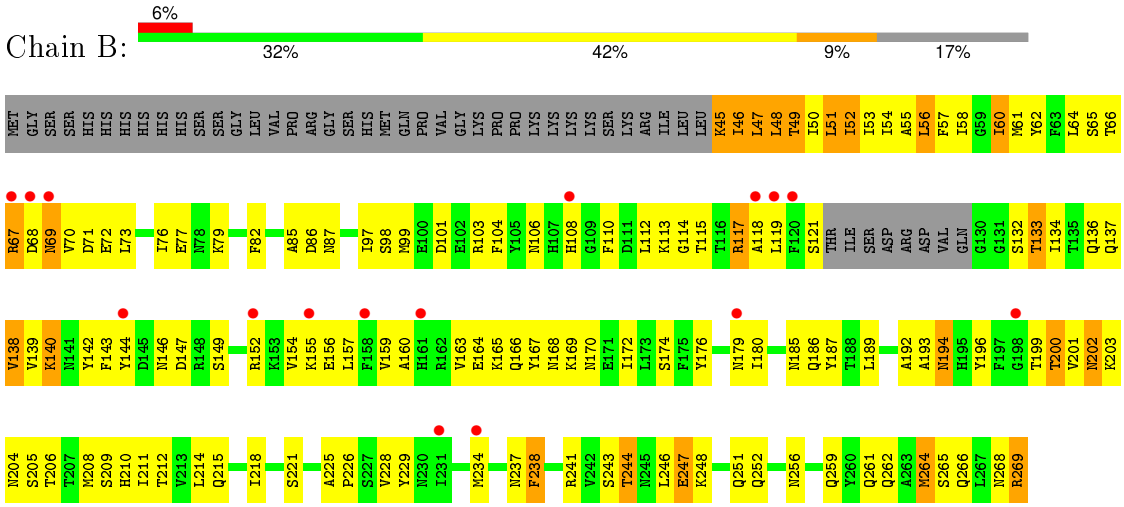
- Molecule 1: Monofunctional glycosyltransferase

Chain A:



- Molecule 1: Monofunctional glycosyltransferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.88Å 67.16Å 140.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 3.20 30.01 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.93-3.20) 99.1 (30.01-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.262 , 0.330 0.243 , 0.319	Depositor DCC
R_{free} test set	522 reflections (4.82%)	DCC
Wilson B-factor (Å^2)	83.7	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 70.0	EDS
Estimated twinning fraction	0.038 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 10845 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	3565	wwPDB-VP
Average B, all atoms (Å^2)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.37	0/1826	0.57	0/2462
1	B	0.30	0/1803	0.49	0/2430
All	All	0.34	0/3629	0.53	0/4892

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	1794	0	1767	154	0
1	B	1771	0	1738	141	0
All	All	3565	0	3505	290	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 41.

All (290) 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:54:ILE:O	1:B:58:ILE:HG23	1.64	0.97
1:B:262:GLN:O	1:B:266:GLN:HG3	1.66	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ARG:HA	1:B:121:SER:HB2	1.47	0.95
1:B:146:ASN:H	1:B:147:ASP:HA	1.33	0.91
1:B:140:LYS:HA	1:B:144:TYR:HB2	1.50	0.90
1:A:101:ASP:HB2	1:A:134:ILE:HG13	1.52	0.89
1:B:79:LYS:HB2	1:B:82:PHE:HB2	1.55	0.88
1:A:149:SER:HB3	1:A:152:ARG:HG2	1.55	0.87
1:A:152:ARG:HA	1:A:155:LYS:HE2	1.56	0.86
1:A:65:SER:O	1:A:68:ASP:HB2	1.77	0.84
1:A:211:ILE:HG13	1:A:215:GLN:HE21	1.42	0.82
1:B:52:ILE:HA	1:B:55:ALA:HB3	1.64	0.79
1:A:180:ILE:O	1:A:187:TYR:HA	1.82	0.79
1:B:211:ILE:HG13	1:B:215:GLN:HE21	1.47	0.79
1:B:65:SER:HB2	1:B:155:LYS:HG3	1.65	0.79
1:A:47:LEU:O	1:A:50:ILE:HG12	1.83	0.79
1:B:67:ARG:N	1:B:68:ASP:HB3	1.97	0.78
1:B:53:ILE:O	1:B:57:PHE:HB2	1.84	0.78
1:B:146:ASN:N	1:B:147:ASP:HA	1.96	0.77
1:A:239:THR:HB	1:A:267:LEU:HD11	1.68	0.76
1:B:47:LEU:H	1:B:47:LEU:HD13	1.51	0.75
1:B:50:ILE:HA	1:B:53:ILE:HB	1.70	0.74
1:A:51:LEU:O	1:A:54:ILE:HG12	1.88	0.74
1:A:257:GLU:O	1:A:261:GLN:HG2	1.87	0.74
1:A:211:ILE:HG13	1:A:215:GLN:NE2	2.04	0.73
1:A:56:LEU:O	1:A:60:ILE:HG12	1.88	0.73
1:A:148:ARG:CG	1:A:148:ARG:HH21	2.02	0.73
1:A:43:LEU:HD22	1:A:44:LEU:N	2.03	0.72
1:B:115:THR:HG23	1:B:119:LEU:HD23	1.70	0.72
1:A:66:THR:CG2	1:A:67:ARG:HG3	2.21	0.71
1:A:112:LEU:O	1:A:116:THR:HG23	1.90	0.71
1:B:55:ALA:O	1:B:58:ILE:HG12	1.90	0.71
1:B:56:LEU:O	1:B:60:ILE:HG22	1.92	0.70
1:A:104:PHE:HE2	1:A:173:LEU:HB2	1.56	0.70
1:A:190:GLU:HA	1:A:190:GLU:OE1	1.92	0.69
1:A:149:SER:HB3	1:A:152:ARG:CG	2.23	0.69
1:A:211:ILE:CG1	1:A:215:GLN:HE21	2.05	0.68
1:A:180:ILE:HD12	1:A:223:VAL:HG21	1.75	0.68
1:B:133:THR:CG2	1:B:136:GLN:HG2	2.25	0.67
1:A:180:ILE:HD12	1:A:223:VAL:CG2	2.25	0.67
1:A:60:ILE:O	1:A:64:LEU:HD13	1.95	0.67
1:A:70:VAL:HG21	1:A:167:TYR:HE2	1.59	0.67
1:B:73:LEU:O	1:B:76:ILE:HG22	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ALA:HA	1:A:249:MET:SD	2.36	0.65
1:A:61:MET:HA	1:A:61:MET:CE	2.26	0.65
1:A:117:ARG:HG3	1:A:122:THR:OG1	1.95	0.65
1:B:66:THR:HG22	1:B:67:ARG:HG2	1.79	0.65
1:B:46:ILE:H	1:B:46:ILE:HD12	1.60	0.65
1:A:46:ILE:O	1:A:50:ILE:HG23	1.96	0.65
1:A:102:GLU:HG3	1:A:252:GLN:NE2	2.11	0.65
1:A:44:LEU:HA	1:A:47:LEU:HD11	1.78	0.65
1:B:47:LEU:HD22	1:B:48:LEU:N	2.13	0.64
1:A:66:THR:HG22	1:A:67:ARG:HG3	1.80	0.64
1:B:70:VAL:HG12	1:B:167:TYR:CE2	2.32	0.64
1:A:137:GLN:O	1:A:141:ASN:ND2	2.30	0.63
1:A:79:LYS:HZ2	1:A:179:ASN:HD22	1.47	0.63
1:B:97:ILE:HG23	1:B:101:ASP:O	1.99	0.62
1:A:104:PHE:CE2	1:A:173:LEU:HB2	2.34	0.62
1:B:115:THR:HA	1:B:118:ALA:HB3	1.81	0.62
1:A:230:ASN:ND2	1:A:232:ASN:H	1.96	0.62
1:A:197:PHE:HE2	1:A:219:LEU:HD11	1.64	0.62
1:B:149:SER:HB3	1:B:152:ARG:HG2	1.80	0.62
1:B:54:ILE:HA	1:B:57:PHE:HB3	1.81	0.62
1:A:133:THR:O	1:A:137:GLN:HG3	2.00	0.61
1:A:250:LYS:HD2	1:A:257:GLU:OE1	2.00	0.61
1:B:133:THR:HG23	1:B:136:GLN:HG2	1.81	0.61
1:A:203:LYS:HG3	1:A:204:ASN:ND2	2.16	0.60
1:A:76:ILE:O	1:A:79:LYS:HG3	2.01	0.60
1:A:135:THR:HG22	1:A:160:ALA:HB1	1.83	0.60
1:B:200:THR:CG2	1:B:208:MET:HB3	2.30	0.60
1:B:117:ARG:CA	1:B:121:SER:HB2	2.25	0.60
1:A:148:ARG:HH21	1:A:148:ARG:HG2	1.65	0.60
1:B:221:SER:O	1:B:225:ALA:HB2	2.01	0.60
1:B:46:ILE:O	1:B:50:ILE:HG23	2.02	0.60
1:B:49:THR:O	1:B:53:ILE:HG12	2.02	0.59
1:B:214:LEU:O	1:B:218:ILE:HG13	2.03	0.59
1:B:144:TYR:HE1	1:B:152:ARG:HB3	1.68	0.59
1:B:112:LEU:HD12	1:B:113:LYS:N	2.18	0.59
1:B:225:ALA:HB1	1:B:229:TYR:HD2	1.67	0.58
1:A:67:ARG:HD2	1:A:69:ASN:HB3	1.85	0.58
1:B:132:SER:OG	1:B:136:GLN:HG3	2.02	0.58
1:A:49:THR:HA	1:A:52:ILE:HD12	1.84	0.58
1:A:90:GLU:H	1:B:269:ARG:NH2	2.02	0.58
1:B:268:ASN:O	1:B:269:ARG:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASP:CB	1:A:134:ILE:HG13	2.29	0.58
1:A:240:GLN:HG3	1:A:240:GLN:O	2.04	0.58
1:B:110:PHE:HE1	1:B:115:THR:H	1.52	0.57
1:B:65:SER:CB	1:B:155:LYS:HG3	2.32	0.57
1:A:57:PHE:CD1	1:A:57:PHE:C	2.77	0.57
1:B:45:LYS:HE3	1:B:46:ILE:HG13	1.85	0.57
1:A:174:SER:O	1:A:178:ASN:HB2	2.04	0.57
1:B:49:THR:O	1:B:52:ILE:HG23	2.05	0.57
1:A:204:ASN:HD22	1:A:204:ASN:N	2.03	0.56
1:B:56:LEU:HD23	1:B:57:PHE:N	2.20	0.56
1:A:230:ASN:HD22	1:A:230:ASN:C	2.08	0.56
1:B:215:GLN:HA	1:B:218:ILE:HD12	1.88	0.56
1:A:230:ASN:C	1:A:230:ASN:ND2	2.59	0.56
1:B:160:ALA:O	1:B:164:GLU:HG2	2.06	0.55
1:A:43:LEU:HD13	1:A:44:LEU:HD13	1.87	0.55
1:A:47:LEU:HD22	1:A:48:LEU:N	2.21	0.55
1:B:168:ASN:O	1:B:172:ILE:HG13	2.06	0.55
1:A:90:GLU:OE2	1:B:262:GLN:HA	2.07	0.55
1:A:247:GLU:OE2	1:A:250:LYS:HE3	2.07	0.55
1:A:79:LYS:NZ	1:A:179:ASN:HD22	2.04	0.54
1:B:200:THR:HG21	1:B:208:MET:HB3	1.88	0.54
1:A:259:GLN:O	1:A:262:GLN:HB3	2.07	0.54
1:A:148:ARG:NH2	1:A:148:ARG:HG2	2.22	0.54
1:B:159:VAL:O	1:B:163:VAL:HG13	2.08	0.54
1:B:65:SER:O	1:B:68:ASP:HB2	2.07	0.53
1:B:225:ALA:HB1	1:B:229:TYR:CD2	2.43	0.53
1:A:69:ASN:O	1:A:72:GLU:HB2	2.09	0.53
1:B:47:LEU:H	1:B:47:LEU:CD1	2.20	0.53
1:B:221:SER:HB3	1:B:241:ARG:HG2	1.90	0.53
1:A:229:TYR:CD2	1:A:238:PHE:CD1	2.96	0.53
1:A:134:ILE:O	1:A:138:VAL:HG23	2.08	0.53
1:B:50:ILE:O	1:B:54:ILE:HG12	2.09	0.53
1:A:148:ARG:HD3	1:A:149:SER:N	2.23	0.53
1:A:67:ARG:HD2	1:A:69:ASN:CB	2.38	0.52
1:A:115:THR:O	1:A:119:LEU:HD13	2.09	0.52
1:B:54:ILE:O	1:B:57:PHE:HB3	2.10	0.52
1:B:133:THR:HG22	1:B:136:GLN:HG2	1.92	0.52
1:A:230:ASN:HD22	1:A:231:ILE:N	2.07	0.52
1:B:160:ALA:O	1:B:163:VAL:HG22	2.10	0.52
1:A:102:GLU:O	1:A:102:GLU:HG2	2.08	0.52
1:B:214:LEU:HG	1:B:218:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LYS:HG3	1:A:204:ASN:HD22	1.74	0.51
1:B:69:ASN:HD22	1:B:69:ASN:C	2.14	0.51
1:B:52:ILE:O	1:B:56:LEU:N	2.37	0.51
1:B:58:ILE:HA	1:B:61:MET:HB2	1.92	0.51
1:A:98:SER:HA	1:A:252:GLN:HE22	1.76	0.51
1:A:148:ARG:C	1:A:148:ARG:HD3	2.30	0.50
1:B:67:ARG:HA	1:B:68:ASP:C	2.30	0.50
1:B:134:ILE:O	1:B:138:VAL:HG23	2.11	0.50
1:A:226:PRO:C	1:A:228:VAL:H	2.15	0.50
1:B:211:ILE:HG13	1:B:215:GLN:HB2	1.94	0.50
1:A:79:LYS:NZ	1:A:179:ASN:ND2	2.59	0.50
1:B:134:ILE:HG23	1:B:176:TYR:CG	2.46	0.50
1:B:110:PHE:CE1	1:B:115:THR:N	2.80	0.50
1:A:229:TYR:HD2	1:A:238:PHE:CD1	2.29	0.50
1:A:148:ARG:NH2	1:A:148:ARG:CG	2.69	0.50
1:A:181:TYR:HE1	1:A:185:ASN:CA	2.25	0.50
1:A:71:ASP:HA	1:A:167:TYR:OH	2.12	0.50
1:A:48:LEU:C	1:A:48:LEU:HD23	2.32	0.50
1:A:148:ARG:NH1	1:A:153:LYS:HB2	2.25	0.50
1:B:76:ILE:HD11	1:B:179:ASN:CB	2.42	0.50
1:A:176:TYR:CD2	1:A:177:LEU:HD12	2.47	0.49
1:A:44:LEU:HA	1:A:47:LEU:CD1	2.42	0.49
1:A:181:TYR:HE1	1:A:185:ASN:N	2.11	0.49
1:A:61:MET:HA	1:A:61:MET:HE3	1.93	0.49
1:B:70:VAL:HG12	1:B:167:TYR:HE2	1.75	0.49
1:B:69:ASN:HD22	1:B:70:VAL:N	2.10	0.49
1:B:154:VAL:HA	1:B:157:LEU:HD13	1.94	0.49
1:A:70:VAL:CG2	1:A:167:TYR:HE2	2.25	0.49
1:A:43:LEU:O	1:A:46:ILE:HG13	2.12	0.49
1:A:47:LEU:O	1:A:51:LEU:HD13	2.13	0.49
1:B:165:LYS:HA	1:B:165:LYS:NZ	2.27	0.49
1:A:90:GLU:OE1	1:A:90:GLU:HA	2.12	0.49
1:A:267:LEU:HD12	1:A:267:LEU:O	2.13	0.49
1:B:114:GLY:O	1:B:118:ALA:N	2.45	0.49
1:B:76:ILE:HD11	1:B:179:ASN:HB2	1.95	0.49
1:B:72:GLU:HB3	1:B:142:TYR:CE1	2.48	0.49
1:B:186:GLN:HA	1:B:186:GLN:OE1	2.13	0.49
1:B:215:GLN:HA	1:B:218:ILE:CD1	2.43	0.49
1:B:247:GLU:O	1:B:251:GLN:HG3	2.13	0.49
1:B:47:LEU:O	1:B:51:LEU:HD13	2.12	0.48
1:A:115:THR:HG22	1:A:119:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ILE:O	1:B:187:TYR:HA	2.13	0.48
1:A:61:MET:HG2	1:A:154:VAL:CG1	2.43	0.48
1:B:103:ARG:HG2	1:B:106:ASN:OD1	2.13	0.48
1:B:53:ILE:HA	1:B:56:LEU:HD22	1.96	0.48
1:B:202:ASN:O	1:B:205:SER:HB3	2.14	0.48
1:B:60:ILE:O	1:B:64:LEU:HB2	2.13	0.48
1:A:43:LEU:CD1	1:A:44:LEU:HD13	2.44	0.48
1:B:243:SER:O	1:B:246:LEU:HB2	2.14	0.48
1:B:72:GLU:HB3	1:B:142:TYR:HE1	1.79	0.47
1:A:109:GLY:O	1:A:133:THR:HG21	2.14	0.47
1:A:50:ILE:O	1:A:54:ILE:HG23	2.13	0.47
1:B:54:ILE:CA	1:B:57:PHE:HB3	2.45	0.47
1:A:134:ILE:HG23	1:A:176:TYR:CG	2.50	0.47
1:A:252:GLN:O	1:A:253:ASN:HB2	2.13	0.47
1:B:67:ARG:N	1:B:68:ASP:CB	2.74	0.47
1:B:202:ASN:O	1:B:210:HIS:CD2	2.68	0.47
1:B:256:ASN:OD1	1:B:259:GLN:HG3	2.15	0.47
1:B:140:LYS:HE3	1:B:140:LYS:HB3	1.79	0.47
1:B:70:VAL:O	1:B:73:LEU:HB2	2.15	0.47
1:A:90:GLU:OE1	1:A:93:LYS:HB2	2.15	0.46
1:B:113:LYS:HD3	1:B:113:LYS:O	2.14	0.46
1:A:156:GLU:HG2	1:A:156:GLU:O	2.16	0.46
1:A:54:ILE:HG13	1:A:55:ALA:N	2.30	0.46
1:A:139:VAL:O	1:A:143:PHE:HD2	1.98	0.46
1:A:260:TYR:HD2	1:A:261:GLN:NE2	2.13	0.46
1:A:110:PHE:HZ	1:A:115:THR:HG21	1.81	0.46
1:A:92:VAL:O	1:A:96:PHE:HD1	1.98	0.46
1:B:52:ILE:HD13	1:B:53:ILE:N	2.31	0.46
1:A:77:GLU:HA	1:A:82:PHE:CD1	2.51	0.46
1:B:237:ASN:HD22	1:B:237:ASN:H	1.64	0.46
1:A:167:TYR:N	1:A:167:TYR:CD2	2.83	0.46
1:A:112:LEU:HD22	1:A:113:LYS:N	2.31	0.46
1:B:140:LYS:CA	1:B:144:TYR:HB2	2.35	0.46
1:B:194:ASN:N	1:B:194:ASN:OD1	2.49	0.45
1:A:152:ARG:HD3	1:A:155:LYS:HZ3	1.80	0.45
1:B:244:THR:O	1:B:248:LYS:HG3	2.15	0.45
1:B:76:ILE:HD12	1:B:142:TYR:CD2	2.52	0.45
1:A:210:HIS:H	1:A:210:HIS:CD2	2.34	0.45
1:A:210:HIS:N	1:A:210:HIS:CD2	2.84	0.45
1:A:71:ASP:C	1:A:73:LEU:N	2.69	0.45
1:B:268:ASN:O	1:B:269:ARG:O	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:TYR:HB3	1:B:143:PHE:CD2	2.52	0.45
1:B:226:PRO:HD2	1:B:229:TYR:CE2	2.51	0.45
1:B:212:THR:H	1:B:215:GLN:NE2	2.14	0.45
1:B:110:PHE:HE1	1:B:115:THR:N	2.12	0.45
1:A:46:ILE:HD12	1:A:47:LEU:N	2.31	0.45
1:A:67:ARG:HB3	1:A:69:ASN:HB3	1.99	0.45
1:B:139:VAL:HB	1:B:156:GLU:OE1	2.17	0.44
1:B:76:ILE:HB	1:B:142:TYR:HE2	1.82	0.44
1:A:105:TYR:CG	1:B:261:GLN:HG3	2.53	0.44
1:B:47:LEU:O	1:B:50:ILE:HG12	2.17	0.44
1:B:54:ILE:HA	1:B:57:PHE:CB	2.46	0.44
1:B:60:ILE:HG12	1:B:60:ILE:O	2.16	0.44
1:A:180:ILE:HG13	1:A:182:PHE:CZ	2.52	0.44
1:A:43:LEU:O	1:A:47:LEU:HD13	2.18	0.44
1:A:69:ASN:O	1:A:69:ASN:OD1	2.36	0.44
1:B:226:PRO:HD2	1:B:229:TYR:CD2	2.53	0.44
1:A:62:TYR:CD1	1:A:62:TYR:C	2.91	0.44
1:B:101:ASP:OD2	1:B:104:PHE:HA	2.18	0.44
1:B:64:LEU:O	1:B:64:LEU:HD13	2.18	0.44
1:B:265:SER:O	1:B:269:ARG:HG3	2.18	0.44
1:A:43:LEU:N	1:A:43:LEU:HD13	2.33	0.44
1:A:242:VAL:O	1:A:245:ASN:HB3	2.18	0.44
1:B:62:TYR:CD1	1:B:62:TYR:C	2.91	0.44
1:B:185:ASN:CG	1:B:185:ASN:O	2.56	0.44
1:A:181:TYR:HE1	1:A:185:ASN:HA	1.83	0.43
1:B:69:ASN:ND2	1:B:71:ASP:H	2.16	0.43
1:A:215:GLN:HA	1:A:218:ILE:HD12	1.99	0.43
1:A:66:THR:HG23	1:A:67:ARG:HG3	1.96	0.43
1:A:48:LEU:HA	1:A:51:LEU:HD22	2.00	0.43
1:B:69:ASN:HD22	1:B:71:ASP:H	1.67	0.43
1:B:269:ARG:NH1	1:B:269:ARG:HB2	2.33	0.43
1:A:185:ASN:ND2	1:A:187:TYR:HE2	2.17	0.43
1:A:44:LEU:HD13	1:A:44:LEU:H	1.83	0.43
1:A:243:SER:C	1:A:245:ASN:N	2.71	0.43
1:A:266:GLN:O	1:A:269:ARG:HB2	2.18	0.43
1:B:98:SER:HA	1:B:252:GLN:HE22	1.84	0.43
1:A:112:LEU:HA	1:A:115:THR:HB	2.01	0.43
1:A:105:TYR:CD1	1:A:169:LYS:HB3	2.53	0.43
1:A:226:PRO:C	1:A:228:VAL:N	2.71	0.43
1:A:252:GLN:HB3	1:A:254:TYR:CE2	2.53	0.43
1:A:253:ASN:HB3	1:B:212:THR:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:SER:HB3	1:A:264:MET:CE	2.49	0.42
1:A:148:ARG:HH21	1:A:148:ARG:HG3	1.83	0.42
1:B:193:ALA:HB1	1:B:199:THR:O	2.19	0.42
1:A:176:TYR:HD2	1:A:177:LEU:CD1	2.32	0.42
1:A:152:ARG:HD3	1:A:155:LYS:NZ	2.34	0.42
1:A:204:ASN:ND2	1:A:204:ASN:N	2.67	0.42
1:A:263:ALA:O	1:A:266:GLN:HB2	2.19	0.42
1:A:69:ASN:O	1:A:69:ASN:CG	2.58	0.42
1:A:105:TYR:CD1	1:B:261:GLN:HG3	2.55	0.42
1:B:76:ILE:HB	1:B:142:TYR:CE2	2.54	0.42
1:A:110:PHE:CZ	1:A:115:THR:HG21	2.55	0.42
1:B:70:VAL:HB	1:B:166:GLN:HE22	1.85	0.42
1:A:56:LEU:HD13	1:A:56:LEU:HA	1.73	0.42
1:B:208:MET:HG2	1:B:209:SER:H	1.83	0.42
1:A:45:LYS:O	1:A:49:THR:HG23	2.19	0.42
1:A:225:ALA:HB1	1:A:229:TYR:CD2	2.53	0.42
1:A:244:THR:O	1:A:248:LYS:HG3	2.20	0.42
1:B:238:PHE:O	1:B:241:ARG:HB3	2.19	0.42
1:B:87:ASN:O	1:B:203:LYS:HG2	2.19	0.41
1:A:181:TYR:CE1	1:A:185:ASN:N	2.88	0.41
1:B:85:ALA:HB3	1:B:170:ASN:HD21	1.85	0.41
1:A:59:GLY:O	1:A:63:PHE:HD1	2.04	0.41
1:B:234:MET:HE2	1:B:234:MET:HB3	1.68	0.41
1:B:179:ASN:HA	1:B:187:TYR:O	2.20	0.41
1:B:101:ASP:HB3	1:B:134:ILE:HG13	2.01	0.41
1:B:192:ALA:O	1:B:196:TYR:HB2	2.21	0.41
1:A:173:LEU:O	1:A:173:LEU:HG	2.19	0.41
1:A:190:GLU:OE1	1:A:201:VAL:HG22	2.21	0.41
1:B:268:ASN:C	1:B:269:ARG:HG3	2.40	0.41
1:A:152:ARG:HH11	1:A:155:LYS:HZ1	1.69	0.41
1:B:48:LEU:HD23	1:B:49:THR:N	2.36	0.41
1:A:248:LYS:O	1:A:252:GLN:HG3	2.21	0.41
1:B:264:MET:HE2	1:B:264:MET:HB3	1.92	0.41
1:B:54:ILE:C	1:B:57:PHE:HB3	2.42	0.40
1:B:169:LYS:HD3	1:B:169:LYS:HA	1.65	0.40
1:A:102:GLU:HG3	1:A:252:GLN:CD	2.41	0.40
1:A:56:LEU:O	1:A:60:ILE:CG1	2.65	0.40
1:A:70:VAL:HG11	1:A:163:VAL:HG12	2.03	0.40
1:A:256:ASN:OD1	1:A:259:GLN:HB2	2.22	0.40
1:B:85:ALA:HB3	1:B:170:ASN:ND2	2.36	0.40
1:A:104:PHE:CE1	1:A:169:LYS:HD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LEU:HG	1:B:201:VAL:HG11	2.04	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	216/263 (82%)	192 (89%)	21 (10%)	3 (1%)	14 57
1	B	213/263 (81%)	188 (88%)	24 (11%)	1 (0%)	34 78
All	All	429/526 (82%)	380 (89%)	45 (10%)	4 (1%)	21 67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	VAL
1	A	172	ILE
1	A	227	SER
1	B	138	VAL

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	200/239 (84%)	173 (86%)	27 (14%)	5 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	197/239 (82%)	166 (84%)	31 (16%)	3 15
All	All	397/478 (83%)	339 (85%)	58 (15%)	4 19

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	44	LEU
1	A	47	LEU
1	A	51	LEU
1	A	52	ILE
1	A	56	LEU
1	A	57	PHE
1	A	61	MET
1	A	69	ASN
1	A	73	LEU
1	A	74	ARG
1	A	103	ARG
1	A	112	LEU
1	A	117	ARG
1	A	119	LEU
1	A	148	ARG
1	A	163	VAL
1	A	184	ASP
1	A	185	ASN
1	A	200	THR
1	A	209	SER
1	A	227	SER
1	A	228	VAL
1	A	230	ASN
1	A	235	SER
1	A	240	GLN
1	A	242	VAL
1	B	45	LYS
1	B	46	ILE
1	B	47	LEU
1	B	48	LEU
1	B	49	THR
1	B	51	LEU
1	B	52	ILE
1	B	56	LEU
1	B	60	ILE

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Mol	Chain	Res	Type
1	B	67	ARG
1	B	69	ASN
1	B	77	GLU
1	B	86	ASP
1	B	99	MET
1	B	108	HIS
1	B	117	ARG
1	B	133	THR
1	B	137	GLN
1	B	140	LYS
1	B	174	SER
1	B	194	ASN
1	B	200	THR
1	B	202	ASN
1	B	204	ASN
1	B	206	THR
1	B	228	VAL
1	B	238	PHE
1	B	244	THR
1	B	247	GLU
1	B	264	MET
1	B	269	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	87	ASN
1	A	106	ASN
1	A	141	ASN
1	A	166	GLN
1	A	179	ASN
1	A	185	ASN
1	A	204	ASN
1	A	210	HIS
1	A	215	GLN
1	A	230	ASN
1	A	233	ASN
1	A	245	ASN
1	A	251	GLN
1	A	252	GLN
1	A	261	GLN

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Mol	Chain	Res	Type
1	A	262	GLN
1	B	69	ASN
1	B	137	GLN
1	B	166	GLN
1	B	170	ASN
1	B	179	ASN
1	B	210	HIS
1	B	215	GLN
1	B	232	ASN
1	B	233	ASN
1	B	237	ASN
1	B	262	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 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	220/263 (83%)	0.07	11 (5%)	32	19	59, 97, 181, 259	0
1	B	217/263 (82%)	0.23	16 (7%)	17	10	58, 138, 253, 395	0
All	All	437/526 (83%)	0.15	27 (6%)	24	13	58, 116, 242, 395	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	69	ASN	5.4
1	B	161	HIS	5.4
1	B	67	ARG	4.0
1	B	68	ASP	3.9
1	A	205	SER	3.7
1	B	144	TYR	3.7
1	B	118	ALA	3.5
1	A	206	THR	3.3
1	A	144	TYR	3.2
1	B	108	HIS	3.0
1	A	66	THR	3.0
1	B	231	ILE	2.9
1	A	67	ARG	2.8
1	A	110	PHE	2.7
1	B	152	ARG	2.7
1	B	198	GLY	2.6
1	B	158	PHE	2.5
1	A	165	LYS	2.4
1	B	120	PHE	2.4
1	A	112	LEU	2.4
1	B	155	LYS	2.3
1	A	121	SER	2.2
1	A	68	ASP	2.1
1	A	146	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	179	ASN	2.0
1	B	119	LEU	2.0
1	B	234	MET	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.