



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:37 AM UTC

PDB ID : 3VMS / pdb_00003vms
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

<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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

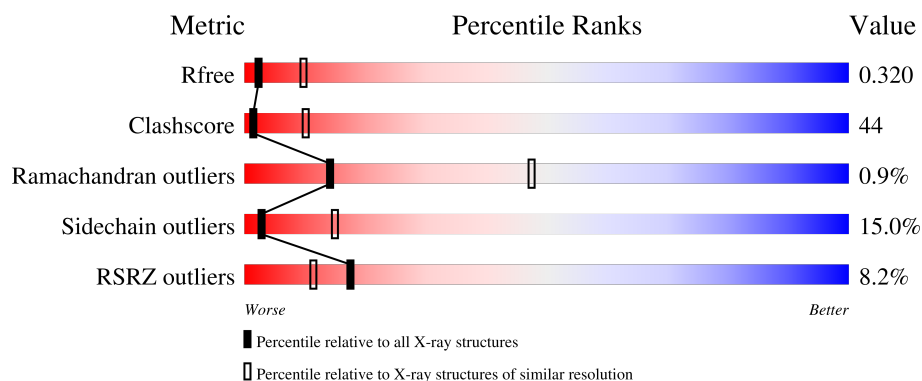
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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 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 $\leq 5\%$. 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	5% 31% 47% 5% 16%
1	B	263	9% 29% 43% 10% 17%

2 Entry composition

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

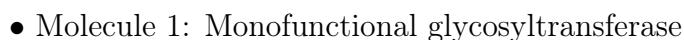
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Chain	Residue	Modelled	Actual	Comment	Reference
B	11	HIS	-	expression tag	UNP Q99T05
B	12	HIS	-	expression tag	UNP Q99T05
B	13	HIS	-	expression tag	UNP Q99T05
B	14	HIS	-	expression tag	UNP Q99T05
B	15	HIS	-	expression tag	UNP Q99T05
B	16	HIS	-	expression 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

i

- Molecule 1: Monofunctional glycosyltransferase



4 Data and refinement statistics

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 29.93 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.93-3.20) 98.9 (29.93-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.262 , 0.330 0.244 , 0.320	Depositor DCC
R_{free} test set	522 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	83.7	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 106.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.46	0/1826	0.88	3/2462 (0.1%)
1	B	0.36	0/1803	0.80	2/2430 (0.1%)
All	All	0.42	0/3629	0.84	5/4892 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	HIS	N-CA-C	-6.03	104.66	112.68
1	A	244	THR	N-CA-C	-5.67	105.47	112.38
1	A	121	SER	N-CA-C	-5.59	106.43	113.20
1	B	148	ARG	N-CA-C	5.27	117.09	108.76
1	A	230	ASN	N-CA-C	5.13	116.66	108.41

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1794	0	1767	161	0
1	B	1771	0	1738	153	0
All	All	3565	0	3505	309	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 44.

All (309) 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
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:243:SER:HB3	1:A:264:MET:HE1	1.56	0.86
1:A:65:SER:O	1:A:68:ASP:HB2	1.77	0.84
1:A:61:MET:HE3	1:A:61:MET:HA	1.59	0.83
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:HD13	1:B:47:LEU:H	1.51	0.75
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:B:50:ILE:HA	1:B:53:ILE:HB	1.70	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:HH21	1:A:148:ARG:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:46:ILE:O	1:A:50:ILE:HG23	1.96	0.65
1:B:46:ILE:HD12	1:B:46:ILE:H	1.60	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:57:PHE:CD1	1:A:57:PHE:C	2.77	0.62
1:A:197:PHE:HE2	1:A:219:LEU:HD11	1.64	0.62
1:A:230:ASN:ND2	1:A:232:ASN:H	1.96	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:230:ASN:ND2	1:A:230:ASN:C	2.59	0.60
1:A:230:ASN:C	1:A:230:ASN:HD22	2.08	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:A:148:ARG:HH21	1:A:148:ARG:HG2	1.65	0.60
1:B:117:ARG:CA	1:B:121:SER:HB2	2.25	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:A:152:ARG:HD3	1:A:155:LYS:HZ3	1.67	0.59
1:B:49:THR:O	1:B:53:ILE:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:49:THR:HA	1:A:52:ILE:HD12	1.84	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:90:GLU:H	1:B:269:ARG:NH2	2.02	0.58
1:A:101:ASP:CB	1:A:134:ILE:HG13	2.29	0.58
1:B:268:ASN:O	1:B:269:ARG:HG3	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:174:SER:O	1:A:178:ASN:HB2	2.04	0.57
1:B:45:LYS:HE3	1:B:46:ILE:HG13	1.85	0.57
1:B:49:THR:O	1:B:52:ILE:HG23	2.05	0.57
1:A:204:ASN:N	1:A:204:ASN:HD22	2.03	0.56
1:B:56:LEU:HD23	1:B:57:PHE:N	2.20	0.56
1:B:215:GLN:HA	1:B:218:ILE:HD12	1.88	0.56
1:B:69:ASN:HD22	1:B:69:ASN:C	2.14	0.56
1:B:67:ARG:HA	1:B:68:ASP:C	2.30	0.55
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:A:148:ARG:HD3	1:A:148:ARG:C	2.30	0.55
1:A:226:PRO:C	1:A:228:VAL:H	2.15	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:48:LEU:C	1:A:48:LEU:HD23	2.32	0.55
1:B:58:ILE:HA	1:B:61:MET:HE3	1.88	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:HG2	1:A:148:ARG:NH2	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:A:229:TYR:CD2	1:A:238:PHE:CD1	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:203:LYS:HG3	1:A:204:ASN:HD22	1.74	0.51
1:A:234:MET:HE2	1:A:239:THR:HG22	1.92	0.51
1:B:52:ILE:O	1:B:56:LEU:N	2.37	0.51
1:A:98:SER:HA	1:A:252:GLN:HE22	1.76	0.51
1:B:58:ILE:HA	1:B:61:MET:HB2	1.92	0.51
1:B:134:ILE:O	1:B:138:VAL:HG23	2.11	0.50
1:A:79:LYS:NZ	1:A:179:ASN:ND2	2.59	0.50
1:B:211:ILE:HG13	1:B:215:GLN:HB2	1.94	0.50
1:B:134:ILE:HG23	1:B:176:TYR:CG	2.46	0.50
1:A:229:TYR:HD2	1:A:238:PHE:CD1	2.29	0.50
1:A:240:GLN:O	1:A:240:GLN:HG3	2.04	0.50
1:B:110:PHE:CE1	1:B:115:THR:N	2.80	0.50
1:A:71:ASP:HA	1:A:167:TYR:OH	2.12	0.50
1:A:148:ARG:CG	1:A:148:ARG:NH2	2.69	0.50
1:A:181:TYR:HE1	1:A:185:ASN:CA	2.25	0.50
1:A:71:ASP:C	1:A:73:LEU:N	2.69	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:B:69:ASN:HD22	1:B:70:VAL:N	2.10	0.49
1:B:70:VAL:HG12	1:B:167:TYR:HE2	1.75	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:NZ	1:B:165:LYS:HA	2.27	0.49
1:A:90:GLU:HA	1:A:90:GLU:OE1	2.12	0.49
1:A:267:LEU:HD12	1:A:267:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ILE:HD11	1:B:179:ASN:HB2	1.95	0.49
1:B:114:GLY:O	1:B:118:ALA:N	2.45	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:A:61:MET:HG2	1:A:154:VAL:CG1	2.43	0.48
1:A:62:TYR:CD1	1:A:62:TYR:C	2.91	0.48
1:A:115:THR:HG22	1:A:119:LEU:HD22	1.95	0.48
1:B:47:LEU:O	1:B:51:LEU:HD13	2.12	0.48
1:B:180:ILE:O	1:B:187:TYR:HA	2.13	0.48
1:B:62:TYR:C	1:B:62:TYR:CD1	2.91	0.48
1:B:185:ASN:O	1:B:185:ASN:CG	2.56	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:A:243:SER:C	1:A:245:ASN:N	2.71	0.48
1:A:109:GLY:O	1:A:133:THR:HG21	2.14	0.47
1:B:72:GLU:HB3	1:B:142:TYR:HE1	1.79	0.47
1:A:50:ILE:O	1:A:54:ILE:HG23	2.13	0.47
1:A:226:PRO:C	1:A:228:VAL:N	2.71	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:54:ILE:CA	1:B:57:PHE:HB3	2.45	0.47
1:A:69:ASN:O	1:A:69:ASN:CG	2.58	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:70:VAL:O	1:B:73:LEU:HB2	2.15	0.47
1:B:140:LYS:HE3	1:B:140:LYS:HB3	1.79	0.47
1:A:90:GLU:OE1	1:A:93:LYS:HB2	2.15	0.46
1:A:156:GLU:O	1:A:156:GLU:HG2	2.16	0.46
1:B:113:LYS:O	1:B:113:LYS:HD3	2.14	0.46
1:B:268:ASN:C	1:B:269:ARG:HG3	2.40	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:B:57:PHE:CG	1:B:61:MET:HE2	2.50	0.46
1:B:57:PHE:CD1	1:B:61:MET:HE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:VAL:O	1:A:96:PHE:HD1	1.98	0.46
1:A:110:PHE:HZ	1:A:115:THR:HG21	1.81	0.46
1:A:260:TYR:HD2	1:A:261:GLN:NE2	2.13	0.46
1:A:77:GLU:HA	1:A:82:PHE:CD1	2.51	0.46
1:B:52:ILE:HD13	1:B:53:ILE:N	2.31	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:OD1	1:B:194:ASN:N	2.49	0.45
1:B:244:THR:O	1:B:248:LYS:HG3	2.15	0.45
1:A:210:HIS:H	1:A:210:HIS:CD2	2.34	0.45
1:A:210:HIS:CD2	1:A:210:HIS:N	2.84	0.45
1:B:76:ILE:HD12	1:B:142:TYR:CD2	2.52	0.45
1:A:102:GLU:HG3	1:A:252:GLN:CD	2.41	0.45
1:B:142:TYR:HB3	1:B:143:PHE:CD2	2.52	0.45
1:B:268:ASN:O	1:B:269:ARG:O	2.33	0.45
1:B:54:ILE:C	1:B:57:PHE:HB3	2.42	0.45
1:B:226:PRO:HD2	1:B:229:TYR:CE2	2.51	0.45
1:B:110:PHE:HE1	1:B:115:THR:N	2.12	0.45
1:B:212:THR:H	1:B:215:GLN:NE2	2.14	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:234:MET:HE2	1:B:234:MET:HB3	1.83	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:A:43:LEU:O	1:A:47:LEU:HD13	2.18	0.44
1:A:46:ILE:HD12	1:A:46:ILE:C	2.43	0.44
1:A:180:ILE:HG13	1:A:182:PHE:CZ	2.52	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:O	1:B:60:ILE:HG12	2.16	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:B:101:ASP:OD2	1:B:104:PHE:HA	2.18	0.44
1:A:43:LEU:HD13	1:A:43:LEU:N	2.33	0.44
1:A:242:VAL:O	1:A:245:ASN:HB3	2.18	0.44
1:B:64:LEU:HD13	1:B:64:LEU:O	2.18	0.44
1:B:265:SER:O	1:B:269:ARG:HG3	2.18	0.44
1:A:181:TYR:HE1	1:A:185:ASN:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:PHE:O	1:A:97:ILE:C	2.60	0.43
1:B:69:ASN:ND2	1:B:71:ASP:H	2.16	0.43
1:A:66:THR:HG23	1:A:67:ARG:HG3	1.96	0.43
1:A:215:GLN:HA	1:A:218:ILE:HD12	1.99	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:A:44:LEU:HD13	1:A:44:LEU:H	1.83	0.43
1:A:185:ASN:ND2	1:A:187:TYR:HE2	2.17	0.43
1:A:266:GLN:O	1:A:269:ARG:HB2	2.18	0.43
1:B:269:ARG:HB2	1:B:269:ARG:NH1	2.33	0.43
1:B:98:SER:HA	1:B:252:GLN:HE22	1.84	0.43
1:A:105:TYR:CD1	1:A:169:LYS:HB3	2.53	0.43
1:A:112:LEU:HA	1:A:115:THR:HB	2.01	0.43
1:A:171:GLU:O	1:A:172:ILE:C	2.61	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
1:A:148:ARG:HH21	1:A:148:ARG:HG3	1.83	0.42
1:B:109:GLY:O	1:B:110:PHE:C	2.61	0.42
1:B:193:ALA:HB1	1:B:199:THR:O	2.19	0.42
1:A:152:ARG:HD3	1:A:155:LYS:NZ	2.34	0.42
1:A:176:TYR:HD2	1:A:177:LEU:CD1	2.32	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: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:B:184:ASP:C	1:B:186:GLN:N	2.78	0.42
1:B:264:MET:HE2	1:B:264:MET:HB3	1.78	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:A:137:GLN:C	1:A:141:ASN:HD22	2.28	0.41
1:B:87:ASN:O	1:B:203:LYS:HG2	2.19	0.41
1:A:59:GLY:O	1:A:63:PHE:HD1	2.04	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:B:137:GLN:O	1:B:138:VAL:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:MET:HE2	1:B:239:THR:HG22	2.02	0.41
1:B:101:ASP:HB3	1:B:134:ILE:HG13	2.01	0.41
1:B:179:ASN:HA	1:B:187:TYR:O	2.20	0.41
1:A:144:TYR:C	1:A:146:ASN:H	2.28	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:A:112:LEU:HD22	1:A:112:LEU:C	2.46	0.41
1:B:135:THR:C	1:B:137:GLN:N	2.77	0.41
1:A:61:MET:HE3	1:A:61:MET:CA	2.41	0.41
1:A:248:LYS:O	1:A:252:GLN:HG3	2.21	0.41
1:B:48:LEU:HD23	1:B:49:THR:N	2.36	0.41
1:B:140:LYS:HD2	1:B:140:LYS:C	2.46	0.40
1:B:169:LYS:HD3	1:B:169:LYS:HA	1.65	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:B:165:LYS:HA	1:B:165:LYS:HZ2	1.86	0.40
1:B:234:MET:HE3	1:B:238:PHE:CG	2.56	0.40
1:B:56:LEU:HD23	1:B:56:LEU:C	2.47	0.40
1:A:104:PHE:CE1	1:A:169:LYS:HD2	2.56	0.40
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%)	9 39
1	B	213/263 (81%)	188 (88%)	24 (11%)	1 (0%)	24 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	429/526 (82%)	380 (89%)	45 (10%)	4 (1%)	14	47

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 ⓘ

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	137/239 (57%)	121 (88%)	16 (12%)	5	23
1	B	197/239 (82%)	163 (83%)	34 (17%)	2	10
All	All	334/478 (70%)	284 (85%)	50 (15%)	3	15

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	ARG
1	A	119	LEU
1	A	148	ARG
1	A	163	VAL
1	A	185	ASN
1	A	200	THR
1	A	209	SER
1	A	213	VAL
1	A	223	VAL
1	A	227	SER
1	A	228	VAL
1	A	235	SER
1	A	240	GLN
1	A	242	VAL

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Mol	Chain	Res	Type
1	A	249	MET
1	A	258	THR
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
1	B	67	ARG
1	B	70	VAL
1	B	77	GLU
1	B	86	ASP
1	B	99	MET
1	B	108	HIS
1	B	115	THR
1	B	117	ARG
1	B	133	THR
1	B	137	GLN
1	B	155	LYS
1	B	159	VAL
1	B	165	LYS
1	B	174	SER
1	B	194	ASN
1	B	200	THR
1	B	204	ASN
1	B	206	THR
1	B	218	ILE
1	B	228	VAL
1	B	237	ASN
1	B	242	VAL
1	B	244	THR
1	B	247	GLU
1	B	264	MET
1	B	269	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	141	ASN

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Mol	Chain	Res	Type
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	232	ASN
1	A	233	ASN
1	A	251	GLN
1	A	252	GLN
1	A	261	GLN
1	B	69	ASN
1	B	137	GLN
1	B	166	GLN
1	B	170	ASN
1	B	179	ASN
1	B	202	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	220/263 (83%)	0.42	13 (5%) 28 18	59, 97, 181, 259	0
1	B	217/263 (82%)	0.58	23 (10%) 11 8	58, 138, 253, 395	0
All	All	437/526 (83%)	0.50	36 (8%) 17 11	58, 116, 242, 395	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	218	ILE	5.4
1	A	189	LEU	5.2
1	A	66	THR	5.1
1	A	92	VAL	4.9
1	A	216	SER	4.5
1	B	156	GLU	4.5
1	B	234	MET	3.9
1	B	198	GLY	3.3
1	A	144	TYR	3.2
1	B	69	ASN	3.0
1	B	161	HIS	3.0
1	B	219	LEU	2.9
1	A	206	THR	2.8
1	A	96	PHE	2.7
1	B	231	ILE	2.6
1	B	203	LYS	2.6
1	B	205	SER	2.6
1	B	210	HIS	2.5
1	A	156	GLU	2.5
1	B	118	ALA	2.5
1	B	109	GLY	2.5
1	B	174	SER	2.5
1	A	257	GLU	2.4
1	A	108	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	177	LEU	2.4
1	B	144	TYR	2.4
1	B	188	THR	2.3
1	B	138	VAL	2.3
1	A	111	ASP	2.2
1	B	145	ASP	2.2
1	B	189	LEU	2.2
1	B	197	PHE	2.2
1	B	110	PHE	2.2
1	B	267	LEU	2.2
1	B	68	ASP	2.1
1	A	261	GLN	2.1

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 oligosaccharides 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.