WORLDWIDE wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 14, 2017 – 02:53 pm GMT

PDB ID	:	3LKD
Title	:	Crystal Structure of the type I restriction-modification system methyltransferase subunit from Streptococcus thermophilus, Northeast Structural Genomics Consortium Target SuR80
Authors	:	Vorobiev, S.; Su, M.; Seetharaman, J.; Mao, M.; Xiao, R.; Foote, E.L.; Ciccosanti, C.; Wang, D.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2010-01-27
Resolution	:	2.25 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.

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 2.25 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	Percentile Ranks	Value
Rfree		0.205
Clashscore		12
Ramachandran outliers		0
Sidechain outliers		4.9%
RSRZ outliers		2.0%

Worse — Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
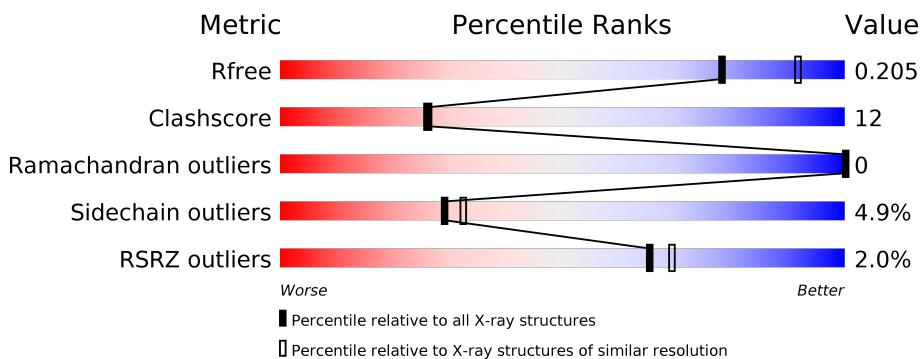
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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	542	2% 66% 18% • 14%
1	B	542	% 67% 19% • 13%
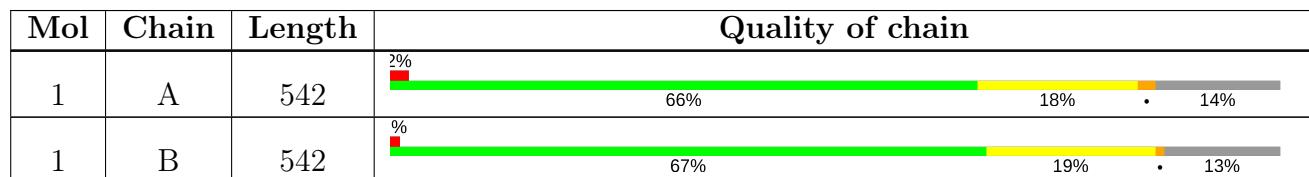
2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 7930 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 Type I restriction-modification system methyltransferase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	Se	0	0	0
			3733	2381	606	731	15			
1	B	472	Total	C	N	O	Se	0	0	0
			3766	2400	612	739	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	535	LEU	-	EXPRESSION TAG	UNP Q5M500
A	536	GLU	-	EXPRESSION TAG	UNP Q5M500
A	537	HIS	-	EXPRESSION TAG	UNP Q5M500
A	538	HIS	-	EXPRESSION TAG	UNP Q5M500
A	539	HIS	-	EXPRESSION TAG	UNP Q5M500
A	540	HIS	-	EXPRESSION TAG	UNP Q5M500
A	541	HIS	-	EXPRESSION TAG	UNP Q5M500
A	542	HIS	-	EXPRESSION TAG	UNP Q5M500
B	535	LEU	-	EXPRESSION TAG	UNP Q5M500
B	536	GLU	-	EXPRESSION TAG	UNP Q5M500
B	537	HIS	-	EXPRESSION TAG	UNP Q5M500
B	538	HIS	-	EXPRESSION TAG	UNP Q5M500
B	539	HIS	-	EXPRESSION TAG	UNP Q5M500
B	540	HIS	-	EXPRESSION TAG	UNP Q5M500
B	541	HIS	-	EXPRESSION TAG	UNP Q5M500
B	542	HIS	-	EXPRESSION TAG	UNP Q5M500

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	205	Total	O	0	0
			205	205		
2	B	226	Total	O	0	0
			226	226		

3 Residue-property plots ⓘ

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

• Molecule 1: Type I restriction-modification system methyltransferase subunit

• Molecule 1: Type I restriction-modification system methyltransferase subunit

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.87Å 83.13Å 96.68Å 90.00° 98.13° 90.00°	Depositor
Resolution (Å)	48.79 – 2.25 48.79 – 2.25	Depositor EDS
% Data completeness (in resolution range)	94.9 (48.79-2.25) 99.5 (48.79-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.49 (at 2.24Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.186 , 0.210 0.187 , 0.205	Depositor DCC
R_{free} test set	2278 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	19.8	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7930	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

---

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0/3800	0.58	0/5124
1	B	0.34	0/3834	0.59	0/5169
All	All	0.34	0/7634	0.59	0/10293

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	3733	0	3593	83	0
1	B	3766	0	3635	92	0
2	A	205	0	0	5	0
2	B	226	0	0	9	0
All	All	7930	0	7228	174	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 12.

All (174) 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:230:MSE:HE3	1:B:236:LEU:HD12	1.27	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:ALA:HA	1:B:161:MSE:HE3	1.36	1.07
1:B:268:MSE:HE2	1:B:280:LEU:HD21	1.39	1.03
1:A:230:MSE:HE3	1:A:236:LEU:HD12	1.44	0.99
1:B:157:VAL:HG12	1:B:161:MSE:HE2	1.44	0.97
1:A:268:MSE:HE2	1:A:280:LEU:HD21	1.47	0.95
1:B:7:THR:HG22	1:B:10:SER:H	1.33	0.93
1:A:201:THR:HG21	1:A:209:MSE:HE1	1.51	0.92
1:B:201:THR:HG21	1:B:209:MSE:HE1	1.52	0.89
1:A:268:MSE:HE3	1:A:278:GLN:HG2	1.55	0.89
1:A:158:ALA:HA	1:A:161:MSE:HE3	1.60	0.84
1:B:230:MSE:CE	1:B:236:LEU:HD12	2.07	0.83
1:A:158:ALA:HA	1:A:161:MSE:CE	2.10	0.80
1:B:205:VAL:HG12	1:B:209:MSE:HE2	1.65	0.79
1:B:268:MSE:HE3	1:B:278:GLN:HG2	1.65	0.78
1:B:206:ALA:HA	1:B:209:MSE:HE3	1.67	0.77
1:B:113:PHE:CE2	1:B:161:MSE:HE1	2.20	0.76
1:B:240:LYS:HE3	1:B:271:HIS:O	1.86	0.75
1:B:7:THR:CG2	1:B:10:SER:H	2.00	0.75
1:B:204:PRO:HB3	1:B:437:ILE:HD11	1.69	0.72
1:B:313:ALA:HB3	1:B:332:LYS:HG2	1.71	0.72
1:A:385:VAL:HG12	1:A:471:ILE:HD11	1.71	0.71
1:B:173:ALA:HA	1:B:176:MSE:HE2	1.71	0.71
1:A:33:SER:HB2	2:A:996:HOH:O	1.90	0.71
1:A:173:ALA:O	1:A:176:MSE:HB2	1.92	0.70
1:B:230:MSE:HE2	1:B:233:GLY:HA2	1.74	0.70
1:A:205:VAL:HG12	1:A:209:MSE:HE2	1.75	0.69
1:A:83:LEU:O	1:A:87:ILE:HG12	1.95	0.67
1:B:176:MSE:HG2	2:B:868:HOH:O	1.95	0.67
1:B:158:ALA:CA	1:B:161:MSE:HE3	2.21	0.66
1:B:230:MSE:HE3	1:B:236:LEU:CD1	2.17	0.66
1:A:230:MSE:CE	1:A:236:LEU:HD12	2.25	0.66
1:A:230:MSE:HE2	1:A:233:GLY:CA	2.25	0.65
1:B:206:ALA:HA	1:B:209:MSE:CE	2.27	0.65
1:A:254:GLN:HE21	1:A:283:ALA:HB3	1.63	0.64
1:A:206:ALA:HA	1:A:209:MSE:HE3	1.79	0.64
1:B:285:THR:HG22	2:B:955:HOH:O	1.96	0.64
1:A:102:THR:O	1:A:106:GLU:HG3	1.98	0.63
1:A:113:PHE:CE2	1:A:161:MSE:HE1	2.34	0.63
1:A:471:ILE:HB	1:A:472:PRO:HD3	1.81	0.63
1:A:285:THR:HG22	2:A:970:HOH:O	1.97	0.63
1:B:149:THR:O	1:B:153:GLN:HG3	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:MSE:HE2	1:A:56:MSE:HA	1.82	0.62
1:B:102:THR:O	1:B:106:GLU:HG3	2.00	0.62
1:B:411:ASN:HB2	2:B:636:HOH:O	1.99	0.62
1:B:230:MSE:HE2	1:B:233:GLY:CA	2.31	0.61
1:A:432:MSE:HE3	1:A:437:ILE:HD11	1.81	0.61
1:A:268:MSE:HE3	1:A:278:GLN:CG	2.28	0.60
1:B:251:TYR:HB2	1:B:268:MSE:HE1	1.83	0.60
1:A:251:TYR:HB2	1:A:268:MSE:HE1	1.84	0.60
1:B:130:GLU:O	1:B:133:GLU:HG2	2.01	0.60
1:A:230:MSE:HE2	1:A:233:GLY:HA2	1.82	0.60
1:A:196:ALA:HA	1:A:199:PHE:CE1	2.38	0.59
1:A:131:LEU:HD21	1:A:275:ILE:HD12	1.85	0.59
1:A:175:ASP:HA	2:A:974:HOH:O	2.01	0.59
1:A:52:VAL:HG22	1:A:87:ILE:HD11	1.84	0.58
1:B:131:LEU:HD22	1:B:275:ILE:HD12	1.84	0.58
1:B:42:LYS:NZ	1:B:46:ASP:OD2	2.36	0.58
1:B:203:GLN:HB3	1:B:204:PRO:HD3	1.86	0.58
1:B:460:GLU:O	1:B:464:GLU:HG3	2.04	0.58
1:A:427:LYS:O	1:A:428:ASN:HB2	2.03	0.57
1:A:107:ARG:NH1	1:A:112:SER:O	2.38	0.57
1:A:206:ALA:HA	1:A:209:MSE:CE	2.34	0.56
1:B:42:LYS:HE3	1:B:164:LEU:O	2.05	0.56
1:B:427:LYS:NZ	1:B:427:LYS:HB2	2.20	0.56
1:B:55:THR:HG22	1:B:56:MSE:CE	2.36	0.56
1:A:95:ILE:HD11	1:A:125:ILE:HD11	1.88	0.56
1:A:196:ALA:HA	1:A:199:PHE:CZ	2.41	0.56
1:A:411:ASN:OD1	1:B:411:ASN:OD1	2.23	0.55
1:A:55:THR:HG22	1:A:56:MSE:HE3	1.88	0.55
1:B:54:GLU:HA	1:B:59:GLU:HG2	1.89	0.55
1:B:7:THR:HG22	1:B:10:SER:N	2.15	0.55
1:A:385:VAL:CG1	1:A:471:ILE:HD11	2.37	0.54
1:A:133:GLU:O	1:A:134:ASN:HB2	2.07	0.54
1:A:158:ALA:HA	1:A:161:MSE:HE2	1.90	0.54
1:A:313:ALA:HB3	1:A:332:LYS:HG2	1.90	0.54
1:A:131:LEU:CD2	1:A:275:ILE:HD12	2.37	0.54
1:A:374:LYS:HE2	1:A:467:TYR:CE2	2.43	0.53
1:B:268:MSE:HE3	1:B:278:GLN:CG	2.36	0.53
1:B:113:PHE:CZ	1:B:161:MSE:HE1	2.43	0.53
1:B:70:TYR:CE2	1:B:97:PRO:HG3	2.43	0.53
1:B:374:LYS:HE2	1:B:467:TYR:CE2	2.44	0.53
1:A:55:THR:HG22	1:A:56:MSE:CE	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:GLY:O	1:B:409:ARG:HD3	2.09	0.53
1:B:115:LEU:HD11	1:B:157:VAL:HG21	1.90	0.53
1:A:198:GLU:HG3	1:A:306:PRO:HG3	1.90	0.52
1:A:113:PHE:CZ	1:A:161:MSE:HE1	2.45	0.52
1:B:133:GLU:O	1:B:134:ASN:HB2	2.09	0.52
1:B:350:ASP:O	1:B:351:ASN:HB2	2.08	0.52
1:B:131:LEU:CD2	1:B:275:ILE:HD12	2.38	0.52
1:B:245:GLN:NE2	2:B:682:HOH:O	2.40	0.52
1:B:427:LYS:HG3	1:B:428:ASN:OD1	2.10	0.51
1:A:268:MSE:CE	1:A:278:GLN:HG2	2.36	0.51
1:A:426:GLY:HA3	1:A:431:ILE:HD13	1.93	0.51
1:A:20:ASP:HA	1:A:23:ARG:HG3	1.93	0.51
1:A:130:GLU:O	1:A:133:GLU:HG2	2.11	0.51
1:B:95:ILE:HG12	1:B:125:ILE:HD11	1.92	0.51
1:B:72:LYS:HE3	1:B:73:TYR:CE2	2.46	0.51
1:B:131:LEU:HD23	1:B:132:TYR:CZ	2.46	0.50
1:B:33:SER:O	1:B:139:ILE:HD11	2.11	0.50
1:B:134:ASN:O	1:B:137:GLU:HG2	2.10	0.50
1:A:72:LYS:HE3	1:A:73:TYR:CE2	2.47	0.49
1:B:107:ARG:NH1	1:B:112:SER:O	2.45	0.49
1:B:347:LEU:HD11	1:B:353:VAL:N	2.26	0.49
1:B:204:PRO:CB	1:B:437:ILE:HD11	2.41	0.49
1:A:147:GLY:HA3	1:A:152:LYS:HG3	1.95	0.49
1:B:96:HIS:CD2	1:B:97:PRO:HD2	2.47	0.49
1:A:367:ASN:O	1:A:370:GLY:N	2.46	0.49
1:B:267:ASN:HD21	1:B:271:HIS:CE1	2.31	0.48
1:B:268:MSE:CE	1:B:278:GLN:HG2	2.40	0.48
1:B:177:LEU:C	1:B:177:LEU:HD13	2.33	0.48
1:B:349:GLN:HA	1:B:407:LYS:HB2	1.94	0.48
1:B:205:VAL:C	1:B:209:MSE:HE2	2.34	0.47
1:A:380:GLY:O	1:A:409:ARG:HD3	2.14	0.47
1:B:55:THR:HG22	1:B:56:MSE:HE2	1.97	0.47
1:A:267:ASN:HD21	1:A:271:HIS:HE1	1.63	0.47
1:B:308:SER:HA	2:B:928:HOH:O	2.14	0.47
1:A:206:ALA:HB1	1:A:238:ASN:ND2	2.31	0.46
1:A:254:GLN:NE2	1:A:283:ALA:HB3	2.27	0.46
1:A:40:PHE:HD1	1:A:270:LEU:HD13	1.81	0.46
1:B:477:THR:O	1:B:477:THR:CG2	2.62	0.46
1:B:153:GLN:O	1:B:157:VAL:HG23	2.16	0.46
1:B:340:LEU:C	1:B:340:LEU:HD23	2.37	0.46
1:A:116:GLU:HG2	1:A:142:TYR:OH	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:MSE:HE2	1:A:233:GLY:HA3	1.97	0.45
1:A:203:GLN:HB3	1:A:204:PRO:HD3	1.99	0.45
1:B:267:ASN:HD21	1:B:271:HIS:HE1	1.65	0.45
1:A:48:MSE:SE	1:A:95:ILE:H	2.51	0.44
1:B:205:VAL:HG12	1:B:209:MSE:CE	2.41	0.44
1:B:305:PRO:HG3	1:B:358:LEU:HD21	1.99	0.44
1:B:166:VAL:HG12	1:B:166:VAL:O	2.18	0.44
1:A:326:PHE:CE1	1:A:376:LEU:HD13	2.52	0.44
1:B:95:ILE:CG1	1:B:125:ILE:HD11	2.47	0.44
1:B:281:HIS:HE1	2:B:962:HOH:O	2.01	0.44
1:B:374:LYS:O	1:B:378:GLU:HG3	2.16	0.44
1:A:42:LYS:HE3	1:A:164:LEU:O	2.18	0.43
1:B:7:THR:N	1:B:176:MSE:SE	3.01	0.43
1:B:21:VAL:O	1:B:25:LYS:HE2	2.18	0.43
1:A:22:LEU:HD13	1:A:31:TYR:HB2	1.99	0.43
1:A:416:PHE:HD2	1:A:471:ILE:HD13	1.83	0.43
1:A:347:LEU:HD11	1:A:353:VAL:N	2.33	0.43
1:A:230:MSE:HE3	1:A:236:LEU:CD1	2.32	0.43
1:A:468:ASN:OD1	1:A:470:ASN:HB2	2.18	0.43
1:A:23:ARG:HG3	1:A:23:ARG:HH11	1.84	0.43
1:B:115:LEU:HD12	1:B:115:LEU:HA	1.92	0.43
1:B:367:ASN:O	1:B:370:GLY:N	2.51	0.43
1:B:59:GLU:O	1:B:60:THR:HG23	2.19	0.43
1:B:16:TRP:CE2	1:B:23:ARG:NH2	2.86	0.42
1:B:267:ASN:ND2	1:B:271:HIS:CE1	2.87	0.42
1:B:427:LYS:HG3	1:B:428:ASN:CG	2.40	0.42
1:A:245:GLN:NE2	2:A:722:HOH:O	2.41	0.42
1:A:340:LEU:C	1:A:340:LEU:HD23	2.40	0.42
1:B:430:ASN:HA	1:B:430:ASN:HD22	1.62	0.42
1:A:50:PHE:O	1:A:54:GLU:HB2	2.19	0.42
1:B:33:SER:HB3	1:B:139:ILE:HD13	2.01	0.42
1:B:258:THR:O	1:B:261:TYR:HB3	2.19	0.42
1:B:247:GLN:NE2	2:B:697:HOH:O	2.52	0.42
1:A:7:THR:HA	1:A:176:MSE:SE	2.70	0.41
1:A:446:SER:HB2	1:A:448:GLU:HG3	2.02	0.41
1:A:177:LEU:C	1:A:177:LEU:HD13	2.41	0.41
1:A:157:VAL:HG12	1:A:161:MSE:HE2	2.03	0.41
1:A:427:LYS:O	1:A:428:ASN:CB	2.68	0.41
1:A:430:ASN:C	1:A:431:ILE:HD12	2.41	0.41
1:B:391:ASN:ND2	2:B:786:HOH:O	2.52	0.41
1:A:367:ASN:O	1:A:368:ALA:C	2.59	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLU:HG3	1:B:59:GLU:HG2	2.03	0.41
1:A:267:ASN:ND2	1:A:271:HIS:CE1	2.89	0.41
1:B:7:THR:N	2:B:975:HOH:O	2.53	0.41
1:A:374:LYS:O	1:A:378:GLU:HG3	2.21	0.40
1:B:95:ILE:HD11	1:B:125:ILE:HD11	2.03	0.40
1:A:196:ALA:HA	1:A:199:PHE:HE1	1.85	0.40
1:A:466:ASP:HB2	2:A:817:HOH:O	2.21	0.40
1:A:31:TYR:HA	1:A:34:TYR:HD1	1.86	0.40
1:B:198:GLU:OE1	1:B:255:GLU:OE1	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	464/542 (86%)	444 (96%)	20 (4%)	0	100	100
1	B	470/542 (87%)	454 (97%)	16 (3%)	0	100	100
All	All	934/1084 (86%)	898 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	399/449 (89%)	381 (96%)	18 (4%)	32	36
1	B	404/449 (90%)	383 (95%)	21 (5%)	27	29
All	All	803/898 (89%)	764 (95%)	39 (5%)	29	32

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	107	ARG
1	A	130	GLU
1	A	203	GLN
1	A	215	LEU
1	A	263	LEU
1	A	267	ASN
1	A	285	THR
1	A	287	ASP
1	A	304	ASN
1	A	337	PHE
1	A	376	LEU
1	A	391	ASN
1	A	425	LYS
1	A	428	ASN
1	A	441	LEU
1	A	466	ASP
1	A	470	ASN
1	B	7	THR
1	B	12	TYR
1	B	24	SER
1	B	61	GLU
1	B	107	ARG
1	B	124	ASP
1	B	164	LEU
1	B	191	ASP
1	B	203	GLN
1	B	215	LEU
1	B	267	ASN
1	B	287	ASP
1	B	288	GLU
1	B	304	ASN
1	B	337	PHE
1	B	376	LEU
1	B	391	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	427	LYS
1	B	441	LEU
1	B	470	ASN
1	B	477	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	96	HIS
1	A	127	GLN
1	A	203	GLN
1	A	238	ASN
1	A	245	GLN
1	A	247	GLN
1	A	254	GLN
1	A	267	ASN
1	A	304	ASN
1	A	391	ASN
1	A	408	ASN
1	A	430	ASN
1	A	470	ASN
1	B	17	ASN
1	B	96	HIS
1	B	127	GLN
1	B	203	GLN
1	B	238	ASN
1	B	245	GLN
1	B	247	GLN
1	B	254	GLN
1	B	267	ASN
1	B	282	ASN
1	B	304	ASN
1	B	351	ASN
1	B	391	ASN
1	B	408	ASN
1	B	430	ASN
1	B	470	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 ⓘ

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, 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(Å²)	Q<0.9
1	A	453/542 (83%)	-0.08	10 (2%)	62	65	9, 23, 45, 68	0
1	B	457/542 (84%)	-0.21	8 (1%)	69	72	9, 20, 36, 49	0
All	All	910/1084 (83%)	-0.14	18 (1%)	65	69	9, 21, 41, 68	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	ALA	4.2
1	A	172	HIS	4.0
1	A	59	GLU	4.0
1	A	197	GLY	3.4
1	B	478	PHE	3.3
1	A	61	GLU	3.1
1	B	191	ASP	3.0
1	A	394	PHE	2.9
1	B	194	LYS	2.8
1	B	477	THR	2.6
1	A	428	ASN	2.6
1	B	195	LYS	2.6
1	B	73	TYR	2.4
1	B	193	GLY	2.3
1	A	287	ASP	2.2
1	A	429	GLN	2.2
1	B	287	ASP	2.0
1	A	427	LYS	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.