



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:31 PM GMT

PDB ID : 4CFO
Title : Structure of Lytic Transglycosylase MltC from Escherichia coli in complex with tetrasaccharide at 2.9 Å resolution.
Authors : Artola-Recolons, C.; Bernardo-Garcia, N.; Mobashery, S.; Hermoso, J.A.
Deposited on : 2013-11-19
Resolution : 2.90 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

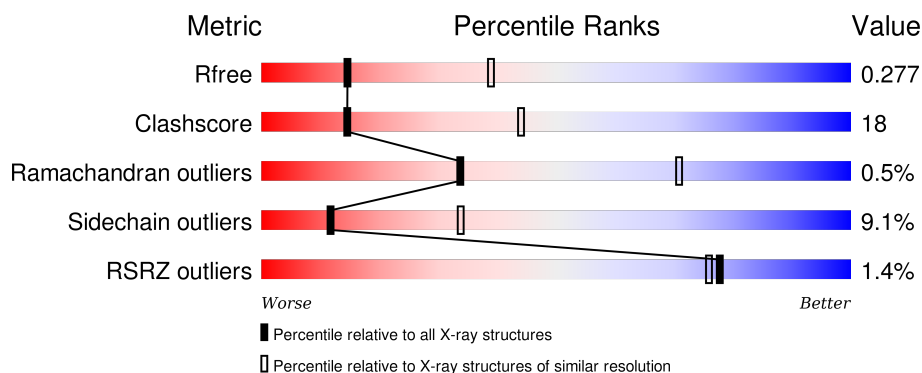
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	341	<div> <div> <div></div> <div>61%</div> <div>32%</div> <div>.</div> <div>.</div> </div> </div>
1	B	341	<div> <div> <div>2%</div> <div>60%</div> <div>32%</div> <div>.</div> <div>.</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5331 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 MLTC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2577	1616	461	492	8			
1	B	327	Total	C	N	O	S	0	0	0
			2577	1616	461	492	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	EXPRESSION TAG	UNP C5A0N2
A	217	GLN	GLU	CONFLICT	UNP C5A0N2
B	19	MET	-	EXPRESSION TAG	UNP C5A0N2
B	217	GLN	GLU	CONFLICT	UNP C5A0N2

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			68	39	6	23		
2	B	4	Total	C	N	O	0	0
			68	39	6	23		

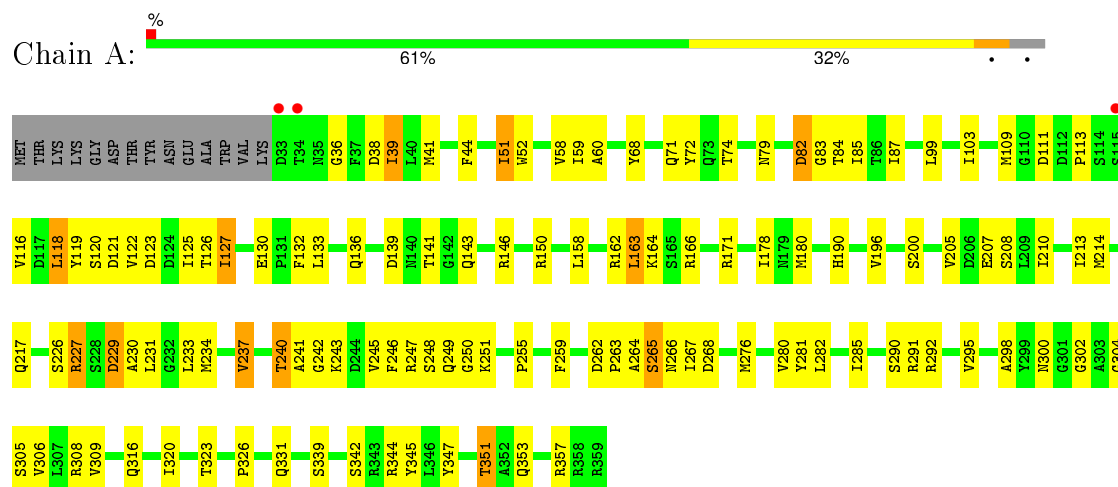
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	21	Total	O	0	0
			21	21		

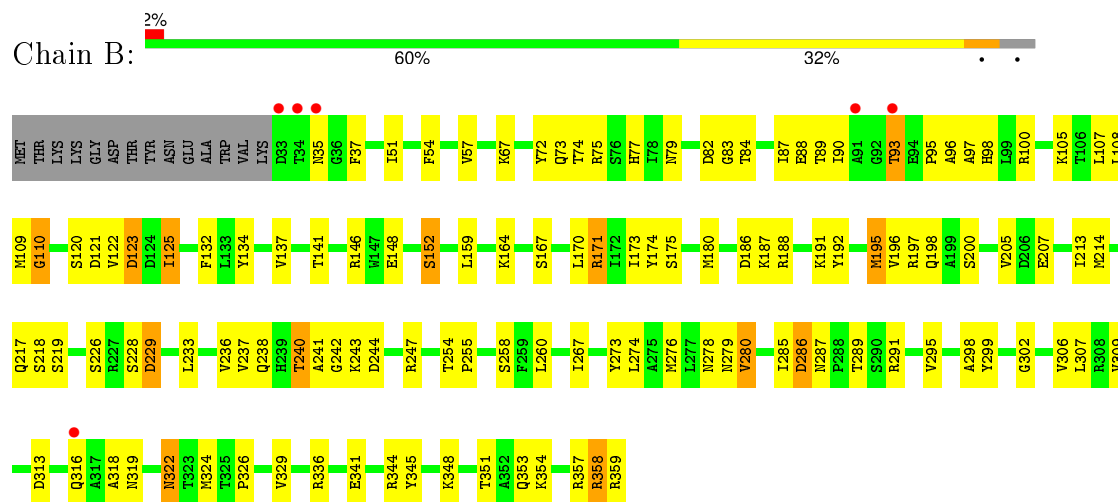
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: MLTC



• Molecule 1: MLTC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.21Å 112.81Å 61.57Å 90.00° 93.52° 90.00°	Depositor
Resolution (Å)	14.93 – 2.90 14.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (14.93-2.90) 99.8 (14.93-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.192 , 0.269 0.199 , 0.277	Depositor DCC
R_{free} test set	741 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 14774 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5331	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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: NM6, NAG, NM9

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.67	0/2628	0.78	1/3559 (0.0%)
1	B	0.57	0/2628	0.73	0/3559
All	All	0.62	0/5256	0.76	1/7118 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	292	ARG	NE-CZ-NH2	-5.65	117.48	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	229	ASP	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2577	0	2547	91	0
1	B	2577	0	2547	92	0
2	A	68	0	54	11	0
2	B	68	0	55	10	0
3	A	20	0	0	1	0
3	B	21	0	0	0	0
All	All	5331	0	5203	188	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 18.

All (188) 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:95:PRO:O	1:B:98:HIS:HB2	1.37	1.19
1:B:228:SER:HB3	2:B:1363:NM9:H3B3	1.52	0.92
1:B:228:SER:CB	2:B:1363:NM9:H3B3	2.05	0.86
1:A:51:ILE:O	1:A:171:ARG:NH2	2.08	0.85
1:B:95:PRO:O	1:B:98:HIS:CB	2.25	0.82
1:B:298:ALA:HB2	1:B:306:VAL:HG21	1.62	0.81
1:A:241:ALA:O	1:A:245:VAL:HG23	1.81	0.81
1:A:234:MET:CE	1:A:267:ILE:HA	2.12	0.79
1:A:109:MET:HB2	1:A:126:THR:HG23	1.64	0.78
1:B:148:GLU:O	1:B:152:SER:OG	2.02	0.77
2:B:1360:NAG:C1	2:B:1361:NM6:HBB1	2.16	0.76
1:A:234:MET:HE2	1:A:267:ILE:HA	1.67	0.76
1:A:226:SER:OG	2:A:1363:NM9:O2B	2.03	0.75
1:A:347:TYR:O	1:A:351:THR:HB	1.86	0.75
1:B:72:TYR:CE1	1:B:121:ASP:HB3	2.22	0.74
1:B:291:ARG:O	1:B:295:VAL:HG23	1.88	0.74
1:A:125:ILE:HD12	1:A:125:ILE:O	1.88	0.73
1:B:107:LEU:HD22	1:B:137:VAL:HG11	1.70	0.73
1:B:213:ILE:HD12	1:B:274:LEU:HD11	1.71	0.71
1:B:96:ALA:HB1	1:B:159:LEU:HD21	1.72	0.70
1:A:58:VAL:O	1:A:68:TYR:OH	2.10	0.69
1:B:226:SER:OG	2:B:1363:NM9:O2B	2.12	0.67
1:A:196:VAL:HG22	1:A:214:MET:HE1	1.76	0.67
1:B:273:TYR:OH	2:B:1361:NM6:O5B	2.09	0.67
1:B:351:THR:HA	1:B:354:LYS:HE2	1.77	0.67
1:B:90:ILE:HG13	1:B:171:ARG:HD3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PRO:HG3	1:B:174:TYR:CE2	2.29	0.67
1:B:90:ILE:CG1	1:B:171:ARG:HD3	2.26	0.66
1:B:96:ALA:O	1:B:97:ALA:HB3	1.95	0.66
1:B:228:SER:HB3	2:B:1363:NM9:C3B	2.23	0.66
1:B:197:ARG:HA	1:B:207:GLU:OE2	1.95	0.65
1:A:207:GLU:OE1	1:B:359:ARG:NH2	2.31	0.64
1:B:200:SER:OG	1:B:205:VAL:O	2.15	0.63
1:A:82:ASP:HB3	1:A:84:THR:HG23	1.79	0.63
1:B:105:LYS:HE3	1:B:125:ILE:HG21	1.82	0.62
1:B:37:PHE:CE1	1:B:229:ASP:HB3	2.34	0.62
1:B:237:VAL:HB	1:B:240:THR:HG22	1.83	0.61
1:B:108:LEU:HD11	1:B:148:GLU:HA	1.83	0.61
1:A:227:ARG:NE	1:A:227:ARG:HA	2.14	0.61
1:A:59:ILE:HG12	1:A:60:ALA:N	2.15	0.61
1:B:132:PHE:O	1:B:191:LYS:NZ	2.34	0.61
1:A:320:ILE:O	1:A:323:THR:HB	2.02	0.60
1:A:120:SER:OG	1:A:122:VAL:HG12	2.01	0.60
2:A:1360:NAG:H61	2:A:1361:NM6:HAT3	1.83	0.60
1:A:111:ASP:HB3	1:A:132:PHE:HB2	1.83	0.60
1:B:228:SER:CB	2:B:1363:NM9:C3B	2.78	0.59
1:A:190:HIS:HB3	3:A:2013:HOH:O	2.03	0.58
2:A:1360:NAG:O5	2:A:1361:NM6:HAT1	2.04	0.58
1:B:87:ILE:O	1:B:175:SER:HA	2.04	0.57
1:B:54:PHE:O	1:B:57:VAL:HG12	2.04	0.57
1:A:285:ILE:O	1:A:291:ARG:NH1	2.37	0.57
1:A:226:SER:HB3	1:A:230:ALA:H	1.69	0.57
1:A:300:ASN:OD1	1:A:342:SER:OG	2.15	0.56
1:A:196:VAL:CG2	1:A:214:MET:HE1	2.36	0.56
1:B:95:PRO:O	1:B:98:HIS:N	2.40	0.55
2:A:1360:NAG:H61	2:A:1361:NM6:C3B	2.35	0.55
1:A:111:ASP:HB3	1:A:132:PHE:CD1	2.42	0.54
1:A:233:LEU:CD1	1:A:263:PRO:HB3	2.36	0.54
1:B:90:ILE:HD12	1:B:173:ILE:HG12	1.89	0.54
1:B:240:THR:HG23	1:B:241:ALA:N	2.23	0.54
1:B:188:ARG:NH1	1:B:219:SER:O	2.39	0.53
2:A:1360:NAG:C6	2:A:1361:NM6:HAT1	2.39	0.53
1:B:196:VAL:HG12	1:B:207:GLU:HG2	1.89	0.53
1:A:227:ARG:HA	1:A:227:ARG:CZ	2.38	0.53
1:A:248:SER:C	1:A:250:GLY:H	2.12	0.53
1:B:73:GLN:HA	1:B:90:ILE:HG22	1.91	0.53
1:A:248:SER:O	1:A:249:GLN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LEU:HD11	1:A:263:PRO:HB3	1.91	0.52
1:B:285:ILE:HB	1:B:291:ARG:HG3	1.90	0.52
1:A:36:GLY:O	1:A:39:ILE:HG22	2.09	0.52
1:A:305:SER:HB3	2:A:1361:NM6:HBE3	1.91	0.52
1:A:262:ASP:OD2	1:A:264:ALA:HB3	2.10	0.52
1:B:96:ALA:C	1:B:98:HIS:H	2.13	0.52
1:B:287:ASN:OD1	1:B:289:THR:N	2.41	0.52
2:A:1363:NM9:H1B2	2:A:1363:NM9:N2A	2.25	0.52
1:B:134:TYR:CD1	1:B:146:ARG:HB3	2.45	0.52
1:A:217:GLN:NE2	1:A:345:TYR:HE2	2.07	0.52
1:A:237:VAL:CG2	1:A:240:THR:OG1	2.58	0.52
1:A:246:PHE:O	1:A:251:LYS:HB2	2.10	0.52
1:A:116:VAL:HG12	1:A:118:LEU:HD13	1.93	0.51
1:B:226:SER:CB	2:B:1363:NM9:O2B	2.58	0.51
1:A:237:VAL:HG22	1:A:240:THR:OG1	2.10	0.51
1:A:280:VAL:HG22	1:A:281:TYR:N	2.24	0.51
1:A:116:VAL:CG1	1:A:118:LEU:HD13	2.41	0.51
1:A:230:ALA:C	1:A:231:LEU:HD12	2.32	0.50
1:B:309:VAL:O	1:B:309:VAL:HG12	2.11	0.50
1:A:226:SER:HB2	1:A:230:ALA:HB3	1.94	0.50
1:B:83:GLY:HA2	1:B:180:MET:SD	2.52	0.50
1:A:298:ALA:HB2	1:A:306:VAL:HG21	1.93	0.49
1:B:319:ASN:HA	1:B:322:ASN:OD1	2.12	0.49
1:A:339:SER:HB3	1:A:342:SER:HB2	1.93	0.49
1:B:51:ILE:HD12	1:B:72:TYR:HB2	1.95	0.49
1:A:158:LEU:HD23	1:A:162:ARG:HG3	1.95	0.49
1:A:291:ARG:O	1:A:295:VAL:HG23	2.11	0.49
1:A:234:MET:HE3	1:A:267:ILE:HA	1.92	0.49
1:A:248:SER:O	1:A:250:GLY:N	2.41	0.49
1:A:87:ILE:CD1	1:A:103:ILE:HA	2.42	0.49
1:B:97:ALA:HA	1:B:100:ARG:HB3	1.95	0.49
1:A:125:ILE:CD1	1:A:125:ILE:O	2.60	0.48
1:A:208:SER:HB2	1:A:353:GLN:HG2	1.94	0.48
1:A:68:TYR:HA	1:A:74:THR:O	2.13	0.48
1:B:354:LYS:O	1:B:358:ARG:NH1	2.46	0.48
1:B:287:ASN:ND2	1:B:326:PRO:HG3	2.28	0.48
1:B:240:THR:CG2	1:B:241:ALA:N	2.77	0.48
1:A:302:GLY:HA3	2:A:1361:NM6:C2A	2.43	0.48
1:B:90:ILE:HD12	1:B:173:ILE:CG1	2.43	0.48
1:B:278:ASN:OD1	1:B:291:ARG:HD2	2.14	0.48
1:A:51:ILE:HG22	1:A:52:TRP:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLY:O	1:A:180:MET:HG3	2.14	0.47
1:A:79:ASN:O	1:A:83:GLY:HA2	2.13	0.47
1:B:236:VAL:HB	1:B:260:LEU:HD13	1.94	0.47
1:B:214:MET:HE1	1:B:267:ILE:HD11	1.96	0.47
1:A:242:GLY:HA3	1:A:255:PRO:HG2	1.97	0.47
1:A:71:GLN:O	1:A:72:TYR:HB2	2.15	0.47
1:A:282:LEU:HB3	1:A:285:ILE:HD12	1.96	0.46
1:A:87:ILE:HD12	1:A:103:ILE:CG1	2.46	0.46
1:A:71:GLN:HA	1:A:121:ASP:OD2	2.16	0.46
1:B:93:THR:HG23	1:B:93:THR:O	2.15	0.46
1:B:79:ASN:ND2	1:B:82:ASP:HB2	2.30	0.46
1:B:242:GLY:CA	1:B:255:PRO:HG3	2.46	0.46
1:A:304:GLY:O	1:A:308:ARG:HB2	2.16	0.46
1:A:139:ASP:OD2	1:A:150:ARG:NH1	2.48	0.46
1:B:276:MET:O	1:B:280:VAL:HB	2.15	0.46
1:B:213:ILE:CD1	1:B:274:LEU:HD21	2.45	0.46
1:A:139:ASP:CB	1:A:141:THR:HB	2.46	0.46
1:A:300:ASN:HA	2:A:1363:NM9:H5A1	1.98	0.46
1:B:313:ASP:HB3	1:B:316:GLN:HB2	1.97	0.46
1:B:240:THR:CG2	1:B:241:ALA:H	2.28	0.45
1:B:353:GLN:O	1:B:357:ARG:N	2.41	0.45
1:B:96:ALA:O	1:B:97:ALA:CB	2.61	0.45
1:B:217:GLN:OE1	1:B:345:TYR:HE1	2.00	0.45
1:B:324:MET:HG3	1:B:329:VAL:HG23	1.98	0.45
1:A:290:SER:OG	1:A:326:PRO:HA	2.17	0.45
2:A:1360:NAG:C6	2:A:1361:NM6:C3B	2.95	0.44
1:A:291:ARG:HH11	1:A:291:ARG:HB2	1.83	0.44
1:A:127:ILE:HA	1:A:127:ILE:HD12	1.86	0.44
1:B:229:ASP:CG	1:B:229:ASP:O	2.55	0.44
1:A:316:GLN:O	1:A:320:ILE:HD12	2.17	0.44
1:B:226:SER:O	1:B:229:ASP:HA	2.17	0.44
1:B:109:MET:O	1:B:110:GLY:C	2.56	0.44
1:B:74:THR:HG22	1:B:89:THR:OG1	2.17	0.44
1:A:210:ILE:O	1:A:214:MET:HB2	2.18	0.44
1:A:230:ALA:HA	1:A:237:VAL:HG12	1.99	0.44
1:A:234:MET:HB2	1:A:266:ASN:OD1	2.18	0.43
1:A:217:GLN:NE2	1:A:345:TYR:CE2	2.86	0.43
1:B:197:ARG:HG2	1:B:207:GLU:OE2	2.19	0.43
1:A:143:GLN:HB2	1:A:150:ARG:HH12	1.83	0.43
1:B:218:SER:HB2	1:B:233:LEU:O	2.19	0.43
1:B:302:GLY:O	1:B:306:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ILE:O	1:A:268:ASP:C	2.55	0.42
1:B:341:GLU:HA	1:B:344:ARG:HH21	1.84	0.42
1:A:217:GLN:HA	1:A:217:GLN:NE2	2.34	0.42
1:B:237:VAL:CG1	1:B:240:THR:HG22	2.49	0.42
1:A:309:VAL:O	1:A:309:VAL:HG12	2.19	0.42
1:A:248:SER:C	1:A:250:GLY:N	2.73	0.42
1:A:133:LEU:HD22	1:A:180:MET:CE	2.49	0.42
1:A:87:ILE:HD12	1:A:103:ILE:HG12	2.02	0.42
1:B:122:VAL:HG12	1:B:123:ASP:N	2.34	0.42
1:B:237:VAL:CB	1:B:240:THR:HG22	2.48	0.42
1:A:136:GLN:O	1:A:180:MET:HB3	2.20	0.42
1:A:41:MET:SD	1:A:227:ARG:NH2	2.93	0.42
1:A:87:ILE:HG22	1:A:99:LEU:CD2	2.49	0.42
1:B:217:GLN:OE1	1:B:345:TYR:CE1	2.73	0.42
1:B:141:THR:O	1:B:141:THR:HG22	2.19	0.42
1:B:307:LEU:C	1:B:309:VAL:H	2.23	0.41
1:A:200:SER:OG	1:A:205:VAL:O	2.29	0.41
1:B:241:ALA:HB1	1:B:273:TYR:CD1	2.55	0.41
1:B:318:ALA:O	1:B:322:ASN:OD1	2.37	0.41
1:B:192:TYR:HA	1:B:195:MET:HG3	2.02	0.41
1:B:226:SER:OG	2:B:1363:NM9:C2A	2.68	0.41
1:B:108:LEU:HD11	1:B:148:GLU:CA	2.50	0.41
1:A:357:ARG:O	1:B:359:ARG:N	2.39	0.41
1:B:67:LYS:O	1:B:75:ARG:HA	2.21	0.41
1:B:336:ARG:HG2	1:B:336:ARG:O	2.21	0.41
1:B:73:GLN:CA	1:B:90:ILE:HG22	2.50	0.41
1:A:59:ILE:CG1	1:A:60:ALA:N	2.84	0.41
1:A:44:PHE:CD1	1:A:119:TYR:O	2.74	0.40
1:B:299:TYR:CZ	2:B:1362:NAG:H82	2.56	0.40
1:B:95:PRO:CB	1:B:174:TYR:CD2	3.04	0.40
1:A:125:ILE:CG1	1:A:125:ILE:O	2.70	0.40
1:A:139:ASP:HB3	1:A:141:THR:HB	2.03	0.40
1:A:259:PHE:CZ	1:A:265:SER:HB3	2.57	0.40
1:A:85:ILE:HB	1:A:178:ILE:HB	2.02	0.40
1:A:240:THR:HG22	2:A:1361:NM6:HBA	2.03	0.40
1:B:146:ARG:HG3	1:B:146:ARG:O	2.21	0.40
1:A:163:LEU:HG	1:A:164:LYS:N	2.37	0.40
1:B:244:ASP:O	1:B:247:ARG:HG2	2.21	0.40
1:B:286:ASP:OD1	1:B:286:ASP:N	2.55	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	325/341 (95%)	303 (93%)	22 (7%)	0	100	100
1	B	325/341 (95%)	288 (89%)	34 (10%)	3 (1%)	21	57
All	All	650/682 (95%)	591 (91%)	56 (9%)	3 (0%)	34	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	93	THR
1	B	280	VAL
1	B	110	GLY

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	279/291 (96%)	255 (91%)	24 (9%)	13	36
1	B	279/291 (96%)	252 (90%)	27 (10%)	10	30
All	All	558/582 (96%)	507 (91%)	51 (9%)	12	34

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	39	ILE
1	A	51	ILE

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Mol	Chain	Res	Type
1	A	82	ASP
1	A	113	PRO
1	A	118	LEU
1	A	123	ASP
1	A	127	ILE
1	A	130	GLU
1	A	146	ARG
1	A	163	LEU
1	A	166	ARG
1	A	213	ILE
1	A	227	ARG
1	A	229	ASP
1	A	237	VAL
1	A	240	THR
1	A	243	LYS
1	A	247	ARG
1	A	265	SER
1	A	276	MET
1	A	331	GLN
1	A	344	ARG
1	A	351	THR
1	B	35	ASN
1	B	77	HIS
1	B	84	THR
1	B	88	GLU
1	B	120	SER
1	B	123	ASP
1	B	125	ILE
1	B	152	SER
1	B	164	LYS
1	B	167	SER
1	B	170	LEU
1	B	171	ARG
1	B	186	ASP
1	B	187	LYS
1	B	195	MET
1	B	198	GLN
1	B	229	ASP
1	B	238	GLN
1	B	240	THR
1	B	243	LYS
1	B	254	THR

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Mol	Chain	Res	Type
1	B	258	SER
1	B	279	ASN
1	B	286	ASP
1	B	322	ASN
1	B	348	LYS
1	B	358	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	GLN
1	B	136	GLN
1	B	235	GLN
1	B	279	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 ⓘ

8 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1360	2	14,14,15	2.81	8 (57%)	15,19,21	3.23	8 (53%)
2	NM6	A	1361	2	19,19,20	3.18	10 (52%)	19,26,28	2.37	6 (31%)
2	NAG	A	1362	2	14,14,15	3.25	10 (71%)	15,19,21	3.28	8 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NM9	A	1363	2	21,21,21	2.42	9 (42%)	26,29,29	3.31	14 (53%)
2	NAG	B	1360	2	14,14,15	2.74	7 (50%)	15,19,21	3.45	9 (60%)
2	NM6	B	1361	2	19,19,20	2.81	6 (31%)	19,26,28	2.82	9 (47%)
2	NAG	B	1362	2	14,14,15	3.10	10 (71%)	15,19,21	3.10	8 (53%)
2	NM9	B	1363	2	21,21,21	2.46	10 (47%)	26,29,29	3.66	14 (53%)

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	NAG	A	1360	2	-	0/6/23/26	0/1/1/1
2	NM6	A	1361	2	-	0/13/31/34	0/1/1/1
2	NAG	A	1362	2	-	0/6/23/26	0/1/1/1
2	NM9	A	1363	2	-	1/15/36/36	0/1/1/1
2	NAG	B	1360	2	-	0/6/23/26	0/1/1/1
2	NM6	B	1361	2	-	0/13/31/34	0/1/1/1
2	NAG	B	1362	2	-	0/6/23/26	0/1/1/1
2	NM9	B	1363	2	-	1/15/36/36	0/1/1/1

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1361	NM6	C3A-C3C	-8.10	1.30	1.52
2	A	1361	NM6	C3A-C3C	-7.78	1.31	1.52
2	B	1363	NM9	O3A-C3A	-7.01	1.28	1.44
2	A	1363	NM9	O3A-C3A	-6.51	1.29	1.44
2	A	1361	NM6	O6-C1	-5.50	1.34	1.43
2	A	1362	NAG	C1-C2	-5.19	1.45	1.52
2	B	1362	NAG	O7-C7	-5.14	1.11	1.23
2	B	1360	NAG	C2-N2	-4.94	1.37	1.46
2	A	1362	NAG	O7-C7	-4.91	1.11	1.23
2	A	1360	NAG	C2-N2	-4.66	1.38	1.46
2	A	1361	NM6	C2-N2A	-4.62	1.38	1.46
2	A	1361	NM6	OAP-C2A	-4.59	1.12	1.23
2	A	1362	NAG	O5-C1	-4.46	1.36	1.43
2	B	1361	NM6	C2-N2A	-4.44	1.38	1.46
2	B	1362	NAG	O3-C3	-4.43	1.32	1.43
2	B	1362	NAG	C1-C2	-4.42	1.46	1.52
2	B	1360	NAG	O7-C7	-4.37	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1362	NAG	O3-C3	-4.28	1.32	1.43
2	A	1363	NM9	C2-N2A	-4.28	1.38	1.45
2	A	1360	NAG	O7-C7	-4.17	1.13	1.23
2	B	1362	NAG	O5-C1	-3.96	1.37	1.43
2	B	1361	NM6	O3A-C3	-3.92	1.34	1.43
2	A	1360	NAG	C1-C2	-3.89	1.47	1.52
2	A	1361	NM6	O3A-C3	-3.87	1.34	1.43
2	B	1363	NM9	C1-C2	-3.80	1.46	1.53
2	B	1360	NAG	C1-C2	-3.71	1.47	1.52
2	B	1361	NM6	OAP-C2A	-3.65	1.14	1.23
2	B	1360	NAG	C4-C5	-3.60	1.45	1.53
2	B	1362	NAG	C6-C5	-3.42	1.39	1.51
2	B	1363	NM9	C2-N2A	-3.41	1.40	1.45
2	A	1362	NAG	C6-C5	-3.40	1.39	1.51
2	A	1362	NAG	C2-N2	-3.40	1.40	1.46
2	A	1362	NAG	C8-C7	-3.35	1.43	1.50
2	A	1360	NAG	C4-C5	-3.28	1.46	1.53
2	A	1360	NAG	O3-C3	-3.27	1.35	1.43
2	B	1362	NAG	C4-C5	-3.22	1.46	1.53
2	A	1360	NAG	O4-C4	-3.20	1.35	1.43
2	A	1363	NM9	C1-C2	-3.18	1.47	1.53
2	B	1362	NAG	C8-C7	-3.18	1.44	1.50
2	A	1362	NAG	C4-C5	-3.14	1.46	1.53
2	B	1361	NM6	O6-C1	-3.11	1.38	1.43
2	A	1363	NM9	O6-C5	-3.10	1.36	1.44
2	B	1363	NM9	O6-C5	-3.02	1.36	1.44
2	B	1360	NAG	O3-C3	-2.91	1.36	1.43
2	A	1363	NM9	O2B-C2A	-2.78	1.16	1.23
2	A	1361	NM6	C2B-C2A	-2.67	1.45	1.50
2	B	1362	NAG	C2-N2	-2.64	1.41	1.46
2	A	1360	NAG	C4-C3	-2.60	1.45	1.52
2	B	1363	NM9	O2B-C2A	-2.57	1.17	1.23
2	A	1363	NM9	C2B-C2A	-2.56	1.45	1.50
2	A	1363	NM9	O3A-C3	-2.50	1.37	1.43
2	B	1360	NAG	C4-C3	-2.49	1.45	1.52
2	A	1360	NAG	O5-C1	-2.46	1.39	1.43
2	A	1361	NM6	C3-C2	-2.38	1.49	1.52
2	B	1360	NAG	O4-C4	-2.37	1.37	1.43
2	A	1361	NM6	O6-C5	-2.36	1.38	1.43
2	B	1363	NM9	O1A-C1B	-2.34	1.33	1.42
2	A	1363	NM9	O1A-C1B	-2.31	1.33	1.42
2	B	1363	NM9	O6-C1	-2.23	1.36	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1363	NM9	OCA-C3E	-2.20	1.19	1.23
2	B	1362	NAG	O6-C6	-2.18	1.32	1.42
2	B	1363	NM9	OCA-C3E	-2.16	1.19	1.23
2	A	1362	NAG	O6-C6	-2.13	1.33	1.42
2	A	1361	NM6	C1-C2	-2.12	1.49	1.52
2	B	1363	NM9	C2B-C2A	-2.12	1.46	1.50
2	B	1361	NM6	C4-C5	-2.07	1.48	1.53
2	B	1362	NAG	O5-C5	-2.05	1.38	1.43
2	B	1363	NM9	O3A-C3	-2.02	1.38	1.43
2	A	1362	NAG	O5-C5	-2.01	1.39	1.43
2	A	1361	NM6	C3C-N3A	2.80	1.38	1.32

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1360	NAG	C3-C2-N2	-6.58	94.79	110.56
2	B	1360	NAG	C3-C2-N2	-6.34	95.38	110.56
2	B	1362	NAG	O5-C5-C6	-5.41	95.63	107.35
2	A	1360	NAG	O4-C4-C3	-5.31	98.38	110.34
2	B	1363	NM9	O5A-C5A-C5	-5.06	94.60	111.33
2	A	1362	NAG	O7-C7-C8	-4.91	113.05	122.06
2	A	1362	NAG	O5-C5-C6	-4.54	97.51	107.35
2	B	1361	NM6	O3B-C3C-N3A	-4.49	116.42	123.08
2	A	1362	NAG	O3-C3-C4	-4.48	100.24	110.34
2	A	1363	NM9	O6-C5-C5A	-4.42	95.18	106.36
2	B	1360	NAG	O6-C6-C5	-4.27	97.22	111.33
2	A	1361	NM6	O3B-C3C-N3A	-4.25	116.78	123.08
2	A	1362	NAG	O6-C6-C5	-4.25	97.30	111.33
2	B	1362	NAG	O3-C3-C4	-4.21	100.87	110.34
2	A	1363	NM9	O5A-C5A-C5	-4.19	97.49	111.33
2	B	1360	NAG	O4-C4-C3	-4.14	101.02	110.34
2	B	1362	NAG	O7-C7-C8	-4.00	114.73	122.06
2	B	1363	NM9	O6-C5-C5A	-3.75	96.88	106.36
2	B	1360	NAG	C6-C5-C4	-3.46	104.47	113.02
2	A	1360	NAG	C6-C5-C4	-3.41	104.61	113.02
2	B	1363	NM9	O6-C1-O1A	-3.35	102.83	110.88
2	B	1362	NAG	C2-N2-C7	-3.30	118.81	123.04
2	A	1363	NM9	O6-C1-C2	-3.24	103.72	110.78
2	A	1363	NM9	C2B-C2A-N2A	-3.18	110.02	116.11
2	A	1362	NAG	C2-N2-C7	-3.15	118.99	123.04
2	B	1362	NAG	O6-C6-C5	-3.10	101.10	111.33
2	B	1361	NM6	O5B-C5B-C5	-3.04	101.30	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1362	NAG	C6-C5-C4	-2.84	106.00	113.02
2	A	1360	NAG	O4-C4-C5	-2.80	101.81	109.24
2	B	1361	NM6	OAP-C2A-C2B	-2.75	117.01	122.06
2	A	1363	NM9	C1-C2-C3	-2.66	105.03	110.13
2	B	1363	NM9	C1-C2-C3	-2.65	105.04	110.13
2	B	1360	NAG	O4-C4-C5	-2.65	102.23	109.24
2	A	1362	NAG	C6-C5-C4	-2.61	106.57	113.02
2	A	1361	NM6	OAP-C2A-C2B	-2.57	117.34	122.06
2	B	1363	NM9	O6-C1-C2	-2.52	105.30	110.78
2	B	1361	NM6	C3-C4-C5	-2.48	103.99	109.61
2	A	1360	NAG	O7-C7-C8	-2.43	117.61	122.06
2	B	1360	NAG	O7-C7-C8	-2.38	117.70	122.06
2	B	1361	NM6	C3B-C3A-C3C	-2.28	105.08	111.05
2	A	1363	NM9	OCA-C3E-C3A	2.02	121.83	118.99
2	B	1363	NM9	O3A-C3-C4	2.21	112.87	107.17
2	A	1363	NM9	C1-O6-C5	2.26	118.12	113.75
2	A	1363	NM9	C1B-O1A-C1	2.38	117.18	113.29
2	A	1363	NM9	O3A-C3A-C3B	2.49	114.75	107.50
2	A	1363	NM9	C3-C2-N2A	2.54	115.50	111.07
2	A	1363	NM9	O2B-C2A-N2A	2.60	127.17	121.86
2	A	1361	NM6	C2B-C2A-N2A	2.66	121.20	116.11
2	B	1363	NM9	C5A-C5-C4	2.70	119.67	113.02
2	B	1361	NM6	C2B-C2A-N2A	2.70	121.28	116.11
2	B	1363	NM9	O4-C4-C3	2.79	116.48	109.87
2	A	1361	NM6	O3A-C3A-C3C	2.86	117.37	111.05
2	B	1363	NM9	O2B-C2A-N2A	3.18	128.35	121.86
2	B	1362	NAG	C8-C7-N2	3.45	122.70	116.11
2	A	1360	NAG	O5-C5-C6	3.47	114.86	107.35
2	A	1360	NAG	C8-C7-N2	3.69	123.17	116.11
2	B	1360	NAG	C8-C7-N2	3.80	123.39	116.11
2	B	1361	NM6	O3A-C3A-C3C	3.83	119.51	111.05
2	A	1362	NAG	C8-C7-N2	4.18	124.10	116.11
2	B	1360	NAG	O5-C5-C6	4.28	116.61	107.35
2	B	1361	NM6	C1-O6-C5	4.47	117.92	112.25
2	B	1363	NM9	OCA-C3E-C3A	4.63	125.49	118.99
2	A	1363	NM9	C2-N2A-C2A	5.09	136.16	123.10
2	A	1363	NM9	C3B-C3A-C3E	5.12	124.45	111.05
2	A	1361	NM6	C3A-C3C-N3A	5.13	124.52	116.92
2	A	1360	NAG	C1-O5-C5	5.13	118.76	112.25
2	A	1361	NM6	C1-O6-C5	5.75	119.54	112.25
2	B	1363	NM9	C3-C2-N2A	5.89	121.33	111.07
2	A	1362	NAG	C1-O5-C5	5.98	119.84	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1362	NAG	C1-O5-C5	6.05	119.92	112.25
2	B	1363	NM9	C3B-C3A-C3E	6.26	127.43	111.05
2	B	1360	NAG	C1-O5-C5	6.31	120.26	112.25
2	B	1363	NM9	C2-N2A-C2A	6.31	139.31	123.10
2	B	1361	NM6	O3B-C3C-C3A	7.19	129.09	118.99
2	B	1363	NM9	O1A-C1-C2	9.83	123.99	108.03
2	A	1363	NM9	O1A-C1-C2	10.99	125.88	108.03

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1363	NM9	C1B-O1A-C1-C2
2	A	1363	NM9	C1B-O1A-C1-C2

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1360	NAG	5	0
2	A	1361	NM6	8	0
2	A	1363	NM9	3	0
2	B	1360	NAG	1	0
2	B	1361	NM6	2	0
2	B	1362	NAG	1	0
2	B	1363	NM9	7	0

5.6 Ligand geometry [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	327/341 (95%)	-0.33	3 (0%) 85 84	17, 28, 51, 93	0
1	B	327/341 (95%)	-0.13	6 (1%) 71 68	18, 40, 68, 100	0
All	All	654/682 (95%)	-0.23	9 (1%) 78 76	17, 32, 65, 100	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	THR	5.9
1	B	35	ASN	3.6
1	B	316	GLN	3.0
1	B	33	ASP	2.9
1	B	93	THR	2.9
1	B	34	THR	2.7
1	A	33	ASP	2.3
1	B	91	ALA	2.2
1	A	115	SER	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](#)

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
2	NM9	A	1363	21/21	0.90	0.20	0.97	0,44,50,54	0
2	NAG	A	1362	14/15	0.94	0.15	0.89	35,39,44,45	0
2	NM6	A	1361	19/20	0.91	0.17	0.24	38,44,49,50	0
2	NAG	B	1362	14/15	0.96	0.14	0.05	34,38,44,45	0
2	NM6	B	1361	19/20	0.91	0.17	0.04	41,45,51,52	0
2	NM9	B	1363	21/21	0.94	0.15	-0.21	35,42,48,50	0
2	NAG	B	1360	14/15	0.94	0.18	-0.32	45,47,49,49	0
2	NAG	A	1360	14/15	0.94	0.15	-0.72	43,45,47,48	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.