



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:00 PM GMT

PDB ID : 3SI1
Title : Structure of glycosylated murine glutaminyl cyclase
Authors : Dambe, T.; Carrillo, D.; Parthier, C.; Stubbs, M.T.
Deposited on : 2011-06-17
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

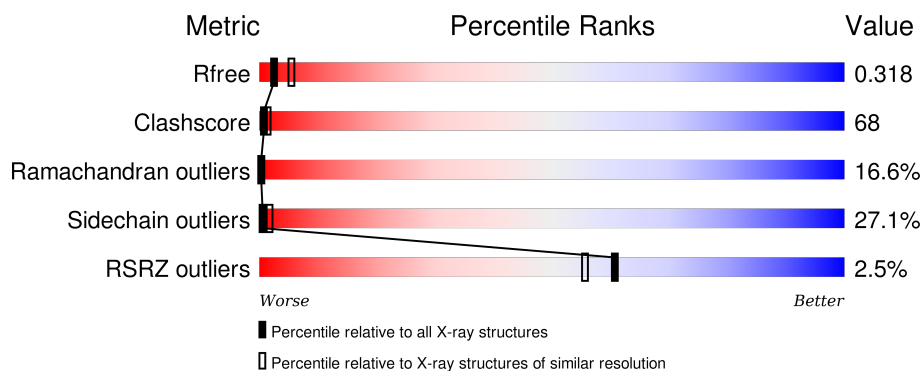
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

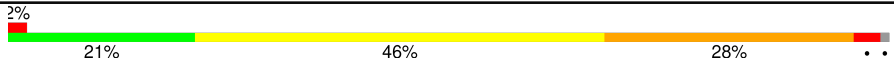
The reported resolution of this entry is 2.90 Å.

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	327	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2712 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 Glutaminyl-peptide cyclotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2631	1682	462	478	9			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

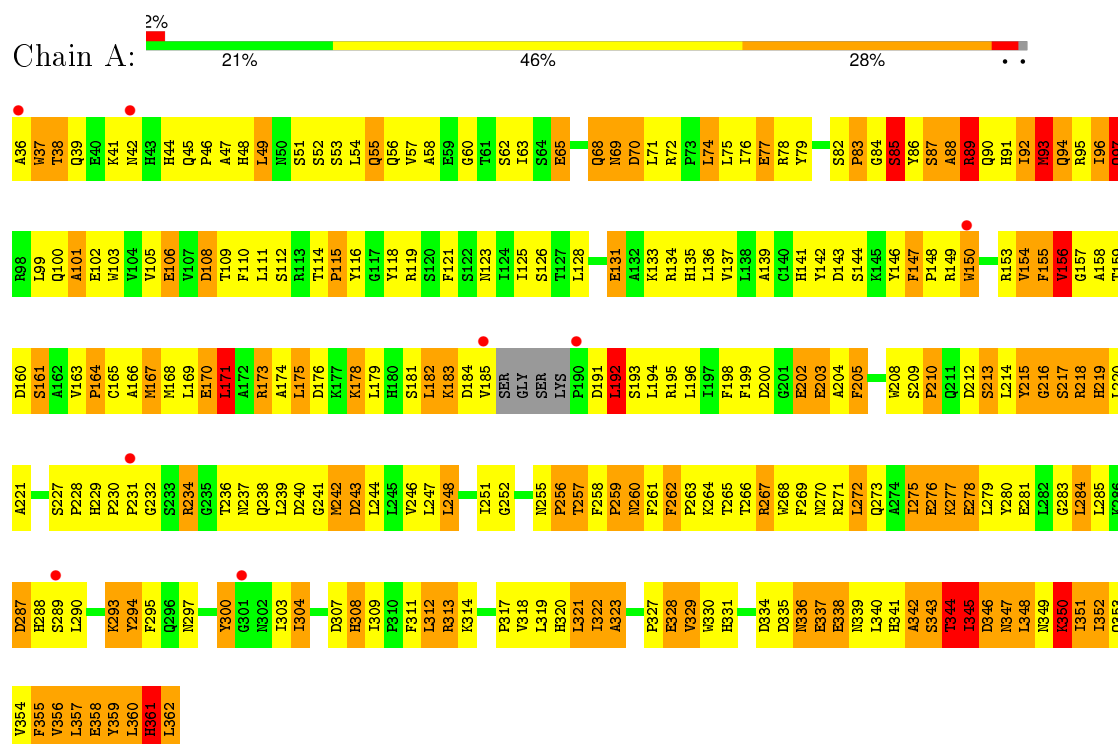
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		

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 ($\text{RSRZ} > 2$). 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: Glutaminy-peptide cyclotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.24Å 86.87Å 97.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.75 – 2.90 19.75 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.75-2.90) 98.9 (19.75-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.83Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.245 , 0.301 0.245 , 0.318	Depositor DCC
R_{free} test set	426 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 68.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Outliers	0 of 9032 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	2712	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% 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: ZN, NAG

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	0.91	0/2707	1.03	3/3675 (0.1%)

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	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	171	LEU	CB-CG-CD2	-6.85	99.35	111.00
1	A	171	LEU	CB-CG-CD1	-6.28	100.32	111.00
1	A	272	LEU	CA-CB-CG	-5.30	103.12	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ALA	Peptide
1	A	313	ARG	Peptide
1	A	321	LEU	Peptide
1	A	361	HIS	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	2631	0	2556	357	0
2	A	1	0	0	0	0
3	A	28	0	25	0	0
4	A	52	0	0	10	0
All	All	2712	0	2581	357	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 68.

All (357) 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:A:171:LEU:O	1:A:175:LEU:HD21	1.37	1.19
1:A:344:THR:O	1:A:348:LEU:HD13	1.42	1.17
1:A:267:ARG:HB2	1:A:267:ARG:HH11	1.08	1.14
1:A:171:LEU:HD11	1:A:352:ILE:HD12	1.33	1.09
1:A:346:ASP:O	1:A:349:ASN:N	1.83	1.09
1:A:175:LEU:HD23	1:A:175:LEU:H	1.16	1.06
1:A:228:PRO:HA	1:A:237:ASN:HA	1.33	1.05
1:A:134:ARG:O	1:A:192:LEU:HA	1.57	1.04
1:A:279:LEU:CD1	1:A:285:LEU:HD13	1.88	1.03
1:A:142:TYR:CE2	1:A:200:ASP:HB2	1.97	0.99
1:A:279:LEU:CD1	1:A:285:LEU:CD1	2.41	0.98
1:A:204:ALA:HB2	1:A:212:ASP:O	1.64	0.97
1:A:280:TYR:HB2	1:A:285:LEU:HD22	1.46	0.96
1:A:78:ARG:NH1	1:A:156:VAL:O	1.98	0.96
1:A:247:LEU:HD22	1:A:308:HIS:HB3	1.48	0.96
1:A:227:SER:HB2	1:A:238:GLN:HE21	1.31	0.95
1:A:281:GLU:HB2	4:A:379:HOH:O	1.67	0.93
1:A:53:SER:HA	1:A:56:GLN:HE21	1.33	0.92
1:A:175:LEU:CD2	1:A:175:LEU:H	1.85	0.89
1:A:277:LYS:C	1:A:279:LEU:H	1.76	0.89
1:A:337:GLU:HA	1:A:340:LEU:HD12	1.54	0.88
1:A:267:ARG:NH1	1:A:267:ARG:HB2	1.89	0.88
1:A:227:SER:HB2	1:A:238:GLN:NE2	1.89	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:HD23	1:A:288:HIS:HD2	1.40	0.87
1:A:260:ASN:HB2	1:A:269:PHE:CD1	2.11	0.86
1:A:342:ALA:O	1:A:343:SER:C	2.13	0.85
1:A:247:LEU:CD2	1:A:308:HIS:HB3	2.05	0.85
1:A:134:ARG:HB3	1:A:243:ASP:OD1	1.76	0.85
1:A:279:LEU:HD12	1:A:285:LEU:CD1	2.06	0.84
1:A:72:ARG:HA	1:A:75:LEU:HD12	1.59	0.83
1:A:171:LEU:C	1:A:175:LEU:HD21	1.98	0.83
1:A:37:TRP:O	1:A:39:GLN:N	2.12	0.82
1:A:204:ALA:CB	1:A:212:ASP:O	2.26	0.82
1:A:279:LEU:HD13	1:A:285:LEU:HD13	1.61	0.82
1:A:218:ARG:HH11	1:A:218:ARG:HB2	1.44	0.81
1:A:139:ALA:O	1:A:247:LEU:HD12	1.81	0.81
1:A:346:ASP:O	1:A:347:ASN:C	2.19	0.80
1:A:102:GLU:HB3	1:A:128:LEU:CD2	2.11	0.80
1:A:112:SER:HB3	1:A:121:PHE:CE2	2.17	0.80
1:A:148:PRO:HB2	1:A:150:TRP:HE1	1.47	0.80
1:A:62:SER:OG	1:A:65:GLU:HB3	1.81	0.80
1:A:344:THR:C	1:A:348:LEU:HD13	2.02	0.80
1:A:347:ASN:HB2	1:A:348:LEU:HD12	1.63	0.80
1:A:133:LYS:H	1:A:191:ASP:HB3	1.46	0.79
1:A:92:ILE:O	1:A:95:ARG:N	2.16	0.78
1:A:99:LEU:HB2	4:A:34:HOH:O	1.83	0.78
1:A:158:ALA:O	1:A:163:VAL:HG23	1.83	0.78
1:A:279:LEU:HD12	1:A:285:LEU:HD11	1.66	0.78
1:A:178:LYS:HZ2	1:A:178:LYS:H	1.32	0.78
1:A:214:LEU:HB3	1:A:217:SER:OG	1.83	0.77
1:A:114:THR:HG21	1:A:119:ARG:HG2	1.65	0.77
1:A:263:PRO:HB3	1:A:300:TYR:OH	1.86	0.76
1:A:123:ASN:OD1	1:A:199:PHE:HA	1.87	0.75
1:A:348:LEU:HA	1:A:351:ILE:HD12	1.69	0.75
1:A:148:PRO:HB2	1:A:150:TRP:NE1	2.02	0.75
1:A:276:GLU:OE1	4:A:377:HOH:O	2.05	0.75
1:A:176:ASP:O	1:A:179:LEU:HB2	1.87	0.74
1:A:311:PHE:O	1:A:313:ARG:N	2.20	0.74
1:A:63:ILE:O	1:A:63:ILE:HG12	1.87	0.74
1:A:114:THR:HG21	1:A:119:ARG:CG	2.18	0.73
1:A:184:ASP:H	1:A:185:VAL:HA	1.53	0.73
1:A:268:TRP:O	1:A:271:ARG:N	2.15	0.72
1:A:360:LEU:O	1:A:362:LEU:N	2.16	0.72
1:A:353:GLN:O	1:A:357:LEU:HD12	1.90	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:HD23	1:A:175:LEU:N	1.96	0.72
1:A:259:PRO:O	1:A:269:PHE:HE1	1.71	0.72
1:A:112:SER:O	1:A:118:TYR:HD1	1.73	0.72
1:A:214:LEU:HD22	1:A:307:ASP:HA	1.70	0.72
1:A:349:ASN:O	1:A:353:GLN:HG3	1.90	0.71
1:A:229:HIS:HA	1:A:230:PRO:C	2.10	0.71
1:A:171:LEU:CD1	1:A:352:ILE:HD12	2.18	0.70
1:A:303:ILE:HG23	1:A:303:ILE:O	1.90	0.70
1:A:103:TRP:HZ3	1:A:194:LEU:O	1.74	0.70
1:A:137:VAL:HG23	1:A:195:ARG:HB3	1.74	0.69
1:A:227:SER:CB	1:A:238:GLN:HE21	2.05	0.69
1:A:270:ASN:HA	1:A:273:GLN:CG	2.23	0.69
1:A:248:LEU:HD12	1:A:248:LEU:N	2.09	0.68
1:A:322:ILE:HG23	1:A:322:ILE:O	1.93	0.68
1:A:72:ARG:HA	1:A:75:LEU:CD1	2.24	0.68
1:A:88:ALA:O	1:A:91:HIS:N	2.27	0.68
1:A:164:PRO:O	1:A:167:MET:HG2	1.94	0.67
1:A:126:SER:HB3	1:A:196:LEU:HB2	1.76	0.67
1:A:88:ALA:O	1:A:89:ARG:C	2.33	0.67
1:A:63:ILE:HD12	1:A:346:ASP:H	1.60	0.67
1:A:167:MET:HB3	1:A:349:ASN:OD1	1.94	0.67
1:A:228:PRO:CA	1:A:237:ASN:HA	2.18	0.66
1:A:137:VAL:HG12	1:A:244:LEU:O	1.96	0.66
1:A:159:THR:O	1:A:161:SER:OG	2.10	0.66
1:A:134:ARG:CB	1:A:243:ASP:OD1	2.44	0.66
1:A:37:TRP:CG	1:A:38:THR:N	2.64	0.66
1:A:102:GLU:HB3	1:A:128:LEU:HD23	1.76	0.66
1:A:259:PRO:O	1:A:269:PHE:CE1	2.48	0.66
1:A:346:ASP:O	1:A:348:LEU:N	2.28	0.65
1:A:280:TYR:HB2	1:A:285:LEU:CD2	2.22	0.65
1:A:96:ILE:HG22	1:A:97:GLN:N	2.10	0.65
1:A:142:TYR:HE2	1:A:200:ASP:HB2	1.56	0.65
1:A:277:LYS:NZ	1:A:281:GLU:OE2	2.29	0.65
1:A:270:ASN:HA	1:A:273:GLN:HG2	1.77	0.65
1:A:53:SER:O	1:A:56:GLN:HG2	1.96	0.65
1:A:214:LEU:O	1:A:215:TYR:C	2.35	0.65
1:A:322:ILE:O	1:A:323:ALA:C	2.34	0.64
1:A:277:LYS:O	1:A:279:LEU:N	2.28	0.64
1:A:275:ILE:O	1:A:279:LEU:HB2	1.97	0.63
1:A:58:ALA:HB3	1:A:284:LEU:HD22	1.79	0.63
1:A:348:LEU:CD1	1:A:348:LEU:H	2.11	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:VAL:HA	1:A:195:ARG:O	1.99	0.62
1:A:263:PRO:HD3	1:A:300:TYR:CE2	2.35	0.62
1:A:356:VAL:O	1:A:360:LEU:HG	2.00	0.62
1:A:336:ASN:HD21	1:A:338:GLU:HB3	1.65	0.62
1:A:96:ILE:HG23	1:A:103:TRP:CD1	2.34	0.62
1:A:57:VAL:O	1:A:57:VAL:HG12	1.99	0.62
1:A:280:TYR:HB3	1:A:290:LEU:HD21	1.81	0.61
1:A:357:LEU:O	1:A:358:GLU:C	2.38	0.61
1:A:353:GLN:O	1:A:357:LEU:CD1	2.47	0.61
1:A:112:SER:O	1:A:118:TYR:CD1	2.53	0.61
1:A:342:ALA:O	1:A:343:SER:O	2.16	0.61
1:A:267:ARG:O	1:A:270:ASN:HB2	2.01	0.61
1:A:262:PHE:N	1:A:262:PHE:CD2	2.67	0.61
1:A:155:PHE:HE1	1:A:335:ASP:HB3	1.65	0.61
1:A:347:ASN:HB2	1:A:348:LEU:CD1	2.29	0.60
1:A:350:LYS:O	1:A:352:ILE:N	2.33	0.60
1:A:348:LEU:N	1:A:348:LEU:CD1	2.65	0.60
1:A:343:SER:O	1:A:346:ASP:HB3	2.02	0.59
1:A:86:TYR:CE2	1:A:90:GLN:HG3	2.37	0.59
1:A:280:TYR:CB	1:A:285:LEU:HD22	2.28	0.59
1:A:58:ALA:CB	1:A:284:LEU:HD22	2.33	0.59
1:A:337:GLU:O	1:A:340:LEU:N	2.36	0.59
1:A:267:ARG:CB	1:A:267:ARG:HH11	2.00	0.59
1:A:295:PHE:HB2	4:A:377:HOH:O	2.03	0.59
1:A:57:VAL:O	1:A:57:VAL:CG1	2.51	0.59
1:A:343:SER:O	1:A:344:THR:C	2.40	0.59
1:A:114:THR:C	1:A:116:TYR:H	2.06	0.58
1:A:336:ASN:ND2	1:A:338:GLU:HB3	2.19	0.58
1:A:86:TYR:CE1	1:A:89:ARG:NH2	2.72	0.58
1:A:279:LEU:HD12	1:A:285:LEU:HD13	1.74	0.58
1:A:354:VAL:O	1:A:355:PHE:C	2.42	0.58
1:A:102:GLU:HG2	1:A:183:LYS:HD2	1.85	0.58
1:A:84:GLY:C	1:A:86:TYR:H	2.07	0.58
1:A:102:GLU:H	1:A:128:LEU:HD21	1.68	0.58
1:A:171:LEU:HG	1:A:353:GLN:HG2	1.84	0.58
1:A:279:LEU:CD1	1:A:285:LEU:HD11	2.22	0.58
1:A:79:TYR:N	1:A:79:TYR:CD1	2.71	0.57
1:A:357:LEU:O	1:A:360:LEU:N	2.38	0.57
1:A:199:PHE:CE1	1:A:220:LEU:HD23	2.40	0.57
1:A:354:VAL:HG12	1:A:355:PHE:N	2.20	0.57
1:A:260:ASN:HB2	1:A:269:PHE:CE1	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ASP:OD1	1:A:347:ASN:N	2.38	0.57
1:A:284:LEU:O	1:A:285:LEU:HD12	2.05	0.57
1:A:163:VAL:HB	1:A:251:ILE:O	2.05	0.56
1:A:70:ASP:OD2	1:A:95:ARG:NH2	2.38	0.56
1:A:279:LEU:N	4:A:379:HOH:O	2.39	0.56
1:A:220:LEU:HB3	1:A:311:PHE:HZ	1.69	0.56
1:A:79:TYR:HD1	1:A:79:TYR:H	1.53	0.56
1:A:146:TYR:OH	1:A:148:PRO:HA	2.05	0.56
1:A:70:ASP:OD1	1:A:169:LEU:HB3	2.06	0.56
1:A:178:LYS:HB2	1:A:178:LYS:HZ3	1.70	0.56
1:A:69:ASN:N	1:A:69:ASN:HD22	2.03	0.56
1:A:92:ILE:HG22	1:A:93:MET:N	2.21	0.55
1:A:161:SER:HB3	1:A:164:PRO:HG2	1.88	0.55
1:A:351:ILE:O	1:A:354:VAL:HB	2.06	0.55
1:A:216:GLY:O	1:A:217:SER:C	2.45	0.55
1:A:84:GLY:O	1:A:86:TYR:N	2.40	0.55
1:A:214:LEU:O	1:A:216:GLY:N	2.40	0.55
1:A:258:PHE:CD2	1:A:294:TYR:HB2	2.42	0.55
1:A:109:THR:HA	1:A:121:PHE:O	2.07	0.54
1:A:57:VAL:HG22	1:A:60:GLY:HA3	1.89	0.54
1:A:287:ASP:OD1	1:A:343:SER:OG	2.24	0.54
1:A:164:PRO:O	1:A:165:CYS:C	2.45	0.54
1:A:243:ASP:HB3	1:A:359:TYR:OH	2.08	0.54
1:A:47:ALA:HB2	1:A:361:HIS:HD2	1.72	0.54
1:A:263:PRO:HB3	1:A:300:TYR:HH	1.71	0.54
1:A:278:GLU:C	4:A:379:HOH:O	2.46	0.53
1:A:279:LEU:HD11	1:A:285:LEU:CD1	2.34	0.53
1:A:348:LEU:N	1:A:348:LEU:HD12	2.23	0.53
1:A:135:HIS:HD2	1:A:194:LEU:N	2.06	0.53
1:A:234:ARG:NH2	4:A:16:HOH:O	2.40	0.53
1:A:106:GLU:HG2	1:A:125:ILE:HD13	1.89	0.53
1:A:285:LEU:HD23	1:A:288:HIS:CD2	2.31	0.53
1:A:114:THR:HG21	1:A:119:ARG:CB	2.37	0.53
1:A:273:GLN:HE22	1:A:297:ASN:HB2	1.74	0.53
1:A:102:GLU:HB3	1:A:128:LEU:HD22	1.90	0.53
1:A:183:LYS:HA	1:A:185:VAL:HG22	1.91	0.53
1:A:82:SER:O	1:A:84:GLY:N	2.42	0.53
1:A:358:GLU:O	1:A:359:TYR:C	2.47	0.53
1:A:92:ILE:O	1:A:95:ARG:HB2	2.09	0.53
1:A:345:ILE:O	1:A:349:ASN:N	2.42	0.53
1:A:158:ALA:HB1	1:A:340:LEU:HD11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:TYR:HB3	1:A:198:PHE:HB3	1.91	0.52
1:A:150:TRP:N	1:A:150:TRP:CD1	2.77	0.52
1:A:277:LYS:C	1:A:279:LEU:N	2.47	0.52
1:A:92:ILE:O	1:A:93:MET:C	2.47	0.52
1:A:173:ARG:O	1:A:174:ALA:C	2.48	0.52
1:A:110:PHE:CD1	1:A:219:HIS:CD2	2.98	0.52
1:A:57:VAL:HA	1:A:60:GLY:H	1.75	0.52
1:A:283:GLY:C	1:A:285:LEU:H	2.12	0.52
1:A:51:SER:HA	1:A:54:LEU:HB2	1.92	0.52
1:A:163:VAL:HG21	1:A:251:ILE:O	2.10	0.51
1:A:115:PRO:HD2	1:A:205:PHE:HD1	1.74	0.51
1:A:86:TYR:CD2	1:A:90:GLN:HG3	2.45	0.51
1:A:163:VAL:HB	1:A:164:PRO:HD3	1.91	0.51
1:A:44:HIS:O	1:A:267:ARG:NH2	2.43	0.51
1:A:91:HIS:C	1:A:91:HIS:CD2	2.84	0.51
1:A:167:MET:O	1:A:171:LEU:N	2.29	0.51
1:A:212:ASP:O	1:A:213:SER:HB3	2.11	0.51
1:A:248:LEU:N	1:A:248:LEU:CD1	2.73	0.51
1:A:311:PHE:C	1:A:313:ARG:N	2.63	0.51
1:A:163:VAL:CB	1:A:251:ILE:O	2.58	0.51
1:A:346:ASP:C	1:A:346:ASP:OD1	2.48	0.51
1:A:198:PHE:CD2	1:A:198:PHE:N	2.78	0.51
1:A:255:ASN:N	1:A:256:PRO:HD3	2.25	0.51
1:A:346:ASP:C	1:A:348:LEU:N	2.63	0.50
1:A:346:ASP:HA	1:A:349:ASN:HB2	1.92	0.50
1:A:63:ILE:CD1	1:A:345:ILE:HB	2.41	0.50
1:A:134:ARG:HG2	1:A:243:ASP:OD1	2.11	0.50
1:A:184:ASP:N	1:A:185:VAL:HA	2.21	0.50
1:A:134:ARG:HG3	1:A:241:GLY:HA2	1.94	0.50
1:A:258:PHE:CD2	1:A:258:PHE:N	2.80	0.50
1:A:288:HIS:CE1	1:A:289:SER:O	2.65	0.50
1:A:79:TYR:HA	1:A:143:ASP:HB2	1.93	0.50
1:A:348:LEU:HD13	1:A:348:LEU:H	1.76	0.50
1:A:362:LEU:HD23	1:A:362:LEU:N	2.27	0.50
1:A:270:ASN:HA	1:A:273:GLN:HG3	1.93	0.50
1:A:68:GLN:NE2	1:A:72:ARG:HD2	2.27	0.49
1:A:262:PHE:HZ	1:A:320:HIS:H	1.60	0.49
1:A:136:LEU:HD21	1:A:356:VAL:HG22	1.94	0.49
1:A:280:TYR:CD2	1:A:290:LEU:HG	2.47	0.49
1:A:354:VAL:HA	1:A:357:LEU:HD12	1.94	0.49
1:A:167:MET:O	1:A:170:GLU:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ASN:C	1:A:353:GLN:HE21	2.15	0.49
1:A:37:TRP:CZ2	1:A:38:THR:HG22	2.48	0.49
1:A:82:SER:O	1:A:83:PRO:C	2.50	0.49
1:A:204:ALA:CB	1:A:208:TRP:HA	2.42	0.49
1:A:112:SER:O	1:A:118:TYR:HA	2.12	0.49
1:A:105:VAL:O	1:A:105:VAL:HG23	2.12	0.49
1:A:70:ASP:O	1:A:74:LEU:HD12	2.13	0.49
1:A:114:THR:HG21	1:A:119:ARG:HB2	1.95	0.48
1:A:350:LYS:O	1:A:353:GLN:N	2.44	0.48
1:A:181:SER:HA	4:A:5:HOH:O	2.13	0.48
1:A:82:SER:O	1:A:85:SER:N	2.46	0.48
1:A:136:LEU:O	1:A:194:LEU:HA	2.14	0.48
1:A:159:THR:HA	1:A:251:ILE:O	2.14	0.48
1:A:213:SER:O	1:A:214:LEU:HB2	2.14	0.48
1:A:260:ASN:ND2	1:A:266:THR:OG1	2.46	0.48
1:A:53:SER:HA	1:A:56:GLN:NE2	2.15	0.48
1:A:191:ASP:O	1:A:192:LEU:HB2	2.14	0.48
1:A:356:VAL:O	1:A:357:LEU:O	2.32	0.48
1:A:102:GLU:HA	1:A:102:GLU:OE2	2.14	0.48
1:A:280:TYR:HD2	1:A:290:LEU:HG	1.79	0.47
1:A:265:THR:O	1:A:268:TRP:HB2	2.14	0.47
1:A:227:SER:O	1:A:237:ASN:HB2	2.15	0.47
1:A:175:LEU:O	1:A:175:LEU:HG	2.14	0.47
1:A:313:ARG:NE	4:A:29:HOH:O	2.31	0.47
1:A:137:VAL:HG23	1:A:195:ARG:O	2.14	0.47
1:A:242:MET:HB3	1:A:242:MET:HE3	1.83	0.47
1:A:337:GLU:O	1:A:338:GLU:C	2.52	0.47
1:A:96:ILE:CG2	1:A:103:TRP:CD1	2.97	0.47
1:A:311:PHE:C	1:A:313:ARG:H	2.18	0.47
1:A:77:GLU:O	1:A:84:GLY:HA3	2.15	0.47
1:A:343:SER:O	1:A:344:THR:O	2.33	0.47
1:A:247:LEU:C	1:A:248:LEU:HD12	2.35	0.47
1:A:141:HIS:CG	1:A:202:GLU:HB2	2.50	0.47
1:A:69:ASN:N	1:A:69:ASN:ND2	2.63	0.47
1:A:354:VAL:O	1:A:357:LEU:HB2	2.15	0.46
1:A:227:SER:O	1:A:238:GLN:HG3	2.15	0.46
1:A:134:ARG:CG	1:A:243:ASP:OD1	2.63	0.46
1:A:171:LEU:O	1:A:171:LEU:HD23	2.16	0.46
1:A:256:PRO:O	1:A:257:THR:HG23	2.16	0.46
1:A:51:SER:O	1:A:52:SER:C	2.53	0.46
1:A:329:VAL:O	1:A:329:VAL:HG23	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HD11	1:A:352:ILE:CD1	2.25	0.46
1:A:354:VAL:CG1	1:A:358:GLU:HG3	2.46	0.46
1:A:149:ARG:CZ	1:A:154:VAL:HG11	2.46	0.46
1:A:72:ARG:C	1:A:74:LEU:H	2.20	0.46
1:A:108:ASP:OD1	1:A:219:HIS:HE1	1.99	0.46
1:A:231:PRO:HA	1:A:232:GLY:HA2	1.71	0.46
1:A:261:PHE:CZ	1:A:304:ILE:HD12	2.51	0.46
1:A:344:THR:O	1:A:345:ILE:C	2.54	0.45
1:A:272:LEU:O	1:A:276:GLU:HB2	2.15	0.45
1:A:147:PHE:HD1	1:A:147:PHE:HA	1.67	0.45
1:A:178:LYS:HB2	1:A:178:LYS:NZ	2.31	0.45
1:A:257:THR:HG22	1:A:294:TYR:HA	1.99	0.45
1:A:37:TRP:CD2	1:A:38:THR:N	2.84	0.45
1:A:311:PHE:O	1:A:312:LEU:C	2.55	0.45
1:A:103:TRP:CZ3	1:A:194:LEU:O	2.64	0.44
1:A:112:SER:HB3	1:A:121:PHE:CZ	2.50	0.44
1:A:112:SER:CB	1:A:121:PHE:CE2	2.96	0.44
1:A:258:PHE:HD2	1:A:294:TYR:HB2	1.80	0.44
1:A:175:LEU:CD2	1:A:175:LEU:N	2.61	0.44
1:A:247:LEU:HD23	1:A:308:HIS:HB3	1.92	0.44
1:A:82:SER:HA	1:A:83:PRO:HD2	1.84	0.44
1:A:237:ASN:N	1:A:240:ASP:OD2	2.50	0.44
1:A:82:SER:C	1:A:84:GLY:N	2.70	0.44
1:A:76:ILE:CD1	1:A:87:SER:OG	2.66	0.44
1:A:178:LYS:NZ	1:A:178:LYS:H	2.10	0.44
1:A:167:MET:C	1:A:169:LEU:N	2.70	0.44
1:A:78:ARG:HG2	1:A:144:SER:HB3	1.99	0.44
1:A:308:HIS:HB2	1:A:318:VAL:HG11	1.99	0.44
1:A:262:PHE:HZ	1:A:320:HIS:N	2.15	0.44
1:A:37:TRP:CE2	1:A:38:THR:HG22	2.53	0.44
1:A:114:THR:HB	1:A:205:PHE:CE1	2.53	0.44
1:A:131:GLU:HG3	1:A:131:GLU:H	1.29	0.43
1:A:227:SER:CB	1:A:238:GLN:NE2	2.70	0.43
1:A:55:GLN:O	1:A:57:VAL:N	2.52	0.43
1:A:202:GLU:HB3	1:A:203:GLU:HG2	1.99	0.43
1:A:327:PRO:C	1:A:329:VAL:H	2.20	0.43
1:A:163:VAL:CG2	1:A:251:ILE:O	2.66	0.43
1:A:277:LYS:HG3	1:A:278:GLU:H	1.82	0.43
1:A:354:VAL:HG12	1:A:358:GLU:HG3	2.01	0.43
1:A:141:HIS:CD2	1:A:143:ASP:O	2.72	0.43
1:A:352:ILE:C	1:A:354:VAL:N	2.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PRO:HA	1:A:237:ASN:CA	2.25	0.43
1:A:218:ARG:NH1	1:A:218:ARG:HB2	2.23	0.43
1:A:110:PHE:CG	1:A:219:HIS:CD2	3.07	0.43
1:A:262:PHE:HA	1:A:263:PRO:HD2	1.69	0.43
1:A:47:ALA:HB2	1:A:361:HIS:CD2	2.53	0.43
1:A:160:ASP:HA	1:A:161:SER:OG	2.19	0.42
1:A:141:HIS:ND1	1:A:202:GLU:HG3	2.34	0.42
1:A:352:ILE:HG13	1:A:352:ILE:H	1.45	0.42
1:A:88:ALA:O	1:A:90:GLN:N	2.52	0.42
1:A:350:LYS:O	1:A:351:ILE:C	2.58	0.42
1:A:134:ARG:HA	1:A:241:GLY:O	2.19	0.42
1:A:354:VAL:HG13	1:A:358:GLU:CG	2.49	0.42
1:A:357:LEU:O	1:A:359:TYR:N	2.52	0.42
1:A:72:ARG:O	1:A:74:LEU:N	2.53	0.42
1:A:275:ILE:HG21	1:A:351:ILE:HA	2.00	0.42
1:A:344:THR:HA	1:A:348:LEU:CD1	2.50	0.42
1:A:110:PHE:CG	1:A:219:HIS:NE2	2.88	0.42
1:A:293:LYS:HG3	1:A:293:LYS:H	1.56	0.42
1:A:94:GLN:OE1	1:A:95:ARG:N	2.52	0.42
1:A:116:TYR:HB3	1:A:119:ARG:HH22	1.84	0.42
1:A:350:LYS:HB2	1:A:351:ILE:H	1.40	0.42
1:A:63:ILE:HD12	1:A:345:ILE:HB	2.01	0.41
1:A:95:ARG:HD2	1:A:95:ARG:HA	1.77	0.41
1:A:262:PHE:CE2	1:A:319:LEU:HA	2.55	0.41
1:A:71:LEU:HD13	1:A:166:ALA:HB2	2.01	0.41
1:A:46:PRO:HB2	1:A:358:GLU:HB3	2.02	0.41
1:A:263:PRO:HD3	1:A:300:TYR:CZ	2.55	0.41
1:A:209:SER:HA	1:A:210:PRO:HD2	1.87	0.41
1:A:63:ILE:HD11	1:A:345:ILE:HB	2.02	0.41
1:A:229:HIS:ND1	1:A:238:GLN:HG2	2.35	0.41
1:A:244:LEU:HD12	1:A:317:PRO:O	2.20	0.41
1:A:355:PHE:O	1:A:356:VAL:C	2.59	0.41
1:A:114:THR:C	1:A:116:TYR:N	2.72	0.41
1:A:96:ILE:CG2	1:A:97:GLN:N	2.72	0.41
1:A:213:SER:O	1:A:218:ARG:NH2	2.53	0.41
1:A:164:PRO:O	1:A:166:ALA:N	2.54	0.41
1:A:72:ARG:HH21	1:A:337:GLU:CD	2.24	0.40
1:A:114:THR:O	1:A:116:TYR:N	2.54	0.40
1:A:330:TRP:O	1:A:331:HIS:HB2	2.22	0.40
1:A:355:PHE:O	1:A:358:GLU:HB2	2.21	0.40
1:A:79:TYR:CZ	1:A:82:SER:HB2	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLY:O	1:A:174:ALA:HB1	2.21	0.40
1:A:36:ALA:N	4:A:363:HOH:O	2.53	0.40
1:A:37:TRP:HZ3	1:A:241:GLY:HA2	1.86	0.40
1:A:345:ILE:HG12	1:A:345:ILE:H	1.53	0.40
1:A:199:PHE:HE1	1:A:220:LEU:HD23	1.84	0.40
1:A:49:LEU:N	1:A:49:LEU:HD23	2.37	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	319/327 (98%)	185 (58%)	81 (25%)	53 (17%)	0 0

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	THR
1	A	85	SER
1	A	92	ILE
1	A	93	MET
1	A	96	ILE
1	A	168	MET
1	A	182	LEU
1	A	215	TYR
1	A	259	PRO
1	A	278	GLU
1	A	312	LEU
1	A	322	ILE
1	A	338	GLU
1	A	341	HIS
1	A	342	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	343	SER
1	A	344	THR
1	A	345	ILE
1	A	346	ASP
1	A	350	LYS
1	A	351	ILE
1	A	357	LEU
1	A	358	GLU
1	A	359	TYR
1	A	361	HIS
1	A	83	PRO
1	A	164	PRO
1	A	192	LEU
1	A	219	HIS
1	A	89	ARG
1	A	97	GLN
1	A	101	ALA
1	A	115	PRO
1	A	217	SER
1	A	264	LYS
1	A	356	VAL
1	A	37	TRP
1	A	88	ALA
1	A	193	SER
1	A	284	LEU
1	A	323	ALA
1	A	337	GLU
1	A	347	ASN
1	A	157	GLY
1	A	173	ARG
1	A	205	PHE
1	A	213	SER
1	A	221	ALA
1	A	210	PRO
1	A	252	GLY
1	A	328	GLU
1	A	216	GLY
1	A	156	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	288 / 291 (99%)	210 (73%)	78 (27%)	0 2

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	42	ASN
1	A	45	GLN
1	A	48	HIS
1	A	49	LEU
1	A	55	GLN
1	A	65	GLU
1	A	68	GLN
1	A	69	ASN
1	A	70	ASP
1	A	74	LEU
1	A	77	GLU
1	A	85	SER
1	A	87	SER
1	A	89	ARG
1	A	93	MET
1	A	94	GLN
1	A	97	GLN
1	A	100	GLN
1	A	106	GLU
1	A	108	ASP
1	A	111	LEU
1	A	131	GLU
1	A	147	PHE
1	A	150	TRP
1	A	153	ARG
1	A	154	VAL
1	A	155	PHE
1	A	156	VAL
1	A	161	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	167	MET
1	A	170	GLU
1	A	171	LEU
1	A	175	LEU
1	A	178	LYS
1	A	182	LEU
1	A	183	LYS
1	A	192	LEU
1	A	202	GLU
1	A	203	GLU
1	A	218	ARG
1	A	234	ARG
1	A	236	THR
1	A	239	LEU
1	A	242	MET
1	A	243	ASP
1	A	246	VAL
1	A	248	LEU
1	A	256	PRO
1	A	257	THR
1	A	260	ASN
1	A	262	PHE
1	A	267	ARG
1	A	275	ILE
1	A	276	GLU
1	A	277	LYS
1	A	287	ASP
1	A	293	LYS
1	A	294	TYR
1	A	300	TYR
1	A	304	ILE
1	A	308	HIS
1	A	309	ILE
1	A	314	LYS
1	A	321	LEU
1	A	328	GLU
1	A	329	VAL
1	A	334	ASP
1	A	336	ASN
1	A	339	ASN
1	A	344	THR
1	A	345	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	348	LEU
1	A	350	LYS
1	A	352	ILE
1	A	355	PHE
1	A	360	LEU
1	A	362	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	48	HIS
1	A	56	GLN
1	A	68	GLN
1	A	69	ASN
1	A	90	GLN
1	A	91	HIS
1	A	135	HIS
1	A	141	HIS
1	A	219	HIS
1	A	238	GLN
1	A	260	ASN
1	A	288	HIS
1	A	331	HIS
1	A	336	ASN
1	A	339	ASN
1	A	353	GLN
1	A	361	HIS

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 ⓘ

2 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$
3	NAG	A	701	1,3	14,14,15	0.70	0	15,19,21	1.53	2 (13%)
3	NAG	A	702	3	14,14,15	0.90	0	15,19,21	3.25	7 (46%)

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
3	NAG	A	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	702	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NAG	O6-C6-C5	-2.09	104.41	111.33
3	A	702	NAG	C8-C7-N2	-2.09	112.11	116.11
3	A	701	NAG	C8-C7-N2	2.08	120.10	116.11
3	A	702	NAG	C3-C4-C5	2.25	114.13	110.20
3	A	702	NAG	O7-C7-N2	2.51	126.98	121.86
3	A	702	NAG	O5-C5-C6	3.19	114.26	107.35
3	A	701	NAG	C1-O5-C5	3.89	117.19	112.25
3	A	702	NAG	C1-O5-C5	4.47	117.92	112.25
3	A	702	NAG	C2-N2-C7	10.03	135.93	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	323/327 (98%)	-0.16	8 (2%) 61 55	21, 47, 69, 84	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	SER	3.7
1	A	36	ALA	2.9
1	A	150	TRP	2.8
1	A	42	ASN	2.3
1	A	301	GLY	2.2
1	A	185	VAL	2.2
1	A	190	PRO	2.2
1	A	231	PRO	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(Å ²)	Q<0.9
3	NAG	A	702	14/15	0.86	0.33	-	57,62,64,67	0
3	NAG	A	701	14/15	0.89	0.23	-	61,62,64,65	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	A	601	1/1	1.00	0.02	-2.61	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.