Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 03:37 AM EDT

PDB ID	:	1YK1
Title	:	structure of natriuretic peptide receptor-C complexed with brain natriuretic peptide
Authors	:	He, X.; Garcia, K.C.
Deposited on	:	2005-01-16
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

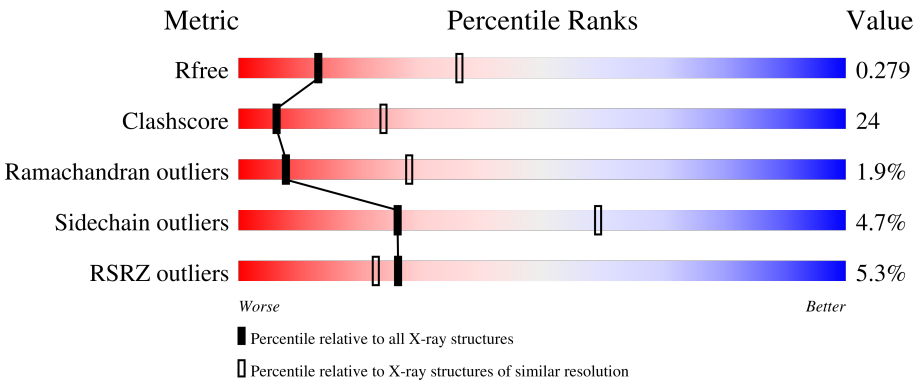
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 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 <=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	479	3%; 47%; 34%; •; 18%
1	B	479	2%; 50%; 30%; •; 18%
2	E	21	95%; 29%; 48%; 19%; 5%
3	C	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	511	X	-	-	-
4	NAG	A	512	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6766 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 Atrial natriuretic peptide clearance receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	394	3111	1972	532	591	16	0	0	0
1	B	394	3111	1972	532	591	16	0	0	0

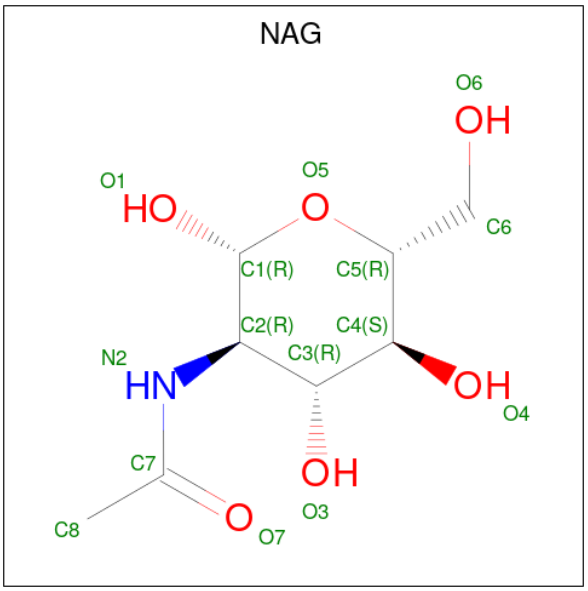
- Molecule 2 is a protein called Natriuretic peptides B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	21	151	91	29	28	3	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
			Total	C	N	O		
4	B	1	14	8	1	5	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	1	1	1	0	0
			Total	Cl		
5	B	1	1	1	0	0

- Molecule 6 is water.

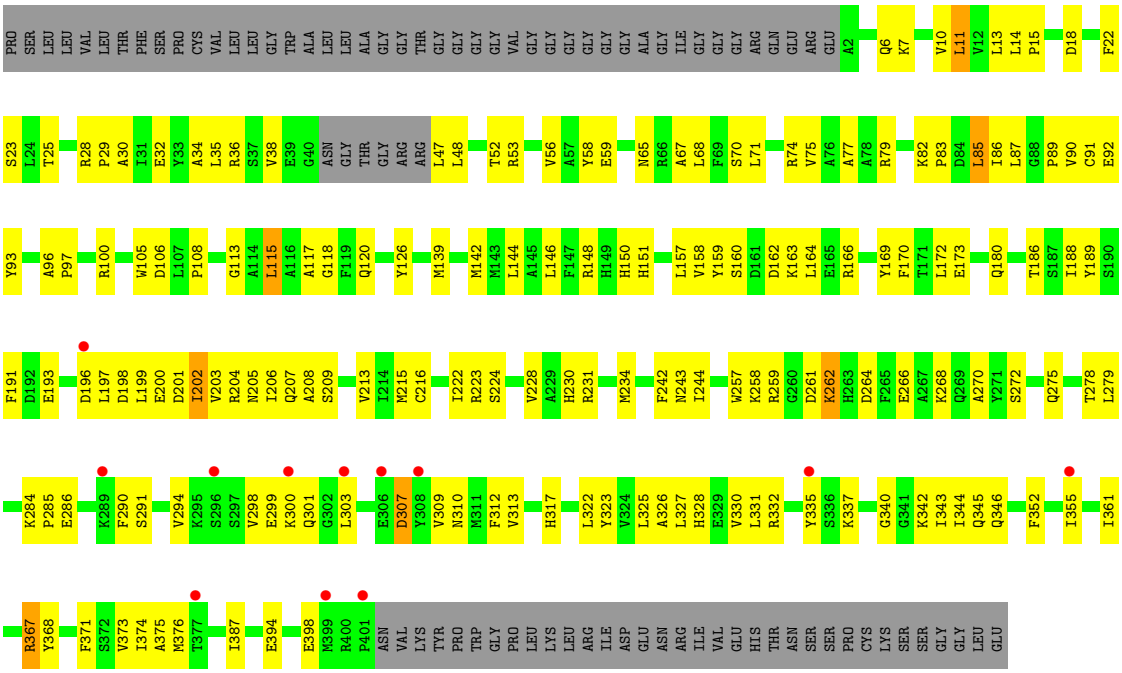
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	167	167	167	0	0
			Total	O		
6	B	151	151	151	0	0
			Total	O		
6	E	3	3	3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

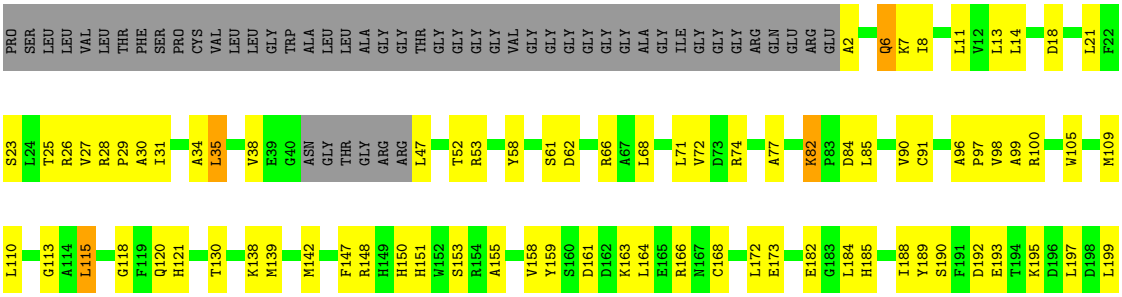
• Molecule 1: Atrial natriuretic peptide clearance receptor

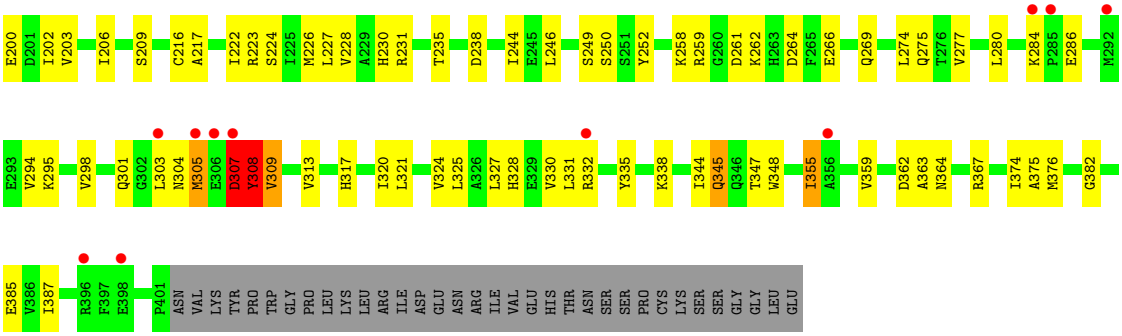
Chain A:



• Molecule 1: Atrial natriuretic peptide clearance receptor

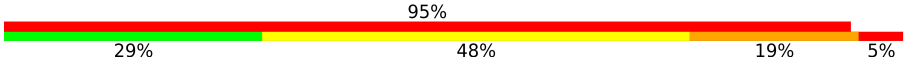
Chain B:

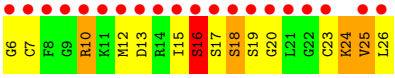




• Molecule 2: Natriuretic peptides B

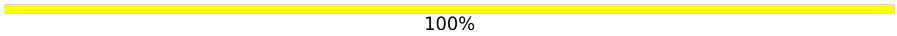
Chain E:





• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.17Å 136.38Å 138.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 48.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.90) 97.3 (48.64-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.54 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.253 , 0.289 0.239 , 0.279	Depositor DCC
R_{free} test set	1153 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	67.3	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 83.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6766	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	0.36	0/3180	0.59	0/4297
1	B	0.34	0/3180	0.60	0/4297
2	E	0.54	0/151	0.68	0/195
All	All	0.35	0/6511	0.59	0/8789

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 (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	3111	0	3013	158	0
1	B	3111	0	3014	143	0
2	E	151	0	155	16	0
3	C	28	0	25	2	0
4	A	28	0	26	0	0
4	B	14	0	13	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	167	0	0	21	0
6	B	151	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	3	0	0	0	0
All	All	6766	0	6246	308	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 24.

All (308) 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:130:THR:HG22	1:B:348:TRP:HE1	1.14	1.09
1:B:38:VAL:HG21	1:B:324:VAL:HG21	1.43	1.00
1:B:189:TYR:HB2	6:B:548:HOH:O	1.66	0.94
1:A:159:TYR:HB3	1:A:172:LEU:HD22	1.49	0.94
1:A:6:GLN:HB2	1:A:52:THR:HG23	1.52	0.89
1:A:10:VAL:HG12	1:A:85:LEU:HB3	1.57	0.86
1:A:146:LEU:HG	6:A:665:HOH:O	1.73	0.86
1:B:90:VAL:HG13	1:B:113:GLY:HA3	1.57	0.86
1:B:130:THR:HG22	1:B:348:TRP:NE1	1.89	0.85
1:A:158:VAL:HG21	1:A:206:ILE:HD11	1.57	0.85
1:B:139:MET:HE1	1:B:244:ILE:HG12	1.59	0.85
1:A:266:GLU:HG3	6:A:548:HOH:O	1.77	0.84
1:B:2:ALA:HB2	6:B:641:HOH:O	1.78	0.82
1:A:53:ARG:HB3	1:A:53:ARG:NH1	1.94	0.82
2:E:15:ILE:HG22	2:E:16:SER:OG	1.81	0.80
1:B:74:ARG:HD3	6:B:606:HOH:O	1.83	0.78
1:A:262:LYS:HB2	1:A:262:LYS:NZ	1.97	0.78
1:A:180:GLN:HB3	6:A:664:HOH:O	1.83	0.77
1:B:148:ARG:HH11	1:B:182:GLU:HG2	1.49	0.77
1:B:375:ALA:HB3	1:B:387:ILE:HD11	1.69	0.73
1:B:91:CYS:HB3	6:B:630:HOH:O	1.86	0.73
1:B:158:VAL:HG21	1:B:206:ILE:HD11	1.73	0.71
1:B:295:LYS:HG3	1:B:305:MET:HG3	1.72	0.71
1:B:199:LEU:HD13	1:B:224:SER:HB3	1.72	0.70
1:A:96:ALA:HB2	2:E:16:SER:HB2	1.73	0.70
1:B:35:LEU:O	1:B:38:VAL:HG12	1.92	0.69
1:A:106:ASP:O	1:A:340:GLY:HA3	1.93	0.69
1:A:298:VAL:HG12	1:A:303:LEU:HB2	1.75	0.68
1:B:110:LEU:HG	1:B:130:THR:OG1	1.92	0.68
1:A:398:GLU:HG3	6:A:575:HOH:O	1.92	0.68
1:A:193:GLU:HA	1:A:197:LEU:HD21	1.76	0.68
1:B:96:ALA:O	1:B:100:ARG:HG3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:TYR:CD1	2:E:16:SER:HA	2.29	0.68
1:B:164:LEU:HB2	6:B:576:HOH:O	1.92	0.68
1:B:192:ASP:HB3	1:B:195:LYS:HG2	1.75	0.67
1:B:193:GLU:HA	1:B:197:LEU:HD21	1.75	0.67
1:B:96:ALA:HB3	1:B:97:PRO:HD3	1.75	0.67
1:A:91:CYS:HB3	6:A:565:HOH:O	1.92	0.67
1:B:148:ARG:HH11	1:B:182:GLU:CG	2.08	0.67
1:A:189:TYR:HE2	1:A:202:ILE:HD13	1.57	0.67
2:E:24:LYS:O	2:E:25:VAL:HB	1.96	0.66
1:B:18:ASP:O	1:B:26:ARG:NH2	2.28	0.65
1:A:223:ARG:HH12	1:A:261:ASP:HB3	1.61	0.65
1:A:322:LEU:HD13	1:A:352:PHE:CE1	2.32	0.65
1:A:70:SER:O	1:A:74:ARG:HG3	1.97	0.64
1:A:323:TYR:HE1	1:A:343:ILE:HD13	1.62	0.64
1:A:162:ASP:O	1:A:164:LEU:HD13	1.96	0.64
1:A:299:GLU:C	1:A:301:GLN:H	1.99	0.64
1:A:28:ARG:HB3	1:A:29:PRO:HD3	1.79	0.64
1:A:326:ALA:O	1:A:330:VAL:HG23	1.98	0.64
1:A:90:VAL:HG13	1:A:113:GLY:HA3	1.78	0.63
1:A:203:VAL:HG21	1:A:228:VAL:HG12	1.80	0.63
1:B:159:TYR:HB3	1:B:172:LEU:HD12	1.81	0.63
1:B:217:ALA:HB3	1:B:222:ILE:CD1	2.29	0.63
1:B:202:ILE:O	1:B:206:ILE:HG12	1.98	0.63
1:A:106:ASP:HB3	6:A:549:HOH:O	1.98	0.62
1:A:199:LEU:HD13	1:A:224:SER:HB3	1.80	0.62
1:B:230:HIS:HA	1:B:235:THR:HG23	1.81	0.61
1:A:242:PHE:HE2	1:A:275:GLN:HE21	1.49	0.61
1:A:290:PHE:O	1:A:294:VAL:HG23	2.00	0.61
1:B:330:VAL:HG22	1:B:335:TYR:HB2	1.82	0.61
1:B:30:ALA:HB2	1:B:313:VAL:HG13	1.82	0.61
1:B:294:VAL:O	1:B:298:VAL:HG23	2.01	0.61
1:A:53:ARG:HB3	1:A:53:ARG:HH11	1.64	0.61
1:A:48:LEU:HD23	1:A:52:THR:HG21	1.84	0.60
1:B:158:VAL:HG21	1:B:206:ILE:CD1	2.31	0.60
1:B:199:LEU:O	1:B:203:VAL:HG23	2.02	0.60
1:B:139:MET:CE	1:B:244:ILE:HG12	2.31	0.59
1:A:30:ALA:HB2	1:A:313:VAL:HG13	1.82	0.59
1:A:6:GLN:HB2	1:A:52:THR:CG2	2.31	0.59
1:B:161:ASP:OD2	1:B:166:ARG:HD2	2.02	0.59
1:B:38:VAL:CG2	1:B:324:VAL:HG11	2.33	0.58
1:A:75:VAL:HG21	1:A:105:TRP:CZ3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ALA:HB2	2:E:16:SER:CB	2.33	0.58
1:A:93:TYR:HD1	2:E:16:SER:HA	1.67	0.58
1:B:321:LEU:O	1:B:325:LEU:HD13	2.03	0.58
1:A:207:GLN:HB3	1:A:234:MET:HE3	1.86	0.58
1:A:262:LYS:HB2	1:A:262:LYS:HZ2	1.69	0.58
1:B:203:VAL:HG21	1:B:228:VAL:CG1	2.34	0.58
1:A:262:LYS:HB2	1:A:262:LYS:HZ3	1.68	0.58
1:B:35:LEU:HA	1:B:38:VAL:HG12	1.86	0.58
1:B:226:MET:HG3	1:B:274:LEU:HD12	1.86	0.58
1:A:85:LEU:HD22	1:A:86:ILE:N	2.19	0.57
2:E:7:CYS:HA	2:E:24:LYS:O	2.04	0.57
1:A:34:ALA:O	1:A:38:VAL:HG13	2.04	0.57
1:A:34:ALA:HB2	1:A:317:HIS:CD2	2.39	0.57
1:A:160:SER:OG	1:A:193:GLU:HG2	2.04	0.57
1:A:224:SER:O	1:A:228:VAL:HG23	2.06	0.56
1:A:118:GLY:N	2:E:15:ILE:HD12	2.20	0.56
1:A:203:VAL:HG21	1:A:228:VAL:CG1	2.36	0.56
1:B:31:ILE:HG23	1:B:320:ILE:HD11	1.86	0.56
1:B:227:LEU:O	1:B:230:HIS:HB3	2.05	0.56
1:A:71:LEU:O	1:A:75:VAL:HG23	2.06	0.56
1:A:242:PHE:CE2	1:A:275:GLN:NE2	2.74	0.56
1:A:47:LEU:N	6:A:630:HOH:O	2.38	0.56
1:B:258:LYS:O	1:B:259:ARG:HG2	2.06	0.56
1:A:343:ILE:HD12	6:A:570:HOH:O	2.06	0.55
1:B:309:VAL:HG12	1:B:313:VAL:HG11	1.87	0.55
1:A:294:VAL:O	1:A:298:VAL:HG23	2.05	0.55
1:A:327:LEU:O	1:A:331:LEU:HD13	2.06	0.55
1:A:309:VAL:HG22	6:A:647:HOH:O	2.05	0.55
1:B:249:SER:HA	1:B:252:TYR:CE2	2.42	0.55
2:E:10:ARG:HH11	2:E:10:ARG:HB2	1.71	0.55
1:A:291:SER:HB2	6:A:647:HOH:O	2.06	0.55
1:B:28:ARG:HB3	1:B:29:PRO:HD3	1.89	0.55
1:B:34:ALA:HB2	1:B:317:HIS:CD2	2.42	0.55
1:A:325:LEU:HB2	6:A:620:HOH:O	2.06	0.55
1:A:345:GLN:NE2	6:A:599:HOH:O	2.34	0.55
1:B:375:ALA:HB3	1:B:387:ILE:CD1	2.37	0.55
1:B:31:ILE:HG23	1:B:320:ILE:CD1	2.37	0.54
1:B:359:VAL:HG13	1:B:367:ARG:CZ	2.37	0.54
1:B:376:MET:HB2	6:B:635:HOH:O	2.08	0.54
1:B:222:ILE:O	1:B:226:MET:HG2	2.08	0.53
1:A:65:ASN:ND2	1:B:100:ARG:HD3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:ILE:HG23	6:B:652:HOH:O	2.07	0.53
1:A:199:LEU:CD1	1:A:224:SER:HB3	2.38	0.53
1:B:7:LYS:HD3	1:B:53:ARG:HB2	1.89	0.53
1:A:367:ARG:HD3	1:A:368:TYR:O	2.09	0.53
1:A:373:VAL:C	1:A:374:ILE:HD12	2.29	0.53
1:B:374:ILE:HG12	6:B:652:HOH:O	2.08	0.53
1:B:266:GLU:O	1:B:269:GLN:HB2	2.09	0.53
1:B:25:THR:HG23	1:B:301:GLN:HG2	1.90	0.53
1:A:15:PRO:HD2	1:A:23:SER:HA	1.92	0.52
1:B:18:ASP:OD2	1:B:25:THR:HB	2.10	0.52
1:B:18:ASP:HA	1:B:23:SER:HB2	1.90	0.52
1:B:327:LEU:O	1:B:330:VAL:HG12	2.09	0.52
1:A:32:GLU:HG2	6:A:648:HOH:O	2.09	0.51
1:B:148:ARG:NH1	1:B:182:GLU:HG2	2.23	0.51
1:A:189:TYR:CE2	1:A:202:ILE:HD13	2.42	0.51
1:A:193:GLU:HA	1:A:197:LEU:CD2	2.40	0.51
1:A:374:ILE:HB	6:A:659:HOH:O	2.11	0.51
1:B:61:SER:O	1:B:66:ARG:HB3	2.11	0.51
1:B:173:GLU:HB3	6:B:618:HOH:O	2.09	0.51
1:A:59:GLU:HG2	1:A:70:SER:HB2	1.93	0.51
1:B:327:LEU:HA	1:B:330:VAL:HG12	1.93	0.51
1:B:13:LEU:O	1:B:14:LEU:HD23	2.11	0.50
2:E:7:CYS:O	2:E:7:CYS:SG	2.69	0.50
1:A:96:ALA:HB3	1:A:97:PRO:CD	2.41	0.50
1:A:213:VAL:HG12	1:A:215:MET:HG3	1.93	0.50
1:A:332:ARG:NH1	6:A:649:HOH:O	2.44	0.50
1:B:244:ILE:N	1:B:244:ILE:HD12	2.26	0.50
1:B:335:TYR:N	6:B:572:HOH:O	2.44	0.50
1:A:205:ASN:O	1:A:208:ALA:HB3	2.12	0.50
1:A:374:ILE:HD12	1:A:374:ILE:N	2.27	0.50
1:B:23:SER:O	1:B:27:VAL:HG23	2.11	0.50
1:B:147:PHE:CE2	1:B:155:ALA:HB2	2.46	0.50
1:A:223:ARG:NH1	1:A:259:ARG:HB2	2.27	0.50
1:B:7:LYS:HA	1:B:53:ARG:O	2.11	0.50
1:A:299:GLU:HA	1:A:303:LEU:O	2.12	0.50
1:B:188:ILE:HG22	1:B:189:TYR:N	2.27	0.50
1:A:198:ASP:OD2	1:A:201:ASP:HB2	2.12	0.49
1:A:166:ARG:HB3	1:A:169:TYR:HB3	1.92	0.49
1:A:74:ARG:HH11	1:A:74:ARG:HB3	1.77	0.49
1:A:310:ASN:OD1	1:A:312:PHE:HB2	2.12	0.49
1:B:190:SER:O	2:E:26:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:ILE:HA	6:B:652:HOH:O	2.12	0.49
1:B:25:THR:CG2	1:B:301:GLN:HG2	2.43	0.49
1:A:53:ARG:HB3	1:A:53:ARG:CZ	2.42	0.49
1:B:71:LEU:HD12	1:B:98:VAL:HG13	1.93	0.49
1:A:284:LYS:HD2	1:A:286:GLU:HB2	1.95	0.49
1:B:6:GLN:NE2	1:B:331:LEU:HD21	2.26	0.49
1:A:77:ALA:C	1:A:79:ARG:H	2.15	0.49
1:A:188:ILE:HD12	1:A:188:ILE:N	2.28	0.48
1:A:215:MET:O	1:A:243:ASN:HA	2.14	0.48
1:A:361:ILE:HD12	1:A:361:ILE:N	2.28	0.48
1:A:47:LEU:O	1:A:328:HIS:ND1	2.47	0.48
1:A:242:PHE:HE2	1:A:275:GLN:NE2	2.12	0.48
1:B:199:LEU:CD1	1:B:224:SER:HB3	2.40	0.48
2:E:17:SER:O	2:E:18:SER:HB3	2.14	0.48
1:A:230:HIS:HB2	1:A:270:ALA:HB2	1.96	0.48
1:B:21:LEU:HG	3:C:1:NAG:H82	1.96	0.48
1:B:138:LYS:HD2	6:B:634:HOH:O	2.14	0.47
1:B:6:GLN:O	1:B:52:THR:HA	2.14	0.47
1:B:8:ILE:HD12	1:B:8:ILE:N	2.29	0.47
1:A:163:LYS:O	1:A:164:LEU:HD12	2.14	0.47
1:A:204:ARG:HG3	1:A:204:ARG:HH11	1.79	0.47
1:B:147:PHE:CZ	1:B:155:ALA:HB2	2.48	0.47
1:A:32:GLU:O	1:A:36:ARG:HG3	2.15	0.47
1:A:189:TYR:CE2	1:A:202:ILE:HA	2.50	0.47
1:A:82:LYS:HB3	1:A:83:PRO:HD2	1.96	0.47
1:A:207:GLN:HB3	1:A:234:MET:CE	2.44	0.47
1:B:280:LEU:O	1:B:280:LEU:HG	2.14	0.47
1:B:130:THR:HG23	1:B:344:ILE:HD12	1.97	0.47
1:A:200:GLU:O	1:A:204:ARG:HD2	2.14	0.47
1:A:299:GLU:C	1:A:301:GLN:N	2.66	0.47
1:A:257:TRP:CE3	1:A:258:LYS:N	2.83	0.46
1:B:163:LYS:HA	1:B:166:ARG:HD3	1.97	0.46
1:B:295:LYS:HG3	1:B:305:MET:CG	2.43	0.46
1:A:163:LYS:HD2	2:E:20:GLY:O	2.16	0.46
1:B:138:LYS:HB3	6:B:619:HOH:O	2.14	0.46
1:B:199:LEU:HA	1:B:202:ILE:HD12	1.97	0.46
1:A:278:THR:OG1	1:A:279:LEU:N	2.47	0.46
1:A:298:VAL:O	1:A:301:GLN:HB3	2.15	0.46
1:B:18:ASP:HA	1:B:23:SER:CB	2.45	0.46
1:B:84:ASP:OD1	1:B:338:LYS:HE2	2.16	0.46
1:B:35:LEU:HD13	1:B:320:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD22	1:B:115:LEU:H	1.81	0.46
1:A:13:LEU:HD23	1:A:59:GLU:HB3	1.98	0.46
1:A:199:LEU:HA	1:A:202:ILE:HG13	1.96	0.46
1:A:216:CYS:HA	6:A:516:HOH:O	2.15	0.46
1:B:99:ALA:HA	1:B:109:MET:SD	2.57	0.46
1:A:18:ASP:OD2	1:A:25:THR:HB	2.16	0.45
1:A:7:LYS:O	1:A:337:LYS:NZ	2.49	0.45
1:A:150:HIS:O	1:A:151:HIS:HB2	2.16	0.45
1:B:284:LYS:HE2	1:B:355:ILE:O	2.16	0.45
1:B:332:ARG:HB2	6:B:562:HOH:O	2.15	0.45
1:A:160:SER:HA	1:A:191:PHE:O	2.17	0.45
1:A:374:ILE:CG1	6:A:659:HOH:O	2.64	0.45
1:A:242:PHE:HA	1:A:275:GLN:O	2.17	0.45
1:A:299:GLU:O	1:A:301:GLN:N	2.50	0.45
1:A:157:LEU:HB3	1:A:172:LEU:HD23	1.99	0.45
1:B:28:ARG:HG3	1:B:58:TYR:CZ	2.51	0.45
1:B:139:MET:HE2	1:B:244:ILE:HG21	1.98	0.45
1:B:90:VAL:HG13	1:B:113:GLY:CA	2.37	0.44
1:A:56:VAL:HG11	1:A:58:TYR:CZ	2.53	0.44
1:B:303:LEU:HD23	1:B:304:ASN:O	2.17	0.44
1:A:47:LEU:O	1:A:48:LEU:HD12	2.18	0.44
1:B:148:ARG:HH21	1:B:148:ARG:HG3	1.83	0.44
1:A:10:VAL:HA	1:A:85:LEU:O	2.17	0.44
1:A:14:LEU:HB3	1:A:15:PRO:CD	2.47	0.44
1:A:70:SER:HB3	6:A:654:HOH:O	2.17	0.44
1:B:130:THR:HG21	1:B:347:THR:OG1	2.18	0.44
1:B:148:ARG:HG3	1:B:148:ARG:NH2	2.33	0.44
1:A:117:ALA:O	1:A:120:GLN:HB2	2.18	0.44
1:A:215:MET:HE2	1:A:222:ILE:HG13	1.99	0.44
1:B:21:LEU:HG	3:C:1:NAG:C8	2.48	0.44
1:B:307:ASP:O	1:B:308:TYR:HB3	2.18	0.44
1:A:272:SER:HA	1:A:376:MET:SD	2.58	0.43
1:B:118:GLY:C	1:B:120:GLN:H	2.21	0.43
2:E:15:ILE:O	2:E:16:SER:CB	2.66	0.43
1:A:59:GLU:HG2	1:A:70:SER:CB	2.47	0.43
1:A:335:TYR:N	1:A:335:TYR:CD1	2.86	0.43
1:B:35:LEU:HA	1:B:35:LEU:HD12	1.87	0.43
1:B:142:MET:CE	1:B:277:VAL:HG11	2.48	0.43
1:A:7:LYS:HB2	1:A:7:LYS:HE3	1.82	0.43
1:B:47:LEU:O	1:B:328:HIS:ND1	2.46	0.43
1:A:13:LEU:O	1:A:89:PRO:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:SER:HA	1:B:184:LEU:HD22	2.01	0.43
1:B:168:CYS:SG	1:B:216:CYS:C	2.97	0.43
1:A:11:LEU:HD12	1:A:71:LEU:HD23	2.00	0.43
1:B:62:ASP:HB3	1:B:66:ARG:HB3	2.01	0.43
1:B:362:ASP:C	1:B:364:ASN:H	2.22	0.43
1:A:113:GLY:C	1:A:115:LEU:HD13	2.39	0.42
1:A:261:ASP:OD1	1:A:262:LYS:N	2.52	0.42
1:A:335:TYR:HD1	1:A:335:TYR:H	1.66	0.42
1:A:22:PHE:CE1	1:A:90:VAL:HB	2.55	0.42
1:A:344:ILE:HD13	1:A:344:ILE:HA	1.89	0.42
1:B:317:HIS:ND1	1:B:317:HIS:C	2.72	0.42
1:A:202:ILE:H	1:A:202:ILE:HG12	1.59	0.42
1:A:139:MET:HA	1:A:371:PHE:CE2	2.54	0.42
1:A:144:LEU:HD11	1:A:148:ARG:CZ	2.50	0.42
1:A:375:ALA:HB3	1:A:387:ILE:HG21	2.02	0.42
1:A:118:GLY:CA	2:E:15:ILE:HD12	2.49	0.42
1:B:375:ALA:HB3	1:B:387:ILE:CG1	2.49	0.42
1:B:274:LEU:HD23	1:B:275:GLN:N	2.35	0.42
1:A:92:GLU:HG3	1:A:170:PHE:CD2	2.55	0.42
1:B:91:CYS:HA	6:B:602:HOH:O	2.20	0.42
1:A:374:ILE:CB	6:A:659:HOH:O	2.65	0.42
1:B:258:LYS:HB2	1:B:258:LYS:HE3	1.88	0.42
1:A:25:THR:HG23	1:A:301:GLN:HG2	2.02	0.42
1:B:139:MET:O	1:B:142:MET:HB3	2.19	0.41
1:B:150:HIS:O	1:B:151:HIS:HB2	2.20	0.41
1:B:230:HIS:HA	1:B:235:THR:CG2	2.48	0.41
1:B:139:MET:CE	1:B:244:ILE:HG21	2.51	0.41
1:B:226:MET:CE	1:B:274:LEU:HB2	2.50	0.41
1:B:244:ILE:CG2	1:B:246:LEU:HG	2.50	0.41
1:B:284:LYS:HE3	1:B:286:GLU:HB3	2.02	0.41
1:A:74:ARG:HB3	1:A:74:ARG:NH1	2.35	0.41
1:A:90:VAL:HG13	1:A:113:GLY:CA	2.47	0.41
2:E:6:GLY:HA2	2:E:25:VAL:HG23	2.02	0.41
1:B:148:ARG:HH11	1:B:182:GLU:CD	2.24	0.41
1:B:376:MET:HE1	1:B:382:GLY:HA2	2.02	0.41
1:A:29:PRO:HB2	1:A:294:VAL:HG13	2.02	0.41
1:B:68:LEU:O	1:B:72:VAL:HG23	2.21	0.41
1:A:35:LEU:O	1:A:38:VAL:HG22	2.20	0.41
1:A:68:LEU:HD13	1:A:97:PRO:HB2	2.01	0.41
1:A:244:ILE:N	1:A:244:ILE:HD12	2.36	0.41
1:A:346:GLN:OE1	1:A:346:GLN:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LYS:HG2	6:B:598:HOH:O	2.20	0.41
1:B:185:HIS:CE1	6:B:623:HOH:O	2.74	0.41
1:A:204:ARG:O	1:A:207:GLN:HG3	2.21	0.41
1:A:394:GLU:H	1:A:394:GLU:HG2	1.66	0.41
1:B:200:GLU:OE2	1:B:231:ARG:NH2	2.53	0.41
1:A:13:LEU:HD13	1:A:67:ALA:HB1	2.02	0.41
1:A:203:VAL:O	1:A:207:GLN:HG2	2.20	0.41
1:B:188:ILE:HG22	1:B:189:TYR:H	1.85	0.41
1:B:261:ASP:OD2	1:B:262:LYS:HG2	2.20	0.41
1:B:308:TYR:N	1:B:308:TYR:CD2	2.89	0.41
1:B:344:ILE:HD13	1:B:344:ILE:HA	1.95	0.41
1:B:345:GLN:NE2	1:B:345:GLN:HA	2.36	0.41
1:B:166:ARG:HA	6:B:647:HOH:O	2.21	0.41
1:B:203:VAL:HG21	1:B:228:VAL:HG12	2.02	0.41
1:A:108:PRO:HB3	1:A:344:ILE:HG12	2.02	0.40
1:A:108:PRO:HD3	1:A:340:GLY:HA2	2.03	0.40
1:B:223:ARG:NH2	1:B:259:ARG:HG3	2.36	0.40
1:A:173:GLU:HB3	6:A:638:HOH:O	2.20	0.40
1:B:121:HIS:ND1	1:B:121:HIS:N	2.69	0.40
1:A:100:ARG:NE	6:A:637:HOH:O	2.54	0.40
1:A:290:PHE:HB2	1:A:355:ILE:HD11	2.03	0.40
1:B:274:LEU:HD23	1:B:274:LEU:C	2.41	0.40
1:A:206:ILE:C	1:A:208:ALA:H	2.23	0.40
1:A:257:TRP:CH2	1:A:268:LYS:HD3	2.56	0.40
1:A:100:ARG:NH2	1:A:126:TYR:OH	2.54	0.40
1:A:223:ARG:CZ	1:A:259:ARG:HG3	2.52	0.40
1:A:284:LYS:O	1:A:285:PRO:C	2.59	0.40
1:B:18:ASP:OD2	1:B:303:LEU:HD12	2.22	0.40
1:B:71:LEU:HD21	1:B:105:TRP:HZ3	1.86	0.40
1:B:385:GLU:C	6:B:652:HOH:O	2.60	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	390/479 (81%)	343 (88%)	43 (11%)	4 (1%)	15	45
1	B	390/479 (81%)	350 (90%)	34 (9%)	6 (2%)	10	34
2	E	19/21 (90%)	7 (37%)	7 (37%)	5 (26%)	0	0
All	All	799/979 (82%)	700 (88%)	84 (10%)	15 (2%)	8	28

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	209	SER
1	B	308	TYR
2	E	13	ASP
2	E	19	SER
1	A	209	SER
1	B	363	ALA
2	E	18	SER
2	E	25	VAL
1	B	264	ASP
1	B	307	ASP
1	A	300	LYS
1	A	307	ASP
1	B	77	ALA
2	E	16	SER
1	A	202	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	329/389 (85%)	316 (96%)	13 (4%)	31	65
1	B	329/389 (85%)	315 (96%)	14 (4%)	29	62
2	E	17/17 (100%)	12 (71%)	5 (29%)	0	1
All	All	675/795 (85%)	643 (95%)	32 (5%)	26	59

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	85	LEU
1	A	87	LEU
1	A	115	LEU
1	A	142	MET
1	A	186	THR
1	A	196	ASP
1	A	231	ARG
1	A	262	LYS
1	A	264	ASP
1	A	307	ASP
1	A	342	LYS
1	A	367	ARG
1	B	6	GLN
1	B	11	LEU
1	B	35	LEU
1	B	82	LYS
1	B	85	LEU
1	B	115	LEU
1	B	238	ASP
1	B	250	SER
1	B	305	MET
1	B	307	ASP
1	B	308	TYR
1	B	309	VAL
1	B	345	GLN
1	B	355	ILE
2	E	10	ARG
2	E	12	MET
2	E	16	SER
2	E	23	CYS
2	E	24	LYS

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

Mol	Chain	Res	Type
1	A	55	GLN
1	A	275	GLN
1	B	205	ASN
1	B	345	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

2 monosaccharides 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	C	1	3,1	14,14,15	0.63	0	17,19,21	0.69	0
3	NAG	C	2	3	14,14,15	0.55	0	17,19,21	0.69	1 (5%)

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	C	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2	NAG	C2-N2-C7	-2.15	119.84	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C8-C7-N2-C2
3	C	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6

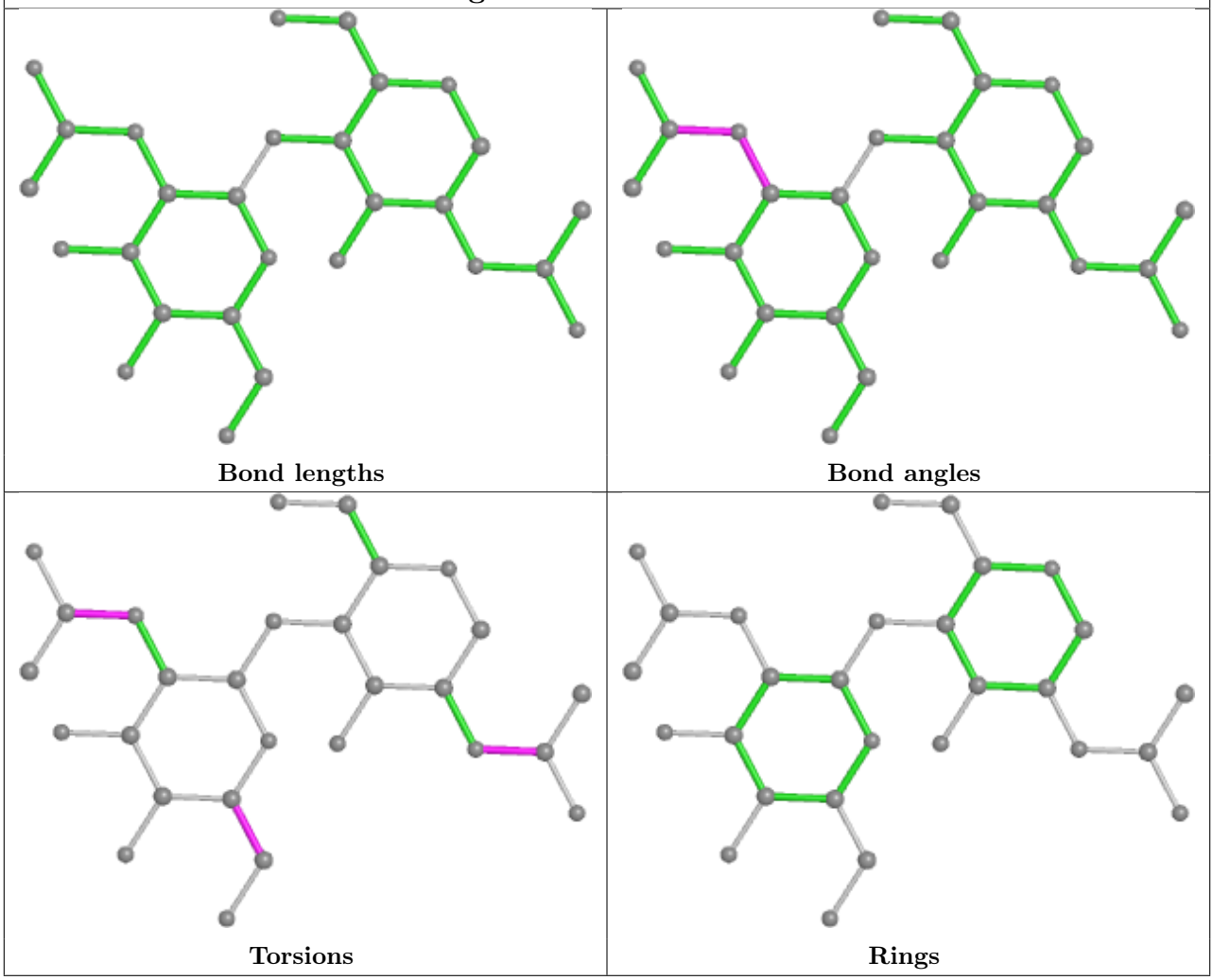
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C



5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	$\#\|Z\| > 2$
4	NAG	B	512	1	14,14,15	0.68	0	17,19,21	0.75	1 (5%)
4	NAG	A	512	1	14,14,15	0.62	0	17,19,21	0.71	0
4	NAG	A	511	1	14,14,15	0.77	0	17,19,21	0.57	0

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
4	NAG	B	512	1	-	2/6/23/26	0/1/1/1
4	NAG	A	512	1	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	A	511	1	1/1/5/7	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	512	NAG	C2-N2-C7	-2.17	119.81	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	511	NAG	C1
4	A	512	NAG	C1

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	511	NAG	C8-C7-N2-C2
4	A	511	NAG	O7-C7-N2-C2
4	A	512	NAG	C8-C7-N2-C2
4	A	512	NAG	O7-C7-N2-C2
4	B	512	NAG	C8-C7-N2-C2
4	B	512	NAG	O7-C7-N2-C2
4	A	511	NAG	O5-C5-C6-O6
4	A	511	NAG	C4-C5-C6-O6
4	A	512	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	394/479 (82%)	0.22	12 (3%)	50	45	40, 65, 109, 124	0
1	B	394/479 (82%)	0.28	11 (2%)	53	49	40, 66, 110, 124	0
2	E	21/21 (100%)	4.22	20 (95%)	0	0	83, 139, 148, 148	0
All	All	809/979 (82%)	0.35	43 (5%)	26	22	40, 67, 116, 148	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	6	GLY	7.4
2	E	26	LEU	6.9
2	E	16	SER	6.3
2	E	13	ASP	5.6
2	E	7	CYS	5.5
2	E	9	GLY	5.3
2	E	25	VAL	5.2
2	E	17	SER	4.9
1	B	303	LEU	4.8
2	E	23	CYS	4.7
1	A	306	GLU	4.2
2	E	11	LYS	4.1
2	E	10	ARG	4.0
2	E	20	GLY	3.9
1	A	303	LEU	3.6
1	A	399	MET	3.5
2	E	18	SER	3.5
1	A	196	ASP	3.5
2	E	12	MET	3.5
1	B	306	GLU	3.4
2	E	15	ILE	3.4
1	B	305	MET	3.3
1	A	300	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	14	ARG	3.2
1	B	396	ARG	3.1
1	B	332	ARG	2.9
1	B	398	GLU	2.9
2	E	22	GLY	2.9
1	B	284	LYS	2.8
1	A	401	PRO	2.8
1	B	307	ASP	2.6
1	A	308	TYR	2.4
2	E	21	LEU	2.4
1	A	296	SER	2.4
1	B	292	MET	2.4
1	B	356	ALA	2.3
2	E	8	PHE	2.3
2	E	19	SER	2.2
1	A	377	THR	2.2
1	A	289	LYS	2.2
1	A	335	TYR	2.1
1	B	285	PRO	2.0
1	A	355	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

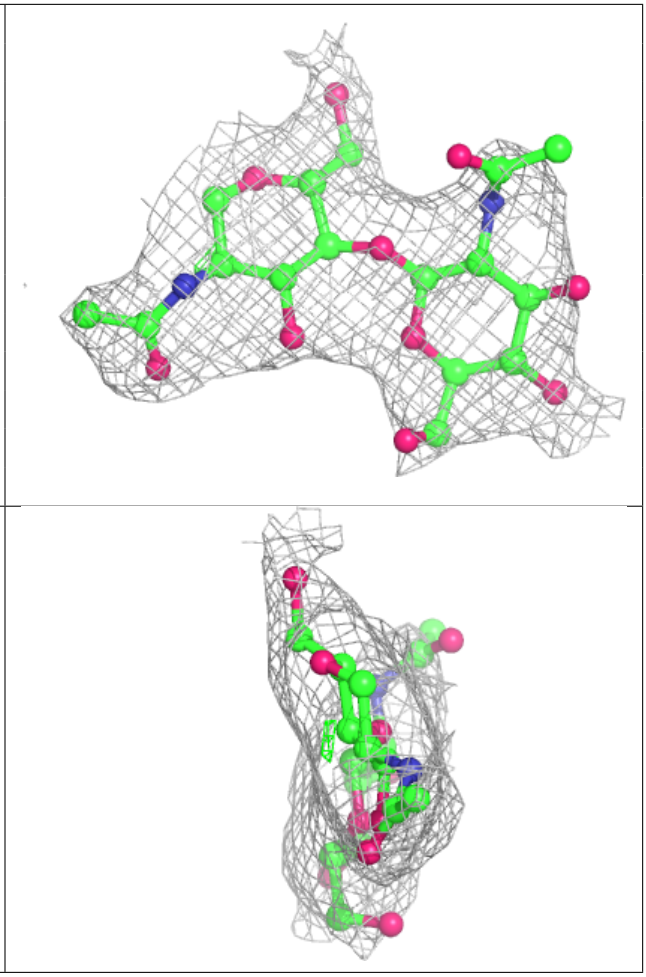
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	C	2	14/15	0.88	0.21	114,117,119,119	0
3	NAG	C	1	14/15	0.94	0.16	67,71,75,81	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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. 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	B-factors(Å^2)	Q<0.9
4	NAG	A	511	14/15	0.64	0.31	117,123,124,124	0
4	NAG	A	512	14/15	0.68	0.35	120,124,124,124	0
4	NAG	B	512	14/15	0.81	0.25	122,124,124,124	0
5	CL	B	513	1/1	0.96	0.10	53,53,53,53	0
5	CL	A	513	1/1	0.97	0.17	54,54,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.