Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:46 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

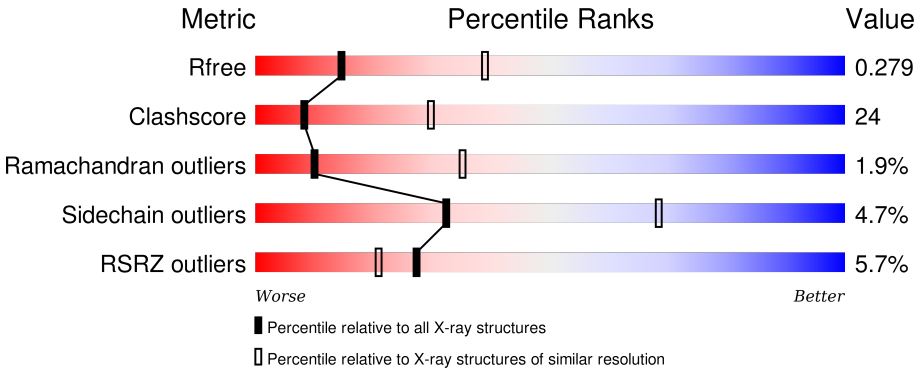
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (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}	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 <=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	3%, 50%, 30%, ·, 18%
2	E	21	95%, 29%, 48%, 19%, 5%

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
3	NAG	A	511	X	-	-	-
3	NAG	A	512	X	-	-	-

2 Entry composition

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.

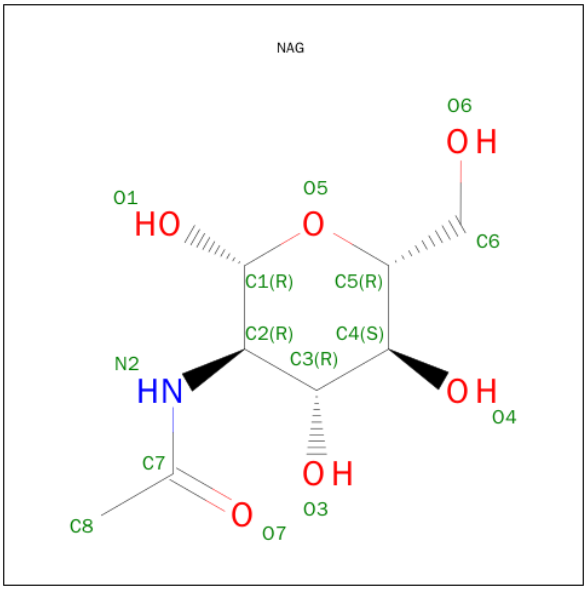
- Molecule 1 is a protein called Atrial natriuretic peptide clearance receptor.

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

- Molecule 2 is a protein called Natriuretic peptides B.

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total C N O 28 16 2 10	0	0

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

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

- Molecule 6 is water.

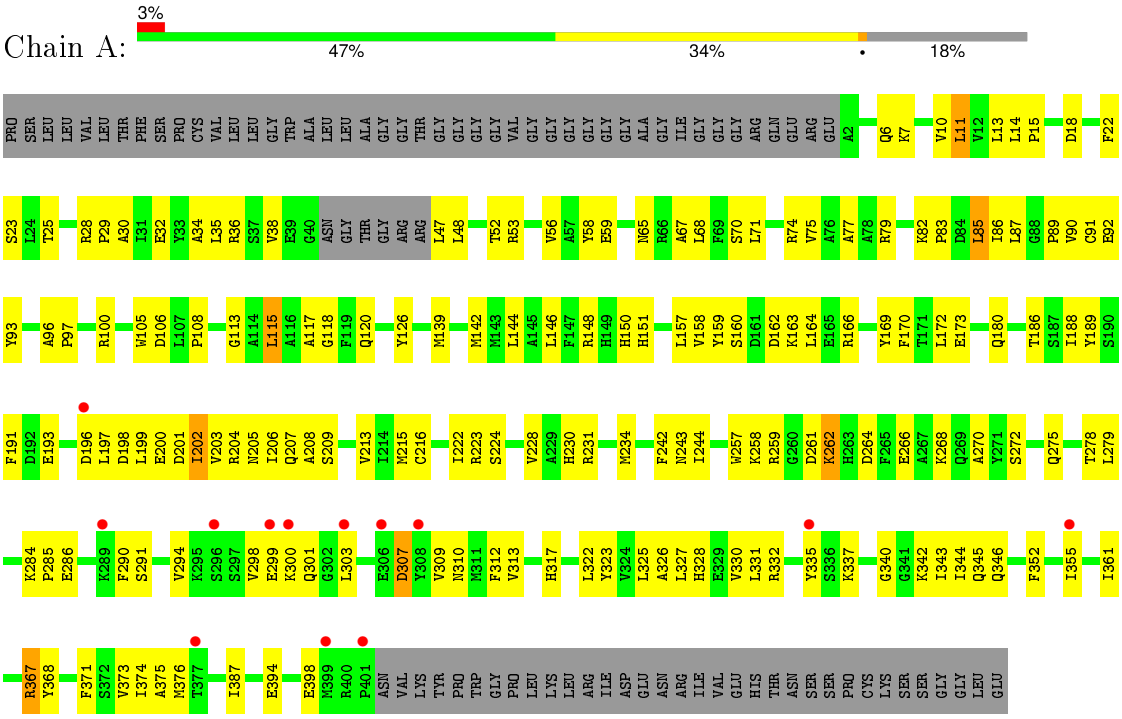
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	167	Total O 167 167	0	0
6	B	151	Total O 151 151	0	0
6	E	3	Total O 3 3	0	0

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 (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.

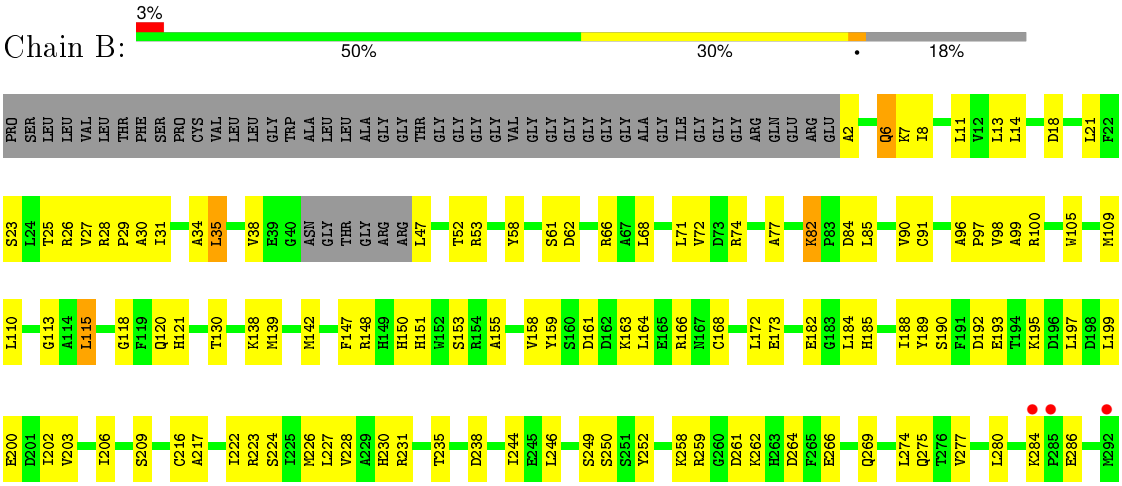
- Molecule 1: Atrial natriuretic peptide clearance receptor

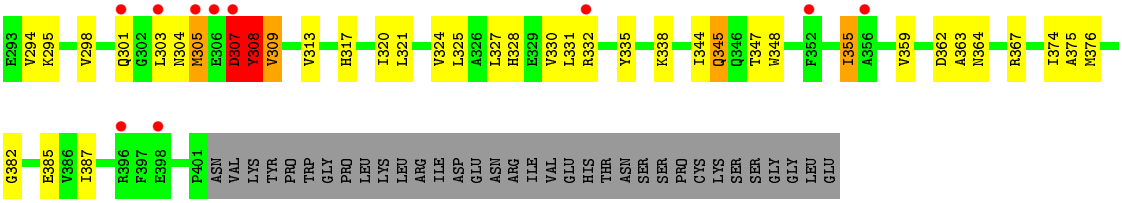
Chain A:



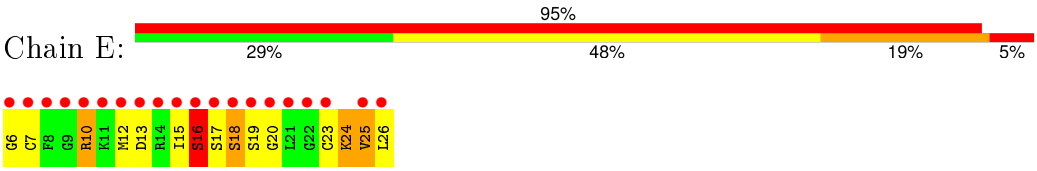
- Molecule 1: Atrial natriuretic peptide clearance receptor

Chain B:





- Molecule 2: Natriuretic peptides B



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%)	DCC
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 , 82.8	EDS
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 23729 reflections	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, 0.375 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: NAG, CL

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

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	A	28	0	26	0	0
3	B	14	0	13	0	0
4	B	28	0	25	2	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:B:96:ALA:O	1:B:100:ARG:HG3	1.94	0.68
1:A:193:GLU:HA	1:A:197:LEU:HD21	1.76	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:B:148:ARG:HH11	1:B:182:GLU:CG	2.08	0.67
1:A:91:CYS:HB3	6:A:565:HOH:O	1.92	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:203:VAL:HG21	1:A:228:VAL:HG12	1.80	0.63
1:A:90:VAL:HG13	1:A:113:GLY:HA3	1.78	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:290:PHE:O	1:A:294:VAL:HG23	2.00	0.61
1:A:242:PHE:HE2	1:A:275:GLN:HE21	1.49	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:HH11	1:A:53:ARG:HB3	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:96:ALA:HB2	2:E:16:SER:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:VAL:HG21	1:A:105:TRP:CZ3	2.38	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: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:207:GLN:HB3	1:A:234:MET:HE3	1.86	0.58
1:B:35:LEU:HA	1:B:38:VAL:HG12	1.86	0.58
1:A:262:LYS:HZ3	1:A:262:LYS:HB2	1.68	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:160:SER:OG	1:A:193:GLU:HG2	2.04	0.57
1:A:34:ALA:HB2	1:A:317:HIS:CD2	2.39	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:242:PHE:CE2	1:A:275:GLN:NE2	2.74	0.56
1:A:71:LEU:O	1:A:75:VAL:HG23	2.06	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:B:375:ALA:HB3	1:B:387:ILE:CD1	2.37	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: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:B:374:ILE:HG12	6:B:652:HOH:O	2.08	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: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:B:18:ASP:OD2	1:B:25:THR:HB	2.10	0.52
1:A:15:PRO:HD2	1:A:23:SER:HA	1.92	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
2:E:7:CYS:SG	2:E:7:CYS:O	2.69	0.50
1:B:13:LEU:O	1:B:14:LEU:HD23	2.11	0.50
1:A:96:ALA:HB3	1:A:97:PRO:CD	2.41	0.50
1:B:244:ILE:HD12	1:B:244:ILE:N	2.26	0.50
1:A:332:ARG:NH1	6:A:649:HOH:O	2.44	0.50
1:A:213:VAL:HG12	1:A:215:MET:HG3	1.93	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:B:23:SER:O	1:B:27:VAL:HG23	2.11	0.50
1:A:374:ILE:N	1:A:374:ILE:HD12	2.27	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:B:188:ILE:HG22	1:B:189:TYR:N	2.27	0.50
1:A:299:GLU:HA	1:A:303:LEU:O	2.12	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:HB3	1:A:74:ARG:HH11	1.77	0.49
1:B:374:ILE:HA	6:B:652:HOH:O	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:A:310:ASN:OD1	1:A:312:PHE:HB2	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:B:6:GLN:NE2	1:B:331:LEU:HD21	2.26	0.49
1:A:284:LYS:HD2	1:A:286:GLU:HB2	1.95	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	4:B:436: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:N	1:B:8:ILE:HD12	2.29	0.47
1:A:204:ARG:HH11	1:A:204:ARG:HG3	1.79	0.47
1:A:163:LYS:O	1:A:164:LEU:HD12	2.14	0.47
1:B:147:PHE:CZ	1:B:155:ALA:HB2	2.48	0.47
1:A:189:TYR:CE2	1:A:202:ILE:HA	2.50	0.47
1:A:32:GLU:O	1:A:36:ARG:HG3	2.15	0.47
1:A:207:GLN:HB3	1:A:234:MET:CE	2.44	0.47
1:B:280:LEU:HG	1:B:280:LEU:O	2.14	0.47
1:A:82:LYS:HB3	1:A:83:PRO:HD2	1.96	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:B:295:LYS:HG3	1:B:305:MET:CG	2.43	0.46
1:B:163:LYS:HA	1:B:166:ARG:HD3	1.97	0.46
1:A:257:TRP:CE3	1:A:258:LYS:N	2.83	0.46
1:A:163:LYS:HD2	2:E:20:GLY:O	2.16	0.46
1:B:199:LEU:HA	1:B:202:ILE:HD12	1.97	0.46
1:B:138:LYS:HB3	6:B:619:HOH:O	2.14	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:A:278:THR:OG1	1:A:279:LEU:N	2.47	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:199:LEU:HA	1:A:202:ILE:HG13	1.96	0.46
1:A:13:LEU:HD23	1:A:59:GLU:HB3	1.98	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:B:284:LYS:HE2	1:B:355:ILE:O	2.16	0.45
1:A:150:HIS:O	1:A:151:HIS:HB2	2.16	0.45
1:B:332:ARG:HB2	6:B:562:HOH:O	2.15	0.45
1:A:7:LYS:O	1:A:337:LYS:NZ	2.49	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:139:MET:HE2	1:B:244:ILE:HG21	1.98	0.45
1:B:28:ARG:HG3	1:B:58:TYR:CZ	2.51	0.45
1:B:90:VAL:HG13	1:B:113:GLY:CA	2.37	0.44
1:B:303:LEU:HD23	1:B:304:ASN:O	2.17	0.44
1:A:56:VAL:HG11	1:A:58:TYR:CZ	2.53	0.44
1:A:47:LEU:O	1:A:48:LEU:HD12	2.18	0.44
1:B:148:ARG:HG3	1:B:148:ARG:HH21	1.83	0.44
1:B:130:THR:HG21	1:B:347:THR:OG1	2.18	0.44
1:A:10:VAL:HA	1:A:85:LEU:O	2.17	0.44
1:B:148:ARG:NH2	1:B:148:ARG:HG3	2.33	0.44
1:A:70:SER:HB3	6:A:654:HOH:O	2.17	0.44
1:A:14:LEU:HB3	1:A:15:PRO:CD	2.47	0.44
1:A:215:MET:HE2	1:A:222:ILE:HG13	1.99	0.44
1:B:21:LEU:HG	4:B:436:NAG:C8	2.48	0.44
1:A:117:ALA:O	1:A:120:GLN:HB2	2.18	0.44
1:B:307:ASP:O	1:B:308:TYR:HB3	2.18	0.44
2:E:15:ILE:O	2:E:16:SER:CB	2.66	0.43
1:B:118:GLY:C	1:B:120:GLN:H	2.21	0.43
1:A:272:SER:HA	1:A:376:MET:SD	2.58	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:HE3	1:A:7:LYS:HB2	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:261:ASP:OD1	1:A:262:LYS:N	2.52	0.42
1:A:113:GLY:C	1:A:115:LEU:HD13	2.39	0.42
1:A:335:TYR:HD1	1:A:335:TYR:H	1.66	0.42
1:A:344:ILE:HD13	1:A:344:ILE:HA	1.89	0.42
1:A:22:PHE:CE1	1:A:90:VAL:HB	2.55	0.42
1:B:317:HIS:C	1:B:317:HIS:ND1	2.72	0.42
1:A:202:ILE:HG12	1:A:202:ILE:H	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:B:91:CYS:HA	6:B:602:HOH:O	2.20	0.42
1:A:92:GLU:HG3	1:A:170:PHE:CD2	2.55	0.42
1:B:258:LYS:HE3	1:B:258:LYS:HB2	1.88	0.42
1:A:374:ILE:CB	6:A:659:HOH:O	2.65	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:230:HIS:HA	1:B:235:THR:CG2	2.48	0.41
1:B:150:HIS:O	1:B:151:HIS:HB2	2.20	0.41
1:B:139:MET:CE	1:B:244:ILE:HG21	2.51	0.41
1:B:244:ILE:CG2	1:B:246:LEU:HG	2.50	0.41
1:B:226:MET:CE	1:B:274:LEU:HB2	2.50	0.41
1:B:284:LYS:HE3	1:B:286:GLU:HB3	2.02	0.41
2:E:6:GLY:HA2	2:E:25:VAL:HG23	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
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:68:LEU:HD13	1:A:97:PRO:HB2	2.01	0.41
1:A:35:LEU:O	1:A:38:VAL:HG22	2.20	0.41
1:A:244:ILE:HD12	1:A:244:ILE:N	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:B:200:GLU:OE2	1:B:231:ARG:NH2	2.53	0.41
1:A:394:GLU:H	1:A:394:GLU:HG2	1.66	0.41
1:B:344:ILE:HA	1:B:344:ILE:HD13	1.95	0.41
1:B:188:ILE:HG22	1:B:189:TYR:H	1.85	0.41
1:A:203:VAL:O	1:A:207:GLN:HG2	2.20	0.41
1:A:13:LEU:HD13	1:A:67:ALA:HB1	2.02	0.41
1:B:308:TYR:CD2	1:B:308:TYR:N	2.89	0.41
1:B:345:GLN:NE2	1:B:345:GLN:HA	2.36	0.41
1:B:261:ASP:OD2	1:B:262:LYS:HG2	2.20	0.41
1:B:203:VAL:HG21	1:B:228:VAL:HG12	2.02	0.41
1:B:166:ARG:HA	6:B:647:HOH:O	2.21	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:B:121:HIS:N	1:B:121:HIS:ND1	2.69	0.40
1:A:173:GLU:HB3	6:A:638:HOH:O	2.20	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:100:ARG:NE	6:A:637:HOH:O	2.54	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:223:ARG:CZ	1:A:259:ARG:HG3	2.52	0.40
1:B:18:ASP:OD2	1:B:303:LEU:HD12	2.22	0.40
1:B:385:GLU:C	6:B:652:HOH:O	2.60	0.40
1:B:71:LEU:HD21	1:B:105:TRP:HZ3	1.86	0.40
1:A:284:LYS:O	1:A:285:PRO:C	2.59	0.40
1:A:100:ARG:NH2	1:A:126:TYR:OH	2.54	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%)	19 54
1	B	390/479 (81%)	350 (90%)	34 (9%)	6 (2%)	13 42
2	E	19/21 (90%)	7 (37%)	7 (37%)	5 (26%)	0 0
All	All	799/979 (82%)	700 (88%)	84 (10%)	15 (2%)	10 35

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%)	38 74
1	B	329/389 (85%)	315 (96%)	14 (4%)	35 71
2	E	17/17 (100%)	12 (71%)	5 (29%)	0 1
All	All	675/795 (85%)	643 (95%)	32 (5%)	32 68

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

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	55	GLN
1	A	275	GLN
1	B	205	ASN
1	B	345	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

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	$\#\|Z\| > 2$
4	NAG	B	436	1,4	14,14,15	0.61	0	15,19,21	0.75	0
4	NAG	B	437	4	14,14,15	0.53	0	15,19,21	0.76	1 (6%)

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	436	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	437	4	-	0/6/23/26	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	437	NAG	C2-N2-C7	-2.49	119.84	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	436	NAG	2	0

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	$\#\|Z\| > 2$
3	NAG	A	511	1	14,14,15	0.77	0	15,19,21	0.63	0
3	NAG	A	512	1	14,14,15	0.60	0	15,19,21	0.73	0
3	NAG	B	512	1	14,14,15	0.67	0	15,19,21	0.85	1 (6%)

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	511	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	512	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	512	1	-	0/6/23/26	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	B	512	NAG	C2-N2-C7	-2.51	119.81	123.04

All (2) chirality outliers are listed below:

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

There are no torsion outliers.

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.24	13 (3%) 50 42	40, 65, 109, 124	0
1	B	394/479 (82%)	0.29	13 (3%) 50 42	40, 66, 110, 124	0
2	E	21/21 (100%)	4.29	20 (95%) 0 0	83, 139, 148, 148	0
All	All	809/979 (82%)	0.37	46 (5%) 27 21	40, 67, 116, 148	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	6	GLY	7.5
2	E	26	LEU	7.0
2	E	16	SER	6.5
2	E	13	ASP	5.8
2	E	7	CYS	5.7
2	E	9	GLY	5.4
2	E	25	VAL	5.2
2	E	17	SER	5.0
1	B	303	LEU	4.9
2	E	23	CYS	4.9
1	A	306	GLU	4.3
2	E	11	LYS	4.2
2	E	20	GLY	4.0
2	E	10	ARG	3.8
1	A	399	MET	3.6
1	A	196	ASP	3.6
1	A	303	LEU	3.6
2	E	18	SER	3.6
2	E	12	MET	3.6
1	B	306	GLU	3.5
1	B	305	MET	3.4
2	E	15	ILE	3.4
1	A	300	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	14	ARG	3.0
1	B	396	ARG	3.0
1	B	398	GLU	2.9
1	A	401	PRO	2.9
1	B	284	LYS	2.9
2	E	22	GLY	2.9
1	B	332	ARG	2.8
1	B	307	ASP	2.7
1	A	308	TYR	2.5
1	A	296	SER	2.5
1	B	292	MET	2.5
2	E	21	LEU	2.4
2	E	19	SER	2.3
1	B	356	ALA	2.3
2	E	8	PHE	2.3
1	A	377	THR	2.3
1	A	289	LYS	2.2
1	A	335	TYR	2.1
1	B	285	PRO	2.1
1	A	299	GLU	2.0
1	A	355	ILE	2.0
1	B	301	GLN	2.0
1	B	352	PHE	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. 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, 95^{th} 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
4	NAG	B	436	14/15	0.94	0.16	-0.68	67,71,75,81	0
4	NAG	B	437	14/15	0.88	0.21	-	114,117,119,119	0

6.4 Ligands

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, 95^{th} 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	511	14/15	0.64	0.31	0.52	117,123,124,124	0
5	CL	A	513	1/1	0.97	0.17	-1.76	54,54,54,54	0
5	CL	B	513	1/1	0.96	0.10	-2.32	53,53,53,53	0
3	NAG	A	512	14/15	0.68	0.35	-	120,124,124,124	0
3	NAG	B	512	14/15	0.81	0.25	-	122,124,124,124	0

6.5 Other polymers

There are no such residues in this entry.