



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:28 pm GMT

PDB ID : 2WIM
Title : CRYSTAL STRUCTURE OF NCAM2 IG1-3
Authors : Kulahin, N.; Kristensen, O.; Rasmussen, K.; Kastrup, J.; Berezin, V.; Bock, E.; Walmod, P.; Gajhede, M.
Deposited on : 2009-05-13
Resolution : 3.00 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

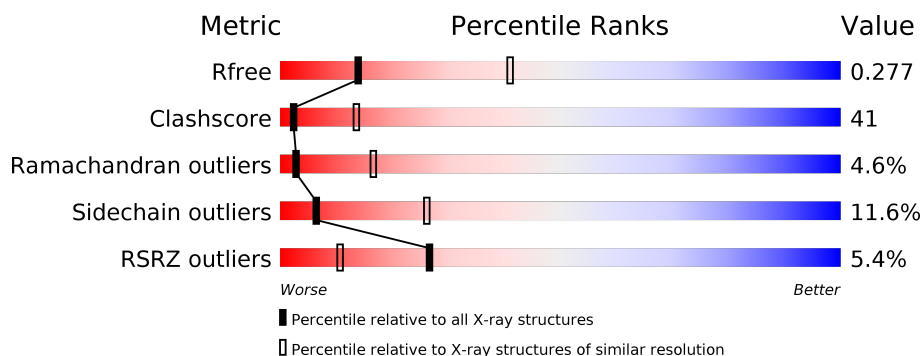
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	291	<div> <div> <div></div> <div>37%</div> <div>46%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	291	<div> <div>9%</div> <div>33%</div> <div>48%</div> <div>9%</div> <div>10%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4281 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.

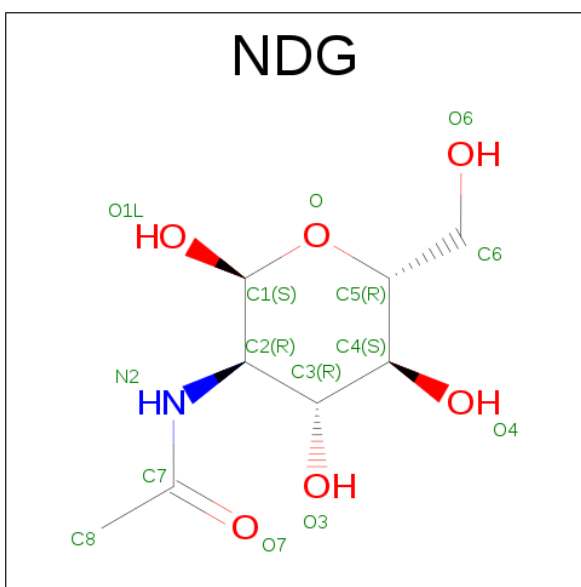
- Molecule 1 is a protein called NEURAL CELL ADHESION MOLECULE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2157	1347	374	427	9			
1	B	263	Total	C	N	O	S	0	0	0
			2050	1279	353	409	9			

There are 16 discrepancies between the modelled and reference sequences:

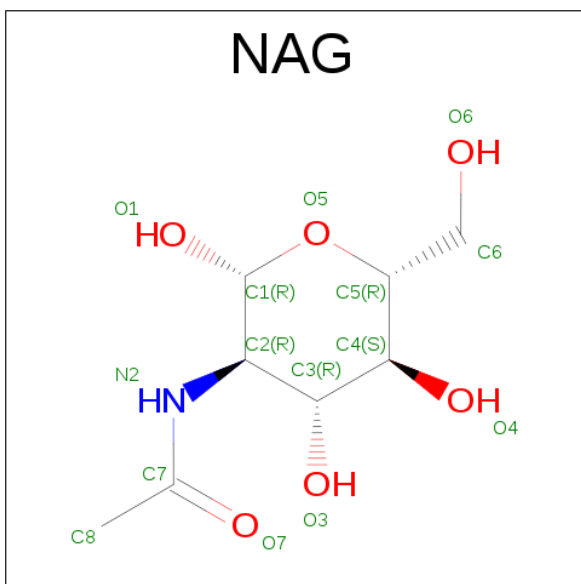
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	SER	-	EXPRESSION TAG	UNP O15394
A	18	MET	-	EXPRESSION TAG	UNP O15394
A	302	HIS	-	EXPRESSION TAG	UNP O15394
A	303	HIS	-	EXPRESSION TAG	UNP O15394
A	304	HIS	-	EXPRESSION TAG	UNP O15394
A	305	HIS	-	EXPRESSION TAG	UNP O15394
A	306	HIS	-	EXPRESSION TAG	UNP O15394
A	307	HIS	-	EXPRESSION TAG	UNP O15394
B	17	SER	-	EXPRESSION TAG	UNP O15394
B	18	MET	-	EXPRESSION TAG	UNP O15394
B	302	HIS	-	EXPRESSION TAG	UNP O15394
B	303	HIS	-	EXPRESSION TAG	UNP O15394
B	304	HIS	-	EXPRESSION TAG	UNP O15394
B	305	HIS	-	EXPRESSION TAG	UNP O15394
B	306	HIS	-	EXPRESSION TAG	UNP O15394
B	307	HIS	-	EXPRESSION TAG	UNP O15394

- Molecule 2 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).



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

- 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		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	18	Total 18	O 18	0	0
5	B	13	Total 13	O 13	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	38.39Å 106.78Å 188.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.57 – 3.00 35.56 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (24.57-3.00) 95.8 (35.56-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 3.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.213 , 0.288 0.220 , 0.277	Depositor DCC
R_{free} test set	781 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	79.1	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 91.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4281	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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, 0.333 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: CA, NAG, NDG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/2191	0.53	0/2965
1	B	0.33	0/2081	0.50	0/2813
All	All	0.33	0/4272	0.52	0/5778

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	SER	Peptide

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	2157	0	2123	160	0
1	B	2050	0	2008	190	0
2	A	14	0	13	1	0
2	B	14	0	13	1	0
3	A	14	0	13	0	0
4	A	1	0	0	0	0
5	A	18	0	0	2	0
5	B	13	0	0	2	0
All	All	4281	0	4170	348	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 41.

All (348) 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:55:ASN:HD21	1:B:59:GLU:HG3	1.22	1.05
1:A:242:ILE:HD12	1:A:264:THR:HG22	1.38	1.02
1:B:162:ARG:H	1:B:162:ARG:HD3	1.28	0.94
1:B:183:ILE:HD11	1:B:200:ASP:HB3	1.49	0.92
1:B:256:LYS:HE2	1:B:257:TYR:HD2	1.34	0.92
1:B:230:PHE:CE1	1:B:294:ALA:HB1	2.05	0.91
1:B:168:ASN:H	1:B:168:ASN:HD22	1.15	0.90
1:A:113:GLN:HG2	1:A:140:SER:HA	1.54	0.89
1:B:256:LYS:HE2	1:B:257:TYR:CD2	2.08	0.88
1:B:232:CYS:HB3	1:B:244:TRP:CZ2	2.10	0.87
1:A:119:GLU:HB2	1:A:137:ARG:HH11	1.38	0.86
1:B:55:ASN:ND2	1:B:59:GLU:HG3	1.93	0.84
1:B:132:ALA:HB3	1:B:173:ILE:HD11	1.61	0.83
1:A:183:ILE:HD12	1:A:183:ILE:H	1.44	0.82
1:A:166:LEU:HB2	1:A:168:ASN:ND2	1.96	0.81
1:A:45:ILE:H	1:A:45:ILE:HD12	1.46	0.80
1:B:256:LYS:HE3	1:B:268:VAL:HG13	1.65	0.79
1:B:84:ASN:OD1	1:B:86:GLU:HG2	1.82	0.78
1:B:98:ALA:O	1:B:99:LYS:HB3	1.83	0.78
1:A:128:GLN:HB2	1:A:207:VAL:HG12	1.63	0.78
1:B:126:PHE:CD2	1:B:132:ALA:HB1	2.18	0.78
1:B:257:TYR:HB3	1:B:268:VAL:HA	1.65	0.78
1:A:38:LYS:HG3	1:B:194:GLY:O	1.86	0.76
1:A:55:ASN:HD21	1:A:59:GLU:HB2	1.50	0.75
1:B:26:SER:HB2	1:B:27:LEU:HD12	1.69	0.75
1:B:56:PRO:HB3	1:B:89:GLY:HA3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:PRO:HB3	1:B:202:ILE:HG13	1.70	0.73
1:A:284:THR:HG22	1:A:289:GLU:HB3	1.68	0.73
1:B:30:VAL:HG11	1:B:40:PHE:HE1	1.53	0.73
1:B:173:ILE:O	1:B:173:ILE:HD12	1.88	0.73
1:B:193:ARG:O	1:B:195:GLU:N	2.19	0.73
1:A:277:GLY:HA2	1:A:295:PHE:CE2	2.25	0.72
1:A:183:ILE:N	1:A:183:ILE:HD12	2.03	0.72
1:B:19:ALA:HB3	1:B:20:LEU:HD22	1.72	0.71
1:B:163:PHE:CD1	1:B:173:ILE:HG22	2.25	0.71
1:A:211:ILE:HG13	1:A:290:ASP:HB3	1.71	0.71
1:A:148:TRP:CD2	1:A:171:LEU:HD22	2.27	0.70
1:A:64:THR:HG22	1:A:66:ARG:H	1.56	0.69
1:A:173:ILE:HB	1:A:176:ILE:HG23	1.74	0.69
1:B:246:ARG:CZ	1:B:251:ILE:HG12	2.22	0.69
1:A:246:ARG:HB2	1:A:251:ILE:HD11	1.74	0.69
1:B:260:LYS:HG3	1:B:261:GLY:H	1.58	0.68
1:B:227:GLU:HG3	1:B:228:MET:H	1.59	0.67
1:A:53:TRP:HB3	1:A:61:ILE:HD12	1.75	0.67
1:B:245:PHE:HA	1:B:251:ILE:HD13	1.76	0.66
1:B:157:THR:C	1:B:158:ILE:HD12	2.15	0.66
1:B:55:ASN:HB2	1:B:56:PRO:HD2	1.78	0.66
1:B:55:ASN:HD21	1:B:59:GLU:CG	2.04	0.66
1:A:119:GLU:HB2	1:A:137:ARG:NH1	2.09	0.66
1:B:162:ARG:HG2	1:B:163:PHE:CE2	2.31	0.65
1:B:33:SER:HB2	5:B:2009:HOH:O	1.96	0.65
1:B:125:GLU:HA	1:B:204:ILE:HG13	1.77	0.64
1:A:21:LEU:HD22	1:A:22:GLN:H	1.63	0.64
1:A:207:VAL:HG22	1:A:237:SER:HB2	1.80	0.64
1:B:202:ILE:HD11	1:B:204:ILE:CG2	2.28	0.64
1:B:202:ILE:HD11	1:B:204:ILE:HG22	1.80	0.63
1:B:168:ASN:H	1:B:168:ASN:ND2	1.90	0.63
1:B:56:PRO:HD3	1:B:91:TYR:CZ	2.34	0.63
1:A:125:GLU:HG2	1:A:204:ILE:HB	1.82	0.62
1:B:258:ILE:O	1:B:259:LEU:HD23	1.99	0.62
1:A:181:GLU:HA	1:A:203:VAL:HG12	1.82	0.62
1:A:32:LEU:HD22	1:A:109:LEU:HD11	1.81	0.61
1:A:146:VAL:HG12	1:A:147:SER:H	1.65	0.61
1:A:32:LEU:H	1:A:32:LEU:HD23	1.64	0.61
1:B:209:PRO:HD3	1:B:285:ASN:HD21	1.65	0.61
1:B:148:TRP:HA	1:B:185:ARG:O	2.00	0.61
1:B:263:ASN:N	1:B:263:ASN:HD22	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ASN:HD22	1:A:287:ALA:H	1.49	0.60
1:B:133:GLU:OE1	1:B:166:LEU:HD11	2.01	0.60
1:A:92:ARG:HG2	1:A:106:THR:HG22	1.82	0.60
1:B:245:PHE:HE1	1:B:250:LEU:HG	1.65	0.60
1:B:51:ILE:H	1:B:71:LYS:NZ	2.00	0.60
1:B:64:THR:HG23	1:B:65:GLN:N	2.17	0.60
1:B:213:MET:SD	1:B:232:CYS:HB2	2.42	0.60
1:B:32:LEU:HD21	1:B:38:LYS:HE2	1.83	0.60
1:B:122:SER:OG	1:B:202:ILE:HG23	2.02	0.60
1:A:21:LEU:CD1	1:A:103:GLN:HB2	2.32	0.59
1:A:32:LEU:CD2	1:A:109:LEU:HD11	2.32	0.59
1:A:67:VAL:HG22	1:A:80:ILE:HG13	1.83	0.59
1:A:261:GLY:O	1:A:264:THR:HG23	2.02	0.59
1:B:209:PRO:HD3	1:B:285:ASN:ND2	2.17	0.59
1:A:146:VAL:HG12	1:A:147:SER:N	2.18	0.59
1:B:260:LYS:CG	1:B:261:GLY:H	2.15	0.59
1:A:21:LEU:HD22	1:A:22:GLN:N	2.18	0.59
1:A:130:GLU:HG2	1:A:176:ILE:HD11	1.85	0.58
1:B:246:ARG:HH22	1:B:251:ILE:HG21	1.69	0.58
1:A:280:VAL:HG22	1:A:293:GLN:HB3	1.86	0.58
1:B:48:PRO:HG2	1:B:74:VAL:HG23	1.85	0.57
1:A:150:TYR:HB3	1:A:151:HIS:CE1	2.40	0.57
1:A:128:GLN:NE2	1:A:177:ASN:HA	2.19	0.57
1:A:84:ASN:O	1:A:111:ILE:HG12	2.04	0.57
1:A:128:GLN:HE22	1:A:177:ASN:HA	1.70	0.56
1:A:66:ARG:NH2	1:A:87:ASP:OD2	2.38	0.56
1:B:125:GLU:HB3	1:B:204:ILE:HD11	1.86	0.56
1:A:209:PRO:HG2	1:A:289:GLU:HA	1.86	0.56
1:B:168:ASN:N	1:B:168:ASN:HD22	1.94	0.56
1:B:131:ASP:HA	1:B:174:LEU:O	2.05	0.56
1:B:240:PRO:HB2	1:B:283:ALA:HB1	1.88	0.56
1:B:46:GLY:C	1:B:48:PRO:HD3	2.26	0.56
1:A:32:LEU:CD2	1:A:32:LEU:H	2.19	0.56
1:A:175:ASN:O	1:A:177:ASN:N	2.39	0.56
1:B:96:THR:HA	1:B:102:THR:HG22	1.87	0.56
1:A:74:VAL:HG13	1:A:74:VAL:O	2.06	0.56
1:B:244:TRP:HB3	1:B:246:ARG:NH1	2.21	0.56
1:A:122:SER:HB3	1:A:123:PRO:CD	2.36	0.55
1:A:181:GLU:HG3	1:A:203:VAL:O	2.05	0.55
1:A:168:ASN:O	1:A:169:ASN:HB2	2.04	0.55
1:B:19:ALA:C	1:B:20:LEU:HD13	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:PRO:HB3	1:A:287:ALA:O	2.05	0.55
1:B:123:PRO:HB3	1:B:202:ILE:CG1	2.37	0.55
1:B:162:ARG:N	1:B:162:ARG:HD3	2.09	0.55
1:A:226:GLU:HB2	1:A:271:ILE:CD1	2.37	0.55
1:A:178:LYS:HE3	5:A:2015:HOH:O	2.06	0.55
1:A:148:TRP:CE3	1:A:171:LEU:HD22	2.41	0.55
1:A:244:TRP:O	1:A:250:LEU:HD12	2.07	0.54
1:A:50:SER:O	1:A:95:ALA:HA	2.08	0.54
1:B:162:ARG:HG2	1:B:163:PHE:CD2	2.41	0.54
1:B:202:ILE:HG13	1:B:202:ILE:O	2.06	0.54
1:A:141:SER:HB3	1:A:142:PRO:HD3	1.90	0.54
1:A:51:ILE:HD13	1:A:71:LYS:HD3	1.89	0.54
1:B:19:ALA:O	1:B:20:LEU:HD13	2.07	0.54
1:B:115:LEU:HA	1:B:140:SER:HB3	1.90	0.54
1:A:168:ASN:HD22	1:A:168:ASN:H	1.56	0.54
1:B:245:PHE:CE1	1:B:250:LEU:HG	2.42	0.54
1:B:236:GLY:CA	1:B:240:PRO:HD3	2.38	0.54
1:A:276:GLY:HA2	1:A:296:LEU:O	2.08	0.53
1:B:99:LYS:HD3	1:B:101:GLN:H	1.73	0.53
1:A:115:LEU:HD23	1:A:140:SER:HB3	1.90	0.53
1:A:113:GLN:HG3	1:A:114:LYS:O	2.09	0.53
1:B:244:TRP:HB3	1:B:246:ARG:HH12	1.72	0.53
1:A:258:ILE:HG23	1:A:267:THR:HB	1.91	0.53
1:B:53:TRP:HB3	1:B:61:ILE:HD13	1.90	0.53
1:A:258:ILE:CG2	1:A:267:THR:HB	2.38	0.52
1:B:245:PHE:CE1	1:B:250:LEU:HA	2.43	0.52
1:B:124:GLN:NE2	1:B:201:ILE:HG21	2.24	0.52
1:B:163:PHE:CE1	1:B:173:ILE:HG22	2.44	0.52
1:B:51:ILE:H	1:B:71:LYS:HZ2	1.57	0.52
1:A:285:ASN:ND2	1:A:287:ALA:H	2.07	0.52
1:B:215:GLN:HG2	1:B:218:PHE:CE1	2.45	0.52
1:B:246:ARG:NH2	1:B:251:ILE:HG12	2.25	0.52
1:A:35:GLY:O	1:A:82:ASN:HA	2.09	0.52
1:A:116:THR:O	1:A:138:VAL:HA	2.09	0.52
1:B:236:GLY:HA3	1:B:240:PRO:HD3	1.92	0.52
1:A:231:SER:HA	1:A:265:GLU:OE2	2.09	0.51
1:B:250:LEU:HD23	1:B:251:ILE:H	1.75	0.51
1:A:122:SER:CB	1:A:123:PRO:CD	2.89	0.51
1:B:260:LYS:HG3	1:B:261:GLY:N	2.23	0.51
1:A:207:VAL:HG23	1:A:236:GLY:HA2	1.92	0.51
1:A:211:ILE:HD11	1:A:290:ASP:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLU:O	1:A:31:GLU:HG3	2.10	0.51
1:B:114:LYS:HG2	5:B:2009:HOH:O	2.10	0.51
1:B:99:LYS:NZ	1:B:101:GLN:HB2	2.26	0.51
1:B:162:ARG:HA	1:B:174:LEU:HD23	1.93	0.51
1:B:173:ILE:HD12	1:B:173:ILE:C	2.31	0.51
1:A:259:LEU:HD13	1:A:263:ASN:OD1	2.11	0.50
1:B:229:THR:HG23	1:B:267:THR:OG1	2.11	0.50
1:A:151:HIS:C	1:A:156:THR:OG1	2.50	0.50
1:A:221:THR:HG22	1:A:226:GLU:HG3	1.93	0.50
1:B:64:THR:HG23	1:B:65:GLN:H	1.76	0.50
1:A:218:PHE:CD1	1:A:218:PHE:N	2.78	0.50
1:B:230:PHE:HB2	1:B:266:LEU:O	2.12	0.50
1:A:253:GLU:O	1:A:254:ASN:HB2	2.11	0.50
1:B:37:SER:OG	1:B:81:TYR:HA	2.11	0.50
1:A:140:SER:OG	1:A:144:PRO:HD3	2.12	0.50
1:A:185:ARG:CZ	1:A:198:PHE:CE1	2.94	0.50
1:B:129:GLY:N	1:B:176:ILE:HD12	2.26	0.50
1:A:255:GLU:O	1:A:269:ARG:HD3	2.10	0.49
1:A:45:ILE:CD1	1:A:45:ILE:H	2.22	0.49
1:A:178:LYS:HB3	2:A:950:NDG:O6	2.12	0.49
1:A:45:ILE:HD12	1:A:45:ILE:N	2.21	0.49
1:B:178:LYS:NZ	1:B:205:VAL:O	2.46	0.49
1:B:242:ILE:HG21	1:B:263:ASN:O	2.13	0.49
1:B:92:ARG:HG2	1:B:106:THR:HG22	1.94	0.49
1:B:99:LYS:C	1:B:99:LYS:HD3	2.33	0.49
1:A:259:LEU:HA	1:A:265:GLU:O	2.13	0.49
1:A:151:HIS:CD2	1:A:156:THR:HA	2.48	0.49
1:B:63:SER:HB3	1:B:69:VAL:CG1	2.43	0.49
1:B:212:SER:HB3	1:B:233:ARG:O	2.13	0.48
1:B:100:GLY:O	1:B:102:THR:HG23	2.13	0.48
1:B:35:GLY:C	1:B:82:ASN:HA	2.34	0.48
1:A:168:ASN:HD22	1:A:168:ASN:N	2.11	0.48
1:B:260:LYS:CG	1:B:261:GLY:N	2.77	0.48
1:A:90:ILE:HG12	1:A:108:VAL:HG22	1.96	0.48
1:B:206:ASN:HD21	1:B:286:LYS:HE3	1.78	0.48
1:B:57:GLN:HA	1:B:57:GLN:NE2	2.29	0.48
1:A:260:LYS:O	1:A:262:SER:N	2.46	0.48
1:A:272:ILE:HD13	1:A:274:SER:H	1.78	0.48
1:B:232:CYS:HB3	1:B:244:TRP:HZ2	1.71	0.47
1:A:259:LEU:O	1:A:259:LEU:HD12	2.15	0.47
1:A:122:SER:O	1:A:123:PRO:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:O	1:A:120:VAL:HG23	2.14	0.47
1:B:219:ASN:HB3	2:B:953:NDG:O	2.15	0.47
1:A:19:ALA:O	1:A:20:LEU:HD22	2.13	0.47
1:A:32:LEU:CD2	1:A:32:LEU:N	2.78	0.47
1:B:215:GLN:HG2	1:B:218:PHE:CZ	2.49	0.47
1:B:121:VAL:O	1:B:124:GLN:HG3	2.15	0.47
1:A:120:VAL:HG12	1:A:137:ARG:H	1.80	0.47
1:A:150:TYR:HB3	1:A:151:HIS:NE2	2.30	0.47
1:A:166:LEU:HB2	1:A:168:ASN:HD21	1.76	0.47
1:A:221:THR:O	1:A:271:ILE:HD11	2.14	0.47
1:B:115:LEU:HD11	1:B:188:GLY:O	2.15	0.47
1:B:125:GLU:HG2	1:B:204:ILE:HG12	1.96	0.46
1:B:63:SER:HB2	1:B:68:VAL:HA	1.97	0.46
1:B:285:ASN:C	1:B:285:ASN:HD22	2.18	0.46
1:B:230:PHE:O	1:B:266:LEU:N	2.49	0.46
1:B:263:ASN:N	1:B:263:ASN:ND2	2.63	0.46
1:A:285:ASN:C	1:A:285:ASN:HD22	2.19	0.46
1:B:173:ILE:HD13	1:B:176:ILE:HG13	1.98	0.46
1:A:149:LEU:HB3	1:A:156:THR:HG22	1.98	0.46
1:A:183:ILE:H	1:A:183:ILE:CD1	2.23	0.46
1:B:39:PHE:HA	1:B:78:LEU:O	2.15	0.46
1:A:24:THR:HG23	1:A:45:ILE:CD1	2.44	0.46
1:B:227:GLU:HG3	1:B:228:MET:N	2.29	0.46
1:A:149:LEU:HD23	1:A:157:THR:HA	1.97	0.46
1:A:177:ASN:OD1	1:A:179:SER:N	2.46	0.46
1:A:19:ALA:C	1:A:20:LEU:HD22	2.36	0.45
1:B:32:LEU:HD21	1:B:38:LYS:CE	2.46	0.45
1:B:202:ILE:HD12	1:B:203:VAL:N	2.31	0.45
1:B:74:VAL:O	1:B:74:VAL:HG13	2.16	0.45
1:A:121:VAL:HG22	1:A:122:SER:N	2.31	0.45
1:A:127:LYS:O	1:A:129:GLY:N	2.50	0.45
1:B:250:LEU:HD23	1:B:251:ILE:N	2.31	0.45
1:B:141:SER:O	1:B:193:ARG:NH2	2.50	0.45
1:A:141:SER:CB	1:A:142:PRO:HD3	2.46	0.45
1:A:51:ILE:HD13	1:A:71:LYS:NZ	2.32	0.45
1:B:174:LEU:N	1:B:174:LEU:HD22	2.32	0.45
1:B:26:SER:OG	1:B:41:THR:N	2.40	0.45
1:A:131:ASP:OD1	1:A:174:LEU:O	2.34	0.45
1:B:246:ARG:NH2	1:B:266:LEU:HD11	2.31	0.45
1:A:221:THR:HG23	1:A:224:ARG:HB2	1.99	0.45
1:A:29:LYS:HE3	1:A:110:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:GLN:CA	1:B:57:GLN:NE2	2.79	0.45
1:A:39:PHE:CD2	1:A:77:ARG:HD3	2.52	0.45
1:A:56:PRO:HD3	1:A:91:TYR:CE2	2.52	0.45
1:B:113:GLN:HE21	1:B:116:THR:HG21	1.81	0.45
1:B:204:ILE:HD12	1:B:204:ILE:O	2.17	0.45
1:B:229:THR:HA	1:B:267:THR:HA	1.99	0.45
1:B:30:VAL:CG1	1:B:40:PHE:HE1	2.26	0.45
1:A:69:VAL:CG2	1:A:78:LEU:HD23	2.47	0.44
1:B:245:PHE:HE1	1:B:250:LEU:HA	1.80	0.44
1:B:133:GLU:HG3	1:B:133:GLU:O	2.16	0.44
1:A:141:SER:CB	1:A:142:PRO:CD	2.95	0.44
1:A:232:CYS:O	1:A:242:ILE:HD13	2.18	0.44
1:A:55:ASN:ND2	1:A:59:GLU:HB2	2.26	0.44
1:B:26:SER:HB2	1:B:27:LEU:CD1	2.43	0.44
1:A:221:THR:HG21	1:A:224:ARG:HD2	1.99	0.44
1:A:69:VAL:HG22	1:A:78:LEU:HD23	1.99	0.44
1:B:212:SER:O	1:B:214:PRO:HD3	2.17	0.44
1:B:57:GLN:HA	1:B:57:GLN:HE21	1.81	0.44
1:A:29:LYS:HG2	5:A:2004:HOH:O	2.16	0.44
1:A:56:PRO:HB3	1:A:89:GLY:HA3	1.99	0.44
1:A:26:SER:O	1:A:27:LEU:HD13	2.18	0.44
1:A:213:MET:HE3	1:A:293:GLN:O	2.18	0.44
1:A:257:TYR:CD1	1:A:268:VAL:HG22	2.53	0.44
1:B:251:ILE:HG23	1:B:257:TYR:CE1	2.52	0.44
1:A:181:GLU:HB2	1:A:205:VAL:HG23	2.00	0.44
1:B:136:CYS:HB2	1:B:148:TRP:CH2	2.53	0.44
1:B:171:LEU:HD12	1:B:172:GLN:H	1.82	0.44
1:B:211:ILE:HG12	1:B:234:ALA:HB2	2.00	0.44
1:A:113:GLN:HE21	1:A:116:THR:HG23	1.82	0.44
1:A:139:SER:HA	1:A:144:PRO:HG3	1.99	0.43
1:A:84:ASN:HD22	1:A:84:ASN:C	2.21	0.43
1:A:213:MET:CE	1:A:216:LYS:HG2	2.48	0.43
1:B:230:PHE:CZ	1:B:294:ALA:HB1	2.51	0.43
1:A:118:ARG:O	1:A:120:VAL:HG13	2.18	0.43
1:B:279:TYR:O	1:B:294:ALA:HB3	2.19	0.43
1:B:246:ARG:HH22	1:B:251:ILE:CG2	2.32	0.43
1:A:30:VAL:HG11	1:A:40:PHE:HE1	1.83	0.43
1:A:37:SER:O	1:A:38:LYS:HB2	2.19	0.43
1:A:219:ASN:HA	1:A:297:GLN:O	2.18	0.43
1:B:49:GLU:HB2	1:B:97:ASP:HA	2.00	0.43
1:A:212:SER:N	1:A:233:ARG:O	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:GLU:HG3	1:B:204:ILE:HA	2.01	0.43
1:B:247:ASN:C	1:B:249:LYS:H	2.22	0.43
1:B:29:LYS:HD2	1:B:108:VAL:O	2.19	0.43
1:A:213:MET:HA	1:A:214:PRO:HD2	1.81	0.43
1:A:256:LYS:HE2	1:A:269:ARG:O	2.19	0.43
1:B:124:GLN:HE21	1:B:201:ILE:HG21	1.83	0.42
1:B:281:CYS:O	1:B:291:GLU:HA	2.18	0.42
1:A:150:TYR:CD2	1:A:184:TYR:CZ	3.08	0.42
1:A:281:CYS:HB3	1:A:292:LYS:O	2.19	0.42
1:B:126:PHE:CE1	1:B:203:VAL:HG13	2.53	0.42
1:B:148:TRP:C	1:B:149:LEU:HG	2.39	0.42
1:A:209:PRO:HD3	1:A:285:ASN:HD21	1.84	0.42
1:A:25:ILE:HG22	1:A:27:LEU:H	1.84	0.42
1:A:50:SER:HB3	1:A:96:THR:HB	2.01	0.42
1:B:145:ALA:O	1:B:188:GLY:HA2	2.18	0.42
1:A:150:TYR:CE2	1:A:184:TYR:CZ	3.07	0.42
1:B:171:LEU:HD12	1:B:172:GLN:N	2.34	0.42
1:B:215:GLN:HB3	1:B:218:PHE:CZ	2.54	0.42
1:B:254:ASN:CB	1:B:257:TYR:CZ	3.02	0.42
1:B:46:GLY:O	1:B:48:PRO:HD3	2.19	0.42
1:B:158:ILE:N	1:B:158:ILE:HD12	2.35	0.42
1:B:38:LYS:HG3	1:B:39:PHE:N	2.34	0.42
1:B:160:ASP:HB3	1:B:161:ASN:H	1.61	0.42
1:B:198:PHE:CD1	1:B:198:PHE:C	2.93	0.42
1:B:209:PRO:HG2	1:B:289:GLU:HA	2.02	0.42
1:A:246:ARG:C	1:A:248:GLY:H	2.22	0.41
1:A:194:GLY:HA2	1:B:39:PHE:CZ	2.55	0.41
1:B:56:PRO:CB	1:B:89:GLY:HA3	2.46	0.41
1:B:97:ASP:OD2	1:B:101:GLN:HB3	2.20	0.41
1:B:56:PRO:HD3	1:B:91:TYR:CE1	2.55	0.41
1:B:56:PRO:HD3	1:B:91:TYR:CE2	2.56	0.41
1:A:256:LYS:HA	1:A:256:LYS:HD3	1.69	0.41
1:B:240:PRO:CB	1:B:283:ALA:HB1	2.49	0.41
1:B:92:ARG:CG	1:B:106:THR:HG22	2.50	0.41
1:B:178:LYS:HA	1:B:205:VAL:HG11	2.03	0.41
1:A:36:GLU:OE1	1:A:36:GLU:HA	2.20	0.41
1:B:26:SER:HG	1:B:41:THR:H	1.62	0.41
1:A:224:ARG:O	1:A:226:GLU:N	2.44	0.41
1:B:251:ILE:HG23	1:B:257:TYR:OH	2.20	0.41
1:A:142:PRO:HD2	1:A:193:ARG:HH12	1.86	0.41
1:B:246:ARG:HD2	1:B:279:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:SER:HB3	1:A:123:PRO:HD3	2.01	0.41
1:A:130:GLU:O	1:A:176:ILE:HD11	2.21	0.41
1:A:168:ASN:ND2	1:A:170:ASN:H	2.18	0.41
1:B:130:GLU:CG	1:B:176:ILE:HD11	2.51	0.41
1:B:25:ILE:HD12	1:B:53:TRP:CH2	2.55	0.41
1:A:113:GLN:HE21	1:A:116:THR:CG2	2.33	0.41
1:A:21:LEU:HD23	1:A:46:GLY:HA3	2.03	0.41
1:B:140:SER:H	1:B:144:PRO:HD3	1.85	0.41
1:B:190:VAL:O	1:B:193:ARG:O	2.39	0.41
1:B:211:ILE:HA	1:B:234:ALA:HA	2.02	0.41
1:B:33:SER:O	1:B:36:GLU:HG2	2.20	0.41
1:B:142:PRO:O	1:B:143:ALA:C	2.58	0.41
1:B:84:ASN:CG	1:B:86:GLU:HG2	2.41	0.41
1:B:37:SER:O	1:B:38:LYS:HB2	2.20	0.41
1:B:54:TYR:CD1	1:B:60:LYS:HA	2.56	0.41
1:B:63:SER:HB3	1:B:69:VAL:HG13	2.03	0.41
1:A:257:TYR:CE1	1:A:268:VAL:HG13	2.56	0.40
1:B:99:LYS:HZ2	1:B:101:GLN:HB2	1.85	0.40
1:B:174:LEU:HA	1:B:174:LEU:HD13	1.91	0.40
1:A:109:LEU:HG	1:A:111:ILE:CD1	2.51	0.40
1:B:140:SER:N	1:B:144:PRO:HD3	2.37	0.40
1:B:173:ILE:CD1	1:B:176:ILE:HG13	2.51	0.40
1:B:63:SER:HB3	1:B:69:VAL:HG12	2.03	0.40
1:A:130:GLU:N	1:A:176:ILE:HD11	2.36	0.40
1:A:146:VAL:CG1	1:A:147:SER:H	2.33	0.40
1:A:84:ASN:O	1:A:87:ASP:HB2	2.21	0.40
1:B:185:ARG:HA	1:B:199:ARG:O	2.22	0.40
1:B:242:ILE:CG2	1:B:243:SER:N	2.85	0.40
1:B:242:ILE:HG23	1:B:243:SER:N	2.36	0.40
1:B:177:ASN:O	1:B:205:VAL:HG21	2.22	0.40
1:B:45:ILE:C	1:B:45:ILE:HD12	2.42	0.40
1:A:151:HIS:HD2	1:A:156:THR:CA	2.35	0.40
1:A:237:SER:HA	1:A:238:PRO:C	2.42	0.40
1:A:280:VAL:HA	1:A:293:GLN:HB3	2.03	0.40
1:B:193:ARG:NH1	1:B:195:GLU:OE1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	272/291 (94%)	230 (85%)	29 (11%)	13 (5%)	2	16
1	B	255/291 (88%)	218 (86%)	26 (10%)	11 (4%)	3	18
All	All	527/582 (90%)	448 (85%)	55 (10%)	24 (5%)	3	16

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	SER
1	A	123	PRO
1	A	128	GLN
1	A	159	SER
1	A	176	ILE
1	A	222	ALA
1	B	192	ALA
1	A	261	GLY
1	B	21	LEU
1	B	159	SER
1	B	160	ASP
1	B	174	LEU
1	B	194	GLY
1	A	130	GLU
1	A	253	GLU
1	B	82	ASN
1	A	141	SER
1	A	226	GLU
1	B	64	THR
1	B	214	PRO
1	B	228	MET
1	B	38	LYS
1	A	225	GLY
1	A	272	ILE

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	238/253 (94%)	212 (89%)	26 (11%)	7	29
1	B	227/253 (90%)	199 (88%)	28 (12%)	5	24
All	All	465/506 (92%)	411 (88%)	54 (12%)	6	26

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	THR
1	A	30	VAL
1	A	32	LEU
1	A	50	SER
1	A	51	ILE
1	A	52	ASP
1	A	63	SER
1	A	71	LYS
1	A	74	VAL
1	A	78	LEU
1	A	84	ASN
1	A	113	GLN
1	A	151	HIS
1	A	168	ASN
1	A	171	LEU
1	A	176	ILE
1	A	177	ASN
1	A	183	ILE
1	A	203	VAL
1	A	254	ASN
1	A	256	LYS
1	A	259	LEU
1	A	260	LYS
1	A	271	ILE
1	A	272	ILE
1	A	285	ASN
1	B	20	LEU

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Mol	Chain	Res	Type
1	B	24	THR
1	B	26	SER
1	B	27	LEU
1	B	30	VAL
1	B	34	VAL
1	B	45	ILE
1	B	47	GLU
1	B	65	GLN
1	B	69	VAL
1	B	70	GLN
1	B	74	VAL
1	B	120	VAL
1	B	134	VAL
1	B	149	LEU
1	B	162	ARG
1	B	168	ASN
1	B	169	ASN
1	B	176	ILE
1	B	189	ARG
1	B	202	ILE
1	B	230	PHE
1	B	232	CYS
1	B	242	ILE
1	B	263	ASN
1	B	265	GLU
1	B	285	ASN
1	B	293	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	113	GLN
1	A	151	HIS
1	A	161	ASN
1	A	168	ASN
1	A	215	GLN
1	A	254	ASN
1	A	285	ASN
1	B	57	GLN
1	B	65	GLN
1	B	101	GLN

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Mol	Chain	Res	Type
1	B	103	GLN
1	B	113	GLN
1	B	168	ASN
1	B	170	ASN
1	B	215	GLN
1	B	263	ASN
1	B	285	ASN
1	B	293	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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is 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	$\# Z > 2$
2	NDG	A	950	1	14,14,15	0.47	0	15,19,21	1.14	1 (6%)
3	NAG	A	951	1	14,14,15	0.54	0	15,19,21	0.89	1 (6%)
2	NDG	B	953	1	14,14,15	0.65	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
2	NDG	A	950	1	-	0/6/23/26	0/1/1/1
3	NAG	A	951	1	-	0/6/23/26	0/1/1/1
2	NDG	B	953	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	953	NDG	C1-O-C5	2.02	114.95	112.17
3	A	951	NAG	C1-O5-C5	2.63	115.79	112.17
2	A	950	NDG	C1-O-C5	3.41	116.87	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	950	NDG	1	0
2	B	953	NDG	1	0

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, 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	276/291 (94%)	0.13	4 (1%) 75 49	58, 87, 130, 152	0
1	B	263/291 (90%)	0.43	25 (9%) 9 3	56, 91, 144, 169	0
All	All	539/582 (92%)	0.28	29 (5%) 26 11	56, 89, 138, 169	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	246	ARG	7.7
1	B	241	ALA	4.9
1	B	284	THR	4.4
1	B	258	ILE	4.4
1	A	296	LEU	4.3
1	B	257	TYR	4.0
1	B	227	GLU	4.0
1	B	253	GLU	3.9
1	B	234	ALA	3.5
1	B	283	ALA	3.4
1	B	243	SER	3.4
1	A	271	ILE	3.2
1	B	230	PHE	3.0
1	A	220	ALA	2.9
1	B	242	ILE	2.9
1	B	232	CYS	2.8
1	B	268	VAL	2.8
1	B	266	LEU	2.7
1	B	267	THR	2.7
1	A	221	THR	2.6
1	B	252	GLU	2.5
1	B	247	ASN	2.4
1	B	244	TRP	2.4
1	B	265	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	218	PHE	2.4
1	B	245	PHE	2.2
1	B	233	ARG	2.2
1	B	279	TYR	2.1
1	B	259	LEU	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](#)

There are no carbohydrates in this entry.

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(Å ²)	Q<0.9
2	NDG	A	950	14/15	0.79	0.47	-	100,138,156,158	0
2	NDG	B	953	14/15	0.74	0.25	-	109,153,164,179	0
3	NAG	A	951	14/15	0.78	0.45	-	134,167,174,178	0
4	CA	A	1299	1/1	0.90	0.39	-	115,115,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.