Full wwPDB X-ray Structure Validation Report (i)

Jun 26, 2024 – 02:10 AM EDT

PDB ID	:	6U3N
Title	:	LS2.8/3.15 - DQ2-P.fluor-alpha1a complex
Authors	:	Petersen, J.; Rossjohn, J.
Deposited on	:	2019-08-22
Resolution	:	2.80 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:

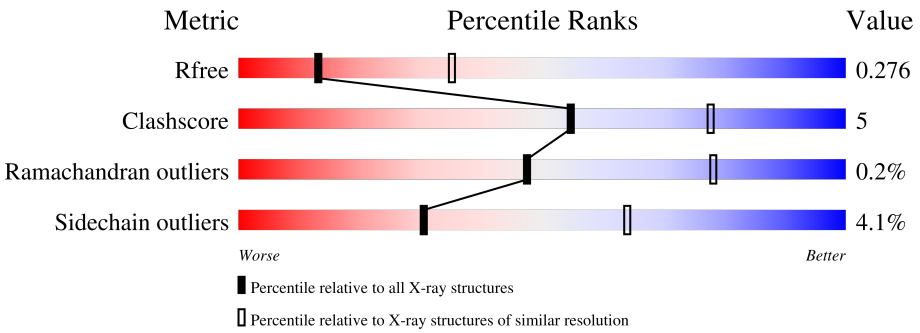
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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%

Mol	Chain	Length	Quality of chain
1	D	206	82% 14% • •
2	E	244	87% 11% ••
3	A	191	73% 21% • 5%
4	B	206	70% 17% 12%
5	C	20	50% 5% 45%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6478 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 T-CELL RECEPTOR, LS2.8/3.15 alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	199	1548	979	253	309	7	0	0	0

- Molecule 2 is a protein called T-CELL RECEPTOR, LS2.8/3.15 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	242	1911	1207	335	364	5	0	0	0

- Molecule 3 is a protein called MHC class II HLA-DQ-alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	181	1445	931	236	276	2	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	SER	CYS	conflict	UNP O19705
A	182	THR	-	expression tag	UNP O19705
A	183	SER	-	expression tag	UNP O19705
A	184	GLY	-	expression tag	UNP O19705
A	185	ASP	-	expression tag	UNP O19705
A	186	ASP	-	expression tag	UNP O19705
A	187	ASP	-	expression tag	UNP O19705
A	188	ASP	-	expression tag	UNP O19705
A	189	LYS	-	expression tag	UNP O19705

- Molecule 4 is a protein called MHC class II HLA-DQ-beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	181	1474	931	261	275	7	0	0	0

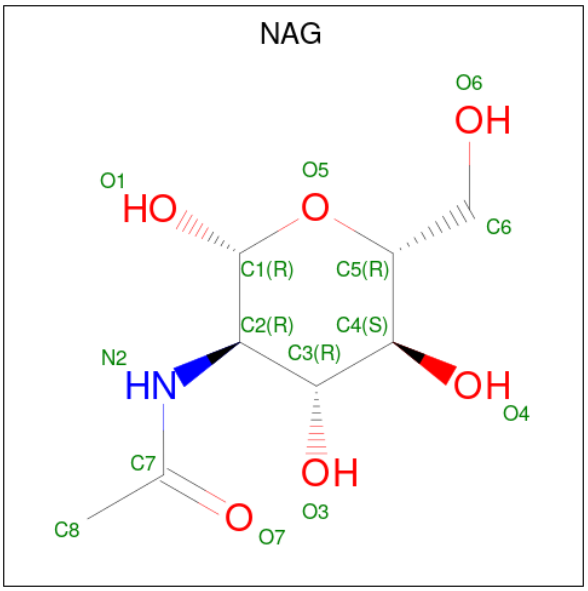
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLY	-	expression tag	UNP O19712
B	-4	GLY	-	expression tag	UNP O19712
B	-3	SER	-	expression tag	UNP O19712
B	-2	GLY	-	expression tag	UNP O19712
B	-1	ALA	-	expression tag	UNP O19712
B	0	SER	-	expression tag	UNP O19712
B	193	THR	-	expression tag	UNP O19712
B	194	GLY	-	expression tag	UNP O19712
B	195	GLY	-	expression tag	UNP O19712
B	196	ASP	-	expression tag	UNP O19712
B	197	ASP	-	expression tag	UNP O19712
B	198	ASP	-	expression tag	UNP O19712
B	199	ASP	-	expression tag	UNP O19712
B	200	LYS	-	expression tag	UNP O19712

- Molecule 5 is a protein called Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	11	85	58	11	14	2	0	0	0

- Molecule 6 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		
6	A	1	14	8	1	5	0	0

- Molecule 7 is water.

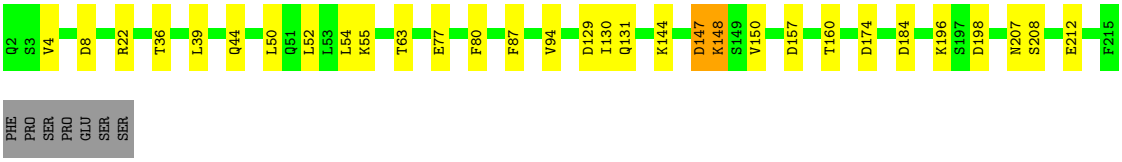
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	C	1	1	1	0	0

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. 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. 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.

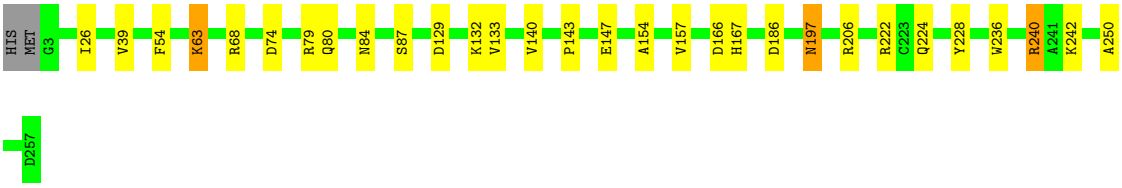
- Molecule 1: T-CELL RECEPTOR, LS2.8/3.15 alpha

Chain D:



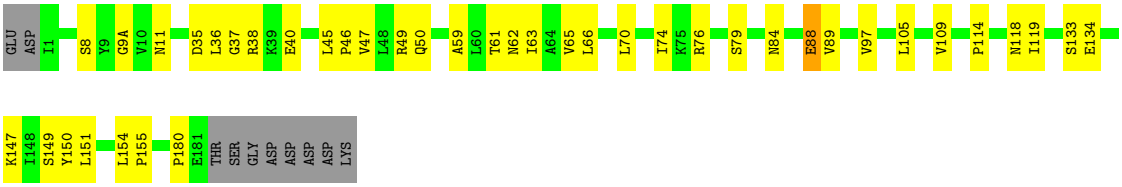
- Molecule 2: T-CELL RECEPTOR, LS2.8/3.15 beta

Chain E:



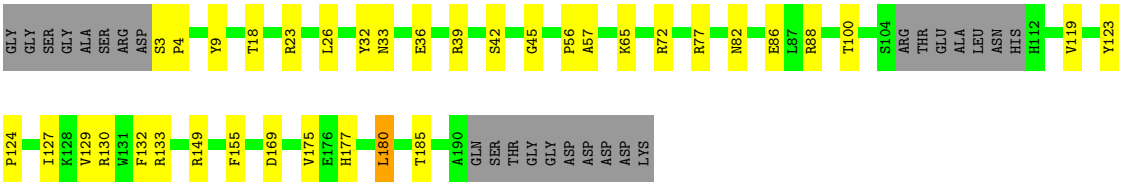
- Molecule 3: MHC class II HLA-DQ-alpha chain

Chain A:



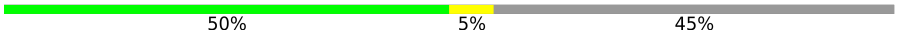
- Molecule 4: MHC class II HLA-DQ-beta-1

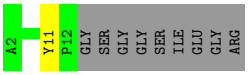
Chain B:



• Molecule 5: Peptide

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	59.98Å 239.47Å 147.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.48 – 2.80 46.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.48-2.80) 99.9 (46.48-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	(Not available) , (Not available) 0.227 , 0.276	Depositor DCC
R_{free} test set	1349 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	76.5	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6478	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 4.07% 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: 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	D	0.26	0/1586	0.44	0/2156
2	E	0.26	0/1964	0.44	0/2673
3	A	0.25	0/1487	0.45	0/2031
4	B	0.23	0/1507	0.41	0/2050
5	C	0.27	0/90	0.42	0/125
All	All	0.25	0/6634	0.44	0/9035

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	D	1548	0	1448	13	0
2	E	1911	0	1805	13	0
3	A	1445	0	1398	24	0
4	B	1474	0	1427	22	0
5	C	85	0	83	1	0
6	A	14	0	13	0	0
7	C	1	0	0	0	0
All	All	6478	0	6174	66	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 5.

All (66) 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)
3:A:38:ARG:NH2	3:A:40:GLU:OE2	2.17	0.78
2:E:133:VAL:O	2:E:240:ARG:NH2	2.21	0.72
3:A:97:VAL:HG11	3:A:180:PRO:HB3	1.73	0.69
1:D:129:ASP:OD2	1:D:131:GLN:NE2	2.26	0.68
3:A:36:LEU:N	3:A:37:GLY:HA3	2.12	0.65
3:A:119:ILE:HD12	3:A:149:SER:HB2	1.78	0.64
2:E:63:LYS:HA	2:E:80:GLN:HB3	1.79	0.63
1:D:63:THR:OG1	1:D:80:PHE:O	2.17	0.62
4:B:129:VAL:HG13	4:B:175:VAL:HG22	1.81	0.62
3:A:11:ASN:HB3	3:A:66:LEU:HD11	1.81	0.61
3:A:50:GLN:OE1	4:B:88:ARG:NH2	2.32	0.61
3:A:45:LEU:HD12	3:A:46:PRO:HD2	1.84	0.59
3:A:70:LEU:HD13	4:B:9:TYR:HB2	1.84	0.59
4:B:177:HIS:H	4:B:180:LEU:HD11	1.67	0.58
1:D:196:LYS:HE3	1:D:198:ASP:OD2	2.05	0.57
2:E:167:HIS:HB3	2:E:228:TYR:HB2	1.85	0.56
4:B:129:VAL:HG22	4:B:175:VAL:HG13	1.88	0.56
4:B:133:ARG:NH1	4:B:169:ASP:OD2	2.38	0.55
4:B:45:GLY:O	4:B:72:ARG:NH1	2.40	0.55
2:E:197:ASN:OD1	2:E:197:ASN:N	2.40	0.54
1:D:207:ASN:N	1:D:207:ASN:OD1	2.42	0.53
2:E:143:PRO:HG3	2:E:154:ALA:HB1	1.92	0.51
4:B:119:VAL:HG11	4:B:127:ILE:HD11	1.92	0.51
1:D:52:LEU:HD21	1:D:55:LYS:HD3	1.94	0.49
4:B:36:GLU:OE2	4:B:39:ARG:HB3	2.12	0.49
2:E:140:VAL:HG23	2:E:250:ALA:HB3	1.95	0.49
3:A:76:ARG:HH12	4:B:56:PRO:HG3	1.78	0.48
2:E:222:ARG:NH1	2:E:224:GLN:OE1	2.43	0.48
2:E:166:ASP:OD1	2:E:166:ASP:N	2.39	0.48
1:D:36:THR:O	4:B:77:ARG:NH1	2.47	0.48
4:B:36:GLU:OE1	4:B:39:ARG:NH2	2.39	0.48
1:D:39:LEU:HD13	1:D:87:PHE:HB2	1.96	0.47
3:A:154:LEU:HD12	3:A:155:PRO:HD2	1.95	0.47
4:B:149:ARG:HG3	4:B:155:PHE:CE2	2.48	0.47
2:E:236:TRP:HB2	2:E:242:LYS:HD3	1.95	0.47
1:D:207:ASN:HA	1:D:208:SER:HA	1.62	0.47
3:A:88:GLU:H	3:A:88:GLU:HG3	1.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:18:THR:HB	4:B:23:ARG:HB3	1.98	0.46
3:A:134:GLU:OE1	3:A:147:LYS:NZ	2.39	0.46
1:D:150:VAL:HG11	2:E:157:VAL:HG11	1.98	0.45
3:A:66:LEU:HD22	4:B:9:TYR:CE2	2.51	0.45
3:A:35:ASP:C	3:A:37:GLY:HA3	2.37	0.44
4:B:26:LEU:HB3	4:B:42:SER:HB3	1.99	0.44
2:E:129:ASP:N	2:E:129:ASP:OD1	2.51	0.44
1:D:8:ASP:OD1	1:D:22:ARG:NH2	2.44	0.43
1:D:44:GLN:HB2	1:D:50:LEU:HD23	2.01	0.43
4:B:32:TYR:HA	4:B:33:ASN:HA	1.76	0.43
2:E:186:ASP:OD1	2:E:206:ARG:NH2	2.42	0.43
4:B:57:ALA:HB2	5:C:11:TYR:CE1	2.54	0.43
4:B:129:VAL:O	4:B:130:ARG:NE	2.52	0.43
3:A:45:LEU:HG	3:A:47:VAL:HG12	2.01	0.43
3:A:59:ALA:O	3:A:63:ILE:HG12	2.19	0.43
3:A:35:ASP:O	3:A:36:LEU:HG	2.19	0.42
3:A:74:ILE:HG23	3:A:79:SER:HA	2.00	0.42
3:A:133:SER:O	3:A:150:TYR:N	2.51	0.42
4:B:123:TYR:CG	4:B:124:PRO:HA	2.54	0.42
3:A:61:THR:O	3:A:65:VAL:HG23	2.20	0.42
1:D:147:ASP:O	1:D:148:LYS:HG3	2.20	0.42
3:A:84:ASN:HA	3:A:114:PRO:HD3	2.02	0.42
3:A:89:VAL:HG22	3:A:109:VAL:HG13	2.02	0.41
3:A:8:SER:C	3:A:9(A):GLY:HA2	2.41	0.41
4:B:82:ASN:O	4:B:86:GLU:HG2	2.20	0.41
3:A:105:LEU:HD12	3:A:151:LEU:HD23	2.03	0.40
1:D:130:ILE:HB	1:D:157:ASP:HA	2.02	0.40
4:B:3:SER:HA	4:B:4:PRO:HD3	1.86	0.40
2:E:39:VAL:HG11	2:E:87:SER:HB2	2.04	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	D	197/206 (96%)	183 (93%)	13 (7%)	1 (0%)	29	61
2	E	240/244 (98%)	231 (96%)	8 (3%)	1 (0%)	34	66
3	A	179/191 (94%)	169 (94%)	10 (6%)	0	100	100
4	B	177/206 (86%)	164 (93%)	13 (7%)	0	100	100
5	C	9/20 (45%)	8 (89%)	1 (11%)	0	100	100
All	All	802/867 (92%)	755 (94%)	45 (6%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	174	ASP
2	E	132	LYS

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	D	171/181 (94%)	161 (94%)	10 (6%)	20	50
2	E	205/211 (97%)	195 (95%)	10 (5%)	25	57
3	A	165/174 (95%)	161 (98%)	4 (2%)	49	81
4	B	163/184 (89%)	158 (97%)	5 (3%)	40	74
5	C	10/15 (67%)	10 (100%)	0	100	100
All	All	714/765 (93%)	685 (96%)	29 (4%)	30	64

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4	VAL
1	D	54	LEU
1	D	77	GLU
1	D	94	VAL
1	D	144	LYS
1	D	147	ASP

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Mol	Chain	Res	Type
1	D	148	LYS
1	D	160	THR
1	D	184	ASP
1	D	212	GLU
2	E	26	ILE
2	E	54	PHE
2	E	63	LYS
2	E	68	ARG
2	E	74	ASP
2	E	79	ARG
2	E	84	ASN
2	E	147	GLU
2	E	197	ASN
2	E	240	ARG
3	A	49	ARG
3	A	62	ASN
3	A	88	GLU
3	A	118	ASN
4	B	65	LYS
4	B	100	THR
4	B	132	PHE
4	B	180	LEU
4	B	185	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	48	GLN
1	D	131	GLN
2	E	152	GLN
2	E	233	ASN
4	B	177	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
6	NAG	A	1001	-	14,14,15	0.19	0	17,19,21	0.45	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
6	NAG	A	1001	-	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1001	NAG	C8-C7-N2-C2
6	A	1001	NAG	O7-C7-N2-C2
6	A	1001	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.