Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2016 – 02:29 PM EST

PDB ID	:	5I78
Title	:	Crystal structure of a beta-1,4-endoglucanase from Aspergillus niger
Authors	:	Liu, W.D.; Yan, J.J.; Li, Y.J.; Zheng, Y.Y.; Chen, C.C.; Guo, R.T.
Deposited on	:	2016-02-17
Resolution	:	1.58 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:

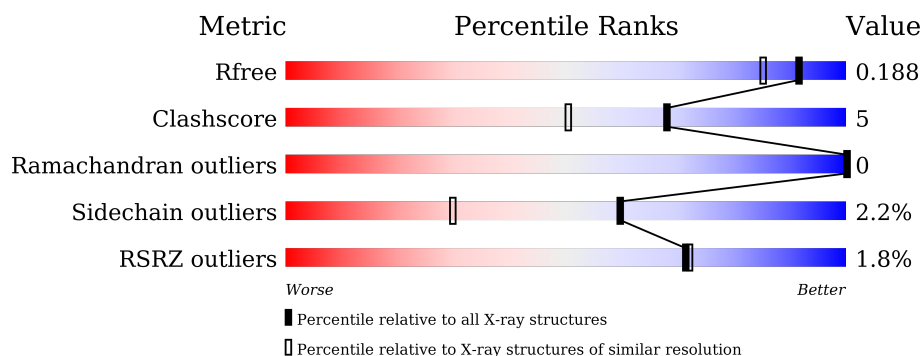|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 1.58 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	3815 (1.60-1.56)
Clashscore	102246	4131 (1.60-1.56)
Ramachandran outliers	100387	4021 (1.60-1.56)
Sidechain outliers	100360	4018 (1.60-1.56)
RSRZ outliers	91569	3823 (1.60-1.56)

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	305	2% — 90% — 10%
1	B	305	2% — 84% — 15% •

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	B	408	-	-	-	X
4	PGE	A	406	-	-	-	X
4	PGE	B	401	-	-	-	X
4	PGE	B	402	-	-	-	X
4	PGE	B	404	-	-	-	X
4	PGE	B	406	-	-	-	X
4	PGE	B	407	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5516 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 Endo-beta-1, 4-glucanase.

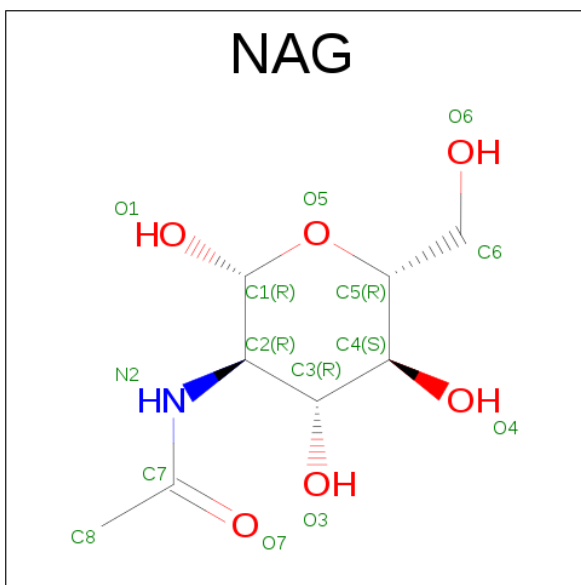| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total 2398	C 1519	N 382	O 484	S 13	0	0	0
1	B	305	Total 2398	C 1519	N 382	O 484	S 13	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ALA	-	expression tag	UNP A0A023UH08
A	29	GLU	-	expression tag	UNP A0A023UH08
A	30	PHE	-	expression tag	UNP A0A023UH08
A	267	ALA	GLU	engineered mutation	UNP A0A023UH08
A	332	LEU	-	expression tag	UNP A0A023UH08
B	28	ALA	-	expression tag	UNP A0A023UH08
B	29	GLU	-	expression tag	UNP A0A023UH08
B	30	PHE	-	expression tag	UNP A0A023UH08
B	267	ALA	GLU	engineered mutation	UNP A0A023UH08
B	332	LEU	-	expression tag	UNP A0A023UH08

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

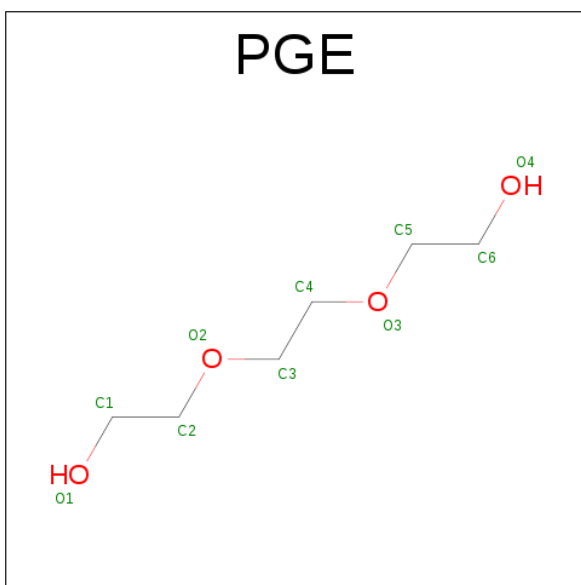| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total 3	Ca 3	0	0

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

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

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 10	C 6	O 4	0	0
4	B	1	Total 10	C 6	O 4	0	0
4	B	1	Total 10	C 6	O 4	0	0
4	B	1	Total 10	C 6	O 4	0	0
4	B	1	Total 10	C 6	O 4	0	0
4	B	1	Total 10	C 6	O 4	0	0
4	B	1	Total 10	C 6	O 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	286	Total 286	O 286	0	0
5	B	305	Total 305	O 305	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 grap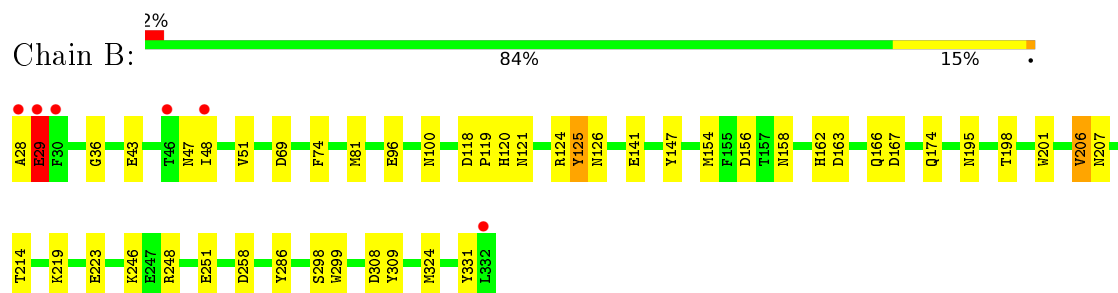hic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor 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: Endo-beta-1, 4-glucanase

• Molecule 1: Endo-beta-1, 4-glucanase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	161.27Å 50.82Å 75.31Å 90.00° 95.08° 90.00°	Depositor
Resolution (Å)	25.00 – 1.58 24.94 – 1.58	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.00-1.58) 99.4 (24.94-1.58)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	7.08 (at 1.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.143 , 0.175 0.157 , 0.188	Depositor DCC
R_{free} test set	4044 reflections (5.13%)	DCC
Wilson B-factor (Å^2)	11.4	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 54.3	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5516	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: CA, PGE, 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	1.19	3/2463 (0.1%)	1.15	9/3355 (0.3%)
1	B	1.26	9/2463 (0.4%)	1.18	12/3355 (0.4%)
All	All	1.23	12/4926 (0.2%)	1.17	21/6710 (0.3%)

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	B	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	298	SER	CB-OG	-7.07	1.33	1.42
1	B	147	TYR	CE1-CZ	6.81	1.47	1.38
1	A	39	GLU	CD-OE2	6.55	1.32	1.25
1	B	309	TYR	CE2-CZ	-6.41	1.30	1.38
1	B	331	TYR	CE1-CZ	-6.21	1.30	1.38
1	A	314	GLU	CD-OE1	6.08	1.32	1.25
1	B	223	GLU	CD-OE1	-5.93	1.19	1.25
1	A	156	ASP	CB-CG	-5.71	1.39	1.51
1	B	206	VAL	CB-CG1	-5.62	1.41	1.52
1	B	125	TYR	CE1-CZ	-5.50	1.31	1.38
1	B	43	GLU	CD-OE2	5.43	1.31	1.25
1	B	286	TYR	CG-CD1	-5.22	1.32	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	VAL	CG1-CB-CG2	-9.69	95.40	110.90
1	B	124	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	B	308	ASP	CB-CG-OD1	7.65	125.19	118.30
1	A	118	ASP	CB-CG-OD2	7.36	124.92	118.30
1	A	94	ASP	CB-CG-OD1	6.62	124.25	118.30
1	A	76	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	B	154	MET	CG-SD-CE	-6.33	90.07	100.20
1	B	69	ASP	CB-CG-OD1	6.33	123.99	118.30
1	B	29	GLU	N-CA-C	6.14	127.58	111.00
1	B	124	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	219	LYS	CD-CE-NZ	-5.82	98.32	111.70
1	A	308	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	32	PHE	CB-CG-CD2	5.62	124.73	120.80
1	B	206	VAL	CA-CB-CG2	5.57	119.25	110.90
1	A	69	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	148	LYS	CD-CE-NZ	-5.26	99.60	111.70
1	A	208	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	A	229	ASP	CB-CG-OD1	5.14	122.93	118.30
1	B	248	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	156	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	258	ASP	CB-CG-OD2	-5.10	113.71	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	29	GLU	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	2398	0	2195	16	1
1	B	2398	0	2195	25	0
2	A	3	0	0	0	0
3	A	28	0	25	2	0
3	B	28	0	26	2	0
4	A	10	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	60	0	84	6	0
5	A	286	0	0	3	4
5	B	305	0	0	9	4
All	All	5516	0	4539	44	6

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 (44) 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:126:ASN:HD22	4:B:406:PGE:H2	1.24	1.01
1:B:167:ASP:OD1	5:B:501:HOH:O	1.81	0.97
1:B:100:ASN:HD22	3:B:403:NAG:H83	1.37	0.88
1:B:174:GLN:HE22	1:B:214:THR:H	1.27	0.83
1:A:100:ASN:HD22	3:A:404:NAG:H83	1.46	0.81
1:A:195:ASN:H	1:A:207:ASN:HD21	1.26	0.81
1:A:174:GLN:HE22	1:A:214:THR:H	1.29	0.80
1:B:195:ASN:H	1:B:207:ASN:HD21	1.29	0.80
4:B:402:PGE:H52	5:B:753:HOH:O	1.82	0.80
1:B:118:ASP:OD2	1:B:120:HIS:HD2	1.66	0.79
1:B:81:MET:H	1:B:121:ASN:HD21	1.35	0.75
1:A:81:MET:H	1:A:121:ASN:HD21	1.36	0.74
1:A:118:ASP:OD2	1:A:120:HIS:HD2	1.74	0.70
1:B:162:HIS:HD2	1:B:163:ASP:OD2	1.75	0.68
1:A:277:ARG:CZ	1:A:327:ILE:HD11	2.23	0.68
4:A:406:PGE:H1	5:A:526:HOH:O	1.94	0.66
1:B:141:GLU:OE1	5:B:503:HOH:O	2.14	0.66
1:A:277:ARG:HD2	5:A:690:HOH:O	1.95	0.64
1:B:100:ASN:ND2	3:B:403:NAG:H83	2.11	0.63
1:B:120:HIS:HE1	5:B:720:HOH:O	1.84	0.60
1:A:166:GLN:HE22	1:A:207:ASN:HD22	1.51	0.57
1:B:166:GLN:HE22	1:B:207:ASN:HD22	1.52	0.57
1:A:81:MET:H	1:A:121:ASN:ND2	2.01	0.57
1:B:81:MET:H	1:B:121:ASN:ND2	2.01	0.56
1:B:162:HIS:HE1	5:B:751:HOH:O	1.89	0.56
1:B:126:ASN:ND2	4:B:406:PGE:H2	2.08	0.55
1:A:195:ASN:N	1:A:207:ASN:HD21	2.01	0.54
4:B:407:PGE:H3	5:B:713:HOH:O	2.09	0.51
1:A:277:ARG:CZ	1:A:327:ILE:CD1	2.90	0.50
1:A:120:HIS:HE1	5:A:731:HOH:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASP:OD2	1:B:120:HIS:CD2	2.56	0.48
1:B:125:TYR:CE2	4:B:406:PGE:H4	2.50	0.47
1:B:299:TRP:CH2	1:B:324:MET:HG2	2.49	0.47
1:B:206:VAL:HG23	5:B:683:HOH:O	2.16	0.46
1:B:47:ASN:C	1:B:48:ILE:HD12	2.38	0.45
4:B:402:PGE:C5	5:B:753:HOH:O	2.55	0.43
1:A:46:THR:O	1:A:48:ILE:HD12	2.18	0.43
1:B:36:GLY:HA3	1:B:74:PHE:O	2.19	0.43
1:A:152:LEU:HG	1:B:28:ALA:HA	2.01	0.43
1:A:118:ASP:OD2	1:A:120:HIS:CD2	2.64	0.42
1:B:48:ILE:N	1:B:48:ILE:HD12	2.35	0.42
1:B:195:ASN:N	1:B:207:ASN:HD21	2.07	0.42
1:A:100:ASN:ND2	3:A:404:NAG:H83	2.24	0.41
1:B:96:GLU:CG	5:B:648:HOH:O	2.67	0.41

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:601:HOH:O	5:B:643:HOH:O[1_554]	1.71	0.49
5:A:662:HOH:O	5:B:683:HOH:O[1_554]	1.81	0.39
5:A:592:HOH:O	5:A:672:HOH:O[4_555]	1.87	0.33
5:B:648:HOH:O	5:B:756:HOH:O[1_565]	2.15	0.05
1:A:237:GLU:OE2	1:A:237:GLU:OE2[2_655]	2.16	0.04
5:A:575:HOH:O	5:B:507:HOH:O[4_546]	2.17	0.03

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	303/305 (99%)	297 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	303/305 (99%)	293 (97%)	10 (3%)	0	100	100
All	All	606/610 (99%)	590 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	252/252 (100%)	249 (99%)	3 (1%)	78	58
1	B	252/252 (100%)	244 (97%)	8 (3%)	46	16
All	All	504/504 (100%)	493 (98%)	11 (2%)	60	30

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	VAL
1	A	158	ASN
1	A	201	TRP
1	B	29	GLU
1	B	51	VAL
1	B	119	PRO
1	B	158	ASN
1	B	198	THR
1	B	201	TRP
1	B	246	LYS
1	B	251	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	121	ASN

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Mol	Chain	Res	Type
1	A	146	GLN
1	A	174	GLN
1	A	207	ASN
1	B	120	HIS
1	B	121	ASN
1	B	126	ASN
1	B	146	GLN
1	B	162	HIS
1	B	174	GLN
1	B	207	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	404	1	14,14,15	1.55	4 (28%)	15,19,21	3.68	6 (40%)
3	NAG	A	405	1,2	14,14,15	0.64	0	15,19,21	1.52	3 (20%)
4	PGE	A	406	-	9,9,9	1.07	0	8,8,8	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	PGE	B	401	-	9,9,9	0.45	0	8,8,8	0.97	1 (12%)
4	PGE	B	402	-	9,9,9	0.78	0	8,8,8	0.66	0
3	NAG	B	403	1	14,14,15	2.23	5 (35%)	15,19,21	2.39	6 (40%)
4	PGE	B	404	-	9,9,9	0.94	0	8,8,8	1.39	2 (25%)
4	PGE	B	405	-	9,9,9	0.58	0	8,8,8	0.79	0
4	PGE	B	406	-	9,9,9	0.95	0	8,8,8	1.07	1 (12%)
4	PGE	B	407	-	9,9,9	1.18	1 (11%)	8,8,8	0.78	0
3	NAG	B	408	1	14,14,15	0.66	0	15,19,21	1.39	2 (13%)

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	404	1	-	0/6/23/26	0/1/1/1
3	NAG	A	405	1,2	-	0/6/23/26	0/1/1/1
4	PGE	A	406	-	-	0/7/7/7	0/0/0/0
4	PGE	B	401	-	-	0/7/7/7	0/0/0/0
4	PGE	B	402	-	-	0/7/7/7	0/0/0/0
3	NAG	B	403	1	-	0/6/23/26	0/1/1/1
4	PGE	B	404	-	-	0/7/7/7	0/0/0/0
4	PGE	B	405	-	-	0/7/7/7	0/0/0/0
4	PGE	B	406	-	-	0/7/7/7	0/0/0/0
4	PGE	B	407	-	-	0/7/7/7	0/0/0/0
3	NAG	B	408	1	-	0/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	403	NAG	C8-C7	-4.86	1.40	1.50
3	A	404	NAG	C1-C2	-2.94	1.48	1.52
3	A	404	NAG	O3-C3	-2.87	1.36	1.43
3	B	403	NAG	C2-N2	-2.65	1.41	1.46
3	B	403	NAG	C1-C2	-2.33	1.49	1.52
3	A	404	NAG	O5-C1	-2.07	1.40	1.43
3	A	404	NAG	C3-C2	2.08	1.57	1.52
4	B	407	PGE	O3-C4	2.21	1.51	1.42
3	B	403	NAG	O4-C4	2.59	1.49	1.43
3	B	403	NAG	O7-C7	4.54	1.33	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	404	NAG	O7-C7-C8	-7.73	107.84	122.07
3	A	404	NAG	O5-C5-C4	-4.29	103.03	110.13
3	A	405	NAG	C6-C5-C4	-3.22	104.92	112.99
3	B	403	NAG	C1-O5-C5	-3.05	107.66	112.14
3	B	408	NAG	O3-C3-C4	-3.00	103.59	110.36
4	B	404	PGE	C3-O2-C2	-2.93	100.79	113.31
3	B	403	NAG	C8-C7-N2	-2.76	110.80	116.10
3	A	405	NAG	O6-C6-C5	-2.53	102.84	111.30
4	B	404	PGE	O3-C4-C3	-2.35	99.99	110.40
3	B	408	NAG	O4-C4-C3	-2.23	105.33	110.36
3	B	403	NAG	O5-C5-C4	-2.19	106.50	110.13
4	B	401	PGE	C5-O3-C4	-2.05	104.55	113.31
3	A	405	NAG	C4-C3-C2	-2.04	108.18	111.34
4	B	406	PGE	O3-C4-C3	2.06	119.52	110.40
3	A	404	NAG	C4-C3-C2	2.20	114.76	111.34
3	B	403	NAG	C3-C4-C5	2.56	114.80	110.23
3	B	403	NAG	O7-C7-N2	3.25	128.47	121.84
3	A	404	NAG	C1-O5-C5	3.54	117.34	112.14
3	B	403	NAG	C2-N2-C7	6.04	130.96	123.11
3	A	404	NAG	O7-C7-N2	6.70	135.50	121.84
3	A	404	NAG	C2-N2-C7	7.26	132.54	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	NAG	2	0
4	A	406	PGE	1	0
4	B	402	PGE	2	0
3	B	403	NAG	2	0
4	B	406	PGE	3	0
4	B	407	PGE	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 (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	305/305 (100%)	-0.16	5 (1%)	74	75	6, 14, 24, 35	0
1	B	305/305 (100%)	-0.22	6 (1%)	68	69	5, 11, 23, 55	0
All	All	610/610 (100%)	-0.19	11 (1%)	71	72	5, 12, 24, 55	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	28	ALA	5.5
1	B	46	THR	5.4
1	B	30	PHE	3.2
1	A	48	ILE	3.2
1	B	29	GLU	3.0
1	A	46	THR	2.9
1	B	48	ILE	2.7
1	B	332	LEU	2.4
1	A	149	ASP	2.4
1	A	239	CYS	2.3
1	A	274	ASP	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)

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
4	PGE	B	401	10/10	0.87	0.20	6.22	31,47,59,60	0
4	PGE	B	407	10/10	0.77	0.18	5.49	31,35,42,45	0
4	PGE	B	404	10/10	0.94	0.11	5.32	9,17,36,42	0
3	NAG	B	408	14/15	0.88	0.17	4.30	15,17,20,21	0
4	PGE	A	406	10/10	0.94	0.11	4.08	10,18,39,40	0
4	PGE	B	402	10/10	0.79	0.14	2.39	34,44,47,47	0
4	PGE	B	406	10/10	0.75	0.19	2.06	39,41,42,45	0
3	NAG	A	404	14/15	0.88	0.11	1.09	19,25,33,39	0
3	NAG	B	403	14/15	0.92	0.08	0.12	10,17,26,28	0
2	CA	A	402	1/1	0.99	0.04	-1.35	14,14,14,14	0
2	CA	A	401	1/1	1.00	0.03	-5.11	14,14,14,14	0
4	PGE	B	405	10/10	0.83	0.16	-	36,44,63,65	0
3	NAG	A	405	14/15	0.87	0.25	-	23,26,32,35	0
2	CA	A	403	1/1	0.99	0.10	-	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.