



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:37 PM UTC

PDB ID : 8HJ6 / pdb_00008hj6
Title : Crystal structure of barley exohydrolase isoform ExoI E220A mutant
Authors : Luang, S.; Streltsov, V.A.; Hrmova, M.
Deposited on : 2022-11-22
Resolution : 1.79 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

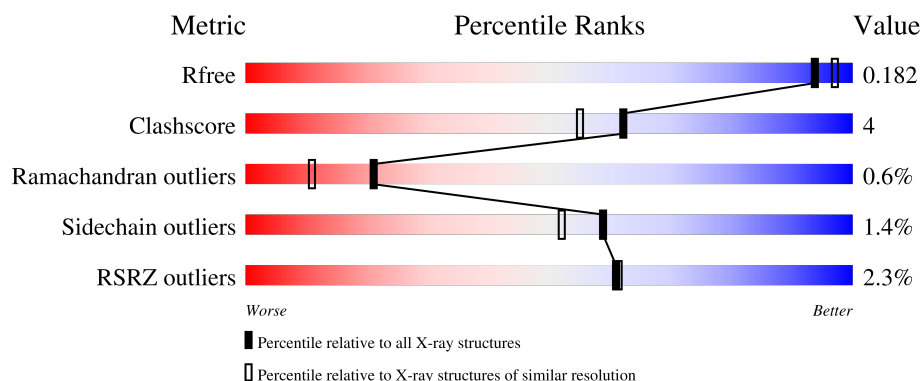
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

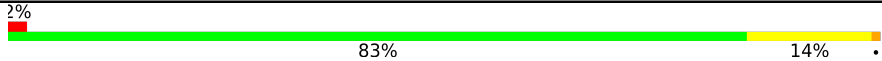
The reported resolution of this entry is 1.79 Å.

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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	609	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5471 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 Glyco_hydro_3 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	606	4617	2918	802	868	29	0	14	0

There are 5 discrepancies between the modelled and reference sequences:

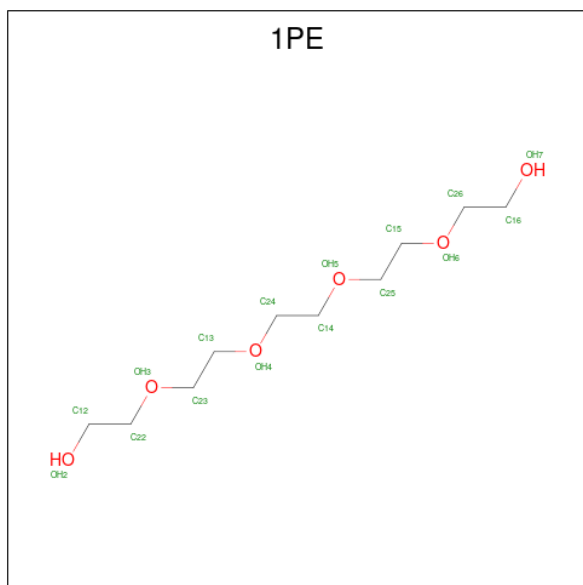
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	expression tag	UNP A0A8I6XKI1
A	-2	HIS	-	expression tag	UNP A0A8I6XKI1
A	-1	ALA	-	expression tag	UNP A0A8I6XKI1
A	220	ALA	GLU	engineered mutation	UNP A0A8I6XKI1
A	320	LYS	ASN	conflict	UNP A0A8I6XKI1

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$) (labeled as "Ligand of Interest" by depositor).



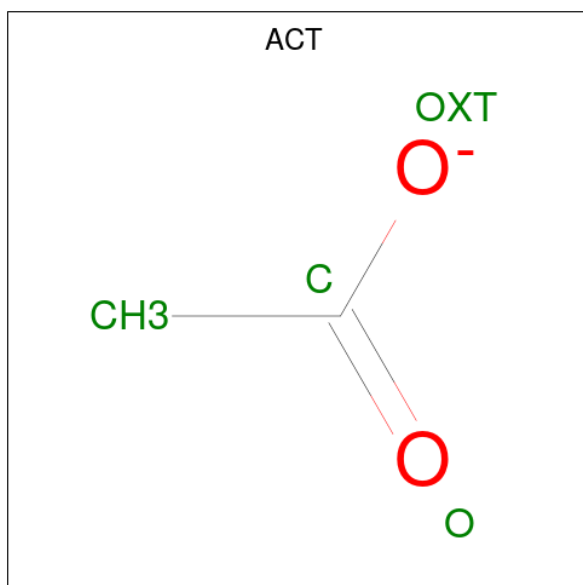
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	7	4		
3	A	1	Total	C	O	0	0
			9	6	3		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

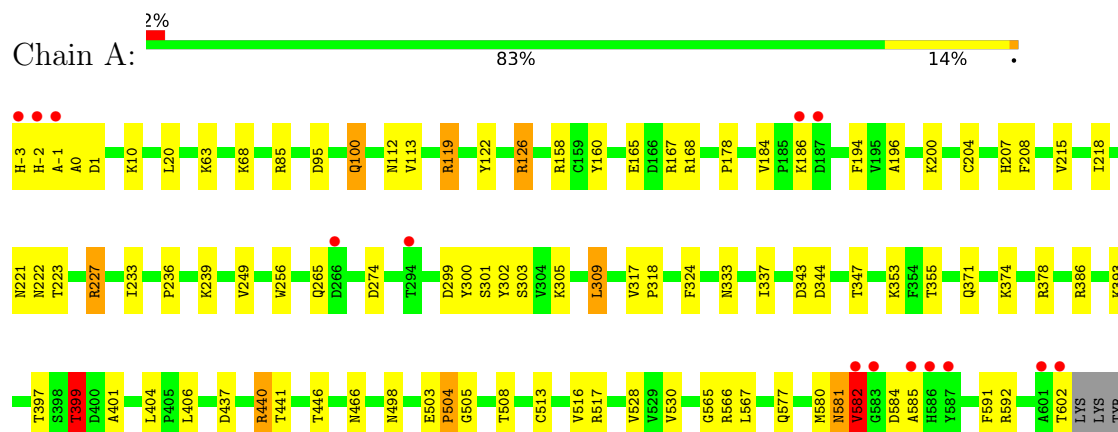
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	695	Total	O	0	0
			695	695		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glyco_hydro_3 domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.23Å 100.23Å 183.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.93 – 1.79 87.93 – 1.79	Depositor EDS
% Data completeness (in resolution range)	95.3 (87.93-1.79) 95.0 (87.93-1.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.79Å)	Xtriage
Refinement program	REFMAC 7.0.005	Depositor
R, R_{free}	0.142 , 0.180 (Not available) , 0.182	Depositor DCC
R_{free} test set	4186 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5471	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4, GOL, ACT, 1PE

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	1.78	66/4769 (1.4%)	1.39	26/6474 (0.4%)

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	4

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	503	GLU	CD-OE2	8.34	1.41	1.25
1	A	126	ARG	CD-NE	-8.32	1.34	1.46
1	A	399	THR	CB-CG2	-7.88	1.26	1.52
1	A	-1	ALA	N-CA	7.86	1.55	1.46
1	A	582	VAL	N-CA	-7.74	1.36	1.46
1	A	440[A]	ARG	CZ-NH1	7.63	1.43	1.32
1	A	1	ASP	CA-C	7.53	1.65	1.52
1	A	355	THR	C-O	7.25	1.32	1.24
1	A	301	SER	CA-CB	7.17	1.64	1.53
1	A	440[A]	ARG	CZ-NH2	7.04	1.42	1.33
1	A	-1	ALA	CA-C	7.03	1.61	1.52
1	A	565	GLY	N-CA	6.91	1.53	1.45
1	A	194	PHE	C-O	-6.75	1.15	1.23
1	A	204	CYS	N-CA	6.70	1.54	1.46
1	A	223	THR	N-CA	-6.65	1.38	1.46
1	A	-2	HIS	N-CA	6.54	1.54	1.46
1	A	233	ILE	CA-CB	-6.40	1.48	1.55
1	A	602	THR	CB-CG2	6.25	1.73	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	ASN	N-CA	6.16	1.54	1.46
1	A	256	TRP	CA-C	6.15	1.59	1.52
1	A	239	LYS	CA-CB	6.09	1.62	1.53
1	A	300	TYR	N-CA	6.08	1.54	1.46
1	A	324	PHE	CA-CB	6.05	1.62	1.53
1	A	517[B]	ARG	NE-CZ	6.02	1.39	1.33
1	A	517[B]	ARG	CZ-NH1	5.93	1.41	1.32
1	A	591	PHE	CA-C	-5.93	1.45	1.52
1	A	303	SER	N-CA	5.92	1.53	1.46
1	A	0	ALA	C-O	-5.88	1.16	1.24
1	A	303	SER	C-O	-5.87	1.17	1.24
1	A	401	ALA	CA-C	5.80	1.59	1.53
1	A	513	CYS	CA-C	5.78	1.60	1.52
1	A	344	ASP	CA-C	5.78	1.60	1.52
1	A	299	ASP	CA-CB	-5.72	1.46	1.53
1	A	337	ILE	N-CA	5.70	1.51	1.46
1	A	528	VAL	C-O	5.58	1.29	1.23
1	A	249	VAL	C-O	5.46	1.29	1.24
1	A	567	LEU	C-N	5.41	1.37	1.33
1	A	302	TYR	CA-CB	5.39	1.61	1.53
1	A	305	LYS	CA-CB	5.38	1.61	1.53
1	A	378	ARG	N-CA	-5.36	1.39	1.46
1	A	371	GLN	CD-NE2	-5.35	1.22	1.33
1	A	517[B]	ARG	CG-CD	5.33	1.68	1.52
1	A	274	ASP	N-CA	5.31	1.53	1.46
1	A	200	LYS	CA-C	5.26	1.59	1.52
1	A	178	PRO	C-O	5.25	1.31	1.24
1	A	167	ARG	CZ-NH1	5.24	1.40	1.32
1	A	337	ILE	CA-C	-5.23	1.48	1.52
1	A	196	ALA	N-CA	-5.22	1.39	1.46
1	A	446	THR	CB-OG1	5.21	1.52	1.43
1	A	440[A]	ARG	NE-CZ	5.21	1.38	1.33
1	A	324	PHE	N-CA	-5.17	1.40	1.46
1	A	393	LYS	N-CA	5.16	1.52	1.45
1	A	309	LEU	C-O	5.15	1.30	1.24
1	A	401	ALA	C-O	-5.14	1.17	1.24
1	A	504	PRO	C-N	-5.13	1.26	1.33
1	A	265	GLN	CD-NE2	-5.12	1.22	1.33
1	A	343	ASP	C-O	5.11	1.30	1.24
1	A	236	PRO	C-O	5.11	1.30	1.24
1	A	233	ILE	CA-C	5.08	1.59	1.52
1	A	184	VAL	N-CA	5.08	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	LYS	CA-C	5.05	1.59	1.52
1	A	126	ARG	NE-CZ	5.04	1.38	1.33
1	A	160	TYR	N-CA	5.03	1.52	1.46
1	A	119	ARG	CZ-NH1	5.03	1.39	1.32
1	A	347	THR	CA-C	5.01	1.59	1.52
1	A	516	VAL	N-CA	-5.00	1.40	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ARG	NE-CZ-NH1	11.46	132.96	121.50
1	A	126	ARG	NE-CZ-NH2	-10.09	110.12	119.20
1	A	440[A]	ARG	CG-CD-NE	-8.98	92.23	112.00
1	A	196	ALA	N-CA-C	7.91	120.99	111.82
1	A	112	ASN	N-CA-C	7.75	120.71	111.33
1	A	126	ARG	CD-NE-CZ	7.60	135.05	124.40
1	A	-2	HIS	N-CA-C	6.25	124.12	110.80
1	A	10	LYS	CA-C-N	6.08	126.02	119.76
1	A	10	LYS	C-N-CA	6.08	126.02	119.76
1	A	399	THR	N-CA-CB	-5.98	101.61	110.53
1	A	440[A]	ARG	NE-CZ-NH2	-5.96	113.83	119.20
1	A	581	ASN	CA-C-N	5.88	132.56	121.97
1	A	581	ASN	C-N-CA	5.88	132.56	121.97
1	A	592	ARG	NE-CZ-NH2	5.85	124.47	119.20
1	A	68	LYS	CD-CE-NZ	5.83	130.55	111.90
1	A	20	LEU	O-C-N	5.47	127.78	122.09
1	A	113	VAL	CB-CA-C	5.41	118.80	111.88
1	A	530	VAL	N-CA-C	5.30	118.83	113.47
1	A	236	PRO	N-CA-C	5.25	121.57	113.75
1	A	301	SER	N-CA-C	5.23	117.39	111.11
1	A	227[A]	ARG	CG-CD-NE	5.13	123.30	112.00
1	A	227[B]	ARG	CG-CD-NE	5.13	123.30	112.00
1	A	208	PHE	CA-C-N	5.07	130.82	121.70
1	A	208	PHE	C-N-CA	5.07	130.82	121.70
1	A	440[A]	ARG	CD-NE-CZ	5.05	131.48	124.40
1	A	85	ARG	N-CA-C	5.01	117.39	111.33

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-3	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	A	581	ASN	Mainchain,Peptide
1	A	582	VAL	Peptide

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	4617	0	4572	35	0
2	A	42	0	39	1	0
3	A	20	0	23	5	0
4	A	24	0	32	3	0
5	A	68	0	51	6	0
6	A	5	0	0	0	0
7	A	695	0	0	10	0
All	All	5471	0	4717	38	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 4.

All (38) 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:A:466[A]:ASN:ND2	1:A:508:THR:OG1	2.10	0.85
1:A:566[B]:ARG:NE	7:A:806:HOH:O	2.15	0.79
1:A:227[A]:ARG:NH1	5:A:724:ACT:OXT	2.14	0.77
5:A:711:ACT:H3	7:A:1123:HOH:O	1.84	0.77
1:A:122:TYR:CE2	1:A:126:ARG:HD2	2.22	0.74
1:A:504:PRO:O	7:A:804:HOH:O	2.07	0.73
1:A:119:ARG:HH21	5:A:718:ACT:H2	1.54	0.72
1:A:566[A]:ARG:NE	7:A:806:HOH:O	2.24	0.70
1:A:566[B]:ARG:CZ	7:A:806:HOH:O	2.43	0.65
1:A:582:VAL:HG13	7:A:1059:HOH:O	1.95	0.65
1:A:158:ARG:HH22	3:A:704:1PE:C26	2.11	0.64
4:A:709:GOL:O2	7:A:805:HOH:O	2.13	0.62
1:A:95:ASP:OD2	3:A:704:1PE:H141	1.99	0.62
1:A:165:GLU:OE2	1:A:582:VAL:HG11	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:GLN:HB3	1:A:580[B]:MET:SD	2.41	0.60
1:A:95:ASP:OD1	3:A:704:1PE:H152	2.04	0.57
5:A:710:ACT:H3	7:A:1380:HOH:O	2.07	0.54
1:A:386:ARG:HH12	5:A:715:ACT:H3	1.74	0.52
1:A:399:THR:HG23	7:A:869:HOH:O	2.10	0.52
1:A:95:ASP:OD2	3:A:704:1PE:C14	2.59	0.51
1:A:158:ARG:NH1	4:A:709:GOL:H2	2.28	0.48
1:A:158:ARG:HH11	4:A:709:GOL:H2	1.81	0.46
1:A:582:VAL:HG22	1:A:582:VAL:O	2.16	0.46
1:A:168:ARG:HH22	5:A:722:ACT:H3	1.80	0.45
1:A:207:HIS:NE2	3:A:704:1PE:C26	2.79	0.45
1:A:227[B]:ARG:NH2	7:A:808:HOH:O	2.37	0.45
1:A:100:GLN:HA	1:A:100:GLN:OE1	2.18	0.44
1:A:397:THR:OG1	1:A:399:THR:HG22	2.18	0.43
1:A:404:LEU:HD23	1:A:406:LEU:HG	1.99	0.43
1:A:122:TYR:O	1:A:126:ARG:HD3	2.19	0.43
1:A:218:ILE:HG22	1:A:221:ASN:HB2	2.01	0.43
1:A:437:ASP:HB3	1:A:441:THR:HG21	2.01	0.42
1:A:215:VAL:HG23	1:A:222:ASN:O	2.20	0.41
1:A:222:ASN:HB2	2:A:701:NAG:H82	2.02	0.40
1:A:122:TYR:CD2	1:A:126:ARG:HD2	2.57	0.40
1:A:309:LEU:HA	1:A:309:LEU:HD23	1.89	0.40
1:A:317:VAL:N	1:A:318:PRO:HA	2.37	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	505/609 (83%)	486 (96%)	16 (3%)	3 (1%)	21 11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	585	ALA
1	A	584	ASP
1	A	505	GLY

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	495/489 (101%)	488 (99%)	7 (1%)	59 52

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	100	GLN
1	A	186[A]	LYS
1	A	374	LYS
1	A	399	THR
1	A	440[A]	ARG
1	A	582	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	375	GLN
1	A	487	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

27 ligands 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	$\# Z > 2$
5	ACT	A	721	-	3,3,3	0.96	0	3,3,3	1.32	0
5	ACT	A	719	-	3,3,3	1.15	0	3,3,3	0.86	0
5	ACT	A	712	-	3,3,3	0.76	0	3,3,3	0.85	0
5	ACT	A	724	-	3,3,3	0.93	0	3,3,3	0.84	0
6	SO4	A	727	-	4,4,4	0.78	0	6,6,6	0.80	0
4	GOL	A	708	-	5,5,5	0.43	0	5,5,5	0.74	0
5	ACT	A	717	-	3,3,3	0.94	0	3,3,3	1.17	0
5	ACT	A	716	-	3,3,3	0.80	0	3,3,3	0.68	0
5	ACT	A	722	-	3,3,3	0.92	0	3,3,3	0.59	0
2	NAG	A	701	1	14,14,15	0.94	1 (7%)	17,19,21	1.95	5 (29%)
2	NAG	A	703	-	14,14,15	1.08	1 (7%)	17,19,21	2.19	5 (29%)
5	ACT	A	720	-	3,3,3	0.87	0	3,3,3	0.72	0
5	ACT	A	715	-	3,3,3	0.59	0	3,3,3	0.94	0
3	1PE	A	704	-	10,10,15	1.21	0	9,9,14	1.75	3 (33%)
5	ACT	A	713	-	3,3,3	0.85	0	3,3,3	0.89	0
4	GOL	A	706	-	5,5,5	0.28	0	5,5,5	0.25	0
5	ACT	A	711	-	3,3,3	0.89	0	3,3,3	0.80	0
5	ACT	A	714	-	3,3,3	0.67	0	3,3,3	1.38	0
4	GOL	A	707	-	5,5,5	0.47	0	5,5,5	1.24	0
5	ACT	A	726	-	3,3,3	1.09	0	3,3,3	0.67	0
4	GOL	A	709	-	5,5,5	0.80	0	5,5,5	1.12	1 (20%)
2	NAG	A	702	-	14,14,15	1.07	1 (7%)	17,19,21	1.70	6 (35%)
3	1PE	A	705	-	8,8,15	0.71	0	7,7,14	0.78	0
5	ACT	A	710	-	3,3,3	1.00	0	3,3,3	0.58	0
5	ACT	A	725	-	3,3,3	0.48	0	3,3,3	2.15	1 (33%)
5	ACT	A	718	-	3,3,3	1.09	0	3,3,3	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	A	723	-	3,3,3	0.76	0	3,3,3	1.61	1 (33%)

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	1PE	A	704	-	-	5/8/8/13	-
2	NAG	A	701	1	-	0/6/23/26	0/1/1/1
2	NAG	A	702	-	-	0/6/23/26	0/1/1/1
3	1PE	A	705	-	-	6/6/6/13	-
4	GOL	A	706	-	-	4/4/4/4	-
4	GOL	A	708	-	-	4/4/4/4	-
2	NAG	A	703	-	-	2/6/23/26	0/1/1/1
4	GOL	A	707	-	-	3/4/4/4	-
4	GOL	A	709	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	702	NAG	C1-C2	3.32	1.56	1.52
2	A	701	NAG	C1-C2	2.51	1.55	1.52
2	A	703	NAG	C1-C2	2.23	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	NAG	O5-C1-C2	-5.63	102.58	111.29
2	A	703	NAG	C2-N2-C7	5.08	129.70	122.90
2	A	703	NAG	C4-C3-C2	3.78	116.56	111.02
2	A	703	NAG	C1-C2-N2	3.76	116.36	110.43
2	A	703	NAG	O5-C5-C6	3.42	114.31	107.66
5	A	725	ACT	O-C-CH3	-2.96	110.39	122.53
3	A	704	1PE	C25-OH5-C14	2.85	125.75	113.26
2	A	702	NAG	C2-N2-C7	2.76	126.59	122.90
2	A	701	NAG	C4-C3-C2	2.66	114.91	111.02
2	A	702	NAG	O6-C6-C5	-2.65	102.31	111.33
2	A	702	NAG	C3-C4-C5	-2.62	105.48	110.23
2	A	701	NAG	C2-N2-C7	2.62	126.41	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	702	NAG	O5-C5-C4	-2.39	105.00	110.83
2	A	702	NAG	C1-C2-N2	2.28	114.02	110.43
2	A	701	NAG	O3-C3-C2	-2.27	104.69	109.40
2	A	702	NAG	O5-C1-C2	-2.26	107.79	111.29
5	A	723	ACT	OXT-C-CH3	2.22	124.35	115.05
3	A	704	1PE	OH4-C24-C14	2.18	120.31	110.35
2	A	701	NAG	C1-O5-C5	-2.17	109.28	112.19
3	A	704	1PE	OH5-C25-C15	2.14	120.12	110.35
4	A	709	GOL	O2-C2-C3	2.07	117.73	109.18
2	A	703	NAG	O5-C5-C4	-2.05	105.84	110.83

There are no chirality outliers.

All (24) torsion outliers are listed below:

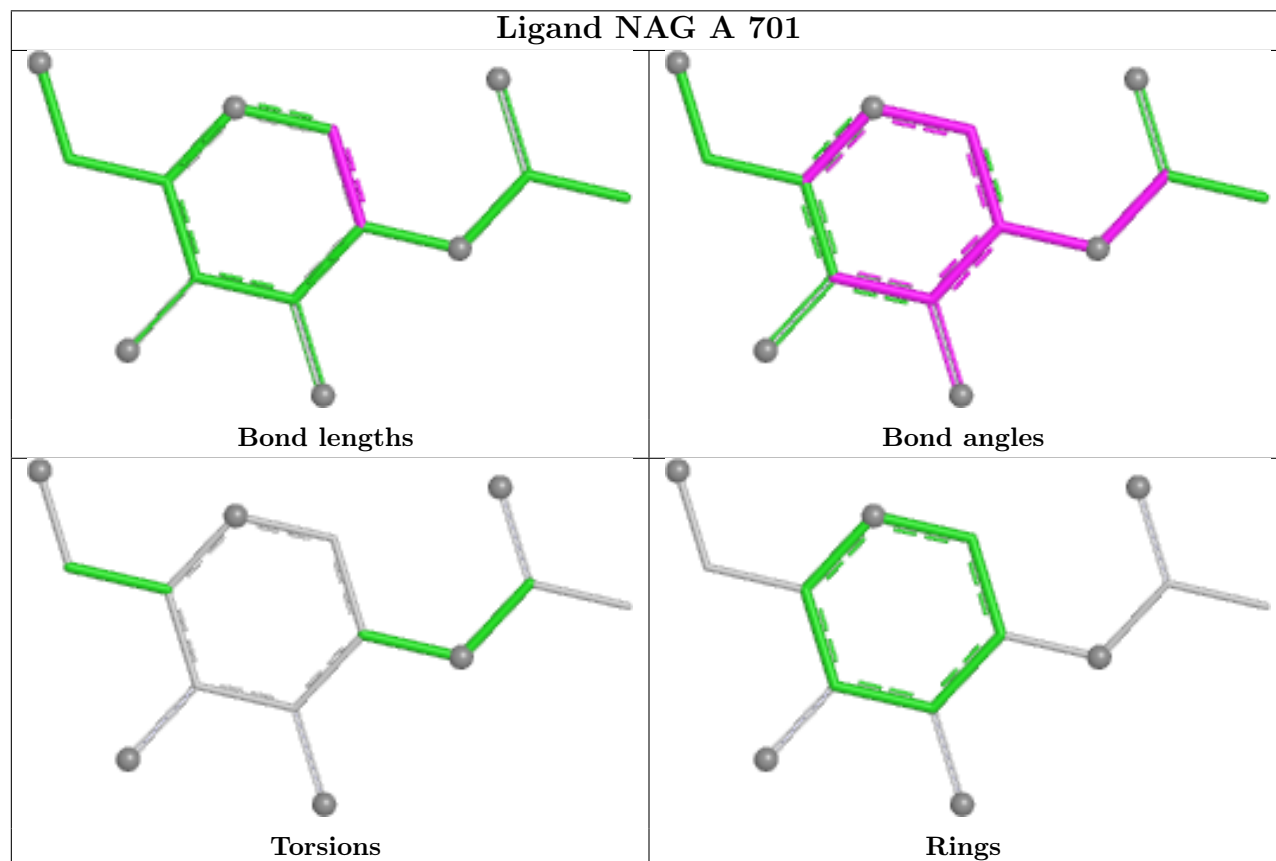
Mol	Chain	Res	Type	Atoms
2	A	703	NAG	C1-C2-N2-C7
4	A	706	GOL	O1-C1-C2-C3
4	A	706	GOL	C1-C2-C3-O3
4	A	708	GOL	O1-C1-C2-O2
4	A	708	GOL	O1-C1-C2-C3
3	A	705	1PE	OH4-C13-C23-OH3
3	A	704	1PE	OH6-C15-C25-OH5
3	A	704	1PE	OH5-C14-C24-OH4
4	A	707	GOL	C1-C2-C3-O3
4	A	708	GOL	C1-C2-C3-O3
4	A	706	GOL	O2-C2-C3-O3
3	A	704	1PE	C15-C25-OH5-C14
3	A	705	1PE	OH2-C12-C22-OH3
4	A	706	GOL	O1-C1-C2-O2
4	A	707	GOL	O2-C2-C3-O3
4	A	708	GOL	O2-C2-C3-O3
3	A	704	1PE	C24-C14-OH5-C25
3	A	704	1PE	C14-C24-OH4-C13
3	A	705	1PE	C23-C13-OH4-C24
3	A	705	1PE	C12-C22-OH3-C23
3	A	705	1PE	C14-C24-OH4-C13
4	A	707	GOL	O1-C1-C2-C3
3	A	705	1PE	C13-C23-OH3-C22
2	A	703	NAG	C4-C5-C6-O6

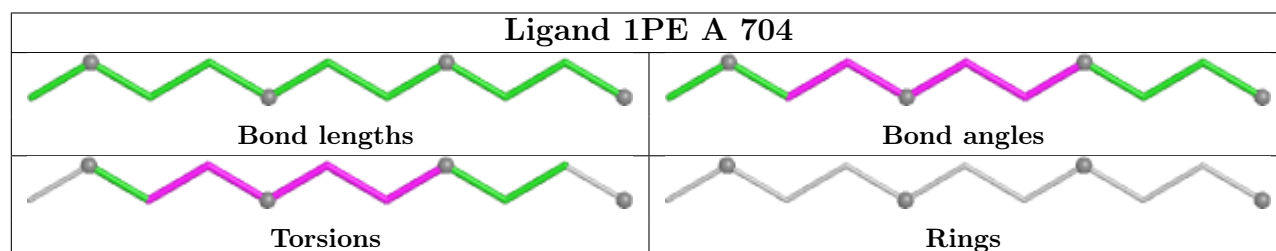
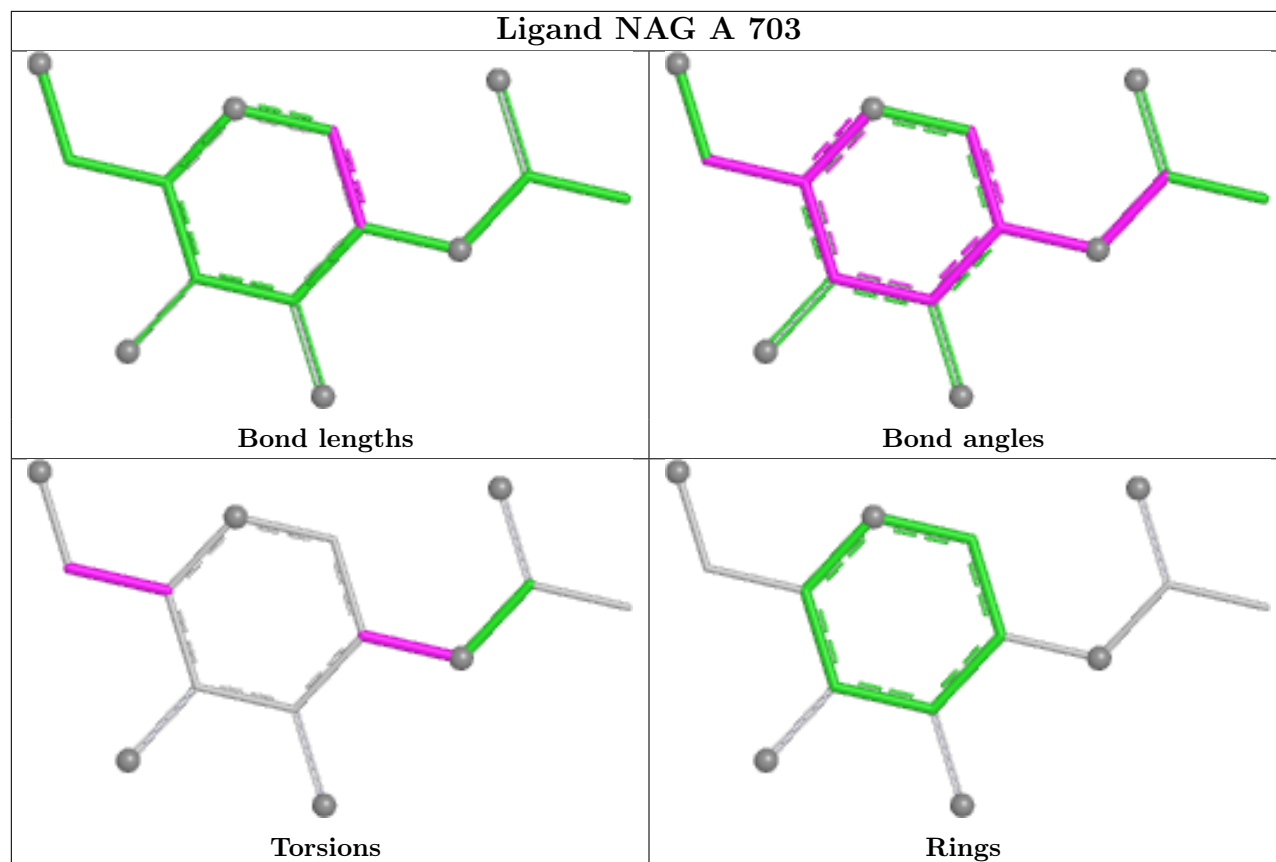
There are no ring outliers.

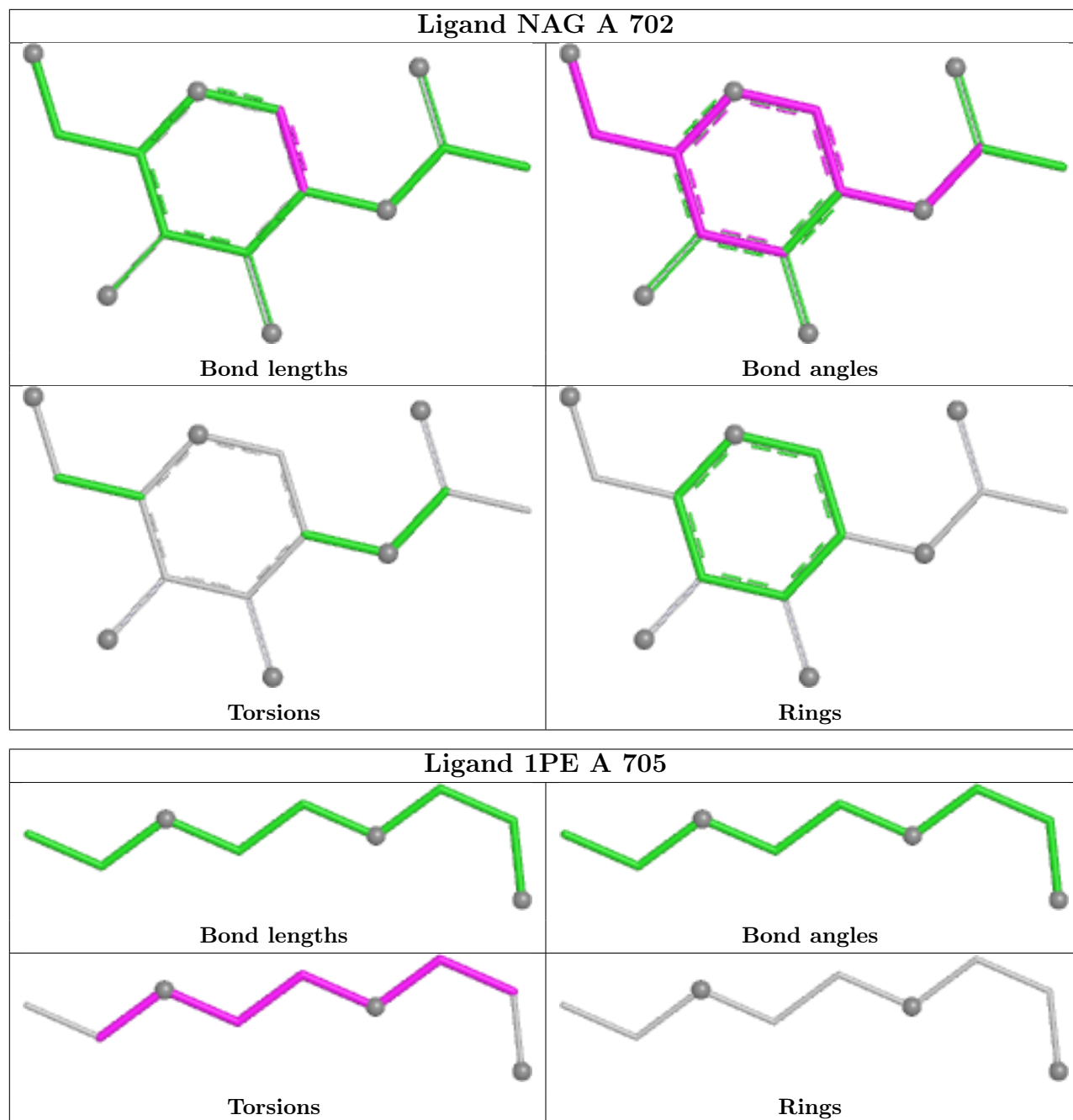
9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	724	ACT	1	0
5	A	722	ACT	1	0
2	A	701	NAG	1	0
5	A	715	ACT	1	0
3	A	704	1PE	5	0
5	A	711	ACT	1	0
4	A	709	GOL	3	0
5	A	710	ACT	1	0
5	A	718	ACT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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	606/609 (99%)	0.03	14 (2%) 61 61	24, 36, 52, 106	8 (1%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-1	ALA	4.7
1	A	582	VAL	4.7
1	A	602	THR	4.3
1	A	-3	HIS	3.9
1	A	-2	HIS	3.6
1	A	585	ALA	3.3
1	A	586	HIS	2.9
1	A	583	GLY	2.8
1	A	186[A]	LYS	2.8
1	A	601	ALA	2.4
1	A	266	ASP	2.4
1	A	587	TYR	2.3
1	A	187	ASP	2.3
1	A	294	THR	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

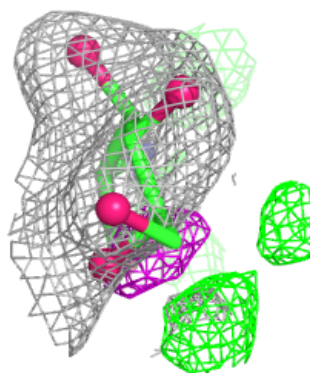
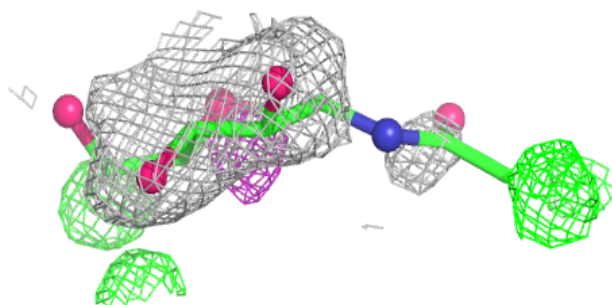
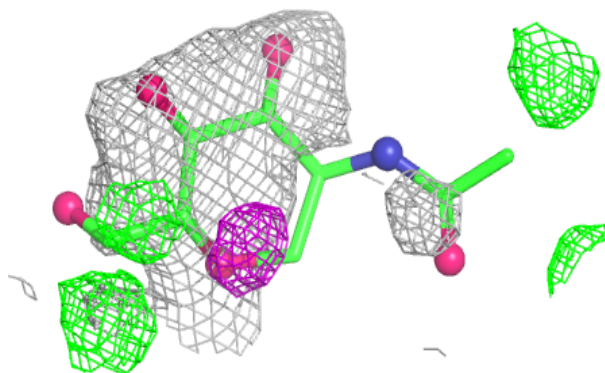
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	A	721	4/4	0.48	0.24	81,81,82,84	0
2	NAG	A	703	14/15	0.56	0.20	87,106,123,124	0
5	ACT	A	723	4/4	0.64	0.23	70,78,82,89	0
5	ACT	A	724	4/4	0.72	0.20	71,80,87,87	0
2	NAG	A	702	14/15	0.73	0.14	82,89,102,103	0
5	ACT	A	726	4/4	0.73	0.26	73,76,79,87	0
5	ACT	A	718	4/4	0.74	0.18	61,70,73,82	0
5	ACT	A	720	4/4	0.75	0.17	77,81,84,89	0
5	ACT	A	722	4/4	0.76	0.17	73,88,90,91	0
5	ACT	A	710	4/4	0.79	0.20	59,81,83,87	0
5	ACT	A	711	4/4	0.80	0.20	61,79,81,89	0
5	ACT	A	717	4/4	0.81	0.16	52,74,79,82	0
5	ACT	A	713	4/4	0.81	0.20	78,84,84,87	0
3	1PE	A	704	11/16	0.82	0.19	28,52,70,85	0
5	ACT	A	725	4/4	0.83	0.18	56,73,75,75	0
3	1PE	A	705	9/16	0.83	0.24	61,77,88,93	0
5	ACT	A	719	4/4	0.84	0.19	63,69,72,74	0
5	ACT	A	712	4/4	0.84	0.17	49,61,63,68	0
5	ACT	A	716	4/4	0.85	0.16	62,68,75,76	0
5	ACT	A	715	4/4	0.86	0.16	62,66,66,73	0
2	NAG	A	701	14/15	0.87	0.13	49,56,82,88	0
4	GOL	A	708	6/6	0.88	0.16	44,61,73,87	0
5	ACT	A	714	4/4	0.89	0.15	60,66,67,68	0
4	GOL	A	706	6/6	0.90	0.16	78,80,85,88	0
4	GOL	A	707	6/6	0.90	0.15	46,74,75,78	0
6	SO4	A	727	5/5	0.91	0.10	40,43,55,56	5
4	GOL	A	709	6/6	0.97	0.10	40,42,44,49	6

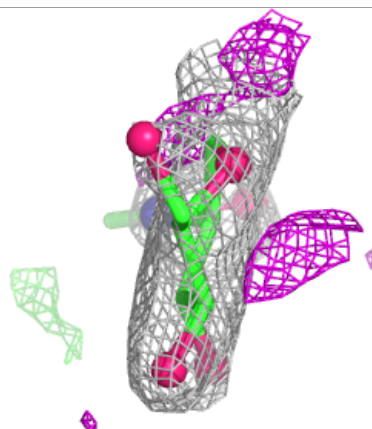
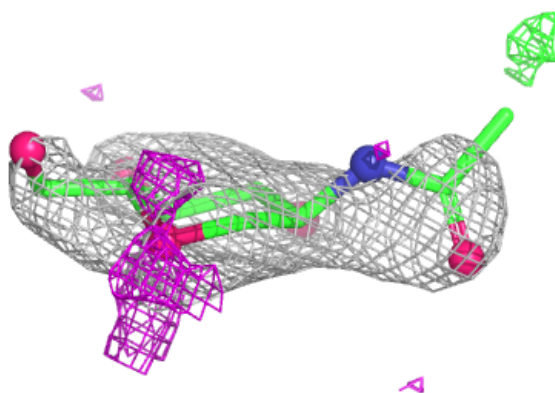
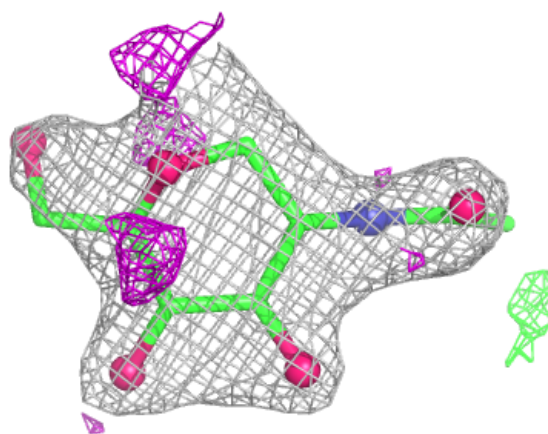
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAG A 703:

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

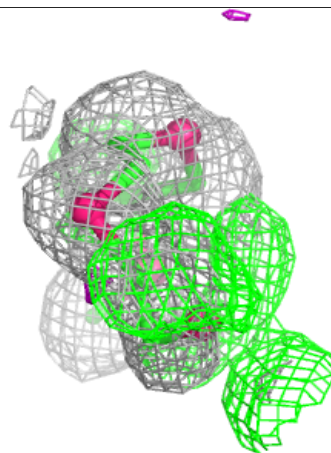
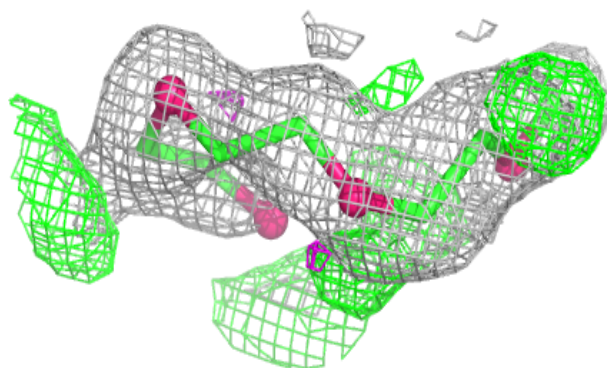
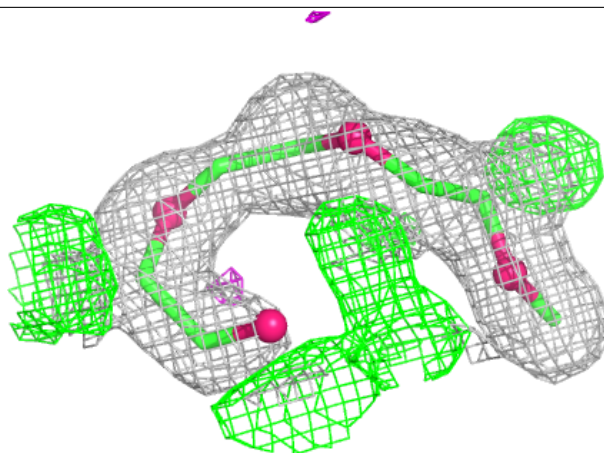
**Electron density around NAG A 702:**

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

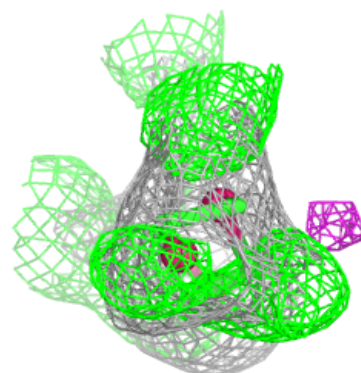
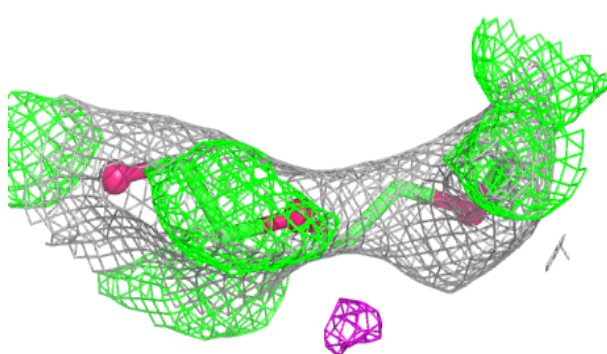
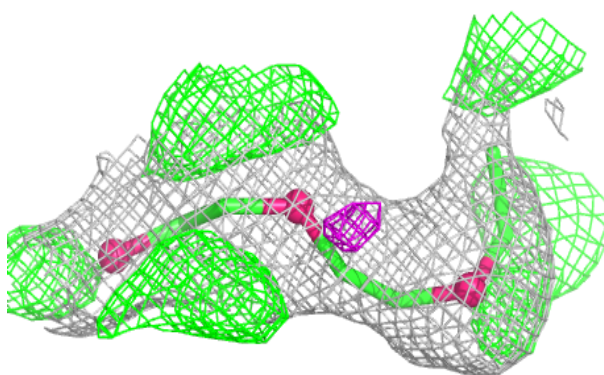


Electron density around 1PE A 704:

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

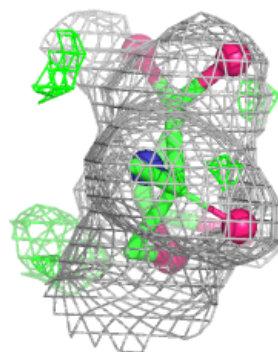
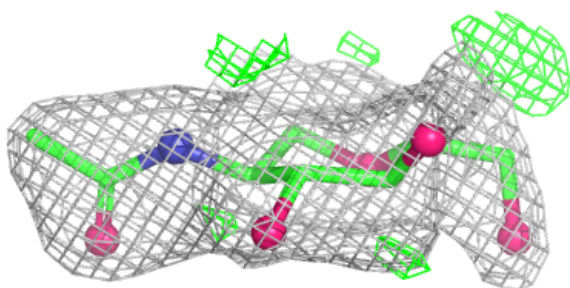
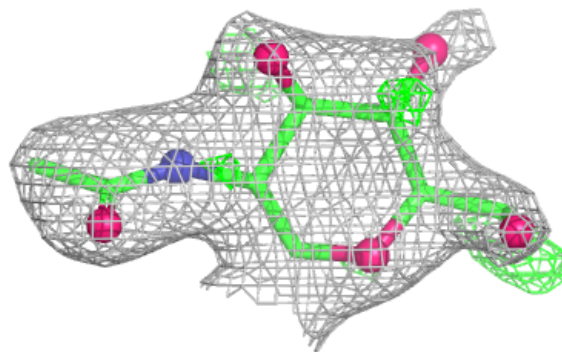
**Electron density around 1PE A 705:**

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



Electron density around NAG A 701:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.