Full wwPDB X-ray Structure Validation Report (i)

May 3, 2025 – 10:21 AM EDT

PDB ID	:	4GTW / pdb_00004gtw
Title	:	Crystal structure of mouse Enpp1 in complex with AMP
Authors	:	Kato, K.; Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on	:	2012-08-29
Resolution	:	2.70 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:

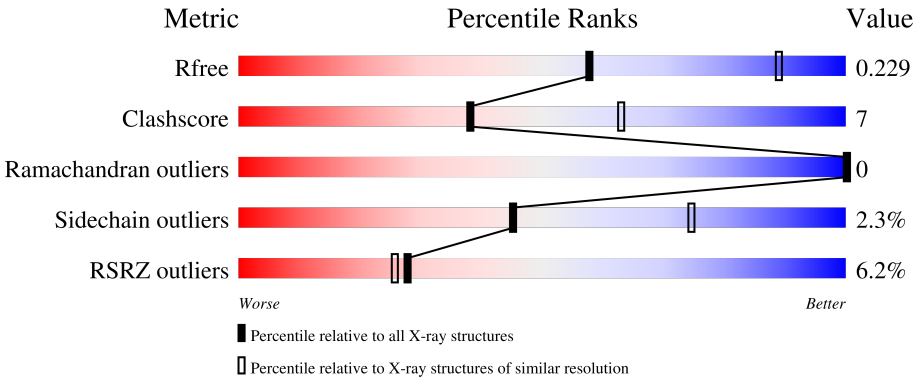
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.70 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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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% 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	823	6% 70% 15% • 14%
1	B	823	5% 70% 13% • 15%
2	C	6	67% 33%
3	D	2	100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11346 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.

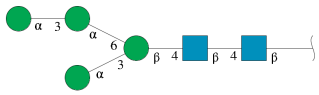
- Molecule 1 is a protein called Ectonucleotide pyrophosphatase/phosphodiesterase family member 2, Alkaline phosphodiesterase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	706	Total	C	N	O	S	Se	0	0	0
			5536	3564	916	1027	17	12			
1	B	697	Total	C	N	O	S	Se	0	0	0
			5481	3527	902	1023	17	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	ARG	LYS	engineered mutation	UNP Q9R1E6
B	59	ARG	LYS	engineered mutation	UNP Q9R1E6

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

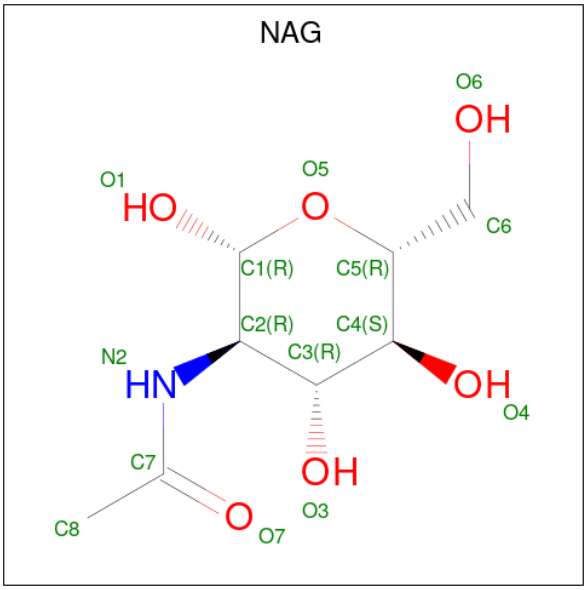


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

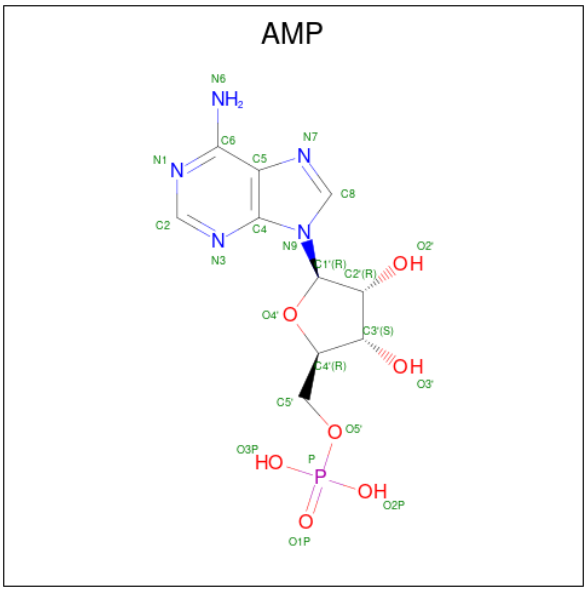
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	2	Total C N O 28 16 2 10	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 23 10 5 7 1	0	0
5	B	1	Total C N O P 23 10 5 7 1	0	0

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Zn 2 2	0	0
6	B	2	Total Zn 2 2	0	0

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	70	Total O 70 70	0	0

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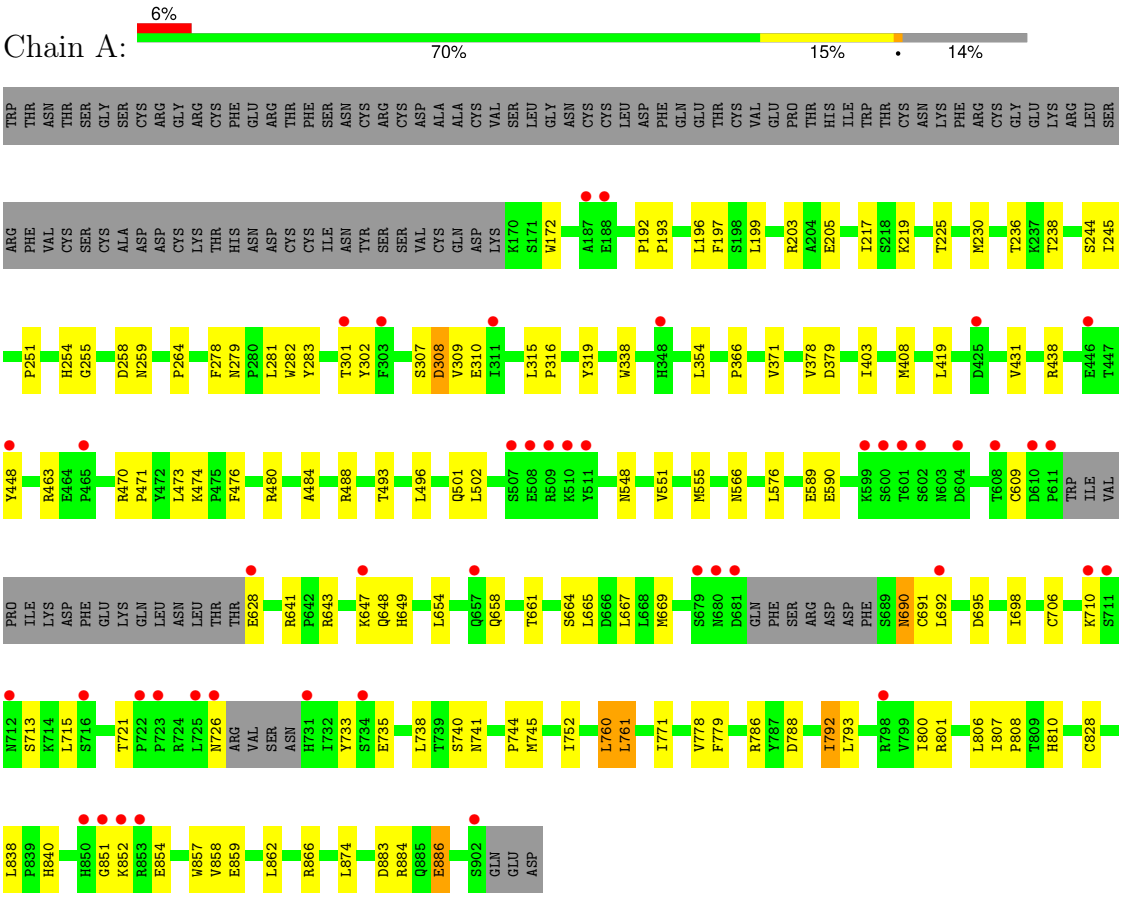
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	51	Total O 51 51	0	0

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 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.

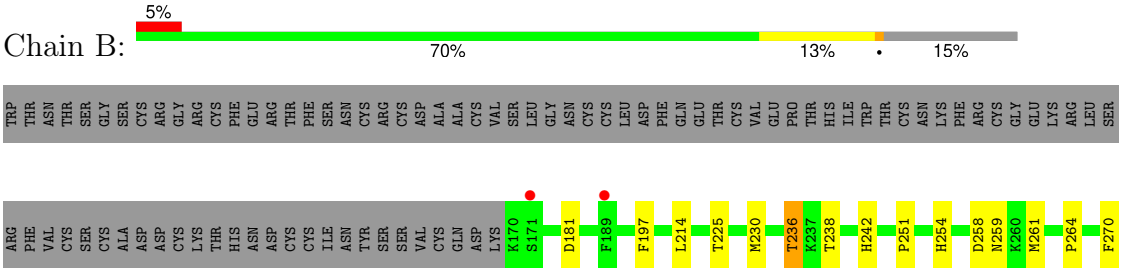
• Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2, Alkaline phosphodiesterase I

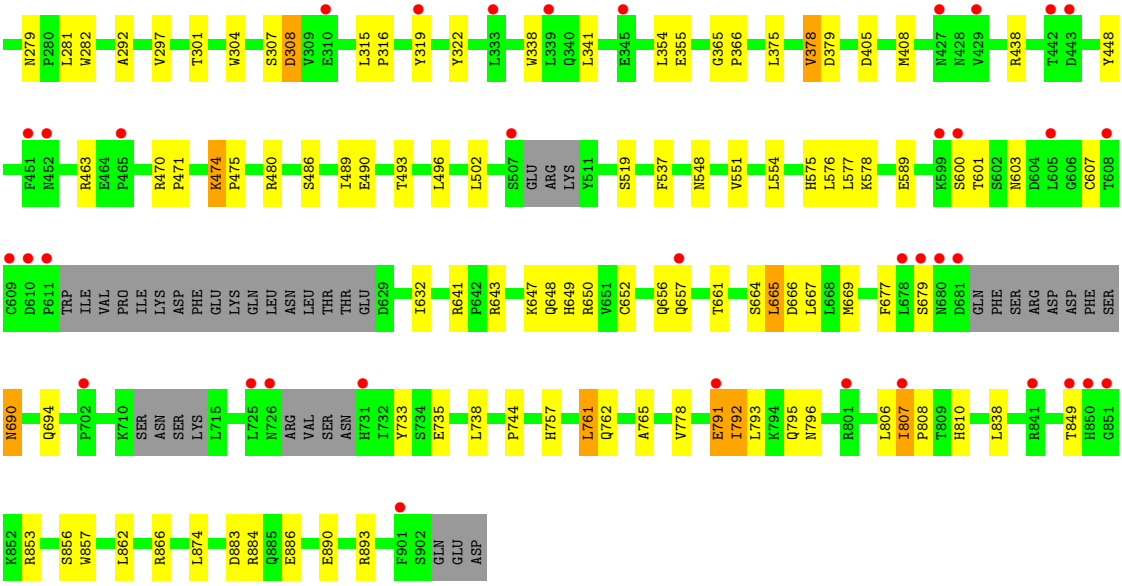
Chain A:



• Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2, Alkaline phosphodiesterase I

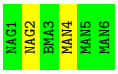
Chain B:





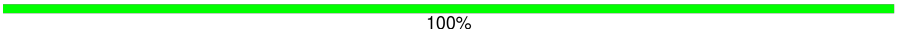
• Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	105.28Å 105.28Å 173.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.88 – 2.70 48.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.88-2.70) 98.4 (48.88-2.70)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.231 , 0.276 0.231 , 0.229	Depositor DCC
R_{free} test set	2916 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l 0.068 for h,-h-k,-l 0.048 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	11346	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, CA, MAN, ZN, NAG, AMP

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	0.29	0/5688	0.75	2/7747 (0.0%)
1	B	0.28	0/5630	0.73	4/7668 (0.1%)
All	All	0.28	0/11318	0.74	6/15415 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	851	GLY	N-CA-C	-7.45	105.61	114.48
1	A	852	LYS	N-CA-C	6.27	120.20	111.74
1	B	474	LYS	CA-C-N	-6.19	113.39	119.64
1	B	474	LYS	C-N-CA	-6.19	113.39	119.64
1	B	365	GLY	CA-C-N	5.12	124.92	119.28
1	B	365	GLY	C-N-CA	5.12	124.92	119.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5536	0	5222	77	0
1	B	5481	0	5156	69	0
2	C	72	0	61	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	28	0	25	0	0
4	A	28	0	26	0	0
4	B	28	0	26	0	0
5	A	23	0	12	2	0
5	B	23	0	12	2	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	70	0	0	3	0
8	B	51	0	0	1	0
All	All	11346	0	10540	147	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 7.

All (147) 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:715:LEU:O	1:A:801:ARG:NH2	2.12	0.83
1:B:650:ARG:NH1	1:B:666:ASP:OD1	2.16	0.78
1:B:230:MSE:HE2	1:B:548:ASN:HA	1.70	0.72
1:B:603:ASN:H	1:B:694:GLN:HE22	1.41	0.69
1:B:225:THR:HG21	1:B:576:LEU:HG	1.75	0.68
1:A:316:PRO:HG2	1:A:319:TYR:HB3	1.75	0.68
1:A:230:MSE:HE2	1:A:548:ASN:HA	1.74	0.68
1:A:225:THR:HG21	1:A:576:LEU:HG	1.78	0.66
1:B:238:THR:OG1	5:B:1005:AMP:P	2.54	0.65
1:A:308:ASP:OD2	1:A:308:ASP:N	2.31	0.64
1:A:838:LEU:HD21	1:A:862:LEU:HD13	1.80	0.63
1:A:238:THR:OG1	5:A:1009:AMP:P	2.57	0.62
1:A:196:LEU:HD22	1:A:555:MSE:HE1	1.80	0.62
1:B:838:LEU:HD11	1:B:862:LEU:HD13	1.81	0.62
1:B:496:LEU:HD21	1:B:502:LEU:HB2	1.81	0.61
1:A:649:HIS:NE2	1:A:664:SER:OG	2.25	0.61
1:B:438:ARG:HG2	1:B:493:THR:HG22	1.82	0.61
1:B:733:TYR:CZ	1:B:735:GLU:HB2	2.35	0.61
1:B:316:PRO:HG2	1:B:319:TYR:HB3	1.82	0.60
1:B:643:ARG:NH2	1:B:883:ASP:OD2	2.34	0.60
1:A:733:TYR:CZ	1:A:735:GLU:HB2	2.37	0.59
1:B:575:HIS:CE1	1:B:893:ARG:HD3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ARG:HG2	1:A:493:THR:HG22	1.84	0.59
1:B:792:ILE:O	1:B:796:ASN:ND2	2.32	0.59
1:A:197:PHE:HE1	1:A:354:LEU:HD13	1.67	0.58
1:B:315:LEU:HD12	1:B:316:PRO:HD2	1.85	0.58
1:B:438:ARG:HB3	1:B:490:GLU:HB2	1.86	0.58
1:A:721:THR:HB	1:A:741:ASN:HD21	1.69	0.57
1:B:649:HIS:HE2	1:B:664:SER:HG	1.51	0.57
1:B:600:SER:OG	1:B:601:THR:N	2.36	0.57
1:A:710:LYS:H	1:A:801:ARG:NH1	2.02	0.57
1:B:735:GLU:HA	1:B:738:LEU:HD13	1.86	0.57
1:A:496:LEU:HD21	1:A:502:LEU:HB2	1.86	0.57
1:A:793:LEU:HD22	1:A:806:LEU:HD21	1.86	0.57
1:A:690:ASN:ND2	1:A:690:ASN:O	2.38	0.57
1:A:643:ARG:NH2	1:A:883:ASP:OD2	2.38	0.56
1:B:264:PRO:HG3	1:B:448:TYR:CZ	2.41	0.56
1:A:698:ILE:HD13	1:A:740:SER:HB3	1.87	0.56
1:B:301:THR:HG21	1:B:307:SER:HB2	1.88	0.55
1:A:501:GLN:NE2	8:A:1138:HOH:O	2.35	0.55
1:A:196:LEU:HD13	1:A:555:MSE:HE1	1.89	0.55
1:A:258:ASP:OD1	1:A:259:ASN:N	2.39	0.54
1:B:258:ASP:OD1	1:B:259:ASN:N	2.40	0.54
1:B:667:LEU:HB3	1:B:669:MSE:HG2	1.89	0.54
1:A:589:GLU:OE2	1:A:641:ARG:NH2	2.41	0.54
1:A:778:VAL:HB	1:A:810:HIS:HB2	1.89	0.54
1:B:744:PRO:HG2	1:B:808:PRO:HD3	1.89	0.54
1:A:301:THR:HG21	1:A:307:SER:HB3	1.89	0.53
1:B:649:HIS:NE2	1:B:664:SER:OG	2.32	0.53
1:B:757:HIS:HA	1:B:761:LEU:HB2	1.90	0.53
1:B:589:GLU:OE2	1:B:641:ARG:NH2	2.42	0.52
1:B:261:MSE:HG3	1:B:270:PHE:HB3	1.90	0.52
1:B:338:TRP:HA	1:B:341:LEU:HD13	1.91	0.52
1:A:760:LEU:HD21	1:A:859:GLU:HG2	1.91	0.52
1:A:649:HIS:HE1	1:A:667:LEU:HD13	1.76	0.51
1:B:890:GLU:HG2	1:B:893:ARG:HH21	1.75	0.51
1:A:735:GLU:HA	1:A:738:LEU:HD13	1.93	0.51
1:A:310:GLU:HB3	1:A:315:LEU:HG	1.91	0.51
1:B:366:PRO:HG3	1:B:408:MSE:HG3	1.92	0.50
1:A:172:TRP:O	1:A:219:LYS:NZ	2.41	0.50
1:A:744:PRO:HG2	1:A:808:PRO:HD3	1.94	0.50
1:A:255:GLY:O	1:A:488:ARG:NH2	2.44	0.49
1:B:197:PHE:HE1	1:B:354:LEU:HD13	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:PHE:HA	1:A:309:VAL:HG22	1.94	0.49
1:A:203:ARG:NH2	1:A:205:GLU:OE1	2.46	0.49
1:A:283:TYR:CE2	1:A:309:VAL:HG21	2.48	0.49
1:A:366:PRO:HG3	1:A:408:MSE:HG3	1.94	0.49
1:A:199:LEU:HD13	1:A:378:VAL:HG11	1.95	0.48
1:A:647:LYS:HA	1:A:648:GLN:HA	1.54	0.48
1:A:264:PRO:HG3	1:A:448:TYR:CZ	2.48	0.48
1:B:607:CYS:HB3	1:B:690:ASN:O	2.13	0.48
1:B:778:VAL:HB	1:B:810:HIS:HB2	1.94	0.48
1:B:486:SER:HB3	1:B:489:ILE:HG13	1.95	0.48
1:A:419:LEU:HD12	1:A:431:VAL:HG21	1.96	0.48
1:B:308:ASP:OD2	1:B:308:ASP:N	2.47	0.47
1:A:566:ASN:ND2	8:A:1108:HOH:O	2.48	0.47
1:B:292:ALA:HB1	1:B:297:VAL:HB	1.97	0.47
1:B:791:GLU:O	1:B:795:GLN:HG3	2.15	0.47
1:A:695:ASP:OD2	1:A:740:SER:OG	2.28	0.46
1:B:649:HIS:HE1	1:B:667:LEU:HD13	1.80	0.46
1:B:537:PHE:O	1:B:578:LYS:NZ	2.36	0.46
1:A:282:TRP:HA	1:A:488:ARG:NH1	2.30	0.46
1:B:214:LEU:HD22	1:B:379:ASP:HB2	1.96	0.46
1:B:853:ARG:O	1:B:856:SER:OG	2.32	0.46
1:A:752:ILE:HG23	1:A:858:VAL:HG13	1.97	0.46
1:B:554:LEU:HD11	1:B:577:LEU:HD21	1.97	0.46
1:B:793:LEU:HD22	1:B:806:LEU:HD21	1.97	0.46
1:A:302:TYR:HD2	1:A:338:TRP:CH2	2.33	0.46
1:A:695:ASP:HB3	1:A:698:ILE:HG12	1.97	0.46
1:B:279:ASN:HB3	1:B:282:TRP:CD1	2.51	0.46
1:B:322:TYR:OH	1:B:355:GLU:OE2	2.31	0.46
1:B:656:GLN:HE22	1:B:661:THR:HG22	1.81	0.46
1:B:251:PRO:HA	1:B:254:HIS:CE1	2.51	0.45
1:B:632:ILE:HG12	1:B:657:GLN:HA	1.98	0.45
1:B:304:TRP:O	1:B:307:SER:OG	2.28	0.45
1:B:677:PHE:HE2	1:B:762:GLN:HA	1.81	0.45
1:A:854:GLU:HA	1:A:857:TRP:NE1	2.31	0.45
1:A:473:LEU:HB2	1:A:476:PHE:CD2	2.51	0.45
1:A:884:ARG:HG3	1:A:886:GLU:HG2	1.97	0.45
1:A:788:ASP:HB3	1:A:792:ILE:HG23	1.98	0.45
1:B:242:HIS:CE1	1:B:405:ASP:HB3	2.51	0.45
1:A:282:TRP:HA	1:A:488:ARG:HH12	1.82	0.44
1:B:603:ASN:N	1:B:694:GLN:HE22	2.11	0.44
1:A:643:ARG:NH1	1:B:181:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:CYS:C	1:A:884:ARG:HH22	2.23	0.44
1:B:677:PHE:CE2	1:B:762:GLN:HA	2.53	0.44
1:A:658:GLN:NE2	1:A:726:ASN:HD22	2.16	0.44
1:A:692:LEU:HD12	1:A:706:CYS:SG	2.58	0.44
1:B:470:ARG:HA	1:B:471:PRO:HD3	1.88	0.44
1:A:366:PRO:O	1:A:371:VAL:HG21	2.18	0.43
1:A:474:LYS:HG2	1:A:484:ALA:HA	1.99	0.43
1:A:245:ILE:HD13	1:A:403:ILE:HD13	2.00	0.43
1:B:474:LYS:HG3	1:B:475:PRO:HD3	2.00	0.43
1:A:807:ILE:HA	1:A:808:PRO:HD3	1.82	0.43
1:B:279:ASN:HB3	1:B:282:TRP:HD1	1.83	0.43
1:A:649:HIS:CE1	1:A:667:LEU:HD13	2.54	0.43
1:B:647:LYS:HA	1:B:648:GLN:HA	1.53	0.43
1:B:375:LEU:O	1:B:378:VAL:HG12	2.19	0.43
1:B:251:PRO:HA	1:B:254:HIS:NE2	2.34	0.43
1:A:480:ARG:HD3	1:A:866:ARG:O	2.19	0.42
1:B:884:ARG:HA	1:B:884:ARG:HD2	1.88	0.42
1:A:251:PRO:HA	1:A:254:HIS:CE1	2.54	0.42
5:A:1009:AMP:N6	8:A:1169:HOH:O	2.32	0.42
1:A:244:SER:OG	1:A:254:HIS:NE2	2.50	0.42
1:B:807:ILE:HA	1:B:808:PRO:HD3	1.83	0.42
1:A:713:SER:HB3	1:A:801:ARG:NH1	2.35	0.42
1:A:217:ILE:HG12	1:A:379:ASP:OD1	2.20	0.42
1:A:669:MSE:SE	1:A:779:PHE:HZ	2.53	0.42
1:B:884:ARG:HG3	1:B:886:GLU:OE1	2.20	0.42
1:B:480:ARG:HD3	1:B:866:ARG:O	2.20	0.41
5:B:1005:AMP:N6	8:B:1149:HOH:O	2.42	0.41
1:A:654:LEU:HB2	1:A:661:THR:HG23	2.01	0.41
1:A:761:LEU:HG	1:A:771:ILE:HD11	2.03	0.41
1:A:172:TRP:CZ3	1:A:219:LYS:HD3	2.55	0.41
1:B:652:CYS:SG	1:B:665:LEU:HD21	2.60	0.41
1:A:470:ARG:HA	1:A:471:PRO:HD3	1.87	0.41
1:A:197:PHE:CE1	1:A:354:LEU:HD13	2.52	0.41
1:A:609:CYS:HA	1:A:691:CYS:HB2	2.03	0.41
1:A:192:PRO:HA	1:A:193:PRO:HD3	1.92	0.41
1:A:715:LEU:HD23	1:A:800:ILE:HD13	2.02	0.41
1:A:786:ARG:HH21	2:C:2:NAG:H62	1.86	0.41
1:B:849:THR:HG23	1:B:857:TRP:NE1	2.36	0.41
1:B:643:ARG:HA	1:B:643:ARG:HD3	1.98	0.40
1:B:677:PHE:CD2	1:B:765:ALA:HB2	2.56	0.40
1:A:745:MSE:HA	1:A:840:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:THR:OG1	1:B:519:SER:O	2.39	0.40
1:A:279:ASN:HB3	1:A:282:TRP:CD1	2.57	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	698/823 (85%)	675 (97%)	23 (3%)	0	100	100
1	B	685/823 (83%)	660 (96%)	25 (4%)	0	100	100
All	All	1383/1646 (84%)	1335 (96%)	48 (4%)	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	600/743 (81%)	586 (98%)	14 (2%)	45	74
1	B	596/743 (80%)	582 (98%)	14 (2%)	45	74
All	All	1196/1486 (80%)	1168 (98%)	28 (2%)	45	74

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	THR
1	A	281	LEU
1	A	308	ASP
1	A	463	ARG
1	A	551	VAL
1	A	590	GLU
1	A	628	GLU
1	A	665	LEU
1	A	690	ASN
1	A	760	LEU
1	A	761	LEU
1	A	792	ILE
1	A	874	LEU
1	A	886	GLU
1	B	236	THR
1	B	281	LEU
1	B	308	ASP
1	B	378	VAL
1	B	463	ARG
1	B	551	VAL
1	B	665	LEU
1	B	679	SER
1	B	690	ASN
1	B	761	LEU
1	B	791	GLU
1	B	792	ILE
1	B	807	ILE
1	B	874	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	ASN
1	A	452	ASN
1	A	525	ASN
1	A	570	HIS
1	A	634	HIS
1	A	658	GLN
1	A	690	ASN
1	A	820	GLN
1	B	293	ASN
1	B	468	HIS
1	B	570	HIS

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Mol	Chain	Res	Type
1	B	583	ASN
1	B	655	GLN
1	B	694	GLN
1	B	820	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)

8 monosaccharides 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	$\#\|Z\| > 2$
2	NAG	C	1	1,2	14,14,15	0.55	0	17,19,21	0.82	0
2	NAG	C	2	2	14,14,15	0.52	0	17,19,21	0.63	0
2	BMA	C	3	2	11,11,12	0.63	0	15,15,17	0.62	0
2	MAN	C	4	2	11,11,12	0.62	0	15,15,17	1.26	2 (13%)
2	MAN	C	5	2	11,11,12	0.57	0	15,15,17	0.73	0
2	MAN	C	6	2	11,11,12	0.63	0	15,15,17	0.46	0
3	NAG	D	1	1,3	14,14,15	0.56	0	17,19,21	0.89	0
3	NAG	D	2	3	14,14,15	0.50	0	17,19,21	0.67	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	2/2/19/22	0/1/1/1
2	MAN	C	5	2	-	1/2/19/22	1/1/1/1
2	MAN	C	6	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4	MAN	C1-O5-C5	2.67	115.76	112.19
2	C	4	MAN	C1-C2-C3	2.32	113.02	109.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	4	MAN	O5-C5-C6-O6
2	C	4	MAN	C4-C5-C6-O6
2	C	5	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

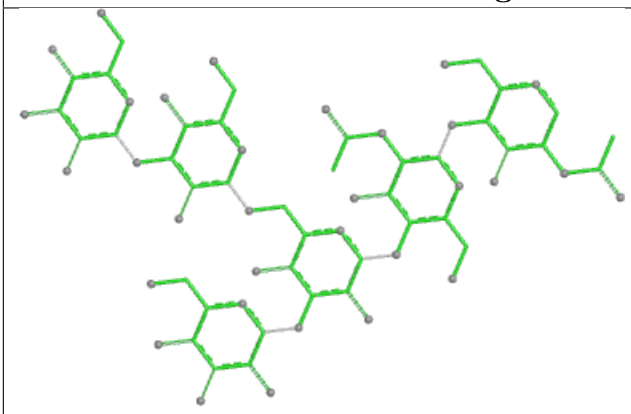
Mol	Chain	Res	Type	Atoms
2	C	5	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 1 short contact:

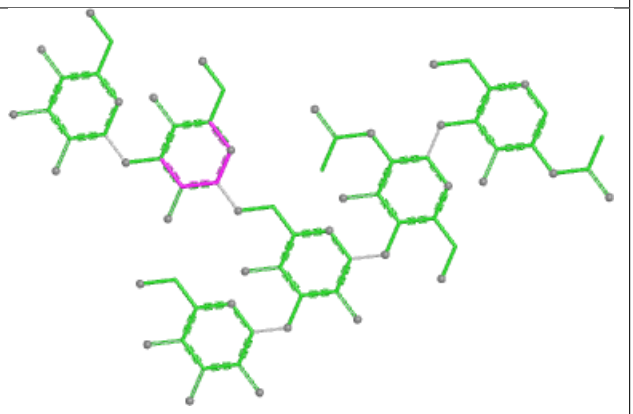
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

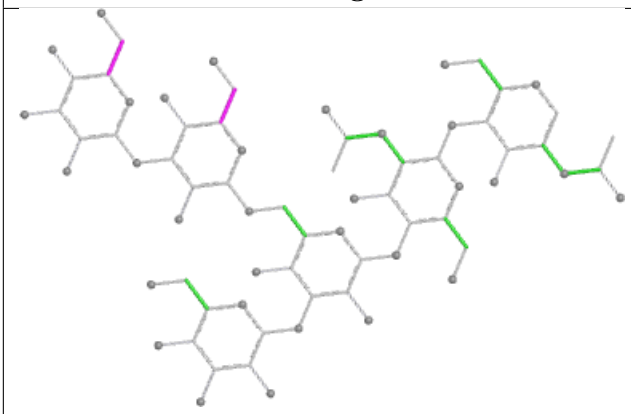
Oligosaccharide Chain C



Bond lengths

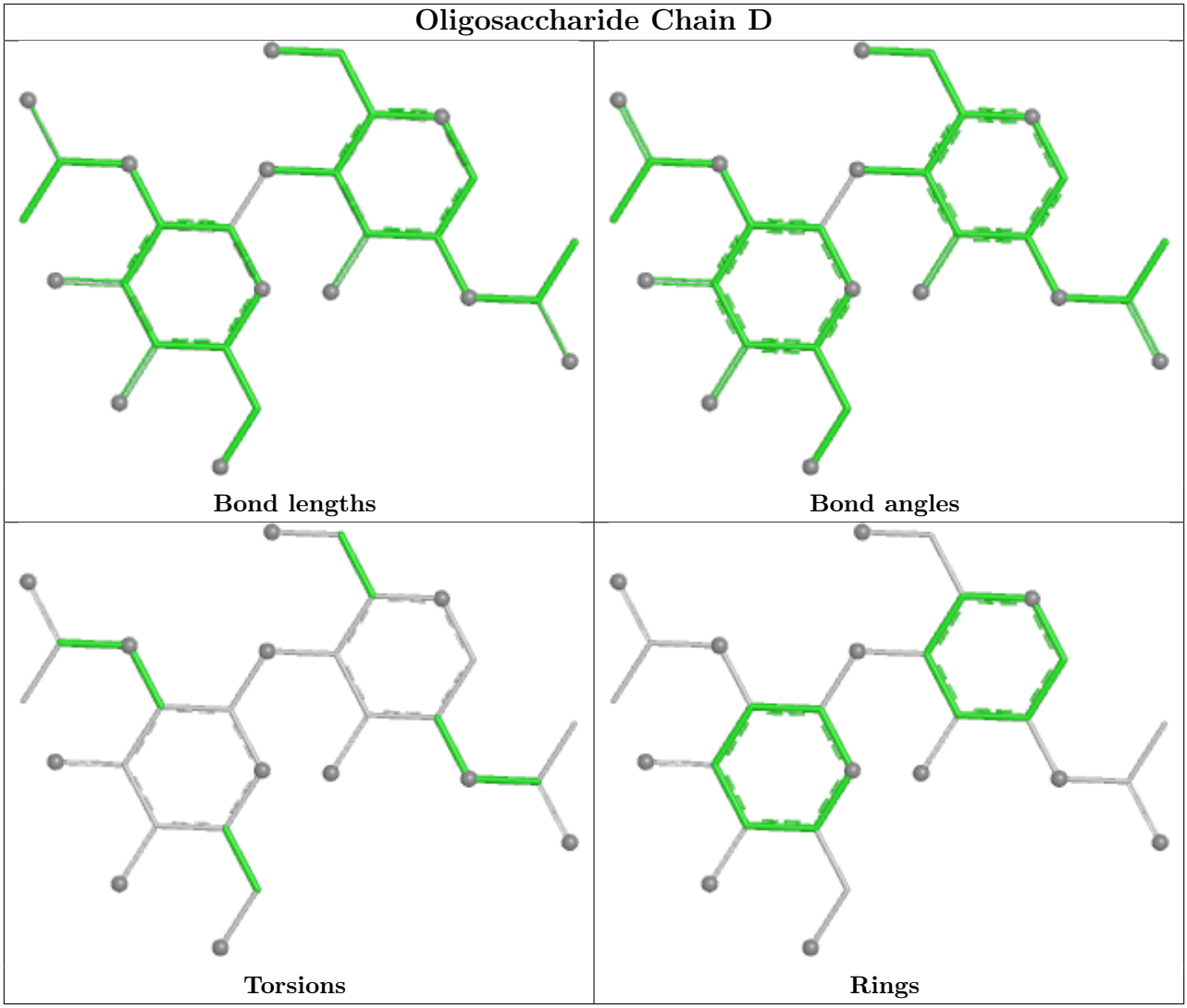


Bond angles



Torsions

Rings



5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
5	AMP	A	1009	6	21,25,25	0.78	0	23,38,38	1.33	3 (13%)
4	NAG	B	1004	1	14,14,15	0.52	0	17,19,21	0.64	0
4	NAG	A	1007	1	14,14,15	0.52	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	A	1008	1	14,14,15	0.51	0	17,19,21	0.66	0
4	NAG	B	1003	1	14,14,15	0.51	0	17,19,21	0.59	0
5	AMP	B	1005	6	21,25,25	0.78	0	23,38,38	1.33	3 (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
5	AMP	A	1009	6	-	0/6/26/26	0/3/3/3
4	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1008	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1003	1	-	0/6/23/26	0/1/1/1
5	AMP	B	1005	6	-	0/6/26/26	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1005	AMP	N3-C2-N1	-3.72	123.62	128.67
5	A	1009	AMP	N3-C2-N1	-3.69	123.67	128.67
5	B	1005	AMP	O3P-P-O5'	-2.78	99.41	106.67
5	A	1009	AMP	C4-C5-N7	-2.68	106.50	109.34
5	A	1009	AMP	O3P-P-O5'	-2.60	99.88	106.67
5	B	1005	AMP	C4-C5-N7	-2.58	106.62	109.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

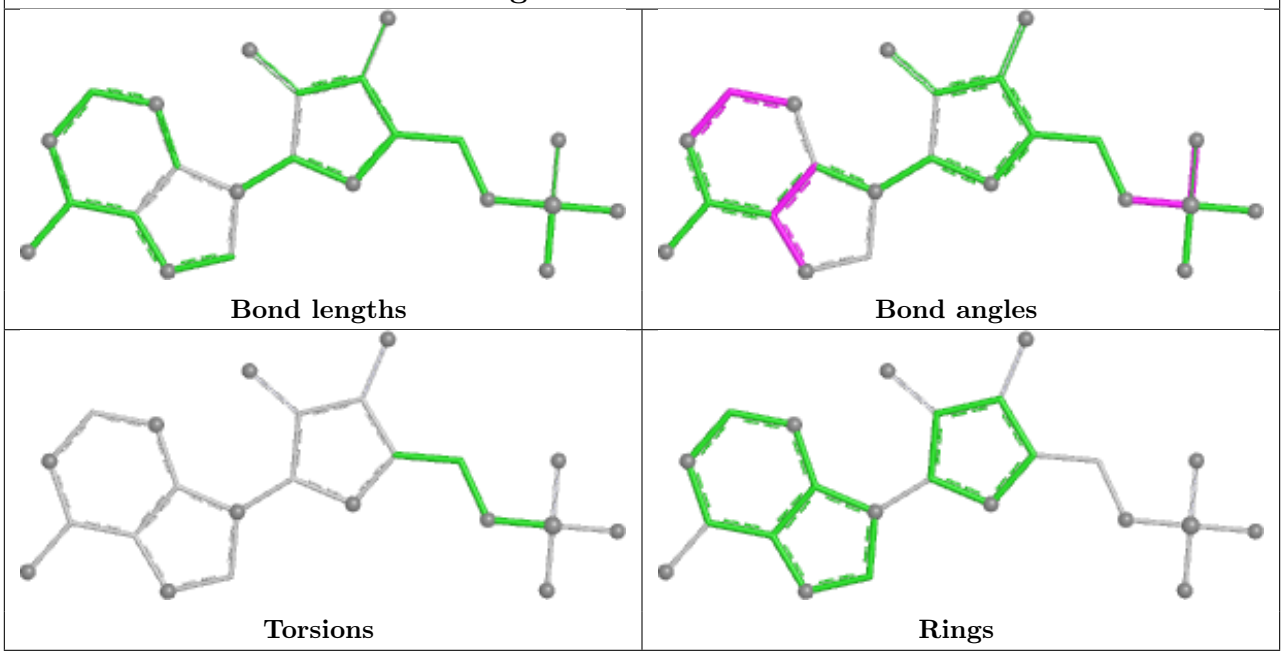
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1009	AMP	2	0
5	B	1005	AMP	2	0

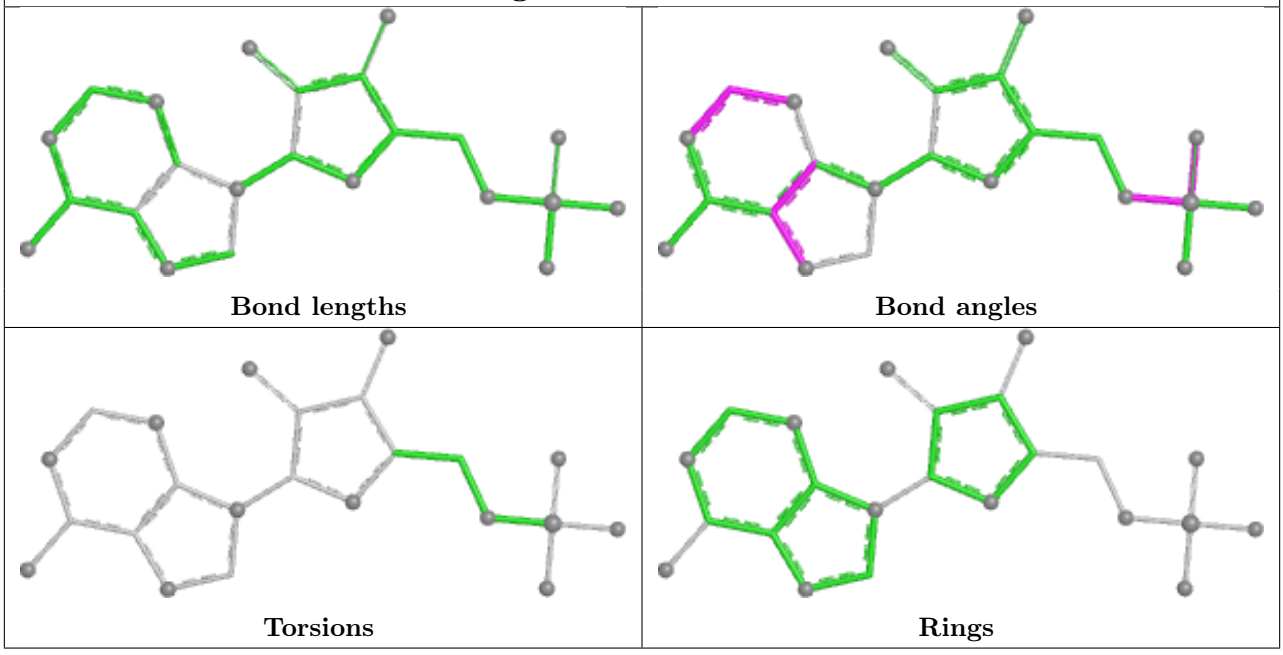
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

Ligand AMP A 1009



Ligand AMP B 1005



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	694/823 (84%)	0.18	46 (6%)	26	24	14, 45, 88, 128	0
1	B	685/823 (83%)	0.20	39 (5%)	30	28	16, 45, 86, 137	0
All	All	1379/1646 (83%)	0.19	85 (6%)	28	26	14, 45, 88, 137	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	ASN	8.4
1	B	507	SER	4.4
1	B	611	PRO	4.4
1	A	712	ASN	4.4
1	B	600	SER	4.1
1	A	853	ARG	4.1
1	A	680	ASN	4.1
1	A	610	ASP	4.0
1	A	647	LYS	4.0
1	B	807	ILE	4.0
1	A	507	SER	3.9
1	B	427	ASN	3.9
1	A	508	GLU	3.8
1	A	600	SER	3.8
1	B	171	SER	3.8
1	A	601	THR	3.6
1	B	610	ASP	3.6
1	B	850	HIS	3.5
1	B	599	LYS	3.4
1	A	725	LEU	3.4
1	B	678	LEU	3.4
1	A	602	SER	3.4
1	B	725	LEU	3.4
1	A	511	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	801	ARG	3.2
1	A	679	SER	3.2
1	A	509	ARG	3.2
1	A	599	LYS	3.2
1	B	731	HIS	3.2
1	A	731	HIS	3.1
1	A	902	SER	3.1
1	A	726	ASN	3.0
1	A	628	GLU	2.9
1	A	710	LYS	2.9
1	B	849	THR	2.9
1	A	611	PRO	2.9
1	A	711	SER	2.8
1	A	303	PHE	2.8
1	B	452	ASN	2.8
1	A	851	GLY	2.7
1	A	510	LYS	2.7
1	A	448	TYR	2.7
1	B	345	GLU	2.7
1	A	301	THR	2.7
1	A	852	LYS	2.6
1	A	798	ARG	2.5
1	A	850	HIS	2.5
1	B	791	GLU	2.5
1	B	609	CYS	2.4
1	B	333	LEU	2.4
1	B	465	PRO	2.4
1	B	901	PHE	2.4
1	B	319	TYR	2.4
1	A	425	ASP	2.4
1	B	657	GLN	2.4
1	A	187	ALA	2.4
1	A	723	PRO	2.3
1	B	429	VAL	2.3
1	B	451	PHE	2.3
1	A	681	ASP	2.3
1	B	702	PRO	2.3
1	B	851	GLY	2.3
1	A	188	GLU	2.2
1	A	465	PRO	2.2
1	B	679	SER	2.2
1	A	692	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	722	PRO	2.2
1	B	189	PHE	2.2
1	A	348	HIS	2.2
1	B	605	LEU	2.2
1	B	442	THR	2.1
1	B	608	THR	2.1
1	B	339	LEU	2.1
1	A	446	GLU	2.1
1	B	310	GLU	2.1
1	A	657	GLN	2.1
1	B	681	ASP	2.1
1	A	608	THR	2.1
1	A	311	ILE	2.1
1	B	841	ARG	2.1
1	B	443	ASP	2.1
1	A	734	SER	2.0
1	B	680	ASN	2.0
1	A	604	ASP	2.0
1	A	716	SER	2.0

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

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

6.3 Carbohydrates (i)

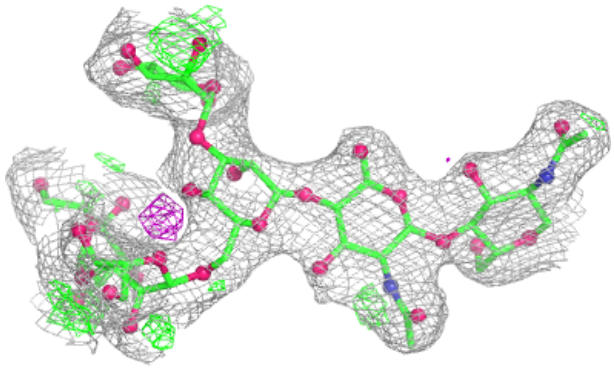
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

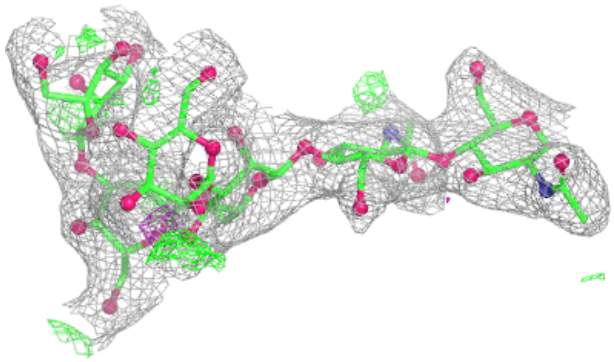
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MAN	C	5	11/12	0.55	0.19	76,95,105,111	0
2	MAN	C	4	11/12	0.74	0.15	53,64,76,88	0
2	MAN	C	6	11/12	0.80	0.12	44,68,81,88	0
2	BMA	C	3	11/12	0.84	0.13	41,58,69,73	0
3	NAG	D	2	14/15	0.86	0.13	49,68,80,82	0
2	NAG	C	2	14/15	0.93	0.08	35,49,57,59	0
3	NAG	D	1	14/15	0.95	0.10	24,36,50,61	0
2	NAG	C	1	14/15	0.95	0.11	17,25,36,45	0

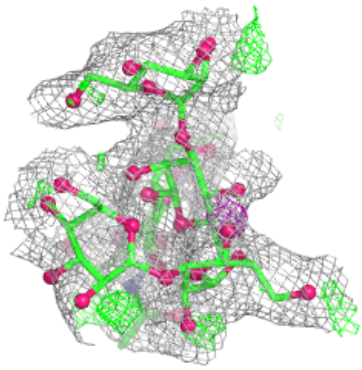
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

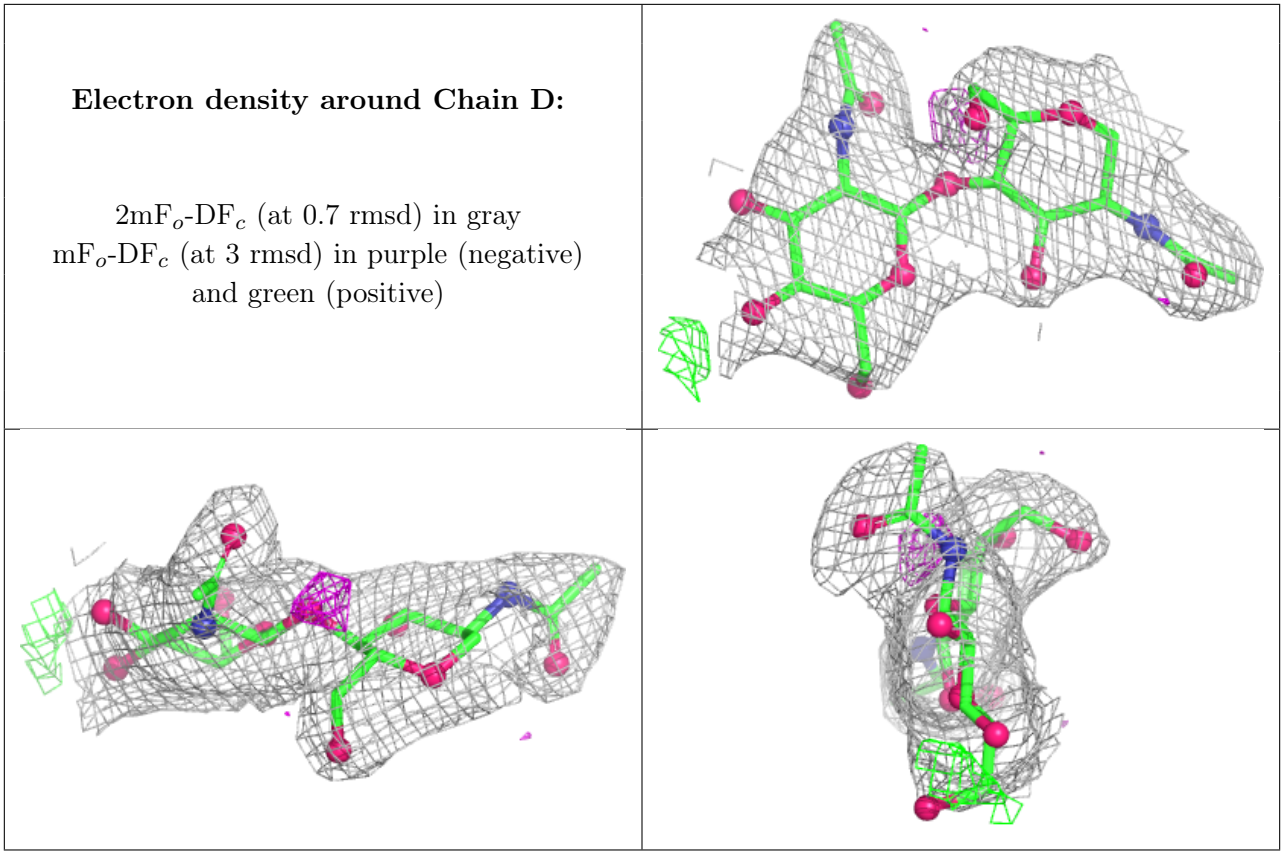






Electron density around Chain D:

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



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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

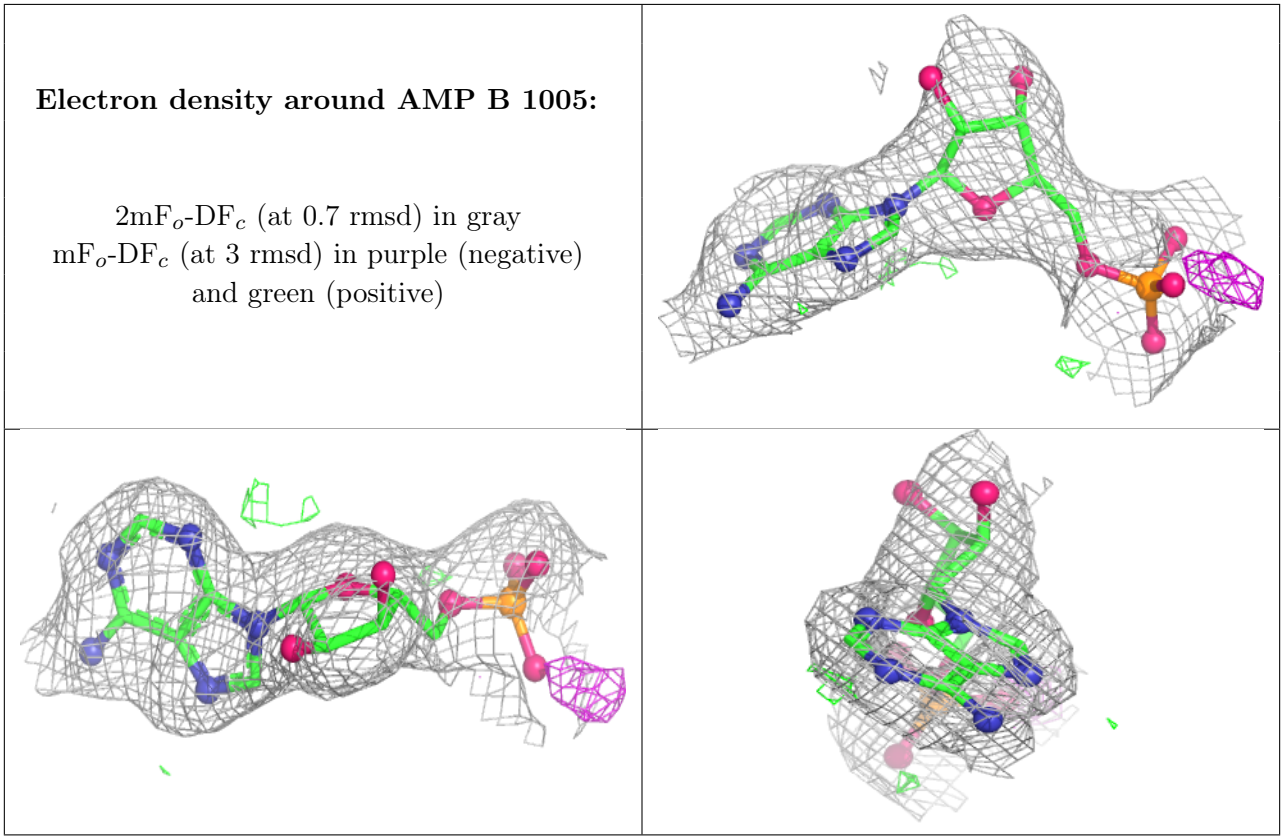
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	B	1004	14/15	0.74	0.16	59,76,84,85	0
4	NAG	B	1003	14/15	0.77	0.16	85,94,98,99	0
4	NAG	A	1007	14/15	0.78	0.15	54,72,85,86	0
4	NAG	A	1008	14/15	0.86	0.11	63,72,81,82	0
5	AMP	B	1005	23/23	0.94	0.10	34,50,69,73	0
5	AMP	A	1009	23/23	0.95	0.07	31,43,54,68	0
6	ZN	B	1007	1/1	0.97	0.04	39,39,39,39	0
6	ZN	A	1010	1/1	0.98	0.03	38,38,38,38	0
7	CA	A	1012	1/1	0.98	0.06	44,44,44,44	0
7	CA	B	1008	1/1	0.98	0.07	54,54,54,54	0
6	ZN	B	1006	1/1	0.99	0.03	43,43,43,43	0
6	ZN	A	1011	1/1	0.99	0.02	45,45,45,45	0

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.

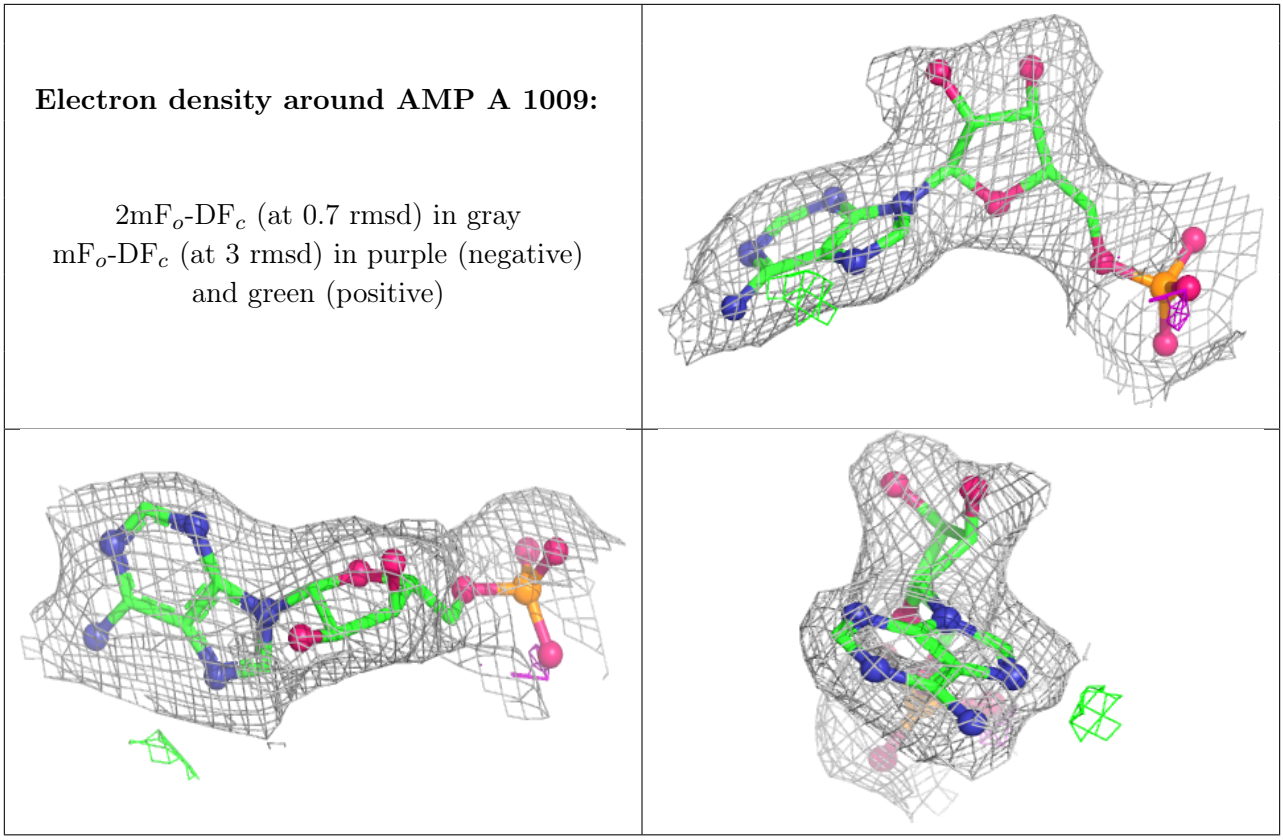
Electron density around AMP B 1005:

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



Electron density around AMP A 1009:

$2mF_o$-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.