



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 02:27 PM BST

PDB ID : 4AZI
Title : Differential inhibition of the tandem GH20 catalytic modules in the pneumococcal exo-beta-D-N-acetylglucosaminidase, StrH
Authors : Pluvinae, B.; Stubbs, K.A.; Vocadlo, D.J.; Boraston, A.B.
Deposited on : 2012-06-26
Resolution : 1.98 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
buster-report : 1.1.7 (2018)
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) : 2.13.1

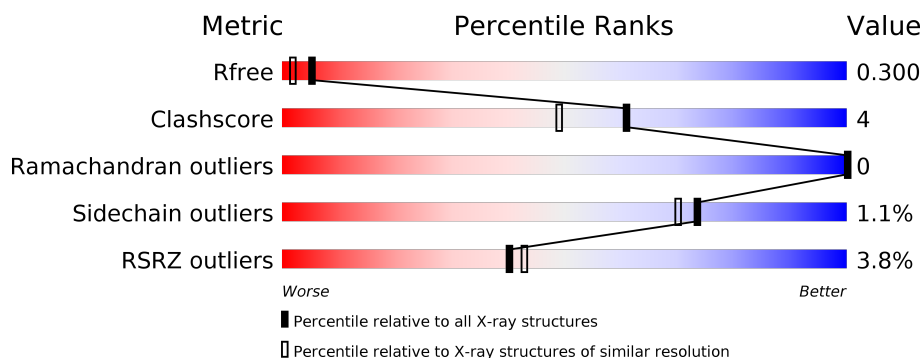
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 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	442	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>
1	B	442	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>8%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7870 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.

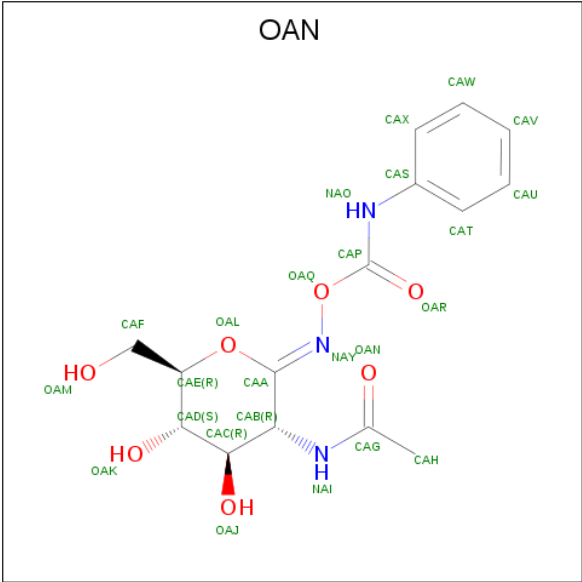
- Molecule 1 is a protein called BETA-N-ACETYLHEXOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	3	5	0
			3293	2113	533	635	12			
1	B	408	Total	C	N	O	S	0	9	0
			3319	2134	535	638	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	623	GLY	-	expression tag	UNP P49610
A	624	SER	-	expression tag	UNP P49610
A	625	HIS	-	expression tag	UNP P49610
A	626	MET	-	expression tag	UNP P49610
A	913	TRP	GLY	engineered mutation	UNP P49610
A	914	TYR	GLY	engineered mutation	UNP P49610
B	623	GLY	-	expression tag	UNP P49610
B	624	SER	-	expression tag	UNP P49610
B	625	HIS	-	expression tag	UNP P49610
B	626	MET	-	expression tag	UNP P49610
B	913	TRP	GLY	engineered mutation	UNP P49610
B	914	TYR	GLY	engineered mutation	UNP P49610

- Molecule 2 is O-(2-ACETAMIDO-2-DEOXY D-GLUCOPYRANOSYLIDENE) AMINO-N-PHENYLCARBAMATE (three-letter code: OAN) (formula: C₁₅H₁₉N₃O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	15	3	7		
2	B	1	Total	C	N	O	0	0
			25	15	3	7		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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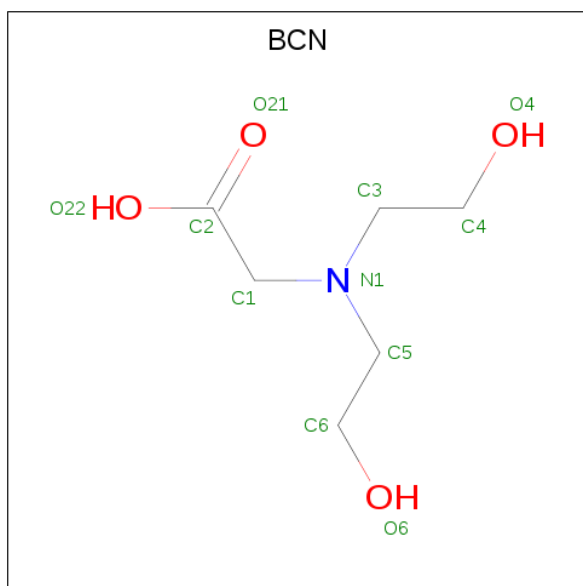
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Br	0	0
			1	1		
4	A	3	Total	Br	0	0
			3	3		

- Molecule 5 is BICINE (three-letter code: BCN) (formula: C₆H₁₃NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			11	6	1	4		
5	B	1	Total	C	N	O	0	0
			11	6	1	4		
5	B	1	Total	C	N	O	0	0
			11	6	1	4		

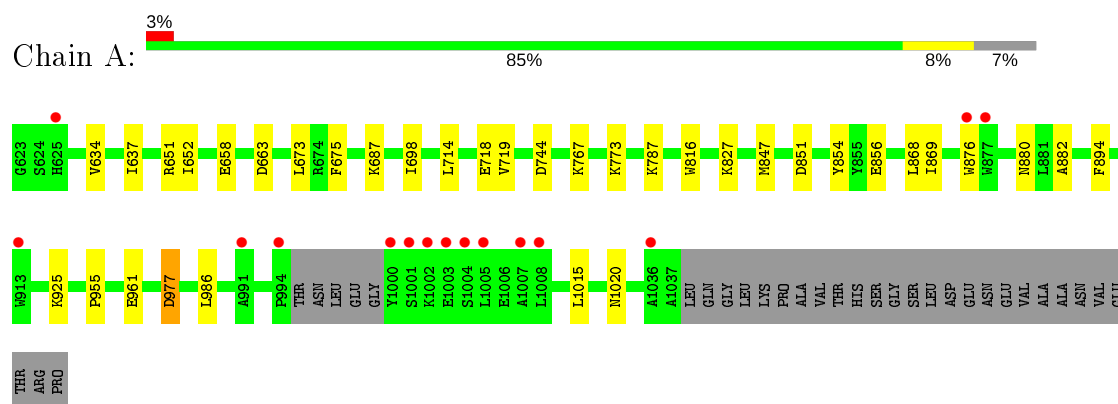
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	570	Total 570	O 570	0	0
6	B	577	Total 577	O 577	0	0

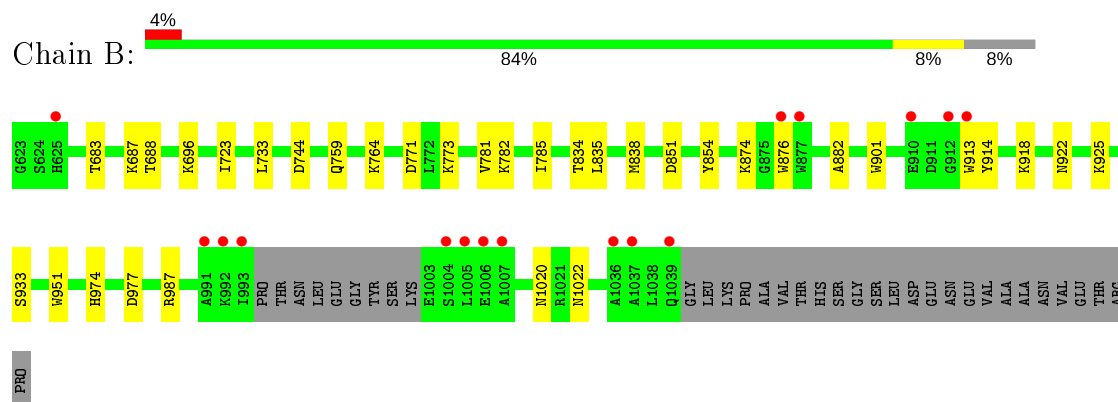
3 Residue-property plots [i](#)

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: BETA-N-ACETYLHEXOSAMINIDASE



• Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.06Å 116.04Å 69.64Å 90.00° 109.57° 90.00°	Depositor
Resolution (Å)	43.47 – 1.98 43.47 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.5 (43.47-1.98) 97.5 (43.47-1.98)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.241 , 0.302 0.241 , 0.300	Depositor DCC
R_{free} test set	3436 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7870	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.88% 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: OAN, BCN, EDO, BR

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	0.64	4/3371 (0.1%)	0.57	1/4562 (0.0%)
1	B	0.53	2/3403 (0.1%)	0.57	0/4608
All	All	0.58	6/6774 (0.1%)	0.57	1/9170 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	925	LYS	CE-NZ	-16.21	1.08	1.49
1	A	827	LYS	CD-CE	-15.70	1.12	1.51
1	A	876	TRP	CD2-CE2	5.20	1.47	1.41
1	A	816	TRP	CD2-CE2	5.08	1.47	1.41
1	B	901	TRP	CD2-CE2	5.08	1.47	1.41
1	B	951	TRP	CD2-CE2	5.01	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	827	LYS	CD-CE-NZ	-6.62	96.48	111.70

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	3293	0	3158	29	1
1	B	3319	0	3167	26	0
2	A	25	0	19	0	0
2	B	25	0	19	2	0
3	A	12	0	18	2	0
3	B	12	0	18	1	0
4	A	3	0	0	1	0
4	B	1	0	0	0	0
5	A	11	0	12	0	0
5	B	22	0	24	4	0
6	A	570	0	0	14	0
6	B	577	0	0	9	1
All	All	7870	0	6435	59	1

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 (59) 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:869:ILE:HB	6:A:3303:HOH:O	1.41	1.17
1:B:834:THR:CG2	6:B:3220:HOH:O	2.14	0.96
1:A:714:LEU:HB3	6:A:3110:HOH:O	1.66	0.93
1:B:834:THR:HG23	6:B:3220:HOH:O	1.70	0.91
1:A:894:PHE:CD1	6:A:3303:HOH:O	2.31	0.82
1:A:673[A]:LEU:HD13	1:A:673[A]:LEU:C	2.00	0.81
1:A:894:PHE:HA	6:A:3303:HOH:O	1.82	0.80
1:A:894:PHE:HD1	6:A:3303:HOH:O	1.68	0.75
1:A:977:ASP:HB3	6:A:3520:HOH:O	1.87	0.74
1:B:834:THR:HG22	6:B:3220:HOH:O	1.85	0.70
1:B:782:LYS:HE2	1:B:834:THR:HG21	1.75	0.67
1:B:838:MET:SD	6:B:3220:HOH:O	2.54	0.66
1:B:771:ASP:OD1	1:B:773:LYS:HG2	1.95	0.65
1:A:719:VAL:HG23	6:A:3110:HOH:O	1.97	0.64
1:A:955:PRO:HD2	4:A:2043:BR:BR	2.53	0.64
1:B:918:LYS:HE2	6:B:3369:HOH:O	1.98	0.63
1:A:673[A]:LEU:CD1	1:A:673[A]:LEU:C	2.69	0.61
1:A:651:ARG:NH1	1:A:961:GLU:OE2	2.36	0.58
1:A:767:LYS:HE3	6:A:3350:HOH:O	2.03	0.58
3:B:2043:EDO:H21	5:B:2046:BCN:H52	1.86	0.57
1:A:869:ILE:O	6:A:3303:HOH:O	2.18	0.54
1:A:718:GLU:HB2	6:A:3110:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2040:OAN:HAX	5:B:2046:BCN:H11	1.90	0.51
1:A:1020:ASN:HD21	3:A:2039:EDO:H11	1.74	0.51
1:B:696:LYS:HD3	6:B:3082:HOH:O	2.10	0.51
1:A:673[A]:LEU:CD1	1:A:673[A]:LEU:O	2.59	0.50
1:A:687:LYS:NZ	6:A:3072:HOH:O	2.43	0.50
1:B:759:GLN:NE2	6:B:3134:HOH:O	2.44	0.49
1:B:922:ASN:OD1	1:B:925:LYS:HE2	2.13	0.49
1:A:673[A]:LEU:HD13	1:A:673[A]:LEU:O	2.13	0.48
1:A:847:MET:HG3	1:A:868:LEU:O	2.14	0.48
3:A:2040:EDO:H22	6:A:3569:HOH:O	2.14	0.47
1:A:977:ASP:OD1	1:A:977:ASP:N	2.38	0.46
6:A:3404:HOH:O	1:B:987:ARG:HD3	2.14	0.46
1:B:974:HIS:ND1	5:B:2045:BCN:H52	2.30	0.46
1:A:856:GLU:HG3	1:A:880:ASN:HB3	1.96	0.45
1:B:854:TYR:O	1:B:882:ALA:HB2	2.17	0.45
1:A:773:LYS:HE3	1:A:773:LYS:HB2	1.84	0.45
1:B:876[B]:TRP:CE3	1:B:876[B]:TRP:HA	2.53	0.44
1:B:687:LYS:NZ	6:B:3071:HOH:O	2.46	0.44
1:B:913[B]:TRP:HB2	1:B:914:TYR:CD2	2.53	0.44
1:A:673[A]:LEU:HD13	1:A:675:PHE:H	1.83	0.43
1:B:874:LYS:HE2	1:B:933:SER:HB2	2.01	0.43
1:A:880:ASN:ND2	6:A:3318:HOH:O	2.51	0.42
1:A:634:VAL:HG22	1:A:663:ASP:HB2	2.01	0.42
1:A:854:TYR:O	1:A:882:ALA:HB2	2.20	0.42
1:A:986:LEU:HD11	1:A:1015:LEU:HD13	2.02	0.42
1:A:637:ILE:HG13	1:A:652:ILE:HD13	2.02	0.41
1:B:1020:ASN:OD1	1:B:1022:ASN:HB2	2.19	0.41
1:B:838:MET:HG3	6:B:3220:HOH:O	2.19	0.41
1:B:781:VAL:O	1:B:785[B]:ILE:HG12	2.20	0.41
1:B:977:ASP:N	1:B:977:ASP:OD1	2.52	0.41
1:B:723:ILE:HG12	1:B:733:LEU:HD22	2.02	0.41
5:B:2046:BCN:H62	5:B:2046:BCN:H32	1.51	0.41
1:B:913[A]:TRP:HZ3	2:B:2040:OAN:HAX	1.85	0.41
1:B:683:THR:HG23	1:B:688:THR:HG22	2.03	0.41
1:A:673[A]:LEU:HD12	1:A:698:ILE:HG21	2.04	0.40
1:B:835[B]:LEU:HA	1:B:835[B]:LEU:HD12	1.64	0.40

All (1) 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)
1:A:787:LYS:NZ	6:B:3413:HOH:O[1_455]	2.14	0.06

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	411/442 (93%)	404 (98%)	7 (2%)	0	100	100
1	B	413/442 (93%)	396 (96%)	17 (4%)	0	100	100
All	All	824/884 (93%)	800 (97%)	24 (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	335/365 (92%)	331 (99%)	4 (1%)	71	67
1	B	336/365 (92%)	333 (99%)	3 (1%)	78	77
All	All	671/730 (92%)	664 (99%)	7 (1%)	73	73

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

Mol	Chain	Res	Type
1	A	658	GLU
1	A	744	ASP
1	A	851	ASP

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Mol	Chain	Res	Type
1	A	977	ASP
1	B	744	ASP
1	B	764	LYS
1	B	851	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	880	ASN
1	A	922	ASN
1	A	1022	ASN
1	B	757	ASN
1	B	814	GLN
1	B	1033	ASN

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](#)

Of 15 ligands modelled in this entry, 4 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	EDO	A	2039	-	3,3,3	0.44	0	2,2,2	0.36	0
5	BCN	B	2045	-	7,10,10	0.59	0	8,11,11	0.54	0
3	EDO	B	2042	-	3,3,3	0.50	0	2,2,2	0.26	0
5	BCN	A	2045	-	7,10,10	0.73	0	8,11,11	1.07	2 (25%)
3	EDO	A	2040	-	3,3,3	0.44	0	2,2,2	0.47	0
3	EDO	B	2043	-	3,3,3	0.49	0	2,2,2	0.18	0
5	BCN	B	2046	-	7,10,10	0.34	0	8,11,11	0.77	0
2	OAN	A	2038	-	24,26,26	1.24	2 (8%)	24,35,35	0.96	1 (4%)
3	EDO	B	2041	-	3,3,3	0.47	0	2,2,2	0.29	0
2	OAN	B	2040	-	24,26,26	1.14	3 (12%)	24,35,35	1.07	2 (8%)
3	EDO	A	2041	-	3,3,3	0.48	0	2,2,2	0.31	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
3	EDO	A	2039	-	-	1/1/1/1	-
5	BCN	B	2045	-	-	1/8/10/10	-
3	EDO	B	2042	-	-	1/1/1/1	-
5	BCN	A	2045	-	-	4/8/10/10	-
3	EDO	A	2040	-	-	1/1/1/1	-
3	EDO	B	2043	-	-	1/1/1/1	-
5	BCN	B	2046	-	-	3/8/10/10	-
2	OAN	A	2038	-	-	3/12/35/35	0/2/2/2
3	EDO	B	2041	-	-	1/1/1/1	-
2	OAN	B	2040	-	-	1/12/35/35	0/2/2/2
3	EDO	A	2041	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2038	OAN	CAS-NAO	-3.46	1.34	1.41
2	A	2038	OAN	OAQ-NAY	-3.36	1.36	1.44
2	B	2040	OAN	OAQ-NAY	-3.07	1.37	1.44
2	B	2040	OAN	CAS-NAO	-2.95	1.35	1.41
2	B	2040	OAN	CAA-NAY	2.07	1.32	1.27

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2040	OAN	CAC-CAB-NAI	-2.44	108.45	112.28
2	B	2040	OAN	OAL-CAA-CAB	2.22	124.38	118.10
2	A	2038	OAN	OAL-CAA-CAB	2.15	124.17	118.10
5	A	2045	BCN	C1-N1-C3	2.09	115.70	111.29
5	A	2045	BCN	C5-N1-C3	2.06	116.35	111.44

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2045	BCN	N1-C3-C4-O4
5	B	2046	BCN	N1-C5-C6-O6
2	A	2038	OAN	CAA-CAB-NAI-CAG
2	B	2040	OAN	CAA-CAB-NAI-CAG
5	A	2045	BCN	C2-C1-N1-C3
5	B	2046	BCN	C6-C5-N1-C3
5	A	2045	BCN	N1-C5-C6-O6
3	A	2040	EDO	O1-C1-C2-O2
5	B	2046	BCN	N1-C3-C4-O4
2	A	2038	OAN	CAT-CAS-NAO-CAP
2	A	2038	OAN	CAX-CAS-NAO-CAP
3	B	2041	EDO	O1-C1-C2-O2
5	B	2045	BCN	C2-C1-N1-C3
3	A	2039	EDO	O1-C1-C2-O2
5	A	2045	BCN	C4-C3-N1-C5
3	B	2042	EDO	O1-C1-C2-O2
3	B	2043	EDO	O1-C1-C2-O2

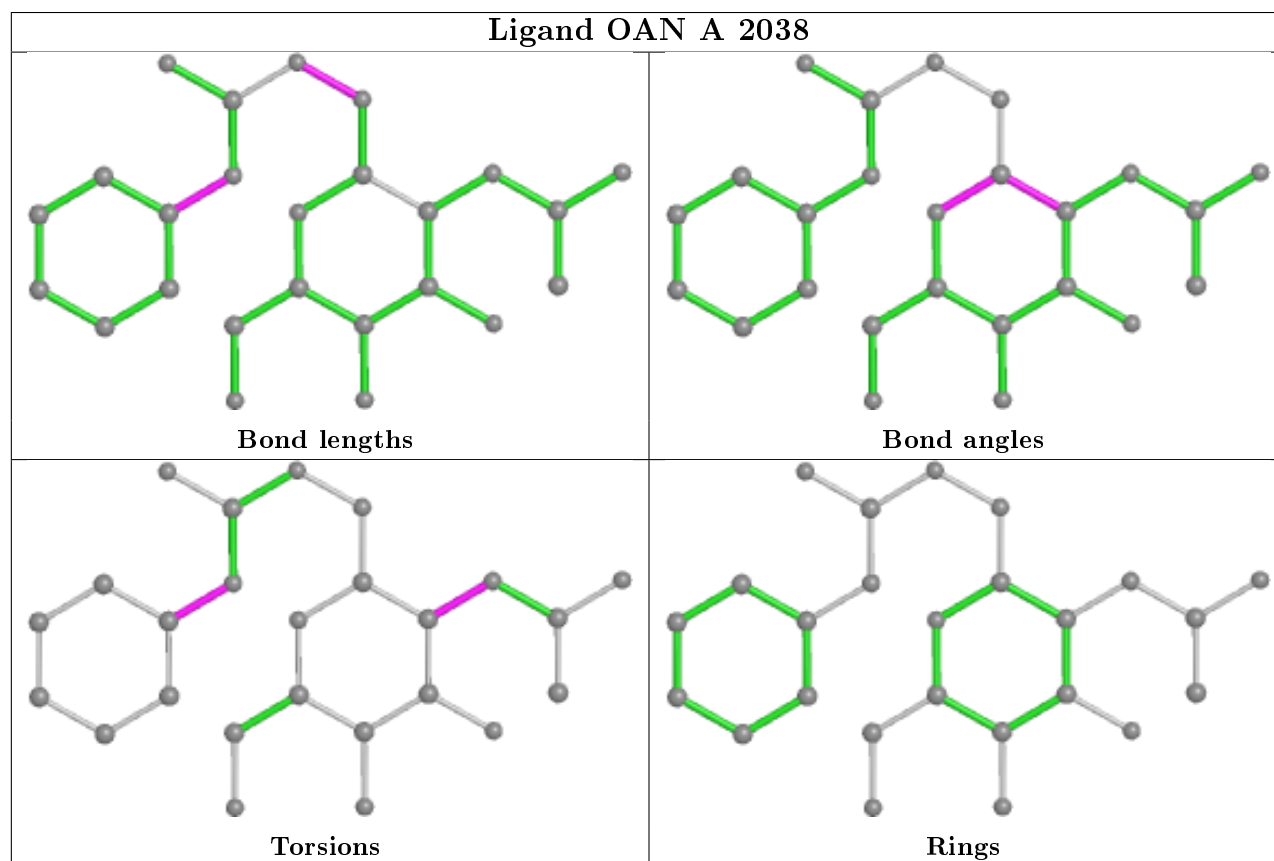
There are no ring outliers.

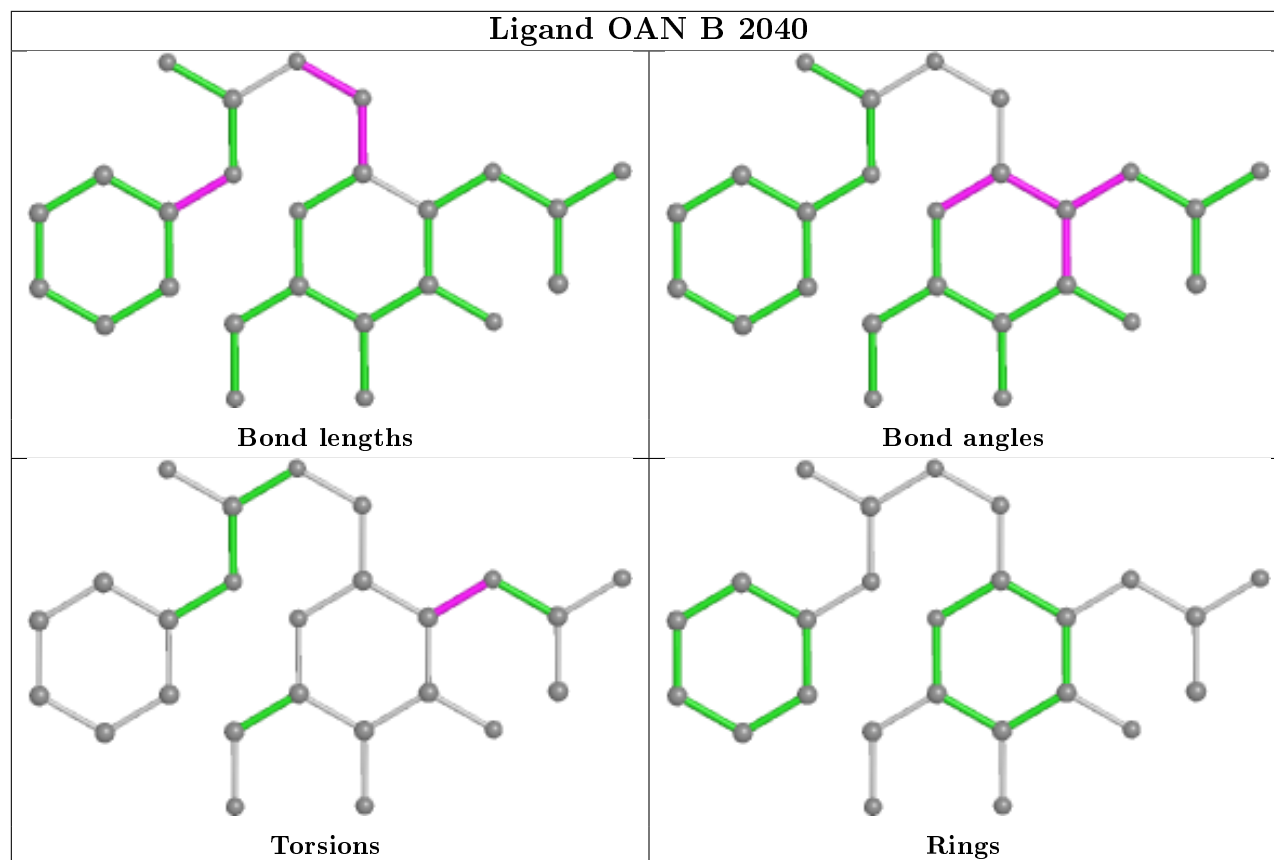
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2039	EDO	1	0
5	B	2045	BCN	1	0
3	A	2040	EDO	1	0
3	B	2043	EDO	1	0
5	B	2046	BCN	3	0
2	B	2040	OAN	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 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	410/442 (92%)	0.27	15 (3%) 41 44	8, 15, 32, 50	7 (1%)
1	B	408/442 (92%)	0.26	16 (3%) 39 42	8, 15, 33, 50	6 (1%)
All	All	818/884 (92%)	0.26	31 (3%) 40 43	8, 15, 33, 50	13 (1%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	877[A]	TRP	7.3
1	B	876[A]	TRP	6.0
1	B	877[A]	TRP	5.5
1	A	876	TRP	4.8
1	B	913[A]	TRP	4.8
1	A	1004	SER	4.7
1	A	1000	TYR	4.3
1	B	1004	SER	4.0
1	A	1007	ALA	3.9
1	A	994	PRO	3.9
1	B	1005	LEU	3.9
1	A	1036	ALA	3.7
1	B	1007	ALA	3.5
1	B	1039	GLN	3.4
1	B	993	ILE	3.4
1	B	992	LYS	3.2
1	A	1001	SER	3.1
1	B	1037	ALA	3.1
1	B	991	ALA	2.9
1	B	625	HIS	2.8
1	A	1002	LYS	2.8
1	B	1006	GLU	2.7
1	A	913	TRP	2.5
1	A	1008	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	912	GLY	2.3
1	A	991	ALA	2.2
1	A	1005	LEU	2.2
1	B	910	GLU	2.1
1	B	1036	ALA	2.1
1	A	1003	GLU	2.1
1	A	625	HIS	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 monosaccharides in this entry.

6.4 Ligands [i](#)

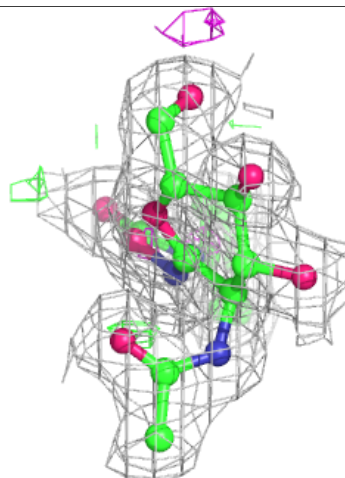
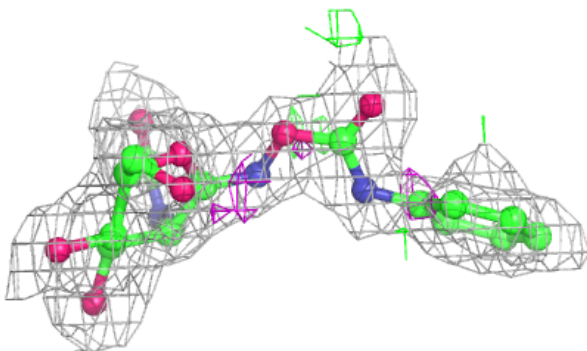
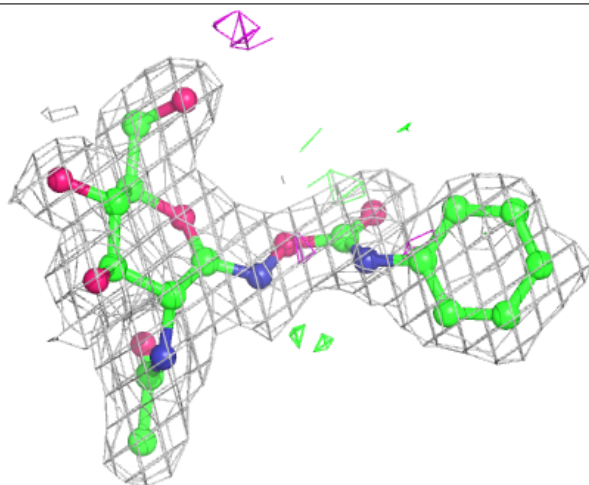
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	BCN	A	2045	11/11	0.56	0.32	33,37,38,39	0
3	EDO	A	2040	4/4	0.70	0.20	28,28,28,29	0
5	BCN	B	2045	11/11	0.71	0.31	41,43,44,45	0
5	BCN	B	2046	11/11	0.78	0.27	26,28,30,32	0
4	BR	B	2044	1/1	0.80	0.21	72,72,72,72	0
3	EDO	B	2041	4/4	0.84	0.14	37,37,38,38	0
3	EDO	B	2042	4/4	0.88	0.14	28,29,29,29	0
3	EDO	A	2039	4/4	0.90	0.14	27,27,27,29	0
2	OAN	A	2038	25/25	0.91	0.12	10,11,17,17	0
2	OAN	B	2040	25/25	0.91	0.12	9,11,17,17	0
3	EDO	B	2043	4/4	0.93	0.13	19,20,20,20	0
4	BR	A	2043	1/1	0.93	0.20	69,69,69,69	0
4	BR	A	2044	1/1	0.96	0.08	32,32,32,32	0
3	EDO	A	2041	4/4	0.97	0.10	17,17,17,17	0
4	BR	A	2042	1/1	0.99	0.09	34,34,34,34	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.

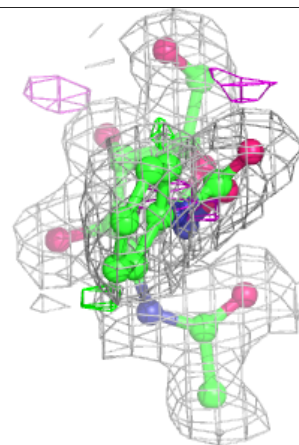
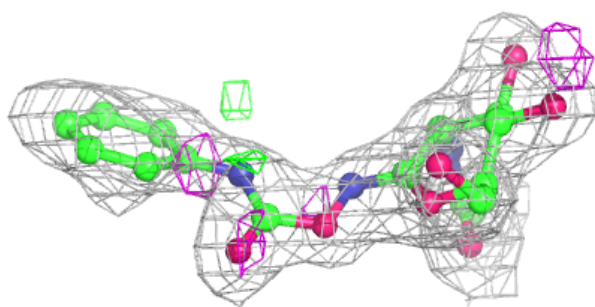
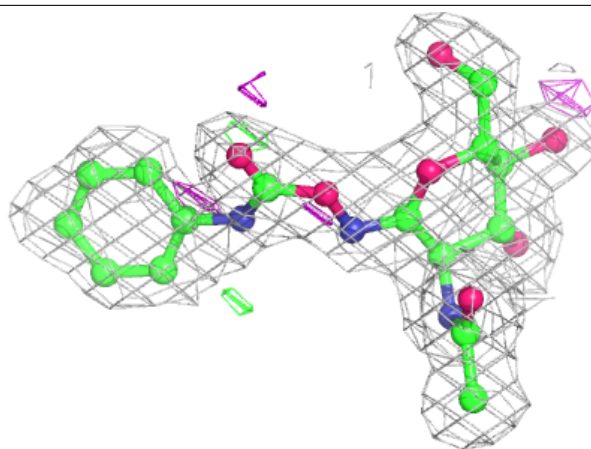
Electron density around OAN A 2038:

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



Electron density around OAN B 2040:

$2mF_o - DF_c$ (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.