



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:00 PM UTC

PDB ID : 5A6B / pdb_00005a6b
Title : GH20C, Beta-hexosaminidase from Streptococcus pneumoniae in complex with PUGNAc
Authors : Cid, M.; Robb, C.S.; Higgins, M.A.; Boraston, A.B.
Deposited on : 2015-06-24
Resolution : 1.77 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

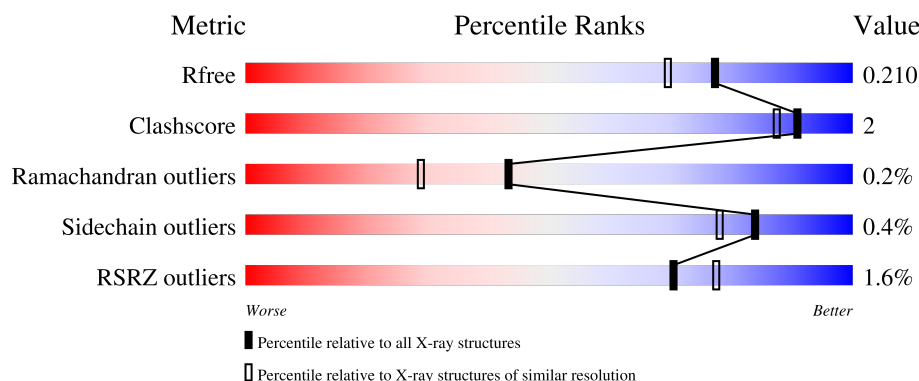
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	649	
1	B	649	
1	C	649	
2	D	648	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21421 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 N-ACETYL-BETA-D-GLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	0	0	0
			4778	3048	800	911	19			
1	B	617	Total	C	N	O	S	0	4	0
			4872	3115	815	922	20			
1	C	610	Total	C	N	O	S	0	1	0
			4822	3075	812	916	19			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP C1CH75
A	-21	GLY	-	expression tag	UNP C1CH75
A	-20	SER	-	expression tag	UNP C1CH75
A	-19	SER	-	expression tag	UNP C1CH75
A	-18	HIS	-	expression tag	UNP C1CH75
A	-17	HIS	-	expression tag	UNP C1CH75
A	-16	HIS	-	expression tag	UNP C1CH75
A	-15	HIS	-	expression tag	UNP C1CH75
A	-14	HIS	-	expression tag	UNP C1CH75
A	-13	HIS	-	expression tag	UNP C1CH75
A	-12	SER	-	expression tag	UNP C1CH75
A	-11	SER	-	expression tag	UNP C1CH75
A	-10	GLY	-	expression tag	UNP C1CH75
A	-9	LEU	-	expression tag	UNP C1CH75
A	-8	VAL	-	expression tag	UNP C1CH75
A	-7	PRO	-	expression tag	UNP C1CH75
A	-6	ARG	-	expression tag	UNP C1CH75
A	-5	GLY	-	expression tag	UNP C1CH75
A	-4	SER	-	expression tag	UNP C1CH75
A	-3	SER	-	expression tag	UNP C1CH75
A	-2	MET	-	expression tag	UNP C1CH75
A	-1	ALA	-	expression tag	UNP C1CH75
A	0	SER	-	expression tag	UNP C1CH75

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Chain	Residue	Modelled	Actual	Comment	Reference
A	9	LEU	PRO	conflict	UNP C1CH75
A	158	VAL	MET	conflict	UNP C1CH75
B	-22	MET	-	expression tag	UNP C1CH75
B	-21	GLY	-	expression tag	UNP C1CH75
B	-20	SER	-	expression tag	UNP C1CH75
B	-19	SER	-	expression tag	UNP C1CH75
B	-18	HIS	-	expression tag	UNP C1CH75
B	-17	HIS	-	expression tag	UNP C1CH75
B	-16	HIS	-	expression tag	UNP C1CH75
B	-15	HIS	-	expression tag	UNP C1CH75
B	-14	HIS	-	expression tag	UNP C1CH75
B	-13	HIS	-	expression tag	UNP C1CH75
B	-12	SER	-	expression tag	UNP C1CH75
B	-11	SER	-	expression tag	UNP C1CH75
B	-10	GLY	-	expression tag	UNP C1CH75
B	-9	LEU	-	expression tag	UNP C1CH75
B	-8	VAL	-	expression tag	UNP C1CH75
B	-7	PRO	-	expression tag	UNP C1CH75
B	-6	ARG	-	expression tag	UNP C1CH75
B	-5	GLY	-	expression tag	UNP C1CH75
B	-4	SER	-	expression tag	UNP C1CH75
B	-3	SER	-	expression tag	UNP C1CH75
B	-2	MET	-	expression tag	UNP C1CH75
B	-1	ALA	-	expression tag	UNP C1CH75
B	0	SER	-	expression tag	UNP C1CH75
B	9	LEU	PRO	conflict	UNP C1CH75
B	158	VAL	MET	conflict	UNP C1CH75
C	-22	MET	-	expression tag	UNP C1CH75
C	-21	GLY	-	expression tag	UNP C1CH75
C	-20	SER	-	expression tag	UNP C1CH75
C	-19	SER	-	expression tag	UNP C1CH75
C	-18	HIS	-	expression tag	UNP C1CH75
C	-17	HIS	-	expression tag	UNP C1CH75
C	-16	HIS	-	expression tag	UNP C1CH75
C	-15	HIS	-	expression tag	UNP C1CH75
C	-14	HIS	-	expression tag	UNP C1CH75
C	-13	HIS	-	expression tag	UNP C1CH75
C	-12	SER	-	expression tag	UNP C1CH75
C	-11	SER	-	expression tag	UNP C1CH75
C	-10	GLY	-	expression tag	UNP C1CH75
C	-9	LEU	-	expression tag	UNP C1CH75
C	-8	VAL	-	expression tag	UNP C1CH75

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	PRO	-	expression tag	UNP C1CH75
C	-6	ARG	-	expression tag	UNP C1CH75
C	-5	GLY	-	expression tag	UNP C1CH75
C	-4	SER	-	expression tag	UNP C1CH75
C	-3	SER	-	expression tag	UNP C1CH75
C	-2	MET	-	expression tag	UNP C1CH75
C	-1	ALA	-	expression tag	UNP C1CH75
C	0	SER	-	expression tag	UNP C1CH75
C	9	LEU	PRO	conflict	UNP C1CH75
C	158	VAL	MET	conflict	UNP C1CH75

- Molecule 2 is a protein called N-ACETYL-BETA-D-GLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	616	Total	C	N	O	S	0	3	0
			4888	3118	820	931	19			

There are 26 discrepancies between the modelled and reference sequences:

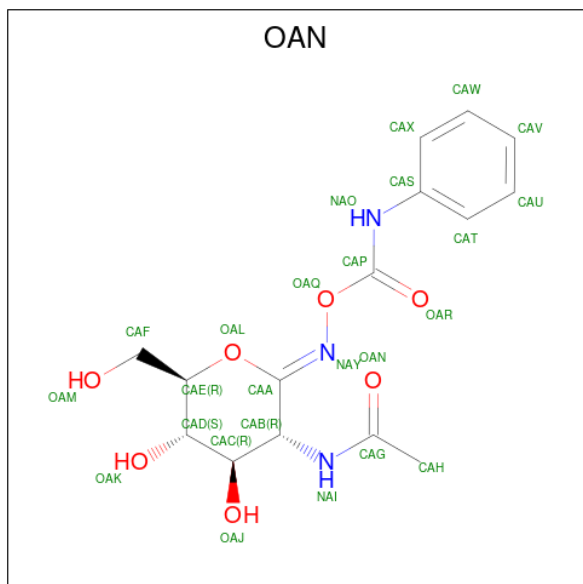
Chain	Residue	Modelled	Actual	Comment	Reference
D	-22	MET	-	expression tag	UNP C1CH75
D	-21	GLY	-	expression tag	UNP C1CH75
D	-20	SER	-	expression tag	UNP C1CH75
D	-19	SER	-	expression tag	UNP C1CH75
D	-18	HIS	-	expression tag	UNP C1CH75
D	-17	HIS	-	expression tag	UNP C1CH75
D	-16	HIS	-	expression tag	UNP C1CH75
D	-15	HIS	-	expression tag	UNP C1CH75
D	-14	HIS	-	expression tag	UNP C1CH75
D	-13	HIS	-	expression tag	UNP C1CH75
D	-12	SER	-	expression tag	UNP C1CH75
D	-11	SER	-	expression tag	UNP C1CH75
D	-10	GLY	-	expression tag	UNP C1CH75
D	-9	LEU	-	expression tag	UNP C1CH75
D	-8	VAL	-	expression tag	UNP C1CH75
D	-7	PRO	-	expression tag	UNP C1CH75
D	-6	ARG	-	expression tag	UNP C1CH75
D	-5	GLY	-	expression tag	UNP C1CH75
D	-4	SER	-	expression tag	UNP C1CH75
D	-3	SER	-	expression tag	UNP C1CH75
D	-2	MET	-	expression tag	UNP C1CH75
D	-1	ALA	-	expression tag	UNP C1CH75

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP C1CH75
D	9	LEU	PRO	conflict	UNP C1CH75
D	158	VAL	MET	conflict	UNP C1CH75
D	?	-	LEU	deletion	UNP C1CH75

- Molecule 3 is O-(2-ACETAMIDO-2-DEOXY D-GLUCOPYRANOSYLIDENE) AMINO-N-PHENYLCARBAMATE (CCD ID: OAN) (formula: $C_{15}H_{19}N_3O_7$).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

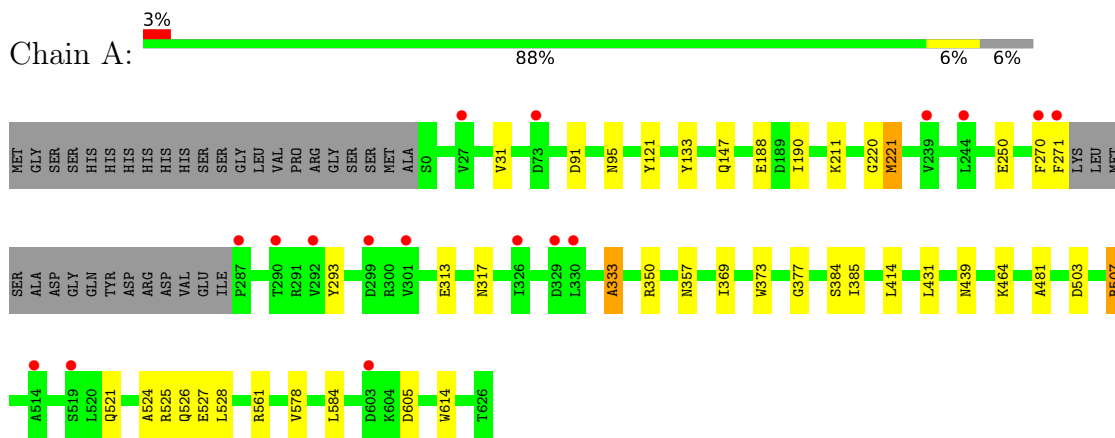
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	425	Total 425	O 425	0	0
5	B	492	Total 492	O 492	0	0
5	C	533	Total 533	O 533	0	0
5	D	508	Total 508	O 508	0	0

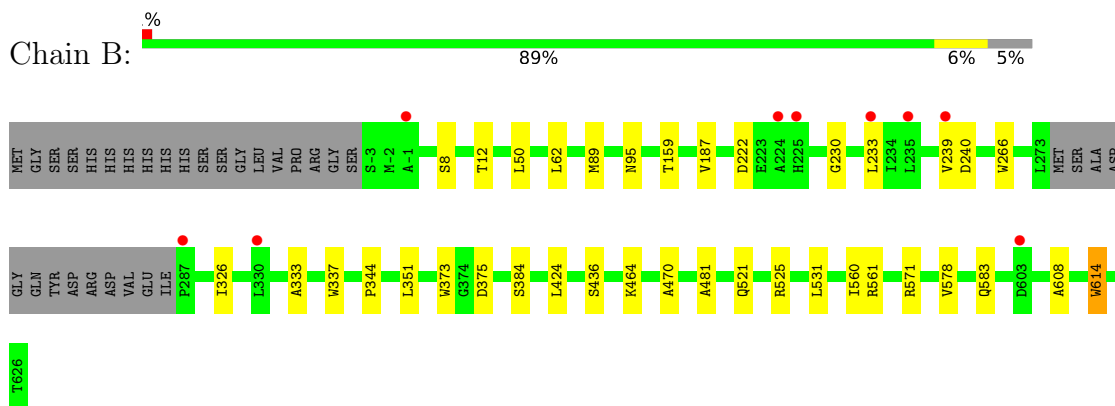
3 Residue-property plots [i](#)

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.

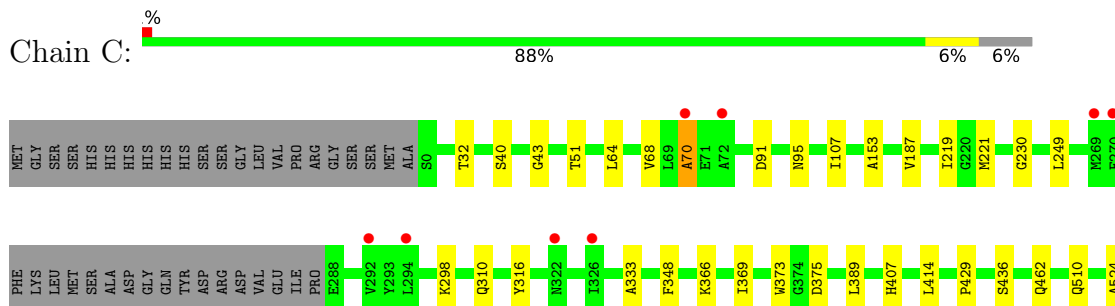
• Molecule 1: N-ACETYL-BETA-D-GLUCOSAMINIDASE



• Molecule 1: N-ACETYL-BETA-D-GLUCOSAMINIDASE



• Molecule 1: N-ACETYL-BETA-D-GLUCOSAMINIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.70Å 136.94Å 201.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.69 – 1.77 38.69 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.69-1.77) 99.6 (38.69-1.77)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.164 , 0.203 0.175 , 0.210	Depositor DCC
R_{free} test set	12474 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21421	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.45% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OAN, MG

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	1.29	9/4879 (0.2%)	1.16	11/6626 (0.2%)
1	B	1.29	7/4994 (0.1%)	1.12	3/6780 (0.0%)
1	C	1.26	7/4926 (0.1%)	1.10	4/6683 (0.1%)
2	D	1.29	14/5003 (0.3%)	1.09	3/6787 (0.0%)
All	All	1.28	37/19802 (0.2%)	1.12	21/26876 (0.1%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	608	ALA	N-CA	7.69	1.56	1.45
1	A	464	LYS	N-CA	-6.81	1.40	1.46
1	B	481	ALA	CA-C	-6.49	1.43	1.52
2	D	161	VAL	CA-C	6.43	1.58	1.52
1	B	608	ALA	N-CA	6.36	1.54	1.45
2	D	528	LEU	C-O	-6.27	1.18	1.24
1	C	510	GLN	N-CA	6.20	1.53	1.46
1	B	614	TRP	C-O	-6.15	1.17	1.24
1	A	133	TYR	N-CA	6.09	1.54	1.46
1	A	384	SER	C-O	5.93	1.31	1.24
2	D	411	ASN	N-CA	-5.88	1.38	1.46
2	D	106	MET	C-O	-5.64	1.17	1.24
2	D	560	ILE	CA-C	5.62	1.59	1.52
2	D	98	LEU	C-O	-5.60	1.16	1.23
1	B	571	ARG	C-O	-5.50	1.17	1.24
1	B	333	ALA	N-CA	5.43	1.52	1.46
2	D	527	GLU	C-O	5.43	1.30	1.24
1	B	531	LEU	N-CA	5.41	1.52	1.46
1	A	190	ILE	N-CA	5.33	1.52	1.46
1	C	575	ARG	CA-C	5.29	1.59	1.52
2	D	116	SER	C-O	5.27	1.31	1.24
1	A	377	GLY	C-O	-5.24	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	414	LEU	CA-C	-5.23	1.46	1.52
2	D	455	ASP	N-CA	5.21	1.52	1.46
1	A	121	TYR	C-O	5.19	1.30	1.24
1	A	350	ARG	N-CA	5.19	1.52	1.46
1	A	357	ASN	CA-C	5.18	1.59	1.52
1	B	470	ALA	C-O	-5.16	1.18	1.24
2	D	317	ASN	N-CA	5.16	1.52	1.46
1	C	568	ARG	CZ-NH1	-5.13	1.25	1.32
2	D	116	SER	CA-C	-5.10	1.45	1.52
2	D	608	ALA	CA-C	-5.09	1.46	1.53
1	C	611	ALA	N-CA	-5.09	1.40	1.46
1	C	249	LEU	C-O	-5.06	1.18	1.24
1	A	333	ALA	N-CA	5.06	1.52	1.46
2	D	301	VAL	C-O	5.02	1.29	1.23
1	C	389	LEU	N-CA	-5.01	1.40	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	524	ALA	N-CA-C	9.53	121.67	111.28
1	A	507	ARG	NE-CZ-NH2	-8.03	111.98	119.20
1	A	431	LEU	CA-C-N	-7.83	112.28	120.03
1	A	431	LEU	C-N-CA	-7.83	112.28	120.03
1	B	326	ILE	N-CA-C	7.54	120.50	112.96
1	A	524	ALA	N-CA-C	7.51	119.47	111.28
1	B	560	ILE	N-CA-C	-6.53	104.40	110.53
2	D	326	ILE	N-CA-C	6.37	119.33	112.96
1	A	528	LEU	CA-C-N	-6.29	112.52	119.19
1	A	528	LEU	C-N-CA	-6.29	112.52	119.19
1	A	220	GLY	N-CA-C	5.70	118.19	111.35
1	C	375	ASP	N-CA-C	5.38	118.27	110.42
1	A	31	VAL	N-CA-C	5.38	116.33	108.53
1	B	424	LEU	N-CA-C	5.33	117.78	111.33
2	D	497	ILE	N-CA-C	5.29	115.50	110.42
1	C	43	GLY	N-CA-C	5.27	117.69	111.63
2	D	9	LEU	N-CA-C	-5.25	105.56	111.28
1	A	507	ARG	NE-CZ-NH1	5.23	126.73	121.50
1	A	439	ASN	N-CA-C	5.19	118.10	109.79
1	A	188	GLU	CB-CA-C	-5.09	110.68	116.54
1	C	70	ALA	N-CA-C	-5.01	103.43	110.50

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	4778	0	4548	17	0
1	B	4872	0	4677	18	0
1	C	4822	0	4659	12	0
2	D	4888	0	4705	12	0
3	A	25	0	19	2	0
3	B	25	0	19	2	0
3	C	25	0	19	0	0
3	D	25	0	19	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	425	0	0	1	0
5	B	492	0	0	4	1
5	C	533	0	0	0	0
5	D	508	0	0	1	1
All	All	21421	0	18665	64	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 2.

All (64) 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)
2:D:521:GLN:HG3	2:D:525:ARG:HD2	1.63	0.79
3:A:1627:OAN:HAT	3:A:1627:OAN:OAR	1.89	0.70
1:B:240:ASP:CB	5:B:2284:HOH:O	2.41	0.68
2:D:8:SER:O	2:D:12:THR:HG23	1.95	0.67
1:A:507:ARG:NH2	1:A:527:GLU:OE1	2.32	0.59
1:B:233:LEU:C	1:B:233:LEU:HD23	2.30	0.57
1:B:240:ASP:CB	5:B:2262:HOH:O	2.51	0.57
1:B:521:GLN:CG	1:B:525:ARG:HD2	2.35	0.57
3:B:1627:OAN:OAR	3:B:1627:OAN:HAX	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ASP:HB3	1:B:266:TRP:CD1	2.42	0.55
1:A:270:PHE:O	1:A:271:PHE:CB	2.56	0.54
1:A:526:GLN:NE2	5:A:2345:HOH:O	2.41	0.54
2:D:521:GLN:HG3	2:D:525:ARG:HH11	1.73	0.53
2:D:521:GLN:OE1	2:D:525:ARG:NH1	2.42	0.53
2:D:232:TYR:CZ	2:D:244:LEU:HD11	2.43	0.53
1:A:578:VAL:HG12	1:A:584:LEU:HG	1.93	0.51
1:B:351:LEU:C	1:B:351:LEU:HD23	2.36	0.51
1:A:313:GLU:HG2	1:A:317:ASN:ND2	2.27	0.49
1:C:68:VAL:O	1:C:70:ALA:O	2.31	0.48
2:D:187:VAL:HB	2:D:230:GLY:HA3	1.96	0.48
3:D:1627:OAN:HAT	3:D:1627:OAN:OAR	2.14	0.48
1:C:219:ILE:HD12	1:C:221:MET:HE3	1.96	0.47
1:A:605:ASP:CG	1:A:605:ASP:O	2.57	0.47
1:B:8:SER:O	1:B:12:THR:HG23	2.15	0.47
1:C:64:LEU:CD2	1:C:407:HIS:CE1	2.97	0.47
1:C:429:PRO:HG2	1:C:462:GLN:HG3	1.95	0.46
1:B:344:PRO:HG3	1:B:384:SER:HB2	1.97	0.46
1:B:521:GLN:HG2	1:B:525:ARG:HD2	1.97	0.46
1:B:89:MET:HE1	1:B:373:TRP:CH2	2.51	0.46
1:B:561:ARG:HG2	1:B:614:TRP:CE2	2.51	0.46
1:C:187:VAL:HB	1:C:230:GLY:HA3	1.97	0.46
1:B:337:TRP:CH2	1:B:436:SER:HB2	2.50	0.45
2:D:60:ARG:O	2:D:64:LEU:HG	2.16	0.45
1:B:187:VAL:HB	1:B:230:GLY:HA3	1.99	0.45
2:D:311:ASP:OD1	2:D:311:ASP:C	2.60	0.45
1:C:333:ALA:HA	1:C:369:ILE:O	2.17	0.45
1:C:91:ASP:HB2	1:C:373:TRP:HA	2.00	0.44
2:D:32:THR:O	2:D:51:THR:HA	2.17	0.44
1:A:147:GLN:NE2	1:A:211:LYS:HB3	2.33	0.43
1:C:32:THR:O	1:C:51:THR:HA	2.18	0.43
1:C:40:SER:HB3	1:C:51:THR:OG1	2.18	0.43
1:A:91:ASP:HB2	1:A:373:TRP:HA	2.01	0.43
1:A:507:ARG:HH22	1:A:527:GLU:CD	2.22	0.43
3:A:1627:OAN:OAR	3:A:1627:OAN:CAT	2.55	0.43
1:C:348:PHE:CZ	1:C:436:SER:HB3	2.53	0.43
2:D:348:PHE:CZ	2:D:436:SER:HB3	2.53	0.43
1:B:50:LEU:C	1:B:50:LEU:HD23	2.45	0.42
1:A:250:GLU:OE1	1:A:293:TYR:OH	2.33	0.42
3:B:1627:OAN:HAU	5:B:2249:HOH:O	2.19	0.42
1:A:561:ARG:HG2	1:A:614:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:GLN:HB2	1:C:316:TYR:CZ	2.54	0.42
1:B:578:VAL:HG13	1:B:583:GLN:HB2	2.02	0.41
1:B:62:LEU:HD23	1:B:62:LEU:HA	1.85	0.41
1:A:503:ASP:CG	1:A:507:ARG:HD3	2.45	0.41
1:B:239:VAL:HG12	1:B:240:ASP:O	2.20	0.41
1:A:521:GLN:HG3	1:A:525:ARG:HD2	2.03	0.41
1:A:147:GLN:HE21	1:A:211:LYS:HB3	1.86	0.41
1:A:414:LEU:HD21	1:A:481:ALA:HA	2.03	0.41
1:B:159:THR:HG23	5:B:2148:HOH:O	2.21	0.41
2:D:510:GLN:HG3	5:D:2419:HOH:O	2.20	0.41
2:D:574:SER:O	2:D:578:VAL:HG23	2.21	0.41
1:A:221:MET:HB3	1:A:221:MET:HE2	1.87	0.40
1:A:333:ALA:HA	1:A:369:ILE:O	2.21	0.40
1:C:107:ILE:HG21	1:C:153:ALA:HA	2.03	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)
5:B:2137:HOH:O	5:D:2042:HOH:O[3_655]	2.13	0.07

5.3 Torsion angles

5.3.1 Protein backbone

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	608/649 (94%)	588 (97%)	19 (3%)	1 (0%)	43	29
1	B	617/649 (95%)	598 (97%)	17 (3%)	2 (0%)	36	22
1	C	607/649 (94%)	587 (97%)	19 (3%)	1 (0%)	43	29
2	D	615/648 (95%)	597 (97%)	16 (3%)	2 (0%)	36	22
All	All	2447/2595 (94%)	2370 (97%)	71 (3%)	6 (0%)	43	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	B	95	ASN
1	C	95	ASN
2	D	95	ASN
1	B	375	ASP
2	D	222	ASP

5.3.2 Protein sidechains ⓘ

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	486/557 (87%)	484 (100%)	2 (0%)	84	78
1	B	505/557 (91%)	504 (100%)	1 (0%)	87	83
1	C	501/557 (90%)	498 (99%)	3 (1%)	78	70
2	D	508/556 (91%)	506 (100%)	2 (0%)	84	78
All	All	2000/2227 (90%)	1992 (100%)	8 (0%)	84	78

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	MET
1	A	385	ILE
1	B	464	LYS
1	C	298	LYS
1	C	366	LYS
1	C	557	THR
2	D	272	LYS
2	D	557	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN

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Mol	Chain	Res	Type
1	A	147	GLN
1	A	363	ASN
1	A	382	GLN
1	A	526	GLN
1	A	534	GLN
1	A	545	GLN
1	A	550	ASN
1	B	49	GLN
1	B	154	GLN
1	B	363	ASN
1	B	382	GLN
1	B	550	ASN
1	C	47	HIS
1	C	324	HIS
1	C	363	ASN
1	C	421	GLN
1	C	469	GLN
1	C	510	GLN
1	C	513	GLN
1	C	544	HIS
1	C	545	GLN
2	D	47	HIS
2	D	147	GLN
2	D	469	GLN
2	D	495	ASN
2	D	522	GLN
2	D	567	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	OAN	A	1627	-	23,26,26	1.81	4 (17%)	24,35,35	1.12	4 (16%)
3	OAN	C	1627	-	23,26,26	1.59	3 (13%)	24,35,35	0.88	1 (4%)
3	OAN	B	1627	-	23,26,26	1.49	1 (4%)	24,35,35	1.28	3 (12%)
3	OAN	D	1627	-	23,26,26	1.49	1 (4%)	24,35,35	1.28	5 (20%)

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	OAN	A	1627	-	-	1/12/35/35	0/2/2/2
3	OAN	C	1627	-	-	1/12/35/35	0/2/2/2
3	OAN	B	1627	-	-	1/12/35/35	0/2/2/2
3	OAN	D	1627	-	-	1/12/35/35	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1627	OAN	OAQ-NAY	-6.90	1.28	1.44
3	B	1627	OAN	OAQ-NAY	-6.06	1.30	1.44
3	D	1627	OAN	OAQ-NAY	-5.72	1.31	1.44
3	C	1627	OAN	OAQ-NAY	-4.75	1.33	1.44
3	C	1627	OAN	CAS-NAO	-2.56	1.36	1.41
3	C	1627	OAN	OAL-CAE	-2.42	1.43	1.46
3	A	1627	OAN	CAS-NAO	-2.34	1.36	1.41
3	A	1627	OAN	CAC-CAB	2.18	1.55	1.52
3	A	1627	OAN	CAP-NAO	-2.18	1.31	1.36

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1627	OAN	OAL-CAE-CAF	-3.13	102.91	106.05
3	B	1627	OAN	OAL-CAA-CAB	2.75	125.83	118.37
3	A	1627	OAN	CAC-CAB-NAI	-2.52	108.20	112.26
3	A	1627	OAN	OAL-CAA-CAB	2.38	124.82	118.37
3	A	1627	OAN	CAS-NAO-CAP	-2.28	122.79	126.39
3	D	1627	OAN	OAL-CAA-CAB	2.27	124.53	118.37
3	D	1627	OAN	CAF-CAE-CAD	2.20	118.43	113.02
3	D	1627	OAN	OAL-CAE-CAF	-2.19	103.85	106.05
3	A	1627	OAN	OAJ-CAC-CAB	2.17	113.37	108.98
3	B	1627	OAN	OAK-CAD-CAC	-2.08	105.48	110.38
3	C	1627	OAN	OAN-CAG-CAH	-2.03	118.45	122.05
3	D	1627	OAN	OAN-CAG-CAH	-2.02	118.45	122.05
3	D	1627	OAN	CAC-CAB-NAI	-2.02	109.02	112.26

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1627	OAN	CAA-CAB-NAI-CAG
3	B	1627	OAN	CAA-CAB-NAI-CAG
3	C	1627	OAN	CAA-CAB-NAI-CAG
3	D	1627	OAN	CAA-CAB-NAI-CAG

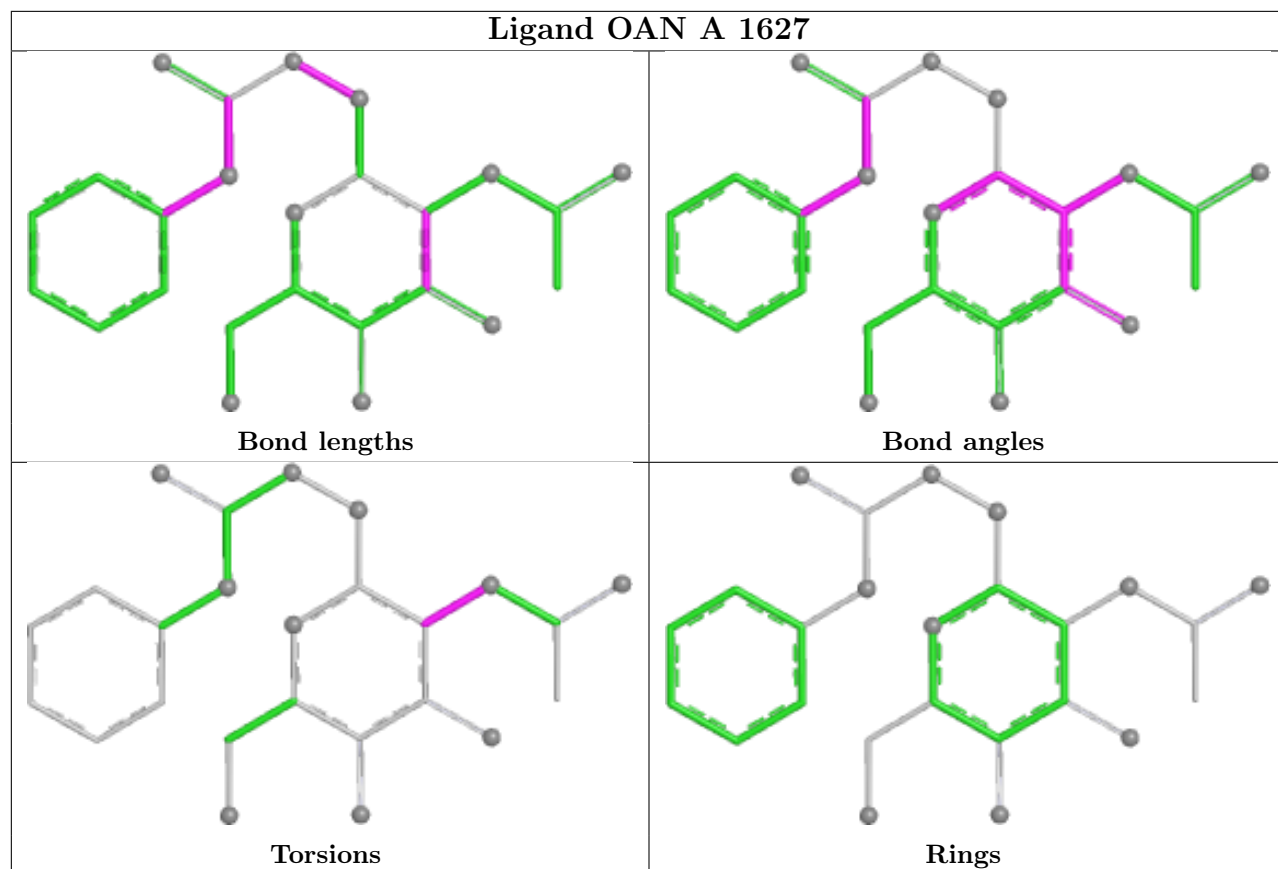
There are no ring outliers.

3 monomers are involved in 5 short contacts:

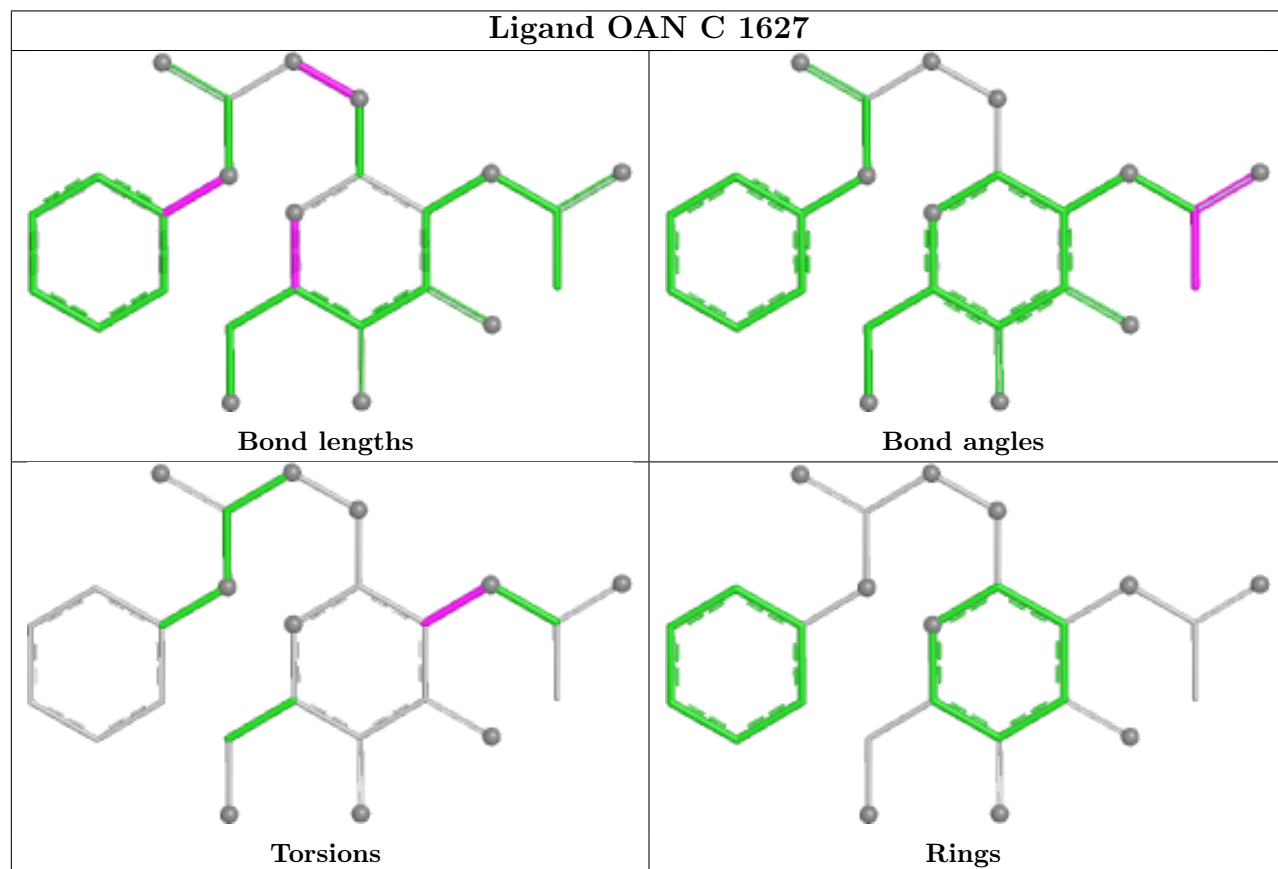
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1627	OAN	2	0
3	B	1627	OAN	2	0
3	D	1627	OAN	1	0

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.

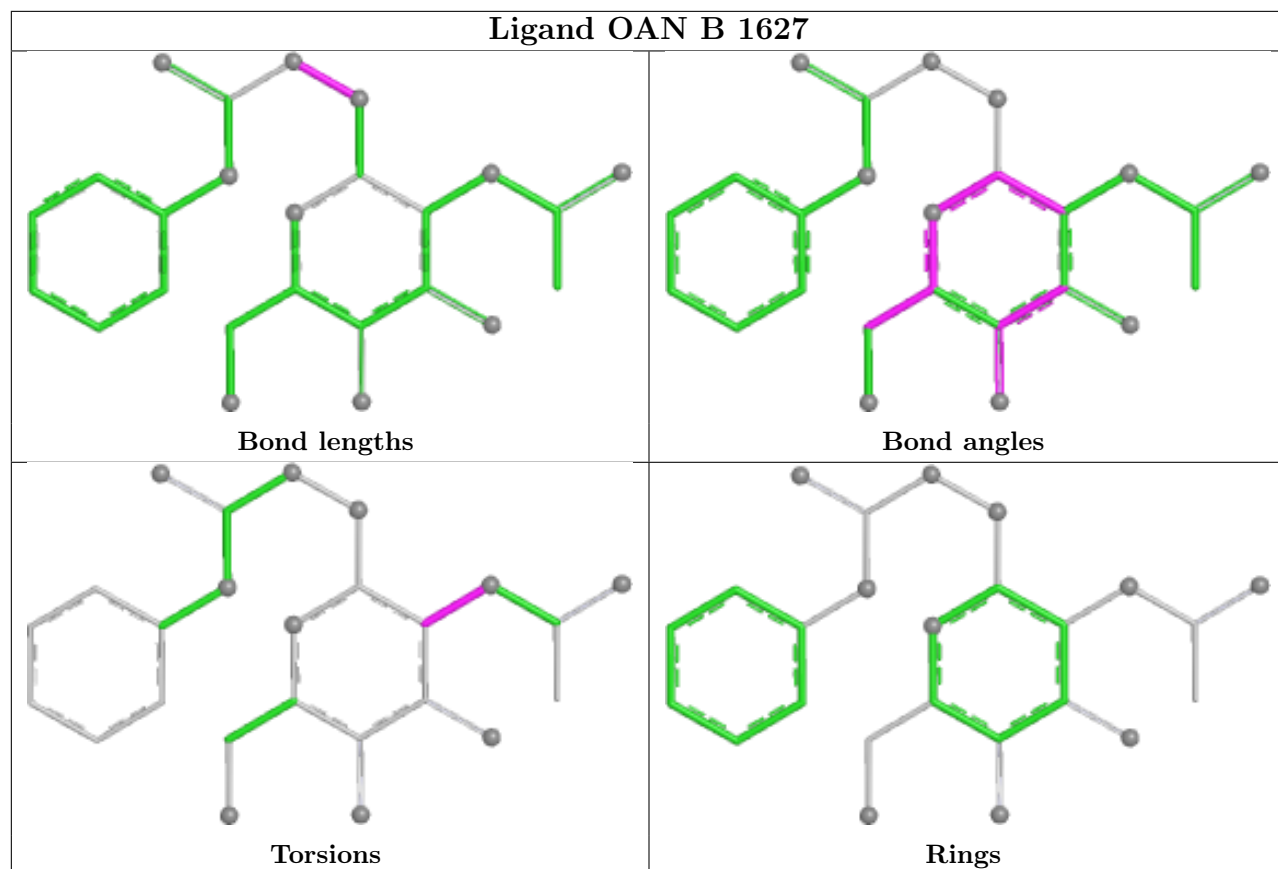
Ligand OAN A 1627



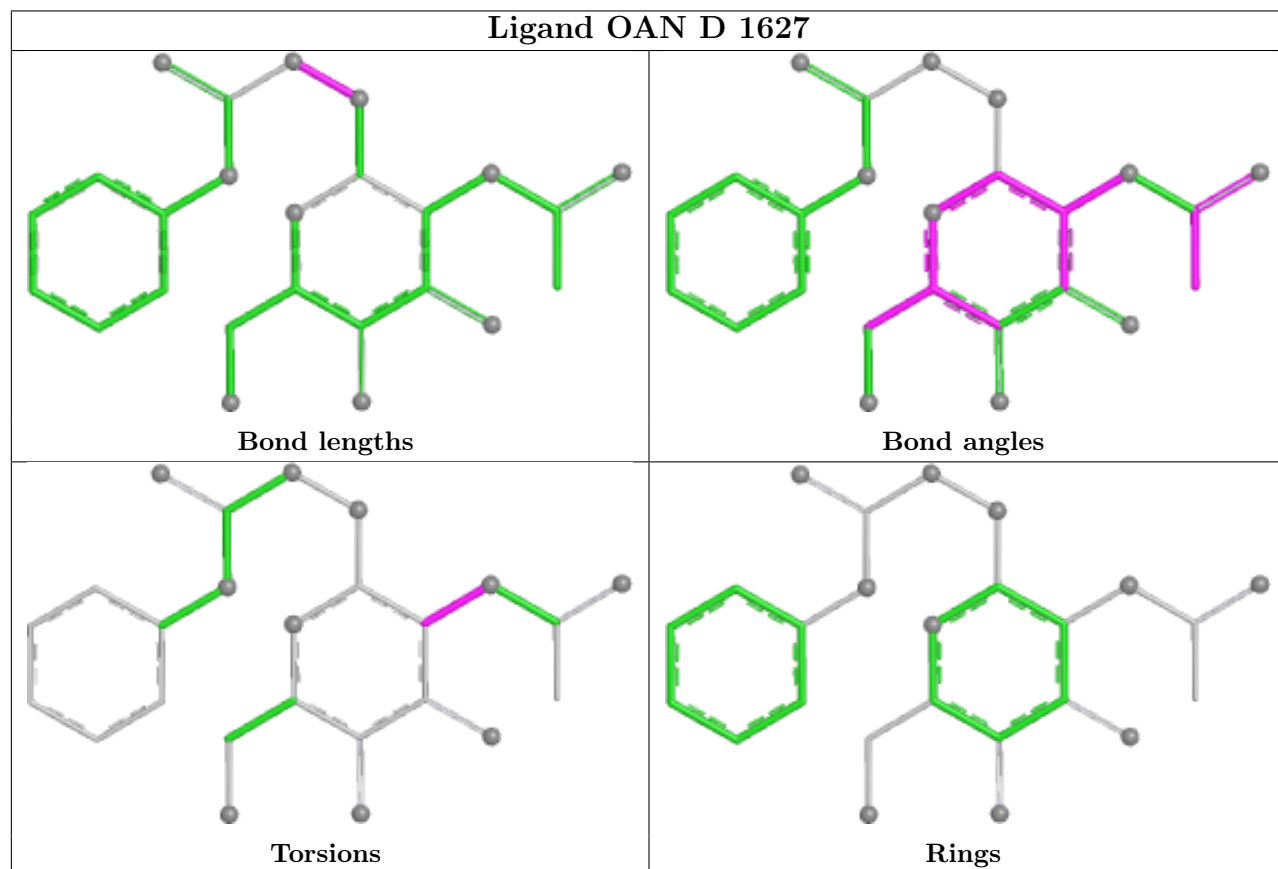
Ligand OAN C 1627



Ligand OAN B 1627



Ligand OAN D 1627



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	612/649 (94%)	0.19	17 (2%) 55 62	13, 27, 44, 59	0
1	B	617/649 (95%)	-0.09	9 (1%) 72 78	12, 22, 38, 57	5 (0%)
1	C	610/649 (93%)	-0.12	8 (1%) 75 81	12, 22, 41, 58	3 (0%)
2	D	616/648 (95%)	-0.15	6 (0%) 79 85	13, 22, 38, 56	3 (0%)
All	All	2455/2595 (94%)	-0.05	40 (1%) 70 77	12, 23, 42, 59	11 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	294	LEU	3.3
1	C	270	PHE	3.2
2	D	222	ASP	3.2
1	A	271	PHE	3.1
1	A	287	PRO	3.1
1	C	70	ALA	3.1
1	B	287	PRO	3.0
1	A	603	ASP	3.0
1	B	-1	ALA	2.9
1	A	73	ASP	2.8
1	A	514	ALA	2.7
2	D	48	TYR	2.6
1	A	519	SER	2.6
1	A	330	LEU	2.5
1	A	239	VAL	2.5
1	C	326	ILE	2.5
1	A	292	VAL	2.5
1	B	224	ALA	2.5
1	A	329	ASP	2.4
1	A	326	ILE	2.4
2	D	286	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	603	ASP	2.4
1	B	233	LEU	2.4
1	B	239	VAL	2.3
1	C	269	MET	2.3
1	A	270	PHE	2.3
1	A	27	VAL	2.3
2	D	27	VAL	2.3
1	B	225	HIS	2.2
1	C	72	ALA	2.2
2	D	70	ALA	2.2
1	B	235	LEU	2.2
1	A	299	ASP	2.1
1	A	290	THR	2.1
2	D	603	ASP	2.1
1	C	322	ASN	2.1
1	B	330	LEU	2.1
1	C	292	VAL	2.0
1	A	244	LEU	2.0
1	A	301	VAL	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 [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($\text{\AA}^2$)	Q<0.9
3	OAN	A	1627	25/25	0.97	0.07	18,24,34,36	9
3	OAN	B	1627	25/25	0.97	0.07	15,19,48,49	0
3	OAN	C	1627	25/25	0.97	0.08	13,18,37,38	8
3	OAN	D	1627	25/25	0.97	0.06	15,18,42,44	0

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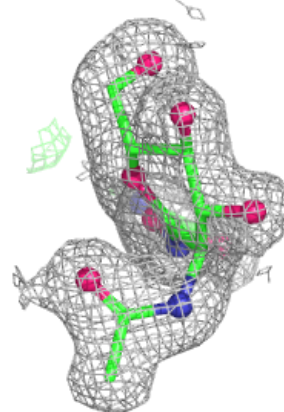
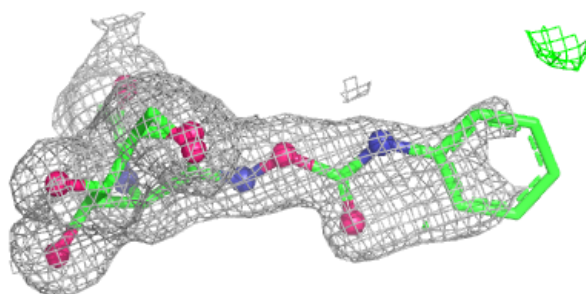
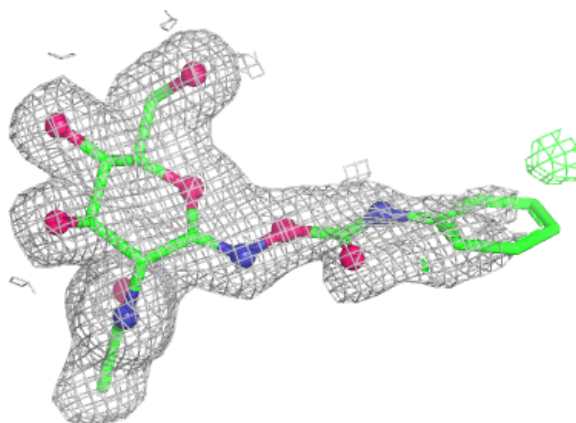
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	1628	1/1	0.98	0.12	27,27,27,27	0
4	MG	B	1628	1/1	0.98	0.10	22,22,22,22	0
4	MG	C	1628	1/1	0.99	0.09	21,21,21,21	0

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.

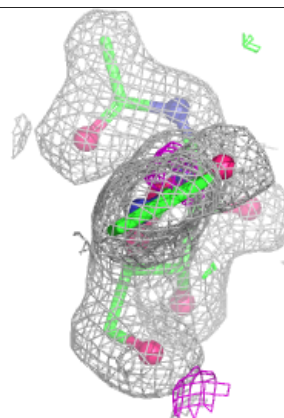
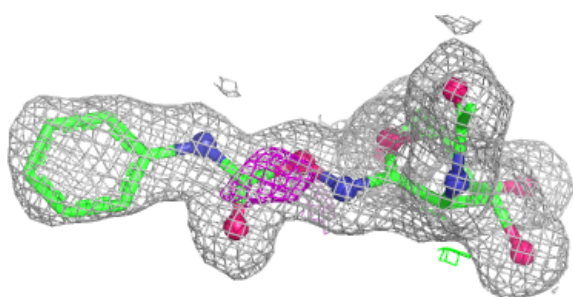
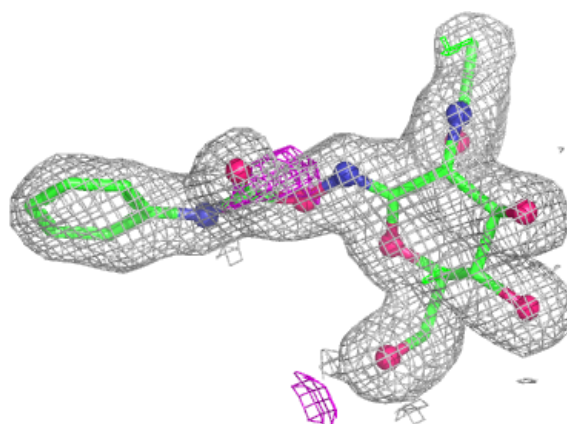
Electron density around OAN A 1627:

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



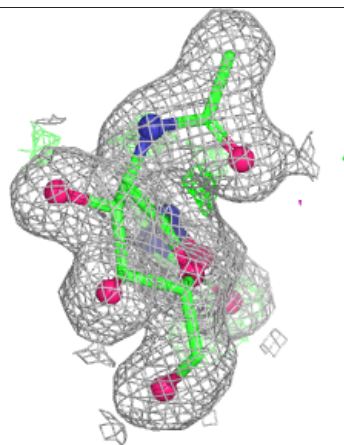
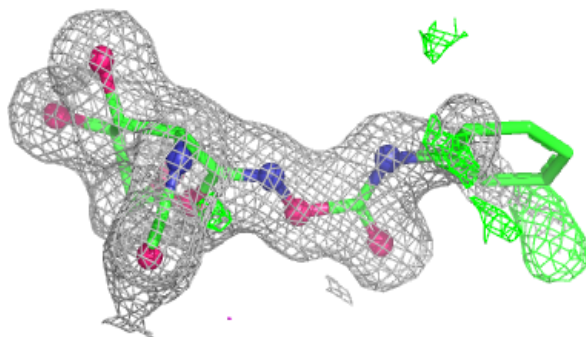
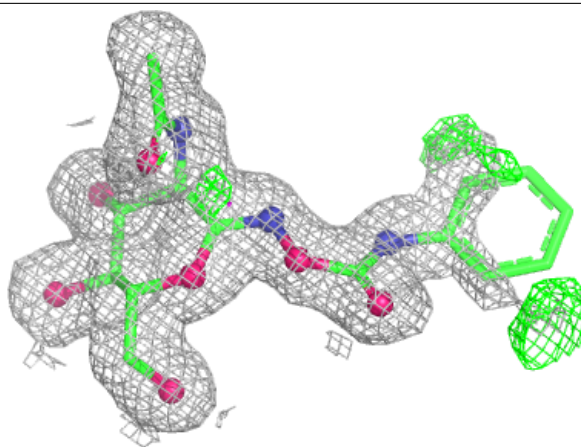
Electron density around OAN B 1627:

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



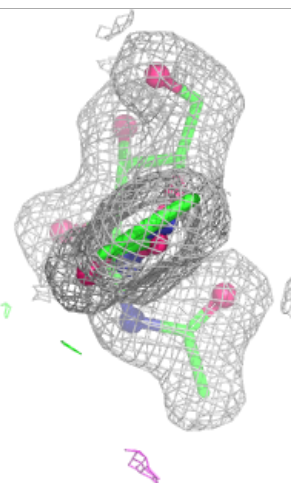
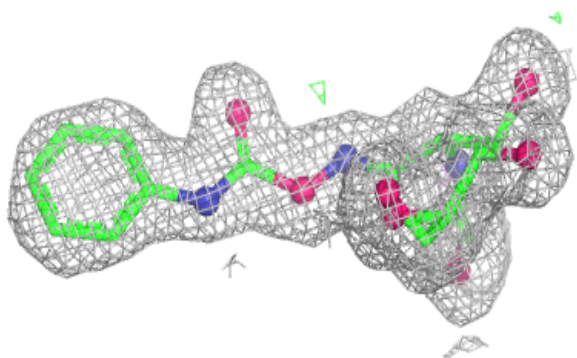
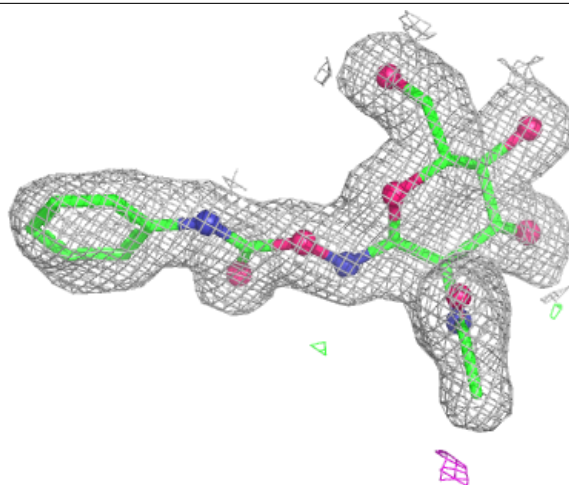
Electron density around OAN C 1627:

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



Electron density around OAN D 1627:

$2mF_o-DF_c$ (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.