Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 12:24 AM EDT

PDB ID	:	5UHO
Title	:	Crystal structure of the core catalytic domain of human O-GlcNAcase complexed with PUGNAc
Authors	:	Klein, D.J.; Elsen, N.L.
Deposited on	:	2017-01-11
Resolution	:	3.21 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:

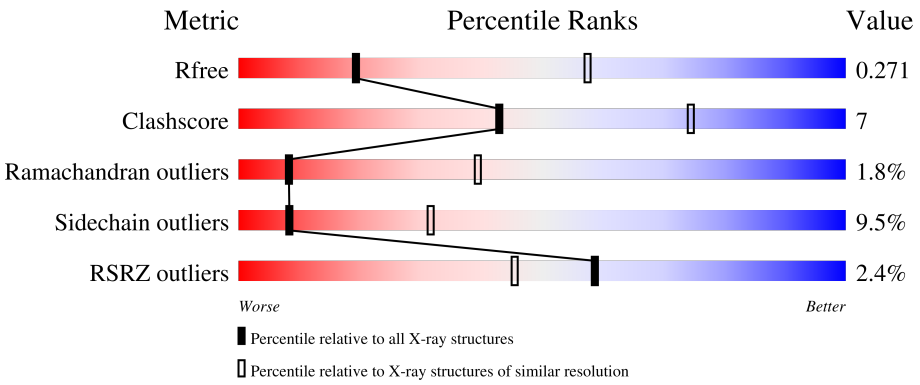
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.21 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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	345	% 70% 17% • 12%
1	C	345	62% 23% • 12%
2	B	163	6% 54% 16% • 26%
2	D	163	5% 55% 17% • 26%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6967 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 O-GlcNAcase TIM-barrel domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	304	2498	1616	413	455	14	0	0	0
1	C	302	2471	1601	405	451	14	0	0	0

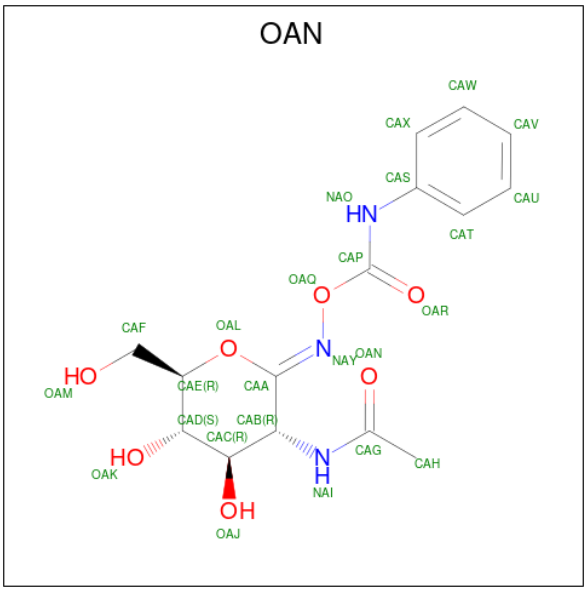
- Molecule 2 is a protein called O-GlcNAcase stalk domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	120	970	627	160	172	11	0	0	0
2	D	120	973	629	160	173	11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	543	MET	-	initiating methionine	UNP O60502
D	543	MET	-	initiating methionine	UNP O60502

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



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

- Molecule 4 is water.

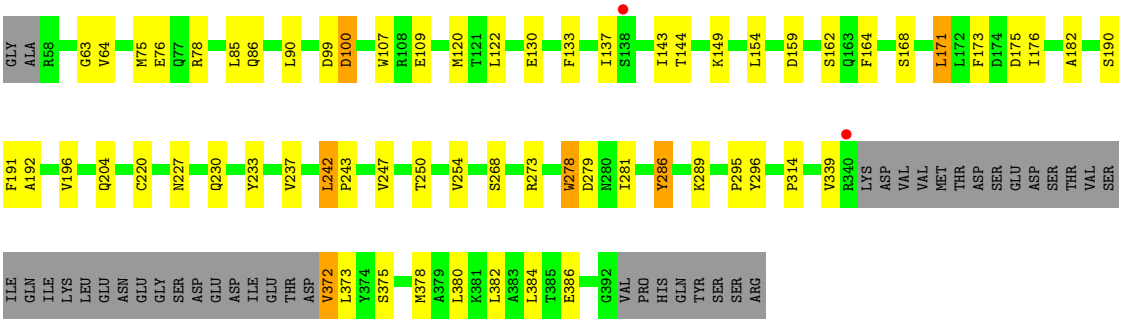
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	1	1	1	0	0
			Total	O		
4	B	1	1	1	0	0
			Total	O		
4	C	3	3	3	0	0

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.

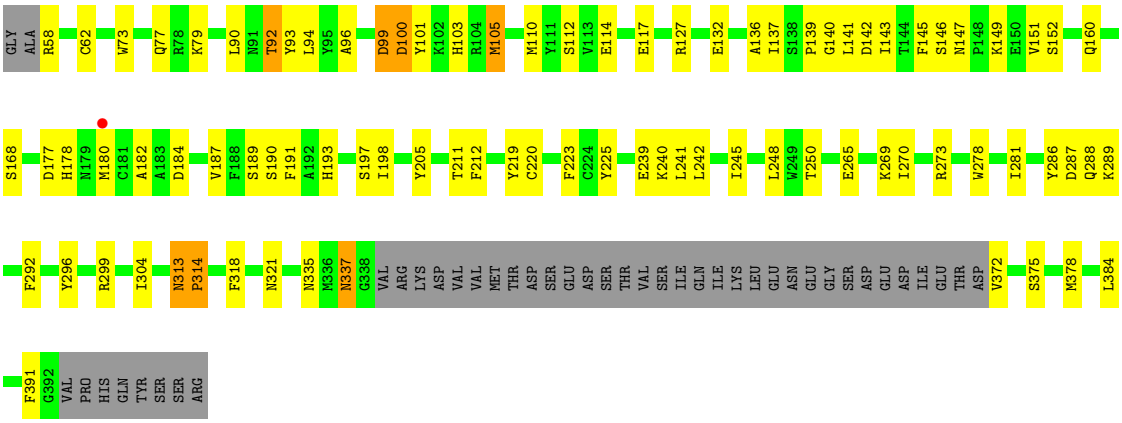
• Molecule 1: O-GlcNAcase TIM-barrel domain

Chain A:



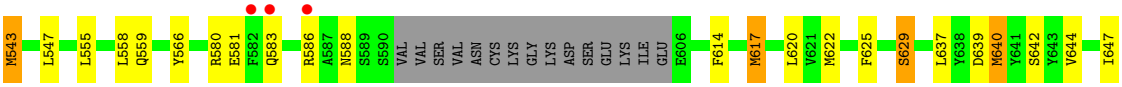
• Molecule 1: O-GlcNAcase TIM-barrel domain

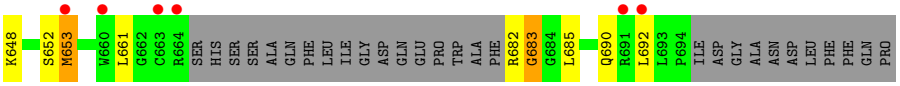
Chain C:



• Molecule 2: O-GlcNAcase stalk domain

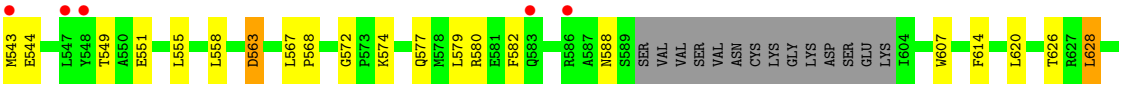
Chain B:

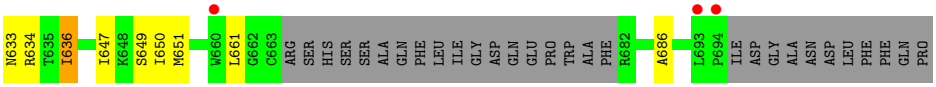




- Molecule 2: O-GlcNAcase stalk domain

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	97.34Å 97.34Å 260.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.38 – 3.21 34.12 – 3.21	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.38-3.21) 100.0 (34.12-3.21)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 3.18Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.197 , 0.259 0.211 , 0.271	Depositor DCC
R_{free} test set	1076 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	103.2	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 92.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6967	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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 (i)

5.1 Standard geometry (i)

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

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	0.55	0/2565	0.77	1/3475 (0.0%)
1	C	0.52	0/2538	0.74	0/3441
2	B	0.50	0/993	0.70	0/1337
2	D	0.52	0/996	0.71	0/1341
All	All	0.53	0/7092	0.74	1/9594 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	278	TRP	N-CA-C	-5.09	97.25	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2498	0	2453	31	0
1	C	2471	0	2420	42	0
2	B	970	0	948	16	0
2	D	973	0	949	17	0
3	A	25	0	17	4	0
3	C	25	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	0	0
All	All	6967	0	6805	94	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 (94) 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:C:110:MET:HB3	1:C:160:GLN:HE22	1.55	0.70
2:B:682:ARG:HG2	2:B:683:GLY:H	1.56	0.70
1:C:62:CYS:SG	1:C:90:LEU:HD22	2.36	0.66
1:A:286:TYR:HB3	3:A:501:OAN:HAW	1.78	0.65
1:C:375:SER:HB3	1:C:378:MET:HB2	1.79	0.64
1:C:219:TYR:HD2	1:C:250:THR:HG1	1.44	0.64
1:C:296:TYR:CZ	1:C:299:ARG:HD3	2.34	0.63
1:A:227:ASN:HD21	1:A:230:GLN:HB2	1.63	0.63
1:C:94:LEU:HD11	1:C:136:ALA:HB2	1.82	0.61
2:B:625:PHE:HD1	2:B:644:VAL:HG12	1.67	0.60
1:A:295:PRO:HD3	1:A:380:LEU:HD22	1.87	0.57
1:A:384:LEU:HD22	2:B:558:LEU:HB3	1.84	0.57
1:A:372:VAL:HG12	1:A:373:LEU:HD12	1.86	0.57
2:B:617:MET:HA	2:B:620:LEU:HD12	1.88	0.56
1:A:254:VAL:HG21	3:A:501:OAN:HAO	1.71	0.56
2:D:563:ASP:HA	2:D:572:GLY:HA3	1.89	0.54
1:A:120:MET:HG2	1:A:164:PHE:HB3	1.89	0.54
2:D:577:GLN:HA	2:D:580:ARG:HE	1.73	0.54
1:C:92:THR:HA	1:C:132:GLU:HB3	1.90	0.54
2:B:629:SER:HA	2:B:637:LEU:HD22	1.90	0.53
1:A:182:ALA:HB3	2:D:543:MET:HB3	1.91	0.53
1:C:239:GLU:HB3	1:C:240:LYS:HE2	1.89	0.53
1:C:286:TYR:CG	3:C:501:OAN:HAW	2.44	0.53
1:C:147:ASN:HD21	1:C:149:LYS:HE3	1.74	0.53
2:B:580:ARG:HA	2:B:583:GLN:HE21	1.74	0.52
1:C:286:TYR:CB	3:C:501:OAN:HAW	2.40	0.52
1:C:180:MET:HG2	1:C:191:PHE:HD1	1.76	0.51
1:C:314:PRO:HB2	1:C:321:ASN:CG	2.32	0.50
1:C:143:ILE:HG23	1:C:145:PHE:CE1	2.46	0.50
1:C:384:LEU:HD22	2:D:558:LEU:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:THR:HG22	1:C:93:TYR:H	1.77	0.49
1:A:220:CYS:HB3	1:A:250:THR:OG1	2.13	0.49
1:A:227:ASN:ND2	1:A:230:GLN:HB2	2.27	0.49
2:B:581:GLU:HB2	2:B:614:PHE:CD2	2.47	0.49
1:C:292:PHE:HE1	2:D:568:PRO:HA	1.78	0.49
1:C:212:PHE:HD2	1:C:245:ILE:HG23	1.78	0.48
1:C:190:SER:OG	1:C:193:HIS:HD2	1.96	0.48
1:C:146:SER:HB2	1:C:187:VAL:HG21	1.96	0.47
1:C:77:GLN:NE2	1:C:318:PHE:HB3	2.28	0.47
2:B:647:ILE:HD12	2:D:686:ALA:HB2	1.96	0.47
1:A:242:LEU:HD23	1:A:243:PRO:HD2	1.97	0.47
2:B:682:ARG:NH1	1:C:287:ASP:HA	2.30	0.47
1:C:99:ASP:O	1:C:100:ASP:C	2.53	0.47
2:B:581:GLU:HB2	2:B:614:PHE:HD2	1.80	0.46
1:C:304:ILE:HD12	1:C:335:ASN:HB3	1.97	0.46
2:D:588:ASN:HB2	2:D:607:TRP:CD1	2.51	0.46
1:C:314:PRO:HB2	1:C:321:ASN:OD1	2.15	0.46
2:D:633:ASN:HD22	2:D:636:ILE:HD11	1.81	0.46
1:C:241:LEU:HD23	1:C:273:ARG:NH2	2.31	0.45
2:B:555:LEU:O	2:B:559:GLN:HG3	2.17	0.45
2:D:647:ILE:O	2:D:651:MET:HB2	2.16	0.45
1:A:64:VAL:HG23	1:A:85:LEU:HD21	1.99	0.45
1:A:133:PHE:O	1:A:168:SER:HB2	2.17	0.45
1:C:101:TYR:HE1	1:C:105:MET:HE1	1.81	0.45
1:A:137:ILE:HG21	1:A:154:LEU:HD11	1.98	0.44
1:C:241:LEU:HD23	1:C:273:ARG:HH22	1.82	0.44
1:A:192:ALA:O	1:A:196:VAL:HG23	2.18	0.44
1:A:233:TYR:O	1:A:237:VAL:HG23	2.17	0.44
2:D:582:PHE:HB2	2:D:614:PHE:CZ	2.52	0.44
1:A:63:GLY:HA2	1:A:90:LEU:HD13	2.00	0.44
1:A:107:TRP:CH2	1:A:143:ILE:HD12	2.52	0.44
1:C:77:GLN:HE21	1:C:318:PHE:HB3	1.82	0.44
1:A:289:LYS:HZ2	2:D:650:ILE:HD11	1.83	0.44
2:B:543:MET:HG2	1:C:182:ALA:HB3	1.98	0.44
2:B:547:LEU:HA	1:C:142:ASP:HB2	1.99	0.44
1:A:247:VAL:HG23	1:A:273:ARG:HD2	2.00	0.44
1:A:279:ASP:OD1	1:A:281:ILE:HG22	2.19	0.43
2:D:636:ILE:H	2:D:636:ILE:HG12	1.53	0.43
1:C:62:CYS:SG	1:C:90:LEU:CD2	3.07	0.42
1:C:205:TYR:C	1:C:205:TYR:CD1	2.91	0.42
2:B:685:LEU:HD23	2:D:647:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:633:ASN:HD22	2:D:636:ILE:CD1	2.32	0.42
1:A:78:ARG:HB3	1:A:122:LEU:HD11	2.01	0.42
1:A:375:SER:HB3	1:A:378:MET:HB2	2.02	0.42
1:C:73:TRP:NE1	1:C:318:PHE:HB2	2.34	0.42
1:C:180:MET:HB3	1:C:184:ASP:HB2	2.02	0.42
1:A:78:ARG:CB	1:A:122:LEU:HD11	2.49	0.42
1:A:286:TYR:CB	3:A:501:OAN:HAW	2.48	0.42
1:C:391:PHE:HE2	2:D:628:LEU:HD21	1.84	0.42
1:A:120:MET:HG2	1:A:164:PHE:CB	2.50	0.42
1:A:254:VAL:HG11	3:A:501:OAN:NAO	2.34	0.41
2:D:567:LEU:HB3	2:D:568:PRO:CD	2.49	0.41
1:C:96:ALA:HA	1:C:103:HIS:CE1	2.55	0.41
1:A:99:ASP:O	1:A:100:ASP:C	2.59	0.41
1:C:168:SER:OG	1:C:211:THR:HB	2.21	0.41
1:C:278:TRP:NE1	1:C:313:ASN:HB2	2.36	0.41
1:A:144:THR:HG21	2:D:544:GLU:HG2	2.03	0.41
1:C:287:ASP:C	1:C:289:LYS:H	2.24	0.41
2:B:653:MET:H	2:B:653:MET:HG2	1.67	0.40
1:A:176:ILE:HD12	1:A:191:PHE:HZ	1.86	0.40
2:B:640:MET:O	2:B:644:VAL:HG23	2.21	0.40
1:C:220:CYS:HB3	1:C:250:THR:OG1	2.20	0.40
1:A:171:LEU:HD23	1:A:173:PHE:CZ	2.57	0.40
1:C:151:VAL:HG22	1:C:198:ILE:HD12	2.03	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	300/345 (87%)	271 (90%)	25 (8%)	4 (1%)	12 46
1	C	298/345 (86%)	267 (90%)	22 (7%)	9 (3%)	4 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	114/163 (70%)	107 (94%)	5 (4%)	2 (2%)	8	39
2	D	114/163 (70%)	108 (95%)	6 (5%)	0	100	100
All	All	826/1016 (81%)	753 (91%)	58 (7%)	15 (2%)	8	39

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	C	140	GLY
1	C	141	LEU
1	C	100	ASP
1	C	337	ASN
1	A	286	TYR
1	C	189	SER
1	A	296	TYR
1	C	223	PHE
2	B	566	TYR
2	B	683	GLY
1	C	288	GLN
1	C	314	PRO
1	A	314	PRO
1	C	139	PRO

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	272/310 (88%)	253 (93%)	19 (7%)	15	47
1	C	268/310 (86%)	244 (91%)	24 (9%)	9	34
2	B	102/141 (72%)	87 (85%)	15 (15%)	3	14
2	D	102/141 (72%)	89 (87%)	13 (13%)	4	19
All	All	744/902 (82%)	673 (90%)	71 (10%)	8	31

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	MET
1	A	76	GLU
1	A	86	GLN
1	A	109	GLU
1	A	130	GLU
1	A	149	LYS
1	A	159	ASP
1	A	162	SER
1	A	171	LEU
1	A	175	ASP
1	A	190	SER
1	A	204	GLN
1	A	242	LEU
1	A	268	SER
1	A	278	TRP
1	A	339	VAL
1	A	372	VAL
1	A	382	LEU
1	A	386	GLU
2	B	543	MET
2	B	586	ARG
2	B	588	ASN
2	B	617	MET
2	B	622	MET
2	B	629	SER
2	B	639	ASP
2	B	640	MET
2	B	642	SER
2	B	648	LYS
2	B	652	SER
2	B	653	MET
2	B	661	LEU
2	B	690	GLN
2	B	692	LEU
1	C	58	ARG
1	C	79	LYS
1	C	92	THR
1	C	99	ASP
1	C	105	MET
1	C	112	SER
1	C	114	GLU
1	C	117	GLU
1	C	127	ARG

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Mol	Chain	Res	Type
1	C	137	ILE
1	C	152	SER
1	C	177	ASP
1	C	178	HIS
1	C	197	SER
1	C	225	TYR
1	C	242	LEU
1	C	248	LEU
1	C	265	GLU
1	C	269	LYS
1	C	270	ILE
1	C	281	ILE
1	C	313	ASN
1	C	337	ASN
1	C	372	VAL
2	D	549	THR
2	D	551	GLU
2	D	555	LEU
2	D	563	ASP
2	D	574	LYS
2	D	579	LEU
2	D	620	LEU
2	D	626	THR
2	D	628	LEU
2	D	634	ARG
2	D	636	ILE
2	D	649	SER
2	D	661	LEU

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

Mol	Chain	Res	Type
1	A	160	GLN
1	A	193	HIS
2	B	583	GLN
1	C	193	HIS
2	D	577	GLN
2	D	633	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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OAN	C	501	-	24,26,26	2.01	7 (29%)	24,35,35	1.96	3 (12%)
3	OAN	A	501	-	24,26,26	1.92	7 (29%)	24,35,35	1.32	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	C	501	-	-	4/12/35/35	0/2/2/2
3	OAN	A	501	-	-	5/12/35/35	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	OAN	CAA-NAY	4.14	1.37	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	OAN	CAP-NAO	4.02	1.44	1.36
3	A	501	OAN	CAP-NAO	3.49	1.43	1.36
3	A	501	OAN	CAC-CAB	3.35	1.57	1.52
3	A	501	OAN	OAR-CAP	3.29	1.27	1.21
3	A	501	OAN	CAA-NAY	3.26	1.35	1.27
3	A	501	OAN	OAJ-CAC	-2.95	1.36	1.43
3	C	501	OAN	OAJ-CAC	-2.78	1.36	1.43
3	C	501	OAN	CAT-CAS	2.67	1.43	1.39
3	C	501	OAN	OAR-CAP	2.55	1.26	1.21
3	C	501	OAN	OAK-CAD	-2.36	1.37	1.43
3	C	501	OAN	OAL-CAA	2.28	1.40	1.36
3	A	501	OAN	OAL-CAA	2.26	1.40	1.36
3	A	501	OAN	OAK-CAD	-2.08	1.38	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	501	OAN	CAS-NAO-CAP	6.23	136.60	126.36
3	C	501	OAN	CAB-NAI-CAG	4.70	129.86	121.84
3	C	501	OAN	OAR-CAP-NAO	3.50	133.72	126.11
3	A	501	OAN	CAS-NAO-CAP	2.91	131.14	126.36
3	A	501	OAN	OAR-CAP-NAO	2.62	131.80	126.11
3	A	501	OAN	CAB-NAI-CAG	2.27	125.71	121.84
3	A	501	OAN	CAF-CAE-CAD	-2.07	108.15	113.00
3	A	501	OAN	OAL-CAE-CAD	2.04	113.36	109.73

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	OAN	OAR-CAP-OAQ-NAY
3	A	501	OAN	NAO-CAP-OAQ-NAY
3	C	501	OAN	OAR-CAP-OAQ-NAY
3	C	501	OAN	NAO-CAP-OAQ-NAY
3	A	501	OAN	OAL-CAE-CAF-OAM
3	A	501	OAN	CAD-CAE-CAF-OAM
3	C	501	OAN	OAL-CAE-CAF-OAM
3	A	501	OAN	CAA-CAB-NAI-CAG
3	C	501	OAN	CAA-CAB-NAI-CAG

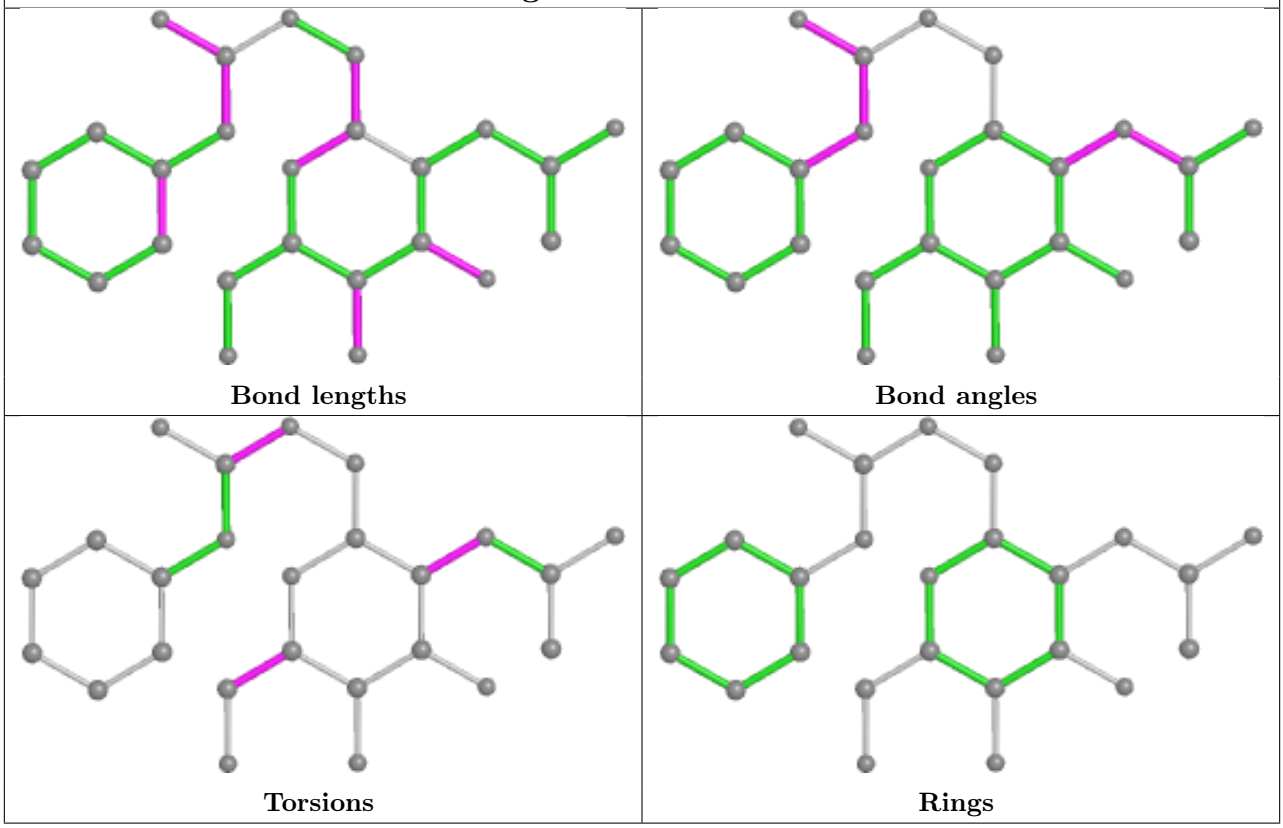
There are no ring outliers.

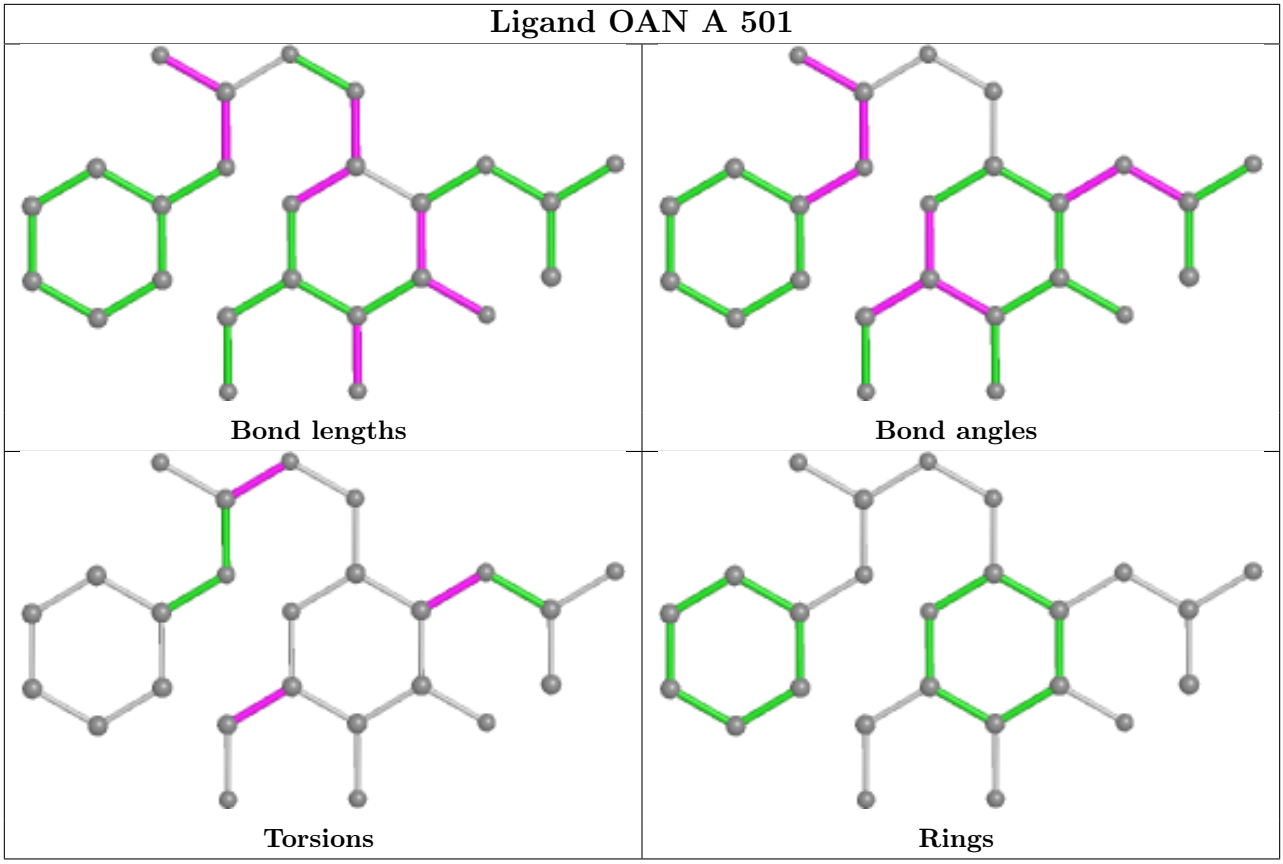
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	OAN	2	0
3	A	501	OAN	4	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 OAN C 501





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	304/345 (88%)	-0.06	2 (0%)	87	82	80, 109, 137, 196	0
1	C	302/345 (87%)	-0.10	1 (0%)	94	92	85, 115, 143, 157	0
2	B	120/163 (73%)	0.21	9 (7%)	14	8	87, 127, 187, 211	0
2	D	120/163 (73%)	0.32	8 (6%)	17	11	84, 116, 153, 170	0
All	All	846/1016 (83%)	0.02	20 (2%)	59	45	80, 114, 153, 211	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	693	LEU	4.0
2	B	664	ARG	3.9
2	B	663	CYS	3.4
1	A	340	ARG	3.0
2	D	583	GLN	2.8
2	B	653	MET	2.8
2	D	586	ARG	2.6
1	A	138	SER	2.5
2	D	660	TRP	2.4
2	D	548	TYR	2.3
2	D	547	LEU	2.3
2	B	660	TRP	2.2
1	C	180	MET	2.2
2	B	582	PHE	2.2
2	B	691	ARG	2.2
2	B	692	LEU	2.1
2	D	543	MET	2.1
2	B	586	ARG	2.1
2	D	694	PRO	2.1
2	B	583	GLN	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)

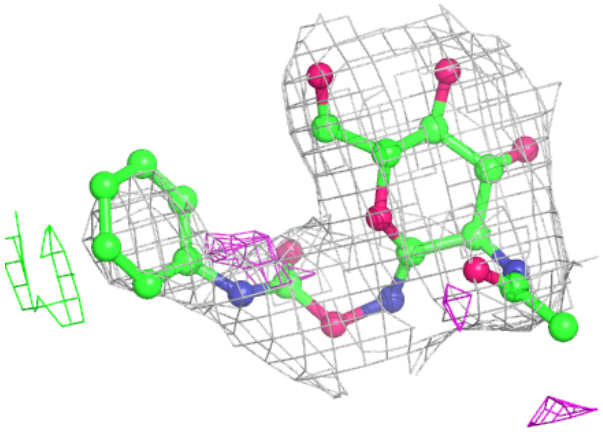
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

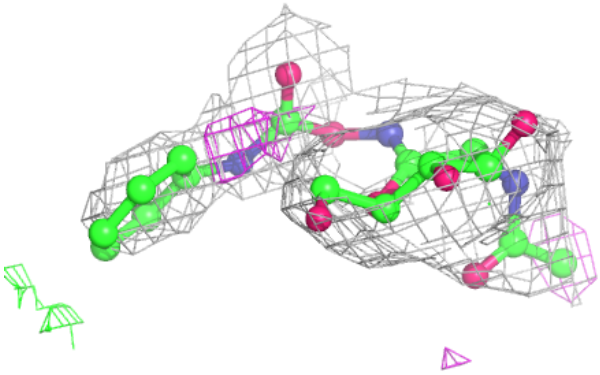
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OAN	A	501	25/25	0.83	0.35	102,102,102,102	0
3	OAN	C	501	25/25	0.84	0.34	118,118,118,118	0

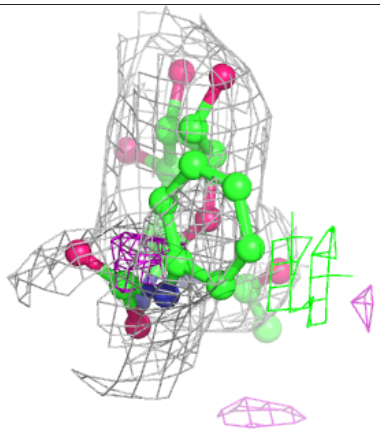
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OAN A 501:

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

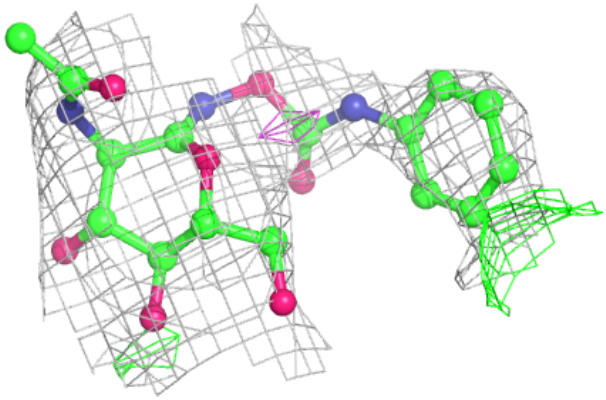


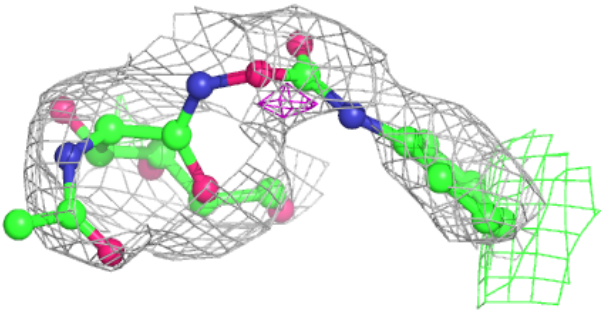


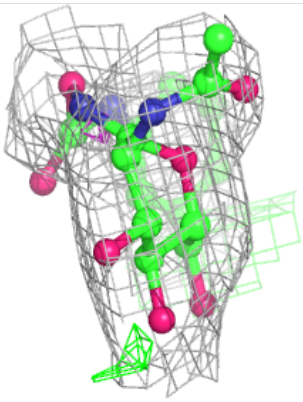


Electron density around OAN C 501:

$2mF_o$-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.