Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 07:04 PM EDT

PDB ID	:	6TBJ
Title	:	Structure of a beta galactosidase with inhibitor
Authors	:	Offen, W.; Davies, G.
Deposited on	:	2019-11-01
Resolution	:	1.50 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:

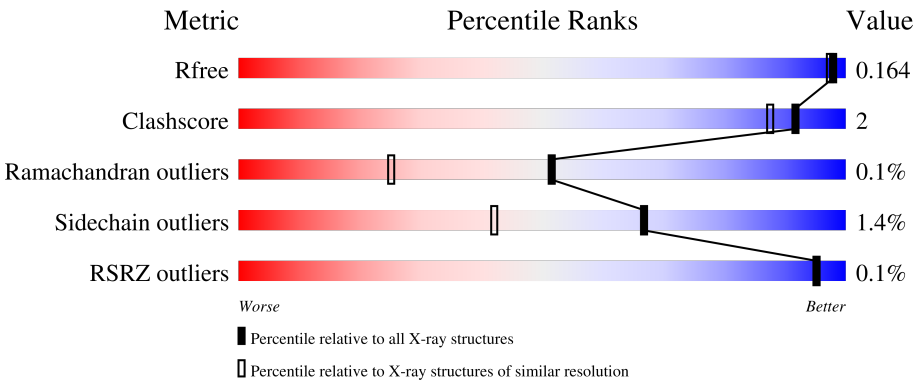
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	550	92% • 5%
1	B	550	90% 5% 5%
1	C	550	% 91% 5% •
1	D	550	91% 5% •
1	E	550	93% • •

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Mol	Chain	Length	Quality of chain
1	F	550	93%
1	G	550	91% 6%
1	H	550	90% 5% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 35492 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-galactosidase, putative, bgl35A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	525	4131	2650	697	767	17	0	3	0
1	B	524	4135	2652	699	769	15	0	2	0
1	C	526	4123	2641	698	769	15	0	1	1
1	D	531	4194	2691	709	779	15	0	4	0
1	E	532	4156	2662	702	777	15	0	0	0
1	F	531	4186	2678	709	784	15	0	3	0
1	G	532	4206	2695	715	780	16	0	5	0
1	H	523	4106	2629	691	771	15	0	5	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	initiating methionine	UNP B3PBE0
A	27	GLY	-	expression tag	UNP B3PBE0
A	28	SER	-	expression tag	UNP B3PBE0
A	29	SER	-	expression tag	UNP B3PBE0
A	30	HIS	-	expression tag	UNP B3PBE0
A	31	HIS	-	expression tag	UNP B3PBE0
A	32	HIS	-	expression tag	UNP B3PBE0
A	33	HIS	-	expression tag	UNP B3PBE0
A	34	HIS	-	expression tag	UNP B3PBE0
A	35	HIS	-	expression tag	UNP B3PBE0
B	26	MET	-	initiating methionine	UNP B3PBE0
B	27	GLY	-	expression tag	UNP B3PBE0
B	28	SER	-	expression tag	UNP B3PBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP B3PBE0
B	30	HIS	-	expression tag	UNP B3PBE0
B	31	HIS	-	expression tag	UNP B3PBE0
B	32	HIS	-	expression tag	UNP B3PBE0
B	33	HIS	-	expression tag	UNP B3PBE0
B	34	HIS	-	expression tag	UNP B3PBE0
B	35	HIS	-	expression tag	UNP B3PBE0
C	26	MET	-	initiating methionine	UNP B3PBE0
C	27	GLY	-	expression tag	UNP B3PBE0
C	28	SER	-	expression tag	UNP B3PBE0
C	29	SER	-	expression tag	UNP B3PBE0
C	30	HIS	-	expression tag	UNP B3PBE0
C	31	HIS	-	expression tag	UNP B3PBE0
C	32	HIS	-	expression tag	UNP B3PBE0
C	33	HIS	-	expression tag	UNP B3PBE0
C	34	HIS	-	expression tag	UNP B3PBE0
C	35	HIS	-	expression tag	UNP B3PBE0
D	26	MET	-	initiating methionine	UNP B3PBE0
D	27	GLY	-	expression tag	UNP B3PBE0
D	28	SER	-	expression tag	UNP B3PBE0
D	29	SER	-	expression tag	UNP B3PBE0
D	30	HIS	-	expression tag	UNP B3PBE0
D	31	HIS	-	expression tag	UNP B3PBE0
D	32	HIS	-	expression tag	UNP B3PBE0
D	33	HIS	-	expression tag	UNP B3PBE0
D	34	HIS	-	expression tag	UNP B3PBE0
D	35	HIS	-	expression tag	UNP B3PBE0
E	26	MET	-	initiating methionine	UNP B3PBE0
E	27	GLY	-	expression tag	UNP B3PBE0
E	28	SER	-	expression tag	UNP B3PBE0
E	29	SER	-	expression tag	UNP B3PBE0
E	30	HIS	-	expression tag	UNP B3PBE0
E	31	HIS	-	expression tag	UNP B3PBE0
E	32	HIS	-	expression tag	UNP B3PBE0
E	33	HIS	-	expression tag	UNP B3PBE0
E	34	HIS	-	expression tag	UNP B3PBE0
E	35	HIS	-	expression tag	UNP B3PBE0
F	26	MET	-	initiating methionine	UNP B3PBE0
F	27	GLY	-	expression tag	UNP B3PBE0
F	28	SER	-	expression tag	UNP B3PBE0
F	29	SER	-	expression tag	UNP B3PBE0
F	30	HIS	-	expression tag	UNP B3PBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	31	HIS	-	expression tag	UNP B3PBE0
F	32	HIS	-	expression tag	UNP B3PBE0
F	33	HIS	-	expression tag	UNP B3PBE0
F	34	HIS	-	expression tag	UNP B3PBE0
F	35	HIS	-	expression tag	UNP B3PBE0
G	26	MET	-	initiating methionine	UNP B3PBE0
G	27	GLY	-	expression tag	UNP B3PBE0
G	28	SER	-	expression tag	UNP B3PBE0
G	29	SER	-	expression tag	UNP B3PBE0
G	30	HIS	-	expression tag	UNP B3PBE0
G	31	HIS	-	expression tag	UNP B3PBE0
G	32	HIS	-	expression tag	UNP B3PBE0
G	33	HIS	-	expression tag	UNP B3PBE0
G	34	HIS	-	expression tag	UNP B3PBE0
G	35	HIS	-	expression tag	UNP B3PBE0
H	26	MET	-	initiating methionine	UNP B3PBE0
H	27	GLY	-	expression tag	UNP B3PBE0
H	28	SER	-	expression tag	UNP B3PBE0
H	29	SER	-	expression tag	UNP B3PBE0
H	30	HIS	-	expression tag	UNP B3PBE0
H	31	HIS	-	expression tag	UNP B3PBE0
H	32	HIS	-	expression tag	UNP B3PBE0
H	33	HIS	-	expression tag	UNP B3PBE0
H	34	HIS	-	expression tag	UNP B3PBE0
H	35	HIS	-	expression tag	UNP B3PBE0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	3	3	3	0	0
2	B	1	1	1	0	0
2	C	3	3	3	0	0
2	D	5	5	5	0	0
2	E	4	4	4	0	0
2	F	4	4	4	0	0
2	G	3	3	3	0	0

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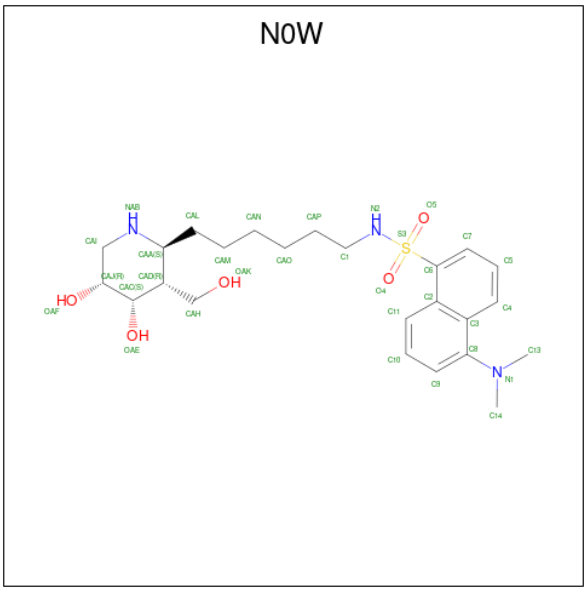
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	4	Total Na 4 4	0	0

- Molecule 3 is 5-(dimethylamino)- {N}-[6-[(2 {S},3 {R},4 {S},5 {R})-3-(hydroxymethyl)-4,5-bis(oxidanyl)piperidin-2-yl]hexyl]naphthalene-1-sulfonamide (three-letter code: N0W) (formula: $C_{24}H_{37}N_3O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 21 13 2 5 1	0	0
3	B	1	Total C N O 13 9 1 3	0	0
3	C	1	Total C N O 12 8 1 3	0	0
3	D	1	Total C N O S 21 13 2 5 1	0	0
3	E	1	Total C N O 15 11 1 3	0	0
3	F	1	Total C N O S 21 13 2 5 1	0	0
3	G	1	Total C N O 15 11 1 3	0	0
3	H	1	Total C N O 15 11 1 3	0	0

- Molecule 4 is water.

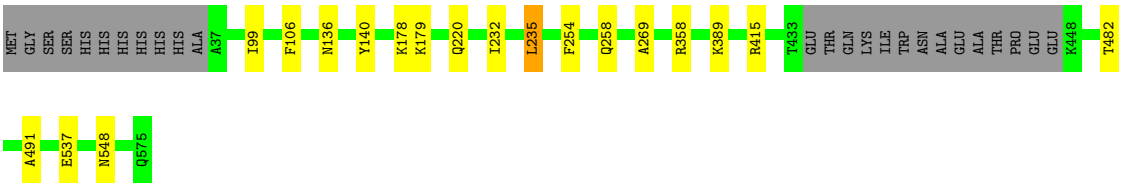
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	220	220	220	0	0
			Total	O		
4	B	254	254	254	0	0
			Total	O		
4	C	238	238	238	0	0
			Total	O		
4	D	307	307	307	0	0
			Total	O		
4	E	301	301	301	0	0
			Total	O		
4	F	274	274	274	0	0
			Total	O		
4	G	291	291	291	0	0
			Total	O		
4	H	210	210	210	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.

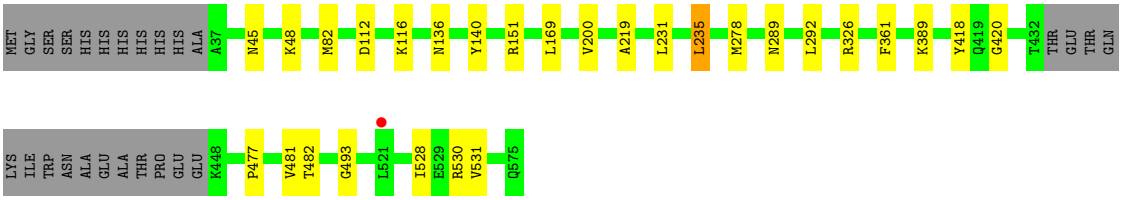
• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain A:



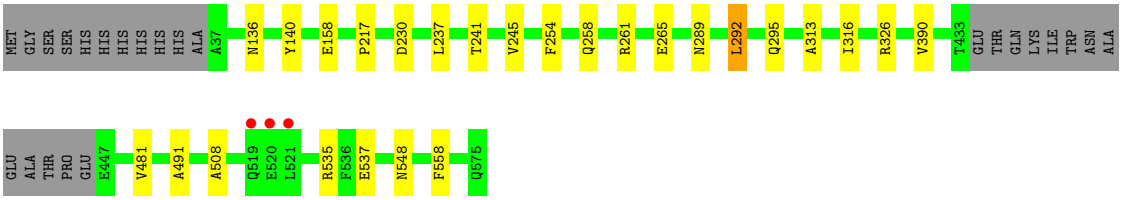
• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain B:



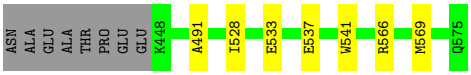
• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain C:



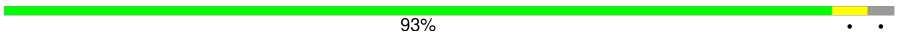
• Molecule 1: Beta-galactosidase, putative, bgl35A

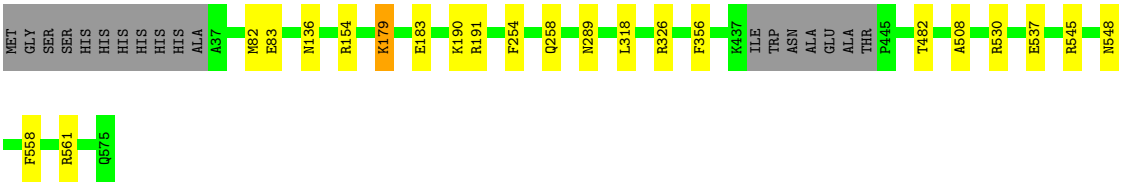
Chain D:



• Molecule 1: Beta-galactosidase, putative, bgl35A

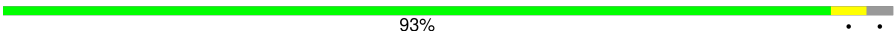
Chain E:

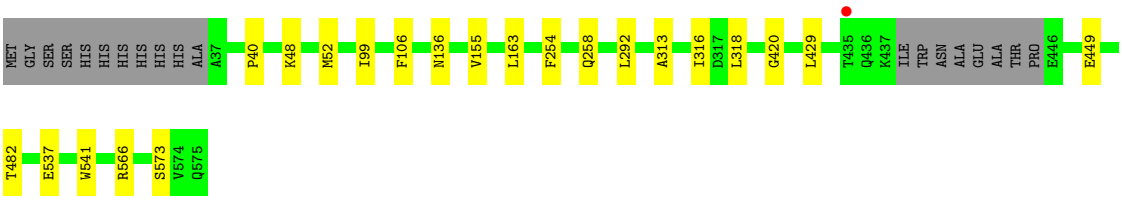




• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain F:





• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain G:

• Molecule 1: Beta-galactosidase, putative, bgl35A

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	99.42Å 115.79Å 116.19Å 89.93° 90.08° 89.99°	Depositor
Resolution (Å)	63.21 – 1.50 63.21 – 1.50	Depositor EDS
% Data completeness (in resolution range)	94.5 (63.21-1.50) 94.5 (63.21-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.145 , 0.164 0.146 , 0.164	Depositor DCC
R_{free} test set	39812 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 27.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	0.249 for h,-l,k 0.249 for h,l,-k 0.186 for h,-k,-l 0.130 for -h,k,-l 0.129 for -h,-k,l 0.136 for -h,-l,-k 0.129 for -h,l,k	Xtriage
Reported twinning fraction	0.582 for H, K, L 0.048 for h,-k,-l 0.089 for H, -L, K 0.281 for H, L, -K	Depositor
Outliers	0 of 793059 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	35492	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: NA, N0W

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	0.81	0/4247	0.94	2/5787 (0.0%)
1	B	0.79	0/4248	0.95	2/5786 (0.0%)
1	C	0.81	0/4233	0.96	1/5771 (0.0%)
1	D	0.85	2/4312 (0.0%)	0.98	0/5877
1	E	0.81	0/4266	0.95	3/5817 (0.1%)
1	F	0.84	0/4299	0.98	0/5859
1	G	0.84	1/4325 (0.0%)	0.99	0/5891
1	H	0.82	1/4225 (0.0%)	0.94	2/5768 (0.0%)
All	All	0.82	4/34155 (0.0%)	0.96	10/46556 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	533	GLU	CD-OE1	-6.49	1.18	1.25
1	H	533	GLU	CD-OE1	-5.58	1.19	1.25
1	G	205	GLU	CD-OE1	-5.45	1.19	1.25
1	D	97	GLU	CD-OE1	-5.21	1.20	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	530	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	C	535	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	H	340	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	E	561	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	151	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	H	340	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	A	415	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	E	545	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	E	154	ARG	NE-CZ-NH2	-5.24	117.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	358	ARG	NE-CZ-NH2	-5.05	117.77	120.30

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	4131	0	3985	8	0
1	B	4135	0	3999	12	0
1	C	4123	0	3960	11	0
1	D	4194	0	4036	19	0
1	E	4156	0	3981	12	0
1	F	4186	0	4014	12	0
1	G	4206	0	4070	18	0
1	H	4106	0	3914	14	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	3	0	0	0	0
2	D	5	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	3	0	0	0	0
2	H	4	0	0	0	0
3	A	21	0	0	0	0
3	B	13	0	0	0	0
3	C	12	0	0	0	0
3	D	21	0	0	0	0
3	E	15	0	0	0	0
3	F	21	0	0	0	0
3	G	15	0	0	0	0
3	H	15	0	0	0	0
4	A	220	0	0	2	0
4	B	254	0	0	1	0
4	C	238	0	0	1	0
4	D	307	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	301	0	0	4	0
4	F	274	0	0	1	0
4	G	291	0	0	3	0
4	H	210	0	0	0	0
All	All	35492	0	31959	102	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 2.

All (102) 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:D:528:ILE:HD13	1:D:569:MET:SD	2.02	0.99
1:D:326:ARG:HG3	1:D:326:ARG:HH21	1.24	0.98
1:A:482:THR:HG22	4:A:724:HOH:O	1.68	0.94
1:H:199:MET:HG2	1:H:277:PRO:HB2	1.52	0.92
1:E:482:THR:HG22	4:E:756:HOH:O	1.89	0.72
1:E:179:LYS:HE3	4:E:953:HOH:O	1.90	0.71
1:G:48:LYS:NZ	1:G:420:GLY:O	2.24	0.70
1:B:326:ARG:NH1	4:B:701:HOH:O	2.26	0.69
1:F:482:THR:HG22	4:F:792:HOH:O	1.94	0.67
1:B:112:ASP:OD1	1:B:116:LYS:HE2	1.94	0.66
1:B:169:LEU:HD12	1:B:219:ALA:HA	1.76	0.66
1:D:326:ARG:NH2	4:D:701:HOH:O	2.28	0.66
1:F:48:LYS:NZ	1:F:420:GLY:O	2.30	0.64
1:A:232:ILE:O	1:A:235:LEU:O	2.15	0.63
1:G:481:VAL:CG2	4:G:969:HOH:O	2.47	0.62
1:G:481:VAL:HG23	4:G:969:HOH:O	2.00	0.62
1:D:326:ARG:HG3	1:D:326:ARG:NH2	2.03	0.60
1:A:179:LYS:NZ	4:A:701:HOH:O	2.31	0.59
1:E:179:LYS:HD2	4:E:784:HOH:O	2.03	0.58
1:H:169:LEU:CD1	1:H:219:ALA:HA	2.33	0.58
1:C:481:VAL:O	1:C:481:VAL:HG22	2.03	0.58
1:E:326:ARG:HG3	1:E:356:PHE:CZ	2.39	0.58
1:B:481:VAL:HG22	1:B:481:VAL:O	2.04	0.57
1:F:541:TRP:CD2	1:F:566:ARG:HD2	2.40	0.57
1:H:541:TRP:CD2	1:H:566:ARG:HD2	2.39	0.57
1:D:326:ARG:HH21	1:D:326:ARG:CG	2.03	0.56
1:D:326:ARG:NH2	1:D:326:ARG:CG	2.67	0.56
1:B:361:PHE:CD2	1:B:493:GLY:HA3	2.41	0.56
1:H:235:LEU:HB3	1:H:237:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LYS:NZ	1:B:420:GLY:O	2.39	0.54
1:B:477:PRO:HD2	1:B:482:THR:HG22	1.88	0.54
1:D:528:ILE:CD1	1:D:569:MET:SD	2.88	0.54
1:D:45:ASN:ND2	4:D:705:HOH:O	2.41	0.54
1:F:318:LEU:C	1:F:318:LEU:HD12	2.28	0.53
1:E:530:ARG:NH1	4:E:701:HOH:O	2.33	0.53
1:E:190:LYS:HG3	1:E:191:ARG:HG2	1.90	0.53
1:F:155:VAL:HG23	1:F:163:LEU:HB2	1.91	0.52
1:C:241:THR:O	1:C:245:VAL:HG13	2.09	0.52
1:G:482[A]:THR:HG23	4:G:785:HOH:O	2.10	0.52
1:E:508:ALA:HB3	1:E:558:PHE:CD1	2.45	0.52
1:G:397:GLU:O	1:G:401:GLN:HG3	2.09	0.51
1:G:157:LYS:HE3	1:G:161:ASP:HB2	1.93	0.51
1:A:140:TYR:CZ	1:C:548:ASN:HB3	2.46	0.51
1:F:155:VAL:CG2	1:F:163:LEU:HB2	2.41	0.51
1:A:254:PHE:O	1:A:258:GLN:HG2	2.11	0.50
1:A:99:ILE:O	1:A:106:PHE:HA	2.11	0.50
1:E:318:LEU:C	1:E:318:LEU:HD12	2.32	0.49
1:D:169:LEU:CD1	1:D:219:ALA:HA	2.42	0.49
1:G:384:TYR:CD1	1:G:385:PRO:HA	2.48	0.49
1:D:390:VAL:HG22	4:D:957:HOH:O	2.13	0.48
1:B:528:ILE:HG21	1:B:531:VAL:HG23	1.95	0.48
1:G:169:LEU:HD13	1:G:219:ALA:HA	1.95	0.48
1:D:318:LEU:HD12	1:D:318:LEU:C	2.32	0.48
1:H:397:GLU:O	1:H:401:GLN:HG3	2.13	0.48
1:C:390:VAL:HG22	4:C:904:HOH:O	2.14	0.47
1:B:231:LEU:HG	1:B:235:LEU:HD22	1.96	0.47
1:H:199:MET:CG	1:H:277:PRO:HB2	2.36	0.47
1:F:254:PHE:O	1:F:258:GLN:HG2	2.13	0.47
1:G:169:LEU:CD1	1:G:219:ALA:HA	2.44	0.47
1:C:508:ALA:HB3	1:C:558:PHE:CD1	2.51	0.46
1:D:83:GLU:HA	1:D:83:GLU:OE1	2.16	0.46
1:D:541:TRP:CE2	1:D:566:ARG:HD3	2.51	0.46
1:G:227:VAL:HB	1:G:232:ILE:HD11	1.99	0.45
1:H:412:GLU:HG2	1:H:536:PHE:CG	2.52	0.45
1:H:528:ILE:HG21	1:H:531:VAL:HG23	1.98	0.45
1:A:178:LYS:HG3	1:A:269:ALA:CB	2.47	0.45
1:D:235:LEU:HB3	1:D:237:LEU:HG	1.98	0.45
1:D:99:ILE:O	1:D:106:PHE:HA	2.17	0.44
1:E:254:PHE:O	1:E:258:GLN:HG2	2.18	0.44
1:G:229:ASP:O	1:G:233:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:95:ALA:O	1:H:98:GLN:HG2	2.18	0.44
1:G:407:ASN:N	1:G:408:PRO:HD2	2.33	0.44
1:D:230:ASP:OD2	1:D:234:LYS:HE3	2.17	0.43
1:G:199:MET:HG2	1:G:277:PRO:HB2	1.99	0.43
1:C:261:ARG:O	1:C:265:GLU:HG3	2.18	0.43
1:D:48:LYS:NZ	1:D:420:GLY:O	2.37	0.43
1:C:254:PHE:O	1:C:258:GLN:HG2	2.19	0.43
1:A:548:ASN:HB3	1:B:140:TYR:CZ	2.53	0.43
1:H:169:LEU:HD13	1:H:219:ALA:HA	1.99	0.43
1:F:313:ALA:HB1	1:F:316:ILE:HD12	2.00	0.42
1:F:541:TRP:CE2	1:F:566:ARG:CD	3.02	0.42
1:G:508:ALA:HB3	1:G:558:PHE:CD1	2.55	0.42
1:D:292:LEU:O	1:D:295:GLN:HB2	2.19	0.42
1:H:99:ILE:O	1:H:106:PHE:HA	2.20	0.42
1:D:140:TYR:CZ	1:E:548:ASN:HB3	2.54	0.42
1:G:477:PRO:HD2	1:G:482[B]:THR:HG22	2.01	0.42
1:B:200:VAL:O	1:B:278:MET:HA	2.20	0.42
1:C:140:TYR:CZ	1:H:548:ASN:HB3	2.55	0.42
1:G:481:VAL:HG22	1:G:481:VAL:O	2.20	0.42
1:C:292:LEU:O	1:C:295:GLN:HB2	2.19	0.42
1:E:179:LYS:HB2	1:E:179:LYS:HE2	1.28	0.42
1:C:292:LEU:HB2	1:C:295:GLN:NE2	2.36	0.41
1:B:45:ASN:OD1	1:B:418:TYR:OH	2.39	0.41
1:E:191:ARG:HD3	1:E:191:ARG:HA	1.89	0.41
1:C:313:ALA:HB1	1:C:316:ILE:HD12	2.01	0.41
1:H:541:TRP:CE2	1:H:566:ARG:CD	3.04	0.41
1:F:40:PRO:HA	1:F:52:MET:O	2.21	0.41
1:F:99:ILE:O	1:F:106:PHE:HA	2.21	0.41
1:F:541:TRP:CE2	1:F:566:ARG:HD3	2.56	0.41
1:G:95:ALA:O	1:G:98:GLN:HG2	2.21	0.41
1:H:407:ASN:N	1:H:408:PRO:HD2	2.36	0.40
1:G:418:TYR:HD2	1:G:419:GLN:HE21	1.70	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	524/550 (95%)	501 (96%)	22 (4%)	1 (0%)	47	23
1	B	522/550 (95%)	499 (96%)	23 (4%)	0	100	100
1	C	523/550 (95%)	501 (96%)	21 (4%)	1 (0%)	47	23
1	D	531/550 (96%)	511 (96%)	19 (4%)	1 (0%)	47	23
1	E	528/550 (96%)	504 (96%)	24 (4%)	0	100	100
1	F	530/550 (96%)	509 (96%)	21 (4%)	0	100	100
1	G	533/550 (97%)	513 (96%)	19 (4%)	1 (0%)	47	23
1	H	524/550 (95%)	504 (96%)	20 (4%)	0	100	100
All	All	4215/4400 (96%)	4042 (96%)	169 (4%)	4 (0%)	51	25

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	491	ALA
1	A	491	ALA
1	G	491	ALA
1	D	491	ALA

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	427/461 (93%)	422 (99%)	5 (1%)	71	48
1	B	429/461 (93%)	423 (99%)	6 (1%)	67	42
1	C	425/461 (92%)	416 (98%)	9 (2%)	53	23
1	D	432/461 (94%)	425 (98%)	7 (2%)	62	36
1	E	427/461 (93%)	420 (98%)	7 (2%)	62	36
1	F	432/461 (94%)	426 (99%)	6 (1%)	67	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	434/461 (94%)	431 (99%)	3 (1%)	84	69
1	H	422/461 (92%)	416 (99%)	6 (1%)	67	42
All	All	3428/3688 (93%)	3379 (99%)	49 (1%)	67	42

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	220	GLN
1	A	235	LEU
1	A	389	LYS
1	A	537	GLU
1	B	82	MET
1	B	136	ASN
1	B	235	LEU
1	B	289	ASN
1	B	292	LEU
1	B	389	LYS
1	C	136	ASN
1	C	158	GLU
1	C	217	PRO
1	C	230	ASP
1	C	237	LEU
1	C	289	ASN
1	C	292	LEU
1	C	326	ARG
1	C	537	GLU
1	D	41	GLU
1	D	76	LYS
1	D	136	ASN
1	D	326	ARG
1	D	419	GLN
1	D	429	LEU
1	D	537	GLU
1	E	82	MET
1	E	83	GLU
1	E	136	ASN
1	E	179	LYS
1	E	183	GLU
1	E	289	ASN
1	E	537	GLU

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Mol	Chain	Res	Type
1	F	136	ASN
1	F	292	LEU
1	F	429	LEU
1	F	449	GLU
1	F	537	GLU
1	F	573	SER
1	G	82	MET
1	G	136	ASN
1	G	537	GLU
1	H	136	ASN
1	H	194[A]	ASP
1	H	194[B]	ASP
1	H	199	MET
1	H	326	ARG
1	H	524	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	289	ASN
1	C	64	GLN
1	C	289	ASN
1	C	451	HIS
1	D	45	ASN
1	F	289	ASN
1	G	289	ASN
1	G	419	GLN
1	H	64	GLN
1	H	289	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 35 ligands modelled in this entry, 27 are monoatomic - leaving 8 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	N0W	D	606	-	21,21,35	2.01	4 (19%)	21,28,49	1.56	4 (19%)
3	N0W	G	604	-	15,15,35	1.24	2 (13%)	13,19,49	1.27	1 (7%)
3	N0W	E	605	-	15,15,35	1.79	5 (33%)	13,19,49	1.04	1 (7%)
3	N0W	B	602	-	13,13,35	1.29	1 (7%)	10,17,49	1.23	1 (10%)
3	N0W	A	604	-	21,21,35	1.76	2 (9%)	21,28,49	3.00	3 (14%)
3	N0W	F	605	-	21,21,35	1.76	3 (14%)	21,28,49	1.72	3 (14%)
3	N0W	H	605	-	15,15,35	1.05	1 (6%)	13,19,49	1.15	1 (7%)
3	N0W	C	604	-	12,12,35	1.70	1 (8%)	11,16,49	0.77	1 (9%)

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	N0W	D	606	-	-	3/13/30/40	0/1/1/3
3	N0W	G	604	-	-	4/7/24/40	0/1/1/3
3	N0W	E	605	-	-	2/7/24/40	0/1/1/3
3	N0W	B	602	-	-	2/5/22/40	0/1/1/3
3	N0W	A	604	-	-	4/13/30/40	0/1/1/3
3	N0W	F	605	-	-	3/13/30/40	0/1/1/3
3	N0W	H	605	-	-	3/7/24/40	0/1/1/3
3	N0W	C	604	-	-	2/4/21/40	0/1/1/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	N0W	C6-S3	-6.93	1.59	1.75
3	F	605	N0W	C6-S3	-6.20	1.61	1.75
3	D	606	N0W	C6-S3	-5.81	1.62	1.75
3	C	604	N0W	CAI-CAJ	4.22	1.56	1.52
3	E	605	N0W	CAD-CAC	-4.21	1.48	1.53
3	D	606	N0W	CAI-CAJ	4.16	1.56	1.52
3	D	606	N0W	CAD-CAC	-3.52	1.49	1.53
3	G	604	N0W	CAI-CAJ	3.34	1.55	1.52
3	F	605	N0W	CAI-CAJ	3.27	1.55	1.52
3	D	606	N0W	CAI-NAB	2.99	1.51	1.47
3	E	605	N0W	CAJ-CAC	2.94	1.57	1.52
3	E	605	N0W	CAL-CAA	2.53	1.58	1.52
3	G	604	N0W	CAA-NAB	2.52	1.51	1.47
3	F	605	N0W	CAD-CAC	2.42	1.55	1.53
3	B	602	N0W	CAA-NAB	2.41	1.51	1.47
3	E	605	N0W	CAI-CAJ	2.38	1.54	1.52
3	E	605	N0W	CAI-NAB	2.26	1.50	1.47
3	A	604	N0W	CAI-CAJ	2.22	1.54	1.52
3	H	605	N0W	CAI-NAB	2.12	1.50	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	604	N0W	O5-S3-O4	-9.63	105.96	118.87
3	A	604	N0W	C6-S3-N2	8.83	113.59	107.82
3	F	605	N0W	CAI-CAJ-CAC	5.25	116.66	110.25
3	D	606	N0W	O5-S3-N2	-4.04	101.71	107.33
3	D	606	N0W	O5-S3-O4	-3.60	114.05	118.87
3	F	605	N0W	O5-S3-O4	-3.34	114.39	118.87
3	H	605	N0W	OAE-CAC-CAD	2.96	115.97	109.94
3	D	606	N0W	O5-S3-C6	2.91	112.87	108.26
3	G	604	N0W	OAF-CAJ-CAI	2.59	114.66	109.65
3	A	604	N0W	O4-S3-N2	2.56	110.90	107.33
3	E	605	N0W	OAE-CAC-CAD	2.49	115.02	109.94
3	D	606	N0W	OAF-CAJ-CAI	-2.45	104.91	109.65
3	F	605	N0W	O5-S3-C6	2.29	111.88	108.26
3	C	604	N0W	OAK-CAH-CAD	2.08	116.14	111.22
3	B	602	N0W	OAF-CAJ-CAC	2.01	114.31	110.15

There are no chirality outliers.

All (23) torsion outliers are listed below:

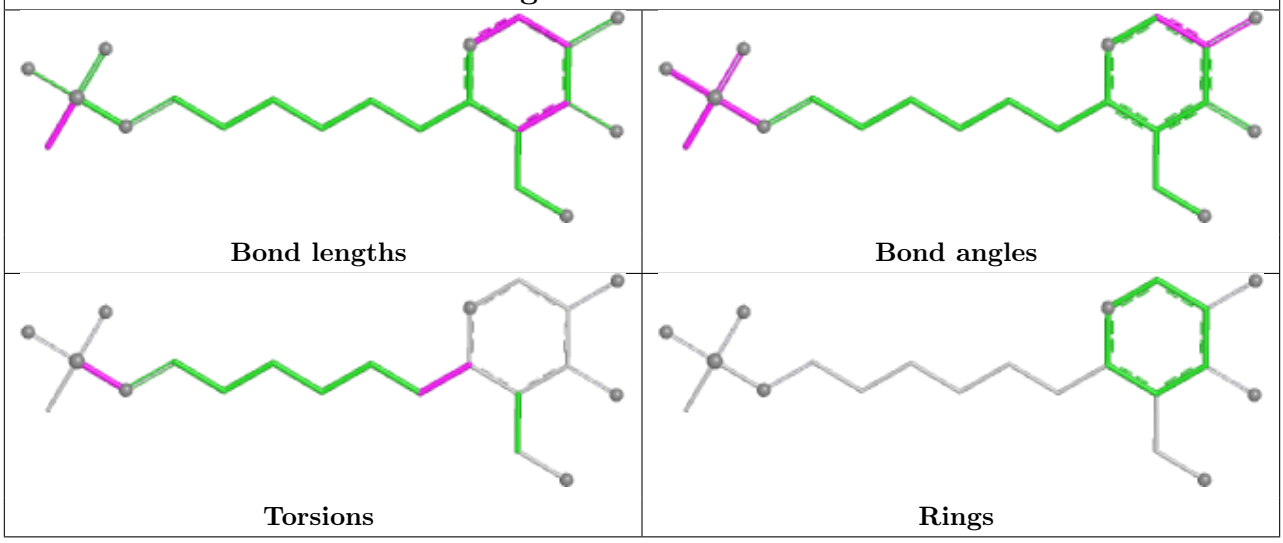
Mol	Chain	Res	Type	Atoms
3	A	604	N0W	C1-N2-S3-O5
3	A	604	N0W	NAB-CAA-CAL-CAM
3	A	604	N0W	CAD-CAA-CAL-CAM
3	B	602	N0W	NAB-CAA-CAL-CAM
3	B	602	N0W	CAD-CAA-CAL-CAM
3	C	604	N0W	NAB-CAA-CAL-CAM
3	D	606	N0W	C1-N2-S3-C6
3	D	606	N0W	NAB-CAA-CAL-CAM
3	D	606	N0W	CAD-CAA-CAL-CAM
3	E	605	N0W	NAB-CAA-CAL-CAM
3	E	605	N0W	CAD-CAA-CAL-CAM
3	F	605	N0W	NAB-CAA-CAL-CAM
3	F	605	N0W	CAD-CAA-CAL-CAM
3	G	604	N0W	NAB-CAA-CAL-CAM
3	H	605	N0W	NAB-CAA-CAL-CAM
3	H	605	N0W	CAD-CAA-CAL-CAM
3	C	604	N0W	CAD-CAA-CAL-CAM
3	A	604	N0W	N2-C1-CAP-CAO
3	G	604	N0W	CAA-CAL-CAM-CAN
3	G	604	N0W	CAM-CAN-CAO-CAP
3	G	604	N0W	CAD-CAA-CAL-CAM
3	F	605	N0W	CAN-CAO-CAP-C1
3	H	605	N0W	CAM-CAN-CAO-CAP

There are no ring outliers.

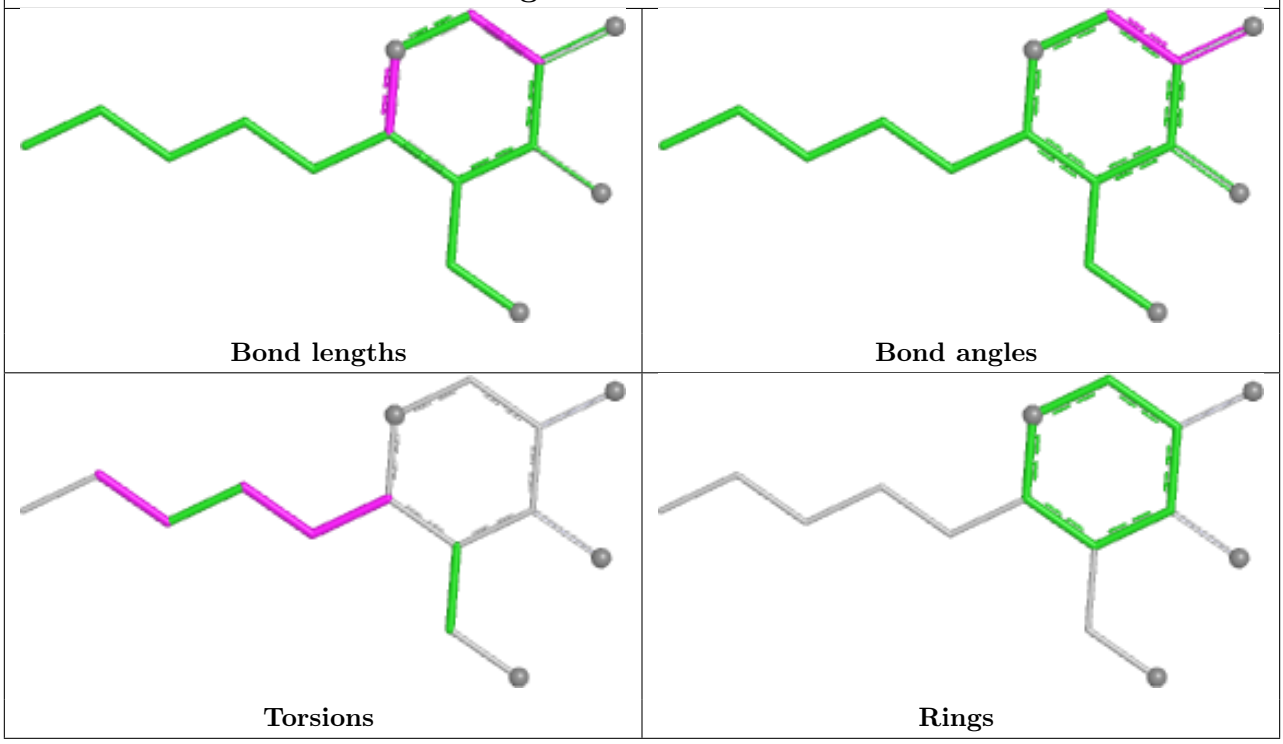
No monomer is involved in short contacts.

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.

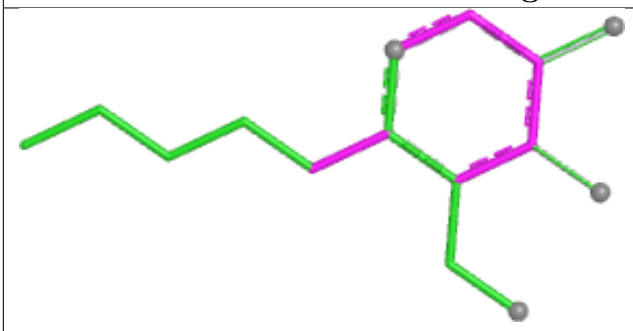
Ligand N0W D 606



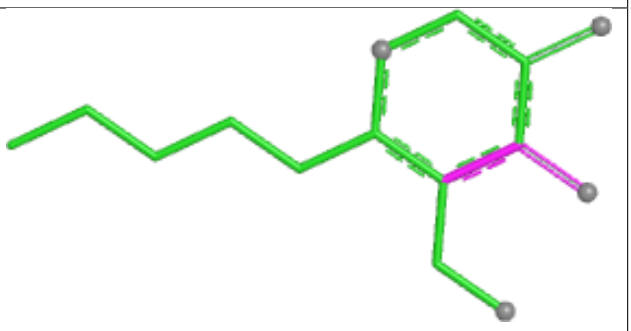
Ligand N0W G 604



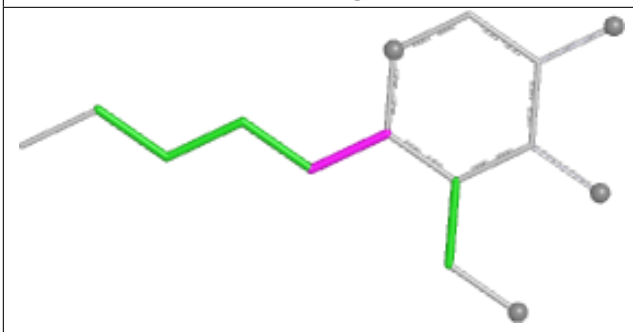
Ligand N0W E 605



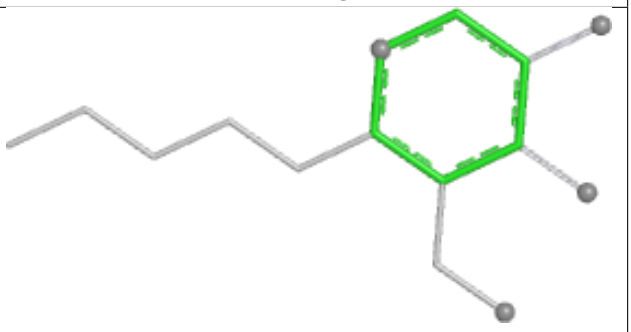
Bond lengths



Bond angles

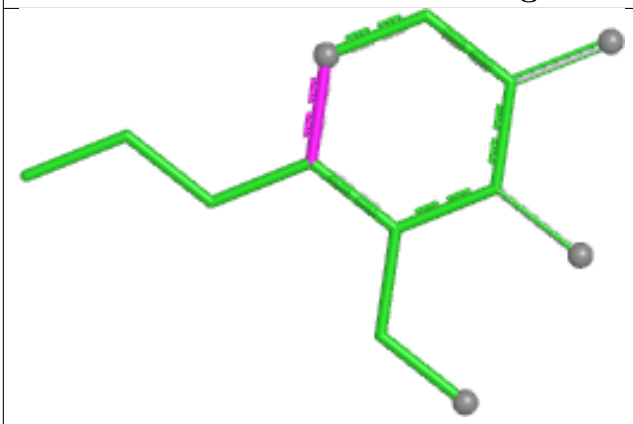


Torsions

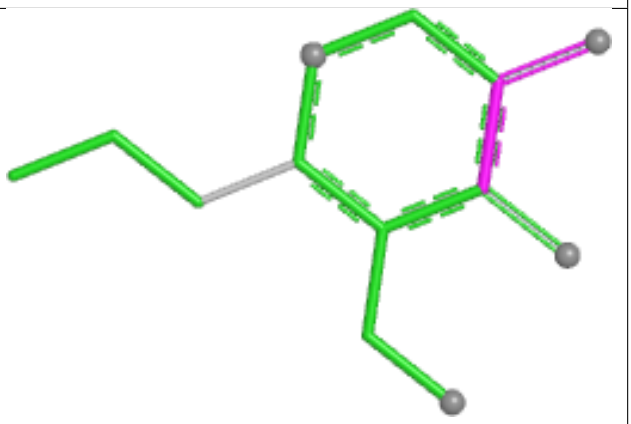


Rings

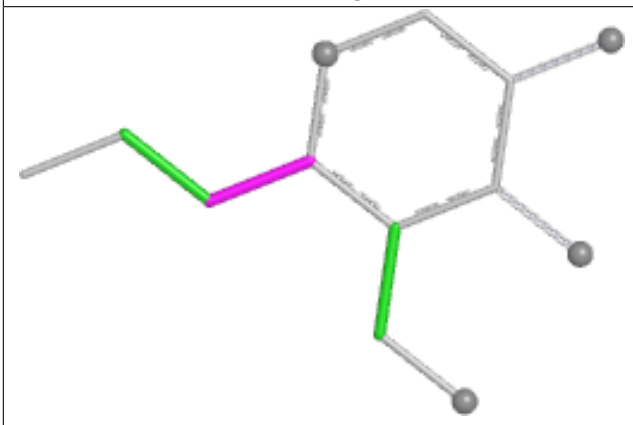
Ligand N0W B 602



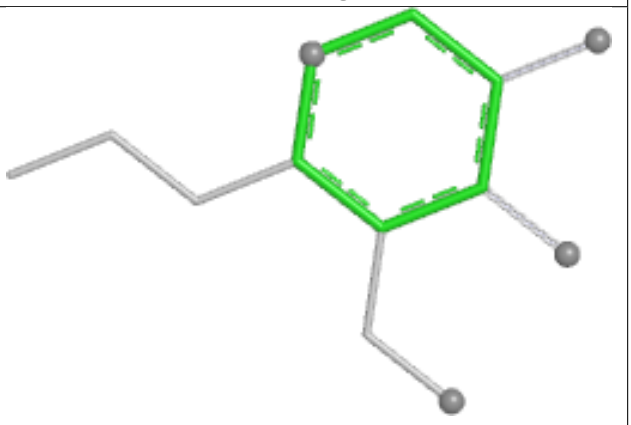
Bond lengths



Bond angles

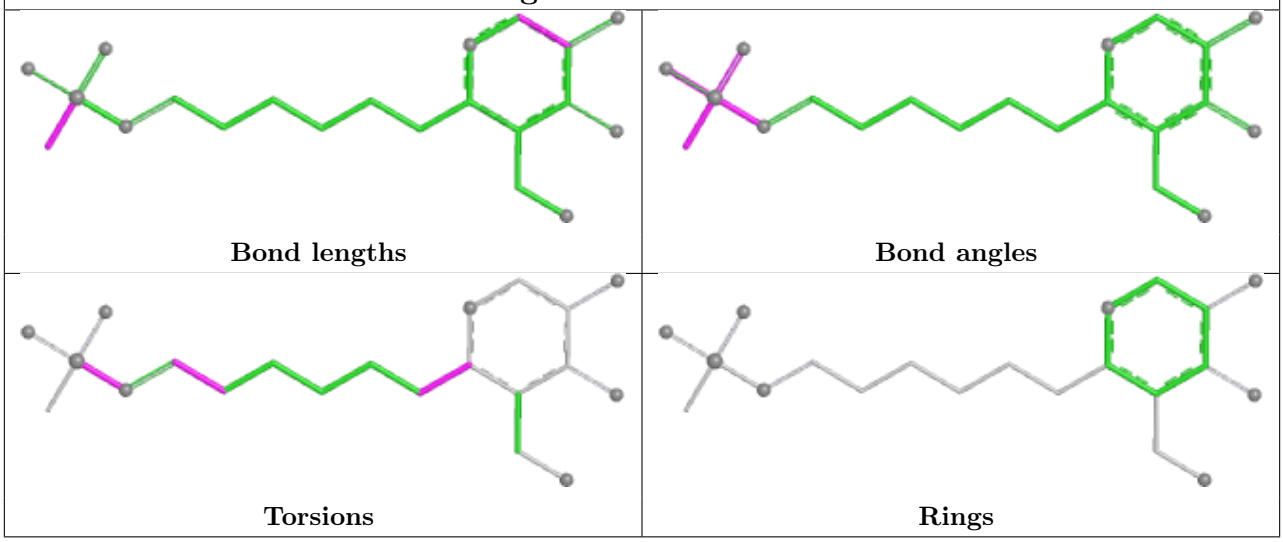


Torsions

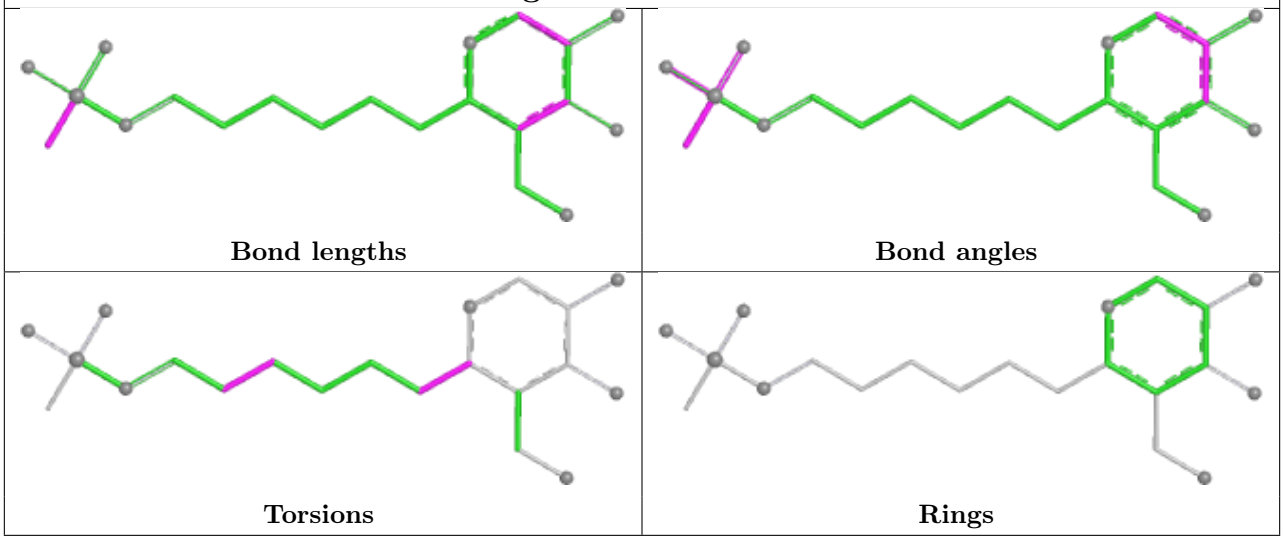


Rings

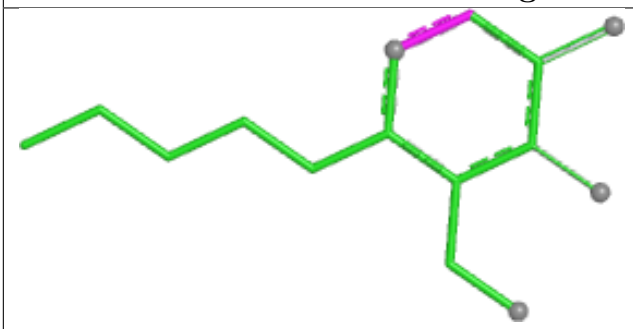
Ligand N0W A 604



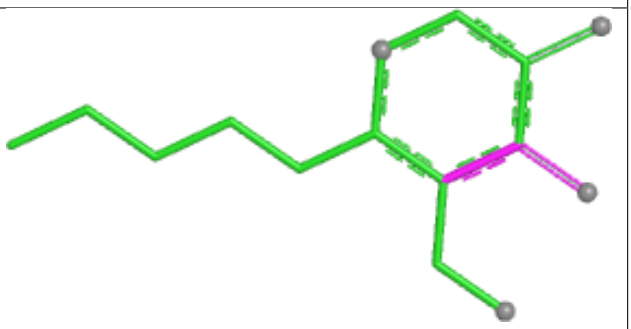
Ligand N0W F 605



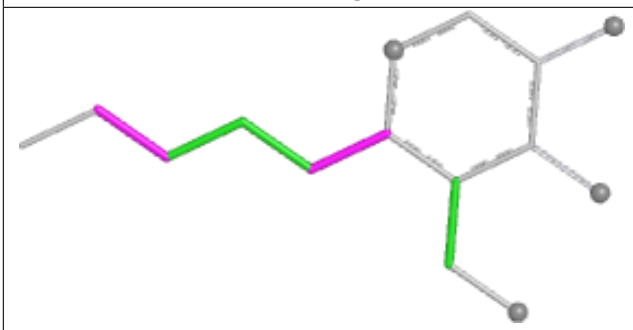
Ligand N0W H 605



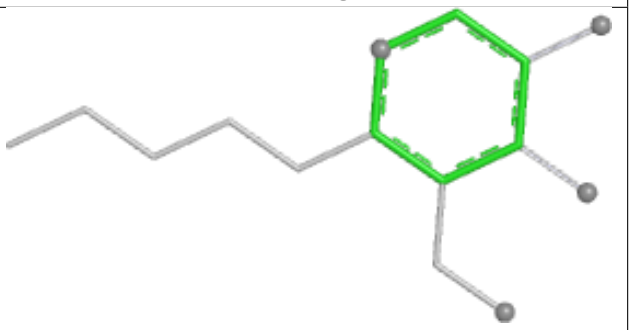
Bond lengths



Bond angles

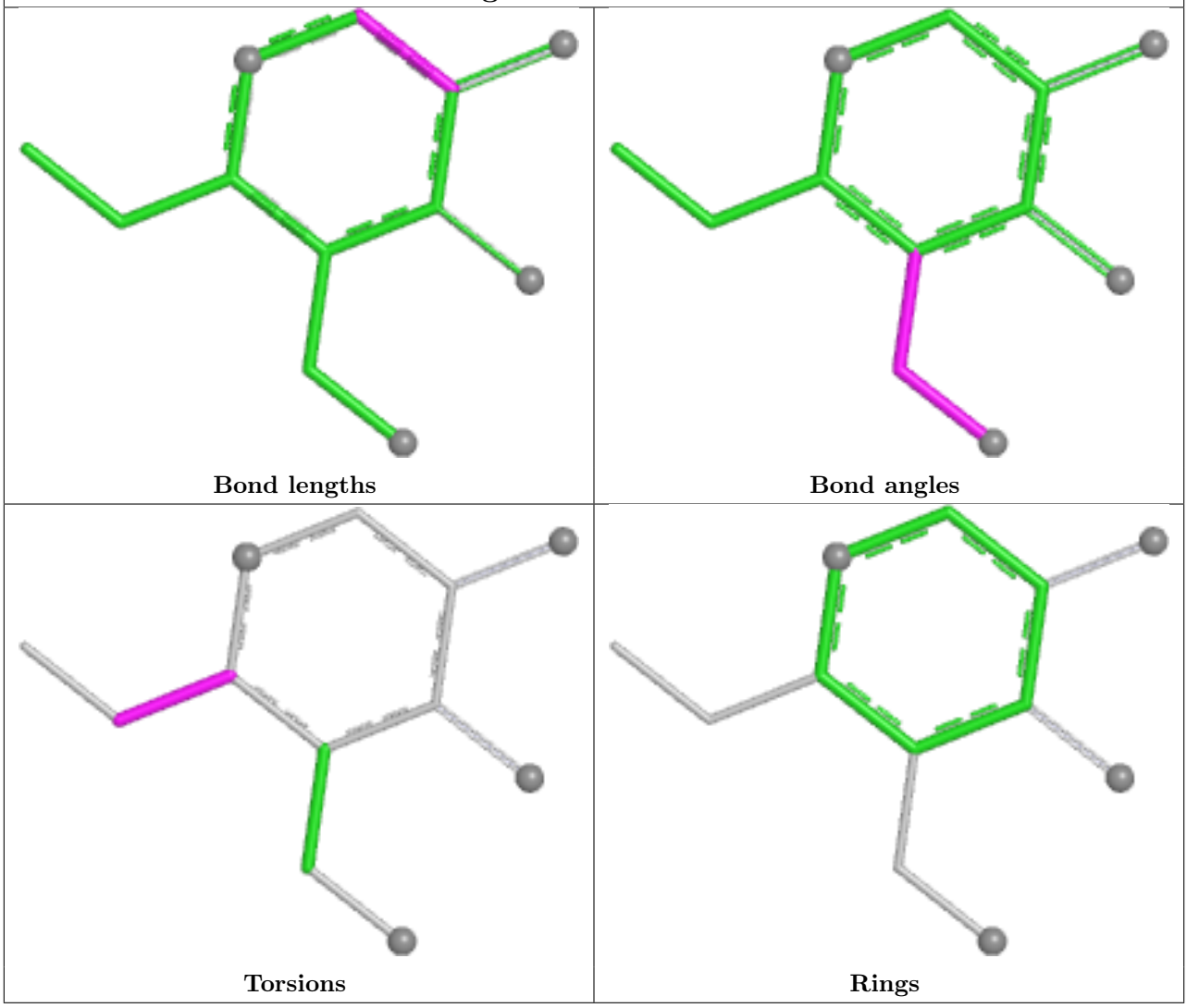


Torsions



Rings

Ligand N0W C 604



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	525/550 (95%)	-0.49	0	100	100	15, 22, 37, 53	3 (0%)
1	B	524/550 (95%)	-0.57	1 (0%)	95	95	15, 21, 31, 45	6 (1%)
1	C	526/550 (95%)	-0.52	3 (0%)	89	91	14, 21, 33, 46	7 (1%)
1	D	531/550 (96%)	-0.54	0	100	100	13, 19, 33, 52	2 (0%)
1	E	532/550 (96%)	-0.56	0	100	100	14, 20, 33, 46	4 (0%)
1	F	531/550 (96%)	-0.51	1 (0%)	95	95	13, 20, 35, 43	2 (0%)
1	G	532/550 (96%)	-0.51	1 (0%)	95	95	13, 19, 34, 47	4 (0%)
1	H	523/550 (95%)	-0.51	0	100	100	15, 22, 34, 49	4 (0%)
All	All	4224/4400 (96%)	-0.53	6 (0%)	95	95	13, 20, 34, 53	32 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	521	LEU	5.0
1	G	36	ALA	4.1
1	B	521	LEU	3.3
1	C	519	GLN	2.2
1	C	520	GLU	2.2
1	F	435	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.

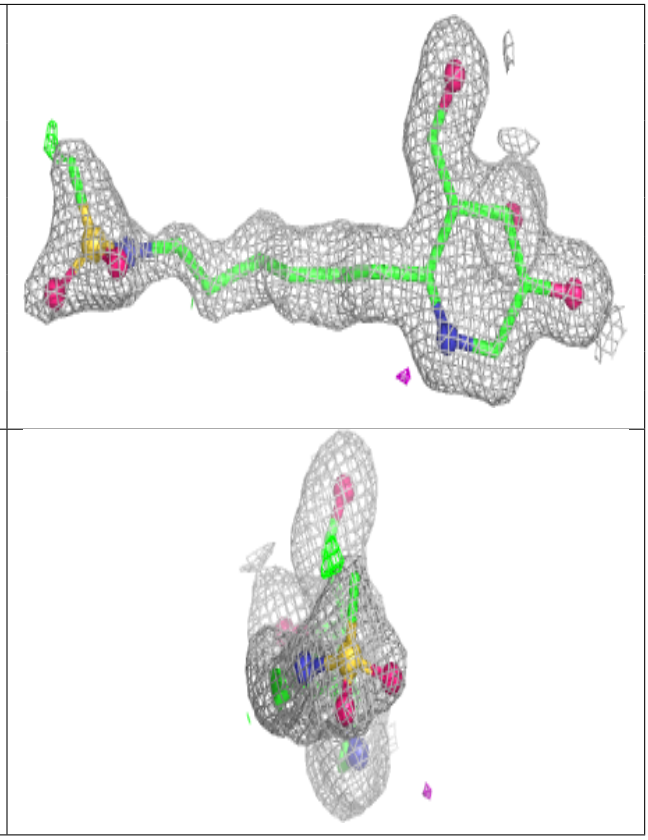
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	A	602	1/1	0.97	0.07	27,27,27,27	0
2	NA	A	603	1/1	0.97	0.06	28,28,28,28	0
3	N0W	A	604	21/33	0.97	0.08	18,20,30,33	7
3	N0W	B	602	13/33	0.97	0.06	17,18,20,25	0
3	N0W	D	606	21/33	0.97	0.07	16,19,32,45	5
3	N0W	F	605	21/33	0.97	0.09	17,19,29,34	7
3	N0W	H	605	15/33	0.97	0.07	16,18,20,24	3
2	NA	F	603	1/1	0.98	0.09	27,27,27,27	0
2	NA	F	604	1/1	0.98	0.05	28,28,28,28	0
2	NA	G	603	1/1	0.98	0.04	27,27,27,27	0
2	NA	C	601	1/1	0.98	0.06	26,26,26,26	0
2	NA	C	602	1/1	0.98	0.06	29,29,29,29	0
3	N0W	C	604	12/33	0.98	0.07	17,18,21,22	0
2	NA	D	605	1/1	0.98	0.08	28,28,28,28	0
3	N0W	E	605	15/33	0.98	0.07	15,16,21,23	3
2	NA	E	603	1/1	0.98	0.04	28,28,28,28	0
3	N0W	G	604	15/33	0.98	0.07	14,17,20,25	3
2	NA	F	602	1/1	0.98	0.03	26,26,26,26	0
2	NA	A	601	1/1	0.99	0.03	30,30,30,30	0
2	NA	H	601	1/1	0.99	0.07	25,25,25,25	0
2	NA	H	603	1/1	0.99	0.03	32,32,32,32	0
2	NA	H	604	1/1	0.99	0.06	29,29,29,29	0
2	NA	B	601	1/1	0.99	0.03	28,28,28,28	0
2	NA	E	604	1/1	0.99	0.06	25,25,25,25	0
2	NA	F	601	1/1	0.99	0.09	21,21,21,21	0
2	NA	C	603	1/1	0.99	0.06	31,31,31,31	0
2	NA	D	601	1/1	0.99	0.04	22,22,22,22	0
2	NA	D	604	1/1	0.99	0.06	26,26,26,26	0
2	NA	G	601	1/1	0.99	0.04	20,20,20,20	0
2	NA	G	602	1/1	0.99	0.05	28,28,28,28	0
2	NA	E	601	1/1	1.00	0.05	21,21,21,21	0
2	NA	E	602	1/1	1.00	0.05	23,23,23,23	0
2	NA	D	602	1/1	1.00	0.05	20,20,20,20	0
2	NA	D	603	1/1	1.00	0.06	24,24,24,24	0
2	NA	H	602	1/1	1.00	0.03	29,29,29,29	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.

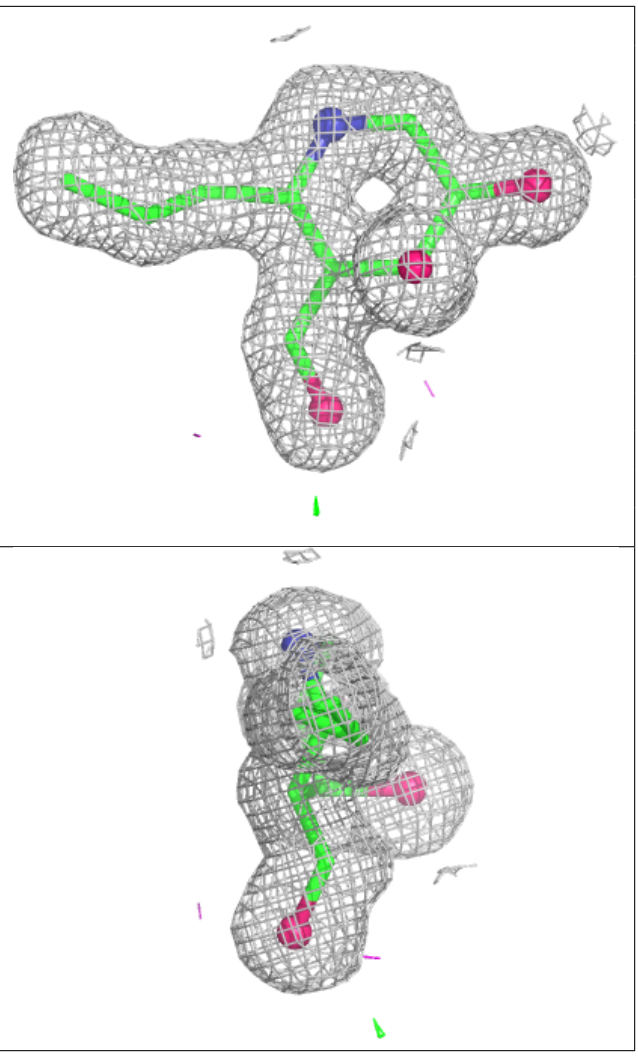
Electron density around N0W A 604:

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



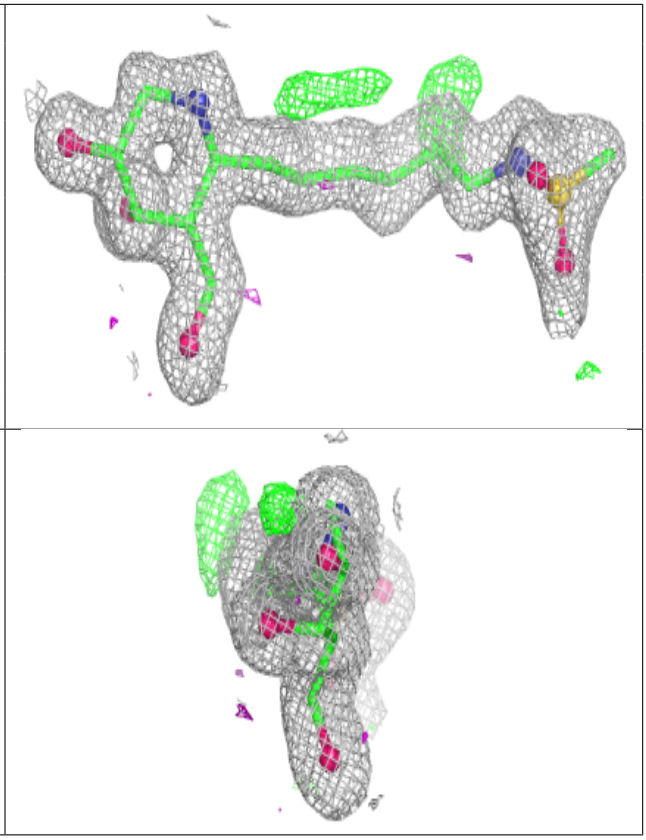
Electron density around N0W B 602:

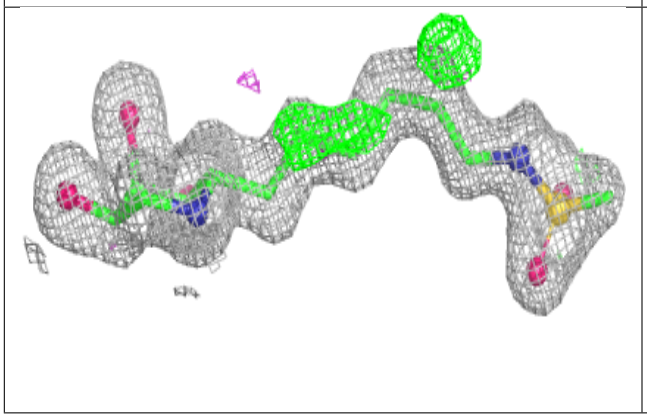
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around N0W D 606:

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





Electron density around N0W F 605:

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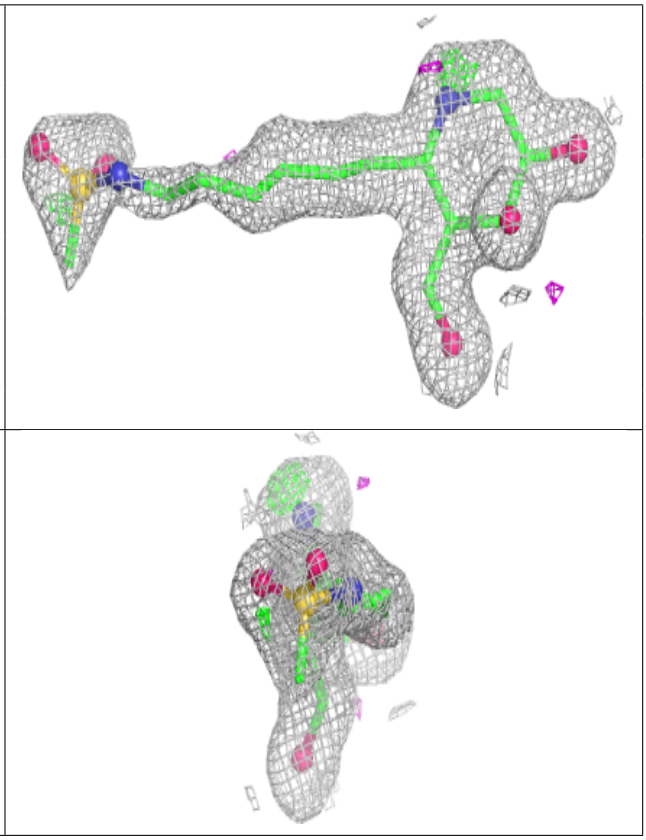
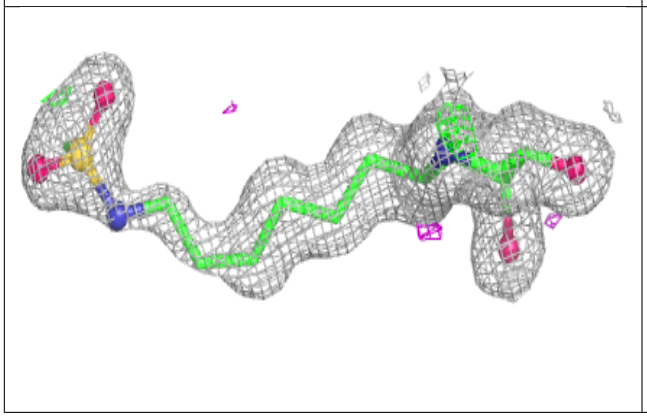
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around N0W H 605:

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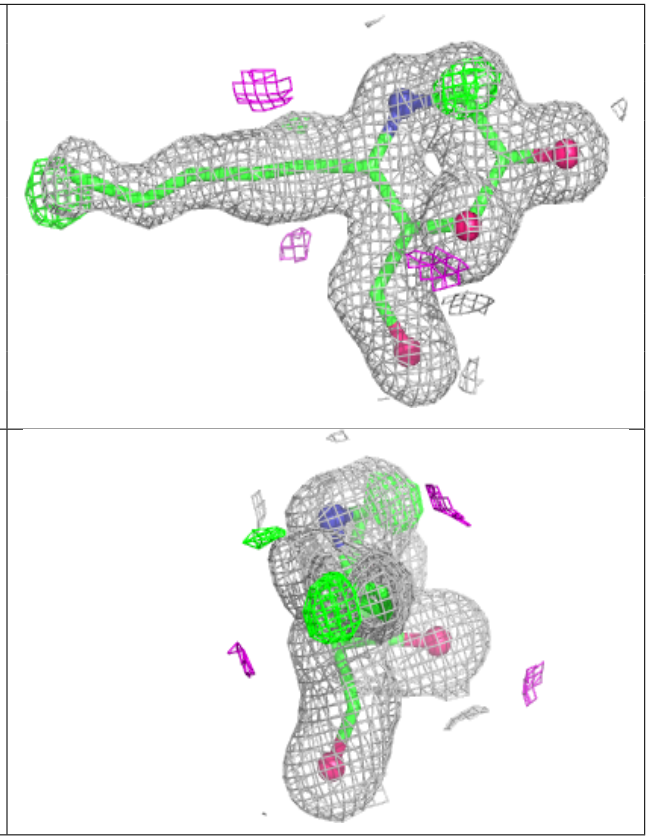
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around N0W C 604:

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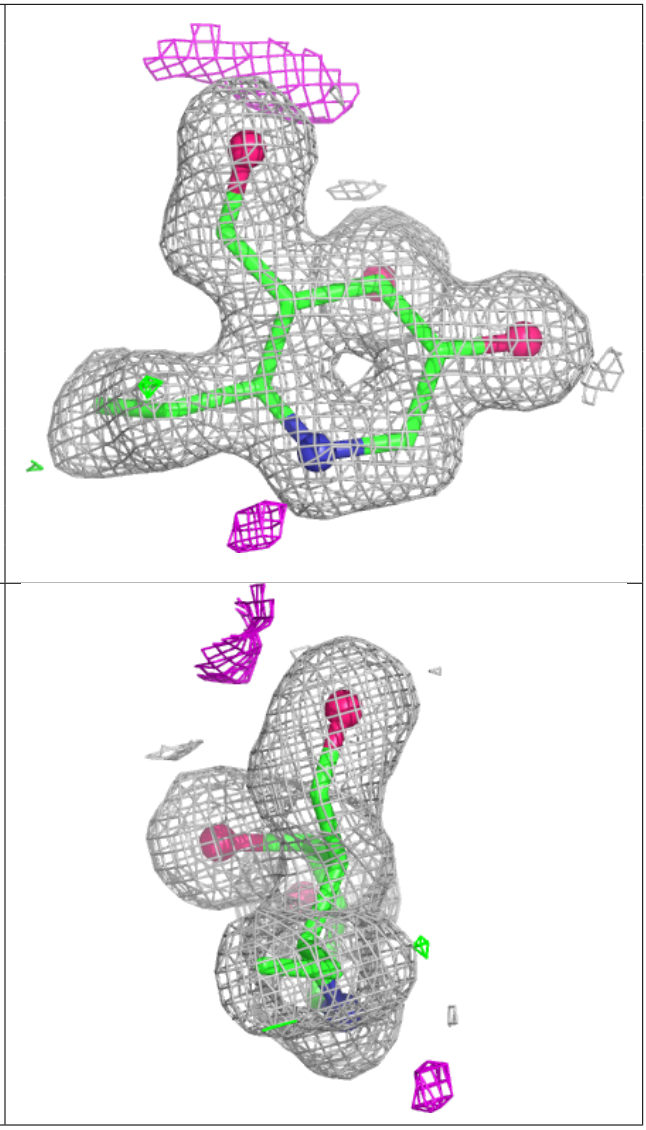
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around N0W E 605:

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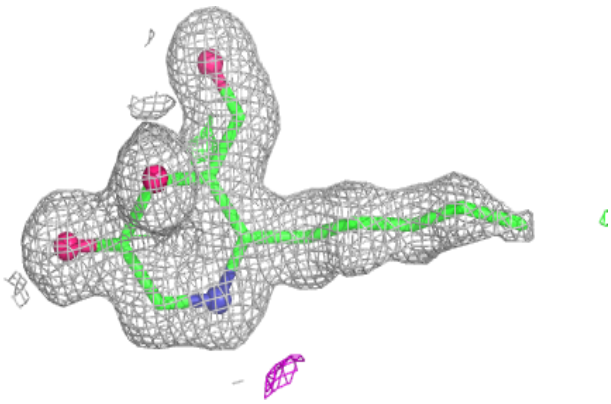
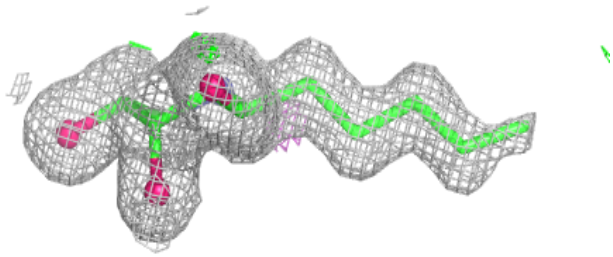
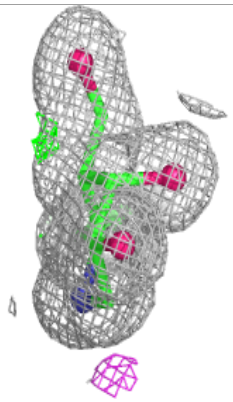
and green (positive)

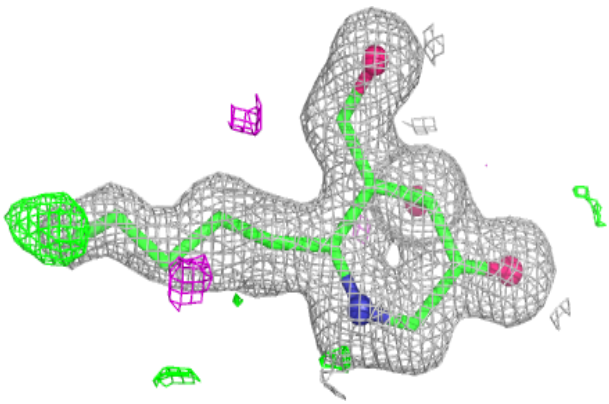


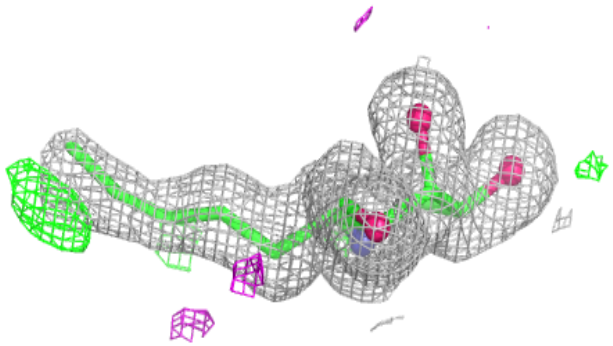


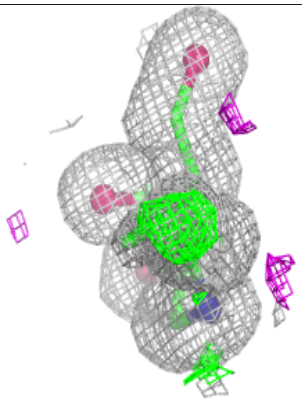


Electron density around N0W G 604:

$2mF_o$-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.