Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2025 – 04:08 pm BST

PDB ID	:	8S6V / pdb_00008s6v
Title	:	Crystal structure of Fab-2D9 chimera complexed to a bis-Tn glycopeptide
Authors	:	Hurtado-Guerrero, R.; Macias-Leon, J.; Gonzalez-Ramirez, A.
Deposited on	:	2024-02-28
Resolution	:	1.95 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:

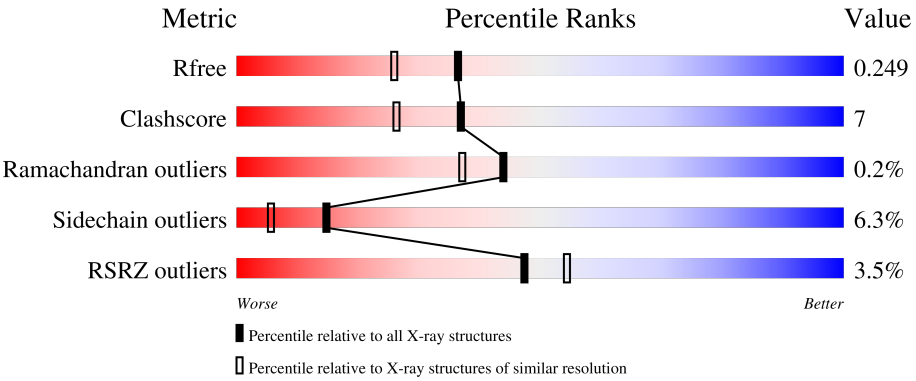
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	216	3% 83% 12%
1	C	216	4% 83% 12%
2	B	217	% 82% 16%
2	D	217	4% 82% 17%
3	M	10	20% 80% 20%

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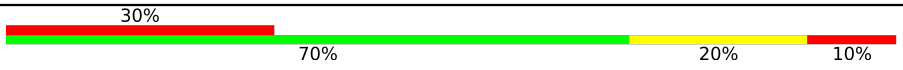
Mol	Chain	Length	Quality of chain
3	N	10	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7355 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 G2D11 (VH-CH1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1600	1018	260	316	6			
1	C	211	Total	C	N	O	S	0	0	0
			1600	1018	260	316	6			

- Molecule 2 is a protein called 2D9 (VL-CL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	3	0
			1702	1064	281	349	8			
2	D	217	Total	C	N	O	S	0	2	0
			1699	1062	281	348	8			

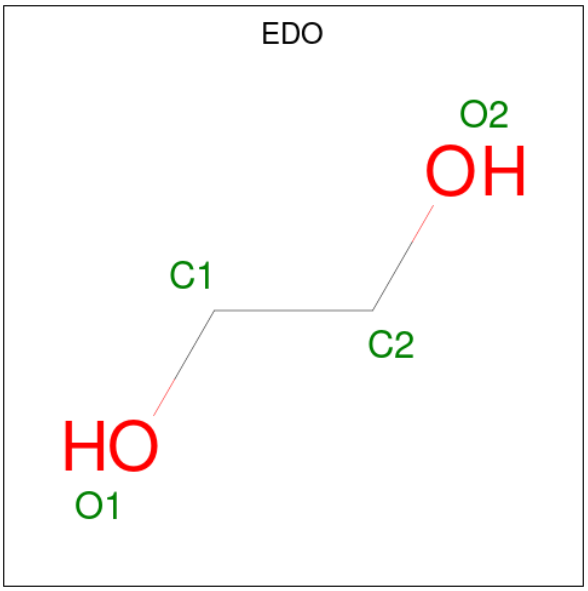
- Molecule 3 is a protein called Mucin-1 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	10	Total	C	N	O	0	0	1
			54	33	10	11			
3	N	10	Total	C	N	O	0	0	1
			54	33	10	11			

There are 2 discrepancies between the modelled and reference sequences:

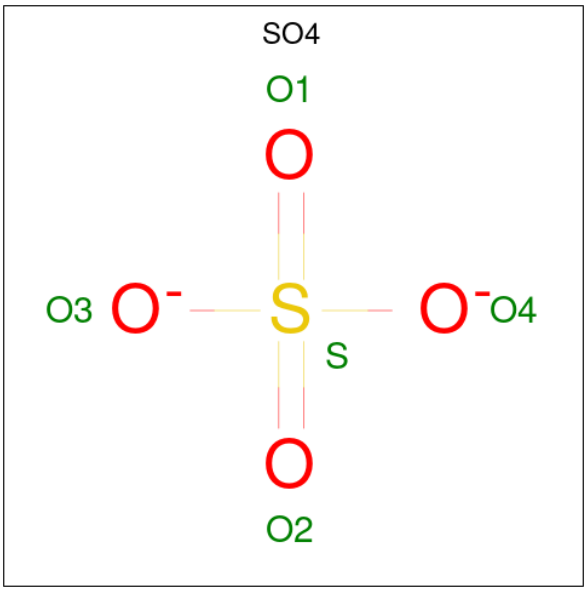
Chain	Residue	Modelled	Actual	Comment	Reference
M	10	NH2	-	amidation	UNP P15941
N	10	NH2	-	amidation	UNP P15941

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



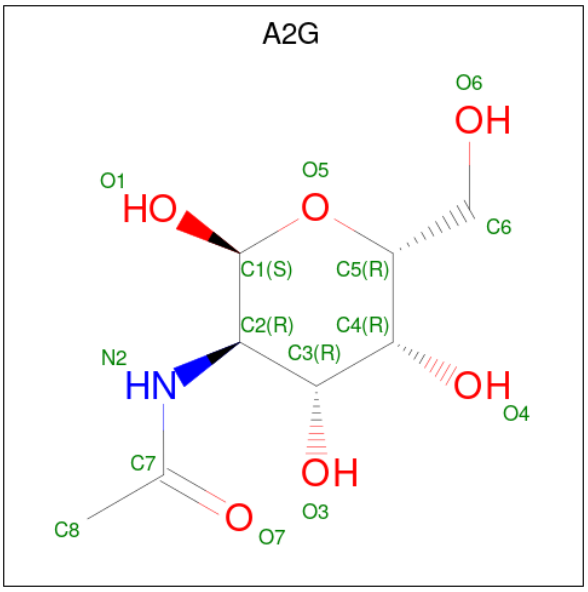
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

- Molecule 6 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (CCD ID: A2G) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	M	1	Total C N O 14 8 1 5	0	0
6	M	1	Total C N O 14 8 1 5	0	0
6	N	1	Total C N O 14 8 1 5	0	0
6	N	1	Total C N O 14 8 1 5	0	0

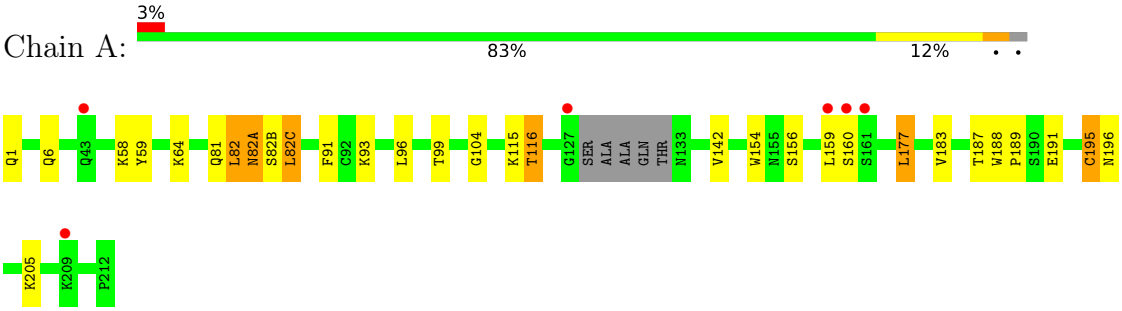
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	124	Total O 124 124	0	0
7	B	138	Total O 138 138	0	0
7	C	126	Total O 126 126	0	0
7	D	113	Total O 113 113	0	0
7	M	11	Total O 11 11	0	0
7	N	9	Total O 9 9	0	0

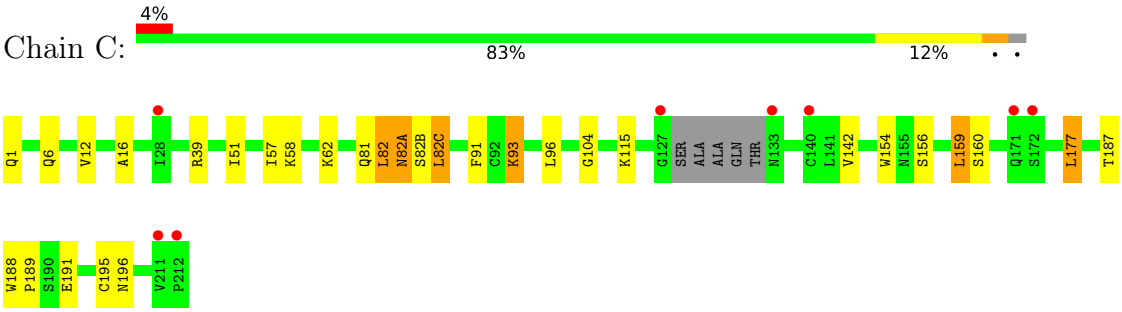
3 Residue-property plots (i)

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.

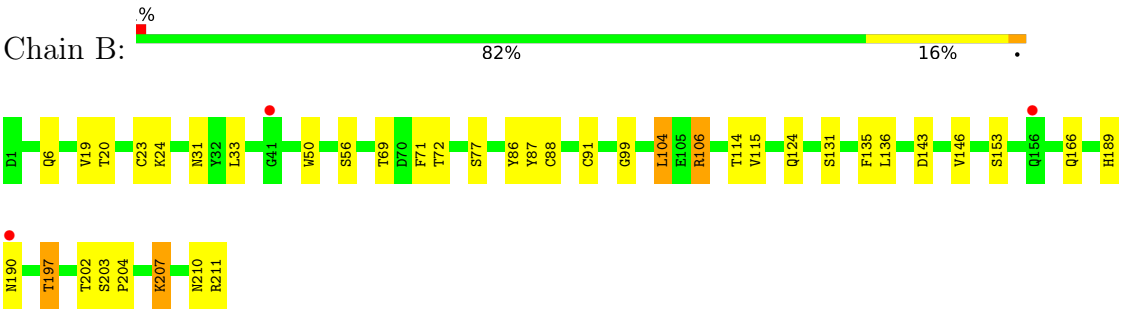
• Molecule 1: G2D11 (VH-CH1)



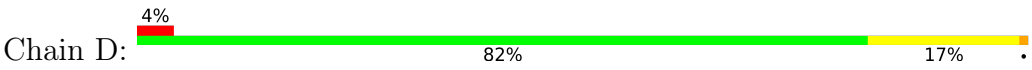
• Molecule 1: G2D11 (VH-CH1)

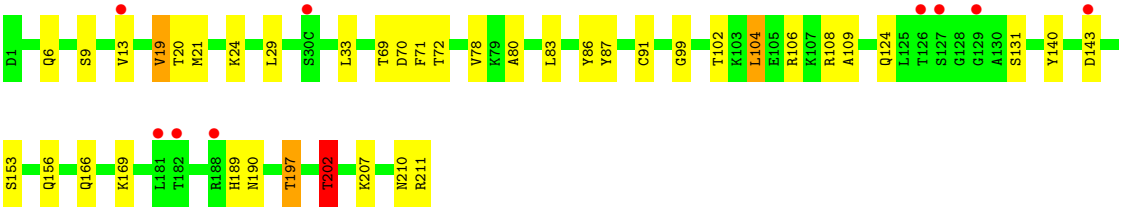


• Molecule 2: 2D9 (VL-CL)

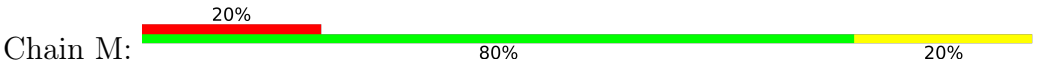


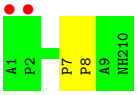
• Molecule 2: 2D9 (VL-CL)



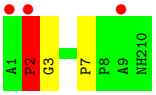


• Molecule 3: Mucin-1 subunit alpha





• Molecule 3: Mucin-1 subunit alpha



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.05Å 111.55Å 134.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.98 – 1.95 85.98 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (85.98-1.95) 99.9 (85.98-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.199 , 0.244 0.207 , 0.249	Depositor DCC
R_{free} test set	3117 reflections (4.18%)	wwPDB-VP
Wilson B-factor (Å^2)	26.4	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 28.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7355	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: EDO, NH2, A2G, SO4

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	0.58	0/1642	0.93	1/2240 (0.0%)
1	C	0.56	0/1642	0.92	0/2240
2	B	0.59	0/1750	0.92	2/2372 (0.1%)
2	D	0.55	0/1744	0.91	2/2364 (0.1%)
3	M	2.16	2/55 (3.6%)	1.80	0/77
3	N	2.31	1/55 (1.8%)	2.28	2/77 (2.6%)
All	All	0.63	3/6888 (0.0%)	0.95	7/9370 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	7	PRO	CA-C	-10.37	1.42	1.52
3	M	7	PRO	CA-C	-9.89	1.45	1.52
3	M	8	PRO	CA-C	-5.82	1.42	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	2	PRO	N-CA-CB	-10.39	91.17	102.60
2	B	202	THR	CB-CA-C	-6.05	99.05	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	2	PRO	N-CA-C	5.83	127.26	112.10
2	D	202	THR	CB-CA-C	5.66	121.81	109.99
2	D	202	THR	N-CA-CB	-5.62	101.23	110.40
2	B	114	THR	CA-CB-OG1	-5.31	101.64	109.60
1	A	116	THR	CB-CA-C	5.09	117.84	109.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	106	ARG	Sidechain
1	C	39	ARG	Sidechain

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	1600	0	1575	17	0
1	C	1600	0	1575	21	0
2	B	1702	0	1643	24	0
2	D	1699	0	1638	29	0
3	M	54	0	51	0	0
3	N	54	0	51	0	0
4	A	8	0	12	2	0
4	B	8	0	12	0	0
4	C	12	0	18	2	0
4	D	16	0	24	5	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
6	M	28	0	24	0	0
6	N	28	0	24	0	0
7	A	124	0	0	3	0
7	B	138	0	0	4	0
7	C	126	0	0	1	0
7	D	113	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	11	0	0	0	0
7	N	9	0	0	0	0
All	All	7355	0	6647	92	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 (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:SER:H	1:A:196:ASN:HD21	1.16	0.94
1:A:81:GLN:HE21	1:A:82(A):ASN:HD21	1.20	0.89
2:B:106:ARG:H	2:B:166:GLN:HE22	1.18	0.88
1:C:81:GLN:HE21	1:C:82(A):ASN:HD21	1.18	0.88
1:C:156:SER:H	1:C:196:ASN:HD21	1.18	0.87
2:D:106:ARG:H	2:D:166:GLN:HE22	1.30	0.79
2:B:197:THR:HG23	7:B:458:HOH:O	1.84	0.76
2:D:202:THR:HG21	7:D:506:HOH:O	1.88	0.73
1:A:156:SER:H	1:A:196:ASN:ND2	1.89	0.69
4:A:302:EDO:H11	7:A:499:HOH:O	1.92	0.69
1:C:156:SER:H	1:C:196:ASN:ND2	1.91	0.68
2:D:197:THR:HG23	7:D:449:HOH:O	1.94	0.67
1:A:142:VAL:HB	1:A:177:LEU:HD22	1.76	0.67
2:B:124:GLN:HE22	2:B:131:SER:H	1.44	0.66
1:C:177:LEU:C	1:C:177:LEU:HD23	2.23	0.63
1:A:177:LEU:C	1:A:177:LEU:HD23	2.25	0.62
2:D:21:MET:HG2	2:D:102:THR:HG21	1.80	0.62
1:C:1:GLN:HB3	7:C:490:HOH:O	2.00	0.61
2:D:108:ARG:HD3	2:D:109:ALA:O	2.01	0.61
2:B:124:GLN:NE2	2:B:131:SER:H	2.01	0.59
2:D:6:GLN:HE22	2:D:87:TYR:HA	1.69	0.58
2:D:80:ALA:O	4:D:302:EDO:H21	2.03	0.58
2:B:33:LEU:HD22	2:B:71:PHE:CG	2.39	0.57
2:D:6:GLN:HE21	2:D:99:GLY:HA3	1.70	0.57
2:D:33:LEU:HD22	2:D:71:PHE:CG	2.40	0.56
1:C:142:VAL:HB	1:C:177:LEU:HD22	1.87	0.56
2:D:197:THR:CG2	7:D:449:HOH:O	2.51	0.55
2:B:136:LEU:HD21	2:B:146:VAL:HG22	1.88	0.55
2:D:91:CYS:CB	4:D:303:EDO:H22	2.36	0.55
2:B:6:GLN:HE22	2:B:87:TYR:HA	1.71	0.55
1:C:12:VAL:CG1	1:C:16:ALA:HB3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:13:VAL:HG21	2:D:19:VAL:HG11	1.88	0.55
1:A:1:GLN:HB3	7:A:493:HOH:O	2.08	0.54
2:D:83:LEU:HB2	4:D:302:EDO:H22	1.89	0.53
1:C:12:VAL:HG12	1:C:16:ALA:HB3	1.90	0.53
1:A:6:GLN:HE21	1:A:104:GLY:HA3	1.74	0.53
2:B:77:SER:N	7:B:402:HOH:O	2.29	0.52
1:A:177:LEU:C	1:A:177:LEU:CD2	2.83	0.52
2:D:124:GLN:NE2	2:D:131:SER:H	2.08	0.52
1:C:177:LEU:C	1:C:177:LEU:CD2	2.83	0.52
1:C:154:TRP:CZ3	1:C:195:CYS:HB3	2.46	0.51
2:B:6:GLN:HE21	2:B:99:GLY:HA3	1.76	0.51
1:C:81:GLN:NE2	1:C:82(A):ASN:HD21	1.99	0.49
2:B:207:LYS:HE3	7:B:482:HOH:O	2.11	0.49
1:C:6:GLN:HE21	1:C:104:GLY:HA3	1.77	0.48
2:B:20:THR:HG23	2:B:72:THR:HG23	1.95	0.48
1:A:154:TRP:CZ3	1:A:195:CYS:HB3	2.49	0.47
1:A:6:GLN:HE22	1:A:91:PHE:HA	1.80	0.46
1:C:82:LEU:HB3	1:C:82(C):LEU:HD21	1.96	0.46
1:C:187:THR:O	1:C:191:GLU:HB2	2.16	0.46
2:B:197:THR:HG22	2:B:204:PRO:HB3	1.96	0.46
2:B:23:CYS:HG	2:B:88:CYS:HG	0.49	0.46
2:B:189:HIS:O	2:B:211:ARG:HD3	2.16	0.46
1:C:51:ILE:HG13	1:C:57:ILE:HG12	1.98	0.46
2:D:190:ASN:O	2:D:210:ASN:HA	2.16	0.46
1:C:6:GLN:HE22	1:C:91:PHE:HA	1.80	0.46
1:C:93:LYS:HE3	4:C:303:EDO:O1	2.16	0.45
2:B:197:THR:CG2	7:B:458:HOH:O	2.54	0.45
2:B:136:LEU:CD2	2:B:146:VAL:HG22	2.47	0.45
1:A:188:TRP:CG	1:A:189:PRO:HA	2.51	0.45
2:D:80:ALA:O	4:D:302:EDO:C2	2.65	0.45
1:C:188:TRP:CG	1:C:189:PRO:HA	2.52	0.45
2:B:86:TYR:CE1	2:B:104:LEU:HD22	2.52	0.44
2:D:86:TYR:CE1	2:D:104:LEU:HD22	2.52	0.44
2:D:202:THR:CG2	7:D:506:HOH:O	2.52	0.44
1:A:82:LEU:HB3	1:A:82(C):LEU:HD21	2.00	0.44
2:D:124:GLN:HE22	2:D:131:SER:H	1.66	0.44
2:D:20:THR:HG23	2:D:72:THR:CG2	2.48	0.44
2:D:124:GLN:NE2	7:D:411:HOH:O	2.49	0.44
2:D:91:CYS:HB2	4:D:303:EDO:H22	2.00	0.43
2:D:13:VAL:HG22	2:D:78:VAL:HG11	1.98	0.43
2:D:108:ARG:HD2	2:D:140:TYR:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:GLN:HE21	1:A:82(A):ASN:ND2	2.02	0.43
2:B:20:THR:HG23	2:B:72:THR:CG2	2.49	0.42
2:B:190:ASN:O	2:B:210:ASN:HA	2.19	0.42
2:B:24:LYS:HA	2:B:69:THR:O	2.20	0.42
2:D:24:LYS:HA	2:D:69:THR:O	2.19	0.42
1:C:159:LEU:HD12	1:C:159:LEU:HA	1.89	0.42
1:A:64:LYS:NZ	7:A:405:HOH:O	2.47	0.42
2:D:13:VAL:HG21	2:D:19:VAL:CG1	2.50	0.42
2:D:20:THR:HG23	2:D:72:THR:HG23	2.00	0.41
2:B:31:ASN:O	2:B:50:TRP:HA	2.20	0.41
1:A:187:THR:O	1:A:191:GLU:HB2	2.20	0.41
2:D:189:HIS:O	2:D:211:ARG:HD3	2.20	0.41
2:B:33:LEU:HD22	2:B:71:PHE:CD1	2.56	0.41
1:C:93:LYS:HE3	4:C:303:EDO:C2	2.50	0.41
1:A:159:LEU:HD21	1:A:183:VAL:HG11	2.03	0.41
2:B:115:VAL:HA	2:B:135:PHE:O	2.21	0.41
2:D:13:VAL:CG2	2:D:78:VAL:HG11	2.51	0.41
1:C:81:GLN:HE21	1:C:82(A):ASN:ND2	2.00	0.40
1:A:59:TYR:CZ	4:A:301:EDO:H22	2.57	0.40
2:B:23:CYS:SG	2:B:88:CYS:CB	3.10	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	207/216 (96%)	205 (99%)	2 (1%)	0	100	100
1	C	207/216 (96%)	205 (99%)	2 (1%)	0	100	100
2	B	218/217 (100%)	214 (98%)	4 (2%)	0	100	100
2	D	217/217 (100%)	211 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	M	8/10 (80%)	7 (88%)	1 (12%)	0	100 100
3	N	8/10 (80%)	6 (75%)	0	2 (25%)	0 0
All	All	865/886 (98%)	848 (98%)	15 (2%)	2 (0%)	44 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	2	PRO
3	N	3	GLY

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	183/186 (98%)	169 (92%)	14 (8%)	10 3
1	C	183/186 (98%)	171 (93%)	12 (7%)	14 5
2	B	198/195 (102%)	189 (96%)	9 (4%)	23 13
2	D	197/195 (101%)	185 (94%)	12 (6%)	15 6
3	M	5/5 (100%)	5 (100%)	0	100 100
3	N	5/5 (100%)	4 (80%)	1 (20%)	1 0
All	All	771/772 (100%)	723 (94%)	48 (6%)	15 6

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	82	LEU
1	A	82(A)	ASN
1	A	82(B)	SER
1	A	82(C)	LEU
1	A	93	LYS
1	A	96	LEU
1	A	99	THR

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Mol	Chain	Res	Type
1	A	115	LYS
1	A	116	THR
1	A	160	SER
1	A	177	LEU
1	A	195	CYS
1	A	205	LYS
2	B	19	VAL
2	B	56	SER
2	B	91	CYS
2	B	104	LEU
2	B	143	ASP
2	B	153	SER
2	B	197	THR
2	B	203	SER
2	B	207	LYS
1	C	58	LYS
1	C	62	LYS
1	C	82	LEU
1	C	82(A)	ASN
1	C	82(B)	SER
1	C	82(C)	LEU
1	C	93	LYS
1	C	96	LEU
1	C	115	LYS
1	C	159	LEU
1	C	160	SER
1	C	177	LEU
2	D	9	SER
2	D	19	VAL
2	D	29	LEU
2	D	70	ASP
2	D	104	LEU
2	D	143	ASP
2	D	153	SER
2	D	156	GLN
2	D	169	LYS
2	D	197	THR
2	D	202	THR
2	D	207	LYS
3	N	2	PRO

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

Mol	Chain	Res	Type
1	A	6	GLN
1	A	81	GLN
1	A	196	ASN
2	B	6	GLN
2	B	124	GLN
2	B	157	ASN
2	B	166	GLN
1	C	6	GLN
1	C	81	GLN
1	C	133	ASN
1	C	196	ASN
2	D	6	GLN
2	D	124	GLN
2	D	166	GLN
2	D	210	ASN

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

20 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	$\#\|Z\|>2$
5	SO4	B	303	-	4,4,4	0.36	0	6,6,6	0.14	0
4	EDO	D	303	-	3,3,3	0.27	0	2,2,2	0.34	0
4	EDO	C	303	-	3,3,3	0.39	0	2,2,2	0.47	0
5	SO4	A	303	-	4,4,4	0.26	0	6,6,6	0.25	0
4	EDO	C	302	-	3,3,3	0.20	0	2,2,2	0.36	0
4	EDO	B	302	-	3,3,3	0.17	0	2,2,2	0.18	0
4	EDO	D	302	-	3,3,3	0.15	0	2,2,2	0.34	0
5	SO4	D	305	-	4,4,4	0.59	0	6,6,6	0.10	0
4	EDO	C	301	-	3,3,3	0.24	0	2,2,2	0.46	0
6	A2G	N	102	3	14,14,15	0.90	1 (7%)	17,19,21	1.51	4 (23%)
6	A2G	M	101	3	14,14,15	1.23	2 (14%)	17,19,21	1.02	1 (5%)
4	EDO	D	304	-	3,3,3	0.28	0	2,2,2	0.26	0
6	A2G	N	101	3	14,14,15	0.79	0	17,19,21	0.96	1 (5%)
4	EDO	A	302	-	3,3,3	0.34	0	2,2,2	0.23	0
4	EDO	A	301	-	3,3,3	0.14	0	2,2,2	0.30	0
4	EDO	B	301	-	3,3,3	0.57	0	2,2,2	0.64	0
6	A2G	M	102	3	14,14,15	1.16	2 (14%)	17,19,21	1.21	1 (5%)
5	SO4	D	306	-	4,4,4	0.21	0	6,6,6	0.12	0
4	EDO	D	301	-	3,3,3	0.20	0	2,2,2	0.19	0
5	SO4	C	304	-	4,4,4	0.32	0	6,6,6	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	301	-	-	0/1/1/1	-
4	EDO	B	301	-	-	0/1/1/1	-
4	EDO	C	302	-	-	1/1/1/1	-
4	EDO	D	303	-	-	1/1/1/1	-
4	EDO	D	304	-	-	0/1/1/1	-
6	A2G	M	102	3	-	0/6/23/26	0/1/1/1
4	EDO	B	302	-	-	1/1/1/1	-
4	EDO	D	302	-	-	1/1/1/1	-
6	A2G	N	101	3	-	0/6/23/26	0/1/1/1
4	EDO	A	302	-	-	0/1/1/1	-
4	EDO	C	301	-	-	0/1/1/1	-
6	A2G	N	102	3	-	0/6/23/26	0/1/1/1
4	EDO	C	303	-	-	1/1/1/1	-
4	EDO	D	301	-	-	1/1/1/1	-
6	A2G	M	101	3	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	101	A2G	C4-C5	2.74	1.58	1.53
6	M	101	A2G	O5-C1	2.28	1.47	1.43
6	N	102	A2G	O3-C3	-2.23	1.37	1.43
6	M	102	A2G	O5-C5	2.14	1.47	1.43
6	M	102	A2G	O3-C3	-2.08	1.38	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	102	A2G	O5-C5-C6	3.08	112.04	107.20
6	N	102	A2G	C3-C4-C5	-2.98	104.92	110.24
6	N	102	A2G	O3-C3-C2	2.28	114.18	109.47
6	M	102	A2G	C4-C3-C2	-2.10	107.94	111.02
6	N	101	A2G	C4-C3-C2	-2.09	107.95	111.02
6	N	102	A2G	C4-C3-C2	-2.06	108.00	111.02
6	M	101	A2G	O5-C5-C6	-2.02	104.03	107.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	302	EDO	O1-C1-C2-O2
4	D	302	EDO	O1-C1-C2-O2
4	C	303	EDO	O1-C1-C2-O2
4	D	301	EDO	O1-C1-C2-O2
6	M	101	A2G	C4-C5-C6-O6
4	C	302	EDO	O1-C1-C2-O2
4	D	303	EDO	O1-C1-C2-O2

There are no ring outliers.

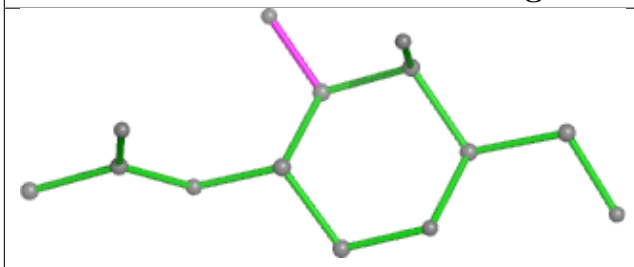
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	303	EDO	2	0
4	C	303	EDO	2	0
4	D	302	EDO	3	0
4	A	302	EDO	1	0
4	A	301	EDO	1	0

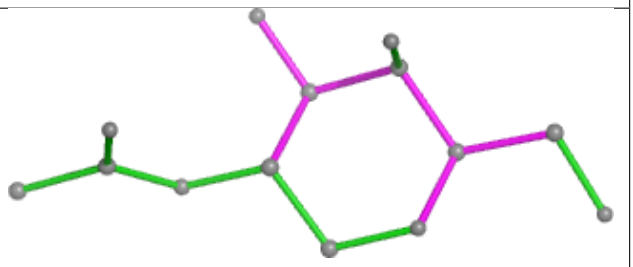
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 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.

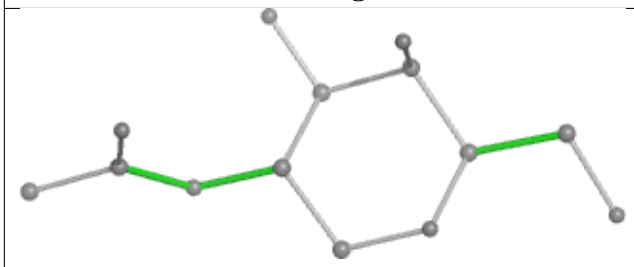
Ligand A2G N 102



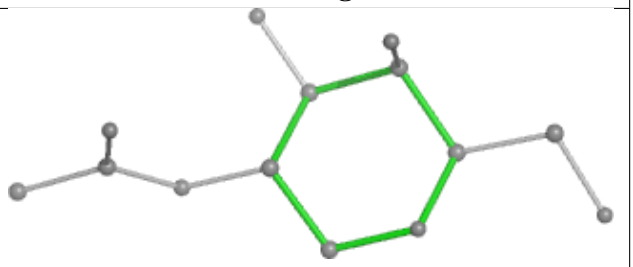
Bond lengths



Bond angles

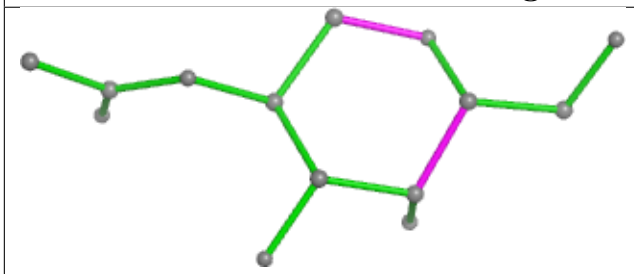


Torsions



Rings

Ligand A2G M 101



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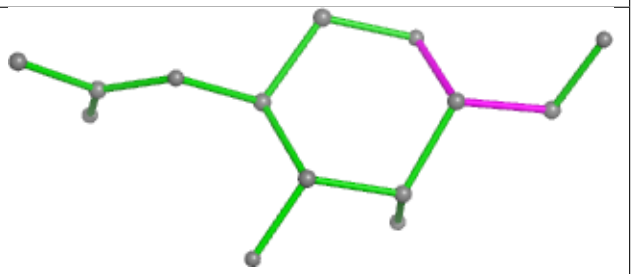
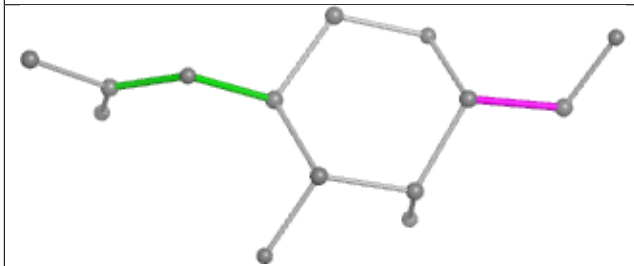


Bond angles



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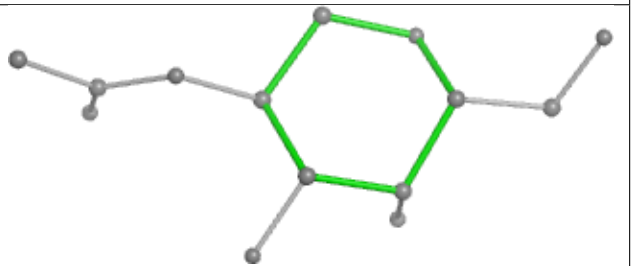
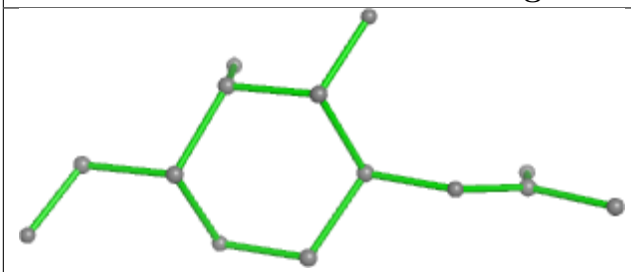
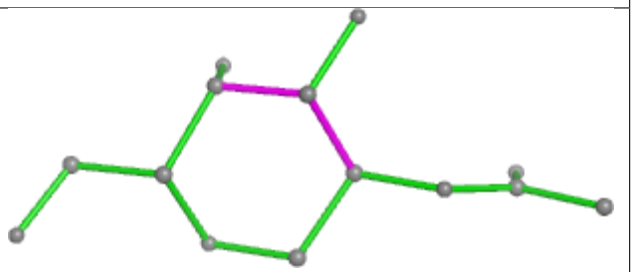


Rings

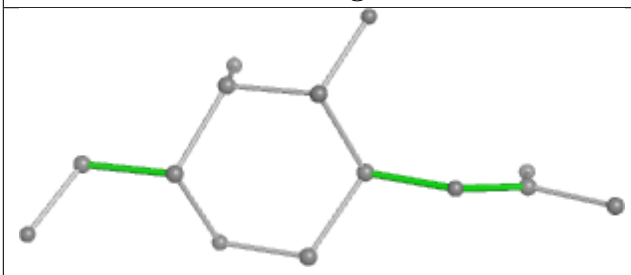
Ligand A2G N 101



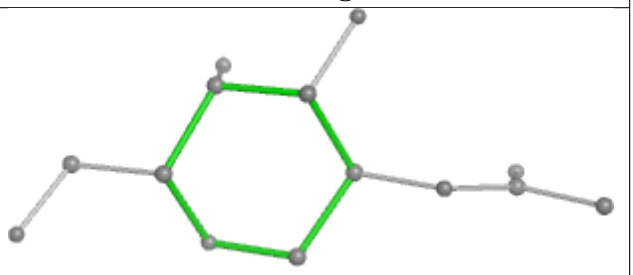
Bond lengths



Bond angles

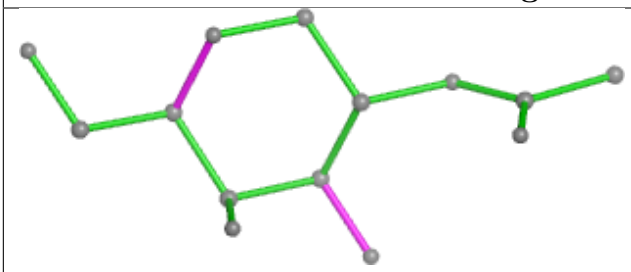


Torsions

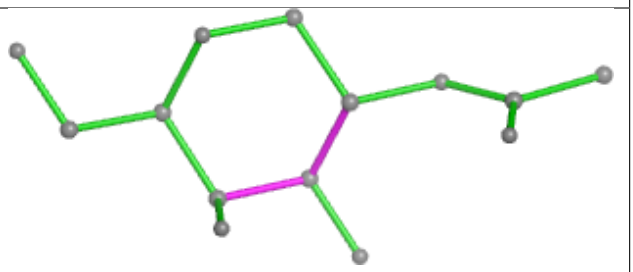


Rings

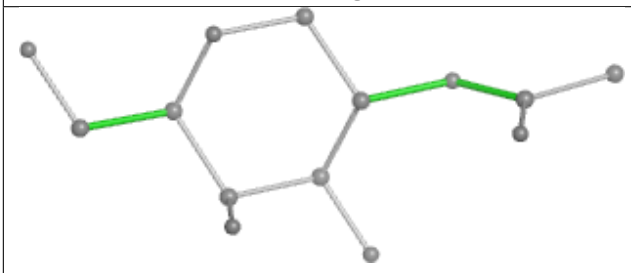
Ligand A2G M 102



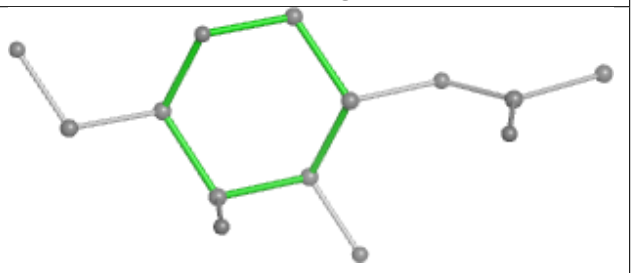
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	211/216 (97%)	0.12	6 (2%)	55	61	21, 29, 52, 69	0
1	C	211/216 (97%)	0.18	8 (3%)	44	51	21, 31, 50, 69	0
2	B	217/217 (100%)	0.08	3 (1%)	73	78	15, 29, 44, 58	3 (1%)
2	D	217/217 (100%)	0.26	9 (4%)	42	49	20, 32, 54, 68	2 (0%)
3	M	9/10 (90%)	0.88	2 (22%)	3	3	28, 31, 72, 85	0
3	N	9/10 (90%)	1.44	3 (33%)	1	1	31, 38, 88, 97	0
All	All	874/886 (98%)	0.18	31 (3%)	47	54	15, 30, 52, 97	5 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	1	ALA	5.0
3	M	2	PRO	4.5
3	M	1	ALA	4.1
2	D	127	SER	4.0
3	N	2	PRO	3.6
1	C	127	GLY	3.5
2	D	126	THR	2.9
1	A	161	SER	2.8
2	D	129	GLY	2.8
3	N	9	ALA	2.8
1	A	127	GLY	2.8
1	C	140	CYS	2.7
1	C	172	SER	2.6
1	C	133	ASN	2.6
1	C	28	ILE	2.6
1	C	211	VAL	2.6
1	C	171	GLN	2.5
2	D	182	THR	2.5
1	A	209	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	190	ASN	2.3
2	D	181	LEU	2.3
2	D	13	VAL	2.2
2	D	30(C)	SER	2.2
1	A	159	LEU	2.2
2	B	41	GLY	2.2
1	C	212	PRO	2.2
2	D	143	ASP	2.1
1	A	43	GLN	2.1
2	B	156	GLN	2.0
1	A	160	SER	2.0
2	D	188	ARG	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	302	4/4	0.59	0.29	80,87,89,104	0
5	SO4	C	304	5/5	0.72	0.18	66,68,93,96	0
4	EDO	A	302	4/4	0.82	0.17	32,37,39,40	0
4	EDO	D	301	4/4	0.85	0.16	51,53,56,57	0
4	EDO	B	301	4/4	0.86	0.16	39,40,41,44	0
4	EDO	D	302	4/4	0.88	0.14	31,39,43,46	0
5	SO4	B	303	5/5	0.89	0.10	65,67,77,81	0
4	EDO	C	303	4/4	0.90	0.14	43,49,49,50	0
5	SO4	D	306	5/5	0.90	0.09	37,43,55,62	0
4	EDO	D	303	4/4	0.92	0.12	27,43,47,55	0
4	EDO	C	302	4/4	0.92	0.10	37,38,38,40	0

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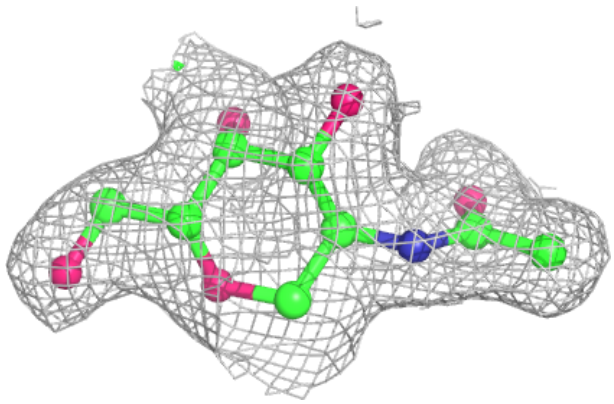
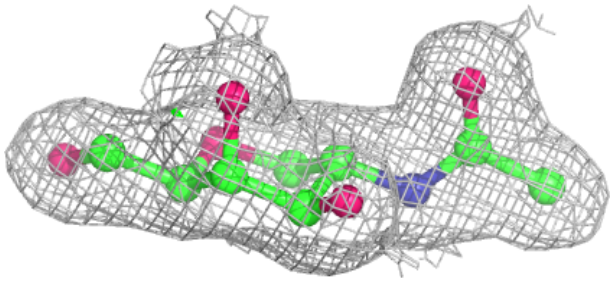
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	A	303	5/5	0.93	0.08	41,46,51,57	0
4	EDO	A	301	4/4	0.93	0.13	31,42,44,52	0
4	EDO	C	301	4/4	0.95	0.07	27,28,30,31	0
4	EDO	D	304	4/4	0.95	0.09	24,30,31,31	0
6	A2G	M	102	14/15	0.95	0.07	23,26,31,33	0
6	A2G	N	102	14/15	0.95	0.07	26,29,36,36	0
6	A2G	N	101	14/15	0.96	0.06	26,31,32,33	0
6	A2G	M	101	14/15	0.96	0.06	25,27,32,35	0
5	SO4	D	305	5/5	0.98	0.06	32,34,38,40	0

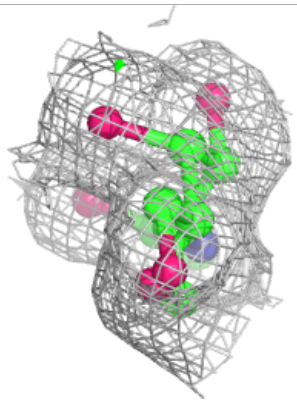
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A2G M 102:

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

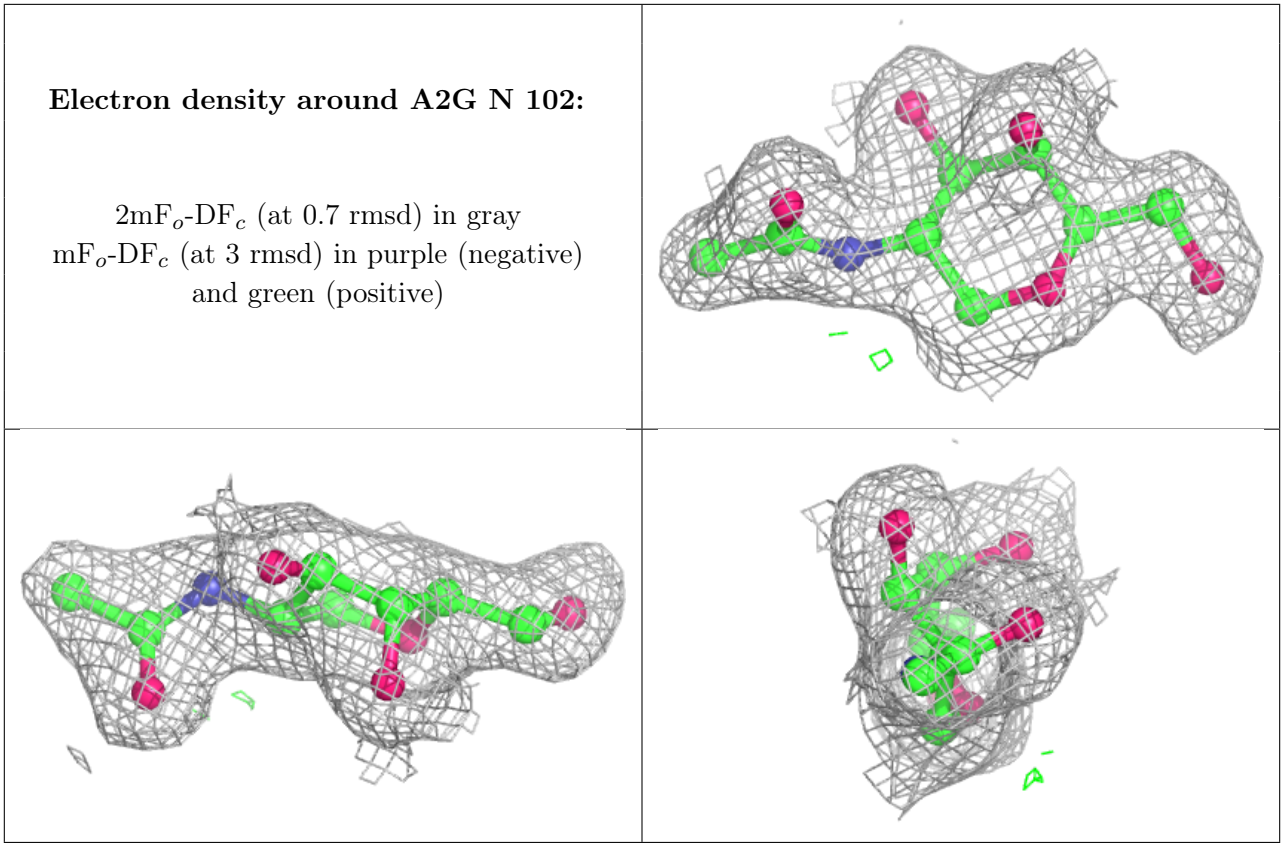






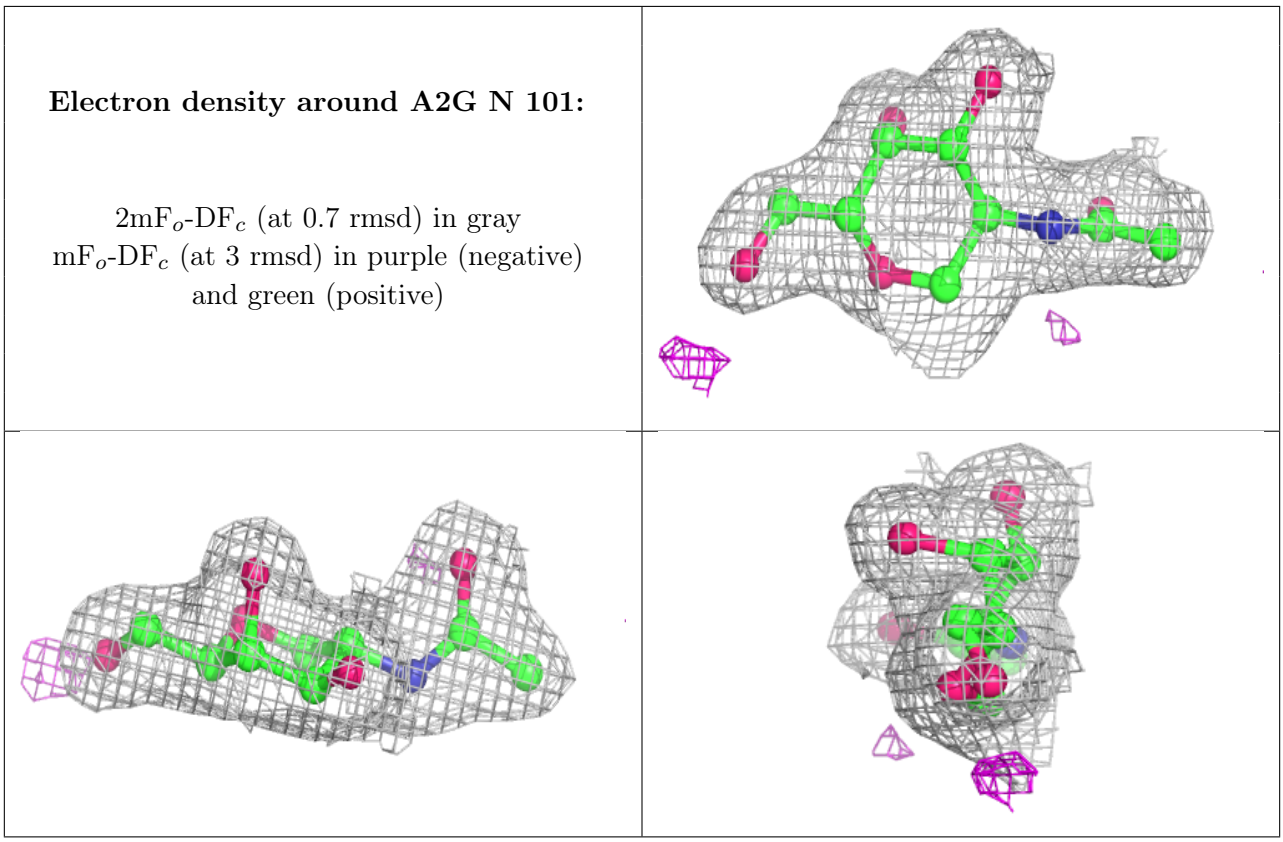
Electron density around A2G N 102:

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



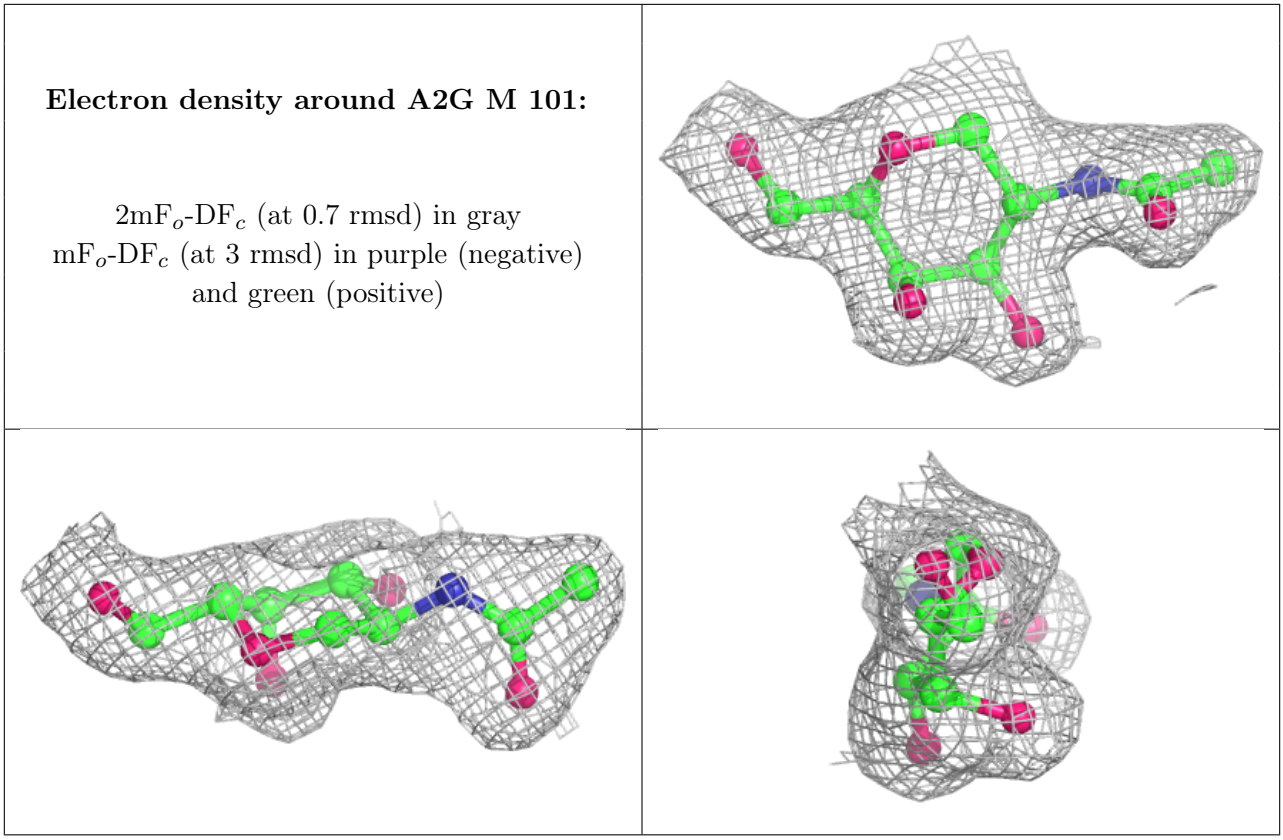
Electron density around A2G N 101:

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



Electron density around A2G M 101:

$2mF_o$-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.