



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2021 – 08:23 PM EDT

PDB ID : 3G82
Title : Complex of GS-alpha with the catalytic domains of mammalian adenylyl cyclase: complex with MANT-ITP and Mn
Authors : Huebner, M.; Mou, T.-C.; Sprang, S.R.; Seifert, R.
Deposited on : 2009-02-11
Resolution : 3.11 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
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) : 2.23.2

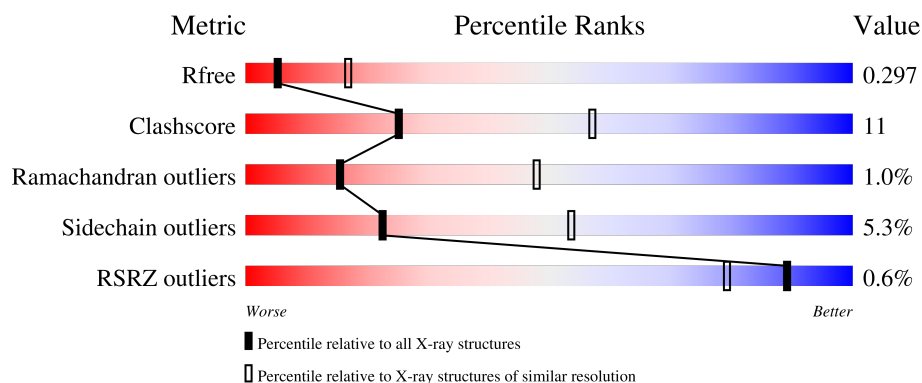
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	225	<div> <div></div> <div>64%</div> <div>18%</div> <div>•</div> <div>16%</div> </div>
2	B	212	<div> <div></div> <div>57%</div> <div>27%</div> <div>5%</div> <div>11%</div> </div>
3	C	394	<div> <div></div> <div>72%</div> <div>11%</div> <div>•</div> <div>16%</div> </div>

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 5755 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 Adenylate cyclase type 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1476	929	259	271	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	MET	-	expression tag	UNP P30803
A	357	HIS	-	expression tag	UNP P30803
A	358	HIS	-	expression tag	UNP P30803
A	359	HIS	-	expression tag	UNP P30803
A	360	HIS	-	expression tag	UNP P30803
A	361	HIS	-	expression tag	UNP P30803
A	362	HIS	-	expression tag	UNP P30803
A	476	MET	VAL	engineered mutation	UNP P30803

- Molecule 2 is a protein called Adenylate cyclase type 2.

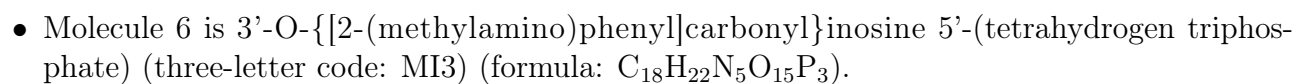
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	189	Total	C	N	O	S	0	0	0
			1467	936	242	279	10			

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	330	Total	C	N	O	S	0	0	0
			2702	1714	470	505	13			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

- Molecule 5 is FORSKOLIN (three-letter code: FOK) (formula: $C_{22}H_{34}O_7$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			41	18	5	15	3		

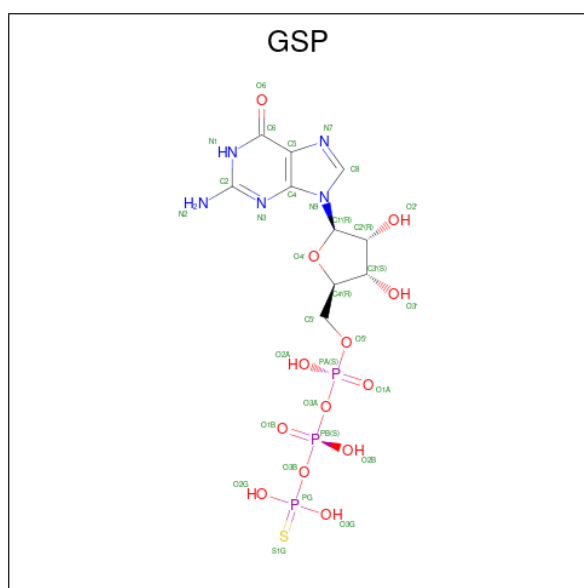
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Cl	0	0
			1	1		

- Molecule 9 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	C	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	2	Total	O	0	0
			2	2		
10	C	1	Total	O	0	0
			1	1		

- Molecule 1: Adenylate cyclase type 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.64Å 133.42Å 70.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.11 15.00 – 3.11	Depositor EDS
% Data completeness (in resolution range)	81.4 (15.00-3.11) 81.4 (15.00-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.237 , 0.294 0.245 , 0.297	Depositor DCC
R_{free} test set	847 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 30.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	5755	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, FOK, CL, MI3, MG, GSP

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	0.33	0/1504	0.51	0/2027
2	B	0.34	0/1492	0.50	0/2014
3	C	0.35	0/2759	0.50	0/3733
All	All	0.34	0/5755	0.50	0/7774

There are no bond length outliers.

There are no bond angle outliers.

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	1476	0	1450	31	0
2	B	1467	0	1470	73	0
3	C	2702	0	2651	18	0
4	A	2	0	0	0	0
5	A	29	0	34	6	0
6	A	41	0	18	5	0
7	C	1	0	0	0	0
8	C	1	0	0	0	0
9	C	32	0	12	0	0
10	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	2	0	0	0	0
10	C	1	0	0	0	0
All	All	5755	0	5635	122	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 11.

All (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:964:ARG:HH11	2:B:964:ARG:CG	1.58	1.16
2:B:964:ARG:HG3	2:B:964:ARG:NH1	1.51	1.08
2:B:953:ILE:HD12	2:B:953:ILE:H	1.16	1.04
2:B:953:ILE:HD12	2:B:953:ILE:N	1.77	0.98
5:A:101:FOK:H173	5:A:101:FOK:H201	1.49	0.92
2:B:953:ILE:H	2:B:953:ILE:CD1	1.87	0.86
2:B:879:HIS:HB3	2:B:1008:GLY:HA3	1.54	0.86
1:A:435:ILE:HD11	1:A:445:VAL:HB	1.59	0.85
2:B:964:ARG:HH11	2:B:964:ARG:HG3	0.71	0.81
2:B:885:VAL:HG12	2:B:886:CYS:N	1.98	0.78
2:B:964:ARG:HG2	2:B:965:GLN:H	1.48	0.78
1:A:470:ILE:HG13	1:A:483:MET:HG2	1.65	0.77
2:B:891:SER:HB3	2:B:943:THR:OG1	1.86	0.76
2:B:886:CYS:HB3	2:B:948:THR:OG1	1.86	0.75
1:A:467:ILE:O	1:A:470:ILE:HG22	1.88	0.74
1:A:452:ARG:HG2	1:A:454:ASP:H	1.54	0.72
3:C:207:ILE:HG12	3:C:224:VAL:HG12	1.70	0.72
2:B:964:ARG:CG	2:B:964:ARG:NH1	2.30	0.70
2:B:915:LEU:HD12	2:B:915:LEU:O	1.94	0.68
2:B:918:ILE:HG12	2:B:986:ILE:HD13	1.75	0.67
2:B:964:ARG:N	2:B:967:MET:HB2	2.10	0.66
2:B:879:HIS:HB2	2:B:1007:ALA:O	1.95	0.66
2:B:879:HIS:CB	2:B:1008:GLY:HA3	2.25	0.66
1:A:403:LEU:HD13	1:A:479:VAL:HG11	1.77	0.66
2:B:928:LYS:HB3	2:B:929:PRO:CD	2.26	0.66
2:B:922:PHE:CD2	2:B:979:LEU:HD22	2.31	0.65
2:B:885:VAL:CG1	2:B:886:CYS:N	2.60	0.64
1:A:420:PHE:HA	1:A:423:PHE:HB2	1.80	0.62
2:B:925:LEU:O	2:B:927:SER:N	2.34	0.61
5:A:101:FOK:H201	5:A:101:FOK:C17	2.29	0.61
2:B:886:CYS:O	2:B:947:ALA:HA	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:928:LYS:HB3	2:B:929:PRO:HD2	1.82	0.60
1:A:477:THR:HB	1:A:479:VAL:HG12	1.83	0.60
1:A:497:LEU:CD1	2:B:915:LEU:HG	2.31	0.60
5:A:101:FOK:H202	5:A:101:FOK:H193	1.85	0.59
6:A:100:MI3:O1G	2:B:1065:LYS:HE3	2.02	0.59
2:B:964:ARG:HG2	2:B:965:GLN:N	2.16	0.59
2:B:885:VAL:CG1	2:B:886:CYS:H	2.16	0.58
2:B:964:ARG:HG2	2:B:965:GLN:HG2	1.83	0.58
5:A:101:FOK:H7	2:B:941:GLY:HA3	1.85	0.58
3:C:364:THR:HA	3:C:371:ASN:HD21	1.69	0.57
1:A:452:ARG:HD3	1:A:454:ASP:HB3	1.86	0.57
2:B:964:ARG:CG	2:B:965:GLN:N	2.65	0.56
1:A:546:CYS:O	1:A:549:GLU:HG2	2.06	0.55
2:B:925:LEU:O	2:B:928:LYS:N	2.31	0.55
2:B:885:VAL:HG12	2:B:886:CYS:H	1.70	0.55
2:B:1033:THR:O	2:B:1059:ARG:NH1	2.38	0.55
3:C:166:SER:HA	3:C:169:TYR:CE2	2.42	0.54
1:A:530:LYS:HD2	1:A:531:ALA:N	2.23	0.54
1:A:508:SER:OG	1:A:511:VAL:HG23	2.09	0.52
3:C:321:PRO:HG2	3:C:324:ALA:HB2	1.91	0.52
2:B:930:LYS:HE3	2:B:931:PHE:CE2	2.44	0.52
2:B:964:ARG:CG	2:B:965:GLN:H	2.12	0.52
1:A:505:ASP:HB3	1:A:507:TRP:CZ2	2.45	0.51
2:B:882:TYR:N	2:B:882:TYR:CD1	2.79	0.51
2:B:1049:LEU:HB3	2:B:1054:TYR:HB2	1.93	0.50
6:A:100:MI3:O1G	2:B:1065:LYS:CE	2.60	0.50
2:B:886:CYS:CB	2:B:948:THR:OG1	2.60	0.50
3:C:143:PRO:O	3:C:146:PHE:HB3	2.12	0.49
2:B:881:SER:HB3	2:B:1006:ILE:HG13	1.94	0.49
2:B:925:LEU:C	2:B:927:SER:N	2.64	0.49
3:C:172:ILE:HD12	3:C:174:CYS:SG	2.52	0.49
2:B:915:LEU:O	2:B:919:ILE:HG12	2.12	0.49
1:A:415:THR:HG21	1:A:477:THR:HG23	1.94	0.49
2:B:905:ASN:OD1	2:B:905:ASN:C	2.50	0.49
2:B:881:SER:C	2:B:882:TYR:HD1	2.17	0.48
6:A:100:MI3:H2	2:B:1019:ILE:O	2.14	0.48
2:B:893:PRO:O	2:B:895:PHE:N	2.47	0.48
2:B:1001:ASN:HB3	2:B:1027:ALA:HB2	1.95	0.48
1:A:494:CYS:HB3	1:A:506:VAL:HG12	1.95	0.48
2:B:915:LEU:HD12	2:B:915:LEU:C	2.34	0.48
2:B:905:ASN:OD1	2:B:905:ASN:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:TYR:N	2:B:882:TYR:HD1	2.12	0.47
3:C:187:GLN:HB2	3:C:190:TYR:HB2	1.96	0.47
2:B:937:ILE:HD13	2:B:937:ILE:N	2.30	0.47
1:A:378:MET:HE1	3:C:284:THR:H	1.80	0.47
1:A:445:VAL:HG11	1:A:448:LEU:HD12	1.97	0.47
5:A:101:FOK:H173	5:A:101:FOK:C20	2.33	0.46
2:B:925:LEU:C	2:B:927:SER:H	2.19	0.46
1:A:400:PHE:N	6:A:100:MI3:O3G	2.49	0.45
2:B:900:THR:O	2:B:905:ASN:ND2	2.49	0.45
2:B:976:ALA:O	2:B:980:VAL:HG23	2.17	0.45
3:C:257:ILE:HD13	3:C:259:GLU:HB2	1.96	0.45
1:A:485:VAL:HB	1:A:526:ILE:HA	1.99	0.45
2:B:1047:LEU:HA	2:B:1050:GLN:HE21	1.81	0.45
3:C:46:LEU:O	3:C:246:PHE:HA	2.16	0.45
1:A:530:LYS:HA	1:A:562:PHE:HE1	1.82	0.45
1:A:493:HIS:CE1	2:B:909:LEU:HD13	2.51	0.44
2:B:912:LEU:O	2:B:916:ASN:N	2.40	0.44
2:B:1062:ILE:HD13	2:B:1062:ILE:HA	1.83	0.44
2:B:1026:VAL:O	2:B:1030:MET:HG2	2.17	0.44
3:C:346:LEU:O	3:C:350:THR:N	2.50	0.44
2:B:940:ILE:HD12	2:B:940:ILE:N	2.32	0.43
6:A:100:MI3:HA3	2:B:1020:TRP:HB3	2.00	0.43
3:C:181:LYS:O	3:C:185:ILE:HG13	2.18	0.43
2:B:921:ASP:OD2	2:B:986:ILE:HD11	2.17	0.43
2:B:928:LYS:CB	2:B:929:PRO:CD	2.94	0.43
2:B:966:TYR:HA	2:B:968:HIS:CE1	2.53	0.43
1:A:390:VAL:HG12	1:A:447:GLY:HA3	1.99	0.43
3:C:331:ASP:HA	3:C:332:PRO:HD2	1.85	0.43
3:C:99:LEU:HD21	3:C:182:ILE:HD13	2.01	0.43
2:B:885:VAL:HG21	2:B:1005:VAL:CG2	2.49	0.42
3:C:257:ILE:HG23	3:C:265:ARG:HG2	2.01	0.42
2:B:881:SER:C	2:B:882:TYR:CD1	2.92	0.42
1:A:501:LYS:HD2	2:B:936:LYS:O	2.20	0.42
5:A:101:FOK:C17	5:A:101:FOK:C20	2.95	0.42
2:B:913:ARG:O	2:B:917:GLU:HG2	2.20	0.42
3:C:103:ILE:HG23	3:C:104:GLU:N	2.35	0.42
2:B:895:PHE:CZ	2:B:915:LEU:HB2	2.54	0.42
1:A:529:THR:HG22	1:A:530:LYS:N	2.34	0.41
2:B:1036:LEU:O	2:B:1037:ASP:HB2	2.21	0.41
1:A:403:LEU:C	1:A:405:SER:H	2.24	0.41
1:A:435:ILE:CG2	1:A:505:ASP:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:TRP:O	1:A:508:SER:HB3	2.21	0.41
2:B:925:LEU:O	2:B:926:LEU:C	2.60	0.41
1:A:378:MET:CE	3:C:284:THR:H	2.34	0.40
1:A:452:ARG:HG2	1:A:454:ASP:N	2.29	0.40
1:A:554:LEU:HA	1:A:559:ILE:HD12	2.03	0.40
2:B:940:ILE:O	2:B:941:GLY:C	2.58	0.40
2:B:995:LYS:HD2	2:B:1037:ASP:OD1	2.22	0.40
1:A:422:ARG:O	1:A:426:LEU:HG	2.22	0.40
3:C:219:PHE:CZ	3:C:380:ARG:HG2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	187/225 (83%)	167 (89%)	20 (11%)	0	100	100
2	B	185/212 (87%)	168 (91%)	13 (7%)	4 (2%)	6	28
3	C	326/394 (83%)	302 (93%)	21 (6%)	3 (1%)	17	51
All	All	698/831 (84%)	637 (91%)	54 (8%)	7 (1%)	15	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	138	PRO
2	B	894	ASP
2	B	926	LEU
3	C	175	ALA
2	B	929	PRO
3	C	59	GLN
2	B	918	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	158/189 (84%)	148 (94%)	10 (6%)	18	47
2	B	162/184 (88%)	151 (93%)	11 (7%)	16	45
3	C	297/351 (85%)	285 (96%)	12 (4%)	31	64
All	All	617/724 (85%)	584 (95%)	33 (5%)	22	53

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	388	ASP
1	A	390	VAL
1	A	403	LEU
1	A	407	CYS
1	A	470	ILE
1	A	476	MET
1	A	477	THR
1	A	500	ARG
1	A	528	ILE
1	A	530	LYS
2	B	882	TYR
2	B	891	SER
2	B	900	THR
2	B	903	ASP
2	B	915	LEU
2	B	936	LYS
2	B	938	LYS
2	B	953	ILE
2	B	964	ARG
2	B	1009	VAL
2	B	1062	ILE
3	C	98	ASN
3	C	139	ASP
3	C	176	GLN
3	C	181	LYS
3	C	205	SER

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Mol	Chain	Res	Type
3	C	211	LYS
3	C	218	ASN
3	C	229	ASP
3	C	235	ILE
3	C	284	THR
3	C	357	HIS
3	C	370	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	385	GLN
1	A	493	HIS
2	B	965	GLN
2	B	1001	ASN
2	B	1050	GLN
3	C	97	ASN
3	C	357	HIS
3	C	371	ASN
3	C	377	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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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
9	GSP	C	395	7	26,34,34	1.20	2 (7%)	28,54,54	2.23	4 (14%)
6	MI3	A	100	4	36,44,44	2.17	6 (16%)	44,67,67	2.34	14 (31%)
5	FOK	A	101	-	28,31,31	1.05	1 (3%)	35,54,54	1.74	7 (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
9	GSP	C	395	7	-	1/17/38/38	0/3/3/3
6	MI3	A	100	4	-	4/28/48/48	0/4/4/4
5	FOK	A	101	-	-	4/7/80/80	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	100	MI3	CA5-CA6	8.87	1.54	1.39
6	A	100	MI3	OA-CA	5.16	1.36	1.22
5	A	101	FOK	O4-C21	4.69	1.45	1.35
6	A	100	MI3	C6-N1	3.99	1.40	1.33
6	A	100	MI3	C2-N1	3.60	1.40	1.33
9	C	395	GSP	C6-N1	3.07	1.38	1.33
9	C	395	GSP	C2'-C1'	-2.30	1.50	1.53
6	A	100	MI3	O4'-C1'	2.14	1.44	1.41
6	A	100	MI3	CA1-CA	2.10	1.54	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	395	GSP	C5-C6-N1	-8.37	111.98	123.43
6	A	100	MI3	O1G-PG-O1B	6.52	126.50	104.64
6	A	100	MI3	O1B-PG-O2G	-6.00	77.90	111.19
9	C	395	GSP	C6-N1-C2	5.72	125.02	115.93
6	A	100	MI3	N3-C2-N1	-5.07	120.76	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	101	FOK	O4-C21-C22	4.79	119.91	111.09
5	A	101	FOK	C13-O1-C8	4.59	127.14	119.84
6	A	100	MI3	O3G-PG-O1B	4.59	120.03	104.64
5	A	101	FOK	C7-O4-C21	-4.28	111.56	117.81
6	A	100	MI3	PB-O1B-PG	-4.21	118.38	132.83
6	A	100	MI3	PB-O1A-PA	-3.90	119.44	132.83
6	A	100	MI3	O3'-CA-CA1	3.77	117.56	111.69
6	A	100	MI3	O4'-C1'-C2'	-3.48	101.84	106.93
5	A	101	FOK	C20-C10-C1	-3.03	103.18	107.68
6	A	100	MI3	CA4-CA5-CA6	-2.88	112.64	118.62
9	C	395	GSP	N3-C2-N1	-2.83	123.45	127.22
9	C	395	GSP	C2-N3-C4	-2.65	112.33	115.36
6	A	100	MI3	CA5-CA6-CA1	2.64	122.86	119.38
5	A	101	FOK	O4-C21-O5	-2.47	118.05	122.96
5	A	101	FOK	C3-C4-C5	2.29	111.26	107.96
6	A	100	MI3	CA1-CA6-NA1	-2.24	118.64	121.25
6	A	100	MI3	CA3-CA4-CA5	2.18	123.52	120.19
6	A	100	MI3	CA5-CA6-NA1	-2.18	118.50	121.23
6	A	100	MI3	O3'-C3'-C4'	-2.10	104.33	109.56
5	A	101	FOK	O7-C11-C12	-2.02	117.84	122.02

There are no chirality outliers.

All (9) torsion outliers are listed below:

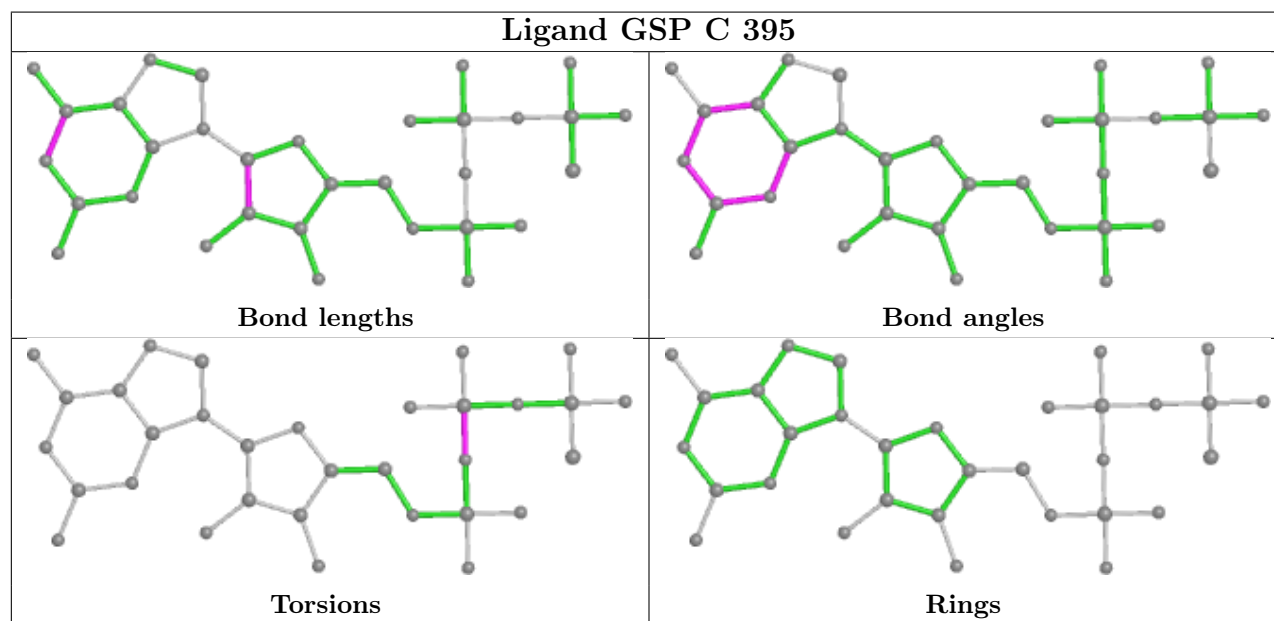
Mol	Chain	Res	Type	Atoms
5	A	101	FOK	O5-C21-O4-C7
5	A	101	FOK	C22-C21-O4-C7
5	A	101	FOK	C16-C13-C14-C15
6	A	100	MI3	C3'-C4'-C5'-O5'
6	A	100	MI3	O4'-C4'-C5'-O5'
6	A	100	MI3	PB-O1B-PG-O1G
9	C	395	GSP	PA-O3A-PB-O2B
5	A	101	FOK	O1-C13-C14-C15
6	A	100	MI3	PA-O1A-PB-O3B

There are no ring outliers.

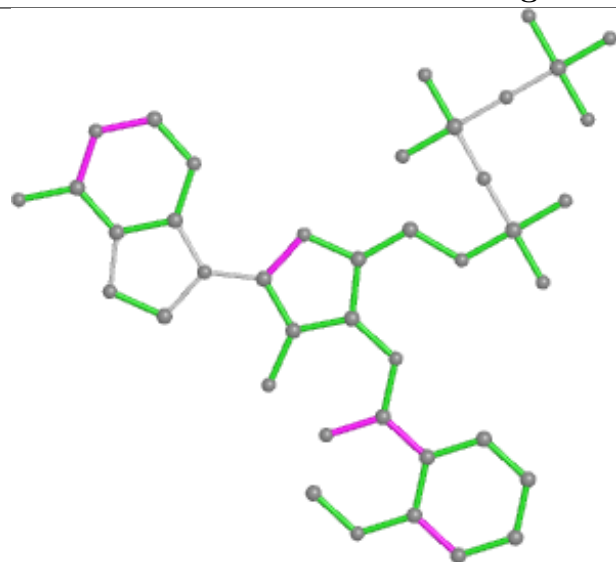
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	100	MI3	5	0
5	A	101	FOK	6	0

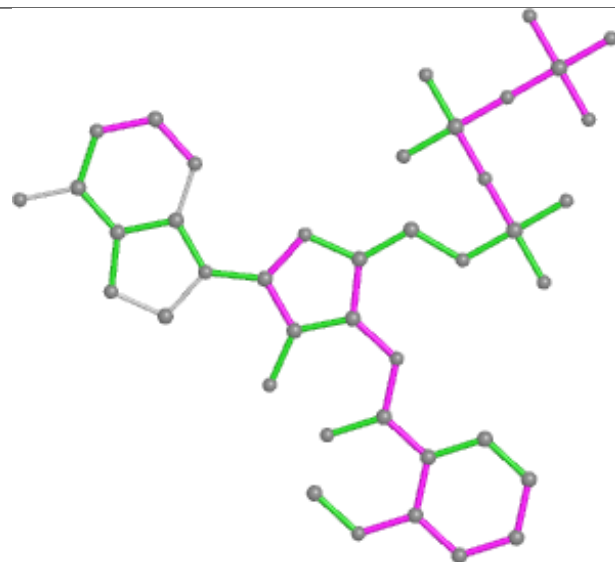
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



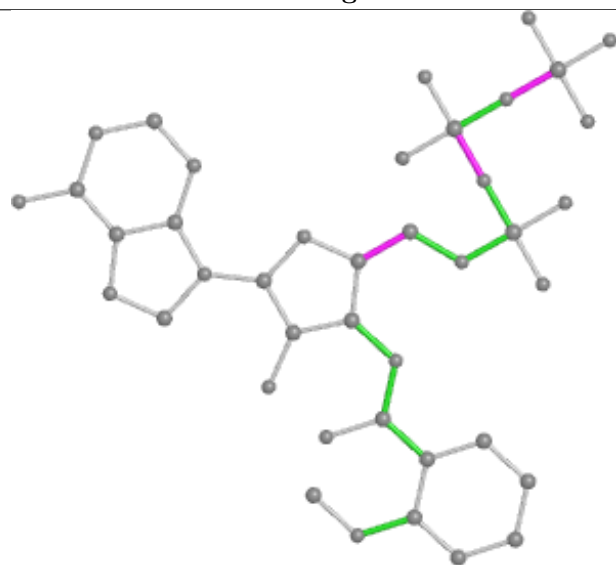
Ligand MI3 A 100



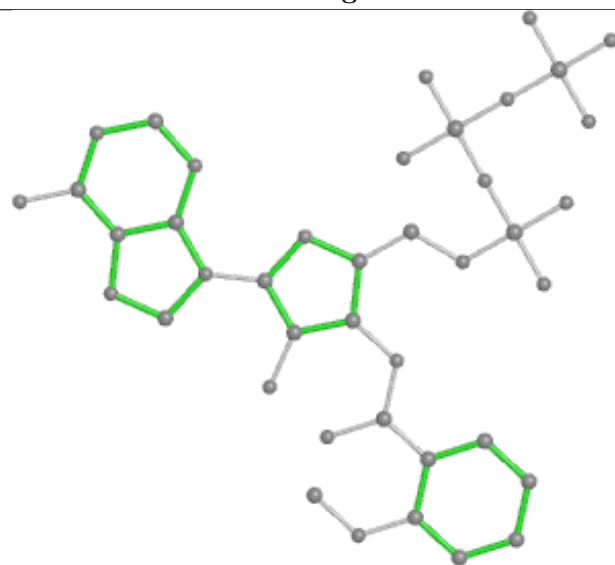
Bond lengths



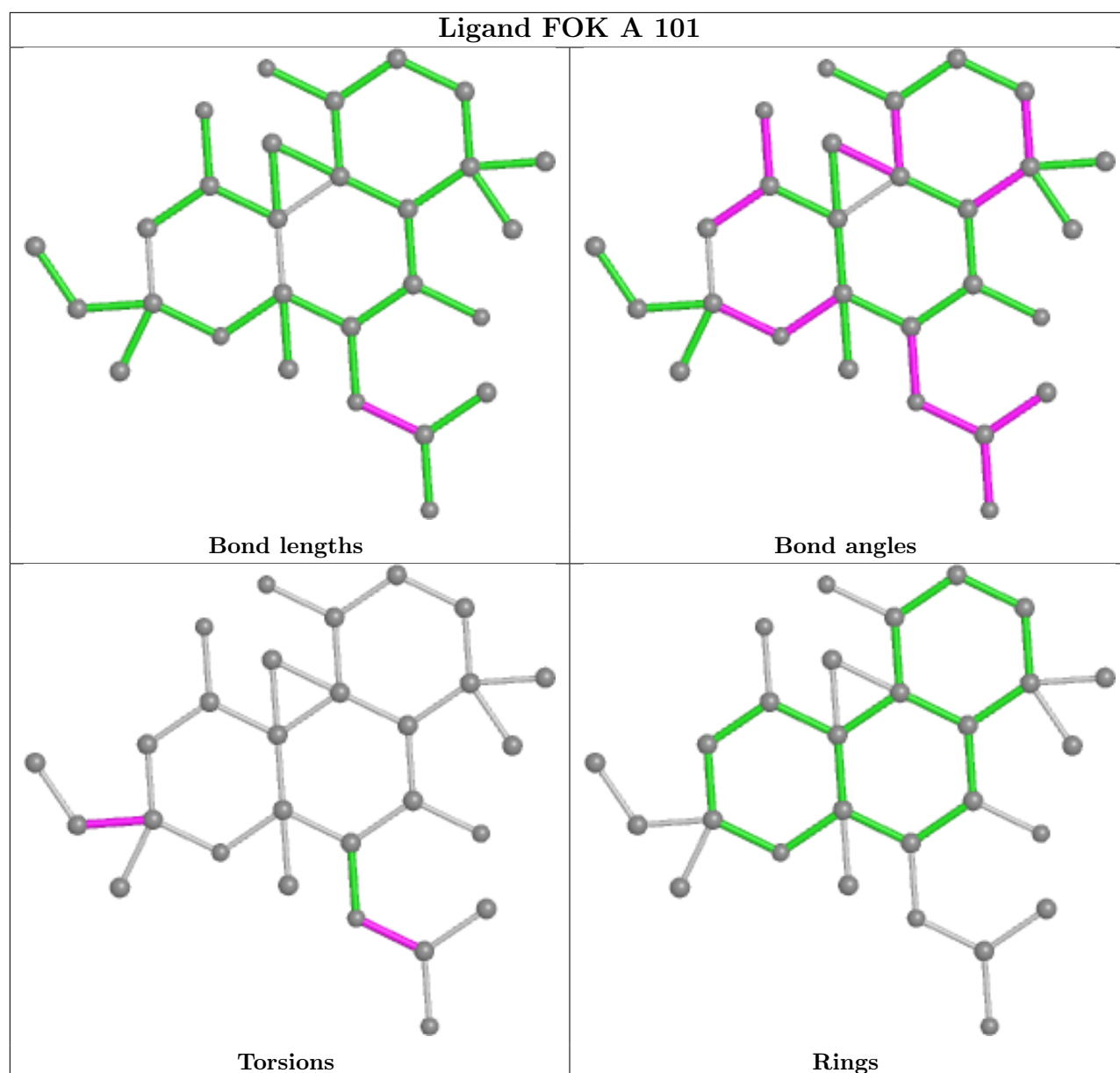
Bond angles



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 [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	189/225 (84%)	-0.20	2 (1%) 80 65	22, 54, 83, 98	0
2	B	189/212 (89%)	-0.51	2 (1%) 80 65	12, 38, 73, 94	0
3	C	330/394 (83%)	-0.40	0 100 100	18, 40, 68, 92	0
All	All	708/831 (85%)	-0.38	4 (0%) 89 79	12, 43, 74, 98	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	953	ILE	3.1
2	B	951	SER	2.2
1	A	480	ASN	2.1
1	A	479	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

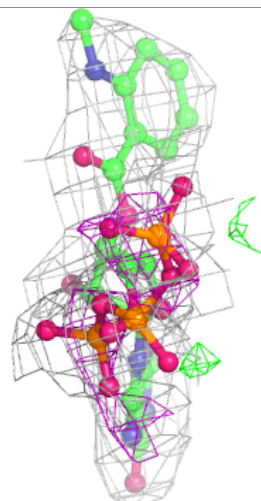
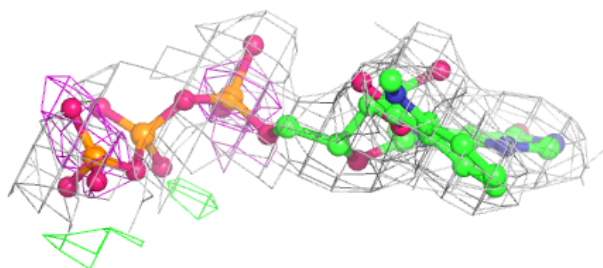
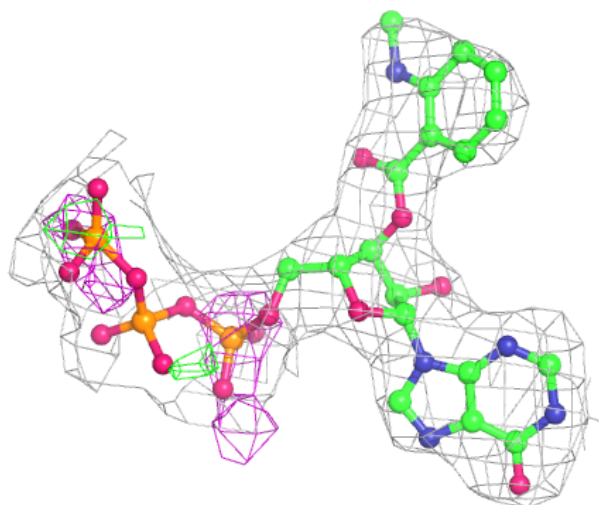
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MG	C	396	1/1	0.84	0.19	11,11,11,11	0
4	MN	A	581	1/1	0.91	0.10	32,32,32,32	0
8	CL	C	397	1/1	0.92	0.23	46,46,46,46	0
6	MI3	A	100	41/41	0.93	0.17	37,41,42,42	0
5	FOK	A	101	29/29	0.94	0.15	26,30,36,40	0
9	GSP	C	395	32/32	0.94	0.17	17,23,36,37	0
4	MN	A	582	1/1	0.95	0.05	37,37,37,37	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.

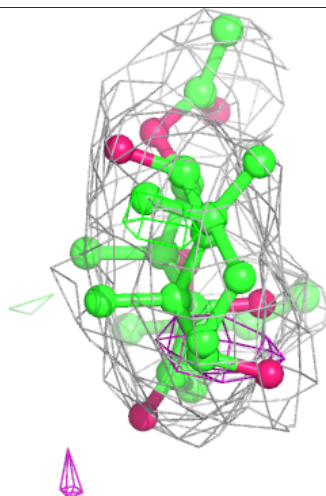
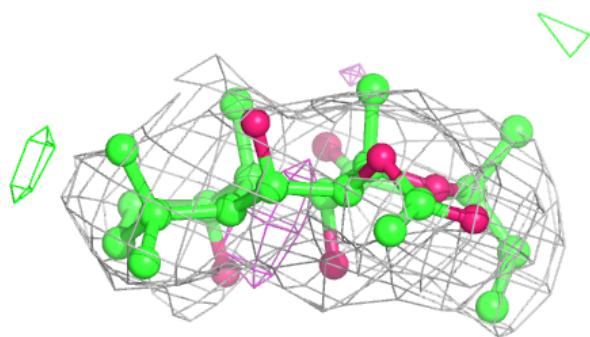
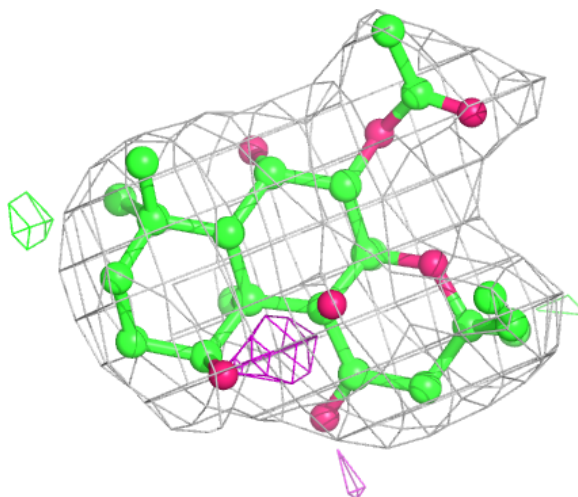
Electron density around MI3 A 100:

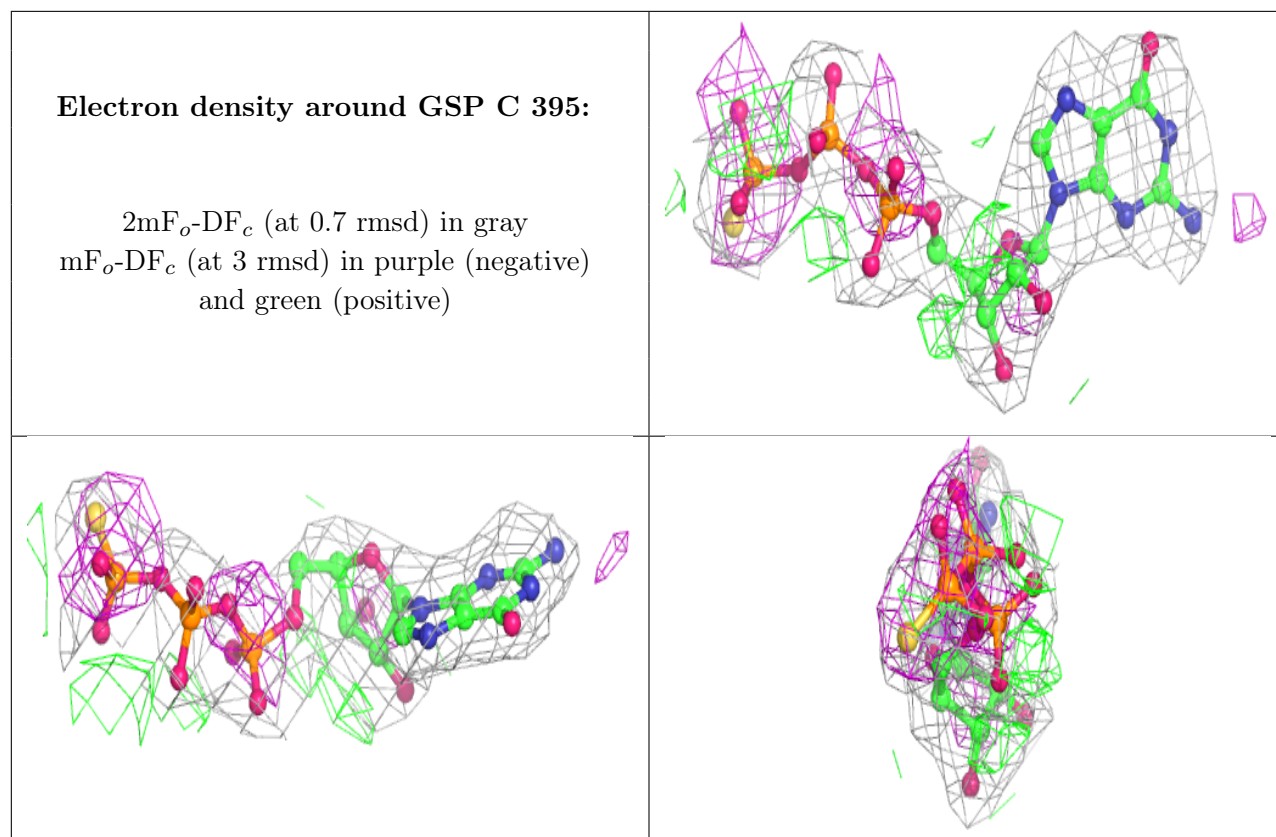
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FOK A 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.