



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2020 – 01:57 PM BST

PDB ID : 5O9A
Title : Crystal structure of the GluA2 ligand-binding domain (S1S2J-L504Y-N775S)
in complex with glutamate and BPAM121 at 1.78 Å resolution
Authors : Laulumaa, S.; Rovinskaja, K.; Frydenvang, K.A.; Kastrup, J.S.
Deposited on : 2017-06-16
Resolution : 1.78 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 : 2.14.3.dev2
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) : 2.14.3.dev2

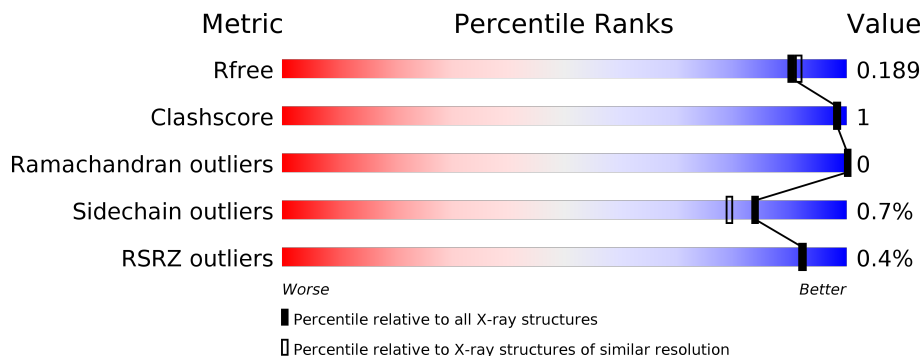
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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 on 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	264	99%
1	B	264	98%
1	C	264	98%
1	D	264	2% (Poor fit), 95%

2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 9878 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 Glutamate receptor 2,Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	2141	1380	347	398	16	0	18	0
1	B	264	2099	1342	345	397	15	0	10	0
1	C	263	2141	1375	350	401	15	0	16	0
1	D	260	2072	1326	340	391	15	0	8	0

There are 24 discrepancies between the modelled and reference sequences:

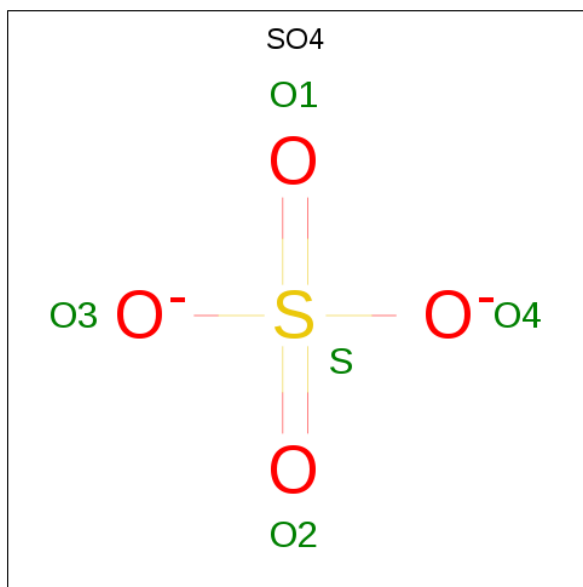
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P19491
A	2	ALA	-	cloning artifact	UNP P19491
A	94	TYR	LEU	engineered mutation	UNP P19491
A	118	GLY	-	linker	UNP P19491
A	119	THR	-	linker	UNP P19491
A	242	SER	ASN	engineered mutation	UNP P19491
B	1	GLY	-	cloning artifact	UNP P19491
B	2	ALA	-	cloning artifact	UNP P19491
B	94	TYR	LEU	engineered mutation	UNP P19491
B	118	GLY	-	linker	UNP P19491
B	119	THR	-	linker	UNP P19491
B	242	SER	ASN	engineered mutation	UNP P19491
C	1	GLY	-	cloning artifact	UNP P19491
C	2	ALA	-	cloning artifact	UNP P19491
C	94	TYR	LEU	engineered mutation	UNP P19491
C	118	GLY	-	linker	UNP P19491
C	119	THR	-	linker	UNP P19491
C	242	SER	ASN	engineered mutation	UNP P19491
D	1	GLY	-	cloning artifact	UNP P19491
D	2	ALA	-	cloning artifact	UNP P19491
D	94	TYR	LEU	engineered mutation	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	118	GLY	-	linker	UNP P19491
D	119	THR	-	linker	UNP P19491
D	242	SER	ASN	engineered mutation	UNP P19491

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



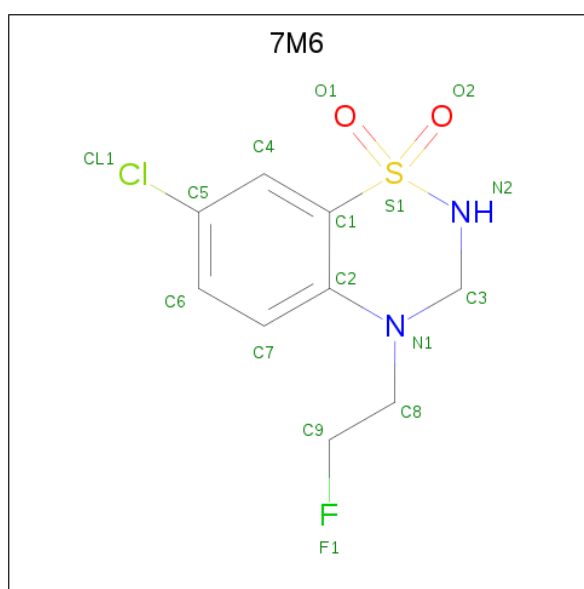
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

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

- Molecule 3 is 7-chloro-4-(2-fluoroethyl)-2,3-dihydro-1,2,4-benzothiadiazine 1,1-dioxide (three-letter code: 7M6) (formula: C₉H₁₀ClFN₂O₂S).

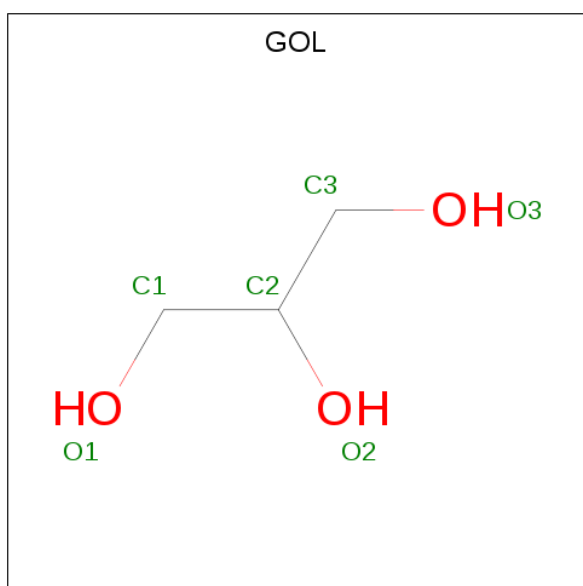


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	S	0	0
			16	9	1	1	2	2	1		
3	B	1	Total	C	Cl	F	N	O	S	0	0
			16	9	1	1	2	2	1		
3	C	1	Total	C	Cl	F	N	O	S	0	0
			16	9	1	1	2	2	1		
3	D	1	Total	C	Cl	F	N	O	S	0	0
			16	9	1	1	2	2	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

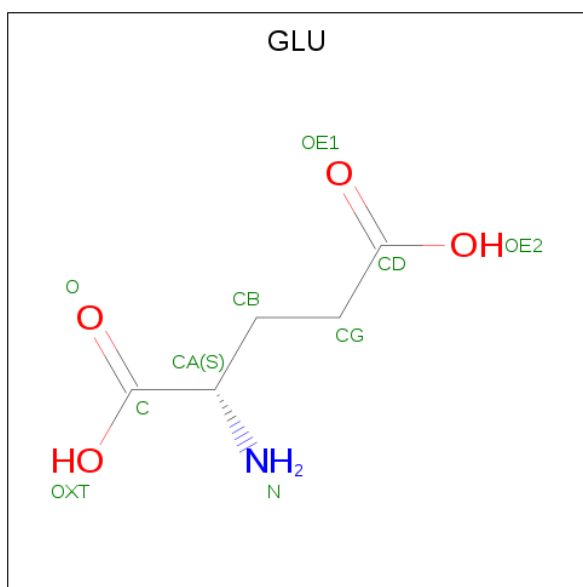
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	3	Total Cl 3 3	0	0
4	D	2	Total Cl 2 2	0	0
4	C	1	Total Cl 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



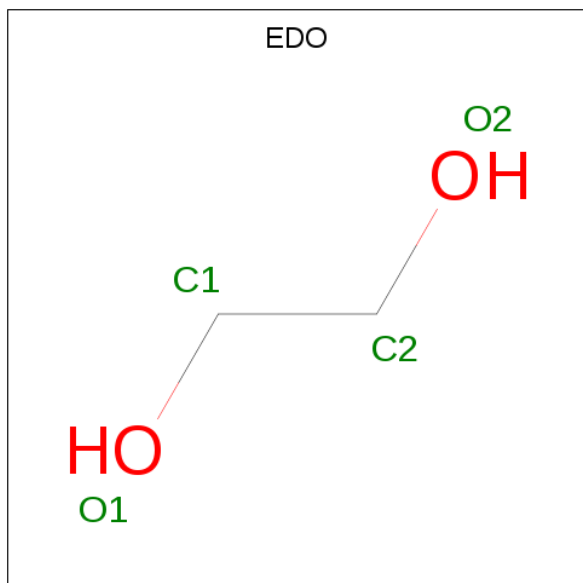
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

- Molecule 6 is GLUTAMIC ACID (three-letter code: GLU) (formula: C₅H₉NO₄).



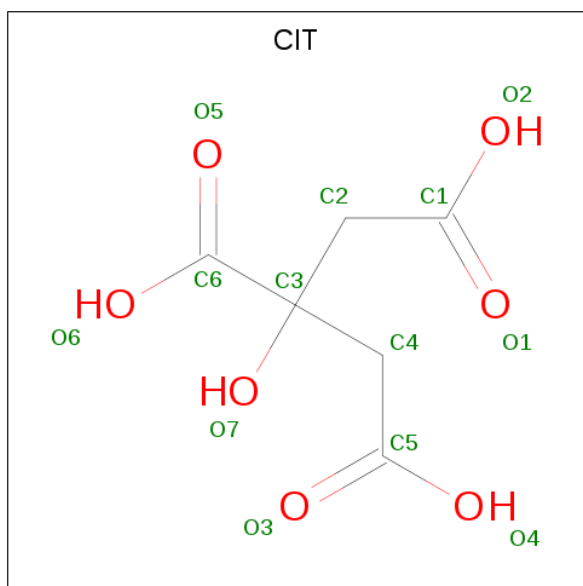
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	10	5	1	4	0	0
6	B	1	10	5	1	4	0	0
6	C	1	10	5	1	4	0	0
6	D	1	10	5	1	4	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



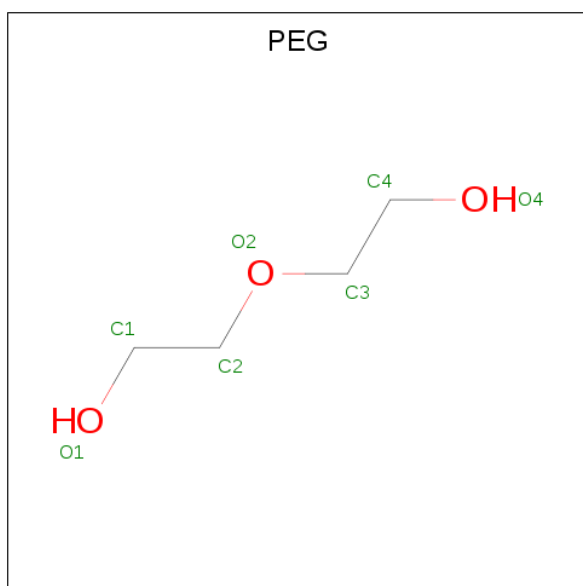
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	311	Total	O	0	7
			316	316		
10	B	245	Total	O	0	9
			253	253		
10	C	323	Total	O	0	11
			331	331		
10	D	281	Total	O	0	7
			286	286		

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: Glutamate receptor 2,Glutamate receptor 2

Chain A:  99%



- Molecule 1: Glutamate receptor 2,Glutamate receptor 2

Chain B:  98%



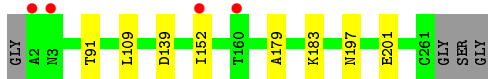
- Molecule 1: Glutamate receptor 2,Glutamate receptor 2

Chain C:  98%



- Molecule 1: Glutamate receptor 2,Glutamate receptor 2

Chain D:  95%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.31Å 98.41Å 121.79Å 90.00° 90.53° 90.00°	Depositor
Resolution (Å)	49.20 – 1.78 49.20 – 1.78	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.20-1.78) 97.4 (49.20-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 1.78Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.153 , 0.179 0.165 , 0.189	Depositor DCC
R_{free} test set	5325 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtrriage
Anisotropy	0.348	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.317 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9878	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.0670e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, CL, EDO, 7M6, SO4, CIT, PEG

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	0/2233	0.52	0/2999
1	B	0.32	0/2166	0.51	0/2911
1	C	0.34	0/2221	0.52	0/2983
1	D	0.32	0/2133	0.50	0/2869
All	All	0.33	0/8753	0.51	0/11762

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	2141	0	2241	1	0
1	B	2099	0	2158	3	0
1	C	2141	0	2221	2	0
1	D	2072	0	2123	5	0
2	A	20	0	0	0	0
2	B	10	0	0	0	0
2	C	30	0	0	0	0
2	D	20	0	0	0	0
3	A	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	0	0	0
3	C	16	0	0	0	0
3	D	16	0	0	0	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	A	12	0	16	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
6	A	10	0	5	1	0
6	B	10	0	5	1	0
6	C	10	0	5	0	0
6	D	10	0	5	1	0
7	B	4	0	6	0	0
8	C	13	0	5	0	0
9	C	7	0	10	1	0
10	A	316	0	0	0	0
10	B	253	0	0	0	0
10	C	331	0	0	0	0
10	D	286	0	0	1	0
All	All	9878	0	8816	10	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 1.

All (10) 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:183:LYS:NZ	10:D:404:HOH:O	2.31	0.62
1:D:197:ASN:O	1:D:201[A]:GLU:HG2	2.11	0.51
1:B:204:LYS:HG3	1:B:260:GLU:HB3	1.97	0.47
1:D:152:ILE:N	1:D:152:ILE:HD12	2.32	0.45
1:A:91:THR:HG1	6:A:310:GLU:N	2.15	0.45
1:B:91:THR:HG1	6:B:307:GLU:N	2.16	0.44
1:C:31:ARG:HH12	9:C:311:PEG:H42	1.83	0.43
1:D:179:ALA:O	1:D:183:LYS:HD3	2.18	0.43
1:B:253:LYS:HD3	1:C:24:GLU:OE2	2.20	0.40
1:D:91:THR:HG1	6:D:308:GLU:N	2.19	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	279/264 (106%)	277 (99%)	2 (1%)	0	100	100
1	B	272/264 (103%)	270 (99%)	2 (1%)	0	100	100
1	C	277/264 (105%)	274 (99%)	3 (1%)	0	100	100
1	D	266/264 (101%)	264 (99%)	2 (1%)	0	100	100
All	All	1094/1056 (104%)	1085 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	237/219 (108%)	236 (100%)	1 (0%)	91	88
1	B	229/219 (105%)	227 (99%)	2 (1%)	78	72
1	C	235/219 (107%)	234 (100%)	1 (0%)	91	88
1	D	226/219 (103%)	224 (99%)	2 (1%)	78	72
All	All	927/876 (106%)	921 (99%)	6 (1%)	84	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	LEU
1	B	109	LEU

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Mol	Chain	Res	Type
1	B	203	ARG
1	C	109	LEU
1	D	109	LEU
1	D	139	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 38 ligands modelled in this entry, 7 are monoatomic - leaving 31 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	$\# Z > 2$
2	SO4	A	301	-	4,4,4	0.15	0	6,6,6	0.23	0
2	SO4	C	302	-	4,4,4	0.12	0	6,6,6	0.11	0
5	GOL	C	310	-	5,5,5	0.38	0	5,5,5	0.27	0
2	SO4	D	302	-	4,4,4	0.15	0	6,6,6	0.07	0
3	7M6	B	304	-	16,17,17	2.06	4 (25%)	21,25,25	3.07	6 (28%)
5	GOL	B	306	-	5,5,5	0.46	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	303	-	4,4,4	0.12	0	6,6,6	0.11	0
2	SO4	C	306	-	4,4,4	0.28	0	6,6,6	0.25	0
3	7M6	A	305	-	16,17,17	1.99	3 (18%)	21,25,25	3.11	7 (33%)
2	SO4	C	301	-	4,4,4	0.14	0	6,6,6	0.22	0
3	7M6	D	305	-	16,17,17	2.19	5 (31%)	21,25,25	3.37	6 (28%)
5	GOL	A	309	-	5,5,5	0.36	0	5,5,5	0.17	0
8	CIT	C	309	-	3,12,12	1.19	0	3,17,17	1.80	1 (33%)
2	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	C	305	-	4,4,4	0.14	0	6,6,6	0.07	0
5	GOL	A	311	-	5,5,5	0.37	0	5,5,5	0.24	0
2	SO4	D	304	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	B	303	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	304	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.14	0
9	PEG	C	311	-	6,6,6	0.44	0	5,5,5	0.50	0
3	7M6	C	307	-	16,17,17	2.11	5 (31%)	21,25,25	2.78	4 (19%)
2	SO4	C	304	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	A	303	-	4,4,4	0.14	0	6,6,6	0.05	0
7	EDO	B	301	-	3,3,3	0.44	0	2,2,2	0.30	0
2	SO4	A	302	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	D	301	-	4,4,4	0.13	0	6,6,6	0.07	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
3	7M6	B	304	-	-	0/3/19/19	0/2/2/2
3	7M6	D	305	-	-	0/3/19/19	0/2/2/2
5	GOL	C	310	-	-	2/4/4/4	-
7	EDO	B	301	-	-	1/1/1/1	-
3	7M6	C	307	-	-	0/3/19/19	0/2/2/2
5	GOL	A	311	-	-	4/4/4/4	-
5	GOL	B	306	-	-	3/4/4/4	-
9	PEG	C	311	-	-	0/4/4/4	-
8	CIT	C	309	-	-	1/6/16/16	-
5	GOL	A	309	-	-	1/4/4/4	-
3	7M6	A	305	-	-	0/3/19/19	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	305	7M6	S1-N2	5.88	1.70	1.63
3	B	304	7M6	S1-N2	5.88	1.70	1.63
3	A	305	7M6	S1-N2	5.36	1.70	1.63
3	C	307	7M6	S1-N2	5.05	1.69	1.63
3	A	305	7M6	O1-S1	3.44	1.47	1.43
3	C	307	7M6	O1-S1	3.32	1.47	1.43
3	D	305	7M6	O1-S1	3.29	1.47	1.43
3	C	307	7M6	O2-S1	3.28	1.47	1.43
3	B	304	7M6	O2-S1	2.71	1.46	1.43
3	A	305	7M6	O2-S1	2.70	1.46	1.43
3	D	305	7M6	O2-S1	2.65	1.46	1.43
3	D	305	7M6	C2-C1	2.62	1.43	1.40
3	B	304	7M6	O1-S1	2.49	1.46	1.43
3	C	307	7M6	C2-C1	2.41	1.43	1.40
3	C	307	7M6	C1-S1	2.23	1.77	1.75
3	D	305	7M6	C1-S1	2.11	1.77	1.75
3	B	304	7M6	C2-C1	2.01	1.42	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	305	7M6	C3-N1-C2	11.81	123.74	110.68
3	B	304	7M6	C3-N1-C2	11.30	123.18	110.68
3	D	305	7M6	C3-N1-C2	11.12	122.98	110.68
3	C	307	7M6	C3-N1-C2	10.52	122.31	110.68
3	D	305	7M6	O1-S1-N2	6.98	114.43	107.92
3	D	305	7M6	C1-S1-N2	-5.52	98.00	102.37
3	C	307	7M6	C1-S1-N2	-4.48	98.82	102.37
3	B	304	7M6	C1-S1-N2	-4.25	99.00	102.37
3	B	304	7M6	O2-S1-N2	-3.90	104.29	107.92
3	A	305	7M6	C1-S1-N2	-3.85	99.32	102.37
3	D	305	7M6	O2-S1-N2	-3.27	104.88	107.92
3	A	305	7M6	O2-S1-O1	3.20	121.73	118.46
3	B	304	7M6	O1-S1-N2	3.12	110.83	107.92
3	D	305	7M6	C4-C1-S1	-3.06	117.31	119.82
3	C	307	7M6	O2-S1-N2	-3.00	105.13	107.92
3	B	304	7M6	O2-S1-C1	2.84	112.79	109.29
3	A	305	7M6	C4-C1-S1	-2.82	117.50	119.82
3	A	305	7M6	O1-S1-C1	-2.65	106.02	109.29
3	B	304	7M6	C4-C1-S1	-2.46	117.80	119.82
3	A	305	7M6	C7-C2-N1	2.34	122.00	118.87
3	A	305	7M6	O1-S1-N2	2.31	110.07	107.92
8	C	309	CIT	C3-C2-C1	-2.06	111.69	114.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	307	7M6	O2-S1-O1	2.05	120.55	118.46
3	D	305	7M6	O2-S1-C1	2.00	111.77	109.29

There are no chirality outliers.

All (12) torsion outliers are listed below:

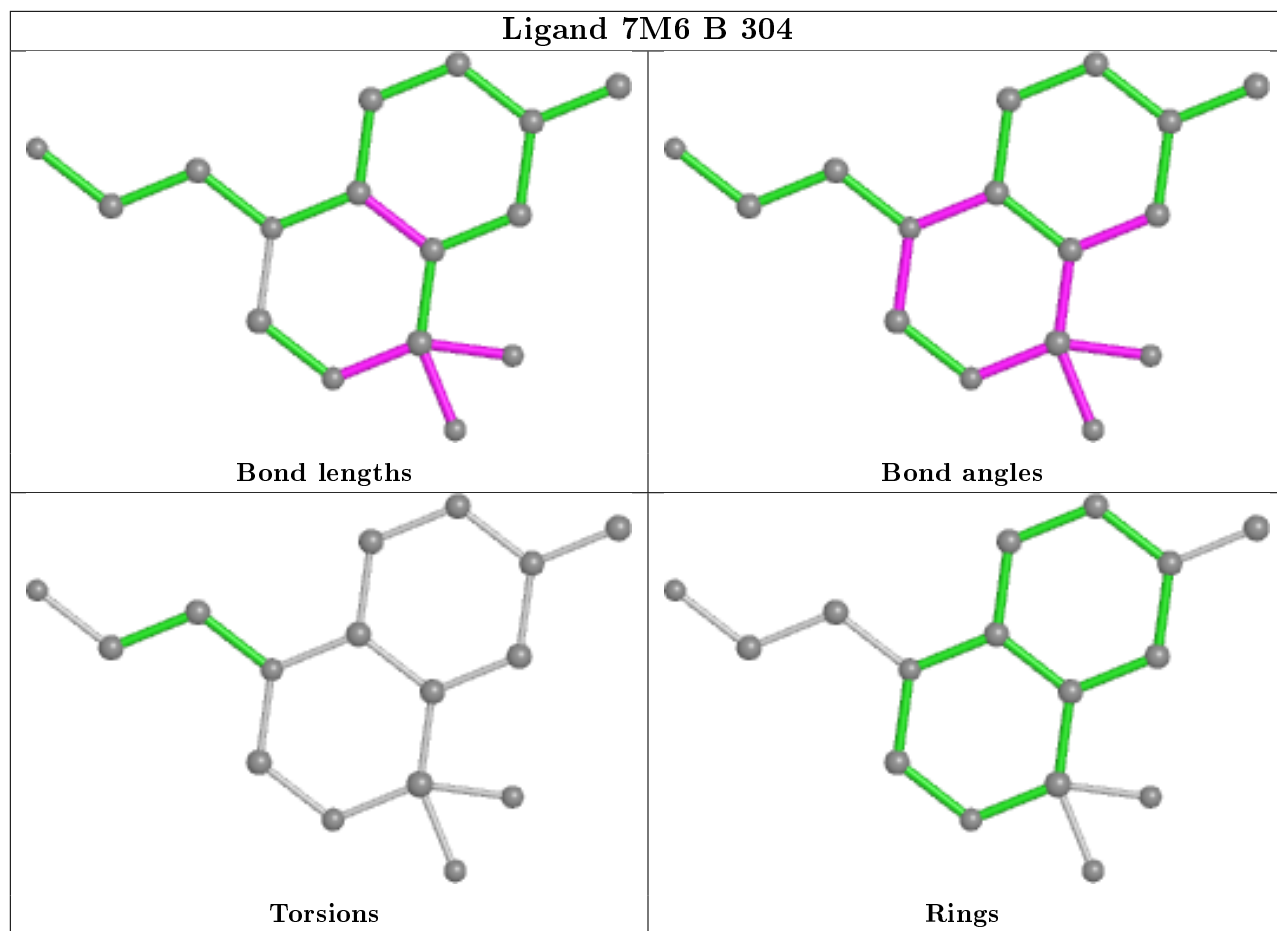
Mol	Chain	Res	Type	Atoms
5	A	311	GOL	C1-C2-C3-O3
5	C	310	GOL	O1-C1-C2-C3
5	B	306	GOL	O1-C1-C2-C3
5	B	306	GOL	C1-C2-C3-O3
5	A	309	GOL	O1-C1-C2-C3
5	A	311	GOL	O1-C1-C2-C3
7	B	301	EDO	O1-C1-C2-O2
5	B	306	GOL	O2-C2-C3-O3
8	C	309	CIT	C1-C2-C3-O7
5	A	311	GOL	O2-C2-C3-O3
5	A	311	GOL	O1-C1-C2-O2
5	C	310	GOL	O1-C1-C2-O2

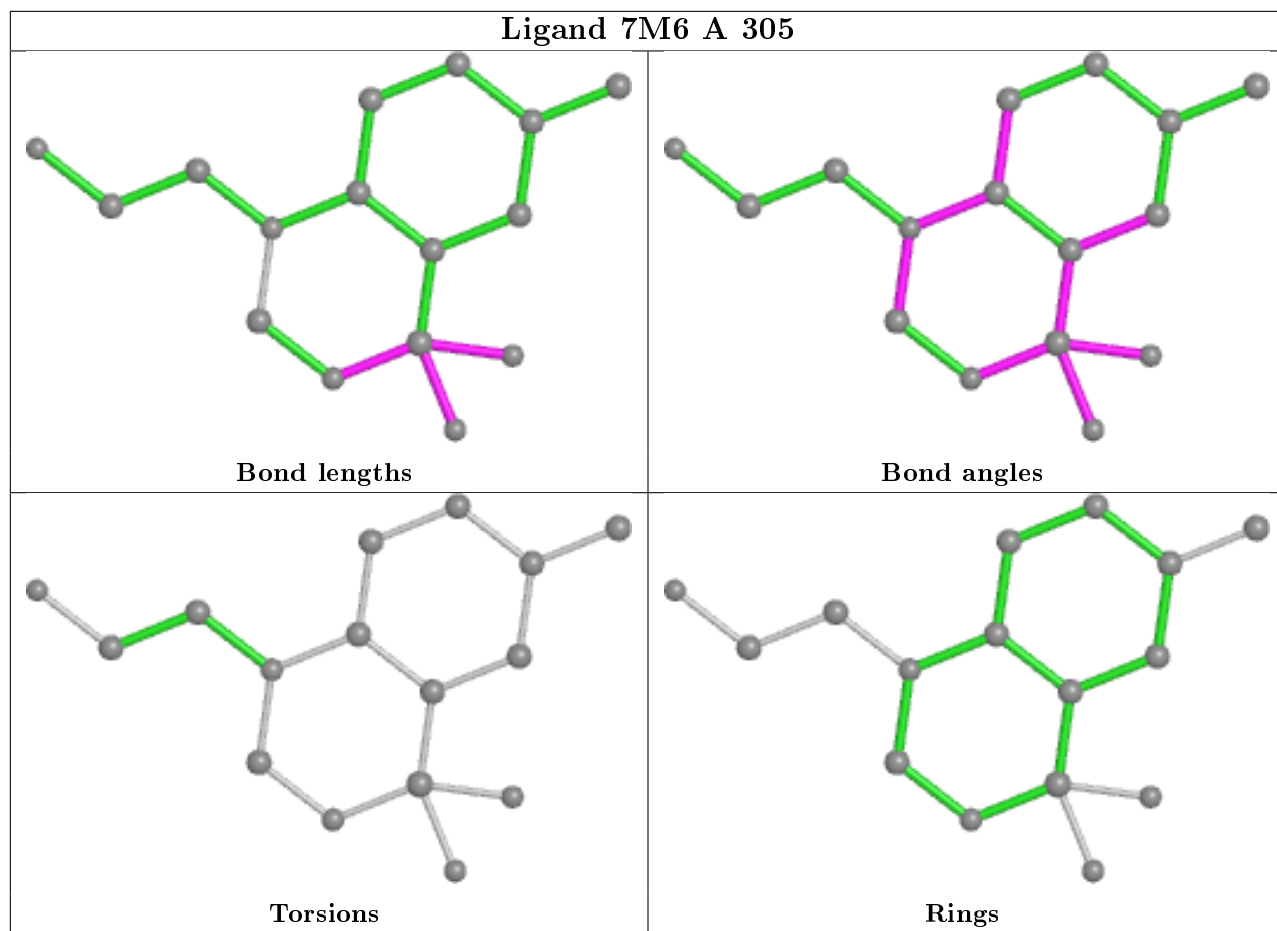
There are no ring outliers.

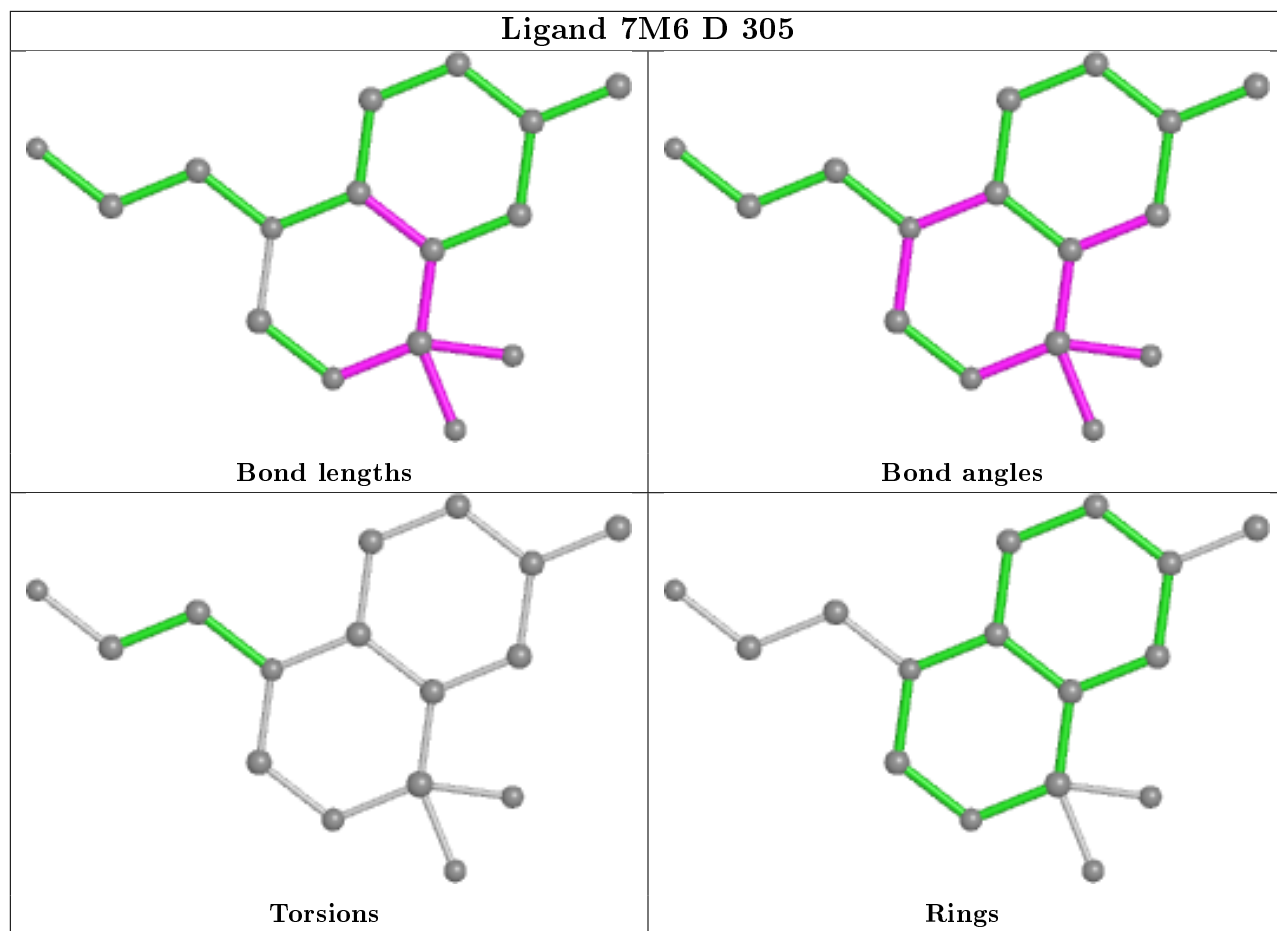
1 monomer is involved in 1 short contact:

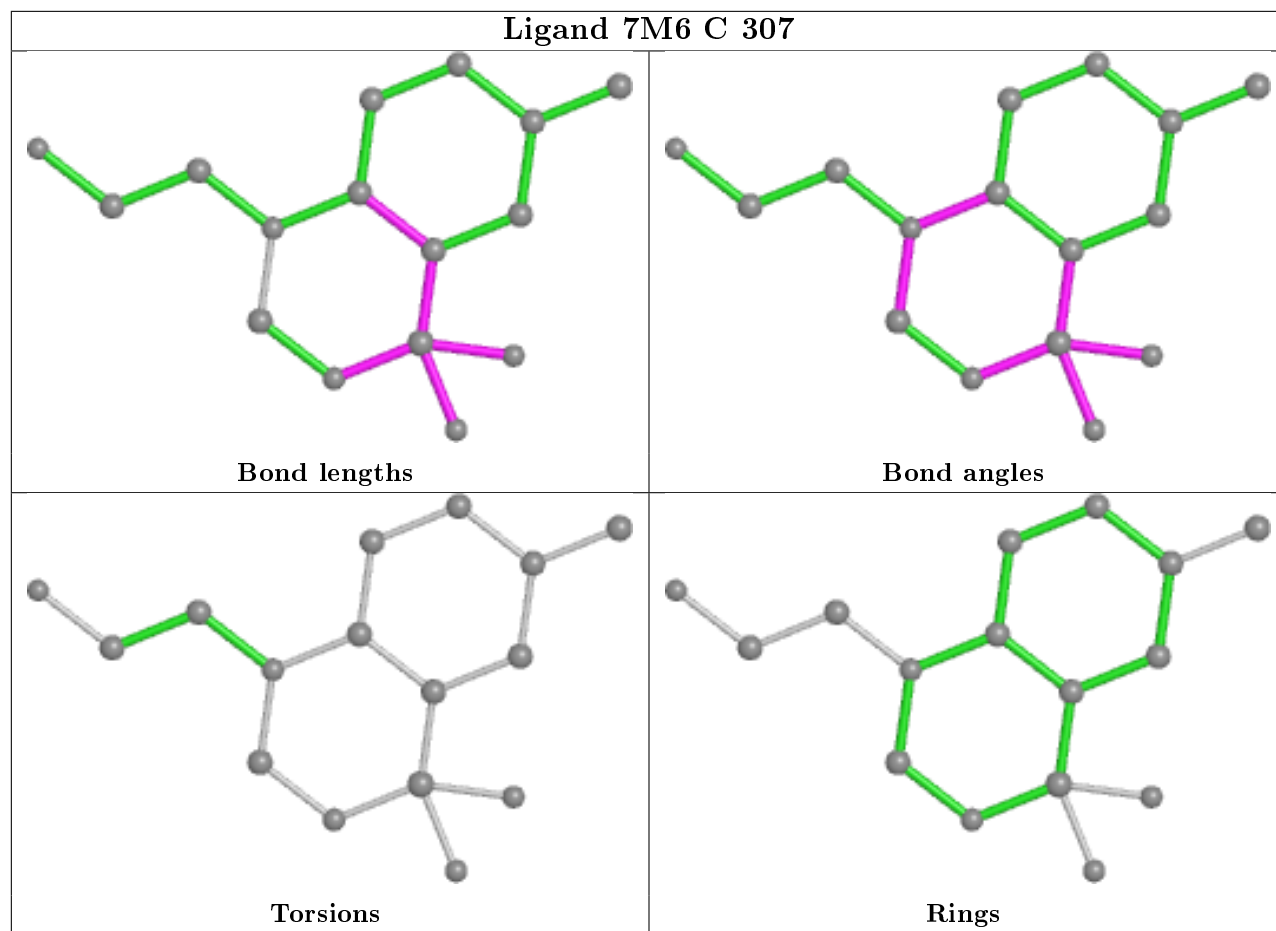
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	311	PEG	1	0

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









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	263/264 (99%)	-0.51	0	100 100	9, 15, 33, 49	0
1	B	264/264 (100%)	-0.18	0	100 100	10, 22, 46, 57	0
1	C	263/264 (99%)	-0.52	0	100 100	8, 14, 32, 52	1 (0%)
1	D	260/264 (98%)	-0.22	4 (1%)	73 73	9, 21, 47, 65	0
All	All	1050/1056 (99%)	-0.36	4 (0%)	92 92	8, 18, 42, 65	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	ASN	2.5
1	D	160	THR	2.2
1	D	2	ALA	2.1
1	D	152	ILE	2.1

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](#)

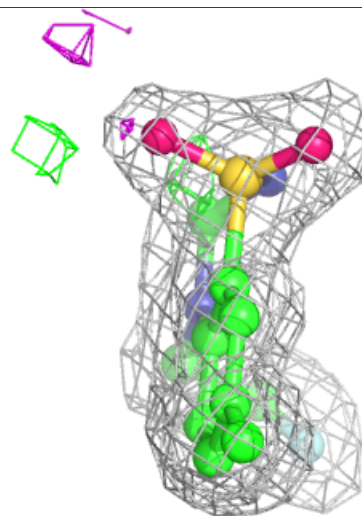
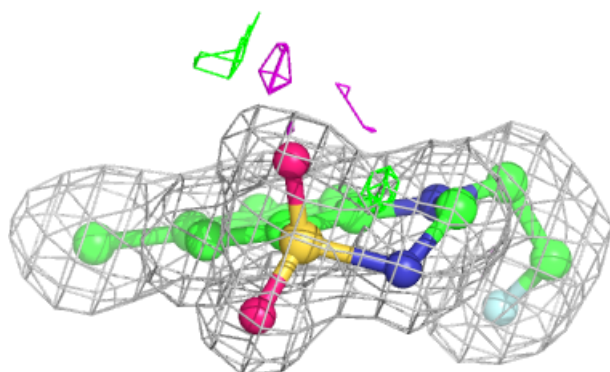
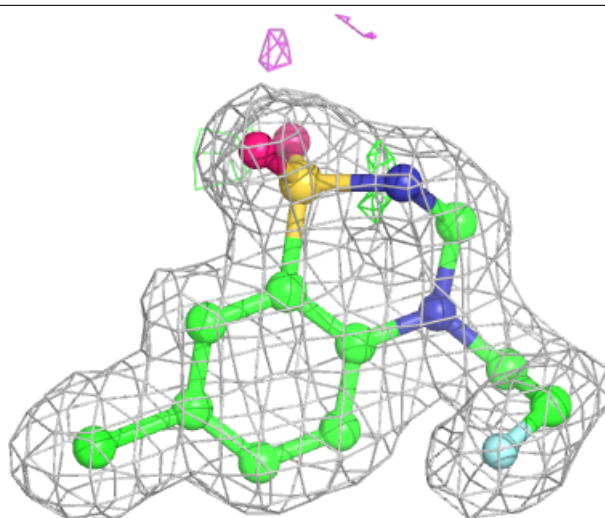
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	PEG	C	311	7/7	0.67	0.17	42,47,49,49	0
5	GOL	B	306	6/6	0.68	0.21	46,48,49,51	0
5	GOL	A	311	6/6	0.69	0.15	43,48,52,58	0
4	CL	D	306	1/1	0.74	0.10	59,59,59,59	0
2	SO4	A	303	5/5	0.77	0.18	111,111,111,112	0
2	SO4	A	304	5/5	0.78	0.21	86,86,87,89	0
5	GOL	A	309	6/6	0.78	0.28	53,54,55,56	0
5	GOL	C	310	6/6	0.78	0.18	38,40,45,47	0
7	EDO	B	301	4/4	0.78	0.14	44,45,45,46	0
2	SO4	B	303	5/5	0.79	0.20	78,80,81,82	0
2	SO4	C	305	5/5	0.84	0.19	78,83,85,85	0
2	SO4	C	303	5/5	0.87	0.15	80,81,82,82	0
4	CL	C	308	1/1	0.87	0.09	44,44,44,44	0
2	SO4	A	302	5/5	0.87	0.16	80,81,81,82	0
2	SO4	D	304	5/5	0.88	0.15	81,83,84,84	0
4	CL	A	307	1/1	0.89	0.14	64,64,64,64	0
2	SO4	D	303	5/5	0.91	0.16	50,52,53,58	5
4	CL	D	307	1/1	0.93	0.09	53,53,53,53	0
8	CIT	C	309	13/13	0.94	0.12	22,29,32,34	0
2	SO4	C	306	5/5	0.94	0.11	19,26,30,32	5
2	SO4	C	302	5/5	0.94	0.10	42,43,49,50	0
4	CL	A	308	1/1	0.96	0.15	53,53,53,53	0
2	SO4	C	304	5/5	0.96	0.10	33,35,39,40	5
2	SO4	B	302	5/5	0.96	0.10	31,33,34,35	5
2	SO4	D	301	5/5	0.96	0.11	50,51,54,58	0
2	SO4	D	302	5/5	0.97	0.12	52,53,54,57	0
6	GLU	D	308	10/10	0.97	0.06	11,12,13,14	0
4	CL	B	305	1/1	0.97	0.05	50,50,50,50	0
6	GLU	A	310	10/10	0.98	0.05	9,11,12,12	0
3	7M6	C	307	16/16	0.98	0.07	11,14,20,22	0
6	GLU	B	307	10/10	0.98	0.06	10,12,14,15	0
3	7M6	B	304	16/16	0.98	0.07	10,13,21,23	0
4	CL	A	306	1/1	0.98	0.06	43,43,43,43	0
6	GLU	C	312	10/10	0.98	0.06	8,9,11,12	0
3	7M6	A	305	16/16	0.98	0.06	11,13,18,20	0
3	7M6	D	305	16/16	0.98	0.08	9,13,19,20	0
2	SO4	C	301	5/5	0.99	0.06	18,18,20,20	0
2	SO4	A	301	5/5	0.99	0.06	21,21,22,23	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.

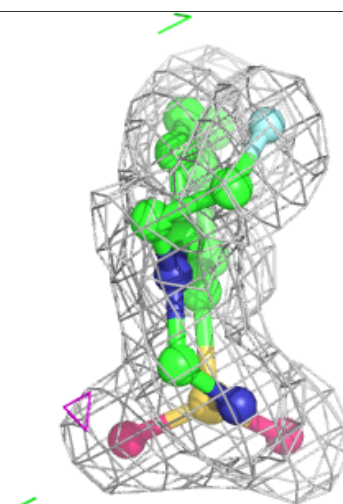
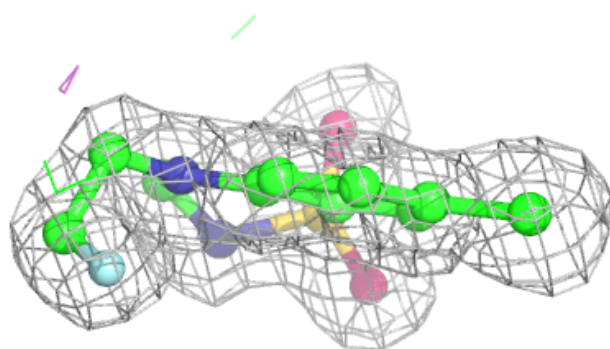
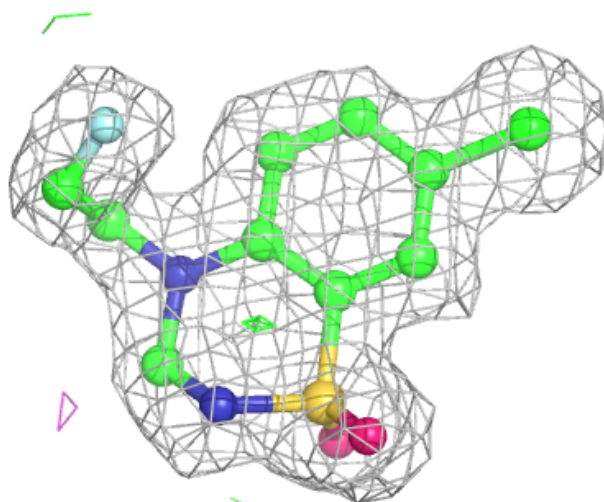
Electron density around 7M6 C 307:

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



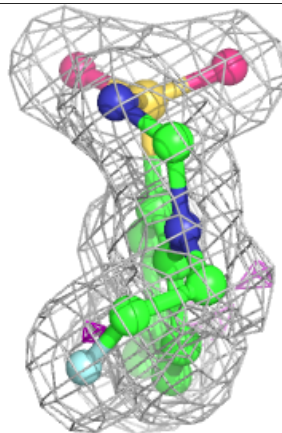
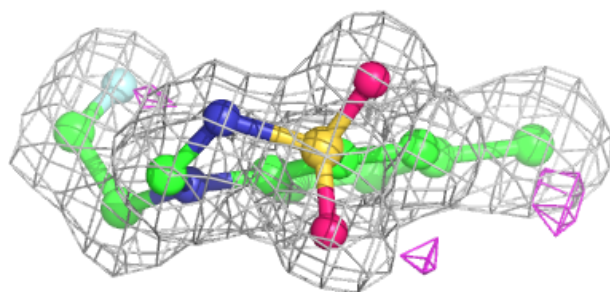
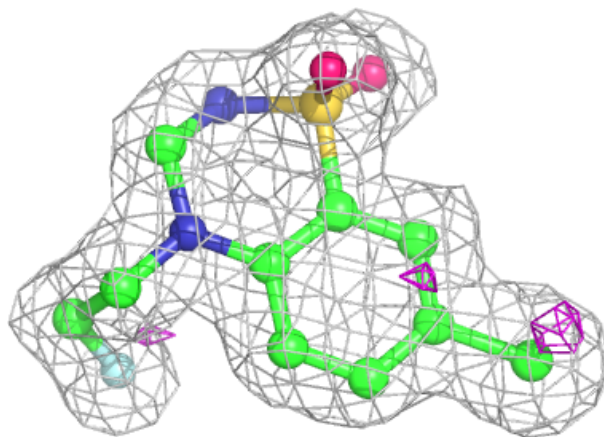
Electron density around 7M6 B 304:

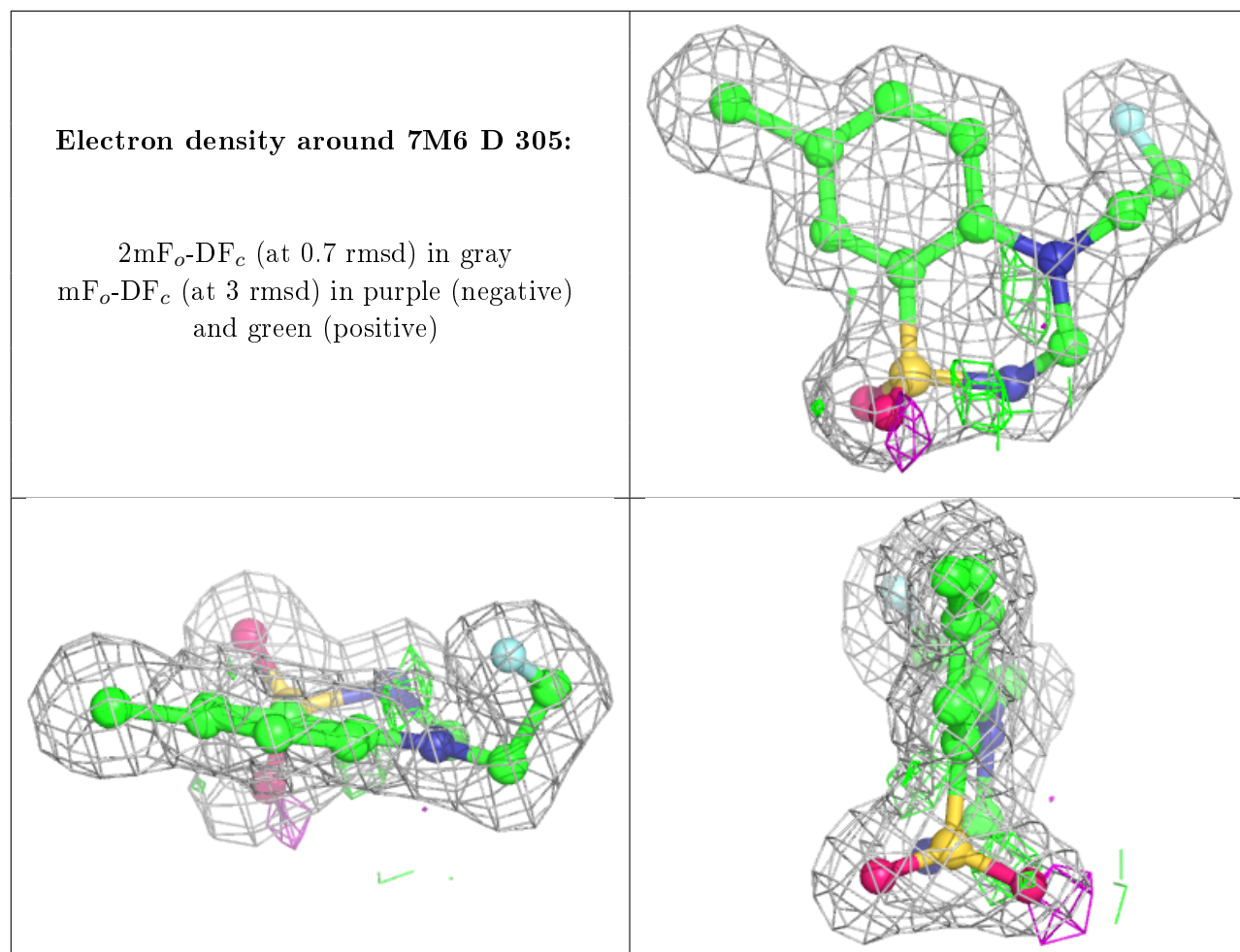
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 7M6 A 305:

$2mF_o-DF_c$ (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.