



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2022 – 01:29 pm BST

PDB ID : 7NBF
Title : Crystal structure of human serine racemase in complex with DSiP fragment
Z126932614, XChem fragment screen.
Authors : Koulouris, C.R.; Roe, S.M.
Deposited on : 2021-01-26
Resolution : 1.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28

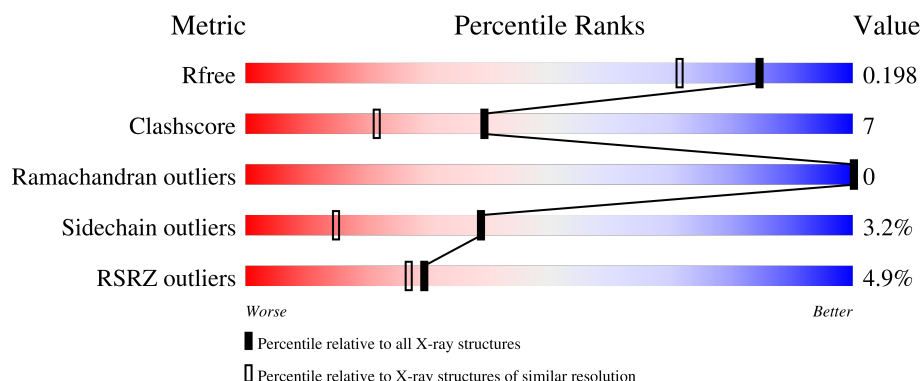
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	AAA	346	<div> <div>3%</div> <div>82%</div> <div>12%</div> <div>7%</div> </div>
1	BBB	346	<div> <div>9%</div> <div>78%</div> <div>11%</div> <div>10%</div> </div>
1	CCC	346	<div> <div>3%</div> <div>85%</div> <div>8%</div> <div>7%</div> </div>
1	DDD	346	<div> <div>3%</div> <div>79%</div> <div>11%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	PGE	CCC	407[A]	-	-	X	-
3	GOL	AAA	403[A]	-	-	X	-
3	GOL	BBB	402	-	-	X	-
3	GOL	CCC	402[B]	-	-	X	-
3	GOL	CCC	405[A]	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 11331 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 Serine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	323	Total	C	N	O	S	0	30	0
			2656	1683	442	519	12			
1	BBB	312	Total	C	N	O	S	0	16	0
			2418	1538	400	469	11			
1	CCC	323	Total	C	N	O	S	0	20	1
			2551	1622	425	492	12			
1	DDD	317	Total	C	N	O	S	0	21	0
			2526	1603	430	480	13			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	2	ASP	CYS	engineered mutation	UNP Q9GZT4
AAA	6	ASP	CYS	engineered mutation	UNP Q9GZT4
AAA	341	HIS	-	expression tag	UNP Q9GZT4
AAA	342	HIS	-	expression tag	UNP Q9GZT4
AAA	343	HIS	-	expression tag	UNP Q9GZT4
AAA	344	HIS	-	expression tag	UNP Q9GZT4
AAA	345	HIS	-	expression tag	UNP Q9GZT4
AAA	346	HIS	-	expression tag	UNP Q9GZT4
BBB	2	ASP	CYS	engineered mutation	UNP Q9GZT4
BBB	6	ASP	CYS	engineered mutation	UNP Q9GZT4
BBB	341	HIS	-	expression tag	UNP Q9GZT4
BBB	342	HIS	-	expression tag	UNP Q9GZT4
BBB	343	HIS	-	expression tag	UNP Q9GZT4
BBB	344	HIS	-	expression tag	UNP Q9GZT4
BBB	345	HIS	-	expression tag	UNP Q9GZT4
BBB	346	HIS	-	expression tag	UNP Q9GZT4
CCC	2	ASP	CYS	engineered mutation	UNP Q9GZT4
CCC	6	ASP	CYS	engineered mutation	UNP Q9GZT4
CCC	341	HIS	-	expression tag	UNP Q9GZT4
CCC	342	HIS	-	expression tag	UNP Q9GZT4
CCC	343	HIS	-	expression tag	UNP Q9GZT4

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	344	HIS	-	expression tag	UNP Q9GZT4
CCC	345	HIS	-	expression tag	UNP Q9GZT4
CCC	346	HIS	-	expression tag	UNP Q9GZT4
DDD	2	ASP	CYS	engineered mutation	UNP Q9GZT4
DDD	6	ASP	CYS	engineered mutation	UNP Q9GZT4
DDD	341	HIS	-	expression tag	UNP Q9GZT4
DDD	342	HIS	-	expression tag	UNP Q9GZT4
DDD	343	HIS	-	expression tag	UNP Q9GZT4
DDD	344	HIS	-	expression tag	UNP Q9GZT4
DDD	345	HIS	-	expression tag	UNP Q9GZT4
DDD	346	HIS	-	expression tag	UNP Q9GZT4

- PLP
-
- The diagram shows the chemical structure of PLP (Pyridoxal phosphate). It consists of a pyridine ring with a nitrogen atom (N1) at the top. The ring is substituted with a hydroxyl group (OH) at C3, an aldehyde group (CHO) at C4, and a phosphate group (PO₃H₂) at C5. The phosphate group is shown as a phosphorus atom (P) bonded to four oxygen atoms: one double-bonded (O1P), and three single-bonded (O2P, O3P, O4P). The aldehyde group is shown as a carbon atom (C4A) double-bonded to an oxygen atom (O4A) and single-bonded to a hydrogen atom (H4A). The hydroxyl group is shown as an oxygen atom (O3) single-bonded to a hydrogen atom (H3).

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	AAA	1	Total	C	O	0	1
			12	6	6		
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	AAA	1	Total	C	O	0	0
			6	3	3		
3	BBB	1	Total	C	O	0	0
			6	3	3		
3	BBB	1	Total	C	O	0	0
			6	3	3		
3	CCC	1	Total	C	O	0	1
			12	6	6		
3	CCC	1	Total	C	O	0	1
			6	3	3		
3	CCC	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	2	Total	Ca	0	0
			2	2		
4	BBB	2	Total	Ca	0	0
			2	2		
4	CCC	1	Total	Ca	0	1
			2	2		

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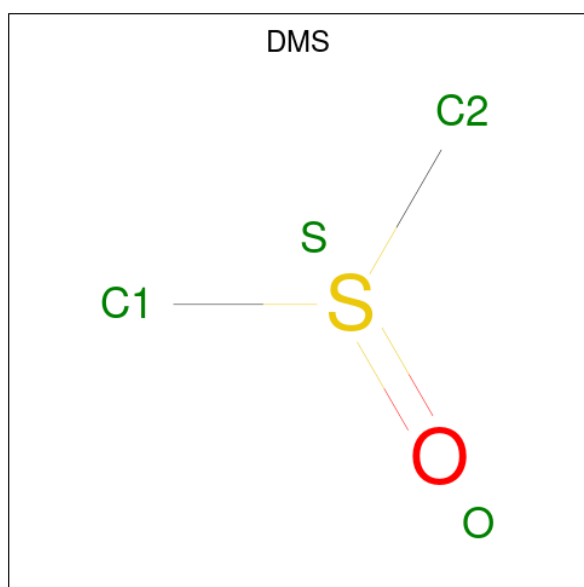
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	DDD	1	Total	Ca	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

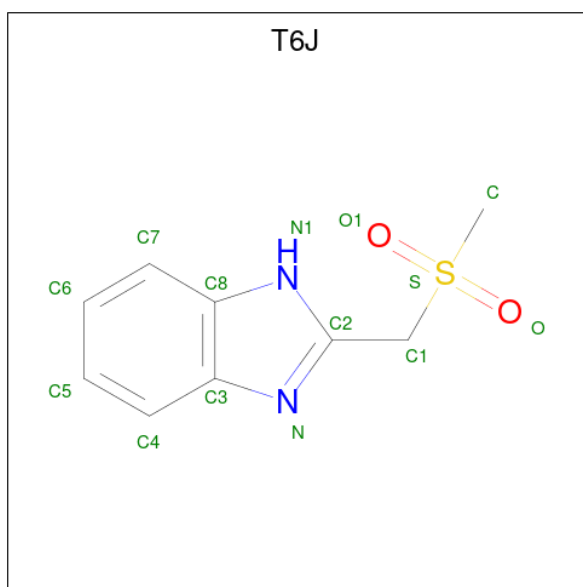
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	1	Total	Mg	0	0
			1	1		
5	DDD	1	Total	Mg	0	0
			1	1		

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is 2-[(methylsulfonyl)methyl]-1H-benzimidazole (three-letter code: T6J) (formula: C₉H₁₀N₂O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	AAA	1	Total	C	N	O	S	0	1
			14	9	2	2	1		
7	BBB	1	Total	C	N	O	S	0	0
			14	9	2	2	1		
7	CCC	1	Total	C	N	O	S	0	1
			14	9	2	2	1		
7	DDD	1	Total	C	N	O	S	0	1
			14	9	2	2	1		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

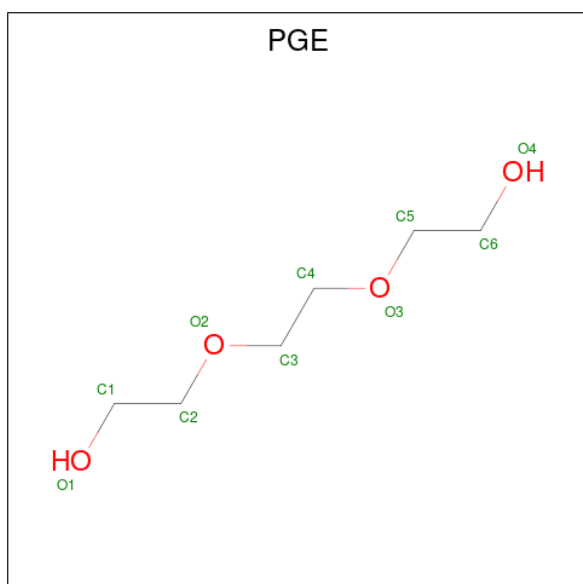
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	1	Total	Na	0	0
			1	1		
8	BBB	1	Total	Na	0	0
			1	1		
8	DDD	2	Total	Na	0	0
			2	2		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	BBB	1	Total	C	O	0	0
			4	2	2		
9	CCC	1	Total	C	O	0	0
			4	2	2		
9	DDD	1	Total	C	O	0	0
			4	2	2		
9	DDD	1	Total	C	O	0	1
			8	4	4		
9	DDD	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	CCC	1	Total	C	O	0	1
			10	6	4		

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	CCC	1	Total	Cl	0	0
			1	1		
11	DDD	1	Total	Cl	0	1
			2	2		

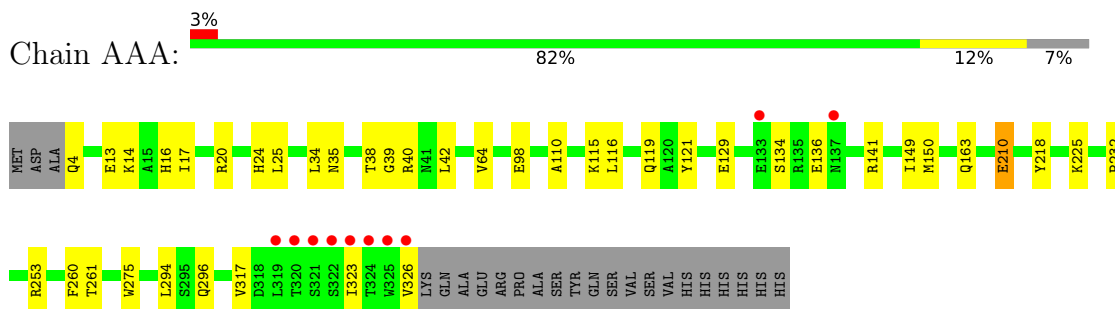
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	AAA	285	Total	O	0	5
			288	288		
12	BBB	162	Total	O	0	1
			162	162		
12	CCC	223	Total	O	0	5
			226	226		
12	DDD	250	Total	O	0	4
			253	253		

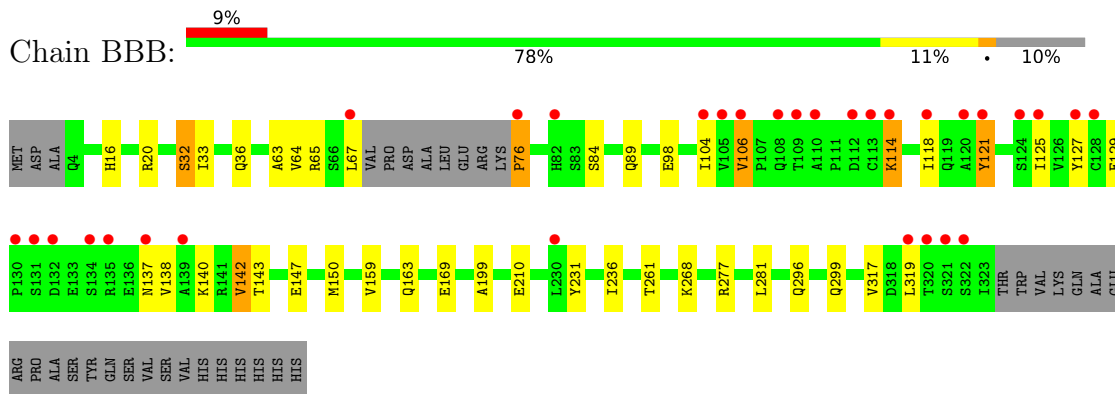
3 Residue-property plots

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.

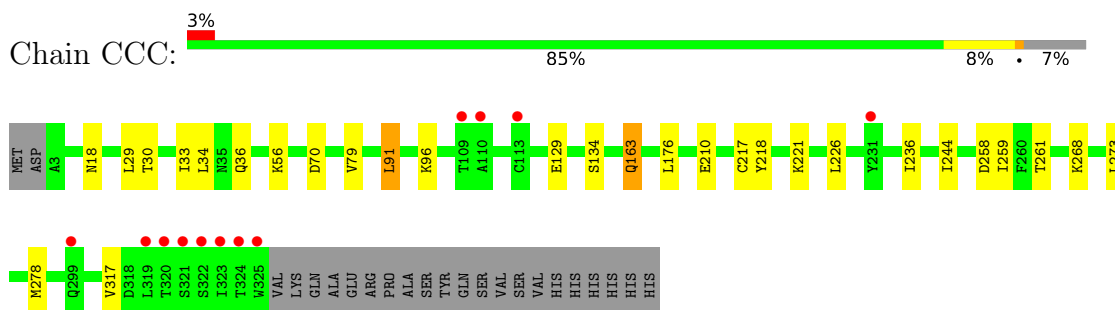
- Molecule 1: Serine racemase



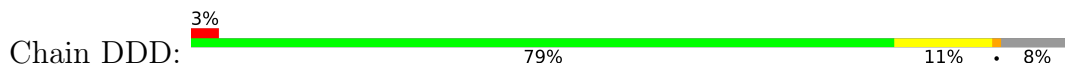
- Molecule 1: Serine racemase

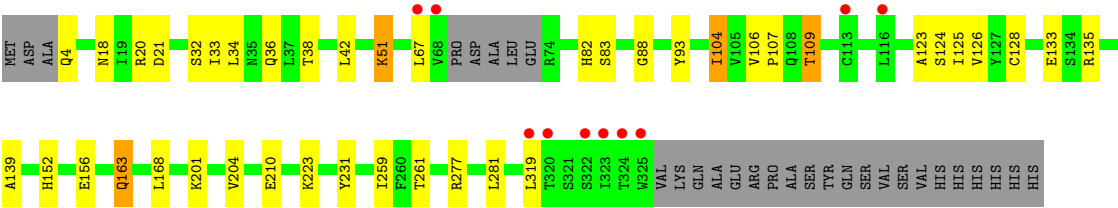


- Molecule 1: Serine racemase



- Molecule 1: Serine racemase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.11Å 154.94Å 85.54Å 90.00° 97.96° 90.00°	Depositor
Resolution (Å)	84.70 – 1.60 84.72 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (84.70-1.60) 97.5 (84.72-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.172 , 0.198 0.172 , 0.198	Depositor DCC
R_{free} test set	7962 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11331	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.66% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NA, CL, PLP, PGE, DMS, T6J, MG, EDO, GOL

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	AAA	0.68	1/2702 (0.0%)	0.98	1/3684 (0.0%)
1	BBB	0.57	1/2459 (0.0%)	0.88	1/3357 (0.0%)
1	CCC	0.59	0/2597	0.88	5/3548 (0.1%)
1	DDD	0.64	0/2570	0.91	2/3505 (0.1%)
All	All	0.63	2/10328 (0.0%)	0.91	9/14094 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	210	GLU	CD-OE2	-6.75	1.18	1.25
1	BBB	169	GLU	CD-OE2	5.34	1.31	1.25

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	20	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	CCC	163	GLN	CB-CG-CD	5.56	126.06	111.60
1	CCC	36[A]	GLN	CB-CG-CD	5.49	125.88	111.60
1	CCC	36[B]	GLN	CB-CG-CD	5.49	125.88	111.60
1	BBB	65	ARG	NE-CZ-NH2	-5.42	117.59	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	AAA	2656	0	2637	30	1
1	BBB	2418	0	2381	34	0
1	CCC	2551	0	2534	39	0
1	DDD	2526	0	2511	45	1
2	AAA	30	0	12	0	0
2	BBB	15	0	6	0	0
2	CCC	15	0	6	1	0
2	DDD	15	0	6	0	0
3	AAA	30	0	40	10	0
3	BBB	12	0	16	5	0
3	CCC	24	0	32	13	0
4	AAA	2	0	0	0	0
4	BBB	2	0	0	0	0
4	CCC	2	0	0	0	0
4	DDD	1	0	0	0	0
5	AAA	1	0	0	0	0
5	DDD	1	0	0	0	0
6	AAA	4	0	6	0	0
7	AAA	14	0	0	1	0
7	BBB	14	0	0	0	0
7	CCC	14	0	0	0	0
7	DDD	14	0	0	0	0
8	AAA	1	0	0	0	0
8	BBB	1	0	0	0	0
8	DDD	2	0	0	0	0
9	BBB	4	0	6	0	0
9	CCC	4	0	6	1	0
9	DDD	16	0	24	0	0
10	CCC	10	0	10	9	0
11	CCC	1	0	0	0	0
11	DDD	2	0	0	0	0
12	AAA	288	0	0	7	0
12	BBB	162	0	0	2	1
12	CCC	226	0	0	3	0
12	DDD	253	0	0	6	2
All	All	11331	0	10233	152	3

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.

The worst 5 of 152 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:DDD:18[B]:ASN:OD1	1:DDD:67:LEU:CD1	1.74	1.35
1:CCC:30:THR:OG1	10:CCC:407[A]:PGE:H12	1.44	1.18
1:DDD:18[B]:ASN:OD1	1:DDD:67:LEU:HD13	1.37	1.17
1:DDD:18[B]:ASN:ND2	12:DDD:501:HOH:O	1.79	1.14
1:DDD:21[B]:ASP:OD1	12:DDD:738[B]:HOH:O	1.71	1.08

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:DDD:608:HOH:O	12:DDD:612:HOH:O[1_455]	1.92	0.28
1:AAA:129[B]:GLU:OE2	1:DDD:231:TYR:OH[1_554]	2.12	0.08
12:BBB:649:HOH:O	12:DDD:681:HOH:O[2_647]	2.16	0.04

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	AAA	351/346 (101%)	344 (98%)	7 (2%)	0	100	100
1	BBB	323/346 (93%)	315 (98%)	8 (2%)	0	100	100
1	CCC	341/346 (99%)	336 (98%)	5 (2%)	0	100	100
1	DDD	334/346 (96%)	324 (97%)	10 (3%)	0	100	100
All	All	1349/1384 (98%)	1319 (98%)	30 (2%)	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	AAA	291/291 (100%)	283 (97%)	8 (3%)	44	20
1	BBB	258/291 (89%)	246 (95%)	12 (5%)	26	7
1	CCC	276/291 (95%)	272 (99%)	4 (1%)	67	47
1	DDD	272/291 (94%)	261 (96%)	11 (4%)	31	10
All	All	1097/1164 (94%)	1062 (97%)	35 (3%)	39	15

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	124	SER
1	DDD	126[A]	VAL
1	DDD	163	GLN
1	BBB	114	LYS
1	BBB	106	VAL

Sometimes 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 44 ligands modelled in this entry, 16 are monoatomic - leaving 28 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	PLP	BBB	401	1	15,15,16	0.78	1 (6%)	20,22,23	0.90	1 (5%)
3	GOL	CCC	405[A]	-	5,5,5	0.15	0	5,5,5	0.44	0
9	EDO	DDD	407[B]	11	3,3,3	0.06	0	2,2,2	0.34	0
2	PLP	DDD	401	1	15,15,16	0.83	1 (6%)	20,22,23	1.25	1 (5%)
9	EDO	DDD	406	-	3,3,3	0.38	0	2,2,2	0.72	0
9	EDO	BBB	407	-	3,3,3	0.14	0	2,2,2	0.33	0
9	EDO	DDD	407[A]	-	3,3,3	0.08	0	2,2,2	0.40	0
7	T6J	DDD	405[A]	-	12,15,15	0.81	0	14,22,22	1.08	1 (7%)
3	GOL	AAA	403[B]	-	5,5,5	0.22	0	5,5,5	0.47	0
3	GOL	CCC	408	-	5,5,5	0.10	0	5,5,5	0.39	0
3	GOL	AAA	403[A]	-	5,5,5	0.12	0	5,5,5	0.71	0
3	GOL	AAA	402	-	5,5,5	0.15	0	5,5,5	0.28	0
3	GOL	CCC	402[B]	-	5,5,5	0.08	0	5,5,5	0.43	0
3	GOL	AAA	404	-	5,5,5	0.17	0	5,5,5	0.29	0
9	EDO	DDD	408	-	3,3,3	0.18	0	2,2,2	0.12	0
7	T6J	AAA	409[B]	-	12,15,15	0.75	0	14,22,22	1.40	2 (14%)
10	PGE	CCC	407[A]	-	9,9,9	0.12	0	8,8,8	0.26	0
2	PLP	CCC	401	1	15,15,16	1.14	1 (6%)	20,22,23	1.33	2 (10%)
6	DMS	AAA	407	-	3,3,3	0.38	0	3,3,3	0.55	0
3	GOL	CCC	402[A]	-	5,5,5	0.08	0	5,5,5	0.36	0
7	T6J	BBB	406	8	12,15,15	0.85	0	14,22,22	1.09	1 (7%)
3	GOL	AAA	408	-	5,5,5	0.23	0	5,5,5	0.63	0
2	PLP	AAA	401[B]	1	15,15,16	0.85	1 (6%)	20,22,23	0.92	1 (5%)
3	GOL	BBB	403	-	5,5,5	0.11	0	5,5,5	0.36	0
2	PLP	AAA	401[A]	1	15,15,16	0.93	1 (6%)	20,22,23	0.87	1 (5%)
7	T6J	CCC	404[A]	8	12,15,15	0.92	0	14,22,22	1.19	1 (7%)
3	GOL	BBB	402	-	5,5,5	0.16	0	5,5,5	0.11	0
9	EDO	CCC	406	-	3,3,3	0.13	0	2,2,2	0.37	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
2	PLP	BBB	401	1	-	0/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	CCC	405[A]	-	-	4/4/4/4	-
9	EDO	DDD	407[B]	11	-	1/1/1/1	-
2	PLP	DDD	401	1	-	0/6/6/8	0/1/1/1
9	EDO	DDD	406	-	-	1/1/1/1	-
9	EDO	BBB	407	-	-	0/1/1/1	-
9	EDO	DDD	407[A]	-	-	1/1/1/1	-
7	T6J	DDD	405[A]	-	-	1/3/5/5	0/2/2/2
3	GOL	AAA	403[B]	-	-	2/4/4/4	-
3	GOL	CCC	408	-	-	3/4/4/4	-
3	GOL	AAA	403[A]	-	-	2/4/4/4	-
3	GOL	AAA	402	-	-	2/4/4/4	-
3	GOL	CCC	402[B]	-	-	0/4/4/4	-
3	GOL	AAA	404	-	-	0/4/4/4	-
9	EDO	DDD	408	-	-	1/1/1/1	-
7	T6J	AAA	409[B]	-	-	0/3/5/5	0/2/2/2
10	PGE	CCC	407[A]	-	-	5/7/7/7	-
2	PLP	CCC	401	1	-	0/6/6/8	0/1/1/1
3	GOL	CCC	402[A]	-	-	0/4/4/4	-
7	T6J	BBB	406	8	-	0/3/5/5	0/2/2/2
3	GOL	AAA	408	-	-	4/4/4/4	-
2	PLP	AAA	401[B]	1	-	0/6/6/8	0/1/1/1
3	GOL	BBB	403	-	-	2/4/4/4	-
2	PLP	AAA	401[A]	1	-	0/6/6/8	0/1/1/1
7	T6J	CCC	404[A]	8	-	0/3/5/5	0/2/2/2
3	GOL	BBB	402	-	-	2/4/4/4	-
9	EDO	CCC	406	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	401[A]	PLP	C4A-C4	-2.76	1.45	1.51
2	DDD	401	PLP	C4A-C4	-2.65	1.46	1.51
2	AAA	401[B]	PLP	C4A-C4	-2.33	1.46	1.51
2	CCC	401	PLP	C3-C2	-2.03	1.38	1.40
2	BBB	401	PLP	C4A-C4	-2.02	1.47	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	401	PLP	O4P-C5A-C5	4.28	117.51	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	401	PLP	C4A-C4-C5	4.11	125.17	120.94
2	AAA	401[B]	PLP	O4P-C5A-C5	3.03	115.12	109.35
7	AAA	409[B]	T6J	O-S-C	-3.00	105.89	108.91
7	CCC	404[A]	T6J	C5-C4-C3	-2.88	115.94	120.08

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	AAA	403[A]	GOL	O1-C1-C2-O2
3	AAA	403[B]	GOL	O1-C1-C2-C3
3	AAA	408	GOL	O1-C1-C2-C3
3	CCC	405[A]	GOL	O1-C1-C2-C3
3	CCC	408	GOL	C1-C2-C3-O3

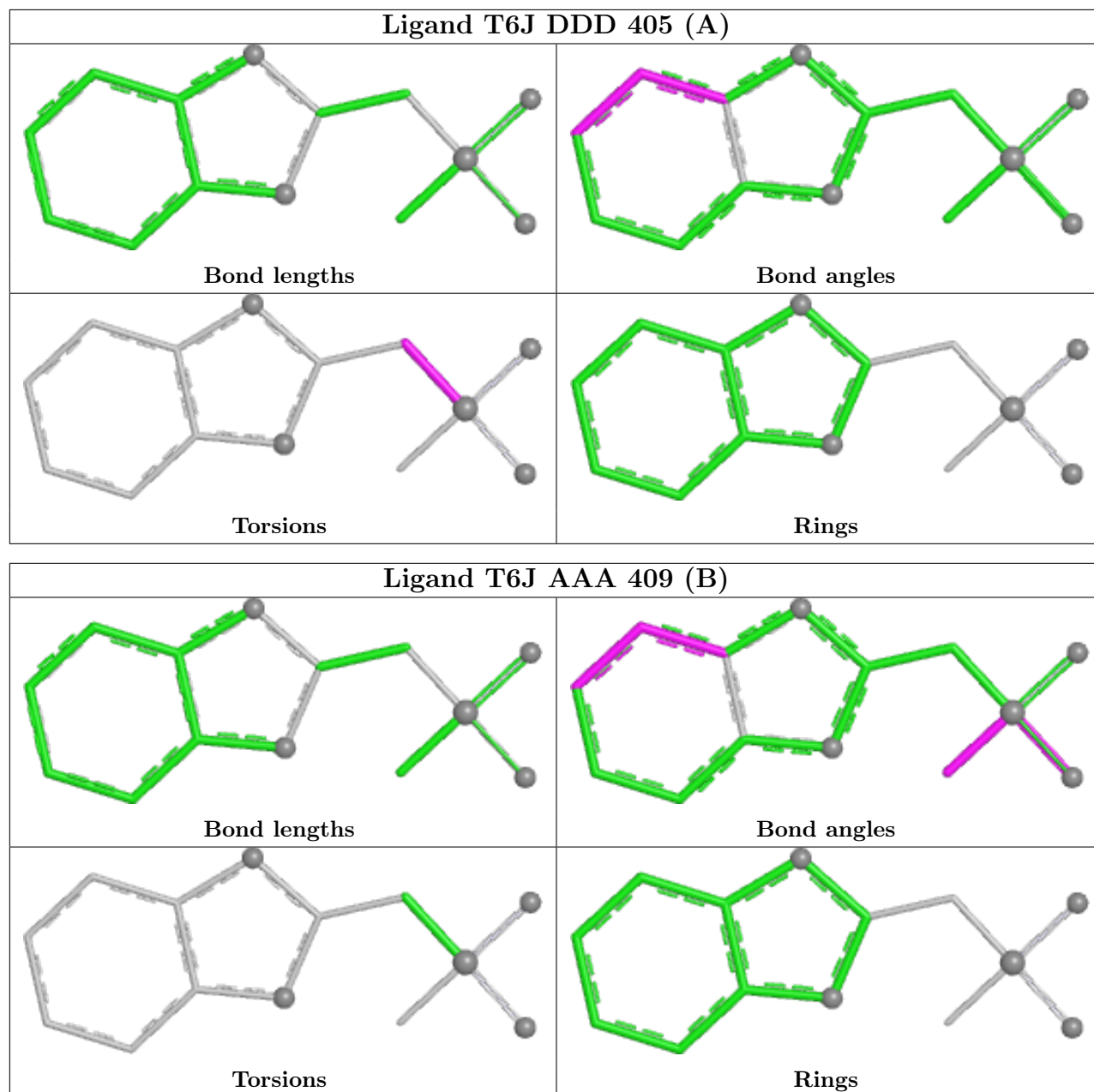
There are no ring outliers.

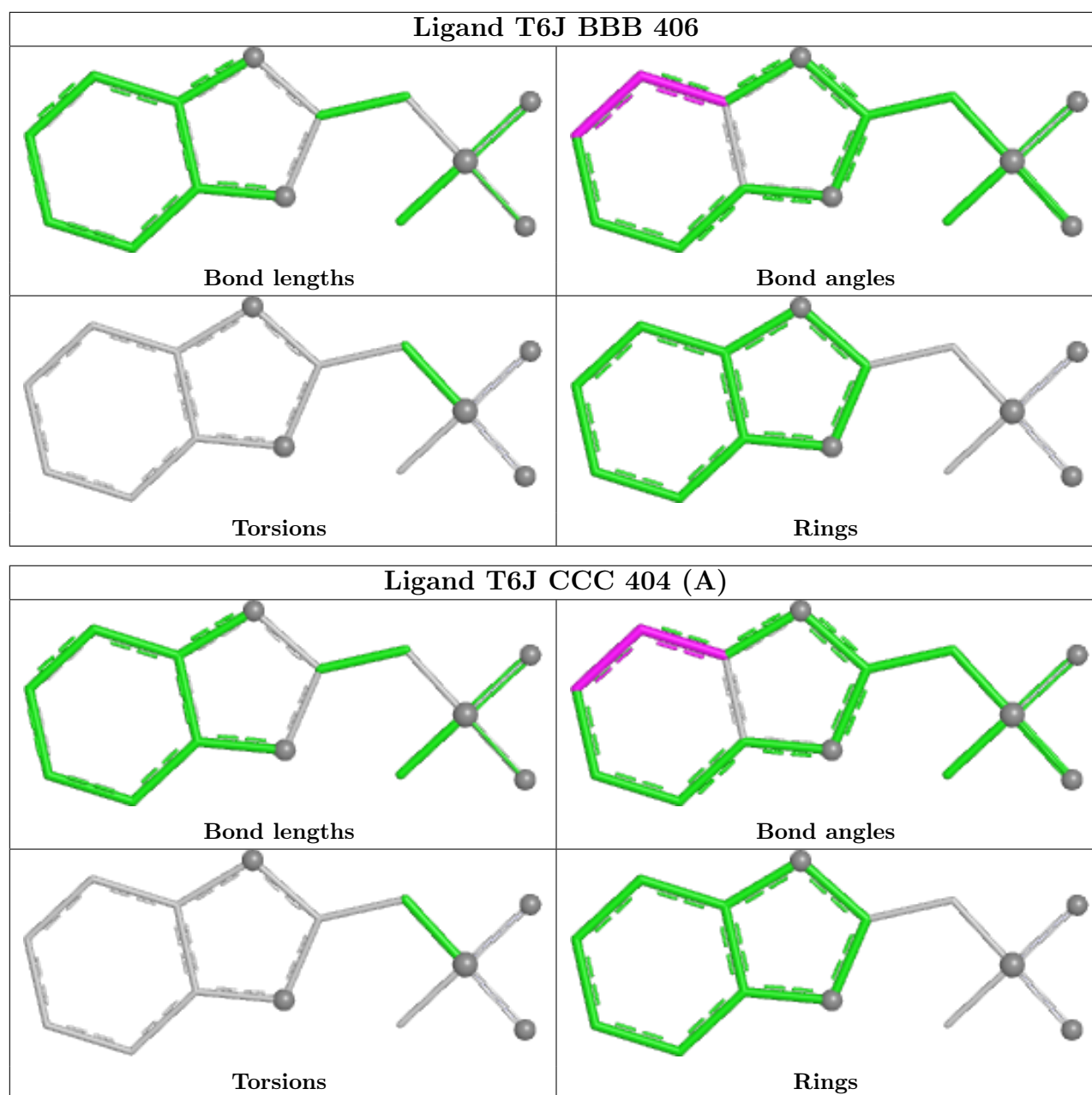
13 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	CCC	405[A]	GOL	5	0
3	AAA	403[B]	GOL	1	0
3	AAA	403[A]	GOL	4	0
3	AAA	402	GOL	2	0
3	CCC	402[B]	GOL	7	0
3	AAA	404	GOL	2	0
7	AAA	409[B]	T6J	1	0
10	CCC	407[A]	PGE	9	0
2	CCC	401	PLP	1	0
3	CCC	402[A]	GOL	1	0
3	AAA	408	GOL	1	0
3	BBB	402	GOL	5	0
9	CCC	406	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 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	AAA	323/346 (93%)	-0.27	10 (3%) 49 46	11, 18, 47, 132	0
1	BBB	312/346 (90%)	0.06	31 (9%) 7 6	16, 27, 88, 122	1 (0%)
1	CCC	323/346 (93%)	-0.22	12 (3%) 41 39	14, 24, 54, 133	0
1	DDD	317/346 (91%)	-0.22	10 (3%) 47 44	13, 20, 66, 126	0
All	All	1275/1384 (92%)	-0.16	63 (4%) 29 27	11, 22, 67, 133	1 (0%)

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	323	ILE	11.2
1	DDD	320	THR	9.3
1	BBB	109	THR	8.5
1	BBB	106	VAL	8.3
1	DDD	319	LEU	8.1

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	EDO	DDD	406	4/4	0.77	0.17	31,32,39,42	0
9	EDO	DDD	407[A]	4/4	0.79	0.17	43,44,44,44	4
9	EDO	DDD	407[B]	4/4	0.79	0.17	46,47,47,48	4
3	GOL	BBB	403	6/6	0.82	0.35	59,69,72,85	0
10	PGE	CCC	407[A]	10/10	0.82	0.26	23,30,36,39	10
9	EDO	DDD	408	4/4	0.83	0.18	42,48,50,54	0
3	GOL	AAA	404	6/6	0.83	0.26	27,38,46,50	0
3	GOL	AAA	403[A]	6/6	0.86	0.22	18,22,26,30	6
3	GOL	AAA	403[B]	6/6	0.86	0.22	17,21,29,37	6
3	GOL	CCC	402[A]	6/6	0.86	0.27	44,49,50,51	6
3	GOL	CCC	402[B]	6/6	0.86	0.27	71,77,79,82	6
3	GOL	CCC	405[A]	6/6	0.86	0.25	22,24,25,28	6
8	NA	DDD	404	1/1	0.87	0.08	43,43,43,43	0
3	GOL	AAA	402	6/6	0.87	0.16	35,45,48,50	0
3	GOL	CCC	408	6/6	0.87	0.15	42,44,54,59	0
3	GOL	BBB	402	6/6	0.90	0.25	48,53,56,61	0
9	EDO	CCC	406	4/4	0.91	0.14	34,34,42,55	0
7	T6J	AAA	409[B]	14/14	0.91	0.17	22,28,30,30	14
3	GOL	AAA	408	6/6	0.92	0.24	37,39,42,50	0
9	EDO	BBB	407	4/4	0.92	0.11	40,44,45,53	0
8	NA	BBB	408	1/1	0.94	0.31	41,41,41,41	0
7	T6J	BBB	406	14/14	0.94	0.10	25,31,33,33	14
8	NA	AAA	411	1/1	0.94	0.20	47,47,47,47	0
7	T6J	DDD	405[A]	14/14	0.95	0.10	26,29,32,32	14
8	NA	DDD	409	1/1	0.96	0.48	44,44,44,44	1
11	CL	DDD	410[A]	1/1	0.96	0.07	25,25,25,25	1
11	CL	DDD	410[B]	1/1	0.96	0.07	31,31,31,31	1
5	MG	DDD	403	1/1	0.97	0.13	31,31,31,31	0
11	CL	CCC	409	1/1	0.97	0.07	34,34,34,34	0
6	DMS	AAA	407	4/4	0.97	0.11	40,42,42,43	0
4	CA	AAA	410	1/1	0.97	0.06	25,25,25,25	1
2	PLP	CCC	401	15/16	0.98	0.06	15,16,18,18	0
4	CA	BBB	405	1/1	0.98	0.07	32,32,32,32	0
7	T6J	CCC	404[A]	14/14	0.98	0.08	20,24,26,26	14
5	MG	AAA	406	1/1	0.98	0.05	21,21,21,21	0
2	PLP	AAA	401[A]	15/16	0.98	0.08	11,11,12,14	15
2	PLP	AAA	401[B]	15/16	0.98	0.08	12,13,16,16	15
2	PLP	DDD	401	15/16	0.99	0.06	12,14,15,16	0
4	CA	BBB	404	1/1	0.99	0.06	23,23,23,23	0
2	PLP	BBB	401	15/16	0.99	0.06	17,17,21,22	0
4	CA	CCC	403[A]	1/1	1.00	0.06	14,14,14,14	1
4	CA	CCC	403[B]	1/1	1.00	0.06	25,25,25,25	1
4	CA	DDD	402	1/1	1.00	0.07	18,18,18,18	0

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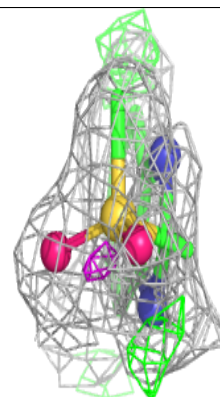
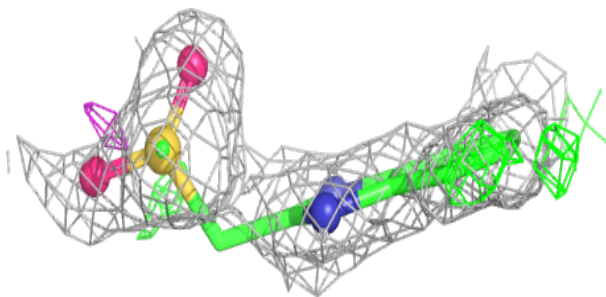
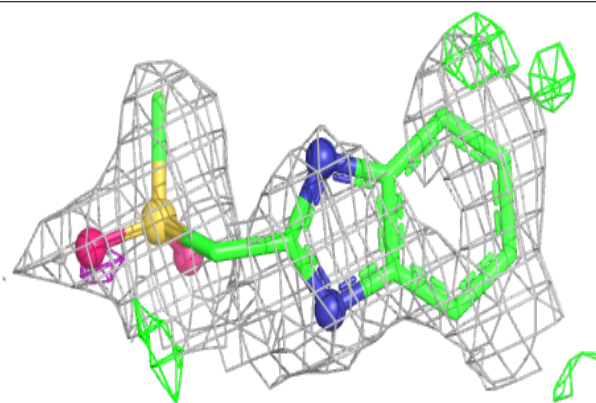
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CA	AAA	405	1/1	1.00	0.08	14,14,14,14	0

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.

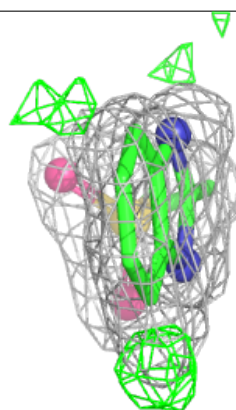
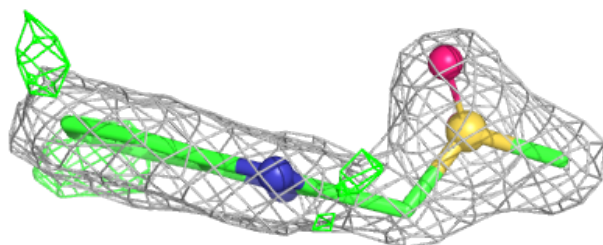
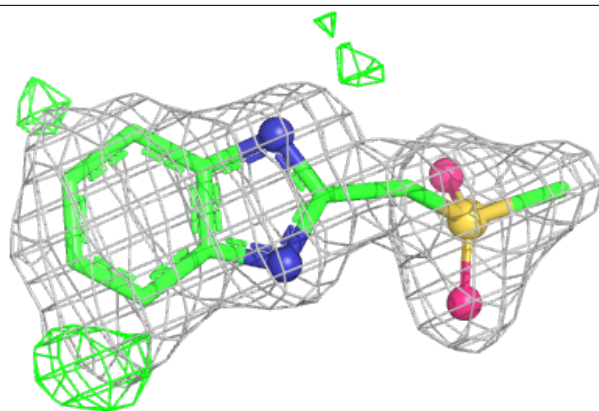
Electron density around T6J AAA 409 (B):

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

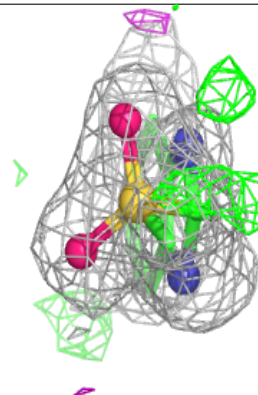
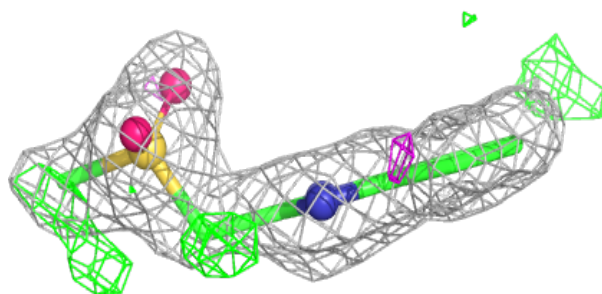
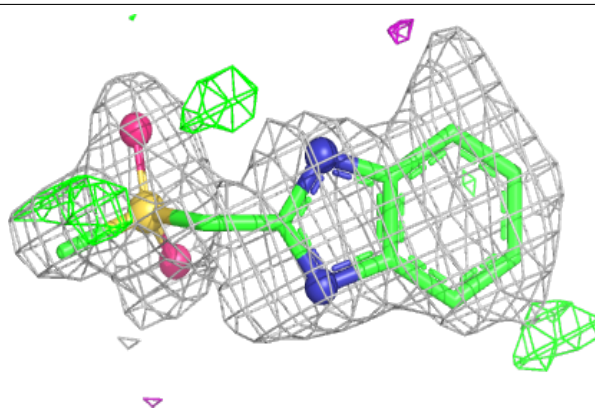


Electron density around T6J BBB 406:

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

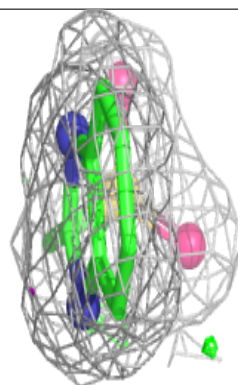
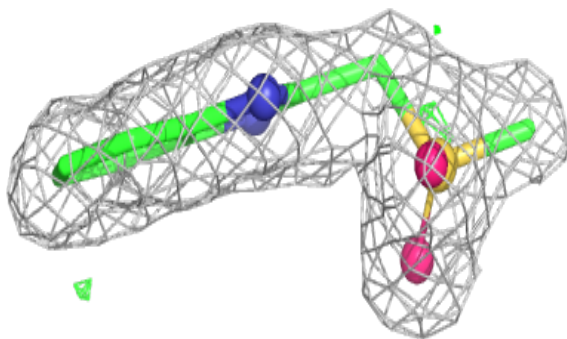
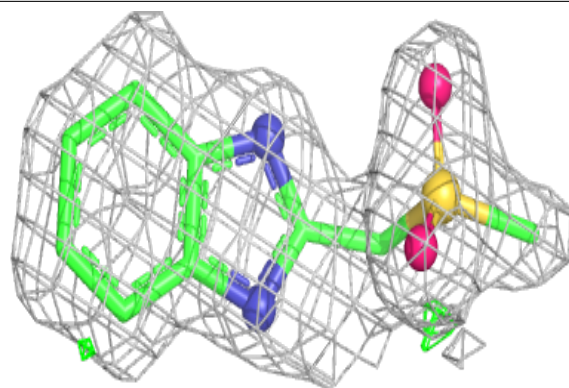
**Electron density around T6J DDD 405 (A):**

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



Electron density around T6J CCC 404 (A):

$2mF_o - DF_c$ (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.