



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2021 – 10:10 AM EDT

PDB ID : 7KA1
Title : 1.60 Angstrom resolution crystal structure of the beta-Q114A mutant Tryptophan Synthase in complex with inhibitor N-(4'-trifluoromethoxybenzenesulfonyl)-2-amino-1-ethylphosphate (F9F) at the alpha-site, aminoacrylate at the beta site, and cesium ion at the metal coordination site
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Deposited on : 2020-09-29
Resolution : 1.60 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 : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

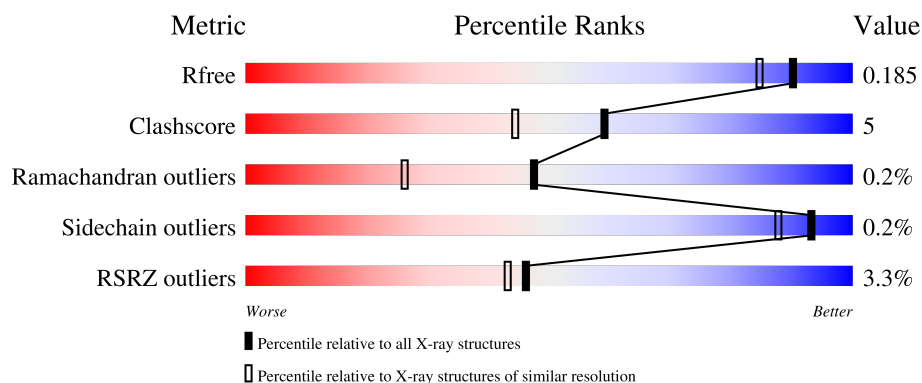
1 Overall quality at a glance

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	A	268	<div> <div>6%</div> <div>89%</div> <div>11%</div> </div>
2	B	397	<div> <div>%</div> <div>92%</div> <div>8%</div> </div>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 6140 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 Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	10	0
			2097	1327	366	396	8			

- Molecule 2 is a protein called Tryptophan synthase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	395	Total	C	N	O	S	0	13	0
			3099	1943	545	591	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	114	ALA	GLN	engineered mutation	UNP P0A2K1

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).

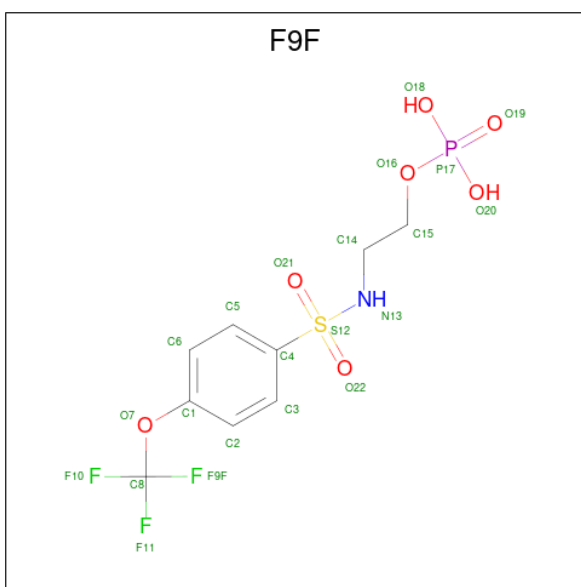


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O S 4 2 1 1	0	0
3	A	1	Total C O S 4 2 1 1	0	0
3	A	1	Total C O S 4 2 1 1	0	0
3	A	1	Total C O S 4 2 1 1	0	0
3	A	1	Total C O S 4 2 1 1	0	0
3	B	1	Total C O S 4 2 1 1	0	0
3	B	1	Total C O S 4 2 1 1	0	0
3	B	1	Total C O S 4 2 1 1	0	0
3	B	1	Total C O S 4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

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

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

- Molecule 5 is 2-([4-(TRIFLUOROMETHOXY)PHENYL]SULFONYL)AMINO)ETHYL DIHYDROGEN PHOSPHATE (three-letter code: F9F) (formula: C₉H₁₁F₃NO₇PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	P	S	
			22	9	3	1	7	1	1	

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

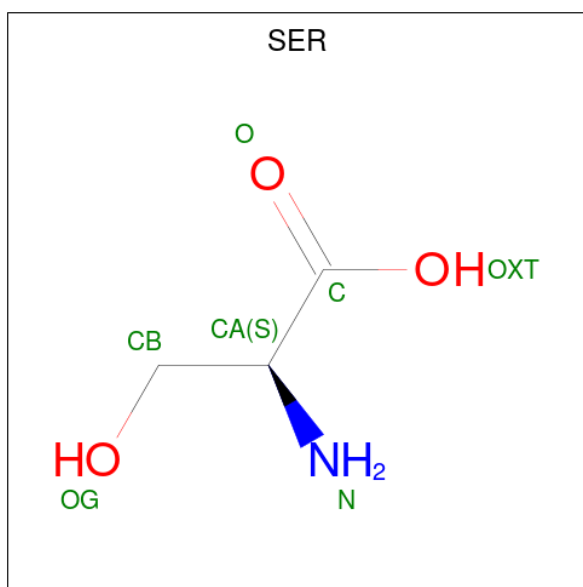
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

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- The chemical structure shows a central pyridine ring (N1) with a phosphate group attached at C5 (C5A, OP4, P, OP2, OP3, OP1) and a carboxylic acid side chain at C4 (C4A, N, CA, CB, C, OXT, O). The pyridine ring has a hydroxyl group at C3 (O3). The phosphate group is a phosphoric acid derivative. The carboxylic acid side chain is a 2-oxo-3-oxopropyl group.

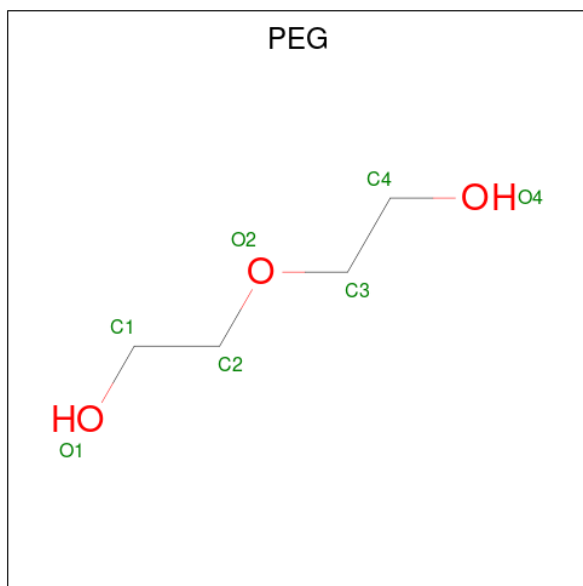
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	2	Total Cs 3 3	0	1

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- WORLD WIDE
PDB
PROTEIN DATA BANK



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

- Molecule 10 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

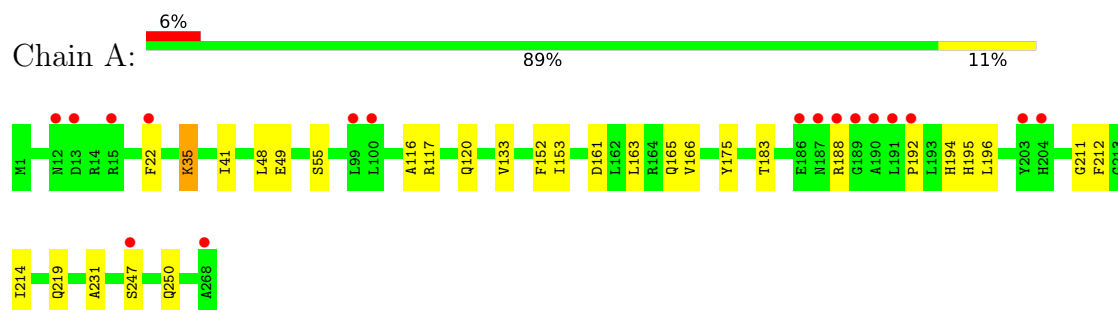
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	271	Total 286	O 286	0	14
11	B	457	Total 490	O 490	0	33

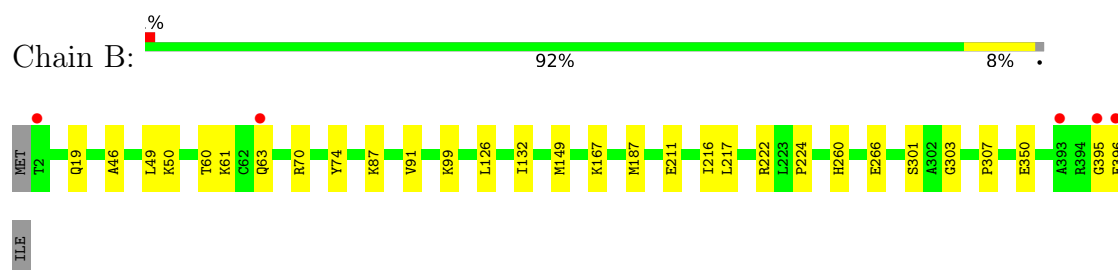
3 Residue-property plots [i](#)

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: Tryptophan synthase alpha chain



- Molecule 2: Tryptophan synthase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.73Å 60.89Å 67.31Å 90.00° 94.85° 90.00°	Depositor
Resolution (Å)	29.35 – 1.60 29.35 – 1.60	Depositor EDS
% Data completeness (in resolution range)	87.9 (29.35-1.60) 87.9 (29.35-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, R_{free}	0.155 , 0.185 0.155 , 0.185	Depositor DCC
R_{free} test set	4274 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6140	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.37% 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: PEG, OJO, F9F, CS, DMS, CL, EDO

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	0.40	0/2138	0.55	0/2905
2	B	0.47	1/3157 (0.0%)	0.68	0/4263
All	All	0.44	1/5295 (0.0%)	0.63	0/7168

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	396	GLU	CD-OE1	-7.36	1.17	1.25

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	2097	0	2089	24	0
2	B	3099	0	3064	24	0
3	A	20	0	30	0	0
3	B	44	0	66	2	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
5	A	22	0	9	2	0
6	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	28	0	42	1	0
7	B	21	0	9	3	0
8	B	3	0	0	0	0
9	B	7	0	4	2	0
10	B	14	0	20	4	0
11	A	286	0	0	1	0
11	B	490	0	0	7	0
All	All	6140	0	5339	50	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 5.

All (50) 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:63[C]:GLN:HG3	10:B:426:PEG:H31	1.54	0.89
1:A:35:LYS:N	1:A:35:LYS:HD3	1.95	0.80
2:B:222:ARG:NH1	11:B:501:HOH:O	2.13	0.78
1:A:161:ASP:O	1:A:165:GLN:HG3	1.89	0.73
2:B:60:THR:HG23	10:B:426:PEG:H21	1.69	0.73
2:B:211:GLU:HG2	6:B:419:EDO:H21	1.71	0.71
2:B:167:LYS:NZ	11:B:509:HOH:O	2.32	0.63
1:A:133[A]:VAL:HG12	1:A:152:PHE:CD1	2.35	0.62
1:A:35:LYS:HD3	1:A:35:LYS:H	1.66	0.61
2:B:61:LYS:O	10:B:426:PEG:H32	2.01	0.60
1:A:214[B]:ILE:HD13	1:A:231:ALA:HB1	1.83	0.60
2:B:217[B]:LEU:HG	11:B:778:HOH:O	2.05	0.57
2:B:132:ILE:HD13	2:B:149:MET:SD	2.46	0.56
1:A:188:ARG:HG3	1:A:219:GLN:NE2	2.26	0.52
1:A:153:ILE:HD13	1:A:175:TYR:HB3	1.92	0.51
2:B:167:LYS:HD2	2:B:307:PRO:HG3	1.91	0.51
2:B:87:LYS:HE3	7:B:401:OJO:N	2.26	0.51
1:A:35:LYS:N	1:A:35:LYS:CD	2.72	0.50
1:A:116:ALA:O	1:A:120[B]:GLN:HG3	2.12	0.50
2:B:260:HIS:HD2	2:B:266:GLU:OE2	1.94	0.50
1:A:194:HIS:HE1	11:A:605:HOH:O	1.95	0.48
2:B:303:GLY:HA2	7:B:401:OJO:CB	2.43	0.48
1:A:183:THR:CG2	5:A:308:F9F:H151	2.44	0.48
1:A:192:PRO:HB2	1:A:194:HIS:HD2	1.79	0.47
1:A:163:LEU:HD21	1:A:196:LEU:HD22	1.97	0.46
10:B:427:PEG:H31	10:B:427:PEG:H11	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:VAL:HG13	2:B:187:MET:CE	2.45	0.46
1:A:133[B]:VAL:HG23	2:B:19:GLN:OE1	2.15	0.46
1:A:152:PHE:HB3	1:A:166[A]:VAL:HG22	1.98	0.46
1:A:41:ILE:HD11	1:A:48:LEU:HD11	1.97	0.46
1:A:211:GLY:O	1:A:212:PHE:HB2	2.16	0.45
2:B:216[A]:ILE:HG21	2:B:224:PRO:HD3	1.99	0.45
1:A:195[B]:HIS:ND1	1:A:195[B]:HIS:N	2.65	0.45
2:B:61:LYS:HB2	2:B:74:TYR:CE2	2.51	0.45
2:B:216[B]:ILE:HG22	2:B:222:ARG:O	2.17	0.45
2:B:70:ARG:NH2	11:B:517:HOH:O	2.50	0.44
7:B:401:OJO:H3	7:B:401:OJO:H4	1.71	0.44
2:B:301[C]:SER:OG	2:B:350:GLU:HG3	2.17	0.44
9:B:425:SER:HB3	11:B:820:HOH:O	2.17	0.43
1:A:55:SER:O	9:B:425:SER:HA	2.19	0.43
1:A:133[A]:VAL:HG12	1:A:152:PHE:HD1	1.81	0.42
1:A:117:ARG:NH1	1:A:120[A]:GLN:OE1	2.53	0.42
2:B:63[C]:GLN:NE2	11:B:516:HOH:O	2.48	0.42
2:B:46:ALA:HB2	3:B:407:DMS:H21	2.02	0.42
2:B:49:LEU:HD12	3:B:407:DMS:H23	2.02	0.41
1:A:247[B]:SER:HB2	1:A:250:GLN:HB3	2.02	0.41
2:B:50:LYS:NZ	11:B:505:HOH:O	2.29	0.41
1:A:22:PHE:HA	1:A:49:GLU:O	2.20	0.41
2:B:99:LYS:HD2	2:B:126:LEU:HB3	2.02	0.40
1:A:175:TYR:CE2	5:A:308:F9F:H3	2.57	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	276/268 (103%)	271 (98%)	5 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	407/397 (102%)	398 (98%)	8 (2%)	1 (0%)	47	26
All	All	683/665 (103%)	669 (98%)	13 (2%)	1 (0%)	47	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	395	GLY

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	218/208 (105%)	217 (100%)	1 (0%)	88	80
2	B	322/310 (104%)	322 (100%)	0	100	100
All	All	540/518 (104%)	539 (100%)	1 (0%)	93	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	HIS
2	B	375	ASN

5.3.3 RNA ⓘ

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 37 ligands modelled in this entry, 8 are monoatomic - leaving 29 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	SER	B	425	-	3,6,6	0.38	0	1,7,7	0.50	0
3	DMS	B	409	-	3,3,3	0.63	0	3,3,3	0.83	0
3	DMS	A	302	-	3,3,3	0.51	0	3,3,3	0.41	0
6	EDO	B	419	-	3,3,3	0.61	0	2,2,2	0.09	0
3	DMS	B	406	-	3,3,3	0.61	0	3,3,3	0.61	0
6	EDO	B	418	-	3,3,3	0.44	0	2,2,2	0.30	0
3	DMS	B	408	-	3,3,3	0.65	0	3,3,3	0.27	0
3	DMS	B	407	-	3,3,3	0.68	0	3,3,3	0.35	0
3	DMS	B	412	-	3,3,3	0.64	0	3,3,3	0.60	0
7	OJO	B	401	-	18,21,21	1.84	1 (5%)	21,30,30	0.58	0
3	DMS	A	304	-	3,3,3	0.65	0	3,3,3	0.34	0
6	EDO	A	309	-	3,3,3	0.39	0	2,2,2	0.23	0
5	F9F	A	308	-	22,22,22	0.31	0	32,33,33	0.34	0
6	EDO	B	421	-	3,3,3	0.50	0	2,2,2	0.25	0
6	EDO	B	423	-	3,3,3	0.59	0	2,2,2	0.26	0
6	EDO	B	420	-	3,3,3	0.34	0	2,2,2	0.51	0
3	DMS	B	404	-	3,3,3	0.65	0	3,3,3	0.51	0
6	EDO	B	424	-	3,3,3	0.45	0	2,2,2	0.37	0
6	EDO	B	422	-	3,3,3	0.46	0	2,2,2	0.54	0
3	DMS	A	303	-	3,3,3	0.63	0	3,3,3	0.53	0
3	DMS	B	411	-	3,3,3	0.69	0	3,3,3	0.64	0
3	DMS	B	413	-	3,3,3	0.62	0	3,3,3	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PEG	B	427	-	6,6,6	0.49	0	5,5,5	0.32	0
10	PEG	B	426	-	6,6,6	0.47	0	5,5,5	0.48	0
3	DMS	B	405	-	3,3,3	0.68	0	3,3,3	0.19	0
3	DMS	A	301	-	3,3,3	0.62	0	3,3,3	0.60	0
3	DMS	B	410	-	3,3,3	0.65	0	3,3,3	0.48	0
3	DMS	A	305	-	3,3,3	0.68	0	3,3,3	0.27	0
3	DMS	B	414	-	3,3,3	0.67	0	3,3,3	0.48	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
6	EDO	B	421	-	-	1/1/1/1	-
6	EDO	B	418	-	-	1/1/1/1	-
6	EDO	B	423	-	-	0/1/1/1	-
6	EDO	B	420	-	-	0/1/1/1	-
9	SER	B	425	-	-	0/2/6/6	-
6	EDO	B	424	-	-	1/1/1/1	-
6	EDO	B	422	-	-	0/1/1/1	-
6	EDO	B	419	-	-	1/1/1/1	-
7	OJO	B	401	-	-	1/9/15/15	0/1/1/1
5	F9F	A	308	-	-	10/20/20/20	0/1/1/1
10	PEG	B	427	-	-	3/4/4/4	-
6	EDO	A	309	-	-	0/1/1/1	-
10	PEG	B	426	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	401	OJO	C-CA	-7.56	1.40	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	308	F9F	C15-O16-P17-O18
5	A	308	F9F	C15-O16-P17-O20

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Mol	Chain	Res	Type	Atoms
6	B	418	EDO	O1-C1-C2-O2
10	B	427	PEG	C1-C2-O2-C3
10	B	426	PEG	O1-C1-C2-O2
10	B	427	PEG	O2-C3-C4-O4
6	B	424	EDO	O1-C1-C2-O2
10	B	427	PEG	O1-C1-C2-O2
5	A	308	F9F	C15-O16-P17-O19
5	A	308	F9F	C5-C4-S12-O21
7	B	401	OJO	C4-C4A-N-CA
6	B	419	EDO	O1-C1-C2-O2
5	A	308	F9F	C3-C4-S12-O21
5	A	308	F9F	C2-C1-O7-C8
5	A	308	F9F	N13-C14-C15-O16
5	A	308	F9F	C6-C1-O7-C8
10	B	426	PEG	O2-C3-C4-O4
6	B	421	EDO	O1-C1-C2-O2
5	A	308	F9F	C5-C4-S12-N13
5	A	308	F9F	C3-C4-S12-N13

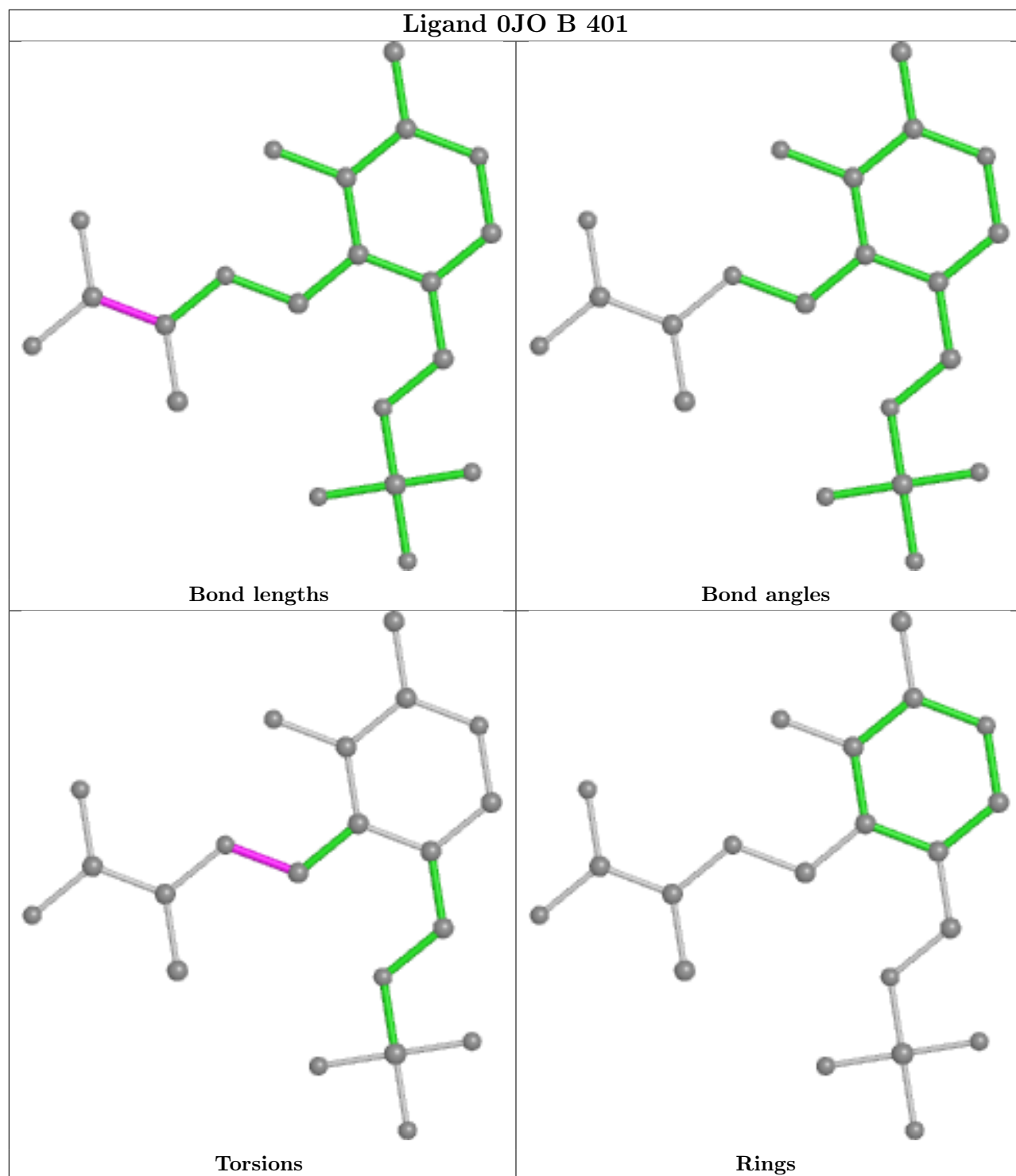
There are no ring outliers.

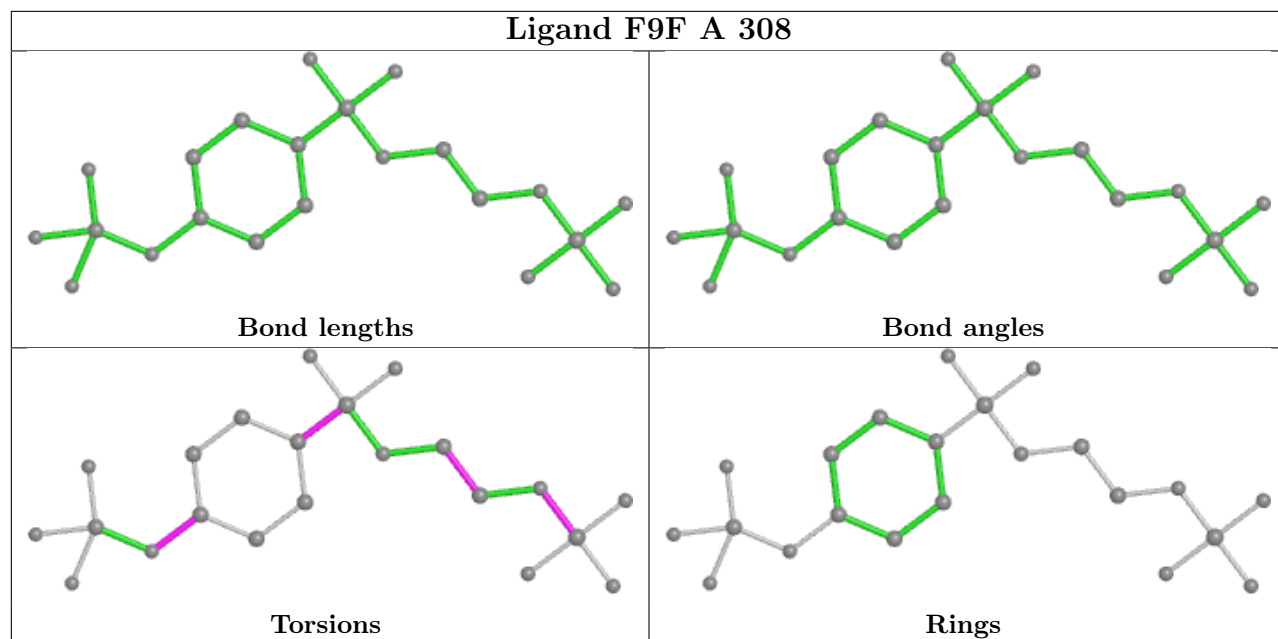
7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	425	SER	2	0
6	B	419	EDO	1	0
3	B	407	DMS	2	0
7	B	401	OJO	3	0
5	A	308	F9F	2	0
10	B	427	PEG	1	0
10	B	426	PEG	3	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

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, 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	268/268 (100%)	0.27	17 (6%) 20 18	15, 24, 44, 75	0
2	B	395/397 (99%)	-0.20	5 (1%) 77 77	11, 16, 27, 57	0
All	All	663/665 (99%)	-0.01	22 (3%) 46 43	11, 19, 38, 75	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	ALA	8.1
1	A	191	LEU	6.6
1	A	189	GLY	4.7
1	A	268	ALA	3.4
1	A	186	GLU	3.3
1	A	13[A]	ASP	3.2
1	A	247[A]	SER	3.0
1	A	192	PRO	2.8
1	A	203	TYR	2.8
1	A	188	ARG	2.7
1	A	15	ARG	2.6
2	B	395	GLY	2.6
1	A	187	ASN	2.6
1	A	100	LEU	2.5
2	B	63[A]	GLN	2.5
2	B	396	GLU	2.5
2	B	393	ALA	2.3
2	B	2	THR	2.3
1	A	22	PHE	2.2
1	A	204	HIS	2.1
1	A	12	ASN	2.1
1	A	99	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DMS	A	301	4/4	0.56	0.23	27,30,43,57	4
6	EDO	B	419	4/4	0.75	0.25	27,27,32,40	0
6	EDO	B	421	4/4	0.78	0.18	31,33,35,47	0
3	DMS	B	411	4/4	0.83	0.21	23,26,30,38	4
10	PEG	B	427	7/7	0.86	0.21	19,24,30,32	7
9	SER	B	425	7/7	0.87	0.14	32,32,35,39	0
6	EDO	B	418	4/4	0.87	0.15	30,33,36,38	0
6	EDO	B	423	4/4	0.88	0.14	22,24,28,35	0
6	EDO	B	424	4/4	0.88	0.10	29,29,39,39	0
3	DMS	B	406	4/4	0.88	0.27	40,40,42,56	0
3	DMS	B	410	4/4	0.88	0.24	36,39,45,54	0
3	DMS	B	412	4/4	0.89	0.37	43,45,56,61	0
4	CL	B	417	1/1	0.91	0.11	66,66,66,66	0
3	DMS	B	407	4/4	0.91	0.19	32,36,43,48	0
3	DMS	A	303	4/4	0.91	0.23	25,36,39,48	0
10	PEG	B	426	7/7	0.91	0.24	17,22,25,25	7
4	CL	A	307	1/1	0.91	0.05	39,39,39,39	0
3	DMS	A	302	4/4	0.92	0.12	27,28,29,33	4
6	EDO	A	309	4/4	0.92	0.17	22,33,33,43	0
6	EDO	B	422	4/4	0.93	0.13	15,28,36,37	0
4	CL	B	416	1/1	0.93	0.07	47,47,47,47	0
3	DMS	B	413	4/4	0.93	0.24	35,44,51,54	0
3	DMS	B	414	4/4	0.94	0.31	39,55,60,60	0
5	F9F	A	308	22/22	0.94	0.11	17,19,27,30	0
3	DMS	A	304	4/4	0.94	0.11	33,34,42,46	0
3	DMS	B	405	4/4	0.94	0.12	13,18,21,22	4
4	CL	B	415	1/1	0.95	0.07	53,53,53,53	0

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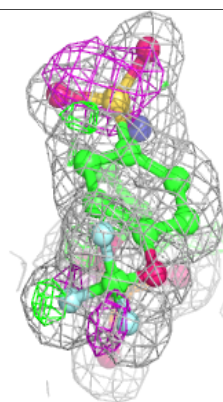
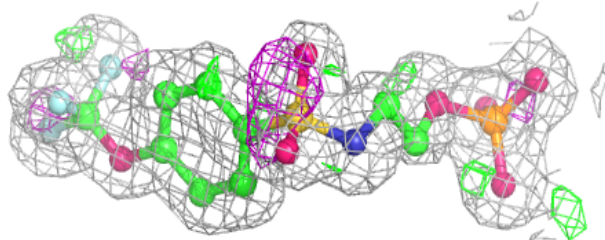
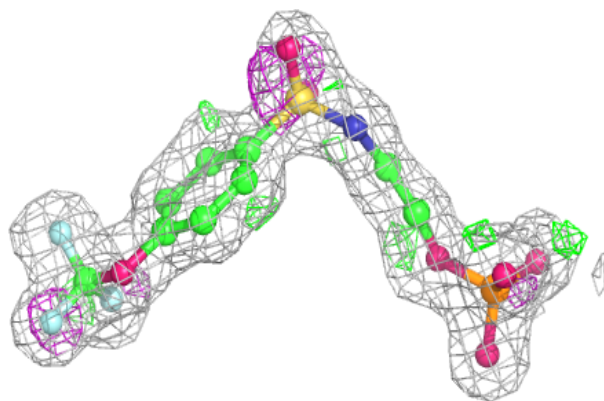
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CL	A	306	1/1	0.95	0.08	54,54,54,54	0
7	OJO	B	401	21/21	0.96	0.11	12,14,16,20	0
3	DMS	B	409	4/4	0.96	0.21	29,34,34,43	0
6	EDO	B	420	4/4	0.96	0.07	15,25,25,36	0
3	DMS	A	305	4/4	0.96	0.17	22,24,28,29	0
3	DMS	B	408	4/4	0.98	0.08	19,19,20,25	4
3	DMS	B	404	4/4	0.99	0.10	23,23,27,28	0
8	CS	B	402[A]	1/1	1.00	0.07	17,17,17,17	1
8	CS	B	402[B]	1/1	1.00	0.07	15,15,15,15	1
8	CS	B	403	1/1	1.00	0.05	20,20,20,20	1

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.

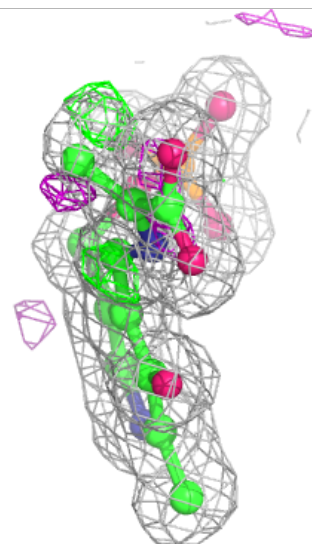
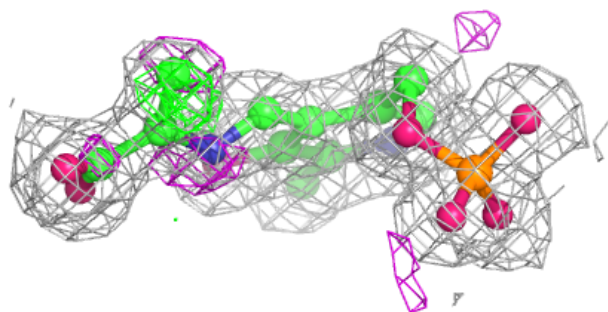
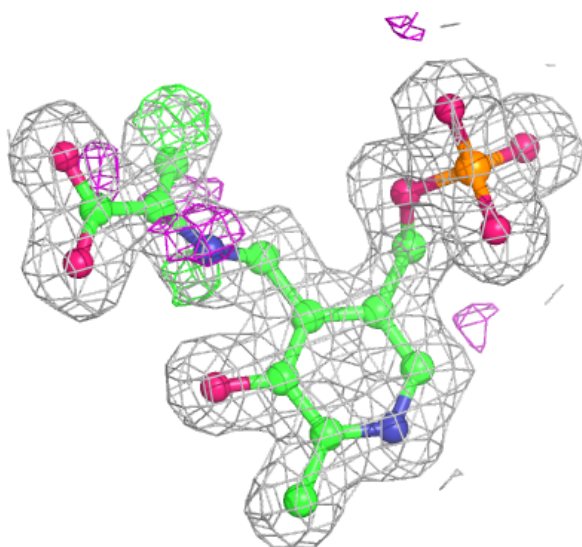
Electron density around F9F A 308:

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



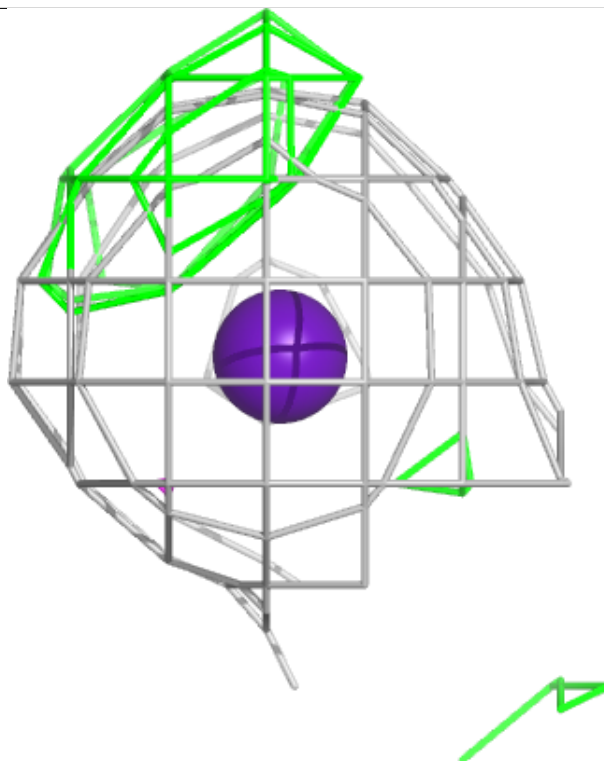
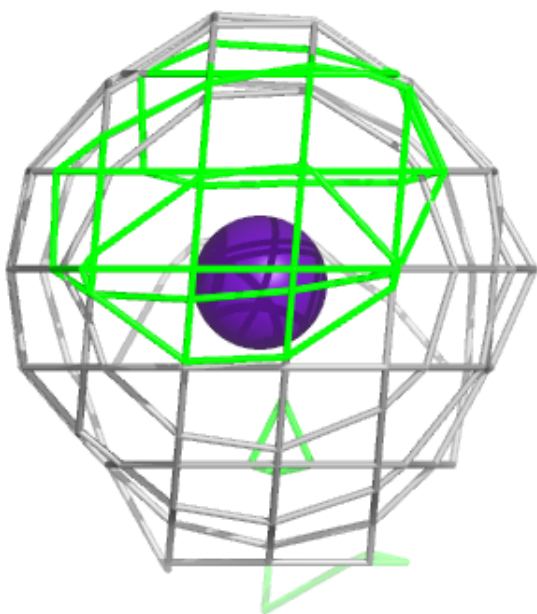
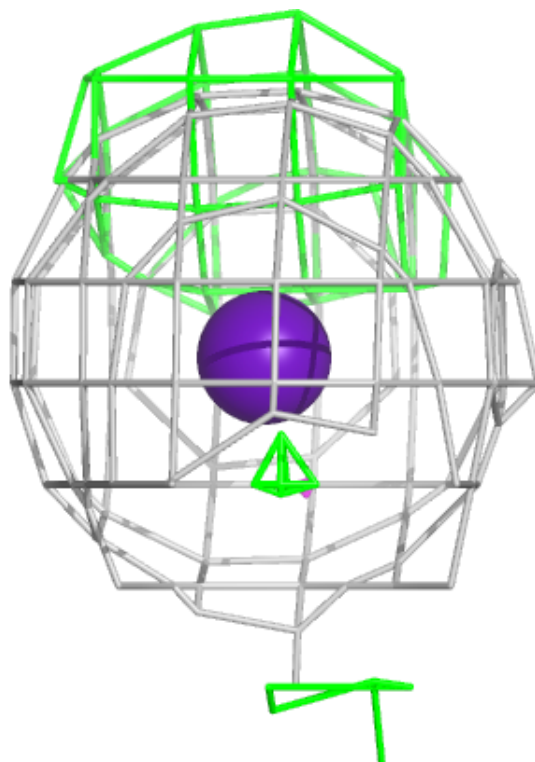
Electron density around 0JO B 401:

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



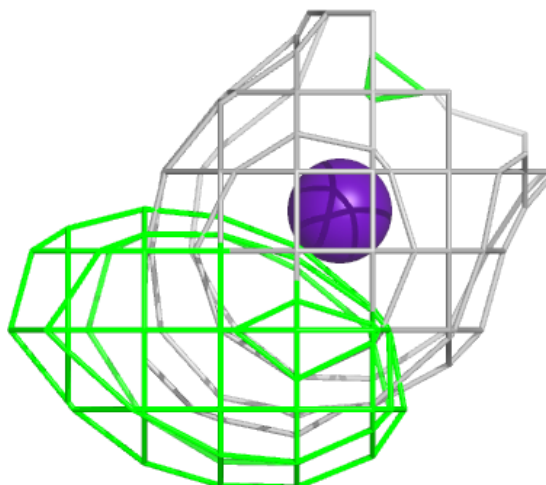
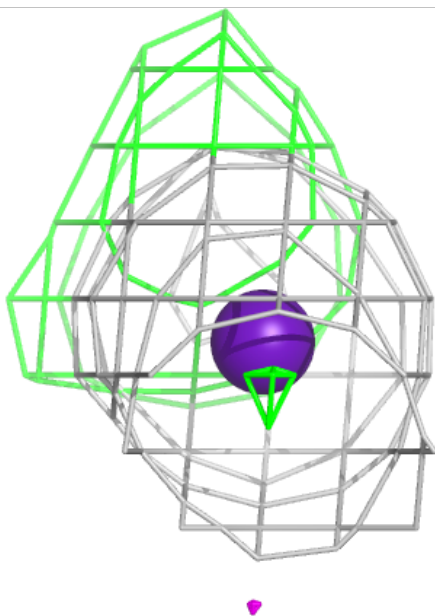
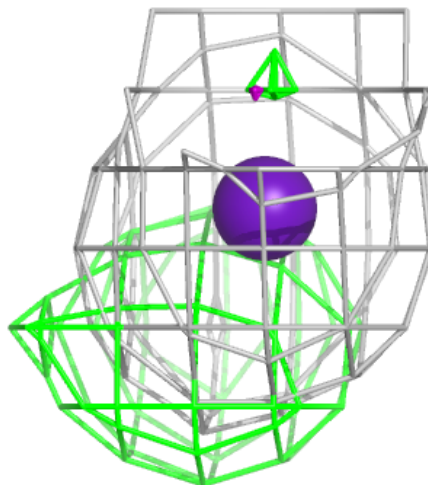
Electron density around CS B 402 (A):

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



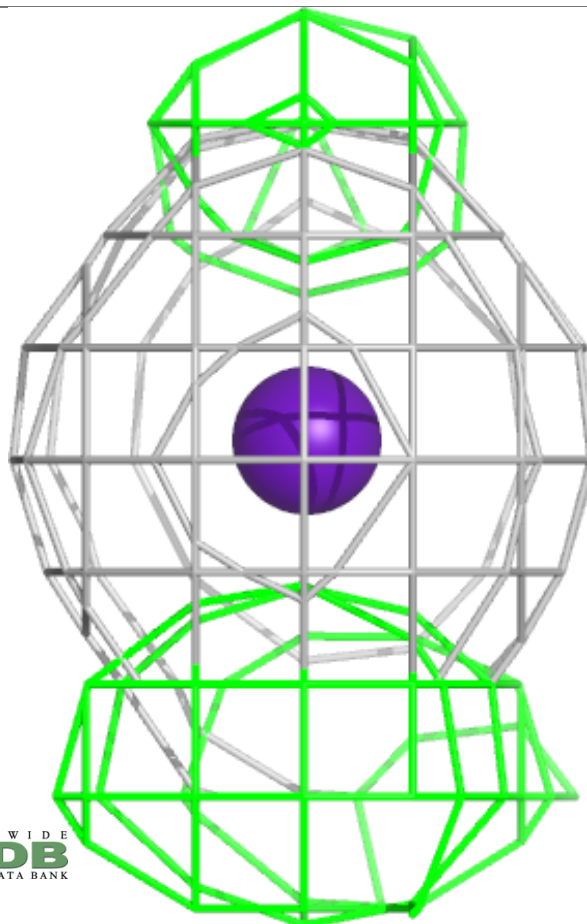
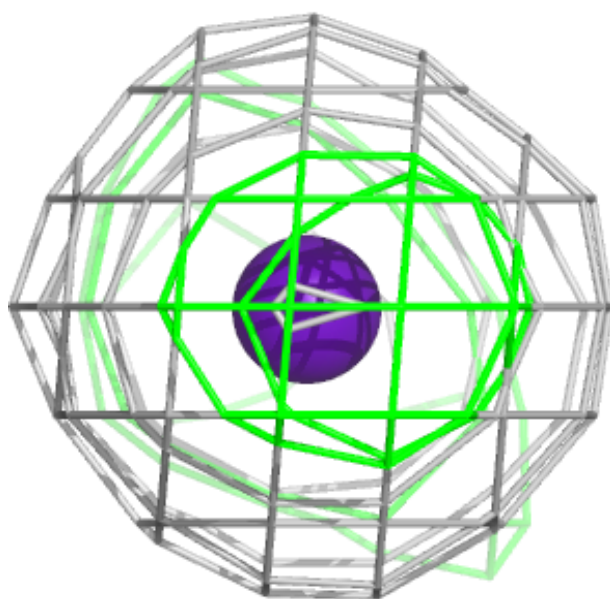
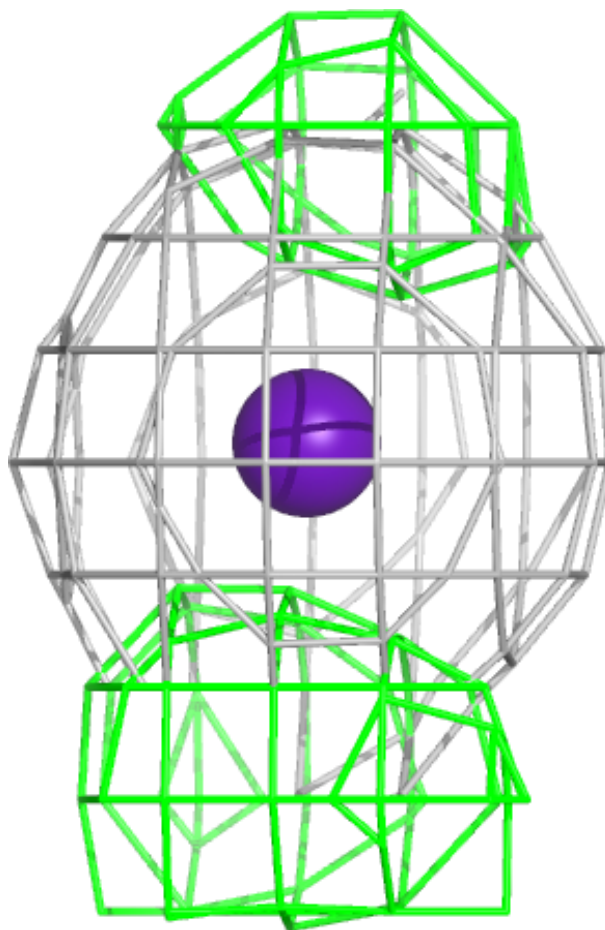
Electron density around CS B 402 (B):

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



Electron density around CS B 403:

$2mF_o-DF_c$ (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.