



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:08 PM UTC

PDB ID : 6KSA / pdb_00006ksa
Title : Crystal Structure of E447A Acyl-CoA Dehydrogenase FadE5 mutant from Mycobacteria smegmatis in complex with C18CoA
Authors : Liu, X.; Chen, X.B.
Deposited on : 2019-08-23
Resolution : 1.77 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

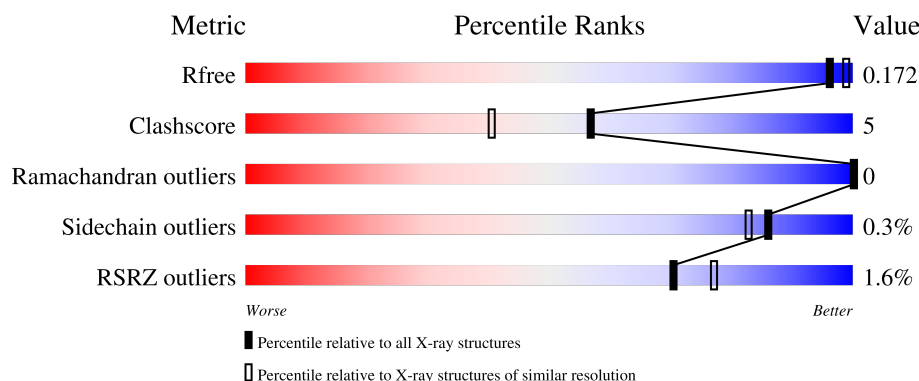
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

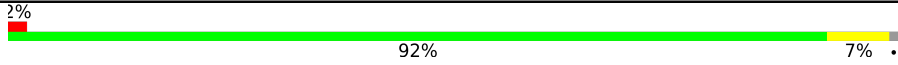
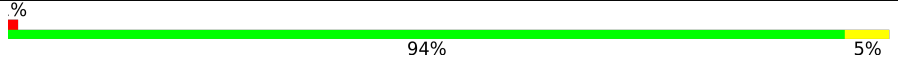
The reported resolution of this entry is 1.77 Å.

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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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 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	614	
1	B	614	

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
4	SO4	A	703	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20114 atoms, of which 9378 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 Acyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	607	Total	C	H	N	O	S	0	0	0
			9228	2949	4578	790	889	22			
1	B	611	Total	C	H	N	O	S	0	0	0
			9286	2964	4607	798	895	22			

There are 8 discrepancies between the modelled and reference sequences:

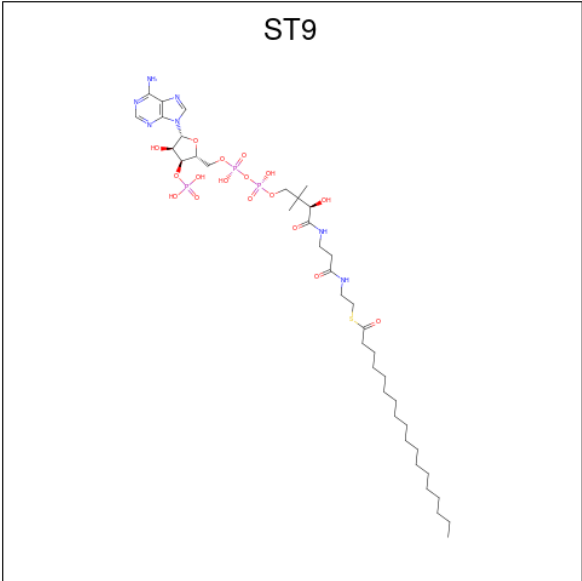
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ARG	-	expression tag	UNP A0A0D6G5A8
A	-1	GLY	-	expression tag	UNP A0A0D6G5A8
A	0	SER	-	expression tag	UNP A0A0D6G5A8
A	447	ALA	GLU	engineered mutation	UNP A0A0D6G5A8
B	-2	ARG	-	expression tag	UNP A0A0D6G5A8
B	-1	GLY	-	expression tag	UNP A0A0D6G5A8
B	0	SER	-	expression tag	UNP A0A0D6G5A8
B	447	ALA	GLU	engineered mutation	UNP A0A0D6G5A8

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	B	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		

- Molecule 3 is STEAROYL-COENZYME A (CCD ID: ST9) (formula: C₃₉H₇₀N₇O₁₇P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	S	0	0
			133	39	66	7	17	3	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	P	S	0	0
			133	39	66	7	17	3	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	557	Total	O	0	0
			557	557		

Continued on next page...

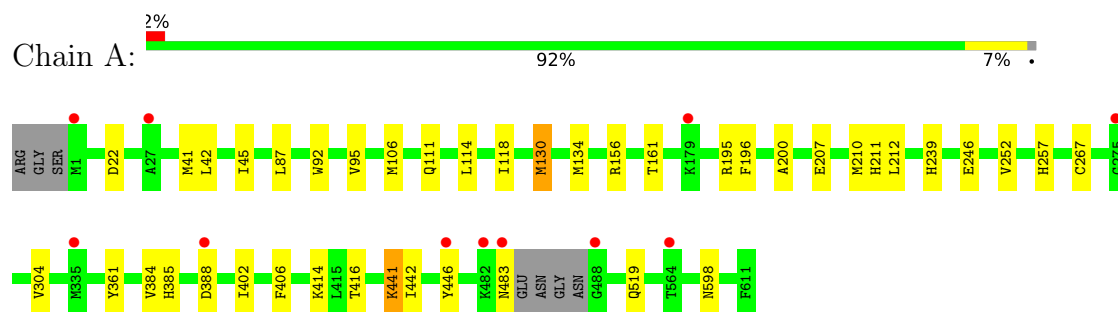
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	593	Total 593	O 593	0	0

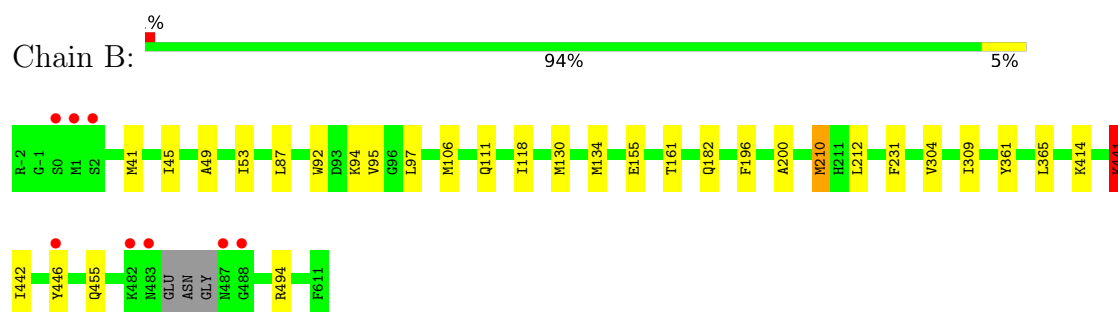
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Acyl-CoA dehydrogenase



- Molecule 1: Acyl-CoA dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.93Å 206.59Å 74.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.68 – 1.77 45.68 – 1.77	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.68-1.77) 98.6 (45.68-1.77)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 1.77Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.149 , 0.171 0.151 , 0.172	Depositor DCC
R_{free} test set	7292 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 43.8	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	20114	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: ST9, FAD, MG, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.66	1/4742 (0.0%)	0.68	1/6415 (0.0%)
1	B	0.68	2/4771 (0.0%)	0.68	0/6453
All	All	0.67	3/9513 (0.0%)	0.68	1/12868 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	MET	SD-CE	5.91	1.94	1.79
1	A	210	MET	SD-CE	5.71	1.93	1.79
1	B	441	LYS	C-O	-5.12	1.17	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	MET	CB-CG-SD	5.12	128.07	112.70

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	A	4650	4578	4583	44	0
1	B	4679	4607	4610	39	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	31	31	5	0
2	B	53	30	31	4	0
3	A	67	66	66	3	0
3	B	67	66	65	6	0
4	A	5	0	0	2	0
4	B	10	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	557	0	0	10	0
6	B	593	0	0	5	0
All	All	10736	9378	9386	87	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 (87) 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)
3:B:702:ST9:O4B	3:B:702:ST9:C1B	1.64	1.20
1:B:134:MET:SD	1:B:212:LEU:HD12	2.05	0.97
1:A:442:ILE:HD11	2:A:701:FAD:HM82	1.48	0.95
1:A:134:MET:SD	1:A:212:LEU:HD12	2.06	0.94
1:B:442:ILE:HG13	1:B:446:TYR:CD2	2.06	0.90
1:B:442:ILE:HD11	2:B:701:FAD:HM82	1.54	0.87
1:A:442:ILE:HG13	1:A:446:TYR:CD2	2.11	0.86
1:A:130:MET:HE2	3:A:702:ST9:H12A	1.59	0.85
4:A:703:SO4:S	6:A:801:HOH:O	2.39	0.80
4:A:703:SO4:O4	6:A:801:HOH:O	2.03	0.75
1:A:598:ASN:ND2	6:A:802:HOH:O	2.19	0.75
1:B:304:VAL:HG22	1:B:446:TYR:HE1	1.50	0.74
1:A:304:VAL:HG22	1:A:446:TYR:HE1	1.53	0.73
1:A:442:ILE:CD1	2:A:701:FAD:HM82	2.18	0.73
1:A:442:ILE:HG13	1:A:446:TYR:CE2	2.24	0.73
1:B:134:MET:HE2	3:B:702:ST9:H11A	1.70	0.73
1:A:134:MET:HE2	3:A:702:ST9:H11A	1.70	0.72
1:A:134:MET:SD	1:A:212:LEU:CD1	2.78	0.72
1:B:442:ILE:HG13	1:B:446:TYR:CE2	2.24	0.71
1:A:442:ILE:HD11	2:A:701:FAD:C8M	2.21	0.70
1:B:442:ILE:CD1	2:B:701:FAD:HM82	2.22	0.70
1:B:442:ILE:CG1	1:B:446:TYR:CD2	2.75	0.69
1:B:134:MET:SD	1:B:212:LEU:CD1	2.80	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:MET:CE	1:A:212:LEU:HD12	2.24	0.67
1:B:304:VAL:CG2	1:B:446:TYR:HE1	2.08	0.65
1:B:442:ILE:HD11	2:B:701:FAD:C8M	2.26	0.64
1:A:442:ILE:CG1	1:A:446:TYR:CD2	2.80	0.64
1:A:195:ARG:NH2	6:A:806:HOH:O	2.33	0.60
1:A:304:VAL:CG2	1:A:446:TYR:HE1	2.16	0.59
1:B:494:ARG:NH2	6:B:809:HOH:O	2.35	0.59
1:B:134:MET:CE	1:B:212:LEU:HD12	2.33	0.58
1:B:155:GLU:OE1	6:B:801:HOH:O	2.17	0.58
1:A:134:MET:HE3	1:A:212:LEU:HD12	1.86	0.57
1:B:442:ILE:CG1	1:B:446:TYR:CE2	2.87	0.57
1:B:455:GLN:OE1	6:B:802:HOH:O	2.17	0.57
1:A:41:MET:HE1	1:A:106:MET:HE1	1.86	0.57
1:A:442:ILE:CG1	1:A:446:TYR:CE2	2.87	0.57
1:A:441:LYS:HA	1:A:441:LYS:HE2	1.88	0.55
1:B:53:ILE:CD1	1:B:87:LEU:HD13	2.40	0.51
1:A:87:LEU:HD11	1:A:118:ILE:HD13	1.91	0.51
1:A:252:VAL:HG13	1:A:267:CYS:HB3	1.93	0.51
1:B:41:MET:HE1	1:B:106:MET:HE1	1.93	0.50
1:B:45:ILE:HD12	1:B:92:TRP:CE3	2.47	0.50
1:A:519:GLN:CD	6:A:817:HOH:O	2.55	0.49
1:A:246:GLU:HG3	6:A:1016:HOH:O	2.11	0.49
1:A:304:VAL:HG22	1:A:446:TYR:CE1	2.41	0.49
1:A:45:ILE:HD12	1:A:92:TRP:CE3	2.48	0.48
1:A:239:HIS:HD2	6:A:1242:HOH:O	1.95	0.48
1:B:455:GLN:CD	6:B:802:HOH:O	2.56	0.47
1:A:196:PHE:O	2:A:701:FAD:C4X	2.63	0.47
1:B:182:GLN:NE2	6:B:814:HOH:O	2.46	0.47
1:B:95:VAL:HG12	1:B:111:GLN:HG3	1.97	0.47
1:B:304:VAL:CG2	1:B:446:TYR:CE1	2.94	0.47
1:A:200:ALA:HB3	1:A:267:CYS:HB2	1.96	0.46
1:B:304:VAL:HG22	1:B:446:TYR:CE1	2.41	0.46
1:A:156:ARG:NE	1:A:207:GLU:OE2	2.49	0.45
1:B:49:ALA:HA	1:B:53:ILE:HB	1.98	0.45
1:B:45:ILE:HD11	1:B:118:ILE:HD11	1.98	0.45
1:A:257:HIS:HE1	6:A:1221:HOH:O	1.98	0.45
1:B:161:THR:HG21	1:B:200:ALA:HA	1.98	0.44
1:A:416:THR:HG23	1:B:441:LYS:HE3	2.00	0.44
1:A:22:ASP:OD1	1:A:22:ASP:N	2.48	0.44
1:B:361:TYR:CE2	1:B:414:LYS:HE3	2.53	0.44
1:A:388:ASP:OD2	6:A:803:HOH:O	2.21	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:VAL:CG2	1:A:446:TYR:CE1	2.99	0.43
2:A:701:FAD:C9	2:A:701:FAD:H2'	2.48	0.43
1:B:446:TYR:CD1	3:B:702:ST9:H3	2.54	0.43
1:A:519:GLN:NE2	6:A:817:HOH:O	2.52	0.43
1:A:95:VAL:HG12	1:A:111:GLN:HG3	2.00	0.43
1:B:196:PHE:O	2:B:701:FAD:C4X	2.67	0.43
1:B:309:ILE:HG12	1:B:365:LEU:HB3	2.00	0.43
1:B:94:LYS:HG2	1:B:97:LEU:HD22	2.02	0.42
1:B:134:MET:HE2	3:B:702:ST9:C11	2.45	0.42
1:A:361:TYR:CE2	1:A:414:LYS:HE3	2.55	0.42
1:A:87:LEU:HD11	1:A:118:ILE:CD1	2.50	0.42
1:A:161:THR:HG21	1:A:200:ALA:HA	2.02	0.42
1:B:53:ILE:HD11	1:B:87:LEU:HD13	2.02	0.41
1:A:384:VAL:HG23	1:A:385:HIS:CD2	2.56	0.41
1:B:210:MET:HE3	1:B:231:PHE:CE1	2.55	0.41
1:A:42:LEU:HD23	1:A:114:LEU:HD23	2.03	0.41
3:B:702:ST9:O5B	3:B:702:ST9:H8AA	2.21	0.41
1:B:53:ILE:HD13	1:B:87:LEU:HD13	2.02	0.41
1:B:210:MET:HE3	1:B:231:PHE:HE1	1.86	0.41
1:A:402:ILE:O	1:A:406:PHE:HB3	2.21	0.41
1:A:130:MET:HE2	3:A:702:ST9:H9	2.03	0.40
1:B:130:MET:HB3	3:B:702:ST9:H12A	2.03	0.40
1:A:161:THR:HG1	1:A:211:HIS:HA	1.86	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	603/614 (98%)	594 (98%)	9 (2%)	0	100	100
1	B	607/614 (99%)	596 (98%)	11 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1210/1228 (98%)	1190 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	475/480 (99%)	473 (100%)	2 (0%)	84	80
1	B	478/480 (100%)	477 (100%)	1 (0%)	87	84
All	All	953/960 (99%)	950 (100%)	3 (0%)	86	83

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	441	LYS
1	A	483	ASN
1	B	441	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	HIS
1	A	318	ASN
1	A	334	GLN
1	A	483	ASN
1	A	598	ASN
1	B	182	GLN
1	B	376	GLN
1	B	396	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	FAD	A	701	-	58,58,58	0.63	2 (3%)	85,89,89	0.54	0
4	SO4	B	703	5	4,4,4	0.54	0	6,6,6	0.44	0
3	ST9	A	702	-	67,69,69	2.28	11 (16%)	89,95,95	1.74	14 (15%)
2	FAD	B	701	-	58,58,58	0.84	2 (3%)	85,89,89	0.62	0
4	SO4	A	703	5	4,4,4	0.90	0	6,6,6	0.63	0
3	ST9	B	702	-	67,69,69	2.47	15 (22%)	89,95,95	1.80	17 (19%)
4	SO4	B	704	-	4,4,4	0.25	0	6,6,6	0.21	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	FAD	A	701	-	-	3/34/50/50	0/6/6/6
3	ST9	B	702	-	-	8/68/84/84	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ST9	A	702	-	-	9/68/84/84	0/3/3/3
2	FAD	B	701	-	-	4/34/50/50	0/6/6/6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	ST9	O4B-C1B	9.84	1.64	1.42
3	B	702	ST9	C2B-C1B	-7.88	1.28	1.53
3	A	702	ST9	O4B-C1B	7.33	1.58	1.42
3	B	702	ST9	O4B-C4B	-6.86	1.29	1.45
3	A	702	ST9	C2B-C1B	-6.73	1.32	1.53
3	A	702	ST9	O4B-C4B	-6.09	1.31	1.45
3	A	702	ST9	P3B-O3B	5.92	1.69	1.59
3	A	702	ST9	P1A-O3A	5.81	1.65	1.59
3	B	702	ST9	C2-C1	5.26	1.56	1.50
3	A	702	ST9	C5P-N4P	4.57	1.44	1.33
3	A	702	ST9	C2-C1	4.54	1.55	1.50
3	B	702	ST9	C5P-N4P	4.51	1.44	1.33
3	B	702	ST9	O2B-C2B	4.27	1.53	1.43
3	B	702	ST9	C9P-N8P	4.13	1.43	1.33
3	B	702	ST9	P1A-O3A	4.07	1.63	1.59
3	A	702	ST9	C9P-N8P	3.85	1.42	1.33
3	B	702	ST9	P3B-O3B	3.73	1.66	1.59
3	A	702	ST9	C6A-N6A	3.46	1.43	1.34
2	B	701	FAD	C4X-N5	3.28	1.37	1.30
2	B	701	FAD	P-O3P	3.27	1.63	1.59
3	B	702	ST9	C6A-N6A	3.23	1.42	1.34
2	A	701	FAD	C4X-N5	2.78	1.36	1.30
3	B	702	ST9	O3B-C3B	-2.77	1.34	1.44
3	A	702	ST9	O2B-C2B	2.63	1.49	1.43
3	A	702	ST9	C8A-N7A	2.48	1.36	1.31
3	B	702	ST9	P2A-O6A	2.32	1.68	1.59
3	B	702	ST9	P2A-O3A	2.17	1.61	1.59
2	A	701	FAD	C5X-N5	-2.15	1.35	1.39
3	B	702	ST9	C2A-N1A	2.13	1.37	1.33
3	B	702	ST9	C6P-C5P	2.02	1.55	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	ST9	N3A-C2A-N1A	-5.44	120.35	128.58
3	B	702	ST9	C5A-C4A-N3A	-5.38	119.31	126.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	ST9	N3A-C2A-N1A	-5.34	120.49	128.58
3	A	702	ST9	O2-C1-S1P	-5.21	116.06	122.68
3	B	702	ST9	O2-C1-C2	5.16	129.93	123.98
3	B	702	ST9	O2-C1-S1P	-4.77	116.62	122.68
3	A	702	ST9	O2-C1-C2	4.48	129.14	123.98
3	A	702	ST9	C5A-C4A-N3A	-4.11	121.06	126.72
3	A	702	ST9	N9A-C8A-N7A	-4.09	108.14	113.94
3	A	702	ST9	P3B-O3B-C3B	-3.78	113.35	123.43
3	B	702	ST9	N3A-C4A-N9A	3.55	133.20	127.17
3	B	702	ST9	N6A-C6A-N1A	-3.45	110.70	118.38
3	B	702	ST9	C2A-N3A-C4A	3.36	120.03	111.83
3	B	702	ST9	N9A-C8A-N7A	-3.19	109.41	113.94
3	A	702	ST9	C2A-N3A-C4A	3.12	119.45	111.83
3	A	702	ST9	C3B-C2B-C1B	3.08	106.67	99.89
3	A	702	ST9	C6P-C7P-N8P	-3.01	105.59	112.00
3	B	702	ST9	C3B-C2B-C1B	2.94	106.36	99.89
3	A	702	ST9	O3B-P3B-O9A	-2.86	99.13	109.33
3	B	702	ST9	C6P-C7P-N8P	-2.84	105.96	112.00
3	A	702	ST9	N6A-C6A-N1A	-2.70	112.37	118.38
3	A	702	ST9	N3A-C4A-N9A	2.68	131.73	127.17
3	B	702	ST9	C4A-N9A-C8A	2.63	108.50	105.74
3	A	702	ST9	C2P-C3P-N4P	-2.51	107.18	112.41
3	A	702	ST9	C4A-N9A-C8A	2.49	108.36	105.74
3	B	702	ST9	P3B-O3B-C3B	-2.45	116.88	123.43
3	B	702	ST9	O5P-C5P-C6P	2.32	126.23	122.02
3	B	702	ST9	O5P-C5P-N4P	-2.30	118.51	123.03
3	B	702	ST9	C3P-N4P-C5P	-2.17	118.78	122.82
3	B	702	ST9	CDP-CBP-CCP	2.15	111.77	108.22
3	B	702	ST9	C4-C3-C2	-2.09	105.45	113.13

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	C2'-C1'-N10-C10
2	B	701	FAD	C2'-C1'-N10-C10
3	B	702	ST9	C6-C7-C8-C9
3	A	702	ST9	C5-C6-C7-C8
3	B	702	ST9	C5-C6-C7-C8
3	A	702	ST9	C6-C7-C8-C9
3	B	702	ST9	C11-C10-C9-C8
3	A	702	ST9	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	702	ST9	C12-C13-C14-C15
3	B	702	ST9	C7-C8-C9-C10
2	A	701	FAD	O2'-C2'-C3'-C4'
3	A	702	ST9	C3-C4-C5-C6
2	B	701	FAD	O2'-C2'-C3'-C4'
2	B	701	FAD	C1'-C2'-C3'-O3'
3	A	702	ST9	CEP-CBP-CCP-O6A
3	A	702	ST9	C12-C13-C14-C15
2	B	701	FAD	O2'-C2'-C3'-O3'
2	A	701	FAD	O2'-C2'-C3'-O3'
3	B	702	ST9	C9-C10-C11-C12
3	B	702	ST9	C15-C16-C17-C18
3	A	702	ST9	CDP-CBP-CCP-O6A
3	A	702	ST9	N8P-C9P-CAP-OAP
3	B	702	ST9	N8P-C9P-CAP-OAP
3	A	702	ST9	CAP-CBP-CCP-O6A

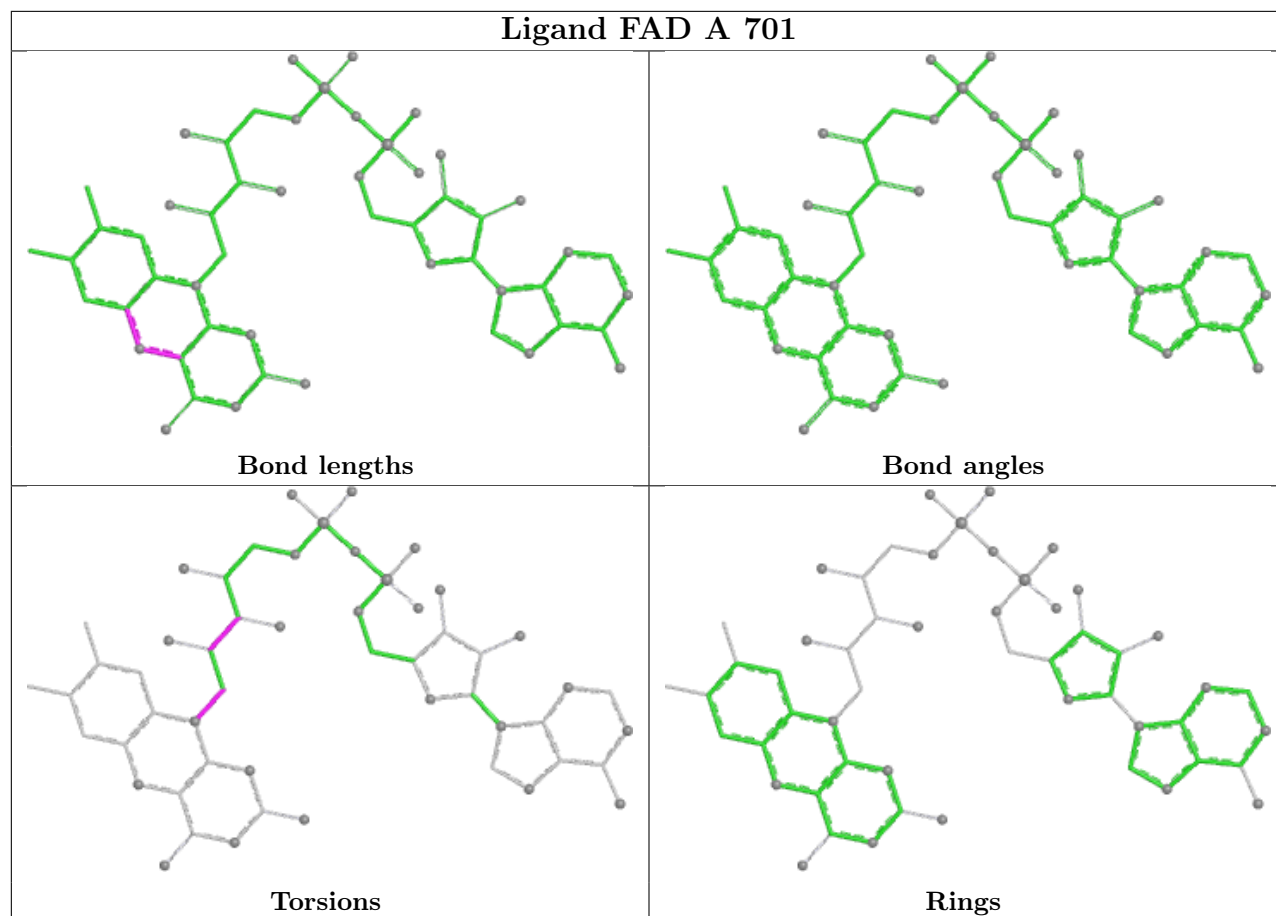
There are no ring outliers.

5 monomers are involved in 20 short contacts:

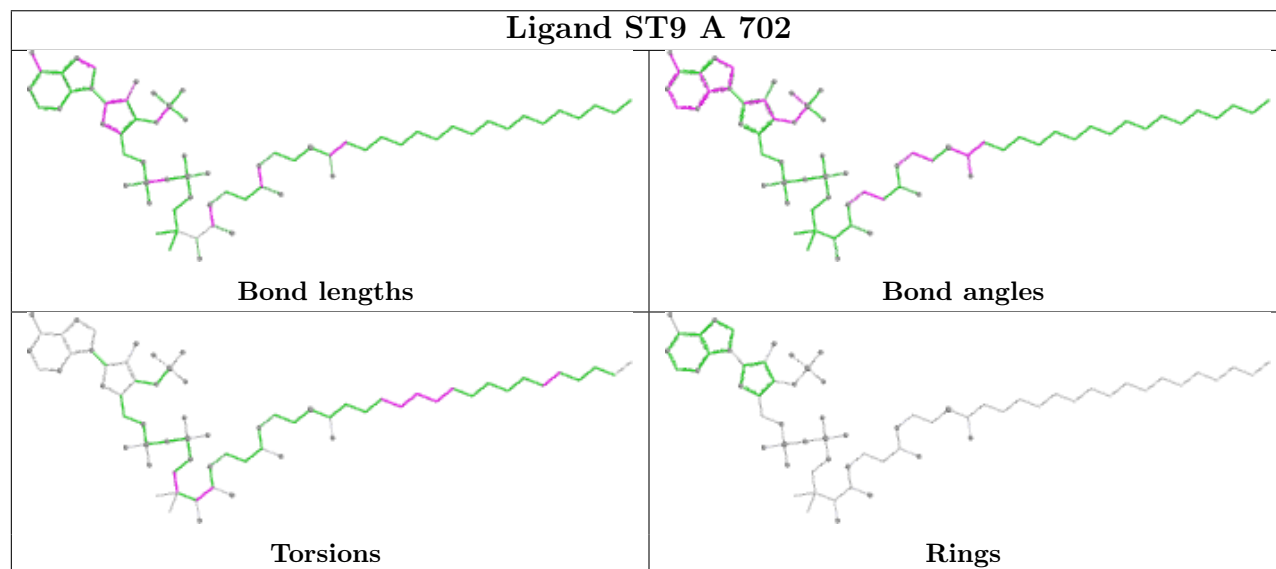
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FAD	5	0
3	A	702	ST9	3	0
2	B	701	FAD	4	0
4	A	703	SO4	2	0
3	B	702	ST9	6	0

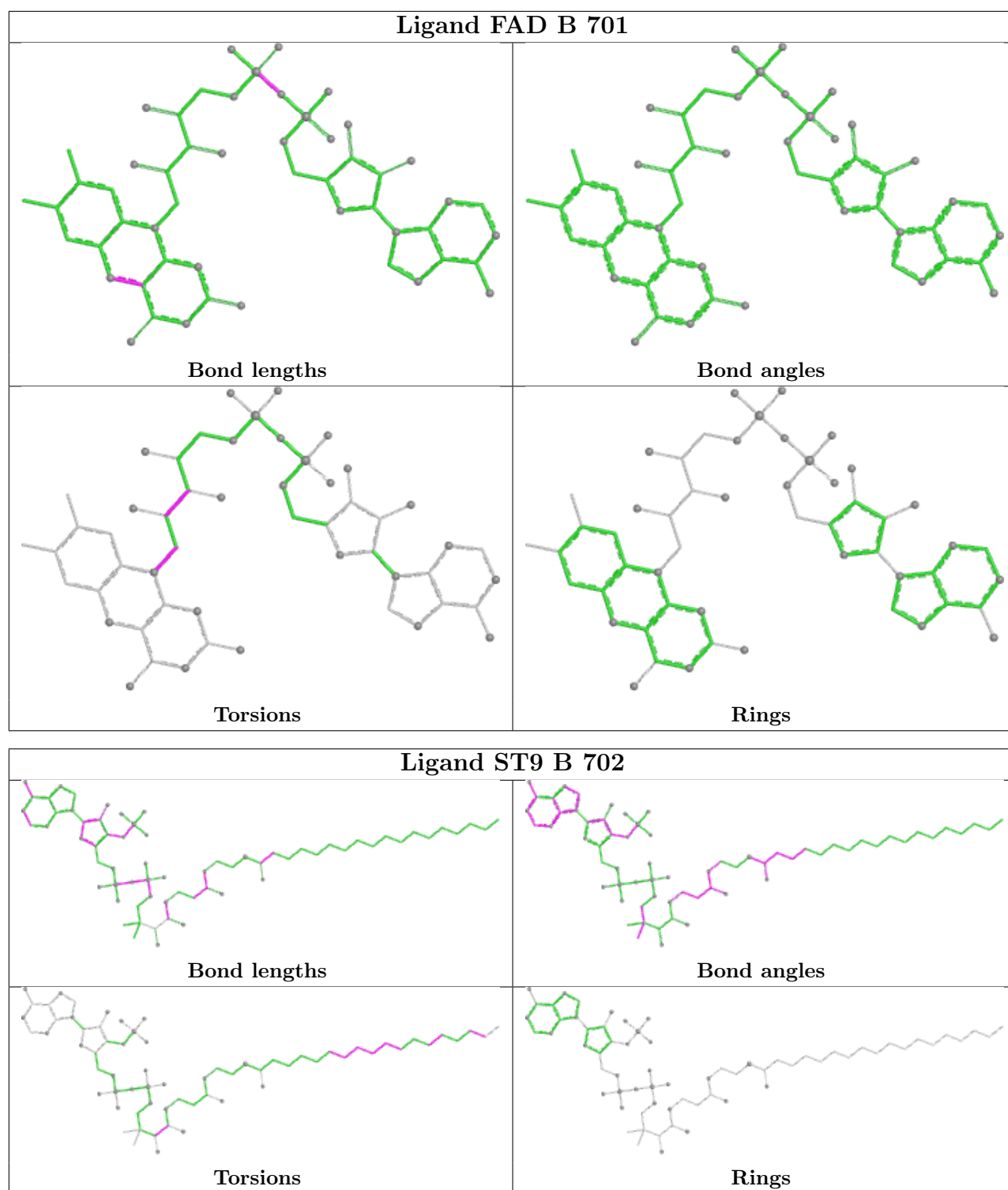
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FAD A 701



Ligand ST9 A 702





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	607/614 (98%)	-0.50	11 (1%) 67 74	14, 23, 43, 82	0
1	B	611/614 (99%)	-0.59	8 (1%) 75 81	14, 22, 41, 128	0
All	All	1218/1228 (99%)	-0.54	19 (1%) 70 77	14, 22, 42, 128	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	487	ASN	6.1
1	B	483	ASN	5.4
1	A	1	MET	5.1
1	A	388	ASP	5.0
1	B	2	SER	4.9
1	A	483	ASN	4.8
1	B	446	TYR	4.0
1	A	446	TYR	3.9
1	A	488	GLY	3.2
1	B	482	LYS	3.0
1	A	179	LYS	2.9
1	B	1	MET	2.6
1	A	335	MET	2.5
1	A	482	LYS	2.4
1	A	27	ALA	2.3
1	B	488	GLY	2.2
1	A	564	THR	2.1
1	B	0	SER	2.1
1	A	275	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

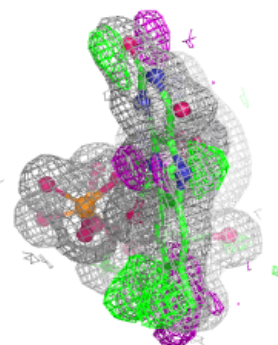
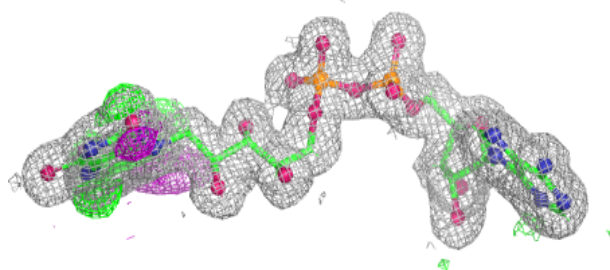
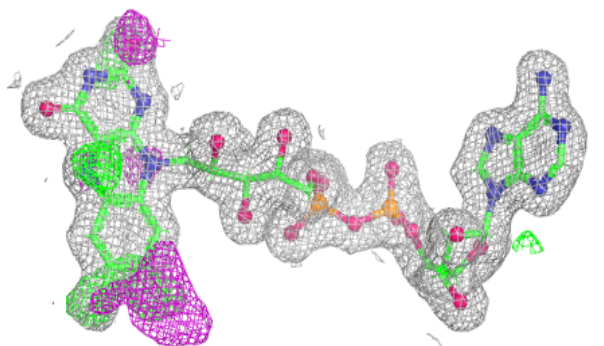
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	703	5/5	0.88	0.10	28,30,48,72	0
4	SO4	A	703	5/5	0.90	0.10	29,33,47,67	0
4	SO4	B	704	5/5	0.91	0.10	30,60,80,82	0
2	FAD	A	701	53/53	0.96	0.07	13,19,28,41	0
2	FAD	B	701	53/53	0.97	0.06	12,17,30,30	0
3	ST9	A	702	67/67	0.97	0.09	18,28,91,101	0
3	ST9	B	702	67/67	0.97	0.08	18,30,59,97	0
5	MG	A	704	1/1	0.97	0.06	32,32,32,32	0
5	MG	B	705	1/1	0.97	0.05	31,31,31,31	0

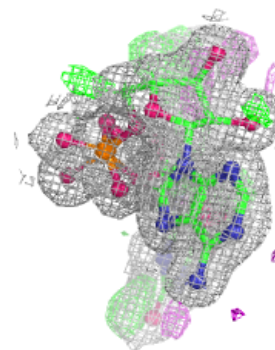
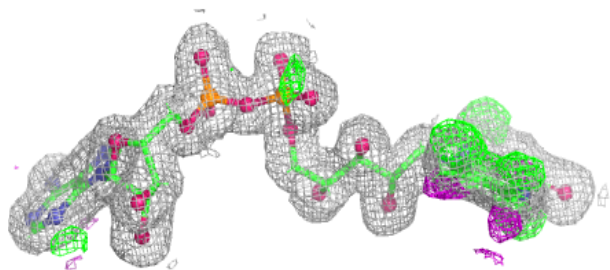
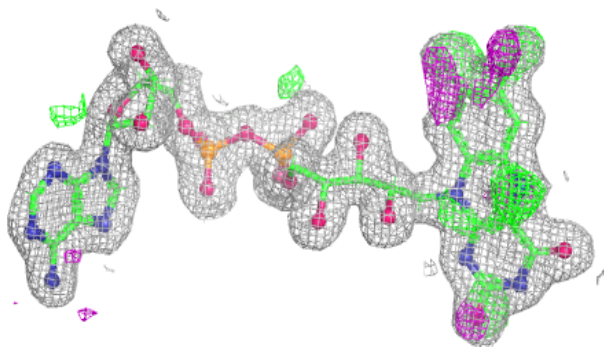
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 701:

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

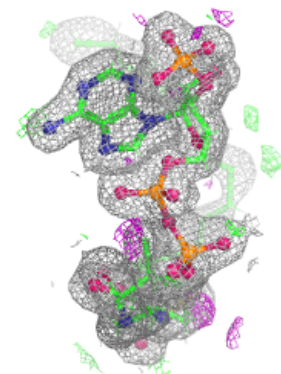
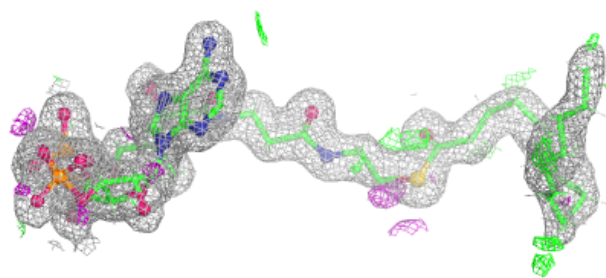
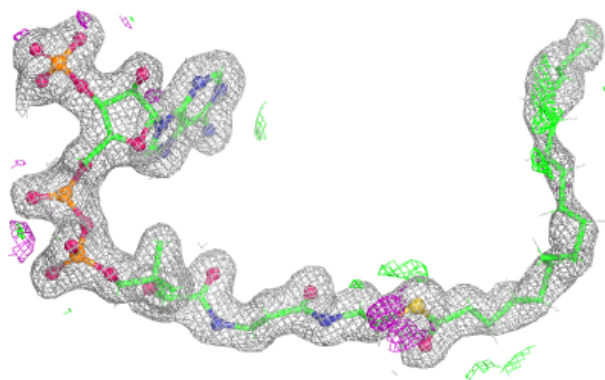
**Electron density around FAD B 701:**

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

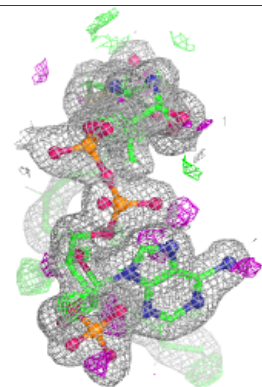
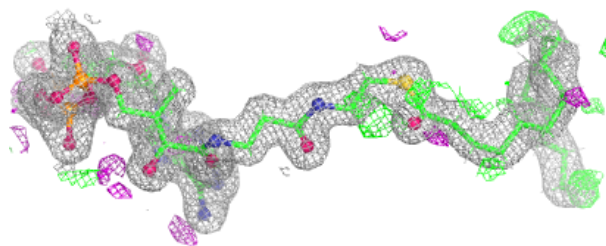
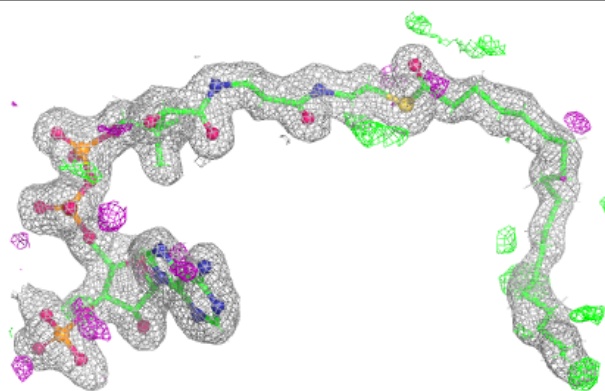


Electron density around ST9 A 702:

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

**Electron density around ST9 B 702:**

$2mF_o-DF_c$ (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.