



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:10 PM UTC

PDB ID : 3E9Y / pdb_00003e9y
Title : Arabidopsis thaliana acetohydroxyacid synthase in complex with monosulfuron
Authors : Guddat, L.W.; Duggleby, R.G.; Wang, J.-G.; Li, Z.-M.
Deposited on : 2008-08-24
Resolution : 3.00 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

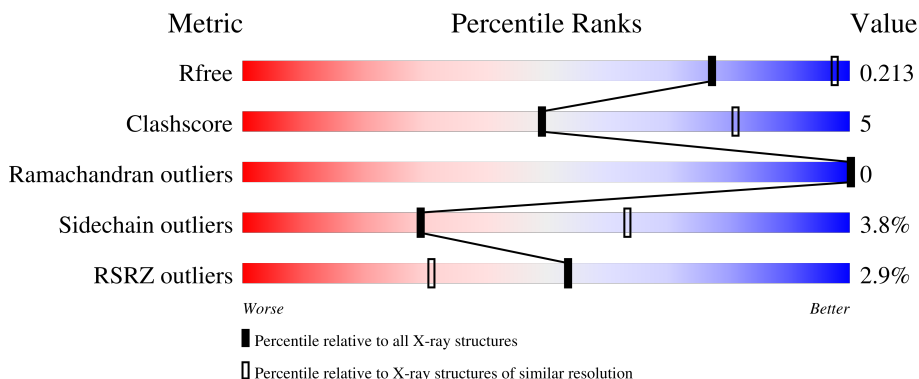
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	584	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4646 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.

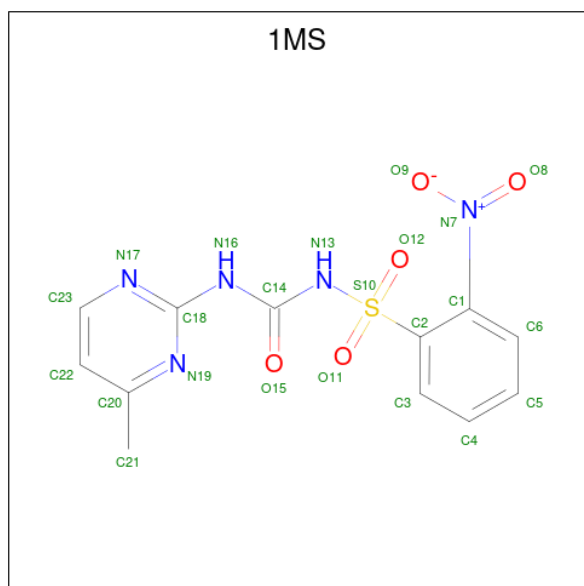
- Molecule 1 is a protein called Acetolactate synthase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	4	0
			4462	2831	767	839	25			

There is a discrepancy between the modelled and reference sequences:

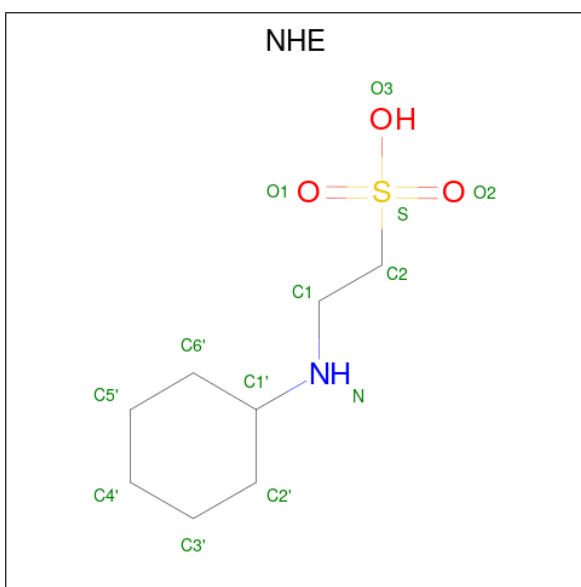
Chain	Residue	Modelled	Actual	Comment	Reference
A	330	THR	SER	conflict	UNP P17597

- Molecule 2 is N-[(4-methylpyrimidin-2-yl)carbamoyl]-2-nitrobenzenesulfonamide (CCD ID: 1MS) (formula: C₁₂H₁₁N₅O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			23	12	5	5	1		

- Molecule 3 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: C₈H₁₇NO₃S).

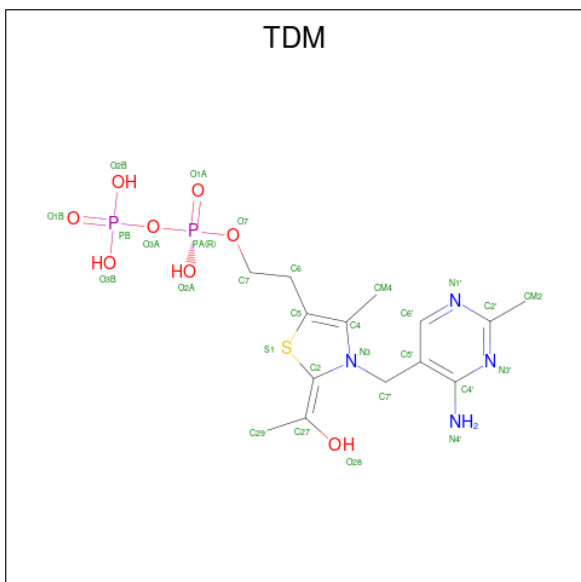


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

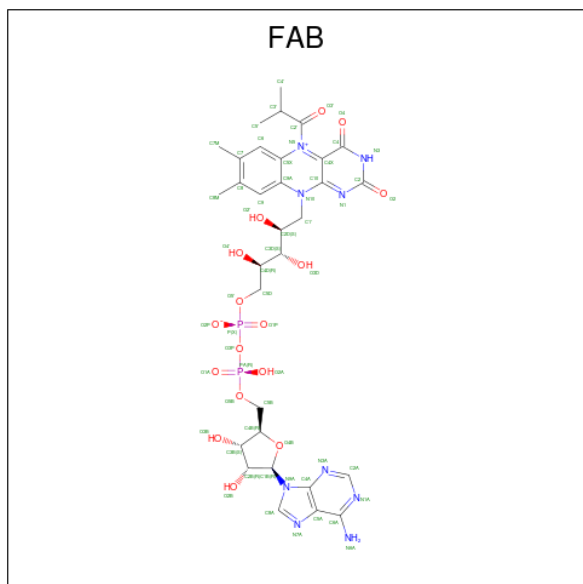
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 2-[(2E)-3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-(1-H YDROXYETHYLIDENE)-4-METHYL-2,3-DIHYDRO-1,3-THIAZOL-5-YL]ETHYL TRIHYDROGEN DIPHOSPHATE (CCD ID: TDM) (formula: C₁₄H₂₂N₄O₈P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	
			29	14	4	8	2	1	
								0	0

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE-N5-ISOBUTYL KETONE (CCD ID: FAB) (formula: $C_{31}H_{39}N_9O_{16}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P		
			53	27	9	15	2		
								0	0

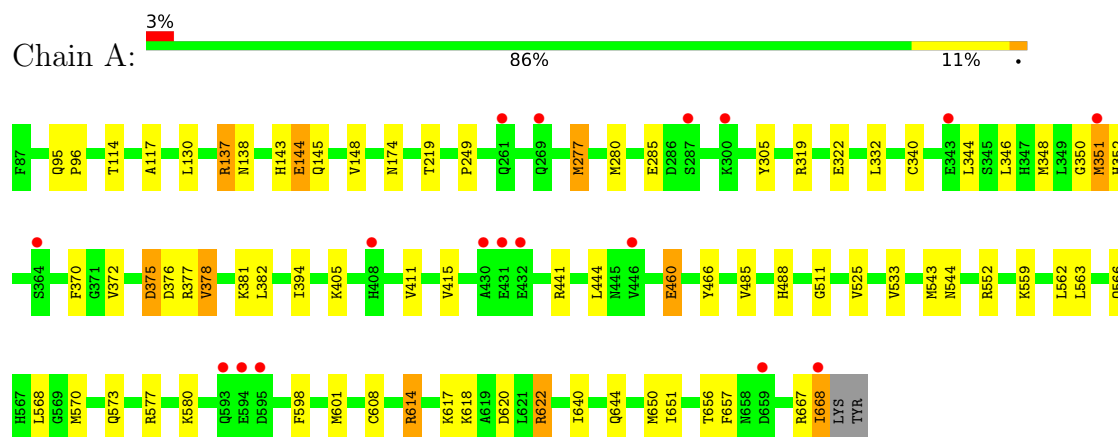
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	65	Total	O		
			65	65		
					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: Acetolactate synthase, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	178.87Å 178.87Å 186.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	89.44 – 3.00 89.44 – 3.00	Depositor EDS
% Data completeness (in resolution range)	80.4 (89.44-3.00) 80.3 (89.44-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.223 (Not available) , 0.213	Depositor DCC
R_{free} test set	1448 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4646	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: CSD, MG, TDM, NHE, 1MS, FAB

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	0.45	0/4556	0.81	1/6190 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	382	LEU	N-CA-C	5.05	116.79	111.28

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	4462	0	4426	45	0
2	A	23	0	11	1	0
3	A	13	0	17	0	0
4	A	1	0	0	0	0
5	A	29	0	19	5	0
6	A	53	0	31	0	0
7	A	65	0	0	2	1
All	All	4646	0	4504	49	1

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 (49) 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:A:622:ARG:HH11	1:A:622:ARG:HG3	1.33	0.92
1:A:644:GLN:HG3	1:A:667:ARG:HG3	1.63	0.81
1:A:143:HIS:HD2	1:A:145:GLN:H	1.30	0.77
1:A:145:GLN:HE21	1:A:544:ASN:HD21	1.33	0.77
1:A:566:GLN:HE22	1:A:598:PHE:H	1.33	0.74
1:A:622:ARG:HH11	1:A:622:ARG:CG	1.98	0.74
1:A:277:MET:HG3	1:A:280:MET:HE2	1.70	0.74
1:A:573:GLN:HE21	1:A:650:MET:HE2	1.53	0.74
1:A:577:ARG:HD2	1:A:650:MET:HE1	1.74	0.70
1:A:543:MET:O	7:A:766:HOH:O	2.12	0.68
1:A:332:LEU:HA	1:A:348:MET:HE2	1.80	0.61
1:A:117:ALA:H	1:A:138:ASN:HD21	1.46	0.61
1:A:350:GLY:HA2	1:A:378:VAL:HA	1.83	0.60
1:A:656:THR:HG22	1:A:657:PHE:N	2.21	0.56
2:A:695:1MS:N13	2:A:695:1MS:O9	2.39	0.55
1:A:394:ILE:HG12	1:A:411:VAL:HB	1.91	0.53
1:A:614:ARG:HD2	1:A:640:ILE:HD11	1.91	0.52
1:A:570:MET:HB3	5:A:700:TDM:S1	2.50	0.52
1:A:376:ASP:OD2	1:A:377:ARG:NH1	2.39	0.51
5:A:700:TDM:C27	5:A:700:TDM:H4'1	2.23	0.51
1:A:144:GLU:HG3	1:A:174:ASN:HB2	1.93	0.50
1:A:375:ASP:OD2	1:A:377:ARG:HB2	2.12	0.50
1:A:656:THR:HG22	1:A:657:PHE:H	1.76	0.49
1:A:622:ARG:CG	1:A:622:ARG:NH1	2.66	0.48
1:A:351[A]:MET:HG3	1:A:651:ILE:O	2.13	0.48
1:A:485:VAL:HG21	1:A:511:GLY:C	2.39	0.47
1:A:144:GLU:H	1:A:144:GLU:HG2	1.37	0.46
1:A:622:ARG:HG3	1:A:622:ARG:NH1	2.13	0.46
1:A:562:LEU:HD21	1:A:601:MET:HG3	1.98	0.45
1:A:346:LEU:HD21	1:A:444:LEU:HD13	1.97	0.45
1:A:305:TYR:CE2	1:A:372:VAL:HG21	2.52	0.44
1:A:460:GLU:HA	1:A:460:GLU:OE2	2.18	0.44
1:A:668:ILE:H	1:A:668:ILE:HD13	1.82	0.44
1:A:114:THR:HG21	1:A:525:VAL:HG11	2.01	0.43
1:A:319:ARG:HA	1:A:322:GLU:HG2	2.01	0.43
1:A:552:ARG:HD3	1:A:552:ARG:O	2.19	0.43
1:A:466:TYR:CE2	1:A:618:LYS:HE3	2.53	0.43
1:A:533:VAL:HG22	1:A:559:LYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:LEU:HD22	5:A:700:TDM:HM43	2.02	0.42
1:A:95:GLN:HA	1:A:96:PRO:HD3	1.87	0.42
5:A:700:TDM:H7'1	5:A:700:TDM:O28	2.19	0.42
1:A:370:PHE:HB3	1:A:415:VAL:HG21	2.02	0.42
1:A:488:HIS:HB2	1:A:563:LEU:HD12	2.02	0.42
5:A:700:TDM:H4'1	5:A:700:TDM:C2	2.33	0.41
1:A:617:LYS:HB2	1:A:620:ASP:OD2	2.20	0.41
1:A:552:ARG:HG2	1:A:608:CYS:O	2.21	0.41
1:A:352:HIS:CE1	1:A:650:MET:HG3	2.56	0.41
1:A:137:ARG:HD2	7:A:717:HOH:O	2.21	0.40
1:A:219:THR:HA	1:A:249:PRO:HG2	2.04	0.40

All (1) 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)
7:A:766:HOH:O	7:A:766:HOH:O[10_665]	1.87	0.33

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	583/584 (100%)	575 (99%)	8 (1%)	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%)	456 (96%)	19 (4%)	28	62

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	LEU
1	A	137	ARG
1	A	144	GLU
1	A	148	VAL
1	A	277	MET
1	A	285	GLU
1	A	344	LEU
1	A	351[A]	MET
1	A	351[B]	MET
1	A	375	ASP
1	A	378	VAL
1	A	381	LYS
1	A	405	LYS
1	A	441	ARG
1	A	460	GLU
1	A	580	LYS
1	A	614	ARG
1	A	622	ARG
1	A	668	ILE

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

Mol	Chain	Res	Type
1	A	138	ASN
1	A	143	HIS
1	A	145	GLN
1	A	174	ASN
1	A	261	GLN
1	A	269	GLN
1	A	288	HIS
1	A	312	ASN
1	A	566	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
1	CSD	A	340	1	4,7,8	2.11	1 (25%)	1,8,10	2.08	1 (100%)

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
1	CSD	A	340	1	-	0/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	340	CSD	OD1-SG	-3.63	1.44	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	CSD	OD1-SG-CB	2.08	109.43	105.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
5	TDM	A	700	4	28,30,30	2.70	9 (32%)	37,45,45	2.34	11 (29%)
6	FAB	A	701	-	58,58,63	2.03	8 (13%)	85,89,97	1.92	19 (22%)
3	NHE	A	696	-	13,13,13	1.52	1 (7%)	16,17,17	1.10	1 (6%)
2	1MS	A	695	-	24,24,24	4.73	11 (45%)	31,34,34	3.39	14 (45%)

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
5	TDM	A	700	4	-	2/17/21/21	0/2/2/2
6	FAB	A	701	-	-	10/34/50/58	0/6/6/6
3	NHE	A	696	-	-	2/7/15/15	0/1/1/1
2	1MS	A	695	-	-	6/17/19/19	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	695	1MS	C3-C2	12.75	1.54	1.39
2	A	695	1MS	O8-N7	11.80	1.43	1.22
2	A	695	1MS	C4-C3	8.95	1.54	1.38
6	A	701	FAB	C2A-N1A	8.36	1.48	1.33
6	A	701	FAB	C2A-N3A	8.34	1.48	1.33
5	A	700	TDM	C2-N3	8.28	1.54	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	700	TDM	O28-C27	8.20	1.53	1.31
2	A	695	1MS	C1-N7	-6.08	1.34	1.45
2	A	695	1MS	O12-S10	5.65	1.50	1.43
2	A	695	1MS	O11-S10	5.24	1.49	1.43
2	A	695	1MS	C21-C20	-4.88	1.39	1.50
6	A	701	FAB	C4X-N5	4.48	1.40	1.30
3	A	696	NHE	C2-S	4.16	1.83	1.77
5	A	700	TDM	PB-O1B	3.64	1.61	1.50
6	A	701	FAB	C10-N1	3.59	1.40	1.33
6	A	701	FAB	C4A-N3A	3.37	1.40	1.34
6	A	701	FAB	C5A-N7A	-3.24	1.33	1.39
2	A	695	1MS	C18-N16	-3.19	1.34	1.38
2	A	695	1MS	C20-N19	3.11	1.40	1.34
5	A	700	TDM	C5-C4	2.92	1.41	1.35
5	A	700	TDM	CM4-C4	2.91	1.54	1.49
5	A	700	TDM	PA-O3A	2.62	1.62	1.59
2	A	695	1MS	C14-N13	-2.29	1.34	1.39
2	A	695	1MS	C18-N19	2.29	1.41	1.34
6	A	701	FAB	C8A-N9A	-2.19	1.33	1.37
5	A	700	TDM	C7'-C5'	2.18	1.55	1.51
5	A	700	TDM	C29-C27	2.11	1.53	1.48
6	A	701	FAB	C4A-N9A	-2.07	1.33	1.37
5	A	700	TDM	C4-N3	-2.03	1.35	1.39

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	701	FAB	N3A-C2A-N1A	-10.96	112.00	128.58
5	A	700	TDM	C5-S1-C2	9.42	96.24	90.80
2	A	695	1MS	O12-S10-O11	-9.26	108.28	119.52
2	A	695	1MS	C23-N17-C18	8.21	122.28	115.42
2	A	695	1MS	N17-C18-N19	-7.45	119.22	126.42
2	A	695	1MS	C2-S10-N13	7.04	114.72	105.96
6	A	701	FAB	C5A-C4A-N3A	-4.35	120.73	126.72
6	A	701	FAB	C2A-N3A-C4A	4.29	122.30	111.83
5	A	700	TDM	C5'-C7'-N3	-4.17	108.10	113.14
2	A	695	1MS	C4-C5-C6	3.68	124.78	120.24
2	A	695	1MS	C18-N16-C14	-3.37	126.87	130.34
6	A	701	FAB	C4-N3-C2	-3.34	119.72	125.64
5	A	700	TDM	C7'-C5'-C4'	3.33	125.93	122.56
5	A	700	TDM	N1'-C2'-N3'	-3.32	120.00	125.53
5	A	700	TDM	C6'-N1'-C2'	3.30	121.49	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	701	FAB	N9A-C8A-N7A	-3.18	109.43	113.94
2	A	695	1MS	C5-C4-C3	-3.12	116.38	120.24
5	A	700	TDM	C29-C27-C2	-2.99	120.58	124.73
5	A	700	TDM	CM2-C2'-N1'	2.95	120.34	117.20
6	A	701	FAB	C5A-N7A-C8A	2.93	108.06	103.45
6	A	701	FAB	C4A-C5A-N7A	-2.90	107.27	110.58
2	A	695	1MS	C5-C6-C1	2.89	123.36	118.60
6	A	701	FAB	C9A-C5X-N5	-2.85	119.43	122.45
2	A	695	1MS	C3-C2-C1	2.85	122.62	119.89
5	A	700	TDM	C7'-C5'-C6'	-2.84	117.23	121.30
6	A	701	FAB	N3A-C4A-N9A	2.78	131.89	127.17
3	A	696	NHE	O2-S-C2	2.76	110.89	106.73
6	A	701	FAB	C10-C4X-N5	-2.74	119.21	124.81
2	A	695	1MS	C3-C2-S10	-2.70	113.64	117.51
6	A	701	FAB	C4X-C4-N3	2.62	119.93	113.25
2	A	695	1MS	C21-C20-N19	2.50	120.34	116.56
2	A	695	1MS	C22-C23-N17	-2.43	120.99	123.97
6	A	701	FAB	C2A-N1A-C6A	2.33	122.56	118.73
2	A	695	1MS	N16-C18-N17	2.33	122.63	116.48
6	A	701	FAB	C6A-C5A-C4A	2.32	120.34	117.18
6	A	701	FAB	O4-C4-C4X	-2.29	120.50	126.53
6	A	701	FAB	C4X-C10-N10	2.25	119.71	116.48
5	A	700	TDM	O2B-PB-O3A	2.20	112.02	104.64
6	A	701	FAB	C4-C4X-C10	2.15	120.61	116.93
2	A	695	1MS	C4-C3-C2	-2.09	115.01	118.76
5	A	700	TDM	O28-C27-C29	2.09	118.75	114.60
6	A	701	FAB	O3P-P-O1P	-2.06	104.49	110.70
5	A	700	TDM	C7'-N3-C2	-2.04	123.61	126.13
6	A	701	FAB	C4A-N9A-C8A	2.03	107.87	105.74
6	A	701	FAB	C4X-C10-N1	-2.03	119.61	124.59

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	696	NHE	N-C1-C2-S
5	A	700	TDM	PA-O3A-PB-O2B
6	A	701	FAB	C1'-C2D-C3D-C4D
6	A	701	FAB	O4'-C4D-C5D-O5'
6	A	701	FAB	C3D-C4D-C5D-O5'
2	A	695	1MS	C14-N13-S10-O11
6	A	701	FAB	O2'-C2D-C3D-C4D

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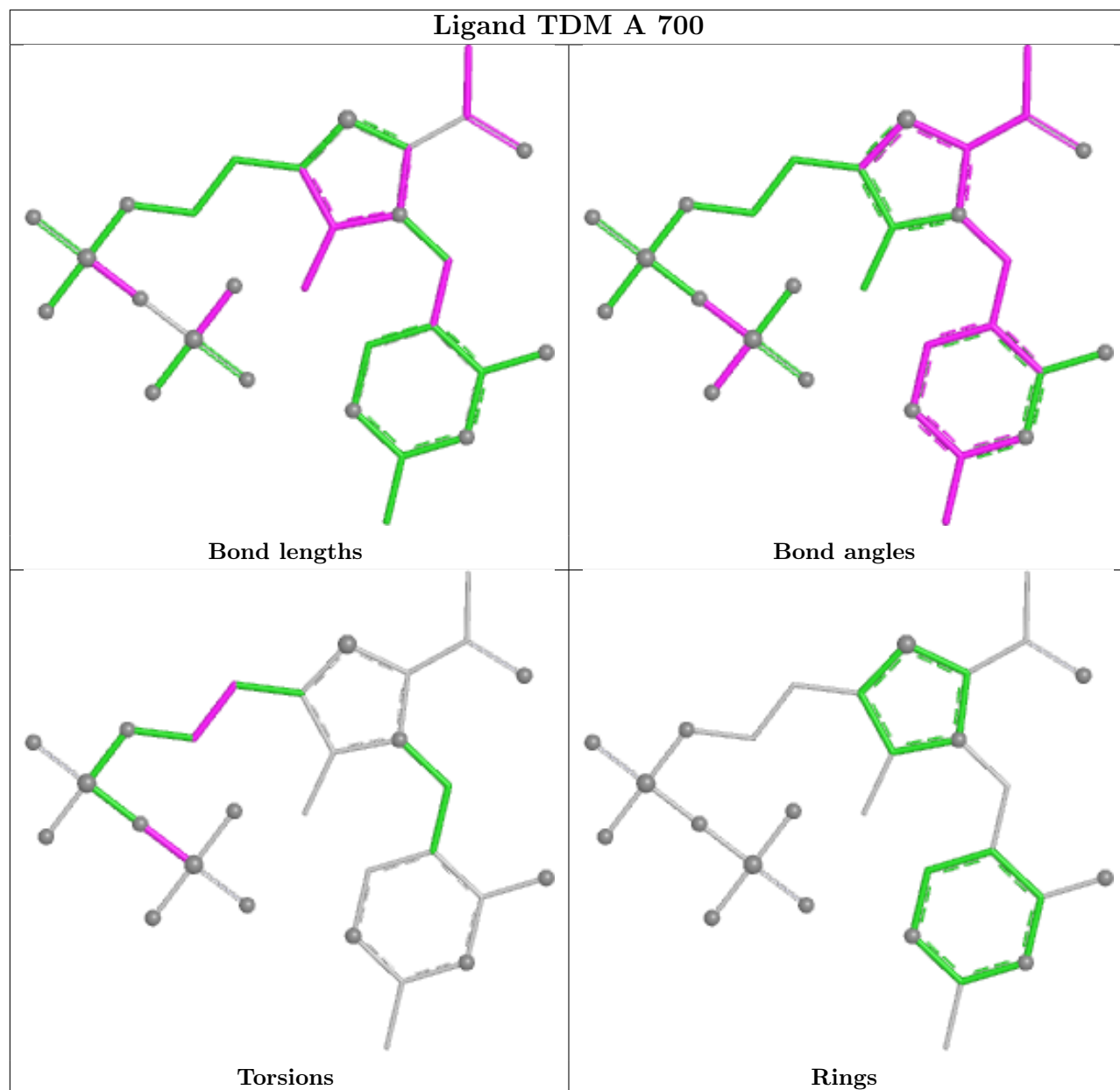
Mol	Chain	Res	Type	Atoms
2	A	695	1MS	C1-C2-S10-O12
6	A	701	FAB	O2'-C2D-C3D-O3D
3	A	696	NHE	C2-C1-N-C1'
2	A	695	1MS	C3-C2-S10-O12
5	A	700	TDM	C5-C6-C7-O7
6	A	701	FAB	O3D-C3D-C4D-C5D
6	A	701	FAB	C1'-C2D-C3D-O3D
2	A	695	1MS	C1-C2-S10-N13
6	A	701	FAB	O4B-C4B-C5B-O5B
2	A	695	1MS	N13-C14-N16-C18
6	A	701	FAB	N10-C1'-C2D-O2'
6	A	701	FAB	C2D-C3D-C4D-O4'
2	A	695	1MS	O15-C14-N16-C18

There are no ring outliers.

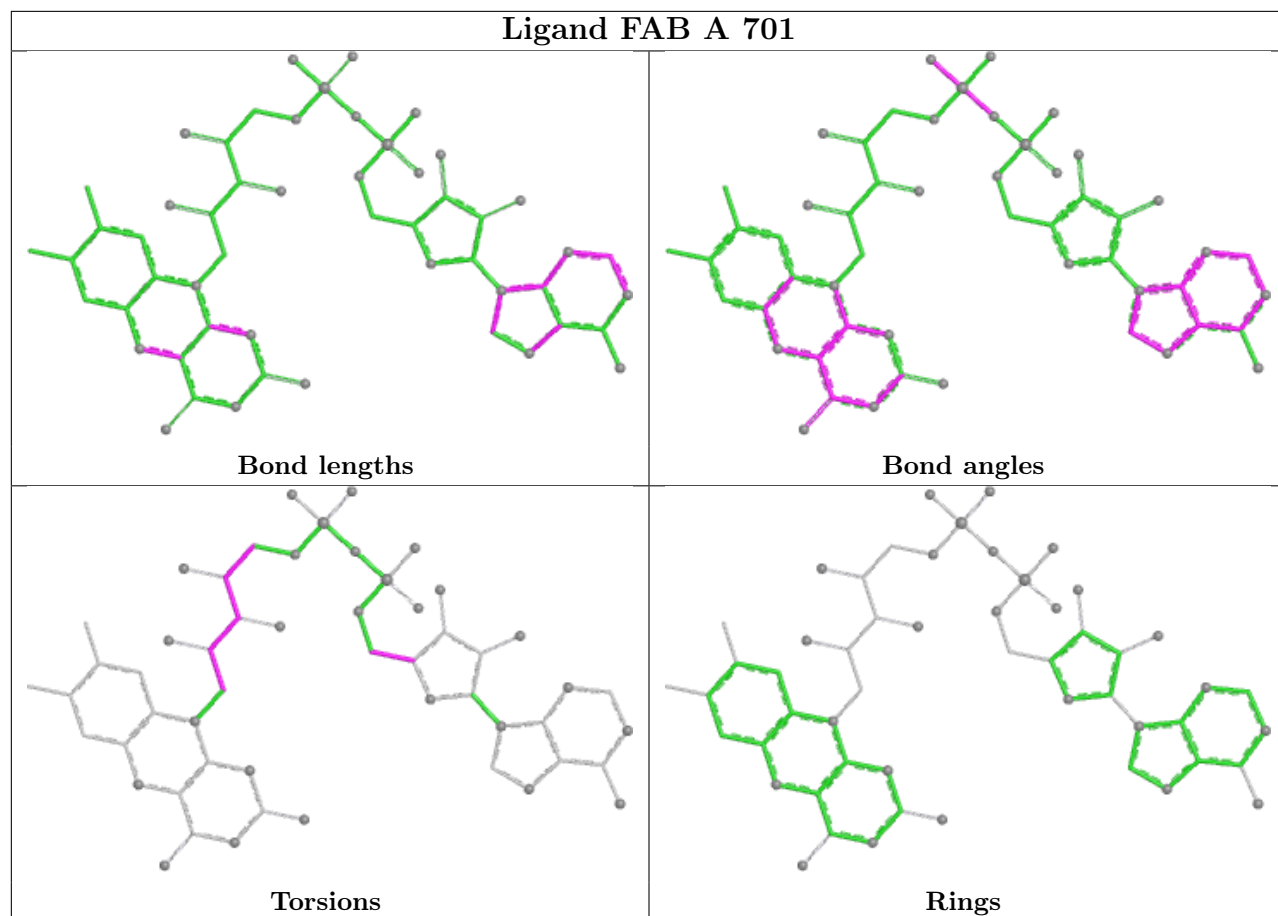
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	700	TDM	5	0
2	A	695	1MS	1	0

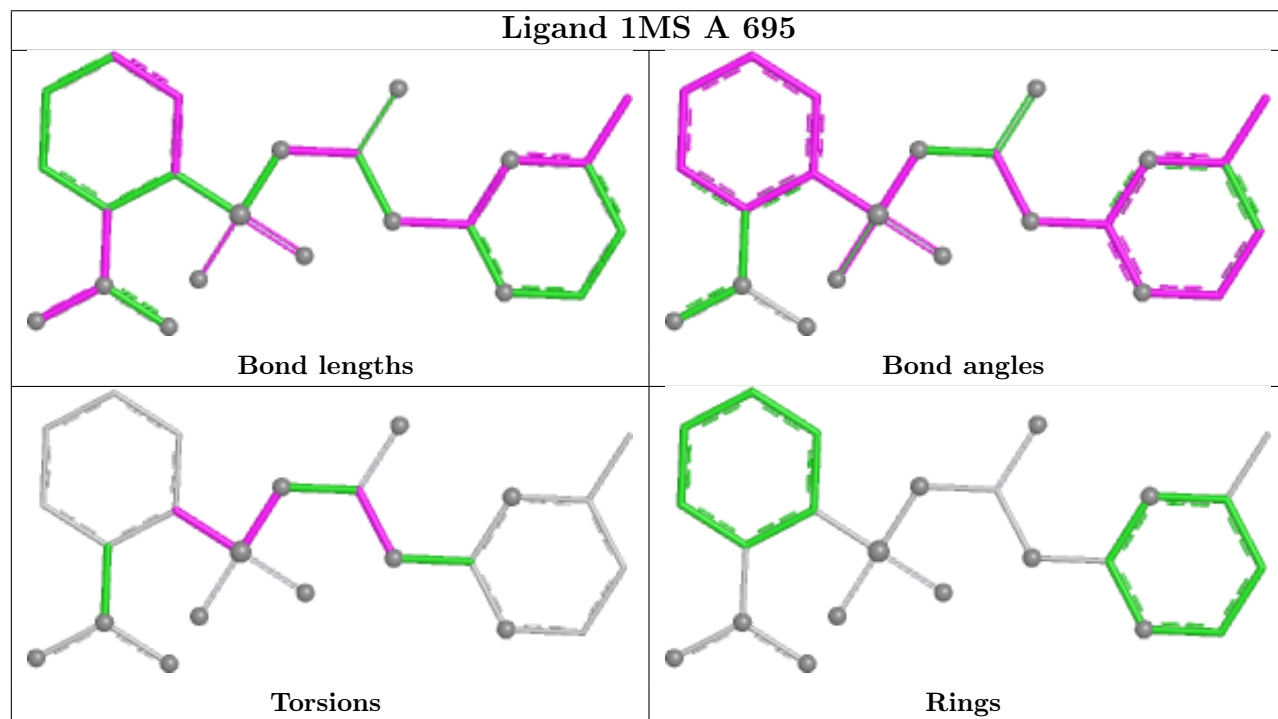
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand FAB A 701



Ligand 1MS A 695



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	581/584 (99%)	0.01	17 (2%) 53 31	26, 49, 71, 79	4 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	668	ILE	7.6
1	A	430	ALA	4.9
1	A	594	GLU	4.0
1	A	351[A]	MET	3.8
1	A	343[A]	GLU	3.5
1	A	408	HIS	2.6
1	A	431	GLU	2.6
1	A	300	LYS	2.5
1	A	432	GLU	2.4
1	A	287	SER	2.2
1	A	595	ASP	2.2
1	A	659	ASP	2.2
1	A	446	VAL	2.1
1	A	269	GLN	2.1
1	A	364	SER	2.1
1	A	261	GLN	2.1
1	A	593	GLN	2.0

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

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
1	CSD	A	340	8/9	0.94	0.13	63,64,65,65	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

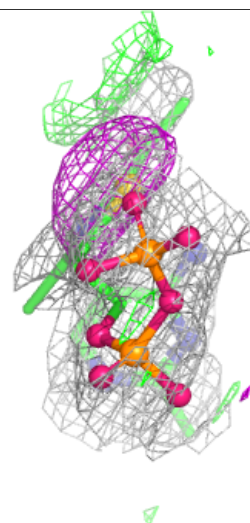
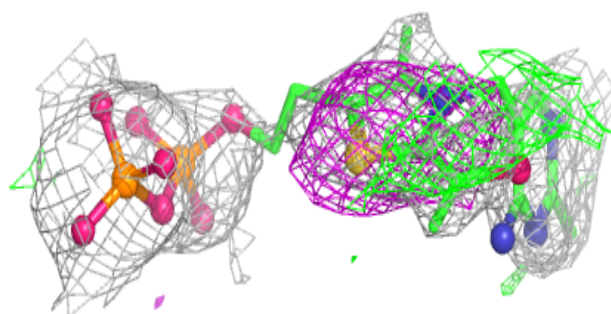
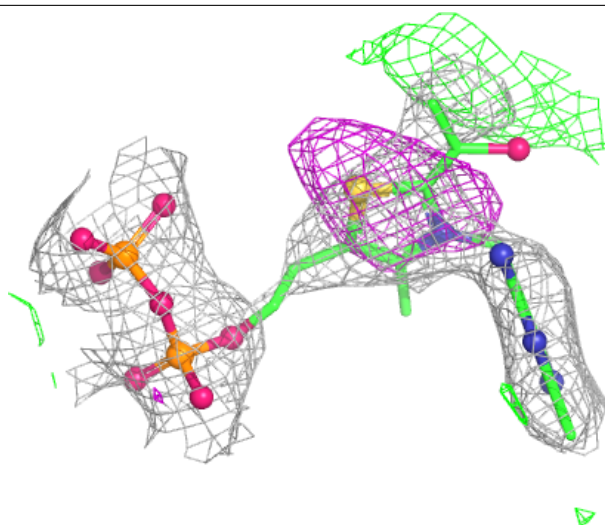
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	A	699	1/1	0.93	0.09	48,48,48,48	0
5	TDM	A	700	29/29	0.93	0.15	53,65,66,66	0
2	1MS	A	695	23/23	0.95	0.14	65,66,67,67	0
3	NHE	A	696	13/13	0.98	0.08	48,48,49,49	0
6	FAB	A	701	53/58	0.98	0.08	32,36,43,43	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.

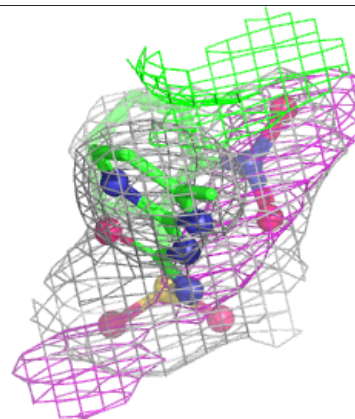
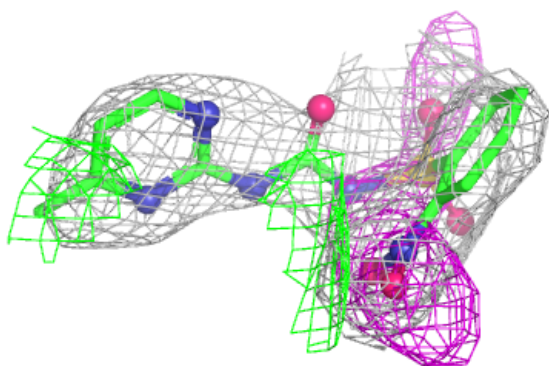
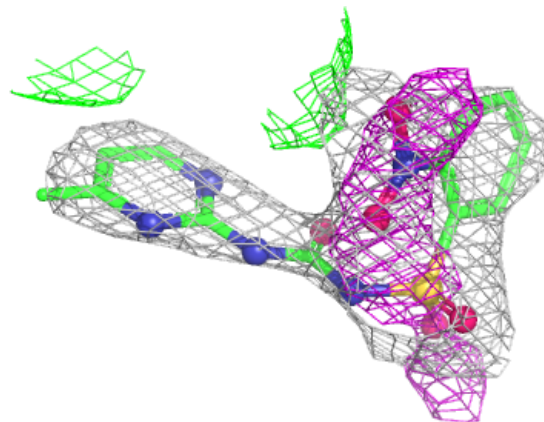
Electron density around TDM A 700:

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

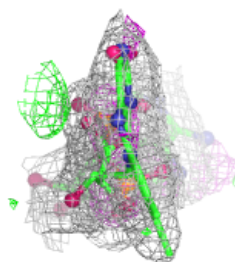
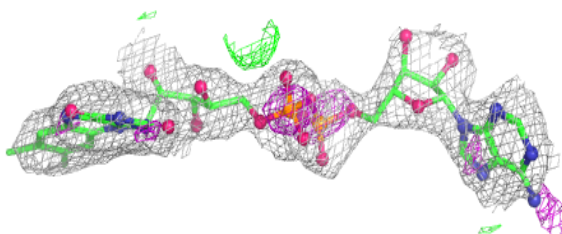
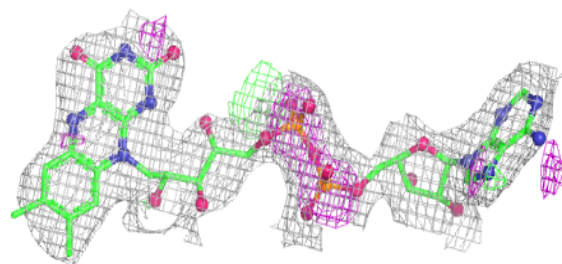


Electron density around 1MS A 695:

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

**Electron density around FAB 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.