



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2022 – 10:05 AM EDT

PDB ID : 7TZZ
Title : Crystal structure of arabidopsis thaliana acetohydroxyacid synthase P197T mutant in complex with bispyribac-sodium
Authors : Guddat, L.W.; Cheng, Y.
Deposited on : 2022-02-16
Resolution : 2.59 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 : 2.28.1
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) : 2.28.1

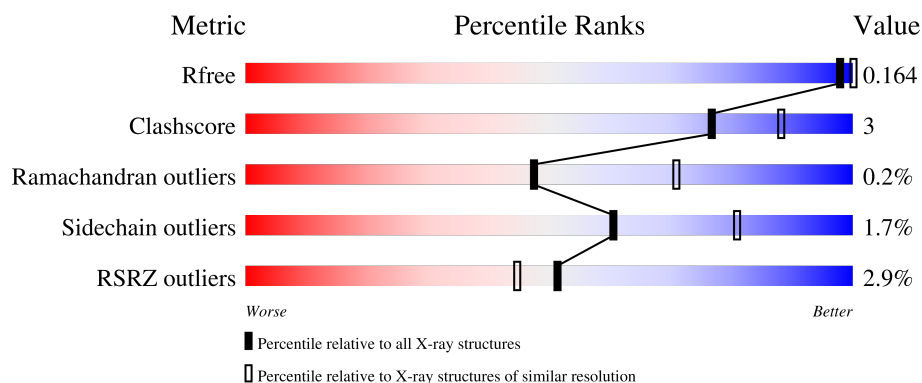
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

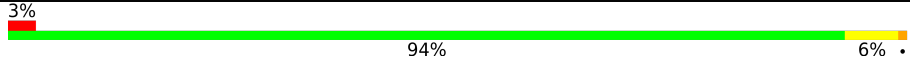
The reported resolution of this entry is 2.59 Å.

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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	582	

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
6	PO4	A	705	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 4907 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
			Total	C	N	O	S			
1	A	582	4480	2839	773	842	26	0	5	0

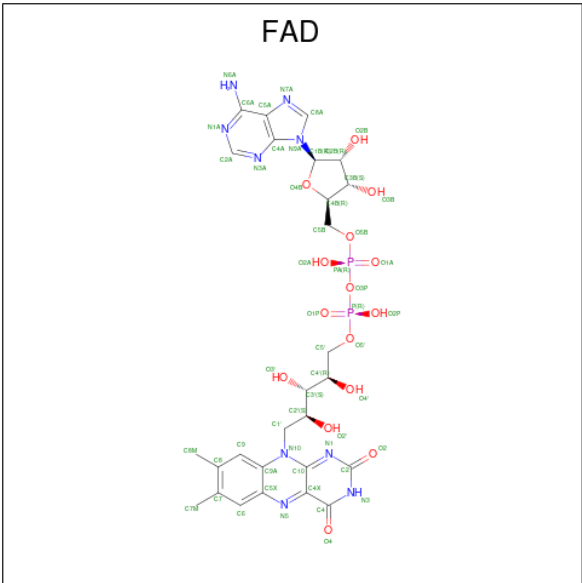
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	THR	PRO	engineered mutation	UNP P17597

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

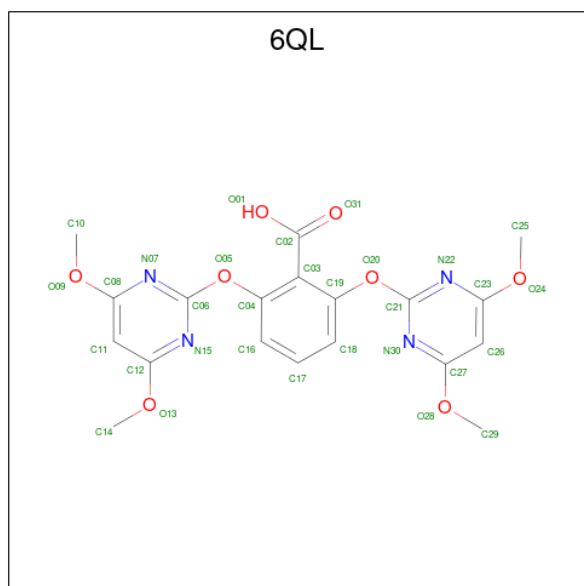
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Mg	0	0
			5	5		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



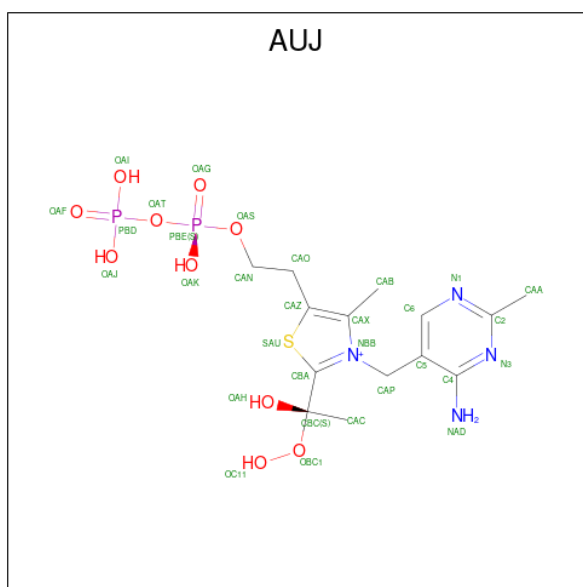
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is 2,6-bis[(4,6-dimethoxypyrimidin-2-yl)oxy]benzoic acid (three-letter code: 6QL) (formula: C₁₉H₁₈N₄O₈).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O		0	0
			31	19	4	8			

- Molecule 5 is 2-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-2-[(1 {S})-1-(dioxidanyl)-1-oxidanyl-ethyl]-4-methyl-1,3-thiazol-5-yl]ethyl phosphono hydrogen phosphate (three-letter code: AUJ) (formula: C₁₄H₂₃N₄O₁₀P₂S).



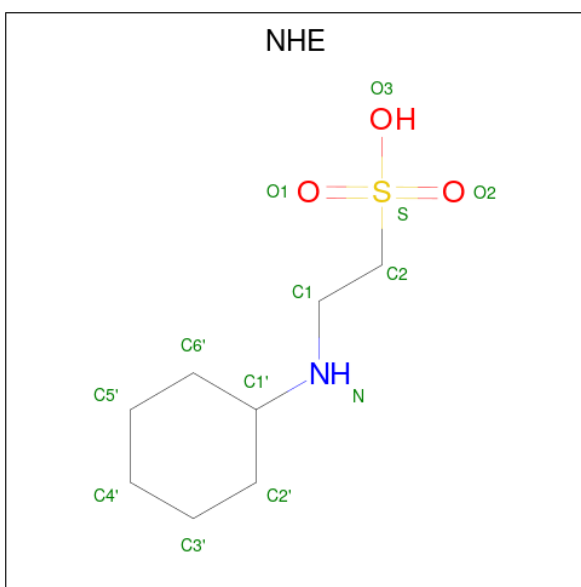
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	
			31	14	4	10	2	1	

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



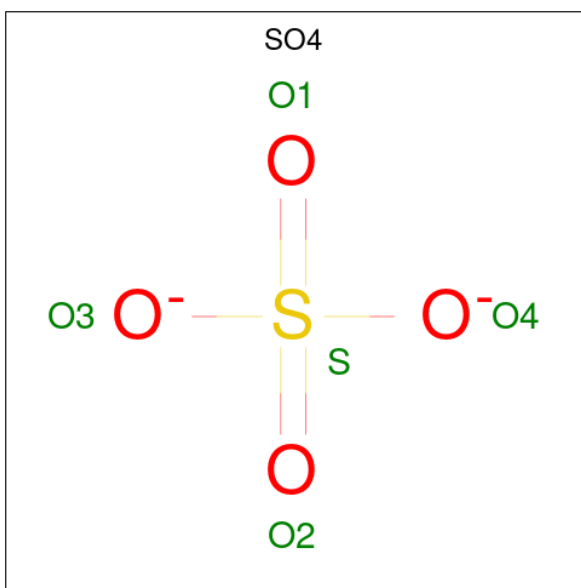
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O P		
			5 4 1		0	0

- Molecule 7 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $C_8H_{17}NO_3S$).



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

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

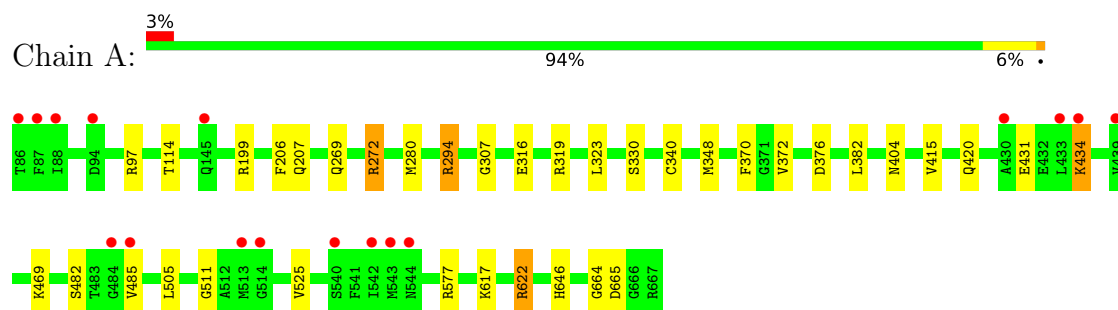
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	284	Total 284	O 284	0	0

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: 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	179.56Å 179.56Å 184.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.89 – 2.59 44.89 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.89-2.59) 99.7 (44.89-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.155 , 0.164 0.154 , 0.164	Depositor DCC
R_{free} test set	1999 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4907	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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, FAD, AUJ, PO4, SO4, 6QL, NHE

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	0.58	0/4576	0.68	1/6213 (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	272	ARG	NE-CZ-NH1	-7.09	116.75	120.30

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	4480	0	4465	25	0
2	A	5	0	0	0	0
3	A	53	0	31	0	0
4	A	31	0	0	1	0
5	A	31	0	0	0	0
6	A	5	0	0	0	0
7	A	13	0	17	1	0
8	A	5	0	0	0	0
9	A	284	0	0	2	0
All	All	4907	0	4513	27	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 3.

All (27) 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:294:ARG:HH21	1:A:294:ARG:HG3	1.23	0.99
1:A:577[B]:ARG:HH11	1:A:577[B]:ARG:HG3	1.42	0.83
1:A:294:ARG:HG3	1:A:294:ARG:NH2	1.99	0.69
1:A:622:ARG:HG2	1:A:622:ARG:HH11	1.61	0.66
1:A:577[B]:ARG:HG3	1:A:577[B]:ARG:NH1	2.14	0.62
1:A:577[B]:ARG:HH21	1:A:664:GLY:HA3	1.69	0.57
1:A:382:LEU:HD11	1:A:404:ASN:HB3	1.86	0.57
1:A:431:GLU:O	1:A:434:LYS:HD2	2.06	0.56
7:A:709:NHE:HC11	9:A:1047:HOH:O	2.06	0.54
1:A:114:THR:HG21	1:A:525:VAL:HG11	1.90	0.53
1:A:370:PHE:HB3	1:A:415:VAL:HG21	1.91	0.53
1:A:294:ARG:HH21	1:A:294:ARG:CG	2.06	0.51
4:A:703:6QL:C02	4:A:703:6QL:C21	2.90	0.50
1:A:577[B]:ARG:HH11	1:A:577[B]:ARG:CG	2.16	0.49
1:A:577[B]:ARG:NH1	1:A:577[B]:ARG:CG	2.73	0.48
1:A:316:GLU:HG2	1:A:420:GLN:HG3	1.95	0.48
1:A:577[B]:ARG:NH2	1:A:664:GLY:HA3	2.28	0.47
1:A:622:ARG:HG2	1:A:622:ARG:NH1	2.30	0.46
1:A:319:ARG:NH2	1:A:323:LEU:HD21	2.31	0.45
1:A:485:VAL:HG21	1:A:511:GLY:C	2.38	0.44
1:A:269:GLN:NE2	9:A:812:HOH:O	2.47	0.43
1:A:307:GLY:HA3	1:A:372:VAL:HG12	2.00	0.43
1:A:482:SER:HA	1:A:505:LEU:O	2.18	0.43
1:A:330:SER:O	1:A:348:MET:HA	2.20	0.41
1:A:206:PHE:CE2	1:A:207:GLN:HG3	2.56	0.41
1:A:646:HIS:CG	1:A:665:ASP:HA	2.55	0.41
1:A:617:LYS:HE2	1:A:617:LYS:HB2	1.76	0.40

There are no symmetry-related clashes.

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	584/582 (100%)	574 (98%)	9 (2%)	1 (0%)	47 71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	LYS

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	480/478 (100%)	472 (98%)	8 (2%)	60 81

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	A	199	ARG
1	A	272	ARG
1	A	280	MET
1	A	294	ARG
1	A	376	ASP
1	A	469	LYS
1	A	622	ARG

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	363	HIS
1	A	626	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	3,7,8	0.89	0	1,8,10	4.69	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	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	CSD	OD1-SG-CB	4.69	114.47	105.54

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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
6	PO4	A	705	-	4,4,4	1.84	2 (50%)	6,6,6	1.61	3 (50%)
5	AUJ	A	704	2	25,32,32	2.67	7 (28%)	30,49,49	2.27	14 (46%)
4	6QL	A	703	-	31,33,33	1.51	4 (12%)	40,45,45	3.22	17 (42%)
8	SO4	A	710	-	4,4,4	0.20	0	6,6,6	0.68	0
3	FAD	A	702	-	51,58,58	2.24	13 (25%)	60,89,89	2.01	15 (25%)
7	NHE	A	709	-	13,13,13	1.84	3 (23%)	16,17,17	3.09	4 (25%)

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
7	NHE	A	709	-	-	6/7/15/15	0/1/1/1
3	FAD	A	702	-	-	7/30/50/50	0/6/6/6
5	AUJ	A	704	2	-	4/17/26/26	0/2/2/2
4	6QL	A	703	-	-	4/16/20/20	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FAD	O4B-C1B	-7.54	1.30	1.41
3	A	702	FAD	C2B-C1B	7.36	1.64	1.53
3	A	702	FAD	O4-C4	6.57	1.41	1.24
5	A	704	AUJ	C6-N1	6.03	1.47	1.34
5	A	704	AUJ	C5-C4	5.86	1.53	1.42
5	A	704	AUJ	C2-N3	5.53	1.43	1.34
5	A	704	AUJ	CAO-CAZ	4.97	1.53	1.50
4	A	703	6QL	C03-C02	4.89	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	709	NHE	C2-S	4.83	1.84	1.77
5	A	704	AUJ	CBA-NBB	4.01	1.44	1.35
4	A	703	6QL	O09-C08	3.45	1.40	1.35
3	A	702	FAD	O3B-C3B	3.40	1.51	1.43
3	A	702	FAD	C5B-C4B	-3.31	1.41	1.51
3	A	702	FAD	C6A-N6A	3.17	1.45	1.34
4	A	703	6QL	O24-C23	3.12	1.40	1.35
5	A	704	AUJ	C4-NAD	3.06	1.41	1.34
6	A	705	PO4	P-O1	2.91	1.57	1.50
7	A	709	NHE	O1-S	2.83	1.53	1.45
4	A	703	6QL	O13-C12	2.67	1.39	1.35
3	A	702	FAD	C3B-C4B	2.51	1.59	1.53
3	A	702	FAD	C2-N1	-2.51	1.33	1.38
3	A	702	FAD	PA-O5B	2.49	1.69	1.59
7	A	709	NHE	O2-S	2.43	1.52	1.45
3	A	702	FAD	O4B-C4B	2.42	1.50	1.45
3	A	702	FAD	C4X-N5	2.29	1.36	1.33
5	A	704	AUJ	CAX-NBB	2.21	1.44	1.39
3	A	702	FAD	O2B-C2B	2.10	1.47	1.43
6	A	705	PO4	P-O4	2.09	1.60	1.54
3	A	702	FAD	C2-N3	-2.08	1.34	1.38

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	709	NHE	O1-S-C2	10.04	119.01	106.92
4	A	703	6QL	C21-N22-C23	8.53	121.58	114.03
4	A	703	6QL	C06-N07-C08	8.02	121.12	114.03
4	A	703	6QL	C06-N15-C12	7.66	120.81	114.03
5	A	704	AUJ	CAA-C2-N1	6.54	124.33	117.14
3	A	702	FAD	C2-N3-C4	6.30	120.46	115.14
3	A	702	FAD	N3A-C2A-N1A	-5.21	120.53	128.68
4	A	703	6QL	C21-N30-C27	5.12	118.56	114.03
4	A	703	6QL	C11-C08-N07	-5.02	118.22	124.08
4	A	703	6QL	C26-C23-N22	-4.86	118.41	124.08
3	A	702	FAD	C5'-C4'-C3'	-4.66	103.21	112.20
4	A	703	6QL	C11-C12-N15	-4.60	118.71	124.08
4	A	703	6QL	C12-C11-C08	4.35	119.16	115.21
7	A	709	NHE	C3'-C2'-C1'	4.16	118.94	111.11
7	A	709	NHE	C4'-C3'-C2'	4.06	119.69	111.42
3	A	702	FAD	O2'-C2'-C1'	3.68	118.46	109.59
3	A	702	FAD	C10-C4X-C4	-3.59	117.58	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	C1'-N10-C9A	3.58	121.11	118.29
3	A	702	FAD	C4A-C5A-N7A	-3.55	105.70	109.40
4	A	703	6QL	C29-O28-C27	-3.54	111.81	117.36
3	A	702	FAD	C9A-N10-C10	-3.54	117.28	121.91
5	A	704	AUJ	OAJ-PBD-OAT	3.50	116.39	104.64
5	A	704	AUJ	CAZ-CAX-NBB	3.34	114.63	107.66
4	A	703	6QL	O20-C19-C03	3.21	122.59	116.88
3	A	702	FAD	C4X-C4-N3	-3.19	119.07	123.43
4	A	703	6QL	C14-O13-C12	-3.09	112.51	117.36
3	A	702	FAD	O2'-C2'-C3'	3.07	116.57	109.10
4	A	703	6QL	C06-O05-C04	-3.03	113.33	118.07
5	A	704	AUJ	C5-C6-N1	-2.97	118.87	123.82
4	A	703	6QL	N15-C06-N07	-2.95	121.96	127.63
3	A	702	FAD	C5X-C9A-N10	2.80	119.75	117.72
5	A	704	AUJ	C5-C4-NAD	-2.78	118.24	122.19
5	A	704	AUJ	C6-N1-C2	2.78	120.69	115.96
5	A	704	AUJ	OAK-PBE-OAG	-2.73	98.75	112.24
3	A	702	FAD	C4-C4X-N5	2.64	121.62	118.60
4	A	703	6QL	C10-O09-C08	-2.63	113.24	117.36
5	A	704	AUJ	OAI-PBD-OAF	-2.61	100.47	110.68
5	A	704	AUJ	CAB-CAX-CAZ	-2.45	122.25	127.60
4	A	703	6QL	N30-C21-N22	-2.40	123.01	127.63
5	A	704	AUJ	CAO-CAZ-CAX	-2.40	125.50	127.43
5	A	704	AUJ	NAD-C4-N3	2.39	120.41	117.03
7	A	709	NHE	O3-S-O2	-2.32	105.60	111.27
3	A	702	FAD	P-O3P-PA	-2.27	125.04	132.83
5	A	704	AUJ	N1-C2-N3	-2.26	121.65	125.54
3	A	702	FAD	C2A-N1A-C6A	2.26	122.61	118.75
4	A	703	6QL	C26-C27-N30	-2.21	121.50	124.08
3	A	702	FAD	O3B-C3B-C4B	-2.17	104.79	111.05
4	A	703	6QL	C21-O20-C19	2.14	121.41	118.07
5	A	704	AUJ	CAP-C5-C6	2.14	124.78	120.69
6	A	705	PO4	O3-P-O2	-2.13	101.13	107.97
6	A	705	PO4	O4-P-O2	2.10	114.72	107.97
6	A	705	PO4	O4-P-O1	2.01	118.26	110.89
5	A	704	AUJ	CAA-C2-N3	-2.01	114.02	117.15

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	FAD	C3'-C4'-C5'-O5'

Continued on next page...

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Mol	Chain	Res	Type	Atoms
3	A	702	FAD	O4'-C4'-C5'-O5'
5	A	704	AUJ	OAS-CAN-CAO-CAZ
5	A	704	AUJ	CAN-CAO-CAZ-CAX
5	A	704	AUJ	CAC-CBC-OBC1-OC11
7	A	709	NHE	N-C1-C2-S
4	A	703	6QL	C18-C19-O20-C21
3	A	702	FAD	O2'-C2'-C3'-C4'
3	A	702	FAD	O2'-C2'-C3'-O3'
7	A	709	NHE	C1-C2-S-O3
7	A	709	NHE	C6'-C1'-N-C1
4	A	703	6QL	C03-C19-O20-C21
7	A	709	NHE	C1-C2-S-O1
3	A	702	FAD	O4B-C4B-C5B-O5B
3	A	702	FAD	O3'-C3'-C4'-C5'
4	A	703	6QL	N30-C21-O20-C19
4	A	703	6QL	N22-C21-O20-C19
3	A	702	FAD	PA-O3P-P-O5'
7	A	709	NHE	C2'-C1'-N-C1
5	A	704	AUJ	CAN-OAS-PBE-OAG
7	A	709	NHE	C1-C2-S-O2

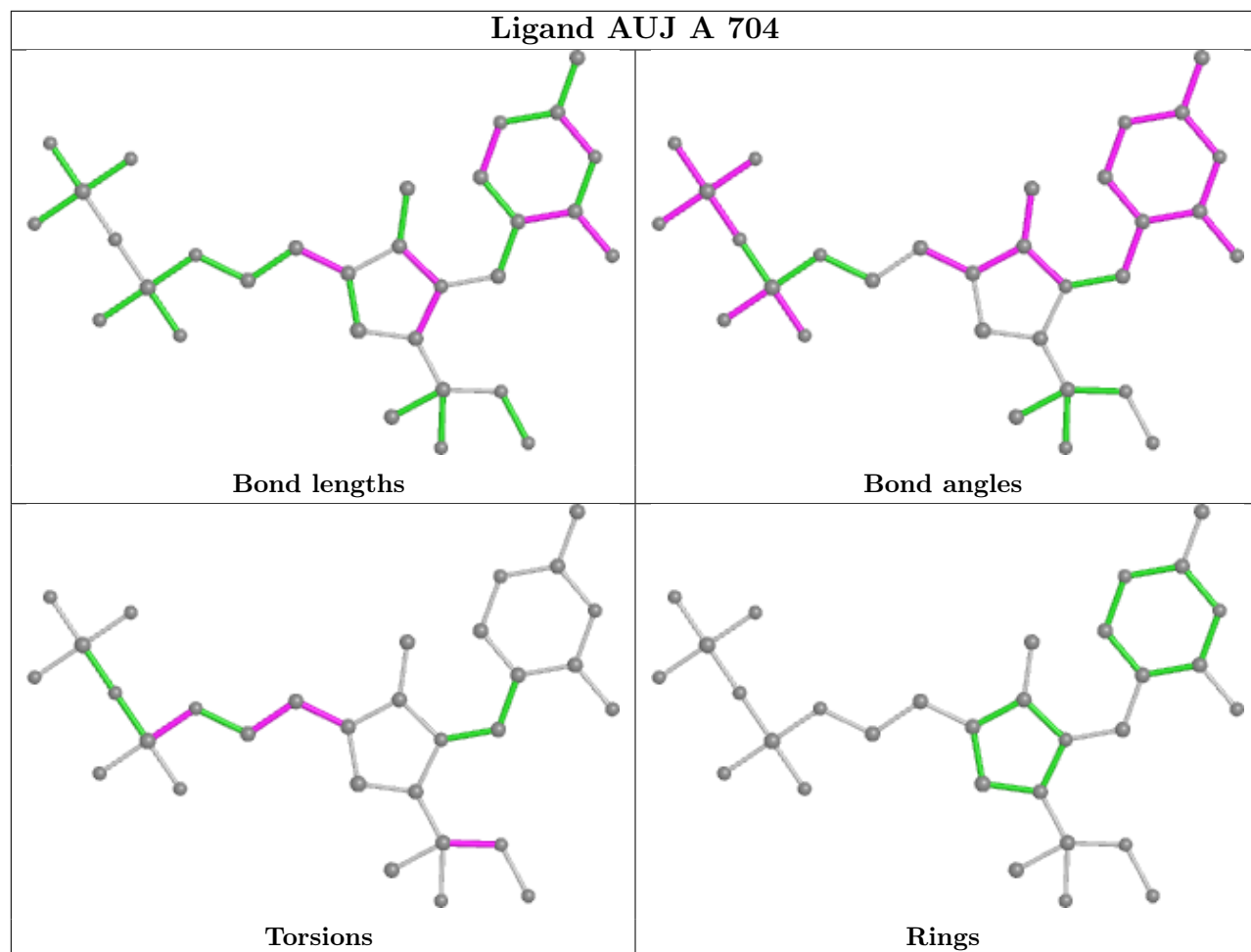
There are no ring outliers.

2 monomers are involved in 2 short contacts:

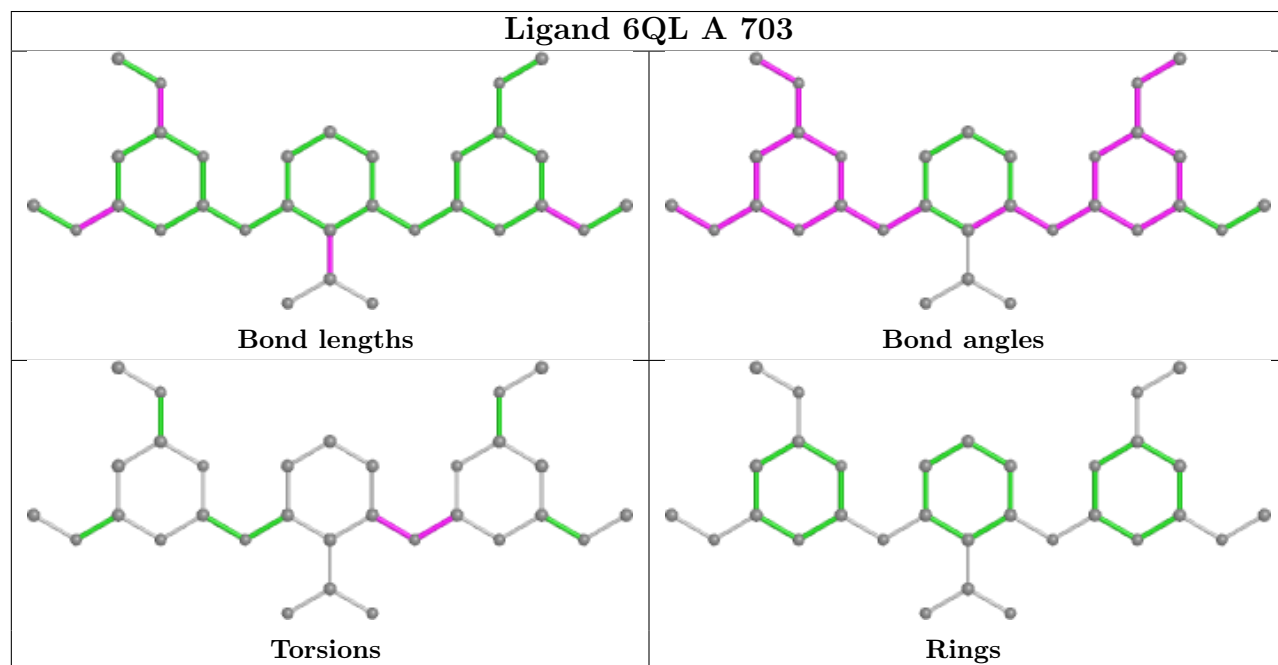
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	6QL	1	0
7	A	709	NHE	1	0

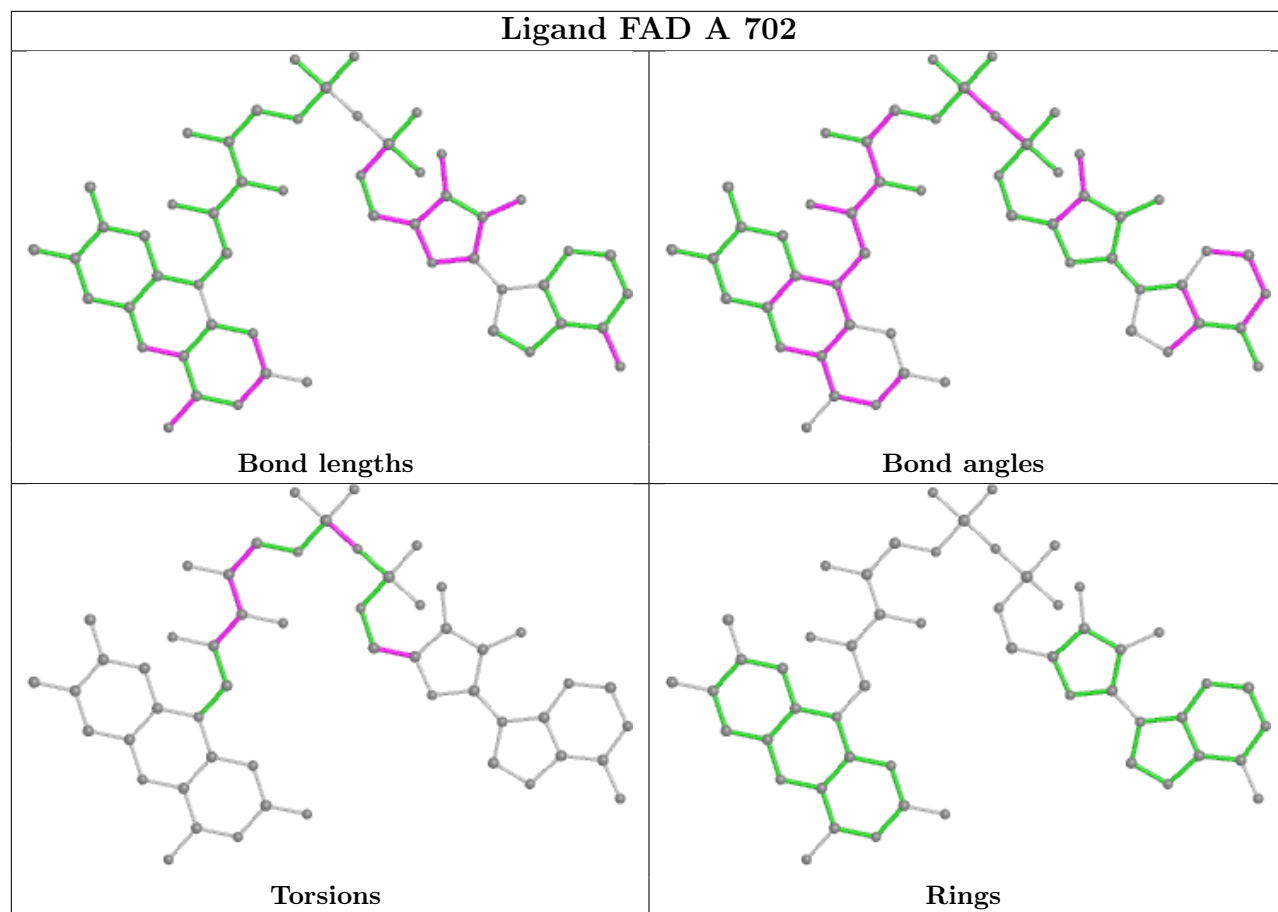
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 AUJ A 704



Ligand 6QL A 703





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	581/582 (99%)	-0.18	17 (2%) 51 45	47, 60, 84, 106	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	THR	3.8
1	A	485	VAL	3.1
1	A	88	ILE	3.0
1	A	87	PHE	2.9
1	A	439	VAL	2.9
1	A	145	GLN	2.7
1	A	430	ALA	2.4
1	A	540	SER	2.4
1	A	484	GLY	2.3
1	A	542	ILE	2.3
1	A	94	ASP	2.3
1	A	513	MET	2.2
1	A	433	LEU	2.2
1	A	544	ASN	2.2
1	A	514	GLY	2.1
1	A	434	LYS	2.0
1	A	543	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	A	340	8/9	0.97	0.10	70,73,91,94	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

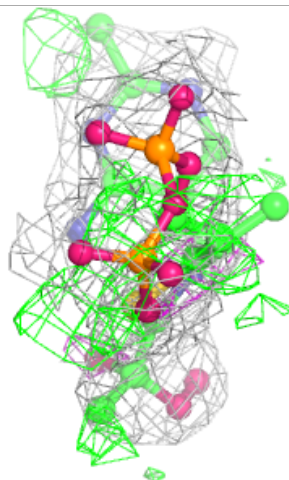
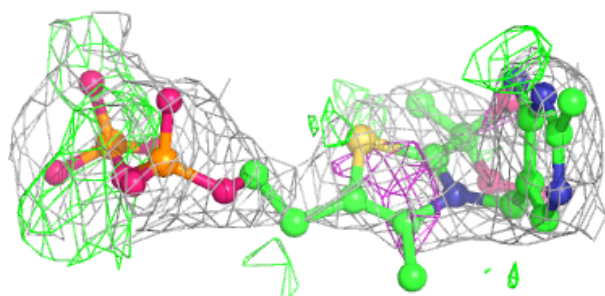
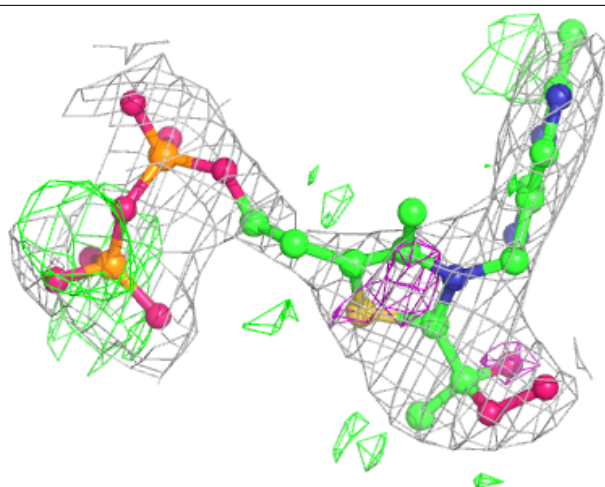
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	PO4	A	705	5/5	0.75	0.17	70,77,87,141	0
2	MG	A	707	1/1	0.76	0.11	121,121,121,121	1
8	SO4	A	710	5/5	0.80	0.35	85,99,109,120	5
5	AUJ	A	704	31/31	0.95	0.28	49,63,73,89	31
2	MG	A	711	1/1	0.96	0.52	87,87,87,87	1
2	MG	A	701	1/1	0.97	0.23	61,61,61,61	0
2	MG	A	708	1/1	0.97	0.12	68,68,68,68	0
4	6QL	A	703	31/31	0.98	0.12	47,51,56,57	0
3	FAD	A	702	53/53	0.98	0.15	45,54,58,60	0
7	NHE	A	709	13/13	0.99	0.15	49,64,71,72	0
2	MG	A	706	1/1	1.00	0.30	55,55,55,55	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.

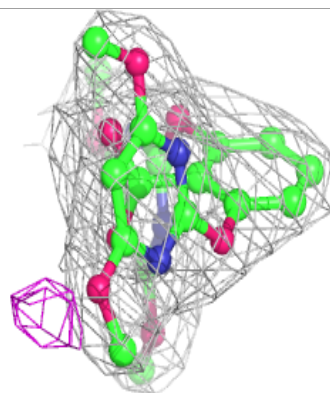
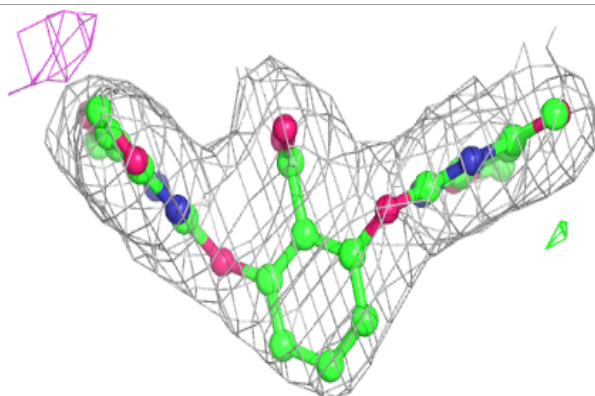
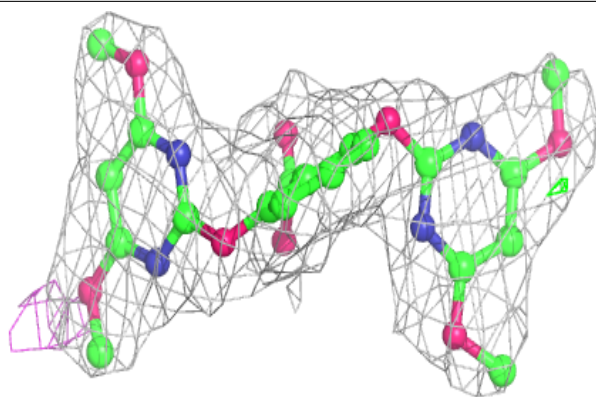
Electron density around AUJ A 704:

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

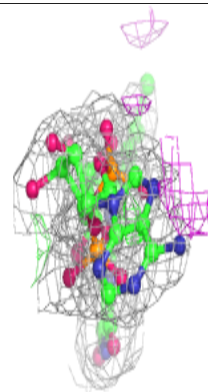
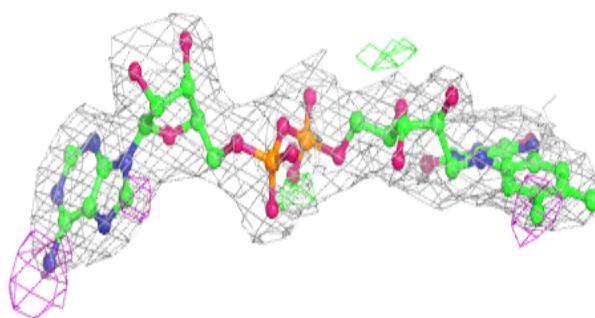
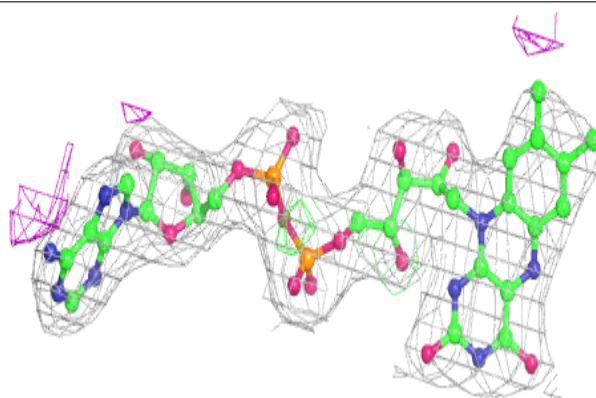


Electron density around 6QL A 703:

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

**Electron density around FAD 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.