



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:35 PM UTC

PDB ID : 5IMS / pdb_00005ims
Title : Saccharomyces cerevisiae acetohydroxyacid synthase
Authors : Guddat, L.W.; Lonhienne, T.
Deposited on : 2016-03-06
Resolution : 1.98 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

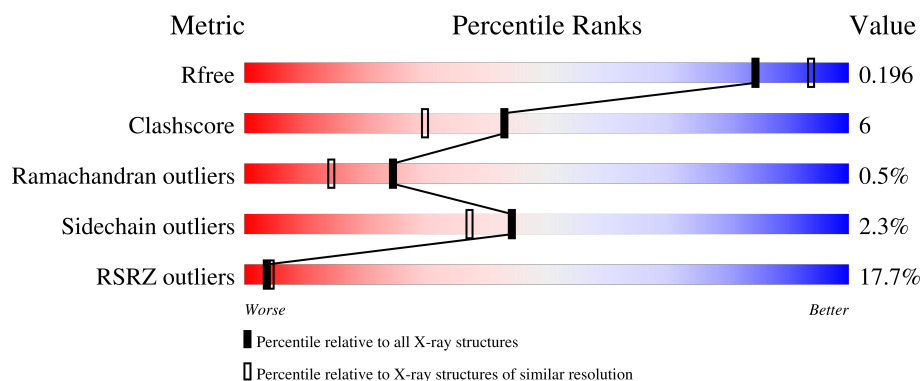
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	677	4% 74% 6% 20%
1	B	677	25% 69% 13% 16%

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
7	ACT	A	708	-	-	X	-
7	ACT	B	712	-	-	X	-
7	ACT	B	713	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9452 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 catalytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	3	0
			4111	2604	709	779	19			
1	B	567	Total	C	N	O	S	0	1	0
			4325	2740	747	818	20			

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	expression tag	UNP P07342
A	12	HIS	-	expression tag	UNP P07342
A	13	HIS	-	expression tag	UNP P07342
A	14	HIS	-	expression tag	UNP P07342
A	15	HIS	-	expression tag	UNP P07342
A	16	HIS	-	expression tag	UNP P07342
A	17	HIS	-	expression tag	UNP P07342
A	18	SER	-	expression tag	UNP P07342
A	19	SER	-	expression tag	UNP P07342
A	20	GLY	-	expression tag	UNP P07342
A	21	LEU	-	expression tag	UNP P07342
A	22	VAL	-	expression tag	UNP P07342
A	23	PRO	-	expression tag	UNP P07342
A	24	ARG	-	expression tag	UNP P07342
A	25	GLY	-	expression tag	UNP P07342
A	26	SER	-	expression tag	UNP P07342
A	27	GLY	-	expression tag	UNP P07342
A	28	MET	-	expression tag	UNP P07342
A	29	LYS	-	expression tag	UNP P07342
A	30	GLU	-	expression tag	UNP P07342
A	31	THR	-	expression tag	UNP P07342
A	32	ALA	-	expression tag	UNP P07342
A	33	ALA	-	expression tag	UNP P07342
A	34	ALA	-	expression tag	UNP P07342
A	35	LYS	-	expression tag	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
A	36	PHE	-	expression tag	UNP P07342
A	37	GLU	-	expression tag	UNP P07342
A	38	ARG	-	expression tag	UNP P07342
A	39	GLN	-	expression tag	UNP P07342
A	40	HIS	-	expression tag	UNP P07342
A	41	MET	-	expression tag	UNP P07342
A	42	ASP	-	expression tag	UNP P07342
A	43	SER	-	expression tag	UNP P07342
A	44	PRO	-	expression tag	UNP P07342
A	45	ASP	-	expression tag	UNP P07342
A	46	LEU	-	expression tag	UNP P07342
A	47	GLY	-	expression tag	UNP P07342
A	48	THR	-	expression tag	UNP P07342
A	49	ASP	-	expression tag	UNP P07342
A	50	ASP	-	expression tag	UNP P07342
A	51	ASP	-	expression tag	UNP P07342
A	52	ASP	-	expression tag	UNP P07342
A	53	LYS	-	expression tag	UNP P07342
A	54	ALA	-	expression tag	UNP P07342
A	55	MET	-	expression tag	UNP P07342
A	56	GLY	-	expression tag	UNP P07342
A	57	SER	-	expression tag	UNP P07342
B	11	MET	-	expression tag	UNP P07342
B	12	HIS	-	expression tag	UNP P07342
B	13	HIS	-	expression tag	UNP P07342
B	14	HIS	-	expression tag	UNP P07342
B	15	HIS	-	expression tag	UNP P07342
B	16	HIS	-	expression tag	UNP P07342
B	17	HIS	-	expression tag	UNP P07342
B	18	SER	-	expression tag	UNP P07342
B	19	SER	-	expression tag	UNP P07342
B	20	GLY	-	expression tag	UNP P07342
B	21	LEU	-	expression tag	UNP P07342
B	22	VAL	-	expression tag	UNP P07342
B	23	PRO	-	expression tag	UNP P07342
B	24	ARG	-	expression tag	UNP P07342
B	25	GLY	-	expression tag	UNP P07342
B	26	SER	-	expression tag	UNP P07342
B	27	GLY	-	expression tag	UNP P07342
B	28	MET	-	expression tag	UNP P07342
B	29	LYS	-	expression tag	UNP P07342
B	30	GLU	-	expression tag	UNP P07342

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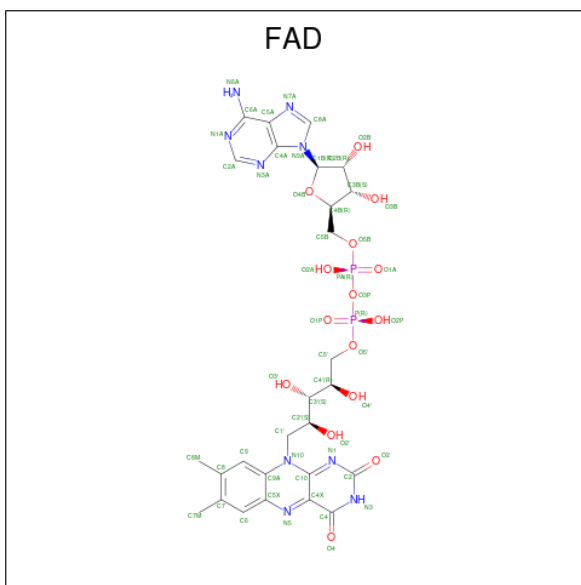
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Chain	Residue	Modelled	Actual	Comment	Reference
B	31	THR	-	expression tag	UNP P07342
B	32	ALA	-	expression tag	UNP P07342
B	33	ALA	-	expression tag	UNP P07342
B	34	ALA	-	expression tag	UNP P07342
B	35	LYS	-	expression tag	UNP P07342
B	36	PHE	-	expression tag	UNP P07342
B	37	GLU	-	expression tag	UNP P07342
B	38	ARG	-	expression tag	UNP P07342
B	39	GLN	-	expression tag	UNP P07342
B	40	HIS	-	expression tag	UNP P07342
B	41	MET	-	expression tag	UNP P07342
B	42	ASP	-	expression tag	UNP P07342
B	43	SER	-	expression tag	UNP P07342
B	44	PRO	-	expression tag	UNP P07342
B	45	ASP	-	expression tag	UNP P07342
B	46	LEU	-	expression tag	UNP P07342
B	47	GLY	-	expression tag	UNP P07342
B	48	THR	-	expression tag	UNP P07342
B	49	ASP	-	expression tag	UNP P07342
B	50	ASP	-	expression tag	UNP P07342
B	51	ASP	-	expression tag	UNP P07342
B	52	ASP	-	expression tag	UNP P07342
B	53	LYS	-	expression tag	UNP P07342
B	54	ALA	-	expression tag	UNP P07342
B	55	MET	-	expression tag	UNP P07342
B	56	GLY	-	expression tag	UNP P07342
B	57	SER	-	expression tag	UNP P07342

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).

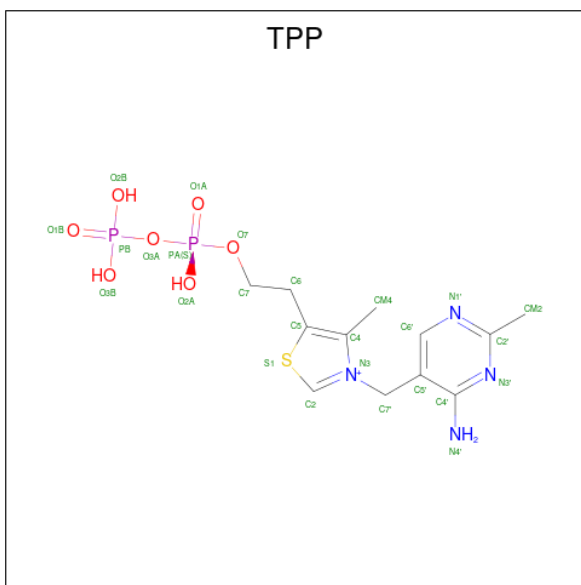


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

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

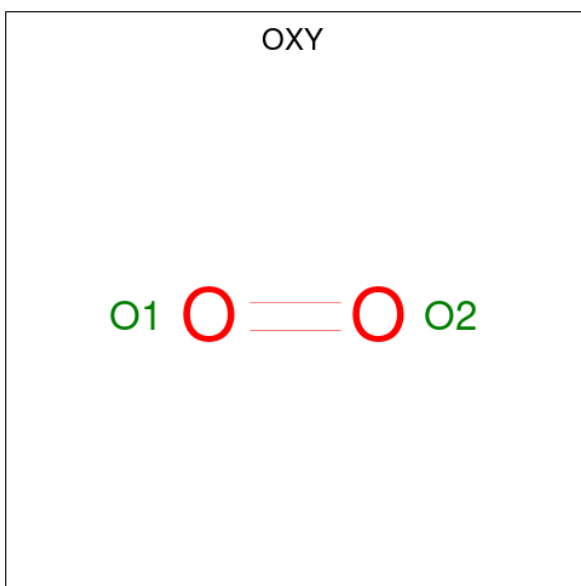
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

- Molecule 5 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $\text{C}_{12}\text{H}_{19}\text{N}_4\text{O}_7\text{P}_2\text{S}$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
5	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 6 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2).



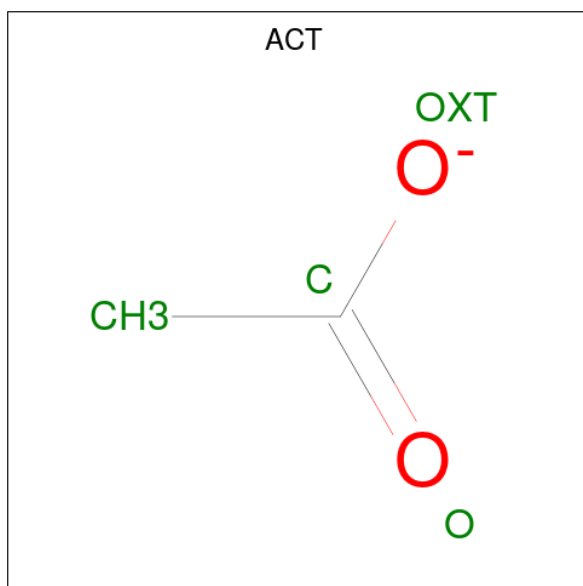
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 2 2	0	0
6	A	1	Total O 2 2	0	0

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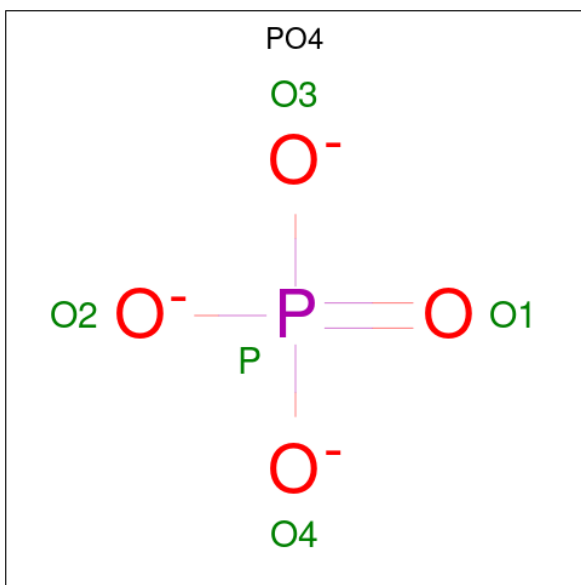
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	O	P	0	0
			5	4	1		

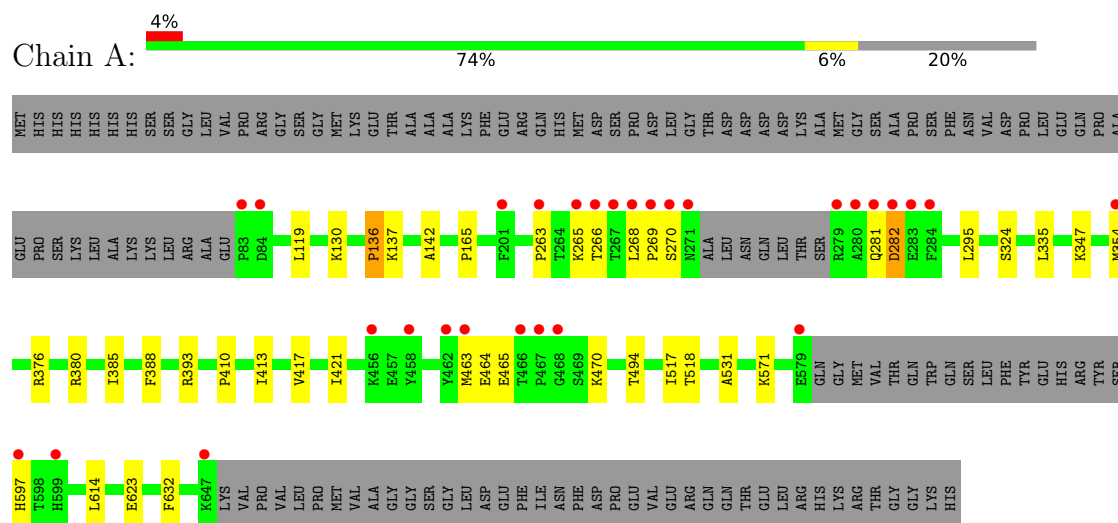
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	492	Total	O	0	0
			492	492		
9	B	327	Total	O	0	0
			327	327		

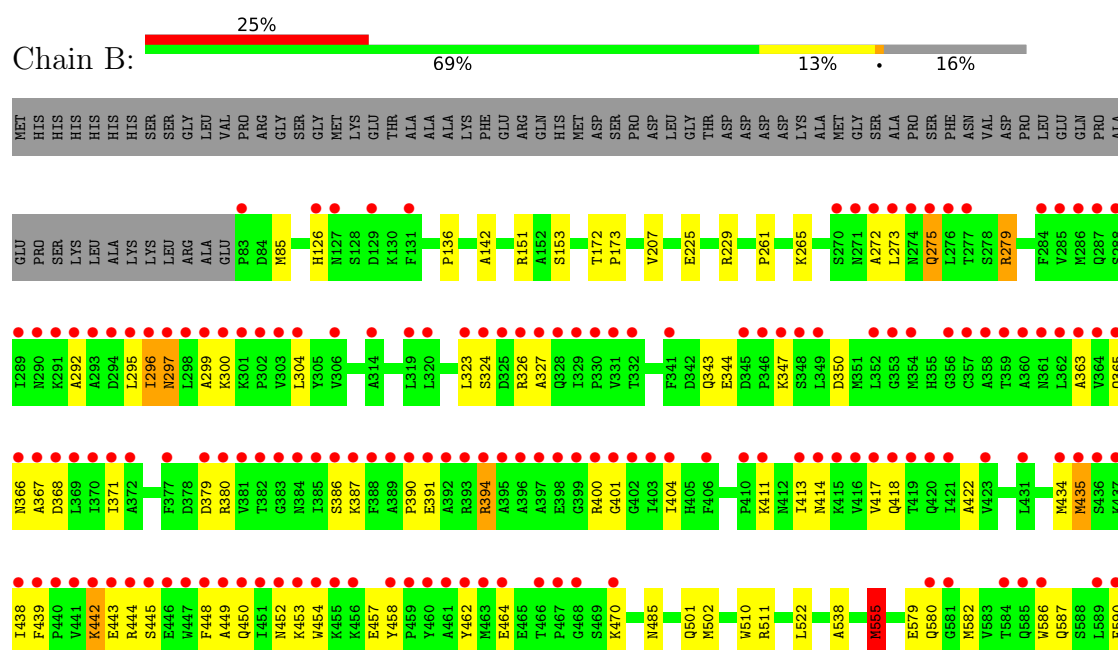
3 Residue-property plots

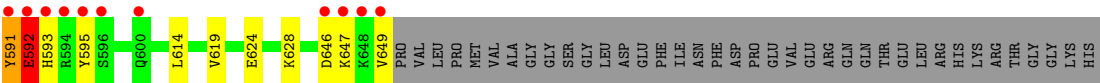
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 catalytic subunit, mitochondrial



- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.68Å 110.18Å 180.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.18 – 1.98 42.18 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.0 (42.18-1.98) 99.0 (42.18-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.166 , 0.193 0.169 , 0.196	Depositor DCC
R_{free} test set	2000 reflections (1.52%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9452	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: OXY, PO4, MG, ACT, TPP, FAD, K

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	0.86	1/4195 (0.0%)	0.92	1/5689 (0.0%)
1	B	0.81	0/4414	0.95	4/5989 (0.1%)
All	All	0.84	1/8609 (0.0%)	0.94	5/11678 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	ALA	CA-CB	5.45	1.61	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	555	MET	CA-CB-CG	-8.19	97.72	114.10
1	B	435	MET	N-CA-C	5.23	117.38	111.11
1	A	281	GLN	CB-CA-C	5.20	118.14	109.56
1	B	458	TYR	CA-C-N	-5.01	115.40	120.21
1	B	458	TYR	C-N-CA	-5.01	115.40	120.21

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	4111	0	4143	26	0
1	B	4325	0	4349	76	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	26	0	16	1	0
5	B	26	0	16	1	0
6	A	6	0	0	1	0
6	B	12	0	0	1	0
7	A	4	0	3	2	0
7	B	8	0	6	2	0
8	B	5	0	0	0	0
9	A	492	0	0	5	1
9	B	327	0	0	11	1
All	All	9452	0	8595	107	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 6.

All (107) 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:B:368:ASP:OD2	1:B:400:ARG:NH2	2.01	0.92
1:B:296:ILE:HD11	1:B:438:ILE:HD12	1.51	0.92
1:B:327:ALA:O	1:B:444:ARG:NH1	2.04	0.89
1:A:388:PHE:O	1:A:393:ARG:NH1	2.09	0.86
1:B:326:ARG:NH2	1:B:438:ILE:O	2.14	0.81
1:B:579:GLU:HB2	1:B:647:LYS:HE2	1.62	0.81
1:B:580:GLN:HB3	1:B:647:LYS:HB3	1.62	0.81
1:B:434:MET:HG2	1:B:438:ILE:HD11	1.64	0.79
1:A:385:ILE:HD11	1:A:417:VAL:HG12	1.64	0.78
6:B:708:OXY:O1	9:B:801:HOH:O	2.03	0.76
1:A:376:ARG:NH2	9:A:801:HOH:O	2.22	0.72
1:B:590:PHE:O	1:B:592:GLU:N	2.20	0.71
1:B:297:ASN:HD21	1:B:439:PHE:H	1.36	0.71
1:B:297:ASN:O	1:B:300:LYS:NZ	2.24	0.70
1:B:450:GLN:O	1:B:452:ASN:N	2.23	0.70
7:B:712:ACT:H2	7:B:713:ACT:H1	1.73	0.69
1:B:279:ARG:HG2	1:B:279:ARG:HH11	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:MET:HE1	1:A:380:ARG:HH11	1.63	0.63
1:B:297:ASN:ND2	1:B:439:PHE:H	1.96	0.63
1:B:587:GLN:NE2	1:B:592:GLU:OE2	2.31	0.63
1:B:85:MET:HE3	1:B:261:PRO:HB2	1.81	0.62
1:B:272:ALA:HA	1:B:275:GLN:HE21	1.64	0.62
1:B:272:ALA:HA	1:B:275:GLN:NE2	2.15	0.62
7:A:708:ACT:H3	9:B:875:HOH:O	2.01	0.60
1:B:582:MET:HG2	9:B:801:HOH:O	2.01	0.60
1:B:442:LYS:HD2	1:B:442:LYS:H	1.66	0.60
1:A:295:LEU:HD12	1:A:421:ILE:HD12	1.84	0.59
1:B:485:ASN:ND2	9:B:806:HOH:O	2.35	0.58
5:B:704:TPP:H2	9:B:875:HOH:O	2.03	0.58
1:B:297:ASN:HD21	1:B:439:PHE:N	2.01	0.58
1:B:151:ARG:NH2	9:B:802:HOH:O	2.09	0.57
1:B:579:GLU:CB	1:B:647:LYS:HE2	2.33	0.57
1:B:443:GLU:CD	1:B:444:ARG:H	2.13	0.57
1:A:385:ILE:HD11	1:A:417:VAL:CG1	2.36	0.56
1:B:391:GLU:OE2	1:B:394:ARG:NH2	2.39	0.56
1:A:130:LYS:HD2	9:A:978:HOH:O	2.07	0.54
1:B:470:LYS:HE3	1:B:646:ASP:HA	1.91	0.53
1:B:324:SER:OG	1:B:347:LYS:HE2	2.08	0.53
1:A:263:PRO:HB3	1:A:265:LYS:HE2	1.92	0.52
1:B:450:GLN:NE2	1:B:454:TRP:HE1	2.08	0.52
1:A:335:LEU:HD22	9:A:1110:HOH:O	2.10	0.52
1:B:296:ILE:CD1	1:B:438:ILE:HD12	2.32	0.51
1:B:300:LYS:HA	1:B:444:ARG:NH2	2.26	0.51
1:B:292:ALA:HB3	1:B:434:MET:HE1	1.93	0.51
1:B:387:LYS:O	1:B:390:PRO:HD3	2.10	0.51
1:B:619:VAL:HG13	1:B:624:GLU:HG3	1.93	0.51
1:B:365:GLN:O	1:B:390:PRO:HD2	2.12	0.50
1:B:435:MET:HA	1:B:435:MET:HE3	1.95	0.49
1:B:442:LYS:HD2	1:B:442:LYS:N	2.27	0.49
1:B:343:GLN:NE2	1:B:510:TRP:H	2.11	0.49
1:B:591:TYR:O	1:B:593:HIS:N	2.46	0.49
1:B:323:LEU:HA	1:B:435:MET:HE1	1.96	0.48
1:B:153:SER:HB3	1:B:538:ALA:HB1	1.95	0.48
1:B:413:ILE:HD13	1:B:422:ALA:HB1	1.96	0.48
1:B:344:GLU:HG3	1:B:511:ARG:NE	2.29	0.47
1:B:449:ALA:O	1:B:453:LYS:HE2	2.14	0.47
1:A:282:ASP:N	1:A:282:ASP:OD1	2.47	0.47
1:B:434:MET:CG	1:B:438:ILE:HD11	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:706:OXY:O1	7:A:708:ACT:O	2.31	0.47
1:A:324:SER:OG	1:A:347:LYS:HE2	2.14	0.47
1:A:597:HIS:HB2	9:A:1116:HOH:O	2.14	0.47
1:B:350:ASP:HB3	9:B:828:HOH:O	2.14	0.47
1:B:586:TRP:CZ3	1:B:595:TYR:CE1	3.03	0.47
1:A:268:LEU:HA	1:A:269:PRO:HD2	1.80	0.46
1:A:463:MET:HE3	1:A:464:GLU:O	2.15	0.46
1:B:501:GLN:HG2	1:B:502:MET:HE2	1.98	0.46
1:B:225:GLU:HG2	1:B:229:ARG:HG2	1.96	0.46
1:B:462:TYR:CE1	1:B:464:GLU:HG2	2.51	0.46
1:B:300:LYS:HA	1:B:444:ARG:HH21	1.81	0.45
1:A:470:LYS:NZ	9:A:812:HOH:O	2.49	0.45
1:B:363:ALA:N	1:B:454:TRP:HZ3	2.15	0.45
1:B:413:ILE:HG22	1:B:414:ASN:ND2	2.32	0.45
1:B:619:VAL:HG22	1:B:628:LYS:HG3	1.99	0.45
1:B:126:HIS:ND1	9:B:804:HOH:O	2.31	0.45
1:A:136:PRO:HG3	1:A:142:ALA:HB2	2.00	0.44
7:B:712:ACT:CH3	7:B:713:ACT:H1	2.43	0.44
1:A:571:LYS:HB3	1:A:632:PHE:CZ	2.52	0.44
1:B:297:ASN:HD22	1:B:297:ASN:HA	1.60	0.44
1:B:299:ALA:O	1:B:300:LYS:HD2	2.18	0.44
1:A:137:LYS:O	1:B:555:MET:HG2	2.17	0.43
1:A:263:PRO:HB2	1:A:266:THR:HG23	2.00	0.43
1:A:335:LEU:HD21	1:A:518:THR:HG21	2.01	0.43
1:B:292:ALA:HB1	1:B:404:ILE:HD13	2.01	0.43
1:B:414:ASN:HA	1:B:417:VAL:O	2.19	0.43
1:B:579:GLU:H	1:B:647:LYS:HE2	1.84	0.42
1:A:410:PRO:HA	1:A:413:ILE:HD12	2.01	0.42
1:B:445:SER:O	1:B:449:ALA:HB3	2.18	0.42
1:B:279:ARG:HH11	1:B:279:ARG:CG	2.30	0.42
1:A:623:GLU:H	1:A:623:GLU:CD	2.27	0.42
1:B:442:LYS:H	1:B:442:LYS:CD	2.32	0.41
1:B:443:GLU:OE2	1:B:448:PHE:HB3	2.18	0.41
1:B:470:LYS:NZ	9:B:805:HOH:O	2.34	0.41
1:A:465:GLU:OE2	1:A:465:GLU:N	2.52	0.41
5:A:704:TPP:H2	9:B:833:HOH:O	2.20	0.41
1:B:379:ASP:HB3	9:B:1065:HOH:O	2.18	0.41
1:B:136:PRO:HG3	1:B:142:ALA:HB2	2.02	0.41
1:B:296:ILE:CD1	1:B:438:ILE:HG23	2.51	0.41
1:B:579:GLU:H	1:B:647:LYS:CE	2.33	0.41
1:A:165:PRO:HD3	1:B:522:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:THR:HG22	1:A:517:ILE:HB	2.03	0.41
1:B:304:LEU:HD23	1:B:371:ILE:HB	2.03	0.41
1:B:418:GLN:OE1	1:B:418:GLN:N	2.54	0.41
1:B:295:LEU:HD21	1:B:401:GLY:HA2	2.02	0.41
1:B:442:LYS:N	1:B:442:LYS:CD	2.84	0.41
1:B:450:GLN:CD	1:B:454:TRP:HE1	2.29	0.41
1:A:385:ILE:HD12	1:A:385:ILE:HA	1.90	0.40
1:B:172:THR:HB	1:B:173:PRO:HD3	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)
9:A:1212:HOH:O	9:B:824:HOH:O[3_544]	2.16	0.04

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	538/677 (80%)	534 (99%)	3 (1%)	1 (0%)	43	35
1	B	566/677 (84%)	544 (96%)	18 (3%)	4 (1%)	18	9
All	All	1104/1354 (82%)	1078 (98%)	21 (2%)	5 (0%)	24	14

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	591	TYR
1	B	592	GLU
1	A	270	SER
1	B	367	ALA
1	B	366	ASN

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	442/556 (80%)	438 (99%)	4 (1%)	70	67
1	B	465/556 (84%)	448 (96%)	17 (4%)	30	20
All	All	907/1112 (82%)	886 (98%)	21 (2%)	44	37

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	136	PRO
1	A	282	ASP
1	A	614	LEU
1	B	207	VAL
1	B	265	LYS
1	B	273	LEU
1	B	275	GLN
1	B	279	ARG
1	B	296	ILE
1	B	297	ASN
1	B	380	ARG
1	B	386	SER
1	B	394	ARG
1	B	411	LYS
1	B	442	LYS
1	B	457	GLU
1	B	555	MET
1	B	592	GLU
1	B	614	LEU
1	B	649	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	ASN

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Mol	Chain	Res	Type
1	A	355	HIS
1	A	501	GLN
1	B	275	GLN
1	B	297	ASN
1	B	580	GLN
1	B	587	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	TPP	A	704	4	26,27,27	1.69	6 (23%)	38,40,40	1.87	8 (21%)
6	OXY	B	709	-	1,1,1	0.04	0	-		
5	TPP	B	704	4	26,27,27	1.60	6 (23%)	38,40,40	1.93	9 (23%)
8	PO4	B	711	-	4,4,4	0.91	0	6,6,6	1.01	0
7	ACT	B	712	-	3,3,3	0.87	0	3,3,3	0.65	0
6	OXY	B	706	-	1,1,1	0.11	0	-		
3	FAD	A	702	-	58,58,58	1.57	11 (18%)	85,89,89	1.70	21 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	OXY	B	707	-	1,1,1	0.12	0	-		
6	OXY	B	708	-	1,1,1	0.01	0	-		
6	OXY	B	710	-	1,1,1	0.07	0	-		
3	FAD	B	702	-	58,58,58	1.59	12 (20%)	85,89,89	1.72	21 (24%)
6	OXY	A	707	-	1,1,1	0.09	0	-		
6	OXY	A	705	-	1,1,1	0.08	0	-		
7	ACT	A	708	-	3,3,3	0.76	0	3,3,3	1.09	0
7	ACT	B	713	-	3,3,3	0.78	0	3,3,3	0.92	0
6	OXY	A	706	-	1,1,1	0.09	0	-		
6	OXY	B	705	-	1,1,1	0.10	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
5	TPP	A	704	4	-	3/17/17/17	0/2/2/2
3	FAD	B	702	-	-	4/34/50/50	0/6/6/6
5	TPP	B	704	4	-	2/17/17/17	0/2/2/2
3	FAD	A	702	-	-	4/34/50/50	0/6/6/6

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FAD	C10-N1	4.61	1.42	1.33
3	B	702	FAD	C4X-N5	4.28	1.40	1.30
3	B	702	FAD	C10-N1	4.25	1.41	1.33
3	A	702	FAD	C4X-N5	4.18	1.39	1.30
5	A	704	TPP	C5-C4	4.10	1.43	1.35
5	B	704	TPP	C5-C4	3.67	1.42	1.35
5	A	704	TPP	C2-S1	3.09	1.78	1.69
5	A	704	TPP	C4'-N4'	2.98	1.41	1.34
5	B	704	TPP	C2-S1	2.97	1.78	1.69
3	B	702	FAD	C9-C9A	2.86	1.44	1.39
3	A	702	FAD	C2'-C3'	2.85	1.58	1.53
3	B	702	FAD	C2'-C3'	2.67	1.58	1.53
3	B	702	FAD	C7M-C7	2.63	1.55	1.51
5	A	704	TPP	C4'-N3'	2.63	1.38	1.35
5	A	704	TPP	C7'-C5'	2.63	1.56	1.51
5	A	704	TPP	C6'-N1'	2.58	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	FAD	C8A-N9A	-2.57	1.33	1.37
5	B	704	TPP	C2'-N1'	2.56	1.38	1.34
3	A	702	FAD	C6A-N6A	2.53	1.40	1.34
3	B	702	FAD	C2-N1	2.49	1.42	1.36
5	B	704	TPP	C7'-C5'	2.41	1.55	1.51
3	B	702	FAD	C8M-C8	2.40	1.55	1.51
3	A	702	FAD	C7M-C7	2.34	1.55	1.51
3	A	702	FAD	PA-O3P	-2.31	1.57	1.59
3	B	702	FAD	C1'-N10	-2.31	1.42	1.47
3	A	702	FAD	C8A-N9A	-2.30	1.33	1.37
3	B	702	FAD	O3'-C3'	-2.27	1.37	1.43
3	B	702	FAD	C4X-C10	-2.25	1.37	1.44
3	A	702	FAD	C1'-N10	-2.21	1.42	1.47
5	B	704	TPP	C4'-N4'	2.13	1.39	1.34
5	B	704	TPP	C4-N3	-2.10	1.35	1.39
3	B	702	FAD	C2B-C1B	-2.08	1.46	1.53
3	A	702	FAD	P-O3P	2.02	1.61	1.59
3	A	702	FAD	C4X-C10	-2.01	1.38	1.44
3	A	702	FAD	C4X-C4	2.00	1.51	1.44

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	704	TPP	CM2-C2'-N1'	6.12	123.71	117.20
5	A	704	TPP	CM2-C2'-N1'	5.07	122.60	117.20
3	B	702	FAD	C5A-C4A-N3A	-4.89	119.99	126.72
3	A	702	FAD	C5A-C4A-N3A	-4.79	120.12	126.72
5	B	704	TPP	N1'-C2'-N3'	-4.44	118.13	125.53
5	A	704	TPP	N1'-C2'-N3'	-4.42	118.17	125.53
3	A	702	FAD	N3A-C2A-N1A	-4.27	122.12	128.58
3	B	702	FAD	N3A-C4A-N9A	3.86	133.74	127.17
3	B	702	FAD	N3A-C2A-N1A	-3.80	122.84	128.58
3	A	702	FAD	O2A-PA-O3P	3.76	117.44	107.27
5	A	704	TPP	C6'-N1'-C2'	3.74	122.22	116.07
3	B	702	FAD	O4-C4-C4X	-3.70	116.77	126.53
3	B	702	FAD	C4A-C5A-N7A	-3.63	106.43	110.58
3	B	702	FAD	C4-N3-C2	-3.61	119.23	125.64
3	B	702	FAD	C5A-N7A-C8A	3.61	109.12	103.45
3	A	702	FAD	N3A-C4A-N9A	3.60	133.29	127.17
5	A	704	TPP	O2A-PA-O3A	3.56	116.89	107.27
3	A	702	FAD	C4A-C5A-N7A	-3.50	106.58	110.58
3	B	702	FAD	N9A-C8A-N7A	-3.44	109.05	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	FAD	C4X-C4-N3	3.43	121.98	113.25
5	B	704	TPP	C6'-N1'-C2'	3.38	121.63	116.07
3	A	702	FAD	C2A-N3A-C4A	3.31	119.92	111.83
3	B	702	FAD	C2A-N3A-C4A	3.27	119.82	111.83
5	A	704	TPP	O2B-PB-O3A	3.27	115.59	104.64
3	B	702	FAD	C4A-N9A-C8A	3.23	109.13	105.74
3	A	702	FAD	C5A-N7A-C8A	3.20	108.47	103.45
3	A	702	FAD	C4X-C10-N10	3.13	120.96	116.48
5	B	704	TPP	CM4-C4-C5	-3.03	119.98	127.75
3	B	702	FAD	C4-C4X-N5	2.98	122.33	118.21
3	A	702	FAD	N9A-C8A-N7A	-2.98	109.71	113.94
3	A	702	FAD	C5'-C4'-C3'	-2.93	106.70	112.22
3	A	702	FAD	O2-C2-N1	-2.91	116.96	121.80
3	B	702	FAD	C10-N1-C2	2.85	123.01	116.85
5	A	704	TPP	CM4-C4-C5	-2.77	120.64	127.75
3	B	702	FAD	O4'-C4'-C3'	2.77	115.73	109.25
3	A	702	FAD	O4-C4-C4X	-2.73	119.31	126.53
3	A	702	FAD	C4A-N9A-C8A	2.72	108.60	105.74
5	B	704	TPP	C7'-N3-C2	-2.67	117.91	123.48
3	A	702	FAD	C4-N3-C2	-2.62	120.98	125.64
3	B	702	FAD	C9A-N10-C10	-2.61	116.77	120.75
5	B	704	TPP	O2A-PA-O3A	2.49	114.01	107.27
3	B	702	FAD	C5'-C4'-C3'	-2.45	107.60	112.22
3	B	702	FAD	C4X-C10-N10	2.41	119.93	116.48
3	A	702	FAD	C5X-C9A-N10	2.35	120.09	117.97
5	A	704	TPP	C7'-N3-C2	-2.30	118.67	123.48
3	A	702	FAD	C4X-C4-N3	2.23	118.93	113.25
3	A	702	FAD	C10-C4X-N5	-2.22	120.28	124.81
5	B	704	TPP	S1-C2-N3	-2.21	109.50	112.30
5	B	704	TPP	C7-C6-C5	-2.20	105.82	112.73
5	B	704	TPP	O3B-PB-O2B	2.18	115.98	107.80
3	B	702	FAD	C9A-C5X-N5	-2.17	120.15	122.45
3	B	702	FAD	C10-C4X-N5	-2.12	120.49	124.81
5	A	704	TPP	CM4-C4-N3	2.10	125.41	120.57
3	B	702	FAD	C4X-C10-N1	-2.09	119.47	124.59
3	A	702	FAD	C4X-C10-N1	-2.07	119.51	124.59
3	A	702	FAD	O2-C2-N3	2.06	122.53	118.58
3	A	702	FAD	C10-N1-C2	2.04	121.28	116.85
3	B	702	FAD	C6A-C5A-N7A	2.02	135.98	132.09
3	A	702	FAD	O3P-PA-O1A	-2.01	104.66	110.70

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	FAD	P-O3P-PA-O5B
3	B	702	FAD	P-O3P-PA-O5B
5	A	704	TPP	PA-O3A-PB-O3B
5	B	704	TPP	PA-O3A-PB-O2B
3	B	702	FAD	C2B-C1B-N9A-C8A
5	A	704	TPP	C7-O7-PA-O1A
3	A	702	FAD	O3'-C3'-C4'-C5'
3	A	702	FAD	C2B-C1B-N9A-C8A
5	B	704	TPP	PA-O3A-PB-O3B
5	A	704	TPP	C5-C6-C7-O7
3	B	702	FAD	O4B-C4B-C5B-O5B
3	A	702	FAD	PA-O3P-P-O2P
3	B	702	FAD	PA-O3P-P-O2P

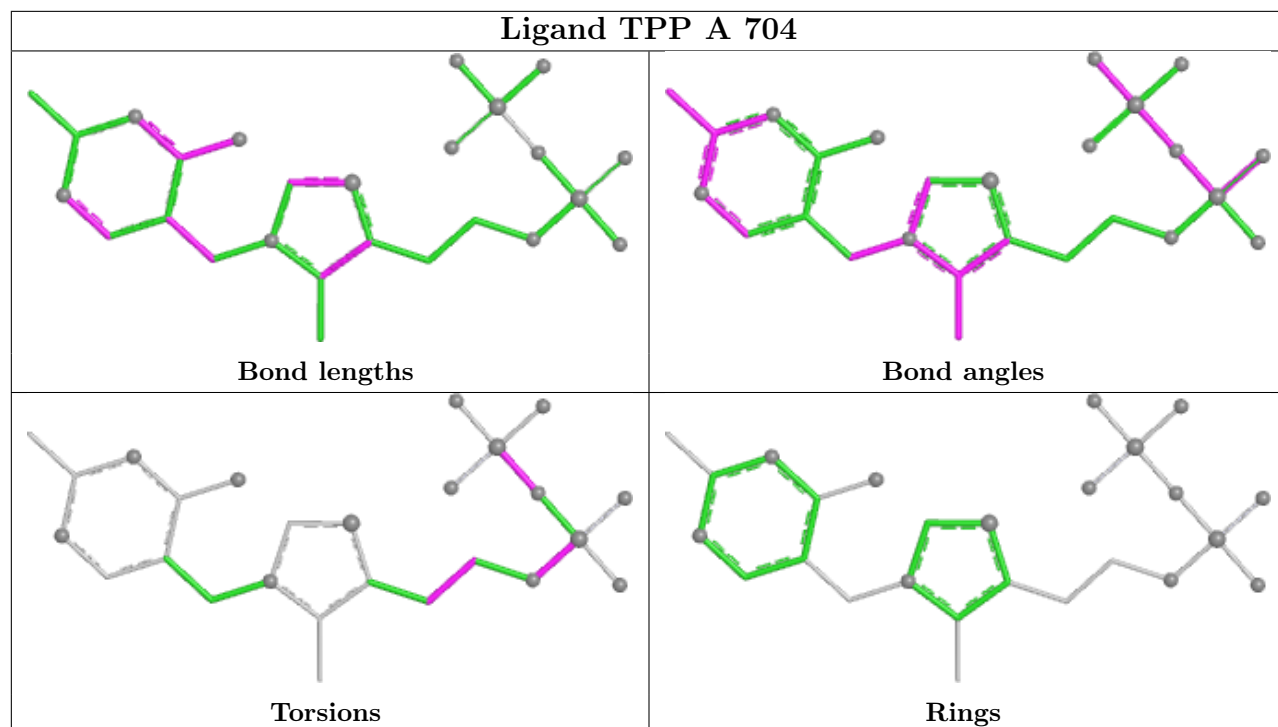
There are no ring outliers.

7 monomers are involved in 7 short contacts:

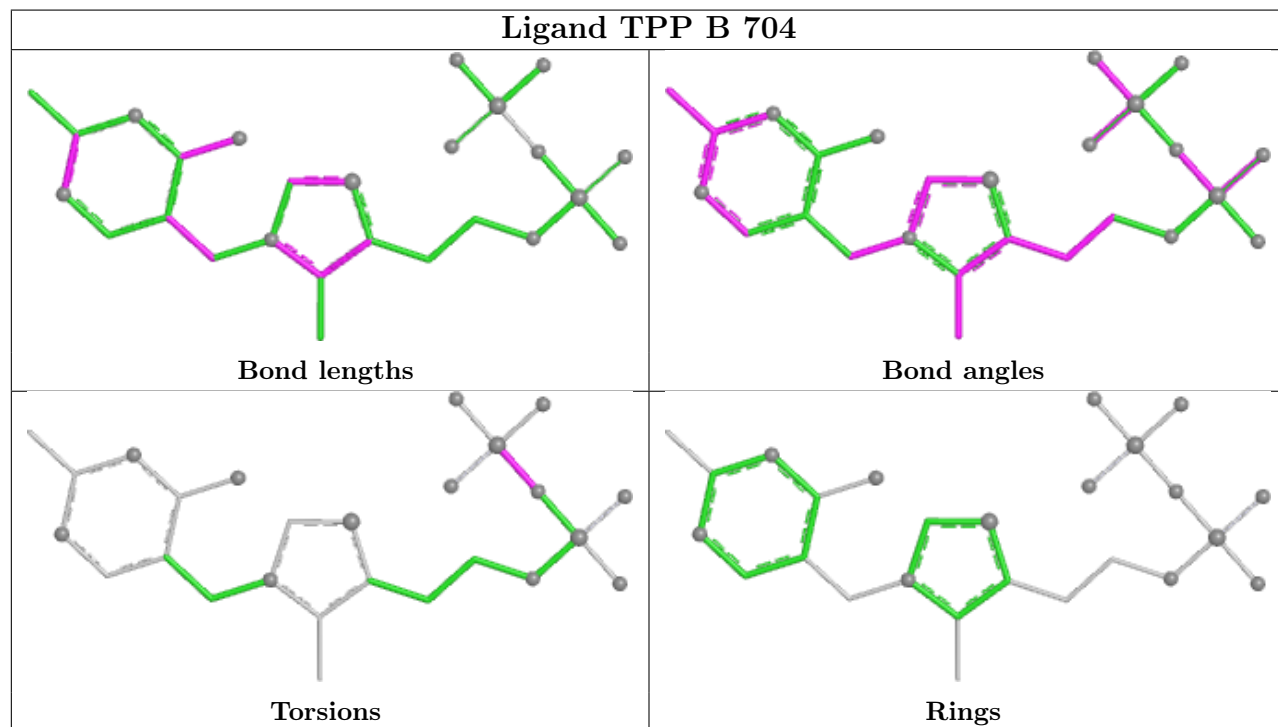
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	704	TPP	1	0
5	B	704	TPP	1	0
7	B	712	ACT	2	0
6	B	708	OXY	1	0
7	A	708	ACT	2	0
7	B	713	ACT	2	0
6	A	706	OXY	1	0

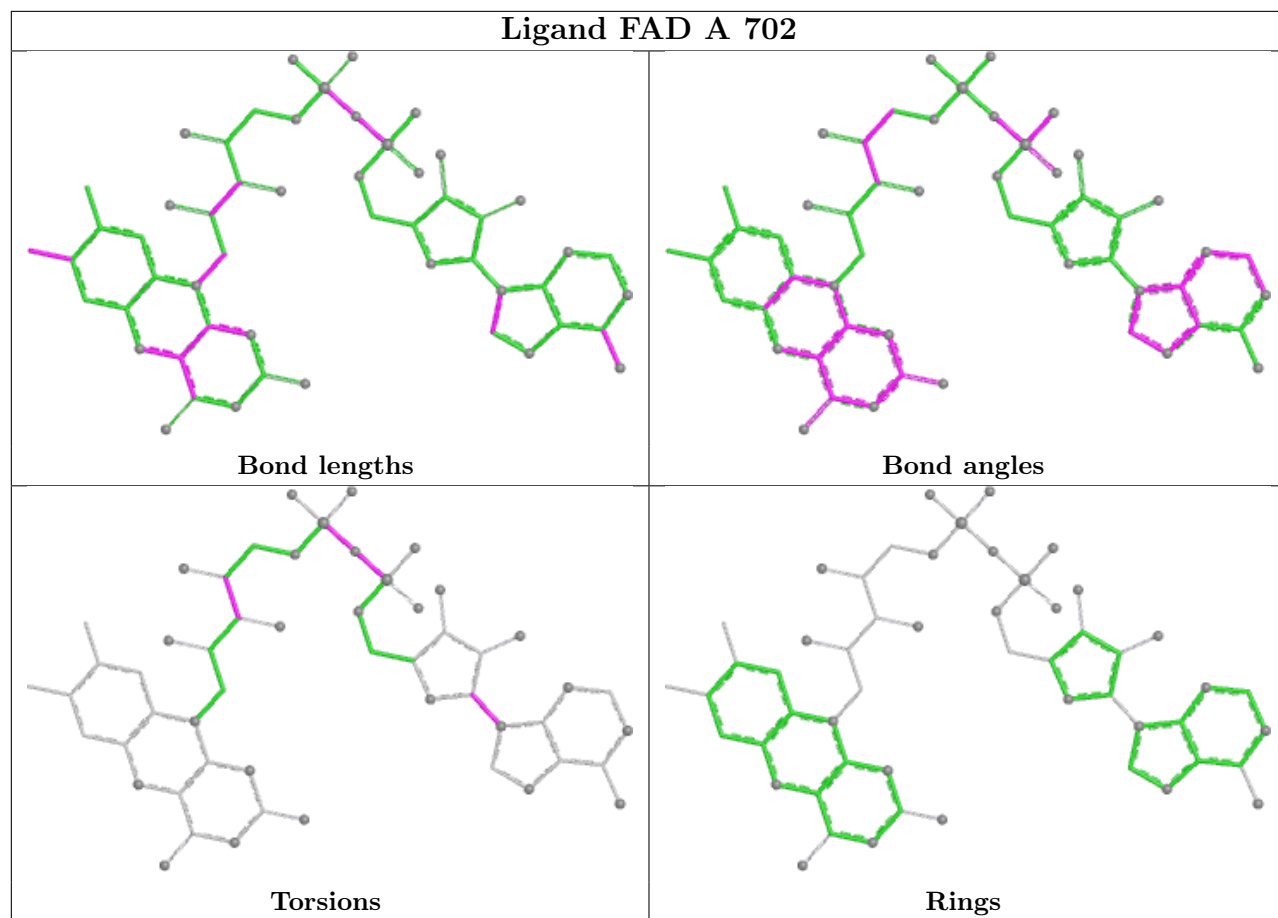
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

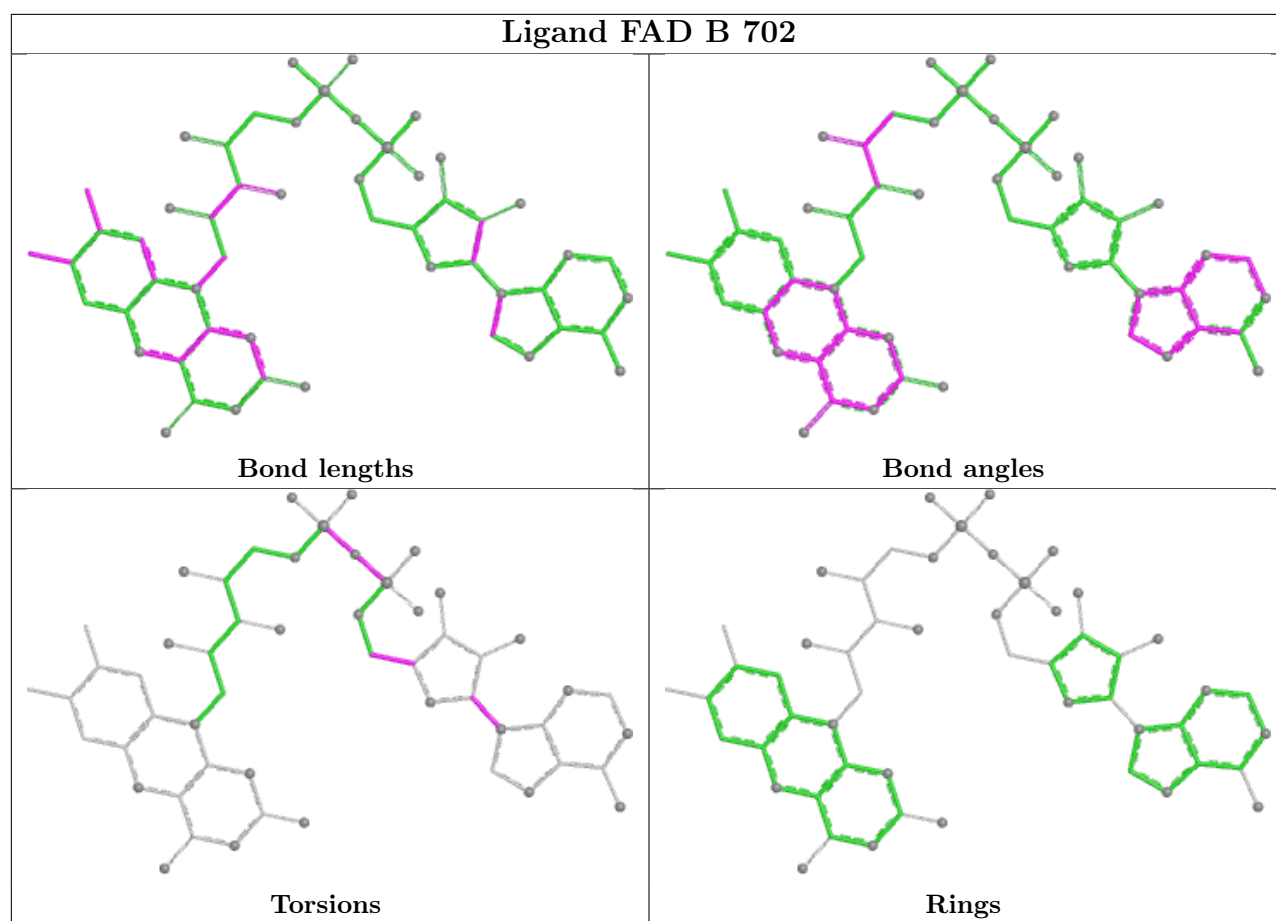
Ligand TPP A 704



Ligand TPP B 704







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	541/677 (79%)	-0.05	29 (5%)	31 40	16, 29, 62, 112	3 (0%)
1	B	567/677 (83%)	1.14	167 (29%)	1 1	14, 37, 117, 144	1 (0%)
All	All	1108/1354 (81%)	0.56	196 (17%)	4 4	14, 32, 105, 144	4 (0%)

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	448	PHE	10.4
1	B	649	VAL	9.5
1	B	447	TRP	8.9
1	B	362	LEU	8.3
1	B	451	ILE	7.7
1	B	296	ILE	7.3
1	B	329	ILE	7.0
1	B	441	VAL	7.0
1	B	367	ALA	6.9
1	B	272	ALA	6.8
1	B	449	ALA	6.8
1	B	358	ALA	6.4
1	B	369	LEU	6.4
1	B	439	PHE	6.4
1	A	83	PRO	6.3
1	B	364	VAL	6.1
1	B	421	ILE	6.1
1	B	395	ALA	6.0
1	B	327	ALA	5.8
1	B	454	TRP	5.8
1	B	295	LEU	5.8
1	B	404	ILE	5.8
1	B	462	TYR	5.6
1	B	303	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	298	LEU	5.5
1	B	458	TYR	5.5
1	B	370	ILE	5.5
1	B	438	ILE	5.4
1	B	83	PRO	5.4
1	B	388	PHE	5.3
1	B	590	PHE	5.2
1	B	273	LEU	5.1
1	B	363	ALA	5.0
1	A	270	SER	5.0
1	A	269	PRO	5.0
1	B	390	PRO	5.0
1	B	302	PRO	4.9
1	B	392	ALA	4.9
1	B	359	THR	4.9
1	B	591	TYR	4.9
1	B	292	ALA	4.9
1	B	385	ILE	4.8
1	A	268	LEU	4.8
1	B	595	TYR	4.7
1	B	380	ARG	4.7
1	B	586	TRP	4.7
1	B	360	ALA	4.6
1	B	371	ILE	4.6
1	B	384	ASN	4.6
1	B	401	GLY	4.6
1	B	366	ASN	4.5
1	B	330	PRO	4.5
1	B	324	SER	4.5
1	B	274	ASN	4.5
1	B	416	VAL	4.4
1	B	647	LYS	4.4
1	B	452	ASN	4.4
1	B	285	VAL	4.4
1	B	304	LEU	4.3
1	B	431	LEU	4.3
1	B	417	VAL	4.3
1	B	383	GLY	4.2
1	B	361	ASN	4.2
1	B	442	LYS	4.2
1	B	397	ALA	4.2
1	B	399	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	301	LYS	4.1
1	B	331	VAL	4.1
1	B	450	GLN	4.1
1	B	445	SER	4.1
1	B	299	ALA	4.1
1	B	463	MET	4.1
1	B	389	ALA	4.0
1	B	403	ILE	4.0
1	B	328	GLN	4.0
1	B	293	ALA	4.0
1	B	440	PRO	4.0
1	B	400	ARG	3.9
1	B	436	SER	3.9
1	B	284	PHE	3.9
1	B	379	ASP	3.9
1	A	579	GLU	3.9
1	B	357	CYS	3.8
1	B	270	SER	3.8
1	A	463	MET	3.8
1	B	460	TYR	3.8
1	B	402	GLY	3.8
1	B	443	GLU	3.8
1	A	280	ALA	3.7
1	B	326	ARG	3.7
1	B	346	PRO	3.7
1	B	275	GLN	3.7
1	B	456	LYS	3.6
1	B	593	HIS	3.6
1	B	323	LEU	3.6
1	B	352	LEU	3.6
1	B	435	MET	3.6
1	B	300	LYS	3.6
1	B	648	LYS	3.6
1	B	398	GLU	3.6
1	B	382	THR	3.6
1	A	281	GLN	3.5
1	B	394	ARG	3.5
1	B	455	LYS	3.5
1	A	599	HIS	3.5
1	B	461	ALA	3.5
1	B	396	ALA	3.5
1	A	597	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	368	ASP	3.4
1	B	365	GLN	3.4
1	B	319	LEU	3.4
1	B	444	ARG	3.4
1	B	289	ILE	3.4
1	B	287	GLN	3.4
1	B	341	PHE	3.4
1	A	279	ARG	3.4
1	B	434	MET	3.4
1	B	453	LYS	3.3
1	B	294	ASP	3.3
1	B	391	GLU	3.3
1	B	418	GLN	3.3
1	B	419	THR	3.3
1	B	377	PHE	3.3
1	B	459	PRO	3.2
1	B	290	ASN	3.2
1	B	581	GLY	3.2
1	B	466	THR	3.2
1	B	646	ASP	3.2
1	B	437	LYS	3.1
1	B	423	VAL	3.1
1	B	387	LYS	3.1
1	B	288	SER	3.1
1	B	348	SER	3.1
1	B	386	SER	3.1
1	B	345	ASP	3.1
1	A	284	PHE	3.1
1	B	297	ASN	3.0
1	B	347	LYS	3.0
1	B	286	MET	3.0
1	B	127	ASN	3.0
1	B	276	LEU	3.0
1	B	349	LEU	3.0
1	B	381	VAL	3.0
1	B	129	ASP	3.0
1	A	467	PRO	3.0
1	A	265	LYS	2.9
1	B	291	LYS	2.9
1	B	411	LYS	2.9
1	B	468	GLY	2.9
1	A	266	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	354	MET	2.7
1	A	271	ASN	2.7
1	B	320	LEU	2.7
1	B	413	ILE	2.7
1	A	647	LYS	2.7
1	B	325	ASP	2.7
1	B	594	ARG	2.6
1	B	584	THR	2.6
1	A	354	MET	2.6
1	B	589	LEU	2.6
1	B	353	GLY	2.6
1	B	410	PRO	2.6
1	B	131	PHE	2.6
1	B	271	ASN	2.6
1	B	406	PHE	2.5
1	A	84	ASP	2.5
1	B	277	THR	2.5
1	A	456	LYS	2.5
1	B	600	GLN	2.4
1	A	267	THR	2.4
1	B	372	ALA	2.4
1	B	356	GLY	2.4
1	B	467	PRO	2.4
1	B	464	GLU	2.4
1	B	393	ARG	2.4
1	B	592	GLU	2.4
1	B	446	GLU	2.3
1	A	458	TYR	2.3
1	A	263	PRO	2.3
1	B	470	LYS	2.3
1	A	282	ASP	2.3
1	B	420	GLN	2.3
1	A	462	TYR	2.3
1	B	306	VAL	2.2
1	A	468	GLY	2.2
1	A	466	THR	2.1
1	B	332	THR	2.1
1	B	596	SER	2.1
1	B	126	HIS	2.1
1	B	415	LYS	2.1
1	B	580	GLN	2.1
1	A	201	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	283	GLU	2.0
1	B	414	ASN	2.0
1	B	314	ALA	2.0
1	B	585	GLN	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(Å ²)	Q<0.9
6	OXY	A	705	2/2	0.76	0.19	55,55,55,60	0
7	ACT	B	712	4/4	0.79	0.20	56,57,63,65	0
6	OXY	B	709	2/2	0.82	0.31	64,64,64,69	0
7	ACT	B	713	4/4	0.83	0.19	57,58,71,73	0
7	ACT	A	708	4/4	0.85	0.19	41,57,57,61	0
6	OXY	B	707	2/2	0.87	0.22	61,61,61,62	0
8	PO4	B	711	5/5	0.89	0.12	57,66,70,71	0
6	OXY	A	706	2/2	0.90	0.27	69,69,69,71	0
6	OXY	B	705	2/2	0.90	0.23	68,68,68,69	0
6	OXY	B	708	2/2	0.91	0.24	59,59,59,61	0
6	OXY	B	706	2/2	0.91	0.40	84,84,84,85	0
6	OXY	B	710	2/2	0.94	0.29	40,40,40,48	0
6	OXY	A	707	2/2	0.95	0.30	48,48,48,53	0
3	FAD	B	702	53/53	0.96	0.09	33,41,66,74	0
5	TPP	A	704	26/26	0.97	0.06	21,30,37,56	0
2	K	B	701	1/1	0.97	0.05	41,41,41,41	0
4	MG	B	703	1/1	0.98	0.03	25,25,25,25	0
3	FAD	A	702	53/53	0.98	0.06	25,31,64,70	0
4	MG	A	703	1/1	0.98	0.07	35,35,35,35	0

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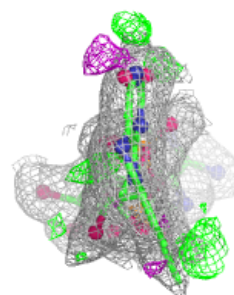
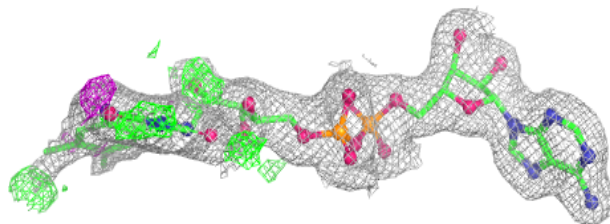
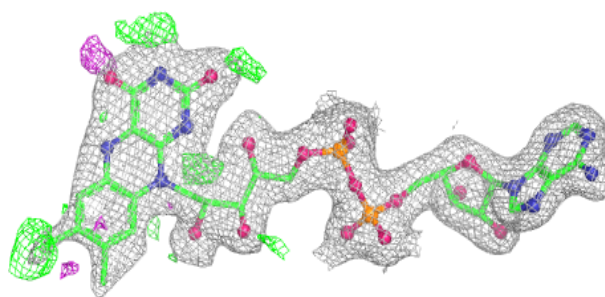
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	TPP	B	704	26/26	0.99	0.04	19,22,26,28	0
2	K	A	701	1/1	0.99	0.05	34,34,34,34	0

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.

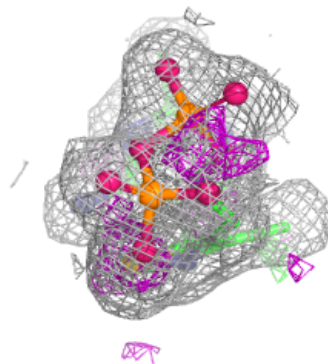
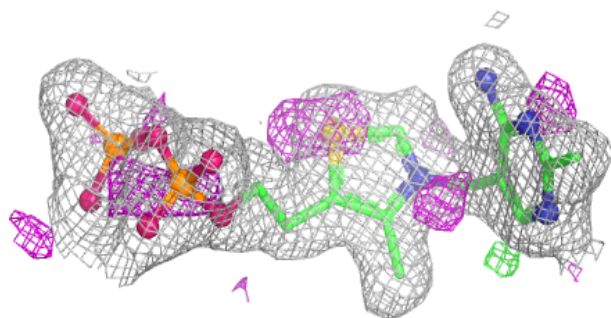
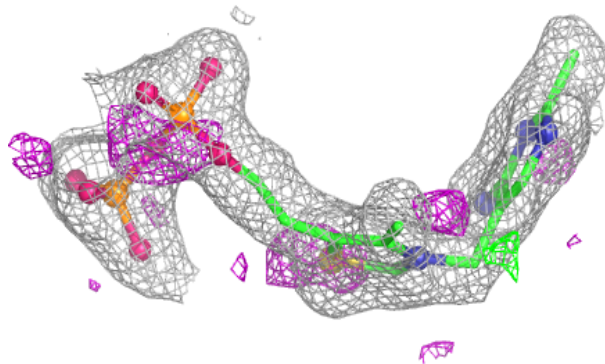
Electron density around FAD B 702:

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

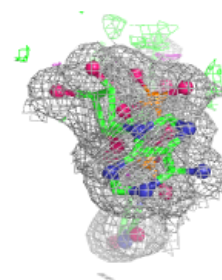
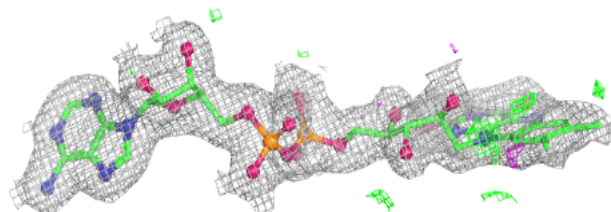
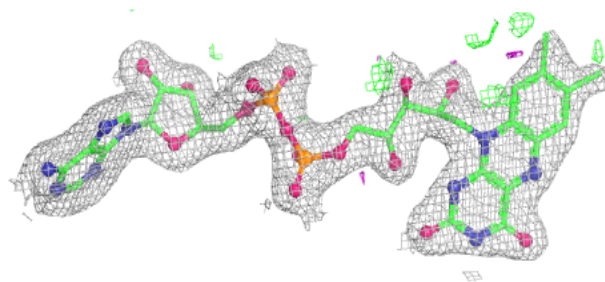


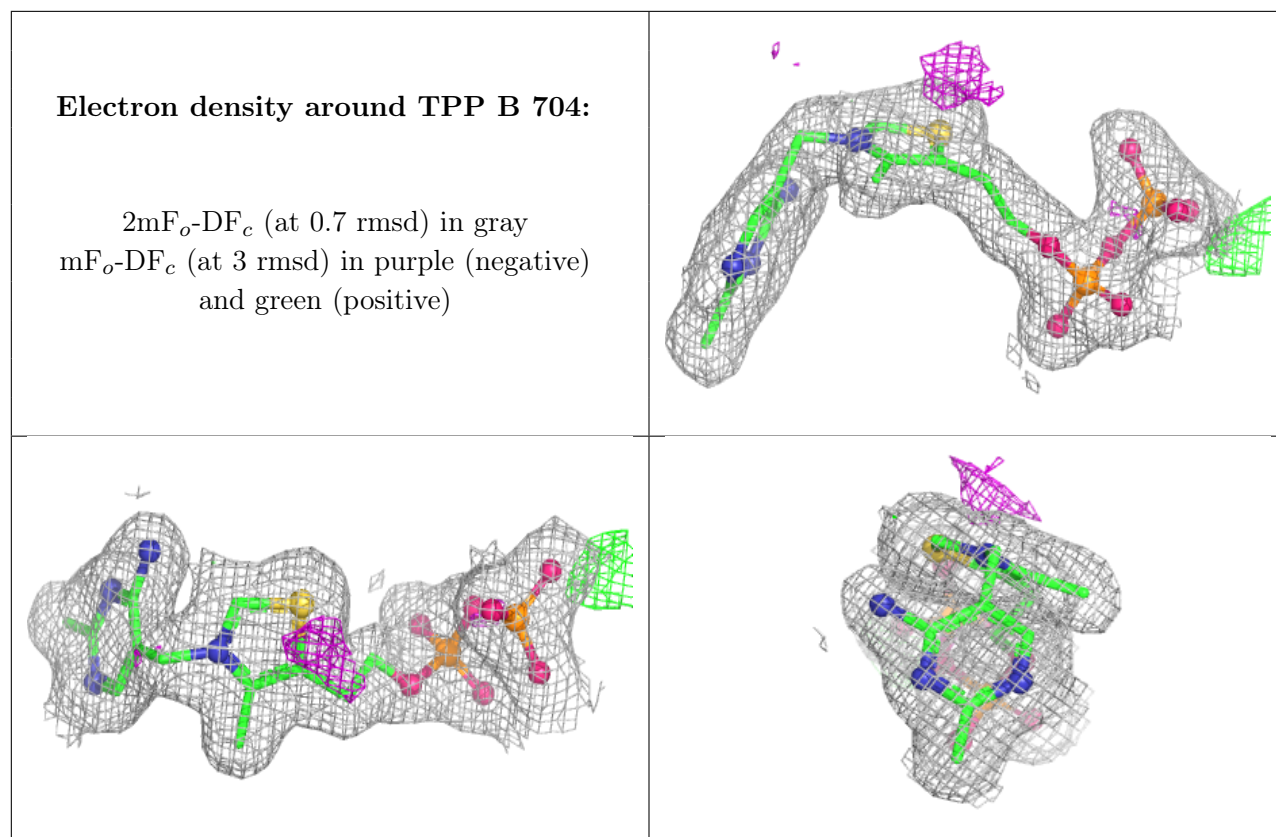
Electron density around TPP A 704:

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

**Electron density around 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.