



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:12 PM UTC

PDB ID : 1JSC / pdb_00001jsc
Title : Crystal Structure of the Catalytic Subunit of Yeast Acetohydroxyacid Synthase: A target for Herbicidal Inhibitors
Authors : Pang, S.S.; Duggleby, R.G.; Guddat, L.W.
Deposited on : 2001-08-17
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

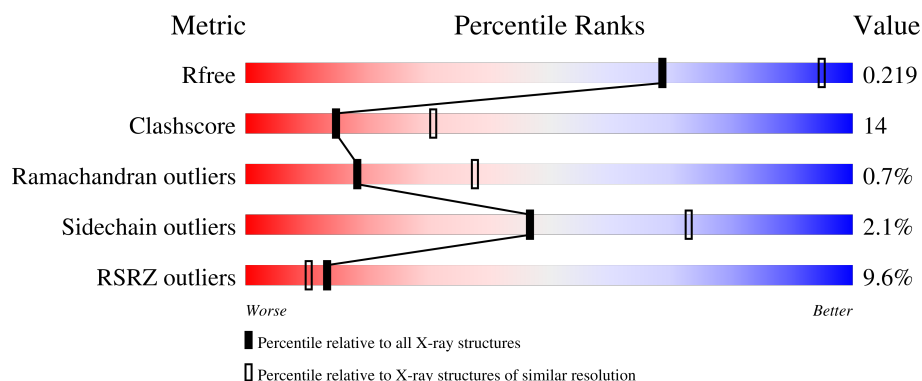
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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	630	 3% 65% 19% 14%
1	B	630	 13% 64% 22% 13%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8628 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 ACETOHYDROXY-ACID SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	0	0
			4071	2577	700	775	19			
1	B	550	Total	C	N	O	S	0	0	0
			4055	2560	692	784	19			

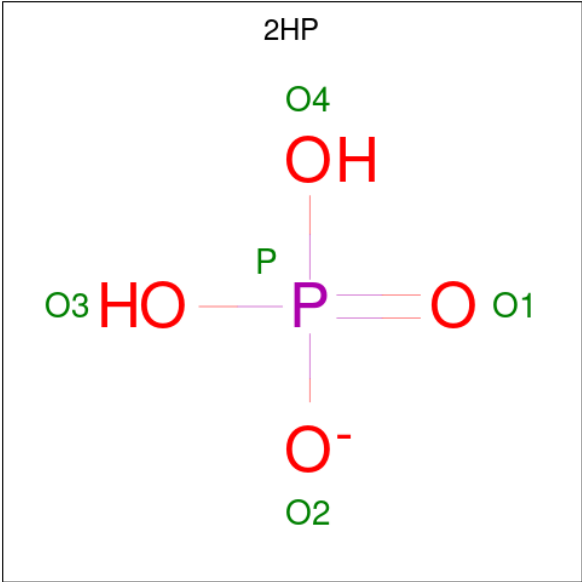
- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

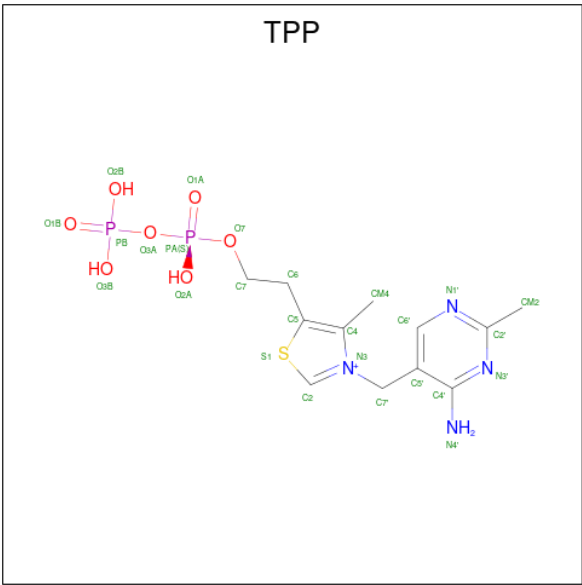
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is DIHYDROGENPHOSPHATE ION (CCD ID: 2HP) (formula: H₂O₄P).



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

- Molecule 5 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



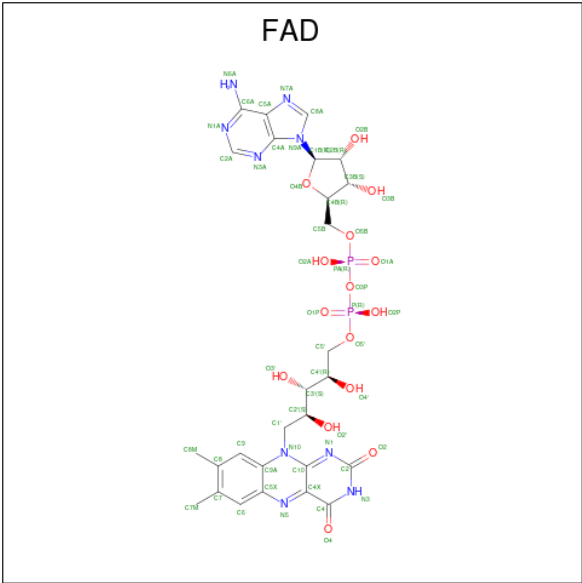
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

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

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

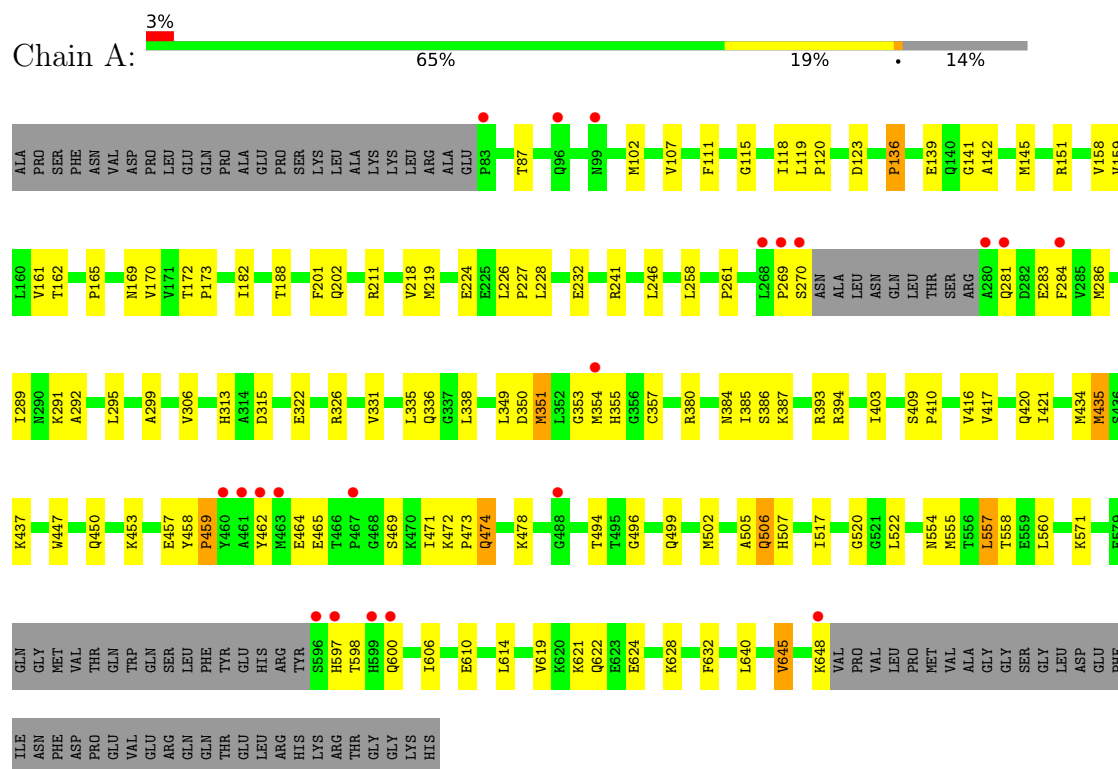
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	203	Total	O	0	0
			203	203		
7	B	122	Total	O	0	0
			122	122		

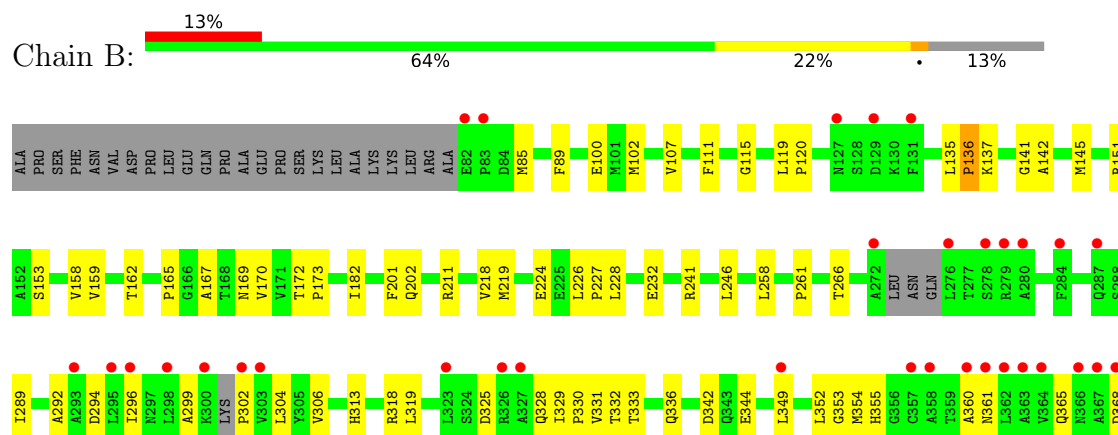
3 Residue-property plots

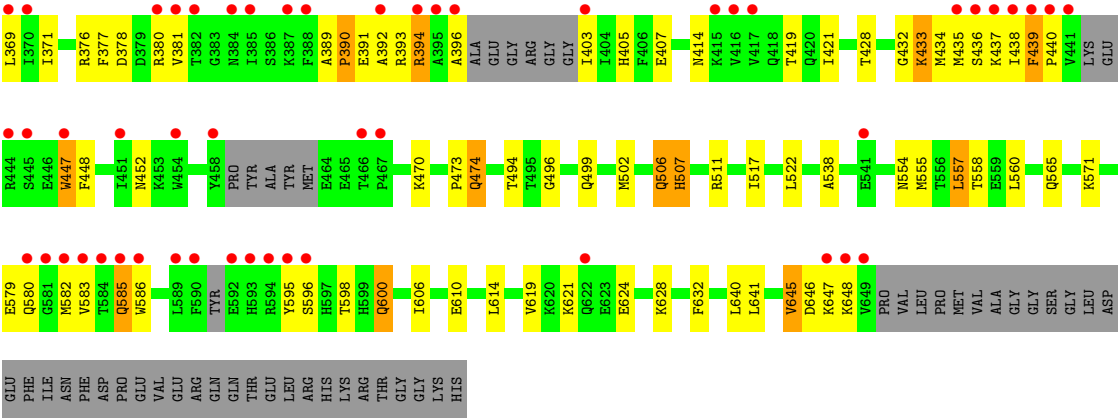
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: ACETOHYDROXY-ACID SYNTHASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.55Å 109.40Å 178.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.60 93.33 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.1 (100.00-2.60) 94.0 (93.33-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.93 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.188 , 0.219 0.188 , 0.219	Depositor DCC
R_{free} test set	5807 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8628	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPP, FAD, K, 2HP, MG

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	0.41	0/4152	0.91	10/5639 (0.2%)
1	B	0.40	0/4131	0.88	7/5619 (0.1%)
All	All	0.41	0/8283	0.90	17/11258 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	507	HIS	N-CA-C	6.12	120.60	113.20
1	B	507	HIS	N-CA-C	6.11	120.59	113.20
1	B	496	GLY	N-CA-C	-5.84	104.15	112.55
1	A	496	GLY	N-CA-C	-5.80	104.20	112.55
1	A	306	VAL	N-CA-C	5.73	116.84	108.53
1	A	506	GLN	N-CA-C	5.65	117.30	111.03
1	B	506	GLN	N-CA-C	5.65	117.30	111.03
1	B	349	LEU	N-CA-C	-5.53	106.30	113.16
1	A	241	ARG	N-CA-C	-5.48	101.62	109.24
1	B	241	ARG	N-CA-C	-5.46	101.65	109.24
1	A	331	VAL	N-CA-C	5.42	115.70	108.11
1	A	353	GLY	N-CA-C	5.39	117.53	112.08
1	A	380	ARG	N-CA-C	-5.23	106.41	112.89
1	A	351	MET	N-CA-C	5.17	117.94	110.28
1	A	435	MET	N-CA-C	5.10	117.23	111.11
1	B	596	SER	N-CA-C	5.08	116.71	109.14
1	B	585	GLN	N-CA-C	-5.05	105.96	112.68

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4071	0	4066	117	0
1	B	4055	0	3938	117	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
5	A	26	0	16	0	0
5	B	26	0	16	1	0
6	A	53	0	31	0	0
6	B	53	0	31	1	0
7	A	203	0	0	6	0
7	B	122	0	0	2	0
All	All	8628	0	8098	226	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 14.

All (226) 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:474:GLN:H	1:A:474:GLN:HE21	1.09	1.01
1:A:403:ILE:H	1:A:420:GLN:HE21	1.07	0.94
1:A:151:ARG:HH22	1:A:336:GLN:HE22	1.20	0.87
1:A:335:LEU:HA	1:A:351:MET:HE2	1.56	0.87
1:B:365:GLN:HA	1:B:390:PRO:HD2	1.56	0.84
1:B:499:GLN:HE22	1:B:580:GLN:NE2	1.77	0.83
1:B:306:VAL:HG13	1:B:333:THR:HG22	1.61	0.82
1:A:474:GLN:H	1:A:474:GLN:NE2	1.76	0.82
1:B:474:GLN:H	1:B:474:GLN:NE2	1.81	0.79
1:A:142:ALA:HA	1:A:145:MET:HE2	1.65	0.78
1:A:151:ARG:NH2	1:A:336:GLN:HE22	1.82	0.77
1:B:142:ALA:HA	1:B:145:MET:HE2	1.67	0.77
1:A:385:ILE:HD11	1:A:417:VAL:CG1	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:HD11	1:A:351:MET:CE	2.16	0.75
1:A:462:TYR:HE2	1:A:478:LYS:HD2	1.51	0.75
1:A:313:HIS:HD2	1:A:315:ASP:H	1.36	0.74
1:B:368:ASP:O	1:B:392:ALA:HA	1.88	0.73
1:B:355:HIS:CB	1:B:502:MET:HE2	2.20	0.72
1:B:352:LEU:HD12	1:B:360:ALA:HB1	1.72	0.71
1:B:435:MET:HE3	1:B:435:MET:HA	1.71	0.70
1:A:403:ILE:N	1:A:420:GLN:HE21	1.87	0.69
1:A:474:GLN:HE21	1:A:474:GLN:N	1.86	0.69
1:B:414:ASN:OD1	1:B:419:THR:HG22	1.92	0.68
1:B:499:GLN:HE22	1:B:580:GLN:HE22	1.41	0.66
1:A:462:TYR:CE2	1:A:478:LYS:HD2	2.31	0.66
1:A:338:LEU:HD11	1:A:351:MET:HE3	1.76	0.66
1:A:450:GLN:HE21	1:A:450:GLN:HA	1.61	0.65
1:A:351:MET:HE1	1:A:505:ALA:HB1	1.78	0.65
1:A:403:ILE:H	1:A:420:GLN:NE2	1.88	0.65
1:B:313:HIS:CD2	1:B:428:THR:HG21	2.31	0.65
1:B:390:PRO:HG2	1:B:391:GLU:H	1.60	0.65
1:A:554:ASN:HA	1:A:557:LEU:HD13	1.79	0.65
1:A:386:SER:HA	1:A:393:ARG:HH22	1.62	0.64
1:A:295:LEU:HD12	1:A:421:ILE:HD12	1.79	0.63
1:B:355:HIS:HB2	1:B:502:MET:HE2	1.80	0.63
1:B:621:LYS:O	1:B:624:GLU:HG2	1.99	0.63
1:A:458:TYR:N	1:A:459:PRO:HD3	2.15	0.62
1:B:226:LEU:HB3	1:B:227:PRO:HD3	1.82	0.62
1:B:302:PRO:O	1:B:330:PRO:HD2	2.00	0.62
1:B:473:PRO:HG3	1:B:645:VAL:HG11	1.81	0.62
1:B:299:ALA:HB1	1:B:368:ASP:OD2	2.00	0.61
1:B:342:ASP:OD2	1:B:344:GLU:HB2	2.00	0.61
1:A:621:LYS:O	1:A:624:GLU:HG2	1.99	0.61
1:B:355:HIS:ND1	1:B:502:MET:HG3	2.16	0.61
1:A:151:ARG:HD2	1:A:182:ILE:CD1	2.31	0.61
1:A:520:GLY:HA3	7:A:1003:HOH:O	2.00	0.61
1:B:228:LEU:O	1:B:232:GLU:HG3	2.02	0.59
1:B:302:PRO:HG2	1:B:329:ILE:HG23	1.84	0.59
1:B:648:LYS:N	1:B:648:LYS:HD2	2.18	0.59
1:B:151:ARG:NH2	7:B:804:HOH:O	2.34	0.59
1:A:226:LEU:HB3	1:A:227:PRO:HD3	1.84	0.59
1:B:554:ASN:HA	1:B:557:LEU:HD13	1.84	0.59
1:A:465:GLU:CD	1:A:472:LYS:H	2.11	0.59
1:B:474:GLN:H	1:B:474:GLN:HE21	1.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:GLY:HA2	1:B:381:VAL:HA	1.84	0.58
1:A:111:PHE:HD2	1:A:145:MET:HE3	1.66	0.58
1:A:385:ILE:HD11	1:A:417:VAL:HG12	1.84	0.58
1:A:151:ARG:NH2	1:A:336:GLN:NE2	2.51	0.58
1:A:322:GLU:OE2	1:A:435:MET:HE2	2.04	0.58
1:A:286:MET:HE3	1:A:286:MET:O	2.03	0.58
1:A:201:PHE:CZ	6:B:1701:FAD:HM82	2.39	0.57
1:B:151:ARG:HD2	1:B:182:ILE:CD1	2.34	0.57
1:A:228:LEU:O	1:A:232:GLU:HG3	2.04	0.57
1:A:141:GLY:O	1:A:145:MET:HG3	2.04	0.57
1:A:606:ILE:O	1:A:610:GLU:HG3	2.04	0.57
1:B:141:GLY:O	1:B:145:MET:HG3	2.05	0.57
1:A:286:MET:HE1	1:A:437:LYS:HE3	1.87	0.57
1:A:87:THR:HG22	1:A:261:PRO:HG3	1.86	0.56
1:B:292:ALA:HB2	1:B:421:ILE:HG21	1.88	0.56
1:B:389:ALA:O	1:B:393:ARG:HB2	2.05	0.56
1:B:389:ALA:HB1	1:B:392:ALA:HB3	1.88	0.56
1:B:606:ILE:O	1:B:610:GLU:HG3	2.05	0.56
1:A:450:GLN:HA	1:A:450:GLN:NE2	2.19	0.55
1:A:619:VAL:HG22	1:A:628:LYS:HG3	1.86	0.55
1:B:111:PHE:HD2	1:B:145:MET:HE3	1.69	0.55
1:A:555:MET:CE	7:A:761:HOH:O	2.54	0.55
1:A:102:MET:HE3	1:A:107:VAL:HG11	1.87	0.55
1:B:355:HIS:HB3	1:B:502:MET:HE2	1.88	0.55
1:B:619:VAL:HG22	1:B:628:LYS:HG3	1.88	0.55
1:B:434:MET:O	1:B:434:MET:HG2	2.04	0.55
1:A:170:VAL:C	1:A:173:PRO:HD2	2.32	0.54
1:B:414:ASN:CG	1:B:419:THR:HG22	2.32	0.54
1:B:439:PHE:CD1	1:B:439:PHE:N	2.75	0.54
1:B:318:ARG:HH21	1:B:319:LEU:HD21	1.71	0.54
1:A:600:GLN:NE2	7:A:759:HOH:O	2.40	0.54
1:B:102:MET:HE3	1:B:107:VAL:HG11	1.89	0.54
1:A:640:LEU:C	1:A:640:LEU:HD23	2.32	0.54
1:B:304:LEU:HD12	1:B:331:VAL:HG22	1.90	0.54
1:B:361:ASN:O	1:B:365:GLN:HG2	2.08	0.54
1:B:170:VAL:C	1:B:173:PRO:HD2	2.33	0.54
1:B:405:HIS:CE1	1:B:407:GLU:HB2	2.43	0.54
1:B:502:MET:O	1:B:506:GLN:HG3	2.08	0.54
1:A:354:MET:HE2	1:A:355:HIS:NE2	2.23	0.53
1:B:354:MET:SD	1:B:380:ARG:CZ	2.96	0.53
1:A:499:GLN:HE22	1:A:648:LYS:CB	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:LEU:C	1:B:640:LEU:HD23	2.33	0.53
1:B:119:LEU:HB3	1:B:120:PRO:HD3	1.90	0.53
1:B:172:THR:HB	1:B:173:PRO:HD3	1.91	0.53
1:B:447:TRP:HA	1:B:447:TRP:CE3	2.43	0.53
1:B:582:MET:HE3	1:B:598:THR:HG22	1.91	0.52
1:B:378:ASP:HB3	1:B:381:VAL:HG23	1.92	0.52
1:A:165:PRO:HD3	1:B:522:LEU:HG	1.91	0.52
1:B:555:MET:CE	7:B:760:HOH:O	2.57	0.52
1:A:471:ILE:HG12	1:A:622:GLN:HG2	1.93	0.51
1:A:289:ILE:HG23	1:A:434:MET:HB2	1.92	0.51
1:A:571:LYS:HB3	1:A:632:PHE:CZ	2.45	0.51
1:A:169:ASN:ND2	1:B:172:THR:OG1	2.43	0.51
1:A:172:THR:HB	1:A:173:PRO:HD3	1.92	0.51
1:A:465:GLU:OE1	1:A:471:ILE:HA	2.11	0.51
1:A:111:PHE:CD2	1:A:145:MET:HE3	2.46	0.51
1:B:571:LYS:HB3	1:B:632:PHE:CZ	2.46	0.50
1:A:246:LEU:C	1:A:246:LEU:HD23	2.37	0.50
1:A:502:MET:O	1:A:506:GLN:HG3	2.11	0.50
1:A:600:GLN:HG3	1:B:137:LYS:HE3	1.92	0.49
1:B:470:LYS:HB3	1:B:646:ASP:HB2	1.94	0.49
1:B:246:LEU:C	1:B:246:LEU:HD23	2.37	0.49
1:A:469:SER:H	1:A:622:GLN:NE2	2.09	0.49
1:A:172:THR:OG1	1:B:169:ASN:ND2	2.45	0.49
1:A:281:GLN:HG3	1:A:284:PHE:HB3	1.94	0.49
1:A:469:SER:H	1:A:622:GLN:HE21	1.59	0.49
1:A:473:PRO:HD3	1:A:645:VAL:HG13	1.95	0.49
1:A:457:GLU:C	1:A:459:PRO:HD3	2.38	0.49
1:B:102:MET:CE	1:B:107:VAL:HG11	2.43	0.48
1:B:448:PHE:HB3	1:B:452:ASN:HD21	1.78	0.48
1:B:432:GLY:C	1:B:434:MET:H	2.21	0.48
1:A:115:GLY:HA3	1:A:162:THR:HB	1.95	0.48
1:A:522:LEU:HG	1:B:165:PRO:HD3	1.95	0.48
1:A:151:ARG:HD2	1:A:182:ILE:HD11	1.94	0.48
1:B:111:PHE:CD2	1:B:145:MET:HE3	2.47	0.48
1:B:85:MET:HE3	1:B:261:PRO:HB2	1.96	0.48
1:B:447:TRP:HA	1:B:447:TRP:HE3	1.79	0.48
1:A:119:LEU:HB3	1:A:120:PRO:HD3	1.96	0.48
1:B:557:LEU:HD23	1:B:558:THR:N	2.29	0.47
1:A:151:ARG:HD2	1:A:182:ILE:HD13	1.97	0.47
1:A:326:ARG:HD3	1:A:435:MET:HE1	1.95	0.47
1:A:349:LEU:O	1:A:350:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASN:ND2	1:A:386:SER:OG	2.46	0.47
1:B:115:GLY:HA3	1:B:162:THR:HB	1.97	0.47
1:B:439:PHE:HD1	1:B:439:PHE:H	1.62	0.47
1:A:102:MET:CE	1:A:107:VAL:HG11	2.45	0.47
1:B:585:GLN:HG3	1:B:586:TRP:HD1	1.80	0.47
1:A:136:PRO:HG3	1:A:142:ALA:HB2	1.96	0.47
1:A:281:GLN:C	1:A:283:GLU:N	2.71	0.46
1:A:434:MET:O	1:A:434:MET:HG2	2.14	0.46
1:B:494:THR:HA	1:B:517:ILE:O	2.15	0.46
1:A:269:PRO:O	1:A:270:SER:HB2	2.15	0.46
1:B:136:PRO:HG3	1:B:142:ALA:HB2	1.97	0.46
1:B:557:LEU:HD23	1:B:557:LEU:C	2.40	0.46
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.80	0.46
1:B:218:VAL:HG22	1:B:219:MET:N	2.30	0.46
1:B:439:PHE:N	1:B:439:PHE:HD1	2.14	0.46
1:A:281:GLN:O	1:A:281:GLN:HG2	2.16	0.46
1:B:394:ARG:C	1:B:396:ALA:H	2.23	0.46
1:A:494:THR:HA	1:A:517:ILE:O	2.16	0.45
1:B:102:MET:HE3	1:B:107:VAL:HG21	1.98	0.45
1:B:211:ARG:HG3	1:B:211:ARG:HH11	1.81	0.45
1:A:218:VAL:HG22	1:A:219:MET:N	2.30	0.45
1:B:153:SER:HB3	1:B:538:ALA:HB1	1.99	0.45
1:A:474:GLN:O	1:A:478:LYS:HG3	2.16	0.45
1:A:102:MET:CE	1:A:158:VAL:HG11	2.47	0.45
1:B:436:SER:C	1:B:438:ILE:H	2.25	0.45
1:A:119:LEU:HD11	1:B:583:VAL:HG13	1.98	0.45
1:A:557:LEU:HD23	1:A:557:LEU:C	2.43	0.44
1:B:289:ILE:HG21	1:B:433:LYS:O	2.17	0.44
1:A:102:MET:HE3	1:A:107:VAL:HG21	1.99	0.44
1:A:292:ALA:HB3	1:A:434:MET:CE	2.47	0.44
1:B:325:ASP:O	1:B:328:GLN:NE2	2.51	0.44
1:B:494:THR:HG22	1:B:517:ILE:HB	1.99	0.44
1:A:557:LEU:HD23	1:A:558:THR:N	2.32	0.44
1:B:151:ARG:HD2	1:B:182:ILE:HD13	1.99	0.44
1:A:416:VAL:HG12	1:A:417:VAL:HG13	2.00	0.44
1:B:329:ILE:HA	1:B:330:PRO:HD3	1.88	0.44
1:B:376:ARG:O	1:B:377:PHE:C	2.61	0.44
1:B:336:GLN:OE1	1:B:336:GLN:HA	2.18	0.43
1:B:365:GLN:CA	1:B:390:PRO:HD2	2.39	0.43
1:B:151:ARG:HD2	1:B:182:ILE:HD11	1.98	0.43
1:B:304:LEU:HD23	1:B:371:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:HG3	1:A:258:LEU:HD11	2.01	0.43
1:B:473:PRO:HG3	1:B:645:VAL:CG1	2.48	0.43
1:B:619:VAL:HG23	1:B:641:LEU:HD11	2.00	0.43
1:A:458:TYR:N	1:A:459:PRO:CD	2.81	0.43
1:B:167:ALA:O	1:B:170:VAL:HG22	2.19	0.43
1:B:344:GLU:HG3	1:B:511:ARG:CZ	2.49	0.43
1:B:645:VAL:HG13	1:B:646:ASP:N	2.33	0.43
1:B:619:VAL:HG13	1:B:624:GLU:HG3	2.00	0.43
1:A:139:GLU:OE2	5:B:1700:TPP:N1'	2.52	0.42
1:A:299:ALA:HB2	7:A:812:HOH:O	2.18	0.42
1:A:384:ASN:ND2	1:A:387:LYS:HG3	2.34	0.42
1:B:89:PHE:HE2	1:B:100:GLU:HG2	1.83	0.42
1:A:161:VAL:CG2	1:A:188:THR:HG22	2.49	0.42
1:B:102:MET:CE	1:B:158:VAL:HG11	2.49	0.42
1:B:579:GLU:HB2	1:B:647:LYS:CB	2.49	0.42
1:A:291:LYS:HB3	1:A:421:ILE:CD1	2.49	0.42
1:A:350:ASP:HB3	7:A:860:HOH:O	2.18	0.42
1:B:369:LEU:HD12	1:B:403:ILE:N	2.35	0.42
1:A:555:MET:HE2	7:A:761:HOH:O	2.19	0.42
1:A:619:VAL:HG13	1:A:624:GLU:HG3	2.01	0.42
1:A:384:ASN:HD22	1:A:387:LYS:HG3	1.85	0.41
1:B:111:PHE:O	1:B:159:VAL:HA	2.20	0.41
1:B:224:GLU:HG3	1:B:258:LEU:HD11	2.02	0.41
1:A:118:ILE:HG13	1:A:118:ILE:O	2.20	0.41
1:A:291:LYS:HB3	1:A:421:ILE:HD13	2.03	0.41
1:A:453:LYS:O	1:A:457:GLU:HB2	2.20	0.41
1:A:494:THR:HG22	1:A:517:ILE:HB	2.01	0.41
1:A:111:PHE:O	1:A:159:VAL:HA	2.20	0.41
1:B:228:LEU:HB2	1:B:266:THR:HB	2.03	0.41
1:A:450:GLN:HE21	1:A:450:GLN:CA	2.28	0.41
1:A:201:PHE:CE2	1:A:202:GLN:HG3	2.56	0.41
1:A:385:ILE:HD12	1:A:385:ILE:HA	1.86	0.41
1:B:294:ASP:C	1:B:296:ILE:N	2.78	0.41
1:B:304:LEU:O	1:B:332:THR:HG22	2.21	0.41
1:A:291:LYS:HD3	1:A:291:LYS:HA	1.90	0.41
1:A:409:SER:HA	1:A:410:PRO:HD3	1.93	0.41
1:B:115:GLY:HA3	1:B:162:THR:CB	2.51	0.41
1:A:119:LEU:HG	1:A:123:ASP:OD2	2.21	0.40
1:A:600:GLN:NE2	1:B:565:GLN:OE1	2.55	0.40
1:B:582:MET:HE2	1:B:600:GLN:HG3	2.02	0.40
1:A:115:GLY:HA3	1:A:162:THR:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ILE:HD11	1:A:417:VAL:HG11	2.01	0.40
1:B:201:PHE:CE2	1:B:202:GLN:HG3	2.57	0.40
1:B:474:GLN:HG3	1:B:507:HIS:CD2	2.56	0.40
1:A:598:THR:HG23	1:B:135:LEU:HD11	2.03	0.40
1:B:365:GLN:O	1:B:390:PRO:HG2	2.22	0.40
1:B:595:TYR:N	1:B:595:TYR:CD1	2.89	0.40
1:A:201:PHE:CZ	1:A:202:GLN:HG3	2.57	0.40
1:A:313:HIS:CD2	1:A:315:ASP:H	2.26	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	535/630 (85%)	517 (97%)	15 (3%)	3 (1%)	21	42
1	B	536/630 (85%)	502 (94%)	29 (5%)	5 (1%)	14	30
All	All	1071/1260 (85%)	1019 (95%)	44 (4%)	8 (1%)	18	38

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	464	GLU
1	B	394	ARG
1	A	597	HIS
1	B	390	PRO
1	B	437	LYS
1	A	459	PRO
1	B	433	LYS
1	B	440	PRO

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	434/518 (84%)	425 (98%)	9 (2%)	47	73
1	B	422/518 (82%)	413 (98%)	9 (2%)	47	73
All	All	856/1036 (83%)	838 (98%)	18 (2%)	47	73

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	PRO
1	A	357	CYS
1	A	394	ARG
1	A	447	TRP
1	A	474	GLN
1	A	557	LEU
1	A	560	LEU
1	A	614	LEU
1	A	645	VAL
1	B	136	PRO
1	B	439	PHE
1	B	447	TRP
1	B	474	GLN
1	B	557	LEU
1	B	560	LEU
1	B	600	GLN
1	B	614	LEU
1	B	645	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	169	ASN
1	A	202	GLN
1	A	313	HIS

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Mol	Chain	Res	Type
1	A	336	GLN
1	A	366	ASN
1	A	384	ASN
1	A	420	GLN
1	A	450	GLN
1	A	474	GLN
1	A	499	GLN
1	A	512	ASN
1	A	536	GLN
1	A	600	GLN
1	A	622	GLN
1	B	106	ASN
1	B	169	ASN
1	B	202	GLN
1	B	313	HIS
1	B	328	GLN
1	B	405	HIS
1	B	418	GLN
1	B	452	ASN
1	B	474	GLN
1	B	499	GLN
1	B	501	GLN
1	B	512	ASN
1	B	536	GLN
1	B	600	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	TPP	B	1700	3	26,27,27	1.42	4 (15%)	38,40,40	1.60	8 (21%)
6	FAD	A	701	-	58,58,58	2.38	20 (34%)	85,89,89	1.19	6 (7%)
4	2HP	B	1698	-	4,4,4	1.69	0	6,6,6	0.46	0
4	2HP	A	698	-	4,4,4	1.67	0	6,6,6	0.47	0
6	FAD	B	1701	-	58,58,58	2.38	21 (36%)	85,89,89	1.16	5 (5%)
5	TPP	A	700	3	26,27,27	1.53	6 (23%)	38,40,40	1.57	8 (21%)
4	2HP	B	1697	-	4,4,4	1.69	0	6,6,6	0.47	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	B	1700	3	-	2/17/17/17	0/2/2/2
6	FAD	A	701	-	-	5/34/50/50	0/6/6/6
6	FAD	B	1701	-	-	2/34/50/50	0/6/6/6
5	TPP	A	700	3	-	1/17/17/17	0/2/2/2

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	701	FAD	C9A-C5X	5.99	1.50	1.41
6	B	1701	FAD	C9A-C5X	5.97	1.50	1.41
6	B	1701	FAD	C9-C8	5.85	1.47	1.39
6	A	701	FAD	C9-C8	5.82	1.47	1.39
6	A	701	FAD	C6-C7	5.50	1.47	1.39
6	B	1701	FAD	C6-C7	5.27	1.46	1.39
6	B	1701	FAD	C9-C9A	5.00	1.47	1.39
6	A	701	FAD	C9-C9A	4.92	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	701	FAD	C8-C7	4.82	1.52	1.40
6	B	1701	FAD	C8-C7	4.63	1.52	1.40
6	A	701	FAD	C6-C5X	4.14	1.46	1.40
6	B	1701	FAD	C5A-C4A	4.11	1.46	1.39
6	B	1701	FAD	C7M-C7	3.98	1.58	1.51
6	A	701	FAD	C7M-C7	3.88	1.58	1.51
6	A	701	FAD	C5A-C4A	3.87	1.46	1.39
6	B	1701	FAD	P-O3P	-3.78	1.55	1.59
6	B	1701	FAD	C6-C5X	3.72	1.45	1.40
6	A	701	FAD	C4X-N5	3.52	1.38	1.30
5	A	700	TPP	C7'-C5'	3.38	1.57	1.51
6	A	701	FAD	C9A-N10	3.26	1.46	1.41
6	B	1701	FAD	C4X-N5	3.24	1.37	1.30
6	A	701	FAD	C10-N1	3.09	1.39	1.33
6	B	1701	FAD	C10-N1	3.07	1.39	1.33
6	B	1701	FAD	C9A-N10	3.05	1.46	1.41
6	B	1701	FAD	C4A-N3A	3.04	1.40	1.34
6	A	701	FAD	O4'-C4'	2.96	1.49	1.43
6	A	701	FAD	C2A-N1A	2.96	1.39	1.33
6	A	701	FAD	P-O3P	-2.91	1.56	1.59
6	B	1701	FAD	C2A-N1A	2.90	1.39	1.33
6	A	701	FAD	C4A-N3A	2.86	1.39	1.34
6	B	1701	FAD	C10-N10	2.75	1.43	1.37
6	A	701	FAD	C8A-N9A	2.59	1.42	1.37
5	B	1700	TPP	C7'-C5'	2.55	1.55	1.51
6	A	701	FAD	C4'-C3'	2.48	1.57	1.53
5	A	700	TPP	C6'-C5'	2.46	1.42	1.37
6	B	1701	FAD	C2A-N3A	2.44	1.38	1.33
6	B	1701	FAD	O4'-C4'	2.44	1.48	1.43
5	A	700	TPP	C2-S1	2.39	1.76	1.69
6	B	1701	FAD	C8A-N9A	2.37	1.41	1.37
5	A	700	TPP	PB-O2B	-2.28	1.46	1.54
5	B	1700	TPP	PB-O2B	-2.27	1.46	1.54
5	B	1700	TPP	C6'-C5'	2.24	1.42	1.37
6	A	701	FAD	C2A-N3A	2.20	1.37	1.33
6	B	1701	FAD	C4-N3	2.17	1.42	1.38
5	B	1700	TPP	C2-S1	2.17	1.75	1.69
6	A	701	FAD	C10-N10	2.13	1.41	1.37
6	B	1701	FAD	C4'-C3'	2.13	1.57	1.53
5	A	700	TPP	PA-O2A	-2.10	1.45	1.55
5	A	700	TPP	C4'-N3'	2.03	1.37	1.35
6	A	701	FAD	C4-N3	2.01	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1701	FAD	P-O2P	-2.01	1.46	1.55

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	700	TPP	C2-S1-C5	-3.96	88.59	91.22
5	B	1700	TPP	C2-S1-C5	-3.63	88.81	91.22
5	A	700	TPP	C6'-N1'-C2'	3.56	121.93	116.07
5	B	1700	TPP	C6'-N1'-C2'	3.56	121.92	116.07
6	A	701	FAD	C9-C9A-N10	3.26	126.23	121.85
5	B	1700	TPP	CM2-C2'-N1'	3.26	120.67	117.20
6	B	1701	FAD	C9-C9A-N10	3.11	126.04	121.85
5	B	1700	TPP	N1'-C2'-N3'	-3.05	120.45	125.53
5	A	700	TPP	CM2-C2'-N1'	2.92	120.31	117.20
5	A	700	TPP	N1'-C2'-N3'	-2.87	120.76	125.53
5	B	1700	TPP	C5'-C6'-N1'	-2.62	119.57	123.83
6	B	1701	FAD	C4A-C5A-N7A	-2.52	107.70	110.58
6	A	701	FAD	O2-C2-N1	-2.49	117.66	121.80
6	A	701	FAD	C4A-C5A-N7A	-2.45	107.78	110.58
5	A	700	TPP	C5'-C6'-N1'	-2.44	119.86	123.83
6	A	701	FAD	O3P-PA-O1A	-2.43	103.40	110.70
6	B	1701	FAD	O2-C2-N1	-2.42	117.77	121.80
6	A	701	FAD	C5A-N7A-C8A	2.40	107.22	103.45
5	A	700	TPP	C7'-N3-C2	-2.38	118.52	123.48
5	B	1700	TPP	C7'-N3-C2	-2.33	118.62	123.48
6	B	1701	FAD	C5A-N7A-C8A	2.33	107.11	103.45
5	B	1700	TPP	CM4-C4-C5	-2.27	121.92	127.75
5	A	700	TPP	C2'-N3'-C4'	2.27	121.59	118.10
6	B	1701	FAD	O3P-PA-O1A	-2.25	103.94	110.70
5	B	1700	TPP	C2'-N3'-C4'	2.24	121.55	118.10
5	A	700	TPP	CM4-C4-C5	-2.22	122.07	127.75
6	A	701	FAD	C4X-C10-N10	2.05	119.42	116.48

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	701	FAD	C2'-C3'-C4'-O4'
6	A	701	FAD	O3'-C3'-C4'-C5'
6	A	701	FAD	C2'-C3'-C4'-C5'
5	B	1700	TPP	PA-O3A-PB-O2B
6	B	1701	FAD	C2B-C1B-N9A-C8A

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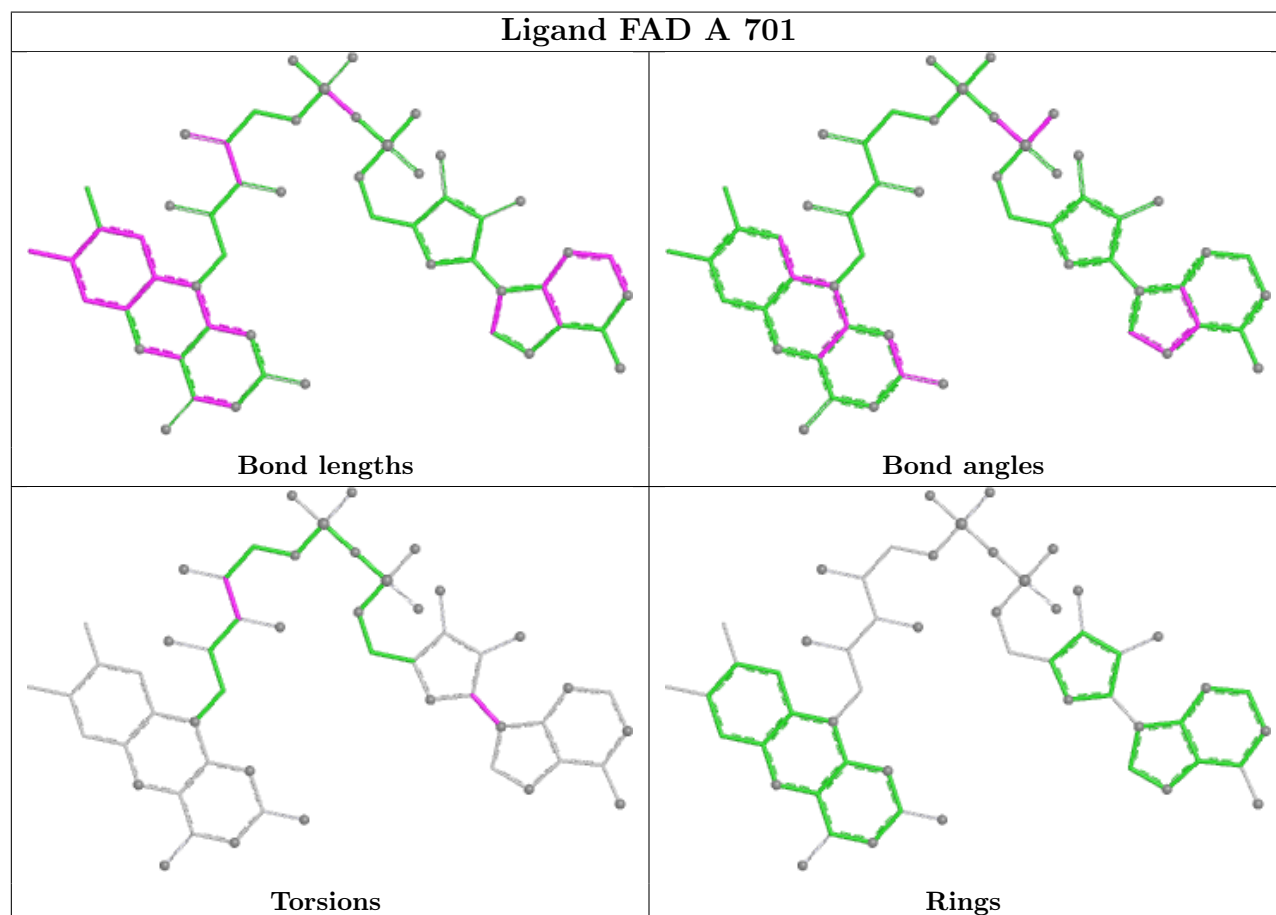
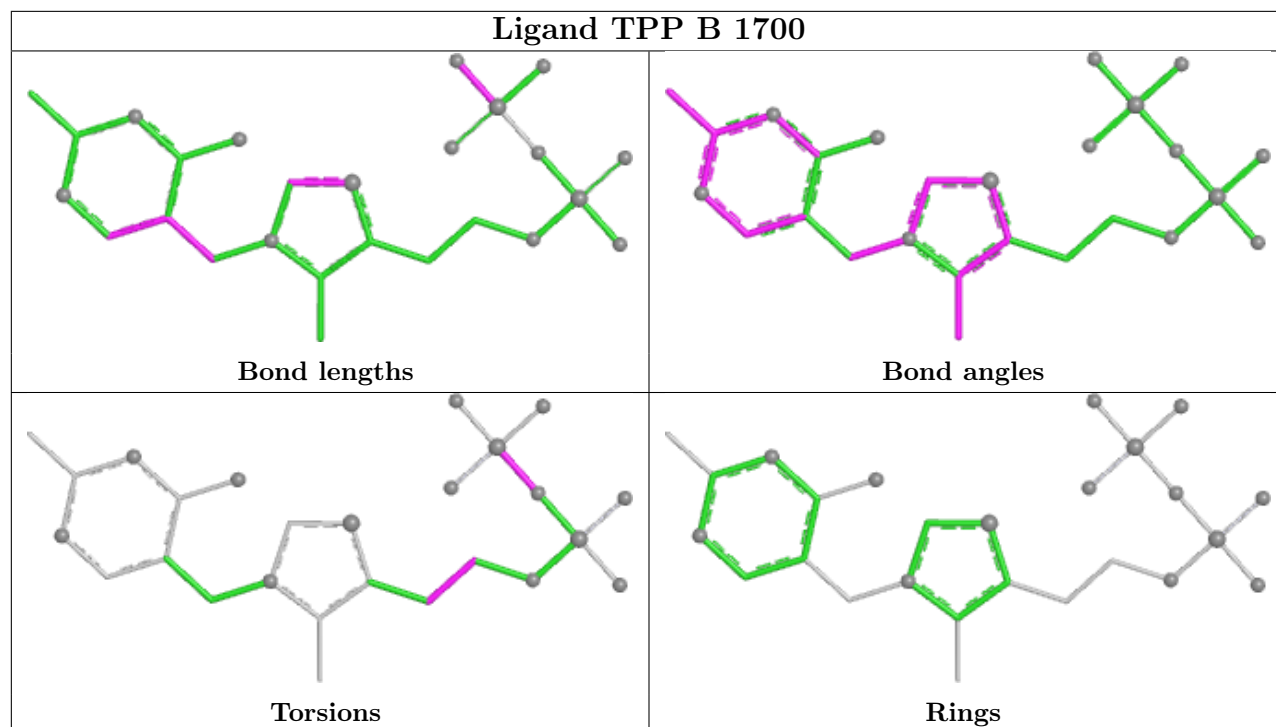
Mol	Chain	Res	Type	Atoms
5	A	700	TPP	C5-C6-C7-O7
5	B	1700	TPP	C5-C6-C7-O7
6	A	701	FAD	C2B-C1B-N9A-C8A
6	A	701	FAD	O3'-C3'-C4'-O4'
6	B	1701	FAD	O4B-C4B-C5B-O5B

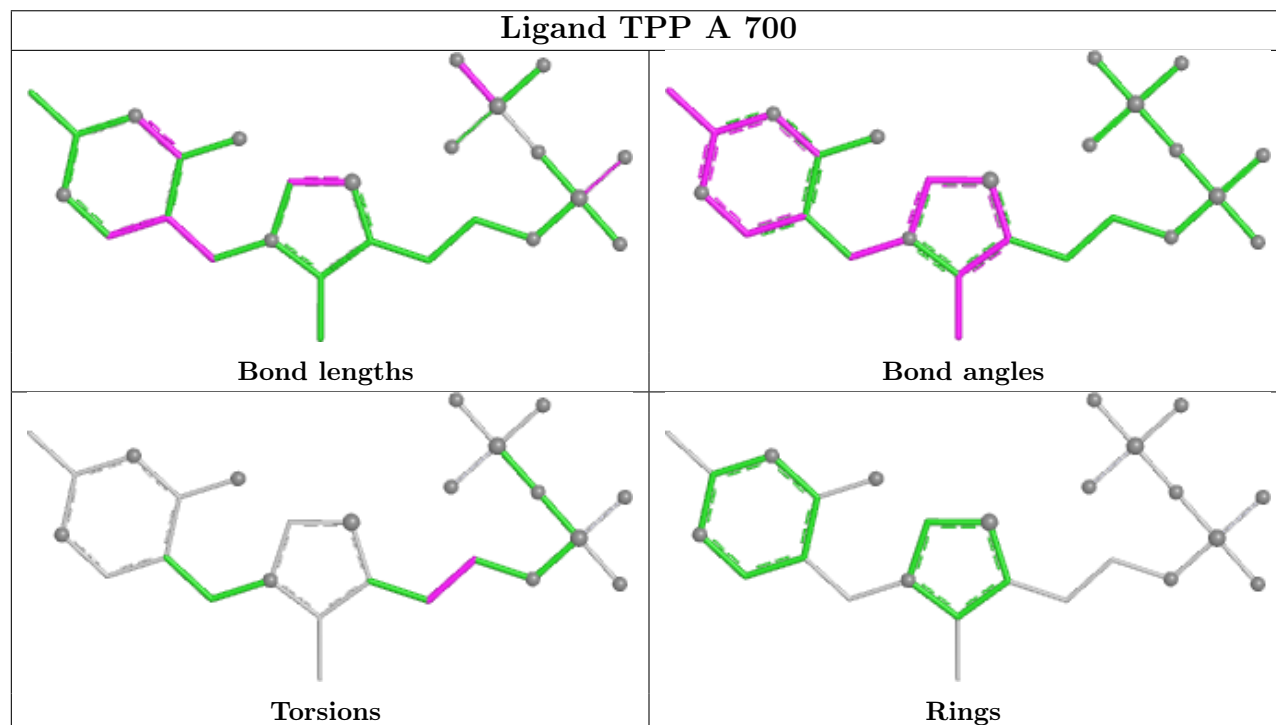
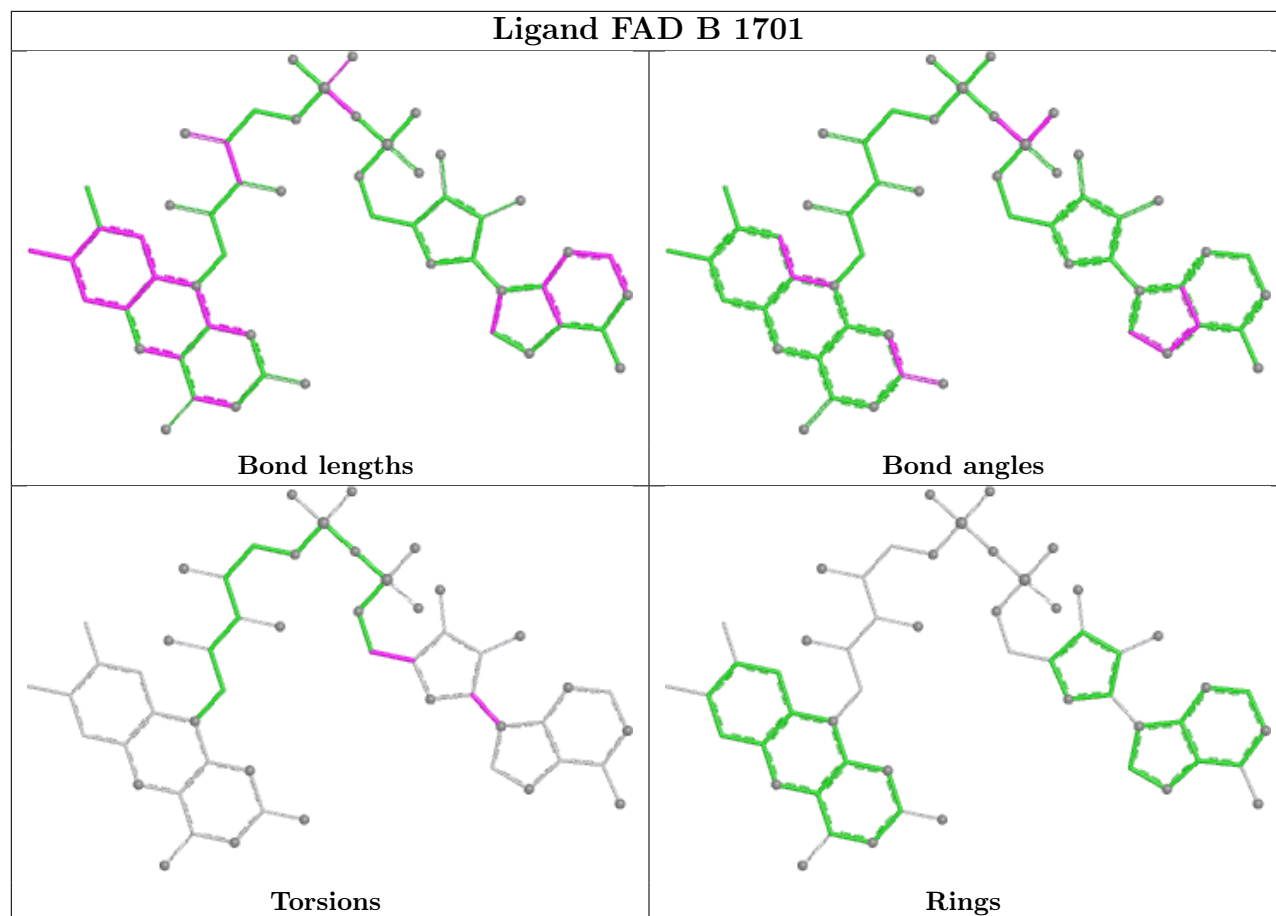
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1700	TPP	1	0
6	B	1701	FAD	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.





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	541/630 (85%)	-0.12	21 (3%) 43 38	33, 48, 90, 140	0
1	B	550/630 (87%)	0.58	84 (15%) 5 4	33, 56, 136, 147	0
All	All	1091/1260 (86%)	0.23	105 (9%) 13 10	33, 50, 125, 147	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	ALA	8.2
1	B	395	ALA	7.7
1	A	596	SER	6.5
1	B	444	ARG	6.4
1	B	441	VAL	6.0
1	B	382	THR	5.7
1	B	454	TRP	5.5
1	A	460	TYR	5.3
1	B	83	PRO	5.3
1	B	581	GLY	5.1
1	B	276	LEU	4.9
1	B	593	HIS	4.9
1	B	366	ASN	4.9
1	B	649	VAL	4.8
1	B	326	ARG	4.4
1	B	364	VAL	4.3
1	B	272	ALA	4.3
1	A	96	GLN	4.3
1	B	595	TYR	4.3
1	B	440	PRO	4.2
1	B	380	ARG	4.2
1	B	385	ILE	4.2
1	A	461	ALA	4.1
1	B	590	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	589	LEU	4.0
1	B	367	ALA	4.0
1	B	437	LYS	3.9
1	B	580	GLN	3.9
1	B	594	ARG	3.9
1	B	467	PRO	3.8
1	B	358	ALA	3.8
1	B	394	ARG	3.8
1	B	384	ASN	3.8
1	B	381	VAL	3.8
1	B	357	CYS	3.7
1	B	362	LEU	3.6
1	B	466	THR	3.5
1	B	127	ASN	3.4
1	B	298	LEU	3.4
1	B	451	ILE	3.4
1	B	586	TRP	3.4
1	A	599	HIS	3.3
1	B	648	LYS	3.3
1	B	592	GLU	3.2
1	B	287	GLN	3.2
1	B	280	ALA	3.1
1	B	447	TRP	3.1
1	A	648	LYS	3.1
1	A	83	PRO	3.1
1	A	281	GLN	3.1
1	B	396	ALA	3.1
1	A	269	PRO	3.1
1	B	369	LEU	3.0
1	B	302	PRO	3.0
1	A	462	TYR	3.0
1	B	323	LEU	2.9
1	B	417	VAL	2.9
1	B	300	LYS	2.9
1	B	647	LYS	2.9
1	B	436	SER	2.8
1	B	584	THR	2.8
1	B	284	PHE	2.8
1	B	279	ARG	2.8
1	B	458	TYR	2.7
1	A	354	MET	2.7
1	B	361	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	438	ILE	2.7
1	B	327	ALA	2.7
1	B	583	VAL	2.7
1	B	416	VAL	2.6
1	B	439	PHE	2.6
1	B	368	ASP	2.6
1	B	585	GLN	2.6
1	B	82	GLU	2.6
1	B	435	MET	2.6
1	B	129	ASP	2.5
1	B	403	ILE	2.5
1	B	303	VAL	2.5
1	B	293	ALA	2.5
1	B	349	LEU	2.4
1	B	622	GLN	2.4
1	A	463	MET	2.3
1	A	268	LEU	2.3
1	A	99	ASN	2.3
1	A	467	PRO	2.3
1	B	388	PHE	2.3
1	B	360	ALA	2.3
1	B	296	ILE	2.3
1	B	582	MET	2.3
1	B	278	SER	2.3
1	B	445	SER	2.2
1	A	284	PHE	2.2
1	B	370	ILE	2.2
1	B	363	ALA	2.2
1	A	270	SER	2.2
1	B	295	LEU	2.2
1	A	488	GLY	2.2
1	A	600	GLN	2.1
1	B	131	PHE	2.1
1	B	392	ALA	2.1
1	B	541	GLU	2.1
1	B	387	LYS	2.1
1	A	597	HIS	2.1
1	B	415	LYS	2.0
1	B	596	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

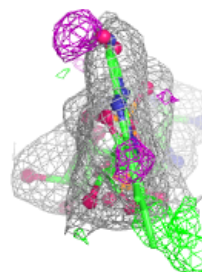
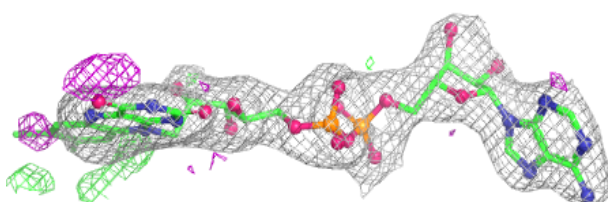
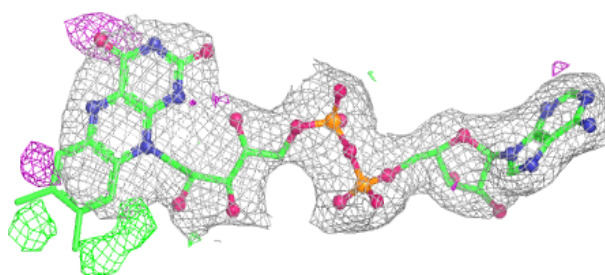
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	2HP	B	1697	5/5	0.83	0.09	115,115,115,115	0
4	2HP	A	698	5/5	0.86	0.15	120,120,121,121	0
4	2HP	B	1698	5/5	0.88	0.17	133,133,133,133	0
6	FAD	B	1701	53/53	0.94	0.12	54,60,86,87	0
5	TPP	A	700	26/26	0.97	0.07	36,46,49,50	0
6	FAD	A	701	53/53	0.97	0.07	40,49,73,74	0
2	K	B	1696	1/1	0.97	0.25	43,43,43,43	0
5	TPP	B	1700	26/26	0.98	0.06	35,42,45,47	0
3	MG	A	699	1/1	0.99	0.03	47,47,47,47	0
2	K	A	696	1/1	0.99	0.23	32,32,32,32	0
3	MG	B	1699	1/1	1.00	0.01	42,42,42,42	0

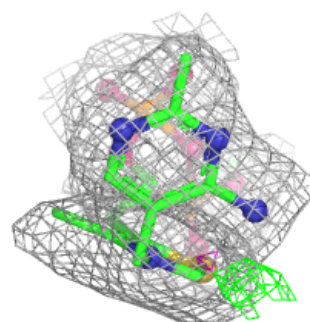
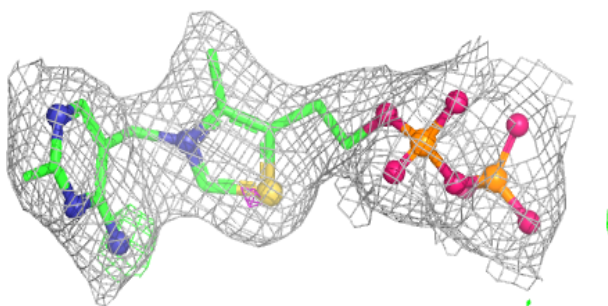
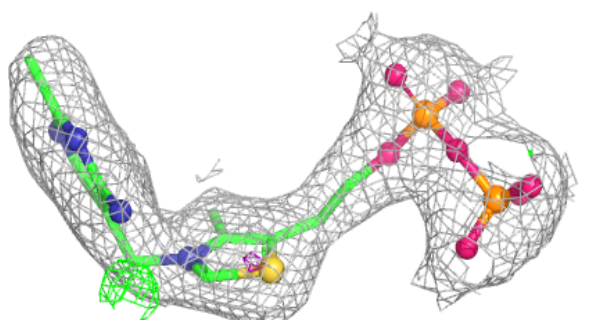
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 1701:

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

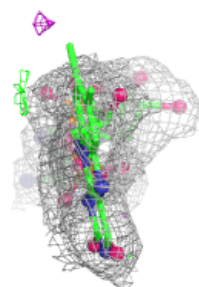
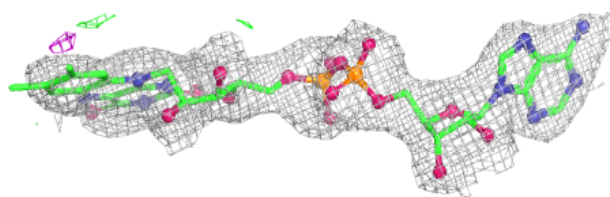
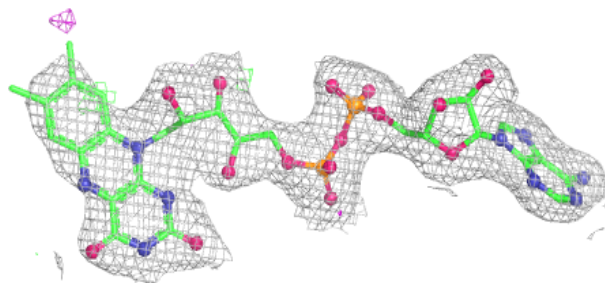
**Electron density around TPP A 700:**

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

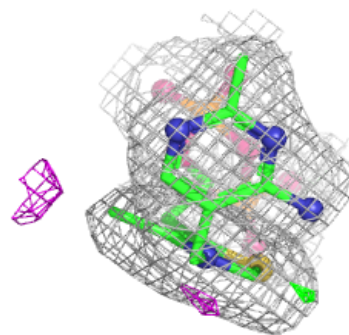
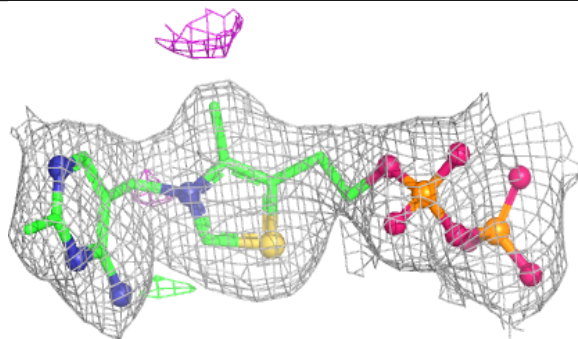
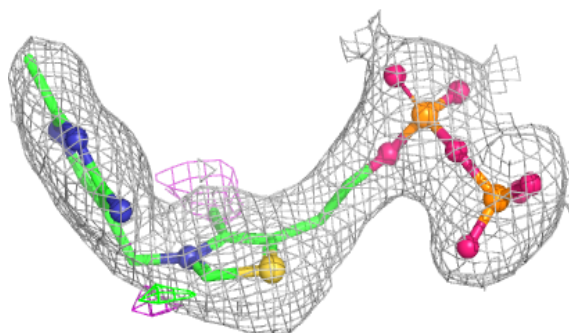


Electron density around FAD A 701:

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

**Electron density around TPP B 1700:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.