



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:13 AM UTC

PDB ID : 8RPJ / pdb_00008rpj
Title : JanthE from Janthinobacterium sp. HH01
Authors : Lanza, L.; Leogrande, C.; Rabe von Pappenheim, F.; Tittmann, K.; Mueller, M.
Deposited on : 2024-01-16
Resolution : 1.90 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

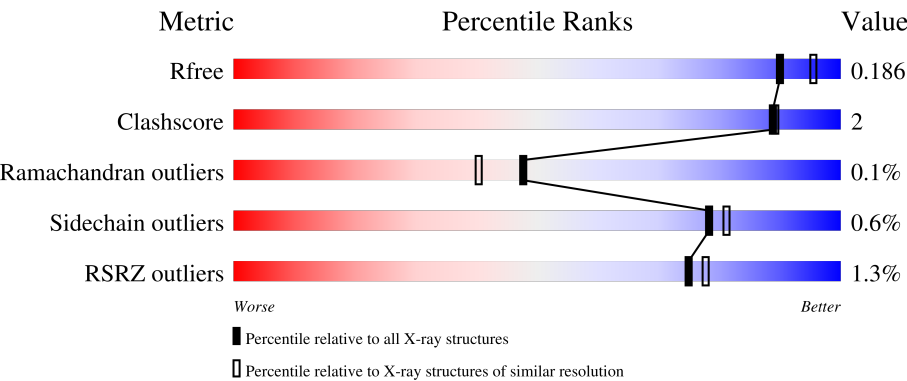
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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.



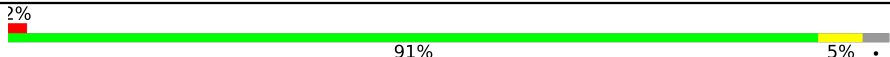
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	619	% 94% 5% 5%
1	B	619	% 95% 5% 5%
1	C	619	% 93% 5% 5%
1	D	619	% 90% 6% 5%
1	E	619	% 93% 5% 5%

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Mol	Chain	Length	Quality of chain
1	F	619	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a small red segment at the beginning labeled '2%', a large green segment in the middle labeled '91%', and a small yellow segment at the end labeled '5%'. A small grey dot is located at the far right end of the bar.

2 Entry composition [i](#)

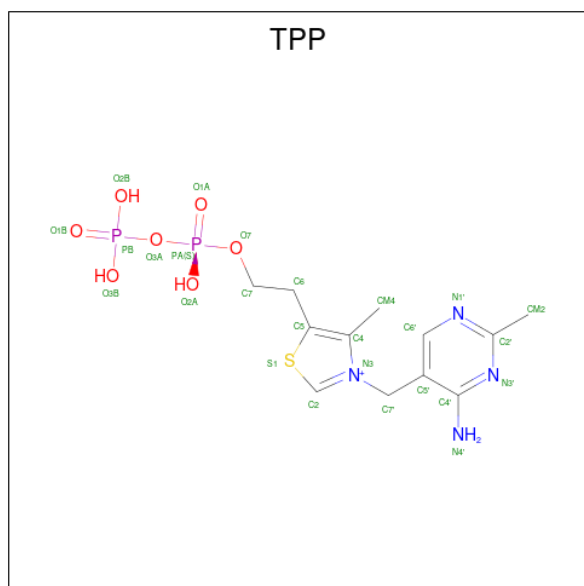
There are 10 unique types of molecules in this entry. The entry contains 58571 atoms, of which 27979 are hydrogens and 0 are deuteriums.

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 Thiamine pyrophosphate-binding protein.

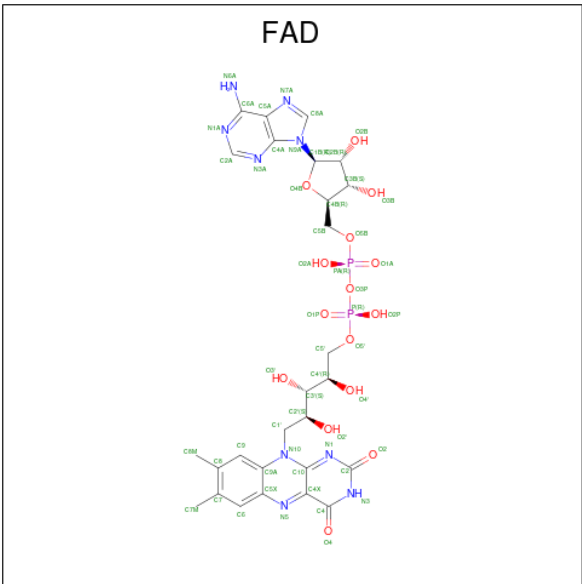
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	605	Total	C	H	N	O	S	0	3	0
			9296	2959	4629	814	862	32			
1	B	608	Total	C	H	N	O	S	0	5	0
			9366	2979	4662	823	870	32			
1	C	607	Total	C	H	N	O	S	0	1	0
			9285	2960	4616	812	865	32			
1	D	591	Total	C	H	N	O	S	0	2	0
			9051	2887	4501	792	841	30			
1	E	608	Total	C	H	N	O	S	0	3	0
			9326	2969	4641	816	868	32			
1	F	598	Total	C	H	N	O	S	0	6	0
			9200	2930	4575	808	856	31			

- Molecule 2 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	D	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	E	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	F	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		

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

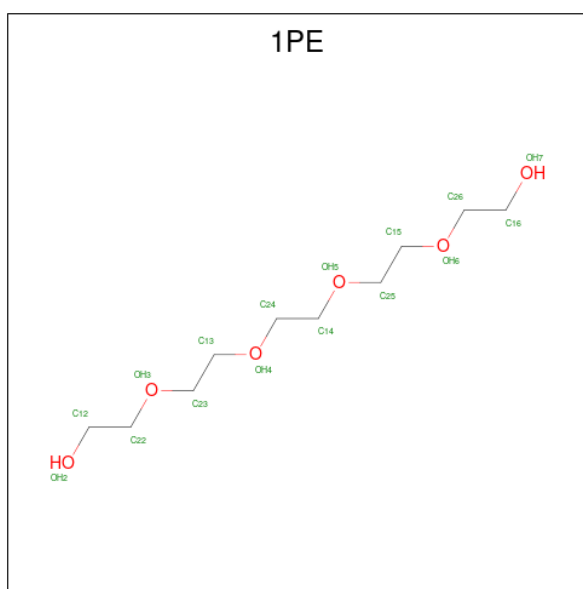


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P		0	0
			84	27	31	9	15	2			
3	B	1	Total	C	H	N	O	P		0	0
			84	27	31	9	15	2			
3	C	1	Total	C	H	N	O	P		0	0
			84	27	31	9	15	2			
3	D	1	Total	C	H	N	O	P		0	0
			84	27	31	9	15	2			
3	E	1	Total	C	H	N	O	P		0	0
			84	27	31	9	15	2			
3	F	1	Total	C	H	N	O	P		0	0
			84	27	31	9	15	2			

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

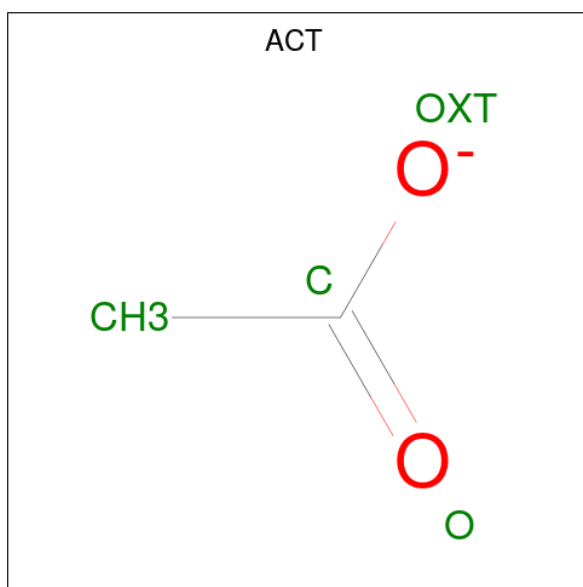
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



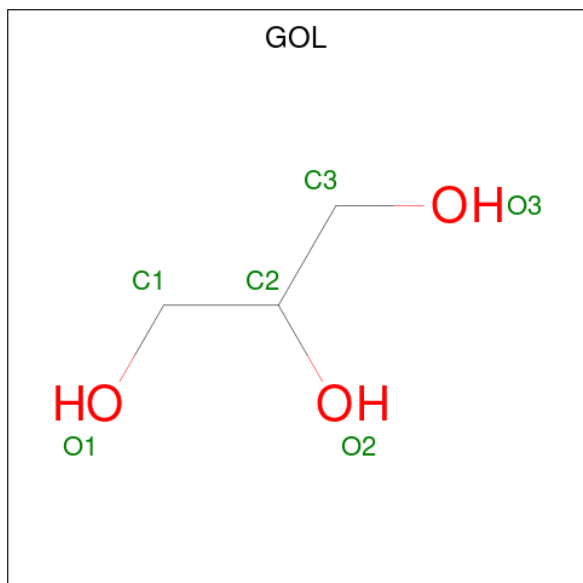
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			38	10	22	6		
5	E	1	Total	C	H	O	0	0
			38	10	22	6		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



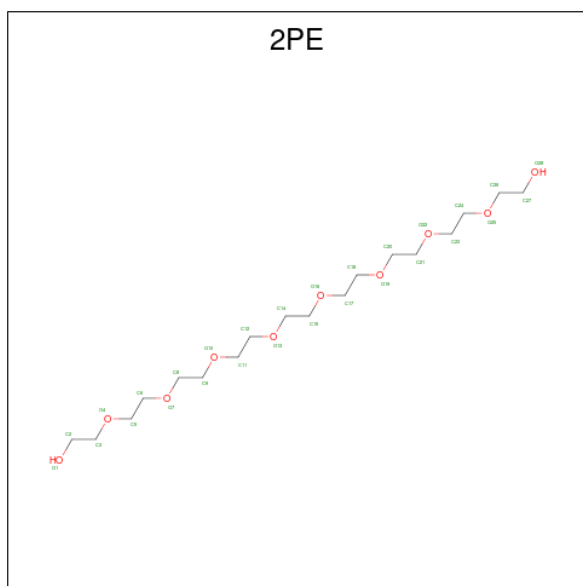
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			7	2	3	2		
6	B	1	Total	C	H	O	0	0
			7	2	3	2		
6	E	1	Total	C	H	O	0	0
			7	2	3	2		
6	F	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



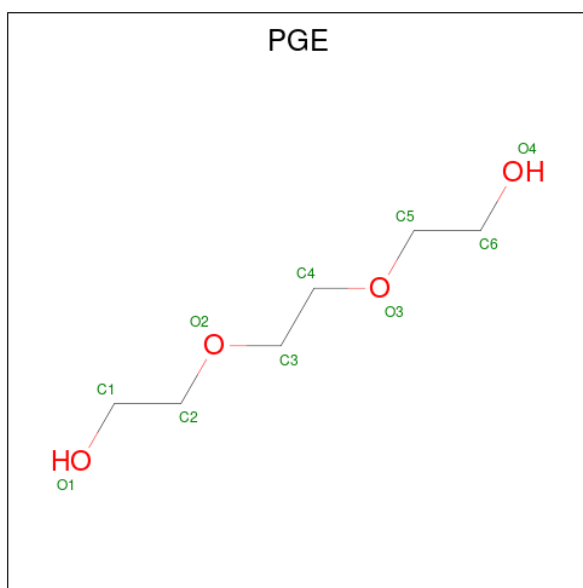
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 8 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			28	18	10		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	E	1	Total	C	H	O	0	0
			19	6	9	4		

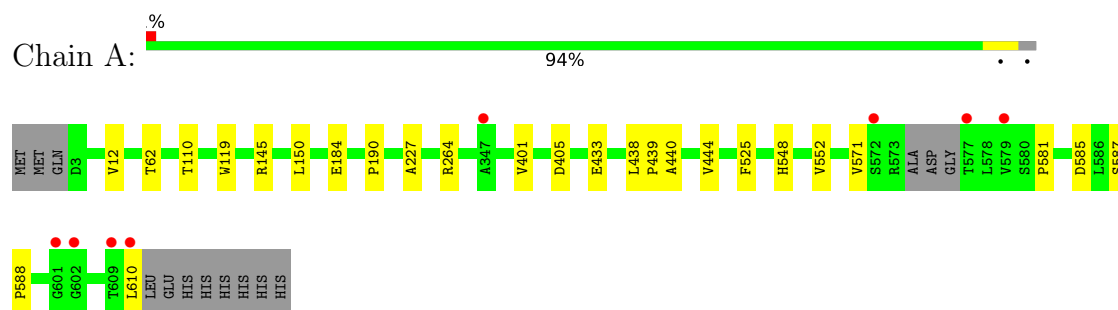
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	377	Total	O	0	0
			377	377		
10	B	417	Total	O	0	0
			417	417		
10	C	352	Total	O	0	0
			352	352		
10	D	285	Total	O	0	0
			285	285		
10	E	411	Total	O	0	0
			411	411		
10	F	278	Total	O	0	0
			278	278		

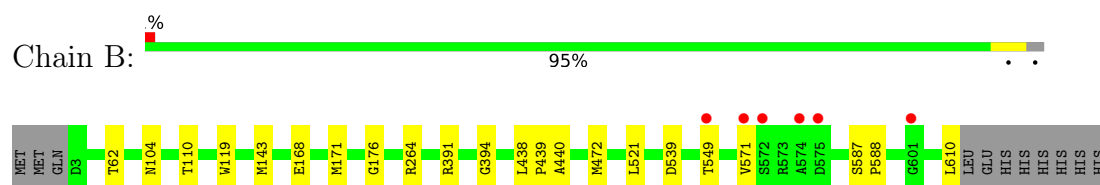
3 Residue-property plots

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.

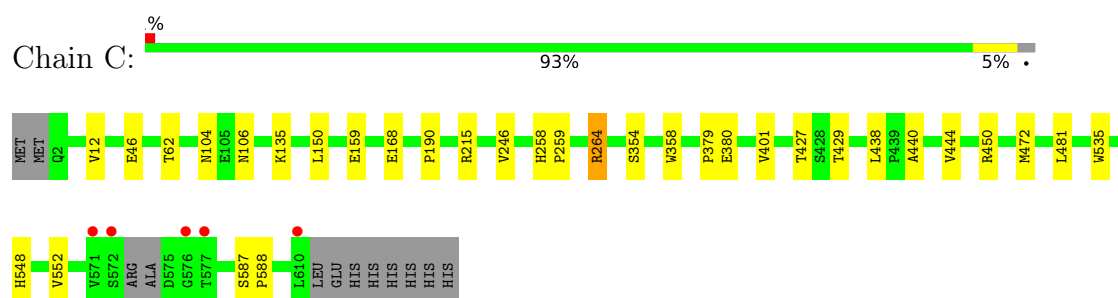
- Molecule 1: Thiamine pyrophosphate-binding protein



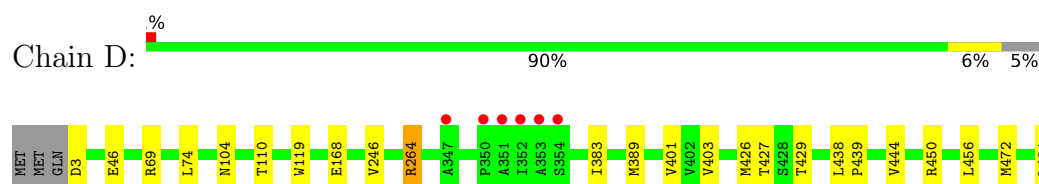
- Molecule 1: Thiamine pyrophosphate-binding protein



- Molecule 1: Thiamine pyrophosphate-binding protein

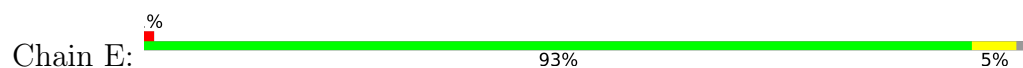


- Molecule 1: Thiamine pyrophosphate-binding protein

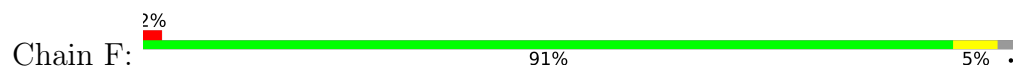




- Molecule 1: Thiamine pyrophosphate-binding protein



- Molecule 1: Thiamine pyrophosphate-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.20Å 105.17Å 193.60Å 90.00° 96.51° 90.00°	Depositor
Resolution (Å)	68.16 – 1.90 68.16 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (68.16-1.90) 99.2 (68.16-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.153 , 0.186 0.154 , 0.186	Depositor DCC
R_{free} test set	14292 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 37.7	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	0.97	EDS
Total number of atoms	58571	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: 2PE, TPP, PGE, MG, 1PE, FAD, GOL, ACT

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	0.22	0/4772	0.46	0/6473
1	B	0.21	0/4810	0.47	0/6525
1	C	0.20	0/4768	0.45	0/6468
1	D	0.19	0/4654	0.43	0/6317
1	E	0.22	0/4794	0.46	0/6504
1	F	0.19	0/4752	0.40	0/6443
All	All	0.21	0/28550	0.45	0/38730

There are no bond length outliers.

There are no bond angle outliers.

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	4667	4629	4637	15	0
1	B	4704	4662	4669	13	0
1	C	4669	4616	4638	20	0
1	D	4550	4501	4510	19	0
1	E	4685	4641	4649	20	0
1	F	4625	4575	4557	18	0
2	A	26	16	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	26	16	16	0	0
2	C	26	16	16	0	0
2	D	26	16	16	0	0
2	E	26	16	16	0	0
2	F	26	16	16	1	0
3	A	53	31	31	1	0
3	B	53	31	31	0	0
3	C	53	31	31	1	0
3	D	53	31	31	1	0
3	E	53	31	31	0	0
3	F	53	31	31	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	B	16	22	22	2	0
5	E	16	22	22	0	0
6	B	8	6	6	1	0
6	E	4	3	3	0	0
6	F	4	3	3	0	0
7	B	6	8	8	0	0
8	C	28	0	38	2	0
9	E	10	9	14	1	0
10	A	377	0	0	0	0
10	B	417	0	0	0	0
10	C	352	0	0	2	0
10	D	285	0	0	1	1
10	E	411	0	0	3	0
10	F	278	0	0	1	0
All	All	30592	27979	28058	108	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 2.

All (108) 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:145:ARG:NH1	1:A:184:GLU:OE1	2.28	0.67
1:D:383:ILE:HD12	1:D:535:TRP:CE2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ARG:HD3	5:B:704:1PE:H221	1.83	0.59
1:E:366[B]:GLU:OE2	10:E:801:HOH:O	2.17	0.58
1:E:114:ASN:O	10:E:802:HOH:O	2.18	0.56
1:E:234:LYS:NZ	10:E:807:HOH:O	2.35	0.55
1:C:62:THR:HG21	1:C:440:ALA:HB1	1.89	0.55
1:E:401:VAL:HG11	1:E:444:VAL:HG11	1.88	0.54
1:A:438:LEU:HB2	1:A:439:PRO:HD3	1.90	0.53
1:C:535:TRP:CD2	8:C:704:2PE:H91	2.44	0.53
1:E:12:VAL:HG13	1:E:150:LEU:CD1	2.39	0.52
1:B:438:LEU:HD22	1:B:472:MET:HE1	1.91	0.52
1:C:587:SER:HA	1:C:588:PRO:C	2.36	0.50
1:B:394:GLY:HA3	5:B:704:1PE:H222	1.94	0.50
1:C:46:GLU:OE2	1:C:450:ARG:NH2	2.45	0.50
1:E:438:LEU:HB2	1:E:439:PRO:HD3	1.95	0.49
1:D:246:VAL:O	1:D:264:ARG:HG3	2.14	0.48
1:D:438:LEU:HD21	1:D:481:LEU:HD22	1.94	0.48
1:E:383:ILE:HG23	1:E:535:TRP:CZ2	2.48	0.48
1:B:438:LEU:HB2	1:B:439:PRO:HD3	1.96	0.48
1:F:271:ARG:NH2	1:F:588:PRO:O	2.44	0.48
1:E:215:ARG:HA	1:E:358:TRP:CD1	2.49	0.48
1:A:587:SER:HA	1:A:588:PRO:C	2.40	0.47
1:D:110:THR:HA	1:D:119:TRP:CE3	2.50	0.47
1:E:62:THR:HG21	1:E:440:ALA:HB1	1.97	0.47
1:E:387:ARG:NH2	9:E:706:PGE:H22	2.29	0.47
1:E:383:ILE:HD12	1:E:535:TRP:CE2	2.50	0.46
1:D:427:THR:HG23	1:D:429:THR:HG23	1.96	0.46
1:F:46:GLU:OE2	1:F:450:ARG:NH2	2.49	0.46
1:F:438:LEU:HD21	1:F:481:LEU:HD22	1.98	0.46
3:F:702:FAD:O2A	3:F:702:FAD:H5'1	2.16	0.46
1:B:62:THR:HG21	1:B:440:ALA:HB1	1.98	0.46
1:C:548:HIS:CB	1:C:552:VAL:HG21	2.46	0.46
1:F:62:THR:HG21	1:F:440:ALA:HB1	1.98	0.46
1:E:105:GLU:HA	1:E:171:MET:HE2	1.98	0.45
1:C:548:HIS:HB2	1:C:552:VAL:HG21	1.98	0.45
1:E:379:PRO:O	1:E:381:GLY:N	2.50	0.45
1:D:587:SER:HA	1:D:588:PRO:C	2.40	0.45
1:D:502:SER:OG	1:D:503:ASP:N	2.50	0.45
1:F:480:LYS:N	1:F:480:LYS:HD2	2.32	0.45
1:F:12:VAL:HG13	1:F:150:LEU:CD1	2.46	0.45
6:B:705:ACT:H1	1:E:196:THR:HG21	1.99	0.44
1:C:438:LEU:HD22	1:C:472:MET:SD	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:438:LEU:HB2	1:D:439:PRO:HD3	1.98	0.44
1:D:438:LEU:HD22	1:D:472:MET:HE1	1.99	0.44
1:A:571:VAL:HG11	1:A:610:LEU:HD13	2.00	0.44
1:A:110:THR:HA	1:A:119:TRP:CE3	2.52	0.44
1:C:106:ASN:HB2	10:C:814:HOH:O	2.17	0.43
8:C:704:2PE:H231	10:C:915:HOH:O	2.17	0.43
1:C:246:VAL:O	1:C:264:ARG:HG3	2.19	0.43
1:E:391:ARG:HD2	1:E:539:ASP:OD1	2.18	0.43
1:F:383:ILE:HD12	1:F:535:TRP:CE2	2.54	0.43
1:F:531:GLN:NE2	10:F:815:HOH:O	2.52	0.43
1:B:391:ARG:HD2	1:B:539:ASP:OD1	2.18	0.43
1:B:104:ASN:HD22	1:B:168:GLU:CD	2.27	0.43
1:A:525:PHE:CE2	1:B:521:LEU:HD21	2.52	0.43
1:C:135:LYS:NZ	1:C:159:GLU:O	2.52	0.43
1:F:383:ILE:HG23	1:F:535:TRP:CZ2	2.54	0.43
1:F:438:LEU:HB2	1:F:439:PRO:HD3	2.01	0.43
1:E:571:VAL:HG21	1:E:610:LEU:HD13	2.01	0.42
2:F:701:TPP:C6'	2:F:701:TPP:HM41	2.49	0.42
1:D:403:VAL:HA	1:D:426:MET:O	2.20	0.42
1:E:215:ARG:HA	1:E:358:TRP:CG	2.55	0.42
1:B:143:MET:CE	1:B:176:GLY:HA3	2.49	0.42
1:E:565:SER:HB2	1:E:566:PRO:HA	2.01	0.42
1:F:110:THR:HA	1:F:119:TRP:CE3	2.54	0.42
1:A:12:VAL:HG13	1:A:150:LEU:CD1	2.50	0.42
1:E:379:PRO:O	1:E:380:GLU:C	2.62	0.42
1:A:433:GLU:O	1:A:433:GLU:HG2	2.19	0.42
1:A:581:PRO:HB2	1:A:585:ASP:HB3	2.00	0.42
1:B:110:THR:HA	1:B:119:TRP:CE3	2.55	0.42
1:D:3:ASP:N	10:D:817:HOH:O	2.52	0.42
1:D:548:HIS:CB	1:D:552:VAL:HG21	2.49	0.42
1:D:593:ASP:OD1	1:D:594:VAL:N	2.52	0.42
1:B:104:ASN:O	1:B:171:MET:HG3	2.20	0.42
1:D:401:VAL:HG11	1:D:444:VAL:HG11	2.02	0.42
1:F:548:HIS:HB2	1:F:552:VAL:HG21	2.02	0.42
1:C:427:THR:HG23	1:C:429:THR:HG23	2.01	0.41
3:D:701:FAD:H9	3:D:701:FAD:H1'1	1.86	0.41
1:C:401:VAL:HG11	1:C:444:VAL:HG11	2.02	0.41
1:F:12:VAL:HG13	1:F:150:LEU:HD11	2.01	0.41
1:F:401:VAL:HG11	1:F:444:VAL:HG11	2.00	0.41
1:C:12:VAL:HG13	1:C:150:LEU:CD1	2.50	0.41
1:C:258:HIS:CG	1:C:259:PRO:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:ARG:HA	1:F:358:TRP:CG	2.55	0.41
1:F:257:SER:OG	1:F:418:ARG:NH1	2.53	0.41
1:A:548:HIS:HB2	1:A:552:VAL:HG21	2.02	0.41
1:C:438:LEU:HD21	1:C:481:LEU:HD22	2.02	0.41
1:E:596:GLU:HB2	1:E:603:MET:HE2	2.02	0.41
1:D:389:MET:HE1	1:D:456:LEU:HD13	2.02	0.41
1:A:62:THR:HG21	1:A:440:ALA:HB1	2.03	0.41
1:C:104:ASN:HD22	1:C:168:GLU:CD	2.28	0.41
1:C:215:ARG:HA	1:C:358:TRP:CG	2.56	0.41
1:C:379:PRO:O	1:C:380:GLU:C	2.63	0.41
1:D:537:GLU:OE1	1:D:537:GLU:N	2.43	0.41
1:A:190:PRO:HB2	1:C:190:PRO:HG2	2.03	0.41
3:C:702:FAD:H1'1	3:C:702:FAD:H9	1.85	0.41
1:B:587:SER:HA	1:B:588:PRO:C	2.46	0.41
1:D:46:GLU:OE2	1:D:450:ARG:NH2	2.53	0.41
1:F:587:SER:HA	1:F:588:PRO:C	2.46	0.41
1:B:571:VAL:HG11	1:B:610:LEU:HD13	2.02	0.40
1:D:548:HIS:HB2	1:D:552:VAL:HG21	2.03	0.40
1:A:227:ALA:HB2	3:A:701:FAD:N6A	2.36	0.40
1:A:401:VAL:HG11	1:A:444:VAL:HG11	2.04	0.40
1:C:438:LEU:HD23	1:C:438:LEU:HA	1.97	0.40
1:D:104:ASN:HD22	1:D:168:GLU:CD	2.30	0.40
1:A:548:HIS:CB	1:A:552:VAL:HG21	2.51	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)
10:D:1066:HOH:O	10:D:1076:HOH:O[2_556]	2.10	0.10

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	604/619 (98%)	590 (98%)	14 (2%)	0	100	100
1	B	611/619 (99%)	597 (98%)	14 (2%)	0	100	100
1	C	604/619 (98%)	590 (98%)	14 (2%)	0	100	100
1	D	589/619 (95%)	574 (98%)	15 (2%)	0	100	100
1	E	609/619 (98%)	594 (98%)	14 (2%)	1 (0%)	43	36
1	F	600/619 (97%)	585 (98%)	14 (2%)	1 (0%)	43	36
All	All	3617/3714 (97%)	3530 (98%)	85 (2%)	2 (0%)	48	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	380	GLU
1	F	380	GLU

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	491/500 (98%)	489 (100%)	2 (0%)	84	87
1	B	494/500 (99%)	492 (100%)	2 (0%)	84	87
1	C	490/500 (98%)	488 (100%)	2 (0%)	84	87
1	D	477/500 (95%)	472 (99%)	5 (1%)	68	70
1	E	492/500 (98%)	490 (100%)	2 (0%)	84	87
1	F	487/500 (97%)	483 (99%)	4 (1%)	73	75
All	All	2931/3000 (98%)	2914 (99%)	17 (1%)	78	81

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	ARG
1	A	405	ASP
1	B	264	ARG

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Mol	Chain	Res	Type
1	B	549	THR
1	C	264	ARG
1	C	354	SER
1	D	69	ARG
1	D	74	LEU
1	D	264	ARG
1	D	491	MET
1	D	549	THR
1	E	264	ARG
1	E	363	ARG
1	F	264	ARG
1	F	354	SER
1	F	491	MET
1	F	580	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	A	470	GLN
1	B	155	HIS
1	B	470	GLN
1	B	476	ASN
1	C	155	HIS
1	C	328	ASN
1	C	470	GLN
1	D	328	ASN
1	D	470	GLN
1	E	155	HIS
1	E	202	GLN
1	E	561	GLN
1	F	328	ASN
1	F	470	GLN

5.3.3 RNA ⓘ

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 27 ligands modelled in this entry, 6 are monoatomic - leaving 21 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TPP	F	701	4	26,27,27	0.72	1 (3%)	38,40,40	0.60	1 (2%)
3	FAD	E	702	-	58,58,58	0.44	0	85,89,89	0.44	0
3	FAD	D	701	-	58,58,58	0.51	1 (1%)	85,89,89	0.45	0
2	TPP	E	701	4	26,27,27	0.34	0	38,40,40	0.47	0
6	ACT	B	705	-	3,3,3	0.98	0	3,3,3	1.60	1 (33%)
2	TPP	A	700	4	26,27,27	0.65	1 (3%)	38,40,40	0.41	0
3	FAD	A	701	-	58,58,58	0.52	1 (1%)	85,89,89	0.41	0
6	ACT	E	705	-	3,3,3	1.04	0	3,3,3	1.60	0
5	1PE	E	704	-	15,15,15	0.14	0	14,14,14	0.10	0
9	PGE	E	706	-	9,9,9	0.10	0	8,8,8	0.35	0
2	TPP	C	701	4	26,27,27	0.65	0	38,40,40	0.65	1 (2%)
7	GOL	B	707	-	5,5,5	1.09	0	5,5,5	1.43	1 (20%)
6	ACT	F	704	-	3,3,3	1.07	0	3,3,3	1.46	0
5	1PE	B	704	-	15,15,15	0.16	0	14,14,14	0.12	0
8	2PE	C	704	-	27,27,27	0.16	0	26,26,26	0.52	0
6	ACT	B	706	-	3,3,3	1.24	0	3,3,3	1.23	0
2	TPP	B	701	4	26,27,27	0.51	0	38,40,40	0.56	1 (2%)
3	FAD	B	702	-	58,58,58	0.53	1 (1%)	85,89,89	0.45	0
2	TPP	D	700	4	26,27,27	0.38	0	38,40,40	0.42	0
3	FAD	C	702	-	58,58,58	0.48	1 (1%)	85,89,89	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	F	702	-	58,58,58	0.51	1 (1%)	85,89,89	0.51	1 (1%)

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	1PE	B	704	-	-	6/13/13/13	-
2	TPP	F	701	4	-	3/17/17/17	0/2/2/2
8	2PE	C	704	-	-	4/25/25/25	-
3	FAD	E	702	-	-	2/34/50/50	0/6/6/6
2	TPP	B	701	4	-	3/17/17/17	0/2/2/2
2	TPP	A	700	4	-	2/17/17/17	0/2/2/2
3	FAD	A	701	-	-	5/34/50/50	0/6/6/6
3	FAD	D	701	-	-	3/34/50/50	0/6/6/6
3	FAD	F	702	-	-	12/34/50/50	0/6/6/6
5	1PE	E	704	-	-	4/13/13/13	-
3	FAD	B	702	-	-	5/34/50/50	0/6/6/6
2	TPP	D	700	4	-	3/17/17/17	0/2/2/2
9	PGE	E	706	-	-	1/7/7/7	-
2	TPP	C	701	4	-	3/17/17/17	0/2/2/2
2	TPP	E	701	4	-	1/17/17/17	0/2/2/2
7	GOL	B	707	-	-	0/4/4/4	-
3	FAD	C	702	-	-	4/34/50/50	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	TPP	PA-O3A	-2.87	1.56	1.59
2	F	701	TPP	PA-O3A	-2.74	1.56	1.59
3	D	701	FAD	C1'-C2'	2.47	1.56	1.52
3	B	702	FAD	C1'-C2'	2.13	1.55	1.52
3	A	701	FAD	C1'-C2'	2.12	1.55	1.52
3	F	702	FAD	C1'-C2'	2.08	1.55	1.52
3	C	702	FAD	C1'-C2'	2.08	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	702	FAD	C4'-C3'-C2'	-3.02	108.55	113.57
7	B	707	GOL	C3-C2-C1	-2.64	102.11	111.80
2	C	701	TPP	O2B-PB-O3A	2.19	111.98	104.64
2	B	701	TPP	O2B-PB-O3A	2.12	111.75	104.64
2	F	701	TPP	O2B-PB-O3A	2.08	111.59	104.64
6	B	705	ACT	OXT-C-O	2.01	129.47	122.03

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	TPP	PA-O3A-PB-O2B
2	B	701	TPP	PA-O3A-PB-O3B
2	C	701	TPP	PA-O3A-PB-O3B
2	D	700	TPP	PA-O3A-PB-O2B
2	E	701	TPP	PA-O3A-PB-O2B
3	A	701	FAD	P-O3P-PA-O5B
3	B	702	FAD	P-O3P-PA-O5B
3	F	702	FAD	P-O3P-PA-O5B
3	F	702	FAD	C3'-C4'-C5'-O5'
3	F	702	FAD	O4'-C4'-C5'-O5'
5	B	704	1PE	OH4-C13-C23-OH3
8	C	704	2PE	C17-C18-O19-C20
5	E	704	1PE	OH7-C16-C26-OH6
5	B	704	1PE	OH2-C12-C22-OH3
8	C	704	2PE	C20-C21-O22-C23
5	B	704	1PE	OH7-C16-C26-OH6
5	E	704	1PE	OH2-C12-C22-OH3
3	F	702	FAD	O3'-C3'-C4'-C5'
3	C	702	FAD	P-O3P-PA-O5B
2	D	700	TPP	PA-O3A-PB-O3B
2	F	701	TPP	PA-O3A-PB-O3B
2	F	701	TPP	C5-C6-C7-O7
3	F	702	FAD	O3'-C3'-C4'-O4'
5	E	704	1PE	OH5-C14-C24-OH4
3	A	701	FAD	PA-O3P-P-O1P
3	B	702	FAD	PA-O3P-P-O1P
3	F	702	FAD	C2'-C3'-C4'-O4'
5	E	704	1PE	C24-C14-OH5-C25
3	F	702	FAD	C5'-O5'-P-O1P
3	F	702	FAD	C5'-O5'-P-O2P
3	F	702	FAD	C5'-O5'-P-O3P
5	B	704	1PE	C12-C22-OH3-C23

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Mol	Chain	Res	Type	Atoms
8	C	704	2PE	O16-C17-C18-O19
8	C	704	2PE	C5-C6-O7-C8
2	F	701	TPP	PA-O3A-PB-O1B
3	B	702	FAD	C4'-C5'-O5'-P
3	C	702	FAD	C4'-C5'-O5'-P
3	F	702	FAD	PA-O3P-P-O1P
3	D	701	FAD	P-O3P-PA-O5B
3	A	701	FAD	C4'-C5'-O5'-P
3	E	702	FAD	C4'-C5'-O5'-P
5	B	704	1PE	OH6-C15-C25-OH5
2	B	701	TPP	PA-O3A-PB-O1B
2	C	701	TPP	PA-O3A-PB-O1B
2	A	700	TPP	PA-O3A-PB-O3B
3	F	702	FAD	C2B-C1B-N9A-C8A
2	B	701	TPP	C5-C6-C7-O7
2	C	701	TPP	C5-C6-C7-O7
2	D	700	TPP	C5-C6-C7-O7
3	B	702	FAD	C2B-C1B-N9A-C8A
3	D	701	FAD	C2B-C1B-N9A-C8A
3	E	702	FAD	C2B-C1B-N9A-C8A
3	A	701	FAD	PA-O3P-P-O2P
3	F	702	FAD	PA-O3P-P-O2P
3	A	701	FAD	C2B-C1B-N9A-C8A
3	C	702	FAD	C2B-C1B-N9A-C8A
9	E	706	PGE	O3-C5-C6-O4
5	B	704	1PE	C16-C26-OH6-C15
3	D	701	FAD	C4'-C5'-O5'-P
3	B	702	FAD	PA-O3P-P-O2P
3	C	702	FAD	PA-O3P-P-O2P

There are no ring outliers.

9 monomers are involved in 11 short contacts:

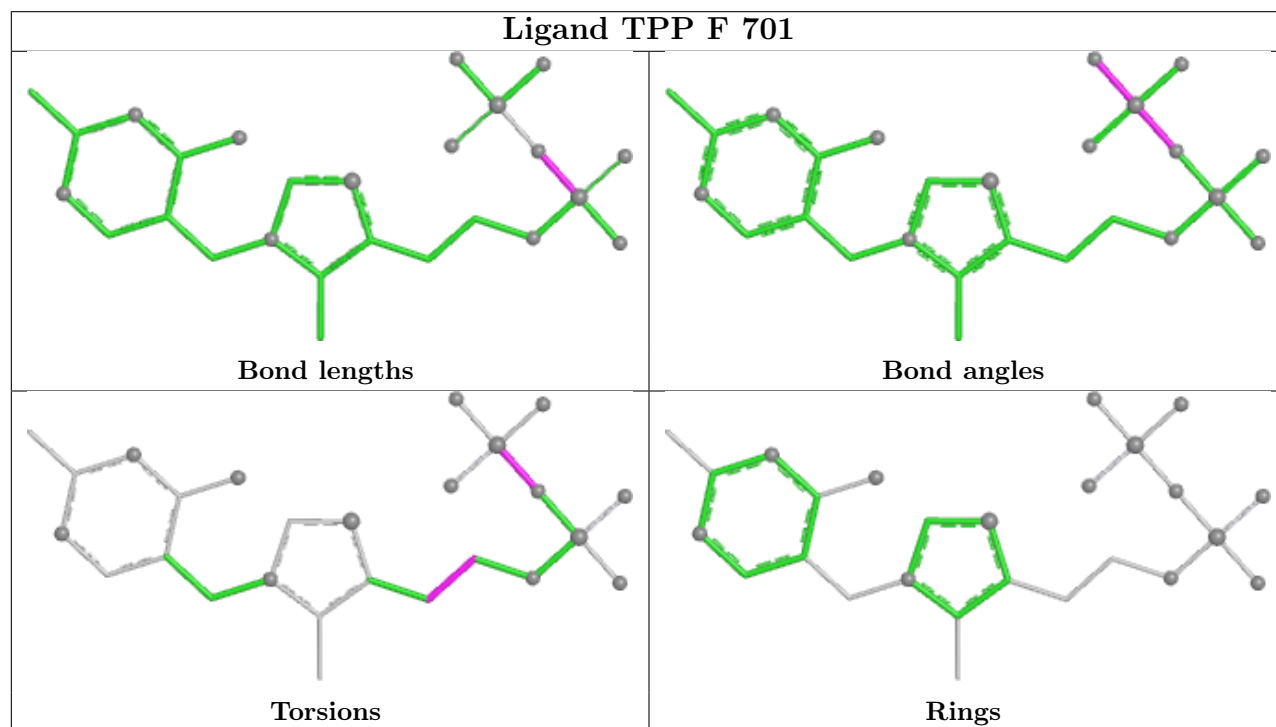
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	701	TPP	1	0
3	D	701	FAD	1	0
6	B	705	ACT	1	0
3	A	701	FAD	1	0
9	E	706	PGE	1	0
5	B	704	1PE	2	0
8	C	704	2PE	2	0
3	C	702	FAD	1	0

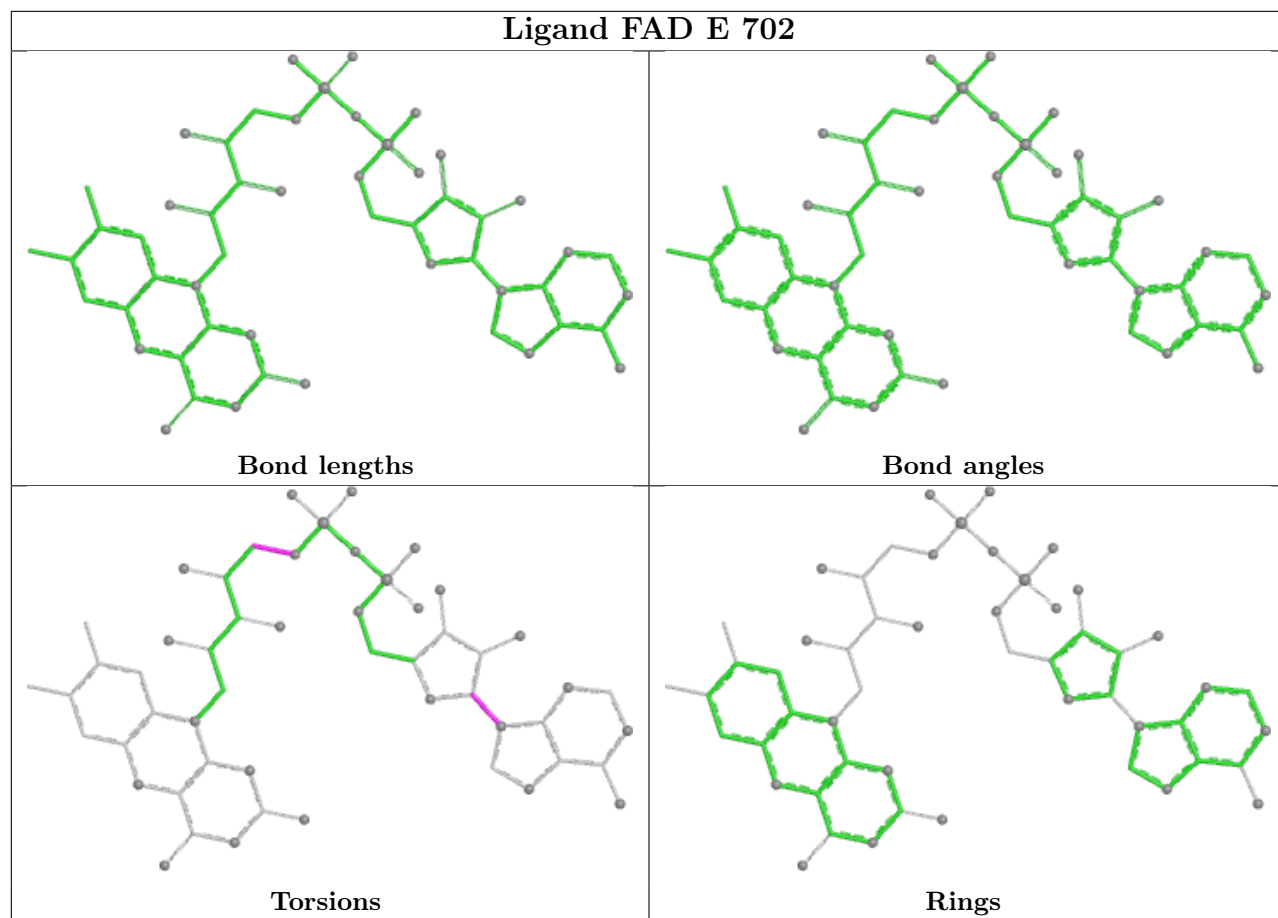
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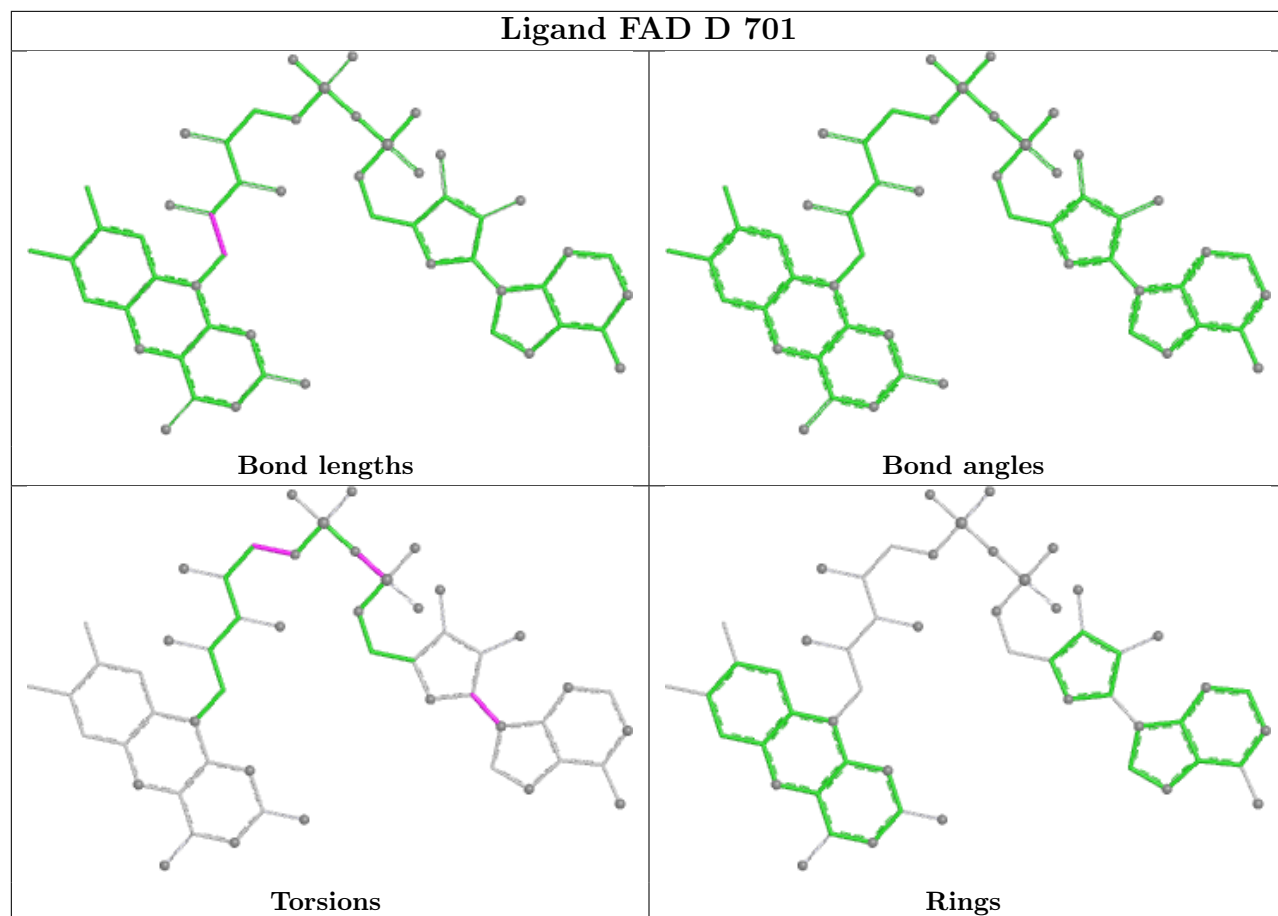
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	702	FAD	1	0

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.

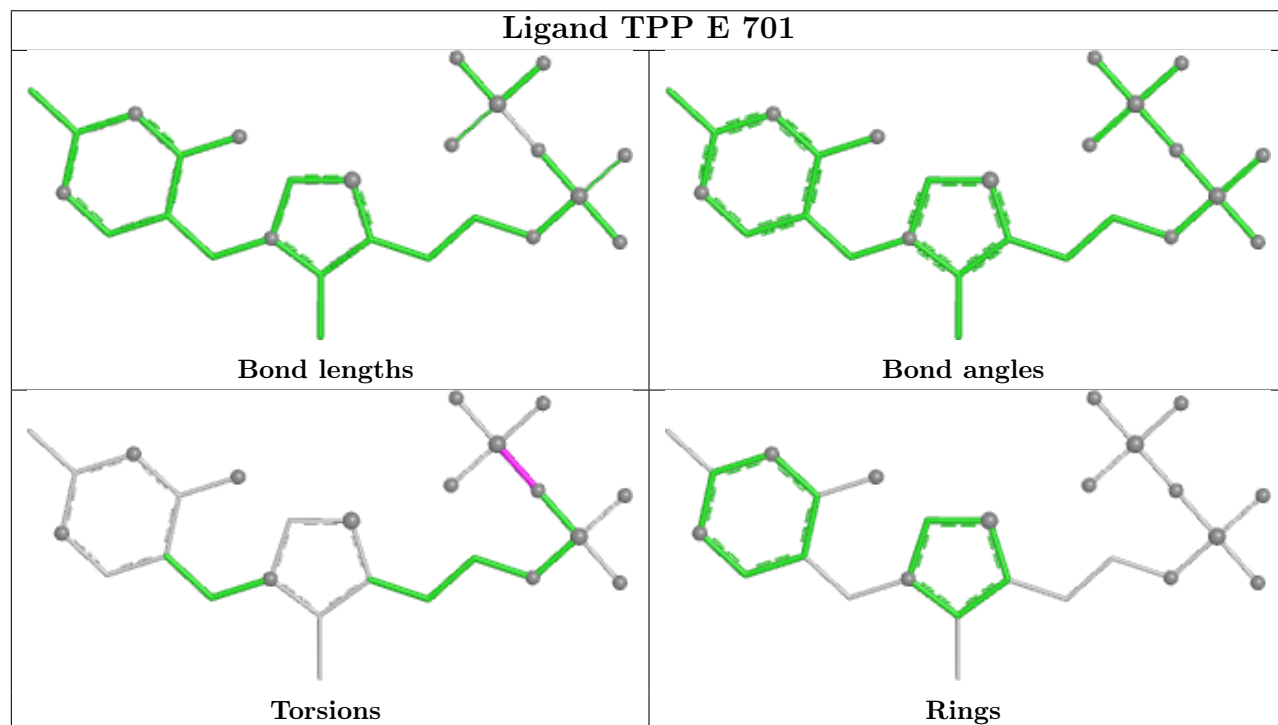


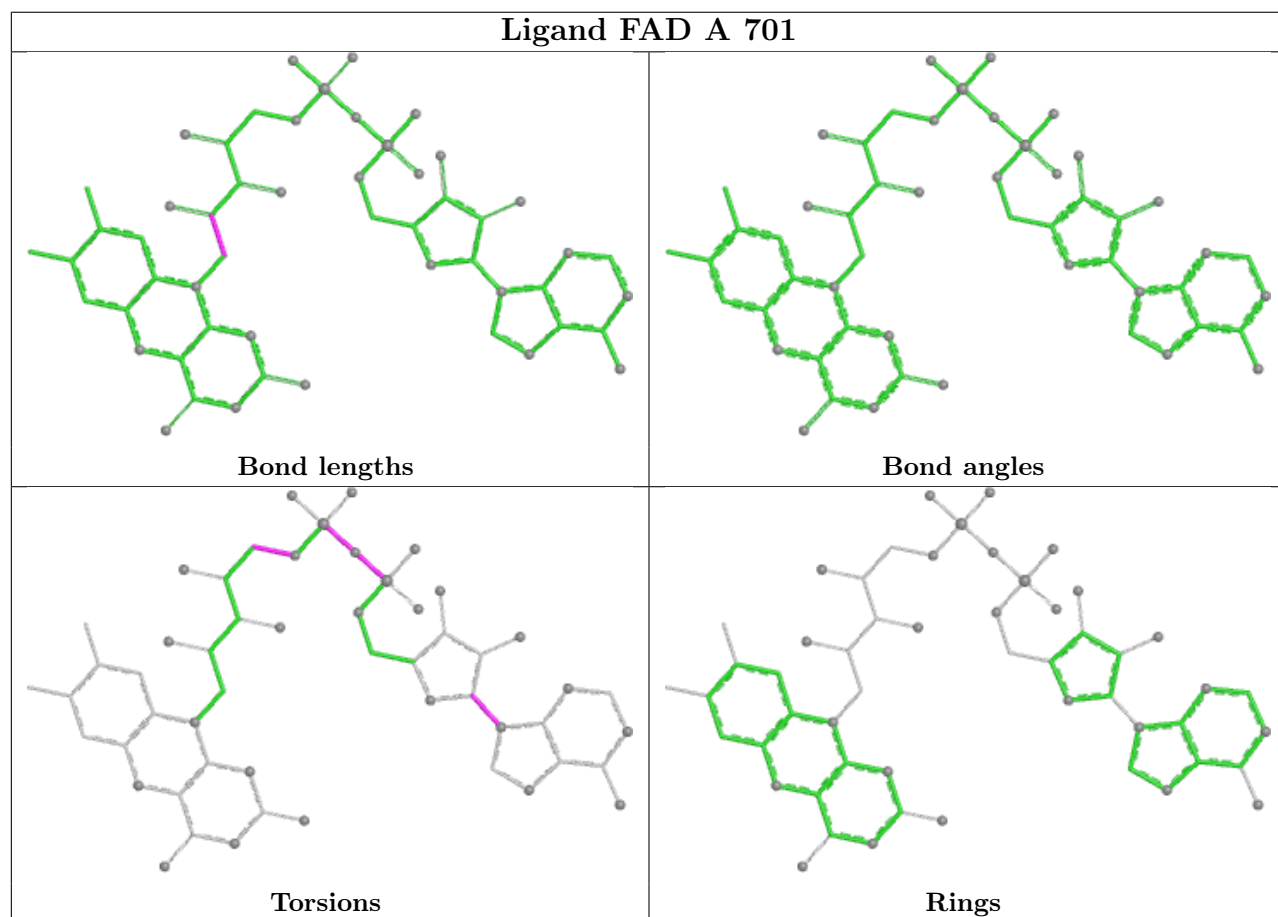
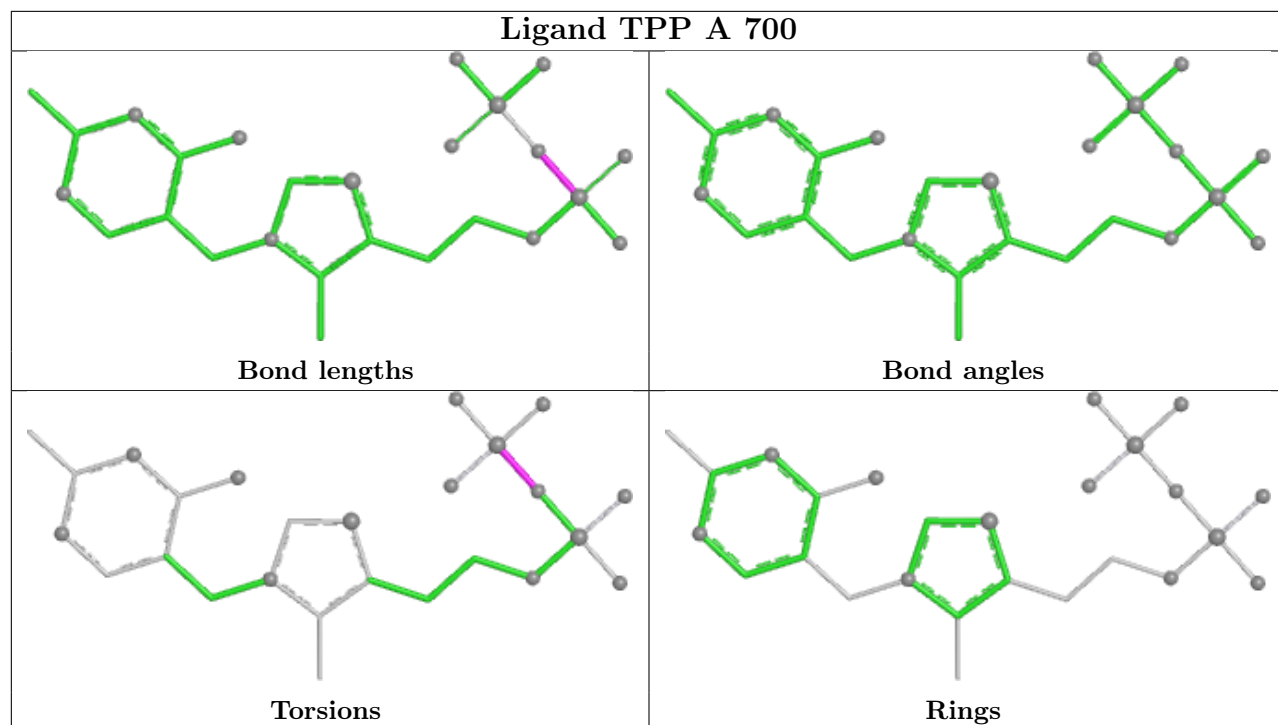


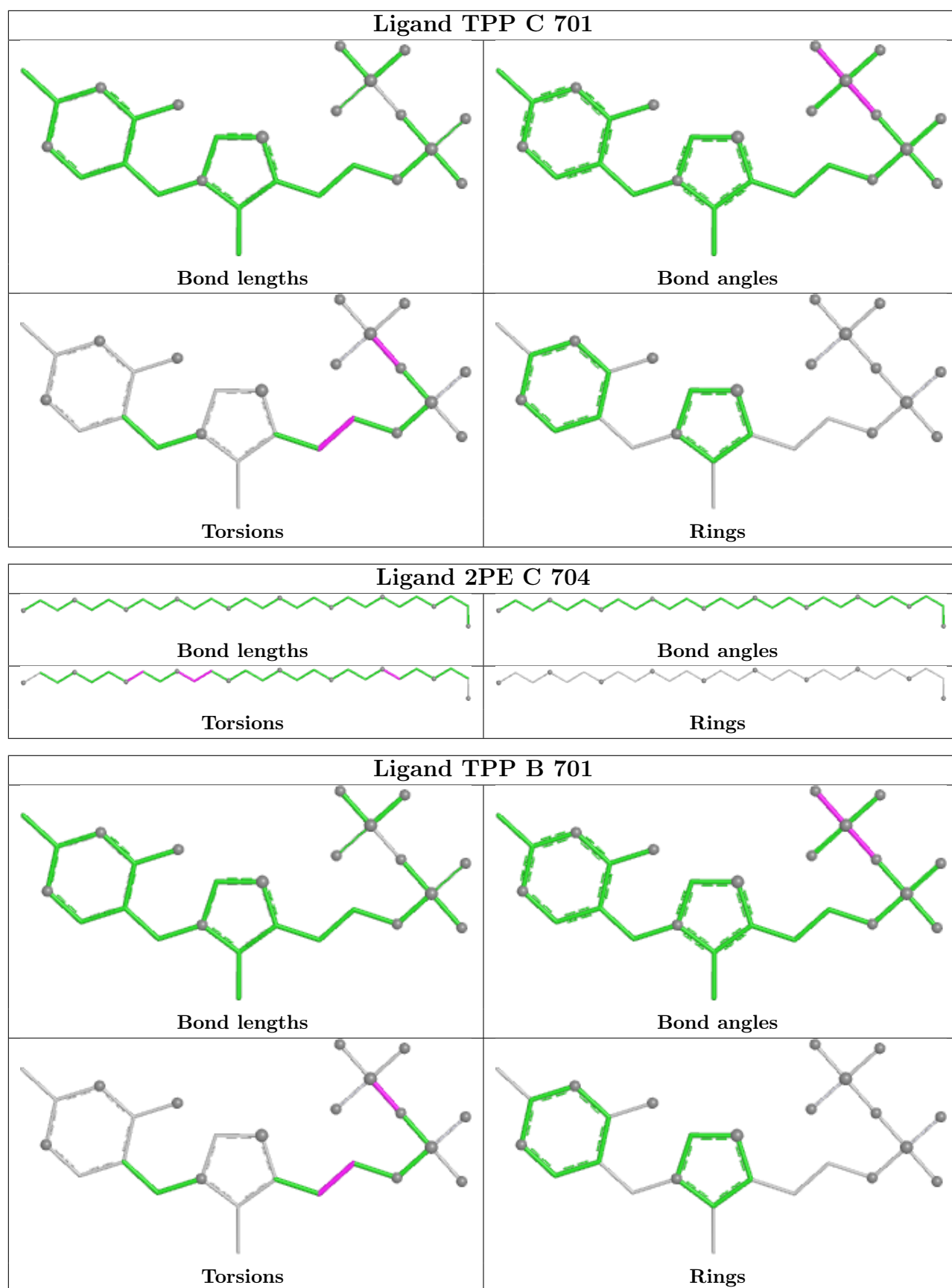
Ligand FAD D 701



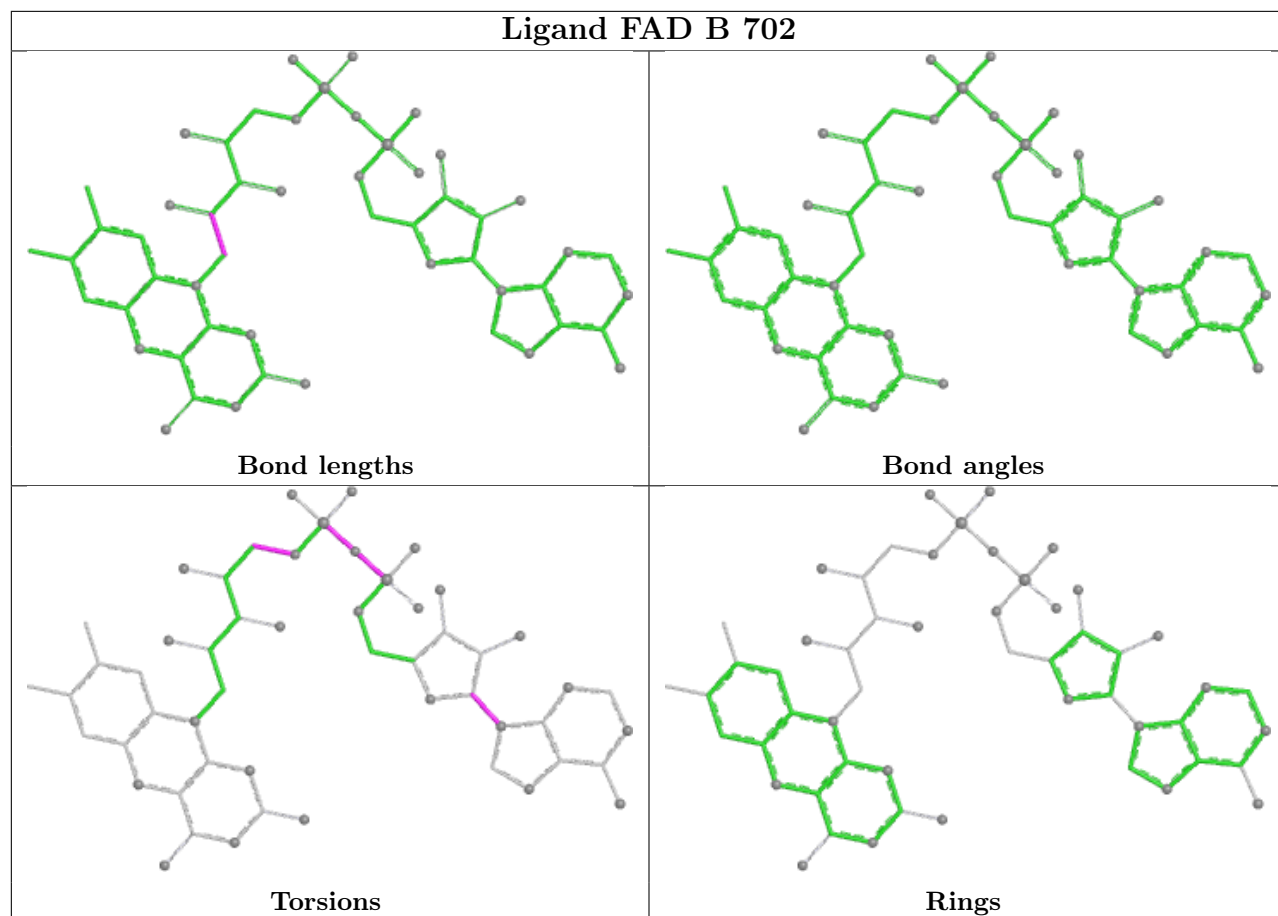
Ligand TPP E 701



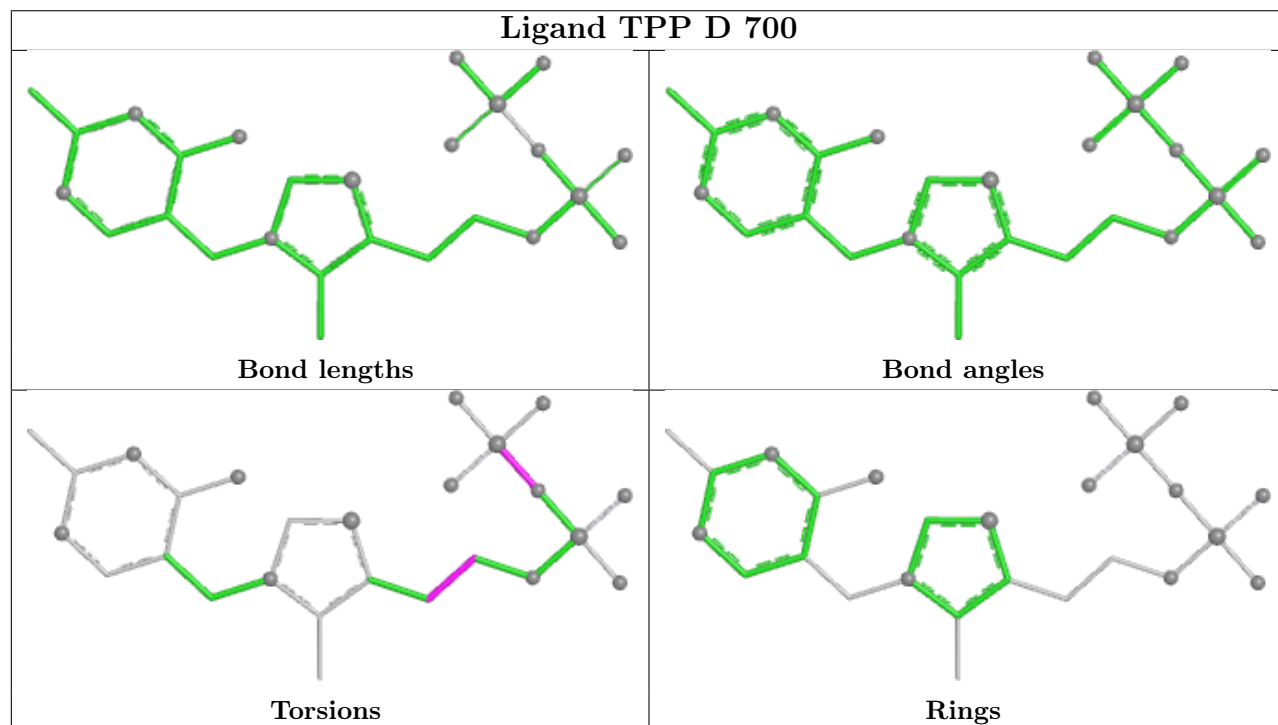


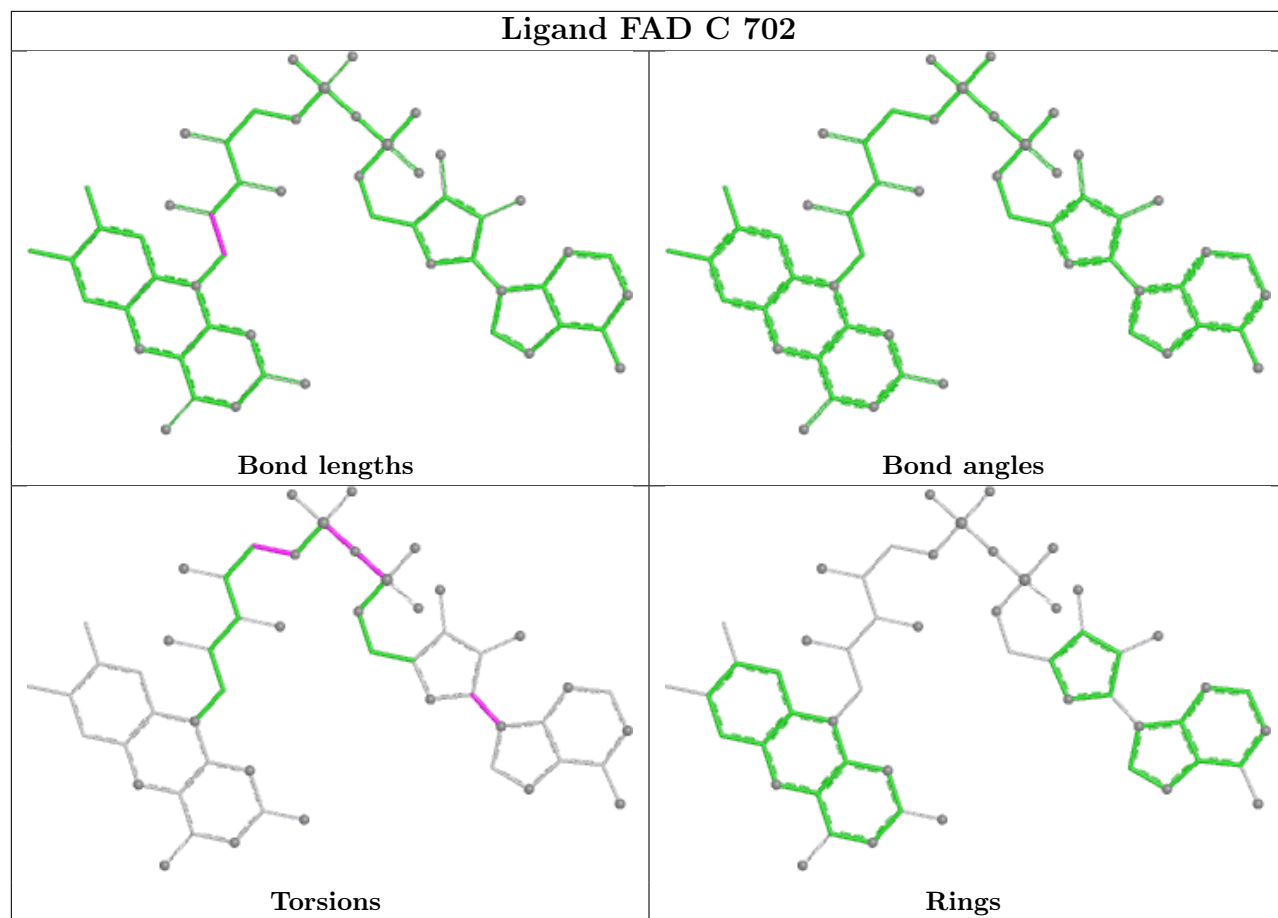


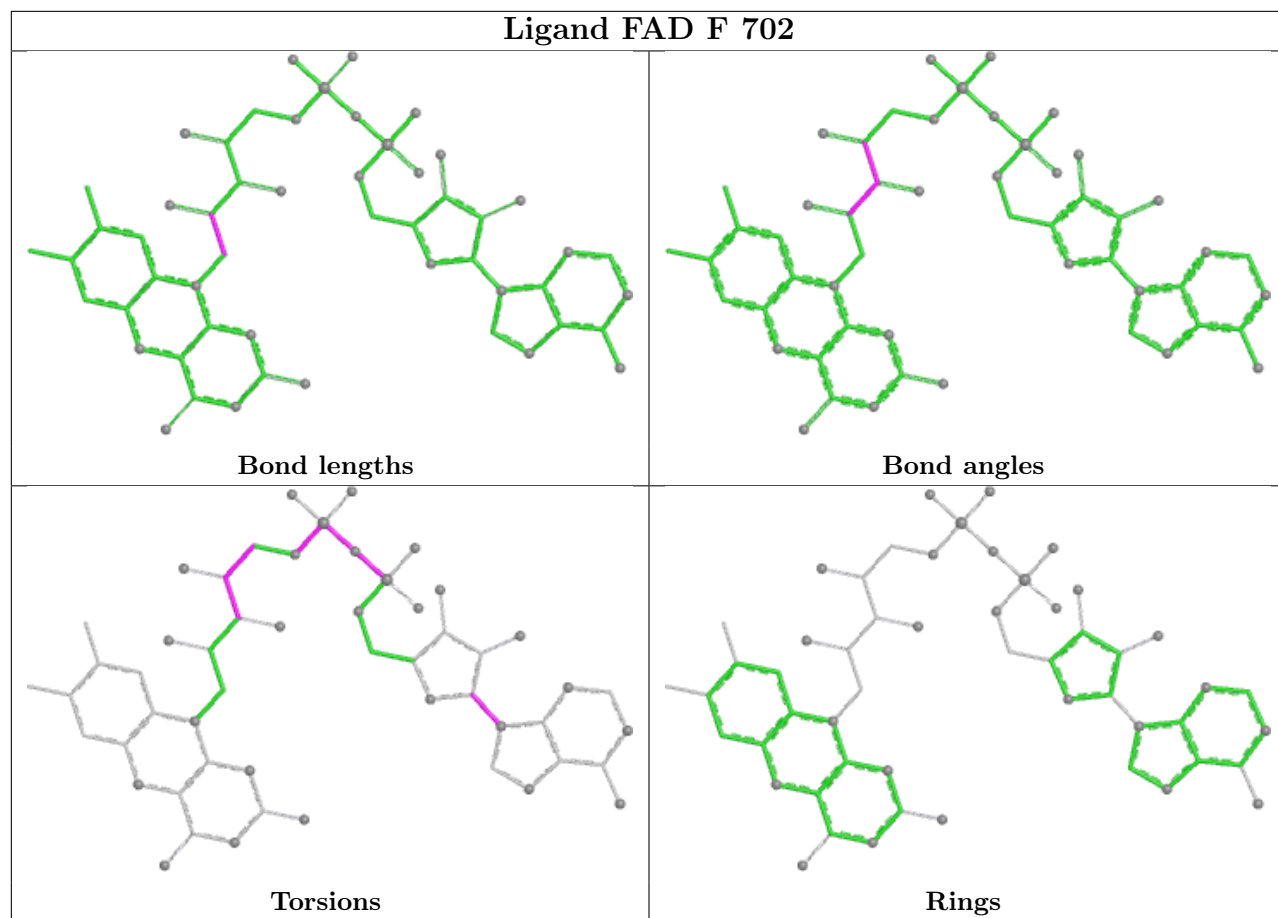
Ligand FAD B 702



Ligand TPP D 700







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	605/619 (97%)	-0.34	8 (1%)	75 78	14, 29, 55, 92	2 (0%)
1	B	608/619 (98%)	-0.43	6 (0%)	79 82	14, 28, 48, 91	4 (0%)
1	C	607/619 (98%)	-0.33	5 (0%)	82 85	15, 30, 54, 81	1 (0%)
1	D	591/619 (95%)	-0.16	9 (1%)	72 75	18, 34, 59, 86	1 (0%)
1	E	608/619 (98%)	-0.43	9 (1%)	72 75	16, 28, 51, 92	2 (0%)
1	F	598/619 (96%)	0.04	11 (1%)	67 71	17, 37, 68, 84	3 (0%)
All	All	3617/3714 (97%)	-0.28	48 (1%)	75 78	14, 31, 57, 92	13 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	570	VAL	5.0
1	B	574	ALA	4.4
1	A	601	GLY	4.0
1	D	601	GLY	4.0
1	E	574	ALA	3.7
1	A	347	ALA	3.6
1	A	609	THR	3.6
1	F	609	THR	3.3
1	C	610	LEU	3.2
1	C	572	SER	3.2
1	F	41[A]	ARG	3.2
1	D	350	PRO	3.1
1	D	353	ALA	3.0
1	A	610	LEU	2.9
1	B	601	GLY	2.8
1	E	111	PHE	2.8
1	B	549	THR	2.8
1	B	575	ASP	2.8
1	F	347	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	383	ILE	2.7
1	D	570	VAL	2.4
1	F	594	VAL	2.4
1	E	575	ASP	2.4
1	A	602	GLY	2.3
1	A	572	SER	2.3
1	D	351	ALA	2.3
1	F	190	PRO	2.3
1	F	591	PRO	2.3
1	B	571	VAL	2.3
1	C	577	THR	2.3
1	E	610	LEU	2.3
1	E	601	GLY	2.2
1	C	576	GLY	2.2
1	D	354	SER	2.2
1	D	347	ALA	2.2
1	F	191	ALA	2.2
1	D	352	ILE	2.1
1	A	579	VAL	2.1
1	B	572	SER	2.1
1	C	571	VAL	2.1
1	E	190	PRO	2.1
1	E	578	LEU	2.1
1	F	383	ILE	2.1
1	F	601	GLY	2.1
1	F	600	ILE	2.0
1	D	579	VAL	2.0
1	A	577	THR	2.0
1	E	4	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

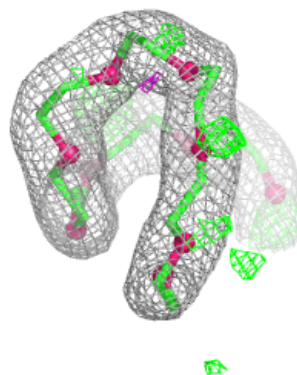
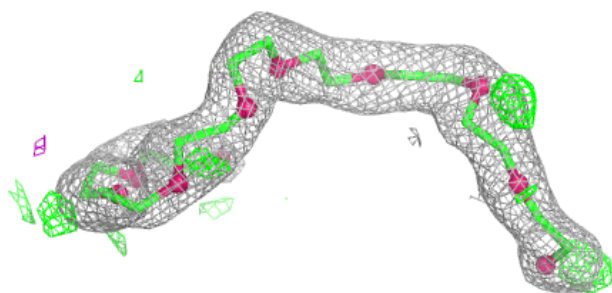
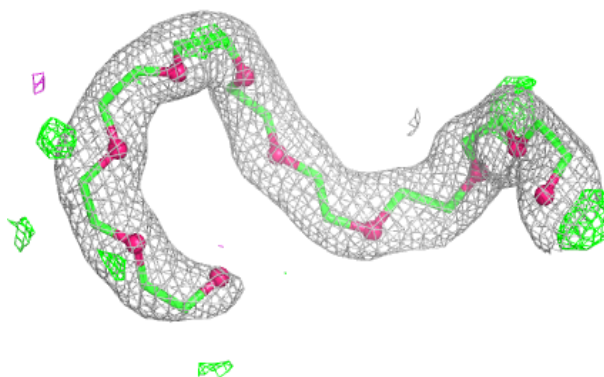
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	PGE	E	706	10/10	0.84	0.13	44,53,56,64	0
6	ACT	E	705	4/4	0.86	0.15	44,47,53,54	0
6	ACT	B	705	4/4	0.86	0.20	45,52,60,60	0
6	ACT	B	706	4/4	0.89	0.13	29,34,41,42	0
6	ACT	F	704	4/4	0.90	0.11	40,47,48,55	0
5	1PE	B	704	16/16	0.90	0.11	39,55,77,86	0
5	1PE	E	704	16/16	0.91	0.09	34,48,63,71	0
8	2PE	C	704	28/28	0.92	0.12	31,38,48,56	0
7	GOL	B	707	6/6	0.94	0.08	29,42,51,53	0
3	FAD	F	702	53/53	0.96	0.07	26,33,50,71	0
2	TPP	F	701	26/26	0.97	0.06	24,31,37,38	0
3	FAD	A	701	53/53	0.97	0.05	19,25,35,36	0
3	FAD	C	702	53/53	0.97	0.06	20,26,34,39	0
3	FAD	D	701	53/53	0.97	0.06	22,30,39,42	0
3	FAD	E	702	53/53	0.97	0.05	18,23,31,31	0
2	TPP	D	700	26/26	0.98	0.06	21,28,33,38	0
3	FAD	B	702	53/53	0.98	0.05	17,22,34,34	0
2	TPP	B	701	26/26	0.98	0.04	17,25,30,34	0
2	TPP	E	701	26/26	0.99	0.04	18,26,32,32	0
2	TPP	C	701	26/26	0.99	0.04	18,25,32,34	0
4	MG	A	702	1/1	0.99	0.06	20,20,20,20	0
4	MG	B	703	1/1	0.99	0.04	21,21,21,21	0
4	MG	C	703	1/1	0.99	0.03	21,21,21,21	0
4	MG	E	703	1/1	0.99	0.04	20,20,20,20	0
4	MG	F	703	1/1	0.99	0.05	27,27,27,27	0
2	TPP	A	700	26/26	0.99	0.04	16,23,30,30	0
4	MG	D	702	1/1	1.00	0.04	22,22,22,22	0

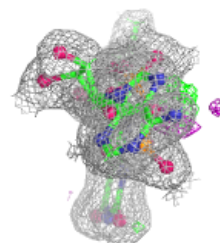
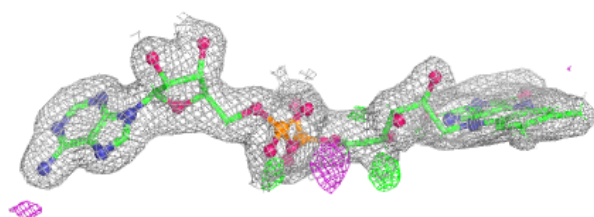
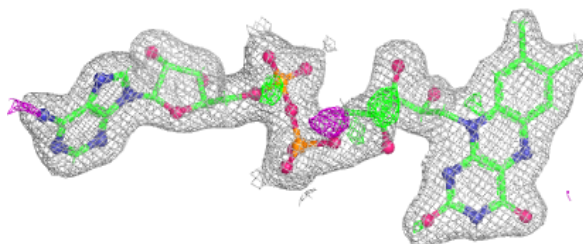
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2PE C 704:

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

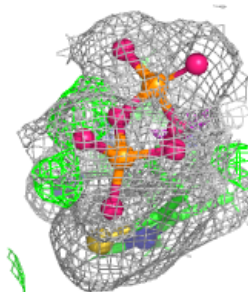
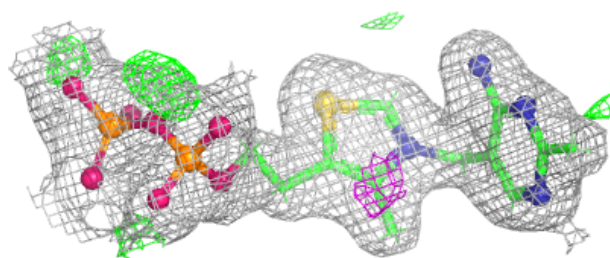
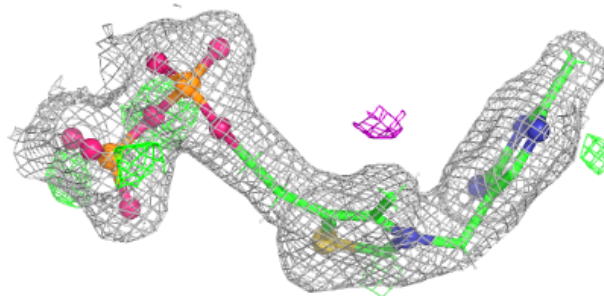
**Electron density around FAD F 702:**

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

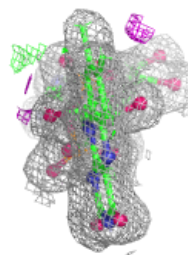
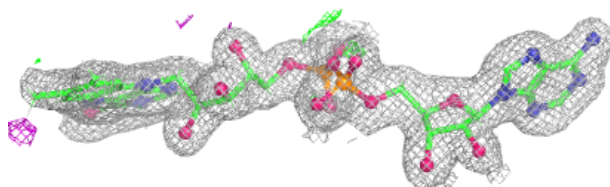
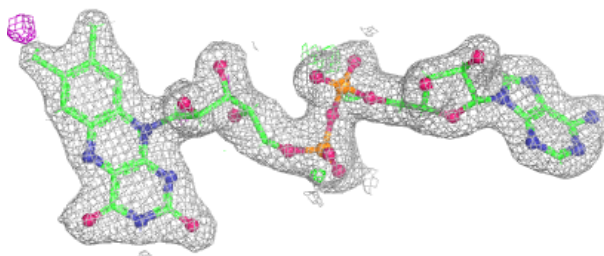


Electron density around TPP F 701:

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

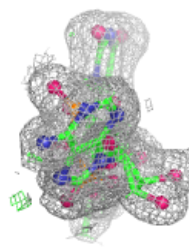
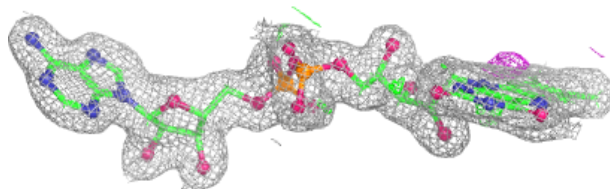
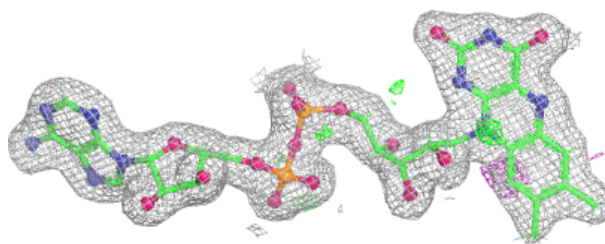
**Electron density around FAD A 701:**

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and green (positive)

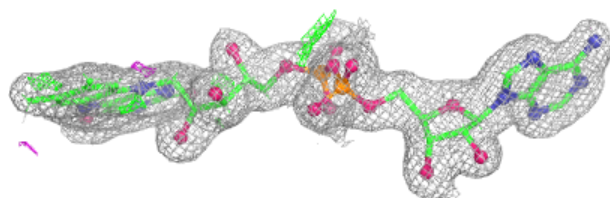
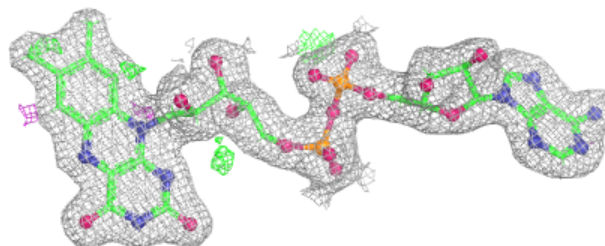


Electron density around FAD C 702:

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

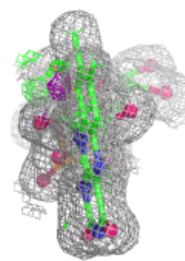
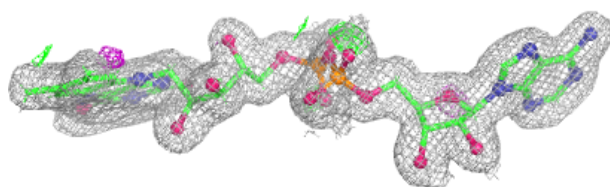
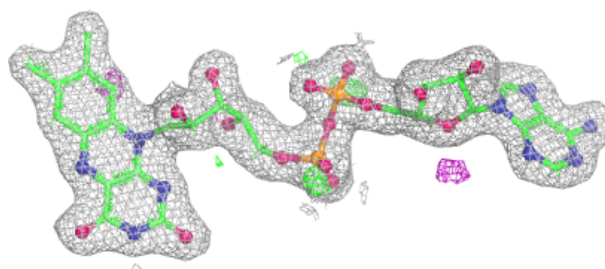
**Electron density around FAD D 701:**

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and green (positive)

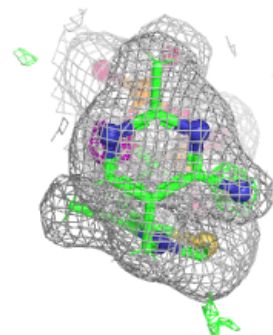
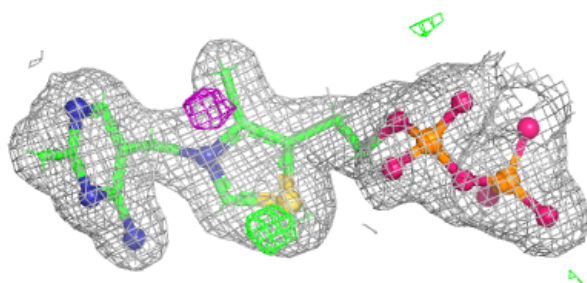
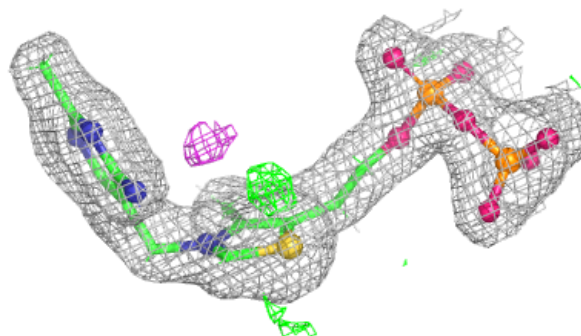


Electron density around FAD E 702:

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

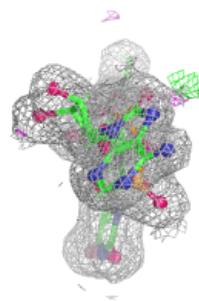
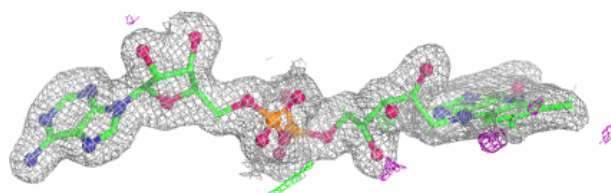
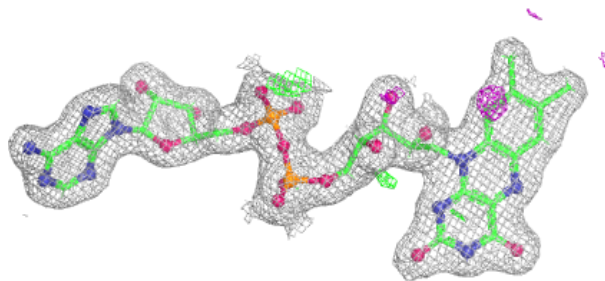
**Electron density around TPP D 700:**

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

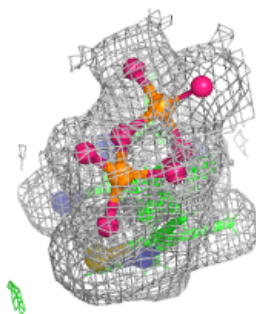
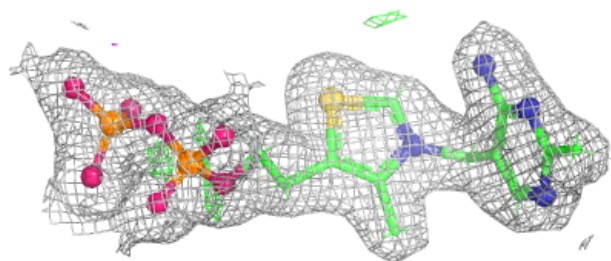
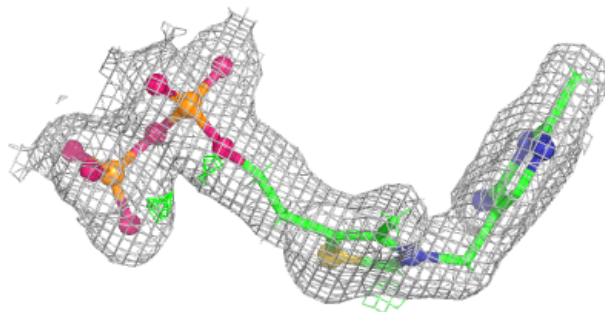


Electron density around FAD B 702:

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

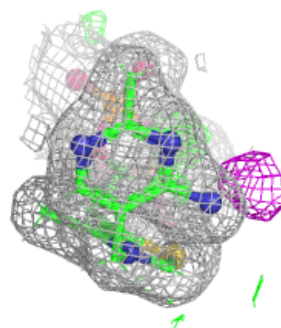
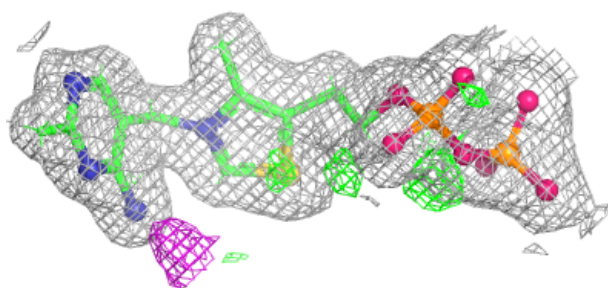
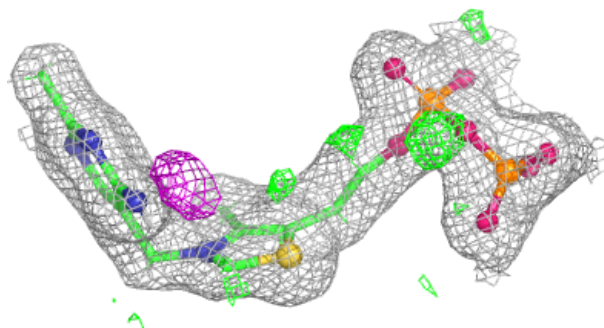
**Electron density around TPP B 701:**

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

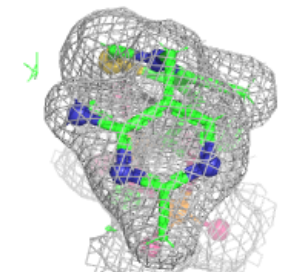
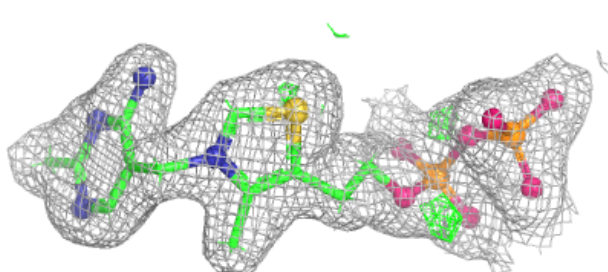
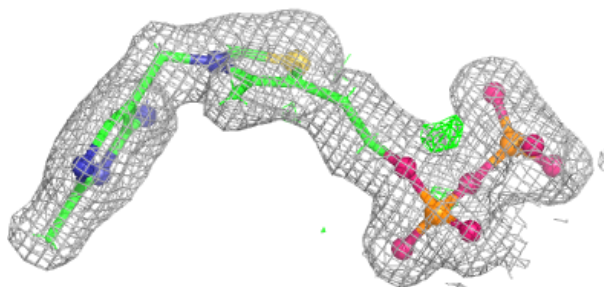


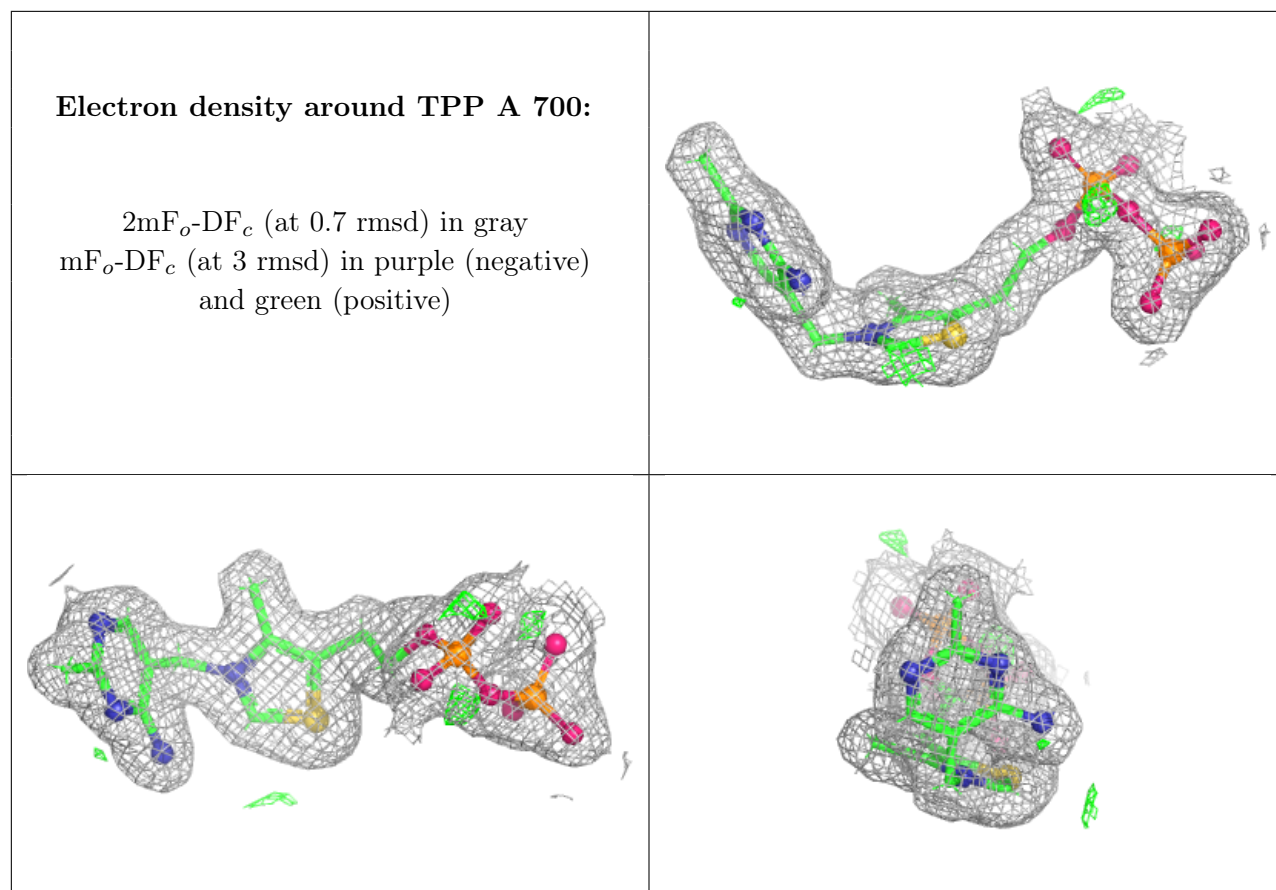
Electron density around TPP E 701:

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

**Electron density around TPP C 701:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.