



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 10:52 am BST

PDB ID : 8RPJ
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

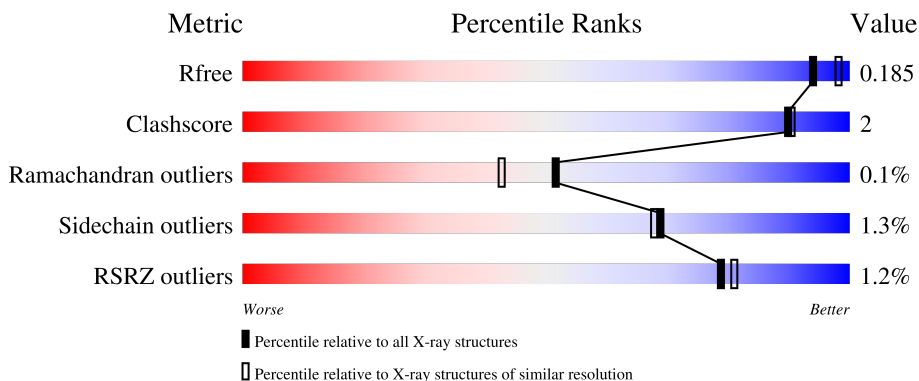
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

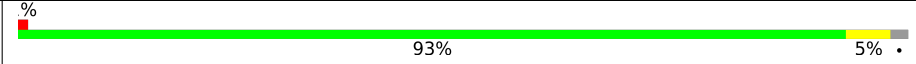
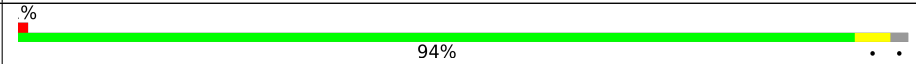
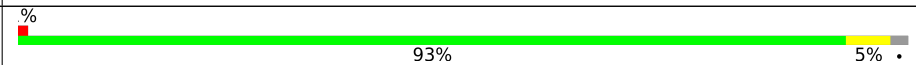
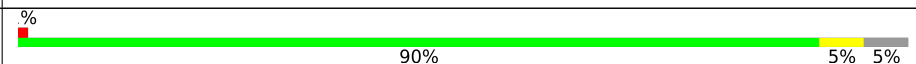
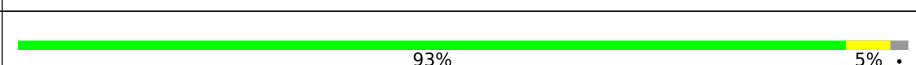
The reported resolution of this entry is 1.90 Å.

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.



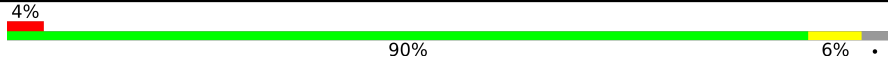
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	 93% 5% .
1	B	619	 94% . .
1	C	619	 93% 5% .
1	D	619	 90% 5% 5%
1	E	619	 93% 5% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	619	 A horizontal bar chart showing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '4%', a large green segment in the middle labeled '90%', a small yellow segment at the end labeled '6%', and a small grey segment at the very end. A small black dot is located at the end of the grey segment.

2 Entry composition [i](#)

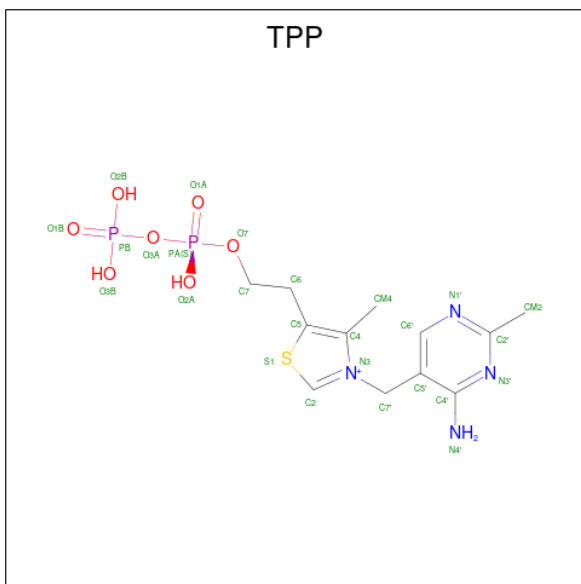
There are 10 unique types of molecules in this entry. The entry contains 58571 atoms, of which 27979 are hydrogens and 0 are deuteriums.

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.

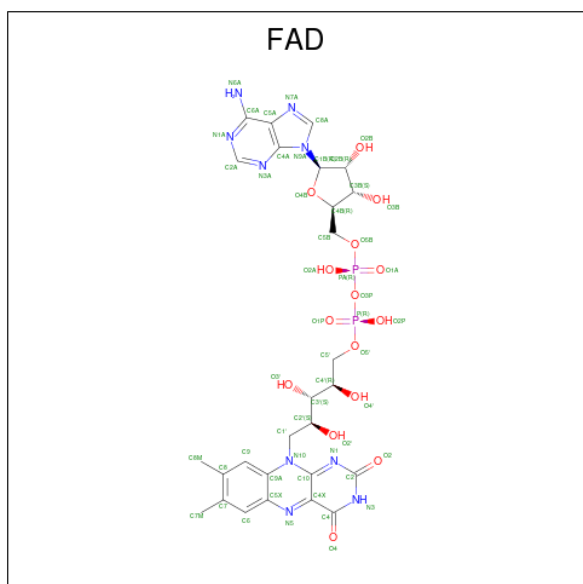
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	605	Total 9296	C 2959	H 4629	N 814	O 862	S 32	0	3	0
1	B	608	Total 9366	C 2979	H 4662	N 823	O 870	S 32	0	5	0
1	C	607	Total 9285	C 2960	H 4616	N 812	O 865	S 32	0	1	0
1	D	591	Total 9051	C 2887	H 4501	N 792	O 841	S 30	0	2	0
1	E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

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S) (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 (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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		

Continued on next page...

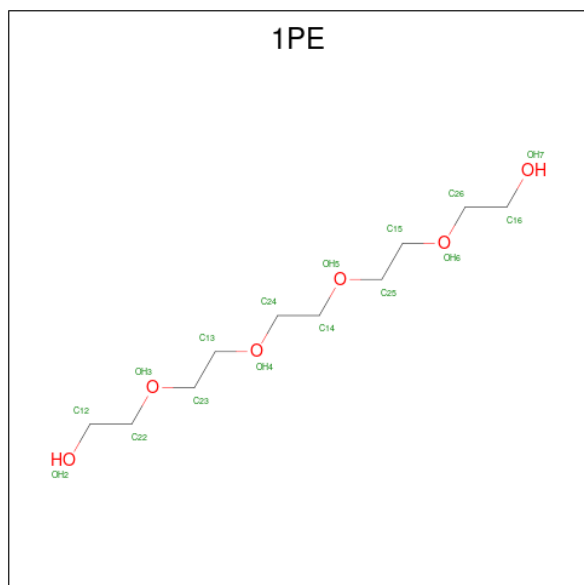
Continued from previous page...

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

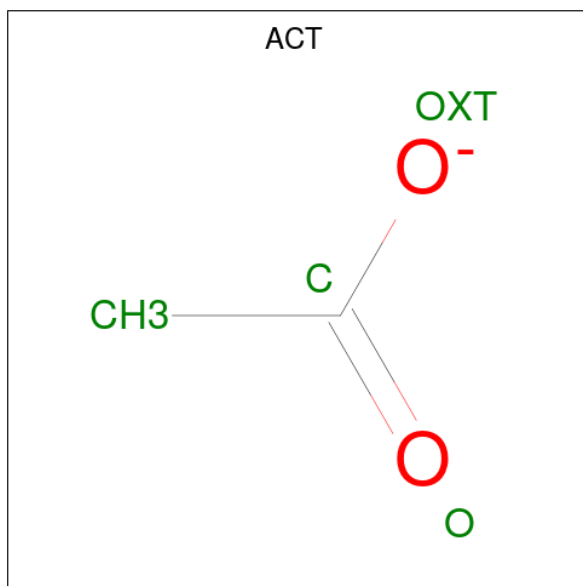
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



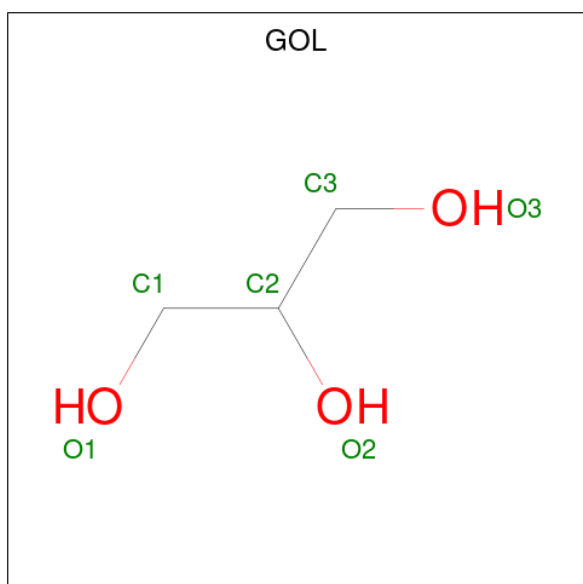
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	B	1	38	10	22	6	0	0
5	E	1	38	10	22	6	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



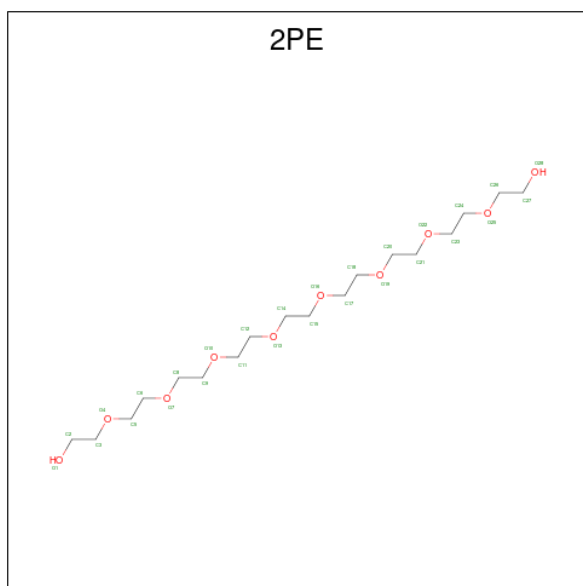
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	B	1	Total 7	C 2	H 3	O 2	0	0
6	B	1	Total 7	C 2	H 3	O 2	0	0
6	E	1	Total 7	C 2	H 3	O 2	0	0
6	F	1	Total 7	C 2	H 3	O 2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



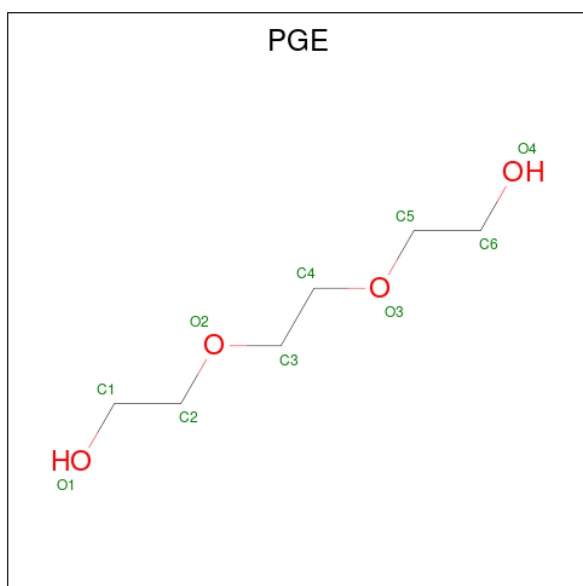
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	B	1	14	3	8	3	0	0

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



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

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: 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		

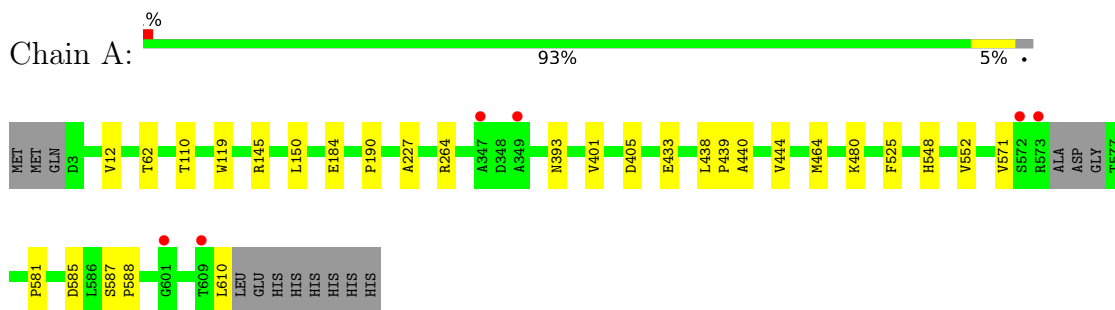
- Molecule 10 is water.

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		

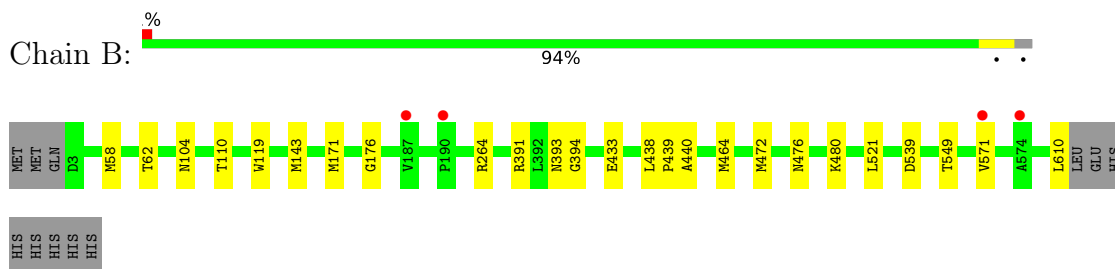
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

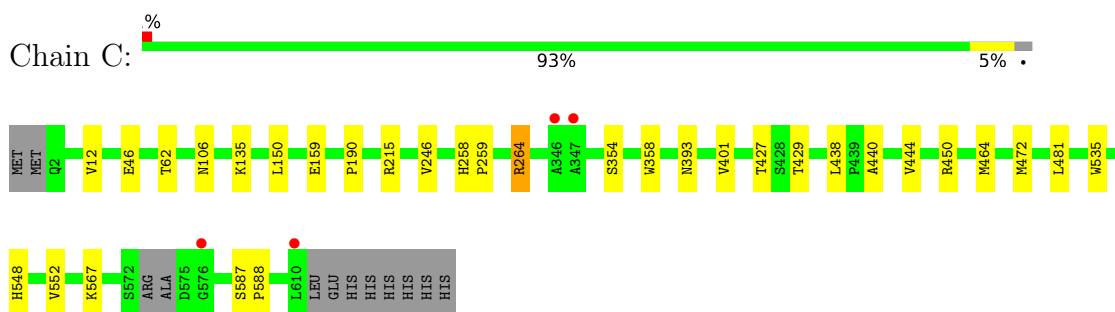
- Molecule 1: Thiamine pyrophosphate-binding protein



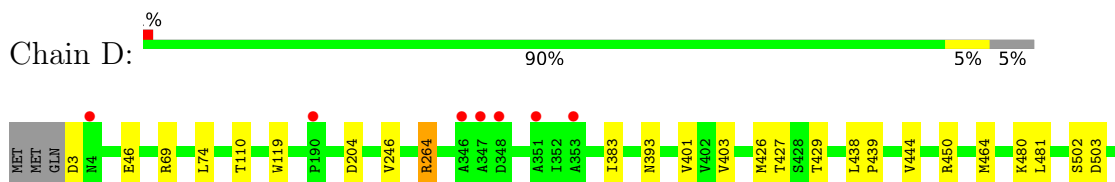
- Molecule 1: Thiamine pyrophosphate-binding protein



- Molecule 1: Thiamine pyrophosphate-binding protein



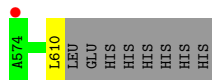
- Molecule 1: Thiamine pyrophosphate-binding protein





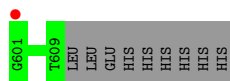
- Molecule 1: Thiamine pyrophosphate-binding protein

Chain E: 93% 5%



- Molecule 1: Thiamine pyrophosphate-binding protein

Chain F: 4% 90% 6%



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 84.34 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (68.16-1.90) 99.3 (84.34-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 1.90Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.153 , 0.186 0.153 , 0.185	Depositor DCC
R_{free} test set	14292 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtrriage
Anisotropy	0.464	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: 1PE, 2PE, PGE, ACT, FAD, TPP, GOL, 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	0.32	0/4772	0.58	0/6473
1	B	0.31	0/4810	0.59	0/6525
1	C	0.31	0/4768	0.57	0/6468
1	D	0.30	0/4654	0.55	0/6317
1	E	0.32	0/4794	0.58	0/6504
1	F	0.30	0/4752	0.55	0/6443
All	All	0.31	0/28550	0.57	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	12	0
1	C	4669	4616	4638	19	0
1	D	4550	4501	4510	16	0
1	E	4685	4641	4649	17	0
1	F	4625	4575	4557	18	0
2	A	26	16	16	0	0

Continued on next page...

Continued from previous page...

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	1	0
2	F	26	16	16	0	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	3	0
10	D	285	0	0	1	1
10	E	411	0	0	2	0
10	F	278	0	0	2	0
All	All	30592	27979	28058	99	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 (99) 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:C:567:LYS:NZ	10:C:801:HOH:O	2.29	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:ILE:HD12	1:D:535:TRP:CE2	2.34	0.62
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: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: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: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:C:587:SER:HA	1:C:588:PRO:C	2.36	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: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
1:B:438:LEU:HD22	1:B:472:MET:HE1	1.98	0.44
1:D:438:LEU:HB2	1:D:439:PRO:HD3	1.98	0.44
1:A:571:VAL:HG11	1:A:610:LEU:HD13	2.00	0.44
1:E:434:MET:SD	2:E:701:TPP:HM42	2.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:142:LYS:NZ	10:F:808:HOH:O	2.44	0.42
1:E:571:VAL:HG21	1:E:610:LEU:HD13	2.01	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:A:587:SER:HA	1:A:588:PRO:C	2.40	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:THR:HG21	1:A:440:ALA:HB1	2.03	0.41
1:C:215:ARG:HA	1:C:358:TRP:CG	2.56	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
1:B:58:MET:HE2	1:B:433:GLU:HG3	2.03	0.41
3:C:702:FAD:H1'1	3:C:702:FAD:H9	1.85	0.41
1:D:46:GLU:OE2	1:D:450:ARG:NH2	2.53	0.41
1:D:587:SER:HA	1:D:588:PRO:C	2.40	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: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%)	47	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	600/619 (97%)	585 (98%)	14 (2%)	1 (0%)	47 38
All	All	3617/3714 (97%)	3530 (98%)	85 (2%)	2 (0%)	51 42

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains [i](#)

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%)	486 (99%)	5 (1%)	76 76
1	B	494/500 (99%)	487 (99%)	7 (1%)	67 65
1	C	490/500 (98%)	485 (99%)	5 (1%)	76 76
1	D	477/500 (95%)	469 (98%)	8 (2%)	60 57
1	E	492/500 (98%)	488 (99%)	4 (1%)	81 82
1	F	487/500 (97%)	476 (98%)	11 (2%)	50 45
All	All	2931/3000 (98%)	2891 (99%)	40 (1%)	69 65

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	ARG
1	A	393	ASN
1	A	405	ASP
1	A	464	MET
1	A	480	LYS
1	B	264	ARG
1	B	393	ASN
1	B	464[A]	MET
1	B	464[B]	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	476	ASN
1	B	480	LYS
1	B	549	THR
1	C	264	ARG
1	C	354	SER
1	C	393	ASN
1	C	464[A]	MET
1	C	464[B]	MET
1	D	69	ARG
1	D	74	LEU
1	D	204	ASP
1	D	264	ARG
1	D	393	ASN
1	D	464	MET
1	D	480	LYS
1	D	549	THR
1	E	74	LEU
1	E	264	ARG
1	E	393	ASN
1	E	464	MET
1	F	74	LEU
1	F	264	ARG
1	F	354	SER
1	F	357	ASP
1	F	393	ASN
1	F	405	ASP
1	F	464	MET
1	F	480	LYS
1	F	501	LYS
1	F	536	ASP
1	F	580	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS

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 monosaccharides 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
3	FAD	D	701	-	53,58,58	0.62	1 (1%)	68,89,89	0.60	1 (1%)
3	FAD	F	702	-	53,58,58	0.58	1 (1%)	68,89,89	0.61	2 (2%)
2	TPP	A	700	4	22,27,27	0.51	0	29,40,40	0.78	1 (3%)
2	TPP	B	701	4	22,27,27	0.67	0	29,40,40	0.90	2 (6%)
2	TPP	F	701	4	22,27,27	0.63	0	29,40,40	0.87	2 (6%)
5	1PE	B	704	-	15,15,15	0.16	0	14,14,14	0.12	0
2	TPP	D	700	4	22,27,27	0.52	0	29,40,40	0.75	1 (3%)
5	1PE	E	704	-	15,15,15	0.15	0	14,14,14	0.11	0
2	TPP	E	701	4	22,27,27	0.48	0	29,40,40	0.78	1 (3%)
3	FAD	B	702	-	53,58,58	0.61	1 (1%)	68,89,89	0.59	1 (1%)
9	PGE	E	706	-	9,9,9	0.11	0	8,8,8	0.34	0
6	ACT	B	705	-	3,3,3	0.92	0	3,3,3	1.62	1 (33%)
6	ACT	B	706	-	3,3,3	1.17	0	3,3,3	1.24	0
3	FAD	E	702	-	53,58,58	0.56	0	68,89,89	0.60	1 (1%)
6	ACT	E	705	-	3,3,3	0.98	0	3,3,3	1.62	0
2	TPP	C	701	4	22,27,27	0.72	0	29,40,40	0.94	2 (6%)
3	FAD	A	701	-	53,58,58	0.61	1 (1%)	68,89,89	0.54	1 (1%)
3	FAD	C	702	-	53,58,58	0.60	1 (1%)	68,89,89	0.59	1 (1%)
6	ACT	F	704	-	3,3,3	1.00	0	3,3,3	1.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	B	707	-	5,5,5	1.05	0	5,5,5	1.33	1 (20%)
8	2PE	C	704	-	27,27,27	0.17	0	26,26,26	0.53	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
2	TPP	D	700	4	-	4/16/17/17	0/2/2/2
3	FAD	A	701	-	-	6/30/50/50	0/6/6/6
3	FAD	D	701	-	-	3/30/50/50	0/6/6/6
3	FAD	F	702	-	-	12/30/50/50	0/6/6/6
2	TPP	A	700	4	-	3/16/17/17	0/2/2/2
3	FAD	C	702	-	-	3/30/50/50	0/6/6/6
5	1PE	E	704	-	-	4/13/13/13	-
9	PGE	E	706	-	-	1/7/7/7	-
7	GOL	B	707	-	-	0/4/4/4	-
2	TPP	B	701	4	-	3/16/17/17	0/2/2/2
2	TPP	F	701	4	-	4/16/17/17	0/2/2/2
2	TPP	E	701	4	-	2/16/17/17	0/2/2/2
3	FAD	E	702	-	-	2/30/50/50	0/6/6/6
3	FAD	B	702	-	-	4/30/50/50	0/6/6/6
2	TPP	C	701	4	-	3/16/17/17	0/2/2/2
8	2PE	C	704	-	-	4/25/25/25	-
5	1PE	B	704	-	-	6/13/13/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	701	FAD	C1'-C2'	2.44	1.56	1.52
3	B	702	FAD	C1'-C2'	2.10	1.55	1.52
3	A	701	FAD	C1'-C2'	2.09	1.55	1.52
3	F	702	FAD	C1'-C2'	2.05	1.55	1.52
3	C	702	FAD	C1'-C2'	2.04	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	707	GOL	C3-C2-C1	-2.47	102.11	111.70
3	E	702	FAD	C5A-C6A-N6A	2.40	123.99	120.35
3	B	702	FAD	C5A-C6A-N6A	2.32	123.88	120.35
3	F	702	FAD	C4'-C3'-C2'	-2.31	108.55	113.36
3	F	702	FAD	C5A-C6A-N6A	2.30	123.85	120.35
3	D	701	FAD	C5A-C6A-N6A	2.27	123.80	120.35
3	C	702	FAD	C5A-C6A-N6A	2.22	123.73	120.35
2	C	701	TPP	O2B-PB-O3A	2.19	111.98	104.64
3	A	701	FAD	C5A-C6A-N6A	2.16	123.63	120.35
2	C	701	TPP	C5-C4-N3	2.15	111.87	107.57
2	B	701	TPP	O2B-PB-O3A	2.12	111.75	104.64
2	F	701	TPP	C5-C4-N3	2.09	111.76	107.57
2	A	700	TPP	C5-C4-N3	2.08	111.74	107.57
2	F	701	TPP	O2B-PB-O3A	2.08	111.59	104.64
2	B	701	TPP	C5-C4-N3	2.07	111.72	107.57
2	E	701	TPP	C5-C4-N3	2.04	111.66	107.57
6	B	705	ACT	OXT-C-O	2.01	129.47	122.05
2	D	700	TPP	C5-C4-N3	2.01	111.59	107.57

There are no chirality outliers.

All (64) 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	C4-C5-C6-C7
2	D	700	TPP	PA-O3A-PB-O2B
2	E	701	TPP	C4-C5-C6-C7
2	E	701	TPP	PA-O3A-PB-O2B
2	F	701	TPP	C4-C5-C6-C7
2	F	701	TPP	C5-C6-C7-O7
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'
3	F	702	FAD	C5'-O5'-P-O3P
5	B	704	1PE	OH4-C13-C23-OH3
8	C	704	2PE	C17-C18-O19-C20
5	E	704	1PE	OH7-C16-C26-OH6
8	C	704	2PE	C20-C21-O22-C23
5	B	704	1PE	OH2-C12-C22-OH3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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
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	C5'-O5'-P-O1P
3	F	702	FAD	C5'-O5'-P-O2P
5	B	704	1PE	C12-C22-OH3-C23
2	A	700	TPP	C4-C5-C6-C7
2	B	701	TPP	C4-C5-C6-C7
2	C	701	TPP	C4-C5-C6-C7
5	E	704	1PE	C24-C14-OH5-C25
3	F	702	FAD	O3'-C3'-C4'-O4'
8	C	704	2PE	O16-C17-C18-O19
3	B	702	FAD	C4'-C5'-O5'-P
3	C	702	FAD	C4'-C5'-O5'-P
8	C	704	2PE	C5-C6-O7-C8
3	F	702	FAD	C2'-C3'-C4'-O4'
3	A	701	FAD	C4'-C5'-O5'-P
2	F	701	TPP	PA-O3A-PB-O1B
3	E	702	FAD	C4'-C5'-O5'-P
3	F	702	FAD	PA-O3P-P-O1P
5	B	704	1PE	OH6-C15-C25-OH5
3	D	701	FAD	P-O3P-PA-O5B
2	B	701	TPP	PA-O3A-PB-O1B
2	C	701	TPP	PA-O3A-PB-O1B
2	D	700	TPP	C5-C6-C7-O7
2	A	700	TPP	PA-O3A-PB-O3B
3	A	701	FAD	O4B-C4B-C5B-O5B
3	C	702	FAD	O4B-C4B-C5B-O5B
3	A	701	FAD	PA-O3P-P-O2P
3	F	702	FAD	PA-O3P-P-O2P
3	D	701	FAD	C4'-C5'-O5'-P
3	B	702	FAD	O4B-C4B-C5B-O5B
3	D	701	FAD	O4B-C4B-C5B-O5B
3	E	702	FAD	O4B-C4B-C5B-O5B
3	F	702	FAD	O4B-C4B-C5B-O5B
5	B	704	1PE	C16-C26-OH6-C15

Continued on next page...

Continued from previous page...

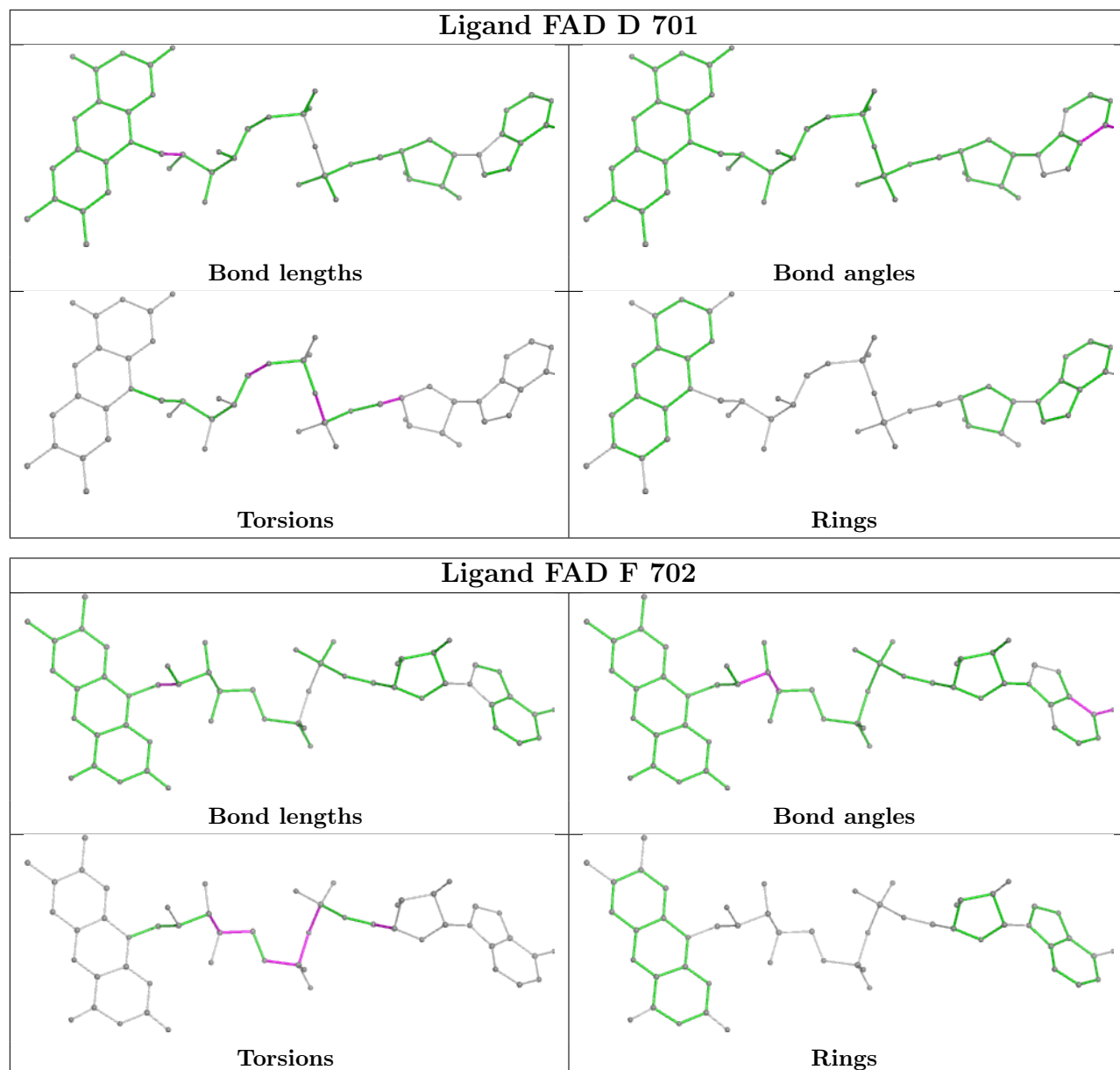
Mol	Chain	Res	Type	Atoms
9	E	706	PGE	O3-C5-C6-O4
3	A	701	FAD	C2'-C1'-N10-C10

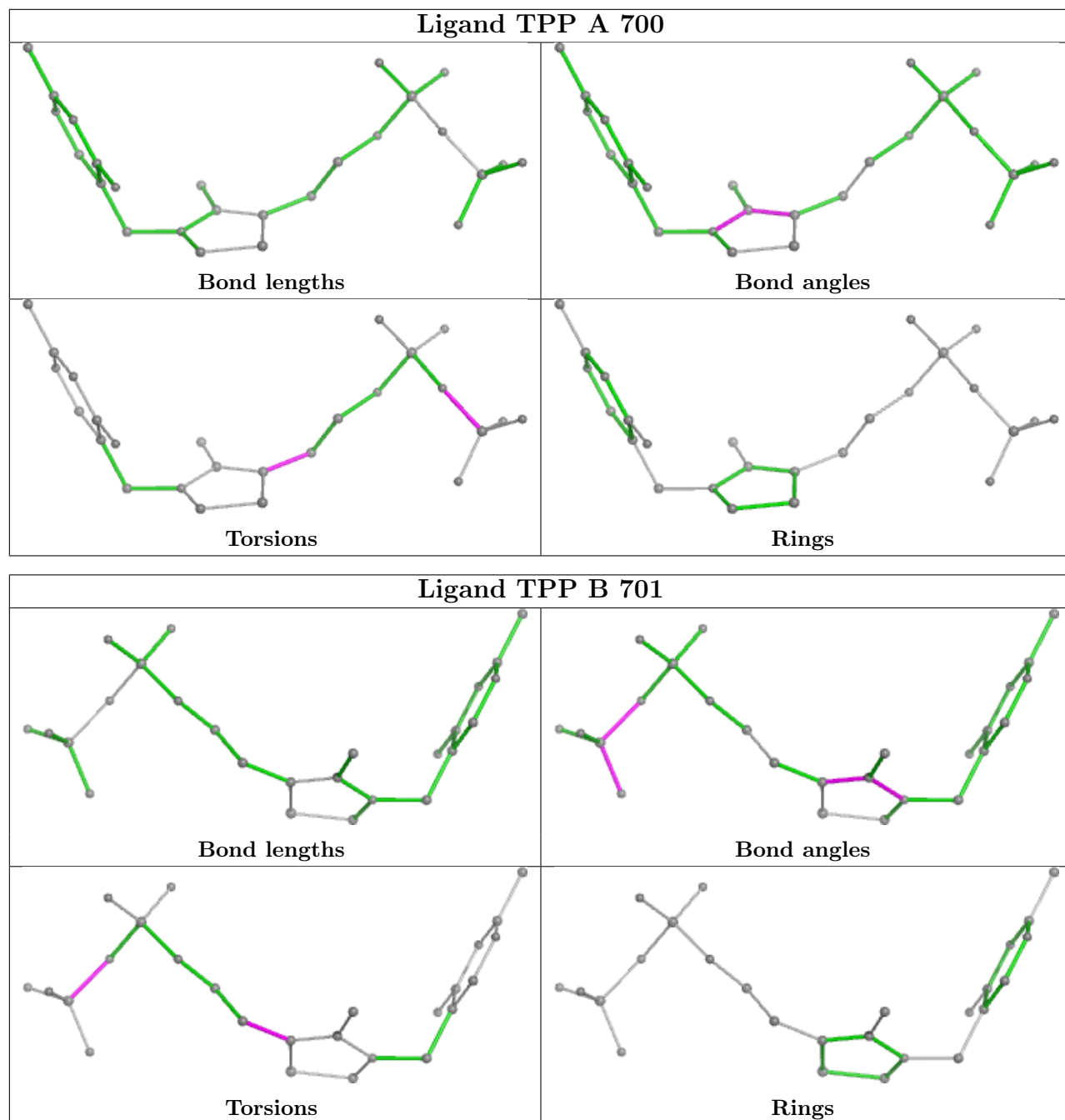
There are no ring outliers.

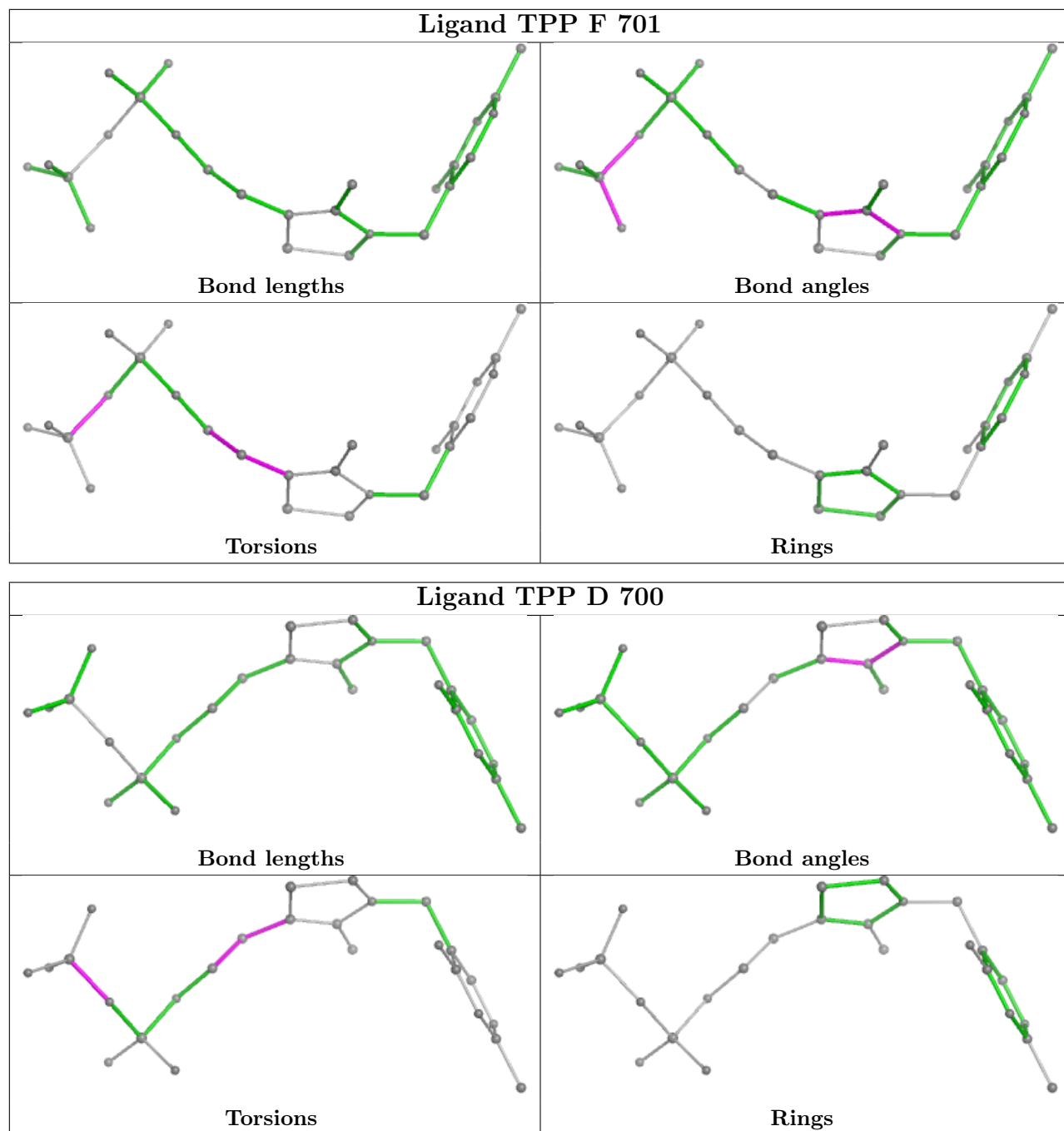
9 monomers are involved in 11 short contacts:

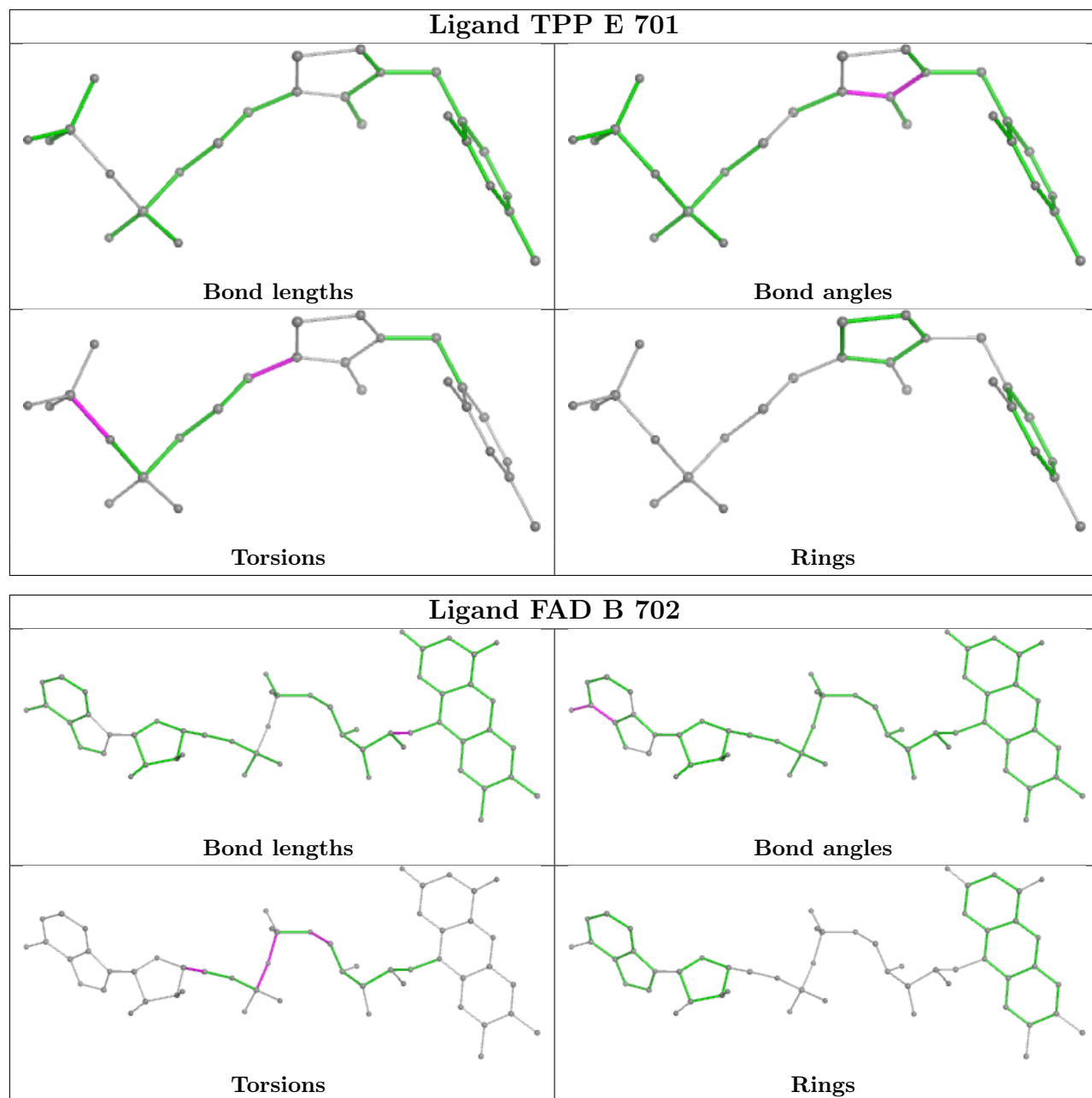
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	701	FAD	1	0
3	F	702	FAD	1	0
5	B	704	1PE	2	0
2	E	701	TPP	1	0
9	E	706	PGE	1	0
6	B	705	ACT	1	0
3	A	701	FAD	1	0
3	C	702	FAD	1	0
8	C	704	2PE	2	0

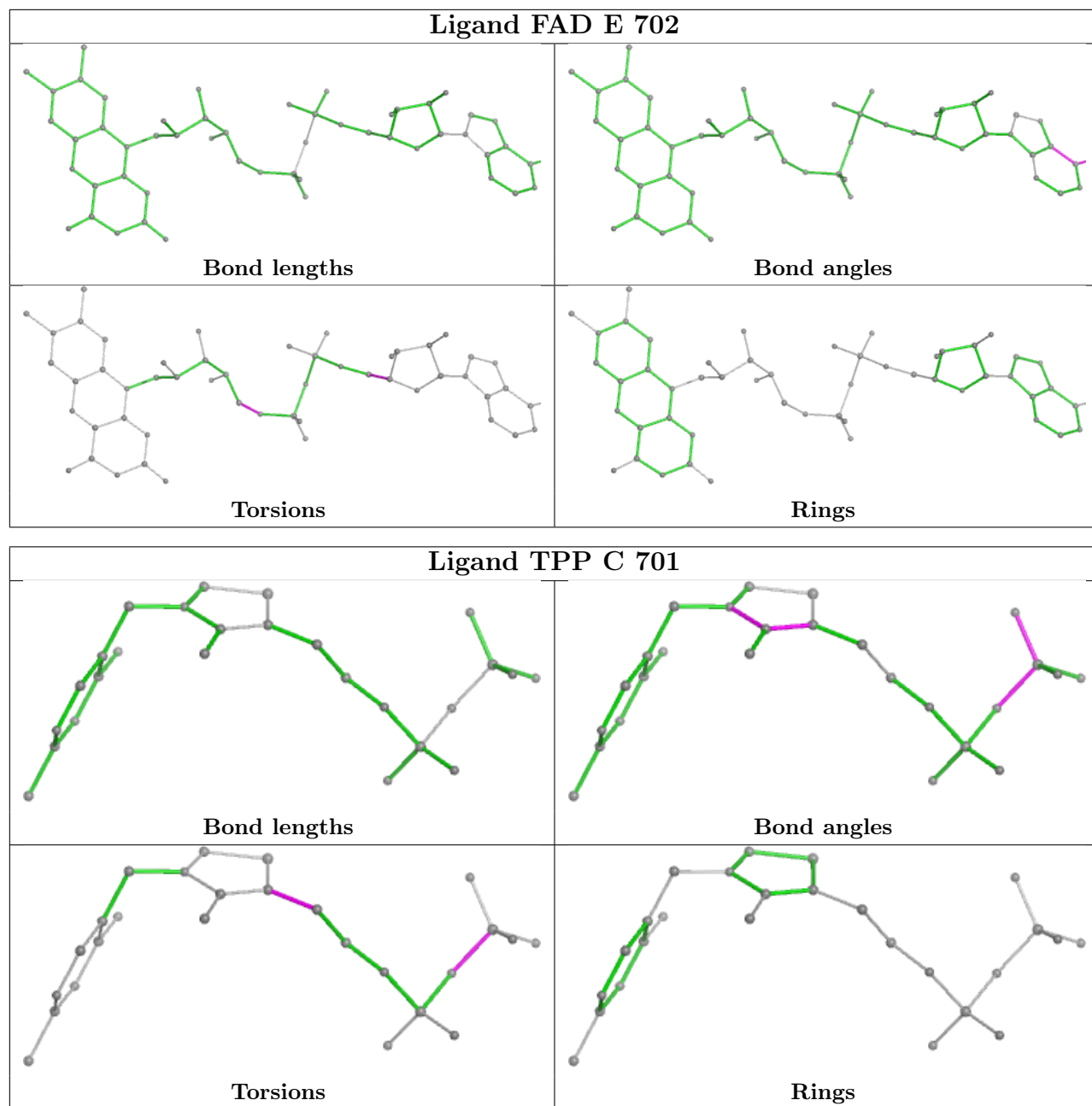
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

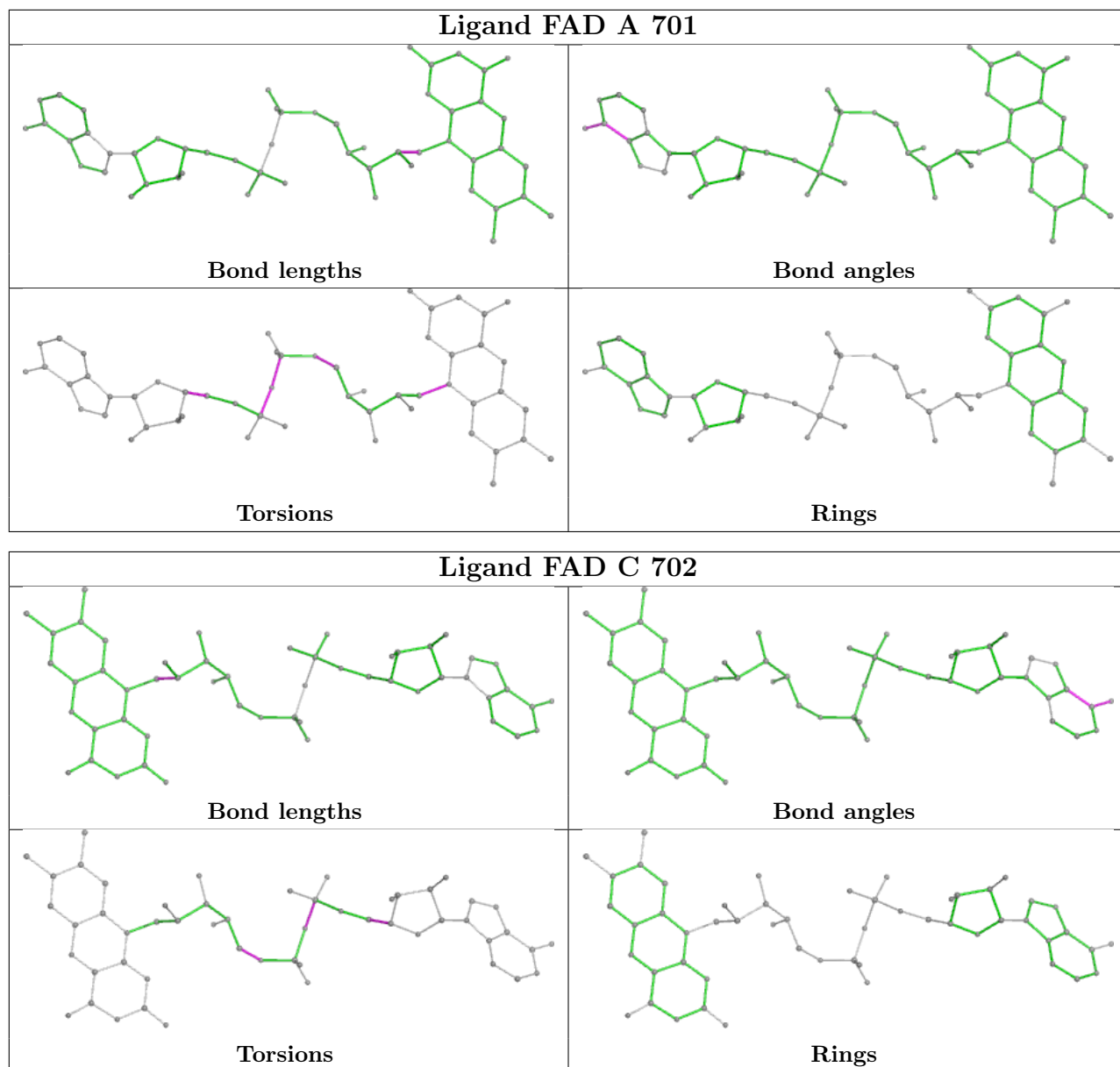


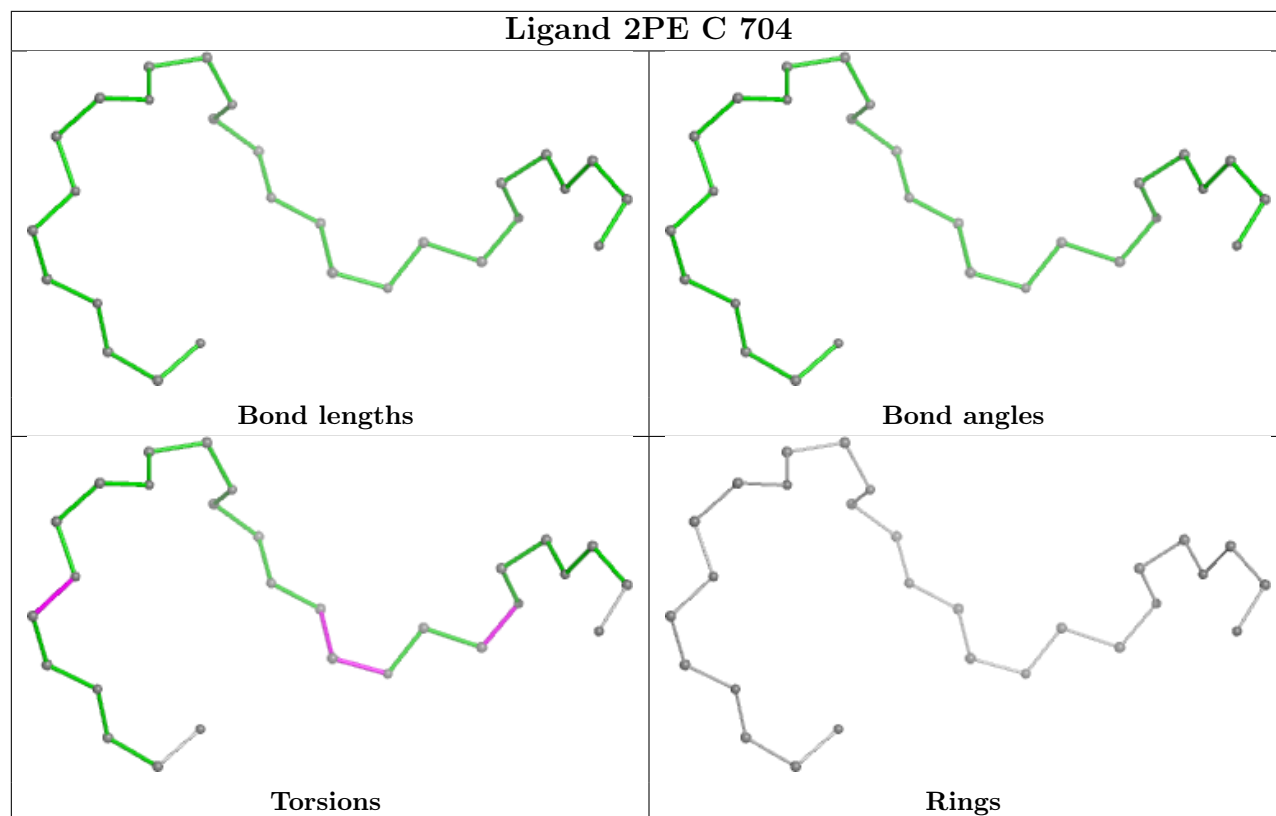












5.7 Other polymers [i](#)

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	605/619 (97%)	-0.23	6 (0%) 82 84	19, 26, 48, 84	0
1	B	608/619 (98%)	-0.29	4 (0%) 87 88	18, 25, 43, 87	0
1	C	607/619 (98%)	-0.17	4 (0%) 87 88	20, 27, 48, 74	0
1	D	591/619 (95%)	-0.22	7 (1%) 79 81	23, 31, 53, 81	0
1	E	608/619 (98%)	-0.28	2 (0%) 94 94	18, 25, 46, 85	0
1	F	598/619 (96%)	0.00	22 (3%) 41 44	22, 34, 60, 77	0
All	All	3617/3714 (97%)	-0.20	45 (1%) 79 81	18, 28, 51, 87	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	574	ALA	8.3
1	A	347	ALA	5.4
1	D	353	ALA	5.2
1	F	190	PRO	4.9
1	D	346	ALA	4.5
1	A	572	SER	4.3
1	F	231	ARG	3.5
1	C	347	ALA	3.3
1	F	601	GLY	3.3
1	D	347	ALA	3.2
1	F	570	VAL	3.2
1	A	609	THR	3.1
1	F	351	ALA	3.1
1	A	601	GLY	3.1
1	F	346	ALA	3.1
1	F	240	LEU	3.1
1	C	346	ALA	3.0
1	C	610	LEU	2.8
1	F	591	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	190	PRO	2.7
1	E	574	ALA	2.7
1	D	190	PRO	2.7
1	F	234	LYS	2.6
1	F	593	ASP	2.6
1	D	348	ASP	2.6
1	F	210	LEU	2.5
1	F	232	LEU	2.4
1	D	351	ALA	2.4
1	F	236	LEU	2.4
1	F	344	LEU	2.3
1	F	594	VAL	2.3
1	A	349	ALA	2.2
1	B	187	VAL	2.2
1	F	191	ALA	2.2
1	B	571	VAL	2.2
1	F	600	ILE	2.2
1	D	4	ASN	2.2
1	F	568	LEU	2.2
1	F	361	LYS	2.2
1	F	383	ILE	2.1
1	C	576	GLY	2.1
1	F	339	ALA	2.1
1	A	573	ARG	2.0
1	F	597	GLN	2.0
1	E	191	ALA	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 monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

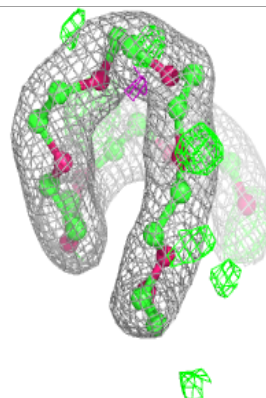
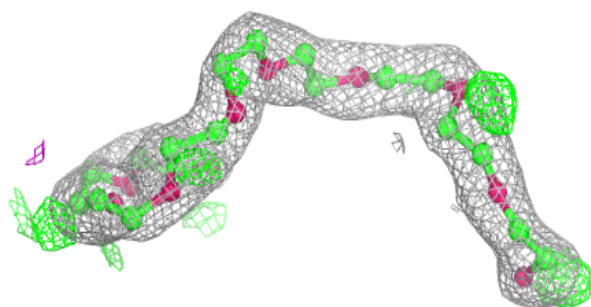
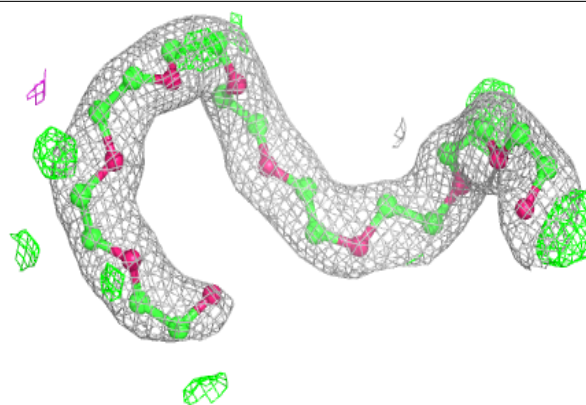
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	1PE	B	704	16/16	0.86	0.20	39,55,77,86	0
9	PGE	E	706	10/10	0.90	0.10	44,53,56,64	0
6	ACT	B	706	4/4	0.91	0.13	29,34,41,42	0
5	1PE	E	704	16/16	0.93	0.12	34,48,63,71	0
6	ACT	B	705	4/4	0.93	0.10	45,52,60,60	0
8	2PE	C	704	28/28	0.94	0.14	31,38,48,56	0
6	ACT	E	705	4/4	0.94	0.08	44,47,53,54	0
6	ACT	F	704	4/4	0.95	0.11	40,47,48,55	0
7	GOL	B	707	6/6	0.96	0.17	29,42,51,53	0
3	FAD	F	702	53/53	0.96	0.10	26,33,50,71	0
4	MG	F	703	1/1	0.96	0.04	27,27,27,27	0
3	FAD	D	701	53/53	0.97	0.09	22,30,39,42	0
3	FAD	A	701	53/53	0.97	0.10	19,25,35,36	0
3	FAD	E	702	53/53	0.98	0.10	18,23,31,31	0
2	TPP	F	701	26/26	0.98	0.10	24,31,37,38	0
2	TPP	B	701	26/26	0.98	0.09	17,25,30,34	0
3	FAD	B	702	53/53	0.98	0.09	17,22,34,34	0
3	FAD	C	702	53/53	0.98	0.10	20,26,34,39	0
2	TPP	D	700	26/26	0.98	0.09	21,28,33,38	0
2	TPP	A	700	26/26	0.99	0.09	16,23,30,30	0
2	TPP	E	701	26/26	0.99	0.10	18,26,32,32	0
2	TPP	C	701	26/26	0.99	0.10	18,25,32,34	0
4	MG	C	703	1/1	0.99	0.11	21,21,21,21	0
4	MG	E	703	1/1	0.99	0.13	20,20,20,20	0
4	MG	D	702	1/1	1.00	0.13	22,22,22,22	0
4	MG	B	703	1/1	1.00	0.14	21,21,21,21	0
4	MG	A	702	1/1	1.00	0.15	20,20,20,20	0

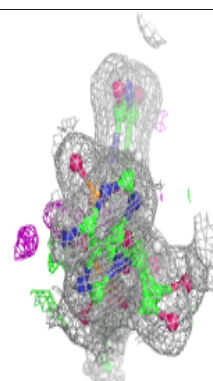
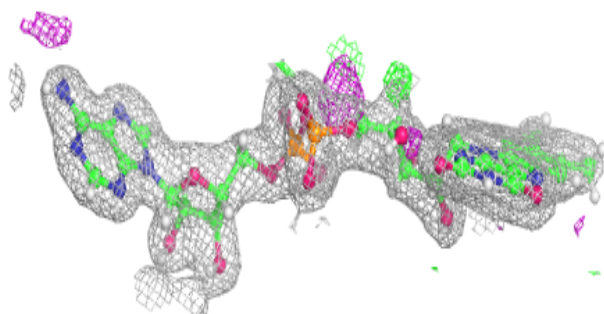
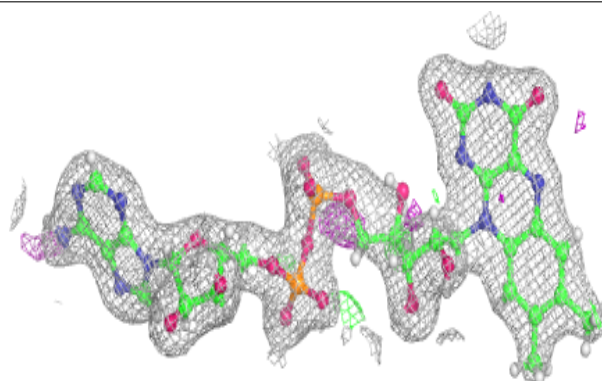
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

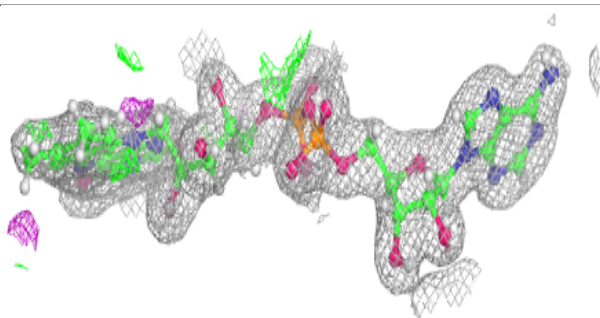
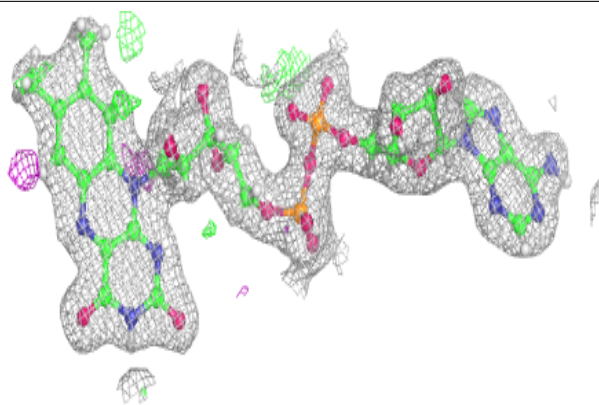
**Electron density around FAD F 702:**

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

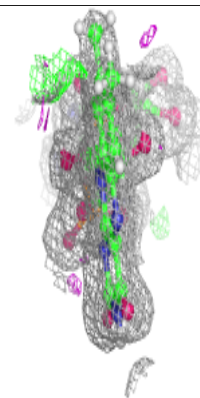
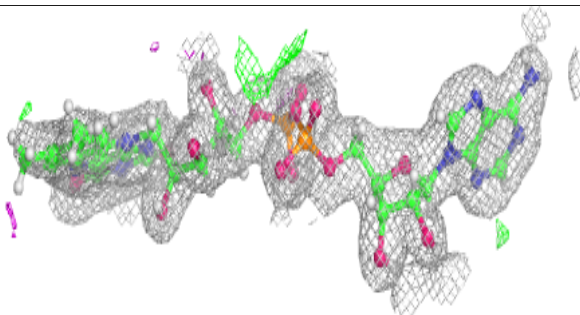
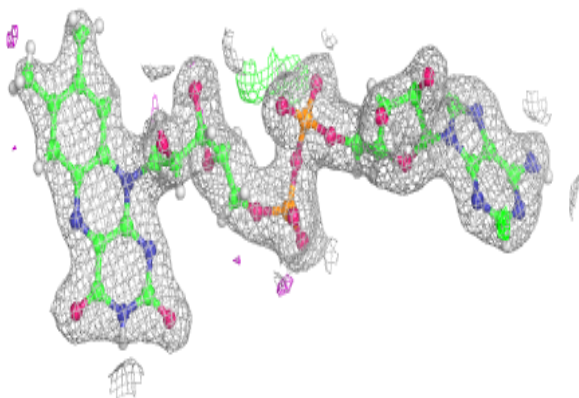


Electron density around FAD D 701:

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

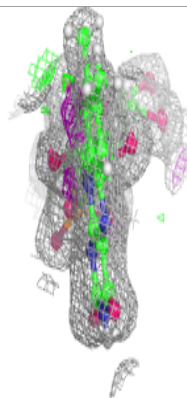
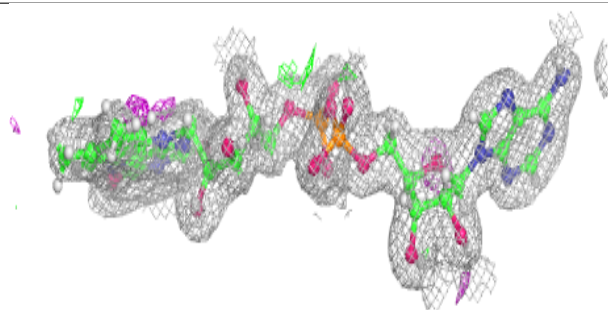
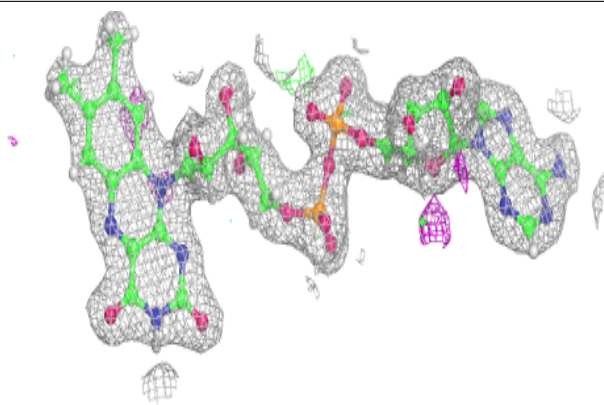
**Electron density around FAD A 701:**

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

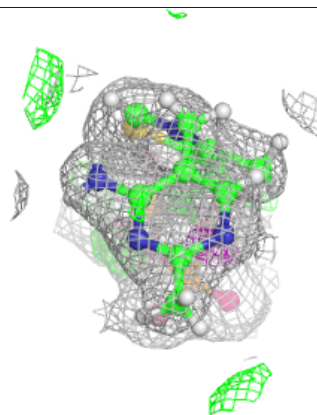
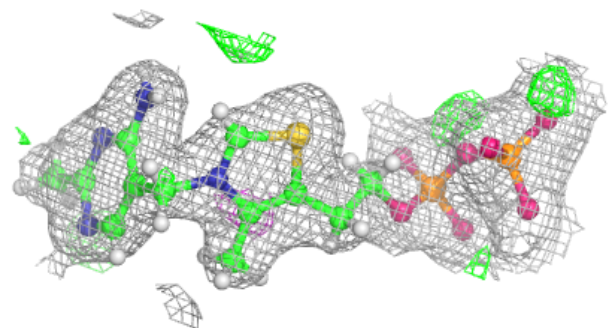
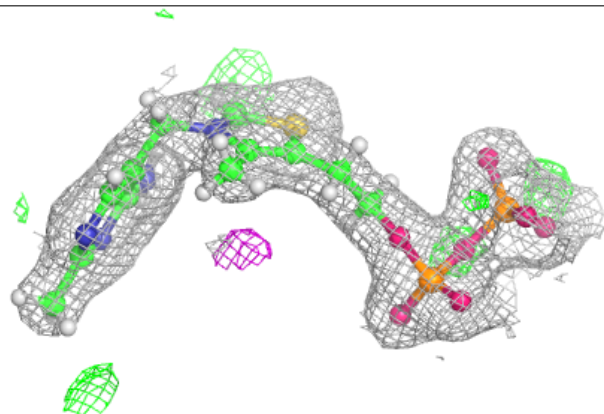


Electron density around FAD E 702:

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

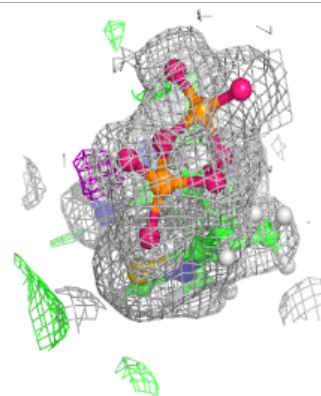
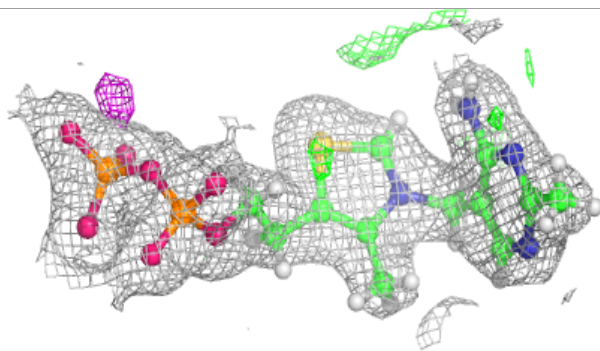
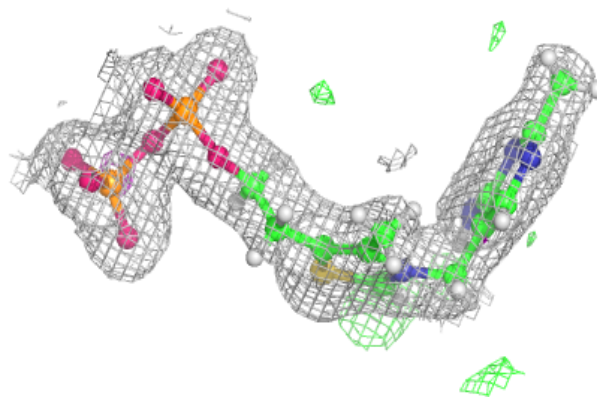
**Electron density around TPP F 701:**

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

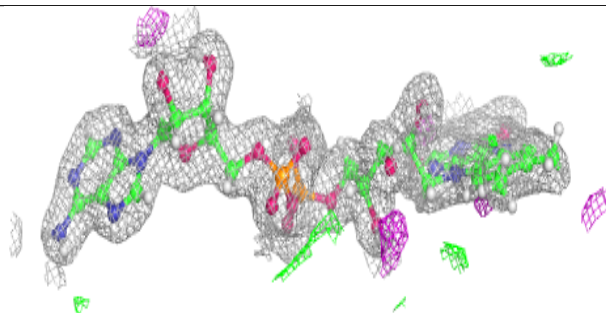
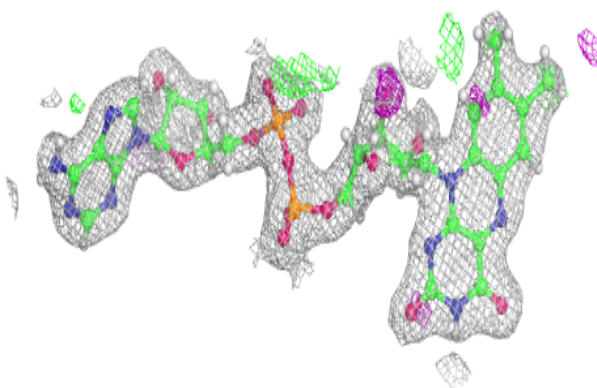


Electron density around TPP B 701:

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

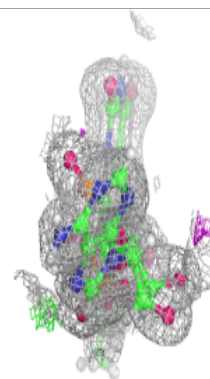
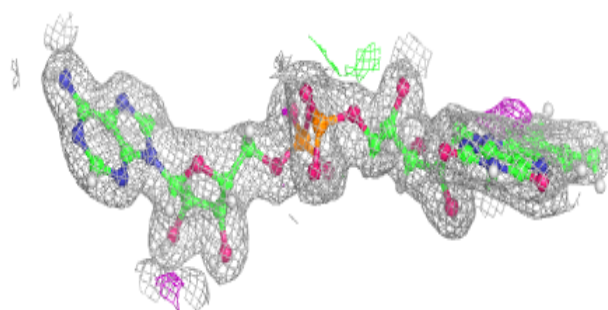
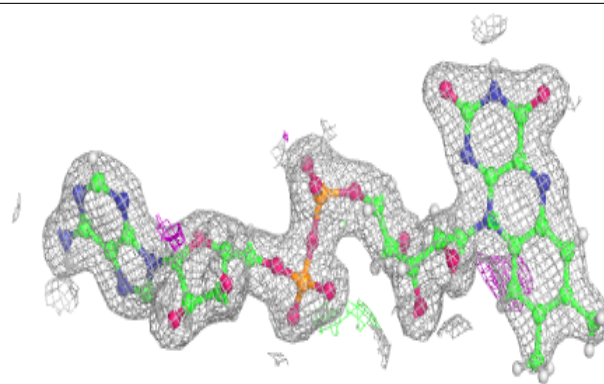
**Electron density around FAD B 702:**

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

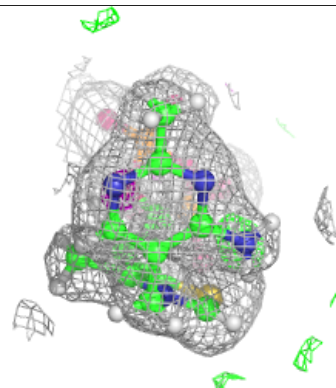
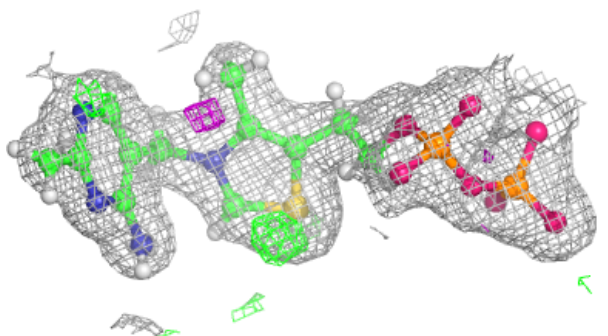
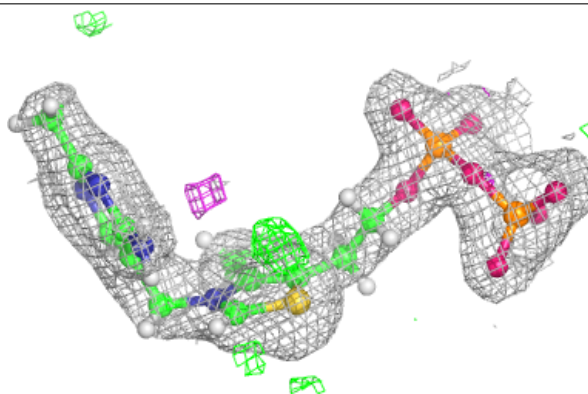


Electron density around FAD C 702:

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

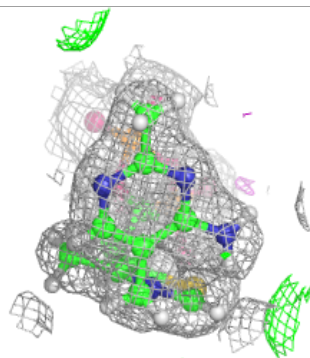
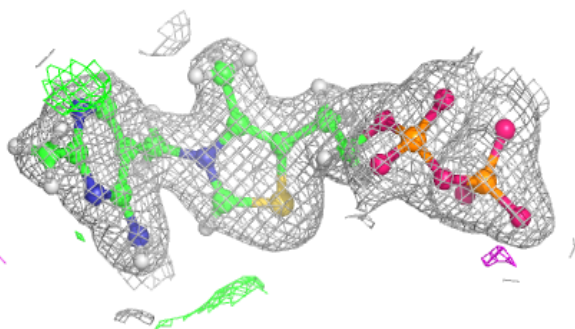
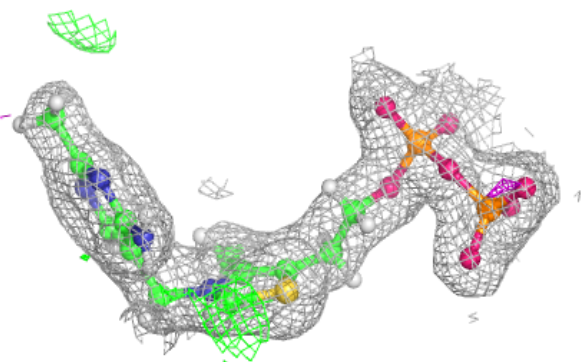
**Electron density around TPP D 700:**

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

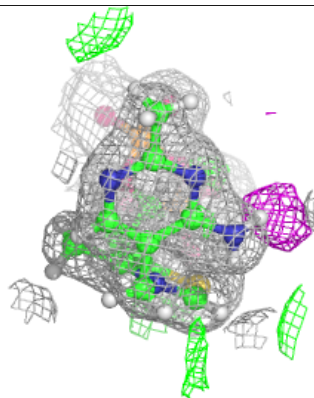
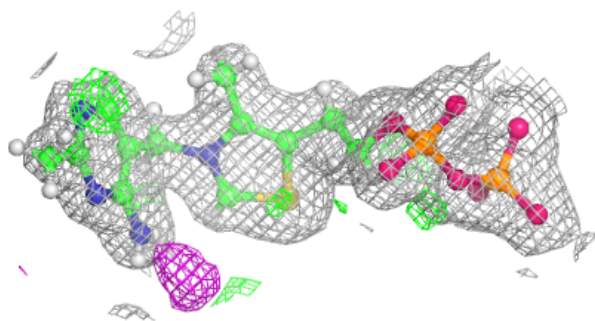
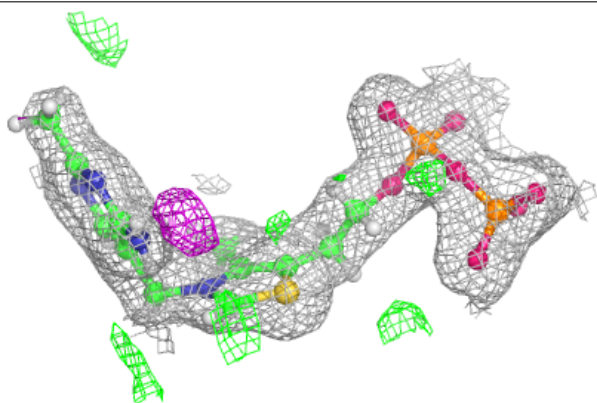


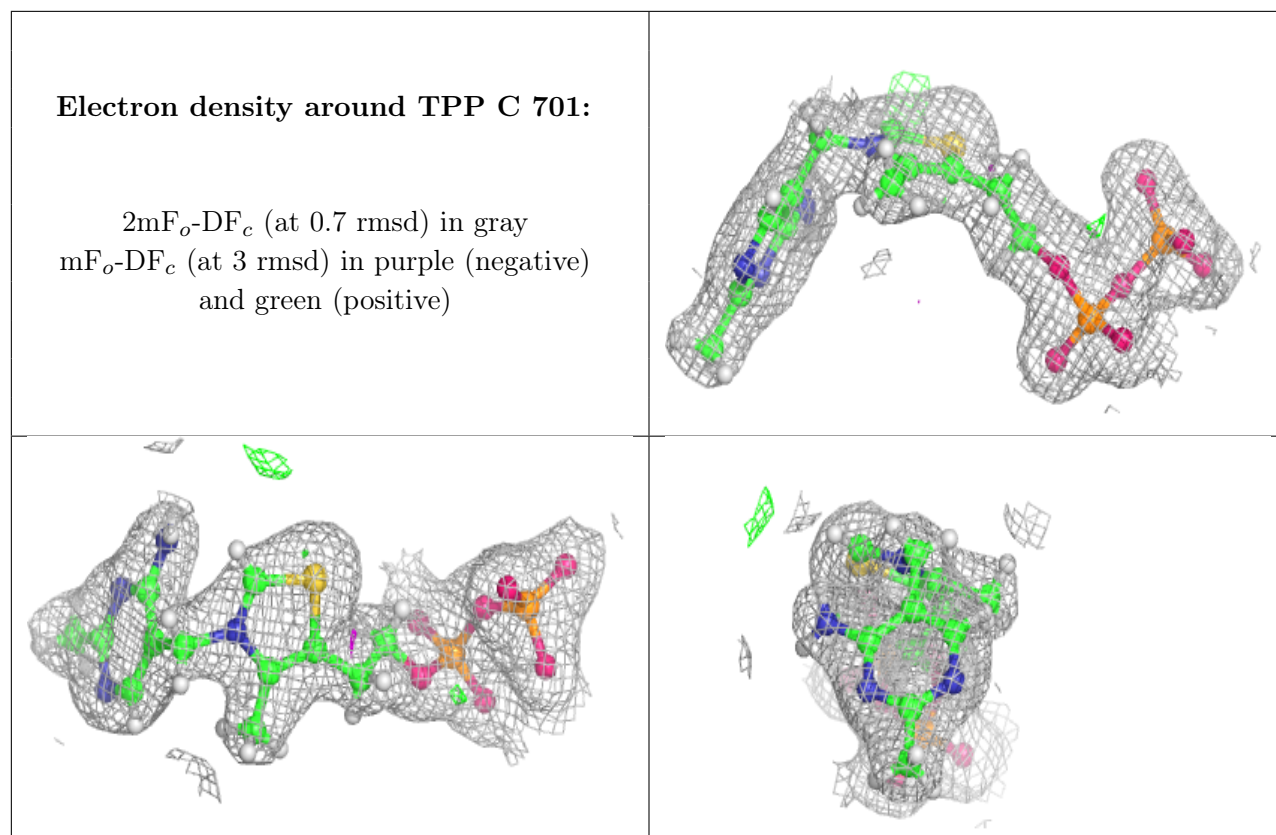
Electron density around TPP A 700:

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

**Electron density around TPP E 701:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.