



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:17 AM UTC

PDB ID : 2CZ8 / pdb_00002cz8
Title : Crystal Structure of tt0972 protein from *Thermus thermophilus*
Authors : Kumei, M.; Inagaki, E.; Nakano, N.; Shinkai, A.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-11
Resolution : 1.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

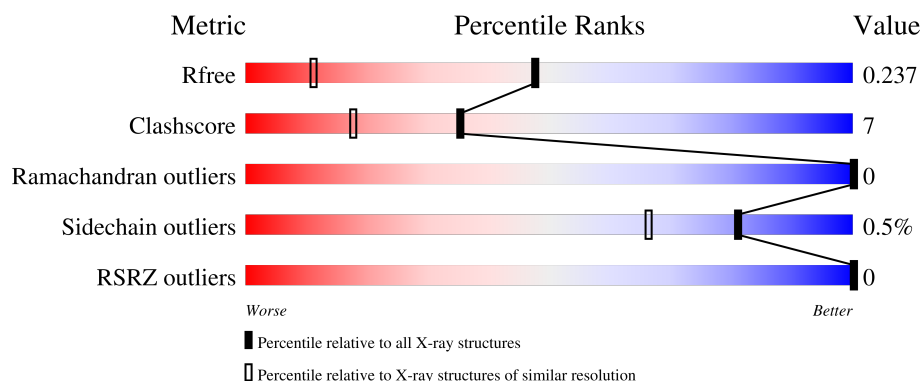
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

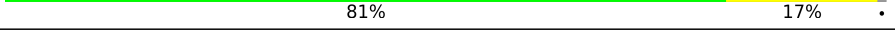
The reported resolution of this entry is 1.50 Å.

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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	69	
1	B	69	
1	C	69	
1	D	69	
1	E	69	

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Mol	Chain	Length	Quality of chain
1	F	69	 91% . .
1	G	69	 83% 14% .
1	H	69	 87% 12% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	D	2102	-	X	-	-
2	PO4	H	2104	-	X	-	-

2 Entry composition

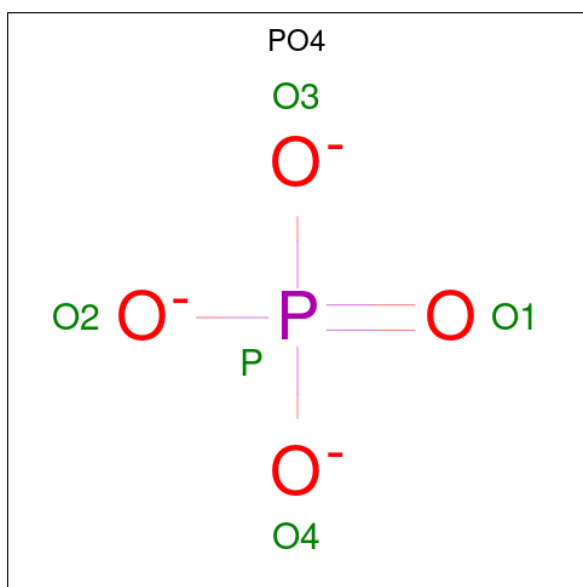
There are 5 unique types of molecules in this entry. The entry contains 5584 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 tt0972 protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	67	Total	C	N	O	0	10	0
			573	361	101	111			
1	B	66	Total	C	N	O	0	5	0
			541	342	93	106			
1	C	67	Total	C	N	O	0	8	0
			562	356	100	106			
1	D	68	Total	C	N	O	0	4	0
			548	347	95	106			
1	E	68	Total	C	N	O	0	10	0
			581	365	102	114			
1	F	66	Total	C	N	O	0	6	0
			543	344	93	106			
1	G	67	Total	C	N	O	0	8	0
			566	361	100	105			
1	H	68	Total	C	N	O	0	3	0
			545	346	95	104			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		
3	E	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total K 1 1	0	0

- # FAD

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	D	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	E	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	F	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	G	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	H	1	Total 53	C 27	N 9	O 15	P 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total 82	O 82	0	3
5	B	82	Total 86	O 86	0	4
5	C	80	Total 82	O 82	0	2
5	D	73	Total 77	O 77	0	4
5	E	84	Total 88	O 88	0	4
5	F	78	Total 83	O 83	0	5
5	G	71	Total 74	O 74	0	3
5	H	80	Total 80	O 80	0	0

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: tt0972 protein

Chain A:  80% 16% . .



- Molecule 1: tt0972 protein

Chain B:  87% 9% .



- Molecule 1: tt0972 protein

Chain C:  87% 10% .



- Molecule 1: tt0972 protein

Chain D:  81% 17% .



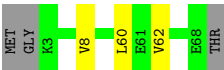
- Molecule 1: tt0972 protein

Chain E:  84% 14% .

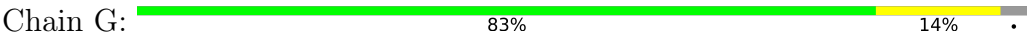


- Molecule 1: tt0972 protein

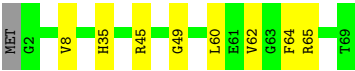
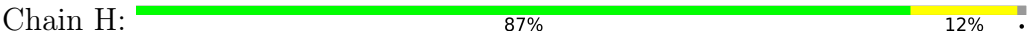
Chain F:  91% . .



● Molecule 1: tt0972 protein



● Molecule 1: tt0972 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	66.36Å 66.36Å 124.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.28 – 1.50 29.28 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.28-1.50) 98.7 (29.28-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 1.25Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.229 0.214 , 0.237	Depositor DCC
R_{free} test set	8414 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	11.5	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.486 for -h,-k,l 0.037 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5584	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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: K, PO4, FAD

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	0.31	0/612	0.81	2/818 (0.2%)
1	B	0.34	0/577	0.81	0/772
1	C	0.36	0/594	0.80	0/794
1	D	0.34	0/578	0.82	0/773
1	E	0.31	0/620	0.80	1/828 (0.1%)
1	F	0.34	0/584	0.80	0/782
1	G	0.35	0/598	0.78	0/800
1	H	0.33	0/569	0.81	0/761
All	All	0.34	0/4732	0.80	3/6328 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	LYS	N-CA-C	-5.06	104.83	111.96
1	A	16	GLU	N-CA-C	5.01	119.39	113.12
1	E	56	TYR	N-CA-C	-5.01	101.54	109.96

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	573	0	574	12	0
1	B	541	0	539	10	0
1	C	562	0	575	8	0
1	D	548	0	554	10	0
1	E	581	0	581	13	0
1	F	543	0	544	3	0
1	G	566	0	582	13	0
1	H	545	0	556	8	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	D	10	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	53	0	31	3	0
4	B	53	0	31	3	0
4	C	53	0	31	4	0
4	D	53	0	31	2	0
4	E	53	0	31	3	0
4	F	53	0	31	1	0
4	G	53	0	31	4	0
4	H	53	0	31	2	0
5	A	82	0	0	2	0
5	B	86	0	0	3	0
5	C	82	0	0	1	0
5	D	77	0	0	0	0
5	E	88	0	0	1	0
5	F	83	0	0	2	0
5	G	74	0	0	3	0
5	H	80	0	0	1	0
All	All	5584	0	4753	73	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 7.

All (73) 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:E:69:THR:HB	1:G:31:LYS:HD3	1.69	0.74
1:A:3:LYS:HB2	1:A:3:LYS:NZ	2.05	0.71
1:G:42:LYS:HE3	1:G:61:GLU:HG3	1.75	0.68
1:D:28:ARG:HD2	1:D:31:LYS:HE2	1.76	0.68
1:D:35:HIS:HB3	4:D:1204:FAD:O2A	1.93	0.68
1:E:42:LYS:HE3	1:E:61:GLU:HG3	1.77	0.67
1:D:37:ASP:OD1	4:D:1204:FAD:H4B	1.95	0.66
1:C:35:HIS:ND1	4:C:1203:FAD:H8A	2.12	0.64
1:B:65:ARG:HB3	1:B:65:ARG:NH2	2.13	0.64
5:A:2158:HOH:O	1:B:68:GLU:HG3	1.97	0.63
1:G:35:HIS:ND1	4:G:1207:FAD:H8A	2.16	0.61
1:D:28:ARG:CD	1:D:31:LYS:HE2	2.30	0.60
1:B:65:ARG:HB3	1:B:65:ARG:HH21	1.67	0.59
1:G:35:HIS:HB3	4:G:1207:FAD:O1A	2.02	0.59
1:F:8[B]:VAL:HG21	5:G:2178[B]:HOH:O	2.03	0.57
1:G:35:HIS:ND1	4:G:1207:FAD:H52A	2.20	0.57
1:E:35:HIS:HB3	4:E:1205:FAD:O1A	2.06	0.55
1:G:28:ARG:NH1	5:G:2145:HOH:O	2.40	0.55
1:C:30:ARG:NH2	1:D:49:GLY:O	2.41	0.54
1:H:35:HIS:HB3	4:H:1208:FAD:O1A	2.08	0.54
1:C:35:HIS:HB3	4:C:1203:FAD:O1A	2.09	0.53
1:A:50[A]:GLU:OE2	1:A:51[A]:ALA:HB2	2.09	0.53
1:G:30:ARG:NH2	1:H:49:GLY:O	2.42	0.52
1:H:8[B]:VAL:HG21	5:H:2142:HOH:O	2.08	0.52
1:C:35:HIS:ND1	4:C:1203:FAD:H52A	2.25	0.52
1:A:35:HIS:HB3	4:A:1201:FAD:O1A	2.09	0.52
1:C:28:ARG:NH1	5:C:1240:HOH:O	2.43	0.52
1:A:65:ARG:HH21	4:A:1201:FAD:H52A	1.76	0.51
1:B:65:ARG:HH21	1:B:65:ARG:CB	2.23	0.51
1:E:60:LEU:HD13	1:E:62:VAL:HG23	1.93	0.50
1:A:3:LYS:HB2	1:A:3:LYS:HZ3	1.74	0.50
1:G:50[B]:GLU:HG2	5:G:2153:HOH:O	2.10	0.50
4:A:1201:FAD:HM81	1:C:11:VAL:HG11	1.94	0.50
1:A:60:LEU:HD13	1:A:62:VAL:HG23	1.95	0.48
1:B:35:HIS:HB3	4:B:1202:FAD:O1A	2.15	0.47
1:B:60:LEU:HD13	1:B:62:VAL:HG23	1.97	0.47
1:H:65:ARG:HH11	4:H:1208:FAD:H52A	1.79	0.47
1:E:60:LEU:O	1:E:60:LEU:HD12	2.14	0.47
5:E:2118:HOH:O	1:G:8[B]:VAL:HG21	2.14	0.47
4:G:1207:FAD:O4	1:H:45:ARG:NE	2.48	0.47
1:A:3:LYS:HB2	1:A:3:LYS:HZ2	1.78	0.47
1:D:60:LEU:CD1	1:D:62:VAL:HG23	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1205:FAD:HM81	1:G:11:VAL:HG11	1.97	0.47
4:C:1203:FAD:O4	1:D:45:ARG:NE	2.47	0.46
1:D:42:LYS:HE3	1:D:61:GLU:HG3	1.97	0.46
1:F:60:LEU:HD12	1:F:60:LEU:O	2.16	0.46
1:E:35:HIS:CE1	4:E:1205:FAD:H8A	2.51	0.46
1:E:11:VAL:HG11	4:F:1206:FAD:HM81	1.97	0.46
1:A:8[B]:VAL:HG23	5:B:2142:HOH:O	2.15	0.46
1:E:8[B]:VAL:HG23	5:F:2145:HOH:O	2.14	0.46
1:B:60:LEU:HD12	1:B:60:LEU:O	2.15	0.45
1:F:60:LEU:HD13	1:F:62:VAL:HG23	1.99	0.45
5:A:2144:HOH:O	1:C:8[B]:VAL:HG23	2.17	0.45
1:A:11:VAL:HG11	4:B:1202:FAD:HM81	1.99	0.44
1:E:68:GLU:O	1:E:69:THR:C	2.60	0.44
1:A:60:LEU:HD12	1:A:60:LEU:O	2.17	0.44
1:B:35:HIS:ND1	4:B:1202:FAD:H52A	2.33	0.43
1:E:60:LEU:HD12	1:E:60:LEU:C	2.43	0.43
1:H:60:LEU:CD1	1:H:62:VAL:HG23	2.48	0.43
1:H:8[A]:VAL:HG13	1:H:64:PHE:HE2	1.84	0.43
1:D:60:LEU:C	1:D:60:LEU:HD12	2.43	0.42
1:D:68:GLU:O	1:D:69:THR:OXT	2.36	0.42
1:E:42:LYS:HE3	1:E:61:GLU:CG	2.45	0.42
1:E:69:THR:CB	1:G:31:LYS:HD3	2.44	0.41
1:B:60:LEU:HD12	1:B:60:LEU:C	2.45	0.41
1:A:8[B]:VAL:HG21	5:B:2126:HOH:O	2.20	0.41
1:G:60:LEU:C	1:G:60:LEU:HD12	2.46	0.41
1:C:36:LEU:HD23	1:C:64:PHE:HB3	2.02	0.41
1:H:60:LEU:C	1:H:60:LEU:HD12	2.45	0.41
1:B:16:GLU:HG2	5:B:2173:HOH:O	2.20	0.41
1:E:8[B]:VAL:HG21	5:F:2127:HOH:O	2.21	0.41
1:G:42:LYS:HE3	1:G:61:GLU:CG	2.48	0.40
1:A:60:LEU:HD12	1:A:60:LEU:C	2.46	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	75/69 (109%)	75 (100%)	0	0	100	100
1	B	69/69 (100%)	68 (99%)	1 (1%)	0	100	100
1	C	73/69 (106%)	72 (99%)	1 (1%)	0	100	100
1	D	70/69 (101%)	69 (99%)	1 (1%)	0	100	100
1	E	76/69 (110%)	76 (100%)	0	0	100	100
1	F	70/69 (101%)	69 (99%)	1 (1%)	0	100	100
1	G	73/69 (106%)	70 (96%)	3 (4%)	0	100	100
1	H	69/69 (100%)	68 (99%)	1 (1%)	0	100	100
All	All	575/552 (104%)	567 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	60/55 (109%)	58 (97%)	2 (3%)	33	8
1	B	58/55 (106%)	58 (100%)	0	100	100
1	C	58/55 (106%)	58 (100%)	0	100	100
1	D	58/55 (106%)	58 (100%)	0	100	100
1	E	61/55 (111%)	61 (100%)	0	100	100
1	F	59/55 (107%)	59 (100%)	0	100	100
1	G	58/55 (106%)	58 (100%)	0	100	100
1	H	57/55 (104%)	57 (100%)	0	100	100
All	All	469/440 (107%)	467 (100%)	2 (0%)	81	71

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	35	HIS
1	F	23	GLN
1	H	35	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	FAD	A	1201	-	58,58,58	1.46	7 (12%)	85,89,89	0.82	1 (1%)
4	FAD	C	1203	-	58,58,58	1.46	8 (13%)	85,89,89	0.82	1 (1%)
2	PO4	G	2109	-	4,4,4	1.67	0	6,6,6	0.46	0
4	FAD	H	1208	-	58,58,58	1.47	8 (13%)	85,89,89	0.82	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	D	2106	-	4,4,4	1.62	0	6,6,6	0.46	0
2	PO4	B	2105	-	4,4,4	1.62	1 (25%)	6,6,6	0.44	0
2	PO4	H	2108	-	4,4,4	1.64	0	6,6,6	0.47	0
2	PO4	H	2104	-	4,4,4	3.06	4 (100%)	6,6,6	0.47	0
4	FAD	E	1205	-	58,58,58	1.46	8 (13%)	85,89,89	0.81	1 (1%)
4	FAD	B	1202	-	58,58,58	1.52	9 (15%)	85,89,89	0.82	1 (1%)
4	FAD	D	1204	-	58,58,58	1.49	9 (15%)	85,89,89	0.81	1 (1%)
2	PO4	A	2101	-	4,4,4	1.72	1 (25%)	6,6,6	0.45	0
2	PO4	E	2103	-	4,4,4	1.73	1 (25%)	6,6,6	0.48	0
4	FAD	G	1207	-	58,58,58	1.46	7 (12%)	85,89,89	0.82	1 (1%)
2	PO4	D	2102	-	4,4,4	3.01	4 (100%)	6,6,6	0.47	0
2	PO4	F	2107	-	4,4,4	1.66	1 (25%)	6,6,6	0.47	0
4	FAD	F	1206	-	58,58,58	1.50	9 (15%)	85,89,89	0.82	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
4	FAD	A	1201	-	-	7/34/50/50	0/6/6/6
4	FAD	C	1203	-	-	8/34/50/50	0/6/6/6
4	FAD	H	1208	-	-	7/34/50/50	0/6/6/6
4	FAD	E	1205	-	-	6/34/50/50	0/6/6/6
4	FAD	B	1202	-	-	8/34/50/50	0/6/6/6
4	FAD	D	1204	-	-	7/34/50/50	0/6/6/6
4	FAD	G	1207	-	-	8/34/50/50	0/6/6/6
4	FAD	F	1206	-	-	6/34/50/50	0/6/6/6

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1201	FAD	C4X-N5	5.55	1.42	1.30
4	C	1203	FAD	C4X-N5	5.53	1.42	1.30
4	G	1207	FAD	C4X-N5	5.50	1.42	1.30
4	F	1206	FAD	C4X-N5	5.50	1.42	1.30
4	B	1202	FAD	C4X-N5	5.47	1.42	1.30
4	E	1205	FAD	C4X-N5	5.44	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1208	FAD	C4X-N5	5.33	1.42	1.30
4	D	1204	FAD	C4X-N5	5.31	1.42	1.30
2	H	2104	PO4	P-O1	4.69	1.61	1.50
2	D	2102	PO4	P-O1	4.64	1.61	1.50
4	D	1204	FAD	C9-C8	4.09	1.45	1.39
4	B	1202	FAD	C9-C8	4.02	1.45	1.39
4	H	1208	FAD	C9-C8	4.01	1.45	1.39
4	F	1206	FAD	C9-C8	3.89	1.44	1.39
4	G	1207	FAD	C9-C8	3.79	1.44	1.39
4	A	1201	FAD	C9-C8	3.75	1.44	1.39
4	E	1205	FAD	C9-C8	3.73	1.44	1.39
4	C	1203	FAD	C9-C8	3.72	1.44	1.39
4	D	1204	FAD	C4A-N3A	3.59	1.41	1.34
4	B	1202	FAD	C4A-N3A	3.58	1.41	1.34
4	F	1206	FAD	C4A-N3A	3.56	1.41	1.34
4	A	1201	FAD	C4A-N3A	3.55	1.41	1.34
4	H	1208	FAD	C4A-N3A	3.47	1.40	1.34
4	C	1203	FAD	C4A-N3A	3.47	1.40	1.34
4	E	1205	FAD	C4A-N3A	3.46	1.40	1.34
4	G	1207	FAD	C4A-N3A	3.42	1.40	1.34
4	D	1204	FAD	C9A-N10	3.23	1.46	1.41
4	F	1206	FAD	C9A-C5X	3.12	1.46	1.41
4	A	1201	FAD	C9A-C5X	3.10	1.46	1.41
4	B	1202	FAD	C9A-C5X	3.04	1.46	1.41
4	H	1208	FAD	C9A-C5X	3.04	1.46	1.41
4	E	1205	FAD	C9A-C5X	3.04	1.46	1.41
4	G	1207	FAD	C9A-N10	3.03	1.46	1.41
4	D	1204	FAD	C9A-C5X	3.03	1.46	1.41
4	H	1208	FAD	C9A-N10	3.00	1.46	1.41
4	E	1205	FAD	C9A-N10	2.99	1.46	1.41
4	B	1202	FAD	C9A-N10	2.98	1.46	1.41
4	A	1201	FAD	C9A-N10	2.96	1.46	1.41
4	C	1203	FAD	C9A-N10	2.95	1.46	1.41
4	G	1207	FAD	C9A-C5X	2.93	1.45	1.41
4	F	1206	FAD	C9A-N10	2.92	1.46	1.41
4	C	1203	FAD	C9A-C5X	2.89	1.45	1.41
4	D	1204	FAD	C6-C5X	2.68	1.44	1.40
4	C	1203	FAD	C6-C5X	2.65	1.44	1.40
4	H	1208	FAD	C6-C5X	2.65	1.44	1.40
4	E	1205	FAD	C6-C5X	2.62	1.44	1.40
4	G	1207	FAD	C10-N1	2.62	1.38	1.33
4	G	1207	FAD	C6-C5X	2.61	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1201	FAD	C6-C5X	2.60	1.43	1.40
4	B	1202	FAD	C6-C5X	2.58	1.43	1.40
4	C	1203	FAD	C10-N1	2.56	1.38	1.33
4	F	1206	FAD	C6-C5X	2.55	1.43	1.40
4	A	1201	FAD	C10-N1	2.54	1.38	1.33
4	D	1204	FAD	C10-N1	2.54	1.38	1.33
4	B	1202	FAD	C10-N1	2.52	1.38	1.33
4	F	1206	FAD	P-O3P	2.51	1.62	1.59
4	E	1205	FAD	C10-N1	2.47	1.38	1.33
4	H	1208	FAD	C10-N1	2.45	1.38	1.33
4	B	1202	FAD	P-O3P	2.45	1.62	1.59
4	F	1206	FAD	C10-N1	2.43	1.38	1.33
2	H	2104	PO4	P-O2	2.31	1.61	1.54
2	H	2104	PO4	P-O3	2.30	1.61	1.54
2	D	2102	PO4	P-O2	2.27	1.61	1.54
2	D	2102	PO4	P-O3	2.26	1.61	1.54
4	E	1205	FAD	P-O3P	2.25	1.61	1.59
4	H	1208	FAD	P-O3P	2.22	1.61	1.59
2	H	2104	PO4	P-O4	-2.17	1.48	1.54
4	B	1202	FAD	PA-O3P	2.15	1.61	1.59
4	C	1203	FAD	P-O3P	2.13	1.61	1.59
2	D	2102	PO4	P-O4	-2.13	1.48	1.54
2	E	2103	PO4	P-O3	-2.08	1.48	1.54
2	A	2101	PO4	P-O2	-2.08	1.48	1.54
4	D	1204	FAD	C2A-N1A	2.05	1.37	1.33
2	B	2105	PO4	P-O2	-2.04	1.48	1.54
4	D	1204	FAD	P-O3P	2.02	1.61	1.59
2	F	2107	PO4	P-O3	-2.01	1.48	1.54
4	F	1206	FAD	PA-O3P	2.01	1.61	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1206	FAD	C4X-C10-N10	2.63	120.24	116.48
4	B	1202	FAD	C4X-C10-N10	2.61	120.22	116.48
4	A	1201	FAD	C4X-C10-N10	2.59	120.19	116.48
4	E	1205	FAD	C4X-C10-N10	2.57	120.16	116.48
4	H	1208	FAD	C4X-C10-N10	2.55	120.14	116.48
4	G	1207	FAD	C4X-C10-N10	2.54	120.12	116.48
4	D	1204	FAD	C4X-C10-N10	2.54	120.12	116.48
4	C	1203	FAD	C4X-C10-N10	2.54	120.11	116.48

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1201	FAD	C4B-C5B-O5B-PA
4	B	1202	FAD	C5B-O5B-PA-O2A
4	B	1202	FAD	C5B-O5B-PA-O3P
4	B	1202	FAD	C4B-C5B-O5B-PA
4	B	1202	FAD	C3B-C4B-C5B-O5B
4	C	1203	FAD	C5B-O5B-PA-O2A
4	C	1203	FAD	C4B-C5B-O5B-PA
4	C	1203	FAD	C3B-C4B-C5B-O5B
4	D	1204	FAD	P-O3P-PA-O5B
4	E	1205	FAD	C4B-C5B-O5B-PA
4	E	1205	FAD	C3B-C4B-C5B-O5B
4	F	1206	FAD	C4B-C5B-O5B-PA
4	G	1207	FAD	C5B-O5B-PA-O2A
4	G	1207	FAD	C5B-O5B-PA-O3P
4	G	1207	FAD	C4B-C5B-O5B-PA
4	G	1207	FAD	C3B-C4B-C5B-O5B
4	H	1208	FAD	C4B-C5B-O5B-PA
4	A	1201	FAD	C3B-C4B-C5B-O5B
4	D	1204	FAD	C3B-C4B-C5B-O5B
4	F	1206	FAD	C3B-C4B-C5B-O5B
4	H	1208	FAD	C3B-C4B-C5B-O5B
4	B	1202	FAD	O4B-C4B-C5B-O5B
4	C	1203	FAD	O4B-C4B-C5B-O5B
4	D	1204	FAD	O4B-C4B-C5B-O5B
4	E	1205	FAD	O4B-C4B-C5B-O5B
4	G	1207	FAD	O4B-C4B-C5B-O5B
4	F	1206	FAD	O4B-C4B-C5B-O5B
4	A	1201	FAD	O4B-C4B-C5B-O5B
4	H	1208	FAD	O4B-C4B-C5B-O5B
4	D	1204	FAD	C4B-C5B-O5B-PA
4	F	1206	FAD	PA-O3P-P-O1P
4	A	1201	FAD	PA-O3P-P-O2P
4	B	1202	FAD	PA-O3P-P-O2P
4	C	1203	FAD	PA-O3P-P-O2P
4	E	1205	FAD	PA-O3P-P-O2P
4	G	1207	FAD	PA-O3P-P-O2P
4	H	1208	FAD	PA-O3P-P-O2P
4	A	1201	FAD	C5'-O5'-P-O1P
4	B	1202	FAD	C5'-O5'-P-O1P
4	C	1203	FAD	C5B-O5B-PA-O3P

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Mol	Chain	Res	Type	Atoms
4	C	1203	FAD	C5'-O5'-P-O1P
4	D	1204	FAD	C5'-O5'-P-O1P
4	E	1205	FAD	C5'-O5'-P-O1P
4	F	1206	FAD	C5'-O5'-P-O1P
4	G	1207	FAD	C5'-O5'-P-O1P
4	H	1208	FAD	C5'-O5'-P-O1P
4	F	1206	FAD	PA-O3P-P-O2P
4	A	1201	FAD	C2B-C1B-N9A-C8A
4	D	1204	FAD	PA-O3P-P-O2P
4	A	1201	FAD	PA-O3P-P-O1P
4	B	1202	FAD	PA-O3P-P-O1P
4	C	1203	FAD	PA-O3P-P-O1P
4	E	1205	FAD	PA-O3P-P-O1P
4	G	1207	FAD	PA-O3P-P-O1P
4	H	1208	FAD	C2B-C1B-N9A-C8A
4	D	1204	FAD	PA-O3P-P-O1P
4	H	1208	FAD	PA-O3P-P-O1P

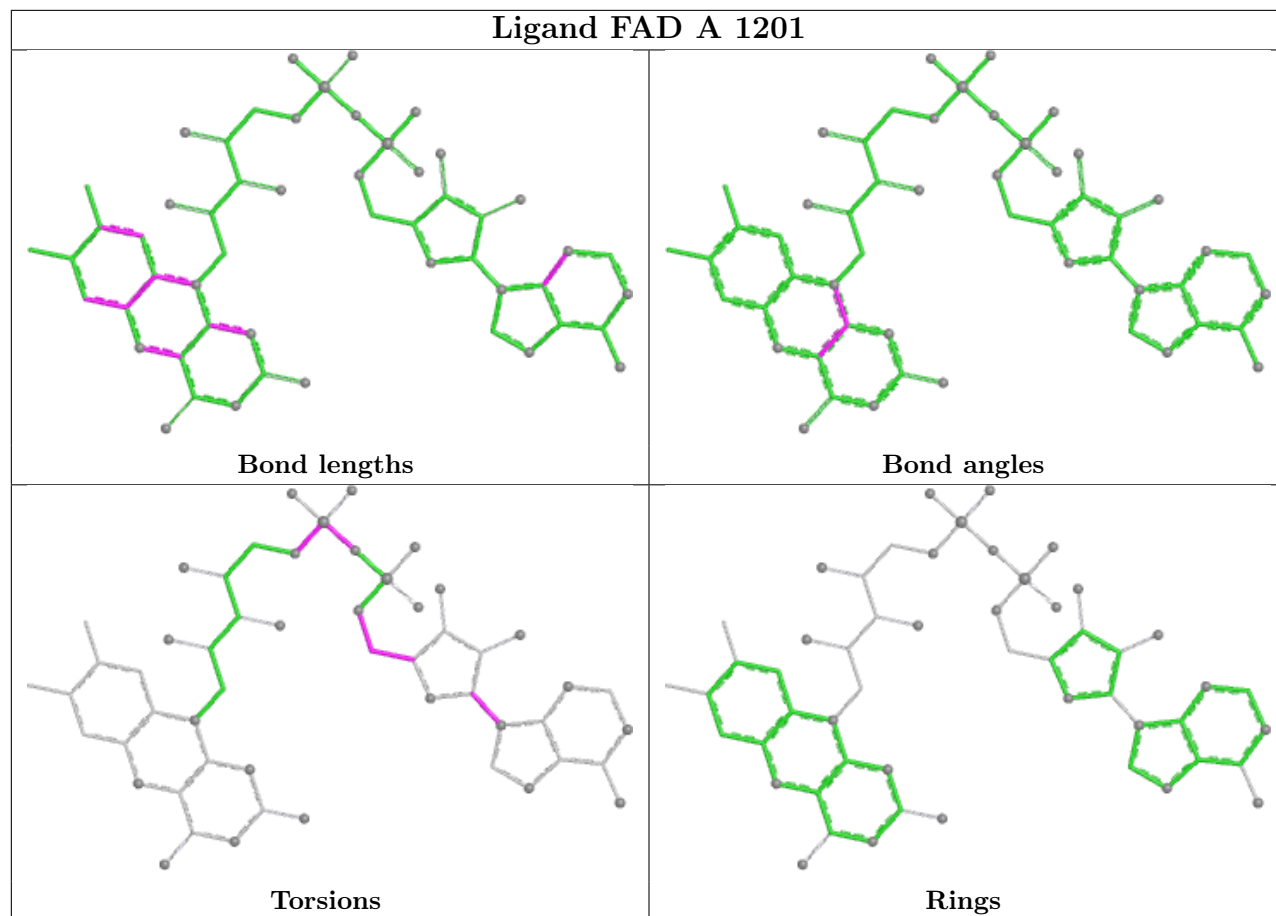
There are no ring outliers.

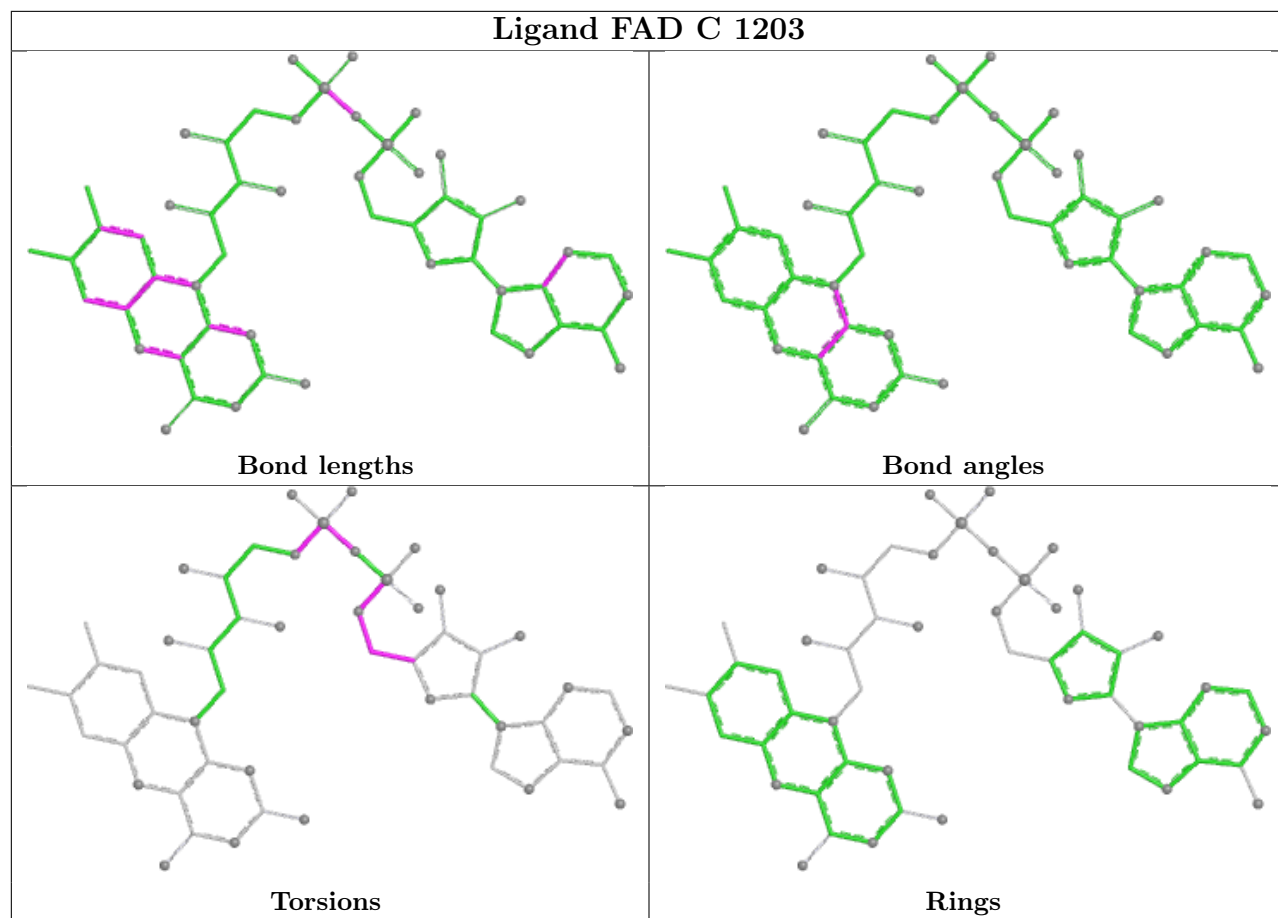
8 monomers are involved in 22 short contacts:

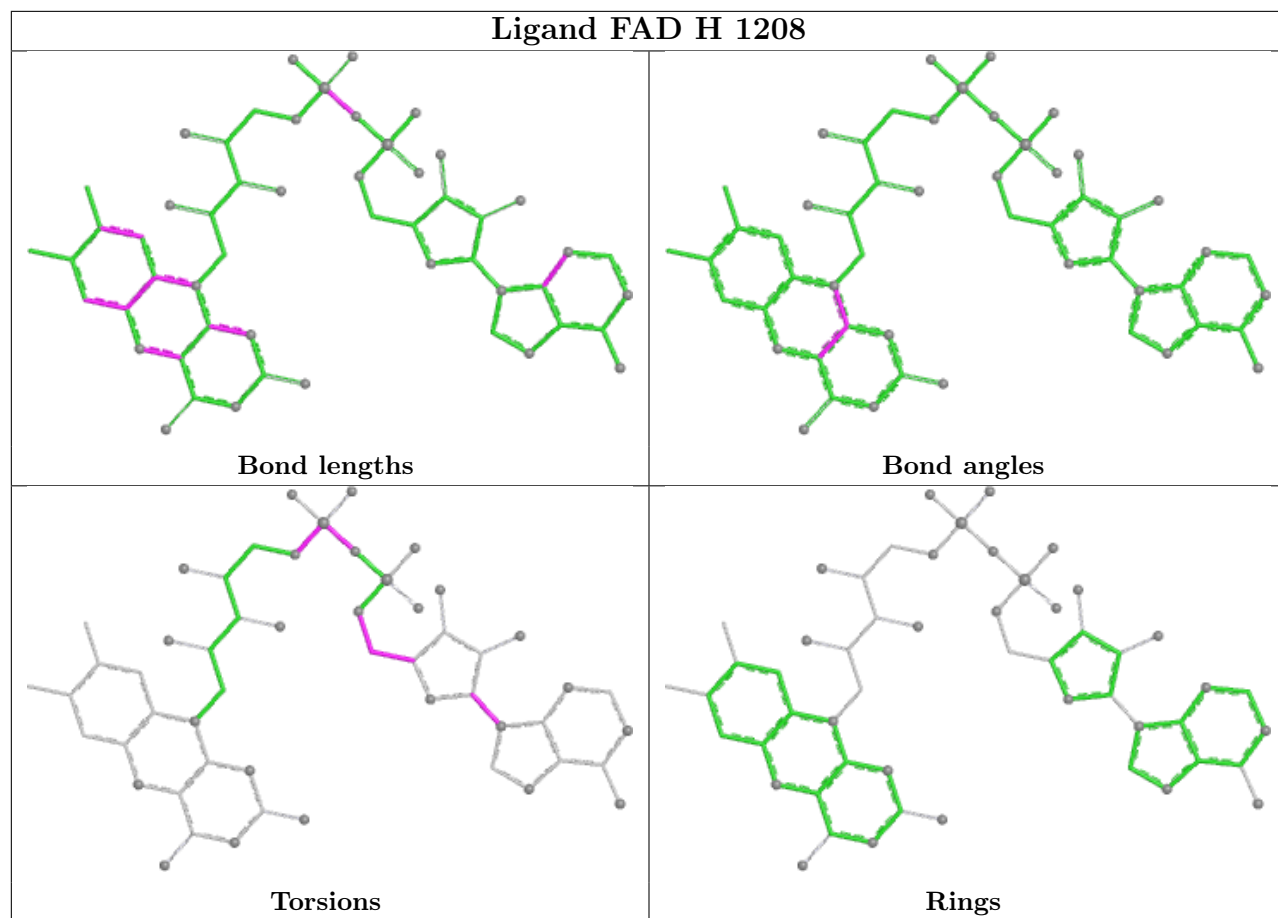
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1201	FAD	3	0
4	C	1203	FAD	4	0
4	H	1208	FAD	2	0
4	E	1205	FAD	3	0
4	B	1202	FAD	3	0
4	D	1204	FAD	2	0
4	G	1207	FAD	4	0
4	F	1206	FAD	1	0

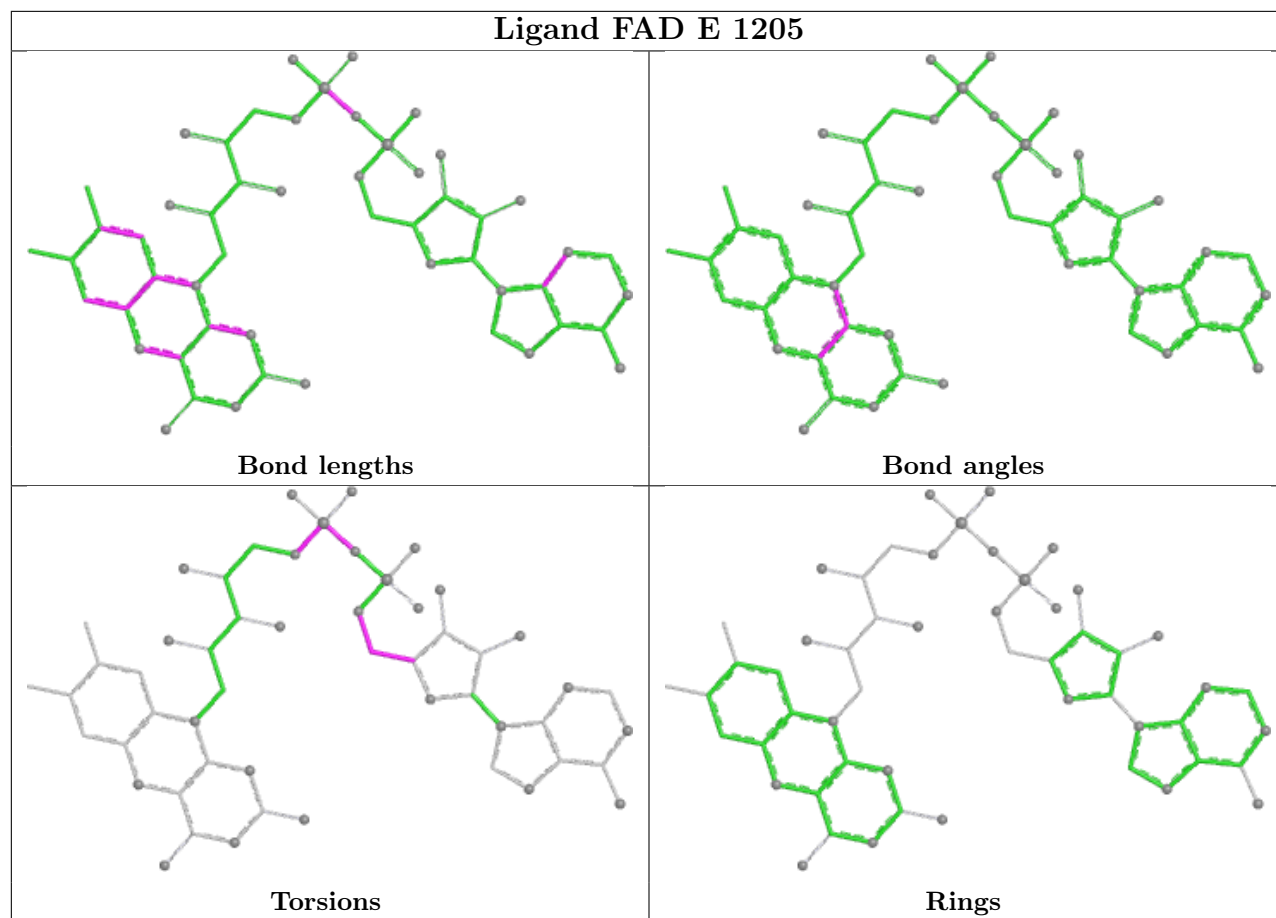
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

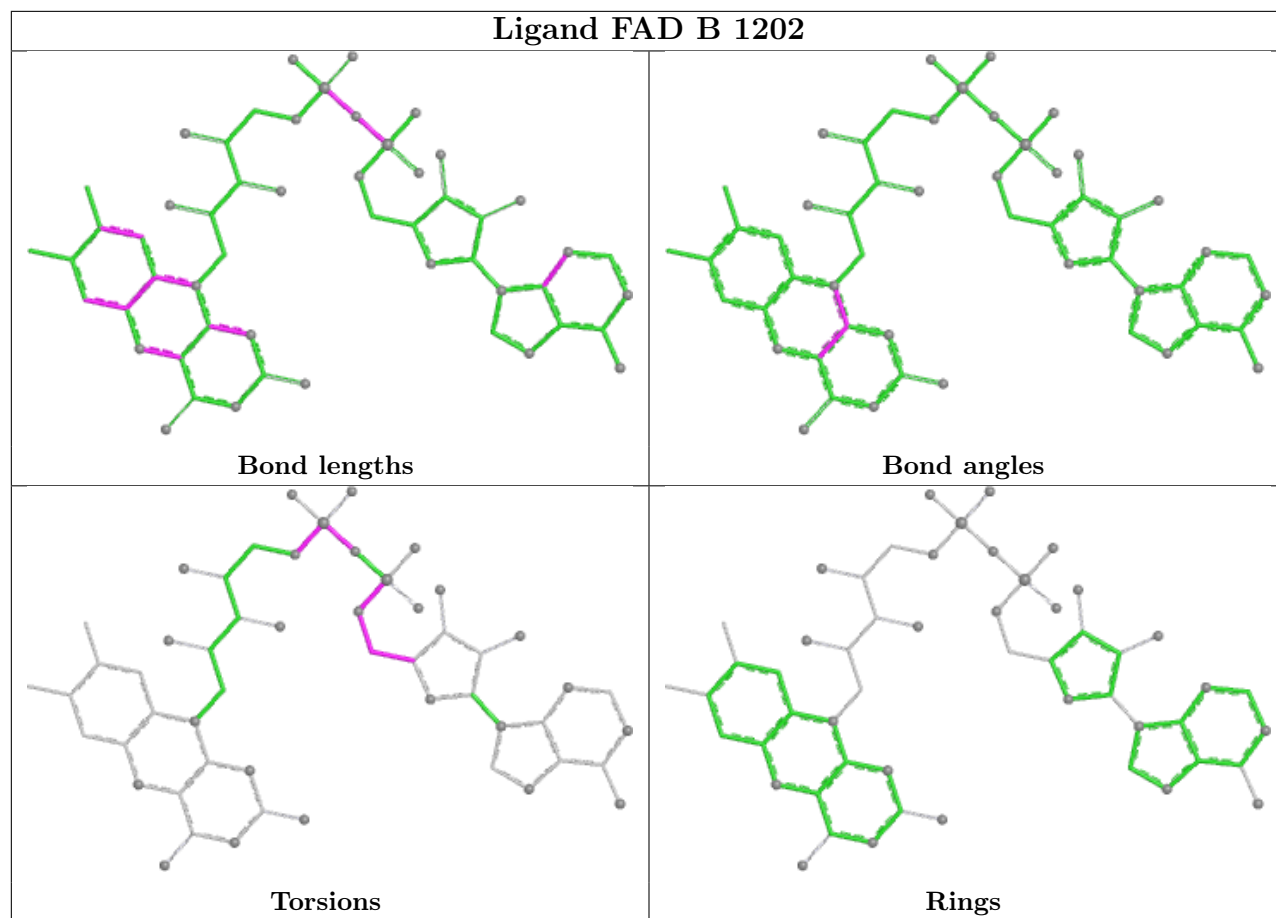
equivalents in the CSD to analyse the geometry.

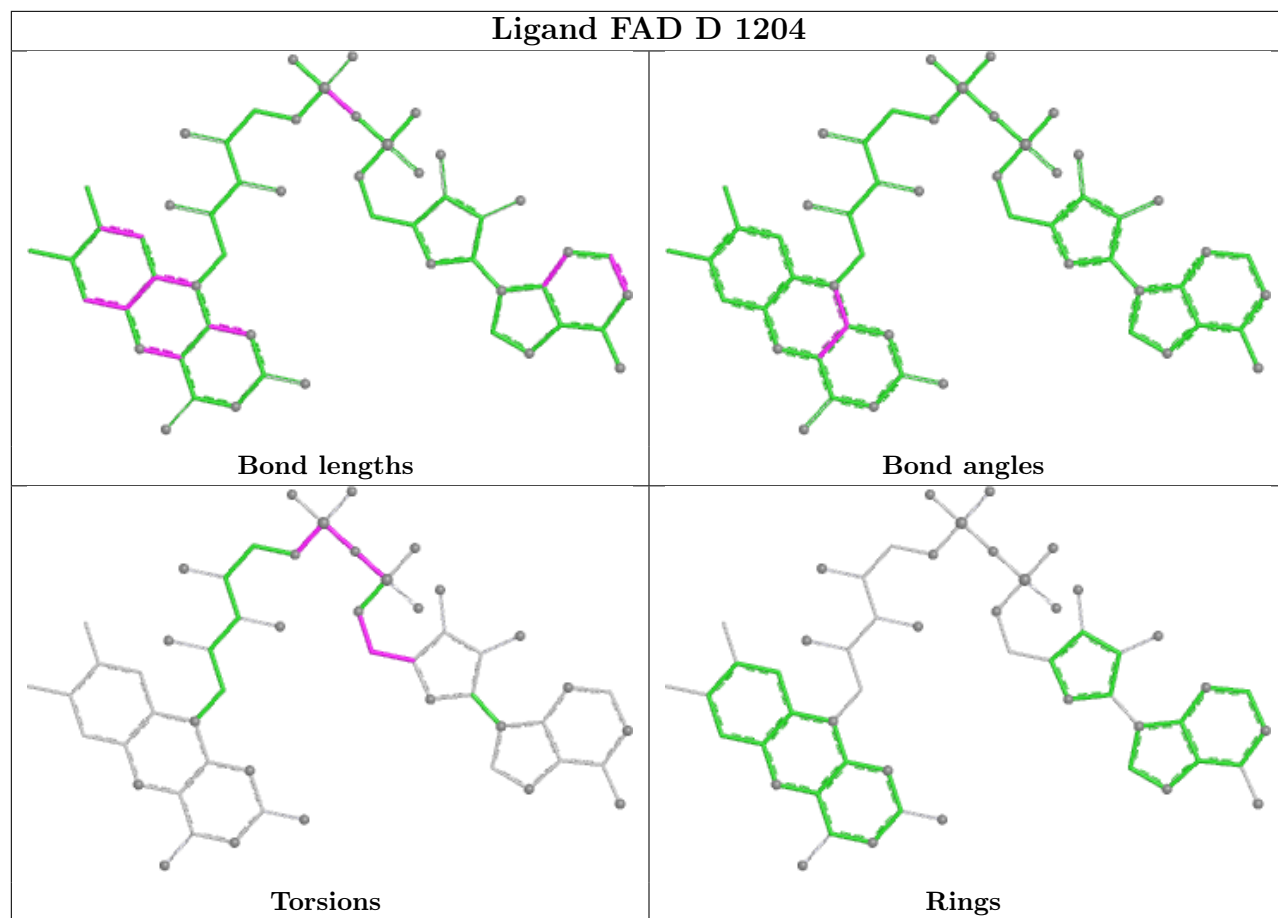


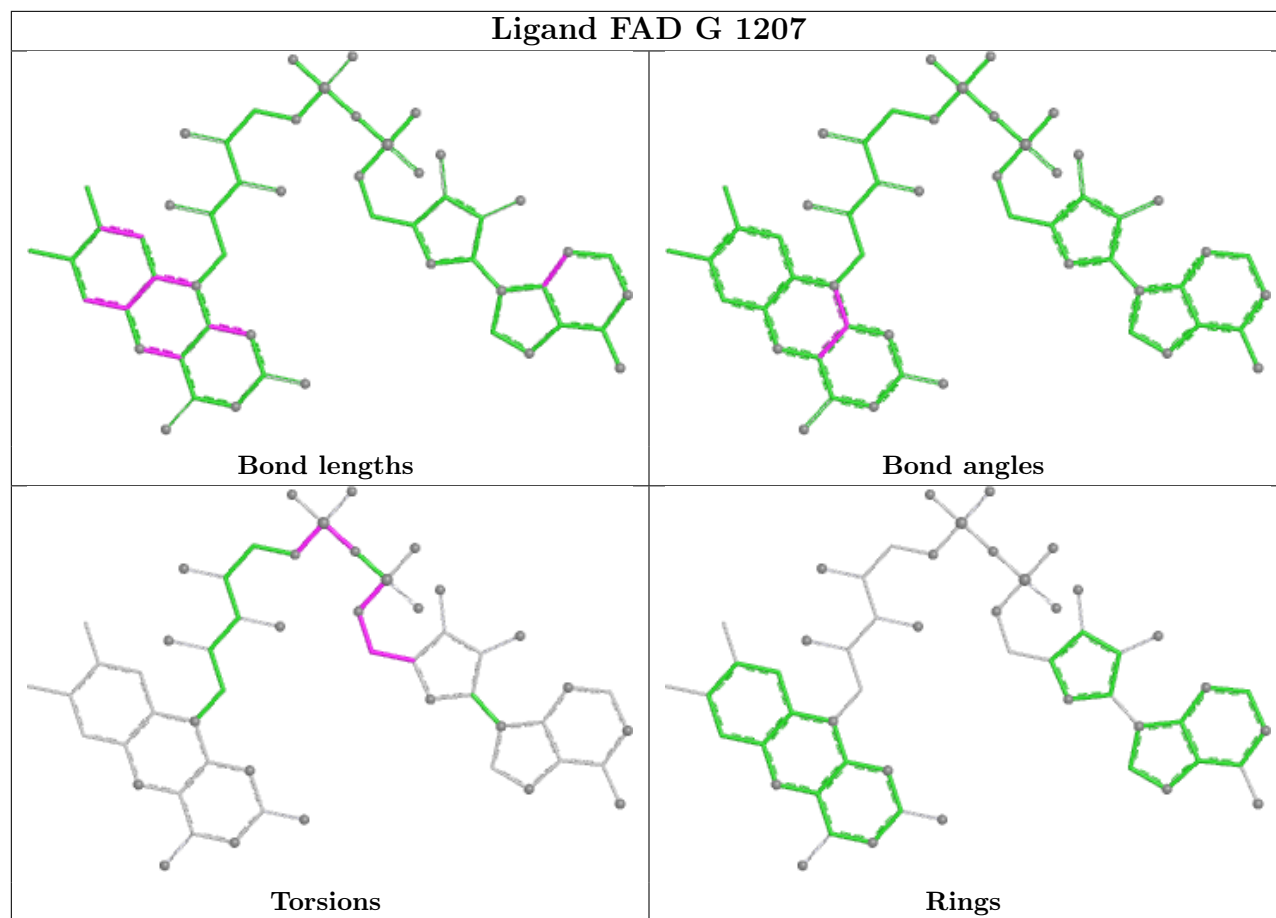


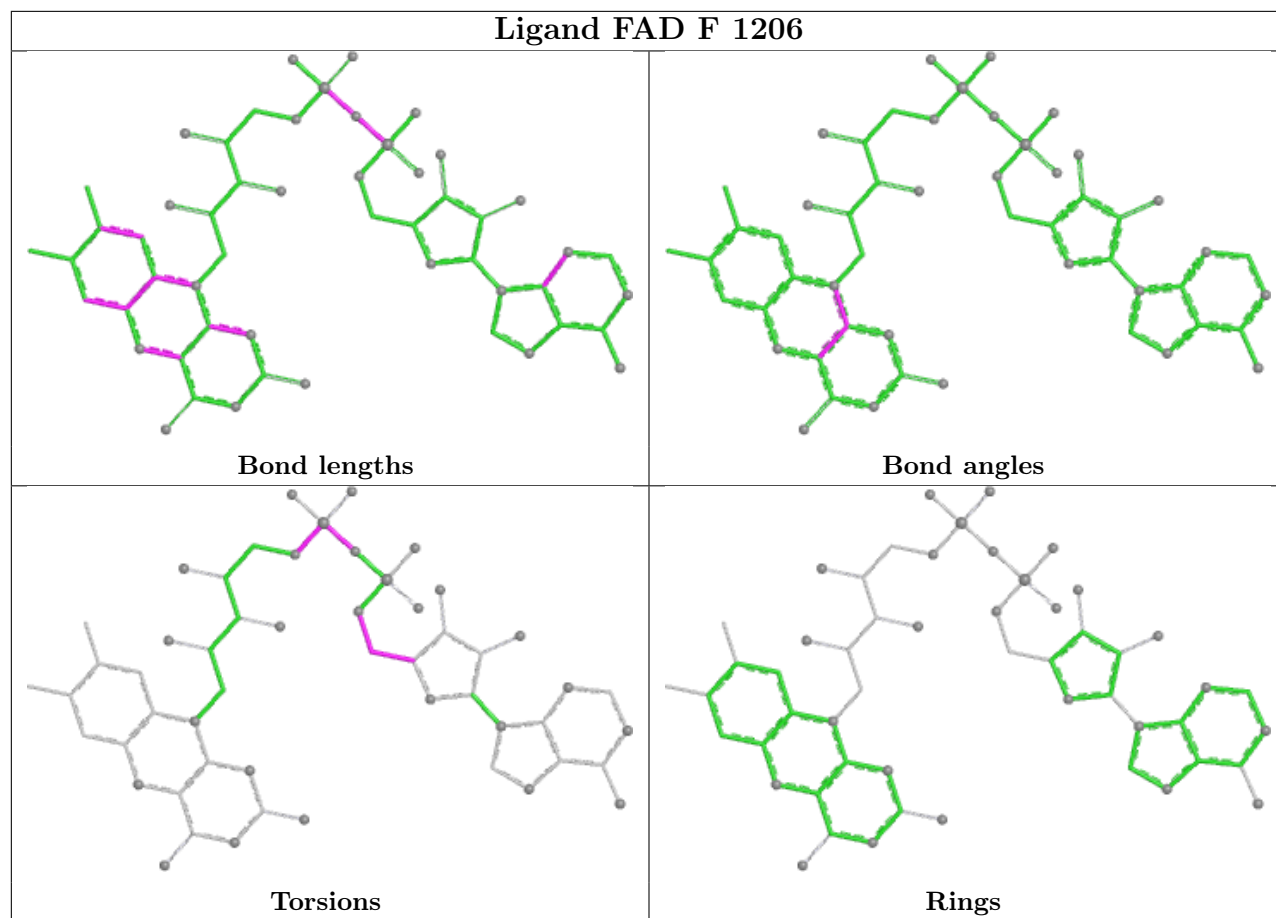












5.7 Other polymers [i](#)

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	67/69 (97%)	-1.00	0 100 100	8, 13, 26, 41	10 (14%)
1	B	66/69 (95%)	-1.05	0 100 100	9, 14, 26, 42	5 (7%)
1	C	67/69 (97%)	-1.01	0 100 100	8, 13, 21, 30	8 (11%)
1	D	68/69 (98%)	-1.06	0 100 100	9, 14, 26, 41	4 (5%)
1	E	68/69 (98%)	-0.98	0 100 100	8, 13, 26, 47	10 (14%)
1	F	66/69 (95%)	-1.06	0 100 100	9, 13, 25, 43	6 (9%)
1	G	67/69 (97%)	-0.99	0 100 100	8, 13, 23, 31	8 (11%)
1	H	68/69 (98%)	-1.01	0 100 100	9, 14, 28, 39	3 (4%)
All	All	537/552 (97%)	-1.02	0 100 100	8, 13, 26, 47	54 (10%)

There are no RSRZ outliers to report.

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](#)

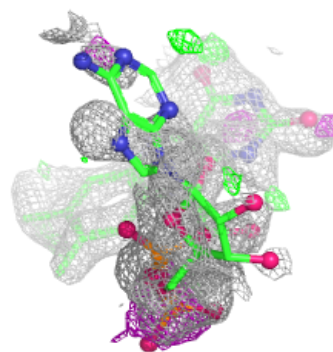
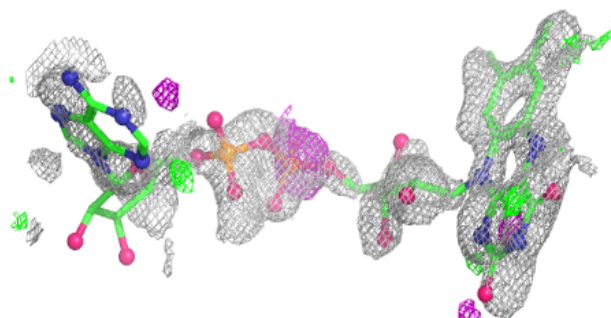
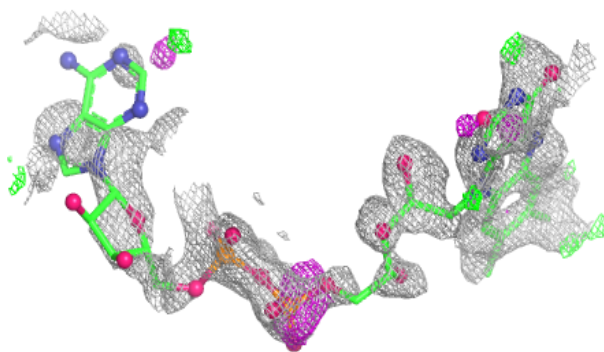
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	FAD	A	1201	53/53	0.95	0.09	34,39,56,56	0
4	FAD	C	1203	53/53	0.95	0.09	24,35,54,55	0
4	FAD	E	1205	53/53	0.95	0.10	34,40,58,58	0
4	FAD	D	1204	53/53	0.96	0.09	24,34,54,54	0
4	FAD	B	1202	53/53	0.96	0.08	29,40,55,56	0
4	FAD	G	1207	53/53	0.96	0.09	25,35,54,55	0
4	FAD	H	1208	53/53	0.96	0.09	23,35,54,55	0
2	PO4	G	2109	5/5	0.97	0.08	27,30,30,31	0
4	FAD	F	1206	53/53	0.97	0.08	28,41,53,54	0
2	PO4	A	2101	5/5	0.98	0.05	24,29,30,31	0
2	PO4	D	2102	5/5	0.98	0.04	38,38,38,38	5
2	PO4	E	2103	5/5	0.98	0.05	25,29,30,31	0
2	PO4	H	2108	5/5	0.99	0.06	18,18,20,20	0
3	K	G	1153	1/1	0.99	0.06	30,30,30,30	0
2	PO4	F	2107	5/5	0.99	0.07	19,19,20,21	0
2	PO4	B	2105	5/5	0.99	0.09	18,19,19,21	0
2	PO4	H	2104	5/5	0.99	0.03	31,31,32,32	5
3	K	A	1150	1/1	1.00	0.09	11,11,11,11	1
3	K	C	1151	1/1	1.00	0.11	29,29,29,29	0
3	K	E	1152	1/1	1.00	0.10	10,10,10,10	1
2	PO4	D	2106	5/5	1.00	0.04	18,18,21,21	0

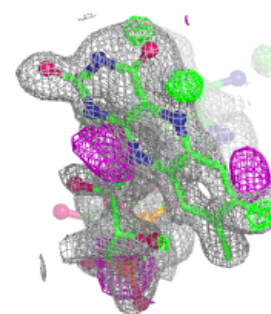
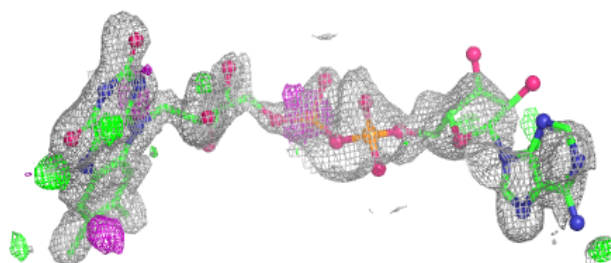
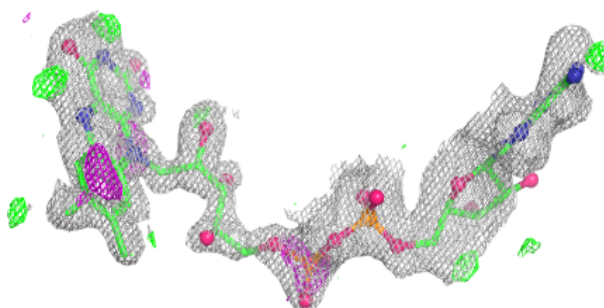
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 1201:

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

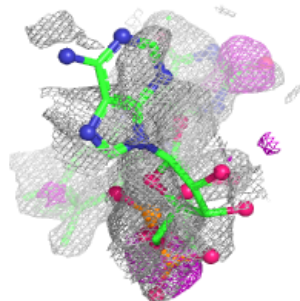
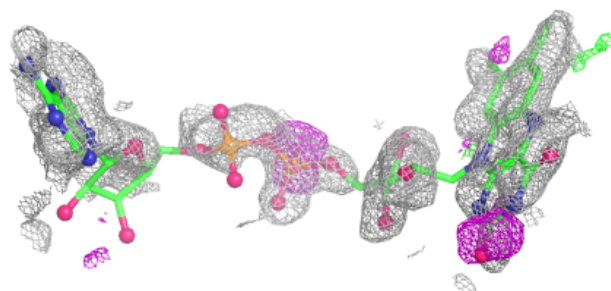
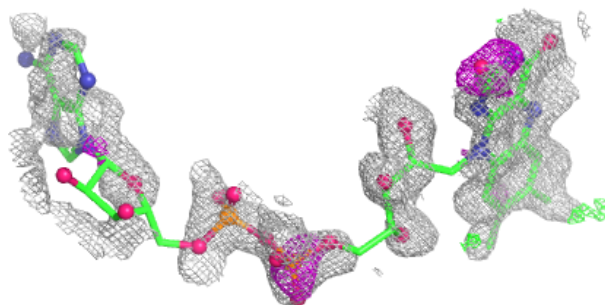
**Electron density around FAD C 1203:**

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

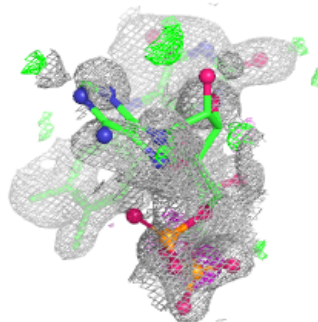
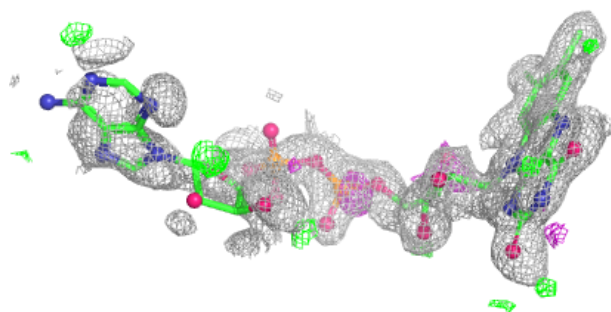
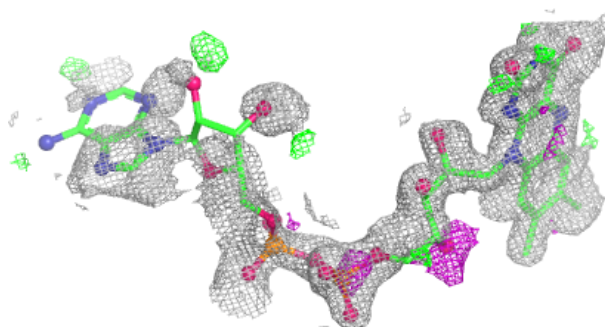


Electron density around FAD E 1205:

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

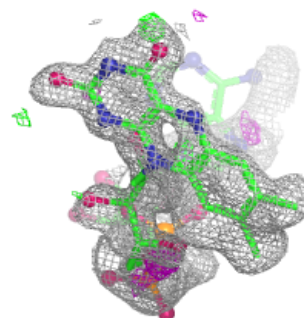
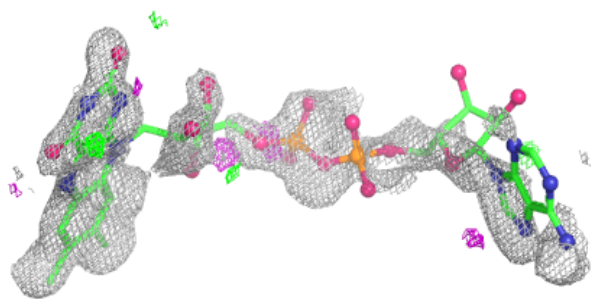
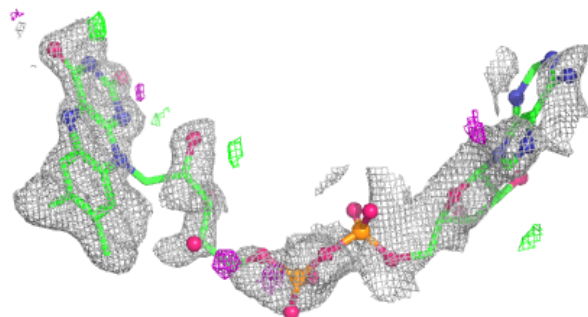
**Electron density around FAD D 1204:**

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

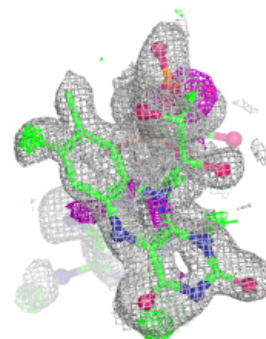
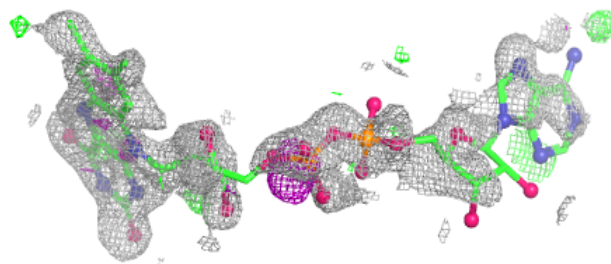
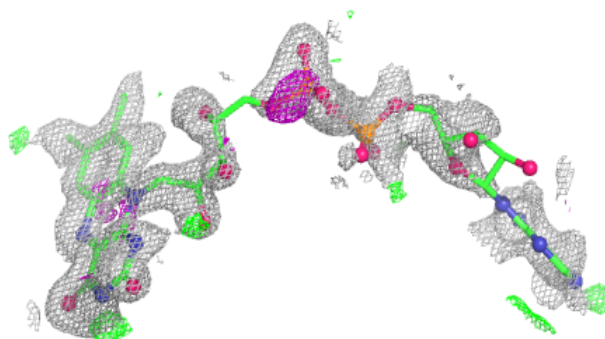


Electron density around FAD B 1202:

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

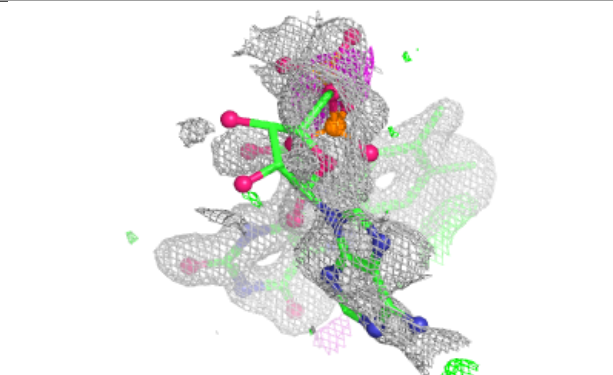
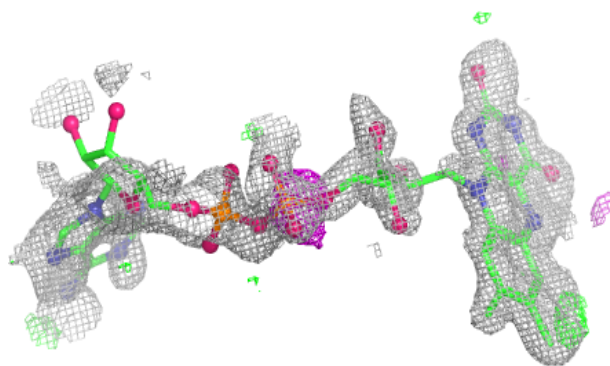
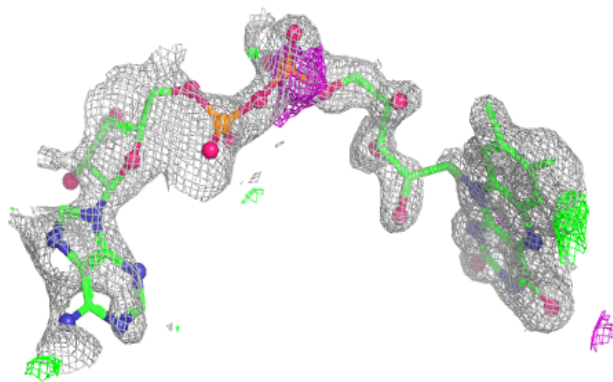
**Electron density around FAD G 1207:**

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

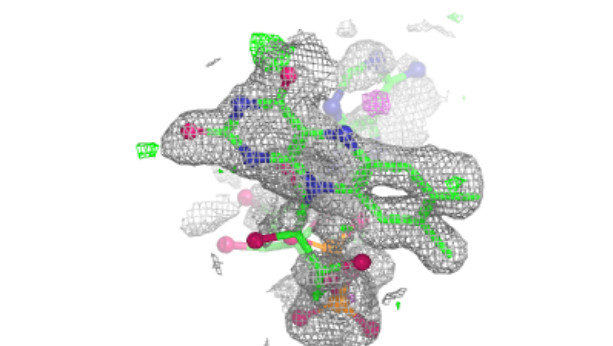
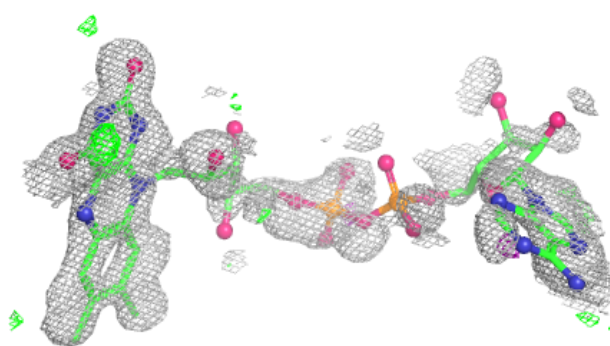
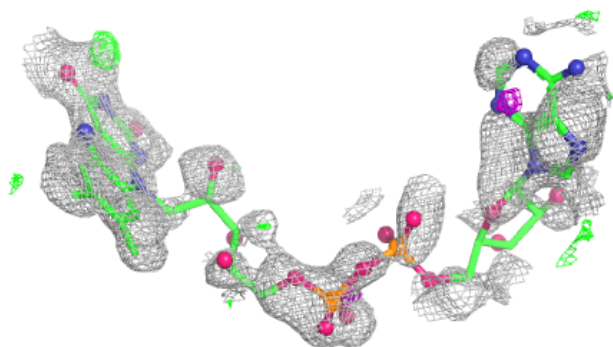


Electron density around FAD H 1208:

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

**Electron density around FAD F 1206:**

$2mF_o-DF_c$ (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.