



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:52 PM UTC

PDB ID : 1O2A / pdb_00001o2a
Title : Crystal structure of Thymidylate Synthase Complementing Protein (TM0449)
from *Thermotoga maritima* with FAD at 1.8 Å resolution
Authors : Mathews, I.I.; Deacon, A.M.; Canaves, J.M.; McMullan, D.; Lesley, S.A.;
Agarwalla, S.; Kuhn, P.; Joint Center for Structural Genomics (JCSG)
Deposited on : 2003-02-18
Resolution : 1.80 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

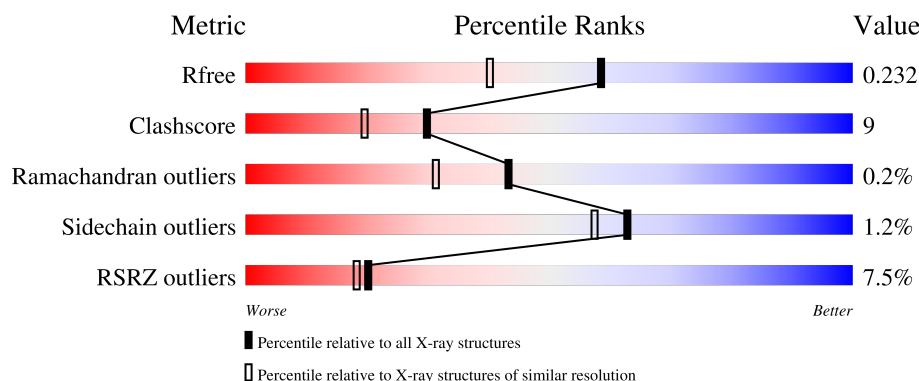
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	232	6% 72% 19% • 9%
1	B	232	7% 74% 17% • 8%
1	C	232	6% 77% 14% • 8%
1	D	232	9% 71% 20% • 8%

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	FAD	A	715	X	-	-	-
2	FAD	B	710	X	-	-	-
2	FAD	C	705	X	-	-	-
2	FAD	D	700	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7668 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 Thymidylate synthase thyX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1764	1148	304	307	5			
1	B	214	Total	C	N	O	S	0	0	0
			1786	1164	307	310	5			
1	C	214	Total	C	N	O	S	0	0	0
			1783	1157	306	315	5			
1	D	213	Total	C	N	O	S	0	5	0
			1815	1179	312	319	5			

There are 48 discrepancies between the modelled and reference sequences:

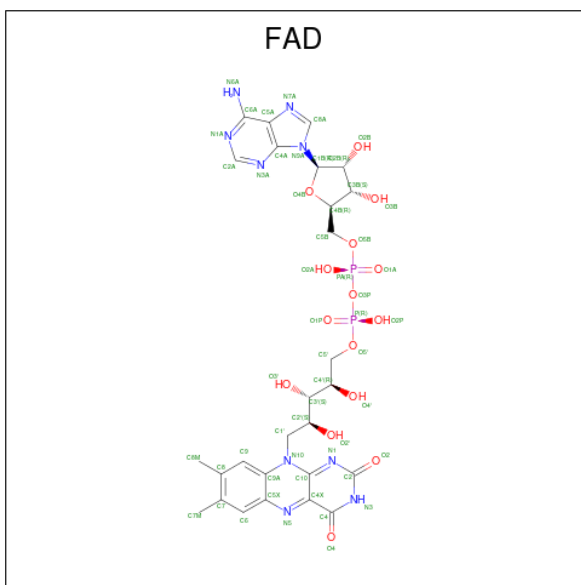
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9WYT0
A	-10	GLY	-	expression tag	UNP Q9WYT0
A	-9	SER	-	expression tag	UNP Q9WYT0
A	-8	ASP	-	expression tag	UNP Q9WYT0
A	-7	LYS	-	expression tag	UNP Q9WYT0
A	-6	ILE	-	expression tag	UNP Q9WYT0
A	-5	HIS	-	expression tag	UNP Q9WYT0
A	-4	HIS	-	expression tag	UNP Q9WYT0
A	-3	HIS	-	expression tag	UNP Q9WYT0
A	-2	HIS	-	expression tag	UNP Q9WYT0
A	-1	HIS	-	expression tag	UNP Q9WYT0
A	0	HIS	-	expression tag	UNP Q9WYT0
B	-11	MET	-	expression tag	UNP Q9WYT0
B	-10	GLY	-	expression tag	UNP Q9WYT0
B	-9	SER	-	expression tag	UNP Q9WYT0
B	-8	ASP	-	expression tag	UNP Q9WYT0
B	-7	LYS	-	expression tag	UNP Q9WYT0
B	-6	ILE	-	expression tag	UNP Q9WYT0
B	-5	HIS	-	expression tag	UNP Q9WYT0
B	-4	HIS	-	expression tag	UNP Q9WYT0
B	-3	HIS	-	expression tag	UNP Q9WYT0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q9WYT0
B	-1	HIS	-	expression tag	UNP Q9WYT0
B	0	HIS	-	expression tag	UNP Q9WYT0
C	-11	MET	-	expression tag	UNP Q9WYT0
C	-10	GLY	-	expression tag	UNP Q9WYT0
C	-9	SER	-	expression tag	UNP Q9WYT0
C	-8	ASP	-	expression tag	UNP Q9WYT0
C	-7	LYS	-	expression tag	UNP Q9WYT0
C	-6	ILE	-	expression tag	UNP Q9WYT0
C	-5	HIS	-	expression tag	UNP Q9WYT0
C	-4	HIS	-	expression tag	UNP Q9WYT0
C	-3	HIS	-	expression tag	UNP Q9WYT0
C	-2	HIS	-	expression tag	UNP Q9WYT0
C	-1	HIS	-	expression tag	UNP Q9WYT0
C	0	HIS	-	expression tag	UNP Q9WYT0
D	-11	MET	-	expression tag	UNP Q9WYT0
D	-10	GLY	-	expression tag	UNP Q9WYT0
D	-9	SER	-	expression tag	UNP Q9WYT0
D	-8	ASP	-	expression tag	UNP Q9WYT0
D	-7	LYS	-	expression tag	UNP Q9WYT0
D	-6	ILE	-	expression tag	UNP Q9WYT0
D	-5	HIS	-	expression tag	UNP Q9WYT0
D	-4	HIS	-	expression tag	UNP Q9WYT0
D	-3	HIS	-	expression tag	UNP Q9WYT0
D	-2	HIS	-	expression tag	UNP Q9WYT0
D	-1	HIS	-	expression tag	UNP Q9WYT0
D	0	HIS	-	expression tag	UNP Q9WYT0

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

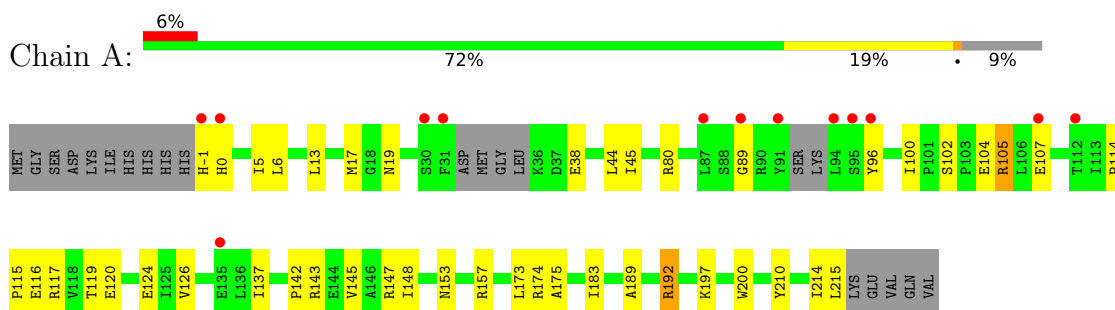
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	82	Total O 82 82	0	0
3	B	80	Total O 80 80	0	0
3	C	72	Total O 72 72	0	0
3	D	74	Total O 74 74	0	0

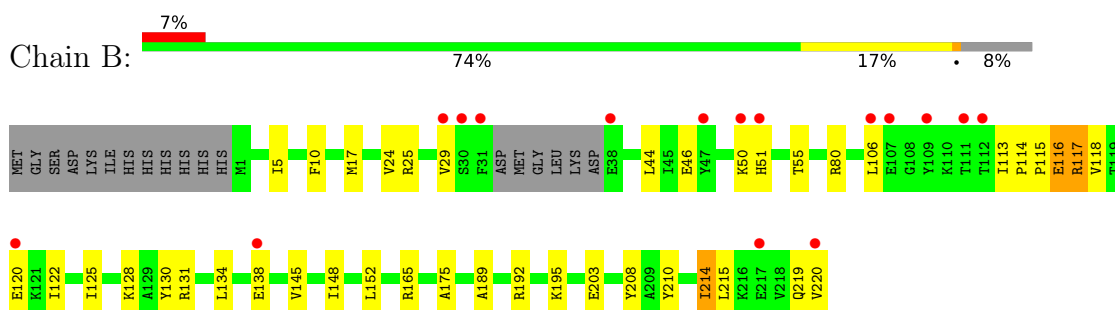
3 Residue-property plots [i](#)

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.

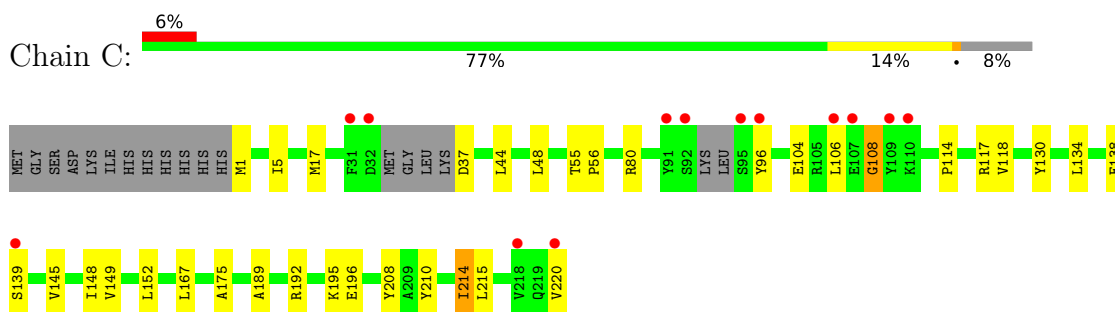
- Molecule 1: Thymidylate synthase thyX



- Molecule 1: Thymidylate synthase thyX

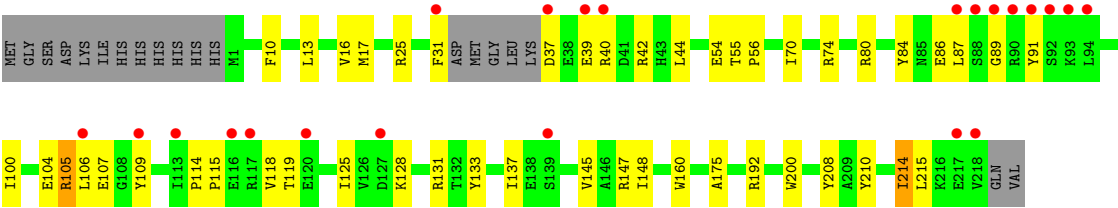


- Molecule 1: Thymidylate synthase thyX



- Molecule 1: Thymidylate synthase thyX





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.50Å 116.95Å 141.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.7 (20.00-1.80) 92.1 (20.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 1.71Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.230 0.204 , 0.232	Depositor DCC
R_{free} test set	4408 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7668	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.34	0/1812	0.83	1/2448 (0.0%)
1	B	0.35	0/1834	0.85	3/2478 (0.1%)
1	C	0.35	0/1829	0.84	3/2470 (0.1%)
1	D	0.34	0/1863	0.83	3/2519 (0.1%)
All	All	0.35	0/7338	0.83	10/9915 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	214	ILE	N-CA-C	8.77	119.56	110.62
1	B	214	ILE	N-CA-C	6.63	118.18	110.62
1	B	80	ARG	N-CA-C	6.48	119.33	111.82
1	D	80	ARG	N-CA-C	6.39	119.23	111.82
1	B	208	TYR	N-CA-C	6.00	121.26	113.88
1	C	208	TYR	N-CA-C	5.62	121.01	114.04
1	D	208	TYR	N-CA-C	5.60	120.98	114.04
1	A	80	ARG	N-CA-C	5.51	118.21	111.82
1	D	214	ILE	N-CA-C	5.43	118.67	111.17
1	C	80	ARG	N-CA-C	5.30	119.01	112.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1764	0	1741	33	0
1	B	1786	0	1784	36	0
1	C	1783	0	1766	28	0
1	D	1815	0	1798	34	0
2	A	53	0	30	1	0
2	B	53	0	30	0	0
2	C	53	0	30	0	0
2	D	53	0	30	0	0
3	A	82	0	0	2	0
3	B	80	0	0	5	0
3	C	72	0	0	1	0
3	D	74	0	0	3	0
All	All	7668	0	7209	124	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 9.

All (124) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:THR:HA	3:B:544:HOH:O	1.64	0.97
1:B:165:ARG:HD2	3:B:544:HOH:O	1.66	0.96
1:A:17:MET:HB2	1:B:17:MET:HB2	1.48	0.94
1:C:17:MET:HB2	1:D:17:MET:HB2	1.56	0.86
1:B:134:LEU:O	1:B:138:GLU:HG2	1.79	0.82
1:B:192:ARG:HG2	1:B:220:VAL:HG12	1.63	0.80
1:B:219:GLN:HG3	1:B:220:VAL:HG23	1.63	0.79
1:B:24:VAL:HG13	1:B:44:LEU:HD23	1.65	0.79
1:C:106:LEU:HD21	1:C:118:VAL:HG11	1.68	0.75
1:D:106:LEU:HD21	1:D:118:VAL:HG11	1.72	0.70
1:D:25:ARG:HH21	1:D:31:PHE:C	2.01	0.67
1:B:195:LYS:HZ3	1:B:220:VAL:HG22	1.61	0.66
1:B:116:GLU:O	1:B:120:GLU:HG3	1.96	0.66
1:C:37:ASP:N	3:C:327:HOH:O	2.30	0.65
1:A:104:GLU:O	1:A:107:GLU:HG3	1.97	0.65
1:B:116:GLU:H	1:B:116:GLU:CD	2.04	0.64
1:B:195:LYS:NZ	1:B:220:VAL:HG22	2.13	0.64
1:B:50:LYS:HG3	1:B:51:HIS:ND1	2.15	0.62
1:A:105:ARG:HD2	1:A:105:ARG:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:SER:HB3	3:A:573:HOH:O	2.01	0.60
1:B:114:PRO:HD2	1:B:117:ARG:HG3	1.83	0.60
1:A:192:ARG:HG2	1:A:192:ARG:HH11	1.65	0.60
1:B:128:LYS:HG2	1:B:131:ARG:HH21	1.67	0.59
1:D:128:LYS:HG2	1:D:131:ARG:HH21	1.69	0.58
1:C:134:LEU:O	1:C:138:GLU:HG3	2.05	0.57
1:D:42:ARG:HG2	1:D:200:TRP:CD2	2.39	0.57
1:D:74:ARG:HD3	3:D:313:HOH:O	2.05	0.56
1:D:86:GLU:HG2	1:D:87[B]:LEU:N	2.21	0.55
1:D:37:ASP:HB3	1:D:40:ARG:HB2	1.87	0.55
1:A:5:ILE:HD11	1:A:189:ALA:HB2	1.88	0.55
1:C:195:LYS:HE2	1:C:220:VAL:HG12	1.88	0.55
1:A:38:GLU:HG3	1:A:200:TRP:CH2	2.42	0.54
1:A:192:ARG:HH11	1:A:192:ARG:CG	2.20	0.54
1:A:174:ARG:HD2	1:A:183:ILE:HD13	1.89	0.53
1:A:19:ASN:HB2	3:A:400:HOH:O	2.08	0.53
1:A:38:GLU:HG3	1:A:200:TRP:CZ2	2.44	0.52
1:D:105:ARG:HD2	1:D:105:ARG:O	2.09	0.52
1:A:5:ILE:HG22	1:A:6:LEU:HG	1.91	0.52
1:D:192:ARG:HH11	1:D:192:ARG:HG3	1.74	0.51
1:B:25:ARG:HD2	3:B:578:HOH:O	2.10	0.51
1:B:5:ILE:HD11	1:B:189:ALA:HB2	1.92	0.51
1:B:122:ILE:O	1:B:125:ILE:HG22	2.10	0.51
1:A:117:ARG:HD3	1:A:120:GLU:OE2	2.11	0.50
1:B:113:ILE:HG12	1:C:139:SER:OG	2.10	0.50
1:A:89:GLY:HA3	1:A:147:ARG:NE	2.27	0.50
1:D:175:ALA:HA	1:D:214:ILE:HD11	1.92	0.49
1:B:175:ALA:HA	1:B:214:ILE:HD11	1.93	0.49
1:A:120:GLU:O	1:A:124:GLU:HG3	2.12	0.49
1:B:165:ARG:NH1	3:B:544:HOH:O	2.46	0.49
1:A:210:TYR:CE2	1:A:215:LEU:HB2	2.48	0.48
1:D:86:GLU:CG	1:D:87[B]:LEU:N	2.76	0.48
1:D:145:VAL:O	1:D:148:ILE:HG12	2.13	0.48
1:C:104:GLU:H	1:C:104:GLU:CD	2.22	0.48
1:A:175:ALA:HA	1:A:214:ILE:HD11	1.94	0.48
1:C:195:LYS:CE	1:C:220:VAL:HG12	2.44	0.47
1:C:192:ARG:HH12	1:C:220:VAL:HG21	1.79	0.47
1:C:220:VAL:HG23	1:C:220:VAL:OXT	2.15	0.47
1:A:104:GLU:HB3	1:A:107:GLU:OE2	2.14	0.47
1:C:96:TYR:HB3	1:C:130:TYR:CE1	2.50	0.46
1:A:137:ILE:HD11	1:A:143:ARG:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:LEU:N	1:D:106:LEU:HD12	2.31	0.46
1:C:55:THR:OG1	1:C:56:PRO:HD3	2.16	0.46
1:B:29:VAL:O	1:B:29:VAL:HG12	2.16	0.46
1:B:145:VAL:O	1:B:148:ILE:HG12	2.16	0.46
1:B:192:ARG:NE	1:B:220:VAL:HG11	2.30	0.46
1:A:116:GLU:H	1:A:116:GLU:CD	2.24	0.46
1:D:133:TYR:CE1	1:D:137:ILE:HD11	2.50	0.45
1:A:45:ILE:HD12	1:A:200:TRP:HE3	1.81	0.45
1:D:86:GLU:HG2	1:D:87[A]:LEU:N	2.31	0.45
1:C:192:ARG:NH2	1:C:220:VAL:HG23	2.31	0.45
1:D:40:ARG:HH11	1:D:40:ARG:HG2	1.82	0.45
1:D:91[A]:TYR:HB2	3:D:539:HOH:O	2.16	0.45
1:D:210:TYR:CE2	1:D:215:LEU:HB2	2.51	0.45
1:D:70:ILE:O	1:D:74:ARG:HG3	2.16	0.45
1:B:114:PRO:O	1:B:117:ARG:HB2	2.17	0.44
1:C:145:VAL:O	1:C:148:ILE:HG12	2.17	0.44
1:D:37:ASP:OD1	1:D:39:GLU:HG2	2.17	0.44
1:A:104:GLU:OE1	1:A:104:GLU:N	2.50	0.44
1:B:46:GLU:O	1:B:50:LYS:HG2	2.17	0.44
1:A:142:PRO:HG3	1:D:109:TYR:CE2	2.52	0.44
1:D:133:TYR:O	1:D:137:ILE:HD13	2.18	0.44
1:A:-1:HIS:O	1:A:0:HIS:HB2	2.18	0.43
1:C:44:LEU:O	1:C:48:LEU:HG	2.19	0.43
1:D:104:GLU:HA	1:D:107:GLU:HG3	2.00	0.43
1:D:25:ARG:HD3	3:D:587:HOH:O	2.18	0.43
1:A:100:ILE:HG22	1:A:119:THR:HG23	1.99	0.42
1:C:1:MET:HE1	1:C:196:GLU:OE1	2.19	0.42
1:D:55:THR:OG1	1:D:56:PRO:HD3	2.18	0.42
1:D:13:LEU:HD11	1:D:16:VAL:CG2	2.50	0.42
1:B:210:TYR:CE2	1:B:215:LEU:HB2	2.54	0.42
1:D:89[B]:GLY:O	1:D:147:ARG:HD2	2.20	0.42
1:B:106:LEU:HD21	1:B:118:VAL:HG11	2.01	0.42
1:B:203:GLU:HG2	3:B:603:HOH:O	2.19	0.42
1:C:175:ALA:HA	1:C:214:ILE:HD11	2.02	0.42
1:A:157:ARG:NH1	1:B:29:VAL:O	2.48	0.42
1:A:173:LEU:HD13	2:A:715:FAD:O3'	2.20	0.42
1:B:130:TYR:O	1:B:134:LEU:HG	2.20	0.42
1:C:210:TYR:CE2	1:C:215:LEU:HB2	2.55	0.42
1:A:192:ARG:CG	1:A:192:ARG:NH1	2.79	0.41
1:C:167:LEU:C	1:C:167:LEU:HD23	2.45	0.41
1:D:86:GLU:CG	1:D:87[A]:LEU:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ILE:HD11	1:C:189:ALA:HB2	2.01	0.41
1:A:145:VAL:O	1:A:148:ILE:HG12	2.20	0.41
1:D:10:PHE:C	1:D:10:PHE:CD2	2.99	0.41
1:A:116:GLU:O	1:A:120:GLU:HG3	2.20	0.41
1:B:10:PHE:CD2	1:B:10:PHE:C	2.98	0.41
1:B:106:LEU:HD12	1:B:106:LEU:N	2.35	0.41
1:C:106:LEU:HD12	1:C:106:LEU:N	2.35	0.41
1:A:114:PRO:HA	1:A:115:PRO:HD3	1.98	0.41
1:B:125:ILE:HG21	1:C:149:VAL:HB	2.01	0.41
1:C:192:ARG:HH22	1:C:220:VAL:HG23	1.86	0.41
1:A:126:VAL:HG21	1:A:153:ASN:HD21	1.86	0.41
1:C:106:LEU:CD2	1:C:118:VAL:HG21	2.50	0.41
1:B:152:LEU:HD23	1:C:152:LEU:HD23	2.03	0.41
1:C:106:LEU:O	1:C:108:GLY:N	2.50	0.41
1:B:114:PRO:HA	1:B:115:PRO:HD3	1.98	0.40
1:C:104:GLU:CD	1:C:104:GLU:N	2.79	0.40
1:D:84:TYR:CE2	1:D:160:TRP:CD1	3.09	0.40
1:D:100:ILE:HG22	1:D:119:THR:HG23	2.04	0.40
1:B:115:PRO:HD2	1:B:116:GLU:OE2	2.20	0.40
1:D:42:ARG:HG2	1:D:200:TRP:CE3	2.57	0.40
1:A:13:LEU:CD2	1:A:197:LYS:HE3	2.52	0.40
1:C:114:PRO:HD2	1:C:117:ARG:HG3	2.03	0.40
1:D:114:PRO:HA	1:D:115:PRO:HD3	1.97	0.40

There are no symmetry-related clashes.

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	205/232 (88%)	198 (97%)	6 (3%)	1 (0%)	24	14
1	B	210/232 (90%)	205 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	208/232 (90%)	198 (95%)	9 (4%)	1 (0%)	24	14
1	D	214/232 (92%)	209 (98%)	5 (2%)	0	100	100
All	All	837/928 (90%)	810 (97%)	25 (3%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	TYR
1	C	108	GLY

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	185/207 (89%)	182 (98%)	3 (2%)	55	47
1	B	189/207 (91%)	187 (99%)	2 (1%)	65	60
1	C	189/207 (91%)	189 (100%)	0	100	100
1	D	191/207 (92%)	187 (98%)	4 (2%)	47	36
All	All	754/828 (91%)	745 (99%)	9 (1%)	63	57

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	105	ARG
1	A	192	ARG
1	B	116	GLU
1	B	117	ARG
1	D	44	LEU
1	D	54	GLU
1	D	105	ARG
1	D	125	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	53	HIS
1	C	185	GLN
1	D	75	GLN
1	D	85	ASN

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](#)

4 ligands are modelled in this entry.

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	FAD	A	715	-	58,58,58	2.89	27 (46%)	85,89,89	2.24	20 (23%)
2	FAD	D	700	-	58,58,58	2.88	26 (44%)	85,89,89	2.25	22 (25%)
2	FAD	B	710	-	58,58,58	2.91	27 (46%)	85,89,89	2.24	22 (25%)
2	FAD	C	705	-	58,58,58	2.89	27 (46%)	85,89,89	2.24	22 (25%)

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	FAD	A	715	-	1/1/9/9	11/34/50/50	0/6/6/6
2	FAD	D	700	-	1/1/9/9	13/34/50/50	0/6/6/6
2	FAD	B	710	-	1/1/9/9	13/34/50/50	0/6/6/6
2	FAD	C	705	-	1/1/9/9	13/34/50/50	0/6/6/6

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	715	FAD	C9A-C5X	7.15	1.52	1.41
2	B	710	FAD	C9A-C5X	7.14	1.52	1.41
2	C	705	FAD	C9A-C5X	7.09	1.52	1.41
2	D	700	FAD	C9A-C5X	6.93	1.52	1.41
2	C	705	FAD	C6-C7	6.70	1.48	1.39
2	D	700	FAD	C6-C7	6.70	1.48	1.39
2	B	710	FAD	C6-C7	6.70	1.48	1.39
2	A	715	FAD	C6-C7	6.66	1.48	1.39
2	D	700	FAD	C9-C9A	6.19	1.49	1.39
2	B	710	FAD	C9-C9A	6.11	1.49	1.39
2	A	715	FAD	C9-C9A	5.99	1.49	1.39
2	D	700	FAD	C4A-N3A	5.95	1.45	1.34
2	C	705	FAD	C9-C9A	5.90	1.49	1.39
2	B	710	FAD	C4A-N3A	5.89	1.45	1.34
2	C	705	FAD	C4A-N3A	5.86	1.45	1.34
2	A	715	FAD	C4A-N3A	5.79	1.45	1.34
2	D	700	FAD	C4X-N5	5.60	1.42	1.30
2	A	715	FAD	C4X-N5	5.59	1.42	1.30
2	B	710	FAD	C4X-N5	5.57	1.42	1.30
2	C	705	FAD	C4X-N5	5.55	1.42	1.30
2	D	700	FAD	C6-C5X	4.92	1.47	1.40
2	A	715	FAD	C6-C5X	4.92	1.47	1.40
2	C	705	FAD	C6-C5X	4.90	1.47	1.40
2	B	710	FAD	P-O3P	-4.83	1.54	1.59
2	D	700	FAD	C10-N1	4.73	1.42	1.33
2	A	715	FAD	C5A-C4A	4.72	1.47	1.39
2	D	700	FAD	P-O3P	-4.72	1.54	1.59
2	C	705	FAD	C5A-C4A	4.71	1.47	1.39
2	B	710	FAD	C6-C5X	4.70	1.47	1.40
2	B	710	FAD	C5A-C4A	4.68	1.47	1.39
2	B	710	FAD	C10-N1	4.61	1.42	1.33
2	A	715	FAD	P-O3P	-4.58	1.54	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	705	FAD	P-O3P	-4.58	1.54	1.59
2	A	715	FAD	C8-C7	4.55	1.51	1.40
2	C	705	FAD	C8-C7	4.54	1.51	1.40
2	D	700	FAD	C5A-C4A	4.53	1.47	1.39
2	A	715	FAD	C10-N1	4.53	1.42	1.33
2	B	710	FAD	C8-C7	4.53	1.51	1.40
2	C	705	FAD	C10-N1	4.51	1.42	1.33
2	D	700	FAD	C8-C7	4.46	1.51	1.40
2	A	715	FAD	C10-N10	4.16	1.46	1.37
2	B	710	FAD	C10-N10	4.06	1.46	1.37
2	C	705	FAD	C10-N10	4.03	1.46	1.37
2	B	710	FAD	PA-O3P	-4.01	1.55	1.59
2	A	715	FAD	C9-C8	3.95	1.45	1.39
2	B	710	FAD	C9-C8	3.94	1.45	1.39
2	D	700	FAD	PA-O3P	-3.93	1.55	1.59
2	B	710	FAD	C2A-N1A	3.91	1.40	1.33
2	D	700	FAD	C10-N10	3.89	1.45	1.37
2	C	705	FAD	C9-C8	3.88	1.44	1.39
2	C	705	FAD	PA-O3P	-3.83	1.55	1.59
2	D	700	FAD	C9-C8	3.80	1.44	1.39
2	C	705	FAD	C2A-N1A	3.75	1.40	1.33
2	A	715	FAD	PA-O3P	-3.70	1.55	1.59
2	D	700	FAD	C2A-N1A	3.64	1.40	1.33
2	A	715	FAD	C2A-N1A	3.53	1.40	1.33
2	C	705	FAD	C4-N3	3.32	1.45	1.38
2	A	715	FAD	C4-N3	3.27	1.45	1.38
2	B	710	FAD	C4-N3	3.26	1.44	1.38
2	D	700	FAD	C4-N3	3.24	1.44	1.38
2	D	700	FAD	C8A-N7A	-3.16	1.25	1.31
2	B	710	FAD	C8A-N7A	-3.10	1.25	1.31
2	C	705	FAD	C8A-N7A	-2.93	1.26	1.31
2	A	715	FAD	C8A-N7A	-2.88	1.26	1.31
2	B	710	FAD	C6A-N1A	2.86	1.43	1.35
2	B	710	FAD	C2A-N3A	2.82	1.38	1.33
2	A	715	FAD	C2B-C1B	2.79	1.62	1.53
2	B	710	FAD	C2B-C1B	2.79	1.62	1.53
2	D	700	FAD	C2A-N3A	2.76	1.38	1.33
2	A	715	FAD	C2A-N3A	2.75	1.38	1.33
2	C	705	FAD	C6A-N1A	2.75	1.43	1.35
2	C	705	FAD	C2B-C1B	2.74	1.62	1.53
2	D	700	FAD	C6A-N1A	2.74	1.43	1.35
2	A	715	FAD	C6A-N1A	2.72	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	705	FAD	C2A-N3A	2.70	1.38	1.33
2	A	715	FAD	C1'-C2'	2.63	1.56	1.52
2	D	700	FAD	C2B-C1B	2.61	1.61	1.53
2	D	700	FAD	P-O5'	-2.57	1.49	1.59
2	C	705	FAD	P-O5'	-2.57	1.49	1.59
2	A	715	FAD	P-O5'	-2.54	1.49	1.59
2	B	710	FAD	P-O5'	-2.52	1.49	1.59
2	C	705	FAD	C2-N3	2.46	1.44	1.39
2	B	710	FAD	C2-N3	2.43	1.44	1.39
2	A	715	FAD	C2-N3	2.42	1.44	1.39
2	A	715	FAD	PA-O5B	-2.41	1.49	1.59
2	C	705	FAD	C1'-C2'	2.40	1.56	1.52
2	B	710	FAD	C1'-C2'	2.36	1.55	1.52
2	B	710	FAD	PA-O5B	-2.35	1.50	1.59
2	C	705	FAD	PA-O5B	-2.34	1.50	1.59
2	C	705	FAD	C5B-C4B	2.33	1.58	1.51
2	C	705	FAD	C8A-N9A	2.30	1.41	1.37
2	A	715	FAD	C8A-N9A	2.30	1.41	1.37
2	D	700	FAD	C8A-N9A	2.28	1.41	1.37
2	D	700	FAD	PA-O5B	-2.27	1.50	1.59
2	D	700	FAD	C2-N3	2.26	1.43	1.39
2	D	700	FAD	C5B-C4B	2.24	1.58	1.51
2	B	710	FAD	C5B-C4B	2.24	1.58	1.51
2	D	700	FAD	O5B-C5B	2.22	1.53	1.44
2	D	700	FAD	C1'-C2'	2.22	1.55	1.52
2	A	715	FAD	C2'-C3'	2.21	1.57	1.53
2	C	705	FAD	C2'-C3'	2.19	1.57	1.53
2	B	710	FAD	C8A-N9A	2.18	1.41	1.37
2	B	710	FAD	C2'-C3'	2.16	1.57	1.53
2	C	705	FAD	O5B-C5B	2.15	1.52	1.44
2	A	715	FAD	C5B-C4B	2.14	1.58	1.51
2	B	710	FAD	O5B-C5B	2.14	1.52	1.44
2	A	715	FAD	O5B-C5B	2.10	1.52	1.44

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	705	FAD	C2B-C1B-N9A	9.95	138.03	113.30
2	B	710	FAD	C2B-C1B-N9A	9.79	137.62	113.30
2	A	715	FAD	C2B-C1B-N9A	9.72	137.46	113.30
2	D	700	FAD	C2B-C1B-N9A	9.67	137.33	113.30
2	B	710	FAD	C3B-C2B-C1B	-6.62	88.93	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	700	FAD	C3B-C2B-C1B	-6.62	88.95	101.46
2	A	715	FAD	C3B-C2B-C1B	-6.59	89.00	101.46
2	C	705	FAD	C3B-C2B-C1B	-6.55	89.07	101.46
2	B	710	FAD	C5A-N7A-C8A	5.42	111.97	103.45
2	C	705	FAD	C5A-N7A-C8A	5.40	111.94	103.45
2	D	700	FAD	C5A-N7A-C8A	5.38	111.91	103.45
2	A	715	FAD	C5A-N7A-C8A	5.36	111.88	103.45
2	D	700	FAD	O2B-C2B-C1B	5.33	128.44	110.10
2	B	710	FAD	O2B-C2B-C1B	5.29	128.32	110.10
2	A	715	FAD	O2B-C2B-C1B	5.26	128.21	110.10
2	C	705	FAD	O2B-C2B-C1B	5.23	128.11	110.10
2	A	715	FAD	O4B-C1B-N9A	4.45	116.63	108.09
2	D	700	FAD	O4B-C1B-N9A	4.41	116.57	108.09
2	B	710	FAD	O4B-C1B-N9A	4.36	116.47	108.09
2	C	705	FAD	O4B-C1B-N9A	4.29	116.33	108.09
2	D	700	FAD	C4B-O4B-C1B	-4.27	100.05	109.47
2	A	715	FAD	C4B-O4B-C1B	-4.21	100.18	109.47
2	B	710	FAD	C4B-O4B-C1B	-4.19	100.22	109.47
2	C	705	FAD	C4B-O4B-C1B	-4.05	100.52	109.47
2	A	715	FAD	C4A-C5A-N7A	-3.93	106.09	110.58
2	C	705	FAD	C4A-C5A-N7A	-3.88	106.14	110.58
2	D	700	FAD	C4A-C5A-N7A	-3.84	106.19	110.58
2	B	710	FAD	C4A-C5A-N7A	-3.82	106.21	110.58
2	C	705	FAD	C4-C4X-N5	3.75	123.39	118.21
2	A	715	FAD	C4-C4X-N5	3.71	123.33	118.21
2	D	700	FAD	C4-C4X-N5	3.70	123.32	118.21
2	B	710	FAD	C4-C4X-N5	3.68	123.29	118.21
2	D	700	FAD	N3A-C2A-N1A	-3.60	123.14	128.58
2	C	705	FAD	N3A-C2A-N1A	-3.58	123.16	128.58
2	B	710	FAD	N3A-C2A-N1A	-3.55	123.20	128.58
2	A	715	FAD	N3A-C2A-N1A	-3.55	123.21	128.58
2	A	715	FAD	C6A-C5A-N7A	3.34	138.53	132.09
2	C	705	FAD	C6A-C5A-N7A	3.28	138.40	132.09
2	D	700	FAD	C6A-C5A-N7A	3.20	138.26	132.09
2	D	700	FAD	N9A-C8A-N7A	-3.17	109.44	113.94
2	B	710	FAD	C6A-C5A-N7A	3.14	138.15	132.09
2	A	715	FAD	N9A-C8A-N7A	-3.11	109.52	113.94
2	C	705	FAD	N9A-C8A-N7A	-3.09	109.55	113.94
2	B	710	FAD	C5B-C4B-C3B	-3.06	104.21	115.21
2	A	715	FAD	C5B-C4B-C3B	-3.05	104.22	115.21
2	C	705	FAD	C5B-C4B-C3B	-3.04	104.27	115.21
2	B	710	FAD	N9A-C8A-N7A	-3.04	109.63	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	700	FAD	C5B-C4B-C3B	-3.00	104.43	115.21
2	A	715	FAD	O3B-C3B-C4B	2.87	119.33	111.08
2	D	700	FAD	O3B-C3B-C4B	2.86	119.29	111.08
2	B	710	FAD	O3B-C3B-C4B	2.83	119.22	111.08
2	A	715	FAD	O4B-C4B-C3B	2.81	110.73	105.15
2	C	705	FAD	O3B-C3B-C4B	2.80	119.13	111.08
2	B	710	FAD	O4B-C4B-C3B	2.79	110.70	105.15
2	A	715	FAD	P-O5'-C5'	2.78	137.29	121.35
2	D	700	FAD	O4B-C4B-C3B	2.76	110.64	105.15
2	C	705	FAD	O4B-C4B-C3B	2.76	110.62	105.15
2	D	700	FAD	C4A-N9A-C8A	2.75	108.62	105.74
2	D	700	FAD	P-O5'-C5'	2.67	136.66	121.35
2	A	715	FAD	C4A-N9A-C8A	2.64	108.51	105.74
2	B	710	FAD	P-O5'-C5'	2.61	136.31	121.35
2	C	705	FAD	P-O5'-C5'	2.58	136.11	121.35
2	D	700	FAD	C9-C9A-N10	2.57	125.30	121.85
2	C	705	FAD	C4A-N9A-C8A	2.55	108.42	105.74
2	B	710	FAD	C4A-N9A-C8A	2.55	108.41	105.74
2	A	715	FAD	C2A-N1A-C6A	2.46	122.77	118.73
2	B	710	FAD	C9-C9A-N10	2.45	125.15	121.85
2	C	705	FAD	C10-C4X-N5	-2.44	119.82	124.81
2	A	715	FAD	C10-C4X-N5	-2.44	119.83	124.81
2	D	700	FAD	C2A-N1A-C6A	2.43	122.73	118.73
2	D	700	FAD	C1'-C2'-C3'	-2.43	103.07	109.66
2	A	715	FAD	C9-C9A-N10	2.43	125.12	121.85
2	D	700	FAD	C10-C4X-N5	-2.43	119.86	124.81
2	B	710	FAD	C10-C4X-N5	-2.42	119.86	124.81
2	A	715	FAD	C10-N1-C2	2.38	122.00	116.85
2	C	705	FAD	C10-N1-C2	2.37	121.97	116.85
2	C	705	FAD	C2A-N1A-C6A	2.37	122.62	118.73
2	B	710	FAD	C10-N1-C2	2.33	121.90	116.85
2	C	705	FAD	C9-C9A-N10	2.32	124.98	121.85
2	B	710	FAD	C2A-N1A-C6A	2.31	122.52	118.73
2	C	705	FAD	C1'-C2'-C3'	-2.31	103.40	109.66
2	D	700	FAD	C10-N1-C2	2.30	121.84	116.85
2	B	710	FAD	C1'-C2'-C3'	-2.29	103.45	109.66
2	B	710	FAD	N3A-C4A-N9A	2.07	130.69	127.17
2	D	700	FAD	N3A-C4A-N9A	2.04	130.63	127.17
2	C	705	FAD	N3A-C4A-N9A	2.01	130.59	127.17

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	715	FAD	C1B
2	B	710	FAD	C1B
2	C	705	FAD	C1B
2	D	700	FAD	C1B

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	715	FAD	C1'-C2'-C3'-O3'
2	A	715	FAD	C1'-C2'-C3'-C4'
2	A	715	FAD	O2'-C2'-C3'-O3'
2	A	715	FAD	O2'-C2'-C3'-C4'
2	A	715	FAD	C3'-C4'-C5'-O5'
2	B	710	FAD	C1'-C2'-C3'-O3'
2	B	710	FAD	C1'-C2'-C3'-C4'
2	B	710	FAD	O2'-C2'-C3'-O3'
2	B	710	FAD	O2'-C2'-C3'-C4'
2	B	710	FAD	C3'-C4'-C5'-O5'
2	C	705	FAD	N10-C1'-C2'-O2'
2	C	705	FAD	N10-C1'-C2'-C3'
2	C	705	FAD	C1'-C2'-C3'-O3'
2	C	705	FAD	C1'-C2'-C3'-C4'
2	C	705	FAD	C3'-C4'-C5'-O5'
2	C	705	FAD	O4'-C4'-C5'-O5'
2	D	700	FAD	C1'-C2'-C3'-O3'
2	D	700	FAD	C1'-C2'-C3'-C4'
2	D	700	FAD	O2'-C2'-C3'-O3'
2	D	700	FAD	O2'-C2'-C3'-C4'
2	D	700	FAD	C3'-C4'-C5'-O5'
2	D	700	FAD	O4'-C4'-C5'-O5'
2	C	705	FAD	O2'-C2'-C3'-C4'
2	C	705	FAD	O2'-C2'-C3'-O3'
2	A	715	FAD	O4'-C4'-C5'-O5'
2	B	710	FAD	O4'-C4'-C5'-O5'
2	A	715	FAD	PA-O3P-P-O1P
2	B	710	FAD	PA-O3P-P-O1P
2	C	705	FAD	PA-O3P-P-O1P
2	D	700	FAD	PA-O3P-P-O1P
2	B	710	FAD	N10-C1'-C2'-O2'
2	D	700	FAD	N10-C1'-C2'-O2'
2	B	710	FAD	C2B-C1B-N9A-C4A
2	C	705	FAD	C2B-C1B-N9A-C4A
2	C	705	FAD	C2B-C1B-N9A-C8A

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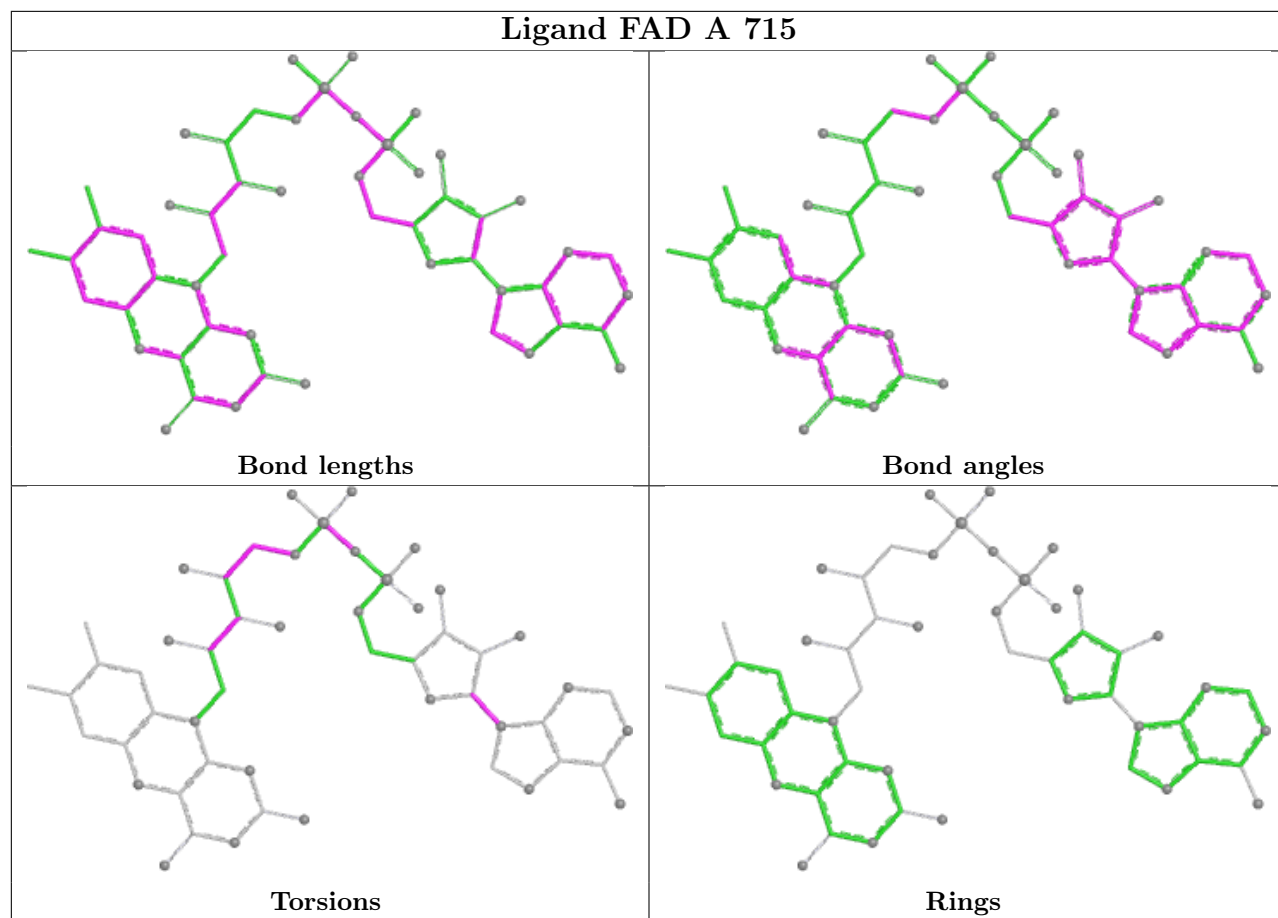
Mol	Chain	Res	Type	Atoms
2	C	705	FAD	C4'-C5'-O5'-P
2	A	715	FAD	C2B-C1B-N9A-C4A
2	D	700	FAD	C2B-C1B-N9A-C4A
2	A	715	FAD	C2B-C1B-N9A-C8A
2	B	710	FAD	C2B-C1B-N9A-C8A
2	D	700	FAD	C2B-C1B-N9A-C8A
2	D	700	FAD	C4'-C5'-O5'-P
2	B	710	FAD	C4'-C5'-O5'-P
2	A	715	FAD	C4'-C5'-O5'-P
2	B	710	FAD	N10-C1'-C2'-C3'
2	D	700	FAD	N10-C1'-C2'-C3'
2	A	715	FAD	PA-O3P-P-O2P
2	B	710	FAD	PA-O3P-P-O2P
2	C	705	FAD	PA-O3P-P-O2P
2	D	700	FAD	PA-O3P-P-O2P

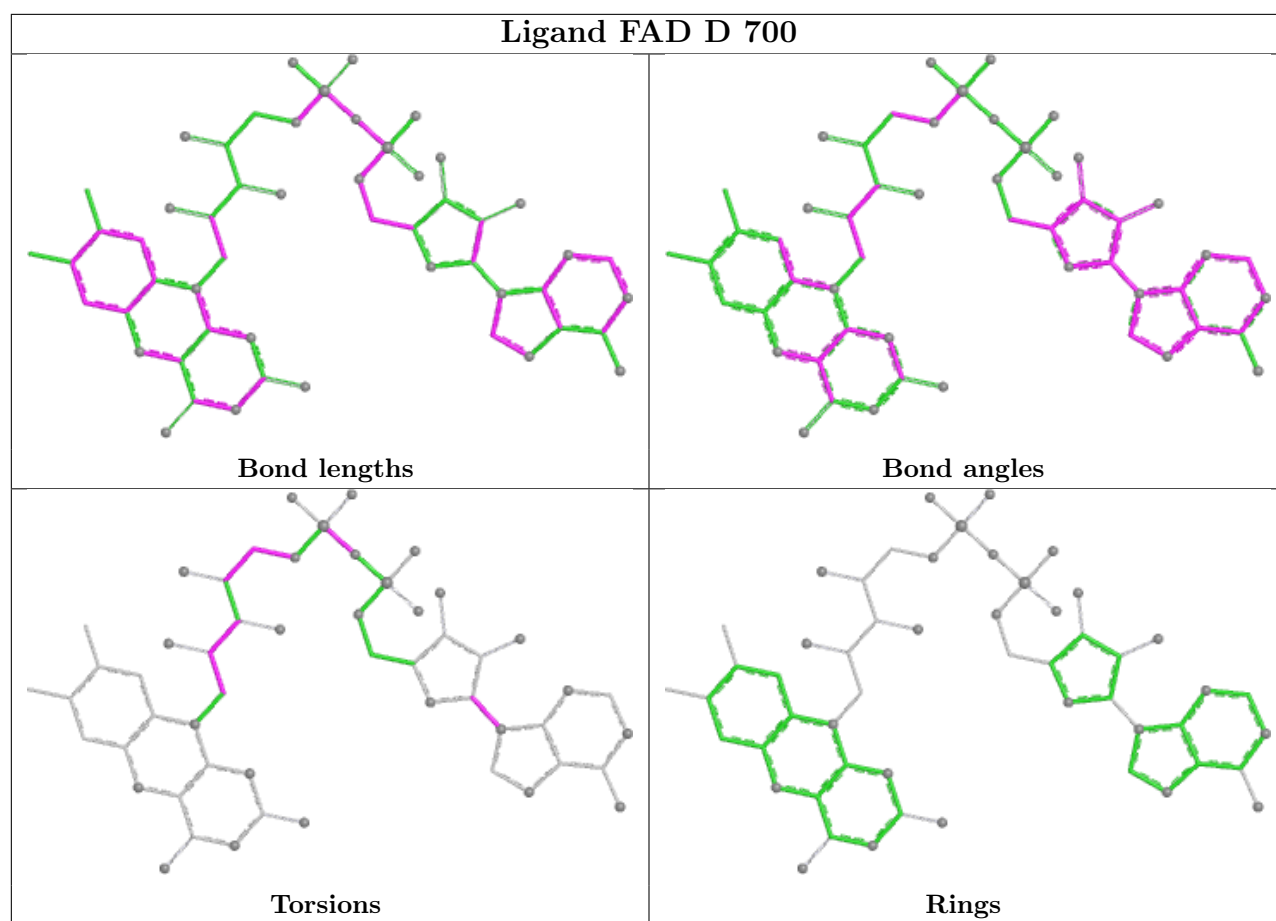
There are no ring outliers.

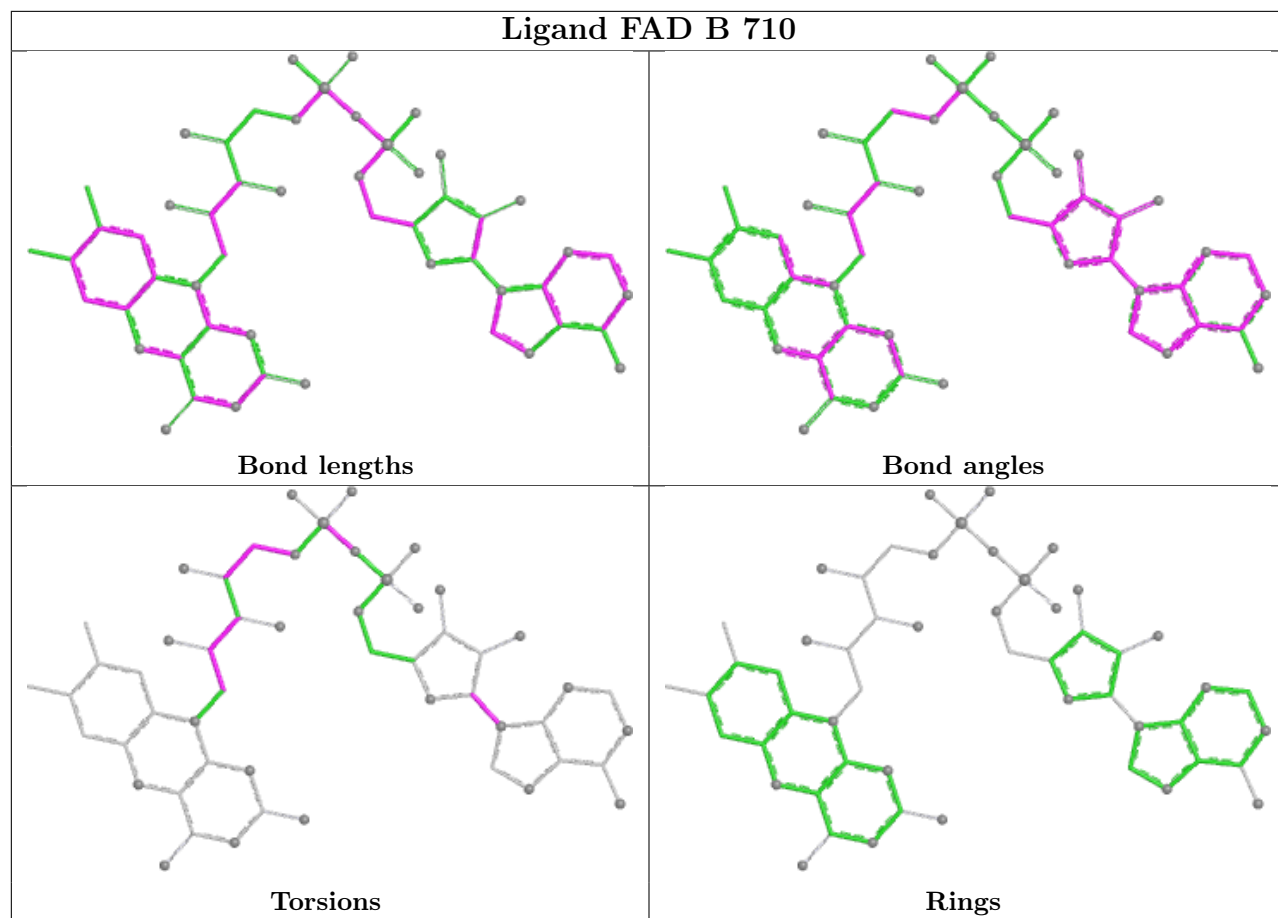
1 monomer is involved in 1 short contact:

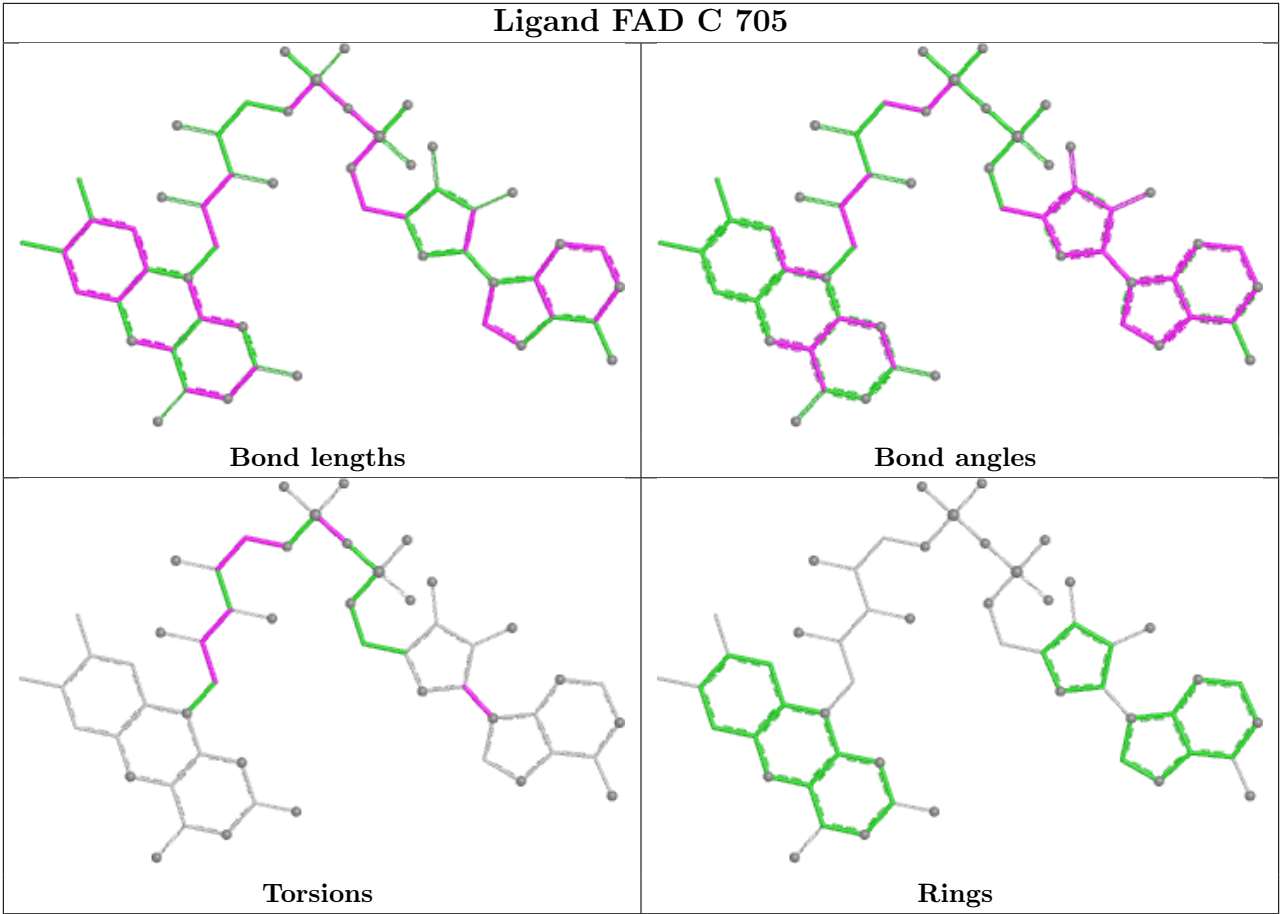
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	715	FAD	1	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	91[B]:TYR	C	92:SER	N	6.85

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	211/232 (90%)	0.32	13 (6%)	26 25	15, 26, 50, 61	0
1	B	214/232 (92%)	0.37	16 (7%)	20 18	16, 28, 53, 58	0
1	C	214/232 (92%)	0.28	13 (6%)	27 25	15, 25, 47, 55	0
1	D	213/232 (91%)	0.56	22 (10%)	12 10	15, 28, 55, 65	5 (2%)
All	All	852/928 (91%)	0.38	64 (7%)	20 18	15, 26, 52, 65	5 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	91[A]	TYR	6.5
1	B	220	VAL	5.8
1	A	91	TYR	4.7
1	A	31	PHE	4.6
1	D	218	VAL	4.5
1	D	31	PHE	4.1
1	D	39	GLU	4.0
1	D	116	GLU	3.9
1	D	93	LYS	3.8
1	B	31	PHE	3.8
1	C	220	VAL	3.8
1	B	107	GLU	3.6
1	D	94	LEU	3.6
1	C	32	ASP	3.5
1	D	90[A]	ARG	3.5
1	C	95	SER	3.5
1	A	95	SER	3.3
1	A	-1	HIS	3.2
1	C	107	GLU	3.2
1	C	91	TYR	3.1
1	C	109	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	0	HIS	3.0
1	D	120	GLU	3.0
1	C	218	VAL	2.9
1	B	29	VAL	2.9
1	B	50	LYS	2.8
1	A	107	GLU	2.8
1	B	120	GLU	2.8
1	B	106	LEU	2.8
1	D	139	SER	2.8
1	A	94	LEU	2.8
1	C	92	SER	2.8
1	D	109	TYR	2.7
1	C	139	SER	2.7
1	D	89[A]	GLY	2.7
1	D	37	ASP	2.6
1	D	87[A]	LEU	2.6
1	A	112	THR	2.6
1	B	30	SER	2.6
1	D	88[A]	SER	2.6
1	D	106	LEU	2.5
1	B	38	GLU	2.5
1	B	138	GLU	2.5
1	D	217	GLU	2.5
1	C	31	PHE	2.4
1	A	30	SER	2.4
1	C	96	TYR	2.4
1	B	51	HIS	2.4
1	C	106	LEU	2.3
1	A	89	GLY	2.3
1	D	92	SER	2.3
1	D	113	ILE	2.3
1	B	109	TYR	2.2
1	C	110	LYS	2.2
1	D	40	ARG	2.2
1	D	117	ARG	2.2
1	B	47	TYR	2.1
1	A	96	TYR	2.1
1	D	127	ASP	2.1
1	B	112	THR	2.1
1	A	135	GLU	2.1
1	A	87	LEU	2.1
1	B	111	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	217	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

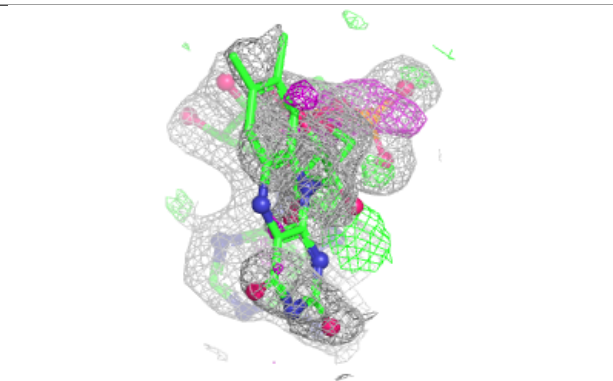
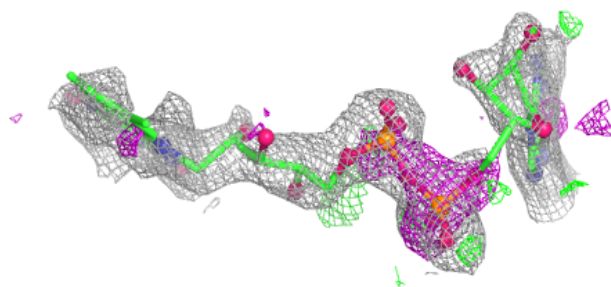
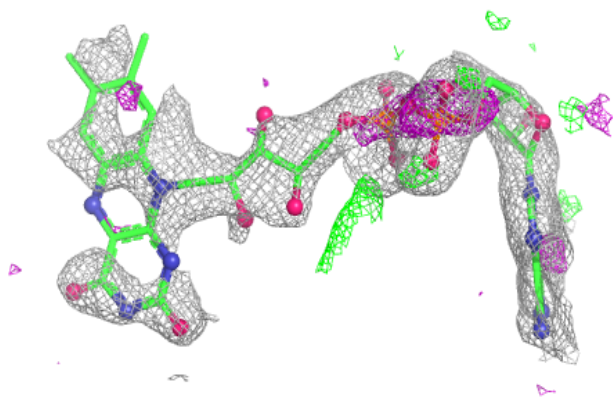
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	B	710	53/53	0.74	0.17	35,52,65,65	0
2	FAD	C	705	53/53	0.75	0.16	33,50,69,69	0
2	FAD	A	715	53/53	0.81	0.15	34,48,68,69	0
2	FAD	D	700	53/53	0.82	0.14	25,39,50,50	0

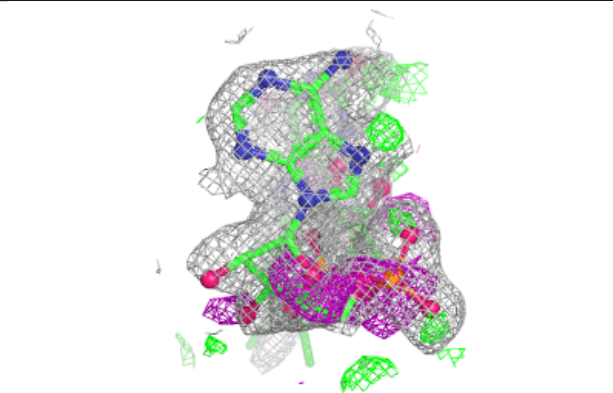
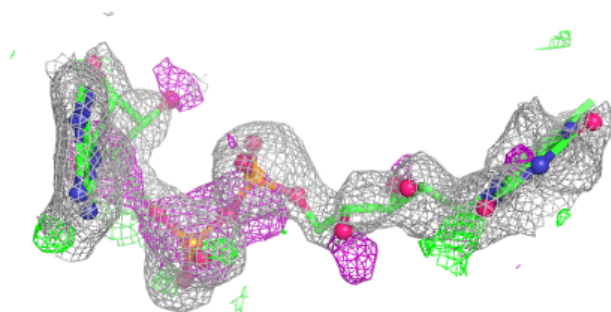
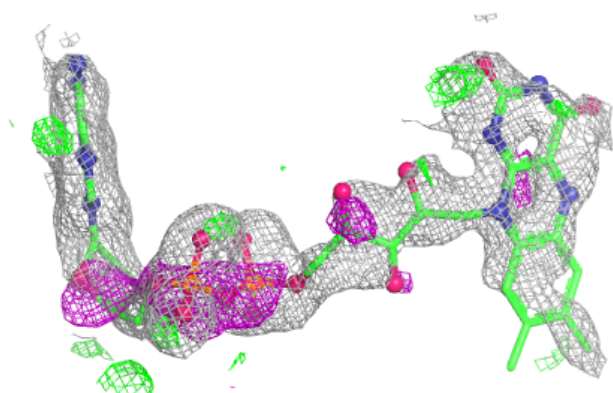
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 710:

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

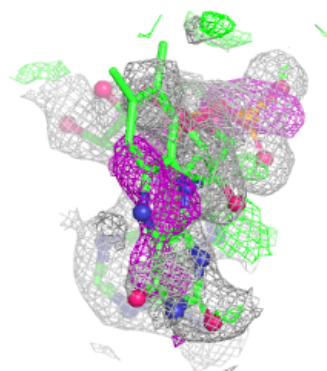
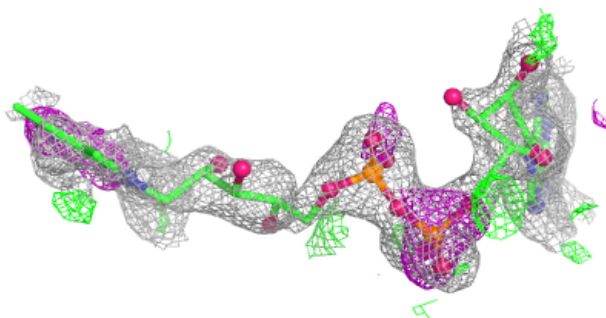
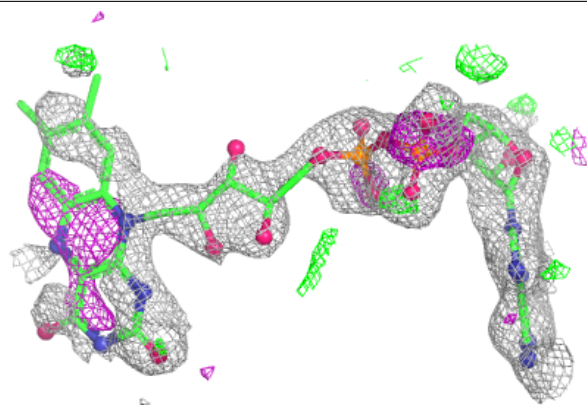
**Electron density around FAD C 705:**

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

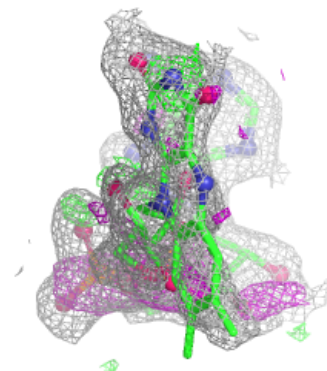
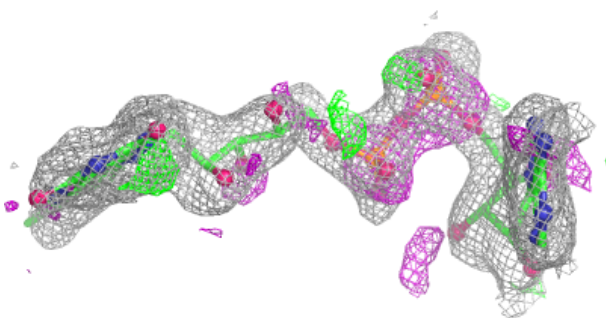
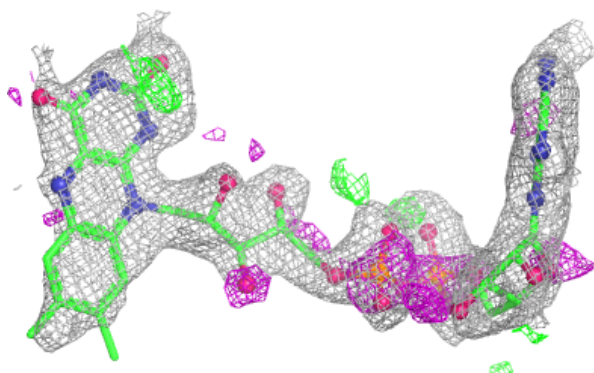


Electron density around FAD A 715:

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

**Electron density around FAD D 700:**

$2mF_o-DF_c$ (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.