Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 03:22 am BST

PDB ID	:	1KQ4
Title	:	CRYSTAL STRUCTURE OF A THY1-COMPLEMENTING PROTEIN (TM0449) FROM THERMOTOGA MARITIMA AT 2.25 A RESOLUTION
Authors	:	Wilson, I.A.; Miller, M.D.; Joint Center for Structural Genomics (JCSG)
Deposited on	:	2002-01-03
Resolution	:	2.25 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 following versions of software and data (see references ⓘ) were used in the production of this report:

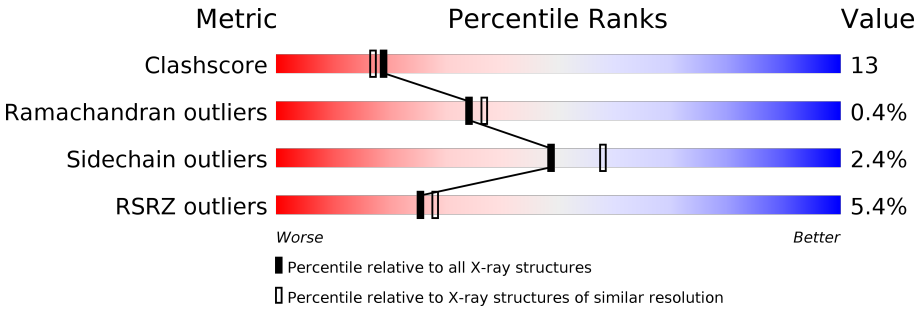
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 on 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 <=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	3% 63% 23% • 13%
1	B	232	5% 69% 20% • 9%
1	C	232	5% 66% 25% • 8%
1	D	232	6% 66% 24% • 9%

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	315	X	-	-	-
2	FAD	B	310	X	-	-	-
2	FAD	C	305	X	-	-	-
2	FAD	D	300	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7467 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 HYPOTHETICAL PROTEIN TM0449.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	Se	0	0	0
			1699	1109	290	295	1	4			
1	B	211	Total	C	N	O	S	Se	0	0	0
			1761	1148	303	305	1	4			
1	C	214	Total	C	N	O	S	Se	0	0	0
			1779	1155	306	313	1	4			
1	D	210	Total	C	N	O	S	Se	0	0	0
			1742	1133	297	307	1	4			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	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
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
A	17	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
A	33	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
A	49	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
A	168	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
B	-11	MSE	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	-2	HIS	-	EXPRESSION TAG	UNP Q9WYT0
B	-1	HIS	-	EXPRESSION TAG	UNP Q9WYT0
B	0	HIS	-	EXPRESSION TAG	UNP Q9WYT0
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
B	17	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
B	33	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
B	49	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
B	168	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
C	-11	MSE	-	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
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
C	17	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
C	33	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
C	49	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
C	168	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
D	-11	MSE	-	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

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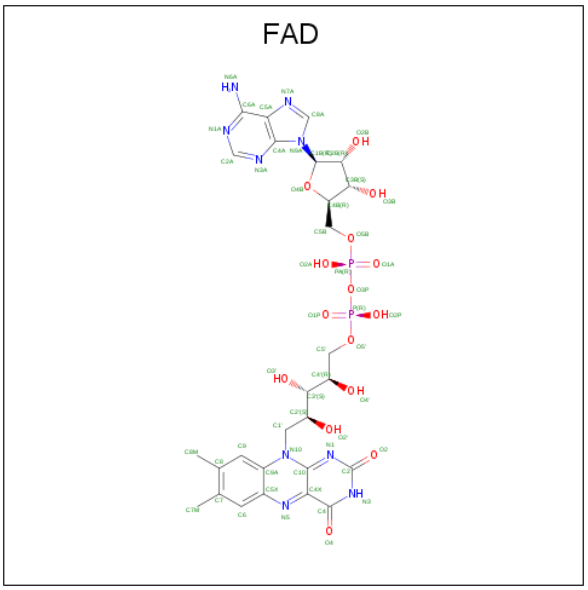
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
D	17	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
D	33	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
D	49	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0
D	168	MSE	MET	MODIFIED RESIDUE	UNP Q9WYT0

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	77	Total	O	0	0
			77	77		
3	B	66	Total	O	0	0
			66	66		

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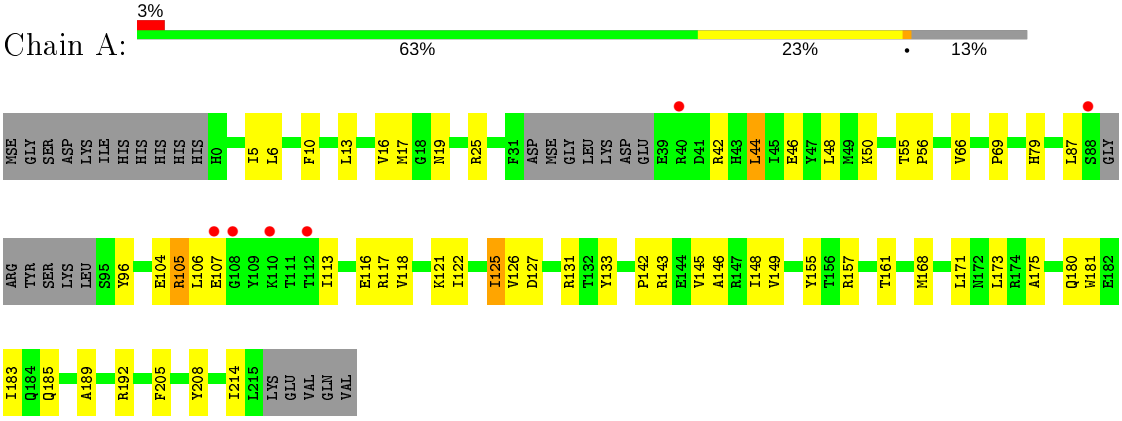
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	67	Total O 67 67	0	0
3	D	64	Total O 64 64	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

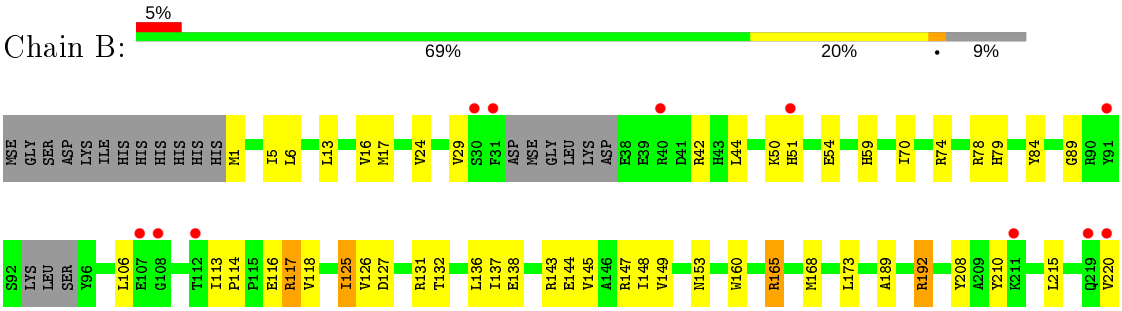
• Molecule 1: HYPOTHETICAL PROTEIN TM0449

Chain A:



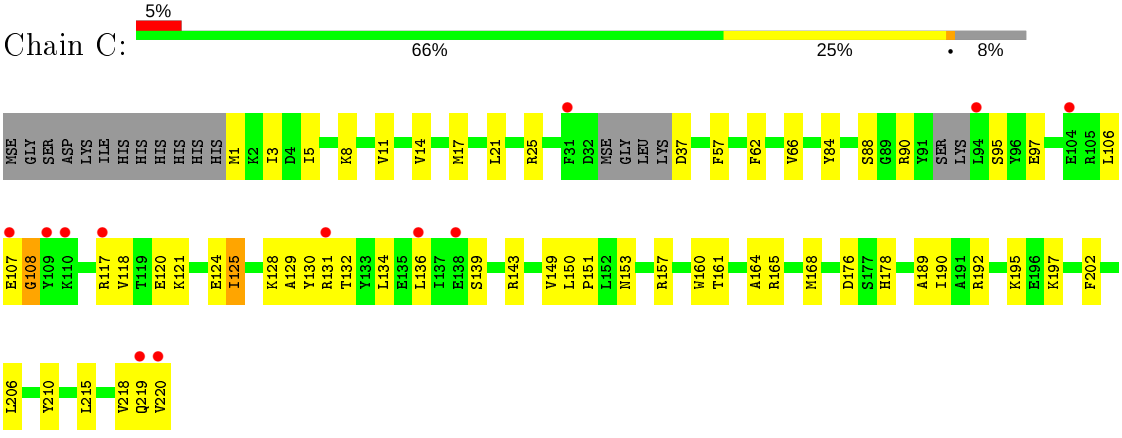
• Molecule 1: HYPOTHETICAL PROTEIN TM0449

Chain B:



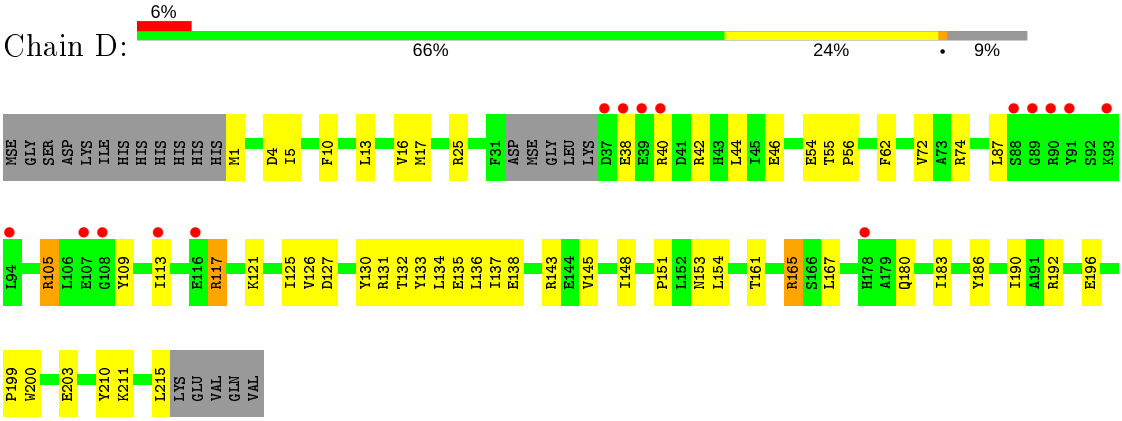
• Molecule 1: HYPOTHETICAL PROTEIN TM0449

Chain C:



• Molecule 1: HYPOTHETICAL PROTEIN TM0449

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.20Å 116.61Å 141.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 19.85 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.25) 99.5 (19.85-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.09Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.192 , 0.240 0.192 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 63.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7467	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 4.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.38	0/1741	0.59	0/2348
1	B	0.38	0/1805	0.60	0/2433
1	C	0.38	0/1822	0.61	0/2455
1	D	0.37	0/1786	0.59	0/2412
All	All	0.38	0/7154	0.60	0/9648

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	1699	0	1689	51	0
1	B	1761	0	1750	54	0
1	C	1779	0	1758	58	0
1	D	1742	0	1718	49	0
2	A	53	0	30	0	0
2	B	53	0	30	1	0
2	C	53	0	30	0	0
2	D	53	0	30	0	0
3	A	77	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	66	0	0	3	0
3	C	67	0	0	1	0
3	D	64	0	0	1	0
All	All	7467	0	7035	185	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 13.

All (185) 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:D:1:MSE:HE1	1:D:196:GLU:HG3	1.49	0.91
1:A:17:MSE:HB2	1:B:17:MSE:HB2	1.51	0.91
1:A:113:ILE:HD13	1:A:121:LYS:HE3	1.53	0.87
1:C:17:MSE:HB2	1:D:17:MSE:HB2	1.57	0.86
1:B:192:ARG:HG2	1:B:220:VAL:HG12	1.57	0.85
1:B:149:VAL:HB	1:C:125:ILE:HD12	1.58	0.83
1:D:133:TYR:CZ	1:D:137:ILE:HD11	2.21	0.74
1:A:146:ALA:O	1:A:149:VAL:HG12	1.89	0.73
1:B:132:THR:HG21	1:C:125:ILE:HD13	1.71	0.71
1:C:37:ASP:N	3:C:347:HOH:O	2.24	0.71
1:B:42:ARG:HH11	1:B:42:ARG:HG3	1.55	0.71
1:B:114:PRO:HD2	1:B:117:ARG:HG3	1.73	0.70
1:C:106:LEU:HD21	1:C:118:VAL:HG11	1.72	0.70
1:A:180:GLN:O	1:A:183:ILE:HG22	1.92	0.70
1:A:122:ILE:HA	1:A:125:ILE:HD11	1.74	0.68
1:C:1:MSE:HE1	1:C:197:LYS:HE2	1.76	0.67
1:A:117:ARG:HD2	3:A:528:HOH:O	1.95	0.67
1:A:125:ILE:HG12	1:D:132:THR:HG21	1.78	0.66
1:D:113:ILE:CG2	1:D:117:ARG:HB3	2.26	0.66
1:B:125:ILE:CD1	1:C:132:THR:HG21	2.25	0.66
1:A:149:VAL:CG2	1:D:125:ILE:HG21	2.26	0.65
1:A:55:THR:OG1	1:A:56:PRO:HD3	1.95	0.65
1:C:202:PHE:CE2	1:C:206:LEU:HD11	2.32	0.65
1:D:134:LEU:O	1:D:138:GLU:HG3	1.98	0.64
1:B:24:VAL:HG22	1:B:44:LEU:HD12	1.80	0.64
1:A:79:HIS:HE1	1:A:173:LEU:HD12	1.61	0.63
1:A:19:ASN:HB2	3:A:426:HOH:O	1.97	0.63
1:B:114:PRO:O	1:B:117:ARG:HB2	1.99	0.62
1:B:116:GLU:H	1:B:116:GLU:CD	2.03	0.61
1:A:122:ILE:O	1:A:125:ILE:HD12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:ARG:HG3	1:D:192:ARG:HH11	1.66	0.60
1:D:72:VAL:HG13	1:D:183:ILE:HD12	1.84	0.60
1:D:132:THR:O	1:D:136:LEU:HG	2.02	0.60
1:D:113:ILE:HG23	1:D:117:ARG:HB3	1.84	0.60
1:B:50:LYS:HB3	1:B:208:TYR:CD2	2.37	0.59
1:C:3:ILE:HD13	1:C:192:ARG:HD2	1.82	0.59
1:B:149:VAL:CB	1:C:125:ILE:HD12	2.30	0.58
1:C:195:LYS:HD3	1:C:220:VAL:HG12	1.84	0.58
1:B:125:ILE:HD12	1:C:149:VAL:HB	1.84	0.58
1:B:132:THR:HG21	1:C:125:ILE:CD1	2.33	0.58
1:C:130:TYR:CE2	1:C:134:LEU:HD11	2.39	0.58
1:D:167:LEU:HD11	1:D:190:ILE:HG21	1.85	0.58
1:C:117:ARG:O	1:C:121:LYS:HG2	2.04	0.57
1:D:167:LEU:HD11	1:D:190:ILE:CG2	2.35	0.57
1:B:137:ILE:HD11	1:B:143:ARG:HG2	1.86	0.57
1:C:106:LEU:HD22	1:C:118:VAL:HG21	1.86	0.57
1:C:143:ARG:HB3	1:C:143:ARG:NH1	2.20	0.57
1:D:130:TYR:O	1:D:133:TYR:HB3	2.04	0.56
1:C:151:PRO:HB2	1:C:153:ASN:OD1	2.06	0.56
1:A:42:ARG:HG2	1:A:42:ARG:HH11	1.71	0.55
1:C:128:LYS:HA	1:C:131:ARG:NH1	2.22	0.55
1:D:38:GLU:HG3	1:D:200:TRP:CH2	2.41	0.55
1:D:40:ARG:HH11	1:D:40:ARG:HG2	1.71	0.55
1:A:149:VAL:HG23	1:D:125:ILE:HG21	1.87	0.55
1:A:5:ILE:HD11	1:A:189:ALA:HB2	1.88	0.55
1:B:210:TYR:CE2	1:B:215:LEU:HB2	2.42	0.54
1:A:25:ARG:NH2	3:A:570:HOH:O	2.39	0.54
1:D:127:ASP:OD1	1:D:131:ARG:HD3	2.07	0.54
1:B:125:ILE:HD11	1:C:132:THR:HG21	1.89	0.54
1:D:126:VAL:HG21	1:D:153:ASN:HD21	1.73	0.54
1:A:106:LEU:HD11	1:A:118:VAL:HG11	1.90	0.54
1:A:104:GLU:HA	1:A:107:GLU:HG3	1.89	0.53
1:D:42:ARG:O	1:D:46:GLU:HG3	2.09	0.53
1:D:145:VAL:O	1:D:148:ILE:HG12	2.07	0.53
1:A:175:ALA:HA	1:A:214:ILE:HD11	1.91	0.53
1:B:125:ILE:HD12	1:C:149:VAL:CG1	2.38	0.53
1:B:144:GLU:HA	1:B:147:ARG:HH11	1.73	0.53
1:B:118:VAL:HG13	1:C:136:LEU:HD22	1.90	0.52
1:D:42:ARG:HG2	1:D:200:TRP:CD2	2.43	0.52
1:B:54:GLU:OE1	1:B:165:ARG:HD3	2.09	0.52
1:D:105:ARG:HD2	1:D:105:ARG:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASP:OD2	1:A:131:ARG:NH1	2.42	0.52
1:A:104:GLU:O	1:A:107:GLU:HG3	2.10	0.52
1:B:5:ILE:HD11	1:B:189:ALA:HB2	1.92	0.52
1:D:199:PRO:O	1:D:203:GLU:HG3	2.09	0.52
1:C:106:LEU:H	1:C:106:LEU:HD12	1.74	0.52
1:C:165:ARG:HA	1:C:168:MSE:HE3	1.92	0.51
1:D:113:ILE:HD13	1:D:121:LYS:HE3	1.93	0.51
1:A:125:ILE:HD12	1:A:126:VAL:H	1.75	0.51
1:C:14:VAL:HG13	1:D:25:ARG:NH2	2.26	0.51
1:D:117:ARG:HD2	1:D:121:LYS:HE2	1.93	0.51
1:D:180:GLN:O	1:D:183:ILE:HG22	2.10	0.51
1:C:3:ILE:CD1	1:C:192:ARG:HD2	2.41	0.51
1:A:105:ARG:HD2	1:A:105:ARG:O	2.11	0.51
1:B:13:LEU:HD21	1:B:16:VAL:CG2	2.41	0.51
1:B:127:ASP:OD2	1:B:131:ARG:NH1	2.39	0.50
1:B:165:ARG:HA	1:B:168:MSE:HE3	1.93	0.50
1:C:106:LEU:O	1:C:108:GLY:N	2.44	0.50
1:D:62:PHE:O	1:D:161:THR:HA	2.11	0.50
1:A:46:GLU:O	1:A:50:LYS:HG3	2.12	0.50
1:B:113:ILE:HG12	1:C:139:SER:OG	2.12	0.50
1:B:125:ILE:HD12	1:C:149:VAL:CB	2.42	0.50
1:B:29:VAL:O	1:B:29:VAL:HG12	2.12	0.50
1:B:79:HIS:HE1	1:B:173:LEU:HD12	1.77	0.49
1:A:127:ASP:O	1:A:131:ARG:HG3	2.11	0.49
1:B:145:VAL:O	1:B:148:ILE:HG12	2.11	0.49
1:A:96:TYR:HH	1:A:133:TYR:HH	1.60	0.49
1:D:4:ASP:O	1:D:5:ILE:HD13	2.13	0.49
1:B:44:LEU:C	1:B:44:LEU:HD13	2.33	0.49
1:C:218:VAL:HG12	1:C:219:GLN:N	2.28	0.48
1:B:89:GLY:O	1:B:147:ARG:HD3	2.14	0.48
1:B:117:ARG:HA	1:B:117:ARG:HE	1.79	0.48
1:D:211:LYS:HB3	1:D:211:LYS:NZ	2.29	0.48
1:A:50:LYS:NZ	3:A:523:HOH:O	2.46	0.48
1:D:1:MSE:HE1	1:D:196:GLU:CG	2.34	0.48
1:C:195:LYS:CE	1:C:220:VAL:HG12	2.44	0.47
1:C:128:LYS:HA	1:C:131:ARG:HH11	1.79	0.47
1:B:132:THR:CG2	1:C:125:ILE:HD13	2.41	0.47
1:A:145:VAL:O	1:A:148:ILE:HG12	2.16	0.46
1:B:50:LYS:HB3	1:B:208:TYR:CG	2.50	0.46
1:D:40:ARG:NH1	1:D:40:ARG:HG2	2.30	0.46
1:B:126:VAL:HG21	1:B:153:ASN:HD21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ARG:HD2	3:B:351:HOH:O	2.14	0.46
1:D:13:LEU:HD11	1:D:16:VAL:CG2	2.46	0.46
1:B:149:VAL:HG11	1:C:125:ILE:HD11	1.98	0.46
1:C:8:LYS:HD3	1:C:97:GLU:OE1	2.16	0.45
1:A:104:GLU:OE1	1:A:104:GLU:N	2.50	0.45
1:A:143:ARG:NH1	3:A:520:HOH:O	2.50	0.45
1:A:50:LYS:HG2	1:A:208:TYR:CD2	2.52	0.45
1:D:137:ILE:HD13	1:D:143:ARG:NH1	2.32	0.45
1:C:90:ARG:O	1:C:143:ARG:HD2	2.16	0.45
1:C:143:ARG:HH11	1:C:143:ARG:CB	2.30	0.45
1:B:125:ILE:HD12	1:C:149:VAL:HG11	1.97	0.45
1:A:161:THR:OG1	1:B:59:HIS:ND1	2.46	0.45
1:A:116:GLU:CD	1:A:116:GLU:H	2.21	0.44
1:C:62:PHE:O	1:C:161:THR:HA	2.17	0.44
1:B:54:GLU:HB3	1:B:165:ARG:HG3	2.00	0.44
1:D:72:VAL:HG13	1:D:183:ILE:CD1	2.46	0.44
1:A:149:VAL:HG22	1:D:125:ILE:HG21	2.00	0.44
1:D:192:ARG:CG	1:D:192:ARG:HH11	2.30	0.44
1:C:117:ARG:HH11	1:C:117:ARG:HG3	1.81	0.44
1:A:121:LYS:HD3	1:D:135:GLU:OE2	2.17	0.44
1:C:210:TYR:CE2	1:C:215:LEU:HB2	2.52	0.44
1:D:74:ARG:HD3	3:D:333:HOH:O	2.17	0.44
1:D:186:TYR:O	1:D:190:ILE:HG12	2.18	0.44
1:D:210:TYR:CE2	1:D:215:LEU:HB2	2.53	0.44
1:B:125:ILE:HG21	1:C:129:ALA:HA	1.99	0.44
1:A:121:LYS:O	1:A:125:ILE:HG13	2.18	0.43
1:A:122:ILE:O	1:A:125:ILE:CD1	2.66	0.43
1:B:42:ARG:HH11	1:B:42:ARG:CG	2.27	0.43
1:A:125:ILE:HD12	1:A:126:VAL:N	2.33	0.43
1:C:143:ARG:CB	1:C:143:ARG:NH1	2.82	0.43
1:C:120:GLU:O	1:C:124:GLU:HG3	2.18	0.42
1:C:66:VAL:O	1:C:157:ARG:HA	2.19	0.42
1:A:66:VAL:O	1:A:157:ARG:HA	2.20	0.42
1:C:11:VAL:HG11	1:C:190:ILE:HD13	2.01	0.42
1:D:54:GLU:HB3	1:D:165:ARG:HG3	2.01	0.42
2:B:310:FAD:O4	1:C:88:SER:HB2	2.19	0.42
1:C:195:LYS:CD	1:C:220:VAL:HG12	2.47	0.42
1:A:44:LEU:O	1:A:48:LEU:HG	2.19	0.42
1:A:5:ILE:HG22	1:A:6:LEU:HG	2.01	0.42
1:D:55:THR:N	1:D:56:PRO:CD	2.83	0.42
1:C:150:LEU:HA	1:C:151:PRO:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:TYR:CE2	1:B:160:TRP:CD1	3.07	0.42
1:A:69:PRO:HD3	1:A:155:TYR:CE2	2.55	0.42
1:A:168:MSE:HB3	1:A:205:PHE:CE1	2.55	0.42
1:A:13:LEU:HD21	1:A:16:VAL:CG2	2.50	0.42
1:B:78:ARG:HD2	1:B:78:ARG:HA	1.90	0.42
1:C:21:LEU:O	1:C:25:ARG:HG3	2.20	0.42
1:A:55:THR:N	1:A:56:PRO:CD	2.83	0.42
1:A:181:TRP:O	1:A:185:GLN:HG2	2.20	0.41
1:C:106:LEU:CD2	1:C:118:VAL:HG21	2.50	0.41
1:A:117:ARG:O	1:A:121:LYS:HG3	2.21	0.41
1:B:192:ARG:HD3	3:B:569:HOH:O	2.21	0.41
1:B:50:LYS:HG3	1:B:51:HIS:ND1	2.35	0.41
1:B:5:ILE:HG22	1:B:6:LEU:HG	2.02	0.41
1:C:106:LEU:N	1:C:106:LEU:HD12	2.35	0.41
1:B:70:ILE:O	1:B:74:ARG:HG3	2.21	0.41
1:B:136:LEU:HD22	1:C:118:VAL:HG13	2.03	0.41
1:C:176:ASP:OD2	1:C:178:HIS:HB2	2.21	0.41
1:A:142:PRO:HG3	1:D:109:TYR:CE2	2.56	0.41
1:B:144:GLU:HA	1:B:147:ARG:NH1	2.36	0.41
1:C:57:PHE:O	1:C:164:ALA:HB3	2.21	0.41
1:B:192:ARG:HG2	1:B:220:VAL:CG1	2.39	0.41
1:B:125:ILE:CD1	1:C:149:VAL:HG11	2.51	0.40
1:C:84:TYR:CE2	1:C:160:TRP:CD1	3.09	0.40
1:D:127:ASP:OD1	1:D:131:ARG:NH1	2.40	0.40
1:A:10:PHE:CD2	1:A:10:PHE:C	2.94	0.40
1:A:104:GLU:CA	1:A:107:GLU:HG3	2.51	0.40
1:D:151:PRO:HG2	1:D:153:ASN:OD1	2.22	0.40
1:D:55:THR:OG1	1:D:56:PRO:HD3	2.20	0.40
1:B:1:MSE:HG3	3:B:498:HOH:O	2.22	0.40
1:C:5:ILE:HD11	1:C:189:ALA:HB2	2.03	0.40
1:A:171:LEU:O	1:A:175:ALA:HB3	2.21	0.40
1:D:10:PHE:C	1:D:10:PHE:CD2	2.95	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	197/232 (85%)	192 (98%)	5 (2%)	0	100 100
1	B	205/232 (88%)	199 (97%)	6 (3%)	0	100 100
1	C	208/232 (90%)	198 (95%)	7 (3%)	3 (1%)	11 7
1	D	206/232 (89%)	202 (98%)	4 (2%)	0	100 100
All	All	816/928 (88%)	791 (97%)	22 (3%)	3 (0%)	34 37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	95	SER
1	C	107	GLU
1	C	108	GLY

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	180/201 (90%)	175 (97%)	5 (3%)	43 52
1	B	185/201 (92%)	179 (97%)	6 (3%)	39 47
1	C	187/201 (93%)	186 (100%)	1 (0%)	88 92
1	D	183/201 (91%)	177 (97%)	6 (3%)	38 46
All	All	735/804 (91%)	717 (98%)	18 (2%)	49 58

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

Mol	Chain	Res	Type
1	A	44	LEU
1	A	87	LEU
1	A	105	ARG

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Mol	Chain	Res	Type
1	A	125	ILE
1	A	192	ARG
1	B	106	LEU
1	B	117	ARG
1	B	125	ILE
1	B	138	GLU
1	B	165	ARG
1	B	192	ARG
1	C	125	ILE
1	D	44	LEU
1	D	87	LEU
1	D	105	ARG
1	D	117	ARG
1	D	154	LEU
1	D	165	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates 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	D	300	-	51,58,58	2.24	15 (29%)	60,89,89	2.07	11 (18%)
2	FAD	C	305	-	51,58,58	2.26	15 (29%)	60,89,89	2.07	11 (18%)
2	FAD	A	315	-	51,58,58	2.32	17 (33%)	60,89,89	2.04	11 (18%)
2	FAD	B	310	-	51,58,58	2.30	14 (27%)	60,89,89	2.07	12 (20%)

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	D	300	-	1/1/9/9	8/30/50/50	0/6/6/6
2	FAD	C	305	-	1/1/9/9	8/30/50/50	0/6/6/6
2	FAD	A	315	-	1/1/9/9	8/30/50/50	0/6/6/6
2	FAD	B	310	-	1/1/9/9	9/30/50/50	0/6/6/6

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	315	FAD	C4X-C10	7.61	1.46	1.38
2	D	300	FAD	C4X-C10	7.45	1.46	1.38
2	B	310	FAD	C4X-C10	7.37	1.46	1.38
2	C	305	FAD	C4X-C10	7.35	1.46	1.38
2	C	305	FAD	C4-N3	5.23	1.42	1.33
2	B	310	FAD	C4A-N3A	5.21	1.42	1.35
2	A	315	FAD	C4-N3	5.05	1.41	1.33
2	B	310	FAD	C4-N3	4.98	1.41	1.33
2	A	315	FAD	C4A-N3A	4.94	1.42	1.35
2	D	300	FAD	C4A-N3A	4.93	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	305	FAD	C4A-N3A	4.85	1.42	1.35
2	D	300	FAD	C4-N3	4.83	1.41	1.33
2	A	315	FAD	C2B-C1B	4.71	1.60	1.53
2	B	310	FAD	C2B-C1B	4.38	1.60	1.53
2	C	305	FAD	C2B-C1B	4.35	1.60	1.53
2	D	300	FAD	C2B-C1B	4.31	1.60	1.53
2	D	300	FAD	C10-N1	4.28	1.38	1.33
2	B	310	FAD	C4X-N5	4.26	1.39	1.33
2	A	315	FAD	C4X-N5	4.06	1.39	1.33
2	A	315	FAD	C10-N1	4.03	1.38	1.33
2	C	305	FAD	C10-N1	3.95	1.38	1.33
2	B	310	FAD	C10-N1	3.91	1.38	1.33
2	C	305	FAD	C4X-N5	3.83	1.38	1.33
2	D	300	FAD	C4X-N5	3.51	1.38	1.33
2	B	310	FAD	C4-C4X	3.37	1.47	1.41
2	D	300	FAD	C8A-N7A	-3.36	1.28	1.34
2	C	305	FAD	C9A-N10	3.20	1.42	1.38
2	A	315	FAD	C9A-N10	3.14	1.42	1.38
2	A	315	FAD	C4-C4X	3.12	1.46	1.41
2	A	315	FAD	C8A-N7A	-3.08	1.29	1.34
2	B	310	FAD	C8A-N7A	-3.05	1.29	1.34
2	C	305	FAD	C4-C4X	3.04	1.46	1.41
2	A	315	FAD	C2A-N3A	3.02	1.37	1.32
2	D	300	FAD	C4-C4X	3.00	1.46	1.41
2	D	300	FAD	C2A-N3A	2.94	1.36	1.32
2	B	310	FAD	C9A-N10	2.92	1.42	1.38
2	D	300	FAD	C9A-N10	2.89	1.42	1.38
2	C	305	FAD	C2A-N3A	2.88	1.36	1.32
2	C	305	FAD	C8A-N7A	-2.85	1.29	1.34
2	B	310	FAD	C2A-N3A	2.78	1.36	1.32
2	C	305	FAD	O4B-C1B	2.65	1.44	1.41
2	B	310	FAD	O4B-C1B	2.43	1.44	1.41
2	B	310	FAD	C8-C7	2.35	1.46	1.40
2	B	310	FAD	C5X-N5	2.33	1.39	1.35
2	C	305	FAD	C8-C7	2.32	1.46	1.40
2	A	315	FAD	O4B-C1B	2.31	1.44	1.41
2	B	310	FAD	C6-C7	2.31	1.43	1.37
2	A	315	FAD	C8-C7	2.29	1.46	1.40
2	D	300	FAD	O5B-C5B	2.20	1.53	1.44
2	A	315	FAD	C6-C7	2.18	1.43	1.37
2	A	315	FAD	C5X-N5	2.13	1.38	1.35
2	D	300	FAD	O4B-C1B	2.13	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	300	FAD	C8-C7	2.12	1.46	1.40
2	A	315	FAD	C2A-N1A	2.11	1.37	1.33
2	A	315	FAD	C5A-C4A	2.09	1.46	1.40
2	C	305	FAD	C5A-C4A	2.07	1.46	1.40
2	A	315	FAD	C9A-C5X	2.06	1.46	1.42
2	C	305	FAD	C6-C7	2.06	1.43	1.37
2	D	300	FAD	C2A-N1A	2.02	1.37	1.33
2	D	300	FAD	C6-C7	2.01	1.42	1.37
2	C	305	FAD	C2A-N1A	2.00	1.37	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	300	FAD	C4-N3-C2	8.37	122.21	115.14
2	B	310	FAD	C4-N3-C2	8.32	122.17	115.14
2	A	315	FAD	C4-N3-C2	8.25	122.11	115.14
2	C	305	FAD	C4-N3-C2	8.11	121.99	115.14
2	C	305	FAD	C3B-C2B-C1B	-7.95	89.01	100.98
2	A	315	FAD	C3B-C2B-C1B	-7.68	89.42	100.98
2	D	300	FAD	C3B-C2B-C1B	-7.60	89.53	100.98
2	B	310	FAD	C3B-C2B-C1B	-7.33	89.94	100.98
2	B	310	FAD	C4X-C4-N3	-4.99	116.60	123.43
2	C	305	FAD	C4X-C4-N3	-4.99	116.61	123.43
2	A	315	FAD	C4X-C4-N3	-4.98	116.62	123.43
2	D	300	FAD	C4X-C4-N3	-4.97	116.63	123.43
2	A	315	FAD	O2B-C2B-C1B	4.42	127.19	110.85
2	D	300	FAD	O2B-C2B-C1B	4.40	127.11	110.85
2	B	310	FAD	O2B-C2B-C1B	4.40	127.09	110.85
2	C	305	FAD	O2B-C2B-C1B	4.39	127.06	110.85
2	B	310	FAD	C1'-N10-C9A	3.68	121.19	118.29
2	C	305	FAD	C1'-N10-C9A	3.59	121.12	118.29
2	A	315	FAD	C1'-N10-C9A	3.16	120.78	118.29
2	B	310	FAD	C4-C4X-C10	-3.14	117.87	119.95
2	D	300	FAD	P-O5'-C5'	3.05	139.58	121.68
2	D	300	FAD	C1'-N10-C9A	3.05	120.69	118.29
2	A	315	FAD	P-O5'-C5'	2.96	139.01	121.68
2	C	305	FAD	P-O3P-PA	2.81	142.49	132.83
2	B	310	FAD	P-O5'-C5'	2.77	137.94	121.68
2	C	305	FAD	P-O5'-C5'	2.76	137.89	121.68
2	D	300	FAD	C4X-N5-C5X	2.75	119.52	116.77
2	A	315	FAD	C4-C4X-C10	-2.74	118.14	119.95
2	C	305	FAD	C4X-N5-C5X	2.71	119.48	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	310	FAD	P-O3P-PA	2.71	142.13	132.83
2	C	305	FAD	C4-C4X-C10	-2.63	118.21	119.95
2	A	315	FAD	C4X-N5-C5X	2.59	119.36	116.77
2	D	300	FAD	P-O3P-PA	2.53	141.50	132.83
2	B	310	FAD	C4X-N5-C5X	2.51	119.28	116.77
2	B	310	FAD	O3B-C3B-C4B	2.51	118.30	111.05
2	B	310	FAD	N3A-C2A-N1A	-2.50	124.77	128.68
2	D	300	FAD	O3B-C3B-C4B	2.49	118.25	111.05
2	D	300	FAD	C4-C4X-C10	-2.49	118.31	119.95
2	D	300	FAD	N3A-C2A-N1A	-2.31	125.07	128.68
2	A	315	FAD	O3B-C3B-C4B	2.29	117.67	111.05
2	A	315	FAD	N3A-C2A-N1A	-2.24	125.18	128.68
2	C	305	FAD	N3A-C2A-N1A	-2.22	125.22	128.68
2	A	315	FAD	P-O3P-PA	2.19	140.35	132.83
2	C	305	FAD	O3B-C3B-C4B	2.07	117.05	111.05
2	B	310	FAD	C4-C4X-N5	2.06	120.96	118.60

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	300	FAD	C1B
2	C	305	FAD	C1B
2	A	315	FAD	C1B
2	B	310	FAD	C1B

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	300	FAD	C1'-C2'-C3'-O3'
2	D	300	FAD	C1'-C2'-C3'-C4'
2	D	300	FAD	O2'-C2'-C3'-O3'
2	D	300	FAD	O2'-C2'-C3'-C4'
2	D	300	FAD	C3'-C4'-C5'-O5'
2	D	300	FAD	O4'-C4'-C5'-O5'
2	C	305	FAD	C1'-C2'-C3'-O3'
2	C	305	FAD	C1'-C2'-C3'-C4'
2	C	305	FAD	O2'-C2'-C3'-O3'
2	C	305	FAD	O2'-C2'-C3'-C4'
2	C	305	FAD	C3'-C4'-C5'-O5'
2	A	315	FAD	C1'-C2'-C3'-O3'
2	A	315	FAD	C1'-C2'-C3'-C4'
2	A	315	FAD	O2'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
2	A	315	FAD	O2'-C2'-C3'-C4'
2	A	315	FAD	C3'-C4'-C5'-O5'
2	B	310	FAD	C1'-C2'-C3'-O3'
2	B	310	FAD	C1'-C2'-C3'-C4'
2	B	310	FAD	O2'-C2'-C3'-O3'
2	B	310	FAD	O2'-C2'-C3'-C4'
2	B	310	FAD	C3'-C4'-C5'-O5'
2	D	300	FAD	C4'-C5'-O5'-P
2	D	300	FAD	PA-O3P-P-O1P
2	C	305	FAD	PA-O3P-P-O1P
2	A	315	FAD	PA-O3P-P-O1P
2	B	310	FAD	PA-O3P-P-O1P
2	A	315	FAD	O4'-C4'-C5'-O5'
2	B	310	FAD	C4'-C5'-O5'-P
2	C	305	FAD	C4'-C5'-O5'-P
2	A	315	FAD	C4'-C5'-O5'-P
2	C	305	FAD	O4'-C4'-C5'-O5'
2	B	310	FAD	O4'-C4'-C5'-O5'
2	B	310	FAD	N10-C1'-C2'-O2'

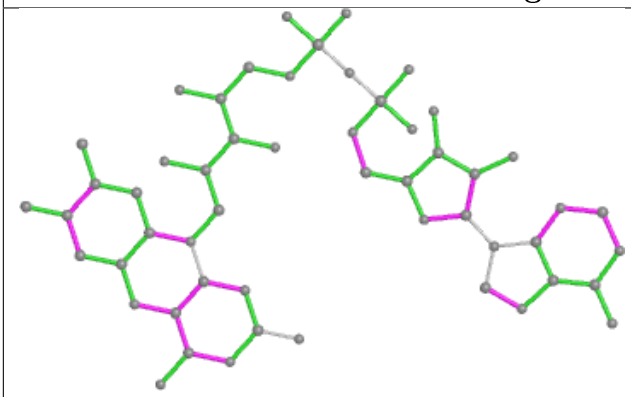
There are no ring outliers.

1 monomer is involved in 1 short contact:

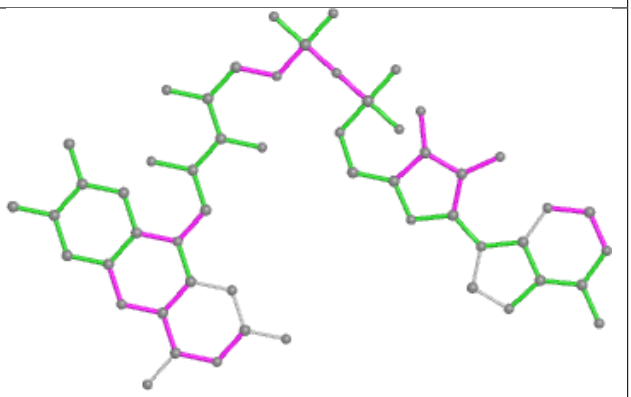
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	310	FAD	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

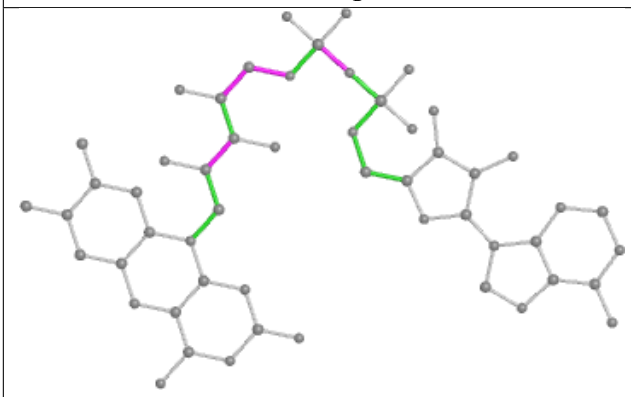
Ligand FAD D 300



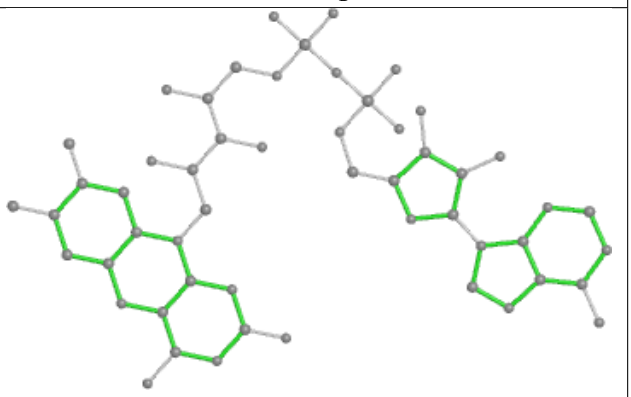
Bond lengths



Bond angles

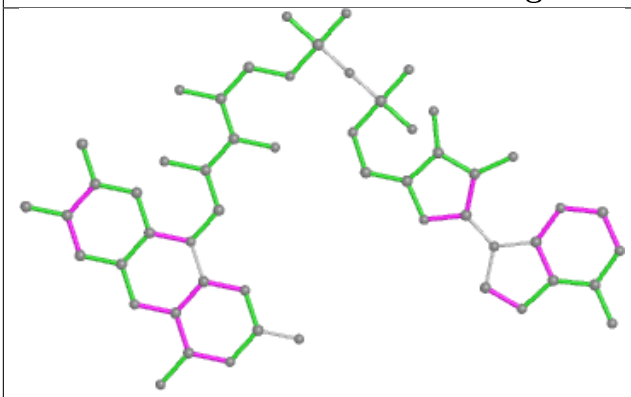


Torsions

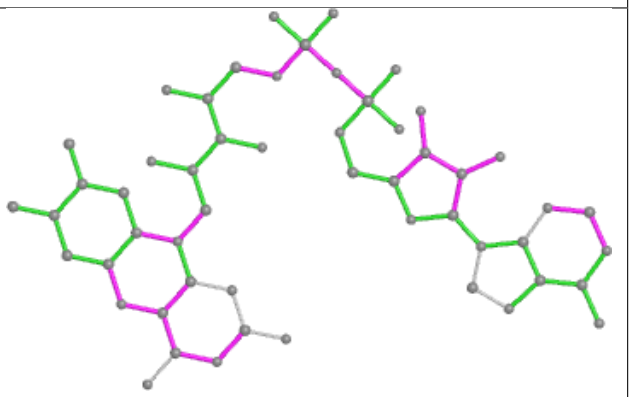


Rings

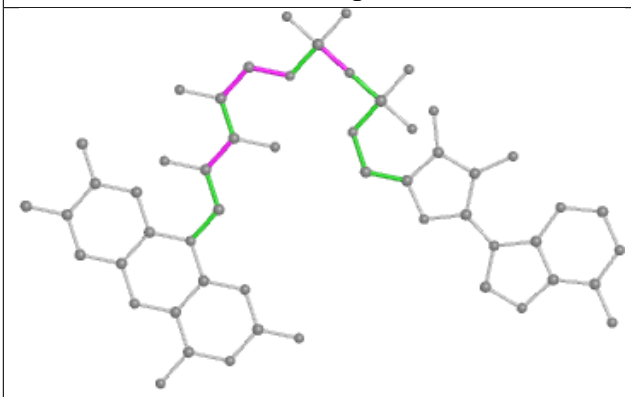
Ligand FAD C 305



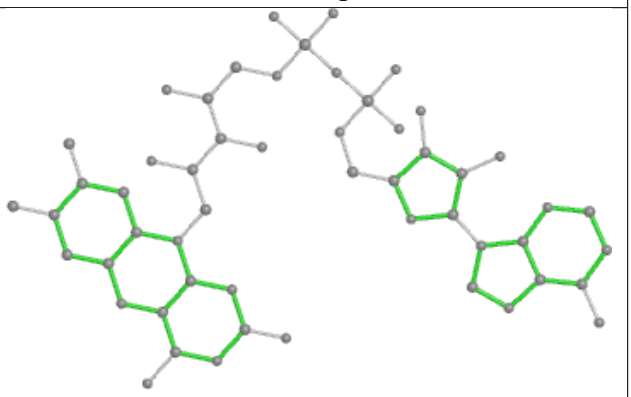
Bond lengths



Bond angles

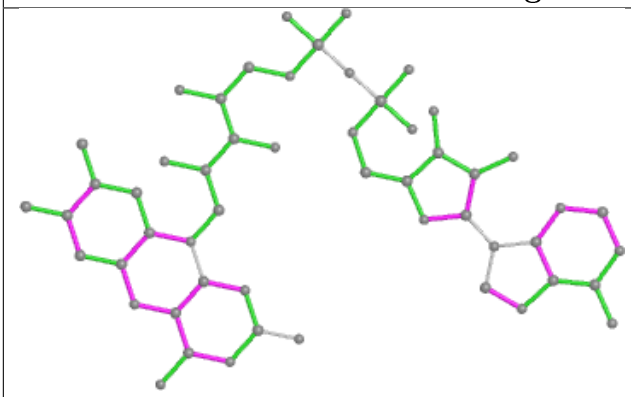


Torsions

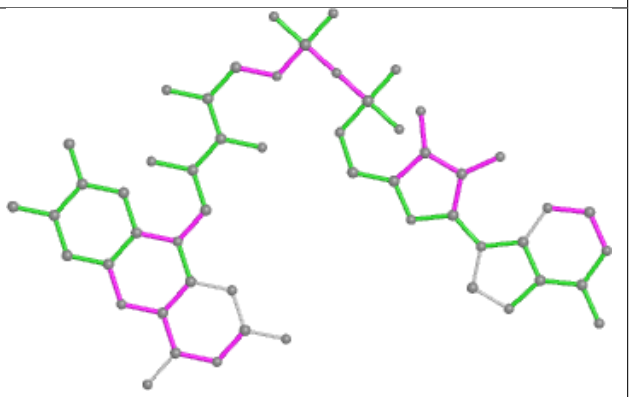


Rings

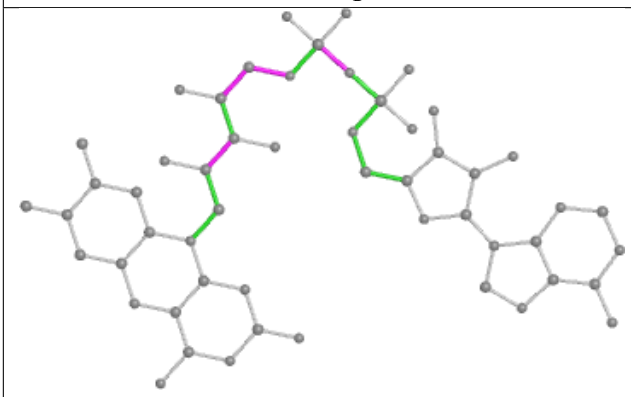
Ligand FAD A 315



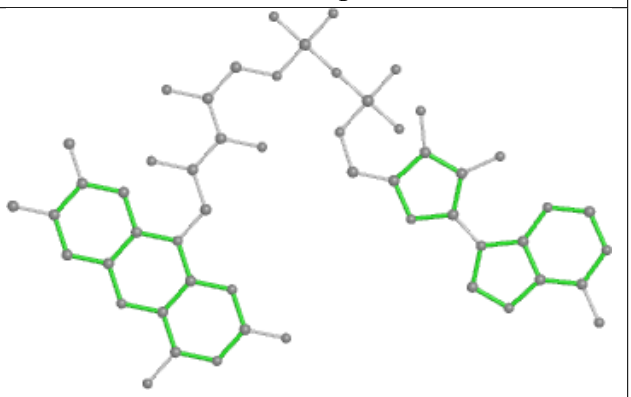
Bond lengths



Bond angles

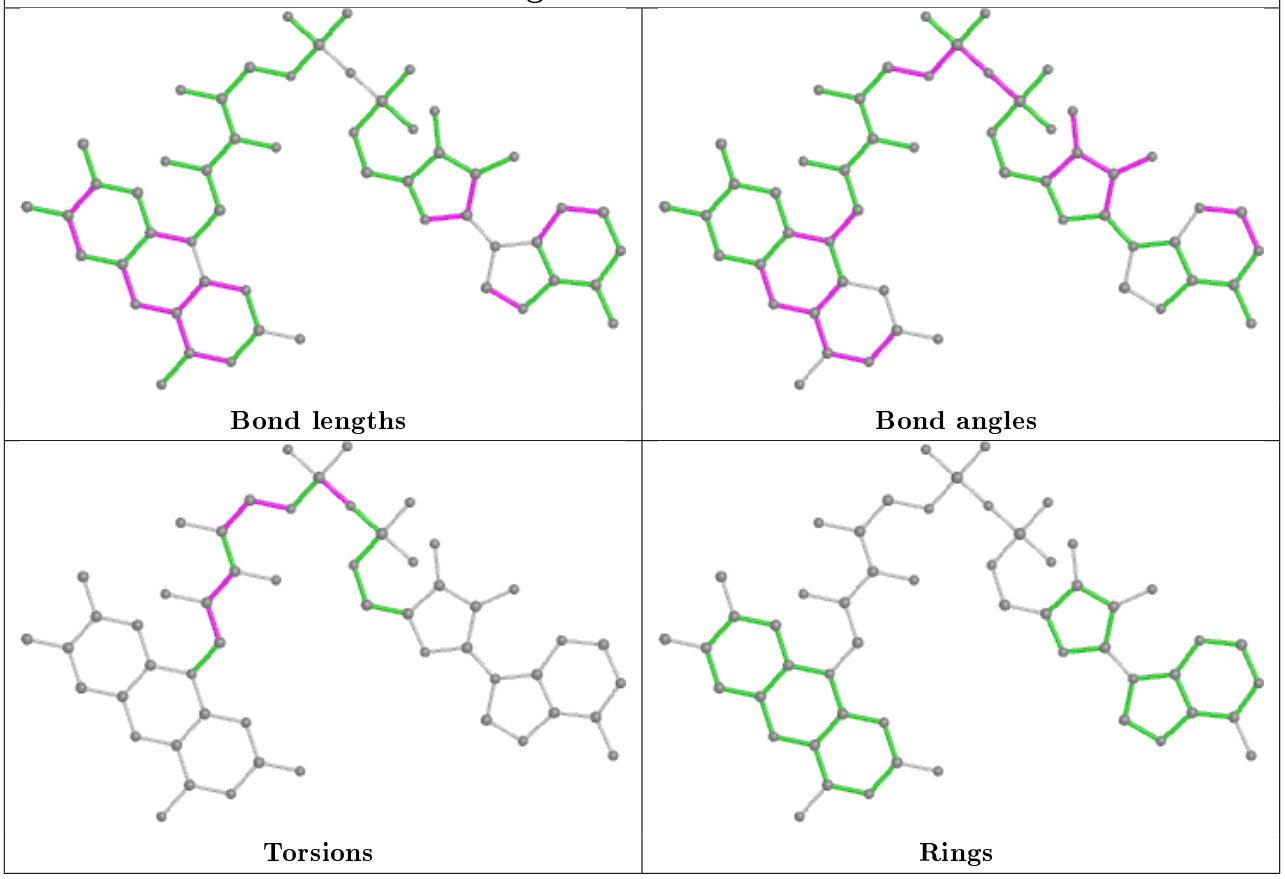


Torsions



Rings

Ligand FAD B 310



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	199/232 (85%)	0.02	6 (3%)	50	53	11, 25, 48, 59	0
1	B	207/232 (89%)	0.11	11 (5%)	26	29	13, 27, 56, 66	0
1	C	210/232 (90%)	0.07	12 (5%)	23	25	11, 24, 52, 66	0
1	D	206/232 (88%)	0.15	15 (7%)	15	15	13, 27, 54, 64	0
All	All	822/928 (88%)	0.09	44 (5%)	25	28	11, 26, 54, 66	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	ARG	4.3
1	B	107	GLU	4.0
1	C	138	GLU	3.7
1	D	40	ARG	3.7
1	B	91	TYR	3.6
1	C	220	VAL	3.6
1	B	219	GLN	3.6
1	A	88	SER	3.5
1	C	107	GLU	3.5
1	B	40	ARG	3.4
1	D	89	GLY	3.3
1	A	110	LYS	3.2
1	D	37	ASP	3.2
1	B	108	GLY	3.2
1	D	94	LEU	3.2
1	C	110	LYS	3.0
1	B	31	PHE	3.0
1	C	31	PHE	3.0
1	D	91	TYR	2.9
1	A	107	GLU	2.8
1	D	39	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	88	SER	2.7
1	D	116	GLU	2.7
1	A	108	GLY	2.7
1	B	220	VAL	2.7
1	B	211	LYS	2.7
1	C	104	GLU	2.6
1	C	109	TYR	2.6
1	D	93	LYS	2.6
1	D	107	GLU	2.5
1	C	136	LEU	2.5
1	D	38	GLU	2.5
1	C	131	ARG	2.2
1	D	178	HIS	2.2
1	D	113	ILE	2.2
1	B	51	HIS	2.2
1	C	219	GLN	2.2
1	A	112	THR	2.1
1	D	108	GLY	2.1
1	D	90	ARG	2.1
1	B	30	SER	2.1
1	C	94	LEU	2.1
1	C	117	ARG	2.1
1	B	112	THR	2.1

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 carbohydrates 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, 95^{th} 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.

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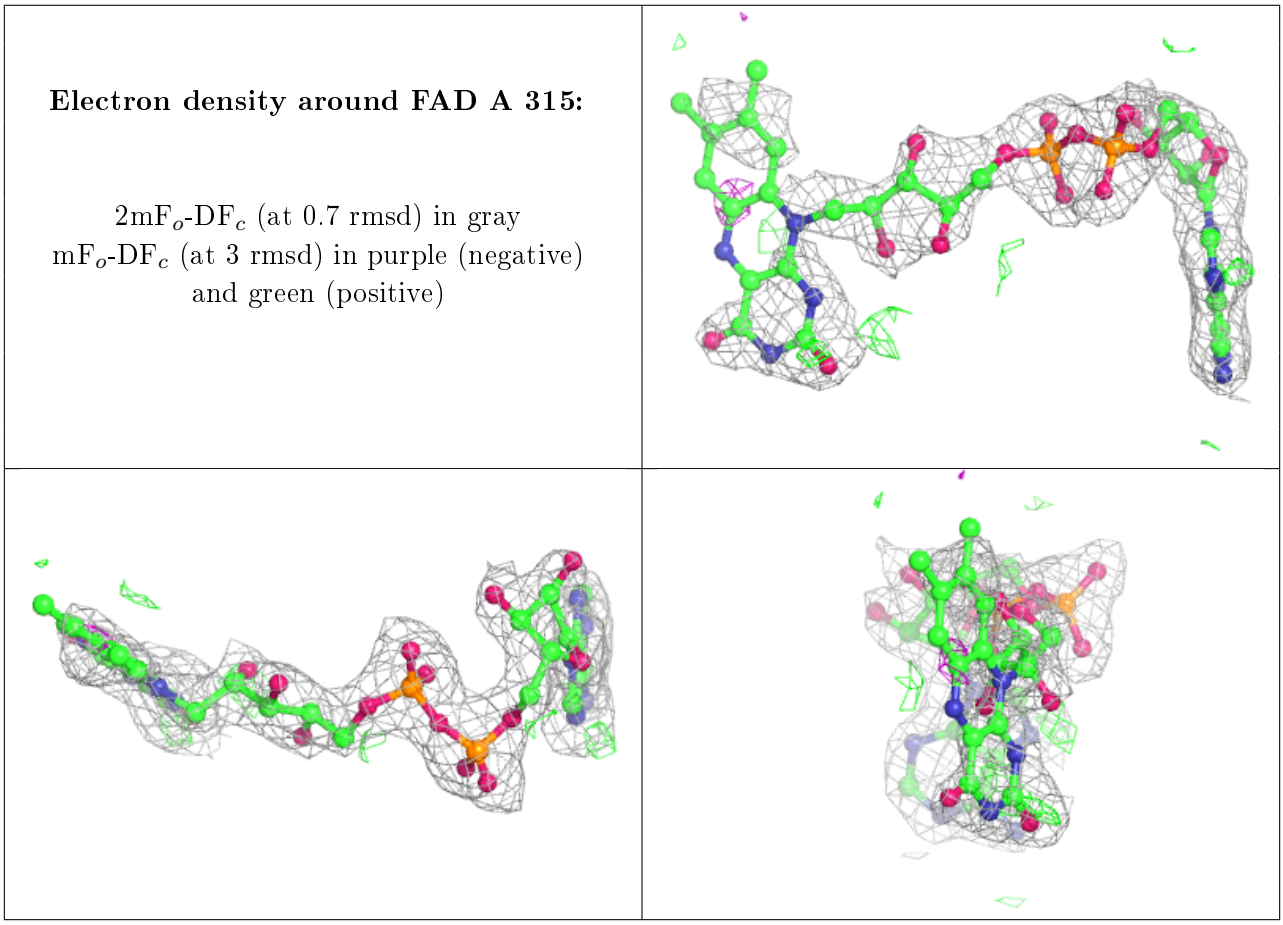
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	A	315	53/53	0.87	0.22	34,45,69,70	0
2	FAD	C	305	53/53	0.88	0.23	30,45,65,66	0
2	FAD	D	300	53/53	0.88	0.21	28,42,64,66	0
2	FAD	B	310	53/53	0.88	0.23	32,45,66,66	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.

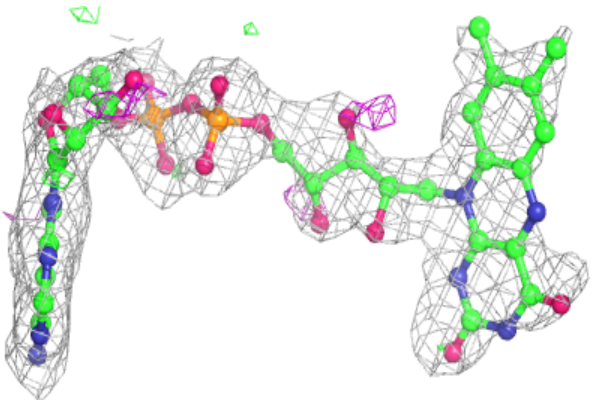
Electron density around FAD A 315:

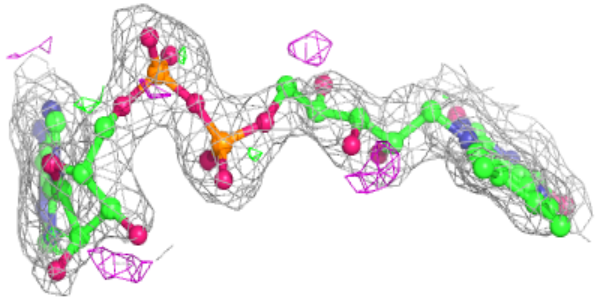
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

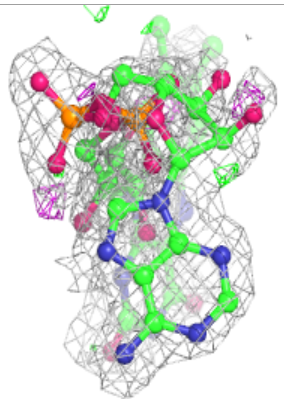


Electron density around FAD C 305:

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

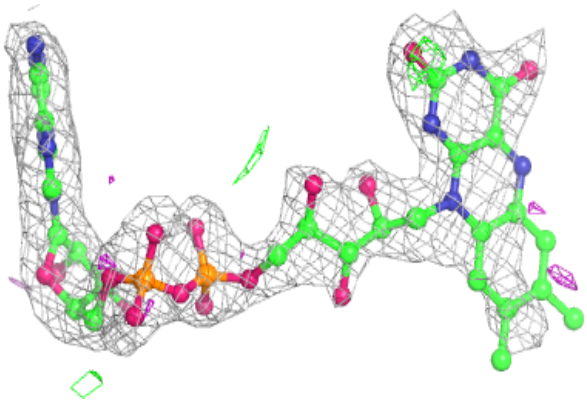


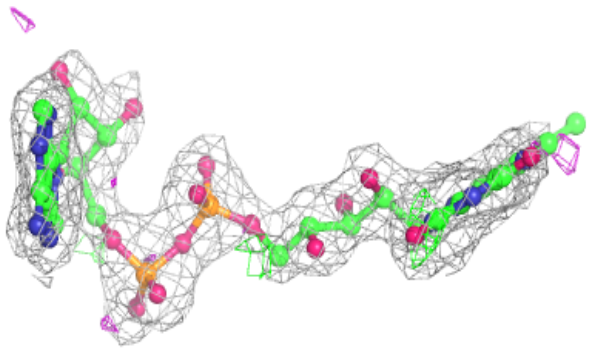




Electron density around FAD D 300:

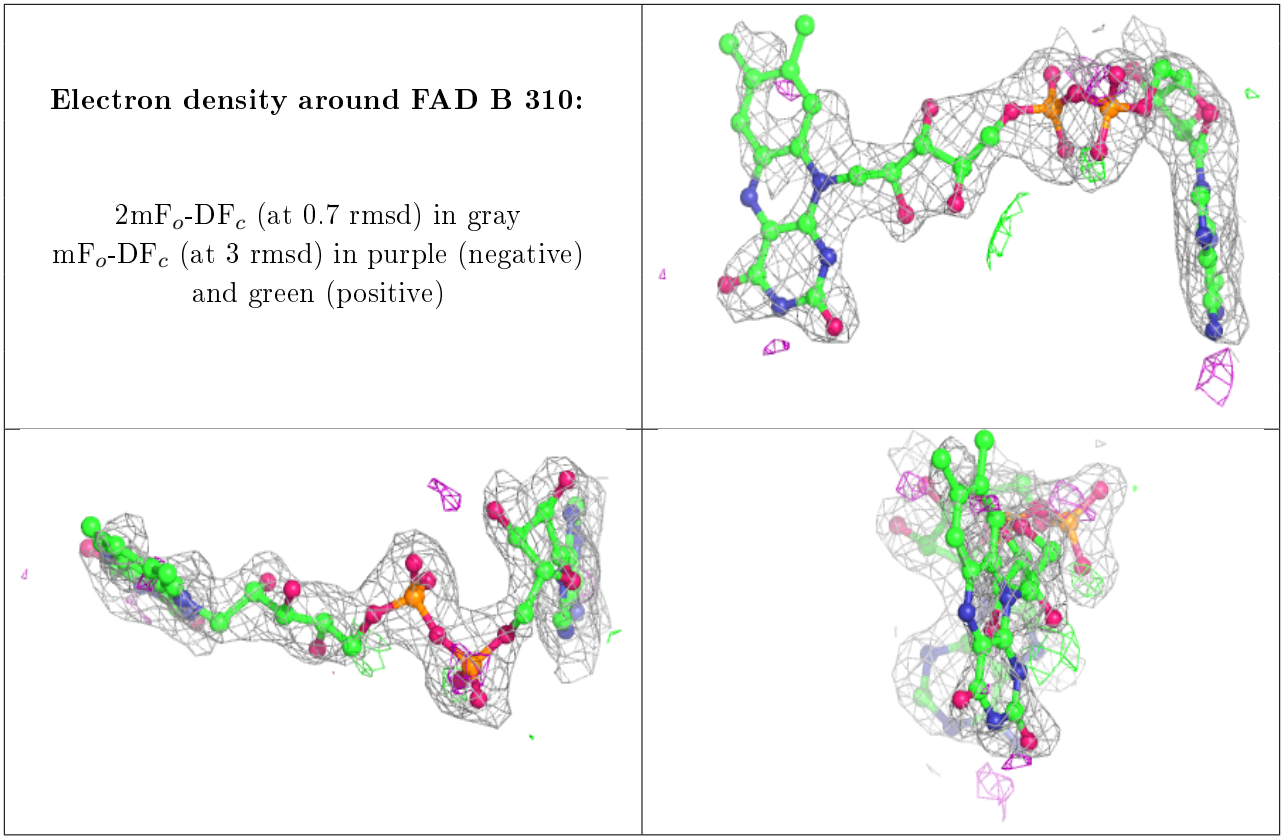
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around FAD B 310:

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



6.5 Other polymers

There are no such residues in this entry.