Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2024 – 01:54 am BST

PDB ID	:	3ZXS
Title	:	Cryptochrome B from Rhodobacter sphaeroides
Authors	:	Geisselbrecht, Y.; Fruhwirth, S.; Pierik, A.J.; Klug, G.; Essen, L.-O.
Deposited on	:	2011-08-15
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

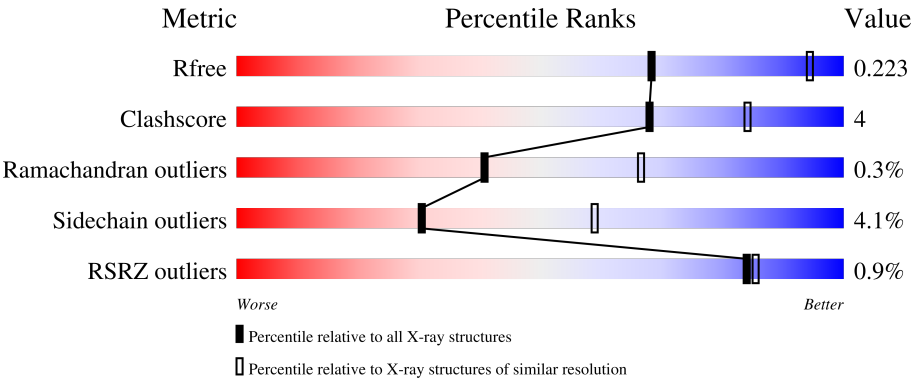
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	522	88% 9% .
1	B	522	87% 9% . .
1	C	522	2% 89% 7% . .

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
5	MG	A	1512	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12654 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 CRYPTOCHROME B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	508	Total	C	N	O	S	0	0	0
			4027	2557	736	711	23			
1	B	508	Total	C	N	O	S	0	0	0
			4015	2544	737	711	23			
1	C	505	Total	C	N	O	S	0	0	0
			3935	2499	706	707	23			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q3IXP1
A	-12	ARG	-	expression tag	UNP Q3IXP1
A	-11	GLY	-	expression tag	UNP Q3IXP1
A	-10	SER	-	expression tag	UNP Q3IXP1
A	-9	HIS	-	expression tag	UNP Q3IXP1
A	-8	HIS	-	expression tag	UNP Q3IXP1
A	-7	HIS	-	expression tag	UNP Q3IXP1
A	-6	HIS	-	expression tag	UNP Q3IXP1
A	-5	HIS	-	expression tag	UNP Q3IXP1
A	-4	HIS	-	expression tag	UNP Q3IXP1
A	-3	GLY	-	expression tag	UNP Q3IXP1
A	-2	ILE	-	expression tag	UNP Q3IXP1
A	-1	ARG	-	expression tag	UNP Q3IXP1
A	0	MET	-	expression tag	UNP Q3IXP1
A	1	LEU	-	expression tag	UNP Q3IXP1
B	-13	MET	-	expression tag	UNP Q3IXP1
B	-12	ARG	-	expression tag	UNP Q3IXP1
B	-11	GLY	-	expression tag	UNP Q3IXP1
B	-10	SER	-	expression tag	UNP Q3IXP1
B	-9	HIS	-	expression tag	UNP Q3IXP1
B	-8	HIS	-	expression tag	UNP Q3IXP1
B	-7	HIS	-	expression tag	UNP Q3IXP1
B	-6	HIS	-	expression tag	UNP Q3IXP1

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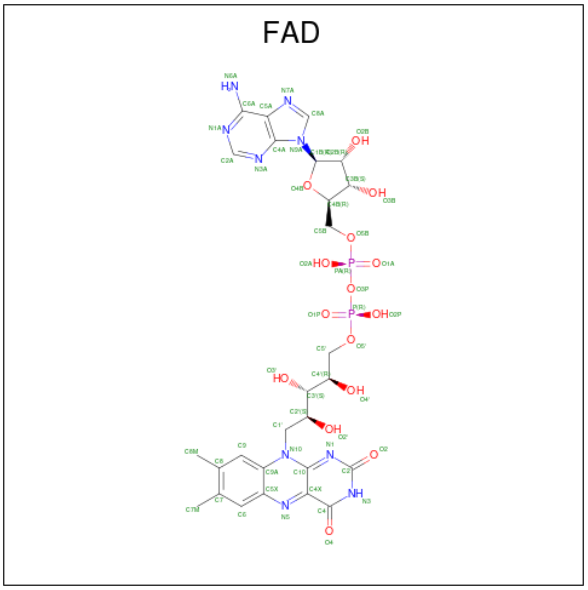
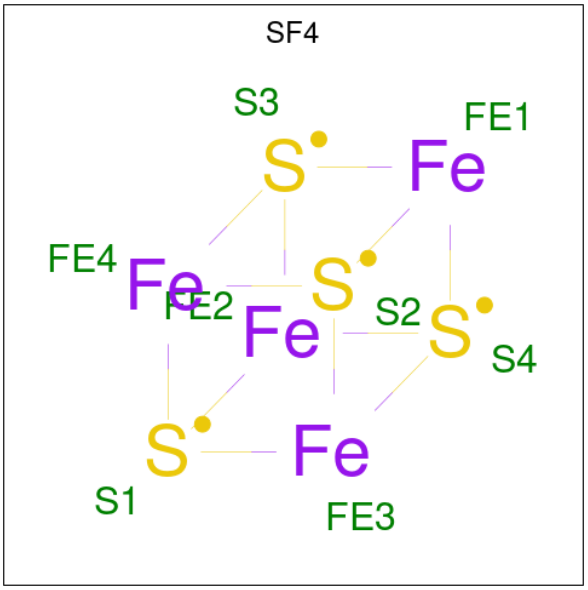
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	expression tag	UNP Q3IXP1
B	-4	HIS	-	expression tag	UNP Q3IXP1
B	-3	GLY	-	expression tag	UNP Q3IXP1
B	-2	ILE	-	expression tag	UNP Q3IXP1
B	-1	ARG	-	expression tag	UNP Q3IXP1
B	0	MET	-	expression tag	UNP Q3IXP1
B	1	LEU	-	expression tag	UNP Q3IXP1
C	-13	MET	-	expression tag	UNP Q3IXP1
C	-12	ARG	-	expression tag	UNP Q3IXP1
C	-11	GLY	-	expression tag	UNP Q3IXP1
C	-10	SER	-	expression tag	UNP Q3IXP1
C	-9	HIS	-	expression tag	UNP Q3IXP1
C	-8	HIS	-	expression tag	UNP Q3IXP1
C	-7	HIS	-	expression tag	UNP Q3IXP1
C	-6	HIS	-	expression tag	UNP Q3IXP1
C	-5	HIS	-	expression tag	UNP Q3IXP1
C	-4	HIS	-	expression tag	UNP Q3IXP1
C	-3	GLY	-	expression tag	UNP Q3IXP1
C	-2	ILE	-	expression tag	UNP Q3IXP1
C	-1	ARG	-	expression tag	UNP Q3IXP1
C	0	MET	-	expression tag	UNP Q3IXP1
C	1	LEU	-	expression tag	UNP Q3IXP1

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



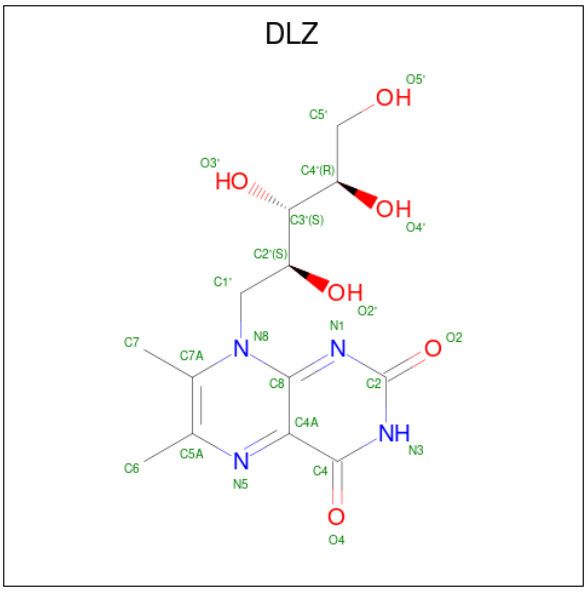
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is 1-deoxy-1-(6,7-dimethyl-2,4-dioxo-3,4-dihydropteridin-8(2H)-yl)-D-ribitol (three-letter code: DLZ) (formula: $C_{13}H_{18}N_4O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 23 13 4 6	0	0
4	B	1	Total C N O 23 13 4 6	0	0
4	C	1	Total C N O 23 13 4 6	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0

- Molecule 6 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Gd 1 1	0	0
6	B	1	Total Gd 1 1	0	0
6	C	1	Total Gd 1 1	0	0

- Molecule 7 is water.

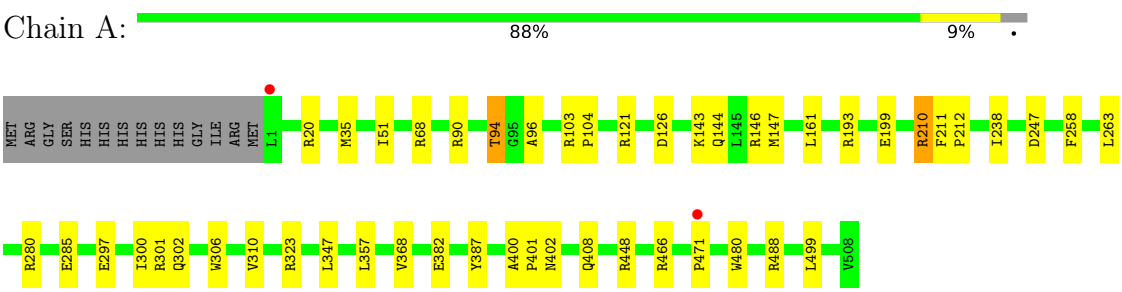
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	179	Total O 179 179	0	0
7	B	146	Total O 148 148	0	2
7	C	92	Total O 92 92	0	0

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.

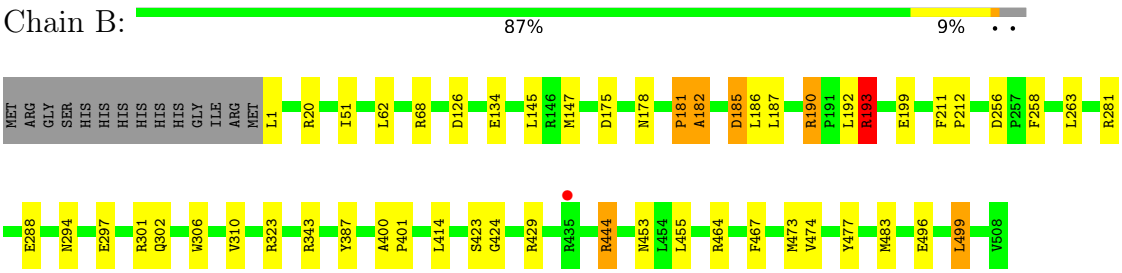
• Molecule 1: CRYPTOCHROME B

Chain A:



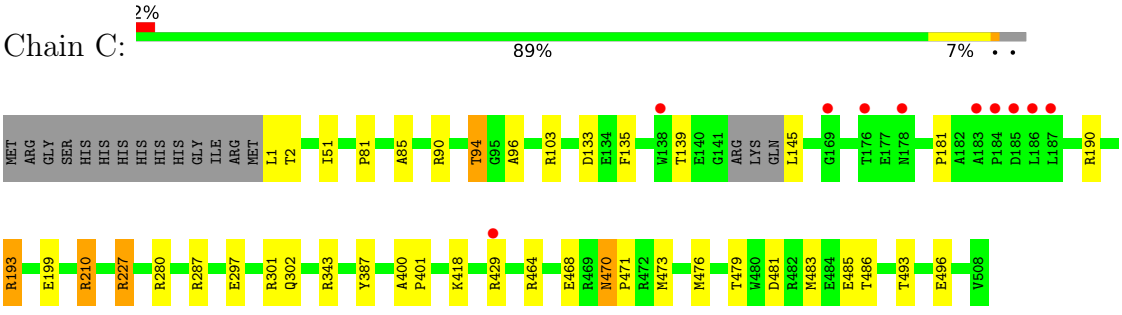
• Molecule 1: CRYPTOCHROME B

Chain B:



• Molecule 1: CRYPTOCHROME B

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	137.84Å 137.84Å 521.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.95 – 2.70 24.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.95-2.70) 99.9 (24.95-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.34 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.198 , 0.228 0.198 , 0.223	Depositor DCC
R_{free} test set	1989 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 35.9	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	0.93	EDS
Total number of atoms	12654	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: DLZ, SF4, MG, GD, 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	0.80	1/4137 (0.0%)	0.78	2/5621 (0.0%)
1	B	0.82	0/4124	0.83	6/5607 (0.1%)
1	C	0.76	0/4042	0.77	2/5502 (0.0%)
All	All	0.79	1/12303 (0.0%)	0.79	10/16730 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	GLU	CD-OE1	5.01	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	175	ASP	CB-CG-OD1	6.54	124.19	118.30
1	B	193	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	190	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	281	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	193	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	181	PRO	N-CA-C	5.27	125.81	112.10
1	B	444	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	227	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	C	227	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	247	ASP	CB-CG-OD1	5.01	122.81	118.30

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	4027	0	3906	27	0
1	B	4015	0	3873	32	0
1	C	3935	0	3753	24	0
2	A	53	0	31	4	0
2	B	53	0	31	2	0
2	C	53	0	31	3	0
3	A	8	0	0	0	0
3	B	8	0	0	0	0
3	C	8	0	0	0	0
4	A	23	0	18	4	0
4	B	23	0	18	6	0
4	C	23	0	18	5	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	179	0	0	2	0
7	B	148	0	0	0	0
7	C	92	0	0	0	0
All	All	12654	0	11679	90	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 4.

All (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:O	1:A:210:ARG:HD3	1.84	0.78
1:C:90:ARG:O	1:C:94:THR:HB	1.84	0.77
1:C:210:ARG:O	1:C:210:ARG:HD3	1.84	0.76
1:B:178:ASN:HD21	1:B:294:ASN:HD22	1.35	0.74
1:C:94:THR:HG22	1:C:96:ALA:H	1.54	0.73
1:C:51:ILE:HD12	4:C:1511:DLZ:H7B	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:ASN:C	1:C:470:ASN:HD22	1.97	0.68
1:C:51:ILE:CD1	4:C:1511:DLZ:H7B	2.24	0.68
1:B:178:ASN:ND2	1:B:294:ASN:HD22	1.92	0.67
1:A:387:TYR:CE1	2:A:1509:FAD:HM73	2.31	0.66
1:B:51:ILE:CD1	4:B:1511:DLZ:H7B	2.27	0.65
1:A:90:ARG:O	1:A:94:THR:HB	1.98	0.63
1:C:297:GLU:OE1	1:C:301:ARG:NH1	2.32	0.62
1:A:51:ILE:CD1	4:A:1511:DLZ:H7B	2.30	0.62
1:B:192:LEU:O	1:B:193:ARG:HD2	2.00	0.61
1:A:402:ASN:HD21	2:A:1509:FAD:H62A	1.48	0.61
1:C:387:TYR:CE1	2:C:1509:FAD:HM73	2.36	0.61
1:B:181:PRO:O	1:B:182:ALA:HB3	2.01	0.61
1:B:467:PHE:CD1	1:B:473:MET:HE2	2.36	0.61
1:C:94:THR:HG22	1:C:96:ALA:N	2.16	0.59
1:B:302:GLN:HB3	2:B:1509:FAD:C8A	2.34	0.57
1:C:302:GLN:HB3	2:C:1509:FAD:C8A	2.33	0.57
1:A:258:PHE:CD1	1:A:263:LEU:HD21	2.40	0.57
1:A:94:THR:HG22	1:A:96:ALA:H	1.68	0.57
1:B:400:ALA:HB3	1:B:401:PRO:HD3	1.87	0.57
1:A:302:GLN:HB3	2:A:1509:FAD:C8A	2.37	0.55
1:B:467:PHE:CD1	1:B:473:MET:CE	2.90	0.54
1:A:51:ILE:HD12	4:A:1511:DLZ:H7B	1.89	0.53
1:A:310:VAL:HG13	1:A:401:PRO:HG2	1.90	0.53
1:B:423:SER:HB2	1:B:453:ASN:HD22	1.75	0.52
1:B:467:PHE:CG	1:B:473:MET:HE2	2.45	0.52
1:B:185:ASP:OD1	1:B:186:LEU:O	2.28	0.52
1:B:467:PHE:CG	1:B:473:MET:CE	2.93	0.52
1:A:258:PHE:CZ	1:A:357:LEU:HD13	2.46	0.51
1:A:20:ARG:NH2	1:A:126:ASP:OD2	2.43	0.51
1:B:464:ARG:HG3	1:B:477:TYR:CE1	2.46	0.50
4:B:1511:DLZ:O4'	4:B:1511:DLZ:O2'	2.16	0.50
1:A:480:TRP:CE2	1:A:488:ARG:HD3	2.46	0.50
1:C:81:PRO:HD2	1:C:85:ALA:CB	2.42	0.50
1:A:94:THR:CG2	1:A:96:ALA:H	2.25	0.50
1:B:455:LEU:HD21	1:B:499:LEU:HD13	1.94	0.49
1:B:444:ARG:NH2	1:B:483:MET:CE	2.75	0.49
1:C:193:ARG:HH11	1:C:193:ARG:HG2	1.77	0.49
1:C:464:ARG:O	1:C:468:GLU:HB2	2.12	0.49
1:C:418:LYS:HE3	1:C:476:MET:HE2	1.95	0.48
4:A:1511:DLZ:O5'	4:A:1511:DLZ:O3'	2.31	0.48
1:B:310:VAL:HG13	1:B:401:PRO:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:PHE:N	1:A:212:PRO:CD	2.76	0.48
1:B:186:LEU:O	1:B:187:LEU:CB	2.59	0.48
1:C:470:ASN:HD22	1:C:471:PRO:N	2.11	0.48
1:A:238:ILE:HG23	1:A:285:GLU:HG3	1.97	0.47
1:B:190:ARG:NH2	1:B:256:ASP:OD1	2.47	0.47
1:B:51:ILE:HD12	4:B:1511:DLZ:H7B	1.95	0.47
1:B:387:TYR:CE1	2:B:1509:FAD:HM73	2.50	0.46
1:A:408:GLN:NE2	7:A:2136:HOH:O	2.40	0.46
1:C:193:ARG:HG2	1:C:193:ARG:NH1	2.31	0.46
1:B:444:ARG:NH2	1:B:483:MET:HE1	2.31	0.46
1:C:135:PHE:O	1:C:139:THR:HG23	2.16	0.46
4:C:1511:DLZ:O4'	4:C:1511:DLZ:O2'	2.26	0.45
4:B:1511:DLZ:H7	4:B:1511:DLZ:H1'	1.76	0.45
1:B:424:GLY:H	1:B:453:ASN:ND2	2.15	0.45
1:A:147:MET:HE2	1:A:306:TRP:CD1	2.53	0.44
1:C:387:TYR:CZ	2:C:1509:FAD:HM73	2.53	0.44
1:A:103:ARG:HA	1:A:104:PRO:HD3	1.83	0.44
4:C:1511:DLZ:H1'	4:C:1511:DLZ:H7	1.62	0.44
1:A:297:GLU:OE1	1:A:301:ARG:NH1	2.50	0.44
1:A:263:LEU:HD12	1:A:263:LEU:N	2.33	0.44
1:B:467:PHE:HB3	1:B:473:MET:HE2	2.00	0.43
1:C:193:ARG:HH11	1:C:193:ARG:CG	2.30	0.43
1:A:400:ALA:HB3	1:A:401:PRO:HD3	1.99	0.43
1:B:193:ARG:HD2	1:B:193:ARG:HA	1.91	0.42
1:A:161:LEU:HD11	1:A:300:ILE:HD12	2.00	0.42
1:C:51:ILE:CD1	4:C:1511:DLZ:C7	2.95	0.42
1:C:470:ASN:C	1:C:470:ASN:ND2	2.68	0.42
1:A:258:PHE:CE1	1:A:263:LEU:HD21	2.54	0.42
1:A:347:LEU:HD23	1:A:368:VAL:HG12	2.01	0.42
1:B:211:PHE:N	1:B:212:PRO:CD	2.83	0.42
1:C:400:ALA:HB3	1:C:401:PRO:HD3	2.02	0.41
4:A:1511:DLZ:O4'	4:A:1511:DLZ:O2'	2.26	0.41
1:B:51:ILE:HD13	4:B:1511:DLZ:H7B	1.99	0.41
1:A:199:GLU:HG3	7:A:2021:HOH:O	2.19	0.41
2:A:1509:FAD:O3P	2:A:1509:FAD:H3B	2.21	0.41
1:B:297:GLU:OE1	1:B:301:ARG:NH1	2.54	0.41
1:A:35:MET:CE	1:A:210:ARG:HD2	2.51	0.41
1:B:51:ILE:HD13	4:B:1511:DLZ:C7	2.50	0.41
1:C:481:ASP:N	1:C:481:ASP:OD1	2.53	0.41
1:C:429:ARG:HG3	1:C:429:ARG:HH11	1.85	0.40
1:B:147:MET:HE2	1:B:306:TRP:NE1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ARG:NH2	1:B:126:ASP:OD2	2.54	0.40
1:B:258:PHE:CE1	1:B:263:LEU:HD21	2.55	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	506/522 (97%)	491 (97%)	14 (3%)	1 (0%)	47 73
1	B	506/522 (97%)	493 (97%)	11 (2%)	2 (0%)	34 60
1	C	501/522 (96%)	482 (96%)	18 (4%)	1 (0%)	47 73
All	All	1513/1566 (97%)	1466 (97%)	43 (3%)	4 (0%)	41 66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	185	ASP
1	A	471	PRO
1	B	182	ALA
1	C	181	PRO

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	400/426 (94%)	388 (97%)	12 (3%)	41 70
1	B	397/426 (93%)	382 (96%)	15 (4%)	33 62
1	C	386/426 (91%)	364 (94%)	22 (6%)	20 44
All	All	1183/1278 (93%)	1134 (96%)	49 (4%)	30 59

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	94	THR
1	A	121	ARG
1	A	143	LYS
1	A	144	GLN
1	A	146	ARG
1	A	210	ARG
1	A	280	ARG
1	A	323	ARG
1	A	448	ARG
1	A	466	ARG
1	A	499	LEU
1	B	1	LEU
1	B	62	LEU
1	B	68	ARG
1	B	134	GLU
1	B	145	LEU
1	B	193	ARG
1	B	199	GLU
1	B	288	GLU
1	B	323	ARG
1	B	343	ARG
1	B	414	LEU
1	B	429	ARG
1	B	474	VAL
1	B	496	GLU
1	B	499	LEU
1	C	1	LEU
1	C	2	THR
1	C	94	THR
1	C	103	ARG
1	C	133	ASP
1	C	145	LEU
1	C	190	ARG

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Mol	Chain	Res	Type
1	C	193	ARG
1	C	199	GLU
1	C	210	ARG
1	C	227	ARG
1	C	280	ARG
1	C	287	ARG
1	C	343	ARG
1	C	470	ASN
1	C	473	MET
1	C	479	THR
1	C	483	MET
1	C	485	GLU
1	C	486	THR
1	C	493	THR
1	C	496	GLU

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

Mol	Chain	Res	Type
1	A	402	ASN
1	B	178	ASN
1	B	453	ASN
1	C	302	GLN
1	C	470	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	A	1509	-	53,58,58	1.29	5 (9%)	68,89,89	1.27	7 (10%)
3	SF4	B	1510	1	0,12,12	-	-	-		
2	FAD	B	1509	-	53,58,58	1.45	8 (15%)	68,89,89	1.28	10 (14%)
3	SF4	C	1510	1	0,12,12	-	-	-		
4	DLZ	C	1511	-	23,24,24	1.72	6 (26%)	29,35,35	2.33	12 (41%)
2	FAD	C	1509	-	53,58,58	1.20	4 (7%)	68,89,89	1.29	7 (10%)
4	DLZ	A	1511	-	23,24,24	1.46	2 (8%)	29,35,35	2.46	11 (37%)
4	DLZ	B	1511	-	23,24,24	1.58	4 (17%)	29,35,35	2.64	14 (48%)
3	SF4	A	1510	1	0,12,12	-	-	-		

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	1509	-	-	2/30/50/50	0/6/6/6
3	SF4	B	1510	1	-	-	0/6/5/5
2	FAD	B	1509	-	-	1/30/50/50	0/6/6/6
3	SF4	C	1510	1	-	-	0/6/5/5
4	DLZ	C	1511	-	-	4/14/14/14	0/2/2/2
2	FAD	C	1509	-	-	2/30/50/50	0/6/6/6
4	DLZ	A	1511	-	-	6/14/14/14	0/2/2/2
4	DLZ	B	1511	-	-	5/14/14/14	0/2/2/2
3	SF4	A	1510	1	-	-	0/6/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1509	FAD	C4X-N5	4.68	1.39	1.30
2	B	1509	FAD	C2A-N3A	4.60	1.39	1.32
2	A	1509	FAD	C4X-N5	4.26	1.39	1.30
2	A	1509	FAD	C2A-N3A	4.06	1.38	1.32
4	B	1511	DLZ	C4'-C3'	-3.52	1.46	1.53
2	C	1509	FAD	C4X-N5	3.48	1.37	1.30
2	C	1509	FAD	C2A-N3A	3.42	1.37	1.32
4	A	1511	DLZ	C8-N8	-3.00	1.33	1.39
4	B	1511	DLZ	C8-N8	-2.99	1.33	1.39
2	B	1509	FAD	C2A-N1A	2.88	1.39	1.33
4	C	1511	DLZ	C7A-N8	-2.88	1.34	1.39
4	C	1511	DLZ	C8-N8	-2.82	1.33	1.39
2	A	1509	FAD	C2B-C1B	-2.66	1.49	1.53
4	B	1511	DLZ	C7A-N8	-2.61	1.35	1.39
2	C	1509	FAD	C2B-C1B	-2.61	1.49	1.53
4	C	1511	DLZ	C2-N3	-2.58	1.33	1.39
4	C	1511	DLZ	C5A-N5	-2.54	1.33	1.39
4	C	1511	DLZ	C4'-C3'	-2.47	1.48	1.53
2	B	1509	FAD	C10-N1	2.46	1.38	1.33
2	A	1509	FAD	C4-N3	-2.33	1.34	1.38
4	A	1511	DLZ	C7A-N8	-2.29	1.35	1.39
2	A	1509	FAD	C4X-C10	-2.26	1.37	1.44
2	B	1509	FAD	C2B-C1B	-2.21	1.50	1.53
2	B	1509	FAD	C4X-C4	-2.16	1.36	1.44
2	B	1509	FAD	C4X-C10	-2.15	1.37	1.44
4	C	1511	DLZ	C4-N3	-2.09	1.35	1.38
4	B	1511	DLZ	C5A-N5	-2.04	1.35	1.39
2	C	1509	FAD	C10-N1	2.01	1.37	1.33
2	B	1509	FAD	C5'-C4'	2.00	1.54	1.51

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1511	DLZ	C6-C5A-N5	6.01	122.00	112.53
4	A	1511	DLZ	C6-C5A-N5	5.76	121.61	112.53
2	A	1509	FAD	N3A-C2A-N1A	-5.13	120.66	128.68
2	C	1509	FAD	N3A-C2A-N1A	-5.05	120.78	128.68
4	C	1511	DLZ	C6-C5A-N5	4.96	120.36	112.53
4	B	1511	DLZ	O3'-C3'-C2'	4.96	120.80	108.81
4	A	1511	DLZ	O3'-C3'-C2'	4.91	120.68	108.81
4	B	1511	DLZ	C7-C7A-C5A	-4.58	116.30	125.26
4	C	1511	DLZ	O3'-C3'-C2'	4.54	119.78	108.81
4	B	1511	DLZ	C7-C7A-N8	4.29	123.49	116.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1511	DLZ	O4'-C4'-C5'	3.96	118.44	109.14
2	B	1509	FAD	N3A-C2A-N1A	-3.92	122.55	128.68
4	A	1511	DLZ	C7-C7A-C5A	-3.76	117.90	125.26
4	B	1511	DLZ	O2'-C2'-C3'	3.65	117.97	109.10
4	A	1511	DLZ	C4-N3-C2	-3.62	118.95	125.64
4	C	1511	DLZ	C5'-C4'-C3'	-3.59	104.63	112.41
4	B	1511	DLZ	O4'-C4'-C3'	-3.55	100.46	109.10
4	A	1511	DLZ	C5'-C4'-C3'	-3.46	104.92	112.41
4	A	1511	DLZ	O4-C4-C4A	-3.45	117.44	126.60
4	C	1511	DLZ	O5'-C5'-C4'	3.32	118.32	111.07
4	C	1511	DLZ	O2'-C2'-C3'	3.27	117.06	109.10
4	A	1511	DLZ	O5'-C5'-C4'	3.26	118.18	111.07
4	A	1511	DLZ	O4'-C4'-C5'	3.21	116.67	109.14
4	B	1511	DLZ	O4'-C4'-C5'	3.19	116.62	109.14
4	B	1511	DLZ	C4-N3-C2	-3.16	119.80	125.64
4	A	1511	DLZ	C4A-C4-N3	3.14	121.17	113.19
4	C	1511	DLZ	C7-C7A-C5A	-3.02	119.34	125.26
2	B	1509	FAD	C4X-C4-N3	2.90	120.55	113.19
2	A	1509	FAD	C4X-C10-N10	2.87	120.67	116.48
2	A	1509	FAD	C4X-C4-N3	2.79	120.28	113.19
4	B	1511	DLZ	O5'-C5'-C4'	2.77	117.10	111.07
2	C	1509	FAD	C4X-C10-N10	2.74	120.49	116.48
4	C	1511	DLZ	C4A-C4-N3	2.73	120.11	113.19
4	A	1511	DLZ	O2'-C2'-C3'	2.69	115.63	109.10
2	B	1509	FAD	C4X-C10-N10	2.66	120.37	116.48
2	B	1509	FAD	C5X-C9A-N10	2.66	120.70	117.95
2	C	1509	FAD	C4-N3-C2	-2.64	120.77	125.64
4	A	1511	DLZ	C7-C7A-N8	2.63	120.95	116.92
4	C	1511	DLZ	C4-N3-C2	-2.49	121.05	125.64
2	B	1509	FAD	O4-C4-C4X	-2.48	120.01	126.60
2	A	1509	FAD	C4-N3-C2	-2.44	121.12	125.64
4	B	1511	DLZ	O4-C4-C4A	-2.42	120.17	126.60
2	C	1509	FAD	C4X-C4-N3	2.39	119.25	113.19
2	A	1509	FAD	C4X-C10-N1	-2.37	119.22	124.73
4	B	1511	DLZ	C4A-C4-N3	2.37	119.21	113.19
2	A	1509	FAD	C3B-C2B-C1B	2.29	104.43	100.98
2	C	1509	FAD	C5X-C9A-N10	2.29	120.32	117.95
2	B	1509	FAD	C4X-C10-N1	-2.28	119.43	124.73
2	B	1509	FAD	C4A-C5A-N7A	-2.25	107.06	109.40
4	C	1511	DLZ	C4-C4A-N5	2.24	121.42	118.23
4	B	1511	DLZ	C4'-C3'-C2'	-2.23	108.72	113.36
2	B	1509	FAD	O4B-C1B-C2B	2.23	110.18	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1509	FAD	C4X-C10-N1	-2.23	119.56	124.73
4	B	1511	DLZ	C5'-C4'-C3'	-2.22	107.60	112.41
2	B	1509	FAD	C4-N3-C2	-2.19	121.60	125.64
2	B	1509	FAD	C10-N1-C2	2.16	121.22	116.90
4	C	1511	DLZ	O2-C2-N3	-2.08	114.60	118.65
2	C	1509	FAD	C9A-C5X-N5	-2.07	120.18	122.43
4	B	1511	DLZ	C8-C4A-N5	-2.06	120.54	124.85
2	A	1509	FAD	C10-C4X-N5	-2.06	120.49	124.86
4	C	1511	DLZ	C7-C7A-N8	2.04	120.05	116.92

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1511	DLZ	C1'-C2'-C3'-O3'
4	A	1511	DLZ	C1'-C2'-C3'-C4'
4	A	1511	DLZ	O2'-C2'-C3'-O3'
4	A	1511	DLZ	O2'-C2'-C3'-C4'
4	B	1511	DLZ	C1'-C2'-C3'-O3'
4	B	1511	DLZ	C1'-C2'-C3'-C4'
4	B	1511	DLZ	O2'-C2'-C3'-O3'
4	B	1511	DLZ	O2'-C2'-C3'-C4'
4	C	1511	DLZ	C1'-C2'-C3'-O3'
4	C	1511	DLZ	C1'-C2'-C3'-C4'
4	C	1511	DLZ	O2'-C2'-C3'-O3'
4	C	1511	DLZ	O2'-C2'-C3'-C4'
2	B	1509	FAD	C4'-C5'-O5'-P
4	A	1511	DLZ	O4'-C4'-C5'-O5'
2	C	1509	FAD	PA-O3P-P-O2P
2	A	1509	FAD	C4'-C5'-O5'-P
2	C	1509	FAD	C4'-C5'-O5'-P
4	A	1511	DLZ	C3'-C4'-C5'-O5'
2	A	1509	FAD	C4B-C5B-O5B-PA
4	B	1511	DLZ	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1509	FAD	4	0
2	B	1509	FAD	2	0

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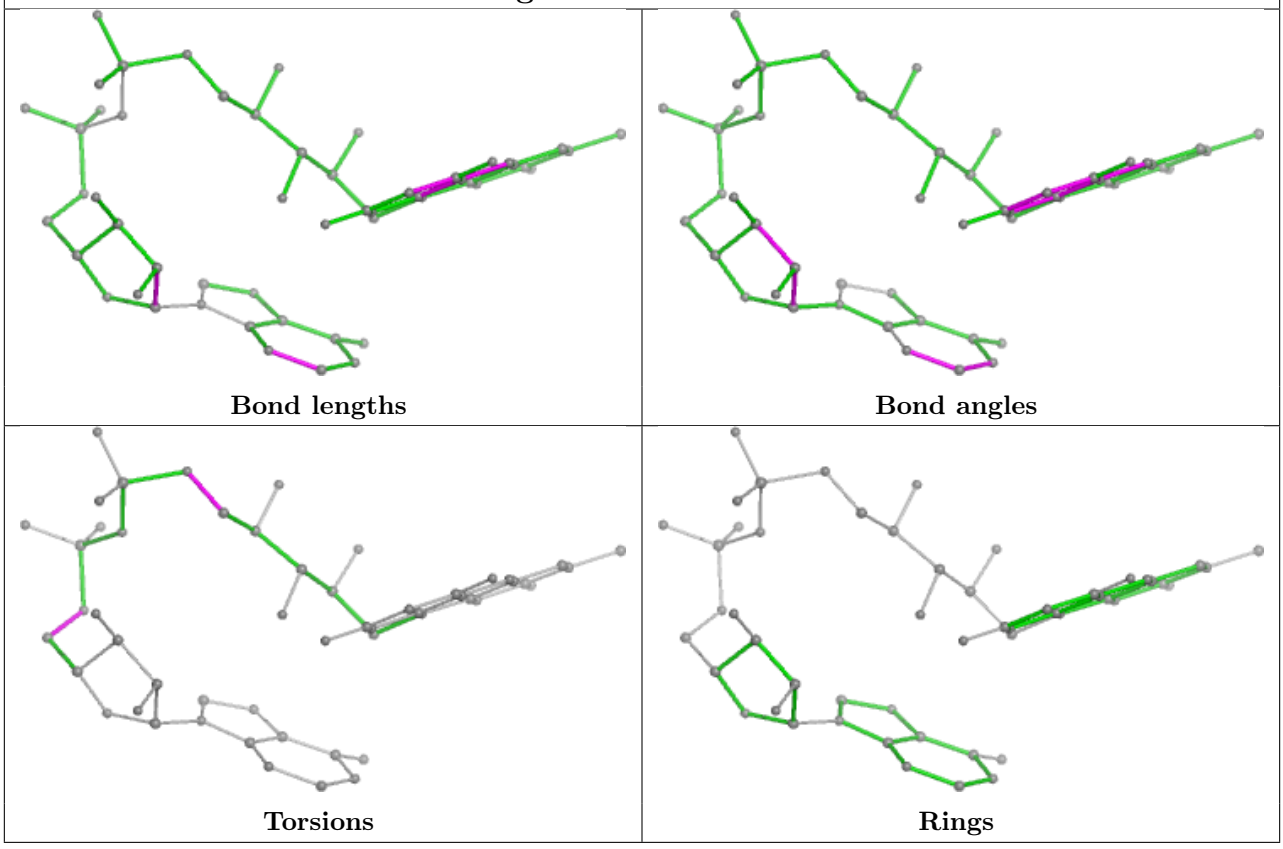
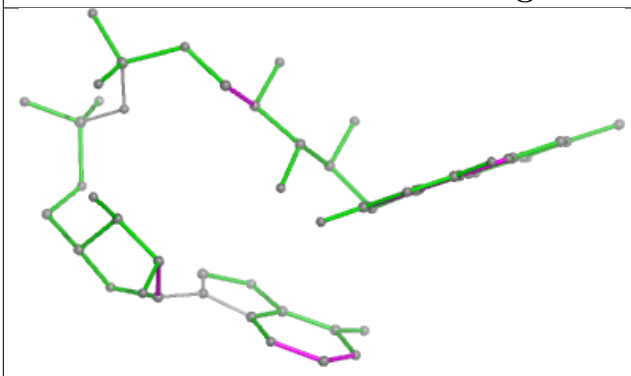
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1511	DLZ	5	0
2	C	1509	FAD	3	0
4	A	1511	DLZ	4	0
4	B	1511	DLZ	6	0

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.

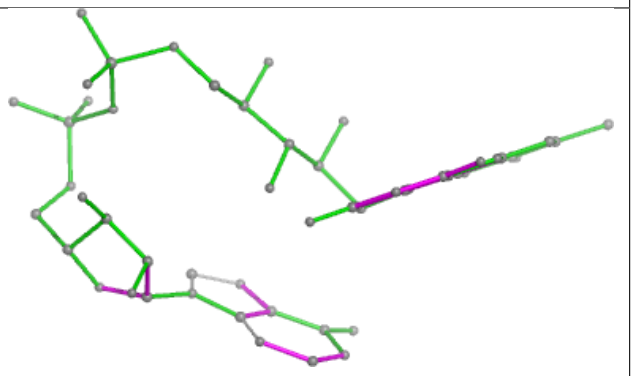
Ligand FAD A 1509



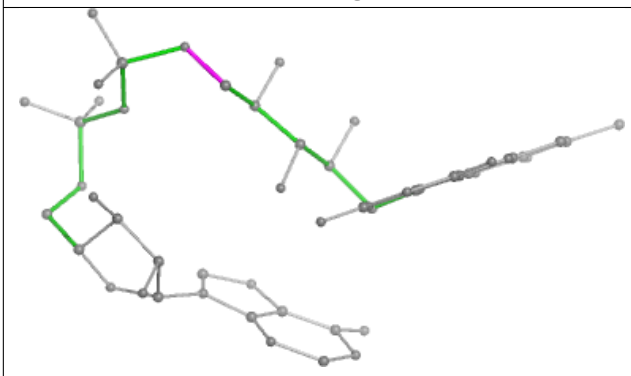
Ligand FAD B 1509



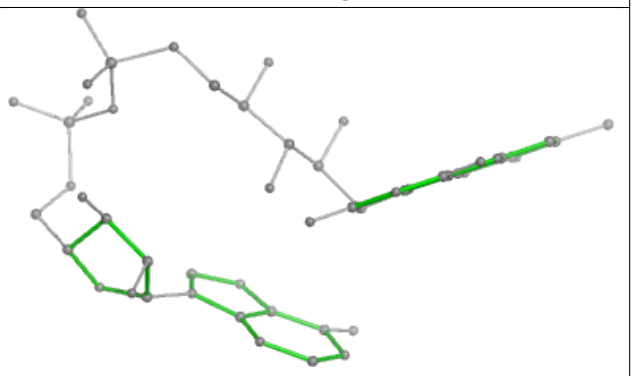
Bond lengths



Bond angles

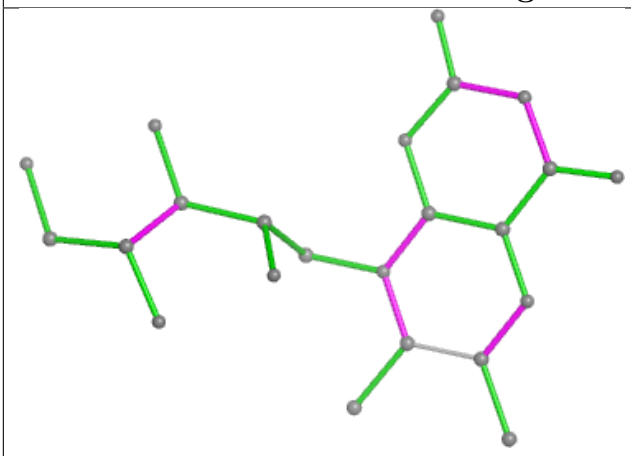


Torsions

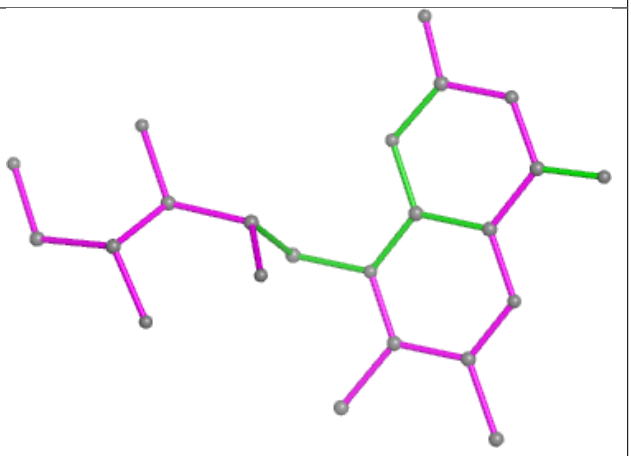


Rings

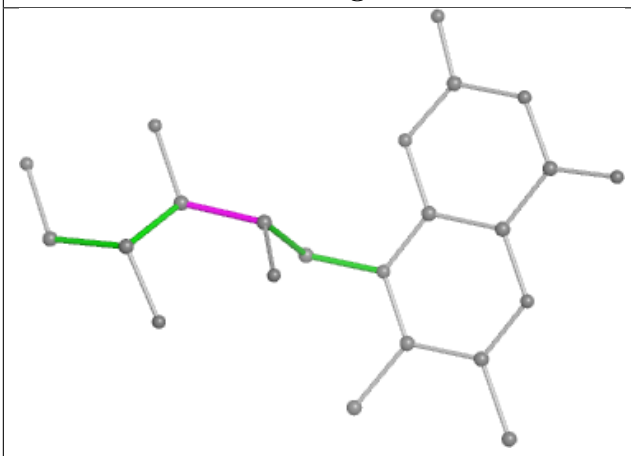
Ligand DLZ C 1511



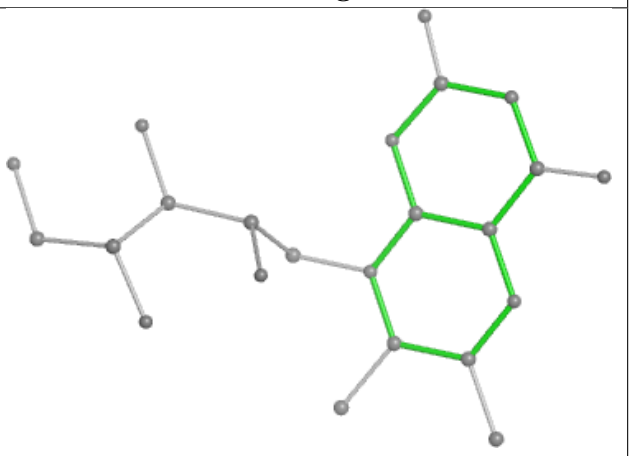
Bond lengths



Bond angles

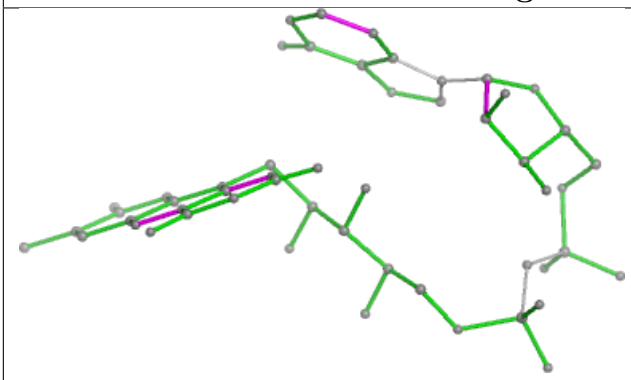


Torsions

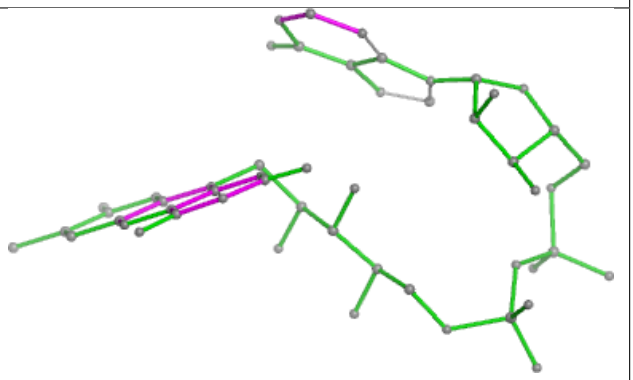


Rings

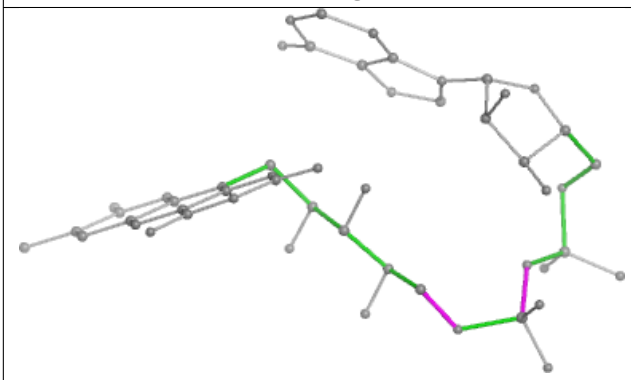
Ligand FAD C 1509



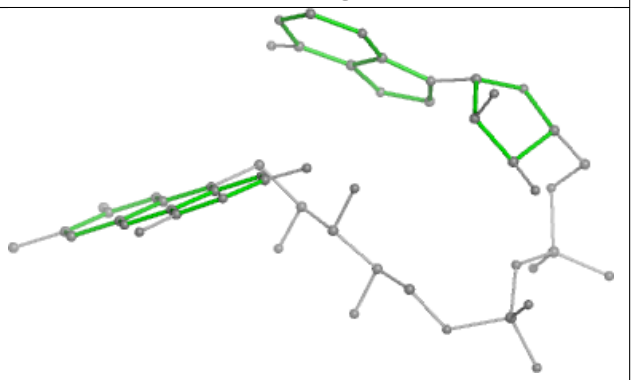
Bond lengths



Bond angles

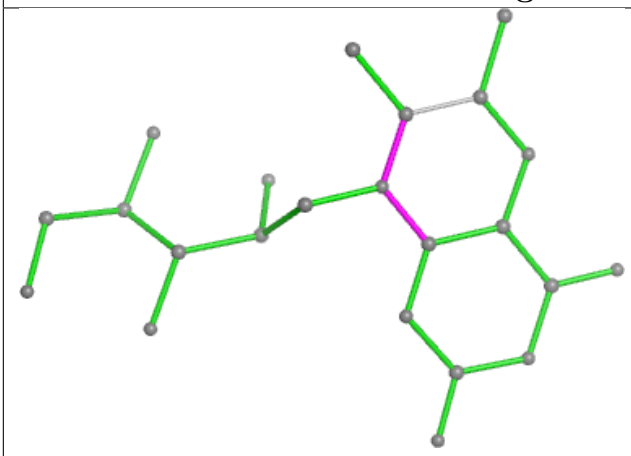


Torsions

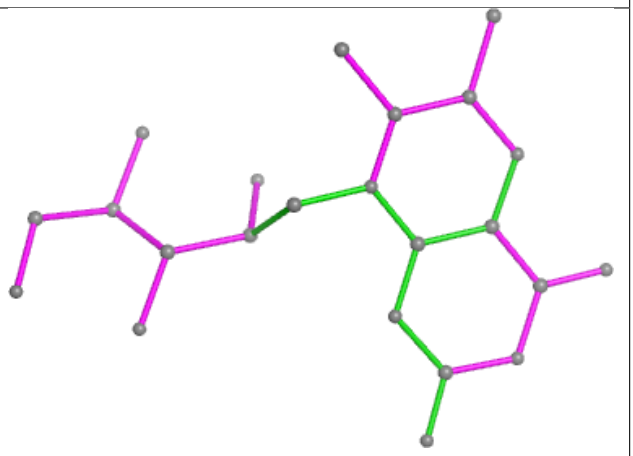


Rings

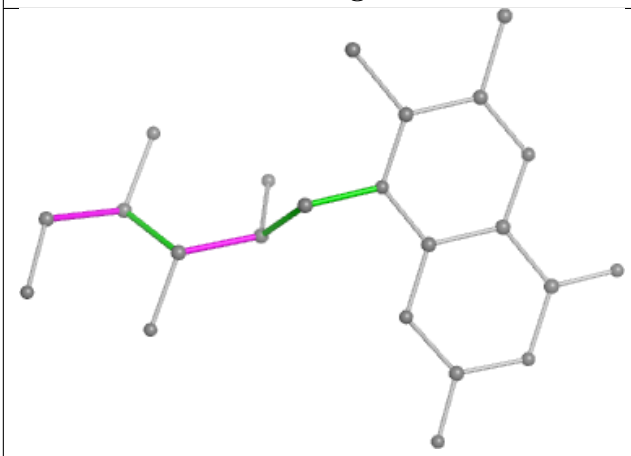
Ligand DLZ A 1511



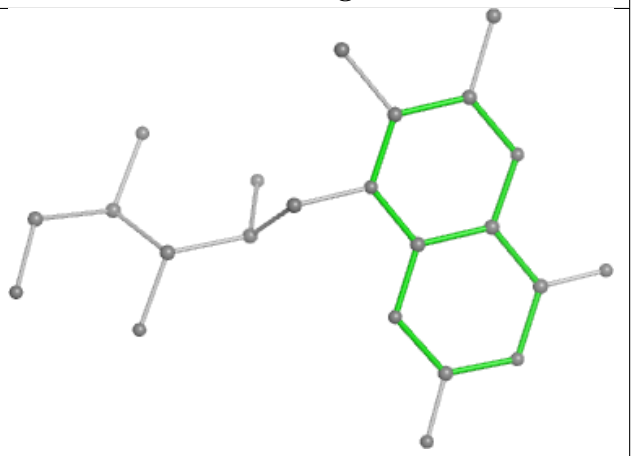
Bond lengths



Bond angles

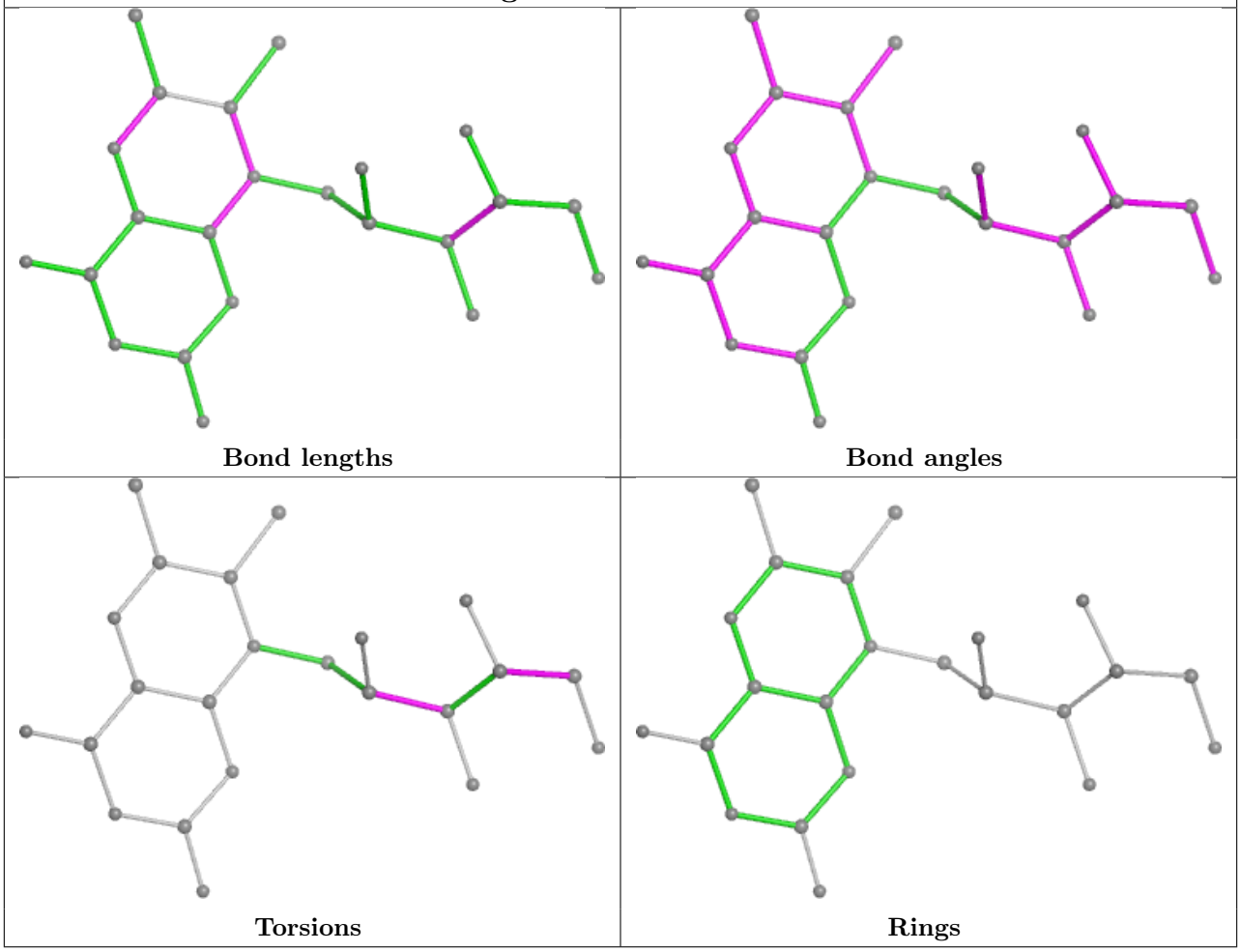


Torsions



Rings

Ligand DLZ B 1511



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	508/522 (97%)	-0.63	2 (0%)	92	93	19, 34, 64, 87	0
1	B	508/522 (97%)	-0.60	1 (0%)	95	96	18, 34, 69, 90	0
1	C	505/522 (96%)	-0.40	10 (1%)	65	67	21, 38, 76, 96	0
All	All	1521/1566 (97%)	-0.55	13 (0%)	84	85	18, 35, 71, 96	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	184	PRO	4.9
1	C	176	THR	3.7
1	C	186	LEU	3.3
1	C	187	LEU	3.1
1	C	178	ASN	2.9
1	B	435	ARG	2.7
1	A	1	LEU	2.7
1	C	138	TRP	2.5
1	A	471	PRO	2.3
1	C	169	GLY	2.2
1	C	185	ASP	2.2
1	C	183	ALA	2.1
1	C	429	ARG	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

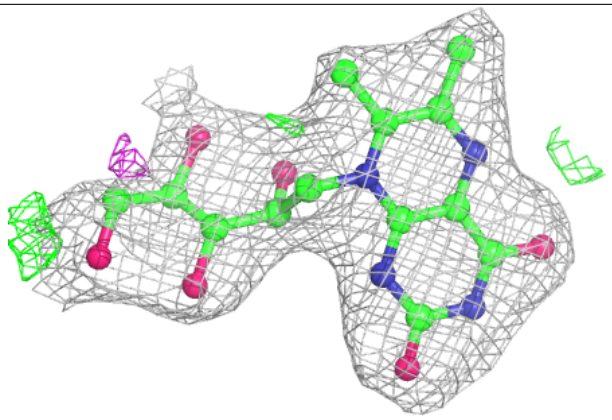
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

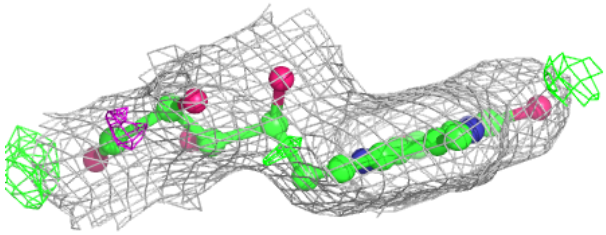
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	1512	1/1	0.72	0.45	54,54,54,54	0
5	MG	C	1512	1/1	0.81	0.36	61,61,61,61	0
5	MG	B	1512	1/1	0.86	0.21	54,54,54,54	0
6	GD	C	1513	1/1	0.92	0.14	98,98,98,98	1
6	GD	A	1513	1/1	0.93	0.10	93,93,93,93	1
4	DLZ	C	1511	23/23	0.96	0.16	26,29,31,33	0
4	DLZ	A	1511	23/23	0.97	0.17	17,25,29,31	0
4	DLZ	B	1511	23/23	0.97	0.17	18,27,34,37	0
2	FAD	C	1509	53/53	0.97	0.12	23,29,32,33	0
6	GD	B	1513	1/1	0.97	0.13	87,87,87,87	1
3	SF4	C	1510	8/8	0.97	0.07	32,37,38,39	0
3	SF4	A	1510	8/8	0.99	0.11	24,26,27,28	0
3	SF4	B	1510	8/8	0.99	0.09	24,26,27,27	0
2	FAD	B	1509	53/53	0.99	0.15	19,21,27,29	0
2	FAD	A	1509	53/53	0.99	0.15	18,21,24,27	0

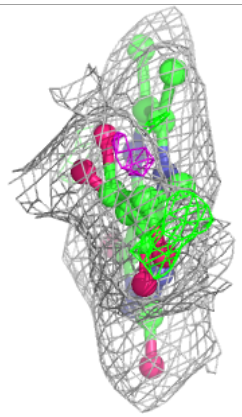
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DLZ C 1511:

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

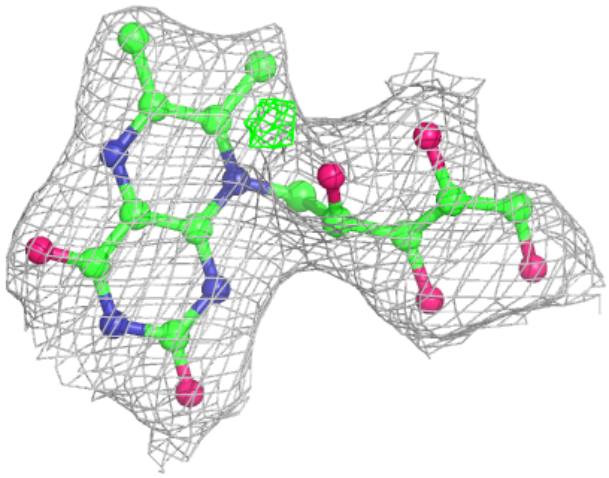


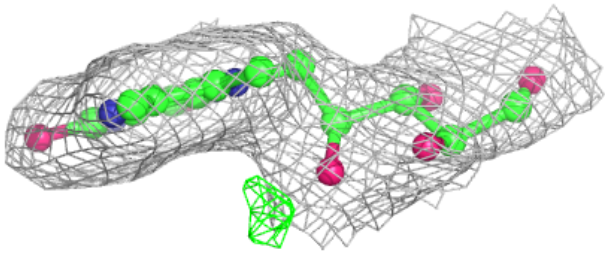


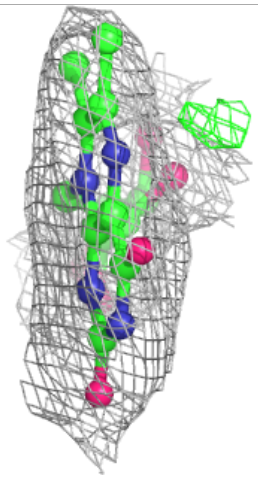


Electron density around DLZ A 1511:

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

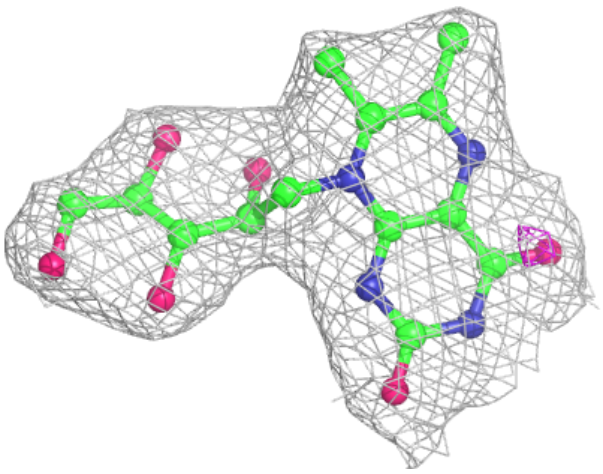


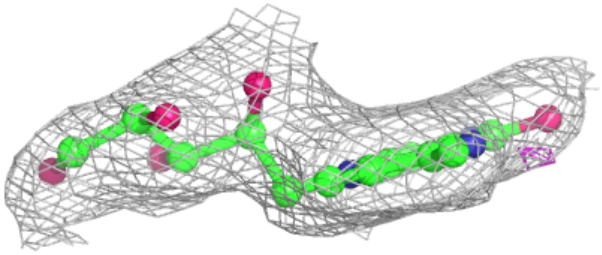


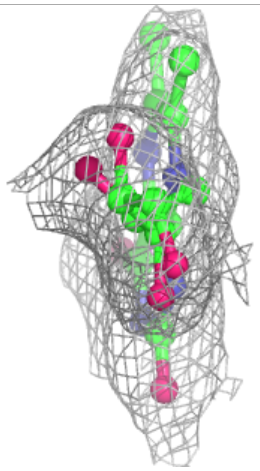


Electron density around DLZ B 1511:

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

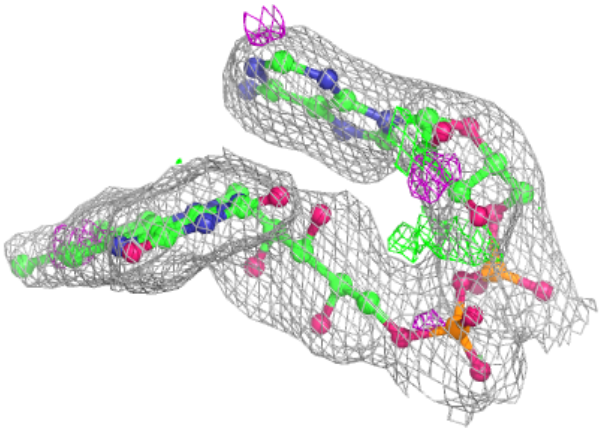


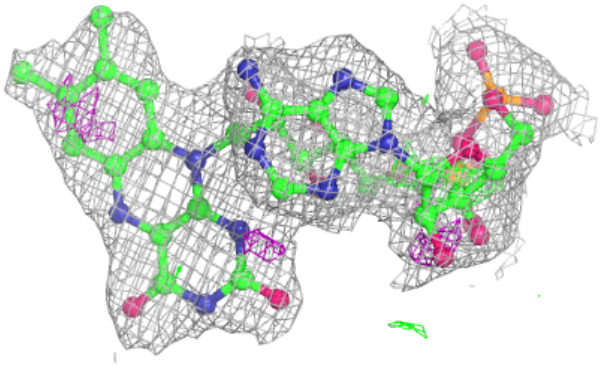


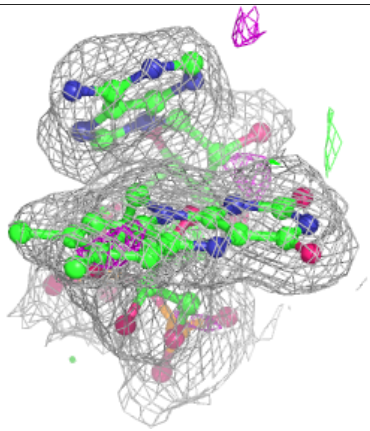


Electron density around FAD C 1509:

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

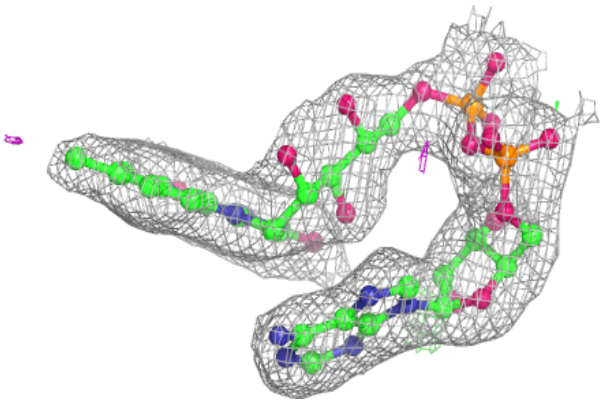


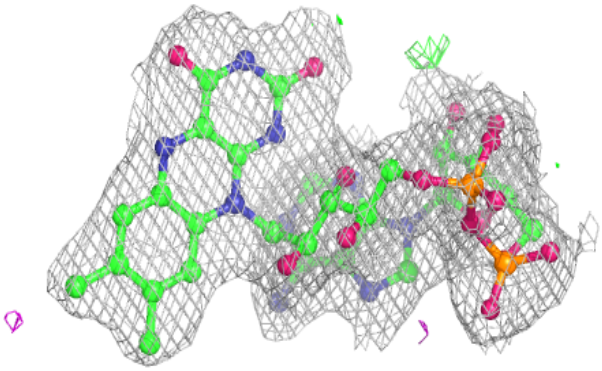


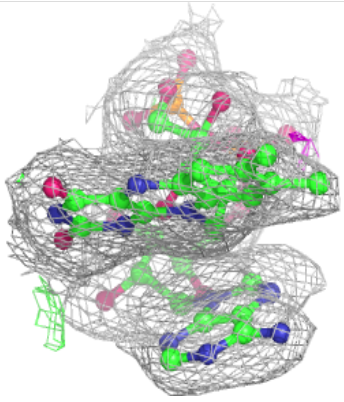


Electron density around FAD B 1509:

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

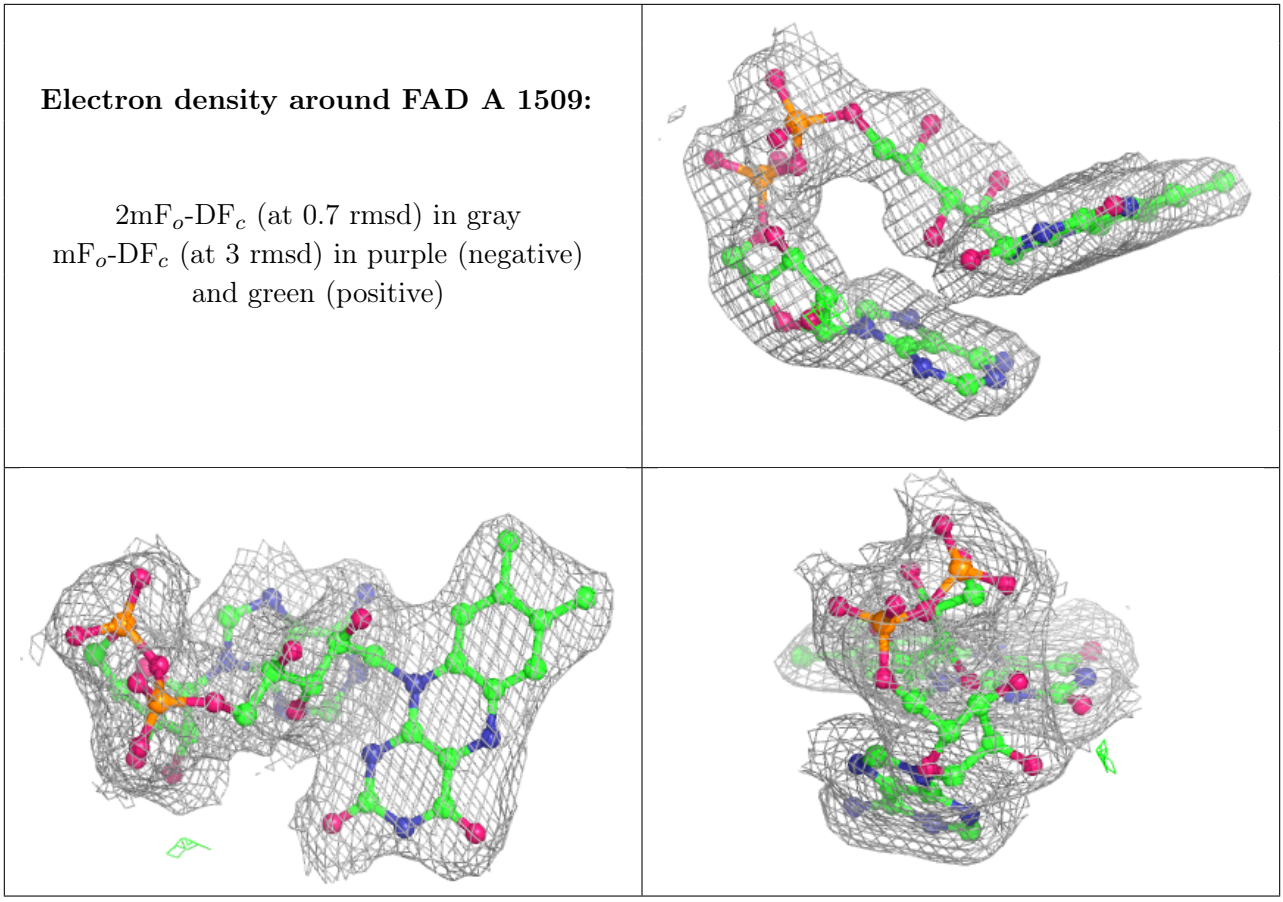






Electron density around FAD A 1509:

$2mF_o$-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.