Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 05:02 AM EDT

PDB ID	:	4GDP
Title	:	Yeast polyamine oxidase FMS1, N195A mutant
Authors	:	Taylor, A.B.; Adachi, M.S.; Hart, P.J.; Fitzpatrick, P.F.
Deposited on	:	2012-08-01
Resolution	:	2.00 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:

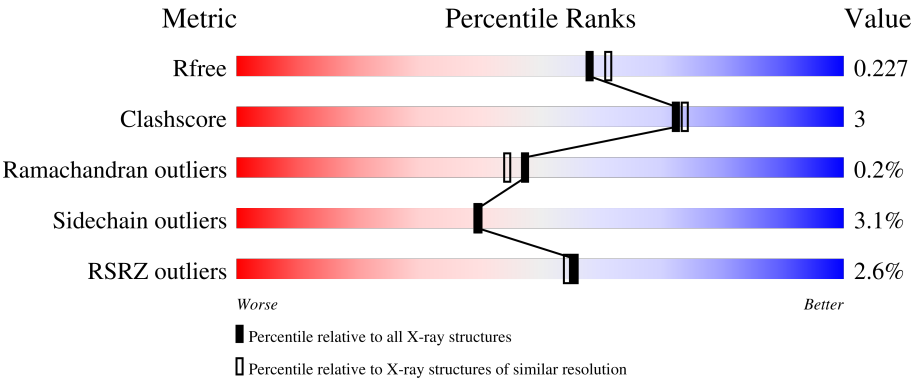
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	516	3% 87% 9% •
1	B	516	3% 88% 9% • •
1	C	516	2% 86% 7% • 5%
1	D	516	2% 84% 12% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16892 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 Polyamine oxidase FMS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	2	0
			3967	2505	689	751	22			
1	B	502	Total	C	N	O	S	0	3	0
			4029	2544	698	763	24			
1	C	488	Total	C	N	O	S	0	1	0
			3916	2474	679	740	23			
1	D	498	Total	C	N	O	S	0	2	0
			3997	2525	693	757	22			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	ALA	ASN	engineered mutation	UNP P50264
A	509	LEU	-	expression tag	UNP P50264
A	510	GLU	-	expression tag	UNP P50264
A	511	HIS	-	expression tag	UNP P50264
A	512	HIS	-	expression tag	UNP P50264
A	513	HIS	-	expression tag	UNP P50264
A	514	HIS	-	expression tag	UNP P50264
A	515	HIS	-	expression tag	UNP P50264
A	516	HIS	-	expression tag	UNP P50264
B	195	ALA	ASN	engineered mutation	UNP P50264
B	509	LEU	-	expression tag	UNP P50264
B	510	GLU	-	expression tag	UNP P50264
B	511	HIS	-	expression tag	UNP P50264
B	512	HIS	-	expression tag	UNP P50264
B	513	HIS	-	expression tag	UNP P50264
B	514	HIS	-	expression tag	UNP P50264
B	515	HIS	-	expression tag	UNP P50264
B	516	HIS	-	expression tag	UNP P50264
C	195	ALA	ASN	engineered mutation	UNP P50264
C	509	LEU	-	expression tag	UNP P50264
C	510	GLU	-	expression tag	UNP P50264

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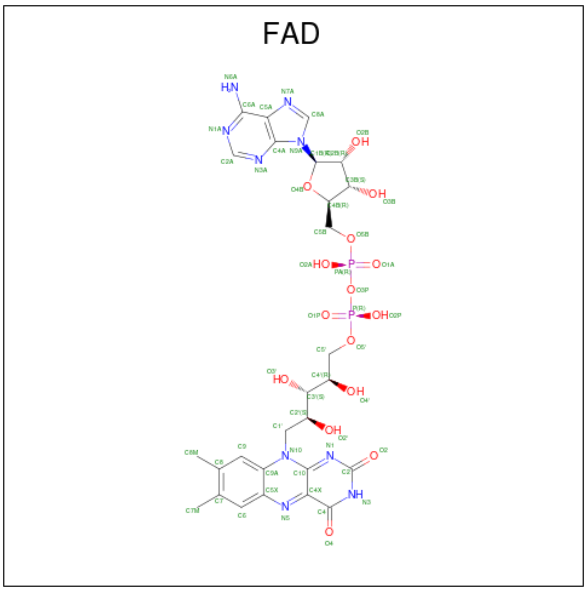
Chain	Residue	Modelled	Actual	Comment	Reference
C	511	HIS	-	expression tag	UNP P50264
C	512	HIS	-	expression tag	UNP P50264
C	513	HIS	-	expression tag	UNP P50264
C	514	HIS	-	expression tag	UNP P50264
C	515	HIS	-	expression tag	UNP P50264
C	516	HIS	-	expression tag	UNP P50264
D	195	ALA	ASN	engineered mutation	UNP P50264
D	509	LEU	-	expression tag	UNP P50264
D	510	GLU	-	expression tag	UNP P50264
D	511	HIS	-	expression tag	UNP P50264
D	512	HIS	-	expression tag	UNP P50264
D	513	HIS	-	expression tag	UNP P50264
D	514	HIS	-	expression tag	UNP P50264
D	515	HIS	-	expression tag	UNP P50264
D	516	HIS	-	expression tag	UNP P50264

- 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		

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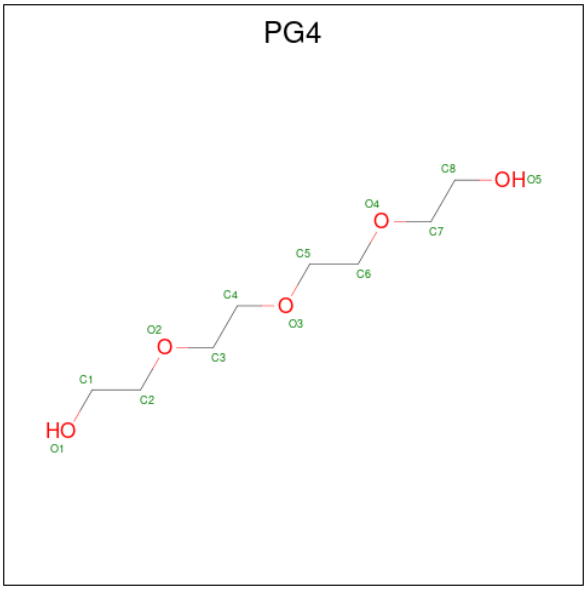
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 8 5	0	0
3	B	1	Total C O 11 7 4	0	0
3	C	1	Total C O 13 8 5	0	0
3	D	1	Total C O 11 8 3	0	0

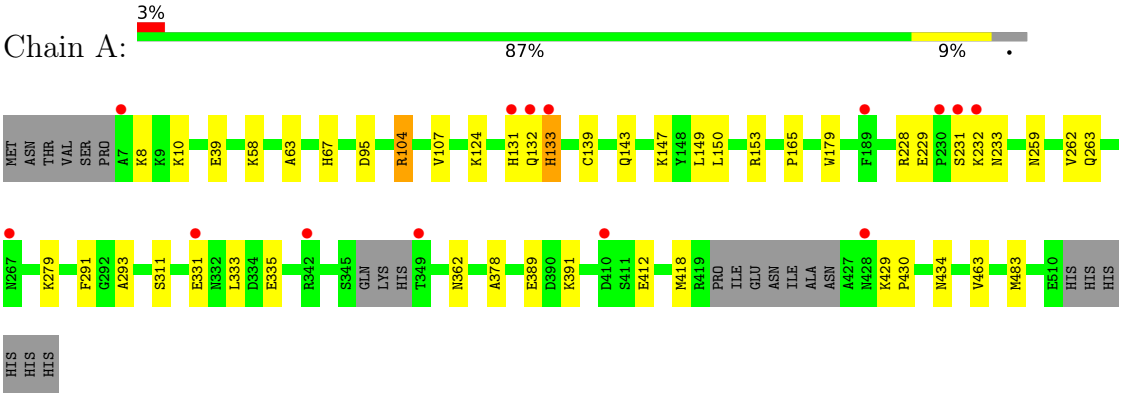
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	163	Total O 163 163	0	0
4	B	199	Total O 199 199	0	0
4	C	161	Total O 161 161	0	0
4	D	200	Total O 200 200	0	0

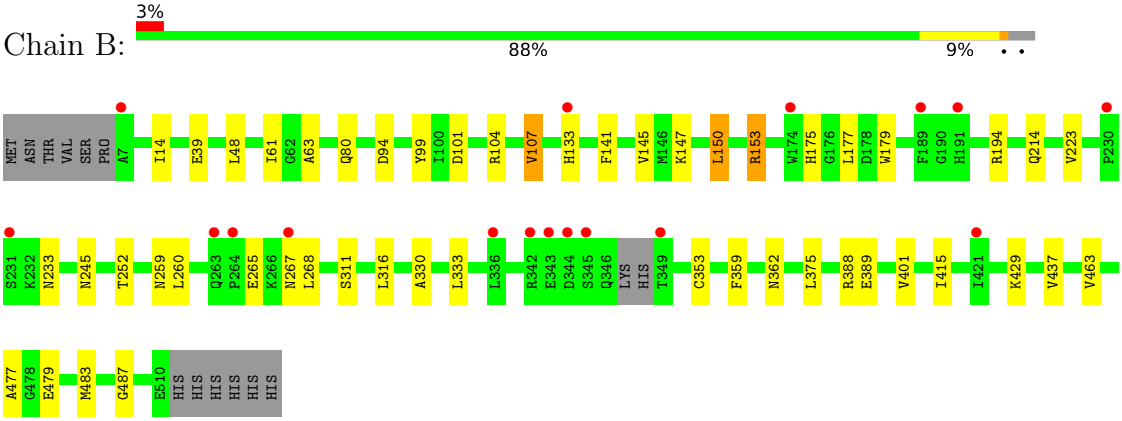
3 Residue-property plots (i)

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.

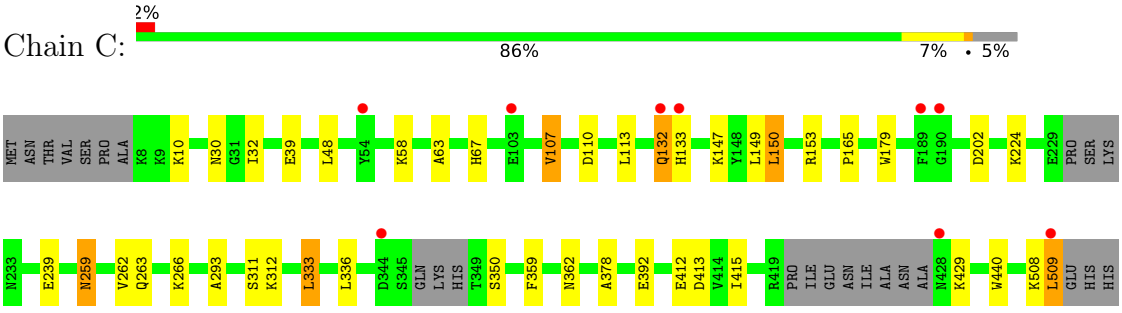
• Molecule 1: Polyamine oxidase FMS1



• Molecule 1: Polyamine oxidase FMS1

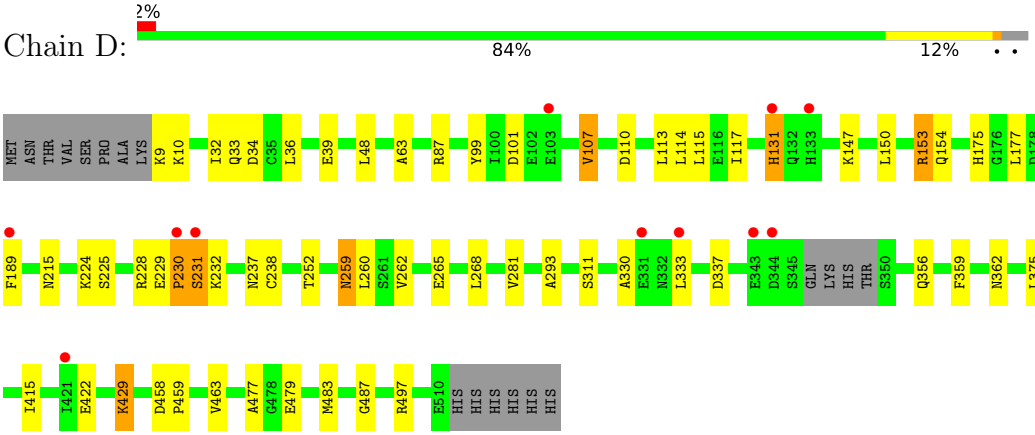


• Molecule 1: Polyamine oxidase FMS1



• Molecule 1: Polyamine oxidase FMS1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.85Å 81.89Å 104.79Å 78.07° 79.51° 78.92°	Depositor
Resolution (Å)	79.07 – 2.00 79.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.9 (79.07-2.00) 88.9 (79.08-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.203 , 0.234 0.196 , 0.227	Depositor DCC
R_{free} test set	1999 reflections (1.34%)	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.138 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16892	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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, PG4

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	0.28	0/4050	0.44	0/5474
1	B	0.28	0/4119	0.44	0/5570
1	C	0.28	0/3996	0.43	0/5399
1	D	0.28	0/4084	0.44	0/5523
All	All	0.28	0/16249	0.44	0/21966

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	3967	0	3885	23	0
1	B	4029	0	3955	26	0
1	C	3916	0	3837	24	0
1	D	3997	0	3921	38	0
2	A	53	0	31	4	0
2	B	53	0	31	2	0
2	C	53	0	31	2	0
2	D	53	0	31	1	0
3	A	13	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	0	13	0	0
3	C	13	0	18	2	0
3	D	11	0	12	0	0
4	A	163	0	0	2	0
4	B	199	0	0	3	0
4	C	161	0	0	1	0
4	D	200	0	0	4	0
All	All	16892	0	15783	110	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 3.

All (110) 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:14:ILE:HD12	1:B:223:VAL:HG21	1.65	0.78
1:C:412:GLU:HG3	1:C:429:LYS:HE3	1.73	0.70
1:D:229:GLU:O	1:D:231:SER:N	2.22	0.70
1:D:9:LYS:N	1:D:34:ASP:O	2.26	0.68
1:A:133:HIS:O	1:D:393:ARG:NH2	2.29	0.65
1:C:67:HIS:HE1	3:C:802:PG4:H71	1.63	0.64
1:C:149:LEU:HD11	1:C:165:PRO:HG3	1.80	0.62
1:D:153:ARG:NH2	1:D:330:ALA:O	2.31	0.62
1:A:279:LYS:NZ	4:A:1048:HOH:O	2.34	0.61
1:C:150:LEU:HD23	1:C:336:LEU:HD22	1.84	0.60
1:C:10:LYS:HE2	1:C:32:ILE:HG23	1.83	0.59
1:A:149:LEU:HD11	1:A:165:PRO:HG3	1.85	0.58
1:C:39:GLU:OE1	2:C:801:FAD:O2B	2.22	0.58
1:B:80:GLN:NE2	4:B:1009:HOH:O	2.34	0.57
1:C:508:LYS:O	1:C:509:LEU:HB2	2.05	0.57
1:A:39:GLU:OE1	2:A:801:FAD:O2B	2.22	0.56
1:B:99:TYR:HB3	1:B:316:LEU:HD21	1.87	0.56
1:B:147:LYS:HG2	1:B:333:LEU:HD11	1.87	0.56
1:C:67:HIS:CE1	3:C:802:PG4:H71	2.40	0.55
1:D:293:ALA:HB3	1:D:378:ALA:HB2	1.89	0.55
1:A:311:SER:HA	1:A:362:ASN:HB3	1.89	0.54
1:C:415:ILE:HD11	1:C:429:LYS:HD3	1.90	0.54
1:A:10:LYS:NZ	4:A:1007:HOH:O	2.40	0.54
1:C:311:SER:HA	1:C:362:ASN:HB3	1.90	0.54
1:B:214:GLN:NE2	4:B:993:HOH:O	2.40	0.54
1:D:497:ARG:NE	4:D:1069:HOH:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ALA:HB3	1:A:378:ALA:HB2	1.90	0.53
1:B:39:GLU:OE1	2:B:801:FAD:O2B	2.27	0.53
1:C:293:ALA:HB3	1:C:378:ALA:HB2	1.91	0.53
1:A:8:LYS:HE2	1:A:233:ASN:HD21	1.75	0.52
1:A:139:CYS:HB2	1:A:143:GLN:OE1	2.10	0.52
1:D:131:HIS:O	1:D:131:HIS:ND1	2.44	0.51
1:B:252:THR:HG22	1:B:477:ALA:HB3	1.92	0.51
1:D:147:LYS:HG2	1:D:333:LEU:HD11	1.93	0.50
1:D:39:GLU:OE1	2:D:801:FAD:O2B	2.29	0.49
1:D:224:LYS:NZ	1:D:238:CYS:O	2.45	0.49
1:B:359:PHE:HD2	1:B:375:LEU:HD22	1.77	0.49
1:B:48:LEU:HD23	1:B:63:ALA:HB3	1.95	0.49
1:C:147:LYS:HG2	1:C:333:LEU:HD21	1.95	0.49
1:D:359:PHE:HD2	1:D:375:LEU:HD22	1.78	0.48
1:D:479:GLU:OE1	1:D:487:GLY:HA2	2.13	0.48
1:B:353:CYS:SG	1:B:401:VAL:HG13	2.53	0.48
1:B:311:SER:HA	1:B:362:ASN:HB3	1.96	0.48
1:A:147:LYS:HD3	1:A:333:LEU:HD11	1.95	0.48
1:B:133:HIS:HD1	1:D:422:GLU:CD	2.17	0.48
1:C:132:GLN:HG3	1:C:133:HIS:CE1	2.49	0.47
1:D:110:ASP:HB3	1:D:113:LEU:HB2	1.95	0.47
1:D:186:ASP:HB2	4:D:1003:HOH:O	2.14	0.47
1:A:8:LYS:HE2	1:A:233:ASN:ND2	2.29	0.47
1:D:48:LEU:CD2	1:D:63:ALA:HB3	2.45	0.47
1:A:463:VAL:HG11	1:A:483:MET:HG2	1.97	0.47
1:A:67:HIS:HE1	3:A:802:PG4:H21	1.80	0.46
1:D:150:LEU:O	1:D:153:ARG:HD2	2.15	0.46
1:D:228:ARG:NE	1:D:232:LYS:O	2.35	0.46
1:D:229:GLU:HA	1:D:230:PRO:HD3	1.82	0.46
1:D:463:VAL:HG11	1:D:483:MET:HG2	1.96	0.46
1:B:48:LEU:CD2	1:B:63:ALA:HB3	2.46	0.46
1:C:58:LYS:NZ	1:C:202:ASP:OD2	2.48	0.45
1:A:228:ARG:HH21	1:A:232:LYS:HA	1.82	0.45
1:D:153:ARG:HG2	1:D:154:GLN:N	2.31	0.45
1:A:132:GLN:HB2	1:A:133:HIS:ND1	2.32	0.45
1:D:311:SER:HA	1:D:362:ASN:HB3	1.98	0.45
1:C:312:LYS:HD2	1:C:359:PHE:CZ	2.52	0.44
1:A:418:MET:HE3	1:A:434:ASN:HA	1.98	0.44
1:D:415:ILE:HD11	1:D:429:LYS:HD3	2.00	0.44
1:C:107:VAL:HG22	1:C:113:LEU:HD13	1.99	0.44
1:C:30:ASN:O	1:C:508:LYS:HE3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:LEU:HD22	1:D:268:LEU:HD13	2.00	0.43
1:A:63:ALA:HA	2:A:801:FAD:C4X	2.48	0.43
1:B:415:ILE:HD11	1:B:429:LYS:HD3	2.00	0.43
1:C:48:LEU:HD22	1:C:63:ALA:HB3	2.00	0.43
1:D:114:LEU:HB3	1:D:117:ILE:HD12	1.99	0.43
1:B:153:ARG:NH2	1:B:330:ALA:O	2.45	0.43
1:D:10:LYS:NZ	1:D:33:GLN:H	2.17	0.43
1:D:215:ASN:ND2	4:D:1056:HOH:O	2.33	0.43
1:A:429:LYS:HA	1:A:430:PRO:HD3	1.89	0.43
1:C:63:ALA:HA	2:C:801:FAD:N5	2.34	0.43
1:D:281:VAL:HG22	4:D:1019:HOH:O	2.18	0.43
1:D:131:HIS:O	1:D:131:HIS:CG	2.72	0.43
1:A:412:GLU:HB3	1:A:429:LYS:HE3	2.01	0.42
1:A:63:ALA:HA	2:A:801:FAD:N5	2.34	0.42
1:C:224:LYS:HE3	1:C:239:GLU:HG2	2.02	0.42
1:D:359:PHE:CD2	1:D:375:LEU:HD22	2.54	0.42
1:D:107:VAL:HG13	1:D:115:LEU:HD12	2.01	0.42
1:D:225:SER:HB2	1:D:237:ASN:HB2	2.01	0.42
1:D:259:ASN:O	1:D:262:VAL:HG22	2.20	0.42
1:B:260:LEU:HD22	1:B:268:LEU:HD13	2.00	0.42
1:C:259:ASN:O	1:C:262:VAL:HG22	2.20	0.42
1:C:413:ASP:O	1:C:429:LYS:HE2	2.20	0.41
1:B:61:ILE:HD12	1:B:61:ILE:HA	1.88	0.41
1:C:440:TRP:HB2	4:C:981:HOH:O	2.19	0.41
1:A:147:LYS:HE2	1:A:147:LYS:HB2	1.60	0.41
1:B:141:PHE:O	1:B:145:VAL:HG23	2.20	0.41
1:D:10:LYS:HD2	1:D:32:ILE:HG23	2.03	0.41
1:A:104:ARG:O	1:A:104:ARG:HG3	2.21	0.41
1:B:94:ASP:OD1	1:B:194:ARG:HB3	2.20	0.41
1:B:104:ARG:HG2	1:B:107:VAL:HG23	2.03	0.41
1:B:150:LEU:HD22	1:B:150:LEU:HA	1.89	0.41
1:B:487:GLY:O	2:B:801:FAD:O3'	2.38	0.41
1:B:479:GLU:OE1	1:B:487:GLY:HA2	2.21	0.41
1:A:259:ASN:O	1:A:262:VAL:HG22	2.21	0.40
1:D:252:THR:HG22	1:D:477:ALA:HB3	2.03	0.40
1:B:388:ARG:HB2	1:B:437:VAL:HB	2.04	0.40
1:B:463:VAL:HG11	1:B:483:MET:HG2	2.02	0.40
2:A:801:FAD:N5	3:A:802:PG4:H51	2.36	0.40
1:D:99:TYR:HB2	1:D:107:VAL:HG12	2.04	0.40
1:D:458:ASP:HA	1:D:459:PRO:HD2	1.83	0.40
1:B:175:HIS:HD2	4:B:955:HOH:O	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ASP:HB3	1:C:113:LEU:HB2	2.03	0.40
1:D:175:HIS:CE1	1:D:189:PHE:HE2	2.40	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	490/516 (95%)	473 (96%)	17 (4%)	0	100	100
1	B	501/516 (97%)	488 (97%)	13 (3%)	0	100	100
1	C	481/516 (93%)	464 (96%)	16 (3%)	1 (0%)	47	44
1	D	496/516 (96%)	480 (97%)	14 (3%)	2 (0%)	34	30
All	All	1968/2064 (95%)	1905 (97%)	60 (3%)	3 (0%)	47	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	132	GLN
1	D	231	SER
1	D	230	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	437/456 (96%)	419 (96%)	18 (4%)	30	28
1	B	445/456 (98%)	433 (97%)	12 (3%)	44	46
1	C	432/456 (95%)	421 (98%)	11 (2%)	47	49
1	D	441/456 (97%)	428 (97%)	13 (3%)	42	43
All	All	1755/1824 (96%)	1701 (97%)	54 (3%)	40	40

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LYS
1	A	95	ASP
1	A	104	ARG
1	A	107	VAL
1	A	124	LYS
1	A	131	HIS
1	A	133	HIS
1	A	150	LEU
1	A	153	ARG
1	A	179	TRP
1	A	229	GLU
1	A	231	SER
1	A	263	GLN
1	A	291	PHE
1	A	331	GLU
1	A	335	GLU
1	A	389	GLU
1	A	391	LYS
1	B	101	ASP
1	B	107	VAL
1	B	150	LEU
1	B	153	ARG
1	B	177	LEU
1	B	179	TRP
1	B	233	ASN
1	B	245	ASN
1	B	259	ASN
1	B	265	GLU
1	B	267	ASN
1	B	389	GLU
1	C	107	VAL
1	C	150	LEU
1	C	153	ARG

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Mol	Chain	Res	Type
1	C	179	TRP
1	C	259	ASN
1	C	263	GLN
1	C	266	LYS
1	C	333	LEU
1	C	350	SER
1	C	392	GLU
1	C	509	LEU
1	D	36	LEU
1	D	87	ARG
1	D	101	ASP
1	D	107	VAL
1	D	131	HIS
1	D	153	ARG
1	D	177	LEU
1	D	179	TRP
1	D	259	ASN
1	D	265	GLU
1	D	337	ASP
1	D	356	GLN
1	D	429	LYS

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	28	HIS
1	A	233	ASN
1	A	245	ASN
1	B	191	HIS
1	C	67	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\| > 2$
3	PG4	C	802	-	12,12,12	0.66	0	11,11,11	1.48	0
3	PG4	B	802	-	10,10,12	0.68	0	9,9,11	1.37	0
2	FAD	C	801	-	53,58,58	1.82	9 (16%)	68,89,89	1.75	14 (20%)
2	FAD	A	801	-	53,58,58	1.82	9 (16%)	68,89,89	1.50	11 (16%)
3	PG4	D	802	-	10,10,12	0.60	0	9,9,11	1.46	0
2	FAD	D	801	-	53,58,58	1.82	9 (16%)	68,89,89	1.50	11 (16%)
3	PG4	A	802	-	12,12,12	0.69	0	11,11,11	1.48	0
2	FAD	B	801	-	53,58,58	1.82	9 (16%)	68,89,89	1.51	11 (16%)

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
3	PG4	C	802	-	-	3/10/10/10	-
3	PG4	B	802	-	-	3/8/8/10	-
2	FAD	C	801	-	-	2/30/50/50	0/6/6/6
2	FAD	A	801	-	-	1/30/50/50	0/6/6/6
3	PG4	D	802	-	-	6/8/8/10	-
2	FAD	D	801	-	-	1/30/50/50	0/6/6/6
3	PG4	A	802	-	-	8/10/10/10	-
2	FAD	B	801	-	-	1/30/50/50	0/6/6/6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FAD	C8M-C8	-5.57	1.39	1.51
2	A	801	FAD	C7M-C7	-5.56	1.39	1.51
2	D	801	FAD	C7M-C7	-5.56	1.39	1.51
2	C	801	FAD	C7M-C7	-5.55	1.39	1.51
2	D	801	FAD	C8M-C8	-5.55	1.39	1.51
2	C	801	FAD	C8M-C8	-5.55	1.39	1.51
2	B	801	FAD	C7M-C7	-5.53	1.40	1.51
2	A	801	FAD	C8M-C8	-5.51	1.40	1.51
2	C	801	FAD	C2A-N3A	4.99	1.40	1.32
2	A	801	FAD	C2A-N3A	4.99	1.40	1.32
2	D	801	FAD	C2A-N3A	4.97	1.40	1.32
2	B	801	FAD	C2A-N3A	4.97	1.40	1.32
2	D	801	FAD	C10-N1	3.52	1.40	1.33
2	A	801	FAD	C10-N1	3.51	1.40	1.33
2	C	801	FAD	C10-N1	3.50	1.40	1.33
2	B	801	FAD	C10-N1	3.49	1.40	1.33
2	B	801	FAD	C9A-N10	-3.48	1.35	1.41
2	D	801	FAD	C9A-N10	-3.48	1.35	1.41
2	A	801	FAD	C9A-N10	-3.47	1.35	1.41
2	C	801	FAD	C9A-N10	-3.45	1.35	1.41
2	D	801	FAD	C2A-N1A	3.28	1.40	1.33
2	A	801	FAD	C2A-N1A	3.26	1.40	1.33
2	B	801	FAD	C2A-N1A	3.26	1.40	1.33
2	C	801	FAD	C2A-N1A	3.24	1.39	1.33
2	A	801	FAD	C5A-C4A	-2.71	1.33	1.40
2	D	801	FAD	C5A-C4A	-2.69	1.33	1.40
2	B	801	FAD	C5A-C4A	-2.69	1.33	1.40
2	C	801	FAD	C5A-C4A	-2.67	1.33	1.40
2	C	801	FAD	C5X-N5	-2.62	1.34	1.39
2	D	801	FAD	C5X-N5	-2.61	1.34	1.39
2	D	801	FAD	C6A-C5A	-2.61	1.33	1.43
2	B	801	FAD	C6A-C5A	-2.60	1.33	1.43
2	C	801	FAD	C6A-C5A	-2.60	1.33	1.43
2	A	801	FAD	C6A-C5A	-2.60	1.33	1.43
2	B	801	FAD	C5X-N5	-2.59	1.34	1.39
2	A	801	FAD	C5X-N5	-2.58	1.34	1.39

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	FAD	N3A-C2A-N1A	-6.77	118.10	128.68
2	D	801	FAD	N3A-C2A-N1A	-6.75	118.12	128.68
2	C	801	FAD	N3A-C2A-N1A	-6.74	118.14	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	FAD	N3A-C2A-N1A	-6.72	118.18	128.68
2	C	801	FAD	O5B-PA-O1A	-5.19	88.80	109.07
2	C	801	FAD	O2A-PA-O5B	-4.66	86.11	107.75
2	C	801	FAD	P-O3P-PA	-3.72	120.06	132.83
2	B	801	FAD	P-O3P-PA	-3.62	120.41	132.83
2	D	801	FAD	P-O3P-PA	-3.62	120.42	132.83
2	A	801	FAD	P-O3P-PA	-3.61	120.44	132.83
2	C	801	FAD	C4-N3-C2	-3.06	119.99	125.64
2	D	801	FAD	C4-N3-C2	-3.04	120.03	125.64
2	B	801	FAD	C4-N3-C2	-3.04	120.03	125.64
2	A	801	FAD	C4-N3-C2	-3.02	120.06	125.64
2	C	801	FAD	C5A-C6A-N6A	-2.69	116.26	120.35
2	C	801	FAD	O4B-C1B-C2B	-2.69	103.00	106.93
2	B	801	FAD	C5A-C6A-N6A	-2.68	116.28	120.35
2	A	801	FAD	C5A-C6A-N6A	-2.68	116.28	120.35
2	A	801	FAD	O4B-C1B-C2B	-2.64	103.06	106.93
2	D	801	FAD	C5A-C6A-N6A	-2.64	116.34	120.35
2	C	801	FAD	C4X-C4-N3	2.63	119.87	113.19
2	B	801	FAD	C4X-C4-N3	2.62	119.85	113.19
2	D	801	FAD	C4X-C4-N3	2.61	119.83	113.19
2	A	801	FAD	C4X-C4-N3	2.59	119.78	113.19
2	B	801	FAD	O4B-C1B-C2B	-2.55	103.19	106.93
2	D	801	FAD	O4B-C1B-C2B	-2.53	103.23	106.93
2	C	801	FAD	C10-C4X-N5	-2.50	119.55	124.86
2	D	801	FAD	C10-C4X-N5	-2.48	119.59	124.86
2	A	801	FAD	C10-C4X-N5	-2.47	119.62	124.86
2	B	801	FAD	C10-C4X-N5	-2.45	119.65	124.86
2	C	801	FAD	C4X-C10-N10	2.40	120.00	116.48
2	B	801	FAD	C4X-C10-N10	2.36	119.93	116.48
2	D	801	FAD	C4X-C10-N10	2.35	119.92	116.48
2	A	801	FAD	C4X-C10-N10	2.33	119.88	116.48
2	A	801	FAD	C9A-C5X-N5	-2.32	119.91	122.43
2	C	801	FAD	C9A-C5X-N5	-2.30	119.93	122.43
2	D	801	FAD	C9A-C5X-N5	-2.29	119.94	122.43
2	B	801	FAD	C9A-C5X-N5	-2.27	119.96	122.43
2	C	801	FAD	O4-C4-C4X	-2.24	120.65	126.60
2	B	801	FAD	O4-C4-C4X	-2.24	120.66	126.60
2	A	801	FAD	O4-C4-C4X	-2.23	120.68	126.60
2	D	801	FAD	O4-C4-C4X	-2.23	120.69	126.60
2	C	801	FAD	O2A-PA-O1A	2.18	123.00	112.24
2	C	801	FAD	C4-C4X-C10	2.15	120.41	116.79
2	A	801	FAD	C4-C4X-C10	2.15	120.40	116.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	801	FAD	C4-C4X-C10	2.14	120.38	116.79
2	B	801	FAD	C4-C4X-C10	2.13	120.37	116.79

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	PG4	C8-C7-O4-C6
3	D	802	PG4	O3-C5-C6-O4
3	A	802	PG4	O4-C7-C8-O5
3	C	802	PG4	O4-C7-C8-O5
3	A	802	PG4	C6-C5-O3-C4
3	C	802	PG4	O1-C1-C2-O2
3	B	802	PG4	O2-C3-C4-O3
3	B	802	PG4	O3-C5-C6-O4
3	D	802	PG4	C8-C7-O4-C6
3	A	802	PG4	O1-C1-C2-O2
3	A	802	PG4	O2-C3-C4-O3
3	D	802	PG4	C4-C3-O2-C2
3	B	802	PG4	C3-C4-O3-C5
3	A	802	PG4	O3-C5-C6-O4
3	A	802	PG4	C1-C2-O2-C3
3	D	802	PG4	C3-C4-O3-C5
3	D	802	PG4	C5-C6-O4-C7
2	C	801	FAD	PA-O3P-P-O5'
3	C	802	PG4	O2-C3-C4-O3
2	A	801	FAD	O4B-C4B-C5B-O5B
2	B	801	FAD	O4B-C4B-C5B-O5B
2	D	801	FAD	O4B-C4B-C5B-O5B
2	C	801	FAD	O4B-C4B-C5B-O5B
3	D	802	PG4	O2-C3-C4-O3
3	A	802	PG4	C4-C3-O2-C2

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	802	PG4	2	0
2	C	801	FAD	2	0
2	A	801	FAD	4	0
2	D	801	FAD	1	0

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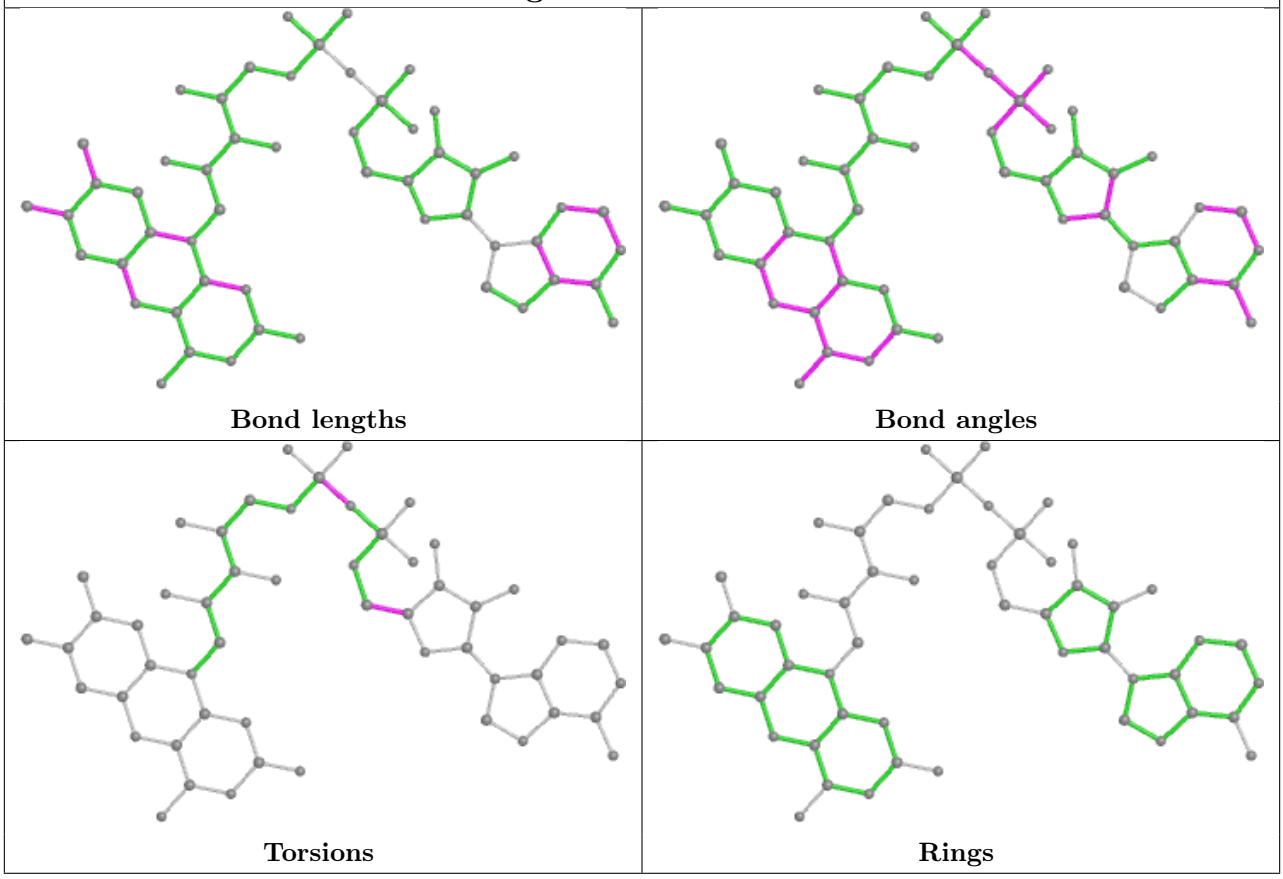
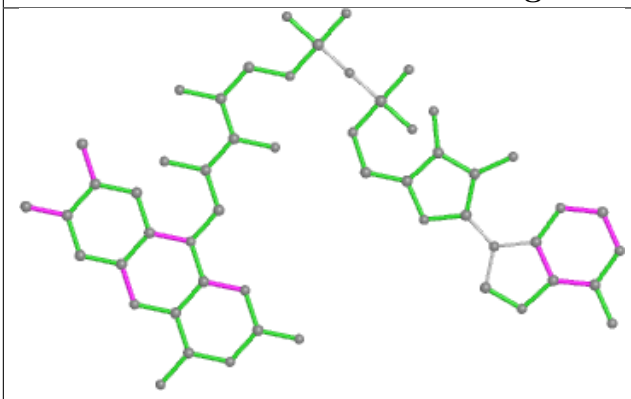
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	PG4	2	0
2	B	801	FAD	2	0

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

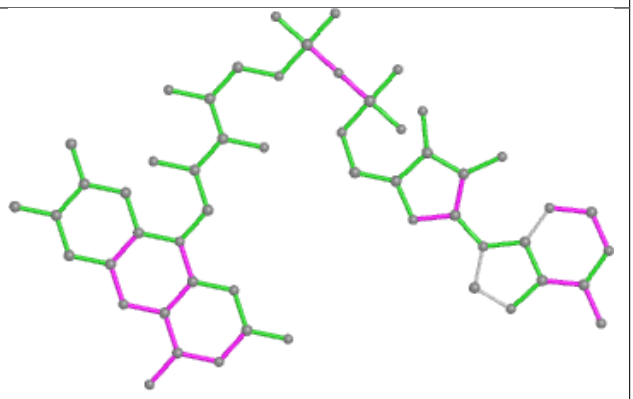
Ligand FAD C 801



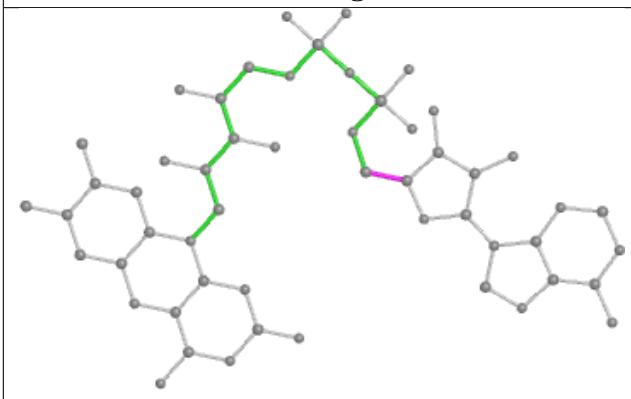
Ligand FAD A 801



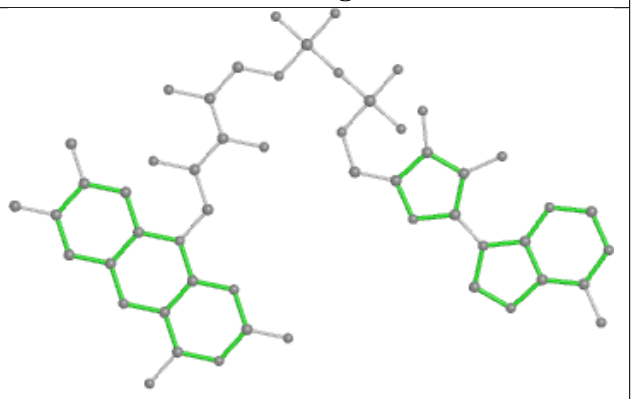
Bond lengths



Bond angles

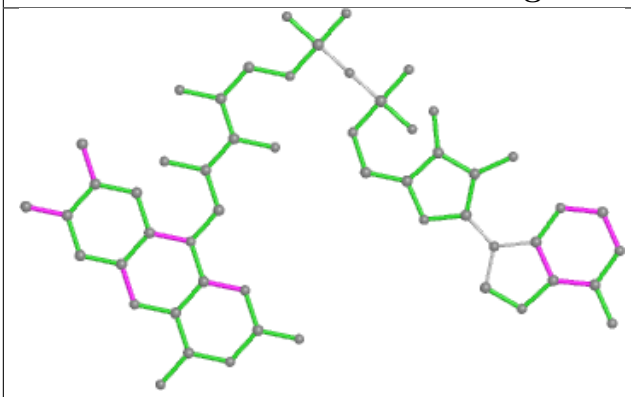


Torsions

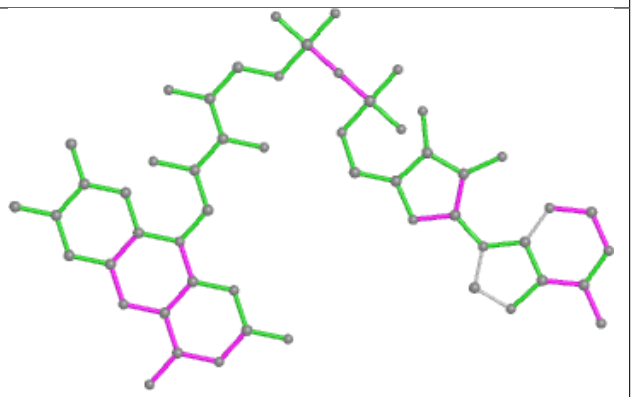


Rings

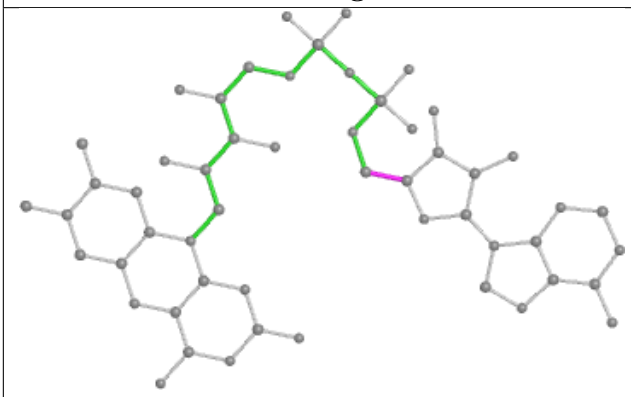
Ligand FAD D 801



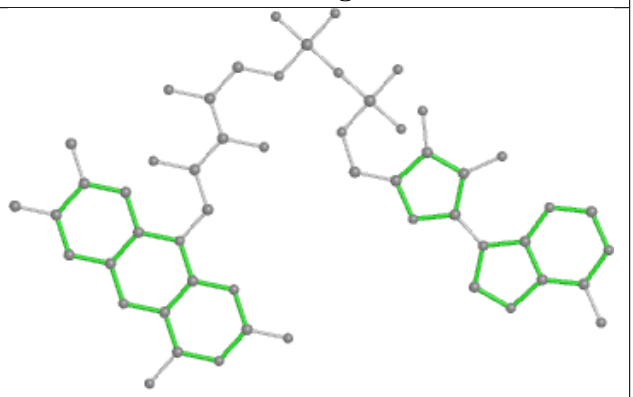
Bond lengths



Bond angles

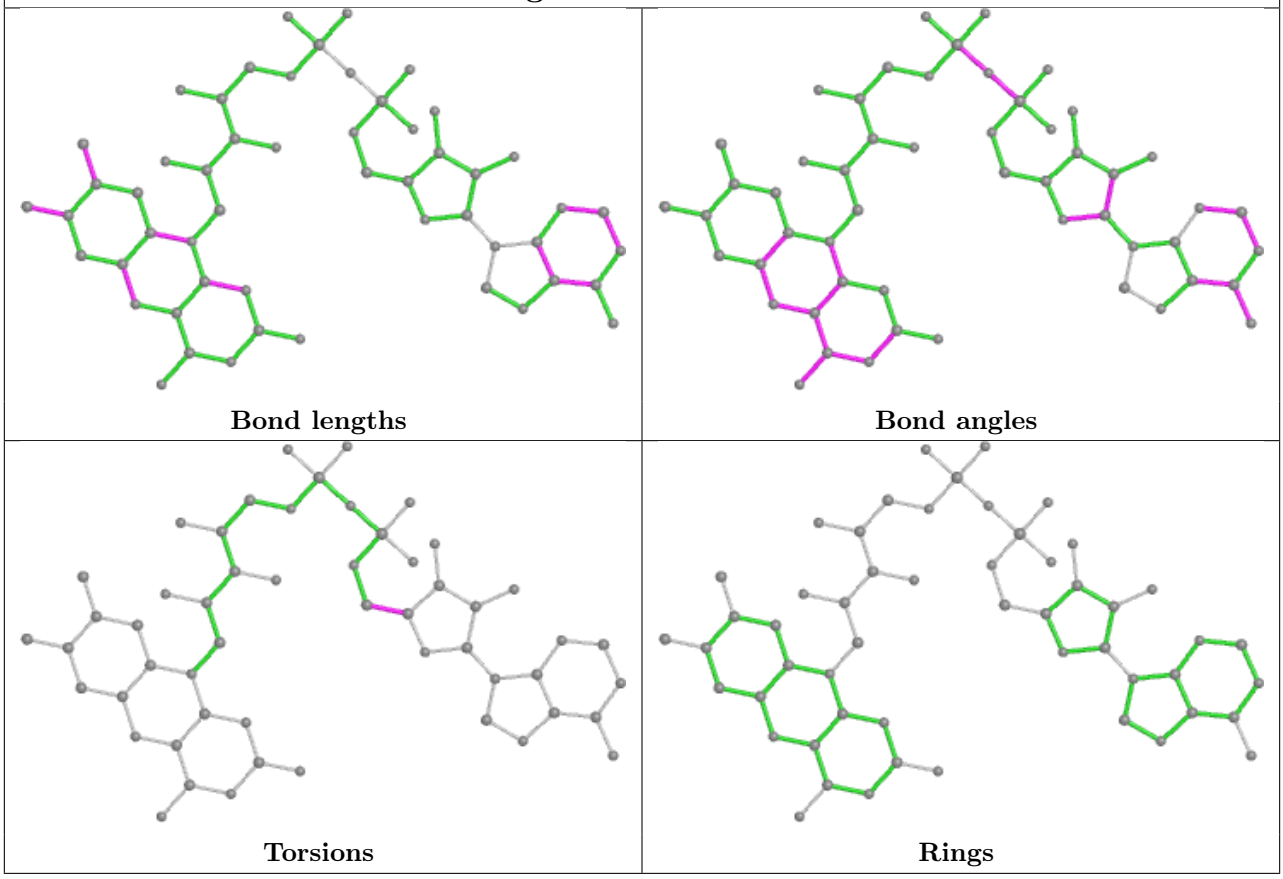


Torsions



Rings

Ligand FAD B 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	494/516 (95%)	0.18	14 (2%) 53 51	18, 31, 53, 77	0
1	B	502/516 (97%)	0.23	17 (3%) 45 44	19, 31, 56, 80	0
1	C	488/516 (94%)	0.14	9 (1%) 68 66	18, 31, 51, 73	0
1	D	498/516 (96%)	0.22	11 (2%) 62 60	17, 30, 55, 82	0
All	All	1982/2064 (96%)	0.19	51 (2%) 56 54	17, 30, 54, 82	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	230	PRO	4.7
1	D	421	ILE	4.2
1	D	230	PRO	4.2
1	A	189	PHE	4.2
1	B	231	SER	4.2
1	A	132	GLN	4.1
1	B	133	HIS	3.8
1	B	421	ILE	3.8
1	B	349	THR	3.7
1	A	232	LYS	3.7
1	C	133	HIS	3.6
1	C	189	PHE	3.3
1	B	264	PRO	3.2
1	A	131	HIS	3.2
1	C	344	ASP	3.1
1	A	428	ASN	3.1
1	C	428	ASN	3.0
1	D	133	HIS	3.0
1	A	7	ALA	3.0
1	C	132	GLN	2.9
1	D	131	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	344	ASP	2.8
1	B	189	PHE	2.8
1	D	343	GLU	2.7
1	B	230	PRO	2.7
1	D	189	PHE	2.6
1	B	174	TRP	2.5
1	B	263	GLN	2.5
1	B	344	ASP	2.5
1	D	103	GLU	2.5
1	B	7	ALA	2.4
1	C	190	GLY	2.4
1	B	342	ARG	2.4
1	A	133	HIS	2.4
1	C	509	LEU	2.3
1	A	231	SER	2.2
1	A	342	ARG	2.2
1	A	267	ASN	2.2
1	D	331	GLU	2.2
1	B	267	ASN	2.1
1	D	231	SER	2.1
1	A	410	ASP	2.1
1	A	331	GLU	2.1
1	B	343	GLU	2.1
1	B	336	LEU	2.1
1	D	333	LEU	2.1
1	C	54	TYR	2.0
1	B	345	SER	2.0
1	A	349	THR	2.0
1	B	191	HIS	2.0
1	C	103	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 monosaccharides in this entry.

6.4 Ligands (i)

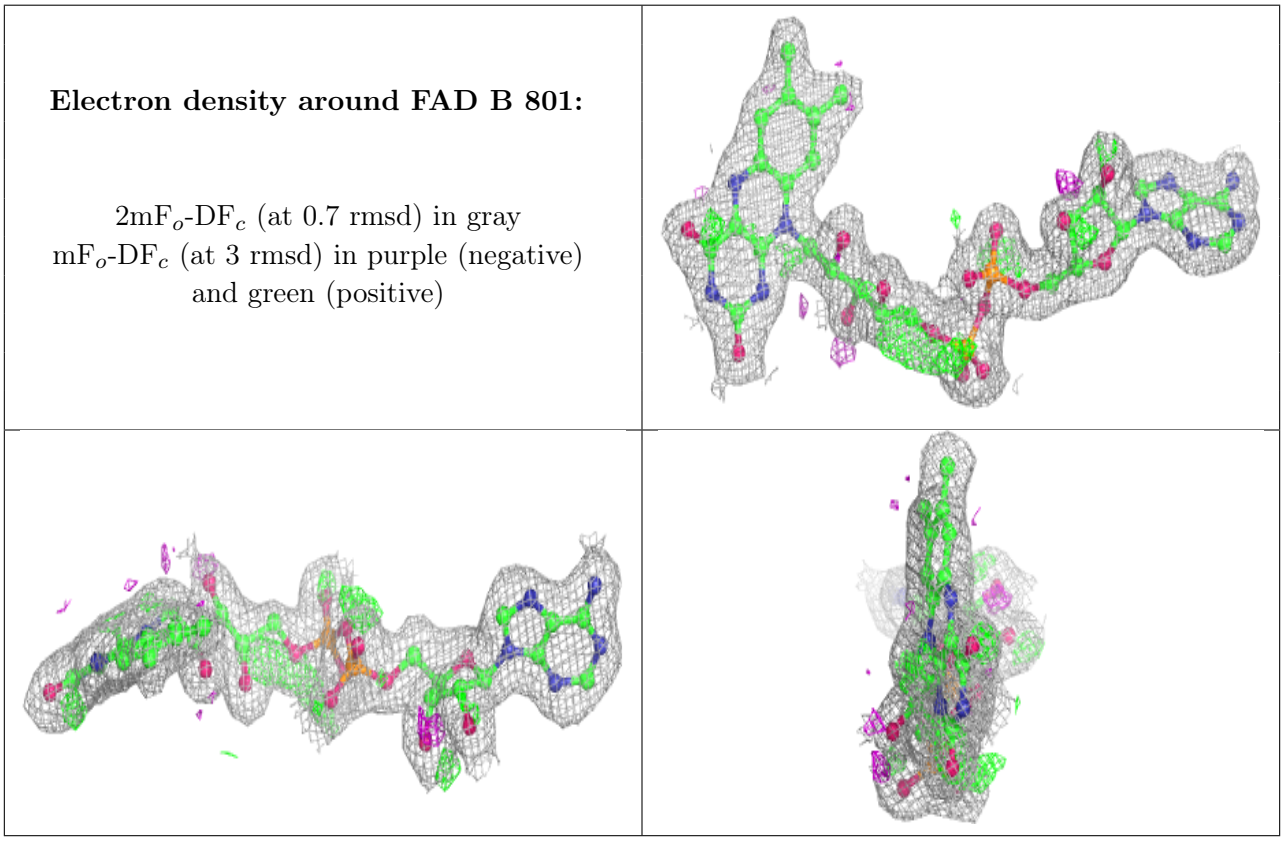
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	PG4	B	802	11/13	0.86	0.14	31,38,45,47	0
3	PG4	A	802	13/13	0.88	0.18	31,37,46,47	0
3	PG4	C	802	13/13	0.88	0.16	29,37,46,64	0
3	PG4	D	802	11/13	0.88	0.18	30,37,43,47	0
2	FAD	B	801	53/53	0.96	0.13	18,21,25,26	0
2	FAD	D	801	53/53	0.96	0.13	15,20,25,25	0
2	FAD	C	801	53/53	0.97	0.11	14,21,25,26	0
2	FAD	A	801	53/53	0.97	0.11	15,20,23,26	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.

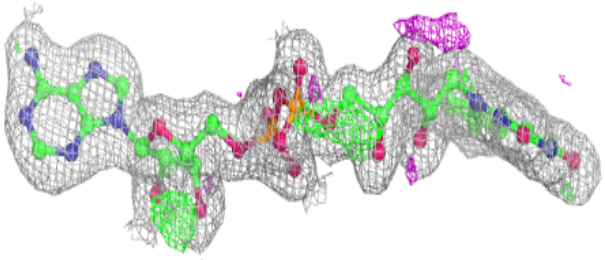
Electron density around FAD B 801:

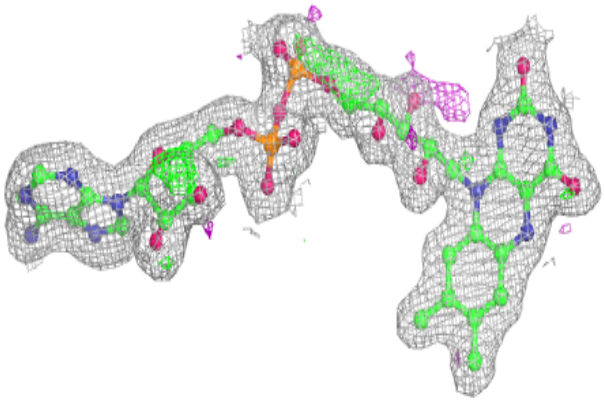
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

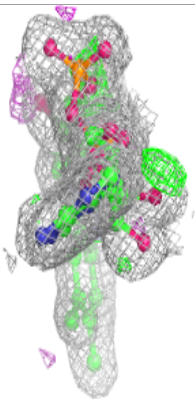


Electron density around FAD D 801:

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

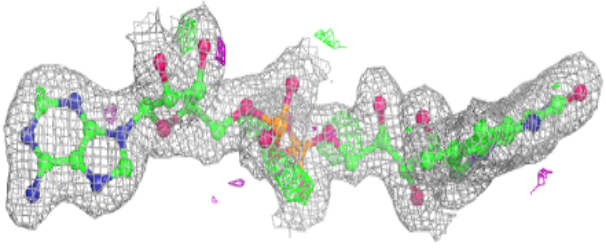


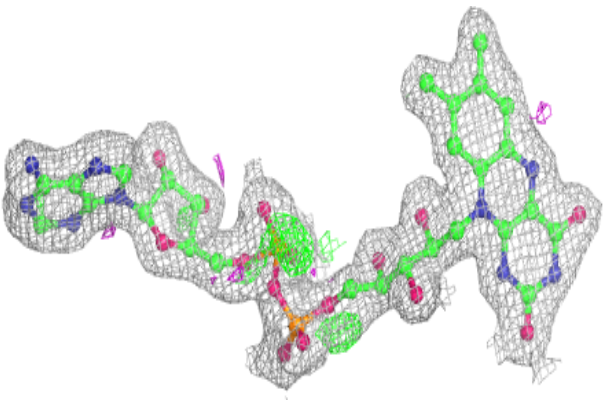


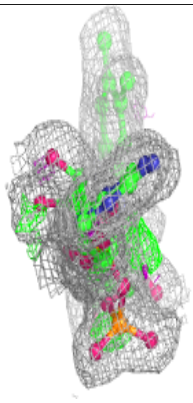


Electron density around FAD C 801:

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

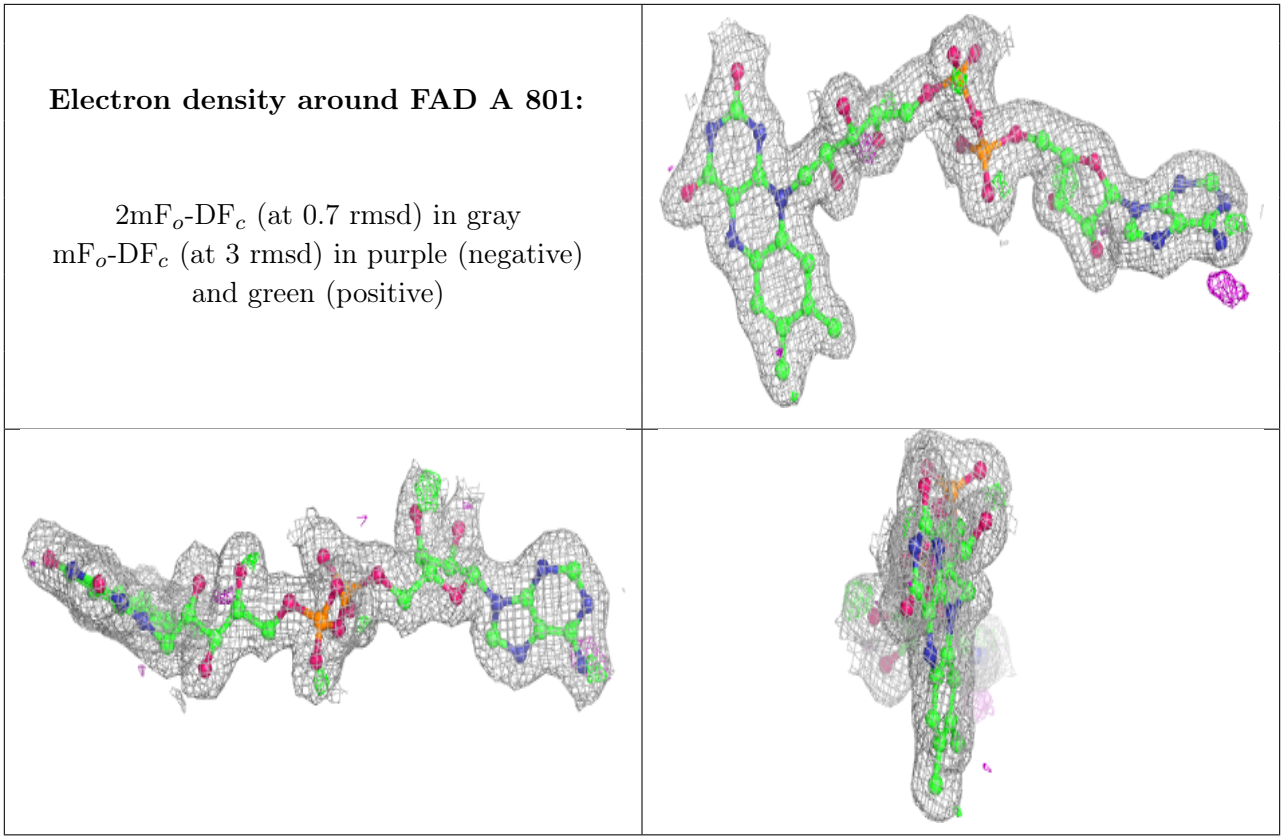






Electron density around FAD A 801:

$2mF_o$-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.