



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:19 AM UTC

PDB ID : 4GDP / pdb_00004gdp
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

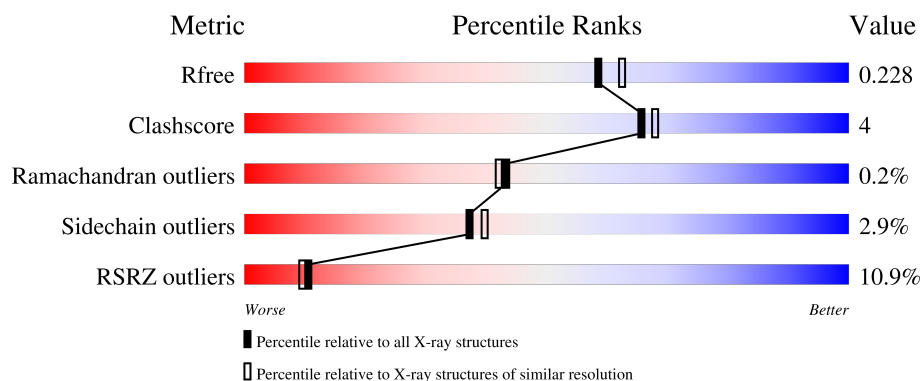
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	516	11% 87% 9% .
1	B	516	12% 87% 9% ..
1	C	516	9% 86% 7% 5%
1	D	516	11% 83% 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:

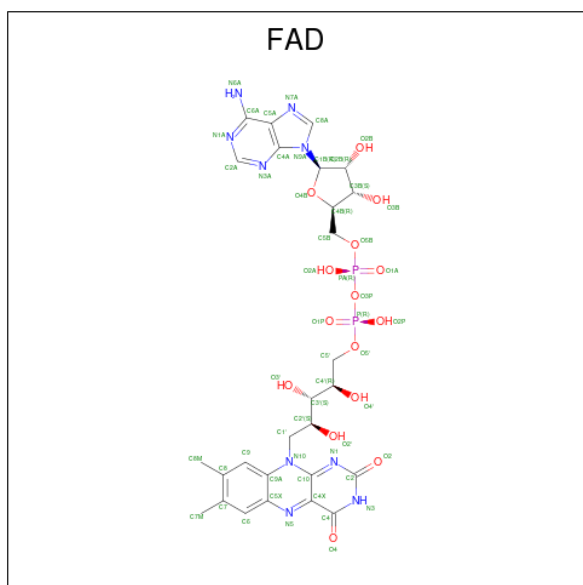
Chain	Residue	Modelled	Actual	Comment	Reference
A	195	ALA	ASN	engineered mutation	UNP P50264
A	509	LEU	-	expression tag	UNP P50264
A	510	GLU	-	expression tag	UNP P50264
A	511	HIS	-	expression tag	UNP P50264
A	512	HIS	-	expression tag	UNP P50264
A	513	HIS	-	expression tag	UNP P50264
A	514	HIS	-	expression 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 (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

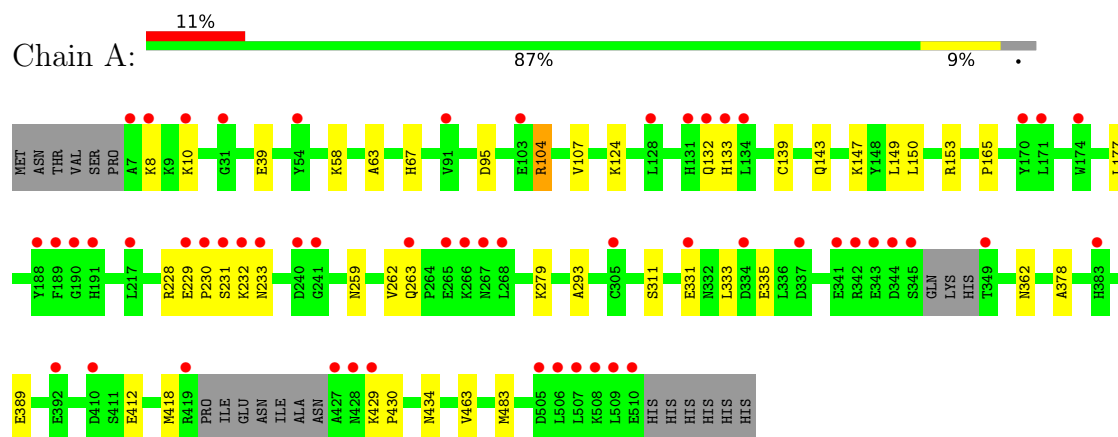
- Molecule 4 is water.

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

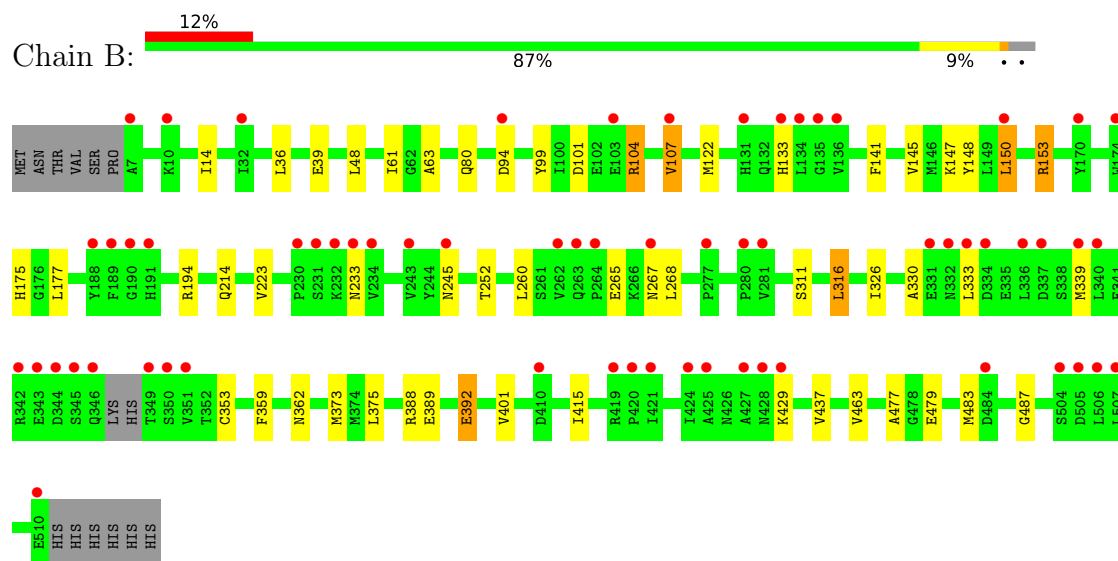
3 Residue-property plots [i](#)

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.

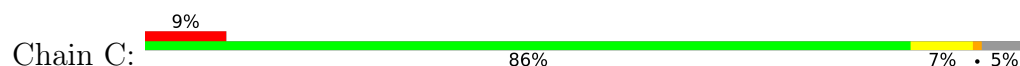
• Molecule 1: Polyamine oxidase FMS1

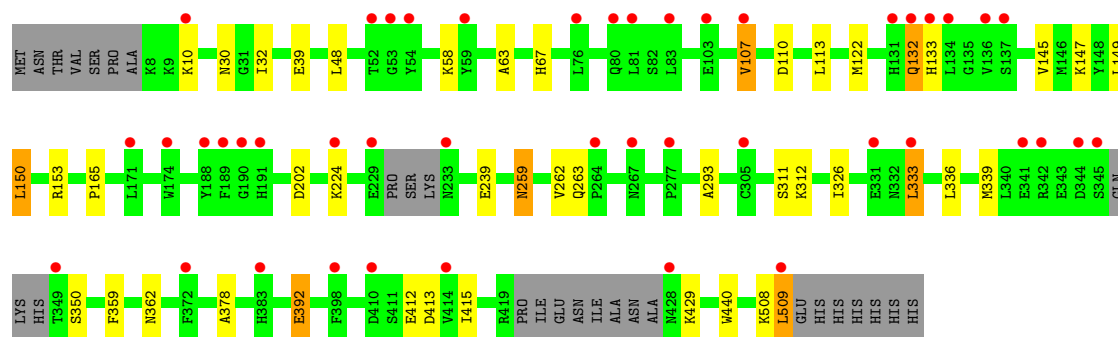


• Molecule 1: Polyamine oxidase FMS1

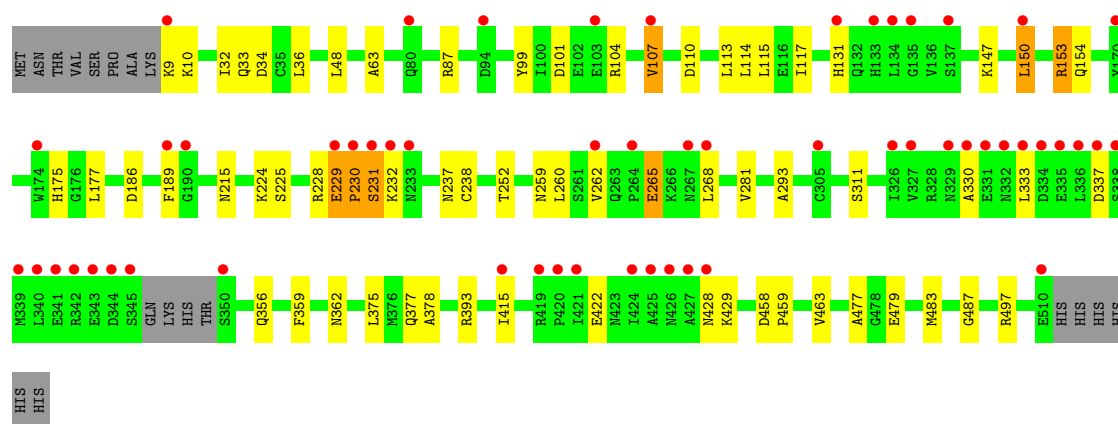
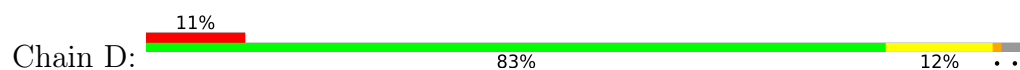


• Molecule 1: Polyamine oxidase FMS1





● Molecule 1: Polyamine oxidase FMS1



4 Data and refinement statistics

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 79.07 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.9 (79.07-2.00) 88.9 (79.07-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.203 , 0.234 0.197 , 0.228	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 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/4050	0.69	0/5474
1	B	0.35	0/4119	0.70	0/5570
1	C	0.35	0/3996	0.69	0/5399
1	D	0.35	0/4084	0.70	2/5523 (0.0%)
All	All	0.35	0/16249	0.69	2/21966 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	229	GLU	CA-C-N	6.00	127.33	119.84
1	D	229	GLU	C-N-CA	6.00	127.33	119.84

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	3967	0	3885	24	0
1	B	4029	0	3955	30	0
1	C	3916	0	3837	27	0
1	D	3997	0	3921	39	0
2	A	53	0	31	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	31	2	0
2	C	53	0	31	2	0
2	D	53	0	31	0	0
3	A	13	0	18	2	0
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	120	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 (120) 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:C:122:MET:HE1	1:C:145:VAL:HG13	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: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:39:GLU:OE1	2:A:801:FAD:O2B	2.22	0.54
1:A:311:SER:HA	1:A:362:ASN:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:326:ILE:HG23	1:C:339:MET:HE2	1.88	0.54
1:D:497:ARG:NE	4:D:1069:HOH:O	2.41	0.54
1:A:293:ALA:HB3	1:A:378:ALA:HB2	1.90	0.53
1:C:293:ALA:HB3	1:C:378:ALA:HB2	1.91	0.53
1:B:133:HIS:HD1	1:D:422:GLU:CD	2.17	0.52
1:B:326:ILE:HG23	1:B:339:MET:HE2	1.92	0.52
1:D:463:VAL:HG21	1:D:483:MET:HE2	1.92	0.52
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: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: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:B:39:GLU:OE1	2:B:801:FAD:O2B	2.27	0.47
1:A:8:LYS:HE2	1:A:233:ASN:ND2	2.29	0.47
1:B:373:MET:HE3	1:B:375:LEU:HD11	1.97	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:A:418:MET:HE3	1:A:434:ASN:HA	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:230:PRO:C	1:A:232:LYS:H	2.25	0.44
1:C:312:LYS:HD2	1:C:359:PHE:CZ	2.52	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:D:265:GLU:H	1:D:265:GLU:CD	2.25	0.44
1:C:30:ASN:O	1:C:508:LYS:HE3	2.18	0.43
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:B:392:GLU:CD	1:B:392:GLU:H	2.27	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:B:122[B]:MET:HE2	1:B:148:TYR:CD2	2.55	0.42
1:C:392:GLU:H	1:C:392:GLU:CD	2.27	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
2:A:801:FAD:O4'	2:A:801:FAD:O2'	2.30	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	43	42
1	D	496/516 (96%)	480 (97%)	14 (3%)	2 (0%)	30	27
All	All	1968/2064 (95%)	1905 (97%)	60 (3%)	3 (0%)	43	42

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 ⓘ

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%)	423 (97%)	14 (3%)	34	35
1	B	445/456 (98%)	431 (97%)	14 (3%)	35	37
1	C	432/456 (95%)	423 (98%)	9 (2%)	47	52
1	D	441/456 (97%)	428 (97%)	13 (3%)	37	40
All	All	1755/1824 (96%)	1705 (97%)	50 (3%)	37	41

All (50) 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	150	LEU
1	A	153	ARG
1	A	177	LEU
1	A	229	GLU
1	A	231	SER
1	A	263	GLN
1	A	331	GLU
1	A	335	GLU
1	A	389	GLU
1	B	36	LEU
1	B	101	ASP
1	B	104	ARG
1	B	107	VAL
1	B	150	LEU

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Mol	Chain	Res	Type
1	B	153	ARG
1	B	177	LEU
1	B	233	ASN
1	B	245	ASN
1	B	265	GLU
1	B	267	ASN
1	B	316	LEU
1	B	389	GLU
1	B	392	GLU
1	C	107	VAL
1	C	150	LEU
1	C	153	ARG
1	C	259	ASN
1	C	263	GLN
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	104	ARG
1	D	107	VAL
1	D	150	LEU
1	D	153	ARG
1	D	177	LEU
1	D	265	GLU
1	D	337	ASP
1	D	356	GLN
1	D	377	GLN
1	D	428	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	120	ASN
1	A	233	ASN
1	A	245	ASN
1	B	80	GLN
1	B	191	HIS
1	B	200	ASN

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Mol	Chain	Res	Type
1	B	206	GLN
1	B	237	ASN
1	B	245	ASN
1	B	259	ASN
1	C	67	HIS
1	C	200	ASN
1	C	428	ASN
1	C	439	ASN
1	D	49	GLN
1	D	80	GLN
1	D	109	HIS
1	D	200	ASN
1	D	237	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	FAD	A	801	-	58,58,58	1.83	12 (20%)	85,89,89	1.66	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	B	801	-	58,58,58	1.83	12 (20%)	85,89,89	1.67	19 (22%)
3	PG4	A	802	-	12,12,12	0.70	0	11,11,11	1.47	0
2	FAD	C	801	-	58,58,58	1.88	13 (22%)	85,89,89	1.91	24 (28%)
3	PG4	C	802	-	12,12,12	0.67	0	11,11,11	1.47	0
2	FAD	D	801	-	58,58,58	1.83	12 (20%)	85,89,89	1.67	19 (22%)
3	PG4	D	802	-	10,10,12	0.61	0	9,9,11	1.46	0
3	PG4	B	802	-	10,10,12	0.70	0	9,9,11	1.37	0

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	801	-	-	1/34/50/50	0/6/6/6
2	FAD	B	801	-	-	1/34/50/50	0/6/6/6
3	PG4	A	802	-	-	8/10/10/10	-
2	FAD	C	801	-	-	2/34/50/50	0/6/6/6
3	PG4	C	802	-	-	3/10/10/10	-
2	FAD	D	801	-	-	1/34/50/50	0/6/6/6
3	PG4	D	802	-	-	6/8/8/10	-
3	PG4	B	802	-	-	3/8/8/10	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FAD	C8M-C8	-5.94	1.39	1.51
2	A	801	FAD	C7M-C7	-5.94	1.39	1.51
2	D	801	FAD	C7M-C7	-5.94	1.39	1.51
2	C	801	FAD	C7M-C7	-5.93	1.39	1.51
2	D	801	FAD	C8M-C8	-5.93	1.39	1.51
2	C	801	FAD	C8M-C8	-5.92	1.39	1.51
2	B	801	FAD	C7M-C7	-5.90	1.40	1.51
2	A	801	FAD	C8M-C8	-5.88	1.40	1.51
2	C	801	FAD	PA-O3P	3.61	1.63	1.59
2	D	801	FAD	C10-N1	3.56	1.40	1.33
2	A	801	FAD	C10-N1	3.55	1.40	1.33
2	B	801	FAD	C9A-N10	-3.55	1.35	1.41
2	D	801	FAD	C9A-N10	-3.55	1.35	1.41
2	A	801	FAD	C9A-N10	-3.54	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	FAD	C10-N1	3.54	1.40	1.33
2	B	801	FAD	C10-N1	3.54	1.40	1.33
2	C	801	FAD	C9A-N10	-3.51	1.35	1.41
2	C	801	FAD	C2A-N3A	3.49	1.40	1.33
2	A	801	FAD	C2A-N3A	3.49	1.40	1.33
2	D	801	FAD	C2A-N3A	3.48	1.40	1.33
2	B	801	FAD	C2A-N3A	3.48	1.40	1.33
2	D	801	FAD	C2A-N1A	3.42	1.40	1.33
2	A	801	FAD	C2A-N1A	3.40	1.40	1.33
2	B	801	FAD	C2A-N1A	3.40	1.40	1.33
2	C	801	FAD	C2A-N1A	3.38	1.39	1.33
2	B	801	FAD	C5A-N7A	-3.08	1.33	1.39
2	C	801	FAD	C5A-N7A	-3.07	1.33	1.39
2	A	801	FAD	C5A-N7A	-3.03	1.33	1.39
2	D	801	FAD	C5A-N7A	-3.02	1.33	1.39
2	A	801	FAD	C5A-C4A	-2.99	1.33	1.39
2	D	801	FAD	C5A-C4A	-2.96	1.33	1.39
2	B	801	FAD	C5A-C4A	-2.96	1.33	1.39
2	C	801	FAD	C5A-C4A	-2.93	1.33	1.39
2	C	801	FAD	C5X-N5	-2.74	1.34	1.39
2	D	801	FAD	C5X-N5	-2.73	1.34	1.39
2	B	801	FAD	C5X-N5	-2.70	1.34	1.39
2	A	801	FAD	C5X-N5	-2.69	1.34	1.39
2	D	801	FAD	C5A-C6A	-2.65	1.33	1.41
2	B	801	FAD	C5A-C6A	-2.65	1.33	1.41
2	C	801	FAD	C5A-C6A	-2.64	1.33	1.41
2	A	801	FAD	C5A-C6A	-2.64	1.33	1.41
2	A	801	FAD	C8A-N9A	-2.50	1.33	1.37
2	D	801	FAD	C8A-N9A	-2.48	1.33	1.37
2	B	801	FAD	C8A-N9A	-2.48	1.33	1.37
2	C	801	FAD	C8A-N9A	-2.44	1.33	1.37
2	D	801	FAD	C4A-N9A	-2.07	1.33	1.37
2	B	801	FAD	C4A-N9A	-2.07	1.33	1.37
2	A	801	FAD	C4A-N9A	-2.01	1.33	1.37
2	C	801	FAD	C4A-N9A	-2.01	1.33	1.37

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FAD	N3A-C2A-N1A	-6.92	118.10	128.58
2	D	801	FAD	N3A-C2A-N1A	-6.91	118.12	128.58
2	C	801	FAD	N3A-C2A-N1A	-6.90	118.14	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	N3A-C2A-N1A	-6.87	118.18	128.58
2	C	801	FAD	O5B-PA-O1A	-5.08	88.80	108.94
2	C	801	FAD	O2A-PA-O5B	-4.73	86.11	107.57
2	D	801	FAD	C5A-C4A-N3A	-4.42	120.63	126.72
2	B	801	FAD	C5A-C4A-N3A	-4.39	120.68	126.72
2	C	801	FAD	C5A-C4A-N3A	-4.38	120.68	126.72
2	A	801	FAD	C5A-C4A-N3A	-4.38	120.68	126.72
2	B	801	FAD	N9A-C8A-N7A	-4.30	107.83	113.94
2	D	801	FAD	N9A-C8A-N7A	-4.30	107.84	113.94
2	C	801	FAD	N9A-C8A-N7A	-4.29	107.84	113.94
2	A	801	FAD	N9A-C8A-N7A	-4.27	107.87	113.94
2	C	801	FAD	O2A-PA-O3P	3.78	117.48	107.27
2	B	801	FAD	C2A-N3A-C4A	3.26	119.80	111.83
2	D	801	FAD	C2A-N3A-C4A	3.26	119.80	111.83
2	C	801	FAD	C2A-N3A-C4A	3.26	119.80	111.83
2	A	801	FAD	C2A-N3A-C4A	3.24	119.74	111.83
2	C	801	FAD	C4-N3-C2	-3.18	119.99	125.64
2	D	801	FAD	C4-N3-C2	-3.16	120.03	125.64
2	B	801	FAD	C4-N3-C2	-3.16	120.03	125.64
2	A	801	FAD	C4-N3-C2	-3.14	120.06	125.64
2	C	801	FAD	C5A-N7A-C8A	3.03	108.21	103.45
2	D	801	FAD	C5A-N7A-C8A	3.02	108.20	103.45
2	A	801	FAD	C5A-N7A-C8A	3.01	108.19	103.45
2	B	801	FAD	C5A-N7A-C8A	3.01	108.18	103.45
2	C	801	FAD	C5A-C6A-N6A	-2.84	116.26	123.29
2	B	801	FAD	C5A-C6A-N6A	-2.83	116.28	123.29
2	A	801	FAD	C5A-C6A-N6A	-2.83	116.28	123.29
2	D	801	FAD	C5A-C6A-N6A	-2.80	116.34	123.29
2	D	801	FAD	C6A-C5A-C4A	2.65	120.79	117.18
2	A	801	FAD	C6A-C5A-C4A	2.62	120.75	117.18
2	C	801	FAD	C4X-C4-N3	2.60	119.87	113.25
2	B	801	FAD	C6A-C5A-C4A	2.60	120.72	117.18
2	B	801	FAD	C4X-C4-N3	2.59	119.85	113.25
2	C	801	FAD	C6A-C5A-C4A	2.59	120.71	117.18
2	D	801	FAD	C4X-C4-N3	2.58	119.83	113.25
2	C	801	FAD	C10-C4X-N5	-2.58	119.55	124.81
2	A	801	FAD	C4X-C4-N3	2.56	119.78	113.25
2	D	801	FAD	N3A-C4A-N9A	2.56	131.52	127.17
2	D	801	FAD	C10-C4X-N5	-2.55	119.59	124.81
2	A	801	FAD	N3A-C4A-N9A	2.54	131.49	127.17
2	B	801	FAD	N3A-C4A-N9A	2.54	131.49	127.17
2	A	801	FAD	C10-C4X-N5	-2.54	119.62	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FAD	N3A-C4A-N9A	2.54	131.48	127.17
2	B	801	FAD	C10-C4X-N5	-2.53	119.65	124.81
2	C	801	FAD	C4X-C10-N10	2.45	120.00	116.48
2	C	801	FAD	O3P-PA-O1A	2.45	118.06	110.70
2	D	801	FAD	C4A-N9A-C8A	2.43	108.29	105.74
2	B	801	FAD	C4A-N9A-C8A	2.42	108.28	105.74
2	C	801	FAD	C4B-O4B-C1B	-2.42	104.12	109.47
2	D	801	FAD	C4A-C5A-N7A	-2.42	107.82	110.58
2	B	801	FAD	C4X-C10-N10	2.41	119.93	116.48
2	A	801	FAD	C4A-N9A-C8A	2.40	108.26	105.74
2	D	801	FAD	C4X-C10-N10	2.40	119.92	116.48
2	A	801	FAD	C9A-C5X-N5	-2.40	119.91	122.45
2	C	801	FAD	C4A-N9A-C8A	2.39	108.25	105.74
2	A	801	FAD	C4A-C5A-N7A	-2.39	107.85	110.58
2	C	801	FAD	C9A-C5X-N5	-2.38	119.93	122.45
2	C	801	FAD	C4A-C5A-N7A	-2.38	107.86	110.58
2	B	801	FAD	C4A-C5A-N7A	-2.37	107.87	110.58
2	A	801	FAD	C4X-C10-N10	2.37	119.88	116.48
2	D	801	FAD	C9A-C5X-N5	-2.36	119.94	122.45
2	C	801	FAD	C4'-C3'-C2'	-2.36	109.65	113.57
2	B	801	FAD	C9A-C5X-N5	-2.35	119.96	122.45
2	D	801	FAD	C4'-C3'-C2'	-2.34	109.68	113.57
2	D	801	FAD	C4B-O4B-C1B	-2.33	104.32	109.47
2	B	801	FAD	C4B-O4B-C1B	-2.32	104.35	109.47
2	A	801	FAD	C4B-O4B-C1B	-2.30	104.38	109.47
2	B	801	FAD	C4'-C3'-C2'	-2.29	109.76	113.57
2	C	801	FAD	O2A-PA-O1A	2.27	123.00	112.44
2	A	801	FAD	C4'-C3'-C2'	-2.26	109.81	113.57
2	C	801	FAD	O4-C4-C4X	-2.23	120.65	126.53
2	B	801	FAD	O4-C4-C4X	-2.22	120.66	126.53
2	A	801	FAD	O4-C4-C4X	-2.22	120.68	126.53
2	D	801	FAD	O4-C4-C4X	-2.21	120.69	126.53
2	C	801	FAD	C4-C4X-C10	2.03	120.41	116.93
2	A	801	FAD	C4-C4X-C10	2.02	120.40	116.93
2	D	801	FAD	C4-C4X-C10	2.01	120.38	116.93
2	B	801	FAD	C4-C4X-C10	2.00	120.37	116.93

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

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Mol	Chain	Res	Type	Atoms
3	D	802	PG4	O3-C5-C6-O4
3	A	802	PG4	O4-C7-C8-O5
3	C	802	PG4	O1-C1-C2-O2
3	C	802	PG4	O4-C7-C8-O5
3	A	802	PG4	C6-C5-O3-C4
3	B	802	PG4	O2-C3-C4-O3
3	B	802	PG4	O3-C5-C6-O4
3	A	802	PG4	O1-C1-C2-O2
3	D	802	PG4	C8-C7-O4-C6
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	D	802	PG4	C3-C4-O3-C5
3	A	802	PG4	C1-C2-O2-C3
3	A	802	PG4	O3-C5-C6-O4
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	O3'-C3'-C4'-C5'
2	B	801	FAD	O3'-C3'-C4'-C5'
3	A	802	PG4	C4-C3-O2-C2
2	D	801	FAD	O3'-C3'-C4'-C5'
3	D	802	PG4	O2-C3-C4-O3
2	C	801	FAD	PA-O3P-P-O2P

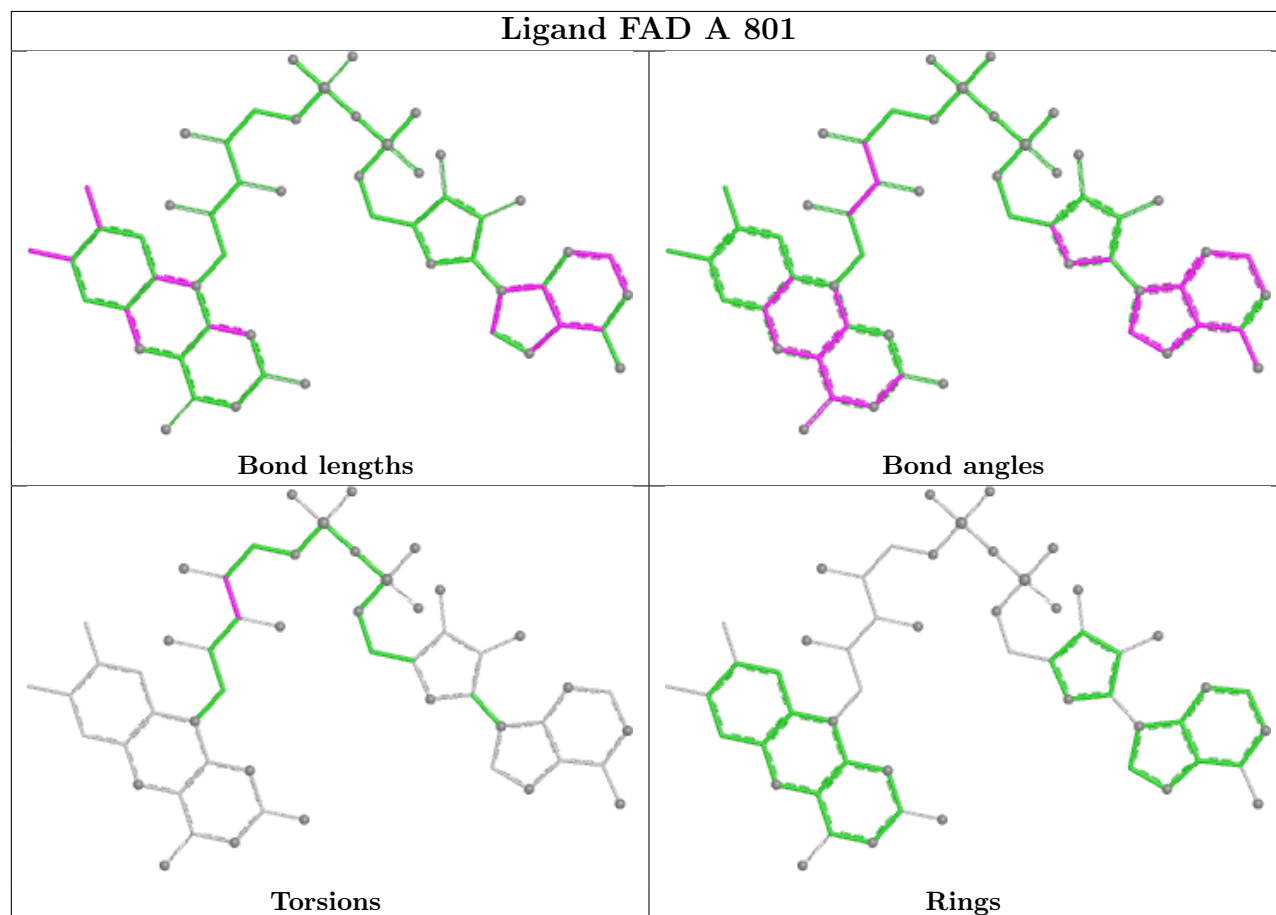
There are no ring outliers.

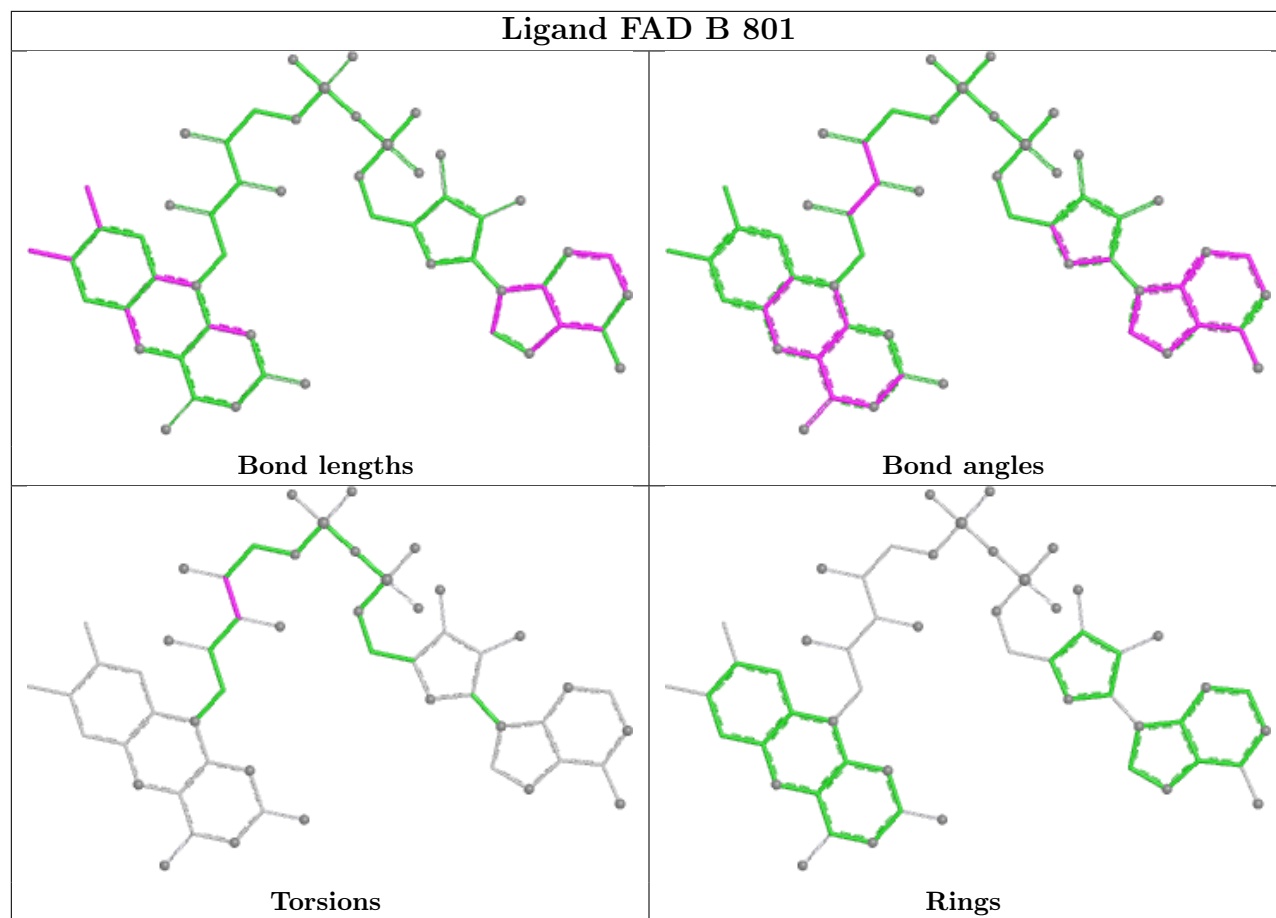
5 monomers are involved in 12 short contacts:

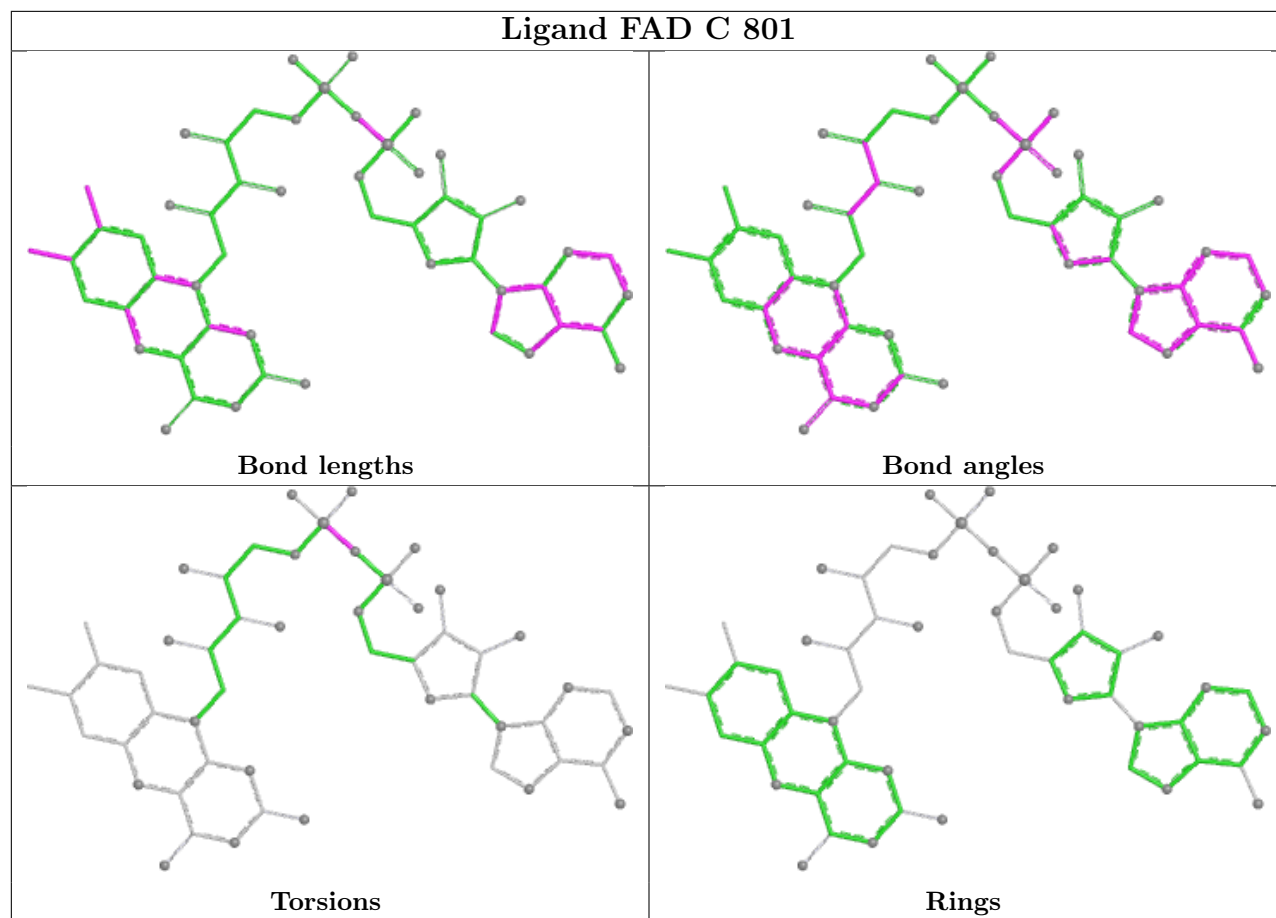
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FAD	5	0
2	B	801	FAD	2	0
3	A	802	PG4	2	0
2	C	801	FAD	2	0
3	C	802	PG4	2	0

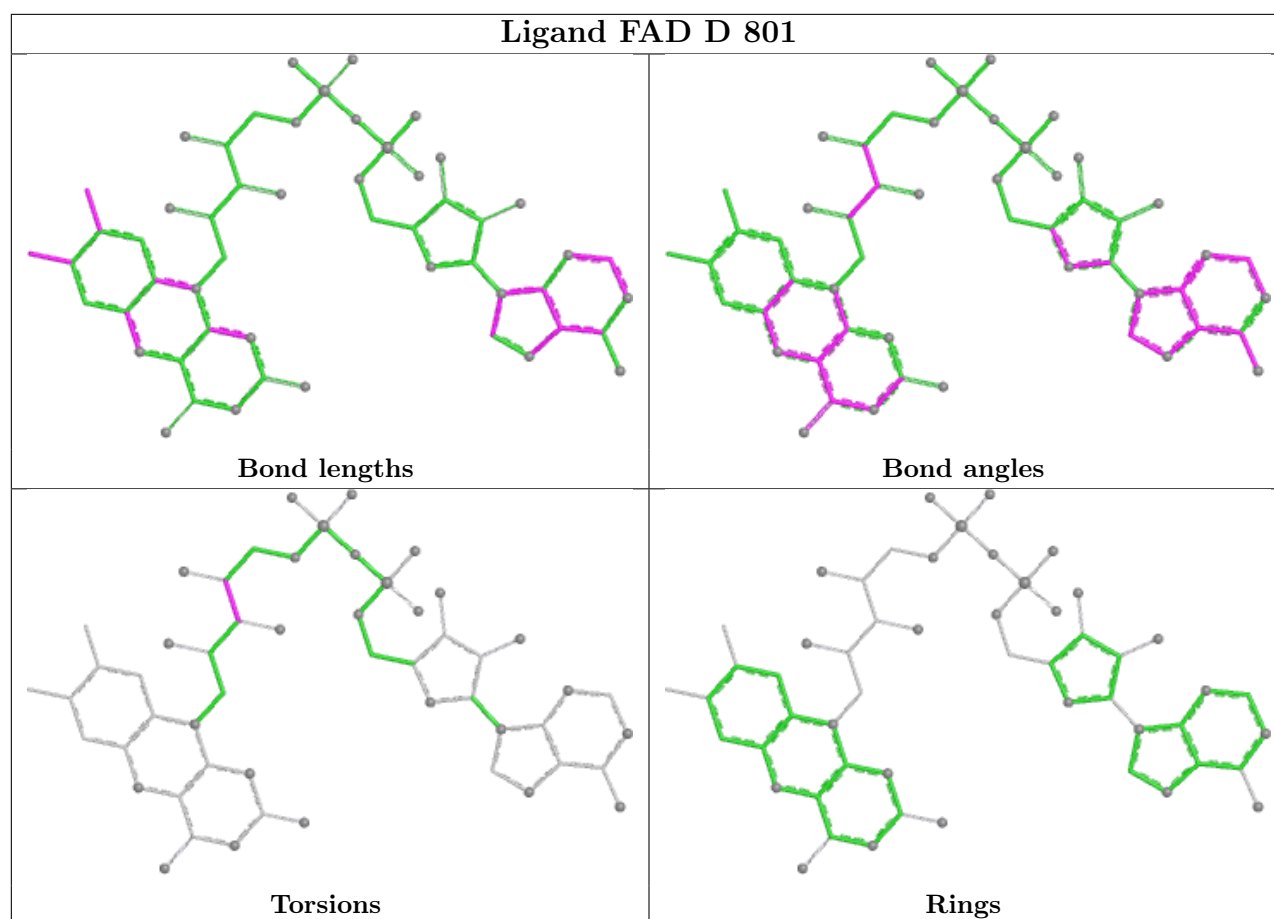
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	494/516 (95%)	0.82	55 (11%) 10 9	16, 31, 53, 77	2 (0%)
1	B	502/516 (97%)	0.86	63 (12%) 8 7	16, 31, 56, 80	3 (0%)
1	C	488/516 (94%)	0.80	44 (9%) 15 14	16, 31, 51, 73	1 (0%)
1	D	498/516 (96%)	0.80	55 (11%) 10 9	17, 30, 55, 82	2 (0%)
All	All	1982/2064 (96%)	0.82	217 (10%) 10 9	16, 30, 54, 82	8 (0%)

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	509	LEU	7.9
1	A	230	PRO	6.5
1	B	230	PRO	5.6
1	A	345	SER	5.4
1	B	349	THR	5.4
1	B	133	HIS	5.1
1	D	131	HIS	5.1
1	B	427	ALA	4.9
1	D	421	ILE	4.9
1	A	189	PHE	4.8
1	C	133	HIS	4.8
1	C	428	ASN	4.8
1	A	132	GLN	4.7
1	D	230	PRO	4.7
1	B	174	TRP	4.6
1	D	345	SER	4.5
1	C	345	SER	4.4
1	D	231	SER	4.4
1	A	232	LYS	4.4
1	A	131	HIS	4.3
1	D	264	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	427	ALA	4.2
1	B	134	LEU	4.1
1	D	343	GLU	4.1
1	D	333	LEU	4.1
1	A	133	HIS	4.0
1	A	188	TYR	4.0
1	D	340	LEU	3.9
1	A	383[A]	HIS	3.9
1	D	332	ASN	3.9
1	C	344	ASP	3.9
1	C	132	GLN	3.8
1	D	103	GLU	3.7
1	D	9	LYS	3.7
1	D	342	ARG	3.7
1	D	189	PHE	3.6
1	D	337	ASP	3.6
1	D	420	PRO	3.6
1	B	504	SER	3.6
1	B	7	ALA	3.5
1	B	336	LEU	3.6
1	B	425	ALA	3.5
1	A	267	ASN	3.5
1	A	231	SER	3.5
1	B	231	SER	3.5
1	C	174	TRP	3.5
1	C	190	GLY	3.5
1	B	340	LEU	3.4
1	A	428	ASN	3.4
1	C	229	GLU	3.4
1	C	189	PHE	3.4
1	C	188	TYR	3.4
1	B	350	SER	3.4
1	C	267	ASN	3.3
1	A	229	GLU	3.3
1	D	334	ASP	3.3
1	D	338	SER	3.3
1	C	54	TYR	3.3
1	D	330	ALA	3.3
1	D	174	TRP	3.3
1	B	189	PHE	3.2
1	A	190	GLY	3.2
1	A	7	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	188	TYR	3.2
1	D	344	ASP	3.2
1	B	170	TYR	3.1
1	A	349	THR	3.1
1	B	135	GLY	3.1
1	B	281	VAL	3.1
1	A	510	GLU	3.0
1	B	346	GLN	3.0
1	B	262	VAL	3.0
1	D	133	HIS	3.0
1	D	135	GLY	3.0
1	D	137	SER	3.0
1	B	232	LYS	3.0
1	D	134	LEU	2.9
1	D	170	TYR	2.9
1	C	349	THR	2.9
1	A	505	ASP	2.9
1	D	107	VAL	2.9
1	B	428	ASN	2.9
1	D	336	LEU	2.9
1	A	331	GLU	2.9
1	B	190	GLY	2.9
1	B	342	ARG	2.9
1	B	136	VAL	2.8
1	B	280	PRO	2.8
1	A	337	ASP	2.8
1	A	343	GLU	2.8
1	C	233	ASN	2.8
1	B	131	HIS	2.8
1	B	277	PRO	2.8
1	B	344	ASP	2.8
1	B	505	ASP	2.8
1	A	171	LEU	2.8
1	B	421	ILE	2.7
1	C	53	GLY	2.7
1	C	305	CYS	2.7
1	A	509	LEU	2.7
1	C	81	LEU	2.7
1	B	267	ASN	2.7
1	A	103	GLU	2.7
1	B	263	GLN	2.7
1	D	331	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	10	LYS	2.7
1	B	233	ASN	2.7
1	B	351	VAL	2.7
1	D	94	ASP	2.6
1	B	264	PRO	2.6
1	D	428	ASN	2.6
1	A	410	ASP	2.6
1	A	266	LYS	2.6
1	D	510	GLU	2.6
1	A	268	LEU	2.6
1	A	507	LEU	2.6
1	B	507	LEU	2.6
1	C	333	LEU	2.6
1	B	484	ASP	2.6
1	D	232	LYS	2.6
1	C	107	VAL	2.6
1	D	350	SER	2.6
1	C	76	LEU	2.5
1	B	191	HIS	2.5
1	C	136	VAL	2.5
1	C	191	HIS	2.5
1	C	383	HIS	2.5
1	A	342	ARG	2.5
1	A	170	TYR	2.5
1	A	506	LEU	2.5
1	C	83	LEU	2.5
1	C	137	SER	2.5
1	D	267	ASN	2.5
1	D	229	GLU	2.5
1	D	425	ALA	2.5
1	A	10	LYS	2.5
1	A	344	ASP	2.5
1	A	54	TYR	2.4
1	C	342	ARG	2.4
1	C	131	HIS	2.4
1	C	134	LEU	2.4
1	B	32	ILE	2.4
1	B	343	GLU	2.4
1	D	415	ILE	2.4
1	A	392	GLU	2.4
1	C	372	PHE	2.4
1	C	410	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	341	GLU	2.4
1	D	262	VAL	2.4
1	D	339	MET	2.4
1	B	419	ARG	2.3
1	D	150	LEU	2.3
1	A	265	GLU	2.3
1	B	331	GLU	2.3
1	A	233	ASN	2.3
1	B	234	VAL	2.3
1	D	419	ARG	2.3
1	C	103	GLU	2.3
1	B	339	MET	2.3
1	B	345	SER	2.3
1	B	245	ASN	2.3
1	C	264	PRO	2.3
1	D	335	GLU	2.2
1	B	94	ASP	2.2
1	B	334	ASP	2.2
1	A	191	HIS	2.2
1	A	128	LEU	2.2
1	A	134	LEU	2.2
1	A	341	GLU	2.2
1	B	333	LEU	2.2
1	A	174	TRP	2.2
1	C	398	PHE	2.2
1	D	424	ILE	2.2
1	A	429	LYS	2.2
1	C	10	LYS	2.2
1	D	327	VAL	2.2
1	A	305	CYS	2.2
1	A	263	GLN	2.2
1	A	31	GLY	2.2
1	A	241	GLY	2.2
1	B	337	ASP	2.2
1	A	508	LYS	2.2
1	B	332	ASN	2.2
1	B	510	GLU	2.2
1	A	91	VAL	2.2
1	C	171	LEU	2.2
1	B	420	PRO	2.2
1	D	233	ASN	2.1
1	D	426	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	326	ILE	2.1
1	A	240	ASP	2.1
1	B	410	ASP	2.1
1	B	107	VAL	2.1
1	D	268	LEU	2.1
1	D	341	GLU	2.1
1	D	427	ALA	2.1
1	D	80	GLN	2.1
1	A	217	LEU	2.1
1	B	506	LEU	2.1
1	C	80	GLN	2.1
1	B	424	ILE	2.1
1	C	52	THR	2.1
1	C	331	GLU	2.1
1	B	243	VAL	2.1
1	C	414	VAL	2.1
1	C	277	PRO	2.1
1	B	150	LEU	2.1
1	D	305	CYS	2.1
1	A	334	ASP	2.1
1	B	103	GLU	2.0
1	A	8	LYS	2.0
1	B	429	LYS	2.0
1	C	224	LYS	2.0
1	D	190	GLY	2.0
1	C	59	TYR	2.0
1	D	329	ASN	2.0
1	A	419	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

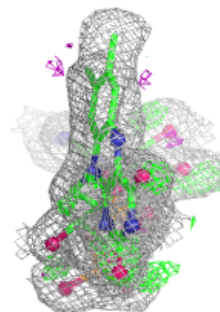
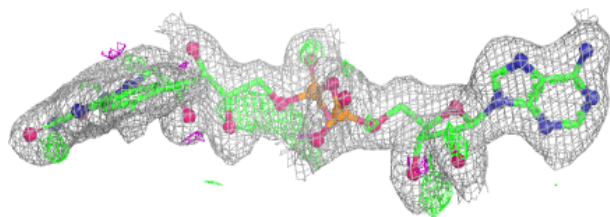
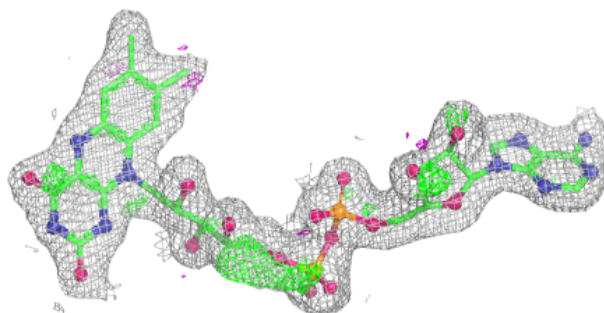
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PG4	B	802	11/13	0.79	0.14	31,38,45,47	0
3	PG4	C	802	13/13	0.81	0.16	29,37,46,64	0
3	PG4	D	802	11/13	0.82	0.16	30,37,43,47	0
3	PG4	A	802	13/13	0.84	0.12	31,37,46,47	0
2	FAD	B	801	53/53	0.95	0.08	18,21,25,26	0
2	FAD	D	801	53/53	0.95	0.08	15,20,25,25	0
2	FAD	C	801	53/53	0.96	0.07	14,21,25,26	0
2	FAD	A	801	53/53	0.96	0.07	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.

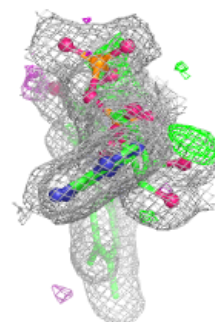
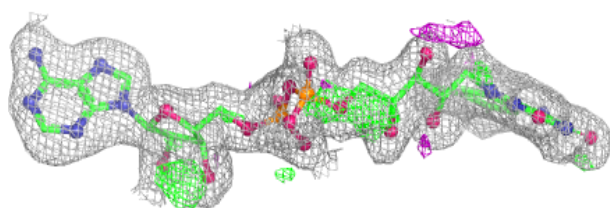
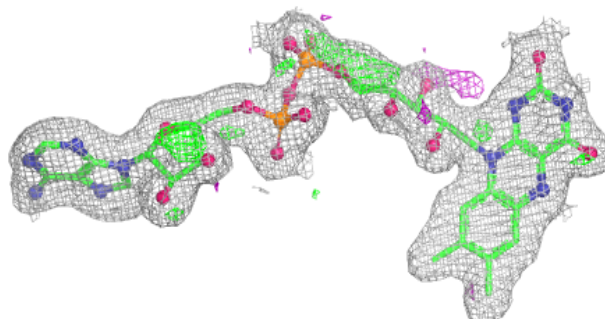
Electron density around FAD B 801:

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

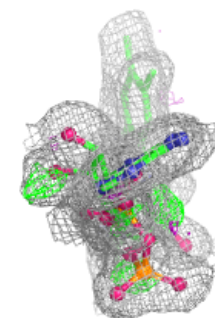
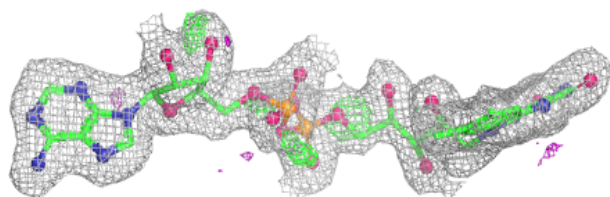
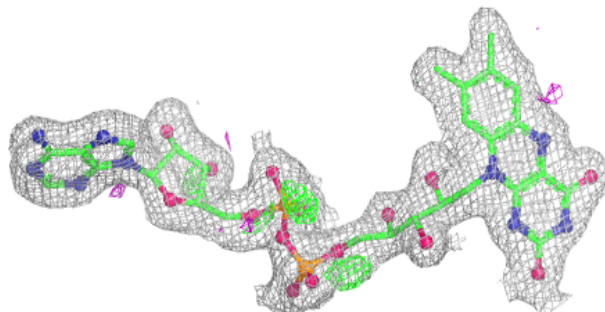


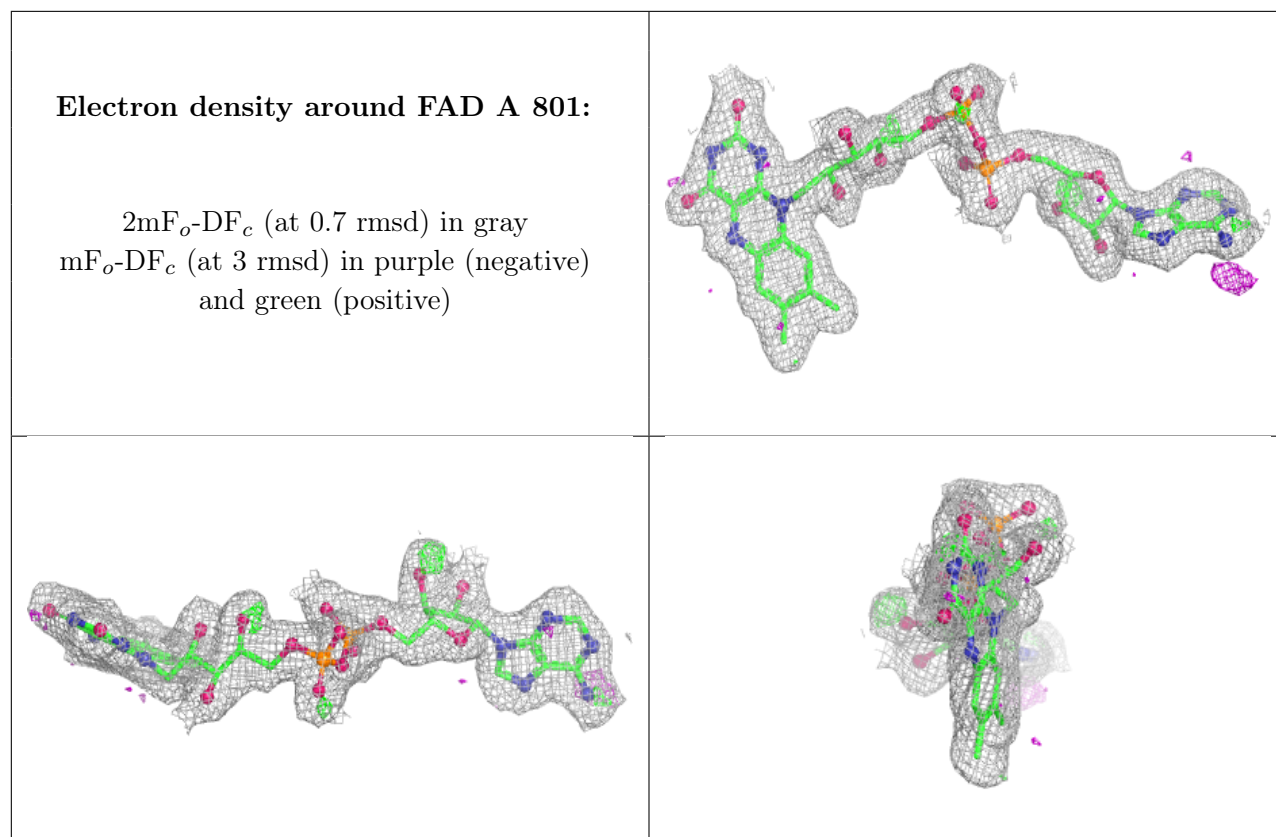
Electron density around FAD D 801:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.