



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:48 PM UTC

PDB ID : 7KAZ / pdb_00007kaz
Title : Crystal structure of OhyA(E82A)-18:1/h18:0-FAD complex from Staphylococcus aureus
Authors : Radka, C.D.; Rock, C.O.
Deposited on : 2020-10-01
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

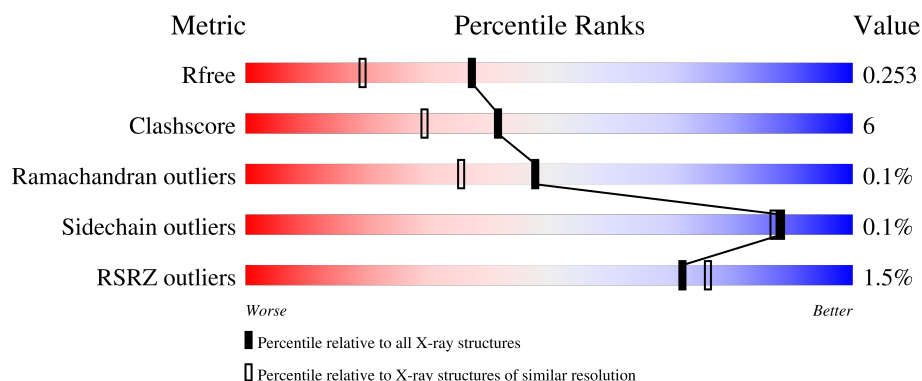
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	611	% 85% 10% 5%
1	B	611	2% 83% 12% .
1	C	611	% 83% 12% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30841 atoms, of which 13849 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 Oleate hydratase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	579	Total	C	H	N	O	S	0	0	0
			9234	2989	4550	772	901	22			
1	B	584	Total	C	H	N	O	S	0	0	0
			9288	3008	4574	778	906	22			
1	A	583	Total	C	H	N	O	S	0	0	0
			9263	3002	4562	776	901	22			

There are 63 discrepancies between the modelled and reference sequences:

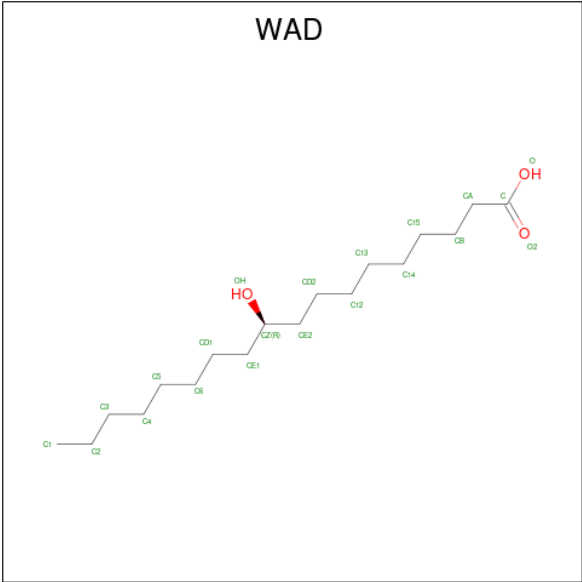
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP A0A0D6GJV1
C	-18	GLY	-	expression tag	UNP A0A0D6GJV1
C	-17	SER	-	expression tag	UNP A0A0D6GJV1
C	-16	SER	-	expression tag	UNP A0A0D6GJV1
C	-15	HIS	-	expression tag	UNP A0A0D6GJV1
C	-14	HIS	-	expression tag	UNP A0A0D6GJV1
C	-13	HIS	-	expression tag	UNP A0A0D6GJV1
C	-12	HIS	-	expression tag	UNP A0A0D6GJV1
C	-11	HIS	-	expression tag	UNP A0A0D6GJV1
C	-10	HIS	-	expression tag	UNP A0A0D6GJV1
C	-9	SER	-	expression tag	UNP A0A0D6GJV1
C	-8	SER	-	expression tag	UNP A0A0D6GJV1
C	-7	GLY	-	expression tag	UNP A0A0D6GJV1
C	-6	LEU	-	expression tag	UNP A0A0D6GJV1
C	-5	VAL	-	expression tag	UNP A0A0D6GJV1
C	-4	PRO	-	expression tag	UNP A0A0D6GJV1
C	-3	ARG	-	expression tag	UNP A0A0D6GJV1
C	-2	GLY	-	expression tag	UNP A0A0D6GJV1
C	-1	SER	-	expression tag	UNP A0A0D6GJV1
C	0	HIS	-	expression tag	UNP A0A0D6GJV1
C	82	ALA	GLU	engineered mutation	UNP A0A0D6GJV1
B	-19	MET	-	initiating methionine	UNP A0A0D6GJV1
B	-18	GLY	-	expression tag	UNP A0A0D6GJV1

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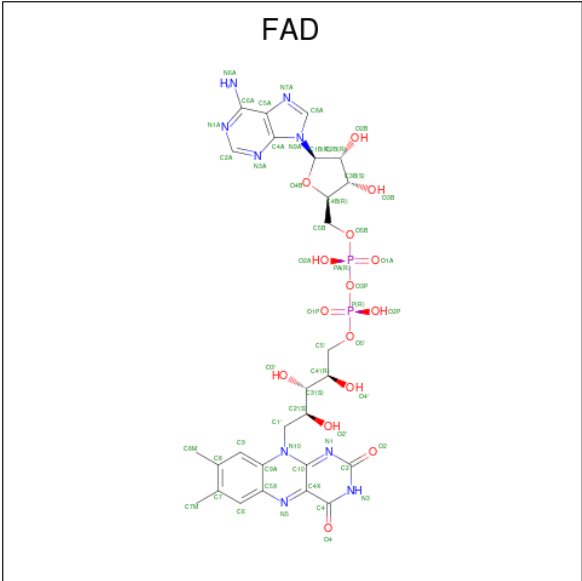
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP A0A0D6GJV1
B	-16	SER	-	expression tag	UNP A0A0D6GJV1
B	-15	HIS	-	expression tag	UNP A0A0D6GJV1
B	-14	HIS	-	expression tag	UNP A0A0D6GJV1
B	-13	HIS	-	expression tag	UNP A0A0D6GJV1
B	-12	HIS	-	expression tag	UNP A0A0D6GJV1
B	-11	HIS	-	expression tag	UNP A0A0D6GJV1
B	-10	HIS	-	expression tag	UNP A0A0D6GJV1
B	-9	SER	-	expression tag	UNP A0A0D6GJV1
B	-8	SER	-	expression tag	UNP A0A0D6GJV1
B	-7	GLY	-	expression tag	UNP A0A0D6GJV1
B	-6	LEU	-	expression tag	UNP A0A0D6GJV1
B	-5	VAL	-	expression tag	UNP A0A0D6GJV1
B	-4	PRO	-	expression tag	UNP A0A0D6GJV1
B	-3	ARG	-	expression tag	UNP A0A0D6GJV1
B	-2	GLY	-	expression tag	UNP A0A0D6GJV1
B	-1	SER	-	expression tag	UNP A0A0D6GJV1
B	0	HIS	-	expression tag	UNP A0A0D6GJV1
B	82	ALA	GLU	engineered mutation	UNP A0A0D6GJV1
A	-19	MET	-	initiating methionine	UNP A0A0D6GJV1
A	-18	GLY	-	expression tag	UNP A0A0D6GJV1
A	-17	SER	-	expression tag	UNP A0A0D6GJV1
A	-16	SER	-	expression tag	UNP A0A0D6GJV1
A	-15	HIS	-	expression tag	UNP A0A0D6GJV1
A	-14	HIS	-	expression tag	UNP A0A0D6GJV1
A	-13	HIS	-	expression tag	UNP A0A0D6GJV1
A	-12	HIS	-	expression tag	UNP A0A0D6GJV1
A	-11	HIS	-	expression tag	UNP A0A0D6GJV1
A	-10	HIS	-	expression tag	UNP A0A0D6GJV1
A	-9	SER	-	expression tag	UNP A0A0D6GJV1
A	-8	SER	-	expression tag	UNP A0A0D6GJV1
A	-7	GLY	-	expression tag	UNP A0A0D6GJV1
A	-6	LEU	-	expression tag	UNP A0A0D6GJV1
A	-5	VAL	-	expression tag	UNP A0A0D6GJV1
A	-4	PRO	-	expression tag	UNP A0A0D6GJV1
A	-3	ARG	-	expression tag	UNP A0A0D6GJV1
A	-2	GLY	-	expression tag	UNP A0A0D6GJV1
A	-1	SER	-	expression tag	UNP A0A0D6GJV1
A	0	HIS	-	expression tag	UNP A0A0D6GJV1
A	82	ALA	GLU	engineered mutation	UNP A0A0D6GJV1

- Molecule 2 is (10R)-10-hydroxyoctadecanoic acid (CCD ID: WAD) (formula: C₁₈H₃₆O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	0	0
			56	18	35	3		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).

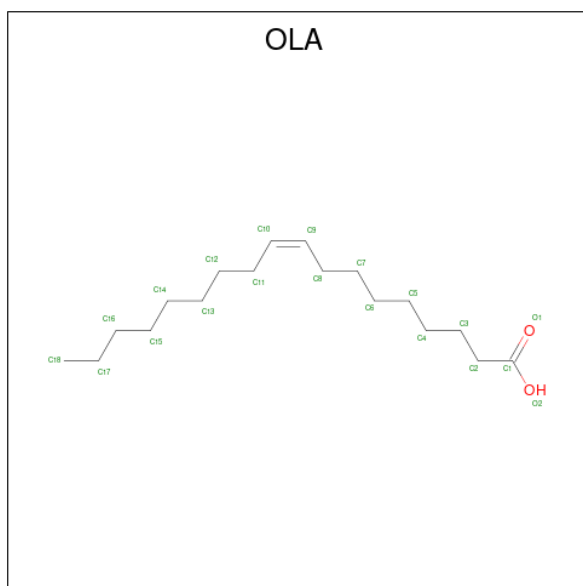


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
3	B	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total K 1 1	0	0

- Molecule 5 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C H O 53 18 33 2	0	0
5	A	1	Total C H O 53 18 33 2	0	0

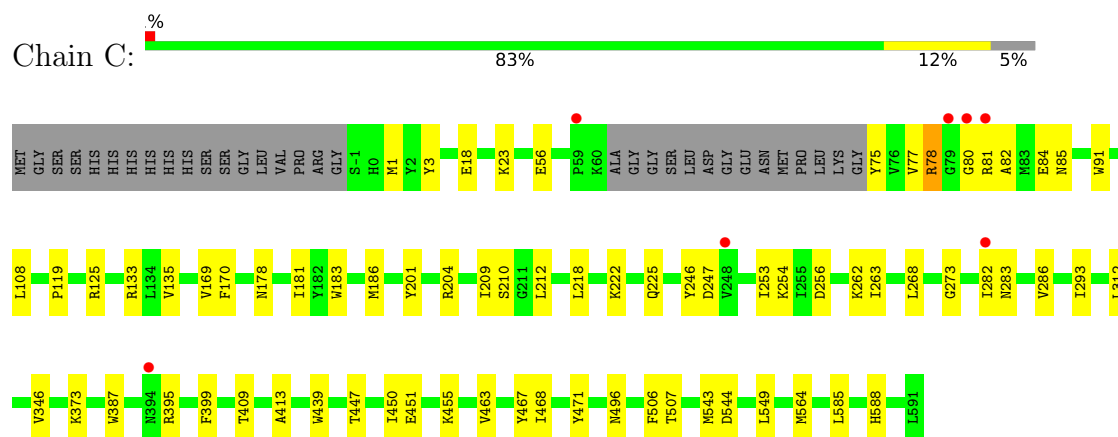
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	917	Total O 917 917	0	0
6	B	908	Total O 908 908	0	0
6	A	900	Total O 900 900	0	0

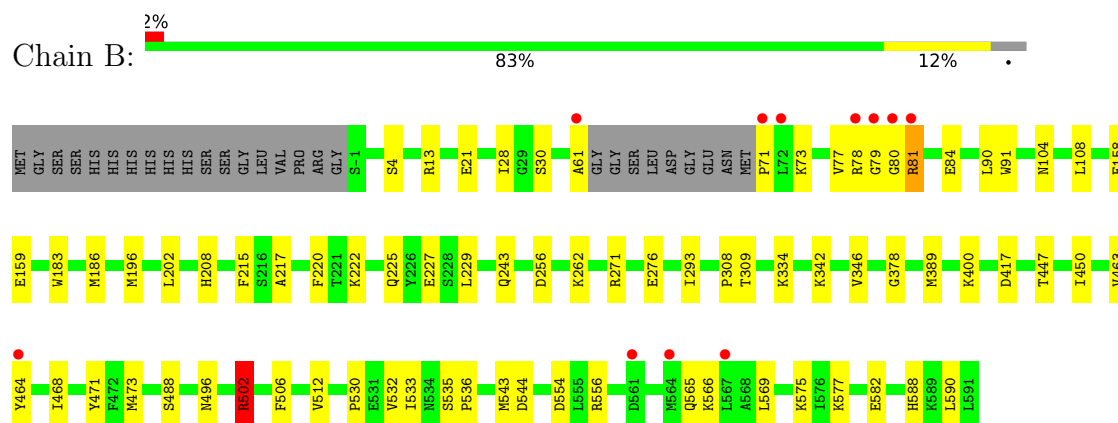
3 Residue-property plots [i](#)

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.

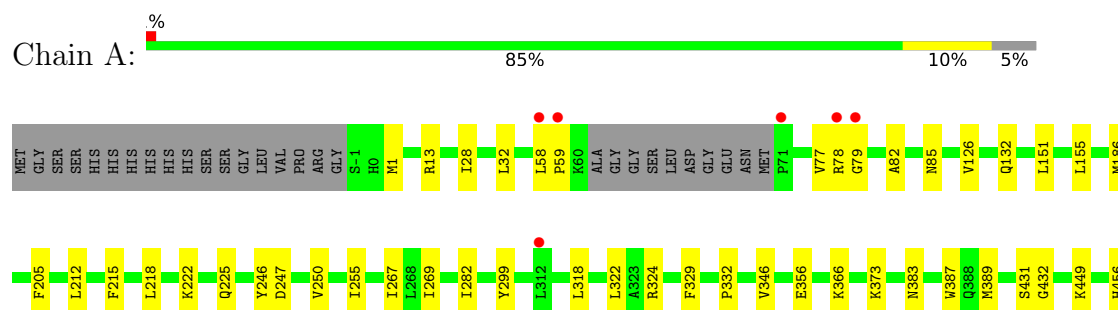
• Molecule 1: Oleate hydratase



• Molecule 1: Oleate hydratase



• Molecule 1: Oleate hydratase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.02Å 113.08Å 118.39Å 90.00° 116.91° 90.00°	Depositor
Resolution (Å)	22.42 – 1.85 22.42 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.5 (22.42-1.85) 98.4 (22.42-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.194 , 0.249 0.200 , 0.253	Depositor DCC
R_{free} test set	2005 reflections (1.07%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	30841	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: WAD, K, FAD, OLA

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	0.63	1/4810 (0.0%)	0.68	0/6519
1	B	0.61	1/4823 (0.0%)	0.72	1/6535 (0.0%)
1	C	0.56	0/4792	0.66	0/6494
All	All	0.60	2/14425 (0.0%)	0.69	1/19548 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	SD-CE	-8.33	1.58	1.79
1	B	506	PHE	C-O	-6.39	1.14	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	502	ARG	N-CA-C	6.41	124.45	110.80

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	4701	4562	4595	56	0
1	B	4714	4574	4608	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4684	4550	4577	55	0
2	C	21	35	0	0	0
3	B	53	31	31	5	0
3	C	53	31	31	4	0
4	C	1	0	0	0	0
5	A	20	33	33	2	0
5	B	20	33	33	0	0
6	A	900	0	0	22	0
6	B	908	0	0	23	0
6	C	917	0	0	14	0
All	All	16992	13849	13908	181	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 6.

All (181) 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:81:ARG:HH22	1:B:378:GLY:HA2	1.22	1.01
1:B:389:MET:SD	6:B:1264:HOH:O	2.21	0.98
1:B:81:ARG:NH2	1:B:378:GLY:HA2	1.85	0.90
1:C:135:VAL:HG23	6:C:775:HOH:O	1.75	0.87
1:A:563:LYS:O	1:A:567:LEU:HD13	1.83	0.78
1:B:256:ASP:CG	6:B:702:HOH:O	2.30	0.74
1:B:473:MET:HE1	6:B:831:HOH:O	1.89	0.73
1:B:225:GLN:NE2	6:B:706:HOH:O	2.25	0.69
1:B:473:MET:CE	6:B:831:HOH:O	2.39	0.68
1:A:132:GLN:NE2	6:A:705:HOH:O	2.27	0.68
1:B:78:ARG:NH2	6:B:710:HOH:O	2.29	0.66
1:B:81:ARG:HH22	1:B:378:GLY:CA	2.03	0.64
1:C:81:ARG:HH21	1:C:225:GLN:H	1.46	0.63
1:B:81:ARG:HB2	1:B:220:PHE:HE2	1.63	0.63
1:A:456:HIS:HB3	6:A:1060:HOH:O	2.00	0.61
1:B:308:PRO:HA	1:B:464:TYR:CE1	2.35	0.61
1:C:282:ILE:H	1:C:282:ILE:HD12	1.65	0.61
1:B:243:GLN:NE2	6:B:715:HOH:O	2.32	0.61
1:B:80:GLY:HA2	3:B:601:FAD:N5	2.16	0.61
1:A:59:PRO:CA	6:A:701:HOH:O	2.48	0.61
1:B:81:ARG:HB2	1:B:220:PHE:CE2	2.36	0.60
1:C:210:SER:HB3	6:C:872:HOH:O	2.02	0.59
1:B:575:LYS:NZ	6:B:709:HOH:O	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:GLN:NE2	6:B:722:HOH:O	2.36	0.59
1:C:312:LEU:HD23	1:C:467:TYR:OH	2.02	0.59
1:A:59:PRO:CB	6:A:701:HOH:O	2.51	0.57
1:A:501:GLU:CG	6:A:733:HOH:O	2.52	0.57
1:B:217:ALA:HB3	6:B:718:HOH:O	2.04	0.57
1:C:119:PRO:HB3	6:C:1142:HOH:O	2.05	0.57
1:B:389:MET:HB3	6:B:1264:HOH:O	2.03	0.57
1:B:79:GLY:O	1:B:81:ARG:HG2	2.05	0.56
1:B:502:ARG:HD2	6:B:1199:HOH:O	2.05	0.56
1:B:575:LYS:HE3	6:B:1239:HOH:O	2.04	0.55
1:C:263:ILE:HD12	6:C:928:HOH:O	2.07	0.55
1:A:28:ILE:HD12	1:A:250:VAL:HG21	1.88	0.55
1:B:30:SER:OG	1:B:61:ALA:HA	2.06	0.55
1:A:299:TYR:CD2	1:A:463:VAL:HG22	2.42	0.55
1:B:309:THR:H	1:B:464:TYR:HE1	1.55	0.55
1:A:78:ARG:HB2	6:A:860:HOH:O	2.08	0.54
1:B:342:LYS:NZ	1:B:417:ASP:OD1	2.40	0.54
1:A:332:PRO:HD2	6:A:744:HOH:O	2.07	0.54
1:C:564:MET:HE3	6:C:1250:HOH:O	2.08	0.54
1:A:534:ASN:ND2	6:A:732:HOH:O	2.41	0.54
1:B:84:GLU:OE1	1:B:208:HIS:CD2	2.60	0.54
1:B:183:TRP:CH2	1:B:202:LEU:HD23	2.43	0.54
1:C:447:THR:HA	1:C:450:ILE:HD12	1.91	0.53
1:B:84:GLU:OE1	1:B:208:HIS:NE2	2.42	0.53
1:A:58:LEU:O	1:A:246:TYR:HB3	2.09	0.53
1:A:186:MET:HE3	1:A:215:PHE:HE1	1.73	0.53
1:C:254:LYS:HE3	1:C:268:LEU:HD21	1.90	0.53
1:B:222:LYS:CD	6:B:913:HOH:O	2.56	0.52
1:A:59:PRO:CG	6:A:701:HOH:O	2.56	0.52
1:B:222:LYS:HD3	6:B:913:HOH:O	2.08	0.52
1:B:80:GLY:HA2	3:B:601:FAD:C5X	2.40	0.52
1:A:59:PRO:N	6:A:701:HOH:O	2.41	0.52
1:A:387:TRP:HE3	1:A:389:MET:HE3	1.75	0.52
1:B:308:PRO:HA	1:B:464:TYR:CD1	2.45	0.51
1:A:373:LYS:HE2	6:A:1218:HOH:O	2.11	0.51
1:B:293:ILE:HD12	3:B:601:FAD:HM82	1.91	0.51
1:B:468:ILE:CD1	3:B:601:FAD:HM82	2.41	0.51
1:A:356:GLU:OE2	1:A:449:LYS:NZ	2.30	0.50
1:C:543:MET:SD	1:C:585:LEU:HD23	2.51	0.50
1:B:159:GLU:H	1:B:159:GLU:CD	2.19	0.50
1:A:566:LYS:NZ	6:A:716:HOH:O	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:GLN:HG3	1:B:229:LEU:HD12	1.93	0.50
1:C:91:TRP:CE3	1:C:108:LEU:HD13	2.47	0.49
1:A:222:LYS:NZ	6:A:739:HOH:O	2.45	0.49
1:B:543:MET:HG2	1:B:590:LEU:HD12	1.95	0.49
1:B:262:LYS:HB2	1:B:488:SER:HA	1.93	0.49
1:B:471:TYR:CE1	1:B:496:ASN:HB2	2.48	0.48
1:C:78:ARG:NE	1:C:81:ARG:HG2	2.27	0.48
1:C:209:ILE:HD11	1:C:549:LEU:HG	1.96	0.48
1:B:334:LYS:NZ	6:B:747:HOH:O	2.46	0.48
1:B:71:PRO:HB3	1:B:73:LYS:HZ1	1.78	0.48
1:B:77:VAL:HG12	1:B:79:GLY:H	1.79	0.48
1:C:178:ASN:HA	1:C:181:ILE:HD12	1.94	0.48
1:B:227:GLU:OE2	1:B:400:LYS:HG3	2.14	0.48
1:B:577:LYS:HE2	6:B:1258:HOH:O	2.13	0.48
1:A:247:ASP:OD1	6:A:701:HOH:O	2.20	0.47
1:B:90:LEU:HA	1:B:512:VAL:HG11	1.96	0.47
1:A:471:TYR:CE1	1:A:496:ASN:HB2	2.50	0.47
1:A:82:ALA:CB	1:A:218:LEU:HD22	2.44	0.47
1:A:255:ILE:HD13	1:A:491:LEU:HD22	1.94	0.47
1:C:23:LYS:HE2	1:C:283:ASN:OD1	2.15	0.47
1:B:256:ASP:CB	6:B:702:HOH:O	2.62	0.47
1:A:318:LEU:O	1:A:322:LEU:HG	2.14	0.47
1:C:125:ARG:O	1:C:125:ARG:HG3	2.13	0.47
1:B:158:GLU:HG3	1:B:196:MET:HG3	1.97	0.47
1:A:13:ARG:HD2	6:A:959:HOH:O	2.15	0.46
1:B:13:ARG:HD3	6:B:1021:HOH:O	2.14	0.46
1:C:80:GLY:HA2	3:C:602:FAD:N5	2.31	0.46
1:A:77:VAL:O	1:A:78:ARG:HB2	2.16	0.46
1:C:387:TRP:HB3	1:C:413:ALA:HB1	1.98	0.45
1:A:151:LEU:O	1:A:155:LEU:HG	2.16	0.45
1:B:556:ARG:HH22	1:B:566:LYS:HG2	1.80	0.45
1:C:186:MET:SD	1:C:212:LEU:CD1	3.05	0.45
1:A:205:PHE:HB3	5:A:600:OLA:H81	1.99	0.45
1:B:4:SER:O	1:B:530:PRO:HA	2.17	0.45
1:C:85:ASN:OD1	1:C:85:ASN:N	2.50	0.45
1:A:32:LEU:HD12	1:A:32:LEU:O	2.17	0.45
1:A:59:PRO:HG3	6:A:701:HOH:O	2.17	0.44
1:B:532:VAL:O	1:B:533:ILE:C	2.60	0.44
1:C:56:GLU:OE2	1:C:56:GLU:HA	2.18	0.44
1:C:82:ALA:HB1	1:C:218:LEU:HD22	1.99	0.44
1:C:77:VAL:O	1:C:78:ARG:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ILE:O	1:B:468:ILE:HG13	2.17	0.44
1:C:451:GLU:OE2	1:C:455:LYS:NZ	2.51	0.44
1:A:562:SER:HB3	1:A:565:GLN:HB2	2.00	0.43
1:B:28:ILE:N	1:B:28:ILE:HD13	2.33	0.43
1:A:501:GLU:CB	6:A:733:HOH:O	2.67	0.43
1:C:225:GLN:HG2	1:C:225:GLN:O	2.17	0.43
1:C:293:ILE:HD13	1:C:471:TYR:CE2	2.53	0.43
1:B:533:ILE:HD12	6:B:1056:HOH:O	2.18	0.43
1:C:18:GLU:OE2	1:C:18:GLU:HA	2.18	0.43
1:C:468:ILE:CD1	3:C:602:FAD:HM82	2.48	0.43
1:C:544:ASP:OD1	1:C:588:HIS:HD2	2.01	0.43
1:B:91:TRP:CE3	1:B:108:LEU:HD13	2.53	0.43
1:A:250:VAL:HG22	1:A:269:ILE:HG22	1.99	0.43
1:A:564:MET:HE1	1:A:567:LEU:HD23	1.99	0.43
1:C:507:THR:HA	3:C:602:FAD:O2	2.18	0.43
1:B:271:ARG:NE	1:B:276:GLU:OE1	2.44	0.43
1:A:151:LEU:HD11	1:A:155:LEU:HD11	2.00	0.43
1:A:387:TRP:CE3	1:A:389:MET:HE3	2.54	0.43
1:C:75:TYR:N	6:C:752:HOH:O	2.51	0.43
1:A:267:ILE:HG22	1:A:269:ILE:CG2	2.49	0.43
1:B:577:LYS:HD2	1:B:582:GLU:OE1	2.19	0.43
1:C:84:GLU:OE2	1:C:204:ARG:NH1	2.52	0.42
1:C:253:ILE:HD13	1:C:286:VAL:HG11	2.01	0.42
1:C:256:ASP:O	1:C:262:LYS:HA	2.19	0.42
1:C:77:VAL:HG13	1:C:399:PHE:CZ	2.54	0.42
1:C:209:ILE:CD1	1:C:549:LEU:HG	2.49	0.42
1:B:21:GLU:H	1:B:21:GLU:CD	2.26	0.42
1:A:126:VAL:CG1	1:A:383:ASN:HB2	2.50	0.42
1:A:324:ARG:HD3	6:A:1219:HOH:O	2.19	0.42
1:A:346:VAL:HA	1:A:463:VAL:O	2.19	0.42
1:C:81:ARG:H	3:C:602:FAD:C4	2.32	0.42
1:C:471:TYR:CZ	1:C:496:ASN:HB2	2.55	0.42
1:B:554:ASP:OD1	1:B:554:ASP:C	2.62	0.42
1:B:91:TRP:CE3	1:B:91:TRP:HA	2.55	0.42
1:B:104:ASN:ND2	6:B:750:HOH:O	2.47	0.42
1:A:85:ASN:OD1	1:A:85:ASN:N	2.53	0.42
1:A:501:GLU:HG2	6:A:733:HOH:O	2.17	0.42
1:C:346:VAL:HA	1:C:463:VAL:O	2.20	0.42
1:C:564:MET:HE3	6:C:1387:HOH:O	2.19	0.42
1:B:544:ASP:OD1	1:B:588:HIS:ND1	2.47	0.42
1:B:566:LYS:HG3	6:B:876:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:GLY:HA2	6:C:725:HOH:O	2.19	0.42
1:A:79:GLY:O	1:A:225:GLN:NE2	2.53	0.42
1:A:574:LYS:N	1:A:574:LYS:HD3	2.35	0.42
1:C:247:ASP:HA	6:C:816:HOH:O	2.19	0.41
1:C:409:THR:HG21	1:C:439:TRP:CZ2	2.54	0.41
1:B:217:ALA:N	6:B:718:HOH:O	2.37	0.41
1:A:59:PRO:HB3	1:A:247:ASP:OD1	2.21	0.41
1:A:431:SER:O	1:A:432:GLY:C	2.63	0.41
1:C:222:LYS:HD2	6:C:712:HOH:O	2.21	0.41
1:C:373:LYS:HE3	6:C:1190:HOH:O	2.20	0.41
1:B:468:ILE:HD11	3:B:601:FAD:HM82	2.03	0.41
1:A:567:LEU:O	1:A:570:ALA:HB3	2.19	0.41
1:B:556:ARG:HD2	1:B:569:LEU:CD2	2.51	0.41
1:A:212:LEU:HD12	5:A:600:OLA:C9	2.50	0.41
1:A:556:ARG:O	1:A:560:LYS:HG2	2.21	0.41
1:C:133:ARG:NH1	6:C:740:HOH:O	2.47	0.41
1:C:222:LYS:HB2	1:C:222:LYS:HE2	1.92	0.41
1:C:543:MET:HE3	1:C:588:HIS:CG	2.55	0.41
1:B:186:MET:HE3	1:B:215:PHE:HE1	1.85	0.41
1:C:246:TYR:HB2	6:C:771:HOH:O	2.20	0.41
1:A:255:ILE:HD12	1:A:329:PHE:CE2	2.55	0.41
1:A:366:LYS:CE	6:A:864:HOH:O	2.69	0.41
1:C:169:VAL:HG23	1:C:170:PHE:CD2	2.56	0.40
1:C:1:MET:HE1	1:C:3:TYR:CE1	2.57	0.40
1:B:535:SER:N	1:B:536:PRO:HD2	2.35	0.40
1:C:183:TRP:CZ2	1:C:201:TYR:HB3	2.56	0.40
1:A:282:ILE:HD11	1:A:489:GLN:HB3	2.04	0.40
1:A:366:LYS:HE2	6:A:864:HOH:O	2.22	0.40
1:C:395:ARG:HG3	6:C:908:HOH:O	2.21	0.40
1:C:496:ASN:OD1	1:C:506:PHE:N	2.55	0.40
1:B:346:VAL:HA	1:B:463:VAL:O	2.21	0.40
1:B:447:THR:HA	1:B:450:ILE:HD12	2.04	0.40
1:B:556:ARG:HD2	1:B:569:LEU:HD23	2.03	0.40
1:A:502:ARG:HD2	6:A:975:HOH:O	2.22	0.40
1:A:564:MET:CE	1:A:567:LEU:HD23	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	579/611 (95%)	557 (96%)	22 (4%)	0	100	100
1	B	580/611 (95%)	558 (96%)	21 (4%)	1 (0%)	43	31
1	C	575/611 (94%)	552 (96%)	22 (4%)	1 (0%)	43	31
All	All	1734/1833 (95%)	1667 (96%)	65 (4%)	2 (0%)	48	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	502	ARG
1	C	78	ARG

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	519/543 (96%)	519 (100%)	0	100	100
1	B	521/543 (96%)	520 (100%)	1 (0%)	87	86
1	C	519/543 (96%)	519 (100%)	0	100	100
All	All	1559/1629 (96%)	1558 (100%)	1 (0%)	88	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	81	ARG

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

Mol	Chain	Res	Type
1	C	274	ASN
1	C	437	GLN
1	C	521	GLN
1	C	565	GLN
1	B	0	HIS
1	B	104	ASN
1	B	130	GLN
1	B	261	GLN
1	B	283	ASN
1	B	383	ASN
1	B	437	GLN
1	B	553	GLN
1	A	53	HIS
1	A	130	GLN
1	A	243	GLN
1	A	261	GLN
1	A	383	ASN
1	A	419	ASN
1	A	437	GLN
1	A	552	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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
5	OLA	B	600	-	19,19,19	0.84	1 (5%)	19,19,19	0.99	1 (5%)
3	FAD	C	602	-	58,58,58	1.47	9 (15%)	85,89,89	1.61	18 (21%)
2	WAD	C	601	-	20,20,20	0.59	0	21,21,21	0.87	1 (4%)
3	FAD	B	601	-	58,58,58	2.00	17 (29%)	85,89,89	1.97	16 (18%)
5	OLA	A	600	-	19,19,19	0.55	0	19,19,19	1.20	2 (10%)

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
5	OLA	B	600	-	-	9/17/17/17	-
3	FAD	C	602	-	-	9/34/50/50	0/6/6/6
2	WAD	C	601	-	-	9/19/19/19	-
3	FAD	B	601	-	-	6/34/50/50	0/6/6/6
5	OLA	A	600	-	-	10/17/17/17	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	FAD	C9A-C5X	5.21	1.49	1.41
3	B	601	FAD	C5A-N7A	-4.83	1.30	1.39
3	C	602	FAD	C5A-C4A	4.62	1.47	1.39
3	B	601	FAD	C8A-N9A	-4.32	1.30	1.37
3	B	601	FAD	C9A-C5X	4.31	1.48	1.41
3	B	601	FAD	PA-O3P	4.12	1.63	1.59
3	B	601	FAD	C5A-C4A	4.02	1.46	1.39
3	C	602	FAD	C8-C7	3.43	1.49	1.40
3	B	601	FAD	C6-C7	-3.37	1.35	1.39
3	B	601	FAD	C7M-C7	-3.28	1.44	1.51
3	B	601	FAD	C4-N3	-3.20	1.32	1.38
3	B	601	FAD	P-O3P	3.16	1.62	1.59
3	B	601	FAD	C5X-N5	-3.06	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	FAD	C6-C5X	-2.93	1.35	1.40
5	B	600	OLA	C10-C9	2.81	1.47	1.31
3	B	601	FAD	P-O2P	-2.79	1.42	1.55
3	B	601	FAD	C9-C8	-2.78	1.35	1.39
3	C	602	FAD	C5A-C6A	2.69	1.48	1.41
3	B	601	FAD	P-O1P	-2.69	1.41	1.50
3	B	601	FAD	C2-N3	-2.65	1.33	1.39
3	B	601	FAD	C1'-N10	-2.60	1.41	1.47
3	B	601	FAD	C4A-N9A	-2.50	1.32	1.37
3	C	602	FAD	C4-N3	-2.41	1.34	1.38
3	C	602	FAD	C8A-N7A	2.38	1.36	1.31
3	C	602	FAD	C5A-N7A	-2.30	1.34	1.39
3	C	602	FAD	C4X-N5	2.24	1.35	1.30
3	C	602	FAD	C5X-N5	-2.01	1.35	1.39

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	FAD	C5A-C4A-N3A	-8.26	115.35	126.72
3	B	601	FAD	N3A-C4A-N9A	6.33	137.93	127.17
3	C	602	FAD	C5A-C4A-N3A	-5.81	118.71	126.72
3	C	602	FAD	N3A-C4A-N9A	4.71	135.17	127.17
3	B	601	FAD	C2A-N3A-C4A	4.52	122.87	111.83
3	B	601	FAD	C6-C7-C8	4.17	125.82	119.69
3	B	601	FAD	C8M-C8-C9	3.99	126.60	119.57
3	C	602	FAD	C2A-N3A-C4A	3.87	121.29	111.83
3	C	602	FAD	N3A-C2A-N1A	-3.72	122.95	128.58
3	B	601	FAD	C4A-C5A-N7A	-3.58	106.49	110.58
3	B	601	FAD	C1B-N9A-C8A	-3.53	119.25	127.09
3	C	602	FAD	C4A-C5A-N7A	-3.46	106.63	110.58
3	B	601	FAD	C4A-N9A-C1B	3.39	134.55	126.63
3	B	601	FAD	C7M-C7-C8	-3.02	114.58	120.76
3	C	602	FAD	C4A-N9A-C8A	2.96	108.85	105.74
3	B	601	FAD	C4X-C4-N3	2.95	120.75	113.25
3	C	602	FAD	C4-C4X-N5	2.86	122.16	118.21
3	B	601	FAD	N3A-C2A-N1A	-2.84	124.28	128.58
5	A	600	OLA	C12-C11-C10	-2.75	97.18	112.60
3	C	602	FAD	C5A-N7A-C8A	2.74	107.75	103.45
5	A	600	OLA	O2-C1-C2	2.56	122.07	114.00
3	B	601	FAD	O4-C4-C4X	-2.51	119.89	126.53
3	C	602	FAD	C4X-C10-N1	-2.44	118.61	124.59
3	B	601	FAD	C8M-C8-C7	-2.41	115.83	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	FAD	C3B-C2B-C1B	2.40	106.01	101.46
3	B	601	FAD	C4'-C3'-C2'	-2.35	109.66	113.57
3	C	602	FAD	N9A-C8A-N7A	-2.31	110.66	113.94
3	C	602	FAD	O4-C4-C4X	-2.23	120.64	126.53
3	B	601	FAD	O5'-P-O1P	2.22	117.72	108.94
2	C	601	WAD	CB-CA-C	-2.19	108.79	114.51
3	C	602	FAD	C4X-C4-N3	2.16	118.75	113.25
3	C	602	FAD	C6A-C5A-N7A	2.14	136.22	132.09
3	C	602	FAD	C4-N3-C2	-2.12	121.88	125.64
3	B	601	FAD	C2'-C1'-N10	2.11	120.15	110.20
3	C	602	FAD	C4X-C10-N10	2.09	119.47	116.48
3	C	602	FAD	C10-N1-C2	2.08	121.35	116.85
3	C	602	FAD	C2A-N1A-C6A	2.08	122.15	118.73
5	B	600	OLA	C3-C2-C1	-2.05	109.15	114.51

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	602	FAD	C5B-O5B-PA-O2A
3	C	602	FAD	C5B-O5B-PA-O3P
3	C	602	FAD	O4B-C4B-C5B-O5B
3	B	601	FAD	C5B-O5B-PA-O1A
3	B	601	FAD	C5B-O5B-PA-O3P
3	B	601	FAD	C3B-C4B-C5B-O5B
3	B	601	FAD	N10-C1'-C2'-O2'
3	C	602	FAD	C3B-C4B-C5B-O5B
3	B	601	FAD	O4B-C4B-C5B-O5B
3	C	602	FAD	C4B-C5B-O5B-PA
5	A	600	OLA	C13-C14-C15-C16
2	C	601	WAD	C14-C15-CB-CA
5	B	600	OLA	C1-C2-C3-C4
2	C	601	WAD	C1-C2-C3-C4
5	B	600	OLA	C11-C10-C9-C8
2	C	601	WAD	C3-C4-C5-C6
5	A	600	OLA	C11-C10-C9-C8
2	C	601	WAD	C5-C6-CD1-CE1
5	A	600	OLA	C3-C4-C5-C6
2	C	601	WAD	C12-C13-C14-C15
5	A	600	OLA	C14-C15-C16-C17
2	C	601	WAD	C4-C5-C6-CD1
5	B	600	OLA	C11-C12-C13-C14

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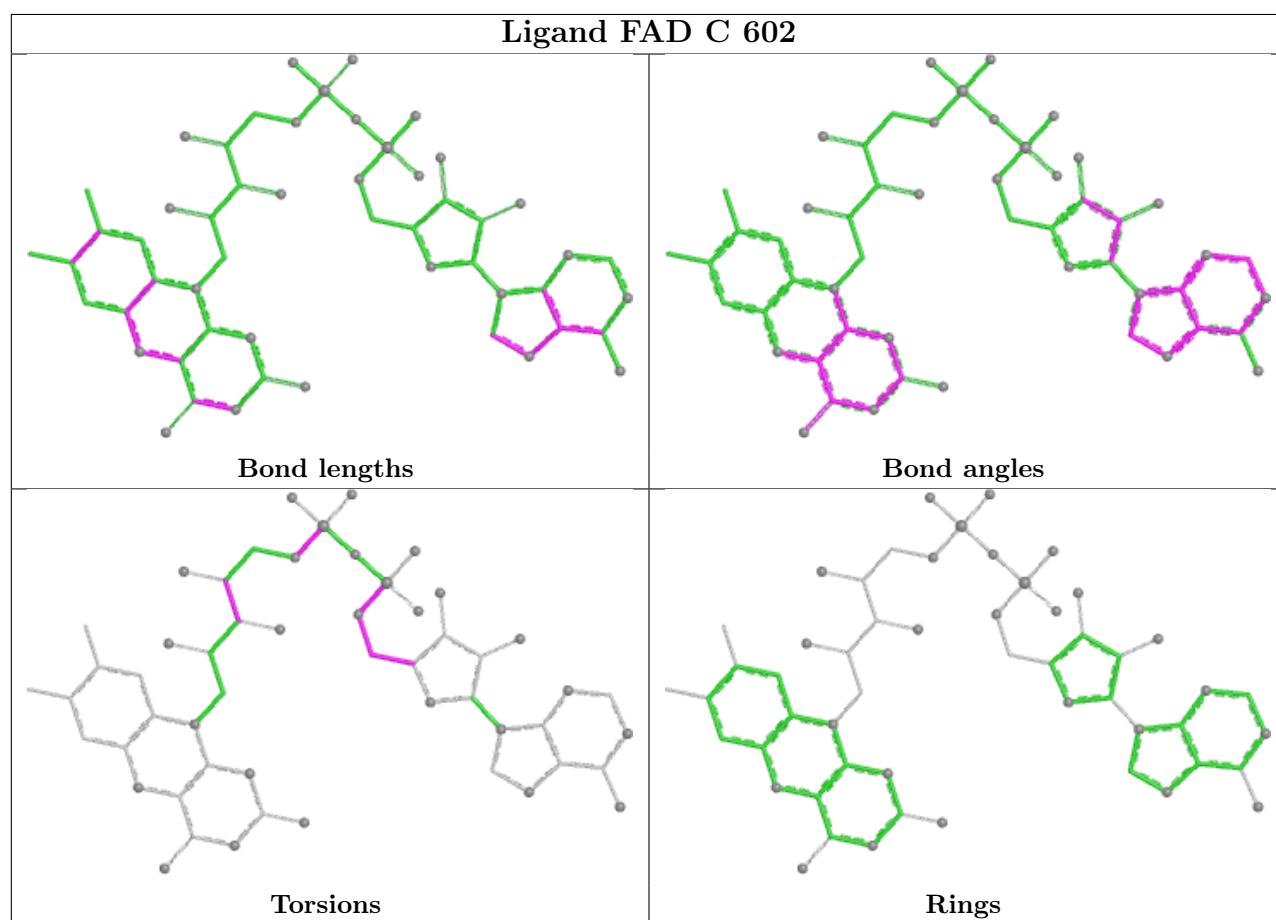
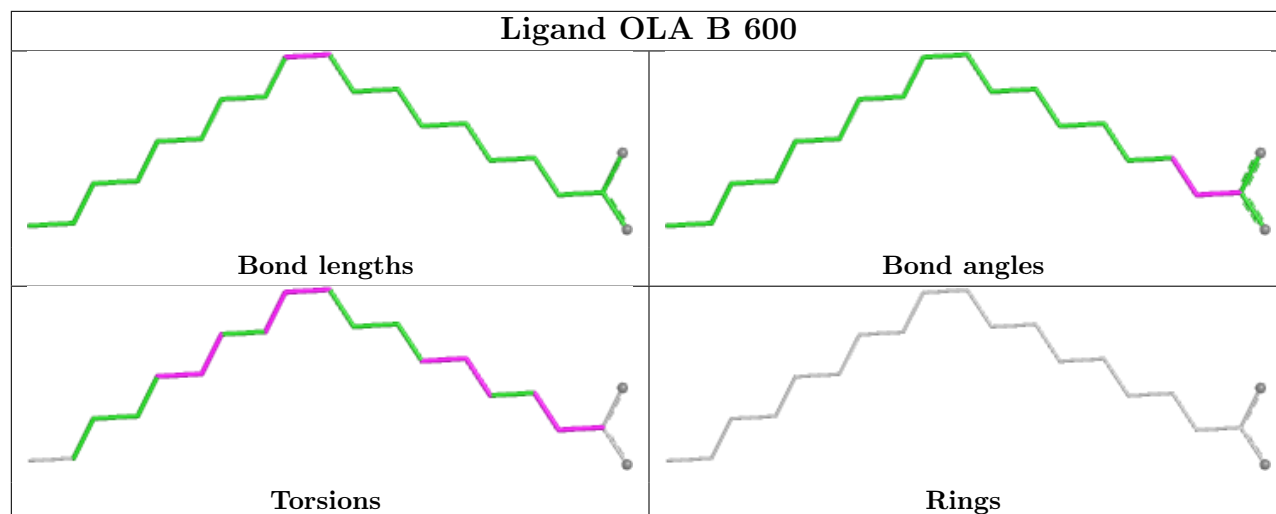
Mol	Chain	Res	Type	Atoms
5	A	600	OLA	C9-C10-C11-C12
3	C	602	FAD	C5'-O5'-P-O3P
5	B	600	OLA	C3-C4-C5-C6
5	A	600	OLA	C12-C13-C14-C15
3	C	602	FAD	C2'-C3'-C4'-O4'
2	C	601	WAD	C12-CD2-CE2-CZ
5	A	600	OLA	C15-C16-C17-C18
5	A	600	OLA	O1-C1-C2-C3
5	B	600	OLA	C12-C13-C14-C15
3	B	601	FAD	C4B-C5B-O5B-PA
5	B	600	OLA	C4-C5-C6-C7
5	A	600	OLA	O2-C1-C2-C3
2	C	601	WAD	C-CA-CB-C15
5	B	600	OLA	C9-C10-C11-C12
5	B	600	OLA	O2-C1-C2-C3
5	B	600	OLA	O1-C1-C2-C3
5	A	600	OLA	C7-C8-C9-C10
3	C	602	FAD	O3'-C3'-C4'-C5'
3	C	602	FAD	O3'-C3'-C4'-O4'
2	C	601	WAD	O-C-CA-CB

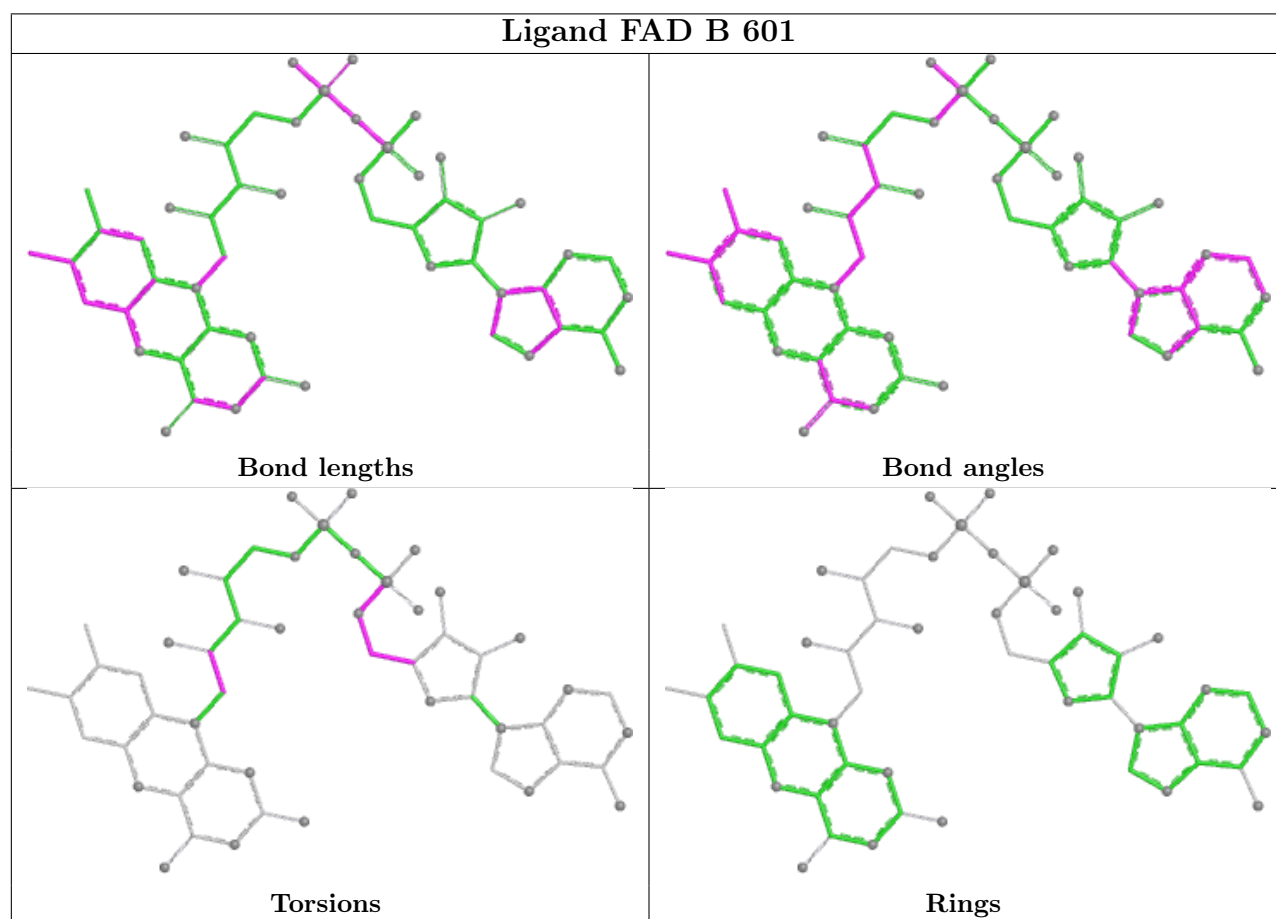
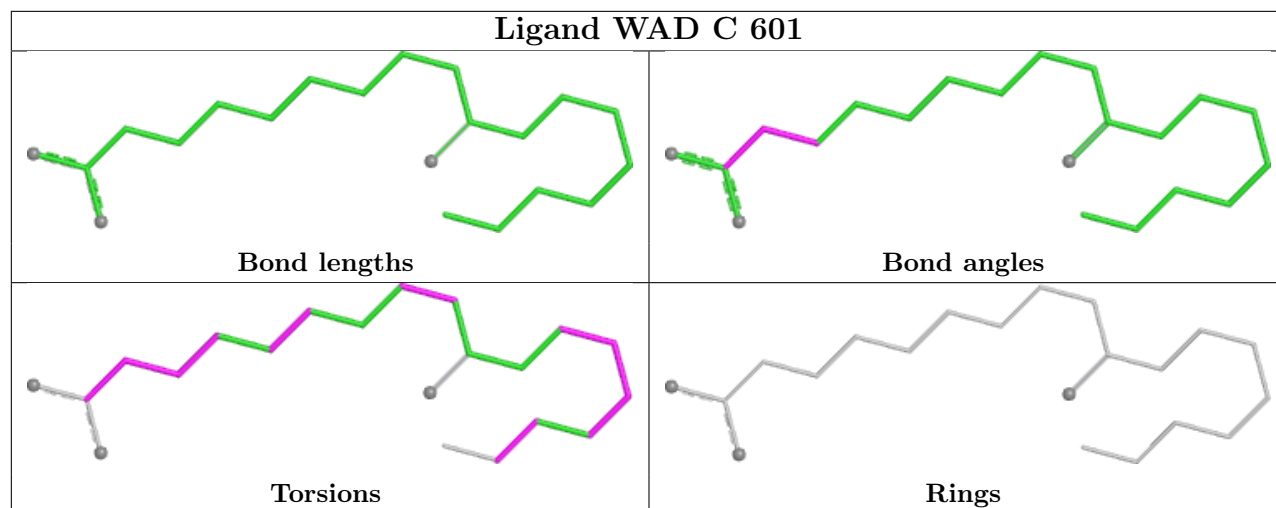
There are no ring outliers.

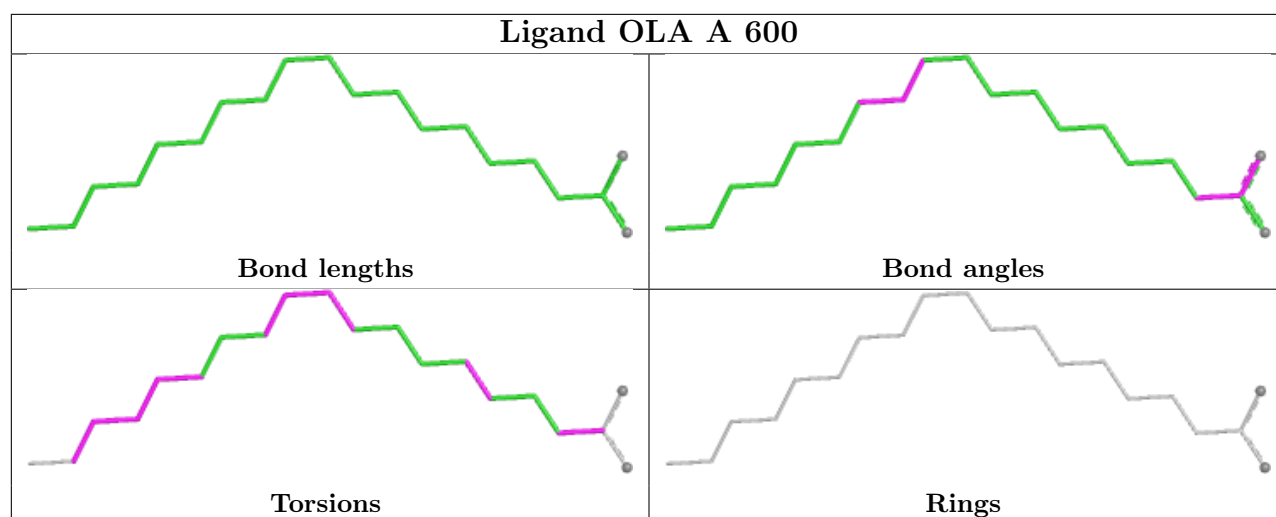
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	FAD	4	0
3	B	601	FAD	5	0
5	A	600	OLA	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	583/611 (95%)	-0.37	8 (1%) 73 77	12, 24, 50, 81	4 (0%)
1	B	584/611 (95%)	-0.35	11 (1%) 66 70	13, 24, 51, 93	3 (0%)
1	C	579/611 (94%)	-0.26	7 (1%) 76 80	13, 27, 51, 84	4 (0%)
All	All	1746/1833 (95%)	-0.33	26 (1%) 72 76	12, 25, 51, 93	11 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	80	GLY	9.0
1	C	79	GLY	6.9
1	A	79	GLY	6.0
1	B	81	ARG	5.2
1	B	71	PRO	4.4
1	C	81	ARG	3.4
1	B	80	GLY	3.3
1	B	72	LEU	3.0
1	B	567	LEU	2.9
1	B	564	MET	2.8
1	A	58	LEU	2.8
1	A	561	ASP	2.7
1	B	79	GLY	2.7
1	C	282	ILE	2.5
1	A	312	LEU	2.5
1	B	464	TYR	2.4
1	A	78	ARG	2.4
1	C	394	ASN	2.3
1	A	564	MET	2.3
1	C	248	VAL	2.3
1	B	561	ASP	2.2
1	A	71	PRO	2.2
1	B	78	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	59	PRO	2.2
1	A	59	PRO	2.2
1	B	61	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

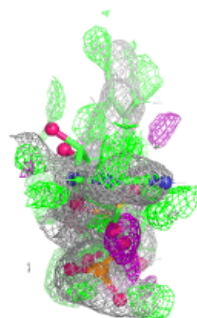
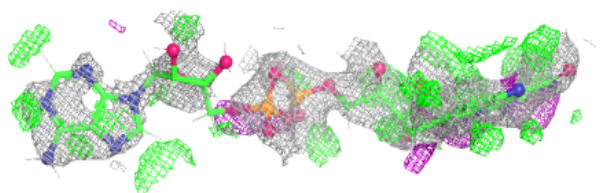
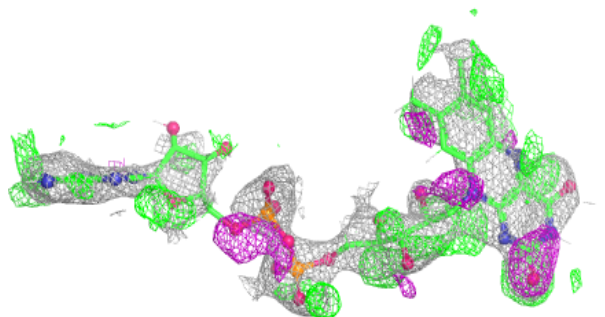
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	FAD	C	602	53/53	0.72	0.21	19,40,53,66	84
5	OLA	A	600	20/20	0.80	0.12	24,33,43,49	0
2	WAD	C	601	21/21	0.81	0.12	21,33,42,47	56
5	OLA	B	600	20/20	0.87	0.10	19,30,41,47	53
3	FAD	B	601	53/53	0.89	0.11	19,34,43,47	84
4	K	C	603	1/1	0.92	0.07	18,18,18,18	1

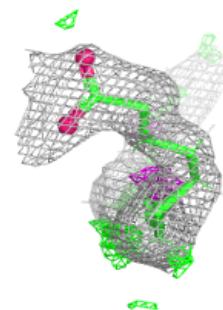
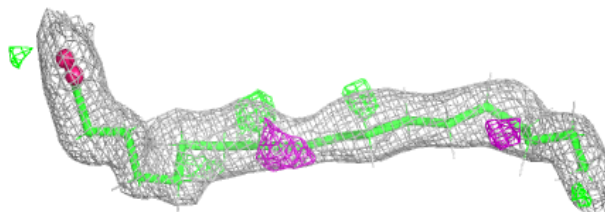
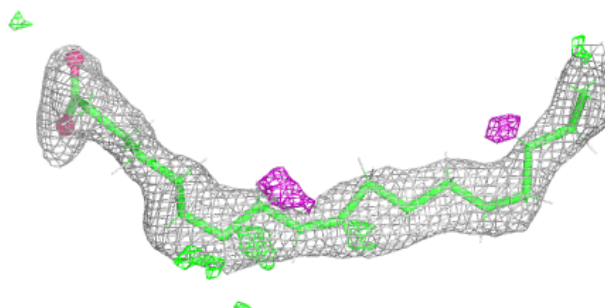
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD C 602:

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

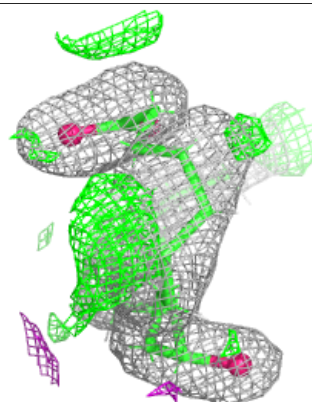
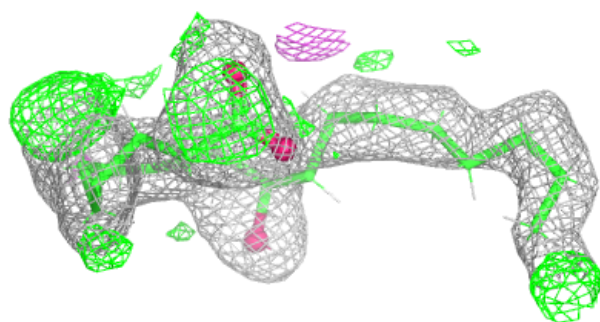
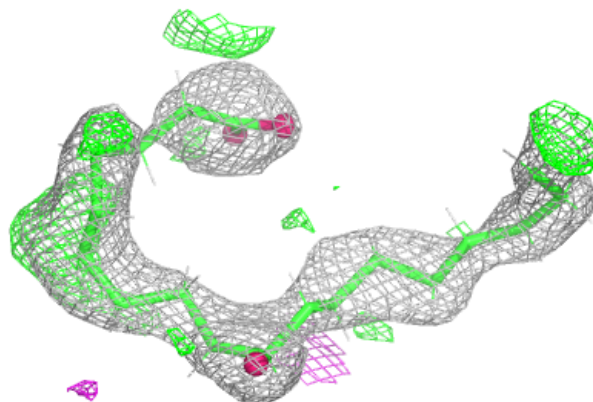
**Electron density around OLA A 600:**

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

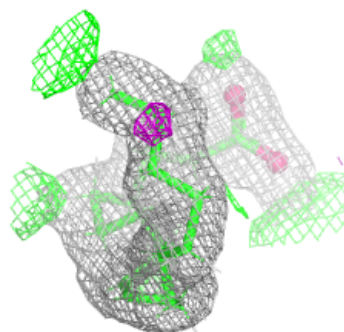
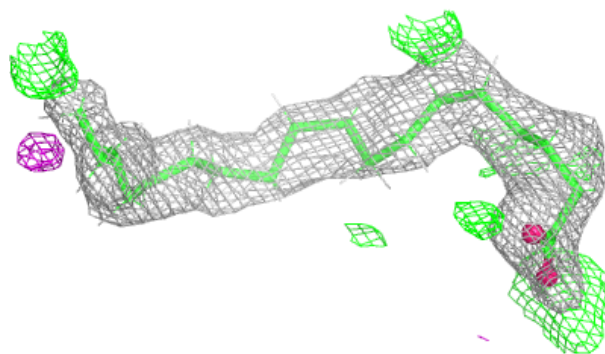
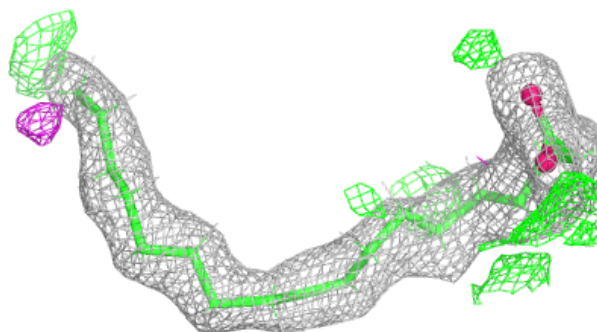


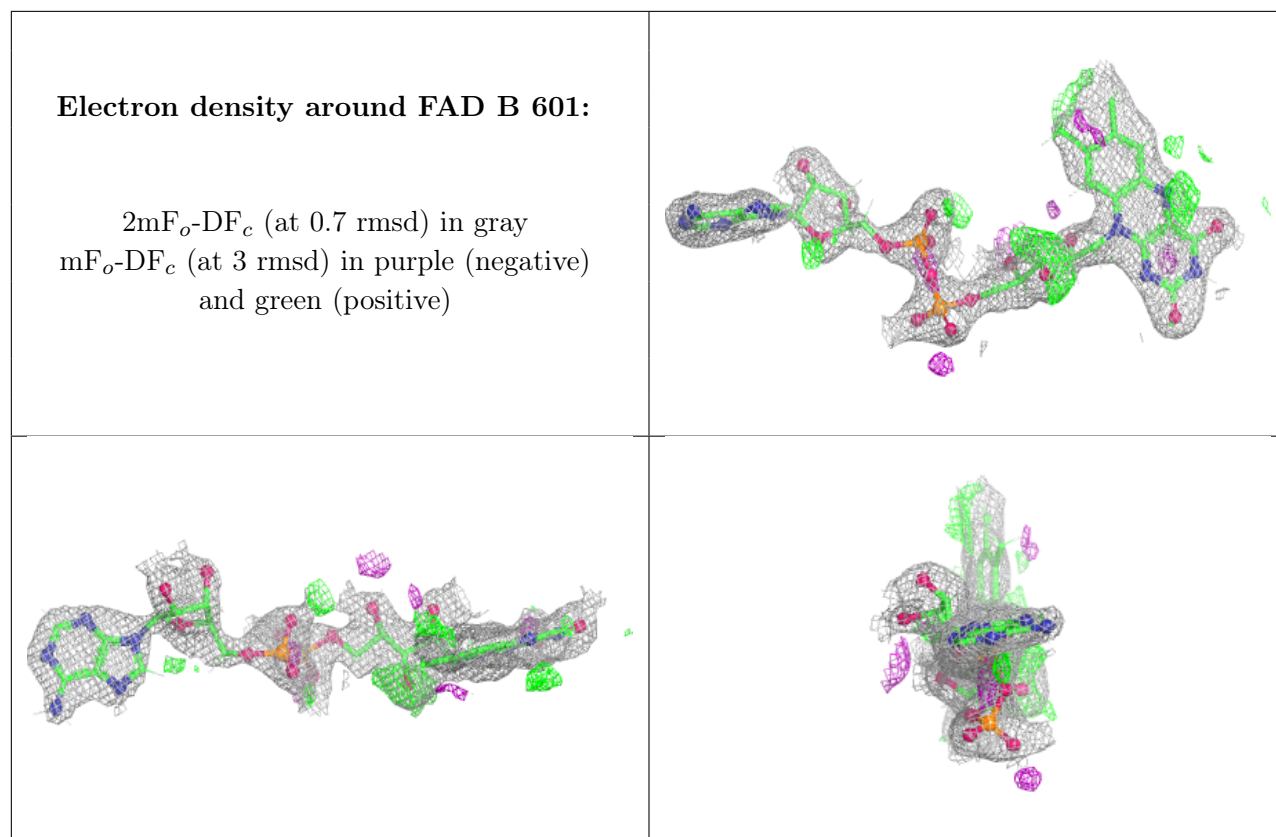
Electron density around WAD C 601:

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

**Electron density around OLA B 600:**

$2mF_o-DF_c$ (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.