



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:49 PM UTC

PDB ID : 6LKD / pdb_00006lkd
Title : in meso full-length rat KMO in complex with a pyrazoyl benzoic acid inhibitor
Authors : Mimasu, S.; Yamagishi, H.; Kiyohara, M.; Kakefuda, K.; Okuda, T.
Deposited on : 2019-12-19
Resolution : 3.00 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

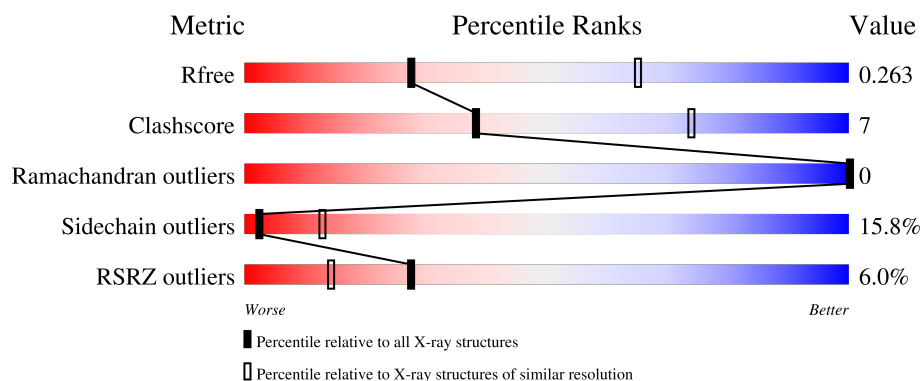
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	495	6% 62% 21% • 14%
1	B	495	4% 64% 18% • 15%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6964 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 Kynurenine 3-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3416	2206	589	591	30			
1	B	421	Total	C	N	O	S	0	0	0
			3362	2170	578	583	31			

There are 34 discrepancies between the modelled and reference sequences:

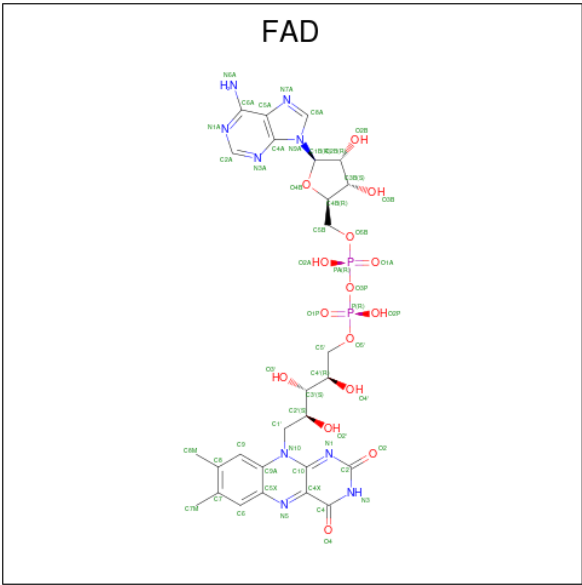
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O88867
A	0	SER	-	expression tag	UNP O88867
A	479	GLU	-	expression tag	UNP O88867
A	480	ASN	-	expression tag	UNP O88867
A	481	LEU	-	expression tag	UNP O88867
A	482	TYR	-	expression tag	UNP O88867
A	483	PHE	-	expression tag	UNP O88867
A	484	GLN	-	expression tag	UNP O88867
A	485	GLY	-	expression tag	UNP O88867
A	486	ASP	-	expression tag	UNP O88867
A	487	TYR	-	expression tag	UNP O88867
A	488	LYS	-	expression tag	UNP O88867
A	489	ASP	-	expression tag	UNP O88867
A	490	ASP	-	expression tag	UNP O88867
A	491	ASP	-	expression tag	UNP O88867
A	492	ASP	-	expression tag	UNP O88867
A	493	LYS	-	expression tag	UNP O88867
B	-1	GLY	-	expression tag	UNP O88867
B	0	SER	-	expression tag	UNP O88867
B	479	GLU	-	expression tag	UNP O88867
B	480	ASN	-	expression tag	UNP O88867
B	481	LEU	-	expression tag	UNP O88867
B	482	TYR	-	expression tag	UNP O88867
B	483	PHE	-	expression tag	UNP O88867
B	484	GLN	-	expression tag	UNP O88867

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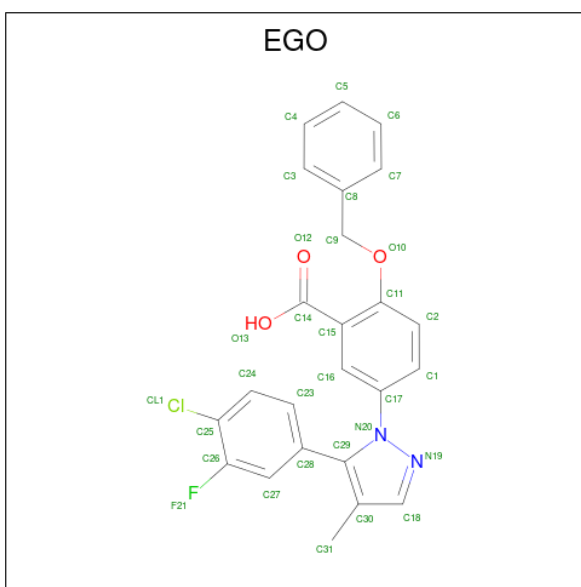
Chain	Residue	Modelled	Actual	Comment	Reference
B	485	GLY	-	expression tag	UNP O88867
B	486	ASP	-	expression tag	UNP O88867
B	487	TYR	-	expression tag	UNP O88867
B	488	LYS	-	expression tag	UNP O88867
B	489	ASP	-	expression tag	UNP O88867
B	490	ASP	-	expression tag	UNP O88867
B	491	ASP	-	expression tag	UNP O88867
B	492	ASP	-	expression tag	UNP O88867
B	493	LYS	-	expression tag	UNP O88867

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



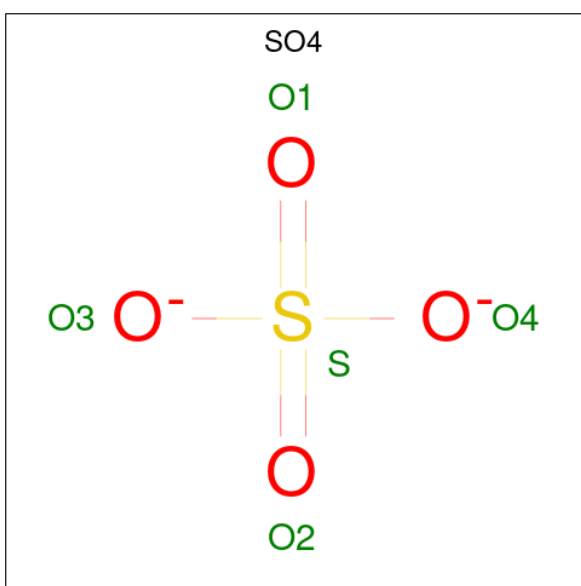
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 5-[5-(4-chloranyl-3-fluoranyl-phenyl)-4-methyl-pyrazol-1-yl]-2-phenylmethoxy-benzoic acid (CCD ID: EGO) (formula: C₂₄H₁₈ClFN₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	0
			31	24	1	1	2	3		
3	B	1	Total	C	Cl	F	N	O	0	0
			31	24	1	1	2	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O S	0	0
			5	4 1		
4	B	1	Total	O S	0	0
			5	4 1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

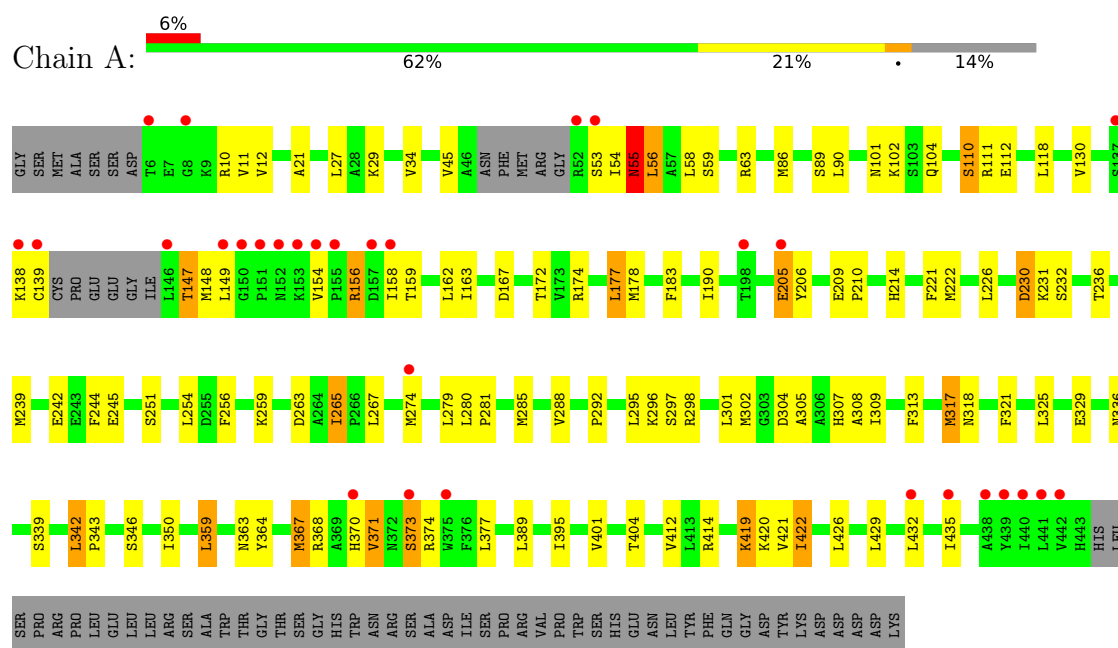
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	O	0	0
			4	4		
6	B	2	Total	O	0	0
			2	2		

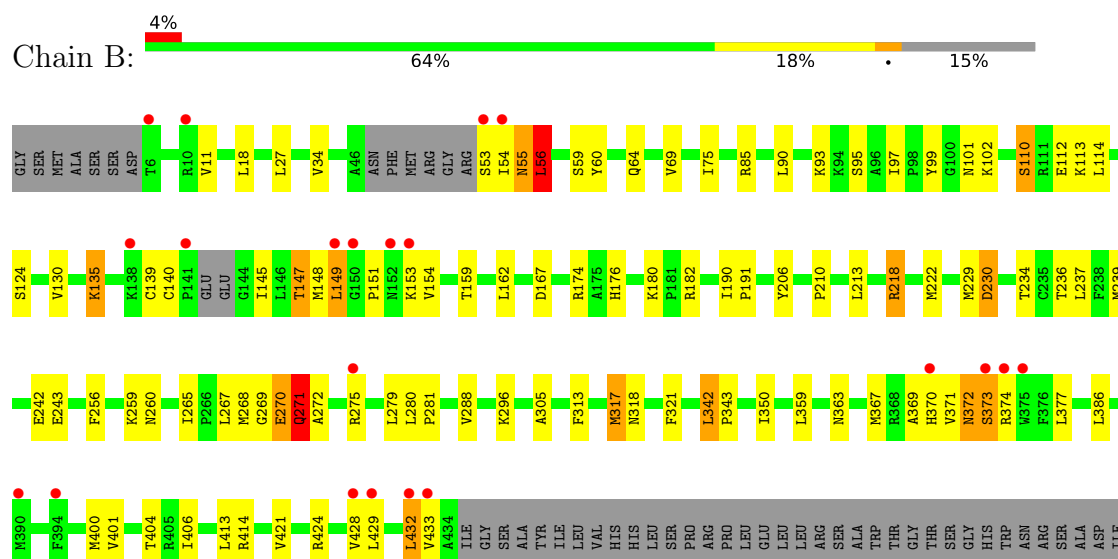
3 Residue-property plots [i](#)

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: Kynurenine 3-monooxygenase



• Molecule 1: Kynurenine 3-monooxygenase



SER
PRO
ARG
VAL
PRO
TRP
SER
HIS
GLU
ASN
LEU
TYR
PHE
GLN
GLY
ASP
TYR
LYS
ASP
ASP
ASP
LYS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.97Å 63.43Å 152.42Å 90.00° 113.52° 90.00°	Depositor
Resolution (Å)	49.25 – 3.00 49.25 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.25-3.00) 100.0 (49.25-3.00)	Depositor EDS
R_{merge}	0.99	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.220 , 0.262 0.224 , 0.263	Depositor DCC
R_{free} test set	1432 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6964	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, CL, SO4, EGO

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	0.85	2/3502 (0.1%)	1.09	7/4727 (0.1%)
1	B	0.87	1/3447 (0.0%)	1.08	9/4653 (0.2%)
All	All	0.86	3/6949 (0.0%)	1.08	16/9380 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	ILE	CA-CB	5.48	1.56	1.54
1	A	147	THR	CA-CB	5.27	1.61	1.53
1	B	147	THR	CA-CB	5.14	1.61	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	ILE	N-CA-CB	8.07	115.93	110.52
1	B	372	ASN	N-CA-C	-6.36	100.56	110.17
1	B	406	ILE	N-CA-C	-6.32	100.83	109.37
1	A	308	ALA	N-CA-C	-6.32	97.97	108.34
1	A	336	ASN	N-CA-C	5.74	119.58	112.24
1	A	55	ASN	CB-CA-C	5.71	119.50	109.80
1	A	265	ILE	CB-CA-C	-5.68	108.30	113.70
1	B	350	ILE	CB-CA-C	-5.64	108.37	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	ASP	N-CA-C	-5.64	103.06	110.33
1	B	56	LEU	N-CA-C	5.45	117.25	109.14
1	A	230	ASP	N-CA-C	-5.44	101.99	110.10
1	A	371	VAL	N-CA-C	-5.27	99.92	107.78
1	B	97	ILE	CB-CA-C	-5.25	104.97	110.53
1	B	101	ASN	N-CA-CB	-5.24	103.44	111.56
1	B	218	ARG	N-CA-C	-5.08	103.34	110.35
1	B	374	ARG	N-CA-C	5.04	119.45	112.45

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	271	GLN	Peptide

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	3416	0	3438	48	0
1	B	3362	0	3380	44	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
3	A	31	0	0	3	0
3	B	31	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	4	0	0	0	0
6	B	2	0	0	0	0
All	All	6964	0	6880	95	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 7.

All (95) 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:55:ASN:C	1:B:55:ASN:HD22	1.73	0.97
1:A:55:ASN:C	1:A:55:ASN:HD22	1.92	0.77
1:B:55:ASN:C	1:B:55:ASN:ND2	2.44	0.75
1:A:304:ASP:HA	1:A:307:HIS:O	1.92	0.69
1:B:367:MET:HA	1:B:371:VAL:HG22	1.75	0.67
1:B:317:MET:HE3	1:B:321:PHE:CD2	2.33	0.64
1:A:156:ARG:O	1:A:156:ARG:NE	2.31	0.62
1:B:149:LEU:HB3	1:B:151:PRO:HD2	1.82	0.62
1:B:149:LEU:HD13	1:B:151:PRO:HD2	1.82	0.61
1:A:178:MET:HA	1:A:183:PHE:CD2	2.36	0.60
1:A:55:ASN:C	1:A:55:ASN:ND2	2.59	0.60
1:A:419:LYS:HA	1:A:422:ILE:HG22	1.87	0.56
1:B:149:LEU:HD12	1:B:154:VAL:HG11	1.88	0.56
1:B:270:GLU:O	1:B:271:GLN:OE1	2.24	0.56
1:A:190:ILE:HD11	1:A:285:MET:HE3	1.89	0.54
1:B:55:ASN:HD22	1:B:56:LEU:N	2.03	0.54
1:B:317:MET:HE2	1:B:318:ASN:N	2.22	0.54
1:A:346:SER:O	1:A:350:ILE:HG13	2.07	0.53
3:A:1002:EGO:C1	3:A:1002:EGO:C27	2.86	0.53
1:A:317:MET:HE2	1:A:318:ASN:N	2.24	0.53
1:A:58:LEU:HD12	1:A:317:MET:HE1	1.90	0.53
1:A:317:MET:HE3	1:A:321:PHE:CD2	2.45	0.52
1:B:239:MET:HE1	1:B:256:PHE:CZ	2.45	0.52
1:B:367:MET:HE3	1:B:371:VAL:HG21	1.90	0.51
1:A:205:GLU:HA	1:A:231:LYS:HD3	1.92	0.51
1:A:56:LEU:HD21	1:A:111:ARG:HD2	1.93	0.51
1:A:177:LEU:HD21	1:A:295:LEU:HB2	1.93	0.50
1:A:55:ASN:HB2	1:A:110:SER:HA	1.93	0.50
1:B:206:TYR:CG	1:B:210:PRO:HB3	2.47	0.49
1:A:206:TYR:CD2	1:A:210:PRO:HB3	2.48	0.49
1:B:218:ARG:NH2	1:B:260:ASN:O	2.44	0.49
1:A:209:GLU:OE1	1:A:209:GLU:N	2.41	0.49
1:A:239:MET:HG3	1:A:244:PHE:CE2	2.48	0.49
1:B:237:LEU:HD21	1:B:239:MET:HE3	1.95	0.48
1:A:325:LEU:O	1:A:329:GLU:HG3	2.13	0.48
1:B:269:GLY:HA3	1:B:272:ALA:HB3	1.95	0.48
1:B:342:LEU:HB2	1:B:343:PRO:HD3	1.96	0.48
1:B:149:LEU:HD13	1:B:151:PRO:CD	2.44	0.47
1:A:230:ASP:O	1:A:232:SER:N	2.46	0.47
1:B:206:TYR:CD2	1:B:210:PRO:HB3	2.50	0.47
1:B:60:TYR:CE1	1:B:64:GLN:NE2	2.82	0.47
1:A:317:MET:HE2	1:A:318:ASN:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:HD13	1:B:317:MET:HG3	1.98	0.47
1:A:317:MET:HE2	1:A:317:MET:C	2.40	0.46
1:B:400:MET:O	1:B:404:THR:OG1	2.31	0.46
1:A:367:MET:HA	1:A:371:VAL:HG22	1.98	0.46
1:A:89:SER:HA	1:A:373:SER:HB3	1.97	0.46
3:A:1002:EGO:C27	3:A:1002:EGO:C17	2.94	0.45
1:B:174:ARG:HD3	1:B:305:ALA:O	2.16	0.45
1:A:174:ARG:HD3	1:A:305:ALA:O	2.17	0.45
1:A:370:HIS:CG	1:A:370:HIS:O	2.68	0.45
1:A:254:LEU:HD13	1:A:274:MET:HE1	1.98	0.45
1:A:154:VAL:HG12	1:A:154:VAL:O	2.17	0.45
1:B:139:CYS:SG	1:B:176:HIS:CD2	3.10	0.45
1:B:280:LEU:HB2	1:B:281:PRO:HD2	2.00	0.44
1:B:317:MET:HE2	1:B:318:ASN:HA	2.00	0.44
1:A:167:ASP:OD2	1:A:172:THR:N	2.51	0.44
1:A:86:MET:HB3	1:A:214:HIS:CD2	2.52	0.44
3:A:1002:EGO:C1	3:A:1002:EGO:C28	2.94	0.43
1:A:206:TYR:CG	1:A:210:PRO:HB3	2.53	0.43
1:A:292:PRO:HA	1:A:350:ILE:CD1	2.48	0.43
1:B:369:ALA:HB3	1:B:370:HIS:CD2	2.54	0.43
1:A:301:LEU:O	1:A:302:MET:HG2	2.18	0.43
1:A:163:ILE:HG22	1:A:298:ARG:O	2.18	0.43
1:A:239:MET:HE1	1:A:256:PHE:CZ	2.54	0.43
1:A:342:LEU:HB2	1:A:343:PRO:HD3	2.01	0.42
1:A:317:MET:HE2	1:A:318:ASN:CA	2.48	0.42
1:B:317:MET:HE2	1:B:317:MET:C	2.43	0.42
1:B:432:LEU:HD23	1:B:433:VAL:HG23	2.01	0.42
1:A:21:ALA:HB1	1:A:118:LEU:HB3	2.01	0.42
1:B:372:ASN:O	1:B:373:SER:C	2.63	0.42
1:B:167:ASP:OD1	1:B:167:ASP:N	2.50	0.42
1:B:110:SER:HG	1:B:113:LYS:H	1.63	0.42
1:A:263:ASP:O	1:A:267:LEU:HD13	2.20	0.42
1:A:297:SER:HB3	1:A:339:SER:HA	2.01	0.42
1:B:151:PRO:O	1:B:154:VAL:HG23	2.19	0.41
1:B:268:MET:O	1:B:269:GLY:C	2.63	0.41
1:A:359:LEU:CD1	1:A:412:VAL:HG22	2.50	0.41
1:A:58:LEU:HG	1:A:63:ARG:HG3	2.02	0.41
1:B:53:SER:HB3	2:B:1001:FAD:C6	2.49	0.41
1:A:10:ARG:NH1	1:A:158:ILE:HG23	2.36	0.41
1:B:239:MET:HE1	1:B:256:PHE:CE1	2.55	0.41
1:B:371:VAL:O	1:B:371:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LEU:HB2	1:A:281:PRO:CD	2.51	0.41
1:B:75:ILE:HD12	1:B:114:LEU:HD12	2.03	0.41
1:B:69:VAL:O	1:B:69:VAL:HG12	2.21	0.41
1:B:85:ARG:HG3	1:B:99:TYR:CZ	2.56	0.41
1:B:190:ILE:HB	1:B:191:PRO:HD2	2.03	0.41
1:B:317:MET:HE2	1:B:318:ASN:CA	2.51	0.41
1:A:242:GLU:O	1:A:245:GLU:HB3	2.22	0.40
1:A:419:LYS:HA	1:A:422:ILE:CG2	2.50	0.40
1:A:55:ASN:HD21	1:A:226:LEU:HB3	1.85	0.40
1:A:190:ILE:HD12	1:A:364:TYR:CZ	2.57	0.40
1:B:229:MET:C	1:B:230:ASP:O	2.58	0.40
1:B:135:LYS:O	1:B:148:MET:N	2.50	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	421/495 (85%)	402 (96%)	19 (4%)	0	100	100
1	B	415/495 (84%)	385 (93%)	30 (7%)	0	100	100
All	All	836/990 (84%)	787 (94%)	49 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	372/431 (86%)	311 (84%)	61 (16%)	2	12
1	B	367/431 (85%)	311 (85%)	56 (15%)	3	14
All	All	739/862 (86%)	622 (84%)	117 (16%)	2	13

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	12	VAL
1	A	27	LEU
1	A	29	LYS
1	A	34	VAL
1	A	45	VAL
1	A	53	SER
1	A	54	ILE
1	A	55	ASN
1	A	56	LEU
1	A	59	SER
1	A	90	LEU
1	A	101	ASN
1	A	102	LYS
1	A	104	GLN
1	A	110	SER
1	A	112	GLU
1	A	130	VAL
1	A	138	LYS
1	A	139	CYS
1	A	147	THR
1	A	148	MET
1	A	149	LEU
1	A	156	ARG
1	A	159	THR
1	A	162	LEU
1	A	177	LEU
1	A	205	GLU
1	A	221	PHE
1	A	222	MET
1	A	236	THR
1	A	251	SER
1	A	259	LYS
1	A	265	ILE

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Mol	Chain	Res	Type
1	A	279	LEU
1	A	288	VAL
1	A	296	LYS
1	A	309	ILE
1	A	313	PHE
1	A	317	MET
1	A	342	LEU
1	A	359	LEU
1	A	363	ASN
1	A	367	MET
1	A	368	ARG
1	A	373	SER
1	A	374	ARG
1	A	377	LEU
1	A	389	LEU
1	A	395	ILE
1	A	401	VAL
1	A	404	THR
1	A	414	ARG
1	A	419	LYS
1	A	420	LYS
1	A	421	VAL
1	A	422	ILE
1	A	426	LEU
1	A	429	LEU
1	A	432	LEU
1	A	435	ILE
1	B	11	VAL
1	B	27	LEU
1	B	34	VAL
1	B	54	ILE
1	B	55	ASN
1	B	56	LEU
1	B	59	SER
1	B	90	LEU
1	B	93	LYS
1	B	95	SER
1	B	102	LYS
1	B	110	SER
1	B	112	GLU
1	B	124	SER
1	B	130	VAL

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Mol	Chain	Res	Type
1	B	135	LYS
1	B	140	CYS
1	B	145	ILE
1	B	147	THR
1	B	149	LEU
1	B	153	LYS
1	B	159	THR
1	B	162	LEU
1	B	180	LYS
1	B	182	ARG
1	B	213	LEU
1	B	222	MET
1	B	234	THR
1	B	236	THR
1	B	242	GLU
1	B	243	GLU
1	B	259	LYS
1	B	265	ILE
1	B	267	LEU
1	B	270	GLU
1	B	271	GLN
1	B	275	ARG
1	B	279	LEU
1	B	288	VAL
1	B	296	LYS
1	B	313	PHE
1	B	317	MET
1	B	342	LEU
1	B	359	LEU
1	B	363	ASN
1	B	373	SER
1	B	377	LEU
1	B	386	LEU
1	B	401	VAL
1	B	413	LEU
1	B	414	ARG
1	B	421	VAL
1	B	424	ARG
1	B	428	VAL
1	B	429	LEU
1	B	432	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	192	HIS
1	A	211	ASN
1	A	214	HIS
1	A	370	HIS
1	A	379	GLN
1	A	409	HIS
1	B	55	ASN
1	B	131	HIS
1	B	176	HIS
1	B	214	HIS
1	B	250	HIS
1	B	258	GLN
1	B	260	ASN
1	B	370	HIS
1	B	379	GLN

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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
4	SO4	B	1003	-	4,4,4	0.64	0	6,6,6	0.55	0
4	SO4	A	1003	-	4,4,4	0.47	0	6,6,6	0.26	0
3	EGO	A	1002	-	34,34,34	0.99	3 (8%)	46,48,48	1.40	6 (13%)
2	FAD	B	1001	-	58,58,58	1.34	10 (17%)	85,89,89	1.77	19 (22%)
2	FAD	A	1001	-	58,58,58	1.47	11 (18%)	85,89,89	1.63	16 (18%)
3	EGO	B	1002	-	34,34,34	1.39	6 (17%)	46,48,48	1.74	10 (21%)

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	1001	-	-	5/34/50/50	0/6/6/6
2	FAD	B	1001	-	-	2/34/50/50	0/6/6/6
3	EGO	A	1002	-	-	4/17/17/17	0/4/4/4
3	EGO	B	1002	-	-	4/17/17/17	0/4/4/4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	FAD	C9A-C5X	4.89	1.49	1.41
3	B	1002	EGO	C28-C29	-4.36	1.42	1.48
2	A	1001	FAD	C5A-C4A	3.69	1.45	1.39
2	B	1001	FAD	C5X-N5	-3.57	1.32	1.39
2	B	1001	FAD	C5A-C4A	3.44	1.45	1.39
2	B	1001	FAD	C5A-N7A	-3.09	1.33	1.39
2	B	1001	FAD	C9A-C5X	3.05	1.46	1.41
2	A	1001	FAD	C8-C7	3.03	1.48	1.40
2	A	1001	FAD	PA-O3P	2.98	1.62	1.59
2	A	1001	FAD	C5X-N5	-2.77	1.34	1.39
2	B	1001	FAD	C8-C7	2.71	1.47	1.40
3	B	1002	EGO	N20-N19	-2.68	1.34	1.38
3	A	1002	EGO	N20-N19	-2.63	1.34	1.38
2	B	1001	FAD	C4A-N9A	-2.58	1.32	1.37
3	A	1002	EGO	C28-C29	-2.54	1.44	1.48
2	A	1001	FAD	C5A-N7A	-2.50	1.34	1.39
3	B	1002	EGO	C17-N20	-2.47	1.38	1.43
3	B	1002	EGO	C18-C30	2.43	1.42	1.40
2	B	1001	FAD	C4-N3	-2.43	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	FAD	P-O3P	2.41	1.62	1.59
2	B	1001	FAD	C8A-N9A	-2.31	1.33	1.37
2	B	1001	FAD	C5A-C6A	2.31	1.47	1.41
2	A	1001	FAD	C4-N3	-2.31	1.34	1.38
3	B	1002	EGO	C29-C30	-2.29	1.37	1.40
2	A	1001	FAD	C8A-N7A	2.19	1.35	1.31
2	A	1001	FAD	C5A-C6A	2.17	1.47	1.41
3	B	1002	EGO	O13-C14	2.12	1.36	1.30
3	A	1002	EGO	C17-N20	-2.06	1.39	1.43
2	B	1001	FAD	C2-N3	-2.05	1.34	1.39
2	A	1001	FAD	C4A-N9A	-2.04	1.33	1.37

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	FAD	C5A-C4A-N3A	-5.87	118.64	126.72
2	A	1001	FAD	C5A-C4A-N3A	-5.45	119.21	126.72
2	B	1001	FAD	N3A-C4A-N9A	4.90	135.50	127.17
3	B	1002	EGO	C9-O10-C11	-4.81	108.23	117.76
2	A	1001	FAD	N3A-C4A-N9A	4.51	134.84	127.17
2	A	1001	FAD	N3A-C2A-N1A	-4.07	122.42	128.58
2	B	1001	FAD	C2A-N3A-C4A	3.92	121.41	111.83
2	A	1001	FAD	C2A-N3A-C4A	3.82	121.17	111.83
3	B	1002	EGO	C24-C25-C26	3.74	122.25	119.04
2	B	1001	FAD	N3A-C2A-N1A	-3.72	122.95	128.58
3	B	1002	EGO	O10-C11-C2	-3.67	115.93	123.95
3	A	1002	EGO	C9-O10-C11	-3.65	110.53	117.76
2	B	1001	FAD	C4'-C3'-C2'	3.31	119.08	113.57
3	A	1002	EGO	O10-C11-C2	-3.30	116.74	123.95
3	B	1002	EGO	C18-N19-N20	-3.29	101.97	104.59
2	B	1001	FAD	C4A-N9A-C8A	3.26	109.17	105.74
2	A	1001	FAD	C4A-N9A-C8A	3.24	109.14	105.74
3	B	1002	EGO	C29-N20-N19	3.16	114.29	112.10
2	B	1001	FAD	C4A-C5A-N7A	-3.15	106.97	110.58
2	B	1001	FAD	O2-C2-N1	-3.10	116.64	121.80
3	A	1002	EGO	C30-C18-N19	-3.05	112.21	113.78
2	A	1001	FAD	C4A-C5A-N7A	-2.95	107.21	110.58
2	A	1001	FAD	O2-C2-N1	-2.88	117.02	121.80
3	A	1002	EGO	C17-N20-C29	-2.83	125.70	129.58
3	A	1002	EGO	O10-C11-C15	2.73	122.97	116.97
2	A	1001	FAD	C4-C4X-N5	2.67	121.90	118.21
2	A	1001	FAD	N9A-C8A-N7A	-2.65	110.17	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	FAD	C5A-N7A-C8A	2.61	107.55	103.45
3	B	1002	EGO	C26-C25-CL1	-2.61	116.50	119.79
2	A	1001	FAD	C5A-N7A-C8A	2.59	107.53	103.45
2	B	1001	FAD	C5X-N5-C4X	2.59	122.28	118.09
2	A	1001	FAD	C6A-C5A-N7A	2.50	136.92	132.09
2	B	1001	FAD	O3'-C3'-C4'	-2.50	103.25	108.93
2	B	1001	FAD	C4X-C10-N1	-2.47	118.53	124.59
2	B	1001	FAD	N9A-C8A-N7A	-2.46	110.44	113.94
2	A	1001	FAD	C10-N1-C2	2.44	122.12	116.85
3	B	1002	EGO	O10-C11-C15	2.43	122.31	116.97
3	B	1002	EGO	O13-C14-C15	-2.39	108.48	115.28
3	B	1002	EGO	C23-C24-C25	-2.38	116.69	119.98
3	A	1002	EGO	C16-C15-C11	2.35	121.47	118.28
2	A	1001	FAD	O4-C4-C4X	-2.33	120.38	126.53
2	A	1001	FAD	C4X-C10-N10	2.31	119.79	116.48
2	B	1001	FAD	O4-C4-C4X	-2.26	120.56	126.53
2	A	1001	FAD	C4X-C10-N1	-2.26	119.06	124.59
2	B	1001	FAD	C4-N3-C2	-2.15	121.83	125.64
2	B	1001	FAD	O4'-C4'-C3'	2.13	114.23	109.25
2	A	1001	FAD	C4A-N9A-C1B	-2.12	121.67	126.63
3	B	1002	EGO	C7-C8-C3	2.10	121.35	118.23
2	B	1001	FAD	N6A-C6A-N1A	2.04	122.91	118.38
2	B	1001	FAD	N3-C2-N1	2.03	123.81	119.50
2	B	1001	FAD	O2A-PA-O1A	2.01	121.78	112.44

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	FAD	C1'-C2'-C3'-C4'
3	A	1002	EGO	O13-C14-C15-C11
2	B	1001	FAD	O4B-C4B-C5B-O5B
3	A	1002	EGO	O12-C14-C15-C11
2	B	1001	FAD	C3B-C4B-C5B-O5B
3	B	1002	EGO	C2-C11-O10-C9
3	A	1002	EGO	C2-C11-O10-C9
2	A	1001	FAD	O2'-C2'-C3'-C4'
3	B	1002	EGO	C15-C11-O10-C9
3	B	1002	EGO	O12-C14-C15-C11
3	B	1002	EGO	O13-C14-C15-C11
3	A	1002	EGO	C15-C11-O10-C9
2	A	1001	FAD	O4B-C4B-C5B-O5B

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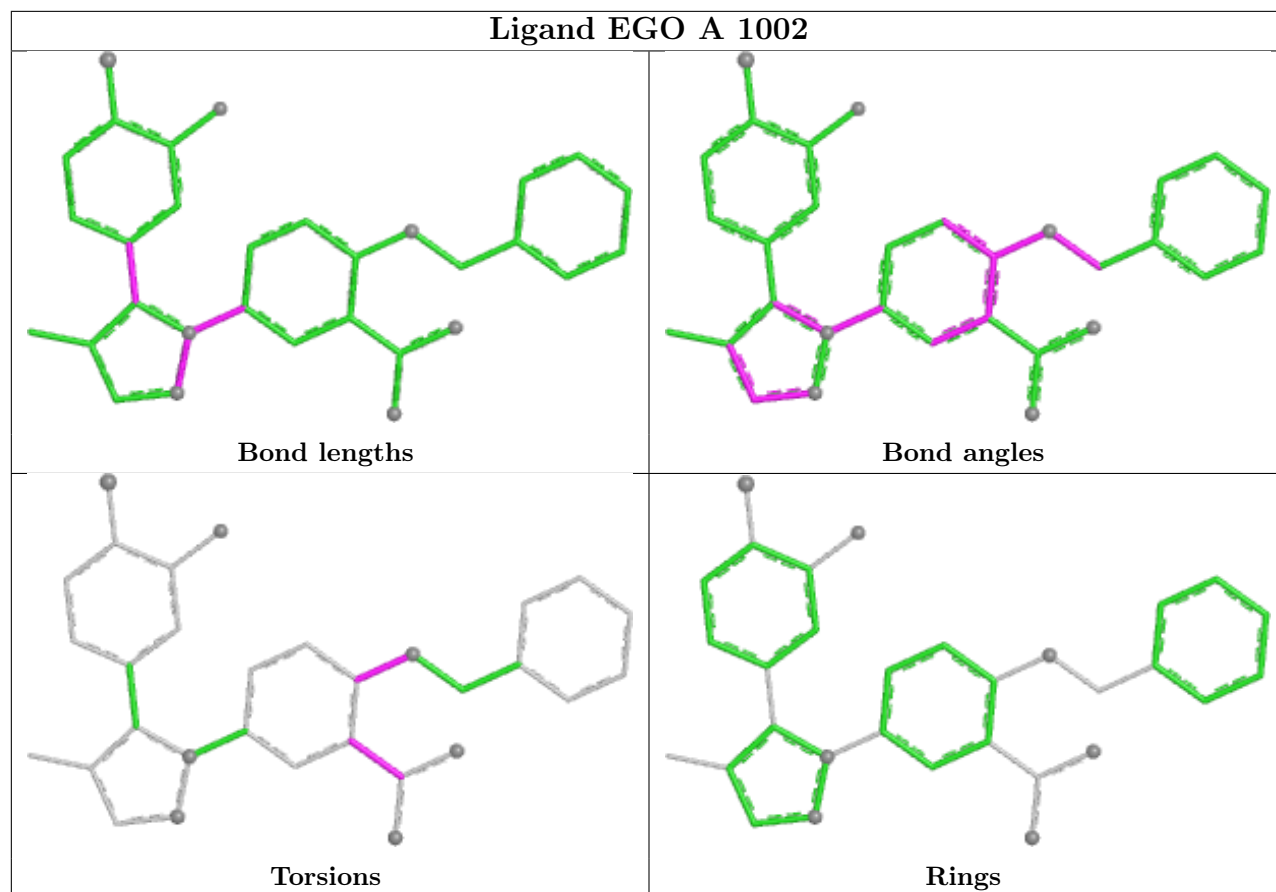
Mol	Chain	Res	Type	Atoms
2	A	1001	FAD	O2'-C2'-C3'-O3'
2	A	1001	FAD	C1'-C2'-C3'-O3'

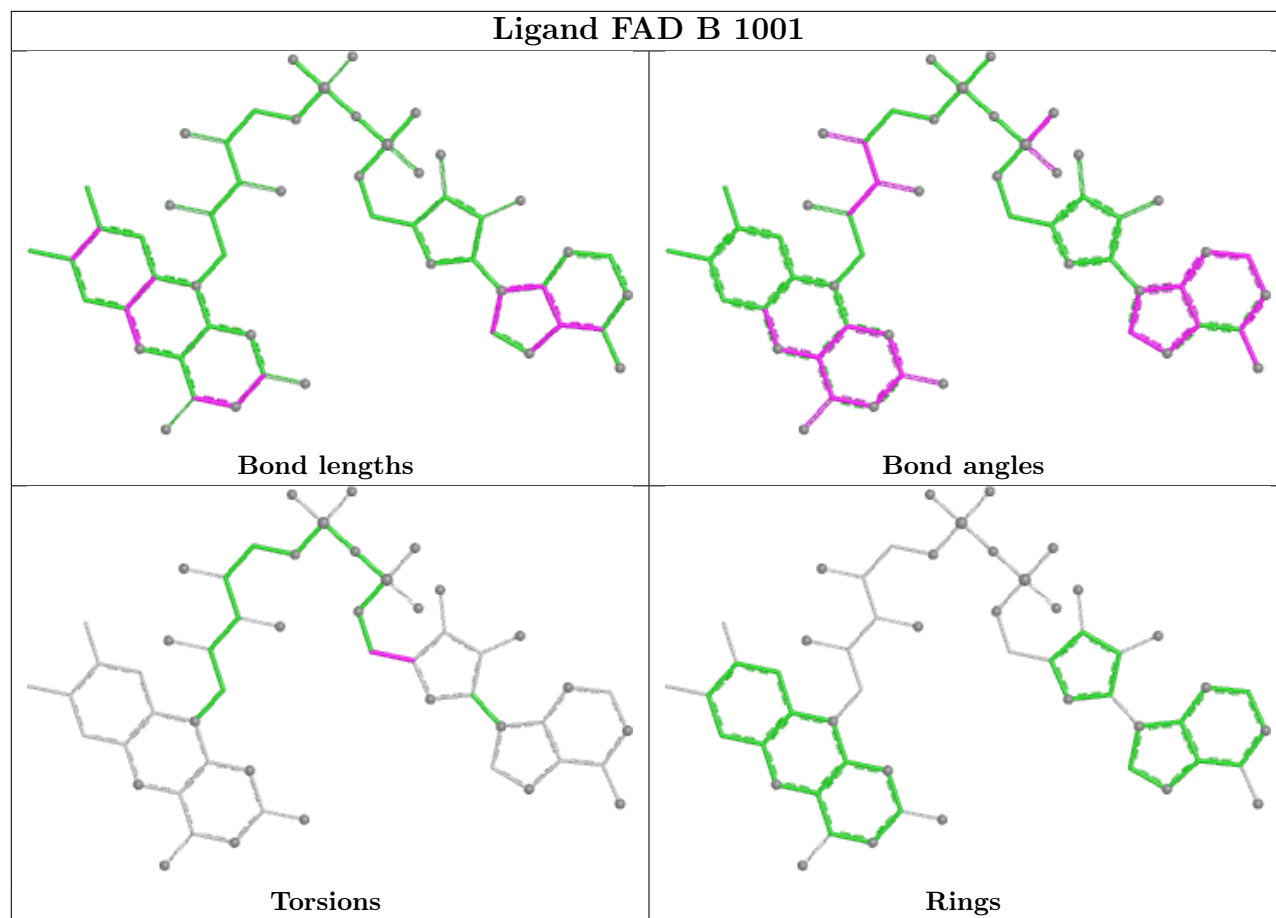
There are no ring outliers.

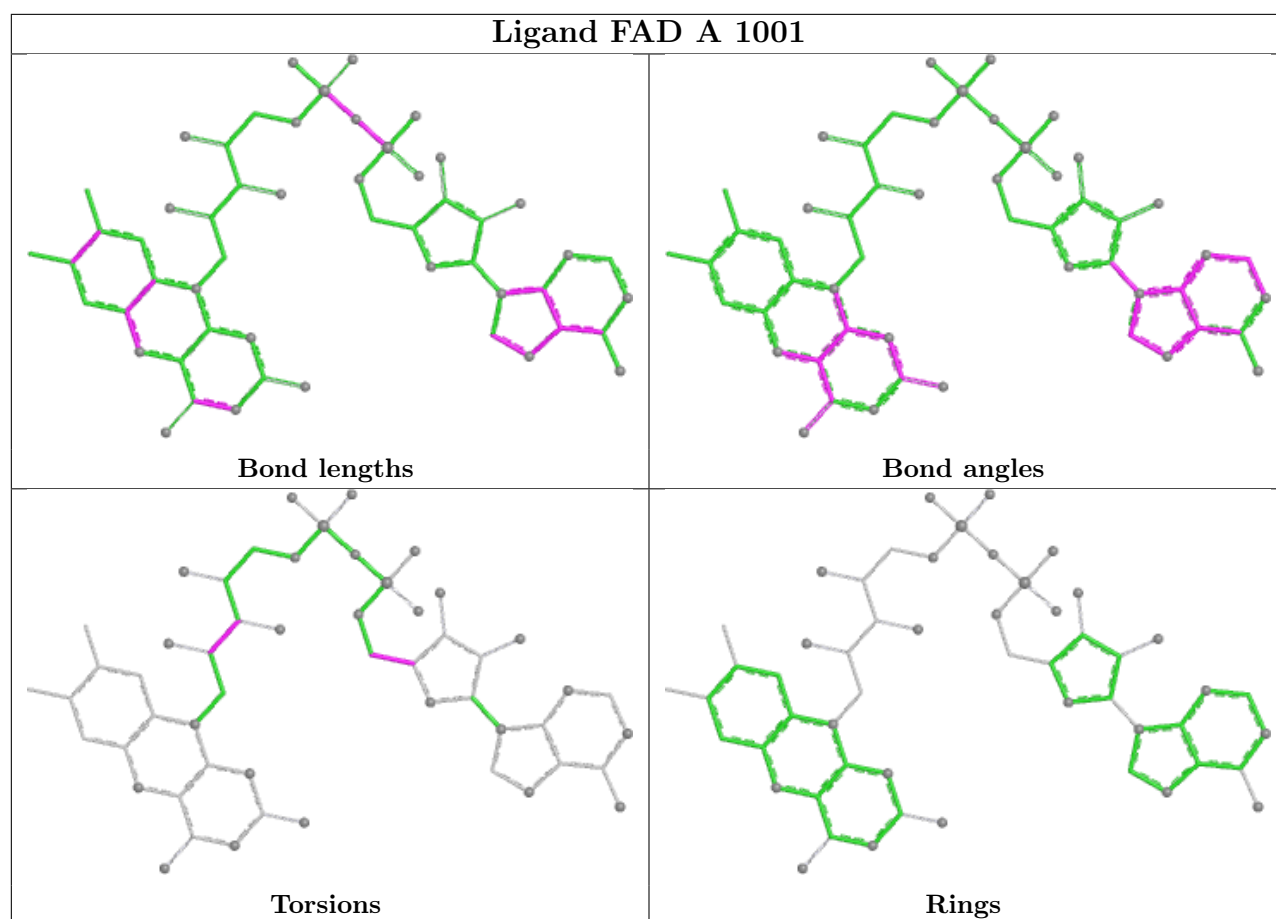
2 monomers are involved in 4 short contacts:

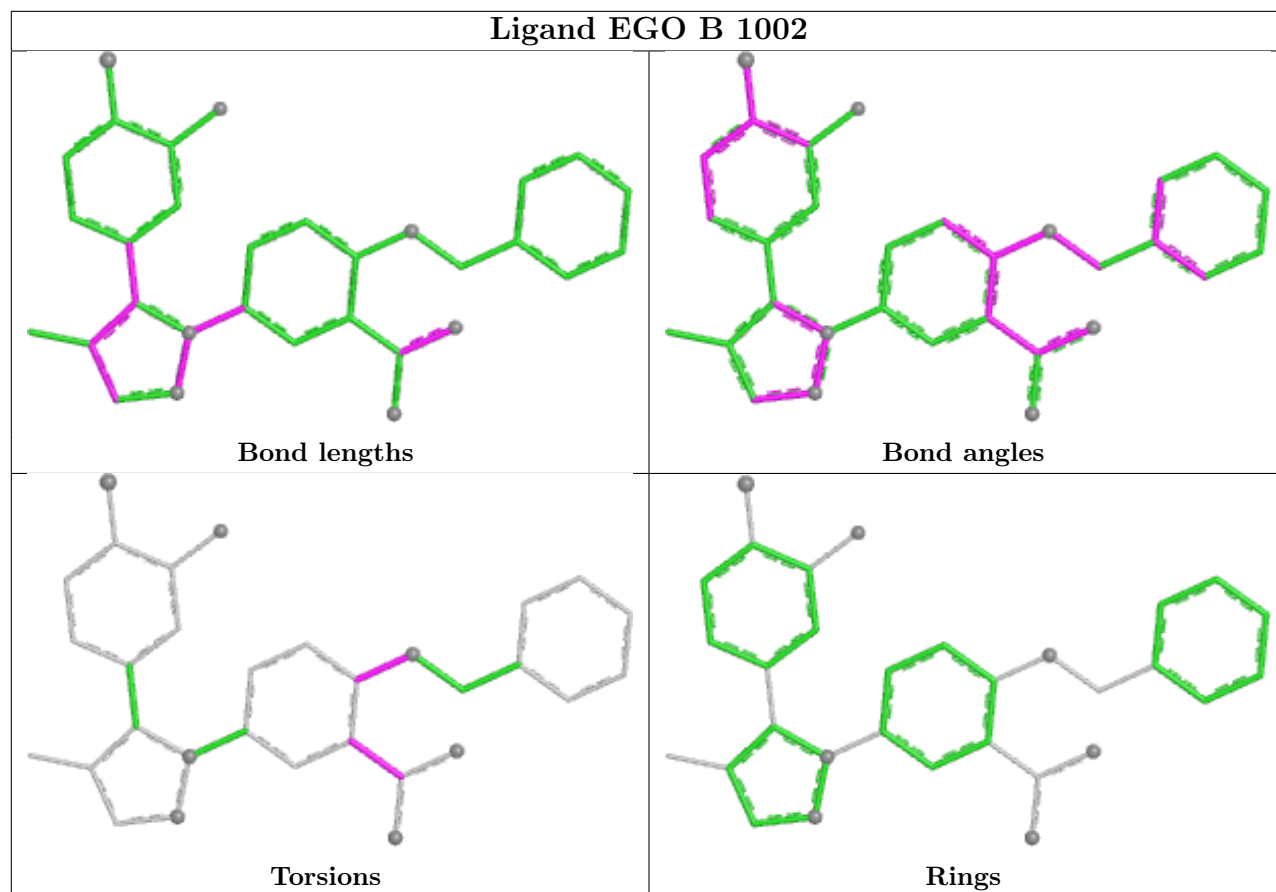
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	EGO	3	0
2	B	1001	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	427/495 (86%)	0.19	30 (7%) 22 12	23, 49, 106, 159	0
1	B	421/495 (85%)	0.06	21 (4%) 34 18	18, 43, 97, 136	0
All	All	848/990 (85%)	0.13	51 (6%) 27 14	18, 46, 103, 159	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	SER	6.1
1	B	141	PRO	4.9
1	A	157	ASP	4.4
1	A	53	SER	4.0
1	B	10	ARG	4.0
1	A	155	PRO	3.9
1	B	152	ASN	3.9
1	A	139	CYS	3.7
1	A	6	THR	3.6
1	A	153	LYS	3.6
1	B	153	LYS	3.6
1	A	149	LEU	3.5
1	B	373	SER	3.3
1	A	205	GLU	3.2
1	B	6	THR	3.2
1	A	8	GLY	3.2
1	A	442	VAL	3.1
1	A	438	ALA	3.1
1	A	151	PRO	3.0
1	B	149	LEU	2.9
1	A	158	ILE	2.9
1	A	373	SER	2.8
1	A	152	ASN	2.8
1	A	137	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	394	PHE	2.7
1	B	275	ARG	2.7
1	A	154	VAL	2.6
1	B	370	HIS	2.6
1	A	52	ARG	2.5
1	A	440	ILE	2.5
1	A	274	MET	2.4
1	A	435	ILE	2.4
1	B	432	LEU	2.4
1	B	150	GLY	2.4
1	A	198	THR	2.3
1	A	138	LYS	2.3
1	B	390	MET	2.3
1	B	429	LEU	2.3
1	B	433	VAL	2.3
1	A	439	TYR	2.3
1	A	375	TRP	2.3
1	B	138	LYS	2.3
1	A	441	LEU	2.2
1	A	432	LEU	2.2
1	A	146	LEU	2.1
1	B	54	ILE	2.1
1	B	428	VAL	2.1
1	B	375	TRP	2.1
1	A	150	GLY	2.1
1	B	374	ARG	2.0
1	A	370	HIS	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,

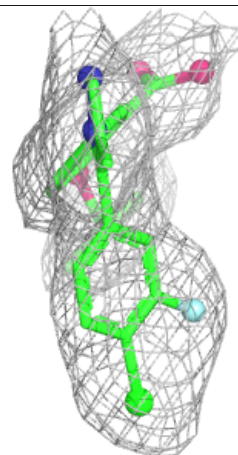
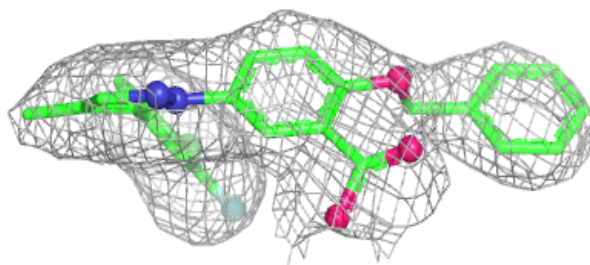
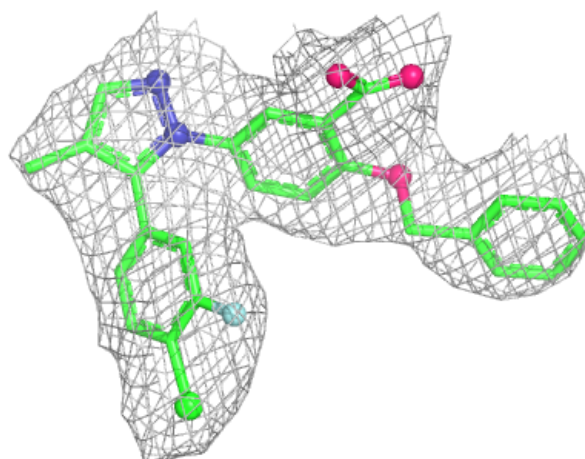
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	1003	5/5	0.94	0.10	53,56,59,62	0
3	EGO	B	1002	31/31	0.96	0.10	28,40,67,68	0
3	EGO	A	1002	31/31	0.96	0.09	31,44,80,83	0
5	CL	A	1004	1/1	0.96	0.08	40,40,40,40	0
4	SO4	A	1003	5/5	0.98	0.07	49,51,51,54	0
2	FAD	A	1001	53/53	0.98	0.06	16,21,37,41	0
2	FAD	B	1001	53/53	0.98	0.06	17,21,25,27	0
5	CL	B	1004	1/1	0.98	0.07	28,28,28,28	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.

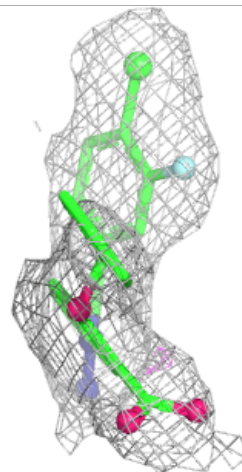
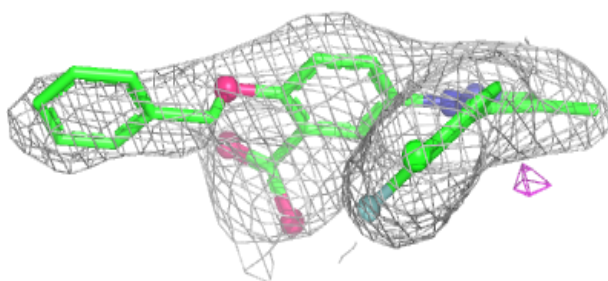
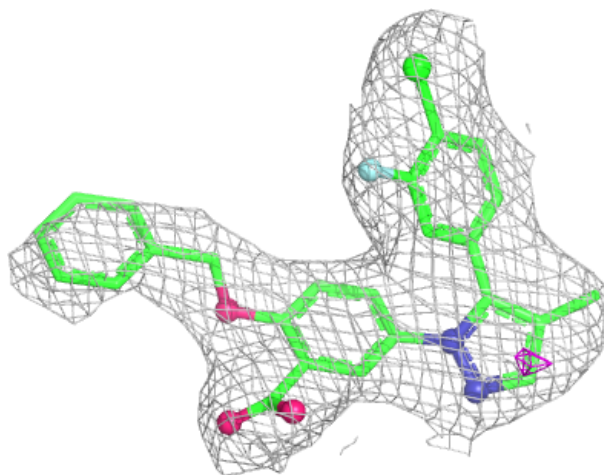
Electron density around EGO B 1002:

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



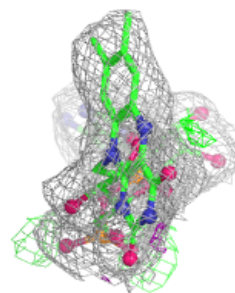
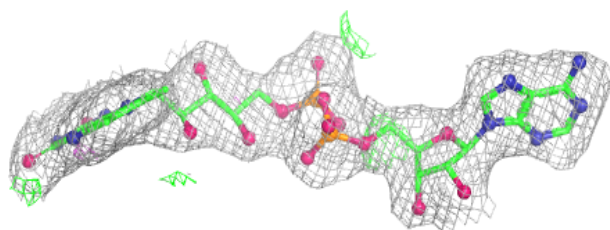
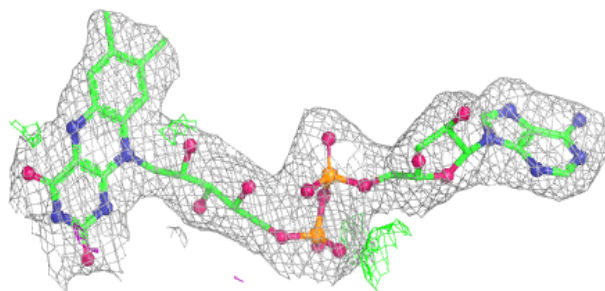
Electron density around EGO A 1002:

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

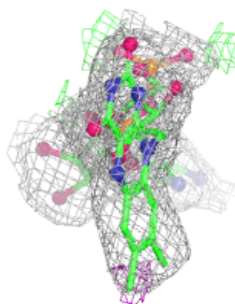
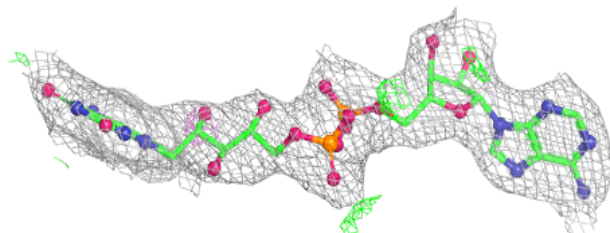
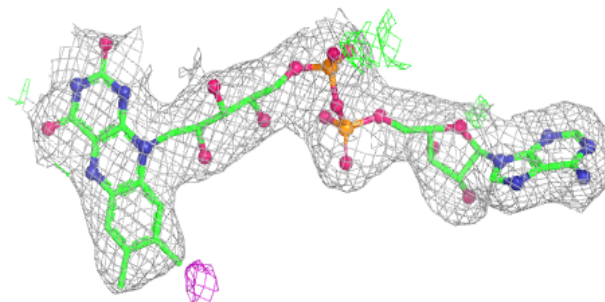


Electron density around FAD A 1001:

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

**Electron density around FAD B 1001:**

$2mF_o-DF_c$ (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.