



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:42 AM UTC

PDB ID : 8ODW / pdb_00008odw
Title : Crystal structure of LbmA Ox-ACP didomain in complex with NADP and ethyl glycinate from the lobatamide PKS (*Gynuella sunshinyii*)
Authors : Francois, R.M.M.; Fraley, A.E.; Piel, J.; Weissman, K.J.; Gruez, A.
Deposited on : 2023-03-09
Resolution : 3.07 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

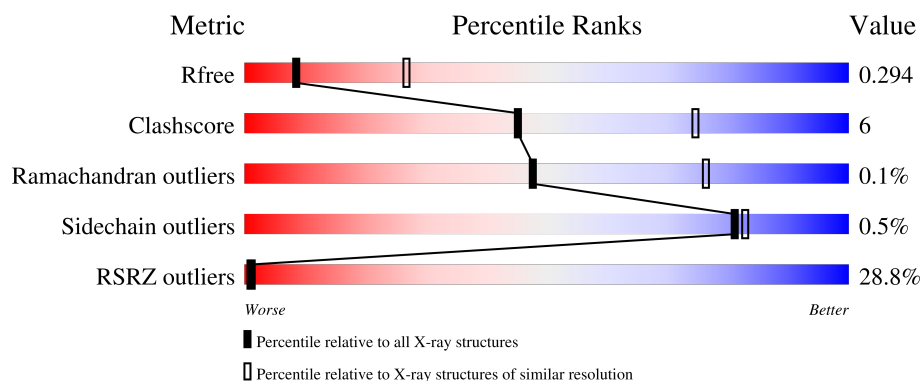
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	639	3% 74% 21% • •
1	B	639	49% 86% • 11%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9771 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.

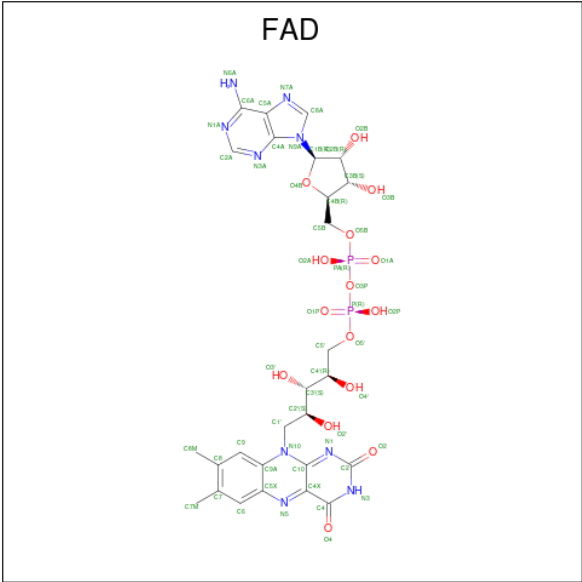
- Molecule 1 is a protein called Polyketide synthase modules-related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	89	0	0
			4878	3098	841	917	22			
1	B	569	Total	C	N	O	S	176	0	0
			4525	2877	778	848	22			

There are 8 discrepancies between the modelled and reference sequences:

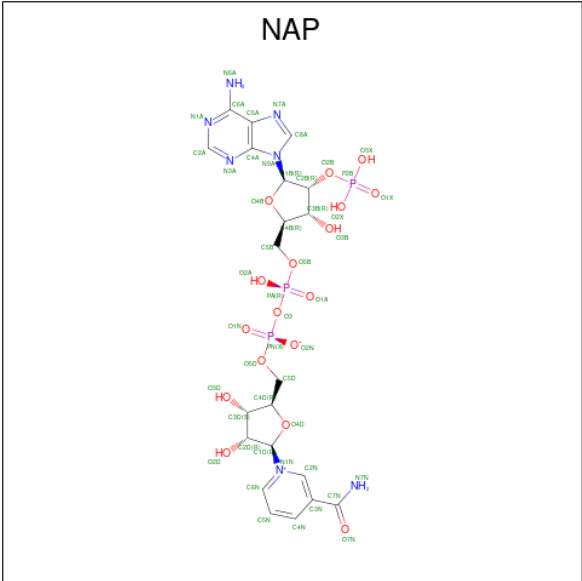
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A0C5VQJ2
A	2	PRO	-	expression tag	UNP A0A0C5VQJ2
A	3	GLY	-	expression tag	UNP A0A0C5VQJ2
A	4	SER	-	expression tag	UNP A0A0C5VQJ2
B	1	GLY	-	expression tag	UNP A0A0C5VQJ2
B	2	PRO	-	expression tag	UNP A0A0C5VQJ2
B	3	GLY	-	expression tag	UNP A0A0C5VQJ2
B	4	SER	-	expression tag	UNP A0A0C5VQJ2

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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 NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



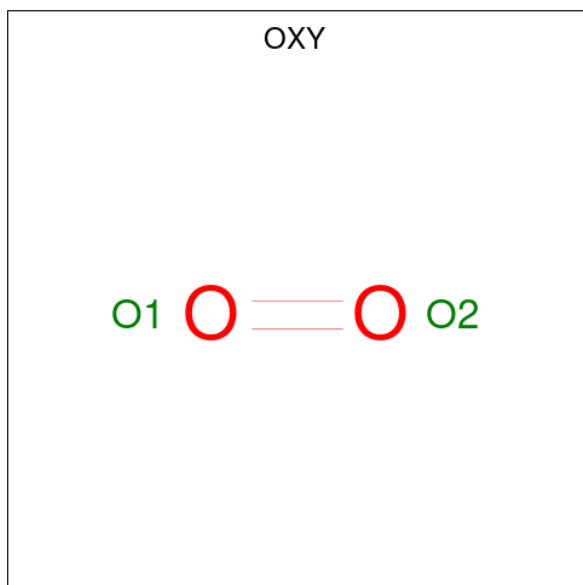
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	2	0
			48	21	7	17	3		

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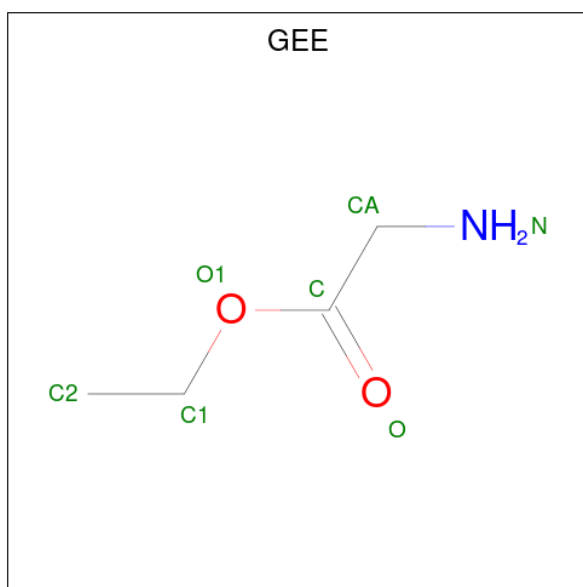
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂) (labeled as "Ligand of Interest" by depositor).



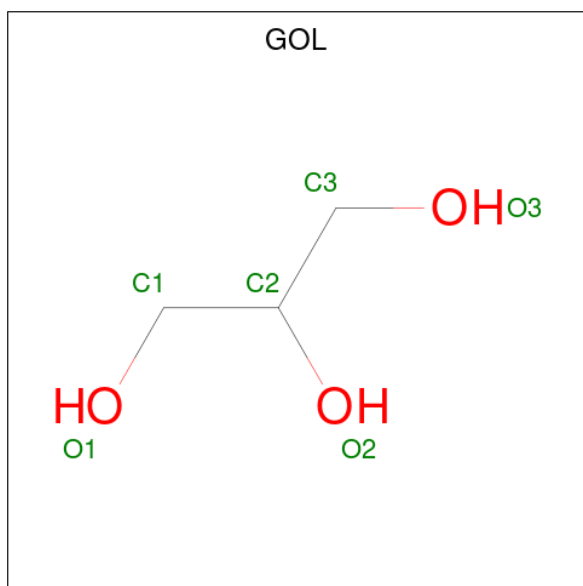
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			2	2		

- Molecule 5 is ethyl glycinate (CCD ID: GEE) (formula: C₄H₉NO₂) (labeled as "Ligand of Interest" by depositor).



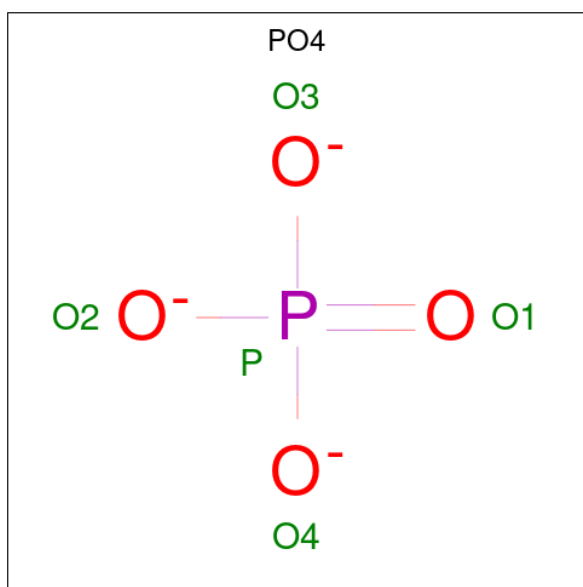
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			7	4	1	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		
7	A	1	Total	O	P	0	0
			5	4	1		
7	A	1	Total	O	P	0	0
			5	4	1		
7	A	1	Total	O	P	0	0
			5	4	1		

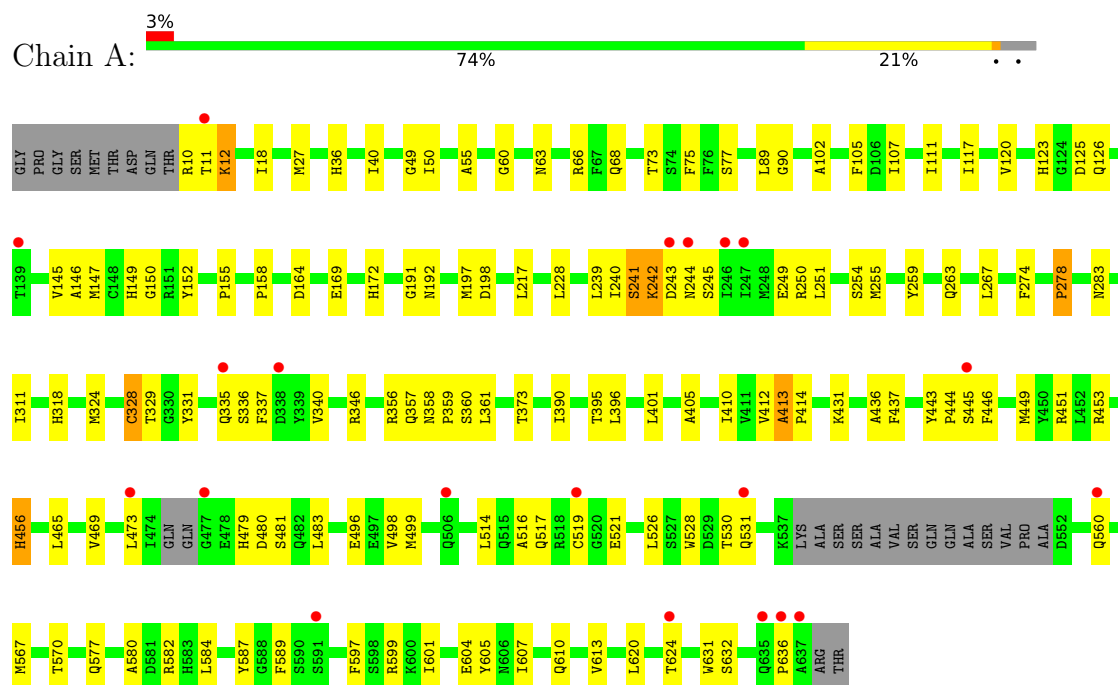
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	121	Total	O	0	0
			121	121		
8	B	10	Total	O	0	0
			10	10		

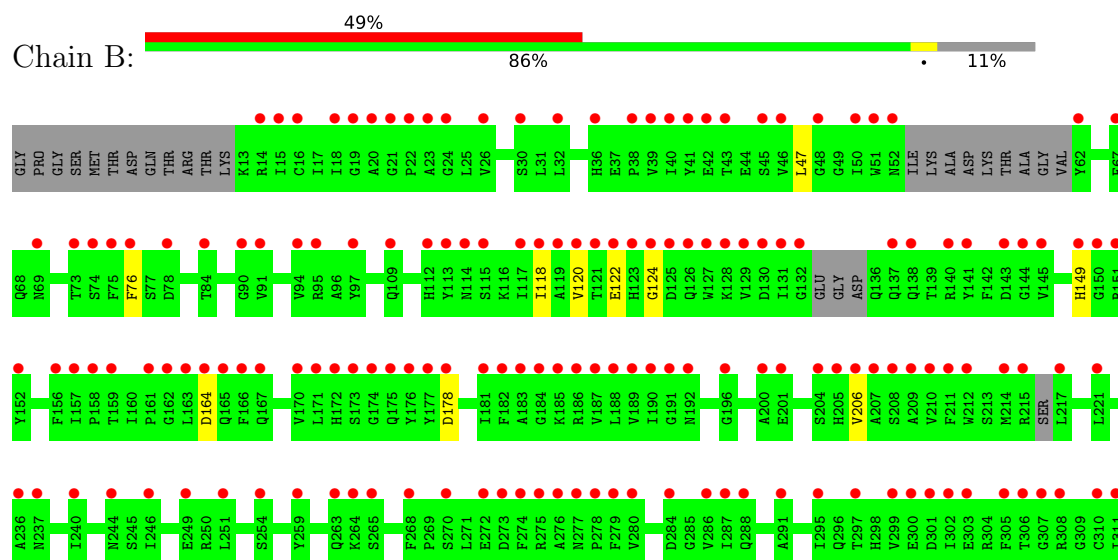
3 Residue-property plots

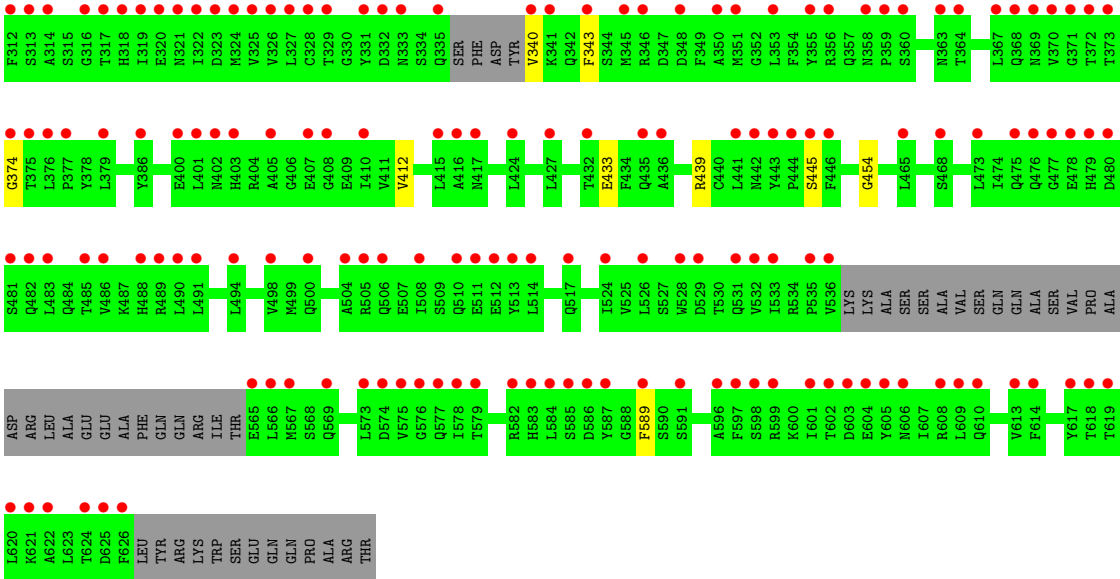
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Polyketide synthase modules-related protein



- Molecule 1: Polyketide synthase modules-related protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	206.75Å 206.75Å 178.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.76 – 3.07 44.76 – 3.07	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.76-3.07) 99.8 (44.76-3.07)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.237 , 0.293 0.237 , 0.294	Depositor DCC
R_{free} test set	2010 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	58.8	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 109.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	9771	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: NAP, PO4, GEE, OXY, FAD, GOL

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	0.56	0/4989	0.83	18/6758 (0.3%)
1	B	0.38	0/4626	0.72	8/6266 (0.1%)
All	All	0.48	0/9615	0.77	26/13024 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	SER	N-CA-C	-11.11	98.02	111.69
1	B	124	GLY	N-CA-C	-10.29	103.35	114.67
1	A	242	LYS	N-CA-C	-9.74	97.95	111.39
1	A	240	ILE	N-CA-C	-8.22	102.32	112.76
1	B	149	HIS	N-CA-C	8.21	121.26	111.33
1	B	445	SER	N-CA-C	-7.20	98.78	109.15
1	A	63	ASN	N-CA-C	6.91	119.70	111.33
1	A	605	TYR	N-CA-C	-6.77	97.87	108.90
1	A	456	HIS	N-CA-C	6.75	120.39	111.28
1	B	122	GLU	N-CA-C	-6.16	101.06	110.30
1	A	49	GLY	N-CA-C	6.00	121.79	111.47
1	A	241	SER	CB-CA-C	-5.94	109.74	116.63
1	A	125	ASP	N-CA-C	-5.82	105.50	113.30
1	B	76	PHE	N-CA-C	5.82	118.89	110.28
1	A	12	LYS	N-CA-C	-5.54	101.99	110.30
1	A	358	ASN	CA-C-N	5.47	126.68	119.84
1	A	358	ASN	C-N-CA	5.47	126.68	119.84
1	B	164	ASP	N-CA-C	-5.34	106.72	113.18
1	A	336	SER	N-CA-C	-5.31	106.83	113.15
1	B	47	LEU	CB-CA-C	-5.28	104.44	111.88
1	A	413	ALA	CA-C-N	-5.26	113.49	119.28
1	A	413	ALA	C-N-CA	-5.26	113.49	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	443	TYR	N-CA-C	-5.24	102.08	110.10
1	B	374	GLY	N-CA-C	5.23	119.26	112.25
1	A	278	PRO	N-CA-C	-5.08	108.17	114.68
1	A	328	CYS	N-CA-C	-5.02	97.83	107.57

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4878	0	4755	102	0
1	B	4525	0	4406	5	0
2	A	53	0	31	3	0
2	B	53	0	31	0	0
3	A	48	0	25	2	0
3	B	48	0	25	0	0
4	A	2	0	0	0	0
5	A	7	0	9	1	0
6	A	6	0	8	1	0
7	A	20	0	0	0	0
8	A	121	0	0	6	0
8	B	10	0	0	1	0
All	All	9771	0	9290	108	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 (108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:THR:HG22	1:A:445:SER:O	1.58	1.04
1:A:50:ILE:CD1	1:A:60:GLY:HA2	1.99	0.92
1:A:373:THR:HG21	1:A:445:SER:HB3	1.69	0.74
1:B:439:ARG:NH1	8:B:801:HOH:O	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ALA:HA	1:A:519:CYS:SG	2.29	0.72
1:A:577:GLN:OE1	1:A:582:ARG:NH2	2.24	0.71
1:A:498:VAL:HG23	8:A:825:HOH:O	1.91	0.71
1:A:610:GLN:HG3	1:A:613:VAL:HG23	1.72	0.70
1:A:50:ILE:HD12	1:A:60:GLY:HA2	1.71	0.70
1:A:105:PHE:HB2	1:A:107:ILE:HD11	1.74	0.69
1:A:239:LEU:C	1:A:241:SER:H	1.98	0.69
1:A:66:ARG:HD2	5:A:704:GEE:H1A	1.74	0.68
1:A:50:ILE:HD11	1:A:60:GLY:N	2.09	0.67
1:A:73:THR:CG2	1:A:445:SER:O	2.38	0.66
1:A:239:LEU:C	1:A:241:SER:N	2.50	0.66
1:B:120:VAL:HG22	1:B:340:VAL:HG12	1.77	0.66
1:A:50:ILE:CD1	1:A:60:GLY:CA	2.75	0.65
1:A:516:ALA:HA	1:A:519:CYS:HG	1.63	0.62
1:A:50:ILE:HD11	1:A:60:GLY:H	1.64	0.61
1:A:479:HIS:O	1:A:480:ASP:C	2.43	0.60
1:B:340:VAL:HB	1:B:343:PHE:HD2	1.66	0.59
1:A:11:THR:O	1:A:12:LYS:C	2.43	0.59
1:A:50:ILE:HD11	1:A:60:GLY:CA	2.31	0.59
1:A:599:ARG:NH1	8:A:801:HOH:O	2.30	0.59
1:A:55:ALA:HA	6:A:705:GOL:H31	1.85	0.58
1:A:36:HIS:CE1	1:A:390:ILE:HG22	2.39	0.58
1:A:242:LYS:O	1:A:243:ASP:C	2.47	0.57
1:A:449:MET:HA	1:A:465:LEU:HD22	1.87	0.57
1:A:412:VAL:HG12	1:A:414:PRO:HD2	1.87	0.57
1:A:50:ILE:HD11	1:A:60:GLY:HA2	1.84	0.56
1:A:251:LEU:HD12	1:A:255:MET:HG3	1.87	0.56
1:A:521:GLU:O	1:A:521:GLU:HG3	2.05	0.56
1:A:66:ARG:HA	1:A:90:GLY:HA2	1.88	0.55
1:A:356:ARG:HG2	1:A:401:LEU:HD23	1.89	0.55
1:A:191:GLY:HA3	1:A:328:CYS:O	2.07	0.54
1:A:241:SER:O	1:A:242:LYS:C	2.51	0.54
1:A:68:GLN:OE1	3:A:702:NAP:H2N	2.08	0.53
1:A:259:TYR:O	1:A:263:GLN:HG3	2.09	0.53
1:A:244:ASN:HB2	1:A:274:PHE:CZ	2.44	0.53
1:A:123:HIS:O	1:A:126:GLN:N	2.42	0.52
1:A:18:ILE:HG13	1:A:117:ILE:HG13	1.91	0.52
1:A:499:MET:HE1	8:A:904:HOH:O	2.10	0.52
1:A:570:THR:HG21	1:A:597:PHE:HA	1.90	0.52
1:A:77:SER:HB2	1:A:451:ARG:HE	1.74	0.52
1:A:359:PRO:C	1:A:361:LEU:N	2.60	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:CYS:SG	1:A:519:CYS:O	2.68	0.51
1:A:451:ARG:NH1	1:A:456:HIS:O	2.44	0.50
1:A:150:GLY:HA3	2:A:701:FAD:O2A	2.12	0.50
1:A:164:ASP:OD1	1:A:164:ASP:N	2.37	0.50
1:A:250:ARG:O	1:A:254:SER:OG	2.28	0.49
1:A:40:ILE:HD12	1:A:111:ILE:HG12	1.95	0.49
1:A:191:GLY:HA2	3:A:702:NAP:H1B	1.95	0.48
1:A:147:MET:HE2	1:A:149:HIS:HE1	1.79	0.48
1:A:431:LYS:HG2	1:A:498:VAL:HG11	1.95	0.48
1:A:278:PRO:HG2	1:A:410:ILE:HD12	1.97	0.47
1:A:357:GLN:HE22	1:B:454:GLY:H	1.61	0.47
1:A:580:ALA:HA	1:A:620:LEU:HD23	1.96	0.47
1:A:514:LEU:O	1:A:517:GLN:HB2	2.14	0.47
1:A:50:ILE:CG1	1:A:60:GLY:HA2	2.44	0.47
1:A:102:ALA:HA	1:A:107:ILE:HD13	1.97	0.47
1:A:584:LEU:HA	1:A:587:TYR:CD2	2.50	0.47
1:A:496:GLU:HA	1:A:499:MET:HE3	1.96	0.46
1:A:158:PRO:HG3	1:A:329:THR:HG21	1.98	0.46
1:A:123:HIS:O	1:A:126:GLN:O	2.34	0.45
1:A:584:LEU:HA	1:A:587:TYR:HD2	1.80	0.45
2:A:701:FAD:N1	2:A:701:FAD:O2'	2.46	0.45
2:A:701:FAD:H1'1	2:A:701:FAD:H9	1.68	0.45
1:A:483:LEU:HA	1:A:483:LEU:HD23	1.79	0.45
1:A:607:ILE:HD11	1:A:631:TRP:HB2	1.99	0.45
1:A:105:PHE:HB2	1:A:107:ILE:CD1	2.45	0.45
1:A:526:LEU:HD22	1:A:530:THR:HG21	2.00	0.44
1:B:340:VAL:HB	1:B:343:PHE:CD2	2.49	0.44
1:A:453:ARG:HD3	8:A:889:HOH:O	2.16	0.44
1:A:444:PRO:HD2	1:A:446:PHE:CE2	2.52	0.43
1:A:436:ALA:O	1:A:437:PHE:C	2.57	0.43
1:A:10:ARG:C	1:A:12:LYS:N	2.76	0.43
1:A:604:GLU:HB3	8:A:804:HOH:O	2.17	0.43
1:A:169:GLU:HB2	1:A:324:MET:HG2	2.01	0.43
1:A:449:MET:HB2	1:A:449:MET:HE3	1.77	0.43
1:A:413:ALA:O	1:A:414:PRO:C	2.60	0.43
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.72	0.43
1:A:597:PHE:O	1:A:601:ILE:HG13	2.19	0.43
1:A:75:PHE:CZ	1:A:89:LEU:HD22	2.54	0.42
1:A:12:LYS:HE3	8:A:839:HOH:O	2.19	0.42
1:A:632:SER:HA	1:A:636:PRO:HG3	2.01	0.42
1:A:267:LEU:HD23	1:A:267:LEU:HA	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ILE:HG12	1:A:318:HIS:HD2	1.84	0.42
1:A:192:ASN:O	1:A:197:MET:HE3	2.20	0.42
1:A:560:GLN:HG3	1:A:624:THR:HG21	2.00	0.42
1:A:249:GLU:OE2	1:A:479:HIS:HE1	2.03	0.42
1:A:567:MET:HE3	1:A:589:PHE:HE2	1.85	0.42
1:A:40:ILE:HB	1:A:111:ILE:HA	2.02	0.41
1:A:198:ASP:OD1	1:A:283:ASN:ND2	2.53	0.41
1:A:217:LEU:HD13	1:A:267:LEU:HA	2.02	0.41
1:A:395:THR:O	1:A:396:LEU:C	2.63	0.41
1:A:120:VAL:HG11	1:A:145:VAL:HG21	2.02	0.41
1:A:480:ASP:O	1:A:481:SER:C	2.60	0.41
1:A:50:ILE:CD1	1:A:60:GLY:N	2.81	0.41
1:A:155:PRO:HB3	1:A:172:HIS:CE1	2.55	0.41
1:A:147:MET:HE1	1:A:340:VAL:HG21	2.03	0.41
1:A:469:VAL:O	1:A:473:LEU:HG	2.20	0.41
1:A:335:GLN:C	1:A:337:PHE:H	2.29	0.41
1:A:359:PRO:O	1:A:360:SER:C	2.63	0.41
1:A:528:TRP:O	1:A:531:GLN:HG2	2.21	0.41
1:A:567:MET:HE3	1:A:589:PHE:CE2	2.55	0.41
1:A:346:ARG:HD2	1:A:405:ALA:O	2.22	0.40
1:A:27:MET:HE3	1:A:146:ALA:HB1	2.04	0.40
1:A:152:TYR:HA	1:A:331:TYR:CG	2.56	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	606/639 (95%)	582 (96%)	24 (4%)	0	100	100
1	B	557/639 (87%)	523 (94%)	33 (6%)	1 (0%)	43	71
All	All	1163/1278 (91%)	1105 (95%)	57 (5%)	1 (0%)	48	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	524/545 (96%)	524 (100%)	0	100	100
1	B	488/545 (90%)	483 (99%)	5 (1%)	68	77
All	All	1012/1090 (93%)	1007 (100%)	5 (0%)	81	83

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	118	ILE
1	B	206	VAL
1	B	412	VAL
1	B	433	GLU
1	B	589	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	263	GLN
1	A	357	GLN
1	A	479	HIS
1	A	484	GLN
1	A	531	GLN
1	A	560	GLN
1	B	149	HIS
1	B	175	GLN
1	B	244	ASN
1	B	263	GLN

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Mol	Chain	Res	Type
1	B	288	GLN
1	B	318	HIS
1	B	321	ASN
1	B	470	GLN
1	B	475	GLN
1	B	484	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 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	$\# Z > 2$
4	OXY	A	703	-	1,1,1	0.10	0	-		
2	FAD	B	701	-	58,58,58	1.43	10 (17%)	85,89,89	1.59	14 (16%)
2	FAD	A	701	-	58,58,58	1.43	11 (18%)	85,89,89	1.65	17 (20%)
7	PO4	A	707	-	4,4,4	0.79	0	6,6,6	0.65	0
5	GEE	A	704	-	6,6,6	0.41	0	5,6,6	1.14	1 (20%)
3	NAP	A	702	-	50,52,52	1.15	5 (10%)	71,80,80	1.49	10 (14%)
6	GOL	A	705	-	5,5,5	1.02	0	5,5,5	1.48	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PO4	A	708	-	4,4,4	0.83	0	6,6,6	0.66	0
3	NAP	B	702	-	50,52,52	1.16	4 (8%)	71,80,80	1.49	8 (11%)
7	PO4	A	709	-	4,4,4	0.88	0	6,6,6	0.67	0
7	PO4	A	706	-	4,4,4	0.94	0	6,6,6	0.72	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	B	701	-	-	7/34/50/50	0/6/6/6
2	FAD	A	701	-	-	8/34/50/50	0/6/6/6
5	GEE	A	704	-	-	4/5/5/5	-
3	NAP	A	702	-	-	10/35/67/67	0/5/5/5
6	GOL	A	705	-	-	2/4/4/4	-
3	NAP	B	702	-	-	14/35/67/67	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FAD	C9A-C5X	4.99	1.49	1.41
3	B	702	NAP	C5A-C4A	4.72	1.47	1.39
2	A	701	FAD	C9A-C5X	4.56	1.48	1.41
2	B	701	FAD	C5A-C4A	4.52	1.47	1.39
3	A	702	NAP	C5A-C4A	4.43	1.47	1.39
2	A	701	FAD	C5A-C4A	4.18	1.46	1.39
2	B	701	FAD	C8-C7	3.29	1.48	1.40
2	A	701	FAD	C8-C7	3.05	1.48	1.40
2	A	701	FAD	C4-N3	-2.93	1.33	1.38
2	B	701	FAD	C4-N3	-2.86	1.33	1.38
3	B	702	NAP	C5A-C6A	2.61	1.48	1.41
2	A	701	FAD	C5A-C6A	2.60	1.48	1.41
2	B	701	FAD	C5A-C6A	2.59	1.48	1.41
3	A	702	NAP	C5A-C6A	2.59	1.48	1.41
2	A	701	FAD	C5A-N7A	-2.52	1.34	1.39
3	B	702	NAP	C5A-N7A	-2.46	1.34	1.39
2	A	701	FAD	C5X-N5	-2.44	1.35	1.39
2	B	701	FAD	C5A-N7A	-2.34	1.34	1.39
3	A	702	NAP	C5A-N7A	-2.29	1.34	1.39
2	A	701	FAD	C4A-N9A	-2.26	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NAP	C8A-N7A	2.26	1.36	1.31
2	B	701	FAD	C8A-N7A	2.25	1.36	1.31
3	A	702	NAP	C4A-N9A	-2.21	1.33	1.37
2	A	701	FAD	C2-N3	-2.18	1.34	1.39
2	B	701	FAD	C5X-N5	-2.17	1.35	1.39
2	B	701	FAD	C2-N3	-2.15	1.34	1.39
3	B	702	NAP	C8A-N7A	2.14	1.35	1.31
2	A	701	FAD	C8A-N7A	2.13	1.35	1.31
2	A	701	FAD	C8A-N9A	-2.12	1.33	1.37
2	B	701	FAD	C4X-N5	2.03	1.35	1.30

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NAP	C5A-C4A-N3A	-5.93	118.55	126.72
2	B	701	FAD	C5A-C4A-N3A	-5.80	118.74	126.72
2	A	701	FAD	C5A-C4A-N3A	-5.78	118.76	126.72
3	A	702	NAP	C5A-C4A-N3A	-5.42	119.26	126.72
2	B	701	FAD	N3A-C4A-N9A	4.79	135.32	127.17
3	B	702	NAP	N3A-C4A-N9A	4.74	135.23	127.17
2	A	701	FAD	N3A-C4A-N9A	4.48	134.79	127.17
3	A	702	NAP	N3A-C4A-N9A	4.39	134.63	127.17
2	A	701	FAD	C4A-C5A-N7A	-3.78	106.26	110.58
2	A	701	FAD	C2A-N3A-C4A	3.75	120.98	111.83
2	A	701	FAD	C4'-C3'-C2'	-3.69	107.43	113.57
3	B	702	NAP	C2A-N3A-C4A	3.66	120.77	111.83
2	B	701	FAD	C2A-N3A-C4A	3.55	120.51	111.83
3	A	702	NAP	C2A-N3A-C4A	3.53	120.46	111.83
3	A	702	NAP	C4A-C5A-N7A	-3.39	106.71	110.58
2	B	701	FAD	C4A-C5A-N7A	-3.35	106.76	110.58
2	A	701	FAD	N3A-C2A-N1A	-3.30	123.58	128.58
3	B	702	NAP	C4A-C5A-N7A	-3.25	106.87	110.58
3	A	702	NAP	C4A-N9A-C8A	3.18	109.07	105.74
3	A	702	NAP	N3A-C2A-N1A	-3.17	123.78	128.58
3	B	702	NAP	C2B-C1B-N9A	-3.17	108.53	113.75
2	B	701	FAD	C4-C4X-N5	3.16	122.57	118.21
2	B	701	FAD	C4A-N9A-C8A	3.16	109.05	105.74
3	B	702	NAP	N3A-C2A-N1A	-3.02	124.00	128.58
2	A	701	FAD	C4A-N9A-C8A	2.99	108.87	105.74
2	B	701	FAD	N3A-C2A-N1A	-2.95	124.12	128.58
2	A	701	FAD	C4X-C10-N1	-2.80	117.72	124.59
2	A	701	FAD	C5A-N7A-C8A	2.71	107.71	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	FAD	C5X-C9A-N10	2.61	120.33	117.97
2	B	701	FAD	C5A-N7A-C8A	2.57	107.49	103.45
6	A	705	GOL	O3-C3-C2	-2.54	98.95	110.38
3	A	702	NAP	C5A-N7A-C8A	2.51	107.39	103.45
2	A	701	FAD	O4-C4-C4X	-2.50	119.93	126.53
5	A	704	GEE	O-C-CA	2.49	125.26	118.99
3	A	702	NAP	C4D-O4D-C1D	-2.39	107.74	109.92
2	A	701	FAD	C10-N1-C2	2.38	121.99	116.85
3	B	702	NAP	C4A-N9A-C8A	2.35	108.20	105.74
2	A	701	FAD	C6A-C5A-N7A	2.32	136.56	132.09
2	A	701	FAD	N9A-C8A-N7A	-2.28	110.70	113.94
3	A	702	NAP	N9A-C8A-N7A	-2.27	110.72	113.94
2	B	701	FAD	C4X-C10-N10	2.27	119.72	116.48
3	B	702	NAP	C5A-N7A-C8A	2.25	106.99	103.45
2	B	701	FAD	N9A-C8A-N7A	-2.24	110.76	113.94
2	A	701	FAD	C4X-C4-N3	2.19	118.82	113.25
3	A	702	NAP	C6A-C5A-N7A	2.19	136.31	132.09
2	B	701	FAD	C4X-C10-N1	-2.18	119.25	124.59
2	B	701	FAD	C4X-C4-N3	2.17	118.78	113.25
2	B	701	FAD	O4B-C1B-N9A	2.15	112.23	108.09
2	A	701	FAD	C4-N3-C2	-2.11	121.90	125.64
2	B	701	FAD	O4-C4-C4X	-2.08	121.03	126.53
2	A	701	FAD	C4-C4X-N5	2.06	121.05	118.21

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	C2'-C1'-N10-C10
2	A	701	FAD	N10-C1'-C2'-O2'
2	A	701	FAD	N10-C1'-C2'-C3'
2	A	701	FAD	C2'-C3'-C4'-O4'
2	A	701	FAD	O3'-C3'-C4'-O4'
2	A	701	FAD	O3'-C3'-C4'-C5'
2	A	701	FAD	PA-O3P-P-O5'
2	B	701	FAD	C5B-O5B-PA-O2A
2	B	701	FAD	C5B-O5B-PA-O3P
2	B	701	FAD	C5'-O5'-P-O3P
3	B	702	NAP	C5B-O5B-PA-O1A
3	B	702	NAP	C5B-O5B-PA-O3
3	B	702	NAP	C3B-C4B-C5B-O5B
3	B	702	NAP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	B	702	NAP	C2N-C3N-C7N-O7N
3	B	702	NAP	C2N-C3N-C7N-N7N
5	A	704	GEE	CA-C-O1-C1
5	A	704	GEE	O-C-CA-N
6	A	705	GOL	C1-C2-C3-O3
3	B	702	NAP	C4N-C3N-C7N-N7N
3	B	702	NAP	C4N-C3N-C7N-O7N
2	A	701	FAD	C2'-C3'-C4'-C5'
3	A	702	NAP	C4D-C5D-O5D-PN
5	A	704	GEE	O1-C-CA-N
5	A	704	GEE	O-C-O1-C1
3	B	702	NAP	O4B-C4B-C5B-O5B
3	A	702	NAP	C3D-C4D-C5D-O5D
6	A	705	GOL	O2-C2-C3-O3
3	A	702	NAP	C2N-C3N-C7N-O7N
3	B	702	NAP	C4D-C5D-O5D-PN
2	B	701	FAD	PA-O3P-P-O5'
3	A	702	NAP	C2N-C3N-C7N-N7N
3	A	702	NAP	O4D-C4D-C5D-O5D
3	B	702	NAP	C4B-C5B-O5B-PA
2	B	701	FAD	C5'-O5'-P-O1P
3	A	702	NAP	C5D-O5D-PN-O3
3	B	702	NAP	C5D-O5D-PN-O1N
3	A	702	NAP	C4N-C3N-C7N-N7N
3	A	702	NAP	C4N-C3N-C7N-O7N
3	B	702	NAP	O4D-C1D-N1N-C2N
3	B	702	NAP	C2B-O2B-P2B-O1X
3	A	702	NAP	O4B-C4B-C5B-O5B
2	B	701	FAD	P-O3P-PA-O2A
2	B	701	FAD	P-O3P-PA-O1A
3	A	702	NAP	PN-O3-PA-O2A

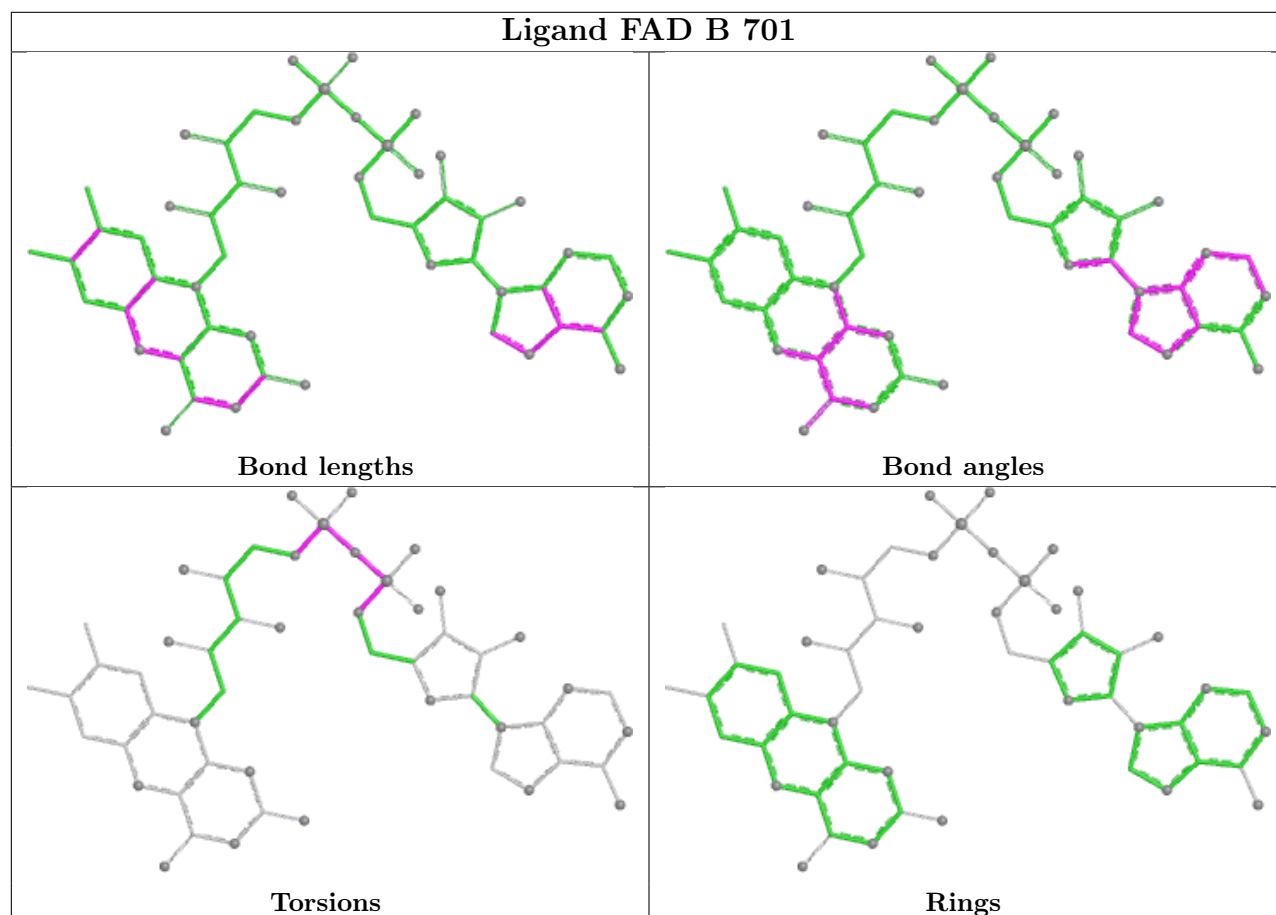
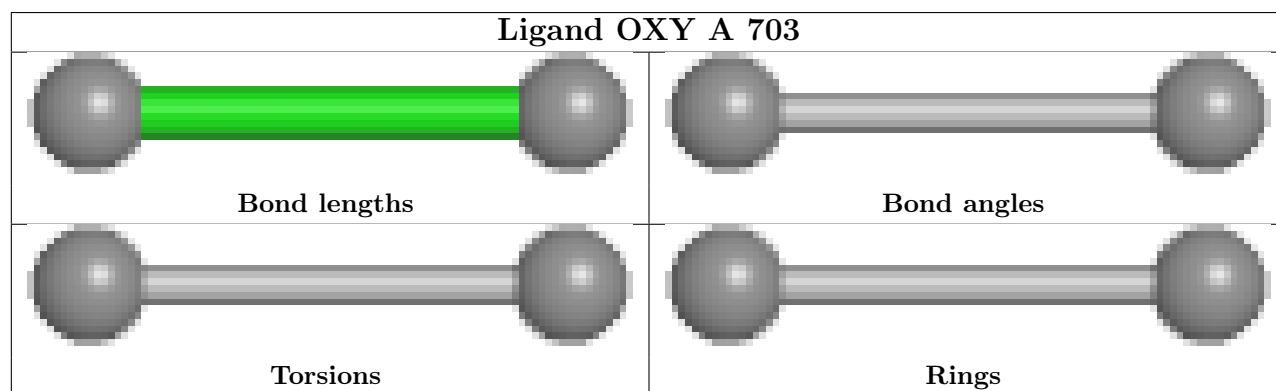
There are no ring outliers.

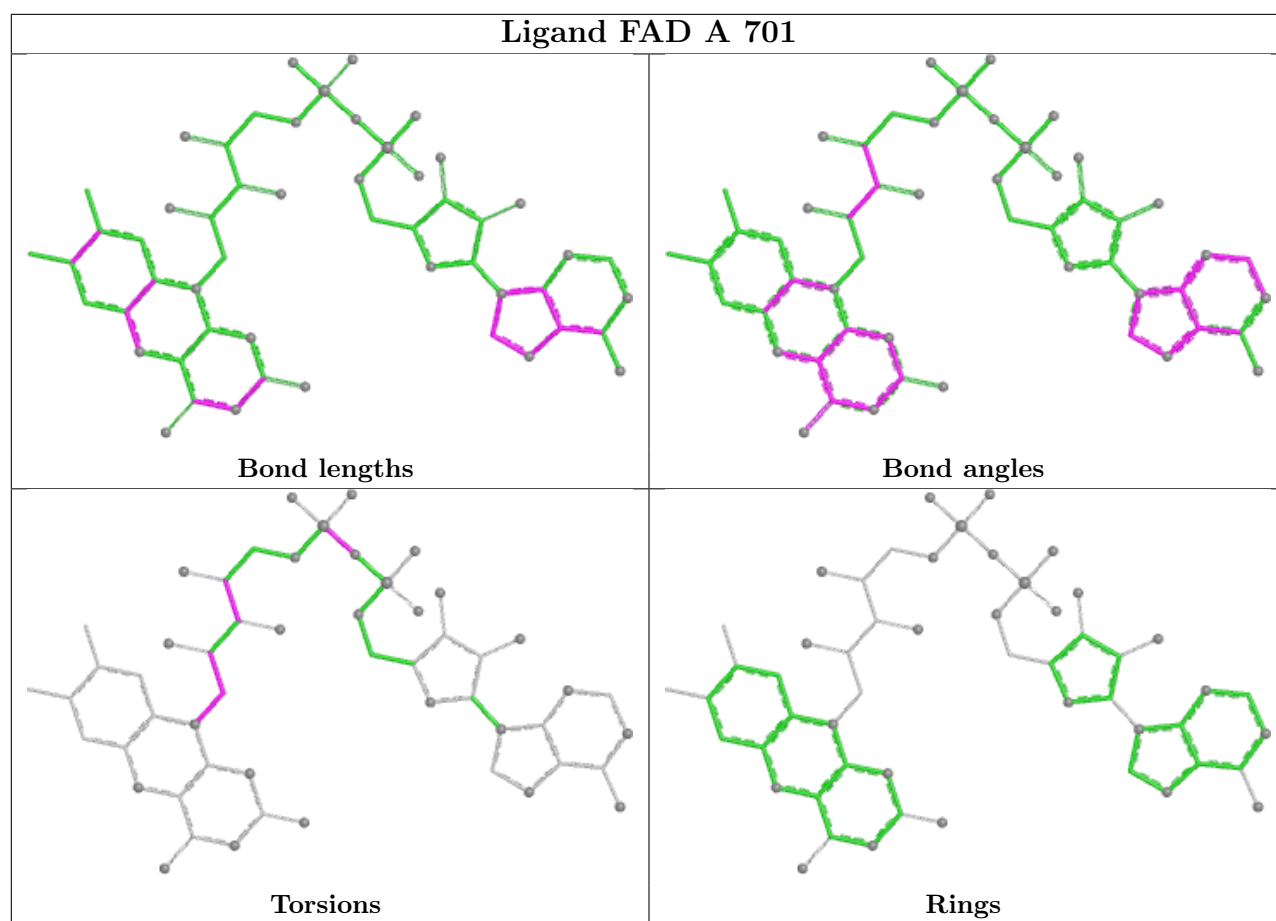
4 monomers are involved in 7 short contacts:

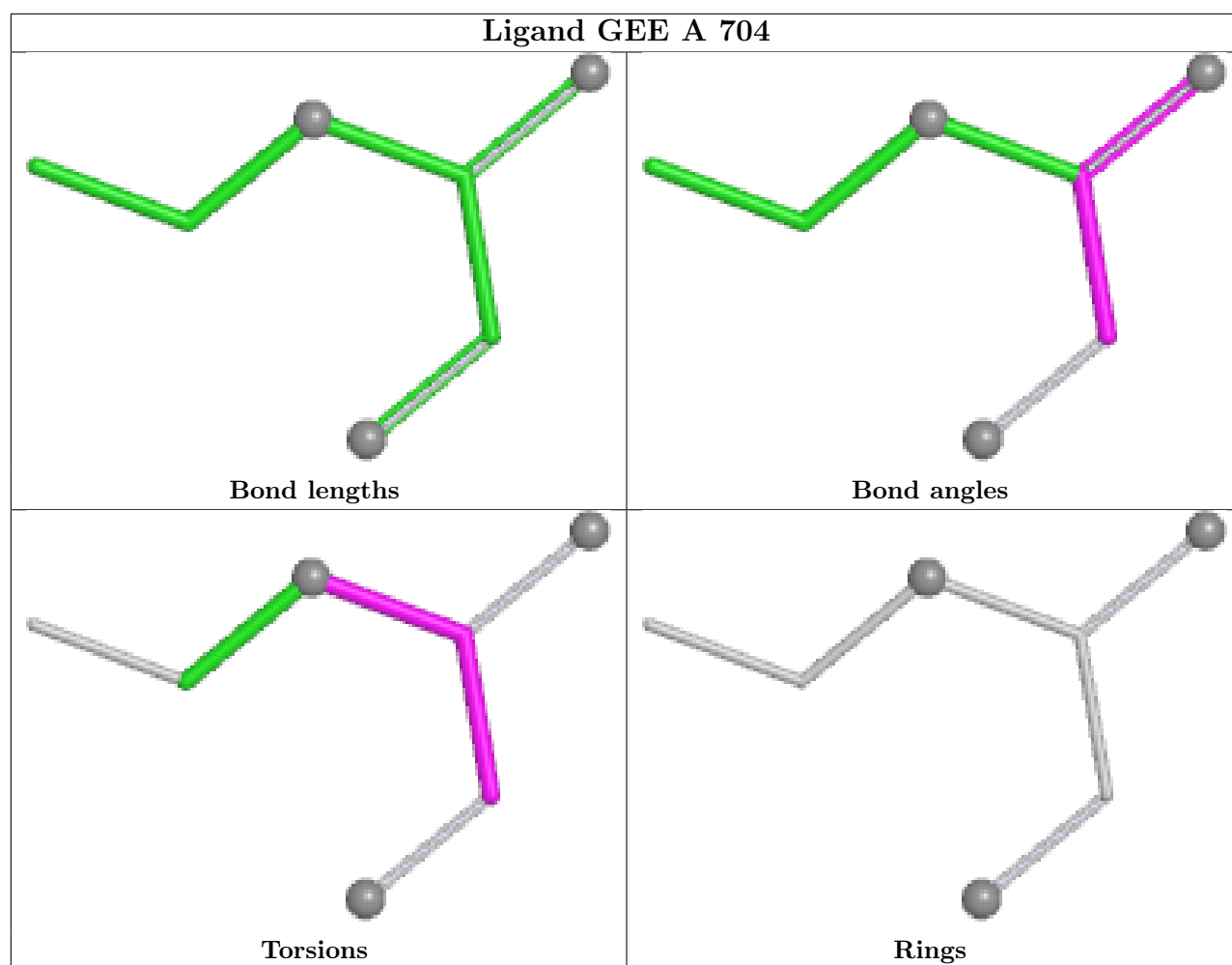
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FAD	3	0
5	A	704	GEE	1	0
3	A	702	NAP	2	0
6	A	705	GOL	1	0

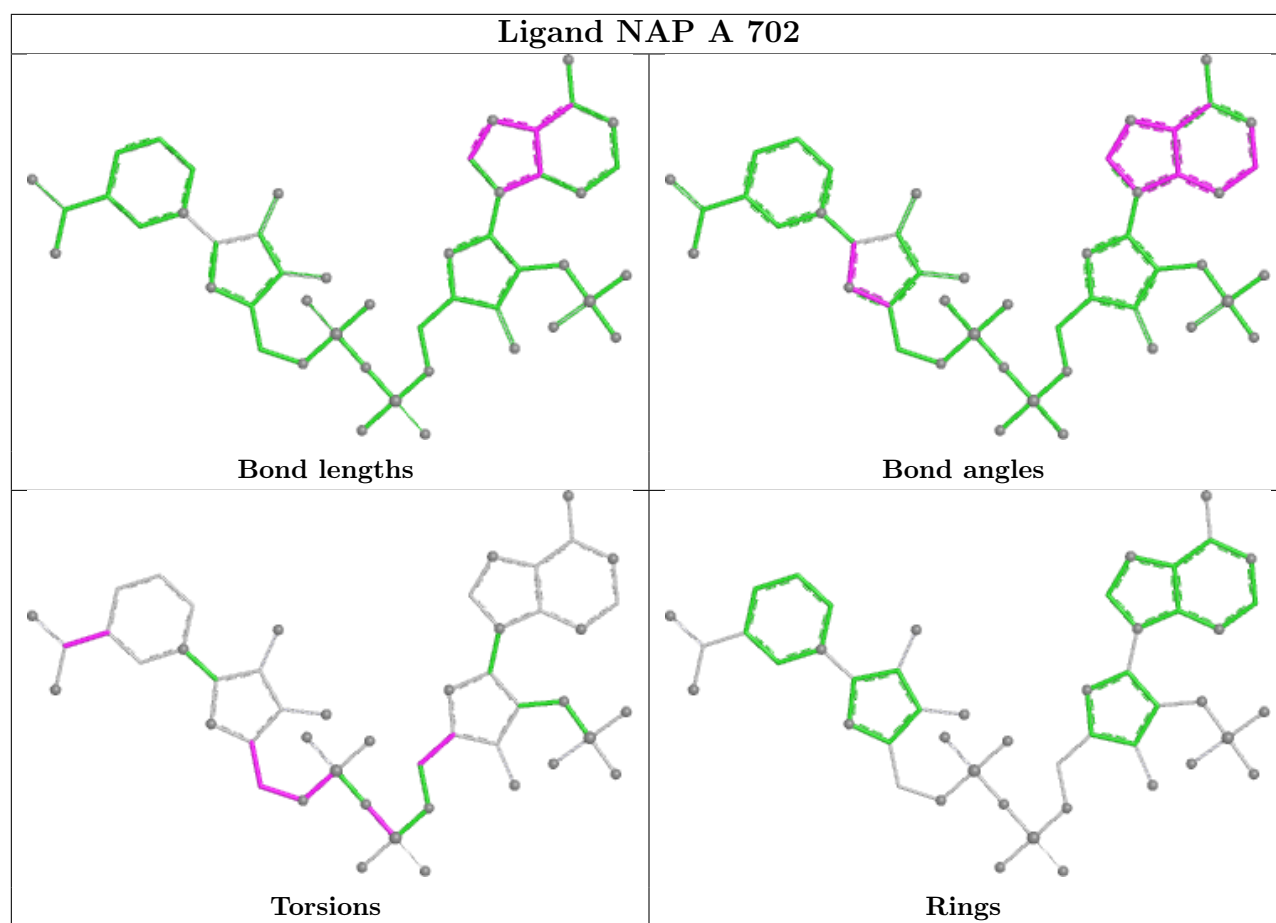
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

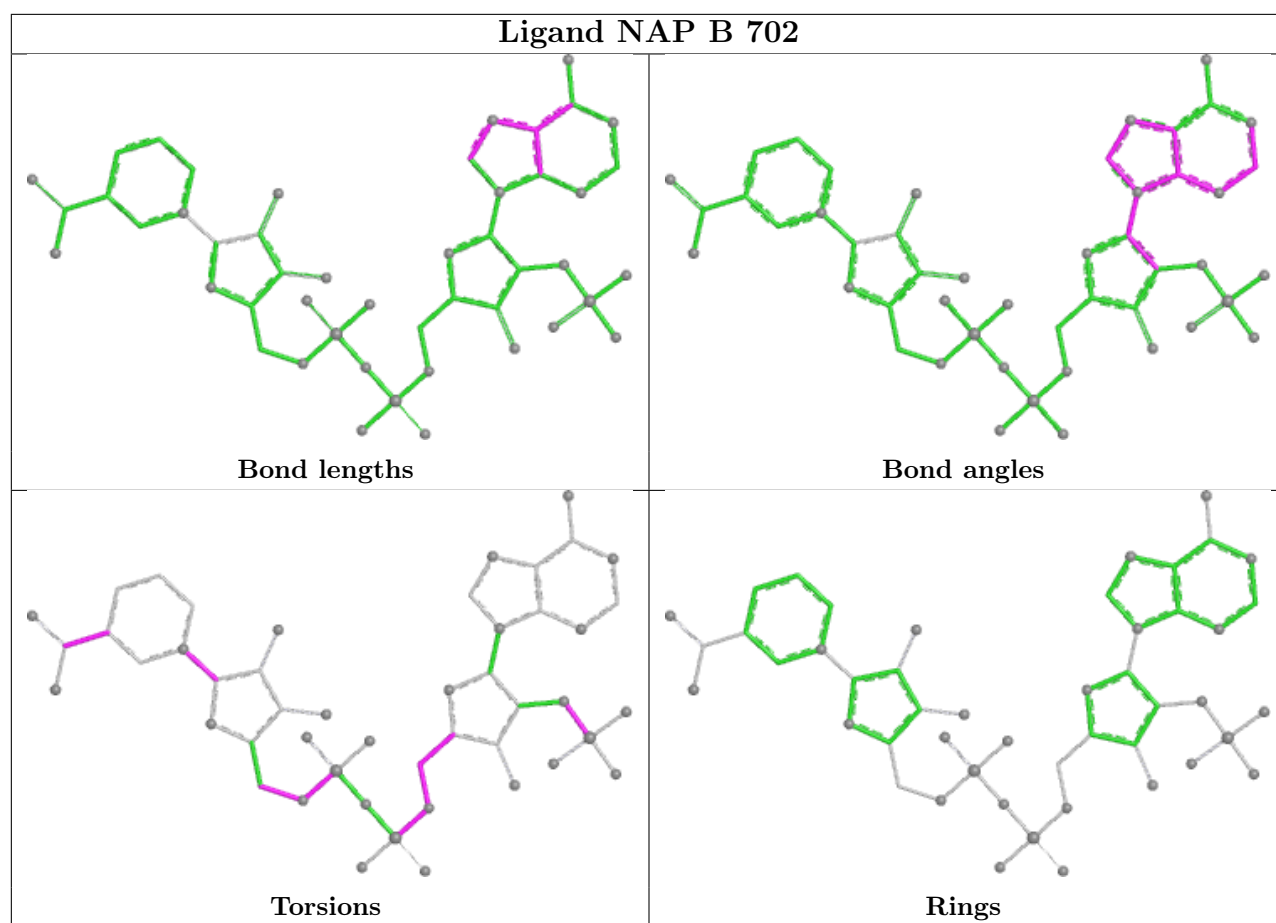
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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	612/639 (95%)	-0.00	20 (3%)	49	28	23, 43, 79, 137	24 (3%)
1	B	556/639 (87%)	2.44	316 (56%)	0	0	5, 24, 42, 131	553 (99%)
All	All	1168/1278 (91%)	1.16	336 (28%)	1	1	5, 34, 72, 137	577 (49%)

All (336) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407	GLU	8.9
1	B	574	ASP	8.8
1	B	165	GLN	7.8
1	B	51	TRP	7.3
1	B	182	PHE	7.3
1	B	322	ILE	7.0
1	B	579	THR	6.7
1	B	18	ILE	6.3
1	B	408	GLY	6.3
1	B	605	TYR	6.2
1	B	482	GLN	6.2
1	B	208	SER	6.2
1	B	318	HIS	6.1
1	B	351	MET	6.0
1	B	328	CYS	6.0
1	B	577	GLN	5.9
1	B	479	HIS	5.8
1	B	618	THR	5.8
1	B	316	GLY	5.8
1	B	476	GLN	5.7
1	B	400	GLU	5.6
1	B	405	ALA	5.6
1	B	424	LEU	5.6
1	B	48	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	619	THR	5.5
1	B	310	CYS	5.4
1	B	150	GLY	5.3
1	B	524	ILE	5.3
1	B	331	TYR	5.3
1	B	19	GLY	5.2
1	B	120	VAL	5.1
1	B	205	HIS	5.1
1	B	442	ASN	5.0
1	B	379	LEU	5.0
1	B	626	PHE	4.9
1	B	118	ILE	4.9
1	B	45	SER	4.9
1	B	567	MET	4.9
1	B	477	GLY	4.9
1	B	403	HIS	4.9
1	B	325	VAL	4.9
1	B	510	GLN	4.8
1	A	11	THR	4.8
1	B	123	HIS	4.8
1	B	596	ALA	4.8
1	B	171	LEU	4.8
1	B	300	GLU	4.8
1	B	152	TYR	4.8
1	B	305	PHE	4.7
1	A	445	SER	4.7
1	B	586	ASP	4.6
1	B	480	ASP	4.6
1	B	620	LEU	4.6
1	A	243	ASP	4.6
1	B	585	SER	4.5
1	B	75	PHE	4.5
1	B	321	ASN	4.5
1	B	97	TYR	4.5
1	B	287	ILE	4.5
1	B	587	TYR	4.5
1	B	584	LEU	4.5
1	B	211	PHE	4.5
1	B	517	GLN	4.4
1	B	185	LYS	4.4
1	B	624	THR	4.4
1	B	324	MET	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	41	TYR	4.2
1	B	355	TYR	4.2
1	B	478	GLU	4.2
1	B	376	LEU	4.1
1	B	279	PHE	4.1
1	B	183	ALA	4.1
1	B	360	SER	4.1
1	B	278	PRO	4.1
1	B	369	ASN	4.1
1	B	181	ILE	4.1
1	B	299	VAL	4.1
1	B	576	GLY	4.1
1	B	622	ALA	4.0
1	B	573	LEU	4.0
1	B	307	GLY	4.0
1	B	306	THR	4.0
1	B	374	GLY	3.9
1	B	617	TYR	3.9
1	B	122	GLU	3.9
1	A	636	PRO	3.9
1	B	263	GLN	3.9
1	B	215	ARG	3.9
1	B	345	MET	3.9
1	B	528	TRP	3.9
1	B	124	GLY	3.8
1	B	272	GLU	3.8
1	B	273	ASP	3.8
1	B	40	ILE	3.8
1	B	117	ILE	3.8
1	B	372	THR	3.8
1	B	582	ARG	3.8
1	B	166	PHE	3.7
1	B	204	SER	3.7
1	B	249	GLU	3.7
1	B	410	ILE	3.7
1	B	367	LEU	3.7
1	B	214	MET	3.7
1	B	16	CYS	3.7
1	B	353	LEU	3.7
1	B	176	TYR	3.7
1	B	575	VAL	3.7
1	B	533	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	46	VAL	3.6
1	B	175	GLN	3.6
1	B	161	PRO	3.6
1	B	240	ILE	3.6
1	B	317	THR	3.6
1	B	500	GLN	3.6
1	B	506	GLN	3.6
1	B	190	ILE	3.6
1	B	583	HIS	3.5
1	B	115	SER	3.5
1	B	443	TYR	3.5
1	B	475	GLN	3.5
1	B	178	ASP	3.5
1	B	264	LYS	3.4
1	B	569	GLN	3.4
1	B	22	PRO	3.4
1	B	311	ILE	3.4
1	B	326	VAL	3.4
1	B	246	ILE	3.4
1	B	184	GLY	3.4
1	B	121	THR	3.4
1	B	138	GLN	3.3
1	B	212	TRP	3.3
1	B	359	PRO	3.3
1	B	177	TYR	3.3
1	B	346	ARG	3.3
1	B	386	TYR	3.2
1	A	519	CYS	3.2
1	B	284	ASP	3.2
1	B	159	THR	3.2
1	B	343	PHE	3.2
1	B	589	PHE	3.2
1	B	526	LEU	3.2
1	B	189	VAL	3.2
1	B	610	GLN	3.2
1	B	151	ARG	3.2
1	B	157	ILE	3.2
1	B	20	ALA	3.2
1	B	370	VAL	3.1
1	B	601	ILE	3.1
1	B	297	THR	3.1
1	B	174	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	402	ASN	3.1
1	B	319	ILE	3.1
1	A	560	GLN	3.1
1	B	21	GLY	3.1
1	B	301	ASP	3.1
1	B	348	ASP	3.1
1	B	602	THR	3.1
1	B	313	SER	3.1
1	B	481	SER	3.1
1	A	635	GLN	3.1
1	B	217	LEU	3.1
1	B	274	PHE	3.1
1	B	62	TYR	3.1
1	B	368	GLN	3.0
1	B	162	GLY	3.0
1	B	23	ALA	3.0
1	B	277	ASN	3.0
1	A	335	GLN	3.0
1	A	244	ASN	3.0
1	B	196	GLY	3.0
1	B	529	ASP	3.0
1	B	52	ASN	3.0
1	B	170	VAL	2.9
1	B	312	PHE	2.9
1	B	302	ILE	2.9
1	B	494	LEU	2.9
1	B	74	SER	2.9
1	B	186	ARG	2.9
1	B	578	ILE	2.9
1	B	188	LEU	2.9
1	B	621	LYS	2.9
1	B	364	THR	2.9
1	B	486	VAL	2.9
1	B	513	TYR	2.9
1	B	127	TRP	2.9
1	B	126	GLN	2.8
1	B	531	GLN	2.8
1	A	473	LEU	2.8
1	B	141	TYR	2.8
1	B	445	SER	2.8
1	B	156	PHE	2.8
1	B	288	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	435	GLN	2.8
1	B	536	VAL	2.8
1	B	207	ALA	2.8
1	B	167	GLN	2.8
1	B	200	ALA	2.8
1	B	504	ALA	2.8
1	B	505	ARG	2.8
1	B	221	LEU	2.8
1	B	566	LEU	2.8
1	B	333	ASN	2.7
1	B	335	GLN	2.7
1	B	131	ILE	2.7
1	B	591	SER	2.7
1	B	604	GLU	2.7
1	B	95	ARG	2.7
1	B	498	VAL	2.7
1	B	323	ASP	2.7
1	B	514	LEU	2.7
1	B	158	PRO	2.7
1	B	270	SER	2.7
1	B	94	VAL	2.7
1	B	209	ALA	2.6
1	B	149	HIS	2.6
1	B	114	ASN	2.6
1	B	275	ARG	2.6
1	B	371	GLY	2.6
1	B	42	GLU	2.6
1	B	201	GLU	2.6
1	B	340	VAL	2.6
1	B	613	VAL	2.6
1	B	508	ILE	2.6
1	B	137	GLN	2.6
1	B	24	GLY	2.6
1	A	624	THR	2.6
1	B	291	ALA	2.6
1	A	246	ILE	2.6
1	B	417	ASN	2.6
1	B	286	VAL	2.6
1	B	237	ASN	2.6
1	B	363	ASN	2.6
1	B	163	LEU	2.6
1	B	109	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	206	VAL	2.5
1	B	608	ARG	2.5
1	B	597	PHE	2.5
1	B	401	LEU	2.5
1	B	308	ARG	2.5
1	B	91	VAL	2.5
1	B	125	ASP	2.5
1	B	164	ASP	2.5
1	B	415	LEU	2.5
1	B	132	GLY	2.5
1	A	139	THR	2.5
1	B	84	THR	2.5
1	B	511	GLU	2.5
1	B	113	TYR	2.5
1	B	432	THR	2.4
1	B	535	PRO	2.4
1	B	265	SER	2.4
1	B	483	LEU	2.4
1	B	490	LEU	2.4
1	B	625	ASP	2.4
1	A	531	GLN	2.4
1	B	67	PHE	2.4
1	B	173	SER	2.4
1	B	468	SER	2.4
1	B	32	LEU	2.4
1	B	43	THR	2.4
1	B	112	HIS	2.4
1	B	314	ALA	2.4
1	B	465	LEU	2.4
1	B	377	PRO	2.4
1	B	69	ASN	2.4
1	B	119	ALA	2.4
1	A	591	SER	2.4
1	B	30	SER	2.4
1	B	244	ASN	2.3
1	B	436	ALA	2.3
1	B	191	GLY	2.3
1	B	129	VAL	2.3
1	B	599	ARG	2.3
1	B	329	THR	2.3
1	B	268	PHE	2.3
1	B	143	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	128	LYS	2.3
1	B	358	ASN	2.3
1	B	140	ARG	2.3
1	A	247	ILE	2.3
1	B	416	ALA	2.3
1	B	192	ASN	2.3
1	B	489	ARG	2.3
1	B	303	GLU	2.2
1	B	295	ILE	2.2
1	B	236	ALA	2.2
1	B	473	LEU	2.2
1	B	488	HIS	2.2
1	B	254	SER	2.2
1	B	603	ASP	2.2
1	B	614	PHE	2.2
1	B	373	THR	2.2
1	B	144	GLY	2.2
1	B	444	PRO	2.2
1	B	375	THR	2.2
1	B	50	ILE	2.2
1	B	327	LEU	2.2
1	B	512	GLU	2.2
1	B	609	LEU	2.2
1	B	38	PRO	2.2
1	B	350	ALA	2.2
1	B	76	PHE	2.2
1	B	73	THR	2.2
1	B	39	VAL	2.2
1	B	491	LEU	2.2
1	B	320	GLU	2.2
1	B	332	ASP	2.2
1	B	485	THR	2.1
1	B	276	ALA	2.1
1	B	14	ARG	2.1
1	B	26	VAL	2.1
1	B	145	VAL	2.1
1	B	210	VAL	2.1
1	B	565	GLU	2.1
1	B	259	TYR	2.1
1	B	598	SER	2.1
1	B	532	VAL	2.1
1	B	36	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	172	HIS	2.1
1	B	341	LYS	2.1
1	B	427	LEU	2.1
1	A	637	ALA	2.1
1	A	477	GLY	2.1
1	B	251	LEU	2.1
1	B	356	ARG	2.1
1	A	506	GLN	2.1
1	B	446	PHE	2.1
1	B	280	VAL	2.0
1	A	338	ASP	2.0
1	B	90	GLY	2.0
1	B	606	ASN	2.0
1	B	78	ASP	2.0
1	B	130	ASP	2.0
1	B	187	VAL	2.0
1	B	441	LEU	2.0
1	B	15	ILE	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
5	GEE	A	704	7/7	0.73	0.37	51,76,88,89	0
3	NAP	B	702	48/48	0.74	0.23	29,76,97,112	48
2	FAD	B	701	53/53	0.81	0.23	25,49,68,73	53
7	PO4	A	707	5/5	0.85	0.22	54,74,106,119	5
4	OXY	A	703	2/2	0.86	0.22	52,52,52,67	0

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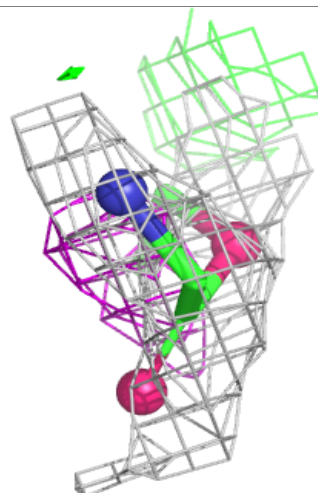
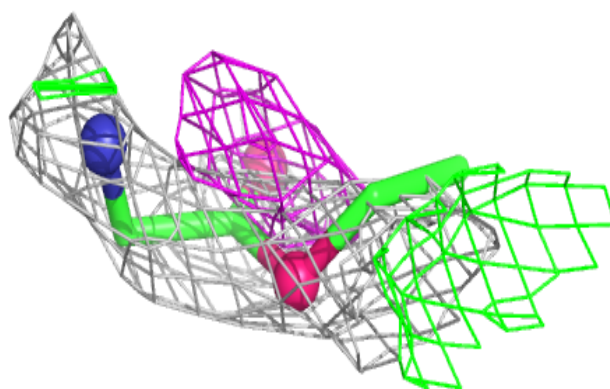
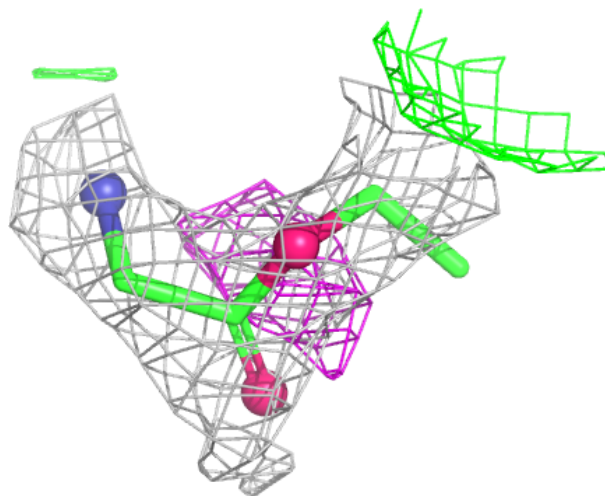
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PO4	A	709	5/5	0.87	0.22	31,43,78,115	5
7	PO4	A	708	5/5	0.92	0.09	37,42,97,98	5
7	PO4	A	706	5/5	0.92	0.17	25,48,71,88	5
3	NAP	A	702	48/48	0.93	0.16	25,45,63,76	25
2	FAD	A	701	53/53	0.97	0.07	17,31,46,50	0
6	GOL	A	705	6/6	0.97	0.09	23,31,34,53	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.

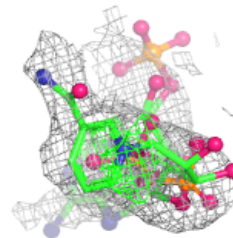
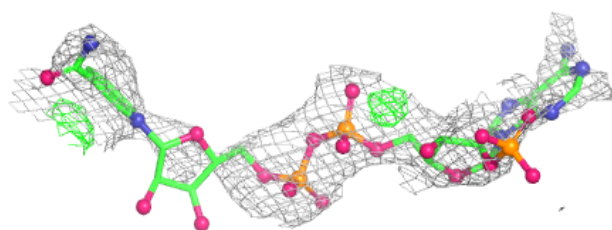
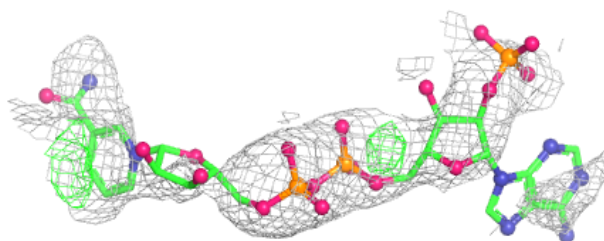
Electron density around GEE A 704:

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

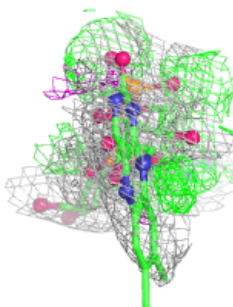
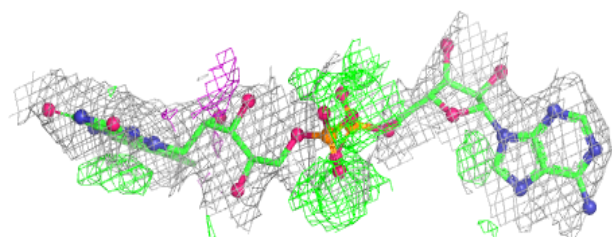
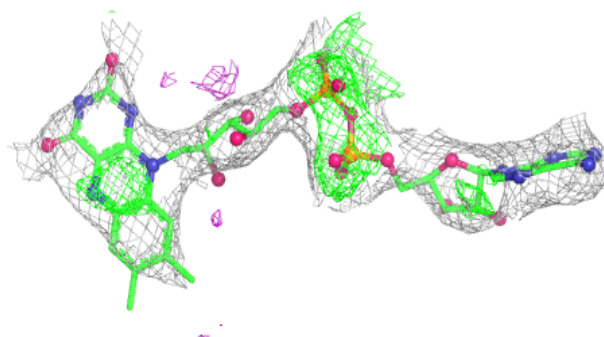


Electron density around NAP B 702:

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

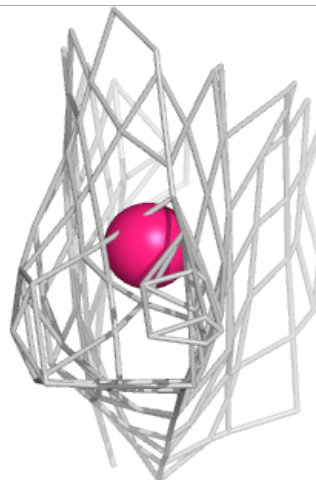
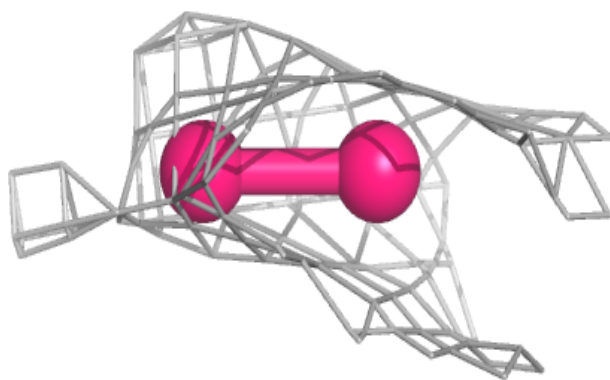
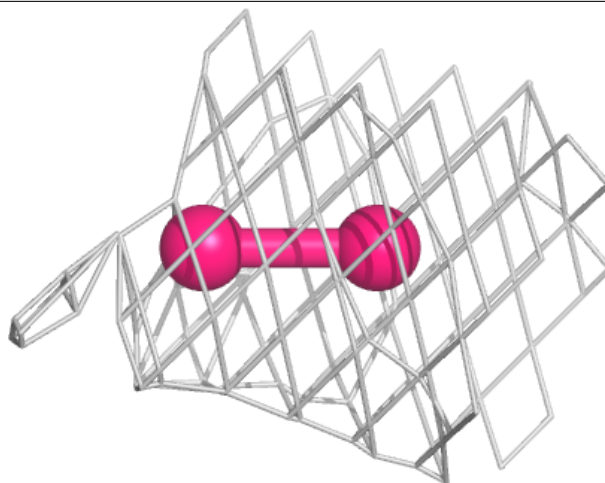
**Electron density around FAD B 701:**

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



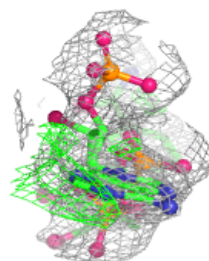
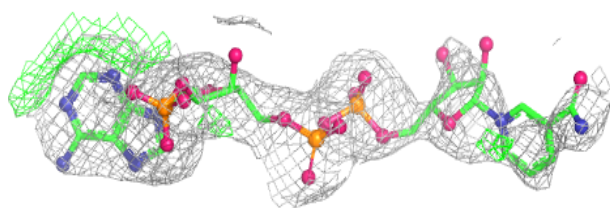
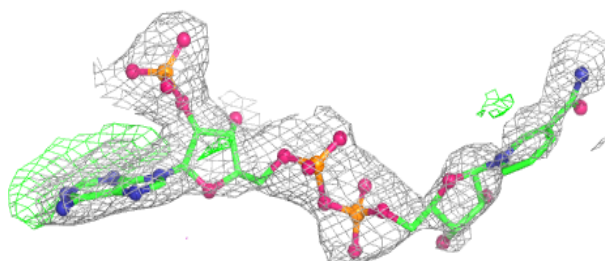
Electron density around OXY A 703:

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

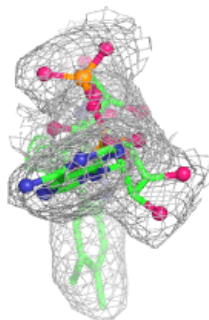
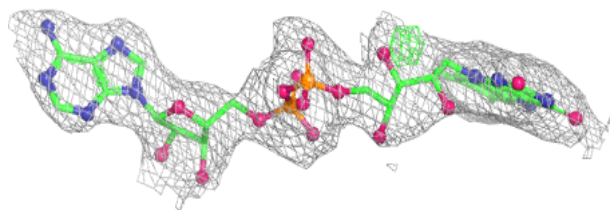
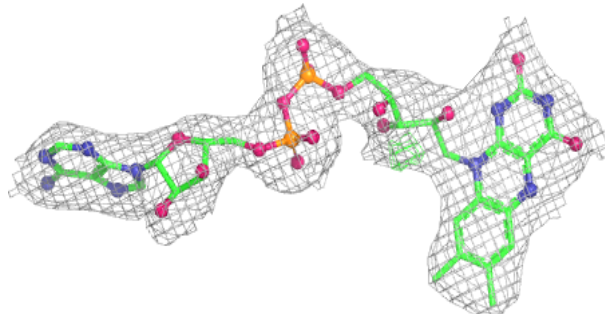


Electron density around NAP A 702:

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

**Electron density around FAD A 701:**

$2mF_o-DF_c$ (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.