Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:52 PM UTC

PDB ID	:	2VQ7 / pdb_00002vq7
Title	:	Bacterial flavin-containing monooxygenase in complex with NADP: native data
Authors	:	Alfieri, A.; Malito, E.; Orru, R.; Fraaije, M.W.; Mattevi, A.
Deposited on	:	2008-03-12
Resolution	:	2.60 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:

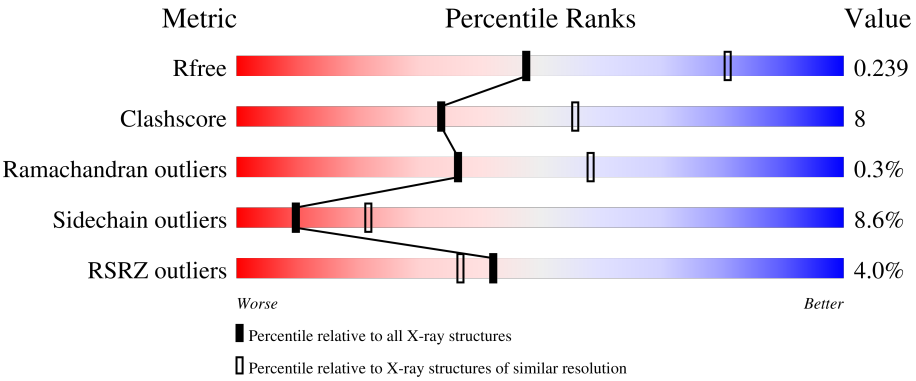
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	461	5% 77% 17%
1	B	461	4% 77% 16%
1	C	461	3% 77% 17%
1	D	461	3% 77% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EPE	C	1456	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15184 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.

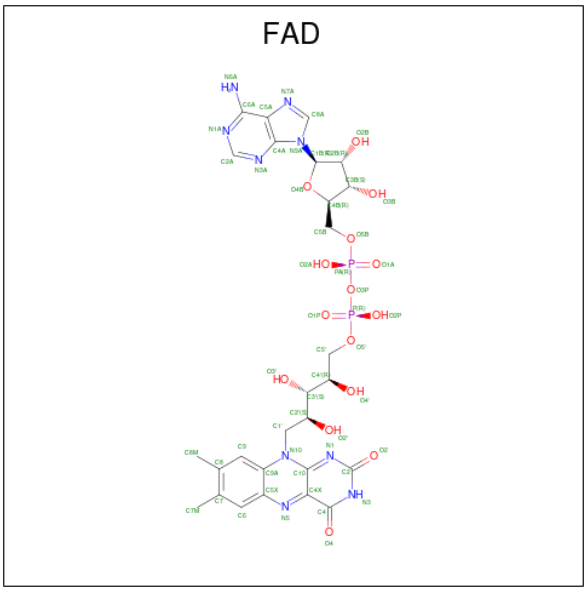
- Molecule 1 is a protein called FLAVIN-CONTAINING MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3638	2335	603	680	20			
1	B	443	Total	C	N	O	S	0	0	0
			3638	2335	603	680	20			
1	C	445	Total	C	N	O	S	0	0	0
			3655	2345	606	684	20			
1	D	443	Total	C	N	O	S	0	0	0
			3638	2335	603	680	20			

There are 8 discrepancies between the modelled and reference sequences:

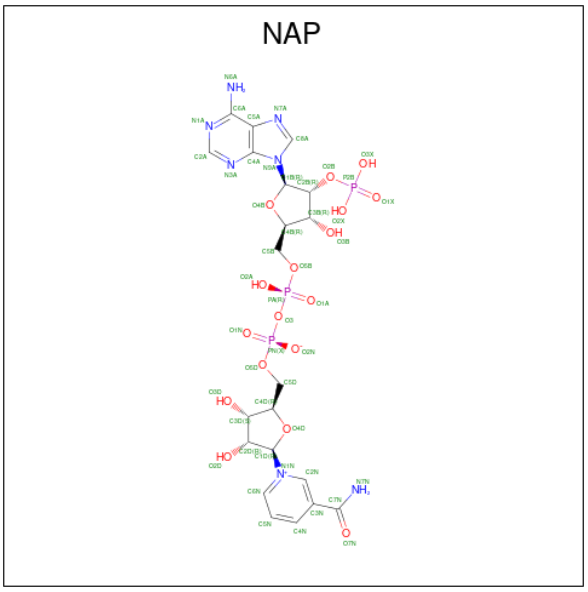
Chain	Residue	Modelled	Actual	Comment	Reference
A	158	ALA	GLU	engineered mutation	UNP Q83XK4
A	159	ALA	GLU	engineered mutation	UNP Q83XK4
B	158	ALA	GLU	engineered mutation	UNP Q83XK4
B	159	ALA	GLU	engineered mutation	UNP Q83XK4
C	158	ALA	GLU	engineered mutation	UNP Q83XK4
C	159	ALA	GLU	engineered mutation	UNP Q83XK4
D	158	ALA	GLU	engineered mutation	UNP Q83XK4
D	159	ALA	GLU	engineered mutation	UNP Q83XK4

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	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: $C_{21}H_{28}N_7O_{17}P_3$).

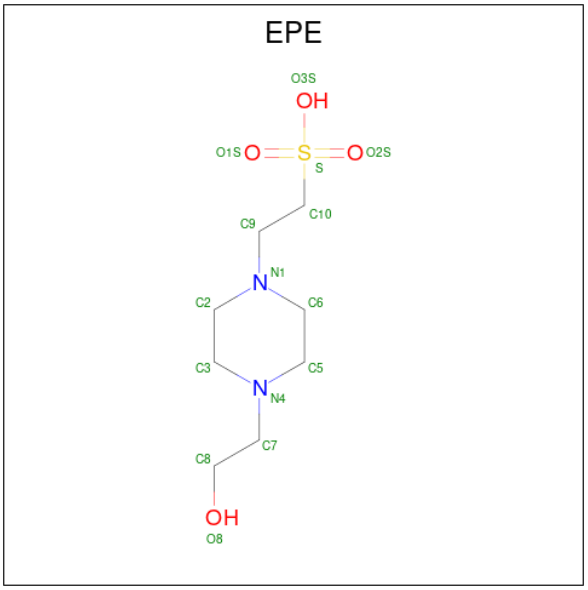


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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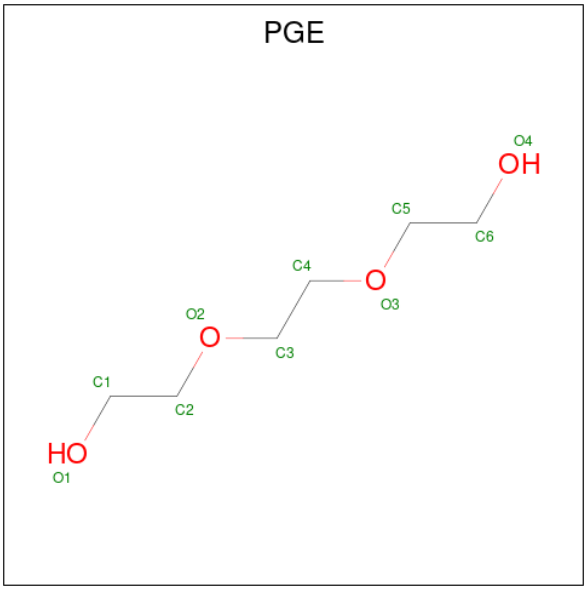
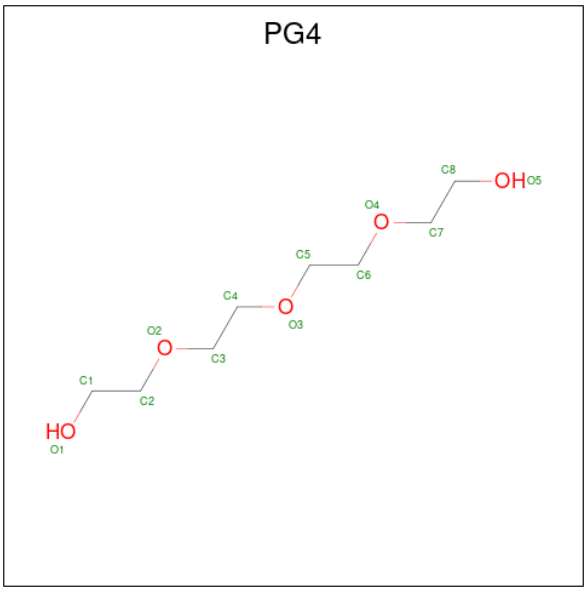
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 13 8 5	0	0

- Molecule 8 is water.

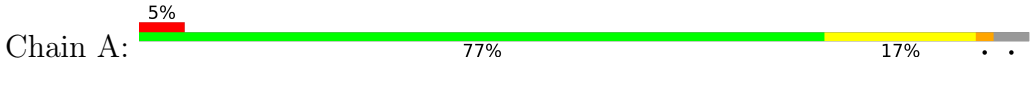
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	41	Total O 41 41	0	0
8	B	33	Total O 33 33	0	0
8	C	26	Total O 26 26	0	0
8	D	24	Total O 24 24	0	0

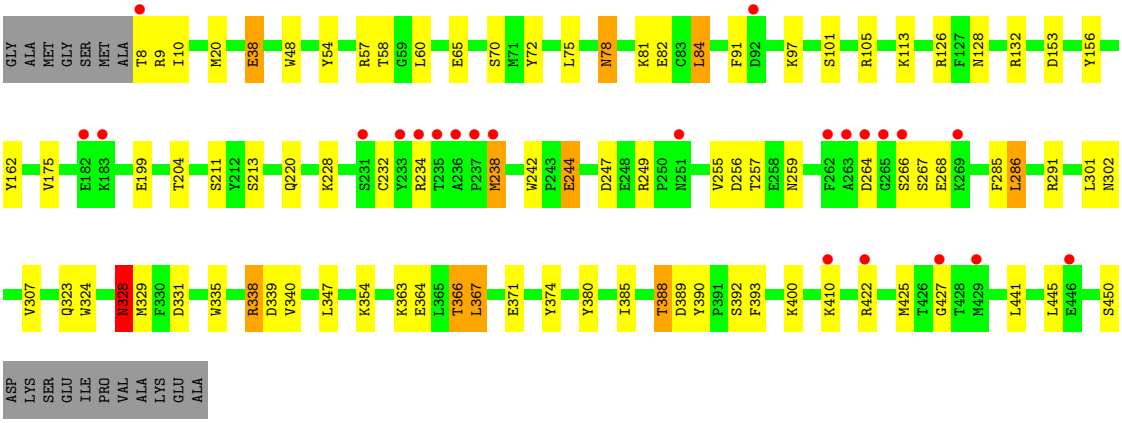
3 Residue-property plots (i)

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: FLAVIN-CONTAINING MONOOXYGENASE

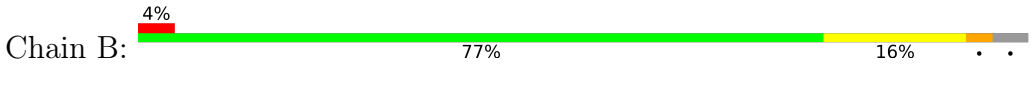
Chain A:

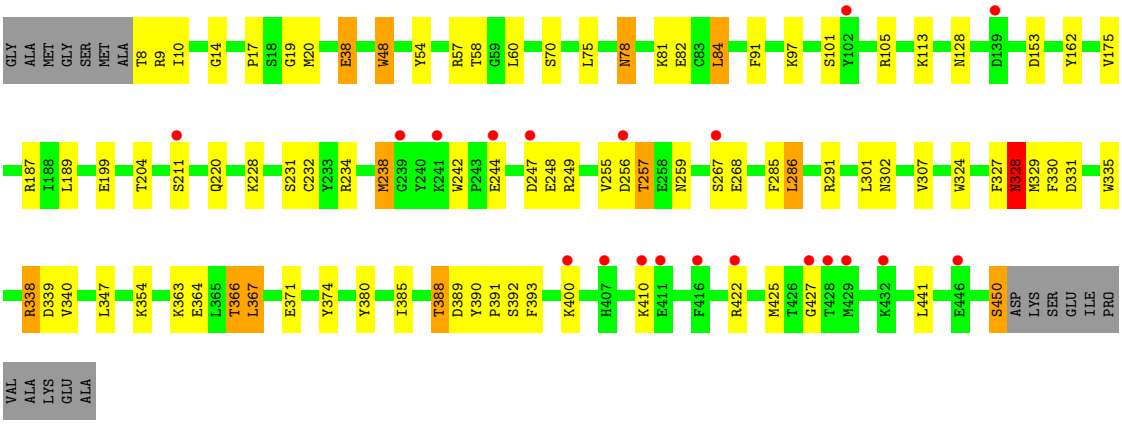




• Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

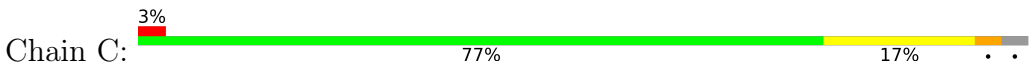
Chain B:

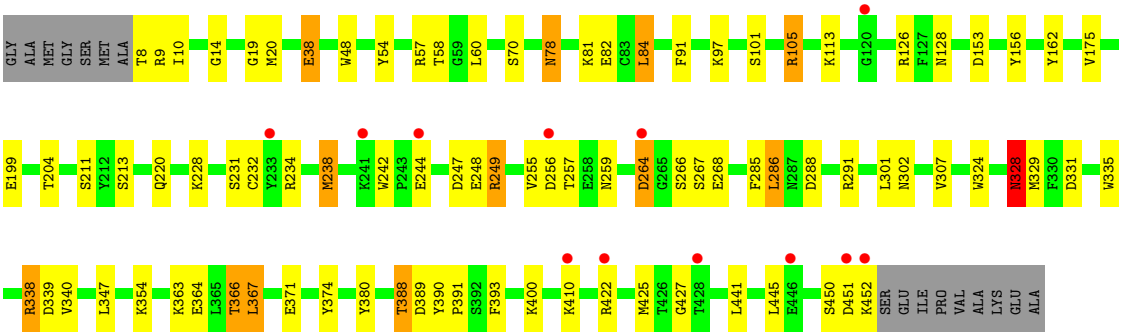




• Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

Chain C:

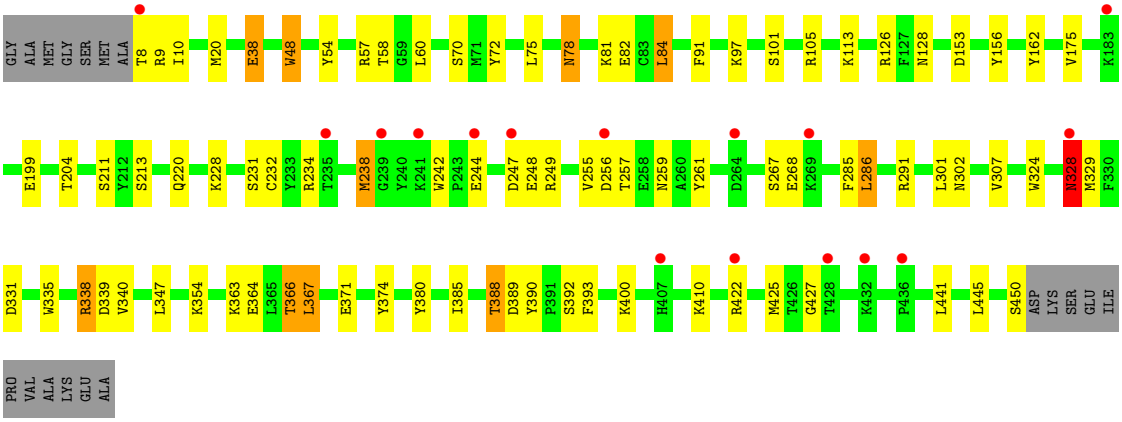




• Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	219.59Å 219.59Å 133.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	188.98 – 2.60 188.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.1 (188.98-2.60) 98.1 (188.98-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.248 , 0.269 0.227 , 0.239	Depositor DCC
R_{free} test set	5539 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	57.5	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 17.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.009 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15184	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.68	0/3752	0.87	3/5095 (0.1%)
1	B	0.69	0/3752	0.87	2/5095 (0.0%)
1	C	0.69	0/3769	0.88	2/5117 (0.0%)
1	D	0.66	0/3752	0.87	2/5095 (0.0%)
All	All	0.68	0/15025	0.87	9/20402 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	324	TRP	N-CA-C	-5.91	103.62	111.96
1	C	324	TRP	N-CA-C	-5.71	103.91	111.96
1	D	328	ASN	N-CA-CB	-5.65	100.93	110.49
1	B	324	TRP	N-CA-C	-5.56	104.12	111.96
1	D	324	TRP	N-CA-C	-5.51	104.19	111.96
1	C	328	ASN	N-CA-CB	-5.28	101.56	110.49
1	A	323	GLN	N-CA-C	5.17	117.07	108.02
1	A	328	ASN	N-CA-CB	-5.13	101.82	110.49
1	B	328	ASN	N-CA-CB	-5.08	101.90	110.49

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	3638	0	3428	57	0
1	B	3638	0	3428	58	0
1	C	3655	0	3445	56	0
1	D	3638	0	3428	52	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0
2	C	53	0	31	1	0
2	D	53	0	31	2	0
3	A	48	0	25	3	0
3	B	48	0	25	1	0
3	C	48	0	25	2	0
3	D	48	0	25	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	30	0	35	10	0
5	C	15	0	17	8	0
5	D	15	0	18	6	0
6	A	10	0	14	0	0
7	B	13	0	18	0	0
8	A	41	0	0	3	0
8	B	33	0	0	2	0
8	C	26	0	0	1	0
8	D	24	0	0	1	0
All	All	15184	0	14055	224	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 8.

All (224) 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)
5:A:1454:EPE:H51	5:A:1454:EPE:O8	1.52	1.08
5:C:1456:EPE:O8	5:C:1456:EPE:C5	2.18	0.90
1:A:388:THR:HG22	1:A:390:TYR:H	1.38	0.88
5:C:1456:EPE:O8	5:C:1456:EPE:H52	1.71	0.88
1:C:388:THR:HG22	1:C:390:TYR:H	1.40	0.86
1:D:388:THR:HG22	1:D:390:TYR:H	1.43	0.81
1:D:285:PHE:CD1	1:D:286:LEU:HD13	2.16	0.81
1:A:390:TYR:O	8:A:2035:HOH:O	2.02	0.78
1:A:285:PHE:CD1	1:A:286:LEU:HD13	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:THR:HG22	1:B:390:TYR:H	1.48	0.76
1:B:285:PHE:CD1	1:B:286:LEU:HD13	2.22	0.75
1:C:285:PHE:CD1	1:C:286:LEU:HD13	2.21	0.75
1:B:390:TYR:O	8:B:2027:HOH:O	2.06	0.74
1:A:388:THR:CG2	1:A:390:TYR:H	2.00	0.72
1:B:57:ARG:NH2	1:C:175:VAL:O	2.22	0.72
1:C:388:THR:CG2	1:C:390:TYR:H	2.03	0.71
1:A:57:ARG:NH2	1:D:175:VAL:O	2.23	0.70
1:D:126:ARG:NH1	5:D:1454:EPE:H91	2.06	0.70
1:A:363:LYS:O	1:A:366:THR:HB	1.93	0.69
1:C:335:TRP:HB3	1:C:388:THR:HG21	1.75	0.69
1:B:175:VAL:O	1:C:57:ARG:NH2	2.26	0.68
1:B:20:MET:HE3	1:B:48:TRP:HB2	1.76	0.68
1:B:363:LYS:O	1:B:366:THR:HB	1.94	0.67
1:C:390:TYR:O	8:C:2024:HOH:O	2.11	0.67
1:D:363:LYS:O	1:D:366:THR:HB	1.95	0.66
1:D:388:THR:CG2	1:D:390:TYR:H	2.07	0.66
1:B:422:ARG:HD3	1:B:427:GLY:O	1.96	0.66
1:B:335:TRP:HB3	1:B:388:THR:HG21	1.78	0.65
1:A:256:ASP:HB3	1:A:259:ASN:H	1.61	0.65
1:C:363:LYS:O	1:C:366:THR:HB	1.96	0.65
1:D:20:MET:HE3	1:D:48:TRP:HB2	1.79	0.65
1:B:388:THR:CG2	1:B:390:TYR:H	2.09	0.65
1:C:422:ARG:HD3	1:C:427:GLY:O	1.96	0.65
1:D:256:ASP:HB3	1:D:259:ASN:H	1.62	0.64
1:A:175:VAL:O	1:D:57:ARG:NH2	2.30	0.64
5:A:1454:EPE:O8	5:A:1454:EPE:C5	2.40	0.64
1:B:256:ASP:HB3	1:B:259:ASN:H	1.62	0.64
1:D:425:MET:HE3	1:D:425:MET:HA	1.79	0.64
1:C:256:ASP:HB3	1:C:259:ASN:H	1.62	0.64
1:C:301:LEU:O	1:C:302:ASN:HB2	1.98	0.63
1:C:81:LYS:HG2	1:C:91:PHE:CE2	2.34	0.63
1:D:335:TRP:HB3	1:D:388:THR:HG21	1.78	0.63
1:A:81:LYS:HG2	1:A:91:PHE:CE2	2.34	0.62
1:A:335:TRP:HB3	1:A:388:THR:HG21	1.80	0.62
5:A:1455:EPE:O8	5:A:1455:EPE:H51	1.99	0.62
1:D:204:THR:HG23	1:D:228:LYS:HB3	1.81	0.62
1:D:422:ARG:HD3	1:D:427:GLY:O	2.00	0.61
1:B:81:LYS:HG2	1:B:91:PHE:CE2	2.35	0.61
1:A:20:MET:HE3	1:A:48:TRP:HB2	1.82	0.61
1:A:422:ARG:HD3	1:A:427:GLY:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:LYS:HG2	1:D:91:PHE:CE2	2.36	0.61
1:D:10:ILE:HD12	1:D:162:TYR:HB2	1.83	0.60
1:D:301:LEU:O	1:D:302:ASN:HB2	2.01	0.60
1:A:204:THR:HG23	1:A:228:LYS:HB3	1.83	0.60
1:B:10:ILE:HD12	1:B:162:TYR:HB2	1.83	0.60
1:A:244:GLU:HG3	8:A:2023:HOH:O	2.02	0.60
1:A:301:LEU:O	1:A:302:ASN:HB2	2.02	0.59
1:D:390:TYR:O	8:D:2020:HOH:O	2.17	0.59
1:C:20:MET:HE3	1:C:48:TRP:HB2	1.85	0.59
1:C:425:MET:HA	1:C:425:MET:HE3	1.85	0.58
1:C:204:THR:HG23	1:C:228:LYS:HB3	1.84	0.58
1:D:338:ARG:NH1	1:D:339:ASP:OD1	2.37	0.58
1:C:70:SER:HB2	2:C:1453:FAD:HM81	1.85	0.58
1:B:329:MET:HE2	1:B:380:TYR:HE2	1.68	0.57
1:A:425:MET:HE3	1:A:425:MET:HA	1.86	0.57
1:B:328:ASN:OD1	1:B:393:PHE:CZ	2.57	0.57
1:C:10:ILE:HD12	1:C:162:TYR:HB2	1.86	0.57
5:C:1456:EPE:O8	5:C:1456:EPE:H51	2.02	0.56
1:A:328:ASN:OD1	1:A:393:PHE:CZ	2.58	0.56
1:A:10:ILE:HD12	1:A:162:TYR:HB2	1.87	0.56
1:B:328:ASN:OD1	1:B:393:PHE:HZ	1.89	0.56
1:B:204:THR:HG23	1:B:228:LYS:HB3	1.87	0.56
1:A:338:ARG:NH1	1:A:339:ASP:OD1	2.39	0.55
1:C:451:ASP:O	1:C:452:LYS:HD2	2.06	0.55
5:A:1455:EPE:O3S	1:B:9:ARG:NH2	2.40	0.55
5:A:1455:EPE:O8	5:A:1455:EPE:C5	2.55	0.55
1:D:285:PHE:HD1	1:D:286:LEU:HD13	1.66	0.54
1:A:285:PHE:HD1	1:A:286:LEU:HD13	1.71	0.54
5:A:1454:EPE:H51	5:A:1454:EPE:HO8	1.65	0.54
5:D:1454:EPE:O8	5:D:1454:EPE:C5	2.55	0.54
1:B:285:PHE:HD1	1:B:286:LEU:HD13	1.68	0.54
1:A:328:ASN:OD1	1:A:393:PHE:HZ	1.89	0.54
1:B:70:SER:HB2	2:B:1451:FAD:HM81	1.90	0.54
1:B:425:MET:HE3	1:B:425:MET:HA	1.89	0.54
1:B:301:LEU:O	1:B:302:ASN:HB2	2.07	0.53
1:A:70:SER:HB2	2:A:1451:FAD:HM81	1.89	0.53
1:B:338:ARG:NH1	1:B:339:ASP:OD1	2.41	0.53
1:C:328:ASN:OD1	1:C:393:PHE:CZ	2.61	0.53
1:D:70:SER:HB2	2:D:1451:FAD:HM81	1.91	0.53
1:C:126:ARG:NH1	5:C:1456:EPE:H91	2.23	0.53
1:D:328:ASN:OD1	1:D:393:PHE:CZ	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:MET:HE3	1:B:242:TRP:CZ2	2.45	0.52
1:D:126:ARG:HH12	5:D:1454:EPE:H91	1.75	0.51
1:A:329:MET:HE2	1:A:380:TYR:HE2	1.75	0.51
1:C:232:CYS:HA	1:C:249:ARG:O	2.11	0.51
1:C:48:TRP:NE1	1:C:113:LYS:HG2	2.26	0.50
1:D:329:MET:HE2	1:D:380:TYR:HE2	1.76	0.50
1:B:231:SER:HB2	1:B:248:GLU:HG2	1.93	0.50
1:B:393:PHE:HB3	1:B:425:MET:HE1	1.93	0.50
1:D:81:LYS:HG2	1:D:91:PHE:CZ	2.47	0.50
1:B:291:ARG:NH2	1:C:153:ASP:OD1	2.41	0.50
1:C:329:MET:HE2	1:C:380:TYR:HE2	1.75	0.50
1:D:78:ASN:HD22	1:D:78:ASN:H	1.60	0.50
1:A:48:TRP:NE1	1:A:113:LYS:HG2	2.27	0.50
1:C:328:ASN:OD1	1:C:393:PHE:HZ	1.92	0.50
1:D:364:GLU:HA	1:D:367:LEU:HD22	1.93	0.50
1:B:81:LYS:HG2	1:B:91:PHE:CZ	2.46	0.50
1:C:285:PHE:HD1	1:C:286:LEU:HD13	1.71	0.50
1:D:231:SER:HB2	1:D:248:GLU:HG2	1.94	0.49
1:A:393:PHE:HB3	1:A:425:MET:HE1	1.95	0.49
1:D:238:MET:HE3	1:D:242:TRP:CZ2	2.48	0.49
1:D:328:ASN:OD1	1:D:393:PHE:HZ	1.94	0.49
1:C:126:ARG:CZ	5:C:1456:EPE:H91	2.43	0.49
1:D:48:TRP:NE1	1:D:113:LYS:HG2	2.28	0.48
1:B:175:VAL:HB	1:C:57:ARG:HH21	1.78	0.48
1:C:156:TYR:CE1	5:C:1456:EPE:H61	2.49	0.48
1:D:81:LYS:O	1:D:84:LEU:HD22	2.12	0.48
1:B:371:GLU:HA	1:B:374:TYR:CZ	2.48	0.48
1:A:81:LYS:HG2	1:A:91:PHE:CZ	2.48	0.48
1:B:329:MET:HE2	1:B:380:TYR:CE2	2.48	0.48
1:B:422:ARG:CD	1:B:427:GLY:O	2.62	0.48
1:D:81:LYS:HB2	1:D:101:SER:O	2.14	0.48
1:D:211:SER:HB3	3:D:1452:NAP:O1N	2.14	0.47
1:A:156:TYR:CE1	5:A:1454:EPE:H52	2.49	0.47
1:C:238:MET:HE3	1:C:242:TRP:CZ2	2.49	0.47
1:D:385:ILE:HD12	1:D:392:SER:HA	1.96	0.47
1:C:81:LYS:HG2	1:C:91:PHE:CZ	2.48	0.47
1:C:338:ARG:NH1	1:C:339:ASP:OD1	2.44	0.47
1:C:371:GLU:HA	1:C:374:TYR:CZ	2.49	0.47
1:A:57:ARG:HH21	1:D:175:VAL:HB	1.80	0.47
1:C:231:SER:HB2	1:C:248:GLU:HG2	1.97	0.47
1:C:329:MET:HE3	1:C:380:TYR:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:LYS:HB2	1:B:101:SER:O	2.15	0.46
5:D:1454:EPE:O8	5:D:1454:EPE:H52	2.15	0.46
1:B:48:TRP:NE1	1:B:113:LYS:HG2	2.31	0.46
1:C:329:MET:HE3	1:C:380:TYR:HD2	1.81	0.46
1:B:81:LYS:O	1:B:84:LEU:HD22	2.15	0.46
1:A:238:MET:HE3	1:A:242:TRP:CZ2	2.50	0.46
1:B:78:ASN:HD22	1:B:78:ASN:H	1.63	0.46
1:D:156:TYR:CE1	5:D:1454:EPE:H61	2.51	0.46
1:A:81:LYS:HB2	1:A:101:SER:O	2.16	0.46
1:B:153:ASP:OD1	1:C:291:ARG:NH2	2.48	0.46
1:C:267:SER:O	1:C:268:GLU:HG2	2.15	0.46
1:D:9:ARG:HG3	1:D:38:GLU:HB2	1.98	0.46
1:D:393:PHE:HB3	1:D:425:MET:HE1	1.97	0.45
1:B:57:ARG:HH21	1:C:175:VAL:HB	1.82	0.45
1:B:267:SER:O	1:B:268:GLU:HG2	2.15	0.45
1:A:156:TYR:CD1	5:A:1454:EPE:H52	2.52	0.45
1:A:211:SER:HB3	3:A:1452:NAP:O1N	2.16	0.45
1:C:422:ARG:CD	1:C:427:GLY:O	2.64	0.45
5:D:1454:EPE:O1S	5:D:1454:EPE:H62	2.17	0.45
1:B:75:LEU:HD11	2:B:1451:FAD:H6	1.98	0.45
1:D:329:MET:HE3	1:D:380:TYR:HD2	1.82	0.45
1:B:329:MET:HE3	1:B:380:TYR:HD2	1.82	0.45
1:C:331:ASP:HB3	1:C:390:TYR:CE1	2.52	0.45
1:C:393:PHE:HB3	1:C:425:MET:HE1	1.99	0.45
1:D:267:SER:O	1:D:268:GLU:HG2	2.17	0.45
1:A:153:ASP:OD1	1:D:291:ARG:NH2	2.47	0.45
1:D:329:MET:HE3	1:D:380:TYR:CD2	2.51	0.45
1:C:81:LYS:O	1:C:84:LEU:HD22	2.17	0.44
1:A:232:CYS:HA	1:A:249:ARG:O	2.18	0.44
1:A:371:GLU:HA	1:A:374:TYR:CZ	2.52	0.44
1:A:78:ASN:H	1:A:78:ASN:HD22	1.64	0.44
1:B:54:TYR:HB2	1:B:105:ARG:CZ	2.47	0.44
1:C:211:SER:HB3	3:C:1454:NAP:O1N	2.17	0.44
1:B:331:ASP:HB3	1:B:390:TYR:CE1	2.53	0.44
1:B:422:ARG:HD3	1:B:427:GLY:C	2.43	0.44
1:B:232:CYS:HA	1:B:249:ARG:O	2.18	0.44
1:B:364:GLU:HA	1:B:367:LEU:HD22	1.99	0.44
1:D:72:TYR:OH	3:D:1452:NAP:H4N	2.17	0.44
1:A:329:MET:HE3	1:A:380:TYR:HD2	1.82	0.43
1:A:385:ILE:HD12	1:A:392:SER:HA	2.00	0.43
1:A:329:MET:HE3	1:A:380:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:MET:HE3	1:C:48:TRP:CG	2.53	0.43
1:D:331:ASP:HB3	1:D:390:TYR:CE1	2.54	0.43
1:B:211:SER:HB3	3:B:1452:NAP:O1N	2.18	0.43
1:B:385:ILE:HD12	1:B:392:SER:HA	1.99	0.43
1:C:78:ASN:H	1:C:78:ASN:HD22	1.65	0.43
1:C:126:ARG:NH2	5:C:1456:EPE:H91	2.34	0.43
1:D:371:GLU:HA	1:D:374:TYR:CZ	2.53	0.43
1:C:9:ARG:HG3	1:C:38:GLU:HB2	2.00	0.43
1:D:75:LEU:HD11	2:D:1451:FAD:H6	2.00	0.43
1:C:81:LYS:HB2	1:C:101:SER:O	2.19	0.43
1:A:75:LEU:HD11	2:A:1451:FAD:H6	2.01	0.43
1:B:329:MET:HE3	1:B:380:TYR:CD2	2.54	0.43
1:A:65:GLU:OE2	1:A:132:ARG:NH2	2.52	0.42
1:D:232:CYS:HA	1:D:249:ARG:O	2.19	0.42
1:A:81:LYS:O	1:A:84:LEU:HD22	2.19	0.42
1:A:126:ARG:NH1	5:A:1454:EPE:H91	2.34	0.42
1:A:213:SER:HA	3:A:1452:NAP:H5N	2.02	0.42
1:B:20:MET:HE3	1:B:48:TRP:CB	2.47	0.42
1:B:390:TYR:HA	1:B:391:PRO:HD3	1.94	0.42
1:C:54:TYR:HB2	1:C:105:ARG:CZ	2.50	0.42
1:B:187:ARG:HD3	1:B:189:LEU:HD22	2.00	0.42
1:D:213:SER:HA	3:D:1452:NAP:H5N	2.02	0.42
1:A:175:VAL:HB	1:D:57:ARG:HH21	1.85	0.42
1:A:364:GLU:HA	1:A:367:LEU:HD22	2.02	0.42
1:A:385:ILE:O	8:A:2035:HOH:O	2.21	0.41
1:B:20:MET:HE3	1:B:48:TRP:CG	2.55	0.41
1:C:264:ASP:HB3	1:C:266:SER:H	1.85	0.41
1:A:9:ARG:HG3	1:A:38:GLU:HB2	2.03	0.41
1:A:267:SER:O	1:A:268:GLU:HG2	2.20	0.41
5:C:1456:EPE:S	5:C:1456:EPE:H62	2.59	0.41
1:A:264:ASP:HB3	1:A:266:SER:H	1.85	0.41
1:D:54:TYR:HB2	1:D:105:ARG:CZ	2.50	0.41
5:A:1455:EPE:H102	5:A:1455:EPE:H62	1.84	0.41
1:A:331:ASP:HB3	1:A:390:TYR:CE1	2.56	0.41
1:B:450:SER:C	8:B:2032:HOH:O	2.63	0.41
1:A:329:MET:HE2	1:A:380:TYR:CE2	2.55	0.41
1:B:9:ARG:HG3	1:B:38:GLU:HB2	2.02	0.41
1:C:288:ASP:OD1	1:C:291:ARG:NH1	2.53	0.41
1:C:390:TYR:HA	1:C:391:PRO:HD3	1.94	0.41
1:A:291:ARG:NH2	1:D:153:ASP:OD1	2.51	0.41
1:C:14:GLY:O	1:C:19:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:GLU:HA	1:C:367:LEU:HD22	2.02	0.41
1:A:54:TYR:HB2	1:A:105:ARG:CZ	2.51	0.40
1:B:256:ASP:OD1	1:B:257:THR:N	2.53	0.40
1:B:327:PHE:HA	1:B:330:PHE:CD2	2.55	0.40
1:C:213:SER:HA	3:C:1454:NAP:H5N	2.02	0.40
1:A:422:ARG:CD	1:A:427:GLY:O	2.69	0.40
1:A:72:TYR:OH	3:A:1452:NAP:H4N	2.21	0.40
1:A:238:MET:HE2	1:A:238:MET:HB2	1.97	0.40
1:D:256:ASP:HB2	1:D:261:TYR:HE1	1.87	0.40
1:B:14:GLY:O	1:B:19:GLY:HA3	2.22	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	441/461 (96%)	414 (94%)	25 (6%)	2 (0%)	24	46
1	B	441/461 (96%)	415 (94%)	25 (6%)	1 (0%)	43	66
1	C	443/461 (96%)	421 (95%)	20 (4%)	2 (0%)	24	46
1	D	441/461 (96%)	416 (94%)	24 (5%)	1 (0%)	43	66
All	All	1766/1844 (96%)	1666 (94%)	94 (5%)	6 (0%)	36	58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	389	ASP
1	B	389	ASP
1	C	389	ASP
1	D	389	ASP
1	C	328	ASN

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Mol	Chain	Res	Type
1	A	328	ASN

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	385/397 (97%)	353 (92%)	32 (8%)	10 23
1	B	385/397 (97%)	352 (91%)	33 (9%)	10 22
1	C	387/397 (98%)	352 (91%)	35 (9%)	9 20
1	D	385/397 (97%)	352 (91%)	33 (9%)	10 22
All	All	1542/1588 (97%)	1409 (91%)	133 (9%)	10 22

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	38	GLU
1	A	58	THR
1	A	60	LEU
1	A	78	ASN
1	A	82	GLU
1	A	84	LEU
1	A	97	LYS
1	A	128	ASN
1	A	199	GLU
1	A	220	GLN
1	A	234	ARG
1	A	238	MET
1	A	244	GLU
1	A	247	ASP
1	A	255	VAL
1	A	257	THR
1	A	286	LEU
1	A	307	VAL
1	A	328	ASN

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Mol	Chain	Res	Type
1	A	338	ARG
1	A	340	VAL
1	A	347	LEU
1	A	354	LYS
1	A	366	THR
1	A	367	LEU
1	A	388	THR
1	A	400	LYS
1	A	410	LYS
1	A	441	LEU
1	A	445	LEU
1	A	450	SER
1	B	8	THR
1	B	17	PRO
1	B	38	GLU
1	B	48	TRP
1	B	58	THR
1	B	60	LEU
1	B	78	ASN
1	B	82	GLU
1	B	84	LEU
1	B	97	LYS
1	B	128	ASN
1	B	199	GLU
1	B	220	GLN
1	B	234	ARG
1	B	238	MET
1	B	244	GLU
1	B	247	ASP
1	B	255	VAL
1	B	257	THR
1	B	286	LEU
1	B	307	VAL
1	B	328	ASN
1	B	338	ARG
1	B	340	VAL
1	B	347	LEU
1	B	354	LYS
1	B	366	THR
1	B	367	LEU
1	B	388	THR
1	B	400	LYS

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Mol	Chain	Res	Type
1	B	410	LYS
1	B	441	LEU
1	B	450	SER
1	C	8	THR
1	C	38	GLU
1	C	58	THR
1	C	60	LEU
1	C	78	ASN
1	C	82	GLU
1	C	84	LEU
1	C	97	LYS
1	C	105	ARG
1	C	128	ASN
1	C	199	GLU
1	C	220	GLN
1	C	234	ARG
1	C	238	MET
1	C	244	GLU
1	C	247	ASP
1	C	249	ARG
1	C	255	VAL
1	C	257	THR
1	C	264	ASP
1	C	286	LEU
1	C	307	VAL
1	C	328	ASN
1	C	338	ARG
1	C	340	VAL
1	C	347	LEU
1	C	354	LYS
1	C	366	THR
1	C	367	LEU
1	C	388	THR
1	C	400	LYS
1	C	410	LYS
1	C	441	LEU
1	C	445	LEU
1	C	450	SER
1	D	8	THR
1	D	38	GLU
1	D	48	TRP
1	D	58	THR

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Mol	Chain	Res	Type
1	D	60	LEU
1	D	78	ASN
1	D	82	GLU
1	D	84	LEU
1	D	97	LYS
1	D	128	ASN
1	D	199	GLU
1	D	220	GLN
1	D	234	ARG
1	D	238	MET
1	D	244	GLU
1	D	247	ASP
1	D	255	VAL
1	D	257	THR
1	D	286	LEU
1	D	307	VAL
1	D	328	ASN
1	D	338	ARG
1	D	340	VAL
1	D	347	LEU
1	D	354	LYS
1	D	366	THR
1	D	367	LEU
1	D	388	THR
1	D	400	LYS
1	D	410	LYS
1	D	441	LEU
1	D	445	LEU
1	D	450	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	78	ASN
1	A	128	ASN
1	A	148	GLN
1	A	169	HIS
1	A	282	HIS
1	A	323	GLN
1	A	328	ASN
1	B	63	ASN

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Mol	Chain	Res	Type
1	B	78	ASN
1	B	128	ASN
1	B	141	GLN
1	B	148	GLN
1	B	282	HIS
1	B	323	GLN
1	B	328	ASN
1	C	63	ASN
1	C	78	ASN
1	C	128	ASN
1	C	148	GLN
1	C	169	HIS
1	C	282	HIS
1	C	323	GLN
1	C	328	ASN
1	D	63	ASN
1	D	78	ASN
1	D	128	ASN
1	D	148	GLN
1	D	169	HIS
1	D	282	HIS
1	D	328	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	EPE	A	1454	-	15,15,15	1.30	1 (6%)	19,20,20	2.15	6 (31%)
5	EPE	C	1456	-	15,15,15	1.22	1 (6%)	19,20,20	2.13	4 (21%)
6	PGE	A	1456	-	9,9,9	0.54	0	8,8,8	0.16	0
3	NAP	A	1452	-	50,52,52	1.61	8 (16%)	71,80,80	1.87	16 (22%)
2	FAD	A	1451	-	58,58,58	1.12	8 (13%)	85,89,89	1.66	18 (21%)
3	NAP	C	1454	-	50,52,52	1.74	9 (18%)	71,80,80	1.85	15 (21%)
7	PG4	B	1453	-	12,12,12	0.62	0	11,11,11	0.24	0
5	EPE	D	1454	-	15,15,15	1.23	1 (6%)	19,20,20	2.24	6 (31%)
2	FAD	B	1451	-	58,58,58	1.10	4 (6%)	85,89,89	1.77	18 (21%)
3	NAP	B	1452	-	50,52,52	1.49	8 (16%)	71,80,80	1.91	18 (25%)
2	FAD	C	1453	-	58,58,58	1.07	5 (8%)	85,89,89	1.75	18 (21%)
5	EPE	A	1455	-	15,15,15	1.14	1 (6%)	19,20,20	2.39	8 (42%)
3	NAP	D	1452	-	50,52,52	1.39	8 (16%)	71,80,80	1.87	19 (26%)
2	FAD	D	1451	-	58,58,58	1.12	5 (8%)	85,89,89	1.67	17 (20%)

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	EPE	A	1454	-	-	7/9/19/19	0/1/1/1
5	EPE	C	1456	-	-	6/9/19/19	0/1/1/1
6	PGE	A	1456	-	-	3/7/7/7	-
3	NAP	A	1452	-	-	9/35/67/67	0/5/5/5
2	FAD	A	1451	-	-	2/34/50/50	0/6/6/6
3	NAP	C	1454	-	-	10/35/67/67	0/5/5/5
7	PG4	B	1453	-	-	3/10/10/10	-
5	EPE	D	1454	-	-	5/9/19/19	0/1/1/1
2	FAD	B	1451	-	-	2/34/50/50	0/6/6/6
3	NAP	B	1452	-	-	8/35/67/67	0/5/5/5
2	FAD	C	1453	-	-	2/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EPE	A	1455	-	-	7/9/19/19	0/1/1/1
3	NAP	D	1452	-	-	9/35/67/67	0/5/5/5
2	FAD	D	1451	-	-	2/34/50/50	0/6/6/6

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1454	NAP	PA-O3	5.75	1.65	1.59
3	C	1454	NAP	PN-O3	5.41	1.65	1.59
3	A	1452	NAP	P2B-O1X	4.39	1.64	1.50
5	A	1454	EPE	C10-S	4.31	1.83	1.77
3	C	1454	NAP	O4D-C1D	4.28	1.46	1.40
3	A	1452	NAP	PA-O3	4.22	1.64	1.59
3	A	1452	NAP	O4D-C1D	4.21	1.46	1.40
3	B	1452	NAP	O4D-C1D	4.19	1.46	1.40
3	A	1452	NAP	PN-O3	4.16	1.64	1.59
5	C	1456	EPE	C10-S	4.15	1.83	1.77
5	D	1454	EPE	C10-S	4.04	1.83	1.77
5	A	1455	EPE	C10-S	3.90	1.83	1.77
3	B	1452	NAP	PN-O3	3.61	1.63	1.59
2	D	1451	FAD	C4X-N5	3.45	1.38	1.30
2	A	1451	FAD	C4X-N5	3.44	1.38	1.30
3	D	1452	NAP	O4D-C1D	3.36	1.45	1.40
2	B	1451	FAD	C4X-N5	3.31	1.37	1.30
2	C	1453	FAD	C4X-N5	3.25	1.37	1.30
3	B	1452	NAP	PA-O3	3.22	1.63	1.59
3	D	1452	NAP	PA-O3	2.99	1.62	1.59
2	D	1451	FAD	C2A-N3A	2.96	1.39	1.33
3	D	1452	NAP	PN-O3	2.92	1.62	1.59
2	B	1451	FAD	C8A-N7A	2.91	1.37	1.31
2	C	1453	FAD	C2A-N3A	2.86	1.39	1.33
3	B	1452	NAP	O4B-C1B	2.83	1.48	1.42
2	D	1451	FAD	C10-N1	2.81	1.38	1.33
2	D	1451	FAD	C8A-N7A	2.74	1.36	1.31
2	B	1451	FAD	C10-N1	2.73	1.38	1.33
3	D	1452	NAP	P2B-O2B	2.70	1.64	1.59
3	A	1452	NAP	C7N-N7N	2.63	1.37	1.33
2	C	1453	FAD	C8A-N7A	2.62	1.36	1.31
3	D	1452	NAP	C6A-N6A	2.53	1.40	1.34
3	B	1452	NAP	P2B-O1X	2.47	1.58	1.50
3	C	1454	NAP	P2B-O2X	2.47	1.64	1.54
3	D	1452	NAP	C2N-C3N	2.44	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1452	NAP	P2B-O3X	2.42	1.63	1.54
3	A	1452	NAP	P2B-O2B	2.41	1.63	1.59
2	B	1451	FAD	C2A-N3A	2.41	1.38	1.33
3	B	1452	NAP	C5A-C4A	2.41	1.43	1.39
2	D	1451	FAD	C2A-N1A	2.38	1.38	1.33
2	A	1451	FAD	C8A-N7A	2.31	1.36	1.31
3	D	1452	NAP	P2B-O2X	2.31	1.63	1.54
2	A	1451	FAD	C2A-N1A	2.28	1.38	1.33
2	A	1451	FAD	C2A-N3A	2.28	1.38	1.33
3	C	1454	NAP	C6A-N6A	2.28	1.40	1.34
3	B	1452	NAP	P2B-O2X	2.26	1.63	1.54
2	A	1451	FAD	C10-N1	2.24	1.37	1.33
3	B	1452	NAP	C6A-N6A	2.23	1.39	1.34
3	C	1454	NAP	C7N-N7N	2.20	1.37	1.33
2	C	1453	FAD	C10-N1	2.19	1.37	1.33
2	C	1453	FAD	PA-O3P	2.15	1.61	1.59
3	D	1452	NAP	C5N-C4N	2.14	1.42	1.38
3	C	1454	NAP	C5A-C4A	2.13	1.42	1.39
3	C	1454	NAP	C5N-C4N	2.13	1.42	1.38
3	C	1454	NAP	C4N-C3N	2.13	1.42	1.39
3	A	1452	NAP	C5A-C4A	2.07	1.42	1.39
2	A	1451	FAD	C5A-N7A	-2.07	1.35	1.39
2	A	1451	FAD	O4B-C4B	-2.04	1.40	1.45
2	A	1451	FAD	C4X-C10	-2.01	1.38	1.44

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1455	EPE	C5-N4-C3	6.71	123.30	108.84
5	D	1454	EPE	C5-N4-C3	6.63	123.11	108.84
5	C	1456	EPE	C5-N4-C3	6.43	122.69	108.84
2	C	1453	FAD	N3A-C2A-N1A	-6.16	119.26	128.58
2	D	1451	FAD	N3A-C2A-N1A	-5.60	120.10	128.58
2	B	1451	FAD	N3A-C2A-N1A	-5.60	120.11	128.58
3	C	1454	NAP	C5A-C4A-N3A	-5.51	119.13	126.72
2	B	1451	FAD	C5A-C4A-N3A	-5.27	119.47	126.72
3	B	1452	NAP	C5A-C4A-N3A	-5.23	119.51	126.72
5	A	1454	EPE	C5-N4-C3	5.12	119.86	108.84
2	A	1451	FAD	N3A-C2A-N1A	-5.01	121.00	128.58
2	C	1453	FAD	C5A-C4A-N3A	-4.95	119.90	126.72
2	A	1451	FAD	C5A-C4A-N3A	-4.94	119.92	126.72
2	D	1451	FAD	C5A-C4A-N3A	-4.77	120.15	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1452	NAP	N3A-C2A-N1A	-4.77	121.37	128.58
3	A	1452	NAP	C5A-C4A-N3A	-4.76	120.17	126.72
3	A	1452	NAP	C3N-C7N-N7N	4.67	123.49	117.74
3	D	1452	NAP	C5A-C4A-N3A	-4.59	120.40	126.72
5	A	1454	EPE	C6-N1-C2	4.52	118.57	108.84
2	B	1451	FAD	N9A-C8A-N7A	-4.49	107.57	113.94
3	C	1454	NAP	N3A-C2A-N1A	-4.44	121.86	128.58
3	D	1452	NAP	N3A-C2A-N1A	-4.28	122.10	128.58
3	D	1452	NAP	N3A-C4A-N9A	4.17	134.26	127.17
2	B	1451	FAD	C5A-N7A-C8A	4.16	109.99	103.45
3	D	1452	NAP	C5A-N7A-C8A	4.12	109.93	103.45
2	A	1451	FAD	C5A-N7A-C8A	4.11	109.90	103.45
2	A	1451	FAD	N9A-C8A-N7A	-4.08	108.15	113.94
2	D	1451	FAD	N9A-C8A-N7A	-4.06	108.17	113.94
3	B	1452	NAP	C3N-C7N-N7N	4.06	122.74	117.74
2	C	1453	FAD	N9A-C8A-N7A	-4.02	108.23	113.94
3	C	1454	NAP	N3A-C4A-N9A	4.01	133.99	127.17
3	C	1454	NAP	C2A-N3A-C4A	3.98	121.56	111.83
3	A	1452	NAP	N3A-C2A-N1A	-3.98	122.56	128.58
3	A	1452	NAP	O4B-C1B-N9A	3.97	115.72	108.09
3	A	1452	NAP	N3A-C4A-N9A	3.95	133.89	127.17
2	C	1453	FAD	C2A-N3A-C4A	3.94	121.45	111.83
3	C	1454	NAP	P2B-O2B-C2B	-3.90	113.00	123.43
3	B	1452	NAP	P2B-O2B-C2B	-3.88	113.08	123.43
3	B	1452	NAP	N3A-C4A-N9A	3.82	133.67	127.17
3	B	1452	NAP	C2A-N3A-C4A	3.79	121.09	111.83
2	B	1451	FAD	C2A-N3A-C4A	3.78	121.06	111.83
2	C	1453	FAD	C5A-N7A-C8A	3.74	109.33	103.45
3	D	1452	NAP	N9A-C8A-N7A	-3.74	108.64	113.94
2	A	1451	FAD	C4A-C5A-N7A	-3.72	106.33	110.58
3	D	1452	NAP	C2B-C1B-N9A	-3.70	107.66	113.75
3	A	1452	NAP	C5A-N7A-C8A	3.70	109.27	103.45
3	B	1452	NAP	O4B-C1B-N9A	3.70	115.20	108.09
3	D	1452	NAP	P2B-O2B-C2B	-3.68	113.62	123.43
2	D	1451	FAD	C2A-N3A-C4A	3.62	120.68	111.83
2	D	1451	FAD	C5A-N7A-C8A	3.57	109.06	103.45
3	C	1454	NAP	O4B-C1B-N9A	3.57	114.95	108.09
3	B	1452	NAP	C5A-N7A-C8A	3.53	108.99	103.45
3	C	1454	NAP	C2B-C1B-N9A	-3.52	107.96	113.75
5	A	1454	EPE	C7-N4-C3	3.48	120.52	111.24
2	B	1451	FAD	C4A-C5A-N7A	-3.41	106.68	110.58
3	C	1454	NAP	C3B-C2B-C1B	-3.41	96.29	102.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1453	FAD	C4X-C10-N10	3.38	121.32	116.48
5	D	1454	EPE	C2-C3-N4	3.37	117.45	110.65
2	C	1453	FAD	C4A-C5A-N7A	-3.37	106.73	110.58
3	C	1454	NAP	C3N-C7N-N7N	3.35	121.87	117.74
5	A	1455	EPE	C6-N1-C2	3.30	115.96	108.84
3	A	1452	NAP	C2A-N3A-C4A	3.30	119.88	111.83
2	A	1451	FAD	C2A-N3A-C4A	3.29	119.86	111.83
2	B	1451	FAD	C4-N3-C2	-3.27	119.83	125.64
3	A	1452	NAP	C2B-C1B-N9A	-3.27	108.37	113.75
2	D	1451	FAD	C4X-C10-N10	3.26	121.15	116.48
5	C	1456	EPE	C7-N4-C3	3.24	119.87	111.24
2	B	1451	FAD	C4X-C10-N10	3.24	121.11	116.48
5	D	1454	EPE	O1S-S-C10	3.24	111.62	106.73
3	D	1452	NAP	C3N-C7N-N7N	3.23	121.72	117.74
5	C	1456	EPE	O1S-S-C10	3.21	111.58	106.73
3	B	1452	NAP	C2B-C1B-N9A	-3.21	108.46	113.75
3	C	1454	NAP	C5A-N7A-C8A	3.20	108.47	103.45
3	D	1452	NAP	C2A-N3A-C4A	3.19	119.62	111.83
3	D	1452	NAP	C4A-N9A-C8A	3.17	109.06	105.74
2	A	1451	FAD	C4X-C10-N10	3.11	120.93	116.48
3	D	1452	NAP	C4A-C5A-N7A	-3.11	107.03	110.58
3	A	1452	NAP	N9A-C8A-N7A	-3.10	109.54	113.94
2	A	1451	FAD	C4-N3-C2	-3.10	120.14	125.64
3	B	1452	NAP	C4A-C5A-N7A	-3.09	107.05	110.58
5	A	1455	EPE	O1S-S-C10	3.08	111.39	106.73
3	A	1452	NAP	C3B-C2B-C1B	-3.08	96.92	102.81
3	C	1454	NAP	C4A-C5A-N7A	-3.06	107.09	110.58
3	D	1452	NAP	O4B-C1B-N9A	3.05	113.94	108.09
2	D	1451	FAD	C4A-C5A-N7A	-3.05	107.10	110.58
2	D	1451	FAD	C4-N3-C2	-3.02	120.27	125.64
3	A	1452	NAP	C4A-C5A-N7A	-2.99	107.17	110.58
3	D	1452	NAP	C3B-C2B-C1B	-2.96	97.14	102.81
3	B	1452	NAP	C3B-C2B-C1B	-2.95	97.16	102.81
5	A	1455	EPE	C6-C5-N4	2.95	116.59	110.65
2	C	1453	FAD	C4-N3-C2	-2.87	120.55	125.64
3	B	1452	NAP	O7N-C7N-N7N	-2.86	118.48	122.62
5	A	1455	EPE	O2S-S-C10	2.85	111.03	106.73
2	B	1451	FAD	N3A-C4A-N9A	2.84	132.00	127.17
2	A	1451	FAD	C4X-C4-N3	2.82	120.44	113.25
3	B	1452	NAP	O3D-C3D-C2D	-2.82	102.77	111.82
3	A	1452	NAP	P2B-O2B-C2B	-2.80	115.96	123.43
2	D	1451	FAD	C4X-C4-N3	2.78	120.32	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1454	EPE	C7-N4-C5	2.77	118.61	111.24
3	B	1452	NAP	N9A-C8A-N7A	-2.76	110.02	113.94
2	B	1451	FAD	C4X-C4-N3	2.75	120.24	113.25
5	C	1456	EPE	C2-C3-N4	2.75	116.19	110.65
2	A	1451	FAD	O4B-C1B-N9A	2.69	113.26	108.09
5	D	1454	EPE	C7-N4-C3	2.68	118.38	111.24
2	B	1451	FAD	C10-C4X-N5	-2.65	119.40	124.81
3	C	1454	NAP	N9A-C8A-N7A	-2.64	110.20	113.94
2	D	1451	FAD	C10-C4X-N5	-2.63	119.44	124.81
2	A	1451	FAD	N3A-C4A-N9A	2.62	131.62	127.17
2	D	1451	FAD	C5A-C4A-N9A	2.59	108.63	105.81
5	D	1454	EPE	C7-N4-C5	2.58	118.11	111.24
5	A	1455	EPE	C7-N4-C5	2.57	118.09	111.24
2	C	1453	FAD	N3A-C4A-N9A	2.56	131.52	127.17
5	A	1455	EPE	C2-C3-N4	2.54	115.78	110.65
2	C	1453	FAD	C4X-C4-N3	2.53	119.70	113.25
2	C	1453	FAD	C10-C4X-N5	-2.51	119.67	124.81
2	C	1453	FAD	C5A-C4A-N9A	2.51	108.55	105.81
3	D	1452	NAP	PN-O5D-C5D	-2.50	107.05	121.35
2	A	1451	FAD	C9A-C5X-N5	-2.49	119.81	122.45
5	A	1454	EPE	O2S-S-C10	2.49	110.49	106.73
2	B	1451	FAD	C5A-C4A-N9A	2.48	108.51	105.81
3	D	1452	NAP	O7N-C7N-N7N	-2.48	119.04	122.62
2	D	1451	FAD	C9A-C5X-N5	-2.45	119.85	122.45
3	C	1454	NAP	PN-O5D-C5D	-2.45	107.33	121.35
2	B	1451	FAD	C9A-C5X-N5	-2.43	119.87	122.45
2	C	1453	FAD	C9A-C5X-N5	-2.43	119.88	122.45
2	A	1451	FAD	C5A-C4A-N9A	2.40	108.42	105.81
2	B	1451	FAD	O4-C4-C4X	-2.38	120.25	126.53
3	B	1452	NAP	PN-O5D-C5D	-2.37	107.75	121.35
2	D	1451	FAD	N3A-C4A-N9A	2.37	131.19	127.17
2	B	1451	FAD	O3P-P-O1P	2.36	117.80	110.70
3	D	1452	NAP	C2A-N1A-C6A	2.34	122.58	118.73
5	A	1454	EPE	O1S-S-C10	2.34	110.27	106.73
2	A	1451	FAD	C10-C4X-N5	-2.32	120.07	124.81
3	A	1452	NAP	PN-O5D-C5D	-2.31	108.13	121.35
2	C	1453	FAD	O2P-P-O3P	2.28	113.45	107.27
3	B	1452	NAP	O3X-P2B-O2B	2.28	114.75	105.85
3	A	1452	NAP	O7N-C7N-N7N	-2.28	119.32	122.62
3	C	1454	NAP	O3D-C3D-C2D	-2.27	104.53	111.82
3	A	1452	NAP	O3D-C3D-C2D	-2.27	104.53	111.82
2	C	1453	FAD	O4B-C1B-N9A	2.26	112.43	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1453	FAD	O4-C4-C4X	-2.24	120.63	126.53
3	A	1452	NAP	C4A-N9A-C8A	2.23	108.08	105.74
2	C	1453	FAD	C5'-C4'-C3'	2.22	116.40	112.22
3	D	1452	NAP	C4B-O4B-C1B	-2.22	104.57	109.47
3	D	1452	NAP	C5N-C4N-C3N	-2.19	118.21	120.36
5	A	1455	EPE	C7-N4-C3	2.18	117.06	111.24
2	D	1451	FAD	O4-C4-C4X	-2.17	120.80	126.53
3	B	1452	NAP	C2A-N1A-C6A	2.17	122.30	118.73
2	A	1451	FAD	O4-C4-C4X	-2.17	120.81	126.53
5	D	1454	EPE	O2S-S-C10	2.16	110.00	106.73
2	D	1451	FAD	C4-C4X-N5	2.13	121.15	118.21
2	A	1451	FAD	C5'-C4'-C3'	2.12	116.22	112.22
3	B	1452	NAP	C6A-C5A-N7A	2.08	136.10	132.09
3	C	1454	NAP	C5N-C4N-C3N	-2.07	118.33	120.36
2	B	1451	FAD	C4-C4X-N5	2.07	121.07	118.21
2	C	1453	FAD	O3P-P-O1P	2.07	116.93	110.70
2	A	1451	FAD	C6A-C5A-C4A	2.07	120.00	117.18
2	B	1451	FAD	C5X-C9A-N10	2.06	119.83	117.97
2	D	1451	FAD	C4X-C10-N1	-2.03	119.61	124.59
2	B	1451	FAD	C4X-C10-N1	-2.03	119.62	124.59
2	D	1451	FAD	C5X-C9A-N10	2.03	119.80	117.97
2	A	1451	FAD	O2P-P-O3P	2.02	112.72	107.27
3	D	1452	NAP	O3D-C3D-C2D	-2.01	105.37	111.82

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1451	FAD	N10-C1'-C2'-O2'
2	A	1451	FAD	N10-C1'-C2'-C3'
2	B	1451	FAD	N10-C1'-C2'-O2'
2	B	1451	FAD	N10-C1'-C2'-C3'
2	C	1453	FAD	N10-C1'-C2'-O2'
2	C	1453	FAD	N10-C1'-C2'-C3'
2	D	1451	FAD	N10-C1'-C2'-O2'
2	D	1451	FAD	N10-C1'-C2'-C3'
3	A	1452	NAP	C5B-O5B-PA-O2A
3	A	1452	NAP	C5B-O5B-PA-O3
3	A	1452	NAP	C5D-O5D-PN-O2N
3	B	1452	NAP	C5B-O5B-PA-O2A
3	B	1452	NAP	C5B-O5B-PA-O3
3	B	1452	NAP	C5D-O5D-PN-O2N

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Mol	Chain	Res	Type	Atoms
3	C	1454	NAP	C5D-O5D-PN-O2N
3	D	1452	NAP	C5B-O5B-PA-O2A
3	D	1452	NAP	C5B-O5B-PA-O3
3	D	1452	NAP	C5D-O5D-PN-O2N
5	A	1454	EPE	C10-C9-N1-C6
5	A	1454	EPE	C8-C7-N4-C5
5	A	1454	EPE	S-C10-C9-N1
5	A	1455	EPE	C10-C9-N1-C6
5	A	1455	EPE	C8-C7-N4-C5
5	A	1455	EPE	S-C10-C9-N1
5	C	1456	EPE	S-C10-C9-N1
5	C	1456	EPE	C9-C10-S-O1S
5	C	1456	EPE	C9-C10-S-O2S
5	C	1456	EPE	C9-C10-S-O3S
5	D	1454	EPE	C8-C7-N4-C5
5	D	1454	EPE	S-C10-C9-N1
5	C	1456	EPE	C8-C7-N4-C5
3	A	1452	NAP	O4B-C4B-C5B-O5B
3	B	1452	NAP	O4B-C4B-C5B-O5B
3	C	1454	NAP	O4B-C4B-C5B-O5B
3	D	1452	NAP	O4B-C4B-C5B-O5B
5	A	1455	EPE	C9-C10-S-O3S
3	C	1454	NAP	C1B-C2B-O2B-P2B
3	D	1452	NAP	C3B-C2B-O2B-P2B
5	A	1454	EPE	N4-C7-C8-O8
5	C	1456	EPE	N4-C7-C8-O8
3	A	1452	NAP	C3B-C4B-C5B-O5B
3	B	1452	NAP	C3B-C4B-C5B-O5B
3	C	1454	NAP	C3B-C4B-C5B-O5B
3	D	1452	NAP	C3B-C4B-C5B-O5B
3	D	1452	NAP	C1B-C2B-O2B-P2B
5	A	1454	EPE	C9-C10-S-O3S
3	A	1452	NAP	C1B-C2B-O2B-P2B
5	D	1454	EPE	C9-C10-S-O3S
3	C	1454	NAP	C3B-C2B-O2B-P2B
5	A	1454	EPE	C9-C10-S-O1S
5	A	1454	EPE	C9-C10-S-O2S
5	A	1455	EPE	C9-C10-S-O1S
5	A	1455	EPE	C9-C10-S-O2S
5	D	1454	EPE	C9-C10-S-O1S
5	D	1454	EPE	C9-C10-S-O2S
6	A	1456	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
3	B	1452	NAP	C1B-C2B-O2B-P2B
3	A	1452	NAP	C5B-O5B-PA-O1A
3	A	1452	NAP	C5D-O5D-PN-O3
3	B	1452	NAP	C5B-O5B-PA-O1A
3	B	1452	NAP	C5D-O5D-PN-O3
3	C	1454	NAP	C5B-O5B-PA-O1A
3	C	1454	NAP	C5B-O5B-PA-O2A
3	C	1454	NAP	C5B-O5B-PA-O3
3	C	1454	NAP	C5D-O5D-PN-O3
3	C	1454	NAP	C5D-O5D-PN-O1N
3	D	1452	NAP	C5B-O5B-PA-O1A
3	D	1452	NAP	C5D-O5D-PN-O3
7	B	1453	PG4	C3-C4-O3-C5
5	A	1455	EPE	N4-C7-C8-O8
6	A	1456	PGE	C6-C5-O3-C4
7	B	1453	PG4	O4-C7-C8-O5
3	A	1452	NAP	C2B-O2B-P2B-O3X
6	A	1456	PGE	C3-C4-O3-C5
7	B	1453	PG4	O1-C1-C2-O2

There are no ring outliers.

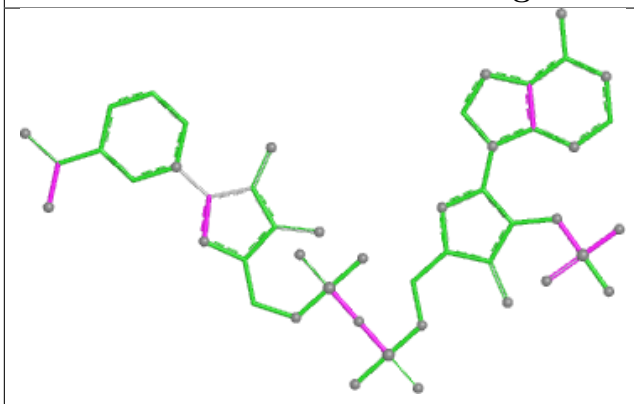
12 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1454	EPE	6	0
5	C	1456	EPE	8	0
3	A	1452	NAP	3	0
2	A	1451	FAD	2	0
3	C	1454	NAP	2	0
5	D	1454	EPE	6	0
2	B	1451	FAD	2	0
3	B	1452	NAP	1	0
2	C	1453	FAD	1	0
5	A	1455	EPE	4	0
3	D	1452	NAP	3	0
2	D	1451	FAD	2	0

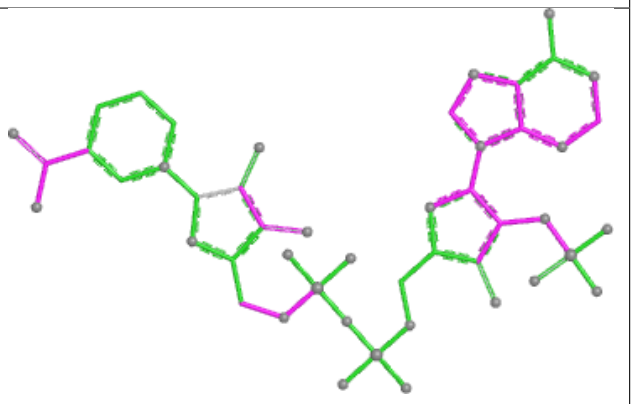
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

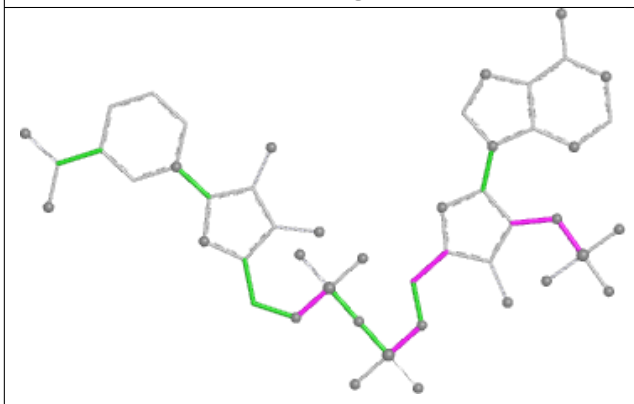
Ligand NAP A 1452



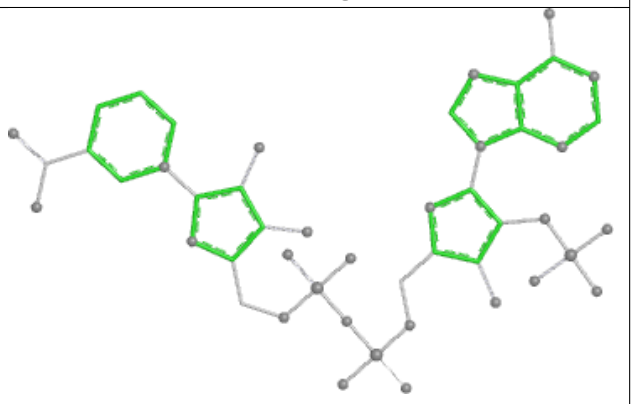
Bond lengths



Bond angles

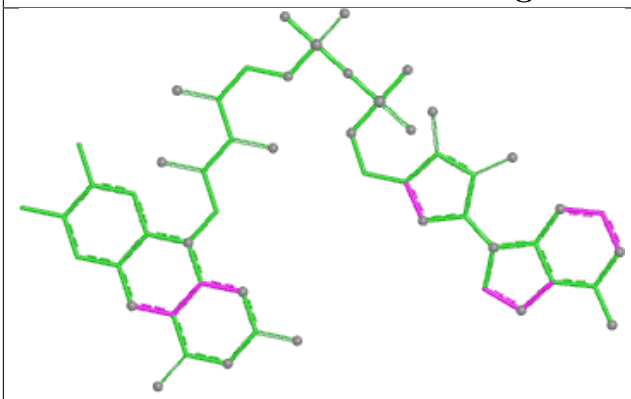


Torsions

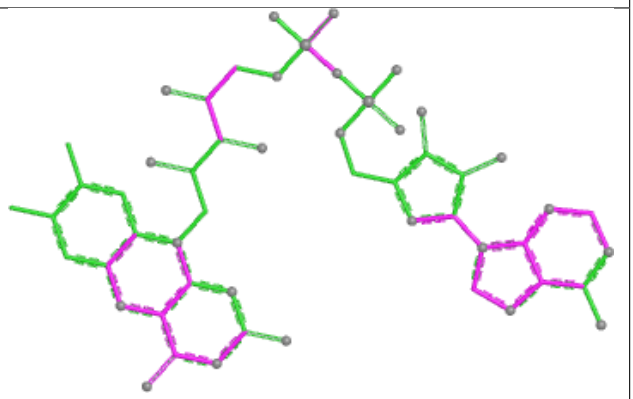


Rings

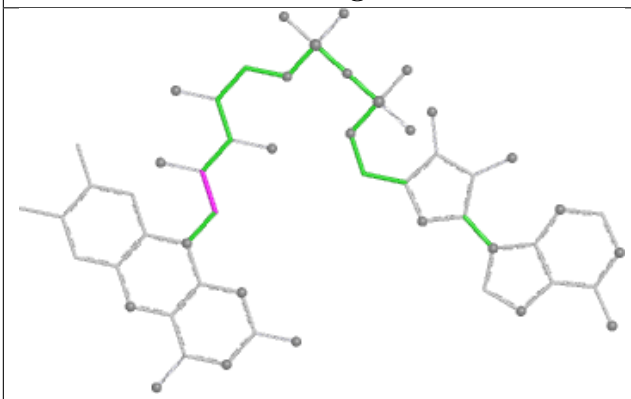
Ligand FAD A 1451



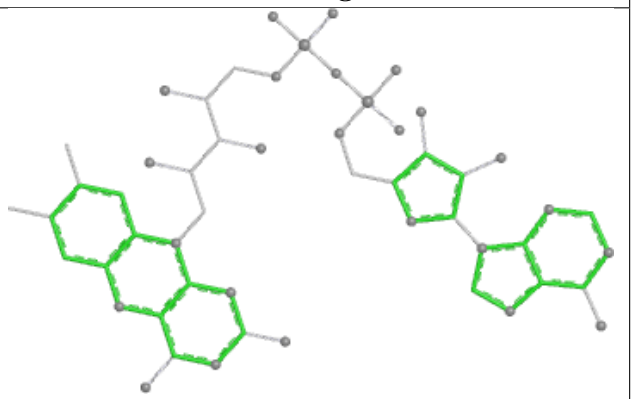
Bond lengths



Bond angles

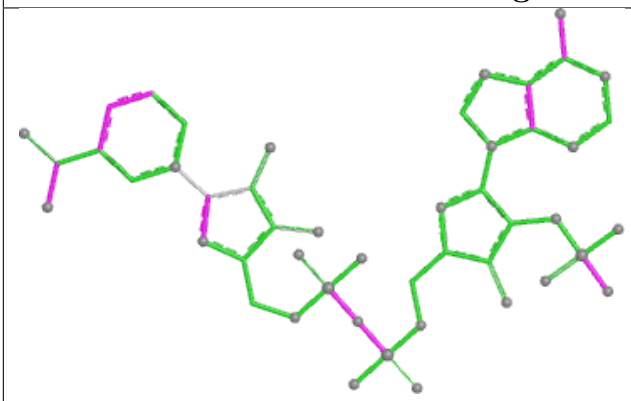


Torsions

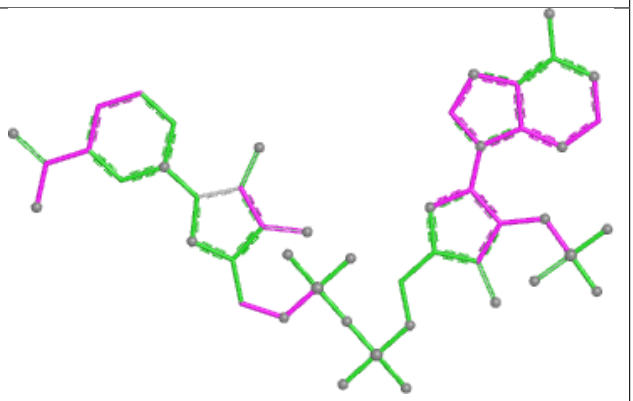


Rings

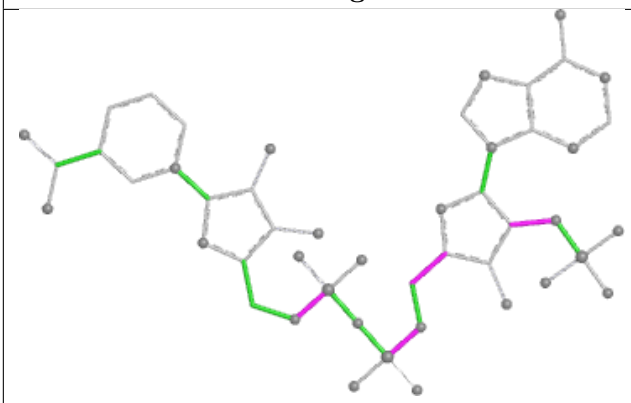
Ligand NAP C 1454



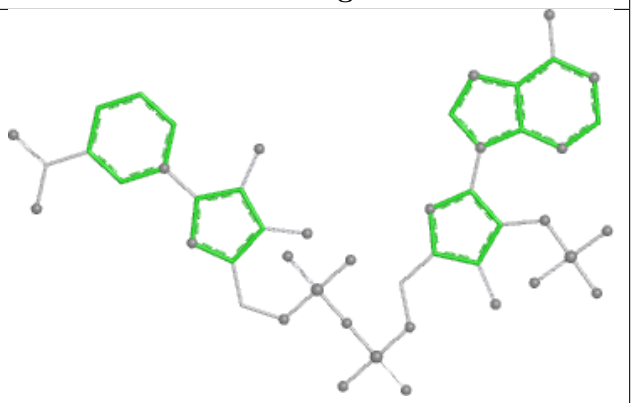
Bond lengths



Bond angles

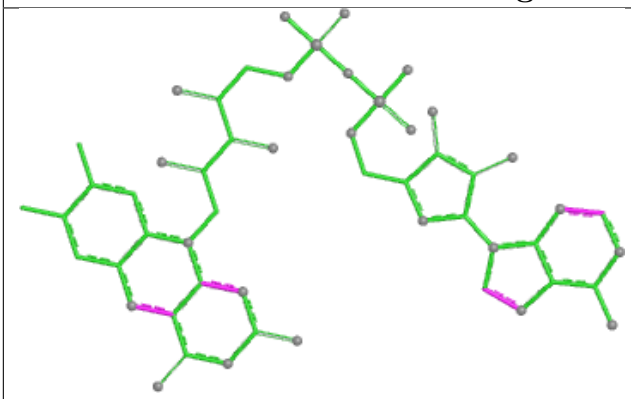


Torsions

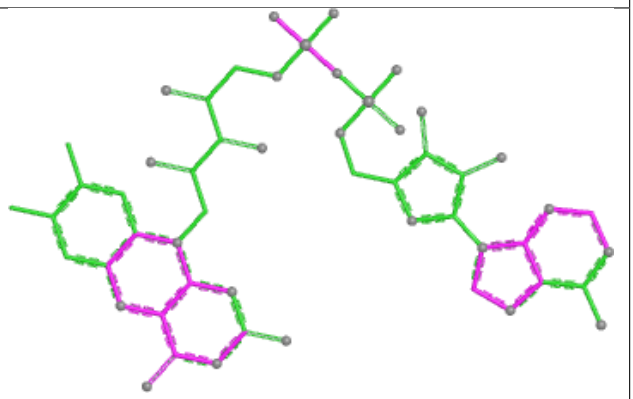


Rings

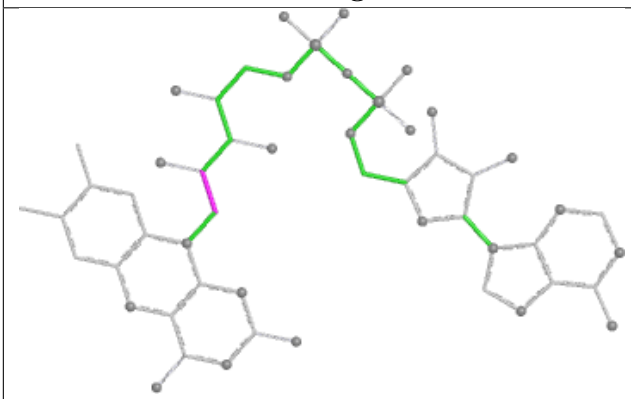
Ligand FAD B 1451



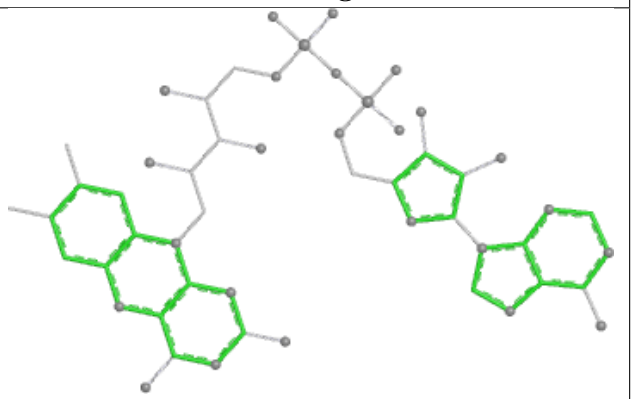
Bond lengths



Bond angles

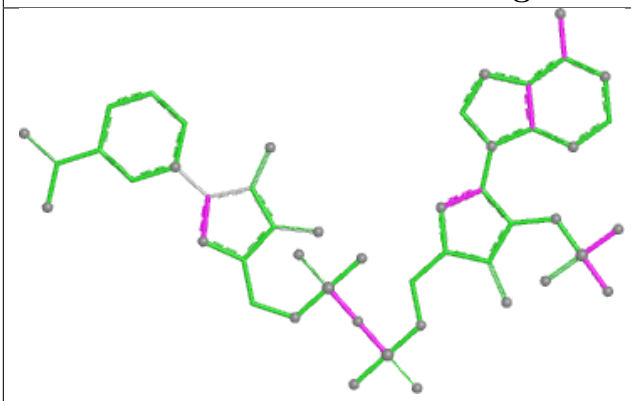


Torsions

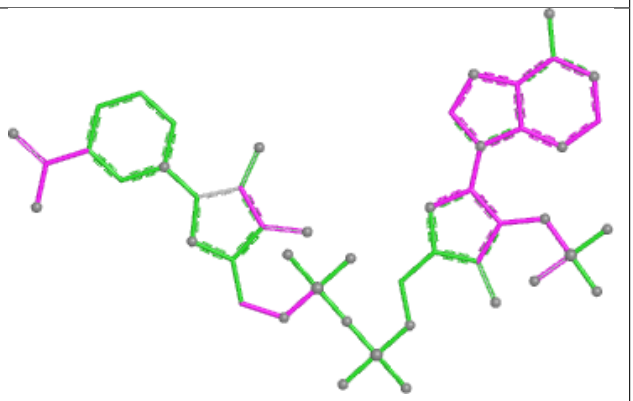


Rings

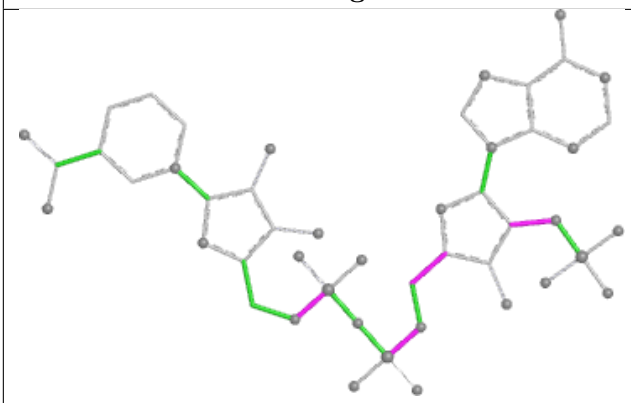
Ligand NAP B 1452



Bond lengths



Bond angles



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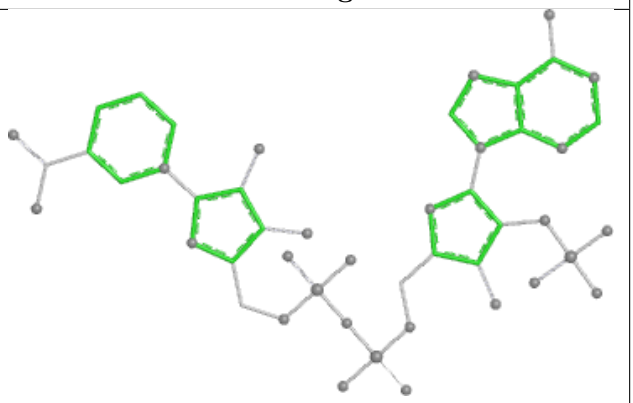
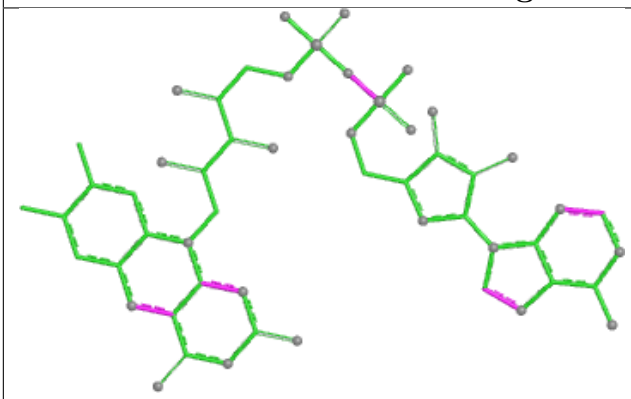


Rings

Ligand FAD C 1453



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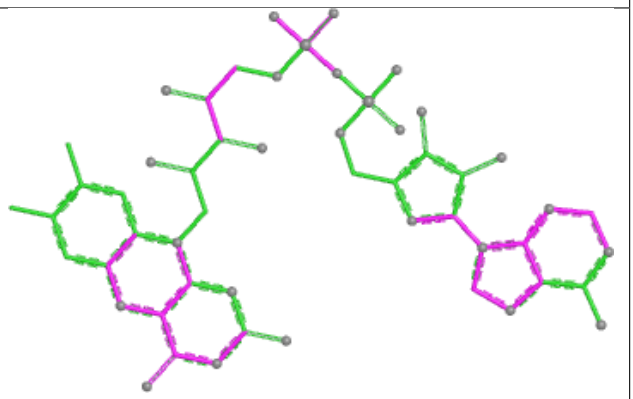
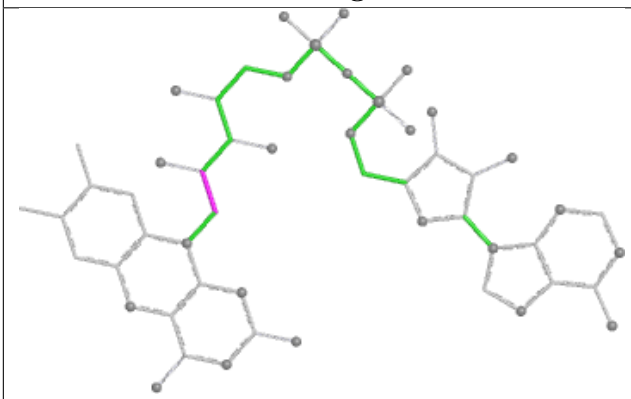


Bond angles



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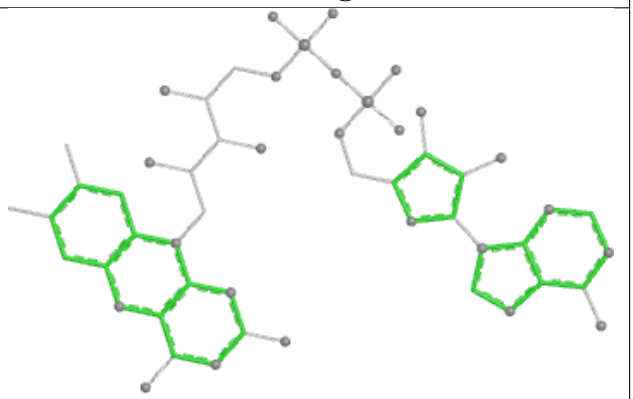
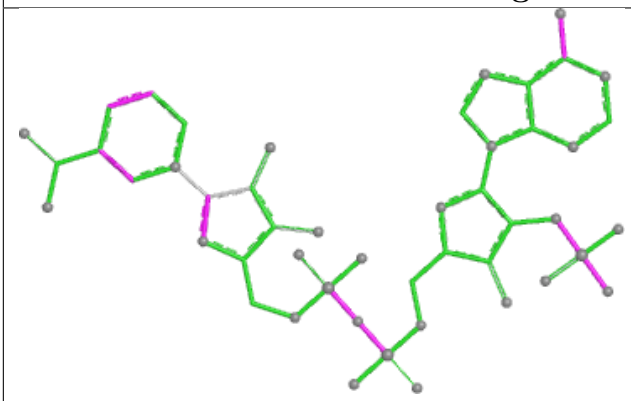
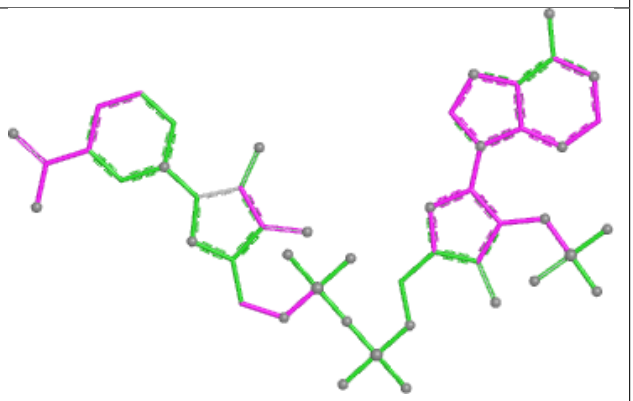


Rings

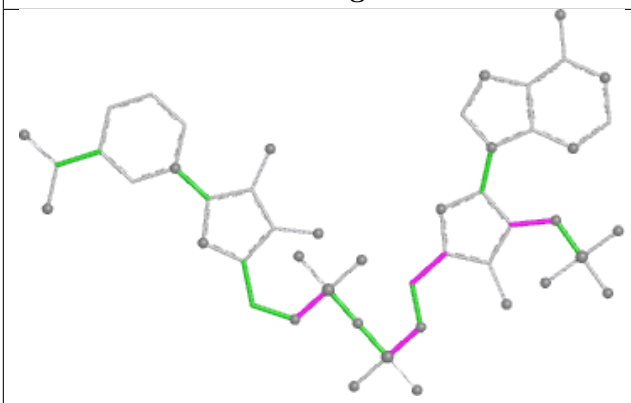
Ligand NAP D 1452



Bond lengths



Bond angles



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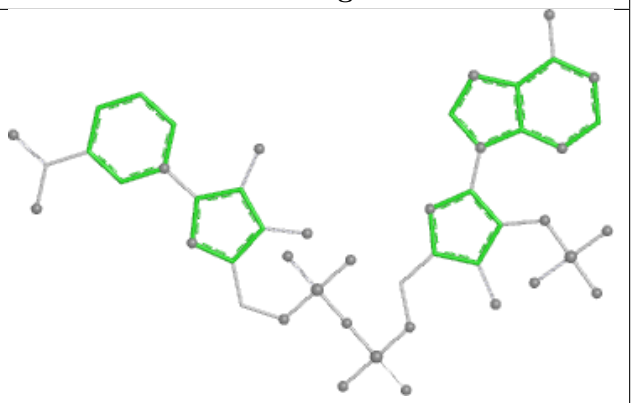
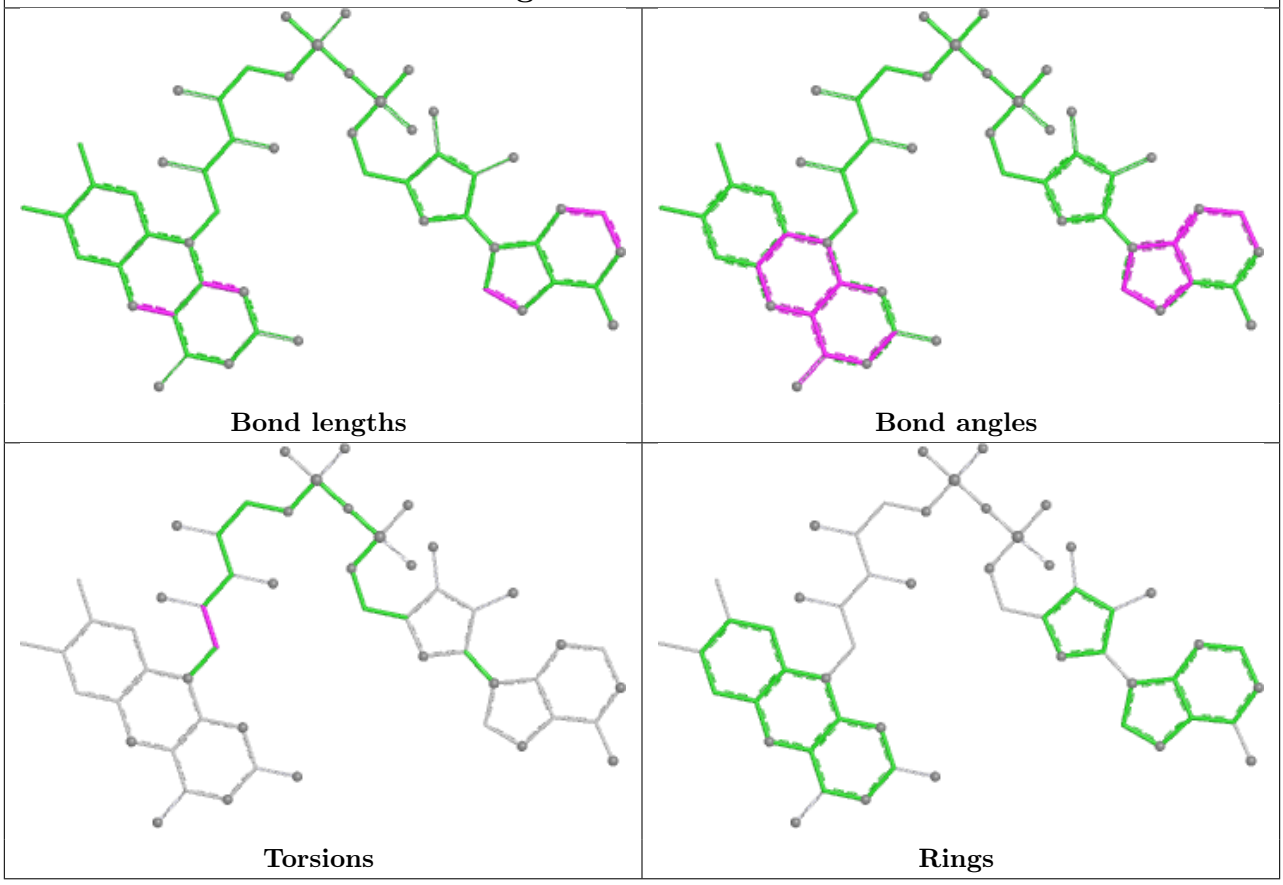


Rings

Ligand FAD D 1451



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	443/461 (96%)	0.42	23 (5%)	33	27	41, 51, 64, 73	0
1	B	443/461 (96%)	0.38	20 (4%)	38	32	41, 51, 65, 73	0
1	C	445/461 (96%)	0.35	12 (2%)	56	50	41, 51, 65, 73	0
1	D	443/461 (96%)	0.41	16 (3%)	46	40	41, 51, 65, 73	0
All	All	1774/1844 (96%)	0.39	71 (4%)	42	37	41, 51, 65, 73	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	236	ALA	5.2
1	D	247	ASP	3.7
1	A	262	PHE	3.6
1	B	427	GLY	3.5
1	C	256	ASP	3.4
1	B	247	ASP	3.4
1	B	244	GLU	3.3
1	C	452	LYS	3.3
1	A	263	ALA	3.2
1	A	237	PRO	3.0
1	B	241	LYS	3.0
1	A	8	THR	3.0
1	D	8	THR	2.9
1	B	400	LYS	2.9
1	C	244	GLU	2.9
1	A	251	ASN	2.9
1	B	432	LYS	2.9
1	A	264	ASP	2.9
1	A	235	THR	2.9
1	B	428	THR	2.9
1	B	267	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	422	ARG	2.8
1	C	241	LYS	2.7
1	A	231	SER	2.7
1	B	410	LYS	2.6
1	D	428	THR	2.6
1	D	407	HIS	2.6
1	D	256	ASP	2.5
1	D	422	ARG	2.5
1	D	244	GLU	2.5
1	B	422	ARG	2.5
1	C	451	ASP	2.5
1	C	428	THR	2.4
1	A	410	LYS	2.4
1	D	235	THR	2.4
1	B	446	GLU	2.4
1	B	239	GLY	2.4
1	D	239	GLY	2.4
1	D	269	LYS	2.3
1	B	411	GLU	2.3
1	B	429	MET	2.3
1	B	211	SER	2.3
1	A	233	TYR	2.3
1	C	233	TYR	2.3
1	C	410	LYS	2.2
1	A	265	GLY	2.2
1	A	427	GLY	2.2
1	C	446	GLU	2.2
1	A	92	ASP	2.2
1	A	269	LYS	2.2
1	A	183	LYS	2.2
1	D	241	LYS	2.2
1	A	429	MET	2.2
1	B	407	HIS	2.2
1	A	182	GLU	2.1
1	D	436	PRO	2.1
1	A	446	GLU	2.1
1	D	432	LYS	2.1
1	C	120	GLY	2.1
1	B	139	ASP	2.1
1	B	256	ASP	2.1
1	C	264	ASP	2.1
1	A	238	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	264	ASP	2.1
1	C	422	ARG	2.1
1	B	102	TYR	2.1
1	B	416	PHE	2.1
1	A	234	ARG	2.0
1	A	266	SER	2.0
1	D	183	LYS	2.0
1	D	328	ASN	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	EPE	C	1456	15/15	0.67	0.33	87,93,105,105	0
5	EPE	D	1454	15/15	0.70	0.28	93,95,106,106	0
5	EPE	A	1454	15/15	0.72	0.24	82,85,99,99	0
5	EPE	A	1455	15/15	0.72	0.25	86,88,100,100	0
6	PGE	A	1456	10/10	0.82	0.24	99,101,103,104	0
7	PG4	B	1453	13/13	0.86	0.17	60,64,72,72	0
3	NAP	A	1452	48/48	0.91	0.10	32,36,44,48	0
3	NAP	D	1452	48/48	0.91	0.11	32,36,44,47	0
3	NAP	C	1454	48/48	0.92	0.10	32,36,44,47	0
3	NAP	B	1452	48/48	0.93	0.09	32,36,44,47	0
4	CL	A	1453	1/1	0.95	0.23	58,58,58,58	0
4	CL	C	1455	1/1	0.95	0.21	56,56,56,56	0
4	CL	D	1453	1/1	0.95	0.26	64,64,64,64	0
2	FAD	B	1451	53/53	0.97	0.08	37,45,46,47	0
2	FAD	C	1453	53/53	0.97	0.08	38,44,46,47	0

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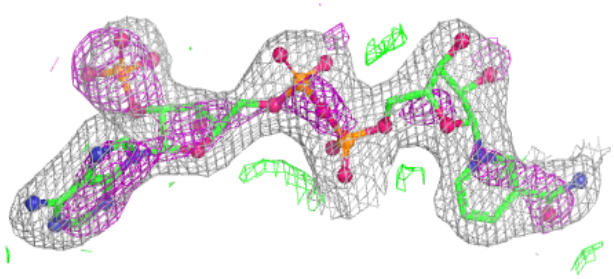
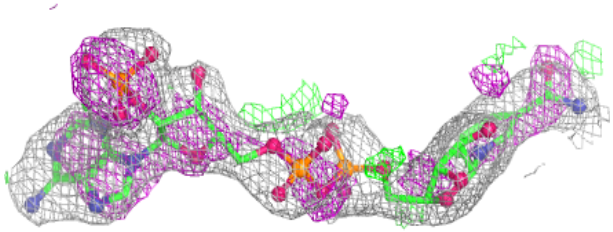
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	D	1451	53/53	0.97	0.08	38,44,46,47	0
2	FAD	A	1451	53/53	0.97	0.08	37,45,46,47	0
4	CL	B	1454	1/1	0.98	0.24	58,58,58,58	0

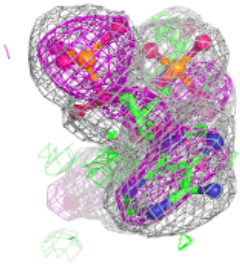
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP A 1452:

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

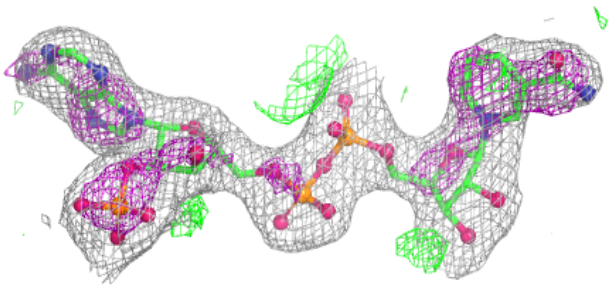


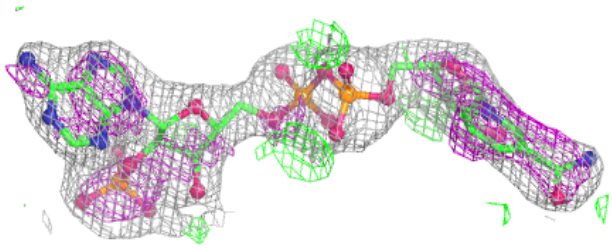


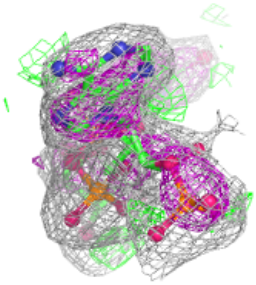


Electron density around NAP D 1452:

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

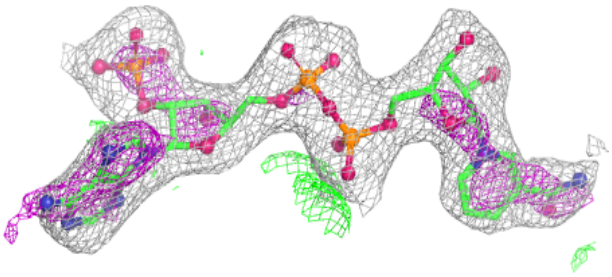


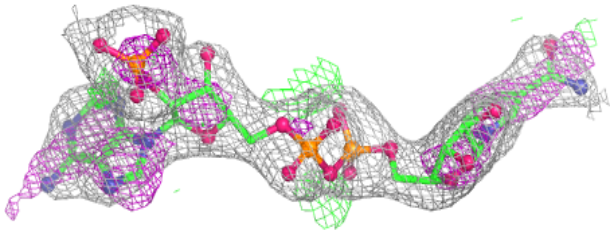


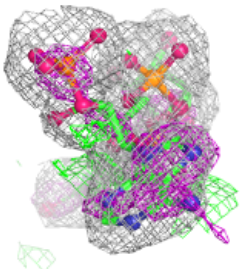


Electron density around NAP C 1454:

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

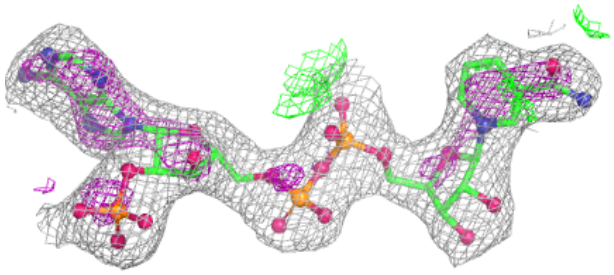


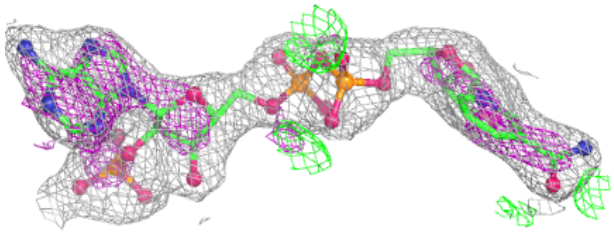


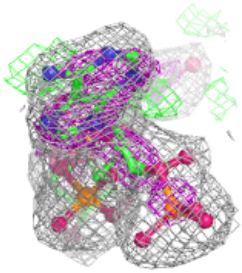


Electron density around NAP B 1452:

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

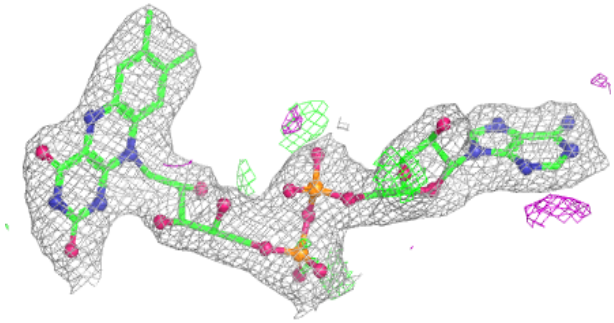


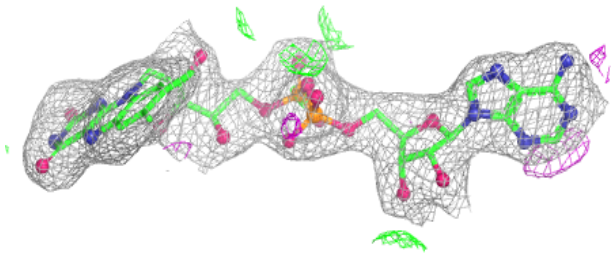


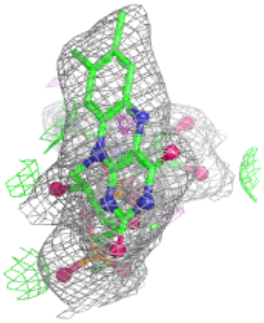


Electron density around FAD B 1451:

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

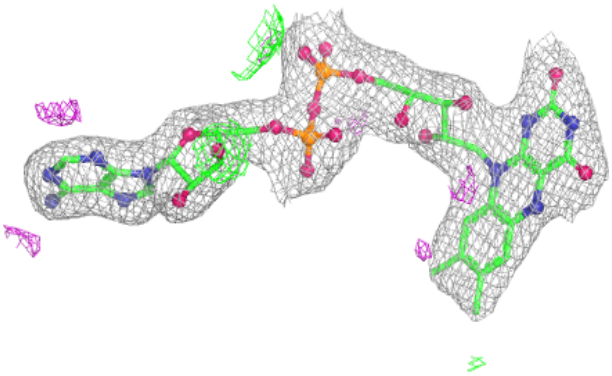


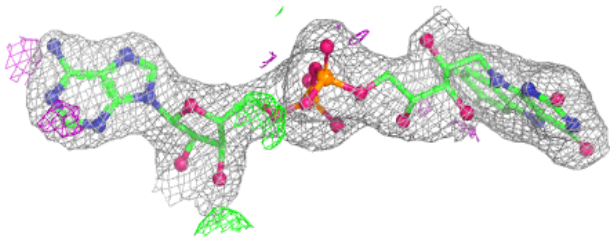


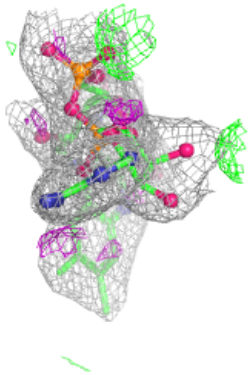


Electron density around FAD C 1453:

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

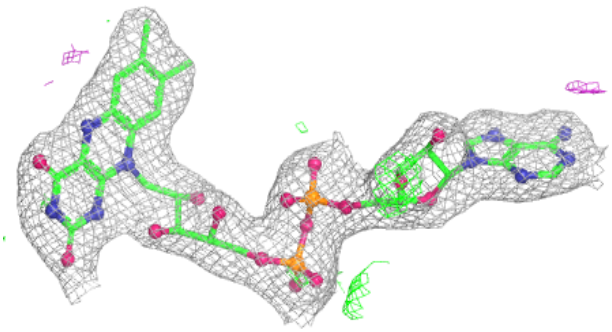


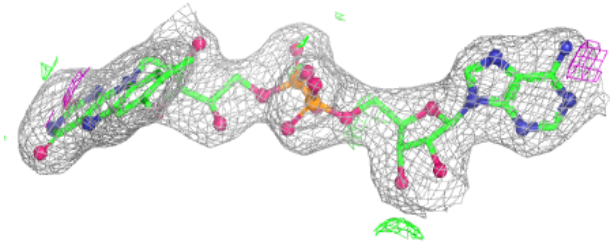


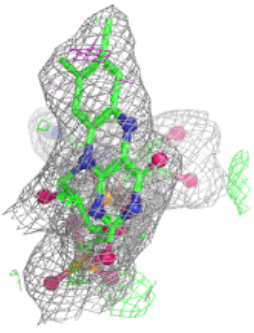


Electron density around FAD D 1451:

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

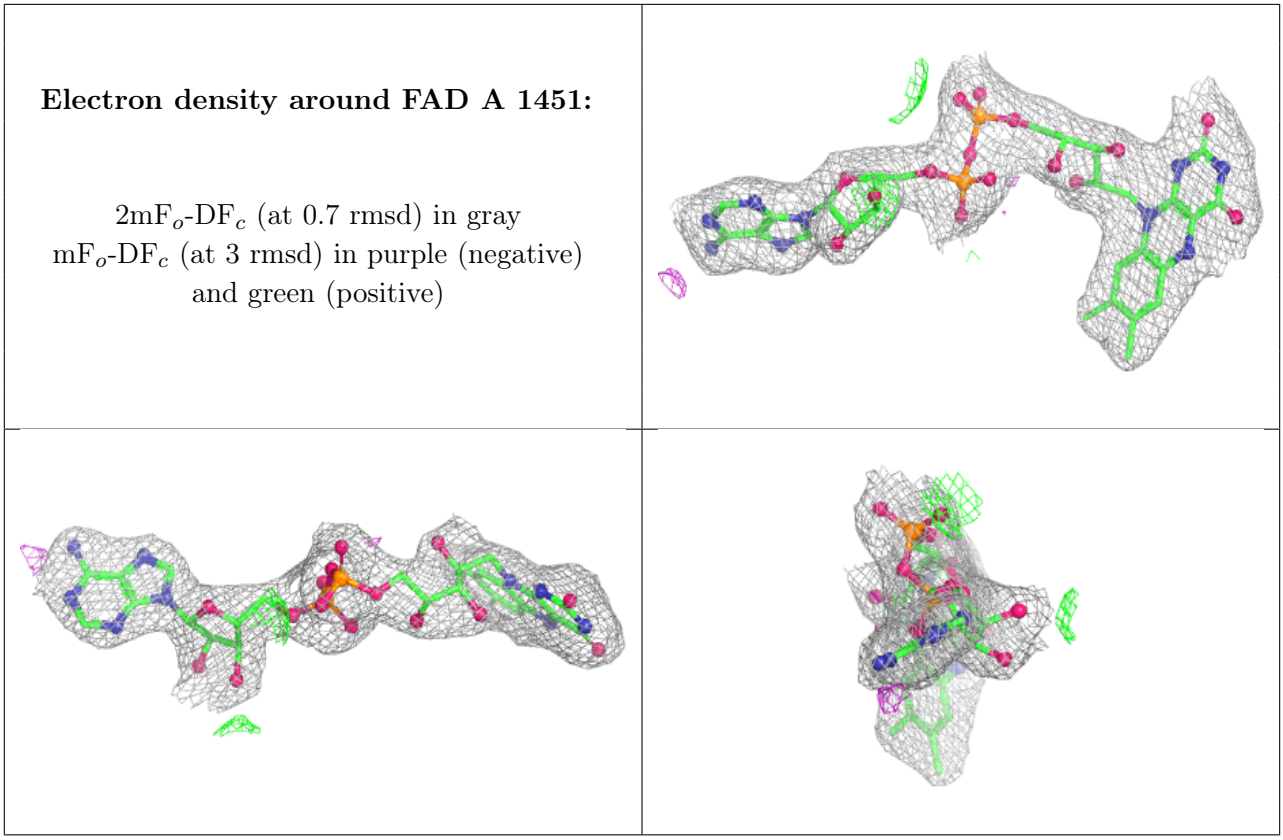






Electron density around FAD A 1451:

$2mF_o$-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.