Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 08:12 pm BST

PDB ID	:	2VQ7
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 following versions of software and data (see references ⓘ) were used in the production of this report:

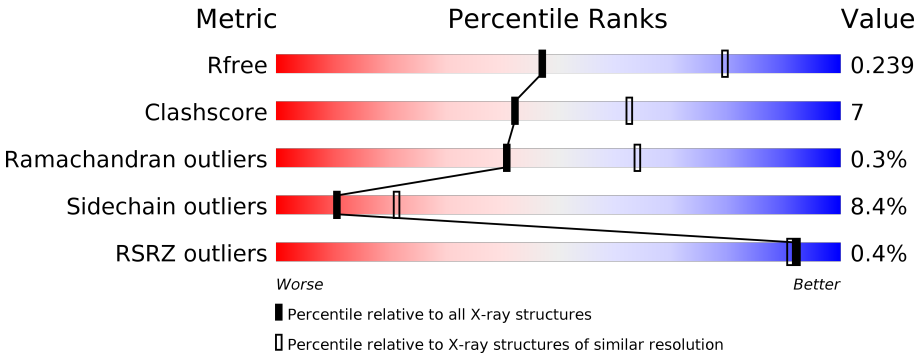
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on 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	78% 15%
1	B	461	78% 16%
1	C	461	79% 15%
1	D	461	78% 15%

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 crite-

ria:

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.

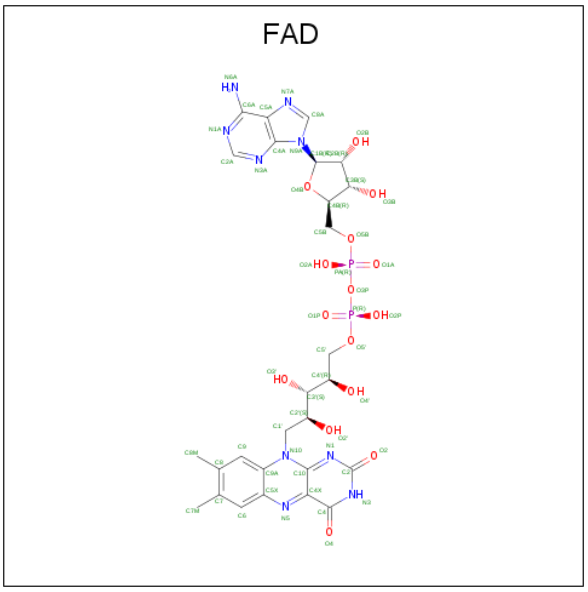
- Molecule 1 is a protein called FLAVIN-CONTAINING MONOOXYGENASE.

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:

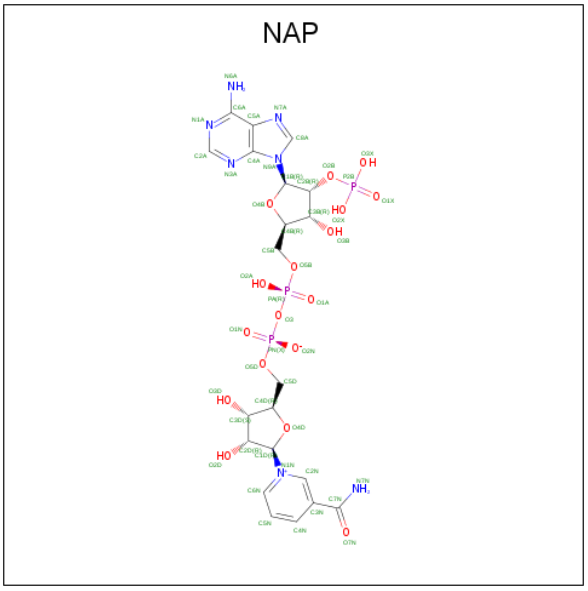
Chain	Residue	Modelled	Actual	Comment	Reference
A	158	ALA	GLU	engineered mutation	UNP Q83XK4
A	159	ALA	GLU	engineered mutation	UNP Q83XK4
B	158	ALA	GLU	engineered mutation	UNP Q83XK4
B	159	ALA	GLU	engineered mutation	UNP Q83XK4
C	158	ALA	GLU	engineered mutation	UNP Q83XK4
C	159	ALA	GLU	engineered mutation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

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: 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 (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

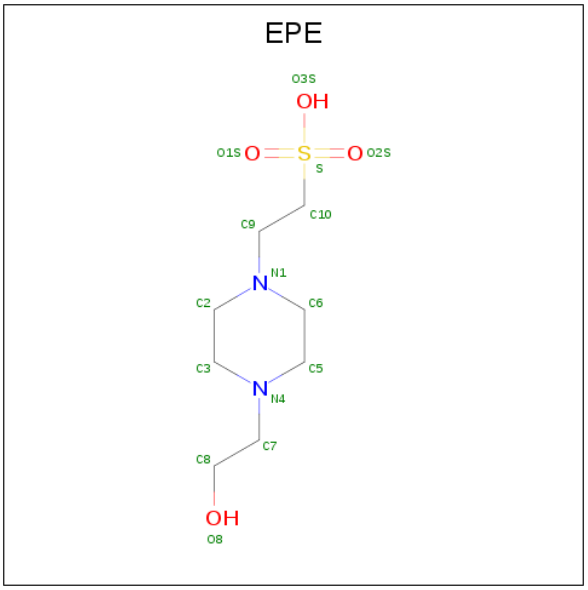


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: 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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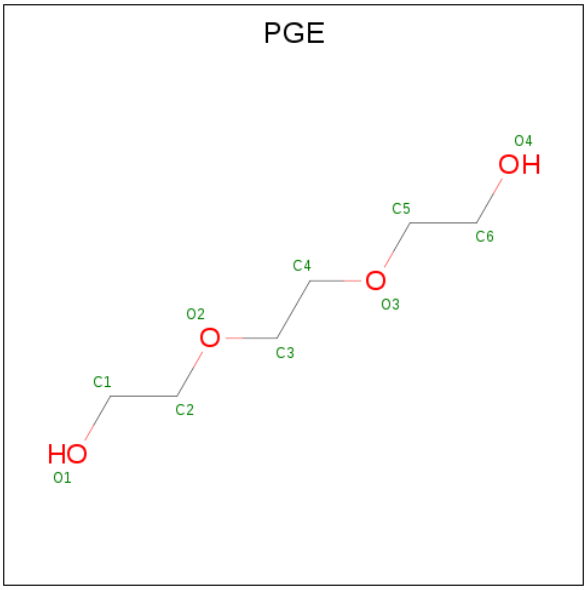
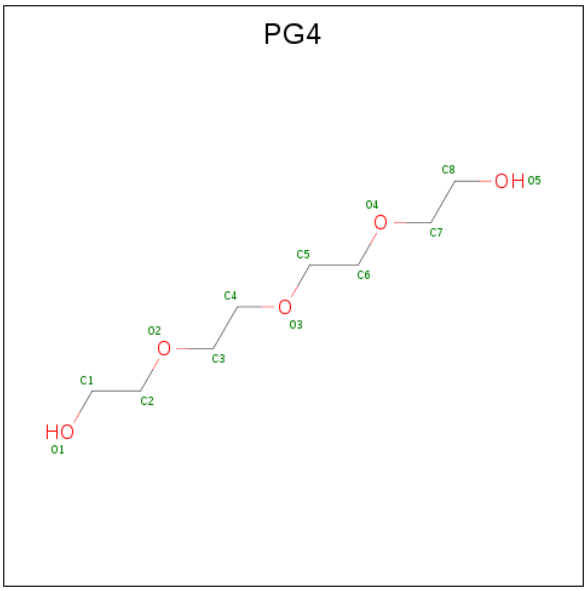
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: 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 (three-letter code: 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.

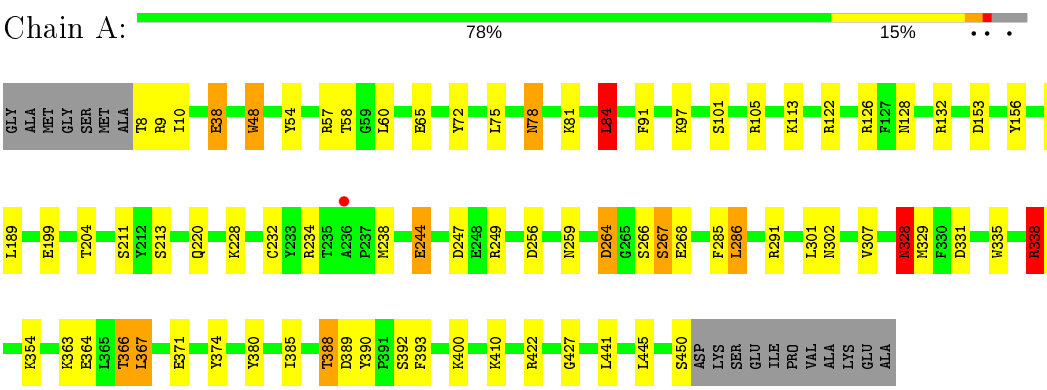
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	41	Total O 41 41	0	0
8	B	33	Total O 33 33	0	0
8	C	26	Total O 26 26	0	0
8	D	24	Total O 24 24	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

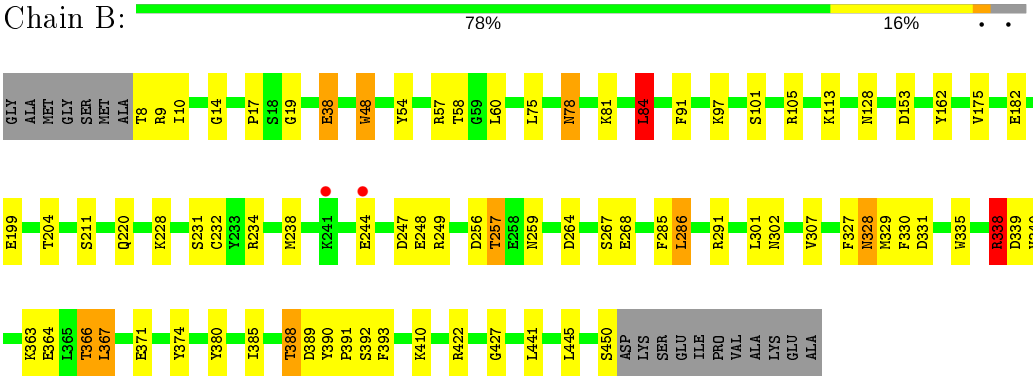
- Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

Chain A:



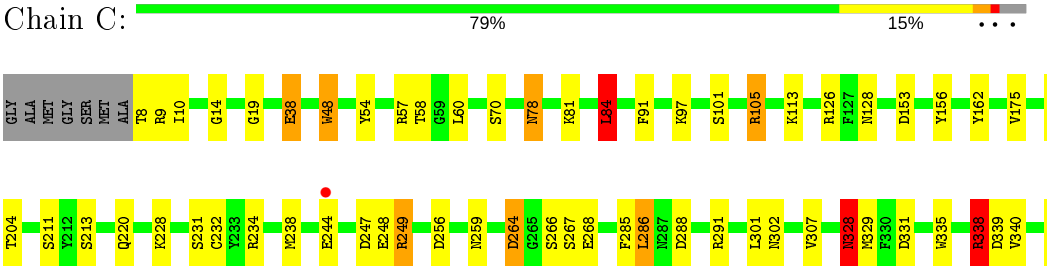
- Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

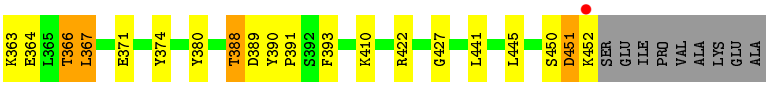
Chain B:



- Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

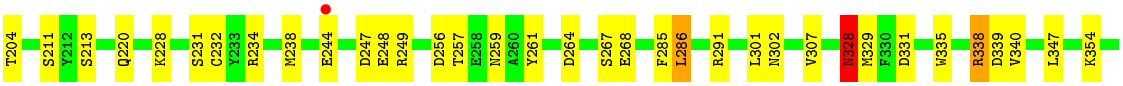
Chain C:

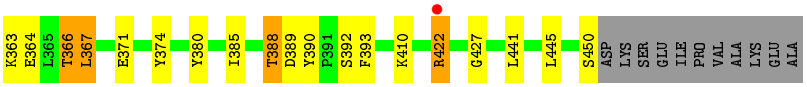




- Molecule 1: FLAVIN-CONTAINING MONOOXYGENASE

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 57.07 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.1 (188.98-2.60) 98.1 (57.07-2.60)	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 0.226 , 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 , 21.9	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: PGE, CL, NAP, PG4, EPE, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.60	0/3752	0.68	4/5095 (0.1%)
1	B	0.60	1/3752 (0.0%)	0.68	3/5095 (0.1%)
1	C	0.60	0/3769	0.68	4/5117 (0.1%)
1	D	0.59	0/3752	0.67	3/5095 (0.1%)
All	All	0.59	1/15025 (0.0%)	0.68	14/20402 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	GLU	CG-CD	5.06	1.59	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	84	LEU	CA-CB-CG	6.49	130.23	115.30
1	A	338	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	C	338	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	445	LEU	CA-CB-CG	6.00	129.11	115.30
1	A	84	LEU	CA-CB-CG	5.93	128.94	115.30
1	D	445	LEU	CA-CB-CG	5.92	128.92	115.30
1	A	445	LEU	CA-CB-CG	5.80	128.65	115.30
1	C	445	LEU	CA-CB-CG	5.76	128.54	115.30
1	B	84	LEU	CA-CB-CG	5.75	128.53	115.30
1	D	84	LEU	CA-CB-CG	5.65	128.30	115.30
1	B	338	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	D	328	ASN	N-CA-CB	-5.37	100.93	110.60
1	A	122	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	328	ASN	N-CA-CB	-5.02	101.56	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3638	0	3428	49	0
1	B	3638	0	3428	48	0
1	C	3655	0	3445	53	0
1	D	3638	0	3428	49	0
2	A	53	0	31	1	0
2	B	53	0	31	1	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	1	0
8	C	26	0	0	1	0
8	D	24	0	0	1	0
All	All	15184	0	14055	200	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (200) 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:C5	5:C:1456:EPE:O8	2.18	0.90
1:A:388:THR:HG22	1:A:390:TYR:H	1.38	0.88
5:C:1456:EPE:H52	5:C:1456:EPE:O8	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
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:D:126:ARG:NH1	5:D:1454:EPE:H91	2.06	0.70
1:A:57:ARG:NH2	1:D:175:VAL:O	2.23	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: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:B:329:MET:HE2	1:B:380:TYR:HE2	1.61	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: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
5:A:1454:EPE:C5	5:A:1454:EPE:O8	2.40	0.64
1:A:175:VAL:O	1:D:57:ARG:NH2	2.30	0.64
1:B:256:ASP:HB3	1:B:259:ASN:H	1.62	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:335:TRP:HB3	1:A:388:THR:HG21	1.80	0.62
1:A:81:LYS:HG2	1:A:91:PHE:CE2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1455:EPE:H51	5:A:1455:EPE:O8	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:422:ARG:HD3	1:A:427:GLY:O	2.01	0.61
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:329:MET:HE2	1:A:380:TYR:HE2	1.67	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: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: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:B:329:MET:HE2	1:B:380:TYR:CE2	2.40	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
1:D:329:MET:HE2	1:D:380:TYR:HE2	1.71	0.55
5:A:1455:EPE:C5	5:A:1455:EPE:O8	2.55	0.55
1:C:329:MET:HE2	1:C:380:TYR:HE2	1.71	0.54
1:D:285:PHE:HD1	1:D:286:LEU:HD13	1.66	0.54
5:A:1454:EPE:H51	5:A:1454:EPE:HO8	1.65	0.54
1:A:285:PHE:HD1	1:A:286:LEU:HD13	1.71	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:301:LEU:O	1:B:302:ASN:HB2	2.07	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: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:D:126:ARG:HH12	5:D:1454:EPE:H91	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:B:231:SER:HB2	1:B:248:GLU:HG2	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:D:78:ASN:H	1:D:78:ASN:HD22	1.60	0.50
1:A:329:MET:HE2	1:A:380:TYR:CE2	2.46	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: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:C:156:TYR:CE1	5:C:1456:EPE:H61	2.49	0.48
1:B:175:VAL:HB	1:C:57:ARG:HH21	1.78	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: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: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:C:231:SER:HB2	1:C:248:GLU:HG2	1.97	0.47
1:A:57:ARG:HH21	1:D:175:VAL:HB	1.80	0.47
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:B:81:LYS:O	1:B:84:LEU:HD22	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:ARG:HG3	1:D:38:GLU:HB2	1.98	0.46
1:B:267:SER:O	1:B:268:GLU:HG2	2.15	0.45
1:B:57:ARG:HH21	1:C:175:VAL:HB	1.82	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:C:331:ASP:HB3	1:C:390:TYR:CE1	2.52	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:C:329:MET:HE3	1:C:380:TYR:HD2	1.82	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:HD22	1:A:78:ASN:H	1.64	0.44
1:B:338:ARG:HG3	1:B:339:ASP:N	2.31	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:C:329:MET:HE2	1:C:380:TYR:CE2	2.51	0.44
1:B:331:ASP:HB3	1:B:390:TYR:CE1	2.53	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:385:ILE:HD12	1:A:392:SER:HA	2.00	0.43
1:C:329:MET:HE3	1:C:380:TYR:CD2	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:126:ARG:NH2	5:C:1456:EPE:H91	2.34	0.43
1:C:78:ASN:H	1:C:78:ASN:HD22	1.65	0.43
1:D:329:MET:HE3	1:D:380:TYR:HD2	1.84	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:D:329:MET:HE2	1:D:380:TYR:CE2	2.52	0.43
1:C:338:ARG:HG3	1:C:339:ASP:N	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:70:SER:HB2	2:C:1453:FAD:HM82	2.02	0.42
1:D:213:SER:HA	3:D:1452:NAP:H5N	2.02	0.42
1:A:364:GLU:HA	1:A:367:LEU:HD22	2.02	0.42
1:A:175:VAL:HB	1:D:57:ARG:HH21	1.85	0.42
1:A:385:ILE:O	8:A:2035:HOH:O	2.21	0.41
1:C:264:ASP:HB3	1:C:266:SER:H	1.85	0.41
1:A:267:SER:O	1:A:268:GLU:HG2	2.20	0.41
1:A:9:ARG:HG3	1:A:38:GLU:HB2	2.03	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:H62	5:A:1455:EPE:H102	1.84	0.41
1:D:329:MET:HE3	1:D:380:TYR:CD2	2.54	0.41
1:A:331:ASP:HB3	1:A:390:TYR:CE1	2.56	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:D:43:GLU:OE2	2:D:1451:FAD:O2B	2.34	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
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: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%)	29	52
1	B	441/461 (96%)	415 (94%)	25 (6%)	1 (0%)	47	71
1	C	443/461 (96%)	421 (95%)	20 (4%)	2 (0%)	29	52
1	D	441/461 (96%)	416 (94%)	24 (5%)	1 (0%)	47	71
All	All	1766/1844 (96%)	1666 (94%)	94 (5%)	6 (0%)	41	64

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
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%)	11	22
1	B	385/397 (97%)	353 (92%)	32 (8%)	11	22
1	C	387/397 (98%)	354 (92%)	33 (8%)	10	21
1	D	385/397 (97%)	353 (92%)	32 (8%)	11	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1542/1588 (97%)	1413 (92%)	129 (8%)	11 21

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	38	GLU
1	A	48	TRP
1	A	58	THR
1	A	60	LEU
1	A	78	ASN
1	A	84	LEU
1	A	97	LYS
1	A	128	ASN
1	A	189	LEU
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	264	ASP
1	A	267	SER
1	A	286	LEU
1	A	307	VAL
1	A	328	ASN
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	450	SER
1	B	8	THR
1	B	17	PRO
1	B	38	GLU
1	B	48	TRP
1	B	58	THR

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Mol	Chain	Res	Type
1	B	60	LEU
1	B	78	ASN
1	B	84	LEU
1	B	97	LYS
1	B	128	ASN
1	B	189	LEU
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	257	THR
1	B	264	ASP
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	410	LYS
1	B	441	LEU
1	B	450	SER
1	C	8	THR
1	C	38	GLU
1	C	48	TRP
1	C	58	THR
1	C	60	LEU
1	C	78	ASN
1	C	84	LEU
1	C	97	LYS
1	C	105	ARG
1	C	128	ASN
1	C	189	LEU
1	C	199	GLU
1	C	220	GLN
1	C	234	ARG
1	C	238	MET

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Mol	Chain	Res	Type
1	C	244	GLU
1	C	247	ASP
1	C	249	ARG
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	410	LYS
1	C	441	LEU
1	C	450	SER
1	C	451	ASP
1	D	8	THR
1	D	38	GLU
1	D	48	TRP
1	D	58	THR
1	D	60	LEU
1	D	78	ASN
1	D	84	LEU
1	D	97	LYS
1	D	128	ASN
1	D	189	LEU
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	257	THR
1	D	264	ASP
1	D	286	LEU
1	D	307	VAL
1	D	328	ASN
1	D	338	ARG
1	D	340	VAL
1	D	347	LEU

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Mol	Chain	Res	Type
1	D	354	LYS
1	D	366	THR
1	D	367	LEU
1	D	388	THR
1	D	410	LYS
1	D	422	ARG
1	D	441	LEU
1	D	450	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	128	ASN
1	A	148	GLN
1	A	328	ASN
1	B	63	ASN
1	B	128	ASN
1	B	148	GLN
1	B	328	ASN
1	C	63	ASN
1	C	78	ASN
1	C	128	ASN
1	C	148	GLN
1	C	328	ASN
1	D	63	ASN
1	D	78	ASN
1	D	128	ASN
1	D	148	GLN
1	D	328	ASN

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 (i)

There are no carbohydrates 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	$\#\|Z\| > 2$
3	NAP	A	1452	-	45,52,52	1.46	6 (13%)	56,80,80	1.59	10 (17%)
5	EPE	A	1455	-	15,15,15	1.13	1 (6%)	18,20,20	2.50	8 (44%)
7	PG4	B	1453	-	12,12,12	0.62	0	11,11,11	0.24	0
3	NAP	D	1452	-	45,52,52	1.29	5 (11%)	56,80,80	1.54	8 (14%)
2	FAD	A	1451	-	51,58,58	1.35	7 (13%)	60,89,89	1.69	9 (15%)
5	EPE	A	1454	-	15,15,15	1.29	1 (6%)	18,20,20	2.25	6 (33%)
3	NAP	C	1454	-	45,52,52	1.40	5 (11%)	56,80,80	1.52	7 (12%)
3	NAP	B	1452	-	45,52,52	1.43	4 (8%)	56,80,80	1.63	9 (16%)
2	FAD	B	1451	-	51,58,58	1.38	5 (9%)	60,89,89	1.82	10 (16%)
6	PGE	A	1456	-	9,9,9	0.54	0	8,8,8	0.16	0
5	EPE	C	1456	-	15,15,15	1.21	1 (6%)	18,20,20	2.24	5 (27%)
2	FAD	C	1453	-	51,58,58	1.31	5 (9%)	60,89,89	1.92	11 (18%)
2	FAD	D	1451	-	51,58,58	1.39	6 (11%)	60,89,89	1.86	11 (18%)
5	EPE	D	1454	-	15,15,15	1.22	1 (6%)	18,20,20	2.35	6 (33%)

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
3	NAP	A	1452	-	-	9/31/67/67	0/5/5/5
5	EPE	A	1455	-	-	7/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PG4	B	1453	-	-	3/10/10/10	-
3	NAP	D	1452	-	-	10/31/67/67	0/5/5/5
2	FAD	A	1451	-	-	3/30/50/50	0/6/6/6
5	EPE	A	1454	-	-	7/9/19/19	0/1/1/1
3	NAP	C	1454	-	-	10/31/67/67	0/5/5/5
3	NAP	B	1452	-	-	9/31/67/67	0/5/5/5
2	FAD	B	1451	-	-	3/30/50/50	0/6/6/6
6	PGE	A	1456	-	-	3/7/7/7	-
5	EPE	C	1456	-	-	6/9/19/19	0/1/1/1
2	FAD	C	1453	-	-	3/30/50/50	0/6/6/6
2	FAD	D	1451	-	-	3/30/50/50	0/6/6/6
5	EPE	D	1454	-	-	5/9/19/19	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1452	NAP	O4B-C1B	5.36	1.48	1.41
2	D	1451	FAD	C2A-N3A	4.40	1.39	1.32
2	D	1451	FAD	C10-N1	4.39	1.38	1.33
5	A	1454	EPE	C10-S	4.31	1.83	1.77
2	C	1453	FAD	C2A-N3A	4.29	1.39	1.32
2	B	1451	FAD	C10-N1	4.27	1.38	1.33
3	A	1452	NAP	P2B-O1X	4.21	1.64	1.50
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	3.91	1.83	1.77
3	C	1454	NAP	O4D-C1D	3.89	1.46	1.41
3	A	1452	NAP	O4D-C1D	3.82	1.46	1.41
3	B	1452	NAP	O4D-C1D	3.81	1.46	1.41
2	B	1451	FAD	C2A-N3A	3.80	1.38	1.32
3	C	1454	NAP	O4B-C1B	3.79	1.46	1.41
3	A	1452	NAP	O4B-C1B	3.73	1.46	1.41
2	A	1451	FAD	C2A-N3A	3.65	1.38	1.32
2	A	1451	FAD	C1'-N10	3.58	1.51	1.48
2	A	1451	FAD	C10-N1	3.49	1.37	1.33
2	C	1453	FAD	C10-N1	3.41	1.37	1.33
2	D	1451	FAD	C4X-N5	3.40	1.38	1.33
2	A	1451	FAD	C4X-N5	3.39	1.38	1.33
2	B	1451	FAD	C4-N3	3.38	1.38	1.33
3	D	1452	NAP	O4B-C1B	3.26	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1451	FAD	C4X-N5	3.19	1.37	1.33
2	C	1453	FAD	C4-N3	3.14	1.38	1.33
2	C	1453	FAD	C4X-N5	3.10	1.37	1.33
2	B	1451	FAD	C1'-N10	3.03	1.51	1.48
3	D	1452	NAP	O4D-C1D	3.02	1.45	1.41
2	D	1451	FAD	C1'-N10	2.87	1.51	1.48
2	D	1451	FAD	C4-N3	2.68	1.37	1.33
3	D	1452	NAP	P2B-O2B	2.62	1.64	1.59
3	A	1452	NAP	C7N-N7N	2.53	1.37	1.33
3	D	1452	NAP	C2N-C3N	2.49	1.42	1.39
2	C	1453	FAD	C5X-N5	2.39	1.39	1.35
3	C	1454	NAP	P2B-O2X	2.37	1.64	1.54
2	A	1451	FAD	C4-N3	2.37	1.37	1.33
3	B	1452	NAP	P2B-O1X	2.36	1.58	1.50
3	A	1452	NAP	P2B-O2B	2.36	1.63	1.59
3	A	1452	NAP	P2B-O3X	2.32	1.63	1.54
2	D	1451	FAD	C2A-N1A	2.29	1.38	1.33
3	D	1452	NAP	P2B-O2X	2.22	1.63	1.54
2	A	1451	FAD	C2A-N1A	2.19	1.38	1.33
3	B	1452	NAP	P2B-O2X	2.17	1.63	1.54
3	C	1454	NAP	C7N-N7N	2.11	1.37	1.33
2	A	1451	FAD	O4B-C4B	-2.03	1.40	1.45
3	C	1454	NAP	C2N-C3N	2.01	1.42	1.39

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1453	FAD	C1'-N10-C9A	6.86	123.69	118.29
2	D	1451	FAD	C1'-N10-C9A	6.62	123.51	118.29
5	A	1455	EPE	C5-N4-C3	6.43	123.30	108.83
2	C	1453	FAD	C4-N3-C2	6.40	120.55	115.14
5	D	1454	EPE	C5-N4-C3	6.35	123.11	108.83
5	C	1456	EPE	C5-N4-C3	6.16	122.69	108.83
2	D	1451	FAD	C4-N3-C2	6.08	120.27	115.14
2	C	1453	FAD	N3A-C2A-N1A	-6.02	119.26	128.68
2	B	1451	FAD	C1'-N10-C9A	5.99	123.01	118.29
2	A	1451	FAD	C4-N3-C2	5.92	120.14	115.14
2	B	1451	FAD	C4-N3-C2	5.55	119.83	115.14
2	D	1451	FAD	N3A-C2A-N1A	-5.49	120.10	128.68
2	B	1451	FAD	N3A-C2A-N1A	-5.48	120.11	128.68
3	C	1454	NAP	PN-O3-PA	-5.36	114.45	132.83
3	B	1452	NAP	PN-O3-PA	-5.33	114.55	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1452	NAP	PN-O3-PA	-5.30	114.63	132.83
2	A	1451	FAD	C1'-N10-C9A	5.07	122.28	118.29
3	A	1452	NAP	PN-O3-PA	-5.03	115.56	132.83
2	A	1451	FAD	N3A-C2A-N1A	-4.91	121.00	128.68
5	A	1454	EPE	C5-N4-C3	4.90	119.86	108.83
3	A	1452	NAP	C3N-C7N-N7N	4.78	123.49	117.75
3	B	1452	NAP	N3A-C2A-N1A	-4.68	121.37	128.68
3	C	1454	NAP	N3A-C2A-N1A	-4.36	121.86	128.68
5	A	1454	EPE	C6-N1-C2	4.33	118.57	108.83
3	D	1452	NAP	N3A-C2A-N1A	-4.21	122.10	128.68
3	B	1452	NAP	C3N-C7N-N7N	4.16	122.74	117.75
3	A	1452	NAP	N3A-C2A-N1A	-3.91	122.56	128.68
5	D	1454	EPE	O1S-S-C10	3.91	111.62	106.92
5	C	1456	EPE	O1S-S-C10	3.88	111.58	106.92
2	D	1451	FAD	C4X-N5-C5X	3.79	120.56	116.77
2	B	1451	FAD	P-O3P-PA	-3.73	120.02	132.83
5	A	1455	EPE	O1S-S-C10	3.71	111.39	106.92
5	A	1454	EPE	C7-N4-C3	3.63	120.52	111.23
2	B	1451	FAD	C4X-N5-C5X	3.55	120.32	116.77
3	C	1454	NAP	C3B-C2B-C1B	-3.51	96.29	102.89
2	A	1451	FAD	C4X-N5-C5X	3.49	120.26	116.77
3	C	1454	NAP	C3N-C7N-N7N	3.43	121.87	117.75
2	A	1451	FAD	P-O3P-PA	-3.43	121.07	132.83
5	A	1455	EPE	O2S-S-C10	3.42	111.03	106.92
5	C	1456	EPE	C7-N4-C3	3.38	119.87	111.23
5	D	1454	EPE	C2-C3-N4	3.32	117.45	110.64
3	D	1452	NAP	C3N-C7N-N7N	3.31	121.72	117.75
2	C	1453	FAD	C4X-N5-C5X	3.29	120.06	116.77
2	D	1451	FAD	P-O3P-PA	-3.23	121.73	132.83
2	C	1453	FAD	P-O3P-PA	-3.22	121.77	132.83
3	A	1452	NAP	C3B-C2B-C1B	-3.18	96.92	102.89
5	A	1455	EPE	C6-N1-C2	3.17	115.96	108.83
3	D	1452	NAP	C3B-C2B-C1B	-3.06	97.14	102.89
3	B	1452	NAP	C3B-C2B-C1B	-3.05	97.16	102.89
5	A	1454	EPE	O2S-S-C10	2.97	110.49	106.92
2	A	1451	FAD	C4A-C5A-N7A	-2.94	106.33	109.40
2	B	1451	FAD	C5X-C9A-N10	2.92	119.83	117.72
5	A	1455	EPE	C6-C5-N4	2.90	116.59	110.64
5	A	1454	EPE	C7-N4-C5	2.88	118.61	111.23
3	B	1452	NAP	O7N-C7N-N7N	-2.88	118.48	122.58
2	D	1451	FAD	C5X-C9A-N10	2.88	119.80	117.72
3	B	1452	NAP	O3D-C3D-C2D	-2.80	102.77	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1454	EPE	C7-N4-C3	2.80	118.38	111.23
5	A	1454	EPE	O1S-S-C10	2.78	110.27	106.92
2	C	1453	FAD	C4X-C4-N3	-2.73	119.70	123.43
5	C	1456	EPE	C2-C3-N4	2.70	116.19	110.64
5	D	1454	EPE	C7-N4-C5	2.69	118.11	111.23
2	B	1451	FAD	C10-C4X-N5	-2.69	119.40	121.26
5	A	1455	EPE	C7-N4-C5	2.68	118.09	111.23
2	D	1451	FAD	C10-C4X-N5	-2.63	119.44	121.26
2	C	1453	FAD	C5X-C9A-N10	2.61	119.61	117.72
2	B	1451	FAD	C4A-C5A-N7A	-2.61	106.68	109.40
2	C	1453	FAD	C4A-C5A-N7A	-2.56	106.73	109.40
5	D	1454	EPE	O2S-S-C10	2.56	110.00	106.92
5	A	1455	EPE	C2-C3-N4	2.50	115.78	110.64
3	D	1452	NAP	PN-O5D-C5D	-2.49	107.05	121.68
3	D	1452	NAP	O7N-C7N-N7N	-2.49	119.04	122.58
3	C	1454	NAP	PN-O5D-C5D	-2.45	107.33	121.68
2	A	1451	FAD	C5X-C9A-N10	2.39	119.45	117.72
3	B	1452	NAP	PN-O5D-C5D	-2.37	107.75	121.68
2	B	1451	FAD	C4X-C4-N3	-2.33	120.24	123.43
3	A	1452	NAP	PN-O5D-C5D	-2.31	108.13	121.68
3	A	1452	NAP	O7N-C7N-N7N	-2.29	119.32	122.58
2	C	1453	FAD	C10-C4X-N5	-2.29	119.67	121.26
5	A	1455	EPE	C7-N4-C3	2.28	117.06	111.23
3	D	1452	NAP	C4A-C5A-N7A	-2.27	107.03	109.40
2	D	1451	FAD	C4X-C4-N3	-2.27	120.32	123.43
3	C	1454	NAP	O3D-C3D-C2D	-2.25	104.53	111.82
3	A	1452	NAP	O3D-C3D-C2D	-2.25	104.53	111.82
3	B	1452	NAP	C4A-C5A-N7A	-2.25	107.05	109.40
3	D	1452	NAP	C2A-N1A-C6A	2.24	122.58	118.75
2	D	1451	FAD	C4-C4X-N5	2.24	121.15	118.60
2	C	1453	FAD	C1'-N10-C10	-2.22	116.42	118.41
3	C	1454	NAP	C4A-C5A-N7A	-2.22	107.09	109.40
2	D	1451	FAD	C4A-C5A-N7A	-2.21	107.10	109.40
2	A	1451	FAD	C4X-C4-N3	-2.19	120.44	123.43
2	C	1453	FAD	C5'-C4'-C3'	2.17	116.40	112.20
2	B	1451	FAD	C4-C4X-N5	2.16	121.07	118.60
3	A	1452	NAP	C4A-C5A-N7A	-2.14	107.17	109.40
2	D	1451	FAD	C9A-N10-C10	-2.09	119.17	121.91
2	A	1451	FAD	C5'-C4'-C3'	2.08	116.22	112.20
3	B	1452	NAP	C2A-N1A-C6A	2.07	122.30	118.75
3	A	1452	NAP	C1B-N9A-C4A	-2.06	123.02	126.64
3	A	1452	NAP	O7N-C7N-C3N	-2.06	117.17	119.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1456	EPE	O2S-S-C10	2.03	109.36	106.92

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1452	NAP	C5B-O5B-PA-O2A
3	A	1452	NAP	C5D-O5D-PN-O3
5	A	1455	EPE	C10-C9-N1-C6
5	A	1455	EPE	C8-C7-N4-C5
5	A	1455	EPE	S-C10-C9-N1
3	D	1452	NAP	C5B-O5B-PA-O2A
3	D	1452	NAP	C5D-O5D-PN-O3
2	A	1451	FAD	N10-C1'-C2'-O2'
5	A	1454	EPE	C10-C9-N1-C6
5	A	1454	EPE	C8-C7-N4-C5
5	A	1454	EPE	S-C10-C9-N1
3	C	1454	NAP	C5D-O5D-PN-O3
3	C	1454	NAP	C5D-O5D-PN-O2N
3	B	1452	NAP	C5B-O5B-PA-O2A
3	B	1452	NAP	C5D-O5D-PN-O3
5	C	1456	EPE	C8-C7-N4-C5
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
2	B	1451	FAD	N10-C1'-C2'-O2'
2	C	1453	FAD	N10-C1'-C2'-O2'
2	D	1451	FAD	N10-C1'-C2'-O2'
5	D	1454	EPE	C8-C7-N4-C5
5	D	1454	EPE	S-C10-C9-N1
3	A	1452	NAP	O4B-C4B-C5B-O5B
3	A	1452	NAP	C3B-C4B-C5B-O5B
3	D	1452	NAP	O4B-C4B-C5B-O5B
3	D	1452	NAP	C3B-C4B-C5B-O5B
3	C	1454	NAP	O4B-C4B-C5B-O5B
3	C	1454	NAP	C3B-C4B-C5B-O5B
3	B	1452	NAP	O4B-C4B-C5B-O5B
3	B	1452	NAP	C3B-C4B-C5B-O5B
3	C	1454	NAP	C1B-C2B-O2B-P2B
3	D	1452	NAP	C3B-C2B-O2B-P2B
5	C	1456	EPE	N4-C7-C8-O8

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Mol	Chain	Res	Type	Atoms
5	A	1455	EPE	C9-C10-S-O3S
5	A	1454	EPE	N4-C7-C8-O8
3	D	1452	NAP	C1B-C2B-O2B-P2B
5	A	1454	EPE	C9-C10-S-O3S
3	A	1452	NAP	C1B-C2B-O2B-P2B
3	C	1454	NAP	C3B-C2B-O2B-P2B
6	A	1456	PGE	O3-C5-C6-O4
3	B	1452	NAP	C1B-C2B-O2B-P2B
3	A	1452	NAP	C5B-O5B-PA-O3
3	D	1452	NAP	C5B-O5B-PA-O3
3	C	1454	NAP	C5B-O5B-PA-O3
3	B	1452	NAP	C5B-O5B-PA-O3
3	A	1452	NAP	C5B-O5B-PA-O1A
3	A	1452	NAP	C5D-O5D-PN-O2N
3	D	1452	NAP	C5B-O5B-PA-O1A
3	D	1452	NAP	C5D-O5D-PN-O2N
3	C	1454	NAP	C5B-O5B-PA-O1A
3	C	1454	NAP	C5B-O5B-PA-O2A
3	C	1454	NAP	C5D-O5D-PN-O1N
3	B	1452	NAP	C5B-O5B-PA-O1A
3	B	1452	NAP	C5D-O5D-PN-O2N
5	D	1454	EPE	C9-C10-S-O3S
5	A	1455	EPE	C9-C10-S-O1S
5	A	1455	EPE	C9-C10-S-O2S
5	A	1454	EPE	C9-C10-S-O1S
5	A	1454	EPE	C9-C10-S-O2S
5	D	1454	EPE	C9-C10-S-O1S
5	D	1454	EPE	C9-C10-S-O2S
2	A	1451	FAD	N10-C1'-C2'-C3'
2	B	1451	FAD	N10-C1'-C2'-C3'
2	C	1453	FAD	N10-C1'-C2'-C3'
2	D	1451	FAD	N10-C1'-C2'-C3'
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
2	B	1451	FAD	O4B-C4B-C5B-O5B
2	C	1453	FAD	O4B-C4B-C5B-O5B
2	D	1451	FAD	O4B-C4B-C5B-O5B
3	A	1452	NAP	C5D-O5D-PN-O1N
3	D	1452	NAP	C5D-O5D-PN-O1N
3	B	1452	NAP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	A	1451	FAD	O4B-C4B-C5B-O5B
6	A	1456	PGE	C3-C4-O3-C5
7	B	1453	PG4	O1-C1-C2-O2

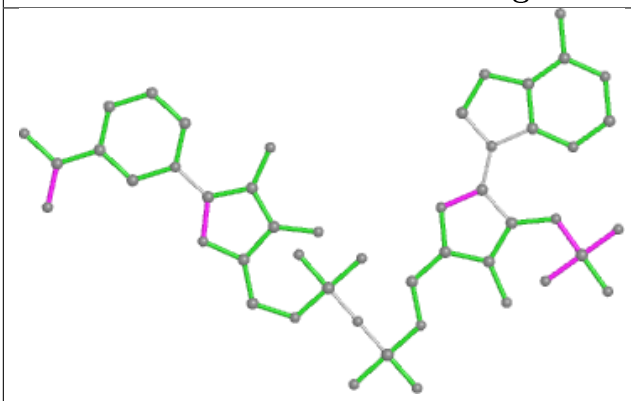
There are no ring outliers.

12 monomers are involved in 38 short contacts:

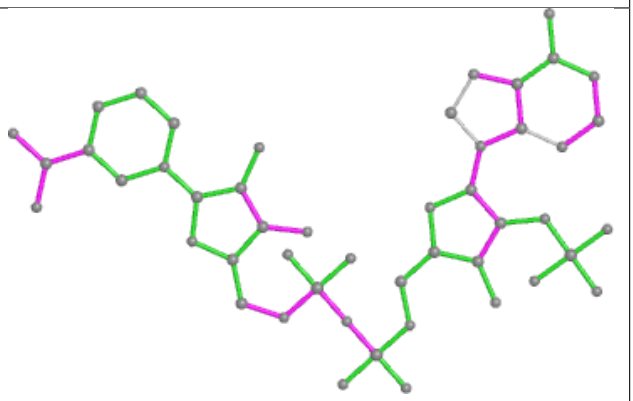
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1452	NAP	3	0
5	A	1455	EPE	4	0
3	D	1452	NAP	3	0
2	A	1451	FAD	1	0
5	A	1454	EPE	6	0
3	C	1454	NAP	2	0
3	B	1452	NAP	1	0
2	B	1451	FAD	1	0
5	C	1456	EPE	8	0
2	C	1453	FAD	1	0
2	D	1451	FAD	2	0
5	D	1454	EPE	6	0

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.

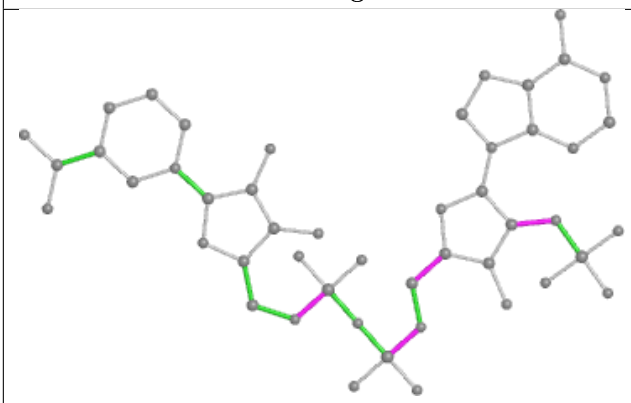
Ligand NAP A 1452



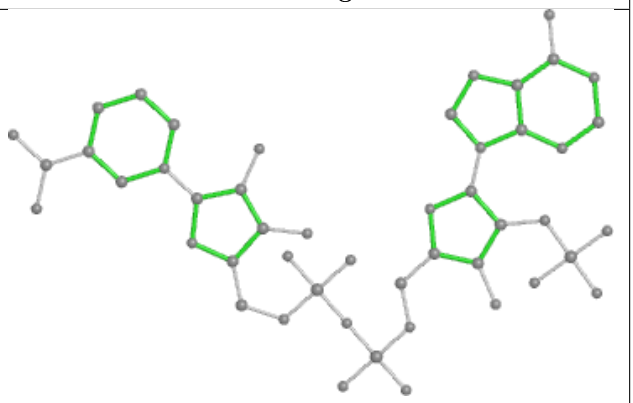
Bond lengths



Bond angles

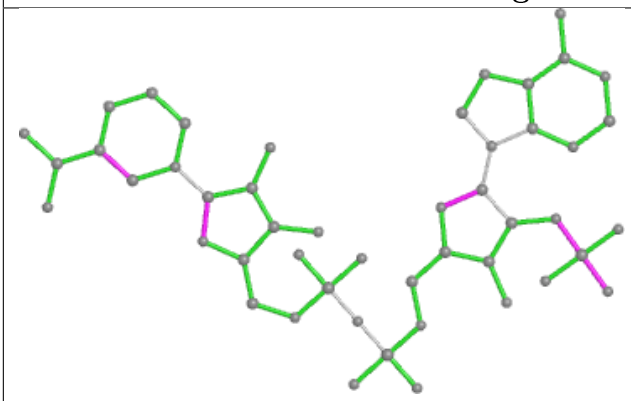


Torsions

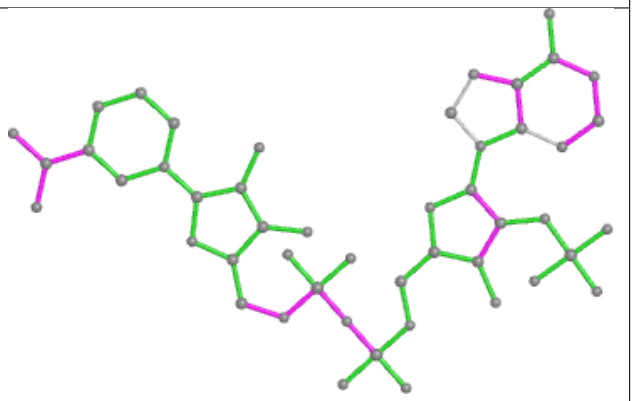


Rings

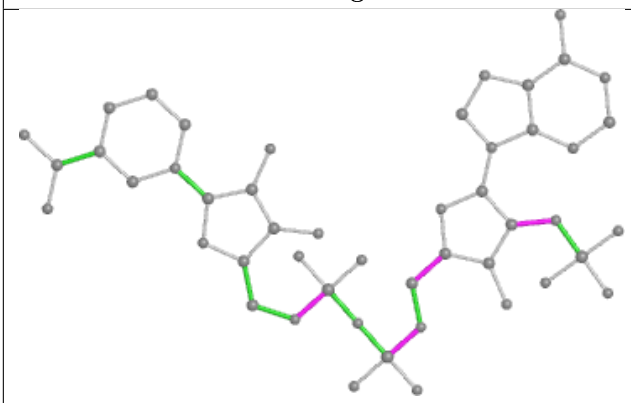
Ligand NAP D 1452



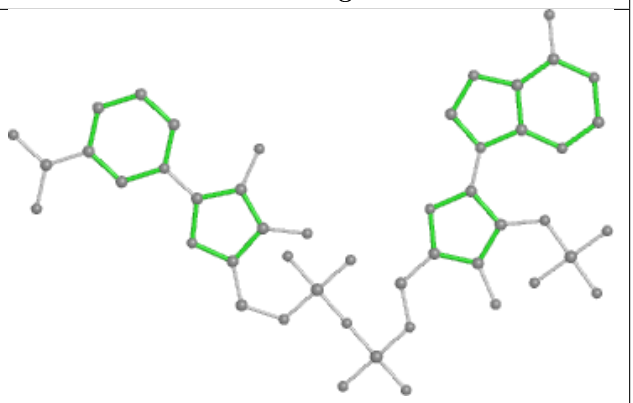
Bond lengths



Bond angles

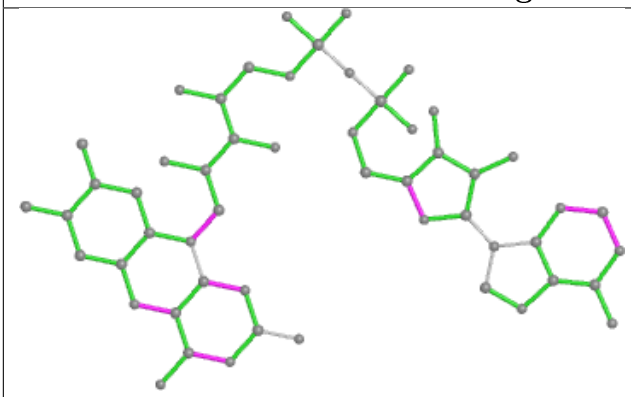


Torsions

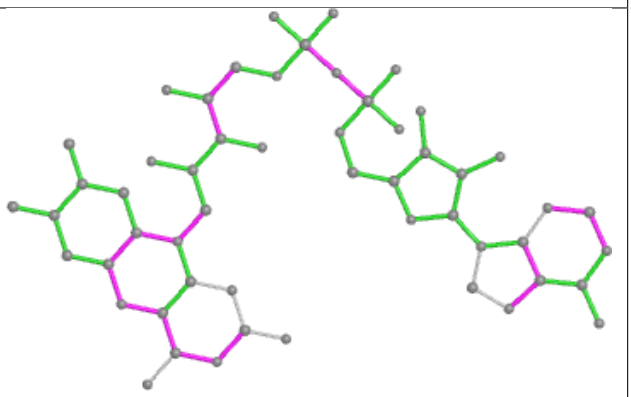


Rings

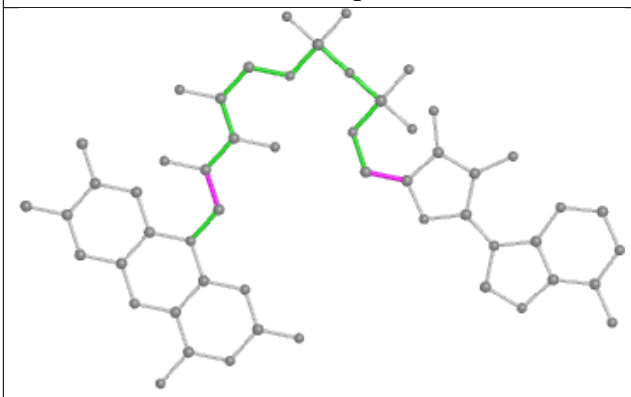
Ligand FAD A 1451



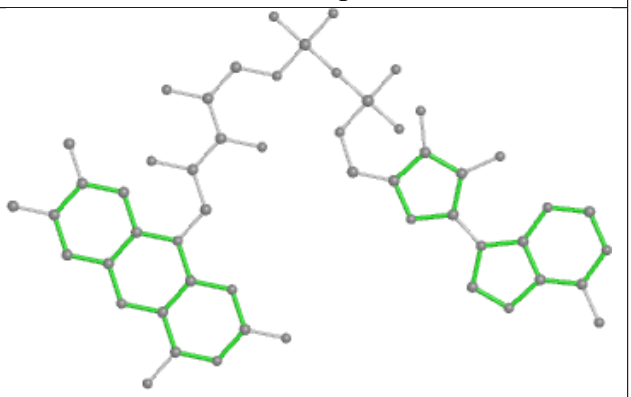
Bond lengths



Bond angles

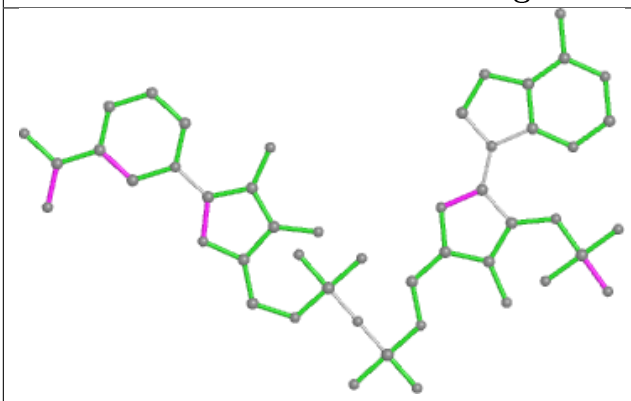


Torsions

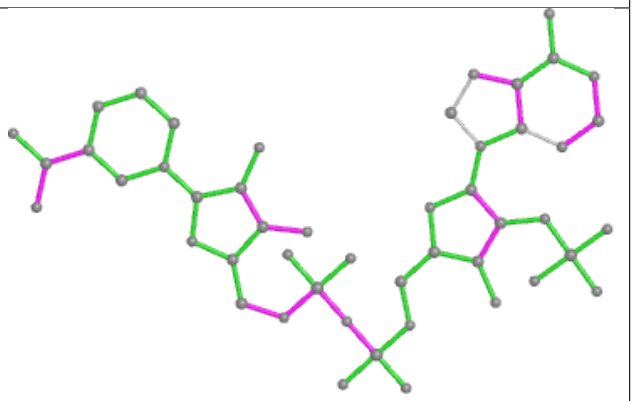


Rings

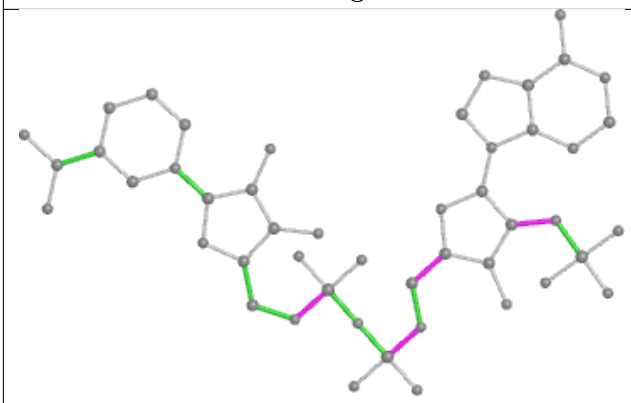
Ligand NAP C 1454



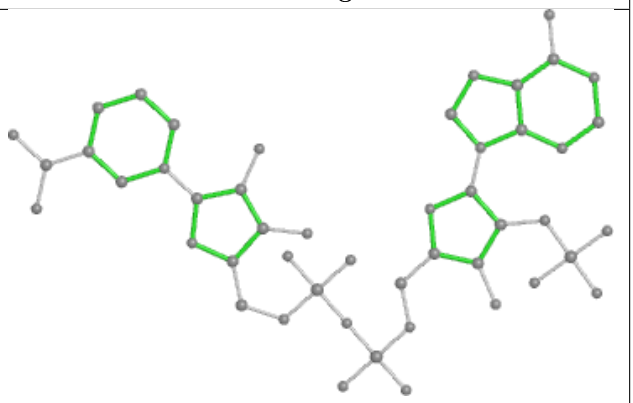
Bond lengths



Bond angles

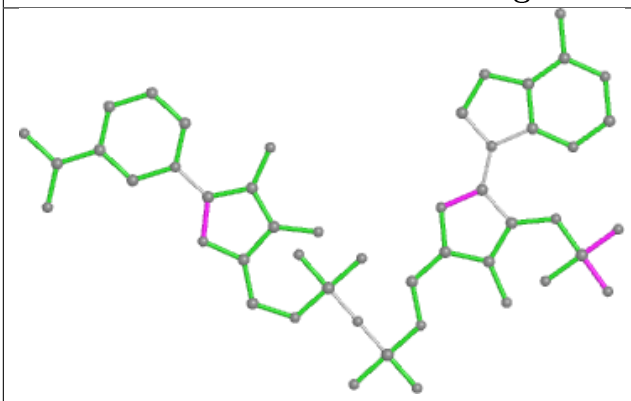


Torsions

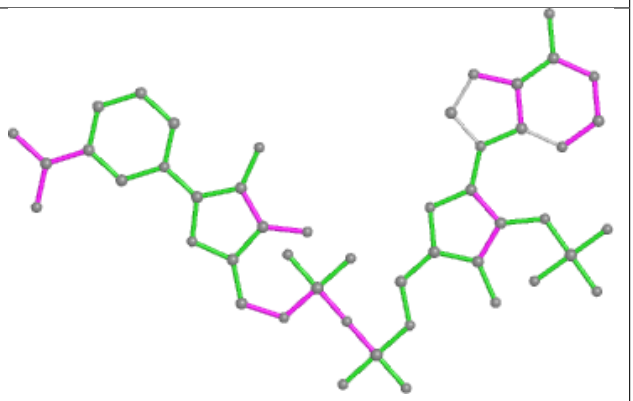


Rings

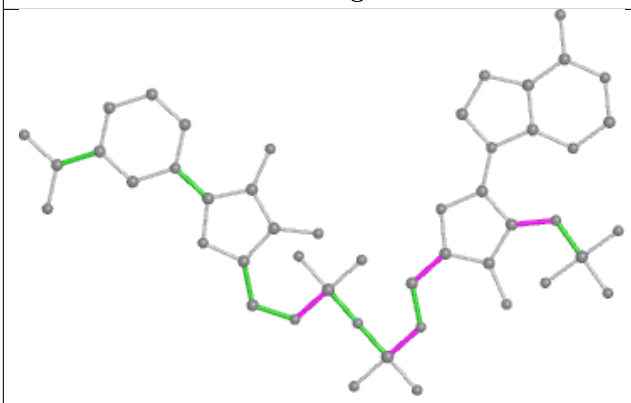
Ligand NAP B 1452



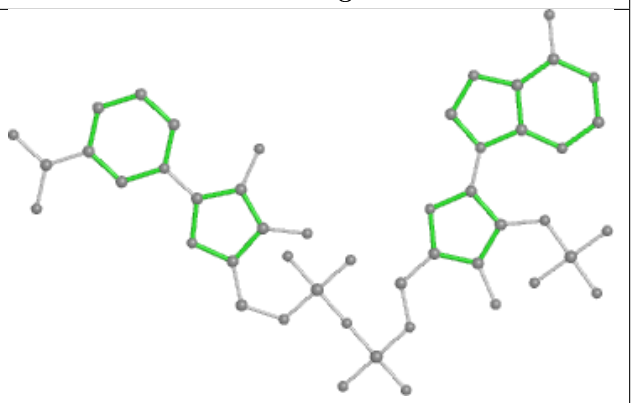
Bond lengths



Bond angles

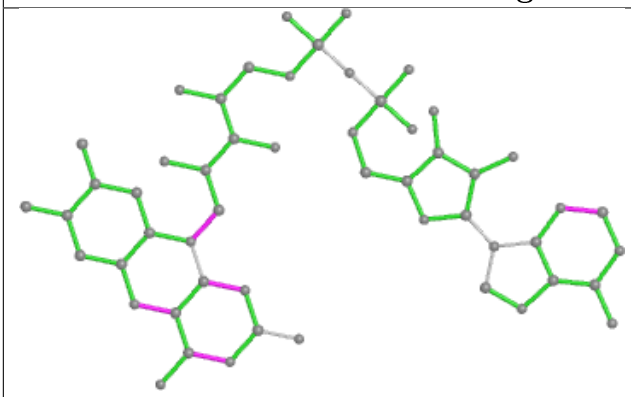


Torsions

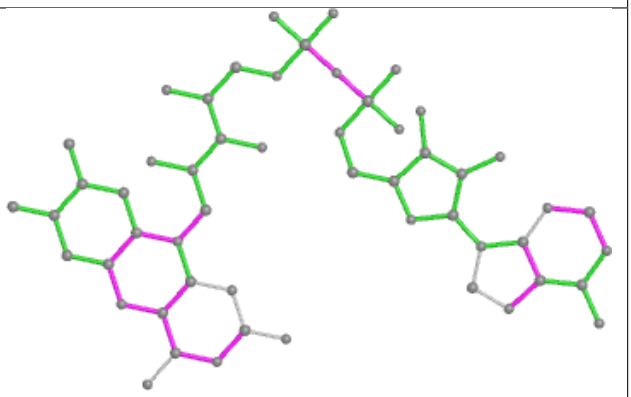


Rings

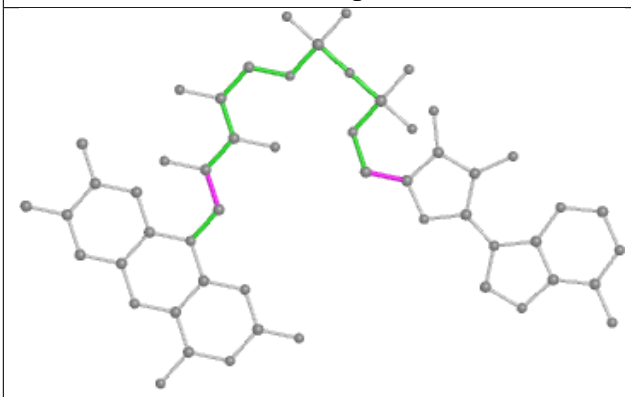
Ligand FAD B 1451



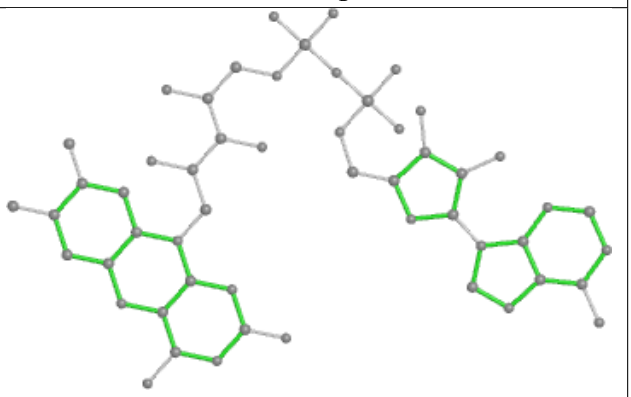
Bond lengths



Bond angles

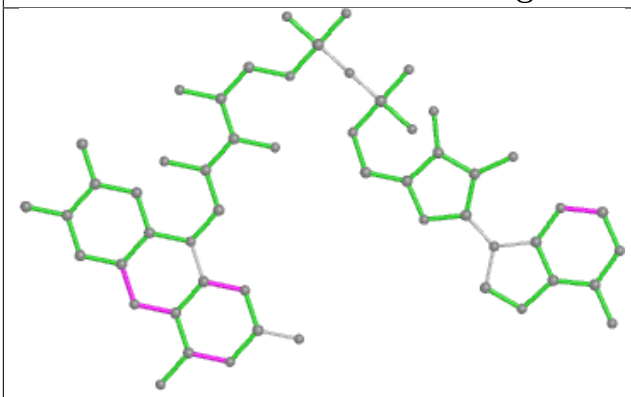


Torsions

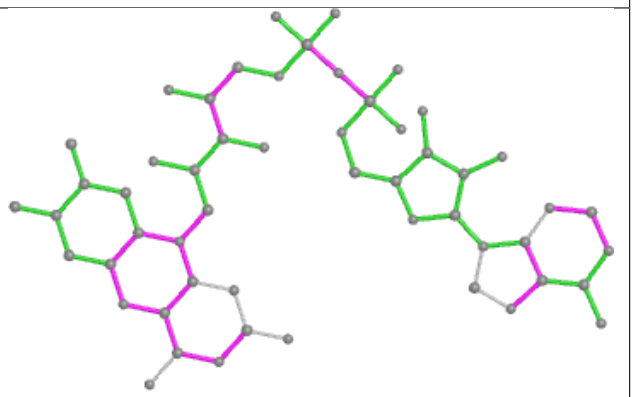


Rings

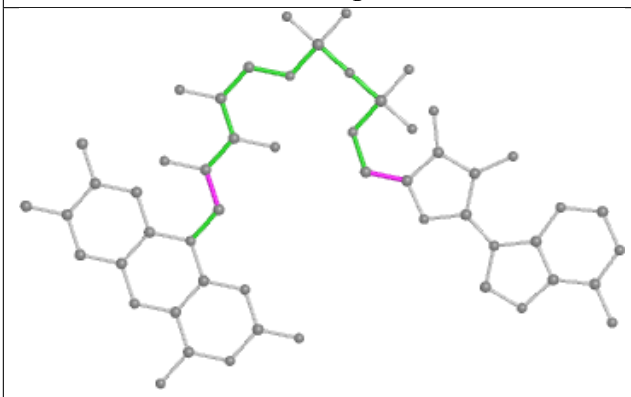
Ligand FAD C 1453



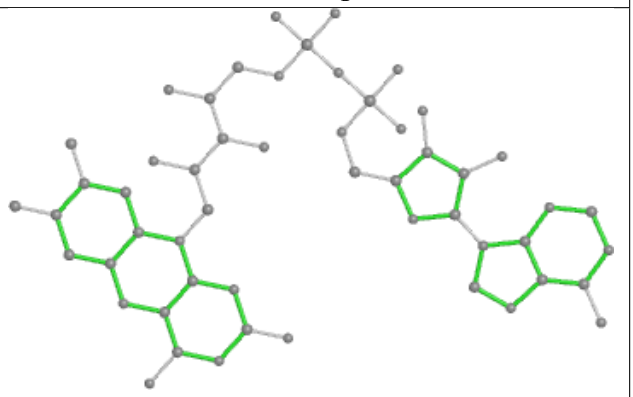
Bond lengths



Bond angles

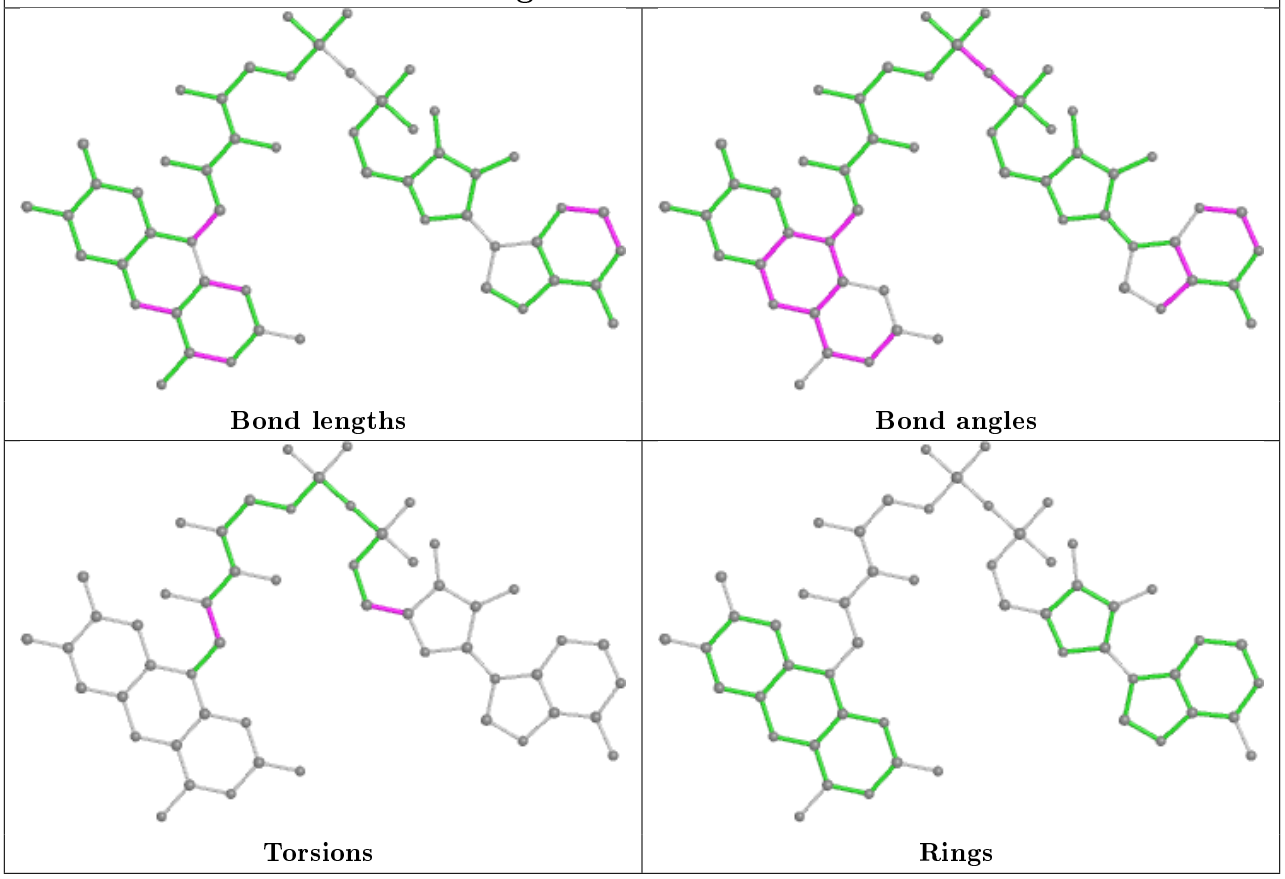


Torsions



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, 95^{th} 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%)	-0.33	1 (0%)	95	95	41, 51, 64, 73	0
1	B	443/461 (96%)	-0.30	2 (0%)	91	89	41, 51, 65, 73	0
1	C	445/461 (96%)	-0.26	2 (0%)	92	91	41, 51, 65, 73	0
1	D	443/461 (96%)	-0.19	2 (0%)	91	89	41, 51, 65, 73	0
All	All	1774/1844 (96%)	-0.27	7 (0%)	92	91	41, 51, 65, 73	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	422	ARG	2.6
1	C	452	LYS	2.5
1	B	241	LYS	2.4
1	B	244	GLU	2.3
1	C	244	GLU	2.1
1	D	244	GLU	2.1
1	A	236	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands (i)

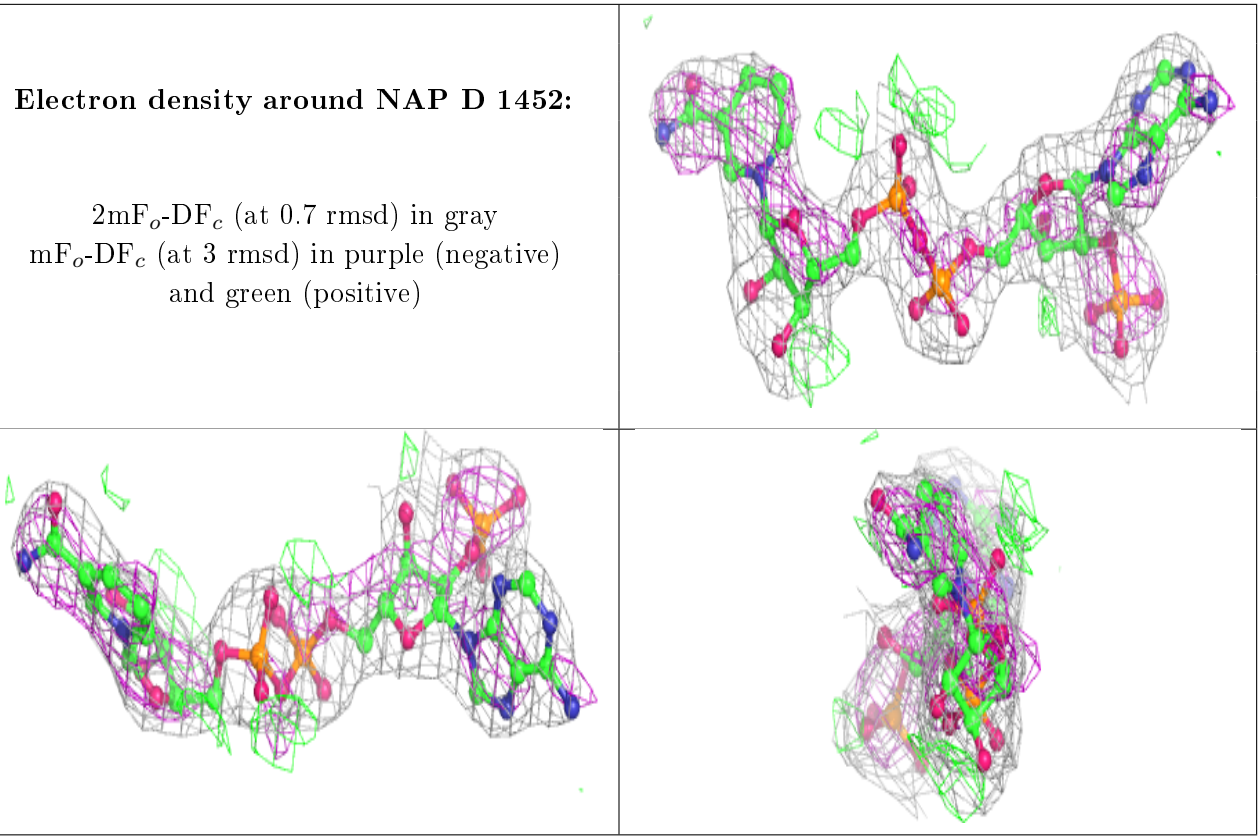
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0.29	87,93,105,105	0
6	PGE	A	1456	10/10	0.73	0.24	99,101,103,104	0
5	EPE	D	1454	15/15	0.73	0.26	93,95,106,106	0
5	EPE	A	1455	15/15	0.74	0.25	86,88,100,100	0
5	EPE	A	1454	15/15	0.76	0.22	82,85,99,99	0
7	PG4	B	1453	13/13	0.87	0.16	60,64,72,72	0
3	NAP	D	1452	48/48	0.94	0.16	32,36,44,47	0
3	NAP	A	1452	48/48	0.95	0.15	32,36,44,48	0
4	CL	A	1453	1/1	0.95	0.31	58,58,58,58	0
3	NAP	C	1454	48/48	0.96	0.13	32,36,44,47	0
3	NAP	B	1452	48/48	0.96	0.15	32,36,44,47	0
2	FAD	A	1451	53/53	0.97	0.15	37,45,46,47	0
4	CL	D	1453	1/1	0.97	0.27	64,64,64,64	0
2	FAD	C	1453	53/53	0.97	0.18	38,44,46,47	0
2	FAD	D	1451	53/53	0.97	0.16	38,44,46,47	0
2	FAD	B	1451	53/53	0.97	0.16	37,45,46,47	0
4	CL	C	1455	1/1	0.98	0.23	56,56,56,56	0
4	CL	B	1454	1/1	0.99	0.35	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.

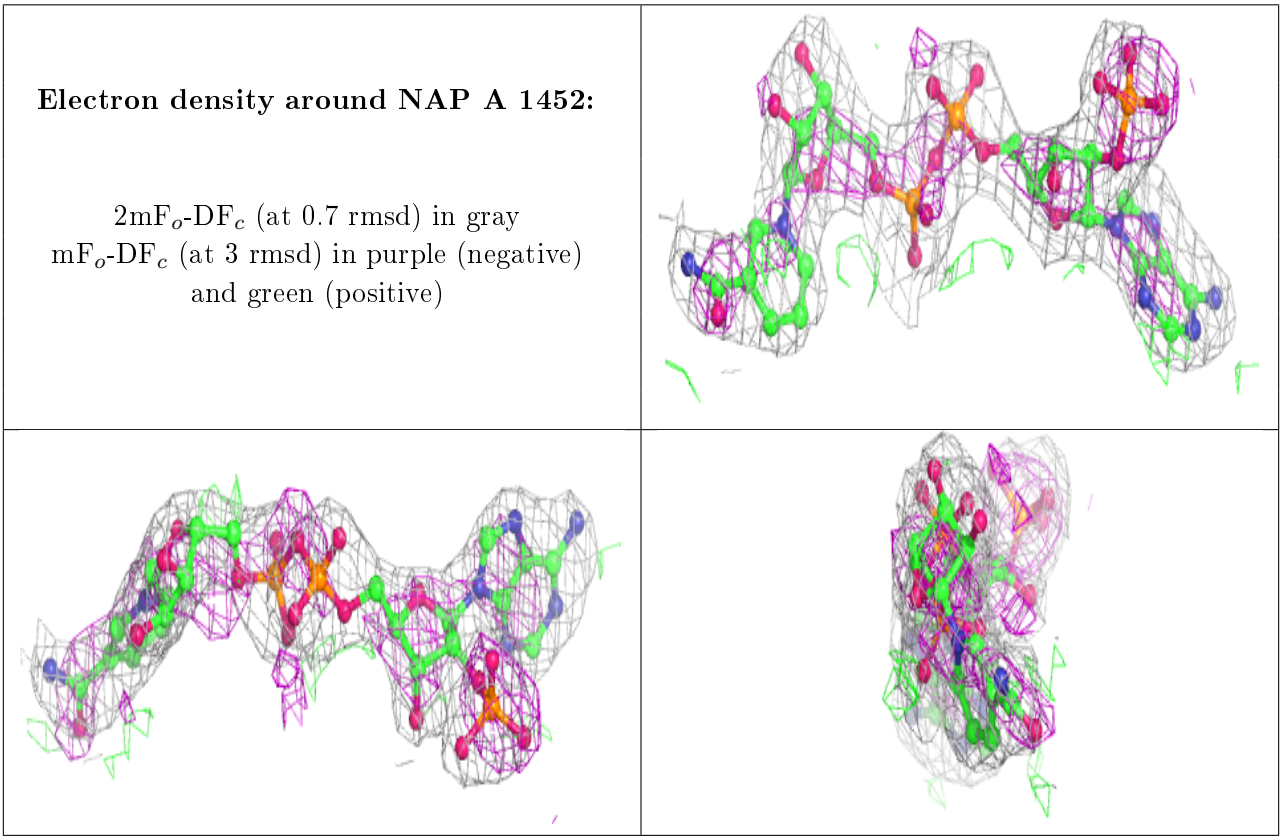
Electron density around NAP D 1452:

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



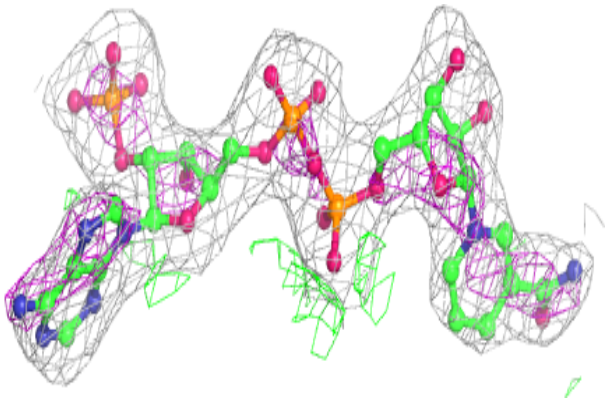
Electron density around NAP A 1452:

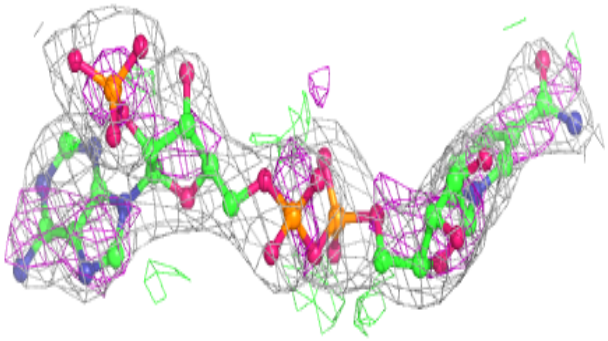
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

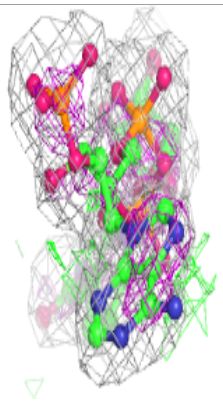


Electron density around NAP C 1454:

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

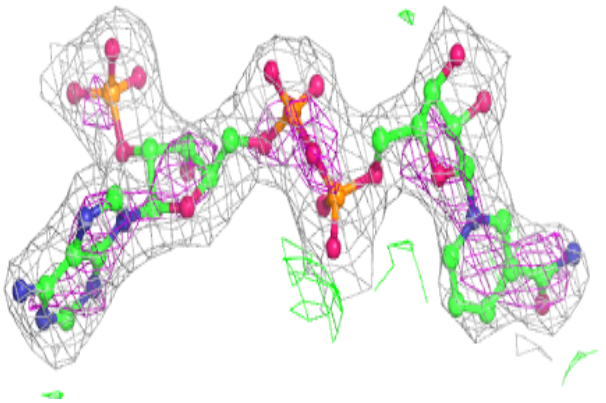


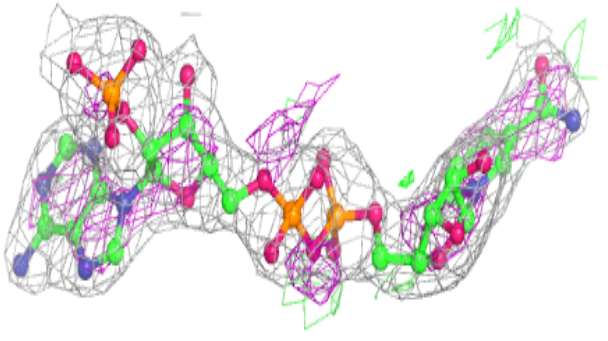


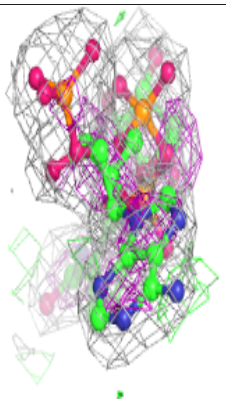


Electron density around NAP B 1452:

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

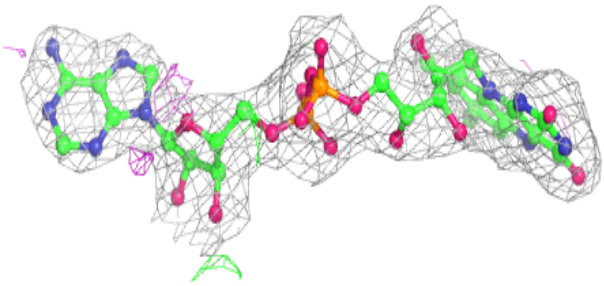


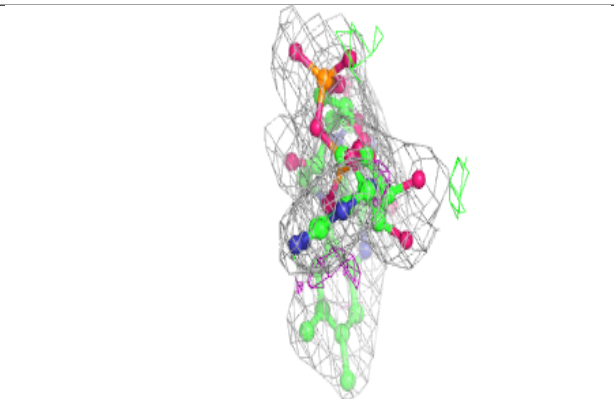




Electron density around FAD A 1451:

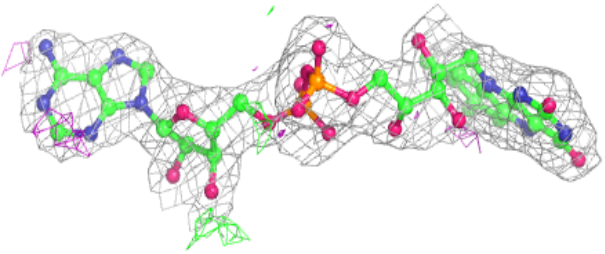
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

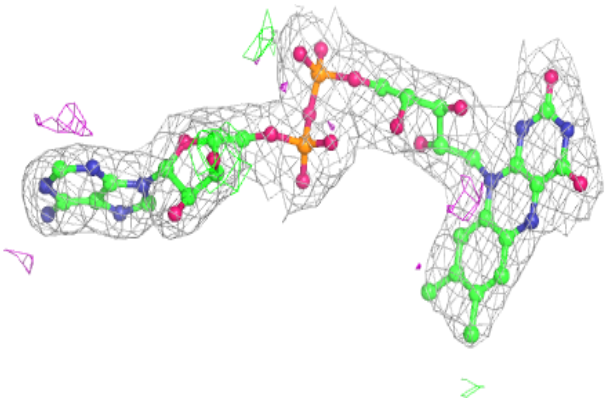


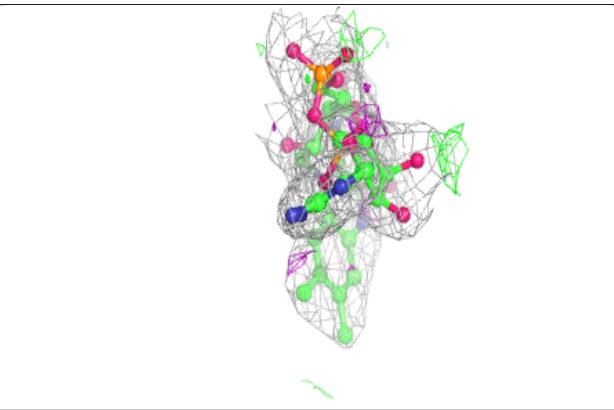


Electron density around FAD C 1453:

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

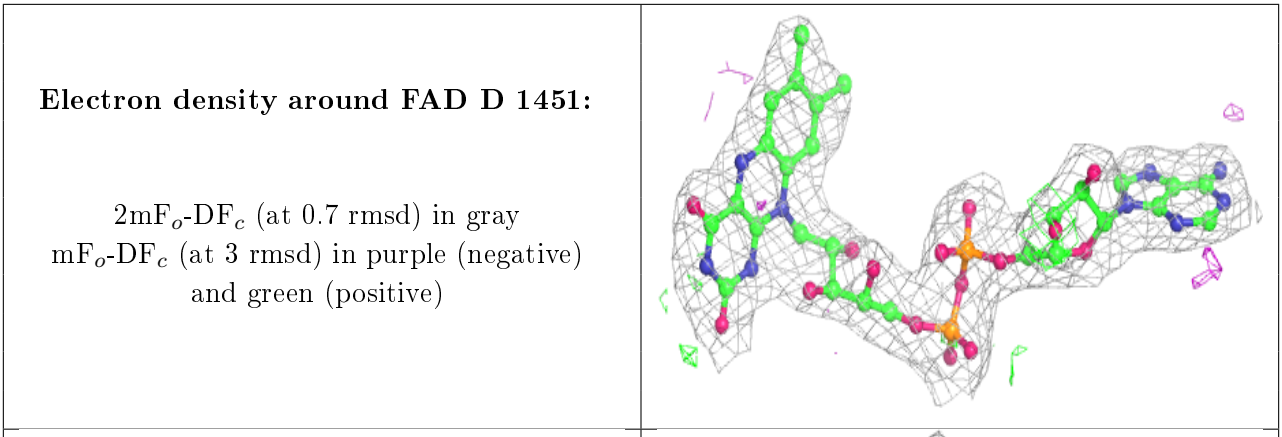






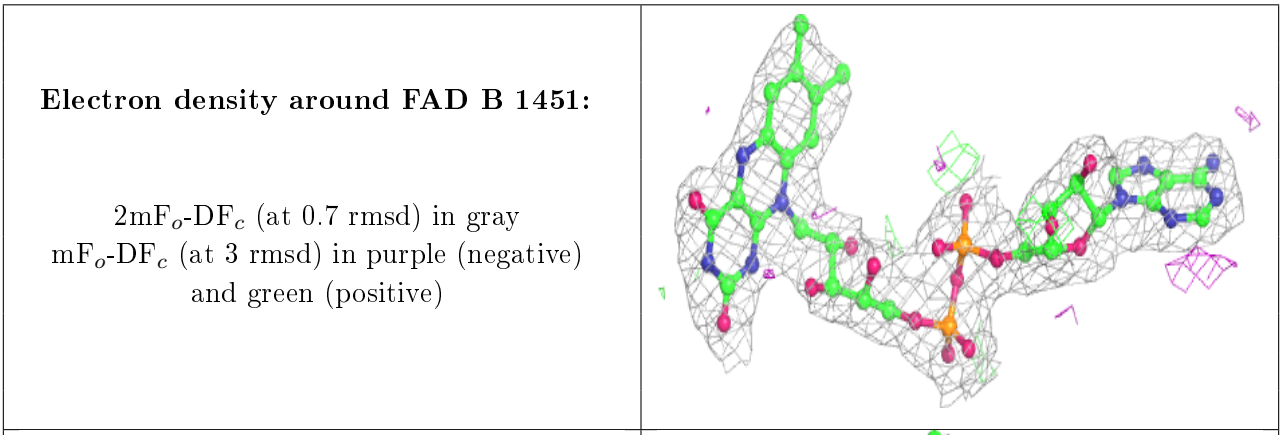
Electron density around FAD D 1451:

$2mF_o$-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 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)



6.5 Other polymers (i)

There are no such residues in this entry.