Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 12:17 PM EDT

PDB ID	:	1QXO
Title	:	Crystal structure of Chorismate synthase complexed with oxidized FMN and EPSP
Authors	:	Maclean, J.; Ali, S.
Deposited on	:	2003-09-08
Resolution	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

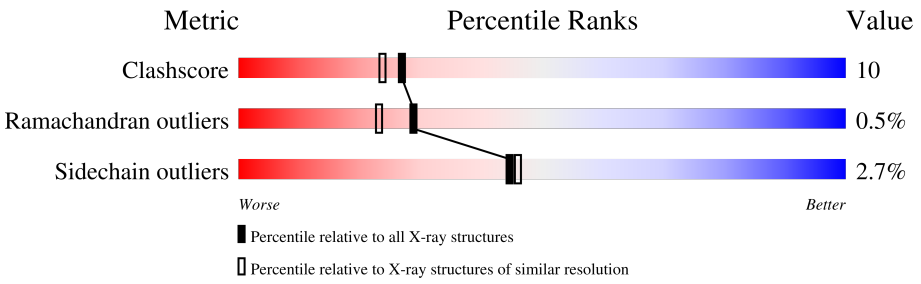
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	388	78% 19% •
1	B	388	82% 15% •
1	C	388	78% 18% • •
1	D	388	73% 21% • •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14427 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 Chorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	388	3037	1892	546	587	12	0	8	0
1	B	388	3043	1892	549	590	12	0	8	0
1	C	388	3035	1893	543	587	12	0	8	0
1	D	388	3022	1884	543	583	12	0	4	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	49	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	74	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	88	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	138	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	155	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	273	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	298	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	310	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	321	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	348	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	350	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	1	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	49	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	74	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	88	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	138	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	155	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	273	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	298	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	310	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6

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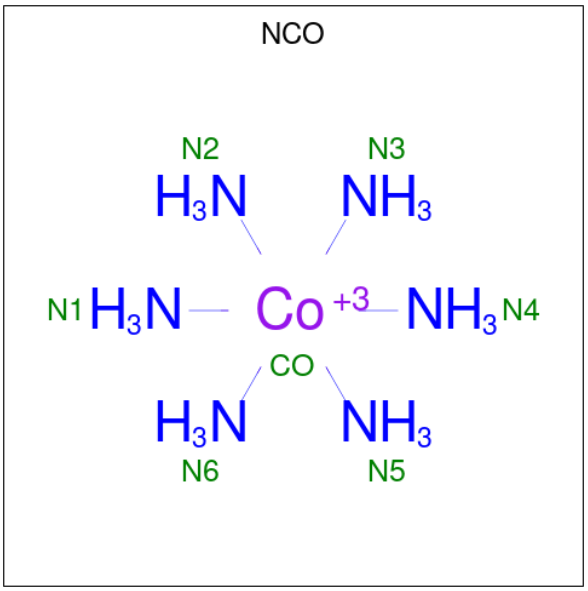
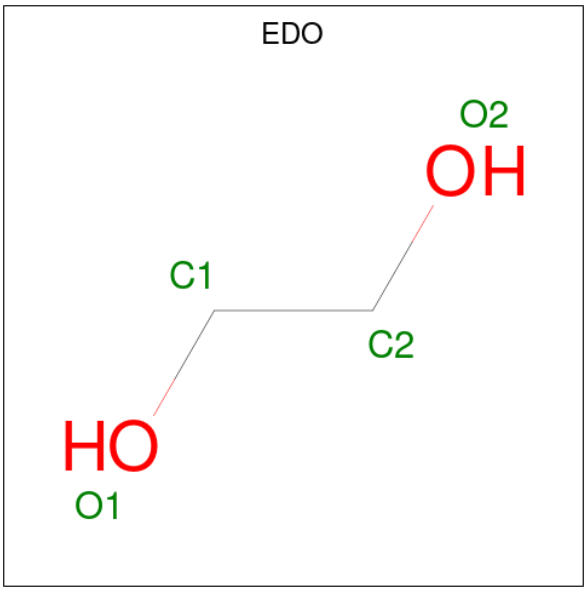
Chain	Residue	Modelled	Actual	Comment	Reference
B	321	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	348	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	350	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	1	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	49	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	74	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	88	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	138	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	155	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	273	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	298	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	310	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	321	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	348	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	350	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	1	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	49	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	74	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	88	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	138	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	155	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	273	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	298	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	310	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	321	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	348	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	350	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6

- Molecule 2 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula: $CoH_{18}N_6$).



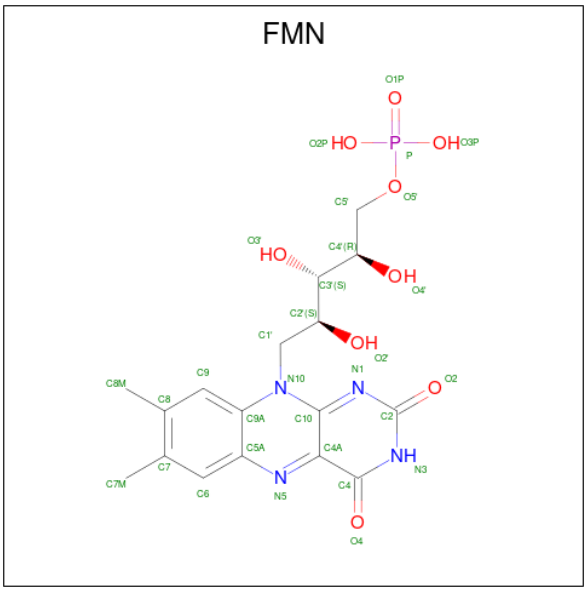
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Co	N		
2	A	1	7	1	6	0	0
2	A	1	7	1	6	0	0
2	A	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	C	1	7	1	6	0	0
2	C	1	7	1	6	0	0
2	D	1	7	1	6	0	0
2	D	1	7	1	6	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



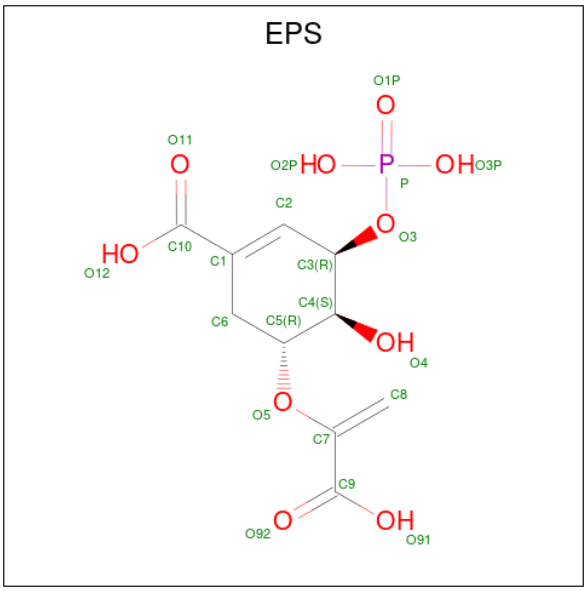
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	C	1	4	2	2	0	0
3	D	1	4	2	2	0	0
3	D	1	4	2	2	0	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 5 is 5-[(1-CARBOXYVINYL)OXY]-4-HYDROXY-3-(PHOSPHONOOXY)CYCLOHEX-1-ENE-1-CARBOXYLIC ACID (three-letter code: EPS) (formula: $C_{10}H_{13}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
5	A	1	21	10	10	1	0	0
			Total	C	O	P		
5	B	1	21	10	10	1	0	0
			Total	C	O	P		
5	C	1	21	10	10	1	0	0
			Total	C	O	P		
5	D	1	21	10	10	1	0	0

- Molecule 6 is water.

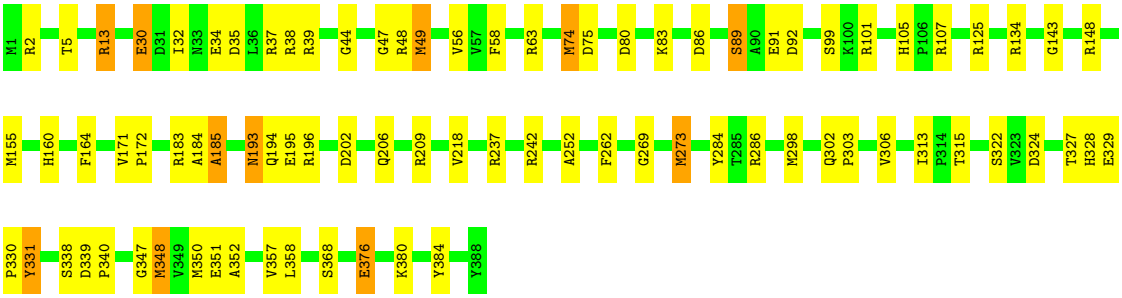
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	453	453	453	0	0
			Total	O		
6	B	528	528	528	0	0
			Total	O		
6	C	469	469	469	0	0
			Total	O		
6	D	479	479	479	0	0

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. 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. 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.

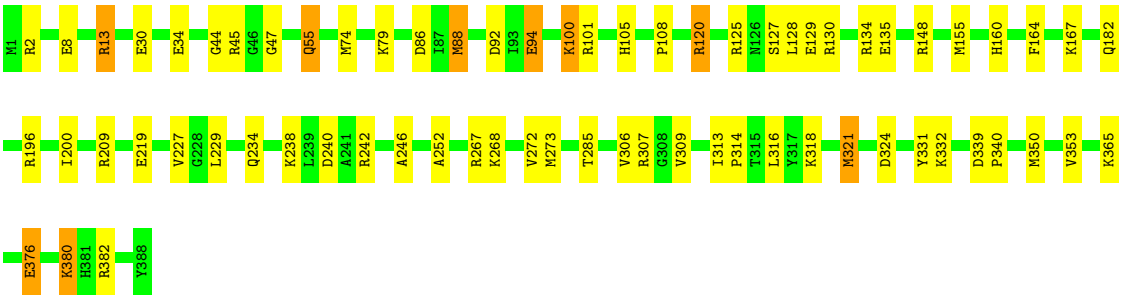
• Molecule 1: Chorismate synthase

Chain A:



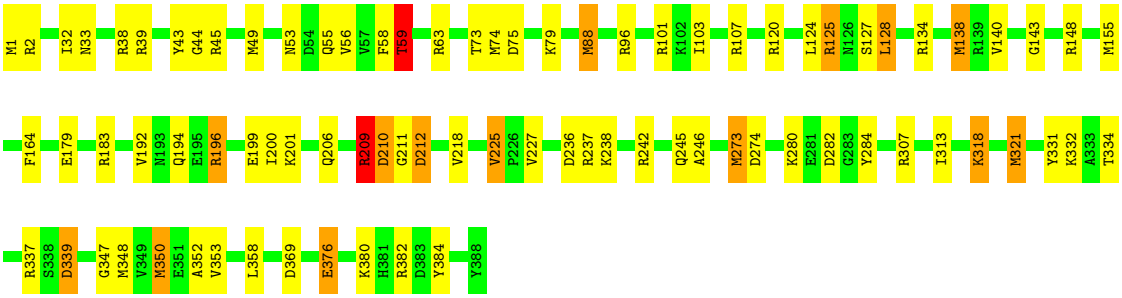
• Molecule 1: Chorismate synthase

Chain B:



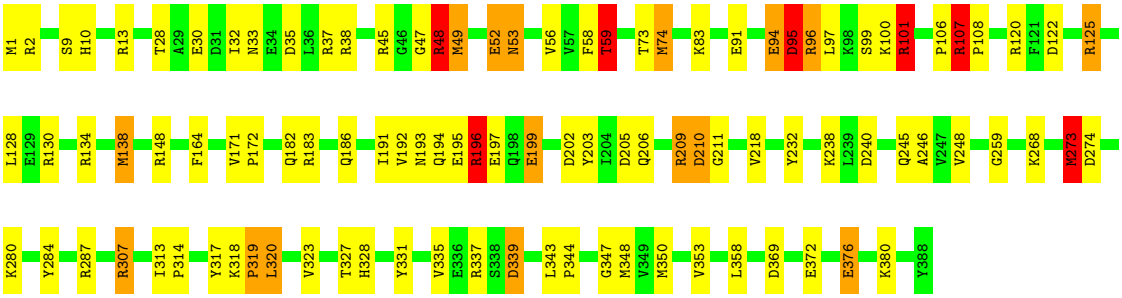
• Molecule 1: Chorismate synthase

Chain C:



• Molecule 1: Chorismate synthase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.06Å 124.58Å 85.16Å 90.00° 115.15° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 24.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.00) 97.4 (24.90-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.30 (at 1.99Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.157 , 0.222 0.145 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	7.9	Xtriage
Anisotropy	0.769	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.31$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	14427	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NCO, EDO, FMN, EPS

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	0.75	5/3115 (0.2%)	1.43	38/4185 (0.9%)
1	B	0.79	4/3119 (0.1%)	1.37	26/4188 (0.6%)
1	C	0.78	8/3111 (0.3%)	1.49	38/4180 (0.9%)
1	D	0.78	4/3078 (0.1%)	1.62	53/4134 (1.3%)
All	All	0.78	21/12423 (0.2%)	1.48	155/16687 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	MSE	CG-SE	13.31	2.40	1.95
1	D	273	MSE	CG-SE	13.14	2.40	1.95
1	C	273	MSE	CG-SE	12.20	2.37	1.95
1	D	49	MSE	CG-SE	9.80	2.28	1.95
1	B	88	MSE	CG-SE	9.58	2.28	1.95
1	C	376	GLU	CD-OE2	9.12	1.35	1.25
1	A	155	MSE	SE-CE	-9.02	1.42	1.95
1	D	376	GLU	CD-OE2	8.49	1.34	1.25
1	A	273	MSE	CG-SE	8.43	2.24	1.95
1	B	376[A]	GLU	CD-OE2	8.34	1.34	1.25
1	B	376[B]	GLU	CD-OE2	8.34	1.34	1.25
1	A	376	GLU	CD-OE2	8.24	1.34	1.25
1	C	321	MSE	CG-SE	7.01	2.19	1.95
1	C	321	MSE	SE-CE	6.37	2.33	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	138	MSE	CG-SE	6.24	2.16	1.95
1	A	348	MSE	SE-CE	5.85	2.29	1.95
1	C	138	MSE	CG-SE	5.75	2.15	1.95
1	C	88	MSE	CG-SE	5.39	2.13	1.95
1	A	49	MSE	CG-SE	5.37	2.13	1.95
1	C	88	MSE	SE-CE	5.36	2.27	1.95
1	C	350	MSE	CG-SE	5.22	2.13	1.95

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	48	ARG	NE-CZ-NH2	-20.75	109.92	120.30
1	D	196	ARG	NE-CZ-NH2	-17.53	111.53	120.30
1	D	196	ARG	NE-CZ-NH1	14.18	127.39	120.30
1	D	2	ARG	NE-CZ-NH1	-13.76	113.42	120.30
1	D	130	ARG	NE-CZ-NH2	-13.60	113.50	120.30
1	C	101	ARG	NE-CZ-NH2	13.29	126.95	120.30
1	A	209	ARG	NE-CZ-NH2	-13.07	113.77	120.30
1	A	286	ARG	NE-CZ-NH1	13.00	126.80	120.30
1	D	134	ARG	NE-CZ-NH2	12.84	126.72	120.30
1	B	209	ARG	CD-NE-CZ	12.33	140.86	123.60
1	C	63	ARG	NE-CZ-NH2	-11.93	114.34	120.30
1	A	2	ARG	NE-CZ-NH1	-11.76	114.42	120.30
1	C	321	MSE	CG-SE-CE	11.72	124.69	98.90
1	D	130	ARG	NE-CZ-NH1	11.70	126.15	120.30
1	D	48	ARG	CD-NE-CZ	11.18	139.25	123.60
1	C	209	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	C	209	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	D	148	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	B	101	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	D	107	ARG	CD-NE-CZ	10.30	138.02	123.60
1	C	2	ARG	NE-CZ-NH1	-10.26	115.17	120.30
1	C	337	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	A	63	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	A	185	ALA	CB-CA-C	9.38	124.18	110.10
1	B	125	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	D	273	MSE	CB-CG-SE	-9.16	85.22	112.70
1	B	209	ARG	NE-CZ-NH2	8.83	124.71	120.30
1	A	75	ASP	CB-CG-OD1	8.70	126.13	118.30
1	A	13	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	C	307	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	C	148	ARG	CD-NE-CZ	8.42	135.38	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	ARG	NE-CZ-NH1	-8.40	116.10	120.30
1	D	59	THR	N-CA-CB	-8.38	94.39	110.30
1	D	48	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	C	242	ARG	NE-CZ-NH1	8.03	124.32	120.30
1	C	382	ARG	NE-CZ-NH1	-7.84	116.38	120.30
1	D	274	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	D	183	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	C	148	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	183	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	C	59	THR	N-CA-CB	-7.51	96.04	110.30
1	A	107	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	C	49	MSE	CG-SE-CE	7.39	115.17	98.90
1	D	101	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	D	125	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	C	339	ASP	CB-CG-OD2	7.27	124.84	118.30
1	A	286	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	C	196	ARG	CG-CD-NE	7.22	126.96	111.80
1	D	183	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	B	92	ASP	CB-CG-OD1	7.21	124.79	118.30
1	B	101	ARG	CD-NE-CZ	7.21	133.69	123.60
1	D	196	ARG	CD-NE-CZ	7.08	133.51	123.60
1	B	125	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	A	48	ARG	NE-CZ-NH1	-6.97	116.81	120.30
1	A	125	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	A	35	ASP	CB-CG-OD2	6.86	124.47	118.30
1	D	199	GLU	OE1-CD-OE2	-6.80	115.14	123.30
1	C	45	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	183	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	D	307	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	B	13	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	107	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	C	134	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	D	273	MSE	CG-SE-CE	-6.71	84.14	98.90
1	D	2	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	D	203	TYR	CB-CG-CD1	-6.62	117.03	121.00
1	A	38	ARG	NE-CZ-NH2	6.61	123.60	120.30
1	A	196	ARG	NE-CZ-NH1	-6.55	117.03	120.30
1	A	38	ARG	CD-NE-CZ	6.54	132.75	123.60
1	A	13	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	C	127	SER	N-CA-CB	6.47	120.20	110.50
1	D	74	MSE	CB-CG-SE	-6.43	93.42	112.70
1	B	380	LYS	CG-CD-CE	6.42	131.17	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	30	GLU	OE1-CD-OE2	-6.42	115.60	123.30
1	C	209	ARG	CA-CB-CG	6.34	127.34	113.40
1	B	240	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	240	ASP	CB-CG-OD1	6.32	123.99	118.30
1	D	45	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	B	148	ARG	CD-NE-CZ	6.27	132.38	123.60
1	D	30	GLU	OE1-CD-OE2	-6.26	115.79	123.30
1	D	287[A]	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	D	287[B]	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	B	45	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	B	130	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	B	321	MSE	CB-CG-SE	-6.21	94.07	112.70
1	B	13	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	324	ASP	CB-CG-OD1	6.17	123.86	118.30
1	D	13	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	D	339	ASP	N-CA-CB	-6.10	99.61	110.60
1	B	101	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	134	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	C	38	ARG	CD-NE-CZ	6.04	132.06	123.60
1	B	88	MSE	CB-CG-SE	-5.99	94.74	112.70
1	C	237	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	A	92	ASP	CB-CG-OD1	5.97	123.67	118.30
1	D	49	MSE	CB-CG-SE	-5.92	94.94	112.70
1	C	273	MSE	CB-CG-SE	-5.91	94.98	112.70
1	C	369	ASP	CB-CG-OD1	5.89	123.60	118.30
1	D	101	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	120	ARG	NE-CZ-NH1	-5.87	117.36	120.30
1	D	209	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	2	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	B	155	MSE	CA-CB-CG	-5.83	103.39	113.30
1	C	274	ASP	CB-CG-OD2	-5.81	113.08	118.30
1	D	1	MSE	CB-CG-SE	-5.79	95.33	112.70
1	D	369	ASP	CB-CG-OD1	5.79	123.51	118.30
1	C	236	ASP	CB-CG-OD1	5.76	123.48	118.30
1	D	107	ARG	CG-CD-NE	-5.74	99.75	111.80
1	A	89	SER	N-CA-CB	-5.71	101.93	110.50
1	C	382	ARG	NH1-CZ-NH2	5.71	125.68	119.40
1	C	125	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	C	212	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	C	75	ASP	CB-CA-C	-5.69	99.02	110.40
1	D	48	ARG	NH1-CZ-NH2	5.69	125.66	119.40
1	A	86	ASP	CB-CG-OD1	5.67	123.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	232	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	A	101	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	39	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	209	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	B	267	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	125	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	2	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	D	232	TYR	CB-CG-CD1	5.57	124.34	121.00
1	C	209	ARG	N-CA-CB	5.52	120.54	110.60
1	D	35	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	1	MSE	CB-CG-SE	-5.51	96.16	112.70
1	B	127	SER	N-CA-CB	5.50	118.75	110.50
1	A	184	ALA	C-N-CA	-5.48	107.99	121.70
1	A	331	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	D	274	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	351	GLU	OE1-CD-OE2	-5.35	116.88	123.30
1	A	49	MSE	CB-CG-SE	-5.30	96.80	112.70
1	C	107	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	D	148	ARG	CD-NE-CZ	5.29	131.00	123.60
1	A	148	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	331	TYR	CA-CB-CG	5.28	123.44	113.40
1	D	52	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	D	38	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	D	13	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	287[A]	ARG	CD-NE-CZ	5.19	130.87	123.60
1	D	287[B]	ARG	CD-NE-CZ	5.19	130.87	123.60
1	C	331	TYR	CA-CB-CG	5.18	123.25	113.40
1	C	55	GLN	CA-CB-CG	5.18	124.80	113.40
1	B	74	MSE	CA-CB-CG	-5.17	104.51	113.30
1	C	88	MSE	CG-SE-CE	-5.16	87.55	98.90
1	C	120	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	202	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	209	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	B	318	LYS	N-CA-CB	5.09	119.76	110.60
1	B	331	TYR	CA-CB-CG	5.09	123.06	113.40
1	C	225	VAL	CA-CB-CG1	5.06	118.49	110.90
1	D	2	ARG	CD-NE-CZ	5.05	130.68	123.60
1	D	74	MSE	CA-CB-CG	-5.03	104.75	113.30
1	A	74	MSE	CA-CB-CG	-5.02	104.76	113.30
1	D	138	MSE	CA-CB-CG	5.00	121.81	113.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	10	HIS	Mainchain
1	D	248	VAL	Mainchain

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	3037	0	3050	49	0
1	B	3043	0	3053	48	0
1	C	3035	0	3054	71	0
1	D	3022	0	3038	86	0
2	A	21	0	0	0	0
2	B	14	0	0	0	0
2	C	14	0	0	0	0
2	D	14	0	0	1	0
3	A	12	0	18	4	0
3	B	4	0	6	1	0
3	C	4	0	6	2	0
3	D	8	0	12	2	0
4	A	31	0	19	5	0
4	B	31	0	19	4	0
4	C	62	0	38	7	0
4	D	62	0	38	6	0
5	A	21	0	8	0	0
5	B	21	0	8	1	0
5	C	21	0	8	0	0
5	D	21	0	8	0	0
6	A	453	0	0	7	0
6	B	528	0	0	12	0
6	C	469	0	0	16	0
6	D	479	0	0	16	0
All	All	14427	0	12383	255	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 10.

All (255) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:MSE:SE	1:D:348:MSE:CE	2.14	1.45
1:C:138:MSE:CG	1:C:138:MSE:SE	2.15	1.45
1:D:273:MSE:SE	1:D:273:MSE:CE	2.14	1.45
1:D:138:MSE:SE	1:D:138:MSE:CG	2.16	1.42
1:B:88:MSE:SE	1:B:88:MSE:CE	2.16	1.42
1:C:348:MSE:CE	1:C:348:MSE:SE	2.19	1.41
1:C:321:MSE:CG	1:C:321:MSE:SE	2.19	1.40
1:A:273:MSE:CG	1:A:273:MSE:SE	2.24	1.36
1:C:88:MSE:SE	1:C:88:MSE:CE	2.27	1.32
1:D:49:MSE:CG	1:D:49:MSE:SE	2.28	1.32
1:B:88:MSE:SE	1:B:88:MSE:CG	2.28	1.31
1:A:348:MSE:SE	1:A:348:MSE:CE	2.29	1.29
1:C:321:MSE:SE	1:C:321:MSE:CE	2.33	1.27
1:C:273:MSE:CG	1:C:273:MSE:SE	2.36	1.23
1:D:273:MSE:SE	1:D:273:MSE:CG	2.40	1.20
1:B:321:MSE:CG	1:B:321:MSE:SE	2.40	1.18
1:C:211:GLY:HA3	1:C:318:LYS:HD3	1.36	1.07
1:C:103[B]:ILE:HG12	1:C:124:LEU:HB2	1.41	1.00
1:A:99:SER:HB2	6:A:5452:HOH:O	1.60	1.00
1:C:284:TYR:HB2	3:C:3003:EDO:H12	1.44	0.97
1:D:202:ASP:HB2	6:D:5444:HOH:O	1.67	0.94
1:D:218[A]:VAL:HG11	1:D:347:GLY:HA2	1.51	0.91
1:A:5:THR:H	1:B:234:GLN:HE22	1.14	0.91
1:C:211:GLY:HA3	1:C:318:LYS:CD	2.05	0.87
1:D:273:MSE:SE	1:D:273:MSE:CB	2.73	0.87
1:C:218[A]:VAL:HG11	1:C:347:GLY:HA2	1.57	0.85
1:D:33:ASN:HD21	1:D:56:VAL:H	1.25	0.84
1:C:32[B]:ILE:HD12	1:C:56:VAL:HG11	1.57	0.84
1:D:284:TYR:HB2	3:D:3004:EDO:H22	1.60	0.82
1:D:32[B]:ILE:HD13	1:D:56:VAL:HG11	1.63	0.81
1:C:33:ASN:HD21	1:C:56:VAL:H	1.24	0.80
1:C:321:MSE:SE	1:C:321:MSE:CB	2.82	0.78
1:C:103[B]:ILE:HD12	1:C:334:THR:HG21	1.66	0.77
1:A:194:GLN:HG3	6:A:5173:HOH:O	1.84	0.77
1:C:321:MSE:SE	1:C:321:MSE:HA	2.36	0.75
1:B:88:MSE:SE	1:B:88:MSE:CB	2.84	0.74
1:D:49:MSE:SE	1:D:49:MSE:CB	2.85	0.74
1:D:122:ASP:HB2	6:D:5336:HOH:O	1.86	0.74
1:B:382[B]:ARG:NH2	6:B:5021:HOH:O	2.21	0.72
1:C:138:MSE:SE	1:C:138:MSE:CB	2.88	0.72
1:D:138:MSE:SE	1:D:138:MSE:CB	2.88	0.71
1:D:83:LYS:HZ3	1:D:337:ARG:HH12	1.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:PRO:O	1:D:320:LEU:HG	1.93	0.68
1:D:32[B]:ILE:HD11	1:D:58:PHE:CZ	2.29	0.68
1:C:273:MSE:SE	1:C:273:MSE:CB	2.91	0.68
1:C:321:MSE:SE	1:C:321:MSE:CA	2.91	0.68
1:A:368:SER:O	3:A:3006:EDO:H11	1.94	0.67
1:B:321:MSE:SE	1:B:321:MSE:CB	2.92	0.67
1:C:103[B]:ILE:HG23	1:C:125:ARG:N	2.11	0.66
6:B:5105:HOH:O	1:D:59:THR:HG23	1.96	0.66
1:A:273:MSE:SE	1:A:273:MSE:CB	2.94	0.65
6:A:5067:HOH:O	1:C:59:THR:HG23	1.97	0.65
1:D:210:ASP:HA	6:D:5243:HOH:O	1.96	0.65
1:C:348:MSE:HB2	6:C:5104:HOH:O	1.97	0.65
1:A:185:ALA:HB2	6:A:5101:HOH:O	1.97	0.64
1:C:210:ASP:HA	6:C:5424:HOH:O	1.96	0.64
1:D:32[B]:ILE:HD11	1:D:58:PHE:HZ	1.61	0.64
1:B:339:ASP:HB3	1:B:340:PRO:HD2	1.80	0.62
1:C:59:THR:HG22	1:C:73:THR:HB	1.80	0.62
1:B:242:ARG:HD2	6:B:5452:HOH:O	1.98	0.62
1:D:194:GLN:C	1:D:196:ARG:H	2.03	0.62
1:D:83:LYS:NZ	1:D:337:ARG:HH12	1.98	0.61
1:D:218[A]:VAL:HG12	1:D:350:MSE:SE	2.49	0.61
1:D:284:TYR:CB	3:D:3004:EDO:H22	2.28	0.61
1:C:196:ARG:O	1:C:200:ILE:HG12	2.00	0.61
1:C:380:LYS:HE3	6:C:5111:HOH:O	1.99	0.60
1:A:32[B]:ILE:HD12	1:A:56:VAL:HG11	1.83	0.60
1:D:194:GLN:C	1:D:196:ARG:N	2.53	0.60
1:D:182:GLN:HG2	6:D:5364:HOH:O	2.02	0.59
1:A:313[A]:ILE:HD12	4:A:4001:FMN:C10	2.32	0.59
1:B:227:VAL:HG21	3:B:3002:EDO:H11	1.84	0.59
1:B:182:GLN:HG3	6:B:5102:HOH:O	2.03	0.58
1:D:238:LYS:HD3	6:D:5363:HOH:O	2.03	0.58
1:A:30:GLU:OE1	1:A:34[B]:GLU:HG3	2.04	0.58
1:C:280:LYS:HG2	6:C:5232:HOH:O	2.02	0.58
1:D:138:MSE:SE	1:D:138:MSE:HA	2.54	0.58
1:D:59:THR:HG22	1:D:73:THR:HB	1.86	0.57
1:B:196:ARG:O	1:B:200:ILE:HG12	2.04	0.57
1:B:285[B]:THR:HG22	6:B:5134:HOH:O	2.03	0.57
1:B:238:LYS:HD3	6:B:5286:HOH:O	2.05	0.57
1:A:44:GLY:O	1:A:340:PRO:HD2	2.03	0.57
1:B:246:ALA:HB1	1:B:353:VAL:CG1	2.35	0.56
1:C:218[B]:VAL:HG23	1:C:350:MSE:SE	2.56	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:HIS:HB3	1:A:331:TYR:CZ	2.41	0.56
1:C:318:LYS:NZ	1:C:318:LYS:HB3	2.21	0.56
1:C:155:MSE:HE3	1:C:225:VAL:HG22	1.87	0.56
1:D:48:ARG:HG3	1:D:49:MSE:HE2	1.87	0.56
1:D:196:ARG:HD2	1:D:199:GLU:OE2	2.06	0.56
1:C:332:LYS:HE3	6:C:5307:HOH:O	2.05	0.56
1:A:193:ASN:ND2	1:A:195:GLU:H	2.03	0.56
1:B:94:GLU:HG2	6:B:5303:HOH:O	2.05	0.56
1:C:138:MSE:SE	1:C:138:MSE:HA	2.56	0.55
1:D:106:PRO:HD2	1:D:323:VAL:O	2.06	0.55
1:B:314:PRO:O	1:B:316:LEU:HD12	2.05	0.55
1:A:32[B]:ILE:HD13	1:A:74:MSE:SE	2.57	0.55
1:C:138:MSE:SE	1:C:138:MSE:CA	3.05	0.55
1:D:273:MSE:SE	1:D:273:MSE:HB3	2.54	0.55
1:C:313:ILE:HG23	4:C:4003:FMN:C2	2.38	0.54
1:A:329[A]:GLU:OE1	1:A:330:PRO:HD2	2.07	0.54
1:D:33:ASN:ND2	1:D:56:VAL:H	2.00	0.54
1:A:80:ASP:O	1:A:83:LYS:HG2	2.08	0.54
1:A:322:SER:HB3	1:A:331:TYR:CZ	2.42	0.54
1:B:272:VAL:HB	1:B:273:MSE:HE2	1.89	0.54
1:D:313:ILE:HG23	4:D:4004:FMN:C2	2.37	0.53
1:C:32[B]:ILE:CD1	1:C:56:VAL:HG11	2.34	0.53
1:C:33:ASN:ND2	1:C:56:VAL:H	2.00	0.52
1:A:49:MSE:HA	1:A:49:MSE:HE2	1.92	0.52
1:D:317:TYR:O	1:D:319:PRO:HD3	2.10	0.52
1:B:246:ALA:HB1	1:B:353:VAL:HG13	1.92	0.51
4:B:4002:FMN:H2'	4:B:4002:FMN:N1	2.25	0.51
1:C:282:ASP:HB2	6:C:5215:HOH:O	2.10	0.51
4:C:4005:FMN:H5'2	2:D:2006:NCO:N2	2.25	0.51
1:A:218[A]:VAL:HG11	1:A:347:GLY:HA2	1.91	0.51
1:C:209:ARG:O	1:C:211:GLY:N	2.43	0.51
1:D:218[B]:VAL:HG23	1:D:350:MSE:SE	2.60	0.51
1:A:322:SER:HB3	1:A:331:TYR:CE2	2.46	0.50
1:C:209:ARG:NH2	6:C:5318:HOH:O	2.44	0.50
1:D:48:ARG:HD2	1:D:52:GLU:HG2	1.93	0.50
1:D:273:MSE:SE	1:D:273:MSE:CA	3.09	0.50
1:C:211:GLY:HA3	1:C:318:LYS:HG3	1.94	0.50
1:D:101:ARG:HA	1:D:101:ARG:NE	2.26	0.50
4:C:4003:FMN:H2'	4:C:4003:FMN:N1	2.26	0.50
1:D:186:GLN:HG2	6:D:5355:HOH:O	2.10	0.50
1:D:138:MSE:SE	1:D:138:MSE:CA	3.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:HIS:HE1	1:B:324:ASP:OD2	1.95	0.49
1:B:321:MSE:CE	1:B:321:MSE:HB2	2.42	0.49
1:D:33:ASN:O	1:D:37:ARG:HG3	2.12	0.49
1:B:30:GLU:O	1:B:34[B]:GLU:HG3	2.12	0.49
1:B:44:GLY:O	1:B:340:PRO:HD2	2.12	0.49
1:D:194:GLN:HG2	1:D:197:GLU:OE1	2.13	0.49
1:B:252:ALA:HA	4:B:4002:FMN:O1P	2.13	0.49
1:D:49:MSE:SE	1:D:49:MSE:HA	2.62	0.49
4:D:4006:FMN:HM82	6:D:5379:HOH:O	2.12	0.49
1:C:211:GLY:HA3	1:C:318:LYS:CG	2.43	0.49
1:A:262:PHE:HA	1:B:309:VAL:HG11	1.95	0.48
1:B:313:ILE:HG23	4:B:4002:FMN:C2	2.43	0.48
1:C:43:TYR:CE1	1:C:201:LYS:HE3	2.49	0.48
1:A:384:TYR:CZ	1:B:120:ARG:HG2	2.48	0.48
1:B:376[A]:GLU:HG3	6:B:5300:HOH:O	2.12	0.48
1:D:9:SER:OG	1:D:48:ARG:NH2	2.46	0.48
1:D:218[A]:VAL:HG11	1:D:347:GLY:CA	2.34	0.48
4:D:4004:FMN:N1	4:D:4004:FMN:H2'	2.29	0.48
1:A:193:ASN:C	1:A:193:ASN:HD22	2.16	0.48
1:C:32[B]:ILE:HD11	1:C:58:PHE:CZ	2.49	0.48
1:B:219:GLU:HB2	1:B:307:ARG:HG2	1.95	0.48
1:D:319:PRO:HG3	1:D:335:VAL:HG22	1.96	0.48
1:A:284:TYR:CB	3:A:3001:EDO:H22	2.44	0.48
1:B:306:VAL:HG13	1:B:350:MSE:HE2	1.96	0.48
1:A:252:ALA:HA	4:A:4001:FMN:O1P	2.14	0.48
1:C:209:ARG:HA	6:C:5353:HOH:O	2.13	0.48
1:B:376[B]:GLU:OE1	1:C:380:LYS:NZ	2.43	0.47
1:C:206:GLN:HG2	6:C:5204:HOH:O	2.14	0.47
1:D:59:THR:HB	6:D:5048:HOH:O	2.14	0.47
1:D:209:ARG:HG3	6:D:5295:HOH:O	2.14	0.47
1:C:245:GLN:HB2	1:D:245:GLN:HB2	1.96	0.47
1:D:191:ILE:HD12	1:D:193:ASN:O	2.14	0.47
1:A:315:THR:HG23	4:A:4001:FMN:O2	2.15	0.47
1:A:327:THR:O	1:A:328:HIS:HB2	2.15	0.47
1:D:107:ARG:HA	1:D:108:PRO:HD3	1.73	0.47
1:D:343:LEU:HB3	1:D:344:PRO:HD3	1.96	0.47
1:D:318:LYS:HG2	1:D:318:LYS:O	2.14	0.46
1:C:313:ILE:HG12	4:C:4003:FMN:C10	2.46	0.46
1:D:101:ARG:HA	1:D:101:ARG:CZ	2.44	0.46
3:A:3006:EDO:H21	6:A:5230:HOH:O	2.14	0.46
1:B:167:LYS:HD2	1:B:200:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LEU:C	1:C:128:LEU:HD23	2.36	0.46
1:C:238:LYS:HD3	6:C:5133:HOH:O	2.16	0.46
1:A:32[B]:ILE:CD1	1:A:74:MSE:SE	3.14	0.46
1:D:58:PHE:CD1	1:D:74:MSE:HG2	2.51	0.45
1:A:105:HIS:HB3	1:A:331:TYR:OH	2.15	0.45
1:B:128:LEU:C	1:B:128:LEU:HD23	2.37	0.45
1:C:32[B]:ILE:HD13	1:C:74:MSE:SE	2.66	0.45
1:C:44:GLY:O	1:C:339:ASP:HB3	2.16	0.45
1:C:212:ASP:OD1	1:D:268:LYS:HE3	2.16	0.45
1:C:384:TYR:CZ	1:D:120:ARG:HG2	2.52	0.45
1:D:307:ARG:NH2	6:D:5144:HOH:O	2.48	0.45
1:B:321:MSE:HE2	1:B:321:MSE:HA	1.98	0.45
1:C:218[A]:VAL:HG12	1:C:350:MSE:SE	2.66	0.45
1:D:28:THR:O	1:D:32[B]:ILE:HD12	2.16	0.45
1:D:259:GLY:O	1:D:307:ARG:NH2	2.46	0.45
1:B:134:ARG:HD3	5:B:5002:EPS:H82	1.99	0.45
1:B:380:LYS:HD2	1:B:380:LYS:HA	1.61	0.45
1:C:196:ARG:HG3	6:C:5227:HOH:O	2.15	0.45
1:B:13:ARG:NH2	1:D:59:THR:HG21	2.32	0.45
1:C:96:ARG:HG3	6:C:5426:HOH:O	2.17	0.44
1:C:227:VAL:HG11	3:C:3003:EDO:H22	1.99	0.44
1:C:376:GLU:HG3	6:C:5145:HOH:O	2.16	0.44
1:A:13:ARG:NH2	1:C:59:THR:HG21	2.33	0.44
1:C:39:ARG:HD3	1:C:140:VAL:HG21	1.99	0.44
1:D:97:LEU:O	1:D:100:LYS:HB2	2.17	0.44
1:A:193:ASN:HD22	1:A:195:GLU:H	1.66	0.44
1:D:49:MSE:SE	1:D:49:MSE:CA	3.16	0.44
1:D:194:GLN:HG3	6:D:5172:HOH:O	2.18	0.44
1:D:205:ASP:O	1:D:209:ARG:HG2	2.18	0.44
4:C:4005:FMN:O2'	4:D:4006:FMN:O2'	2.28	0.44
1:A:284:TYR:HB3	3:A:3001:EDO:H22	1.99	0.43
1:A:380:LYS:NZ	1:D:376:GLU:OE1	2.51	0.43
1:C:143:GLY:HA3	1:C:352:ALA:HB1	2.00	0.43
1:A:5:THR:N	1:B:234:GLN:HE22	1.98	0.43
1:B:8:GLU:HB3	1:B:129:GLU:HB3	2.01	0.43
1:B:135:GLU:HB3	6:B:5124:HOH:O	2.17	0.43
1:A:206:GLN:HG2	6:A:5419:HOH:O	2.17	0.43
1:D:171:VAL:HG22	1:D:192:VAL:CG2	2.49	0.43
4:C:4005:FMN:H5'1	6:C:5376:HOH:O	2.19	0.43
1:D:246:ALA:HB1	1:D:353:VAL:CG1	2.49	0.43
1:A:44:GLY:O	1:A:339:ASP:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:VAL:HG13	1:A:350:MSE:HE2	2.01	0.43
1:D:209:ARG:O	1:D:211:GLY:N	2.52	0.43
1:D:53:ASN:C	1:D:53:ASN:HD22	2.22	0.42
1:B:79:LYS:HB3	6:B:5323:HOH:O	2.18	0.42
1:C:53:ASN:HB3	1:C:79:LYS:NZ	2.34	0.42
1:C:192:VAL:HG22	6:C:5027:HOH:O	2.19	0.42
1:D:339:ASP:HA	6:D:5436:HOH:O	2.18	0.42
1:D:337:ARG:HG2	6:D:5208:HOH:O	2.18	0.42
4:D:4006:FMN:H2'	4:D:4006:FMN:H9	2.01	0.42
1:A:376:GLU:OE1	1:D:380:LYS:NZ	2.52	0.42
1:B:332:LYS:HE3	6:B:5390:HOH:O	2.19	0.42
1:A:91:GLU:CD	1:A:91:GLU:H	2.22	0.42
1:C:179:GLU:O	1:C:183:ARG:HG3	2.20	0.42
4:D:4006:FMN:H9	6:D:5217:HOH:O	2.19	0.42
1:A:37:ARG:HD3	6:A:5121:HOH:O	2.20	0.42
1:A:269:GLY:O	1:A:273:MSE:HG2	2.20	0.42
1:C:318:LYS:NZ	1:C:318:LYS:CB	2.81	0.42
1:D:327:THR:O	1:D:328:HIS:HB2	2.19	0.42
4:A:4001:FMN:H9	4:A:4001:FMN:H1'1	1.92	0.41
1:D:96:ARG:H	1:D:96:ARG:HG3	1.52	0.41
1:B:268:LYS:NZ	6:B:5396:HOH:O	2.53	0.41
1:B:55:GLN:HE21	1:B:55:GLN:HB3	1.70	0.41
1:D:128:LEU:C	1:D:128:LEU:HD23	2.40	0.41
1:C:273:MSE:SE	1:C:273:MSE:CA	3.18	0.41
1:D:125:ARG:HD2	6:D:5046:HOH:O	2.19	0.41
1:B:88:MSE:SE	1:B:88:MSE:HB3	2.71	0.41
1:A:273:MSE:SE	1:A:273:MSE:CA	3.18	0.41
4:B:4002:FMN:H9	4:B:4002:FMN:H1'1	1.86	0.41
1:D:195:GLU:HB2	6:D:5327:HOH:O	2.21	0.41
1:C:211:GLY:O	1:C:318:LYS:HG3	2.20	0.41
1:D:94:GLU:O	1:D:95:ASP:C	2.59	0.41
1:D:171:VAL:HG22	1:D:192:VAL:HG22	2.02	0.41
1:B:86:ASP:OD2	1:B:100:LYS:NZ	2.42	0.41
1:C:194:GLN:HG3	6:C:5065:HOH:O	2.20	0.41
4:C:4005:FMN:H1'1	4:C:4005:FMN:H4'	1.82	0.41
1:D:319:PRO:HG3	1:D:335:VAL:CG2	2.50	0.41
1:A:171:VAL:HA	1:A:172:PRO:HD3	2.01	0.41
1:A:242[B]:ARG:HD3	1:A:357:VAL:HG13	2.03	0.41
1:B:120:ARG:NH1	1:D:372:GLU:OE1	2.44	0.41
1:C:196:ARG:HD2	1:C:199:GLU:OE2	2.21	0.41
1:A:143:GLY:HA3	1:A:352:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:LEU:HD23	1:B:365:LYS:HD3	2.03	0.40
1:A:298:MSE:HE3	1:A:298:MSE:HB2	1.94	0.40
1:A:302:GLN:HB3	1:A:303:PRO:HD2	2.03	0.40
1:D:171:VAL:HA	1:D:172:PRO:HD3	1.95	0.40
1:D:313:ILE:HA	1:D:314:PRO:HD3	1.96	0.40
1:A:32[B]:ILE:HD11	1:A:58:PHE:CZ	2.56	0.40
1:C:246:ALA:HB1	1:C:353:VAL:HG13	2.03	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	394/388 (102%)	386 (98%)	7 (2%)	1 (0%)	41	37
1	B	394/388 (102%)	387 (98%)	6 (2%)	1 (0%)	41	37
1	C	394/388 (102%)	383 (97%)	10 (2%)	1 (0%)	41	37
1	D	390/388 (100%)	375 (96%)	10 (3%)	5 (1%)	12	6
All	All	1572/1552 (101%)	1531 (97%)	33 (2%)	8 (0%)	29	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	GLY
1	D	319	PRO
1	D	47	GLY
1	D	320	LEU
1	C	210	ASP
1	D	95	ASP
1	D	210	ASP
1	B	47	GLY

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	327/308 (106%)	321 (98%)	6 (2%)	59	63
1	B	327/308 (106%)	321 (98%)	6 (2%)	59	63
1	C	327/308 (106%)	321 (98%)	6 (2%)	59	63
1	D	323/308 (105%)	307 (95%)	16 (5%)	24	20
All	All	1304/1232 (106%)	1270 (97%)	34 (3%)	44	48

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	SER
1	A	160	HIS
1	A	164	PHE
1	A	193	ASN
1	A	338	SER
1	A	358	LEU
1	B	55	GLN
1	B	94	GLU
1	B	100	LYS
1	B	108	PRO
1	B	160	HIS
1	B	164	PHE
1	C	59	THR
1	C	128	LEU
1	C	164	PHE
1	C	209	ARG
1	C	318	LYS
1	C	358	LEU
1	D	48	ARG
1	D	53	ASN
1	D	59	THR
1	D	91	GLU
1	D	94	GLU
1	D	95	ASP

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Mol	Chain	Res	Type
1	D	96	ARG
1	D	99	SER
1	D	101	ARG
1	D	107	ARG
1	D	164	PHE
1	D	196	ARG
1	D	206	GLN
1	D	273	MSE
1	D	280	LYS
1	D	358	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	194	GLN
1	B	55	GLN
1	B	105	HIS
1	B	186	GLN
1	B	194	GLN
1	B	234	GLN
1	C	33	ASN
1	C	182	GLN
1	D	33	ASN
1	D	53	ASN
1	D	55	GLN
1	D	182	GLN
1	D	194	GLN
1	D	302	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

26 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EPS	B	5002	-	20,21,21	4.31	15 (75%)	26,31,31	5.00	18 (69%)
2	NCO	B	2008	-	6,6,6	0.52	0	-		
4	FMN	A	4001	-	33,33,33	1.45	5 (15%)	48,50,50	1.48	8 (16%)
2	NCO	C	2005	-	6,6,6	0.63	0	-		
3	EDO	A	3006	-	3,3,3	0.76	0	2,2,2	1.16	0
3	EDO	D	3004	-	3,3,3	0.51	0	2,2,2	0.11	0
4	FMN	B	4002	-	33,33,33	1.36	4 (12%)	48,50,50	1.76	13 (27%)
5	EPS	D	5004	-	20,21,21	4.22	14 (70%)	26,31,31	4.45	17 (65%)
4	FMN	C	4005	-	33,33,33	1.20	5 (15%)	48,50,50	1.55	10 (20%)
2	NCO	A	2002	-	6,6,6	0.55	0	-		
3	EDO	D	3007	-	3,3,3	0.51	0	2,2,2	0.61	0
2	NCO	B	2003	-	6,6,6	0.69	0	-		
2	NCO	D	2006	-	6,6,6	0.54	0	-		
3	EDO	B	3002	-	3,3,3	0.52	0	2,2,2	0.70	0
4	FMN	C	4003	-	33,33,33	1.43	4 (12%)	48,50,50	1.72	11 (22%)
2	NCO	A	2004	-	6,6,6	0.51	0	-		
5	EPS	C	5003	-	20,21,21	4.34	14 (70%)	26,31,31	4.37	17 (65%)
5	EPS	A	5001	-	20,21,21	4.34	14 (70%)	26,31,31	4.12	15 (57%)
3	EDO	C	3003	-	3,3,3	0.44	0	2,2,2	0.60	0
4	FMN	D	4004	-	33,33,33	1.24	2 (6%)	48,50,50	1.70	15 (31%)
3	EDO	A	3005	-	3,3,3	0.65	0	2,2,2	0.52	0
2	NCO	D	2009	-	6,6,6	0.65	0	-		
2	NCO	C	2001	-	6,6,6	0.75	0	-		
4	FMN	D	4006	-	33,33,33	1.30	4 (12%)	48,50,50	1.56	8 (16%)
2	NCO	A	2007	-	6,6,6	0.57	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	A	3001	-	3,3,3	0.49	0	2,2,2	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	3007	-	-	1/1/1/1	-
4	FMN	D	4006	-	-	1/18/18/18	0/3/3/3
3	EDO	A	3006	-	-	1/1/1/1	-
4	FMN	D	4004	-	-	1/18/18/18	0/3/3/3
3	EDO	D	3004	-	-	0/1/1/1	-
4	FMN	B	4002	-	-	1/18/18/18	0/3/3/3
5	EPS	B	5002	-	-	0/15/33/33	0/1/1/1
5	EPS	D	5004	-	-	0/15/33/33	0/1/1/1
3	EDO	B	3002	-	-	1/1/1/1	-
4	FMN	C	4005	-	-	11/18/18/18	0/3/3/3
4	FMN	C	4003	-	-	0/18/18/18	0/3/3/3
5	EPS	C	5003	-	-	0/15/33/33	0/1/1/1
4	FMN	A	4001	-	-	1/18/18/18	0/3/3/3
5	EPS	A	5001	-	-	0/15/33/33	0/1/1/1
3	EDO	C	3003	-	-	1/1/1/1	-
3	EDO	A	3005	-	-	1/1/1/1	-
3	EDO	A	3001	-	-	0/1/1/1	-

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	5003	EPS	C7-C9	-10.49	1.39	1.49
5	A	5001	EPS	C7-C9	-10.40	1.39	1.49
5	B	5002	EPS	C7-C9	-10.07	1.39	1.49
5	D	5004	EPS	C7-C9	-9.81	1.39	1.49
5	B	5002	EPS	O11-C10	6.18	1.37	1.22
5	D	5004	EPS	C3-C2	-5.88	1.41	1.50
5	C	5003	EPS	C3-C2	-5.78	1.41	1.50
5	A	5001	EPS	C3-C2	-5.71	1.41	1.50
5	B	5002	EPS	O4-C4	-5.52	1.29	1.43
5	D	5004	EPS	C4-C5	-5.50	1.41	1.53
5	B	5002	EPS	C2-C1	5.43	1.45	1.33
5	D	5004	EPS	C2-C1	5.41	1.45	1.33
5	A	5001	EPS	C4-C3	-5.30	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	5002	EPS	C3-C2	-5.16	1.42	1.50
5	B	5002	EPS	C4-C5	-5.09	1.42	1.53
5	A	5001	EPS	O4-C4	-5.09	1.30	1.43
5	D	5004	EPS	O11-C10	4.96	1.34	1.22
5	C	5003	EPS	O11-C10	4.93	1.34	1.22
5	C	5003	EPS	C2-C1	4.87	1.44	1.33
5	A	5001	EPS	C8-C7	4.85	1.44	1.31
5	C	5003	EPS	O4-C4	-4.84	1.31	1.43
5	C	5003	EPS	C6-C5	-4.73	1.42	1.53
5	D	5004	EPS	O4-C4	-4.71	1.31	1.43
5	C	5003	EPS	C4-C5	-4.64	1.43	1.53
5	C	5003	EPS	C4-C3	-4.57	1.44	1.52
5	A	5001	EPS	C6-C5	-4.54	1.43	1.53
5	C	5003	EPS	O5-C5	-4.52	1.38	1.46
5	C	5003	EPS	C8-C7	4.51	1.43	1.31
5	B	5002	EPS	C8-C7	4.46	1.43	1.31
5	A	5001	EPS	O5-C5	-4.44	1.38	1.46
4	A	4001	FMN	C4-N3	-4.38	1.30	1.38
5	A	5001	EPS	C2-C1	4.37	1.43	1.33
5	A	5001	EPS	C4-C5	-4.37	1.43	1.53
5	B	5002	EPS	C6-C5	-4.35	1.43	1.53
5	A	5001	EPS	C6-C1	-4.35	1.44	1.51
4	D	4004	FMN	C4-N3	-4.35	1.30	1.38
5	A	5001	EPS	O11-C10	4.31	1.33	1.22
5	D	5004	EPS	C6-C5	-4.26	1.43	1.53
5	C	5003	EPS	C6-C1	-4.20	1.44	1.51
5	D	5004	EPS	C8-C7	4.17	1.42	1.31
5	D	5004	EPS	C6-C1	-4.17	1.44	1.51
5	D	5004	EPS	O5-C5	-4.00	1.39	1.46
5	B	5002	EPS	C4-C3	-3.87	1.46	1.52
4	D	4006	FMN	C4-N3	-3.87	1.31	1.38
5	C	5003	EPS	O92-C9	3.82	1.32	1.22
5	B	5002	EPS	O5-C5	-3.79	1.39	1.46
5	D	5004	EPS	O92-C9	3.75	1.31	1.22
5	B	5002	EPS	C6-C1	-3.69	1.45	1.51
5	A	5001	EPS	O92-C9	3.66	1.31	1.22
5	D	5004	EPS	C4-C3	-3.57	1.46	1.52
4	C	4003	FMN	C4-N3	-3.53	1.32	1.38
4	C	4005	FMN	C4-N3	-3.50	1.32	1.38
5	A	5001	EPS	P-O3P	3.42	1.67	1.54
5	A	5001	EPS	C10-C1	-3.37	1.41	1.49
5	D	5004	EPS	C10-C1	-3.26	1.41	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	5002	EPS	O92-C9	3.25	1.30	1.22
5	C	5003	EPS	P-O3P	3.01	1.66	1.54
5	B	5002	EPS	P-O3P	3.00	1.65	1.54
5	C	5003	EPS	C10-C1	-2.99	1.42	1.49
5	B	5002	EPS	C10-C1	-2.96	1.42	1.49
4	B	4002	FMN	C4-N3	-2.84	1.33	1.38
4	C	4003	FMN	C7M-C7	2.79	1.56	1.51
4	A	4001	FMN	C7M-C7	2.76	1.56	1.51
4	B	4002	FMN	C6-C7	-2.75	1.35	1.39
5	D	5004	EPS	P-O3P	2.53	1.64	1.54
4	D	4006	FMN	C6-C5A	2.52	1.43	1.40
5	B	5002	EPS	P-O1P	2.44	1.58	1.50
4	A	4001	FMN	C2'-C3'	2.41	1.57	1.53
4	C	4003	FMN	C2'-C3'	2.40	1.57	1.53
4	B	4002	FMN	C6-C5A	2.33	1.43	1.40
4	D	4006	FMN	C7M-C7	2.29	1.55	1.51
4	C	4003	FMN	C6-C5A	2.28	1.43	1.40
4	A	4001	FMN	O3'-C3'	2.22	1.48	1.43
4	C	4005	FMN	O2-C2	-2.20	1.20	1.24
4	D	4004	FMN	C2'-C3'	2.19	1.57	1.53
4	B	4002	FMN	O2-C2	-2.18	1.20	1.24
4	A	4001	FMN	C1'-C2'	-2.15	1.49	1.52
4	C	4005	FMN	C7M-C7	2.14	1.55	1.51
4	D	4006	FMN	C6-C7	-2.13	1.36	1.39
4	C	4005	FMN	C6-C7	-2.05	1.36	1.39
4	C	4005	FMN	C6-C5A	2.01	1.43	1.40

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	5002	EPS	C2-C1-C10	13.19	138.02	119.99
5	B	5002	EPS	O12-C10-O11	-10.83	98.13	123.90
5	D	5004	EPS	O12-C10-O11	-10.62	98.61	123.90
5	D	5004	EPS	C2-C1-C10	10.20	133.93	119.99
5	B	5002	EPS	O12-C10-C1	10.00	136.55	115.43
5	C	5003	EPS	C2-C1-C10	9.78	133.35	119.99
5	C	5003	EPS	O12-C10-O11	-9.74	100.72	123.90
5	A	5001	EPS	O12-C10-O11	-9.11	102.20	123.90
5	A	5001	EPS	C2-C1-C10	8.75	131.95	119.99
5	A	5001	EPS	P-O3-C3	-8.56	99.96	122.25
5	C	5003	EPS	P-O3-C3	-7.66	102.29	122.25
5	D	5004	EPS	P-O3-C3	-7.40	102.98	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	5002	EPS	P-O3-C3	-7.33	103.15	122.25
5	A	5001	EPS	O12-C10-C1	7.27	130.78	115.43
5	C	5003	EPS	O12-C10-C1	7.00	130.21	115.43
5	D	5004	EPS	O11-C10-C1	6.41	132.88	121.64
5	D	5004	EPS	O12-C10-C1	6.19	128.51	115.43
5	B	5002	EPS	C6-C1-C2	-5.74	115.17	122.25
5	B	5002	EPS	C6-C1-C10	-5.57	106.77	116.99
5	C	5003	EPS	C6-C1-C2	-5.48	115.49	122.25
5	D	5004	EPS	C6-C1-C2	-5.46	115.51	122.25
4	C	4003	FMN	C4-C4A-N5	4.95	125.04	118.21
5	C	5003	EPS	O91-C9-C7	4.88	122.23	113.91
4	C	4003	FMN	C5A-C9A-N10	-4.80	113.62	117.97
5	C	5003	EPS	O91-C9-O92	-4.56	113.05	123.90
5	A	5001	EPS	C8-C7-C9	-4.49	114.44	122.73
4	B	4002	FMN	C4-C4A-N5	4.41	124.30	118.21
5	C	5003	EPS	O5-C7-C9	4.30	126.30	115.59
5	C	5003	EPS	C6-C1-C10	-4.29	109.11	116.99
5	B	5002	EPS	O3-C3-C2	4.25	118.36	108.09
5	C	5003	EPS	O11-C10-C1	4.24	129.06	121.64
5	A	5001	EPS	C6-C1-C2	-4.21	117.05	122.25
5	B	5002	EPS	C3-C2-C1	4.13	129.09	122.66
5	B	5002	EPS	O91-C9-C7	4.11	120.93	113.91
5	D	5004	EPS	C8-C7-C9	-4.11	115.14	122.73
4	C	4005	FMN	O3'-C3'-C2'	4.05	118.14	108.93
4	D	4006	FMN	C5'-C4'-C3'	3.98	119.73	112.22
5	B	5002	EPS	O4-C4-C5	3.96	119.09	109.32
4	D	4006	FMN	O4-C4-C4A	-3.94	116.14	126.53
5	D	5004	EPS	C3-C2-C1	3.86	128.66	122.66
5	A	5001	EPS	O91-C9-C7	3.85	120.48	113.91
5	D	5004	EPS	O91-C9-O92	-3.82	114.80	123.90
5	A	5001	EPS	C6-C1-C10	-3.78	110.06	116.99
5	A	5001	EPS	O2P-P-O1P	3.75	125.44	110.83
5	D	5004	EPS	C6-C1-C10	-3.71	110.17	116.99
5	A	5001	EPS	O5-C7-C9	3.69	124.77	115.59
5	D	5004	EPS	O4-C4-C3	-3.68	102.28	110.36
5	B	5002	EPS	C8-C7-C9	-3.65	115.98	122.73
5	A	5001	EPS	O91-C9-O92	-3.49	115.59	123.90
5	A	5001	EPS	O4-C4-C5	3.48	117.90	109.32
5	C	5003	EPS	C3-C2-C1	3.34	127.85	122.66
4	D	4004	FMN	C4'-C3'-C2'	3.33	119.10	113.57
4	B	4002	FMN	C8M-C8-C9	3.29	125.37	119.57
5	D	5004	EPS	O91-C9-C7	3.28	119.51	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	4002	FMN	C5A-C9A-N10	-3.28	115.01	117.97
4	D	4006	FMN	O4-C4-N3	3.27	126.26	120.11
5	D	5004	EPS	O5-C7-C9	3.25	123.67	115.59
5	D	5004	EPS	O4-C4-C5	3.25	117.32	109.32
5	C	5003	EPS	C8-C7-C9	-3.22	116.77	122.73
4	A	4001	FMN	C4-C4A-N5	3.19	122.61	118.21
4	D	4004	FMN	C8M-C8-C9	3.14	125.10	119.57
4	D	4004	FMN	C5'-C4'-C3'	3.13	118.12	112.22
4	A	4001	FMN	C1'-C2'-C3'	3.13	118.14	109.66
5	B	5002	EPS	O91-C9-O92	-3.11	116.50	123.90
5	A	5001	EPS	O11-C10-C1	3.07	127.02	121.64
4	B	4002	FMN	C10-N1-C2	3.01	123.36	116.85
5	C	5003	EPS	O3-C3-C4	-2.97	100.89	106.80
4	A	4001	FMN	O4-C4-N3	2.91	125.59	120.11
4	B	4002	FMN	C9A-N10-C10	2.89	125.15	120.75
4	D	4004	FMN	C9A-C9-C8	2.83	124.92	119.22
4	C	4003	FMN	C9A-C5A-N5	2.83	125.45	122.45
4	A	4001	FMN	C5'-C4'-C3'	2.82	117.53	112.22
5	B	5002	EPS	O3-C3-C4	-2.81	101.20	106.80
4	B	4002	FMN	O2'-C2'-C3'	-2.81	102.67	109.25
4	D	4004	FMN	O2'-C2'-C3'	-2.80	102.71	109.25
4	C	4003	FMN	C4A-C4-N3	2.77	120.30	113.25
5	A	5001	EPS	O3P-P-O2P	-2.76	97.44	107.80
4	B	4002	FMN	O4-C4-C4A	-2.73	119.31	126.53
4	D	4004	FMN	C9-C9A-N10	2.72	125.52	121.85
4	C	4003	FMN	C10-N1-C2	2.69	122.67	116.85
5	C	5003	EPS	O4-C4-C5	2.65	115.86	109.32
4	C	4003	FMN	O2P-P-O5'	2.65	113.58	106.67
4	D	4004	FMN	O4-C4-N3	2.64	125.09	120.11
4	C	4005	FMN	C1'-C2'-C3'	2.63	116.80	109.66
4	C	4003	FMN	O2'-C2'-C3'	-2.63	103.10	109.25
4	C	4005	FMN	C5A-C9A-N10	-2.59	115.62	117.97
4	D	4004	FMN	C5A-C9A-N10	-2.59	115.63	117.97
5	D	5004	EPS	O92-C9-C7	2.59	125.69	121.79
4	A	4001	FMN	O3'-C3'-C4'	-2.58	103.06	108.93
4	B	4002	FMN	C5'-C4'-C3'	2.58	117.08	112.22
4	C	4005	FMN	O5'-C5'-C4'	2.54	116.13	109.36
5	C	5003	EPS	O4-C4-C3	-2.52	104.83	110.36
5	B	5002	EPS	O5-C7-C9	2.51	121.83	115.59
5	C	5003	EPS	O2P-P-O1P	2.49	120.53	110.83
5	A	5001	EPS	O4-C4-C3	-2.43	105.03	110.36
5	B	5002	EPS	O3P-P-O2P	-2.43	98.69	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	4004	FMN	C9A-C5A-N5	2.42	125.02	122.45
5	B	5002	EPS	O2P-P-O1P	2.40	120.19	110.83
4	D	4004	FMN	C9-C8-C7	-2.39	116.18	119.69
5	B	5002	EPS	O3P-P-O1P	-2.39	101.52	110.83
4	C	4005	FMN	O4'-C4'-C5'	2.37	115.22	109.99
4	A	4001	FMN	O4-C4-C4A	-2.37	120.28	126.53
4	C	4003	FMN	C4'-C3'-C2'	2.37	117.51	113.57
4	C	4005	FMN	C4-C4A-N5	2.34	121.44	118.21
5	C	5003	EPS	O3P-P-O2P	-2.32	99.12	107.80
4	D	4004	FMN	C4-N3-C2	2.31	129.74	125.64
4	B	4002	FMN	O3P-P-O2P	2.29	116.40	107.80
4	B	4002	FMN	C4A-C4-N3	2.25	118.97	113.25
4	D	4006	FMN	C9A-C9-C8	2.24	123.72	119.22
4	C	4003	FMN	C9-C9A-N10	2.23	124.86	121.85
4	D	4004	FMN	C1'-N10-C9A	2.23	124.96	120.63
4	C	4005	FMN	O4-C4-C4A	-2.23	120.66	126.53
4	C	4005	FMN	C4'-C3'-C2'	-2.23	109.87	113.57
4	C	4005	FMN	C10-N1-C2	2.22	121.65	116.85
5	D	5004	EPS	O2P-P-O1P	2.22	119.48	110.83
4	A	4001	FMN	O3P-P-O5'	-2.21	100.90	106.67
5	D	5004	EPS	O3-C3-C4	-2.20	102.42	106.80
4	D	4006	FMN	O4'-C4'-C5'	-2.16	105.22	109.99
4	D	4006	FMN	C10-N1-C2	2.16	121.52	116.85
4	D	4004	FMN	O3P-P-O2P	2.14	115.83	107.80
4	A	4001	FMN	O3'-C3'-C2'	2.13	113.78	108.93
4	C	4003	FMN	C5'-C4'-C3'	2.13	116.23	112.22
4	C	4005	FMN	O2'-C2'-C3'	-2.11	104.30	109.25
4	C	4003	FMN	C10-C4A-N5	-2.10	120.51	124.81
5	B	5002	EPS	O11-C10-C1	2.10	125.32	121.64
4	D	4004	FMN	C4-C4A-N5	2.10	121.11	118.21
4	D	4006	FMN	C5A-C9A-N10	-2.09	116.08	117.97
4	B	4002	FMN	O2P-P-O5'	2.08	112.09	106.67
4	D	4006	FMN	O3P-P-O2P	2.07	115.57	107.80
4	D	4004	FMN	C1'-C2'-C3'	2.02	115.15	109.66
4	B	4002	FMN	O3'-C3'-C4'	-2.00	104.38	108.93
4	B	4002	FMN	C10-C4A-N5	-2.00	120.72	124.81

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	4005	FMN	C1'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
4	C	4005	FMN	C1'-C2'-C3'-C4'
4	C	4005	FMN	O2'-C2'-C3'-O3'
4	C	4005	FMN	O2'-C2'-C3'-C4'
4	C	4005	FMN	C2'-C3'-C4'-O4'
4	C	4005	FMN	O3'-C3'-C4'-O4'
4	C	4005	FMN	O3'-C3'-C4'-C5'
4	C	4005	FMN	C5'-O5'-P-O2P
4	C	4005	FMN	C5'-O5'-P-O3P
4	C	4005	FMN	C2'-C3'-C4'-C5'
3	C	3003	EDO	O1-C1-C2-O2
4	D	4006	FMN	C2'-C1'-N10-C9A
4	C	4005	FMN	C5'-O5'-P-O1P
4	B	4002	FMN	C2'-C1'-N10-C10
3	A	3005	EDO	O1-C1-C2-O2
3	A	3006	EDO	O1-C1-C2-O2
4	A	4001	FMN	C4'-C5'-O5'-P
3	B	3002	EDO	O1-C1-C2-O2
4	D	4004	FMN	C5'-O5'-P-O3P
3	D	3007	EDO	O1-C1-C2-O2

There are no ring outliers.

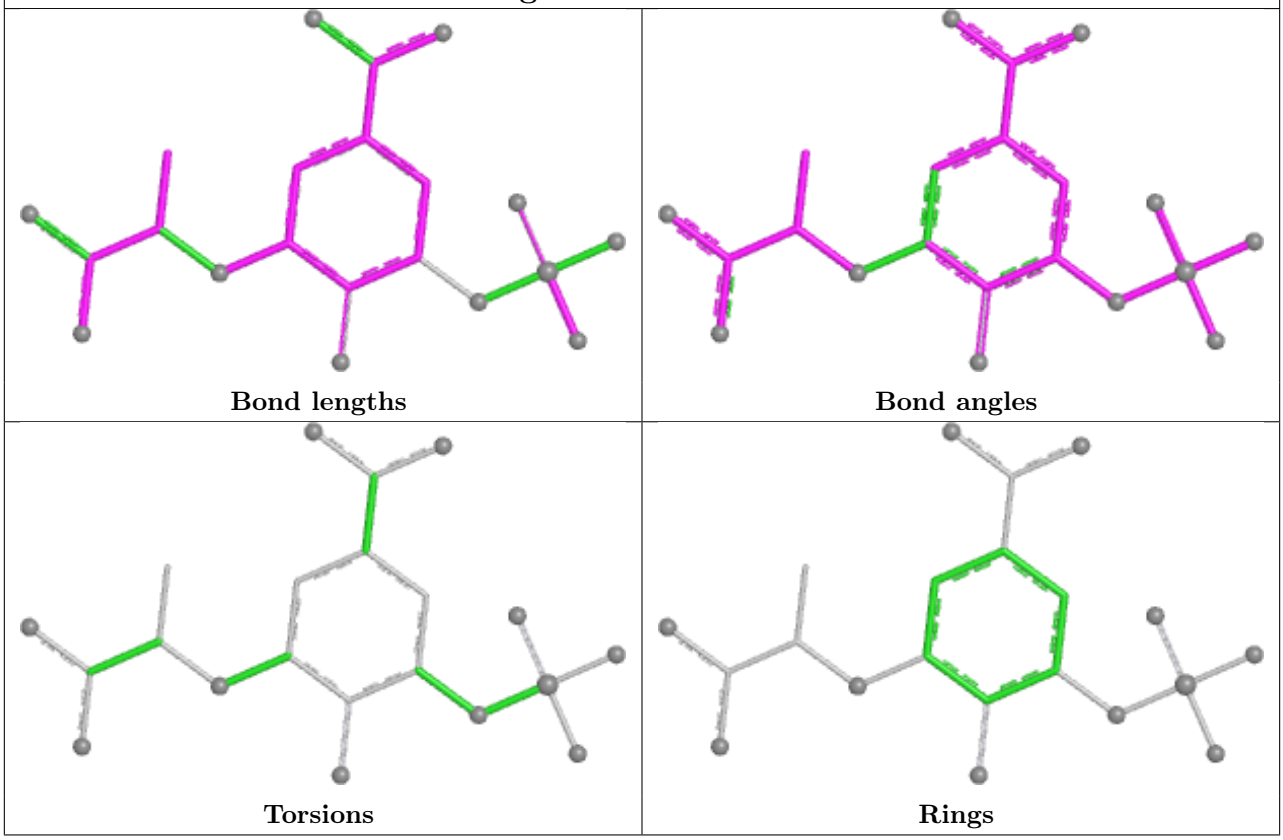
13 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5002	EPS	1	0
4	A	4001	FMN	5	0
3	A	3006	EDO	2	0
3	D	3004	EDO	2	0
4	B	4002	FMN	4	0
4	C	4005	FMN	4	0
2	D	2006	NCO	1	0
3	B	3002	EDO	1	0
4	C	4003	FMN	3	0
3	C	3003	EDO	2	0
4	D	4004	FMN	2	0
4	D	4006	FMN	4	0
3	A	3001	EDO	2	0

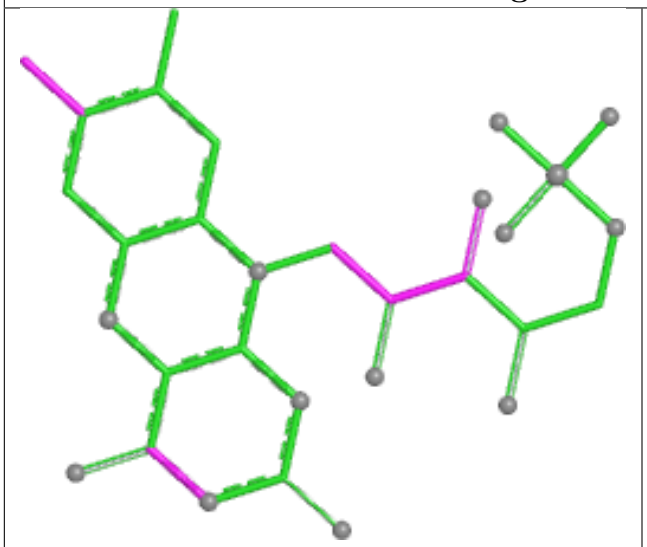
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

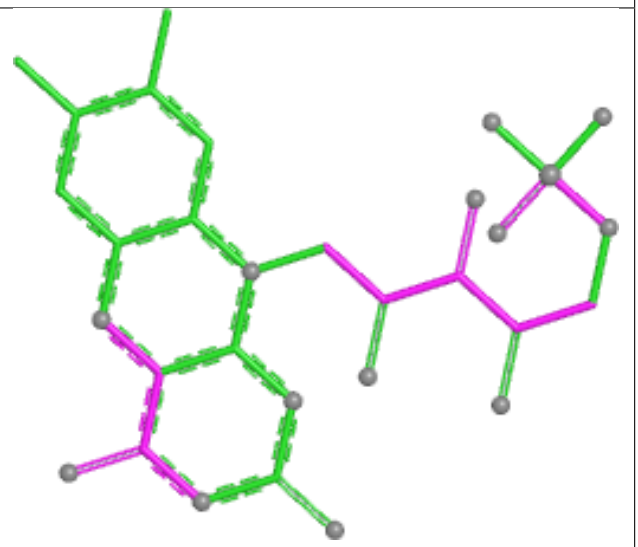
Ligand EPS B 5002



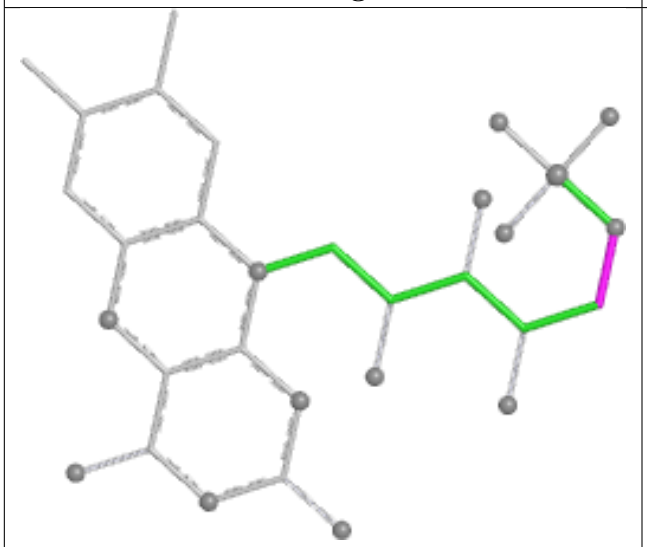
Ligand FMN A 4001



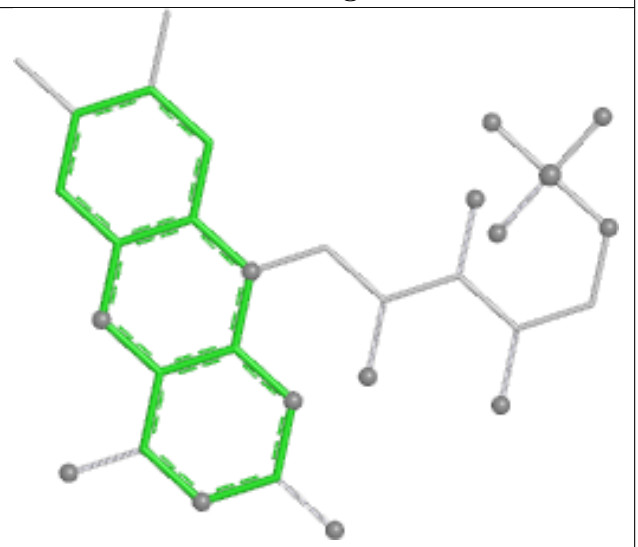
Bond lengths



Bond angles

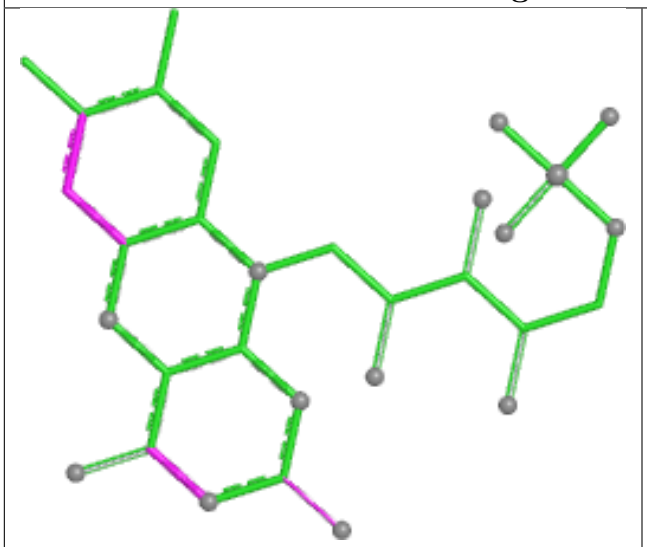


Torsions

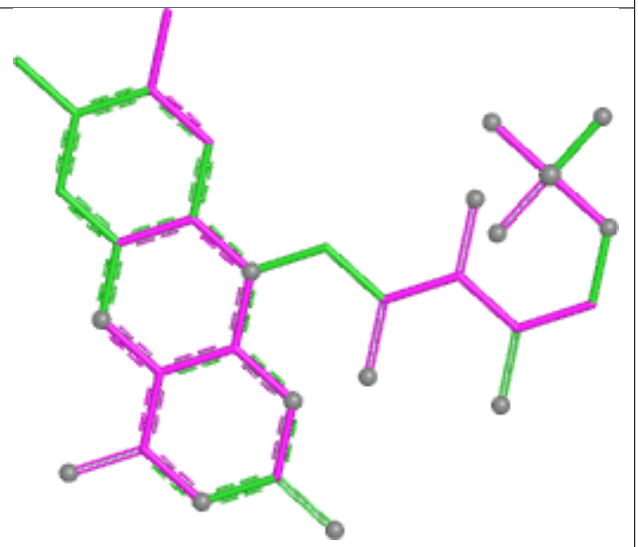


Rings

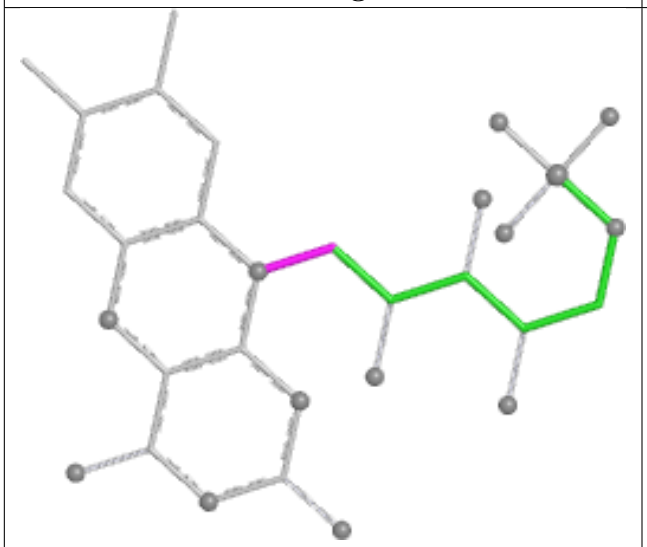
Ligand FMN B 4002



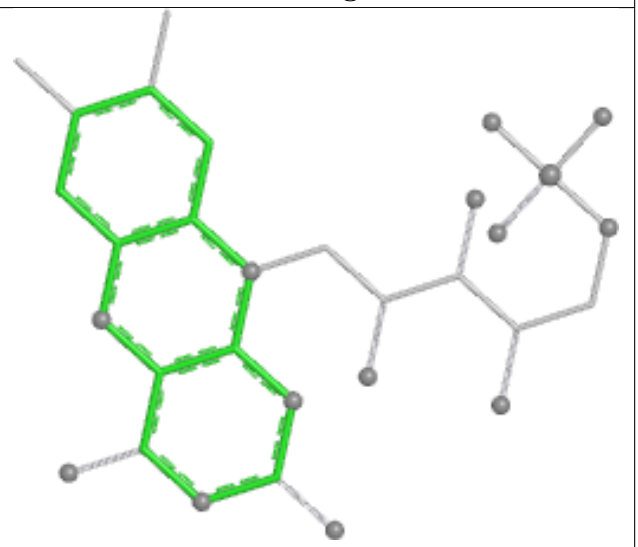
Bond lengths



Bond angles

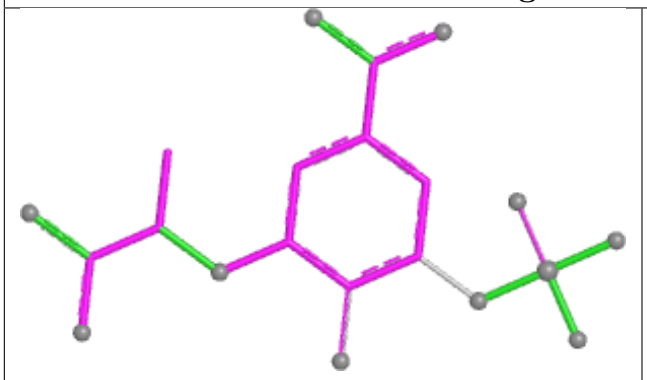


Torsions

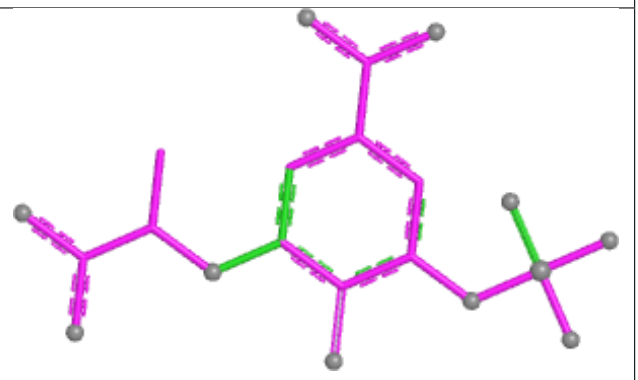


Rings

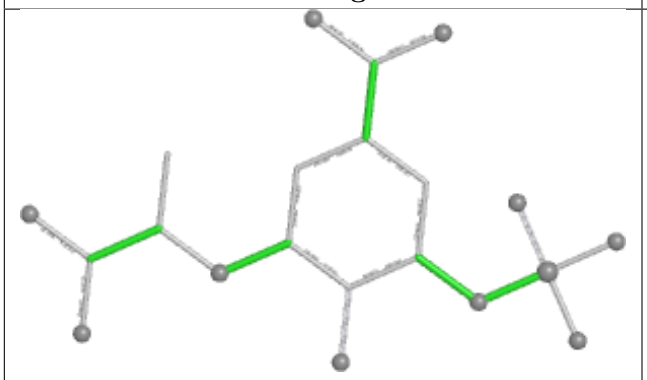
Ligand EPS D 5004



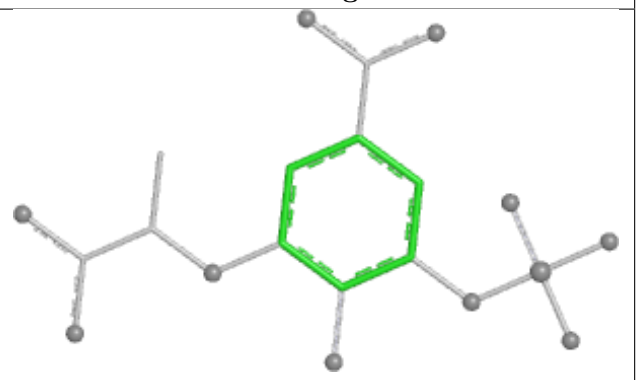
Bond lengths



Bond angles

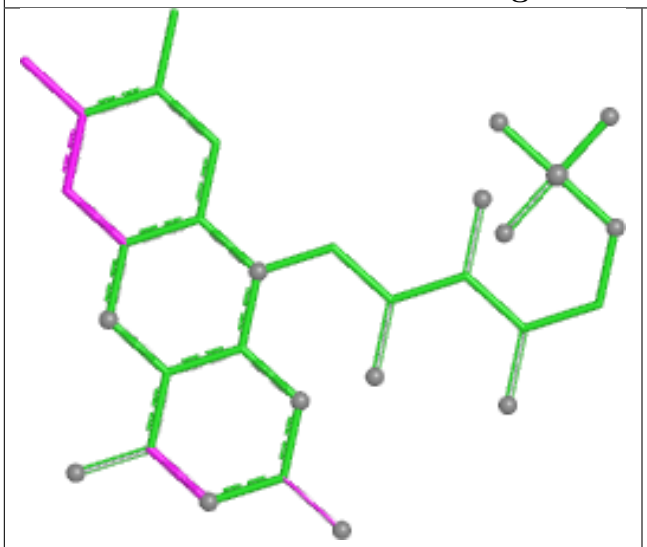


Torsions

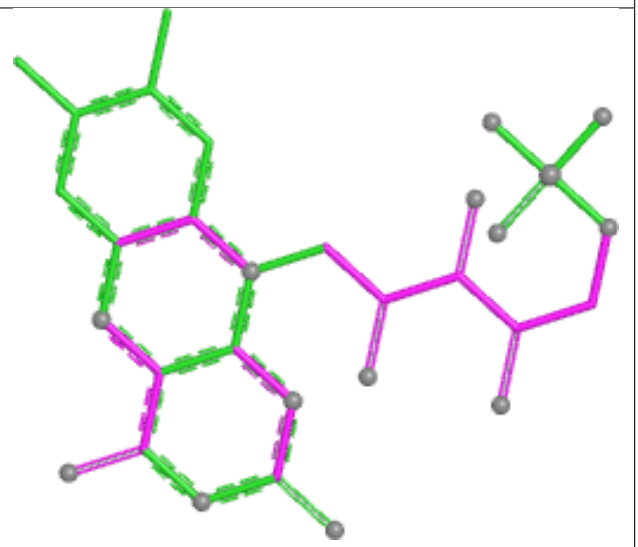


Rings

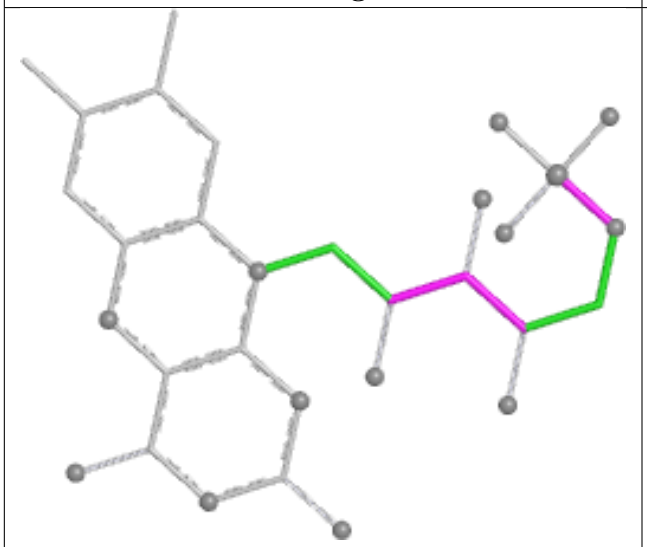
Ligand FMN C 4005



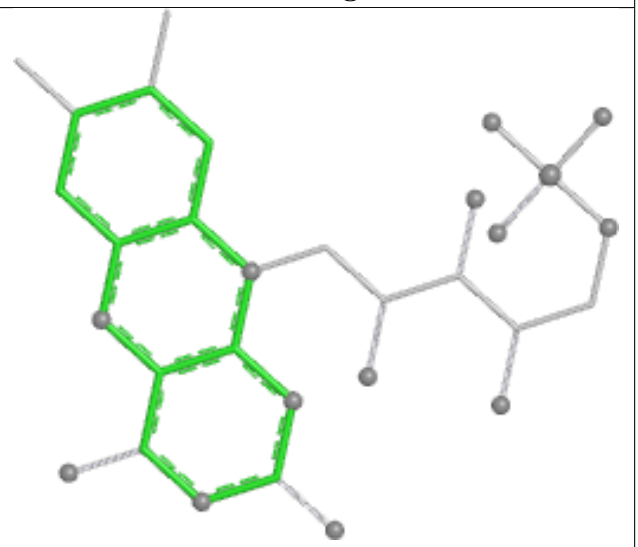
Bond lengths



Bond angles

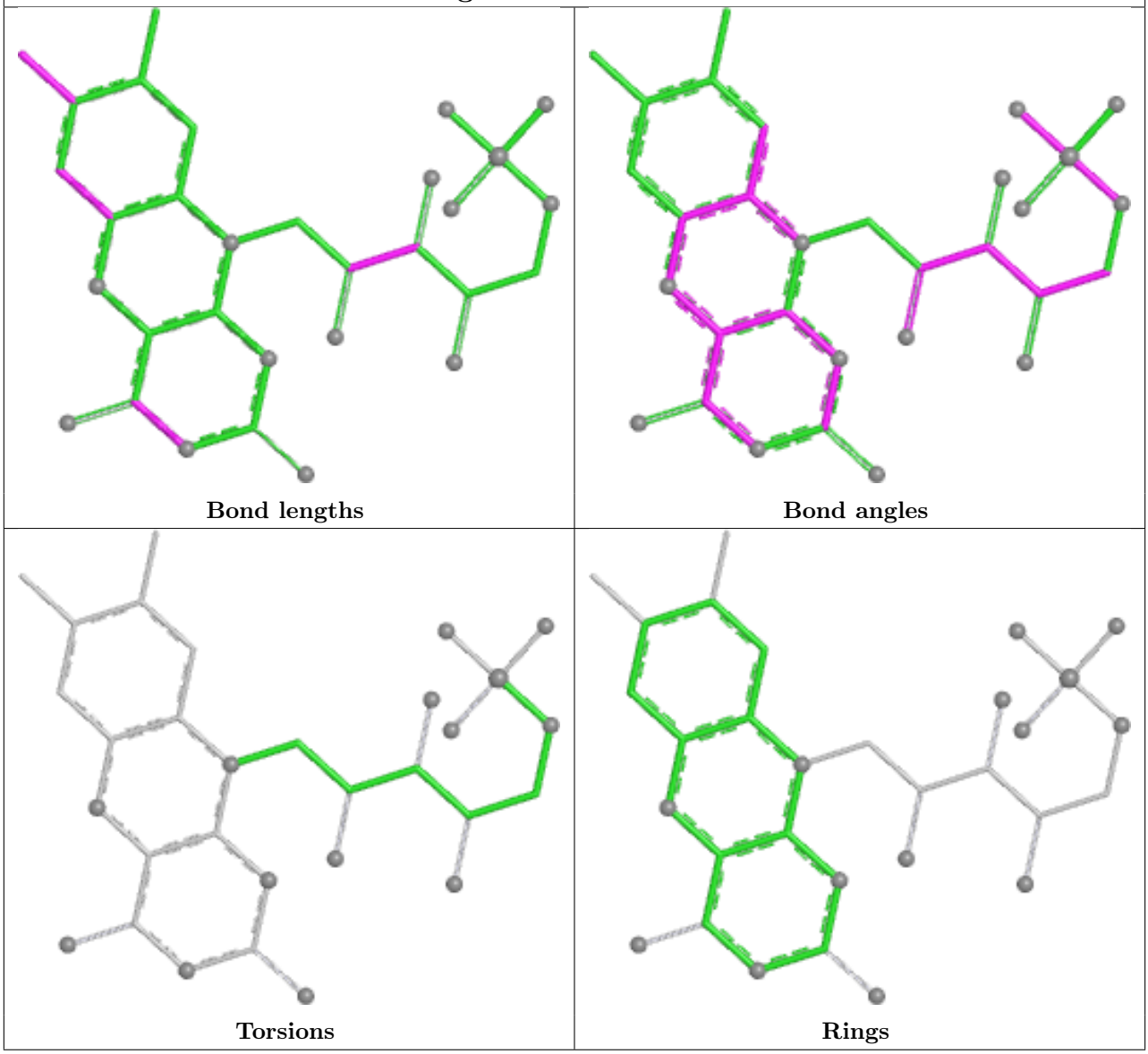


Torsions

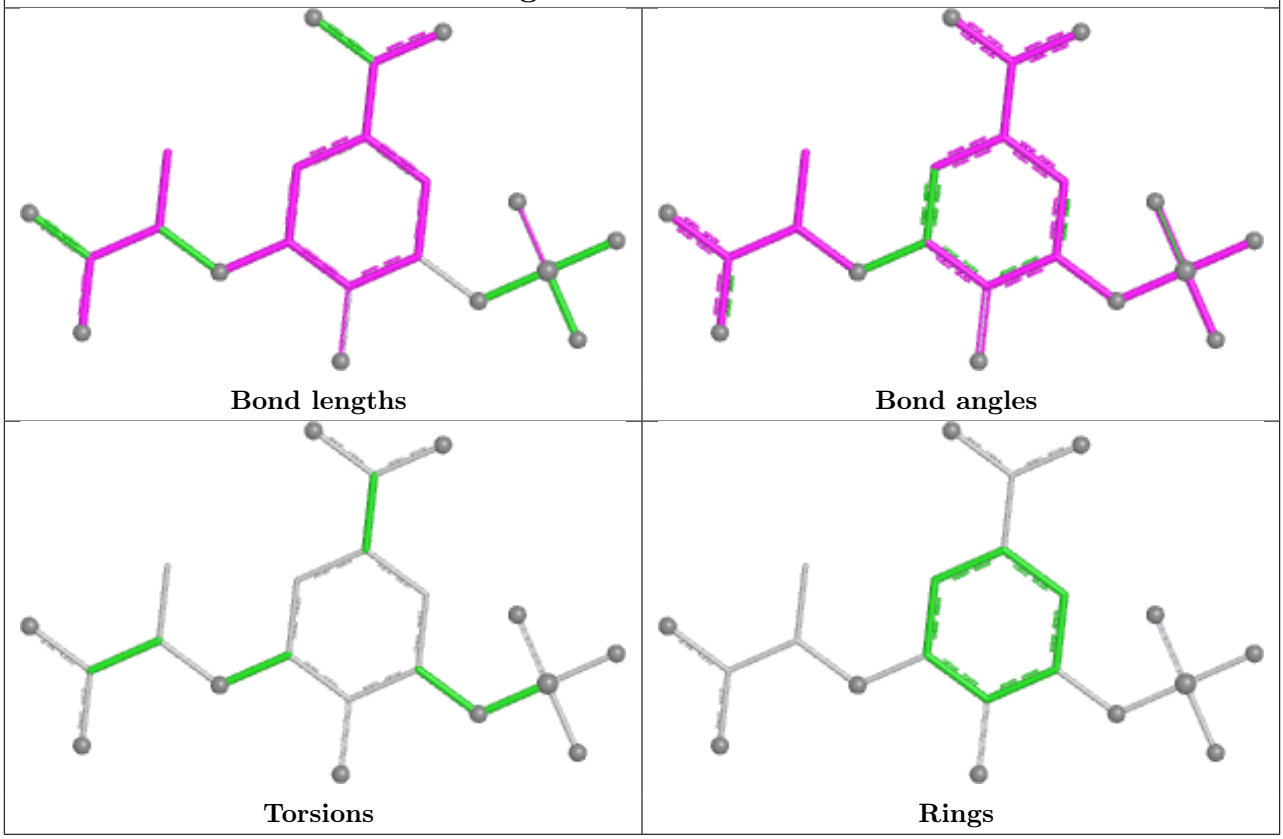


Rings

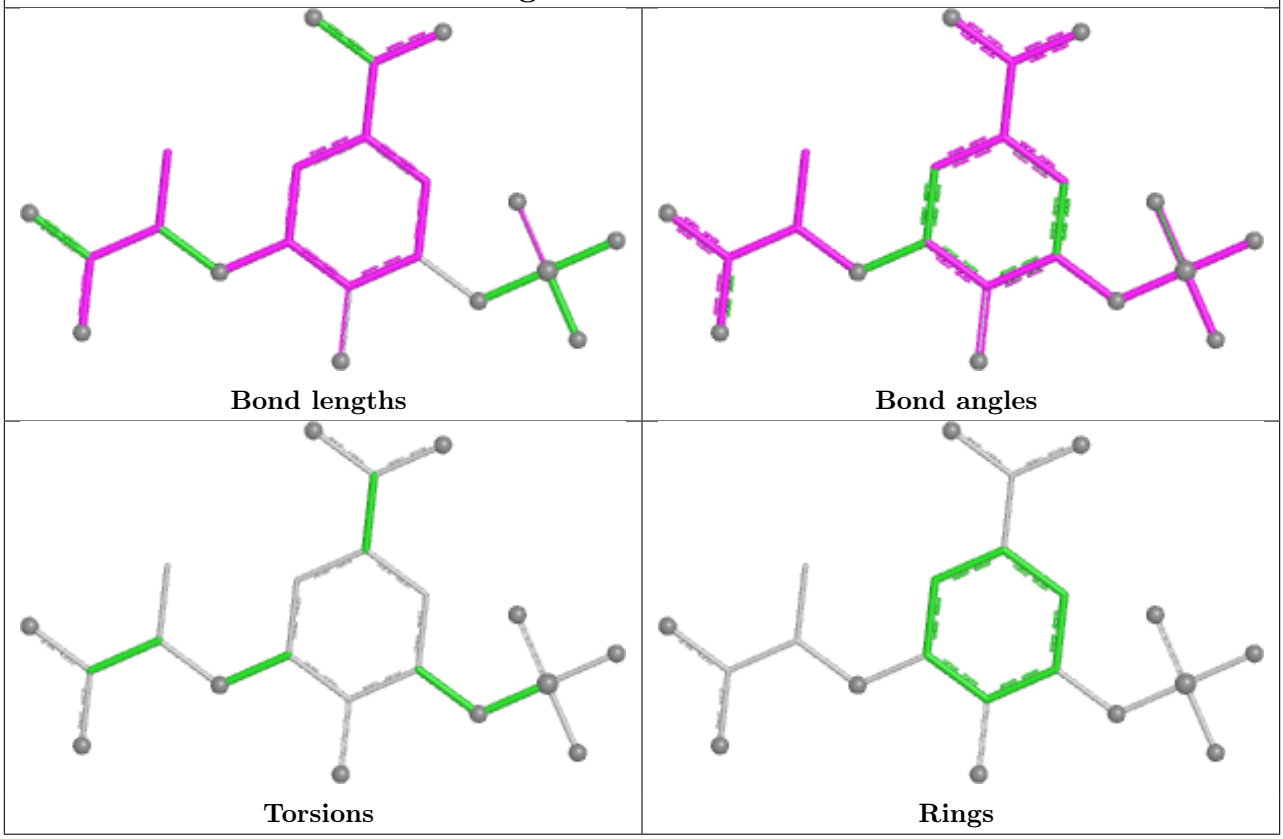
Ligand FMN C 4003



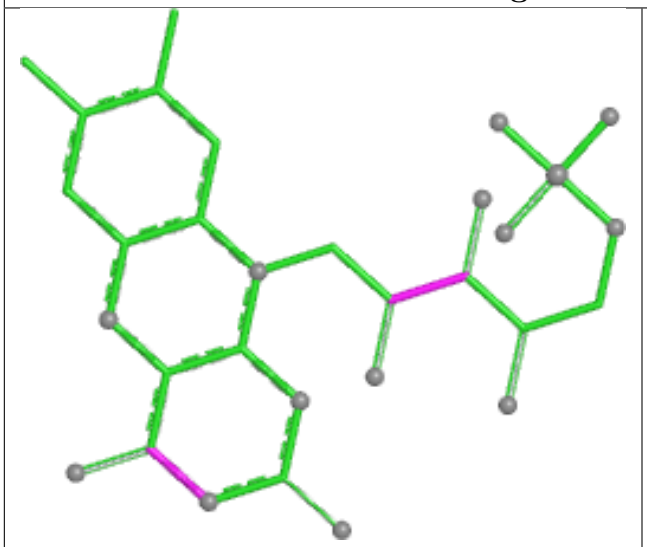
Ligand EPS C 5003



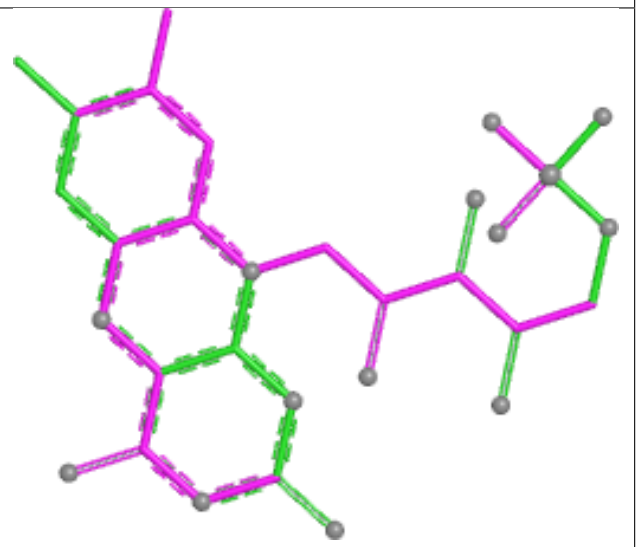
Ligand EPS A 5001



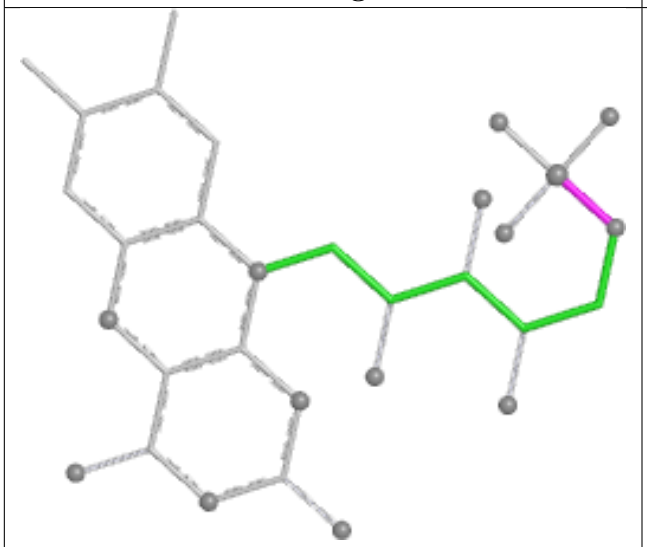
Ligand FMN D 4004



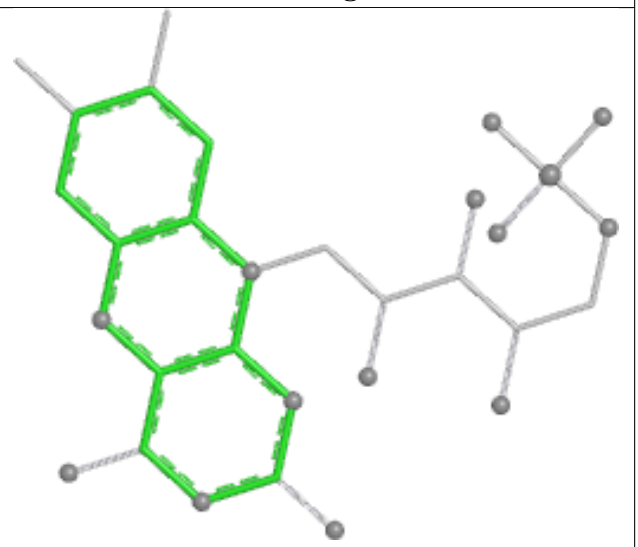
Bond lengths



Bond angles

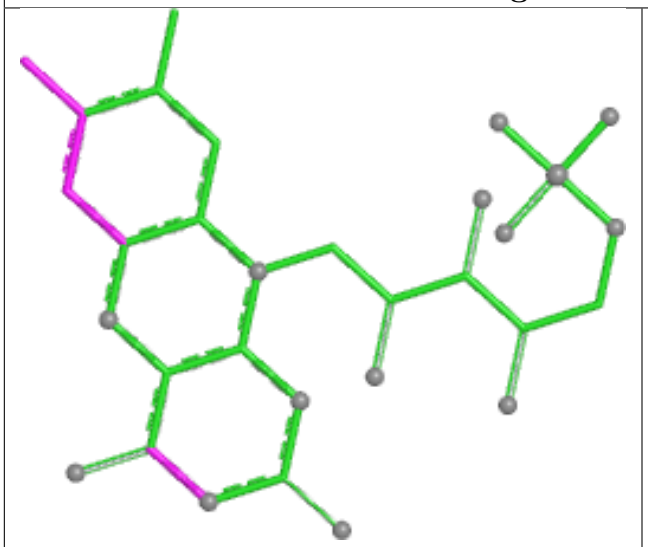


Torsions

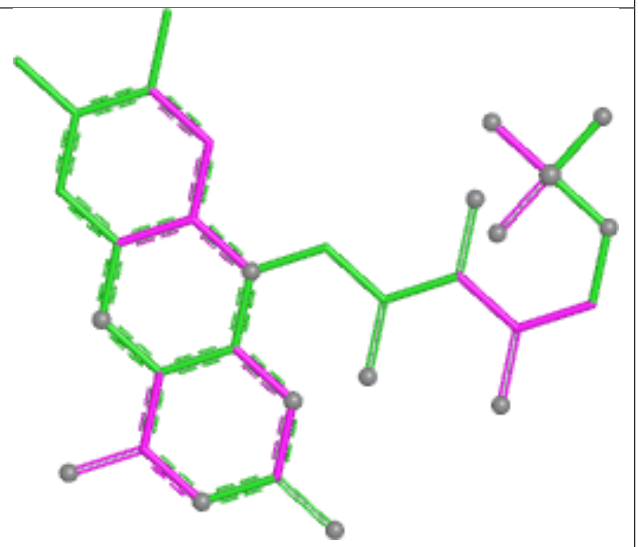


Rings

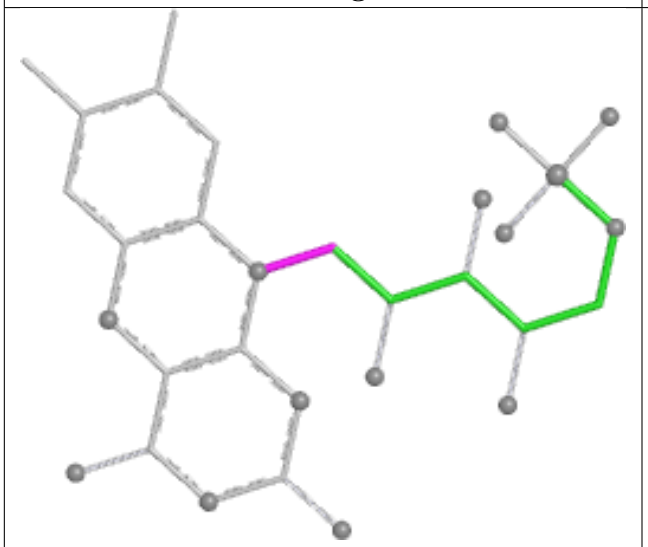
Ligand FMN D 4006



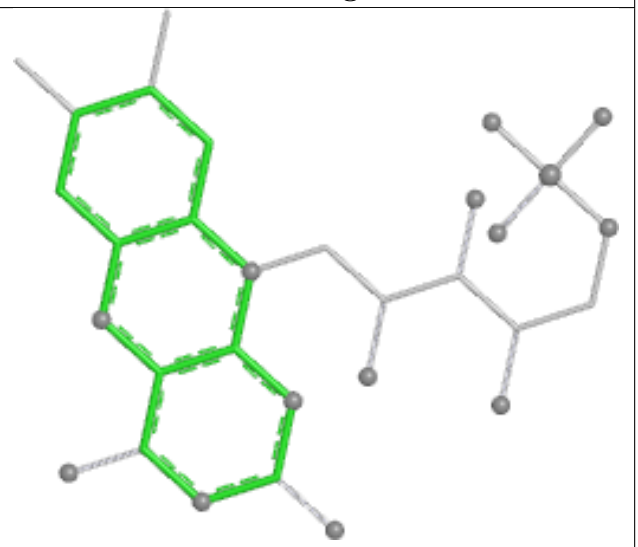
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

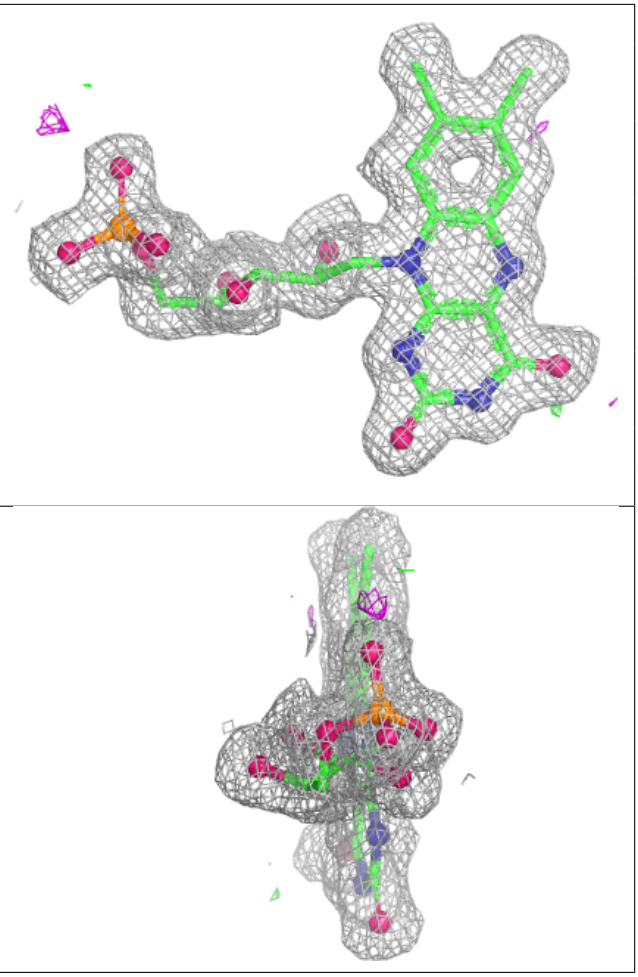
6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

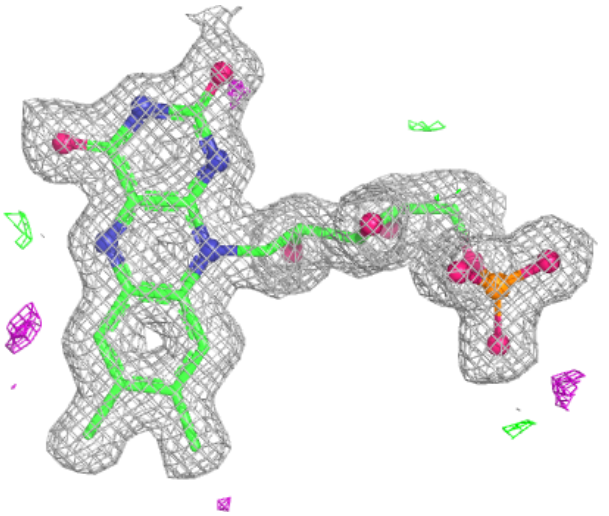
Electron density around FMN A 4001:

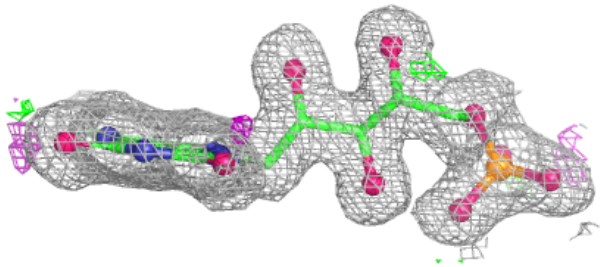
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

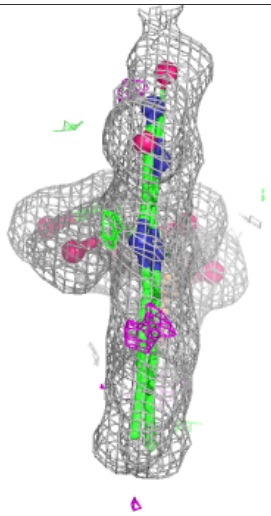


Electron density around FMN B 4002:

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

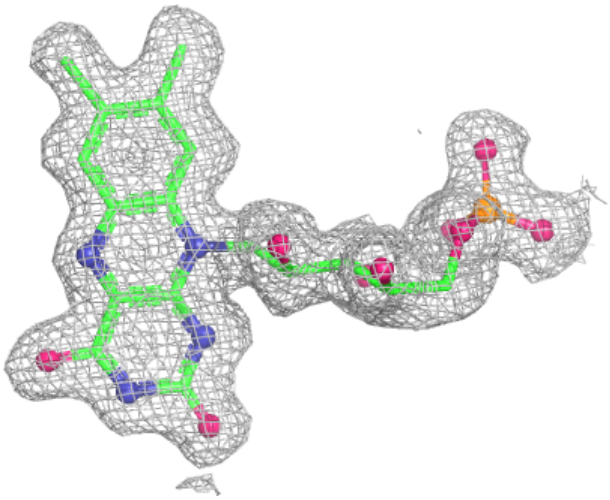


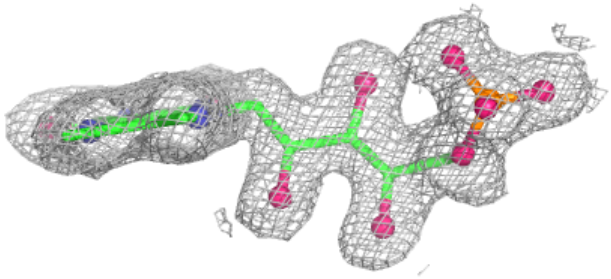


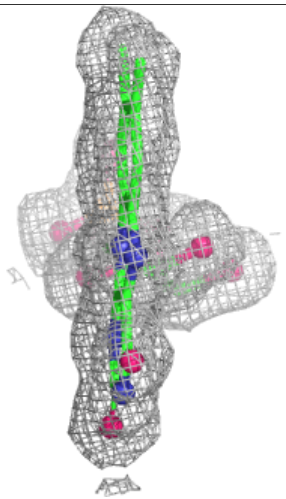


Electron density around FMN C 4003:

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

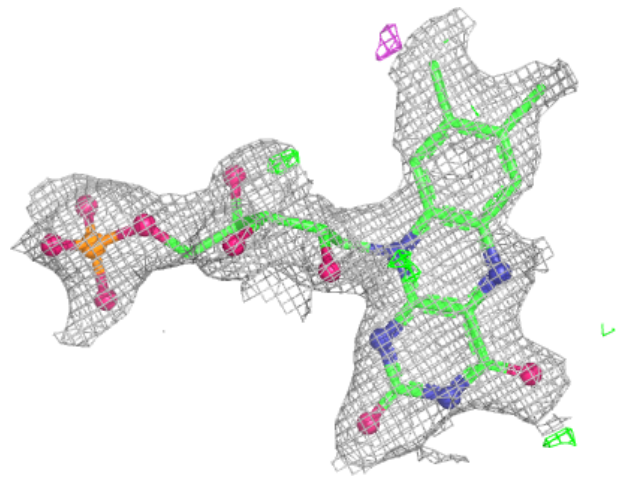


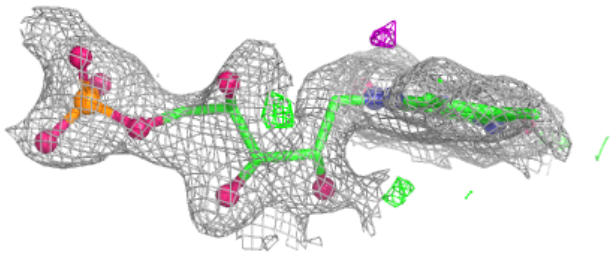


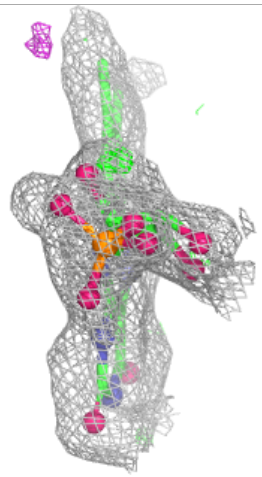


Electron density around FMN C 4005:

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

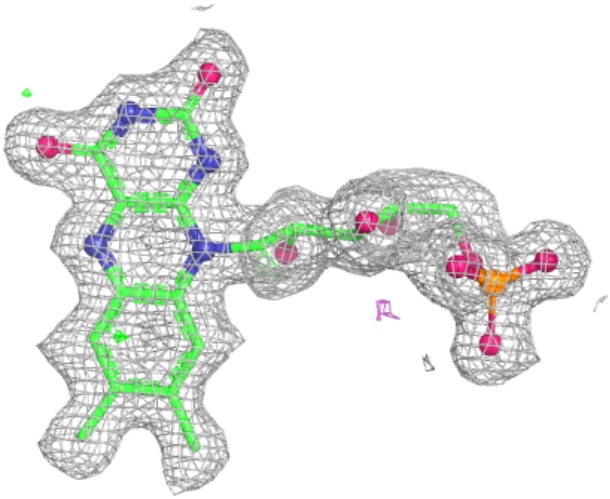


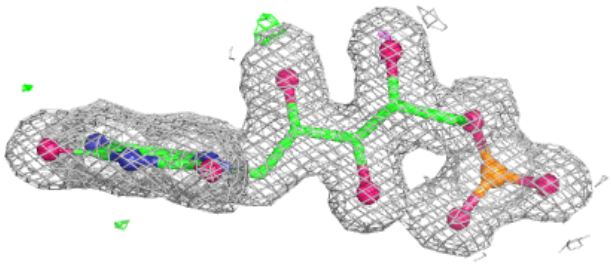


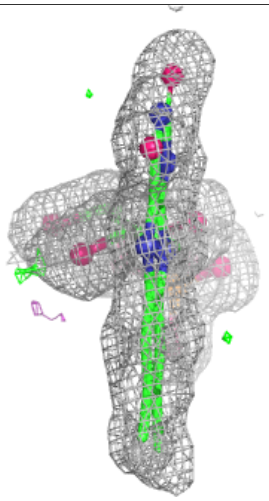


Electron density around FMN D 4004:

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







Electron density around FMN D 4006:

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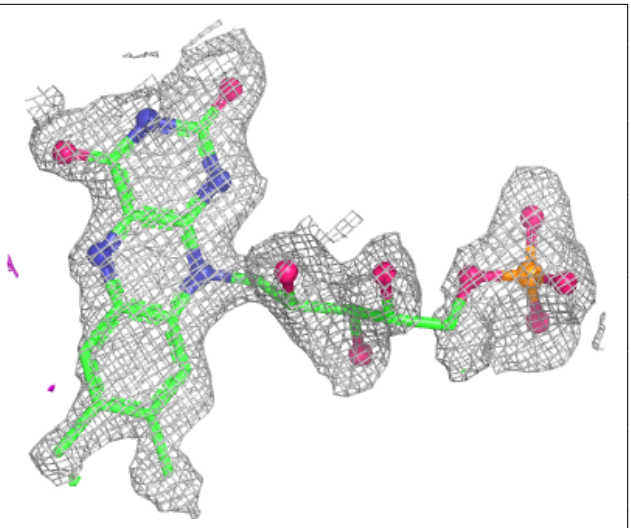
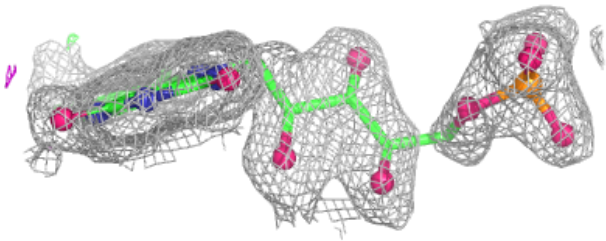
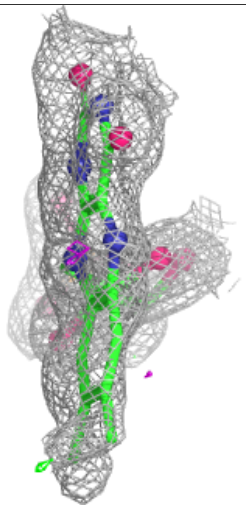
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

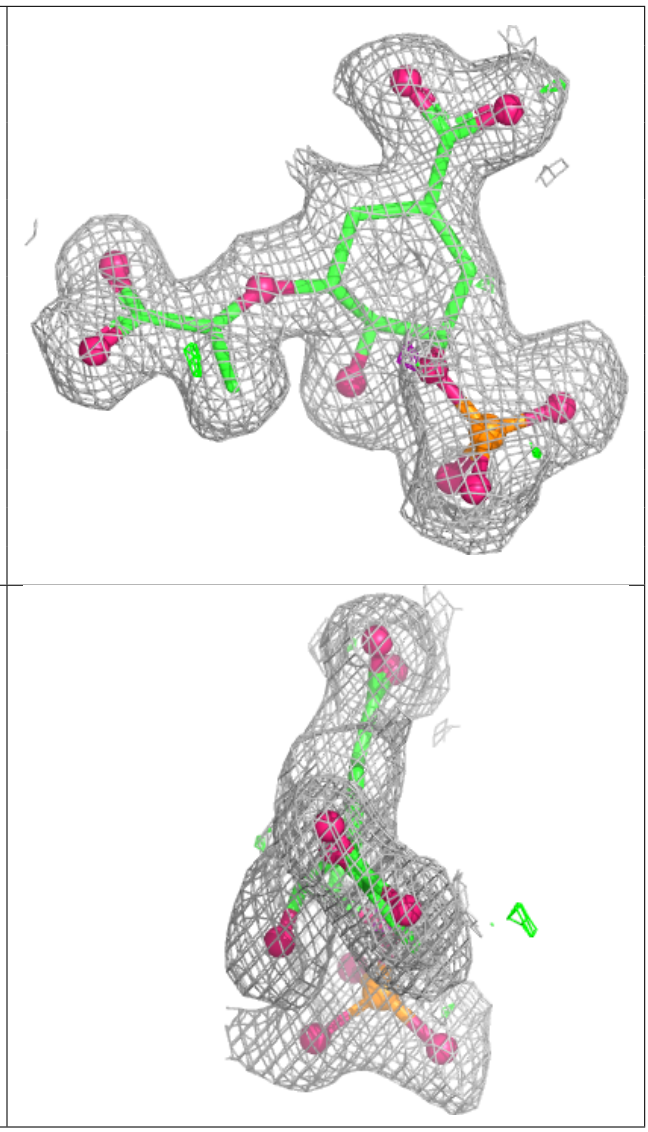






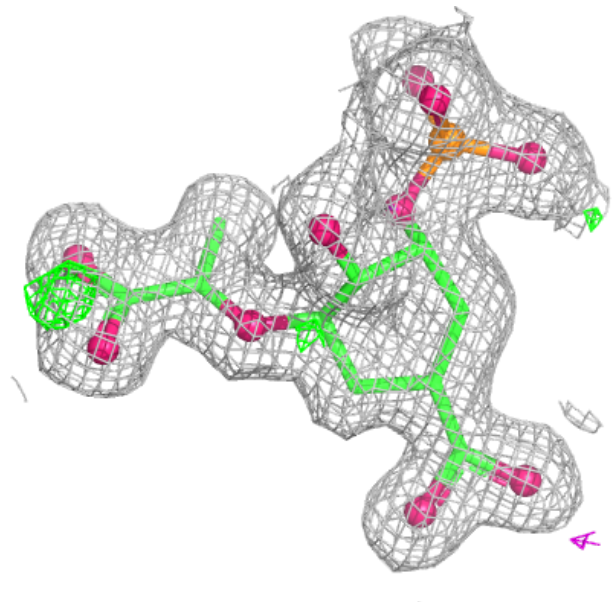
Electron density around EPS A 5001:

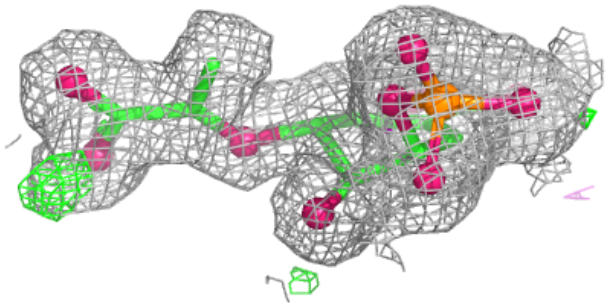
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

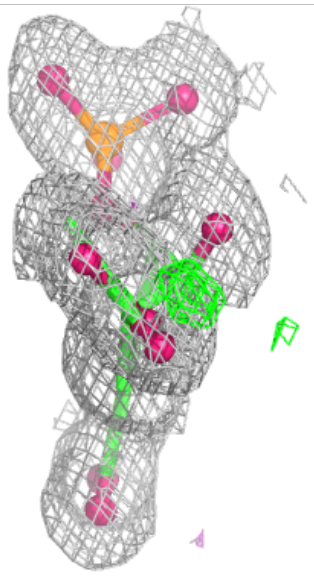


Electron density around EPS B 5002:

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

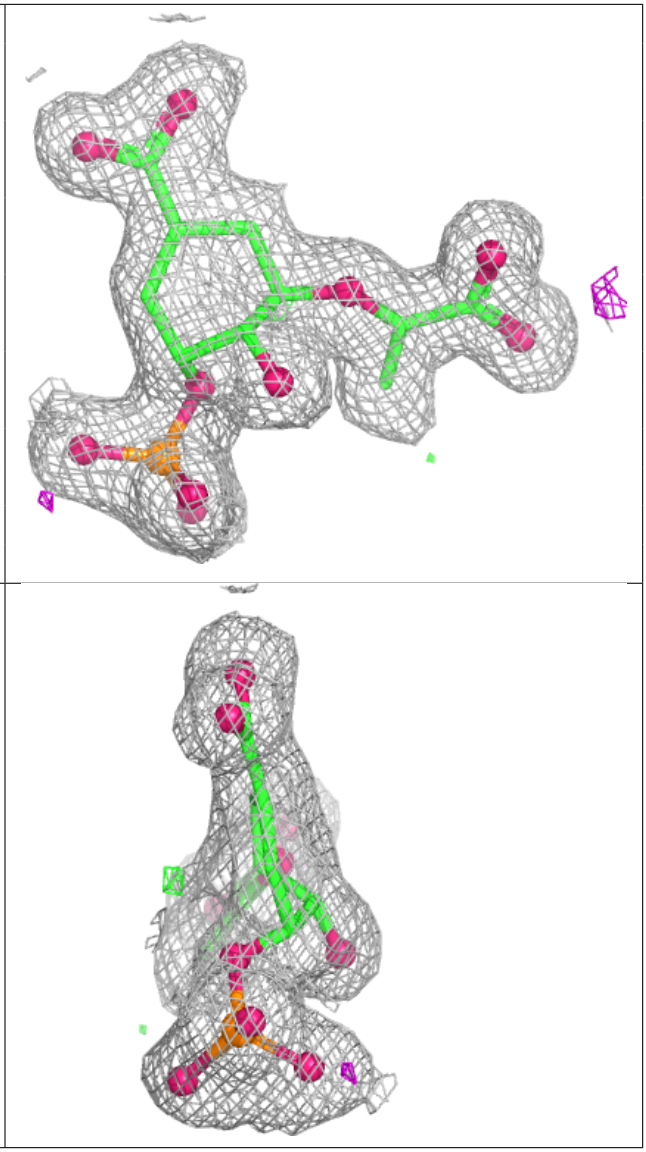






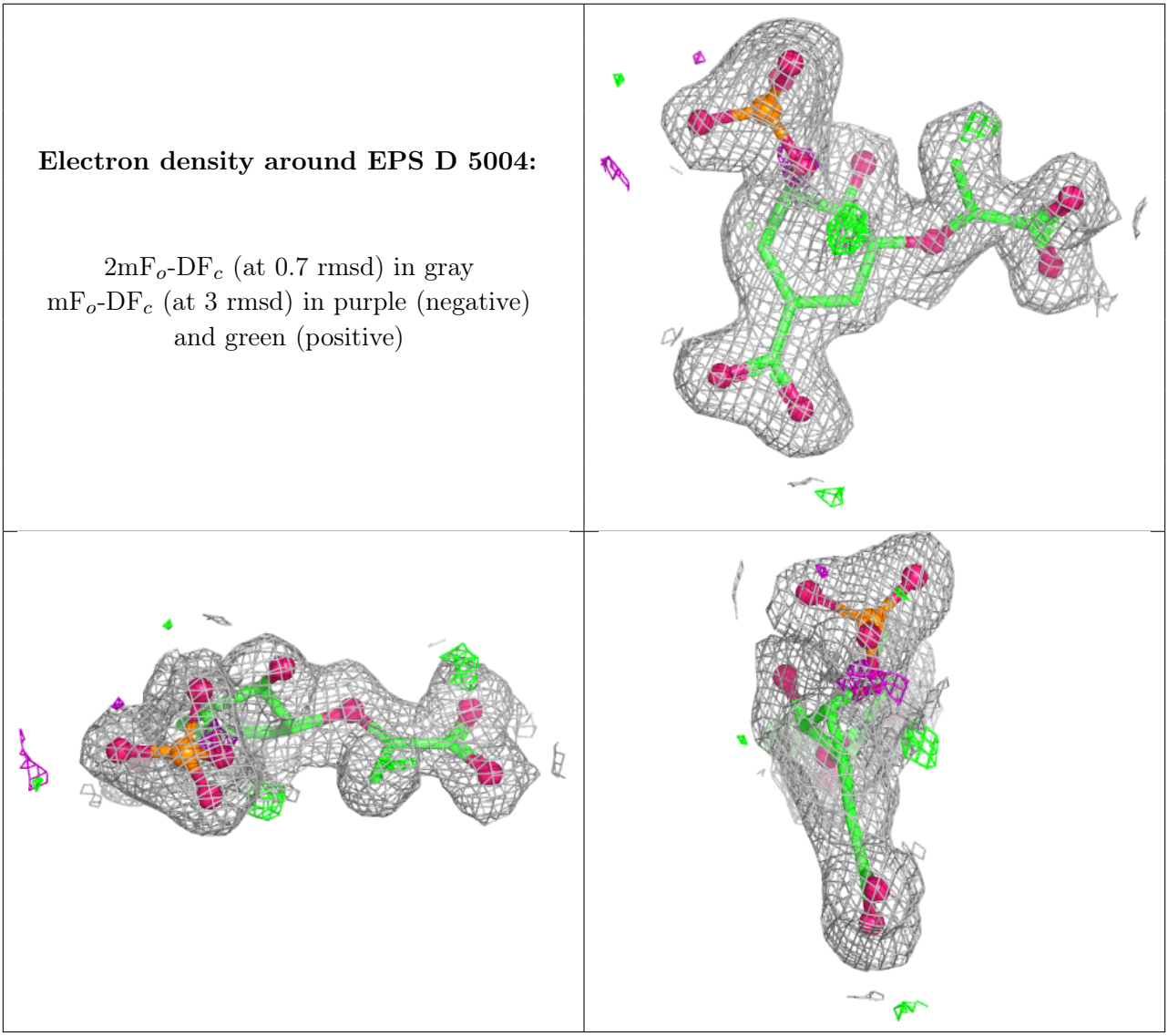
Electron density around EPS C 5003:

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



Electron density around EPS D 5004:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.