



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:11 PM UTC

PDB ID : 1F76 / pdb_00001f76
Title : ESCHERICHIA COLI DIHYDROOROTATE DEHYDROGENASE
Authors : Norager, S.; Jensen, K.F.; Bjornberg, O.; Larsen, S.
Deposited on : 2000-06-26
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

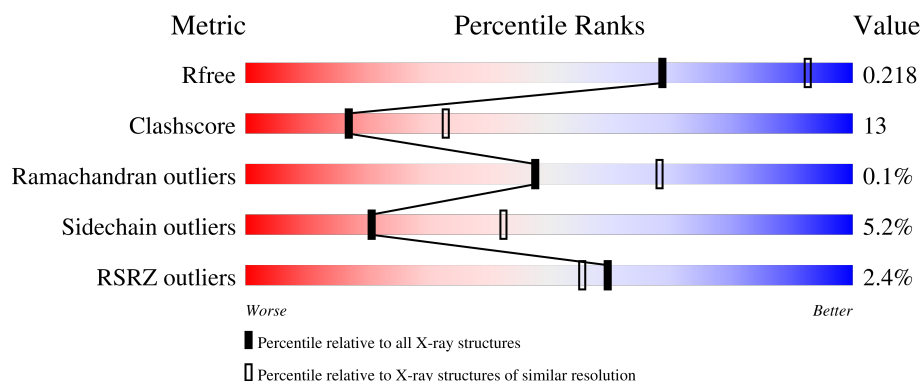
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	336	0% 72% 24% .
1	B	336	3% 72% 25% .
1	D	336	3% 69% 29% .
1	E	336	3% 72% 26% .

2 Entry composition [i](#)

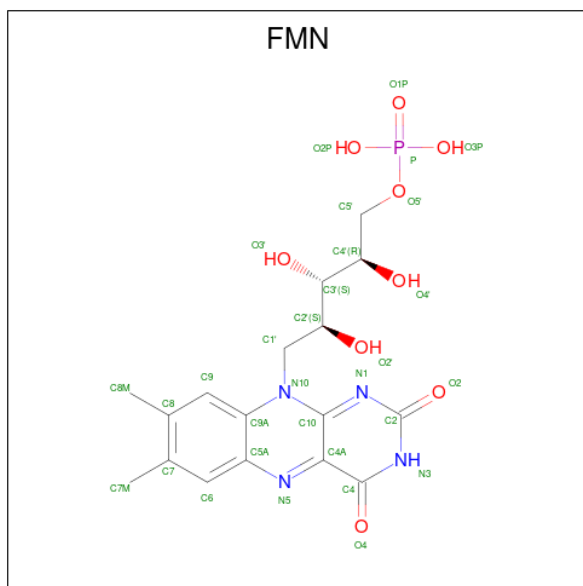
There are 5 unique types of molecules in this entry. The entry contains 11612 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dihydroorotate dehydrogenase (quinone).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	Se	0	2	0
			2595	1647	453	484	4	7			
1	B	336	Total	C	N	O	S	Se	0	2	0
			2595	1648	453	482	4	8			
1	D	336	Total	C	N	O	S	Se	0	0	0
			2586	1642	452	481	4	7			
1	E	336	Total	C	N	O	S	Se	0	3	0
			2601	1650	457	483	4	7			

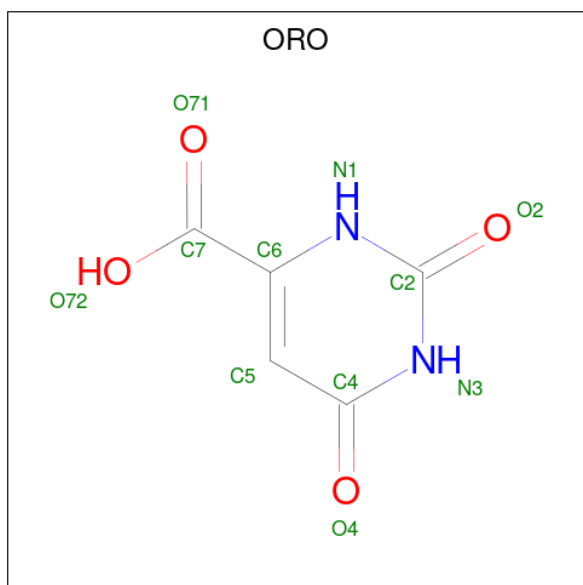
- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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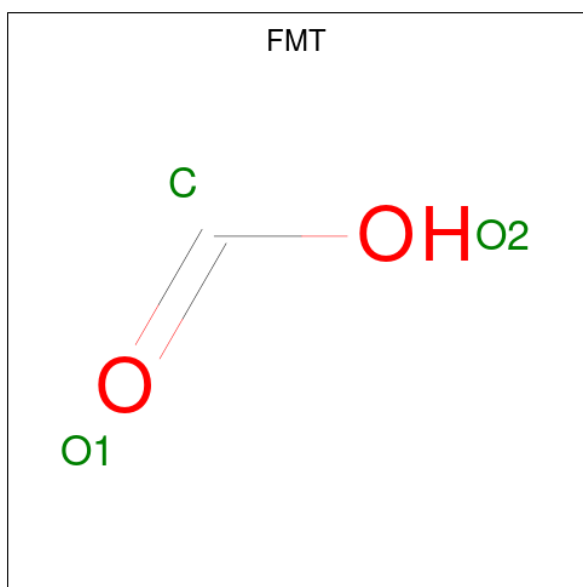
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is OROTIC ACID (CCD ID: ORO) (formula: $C_5H_4N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	5	2	4		
3	A	1	Total	C	N	O	0	1
			22	10	4	8		
3	D	1	Total	C	N	O	0	0
			11	5	2	4		

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



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

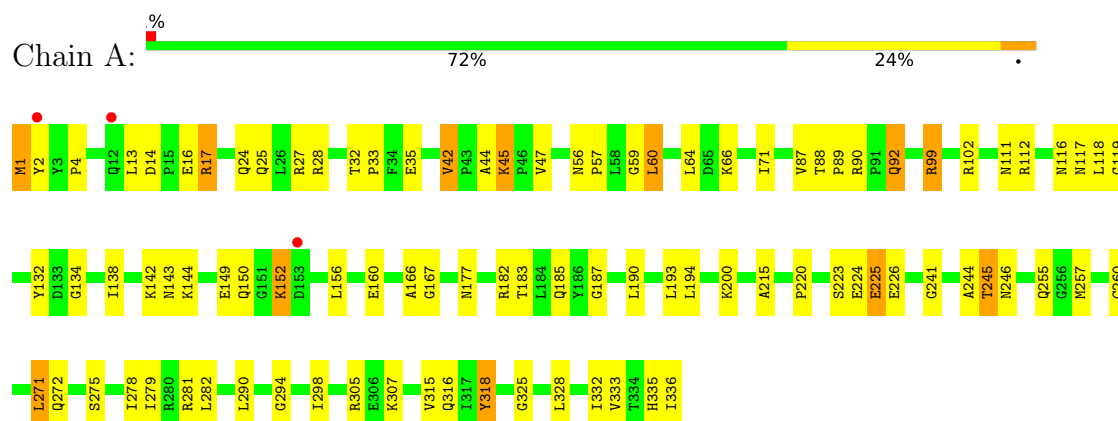
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	340	Total	O	0	0
			340	340		
5	B	231	Total	O	0	0
			231	231		
5	D	180	Total	O	0	0
			180	180		
5	E	292	Total	O	0	0
			292	292		

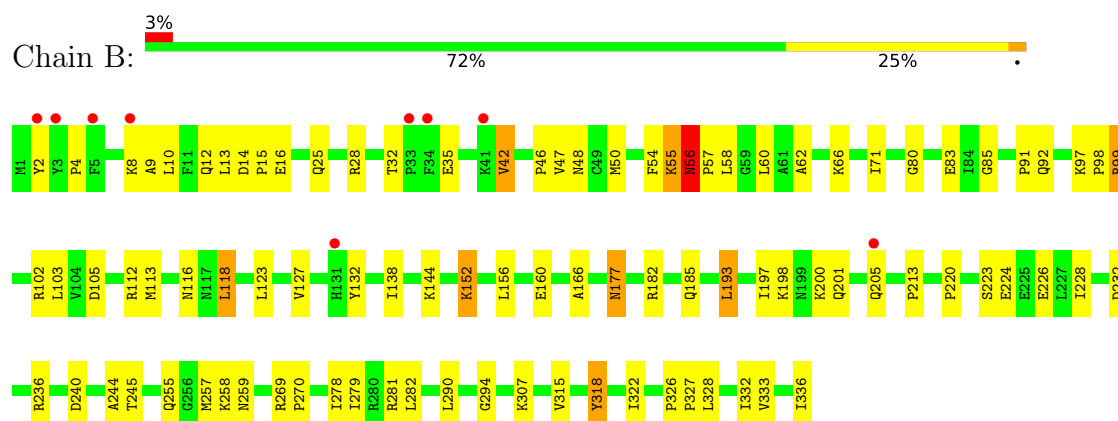
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

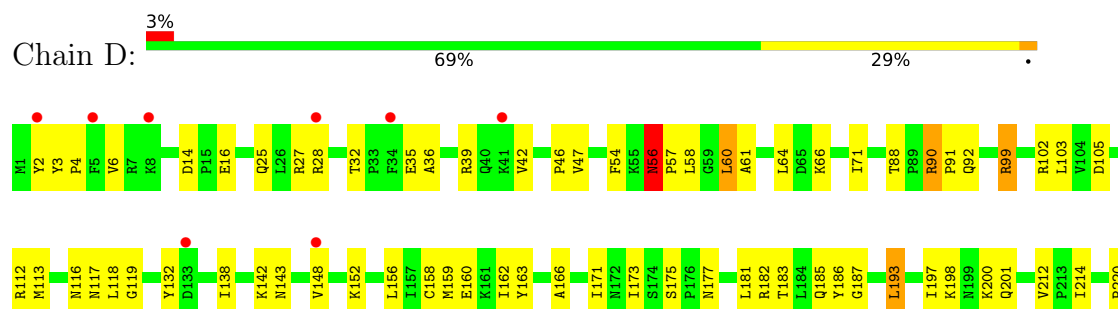
- Molecule 1: Dihydroorotate dehydrogenase (quinone)

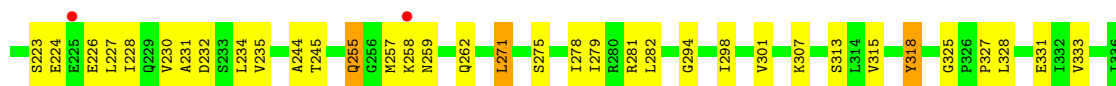


- Molecule 1: Dihydroorotate dehydrogenase (quinone)

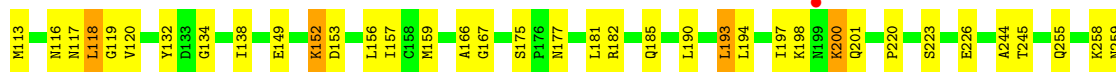


- Molecule 1: Dihydroorotate dehydrogenase (quinone)





- Molecule 1: Dihydroorotate dehydrogenase (quinone)



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.70Å 119.70Å 295.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (20.00-2.50) 98.2 (20.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.05 (at 2.50Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.177 , 0.217 0.179 , 0.218	Depositor DCC
R_{free} test set	7460 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11612	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, ORO, FMT

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	0.42	1/2642 (0.0%)	0.97	15/3564 (0.4%)
1	B	0.37	0/2642	0.92	11/3563 (0.3%)
1	D	0.36	0/2625	0.93	9/3541 (0.3%)
1	E	0.38	0/2652	0.93	6/3577 (0.2%)
All	All	0.39	1/10561 (0.0%)	0.94	41/14245 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	ASN	CG-OD1	5.20	1.33	1.23

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	255	GLN	OE1-CD-NE2	-10.47	112.12	122.60
1	B	255	GLN	OE1-CD-NE2	-10.42	112.18	122.60
1	D	255	GLN	OE1-CD-NE2	-10.00	112.60	122.60
1	A	255	GLN	OE1-CD-NE2	-9.23	113.36	122.60
1	A	167	GLY	N-CA-C	-7.55	103.35	112.49
1	B	255	GLN	CG-CD-NE2	7.35	127.42	116.40
1	A	325	GLY	CA-C-N	6.99	127.58	120.38
1	A	325	GLY	C-N-CA	6.99	127.58	120.38
1	D	56	ASN	CA-C-N	6.83	126.53	119.56
1	D	56	ASN	C-N-CA	6.83	126.53	119.56
1	E	255	GLN	CG-CD-NE2	6.68	126.43	116.40
1	D	255	GLN	CG-CD-NE2	6.53	126.19	116.40
1	A	255	GLN	CG-CD-NE2	6.36	125.94	116.40
1	A	45	LYS	CA-C-N	5.93	126.27	119.93
1	A	45	LYS	C-N-CA	5.93	126.27	119.93
1	B	9	ALA	N-CA-C	-5.71	104.67	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	LEU	CA-C-N	5.59	125.90	119.92
1	A	290	LEU	C-N-CA	5.59	125.90	119.92
1	B	177	ASN	N-CA-C	5.54	119.74	112.92
1	E	325	GLY	CA-C-N	5.36	125.90	120.38
1	E	325	GLY	C-N-CA	5.36	125.90	120.38
1	A	187	GLY	N-CA-C	5.32	120.94	111.73
1	A	272	GLN	N-CA-C	5.30	117.49	111.02
1	E	85	GLY	N-CA-C	-5.27	104.62	111.52
1	A	56	ASN	CA-C-N	5.26	125.34	119.87
1	A	56	ASN	C-N-CA	5.26	125.34	119.87
1	B	92	GLN	CA-C-N	5.24	124.75	119.19
1	B	92	GLN	C-N-CA	5.24	124.75	119.19
1	B	85	GLY	N-CA-C	-5.23	104.29	111.76
1	A	92	GLN	CA-C-N	5.22	124.73	119.19
1	A	92	GLN	C-N-CA	5.22	124.73	119.19
1	D	313	SER	N-CA-C	-5.18	107.09	113.41
1	D	325	GLY	CA-C-N	5.18	125.72	120.38
1	D	325	GLY	C-N-CA	5.18	125.72	120.38
1	B	56	ASN	CA-C-N	5.14	124.86	119.82
1	B	56	ASN	C-N-CA	5.14	124.86	119.82
1	E	167	GLY	N-CA-C	-5.03	101.25	113.18
1	D	92	GLN	CA-C-N	5.02	124.51	119.19
1	D	92	GLN	C-N-CA	5.02	124.51	119.19
1	B	290	LEU	CA-C-N	5.01	125.28	119.92
1	B	290	LEU	C-N-CA	5.01	125.28	119.92

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2595	0	2657	63	0
1	B	2595	0	2662	73	0
1	D	2586	0	2653	70	0
1	E	2601	0	2666	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	31	0	19	0	0
2	B	31	0	19	0	0
2	D	31	0	19	0	0
2	E	31	0	19	0	0
3	A	33	0	9	1	0
3	D	11	0	3	0	0
4	B	9	0	3	1	0
4	D	6	0	2	1	0
4	E	9	0	3	2	0
5	A	340	0	0	7	0
5	B	231	0	0	5	0
5	D	180	0	0	3	0
5	E	292	0	0	7	0
All	All	11612	0	10734	270	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 13.

All (270) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50[B]:MSE:HE2	1:B:213:PRO:HB2	1.32	1.08
1:A:220:PRO:HB3	1:A:245:THR:HG21	1.36	1.03
1:A:1:MSE:N	3:A:1339[A]:ORO:O71	1.99	0.95
1:A:90:ARG:H	1:A:143:ASN:HD21	1.17	0.93
1:A:92:GLN:HE22	1:A:144:LYS:H	1.16	0.89
1:B:56:ASN:HD22	1:B:58:LEU:H	1.33	0.77
1:A:13:LEU:HD22	1:A:17:ARG:NH1	2.01	0.75
1:D:56:ASN:HD22	1:D:58:LEU:H	1.35	0.74
1:A:13:LEU:HD22	1:A:17:ARG:HH12	1.53	0.74
1:A:220:PRO:HB3	1:A:245:THR:CG2	2.17	0.74
1:E:198:LYS:NZ	1:E:201:GLN:HE22	1.85	0.73
1:E:66:LYS:HE2	1:E:116:ASN:OD1	1.89	0.73
1:A:149:GLU:HG3	5:A:1676:HOH:O	1.88	0.72
1:B:50[B]:MSE:HE3	1:B:240:ASP:HB2	1.75	0.69
1:D:223:SER:OG	1:D:226:GLU:HG3	1.93	0.68
1:D:182:ARG:O	1:D:185:GLN:HG2	1.94	0.68
1:E:42:VAL:CG1	1:E:333:VAL:HG11	2.23	0.68
1:E:198:LYS:HZ2	1:E:201:GLN:HE22	1.41	0.67
1:D:66:LYS:HE3	5:D:1545:HOH:O	1.95	0.67
1:E:66:LYS:HE3	5:E:1721:HOH:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ARG:HA	1:D:177:ASN:CG	2.20	0.66
1:B:42:VAL:CG1	1:B:333:VAL:HG11	2.26	0.66
1:B:28:ARG:HH12	1:E:8:LYS:HE3	1.59	0.65
1:D:327:PRO:O	1:D:331:GLU:HG3	1.98	0.64
1:B:182:ARG:O	1:B:185:GLN:HG2	1.98	0.63
1:B:66:LYS:HE2	1:B:116:ASN:OD1	1.99	0.63
1:E:55:LYS:HG3	5:E:1720:HOH:O	1.98	0.63
1:E:32:THR:O	1:E:35:GLU:HB2	1.98	0.63
1:A:66:LYS:HE2	1:A:116:ASN:OD1	1.97	0.62
1:E:16:GLU:OE1	1:E:99:ARG:HD2	2.00	0.62
1:D:156:LEU:O	1:D:160:GLU:HG3	2.00	0.61
1:E:117:ASN:ND2	1:E:119:GLY:H	1.98	0.61
1:B:156:LEU:O	1:B:160:GLU:HG3	2.01	0.61
1:D:66:LYS:HE2	1:D:116:ASN:OD1	2.00	0.61
1:A:112:ARG:HA	1:A:177:ASN:CG	2.26	0.60
1:A:42:VAL:CG1	1:A:333:VAL:HG11	2.31	0.60
1:A:245:THR:HG23	1:A:246:ASN:O	2.02	0.60
1:E:182:ARG:O	1:E:185:GLN:HG2	2.02	0.59
1:B:112:ARG:HA	1:B:177:ASN:CG	2.27	0.59
1:D:56:ASN:ND2	1:D:58:LEU:H	1.98	0.59
1:A:138:ILE:HD12	1:A:166:ALA:HB2	1.83	0.59
1:A:24:GLN:OE1	1:A:27:ARG:NH2	2.35	0.59
1:B:56:ASN:ND2	1:B:58:LEU:H	1.98	0.59
1:D:42:VAL:CG1	1:D:333:VAL:HG11	2.33	0.59
1:D:232:ASP:HB3	5:D:1687:HOH:O	2.03	0.58
1:B:42:VAL:HG13	1:B:333:VAL:HG11	1.85	0.58
1:D:298:ILE:HD11	1:D:307:LYS:HG3	1.85	0.58
1:E:39[B]:ARG:NH1	1:E:39[B]:ARG:HB2	2.19	0.58
1:A:271:LEU:HD22	1:A:275:SER:HB2	1.84	0.58
1:E:111:ASN:HD21	4:E:1639:FMT:C	2.16	0.58
1:A:47:VAL:HG21	1:A:57:PRO:HG3	1.86	0.58
1:D:198:LYS:NZ	1:D:201:GLN:HE22	2.01	0.57
1:A:17:ARG:NH1	5:A:1556:HOH:O	2.37	0.57
1:A:66:LYS:HE3	5:A:1423:HOH:O	2.04	0.57
1:E:152:LYS:O	1:E:156:LEU:HG	2.03	0.57
1:B:56:ASN:HD22	1:B:56:ASN:C	2.12	0.57
1:B:223:SER:OG	1:B:226:GLU:HG3	2.05	0.57
1:B:16:GLU:OE1	1:B:99:ARG:HD2	2.04	0.57
1:B:8:LYS:HZ1	1:E:28:ARG:HH11	1.53	0.57
1:B:66:LYS:HE3	5:B:1583:HOH:O	2.04	0.56
1:D:262:GLN:HE21	1:D:262:GLN:HA	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LYS:NZ	1:E:28:ARG:NH1	2.53	0.56
1:E:13:LEU:HD22	1:E:17:ARG:HD3	1.87	0.56
1:D:56:ASN:HD22	1:D:56:ASN:C	2.13	0.56
1:B:198:LYS:NZ	1:B:201:GLN:HE22	2.03	0.56
1:A:281:ARG:NH1	5:A:1666:HOH:O	2.38	0.55
1:B:13:LEU:HD23	1:E:13:LEU:HD23	1.88	0.55
1:D:46:PRO:HA	1:D:54:PHE:O	2.06	0.55
1:A:156:LEU:O	1:A:160:GLU:HG3	2.07	0.55
1:B:152:LYS:O	1:B:156:LEU:HG	2.07	0.55
1:D:88:THR:H	1:D:117:ASN:HD21	1.54	0.55
1:D:318:TYR:C	1:D:318:TYR:HD1	2.15	0.54
1:A:16:GLU:OE1	1:A:99:ARG:HD2	2.07	0.54
1:D:16:GLU:OE1	1:D:99:ARG:HD2	2.08	0.54
1:A:245:THR:HG23	1:A:246:ASN:N	2.23	0.53
1:B:138:ILE:HD12	1:B:166:ALA:HB2	1.90	0.53
1:D:175:SER:HB3	1:D:181:LEU:HD23	1.91	0.53
1:E:112:ARG:HA	1:E:177:ASN:CG	2.34	0.53
1:E:244:ALA:HB1	1:E:245:THR:HG22	1.91	0.53
1:E:280:ARG:NH2	5:E:1683:HOH:O	2.39	0.53
1:D:231:ALA:O	1:D:235:VAL:HG23	2.10	0.52
1:D:56:ASN:ND2	1:D:56:ASN:C	2.68	0.52
1:B:102:ARG:C	1:B:103:LEU:HD12	2.35	0.52
1:B:32:THR:O	1:B:35:GLU:HB2	2.09	0.52
1:E:102:ARG:C	1:E:103:LEU:HD12	2.35	0.52
1:B:55:LYS:HG3	1:B:80:GLY:HA2	1.92	0.52
1:E:138:ILE:HD12	1:E:166:ALA:HB2	1.90	0.52
1:B:294:GLY:O	1:B:315:VAL:HA	2.10	0.51
1:D:318:TYR:C	1:D:318:TYR:CD1	2.87	0.51
1:D:262:GLN:HA	1:D:262:GLN:NE2	2.25	0.51
1:E:117:ASN:HD22	1:E:119:GLY:H	1.59	0.51
1:A:220:PRO:O	1:A:278:ILE:HD11	2.10	0.51
1:D:294:GLY:O	1:D:315:VAL:HA	2.09	0.51
1:B:318:TYR:C	1:B:318:TYR:HD1	2.19	0.51
1:B:258:LYS:O	1:B:259:ASN:HB2	2.11	0.50
1:E:318:TYR:CD1	1:E:318:TYR:C	2.90	0.50
1:D:60:LEU:HD11	1:D:64:LEU:HD23	1.93	0.50
1:B:244:ALA:HB1	1:B:245:THR:HG22	1.94	0.50
1:D:88:THR:H	1:D:117:ASN:ND2	2.10	0.50
1:D:227:LEU:HD13	1:D:227:LEU:O	2.12	0.50
1:B:318:TYR:HE1	1:B:322:ILE:HD11	1.76	0.50
1:D:220:PRO:O	1:D:278:ILE:HD11	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ARG:HD3	1:D:113:MSE:SE	2.61	0.50
1:E:27:ARG:HD3	5:E:1882:HOH:O	2.11	0.49
1:A:318:TYR:CD1	1:A:318:TYR:C	2.91	0.49
1:E:318:TYR:C	1:E:318:TYR:HD1	2.20	0.49
1:B:113:MSE:HB2	4:B:1440:FMT:C	2.42	0.49
1:D:255:GLN:HA	1:D:255:GLN:OE1	2.13	0.49
1:A:102:ARG:NH1	5:A:1354:HOH:O	2.43	0.49
1:D:138:ILE:HD12	1:D:166:ALA:HB2	1.93	0.49
1:E:1:MSE:HG2	5:E:1899:HOH:O	2.12	0.49
1:D:112:ARG:HA	1:D:177:ASN:ND2	2.28	0.49
1:E:321:PHE:CE1	1:E:329:ILE:HD11	2.47	0.49
1:A:27:ARG:HG2	5:A:1383:HOH:O	2.13	0.49
1:A:89:PRO:HD2	1:A:143:ASN:ND2	2.27	0.48
1:B:46:PRO:HA	1:B:54:PHE:O	2.13	0.48
1:D:262:GLN:HE21	1:D:262:GLN:CA	2.26	0.48
1:B:318:TYR:C	1:B:318:TYR:CD1	2.89	0.48
1:A:117:ASN:ND2	1:A:119:GLY:H	2.12	0.48
1:D:117:ASN:ND2	1:D:119:GLY:H	2.11	0.48
1:A:25:GLN:O	1:A:28:ARG:HB3	2.13	0.48
1:A:42:VAL:HG13	1:A:333:VAL:HG11	1.96	0.48
1:D:258:LYS:O	1:D:259:ASN:HB2	2.13	0.48
1:B:99:ARG:HG3	5:B:1481:HOH:O	2.14	0.48
1:D:224:GLU:O	1:D:228:ILE:HG13	2.14	0.48
1:A:318:TYR:C	1:A:318:TYR:HD1	2.21	0.48
1:D:60:LEU:HD22	1:D:61:ALA:O	2.14	0.48
1:E:25:GLN:O	1:E:28:ARG:HB3	2.13	0.48
1:B:152:LYS:NZ	1:B:152:LYS:HB3	2.29	0.47
1:E:42:VAL:HG11	1:E:333:VAL:HG11	1.96	0.47
1:B:56:ASN:ND2	1:B:56:ASN:C	2.72	0.47
1:E:318:TYR:HE1	1:E:322:ILE:HD11	1.79	0.47
1:D:113:MSE:HB2	4:D:1539:FMT:C	2.44	0.47
1:E:280:ARG:O	1:E:284:LEU:HD22	2.15	0.47
1:B:28:ARG:NH1	1:E:8:LYS:HE3	2.29	0.47
1:B:91:PRO:HB3	1:B:118:LEU:C	2.39	0.47
1:E:223:SER:OG	1:E:226:GLU:HG3	2.15	0.47
1:B:144:LYS:NZ	5:B:1556:HOH:O	2.47	0.46
1:D:230:VAL:O	1:D:234:LEU:HG	2.14	0.46
1:E:5:PHE:O	1:E:8:LYS:HB3	2.16	0.46
1:B:62:ALA:HB2	1:B:83:GLU:HG2	1.97	0.46
1:D:152:LYS:O	1:D:156:LEU:HG	2.15	0.46
1:E:220:PRO:O	1:E:278:ILE:HD11	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:ASP:HB2	1:D:257:MSE:HE2	1.97	0.46
1:B:15:PRO:HG3	1:B:102:ARG:HG3	1.96	0.46
1:D:244:ALA:O	1:D:294:GLY:HA2	2.15	0.46
1:E:193:LEU:HD22	1:E:197:ILE:CD1	2.46	0.46
1:E:46:PRO:HA	1:E:54:PHE:O	2.16	0.46
1:A:142:LYS:HG2	1:A:143:ASN:O	2.15	0.46
1:E:190:LEU:O	1:E:194:LEU:HG	2.16	0.46
1:A:32:THR:HB	1:A:33:PRO:HD2	1.98	0.46
1:B:42:VAL:HG11	1:B:333:VAL:HG11	1.96	0.46
1:D:47:VAL:HG21	1:D:57:PRO:HG3	1.97	0.46
1:E:258:LYS:O	1:E:259:ASN:HB2	2.16	0.45
1:D:71:ILE:HG22	1:D:132:TYR:HB2	1.98	0.45
1:B:10:LEU:C	1:B:12:GLN:H	2.23	0.45
1:D:159:MSE:HE3	1:D:214:ILE:HD11	1.98	0.45
1:D:271:LEU:HD22	1:D:275:SER:HB2	1.98	0.45
1:B:279:ILE:HD12	1:B:307:LYS:HD2	1.97	0.45
1:E:332:ILE:O	1:E:336:ILE:HB	2.16	0.45
1:A:220:PRO:HA	1:A:278:ILE:HD13	1.99	0.45
1:A:298:ILE:HD11	1:A:307:LYS:HG3	1.99	0.45
1:B:8:LYS:NZ	1:E:25:GLN:OE1	2.47	0.45
1:A:60:LEU:HD11	1:A:64:LEU:HD23	1.98	0.45
1:A:225:GLU:OE1	1:A:225:GLU:HA	2.17	0.45
1:E:91:PRO:HG3	1:E:118:LEU:O	2.17	0.45
1:E:93:PRO:O	1:E:99:ARG:NH2	2.49	0.45
1:A:220:PRO:HA	1:A:278:ILE:CD1	2.46	0.45
1:E:42:VAL:HG13	1:E:333:VAL:HG11	1.99	0.45
1:E:156:LEU:HB3	1:E:200:LYS:HD2	1.99	0.45
1:A:279:ILE:HD12	1:A:307:LYS:HD2	1.98	0.45
1:A:279:ILE:CD1	1:A:307:LYS:HD2	2.46	0.44
1:A:71:ILE:HG22	1:A:132:TYR:HB2	1.99	0.44
1:A:244:ALA:HA	1:A:245:THR:HA	1.68	0.44
1:B:8:LYS:HZ3	1:E:28:ARG:NH1	2.15	0.44
1:B:205[A]:GLN:NE2	5:B:1586:HOH:O	2.42	0.44
1:D:193:LEU:HD22	1:D:197:ILE:CD1	2.47	0.44
1:D:198:LYS:HZ2	1:D:201:GLN:HE22	1.64	0.44
1:E:175:SER:HB3	1:E:181:LEU:HD23	1.99	0.44
1:E:113:MSE:HB2	4:E:1638:FMT:C	2.47	0.44
1:E:245:THR:O	1:E:295:VAL:HG13	2.17	0.44
1:A:182:ARG:O	1:A:185:GLN:HG2	2.17	0.44
1:D:279:ILE:HD12	1:D:307:LYS:HD2	1.99	0.44
1:A:294:GLY:O	1:A:315:VAL:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LYS:HA	1:B:98:PRO:C	2.43	0.44
1:D:90:ARG:HB3	1:D:91:PRO:HD2	2.00	0.44
1:A:152:LYS:O	1:A:156:LEU:HG	2.17	0.44
1:B:8:LYS:HZ1	1:E:28:ARG:NH1	2.14	0.44
1:D:102:ARG:C	1:D:103:LEU:HD12	2.43	0.44
1:D:163:TYR:CE1	1:D:212:VAL:HB	2.53	0.44
1:B:71:ILE:HG22	1:B:132:TYR:HB2	1.99	0.43
1:B:112:ARG:HA	1:B:177:ASN:OD1	2.18	0.43
1:A:88:THR:H	1:A:117:ASN:HD21	1.64	0.43
1:B:232:ASP:O	1:B:236:ARG:HG3	2.18	0.43
1:E:99:ARG:HG3	5:E:1695:HOH:O	2.16	0.43
1:A:32:THR:O	1:A:35:GLU:HB2	2.18	0.43
1:B:47:VAL:HG21	1:B:57:PRO:HG3	1.99	0.43
1:B:55:LYS:H	1:B:55:LYS:HG2	1.62	0.43
1:E:271:LEU:HD22	1:E:275:SER:HB2	2.00	0.43
1:A:183:THR:HB	1:B:48:ASN:CG	2.44	0.43
1:E:286:LEU:HD12	1:E:292:ILE:HD11	2.01	0.43
1:A:13:LEU:O	1:A:102:ARG:NH2	2.50	0.43
1:B:123:LEU:O	1:B:127:VAL:HG23	2.18	0.43
1:B:269:ARG:HB3	1:B:270:PRO:HD3	2.01	0.43
1:A:44:ALA:C	1:A:45:LYS:HG2	2.43	0.43
1:B:279:ILE:CD1	1:B:307:LYS:HD2	2.49	0.43
1:E:2:TYR:CG	1:E:4:PRO:HD2	2.54	0.43
1:E:45:LYS:O	1:E:56:ASN:HA	2.19	0.43
1:B:2:TYR:CG	1:B:4:PRO:HD2	2.53	0.42
1:D:183:THR:HA	1:D:186:TYR:CD1	2.53	0.42
1:A:332:ILE:O	1:A:336:ILE:HB	2.19	0.42
1:D:224:GLU:HG2	1:D:281:ARG:HH11	1.83	0.42
1:E:27:ARG:NH2	5:E:1929:HOH:O	2.51	0.42
1:D:36:ALA:HA	1:D:39:ARG:NH1	2.34	0.42
1:E:294:GLY:O	1:E:315:VAL:HA	2.19	0.42
1:A:90:ARG:HG2	5:A:1608:HOH:O	2.18	0.42
1:B:193:LEU:HD22	1:B:197:ILE:CD1	2.50	0.42
1:B:12:GLN:O	1:E:17:ARG:NH2	2.51	0.42
1:D:27:ARG:NH1	5:D:1604:HOH:O	2.52	0.42
1:E:88:THR:H	1:E:117:ASN:HD21	1.68	0.42
1:A:215:ALA:HA	1:A:241:GLY:O	2.20	0.42
1:B:220:PRO:O	1:B:278:ILE:HD11	2.19	0.42
1:D:3:TYR:O	1:D:6:VAL:N	2.53	0.42
1:E:329:ILE:O	1:E:333:VAL:HG23	2.20	0.42
1:B:224:GLU:O	1:B:228:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:PRO:C	1:E:35:GLU:H	2.26	0.41
1:E:132:TYR:CZ	1:E:134:GLY:HA3	2.55	0.41
1:E:198:LYS:NZ	1:E:201:GLN:NE2	2.62	0.41
1:A:152:LYS:NZ	1:A:152:LYS:HB3	2.36	0.41
1:B:42:VAL:HG13	1:B:333:VAL:CG1	2.48	0.41
1:B:326:PRO:N	1:B:327:PRO:CD	2.84	0.41
1:D:158:CYS:O	1:D:162:ILE:HG12	2.20	0.41
1:E:159:MSE:SE	1:E:197:ILE:HG23	2.70	0.41
1:A:190:LEU:O	1:A:194:LEU:HG	2.21	0.41
1:A:257:MSE:O	1:A:260:CYS:HB3	2.21	0.41
1:B:198:LYS:HZ2	1:B:201:GLN:HE22	1.67	0.41
1:D:244:ALA:HA	1:D:245:THR:HA	1.59	0.41
1:B:332:ILE:O	1:B:336:ILE:HB	2.21	0.41
1:D:2:TYR:CG	1:D:4:PRO:HD2	2.56	0.41
1:D:171:ILE:HG22	1:D:173:ILE:HG23	2.03	0.41
1:D:32:THR:O	1:D:35:GLU:HB2	2.20	0.41
1:D:142:LYS:HG2	1:D:143:ASN:O	2.20	0.41
1:E:42:VAL:HG13	1:E:333:VAL:CG1	2.50	0.41
1:A:305:ARG:NH2	1:A:335:HIS:O	2.54	0.41
1:B:10:LEU:C	1:B:12:GLN:N	2.78	0.41
1:D:42:VAL:HG11	1:D:333:VAL:HG11	2.02	0.41
1:A:2:TYR:CG	1:A:4:PRO:HD2	2.56	0.41
1:D:227:LEU:HD13	1:D:227:LEU:C	2.46	0.41
1:E:88:THR:H	1:E:117:ASN:ND2	2.18	0.41
1:E:149:GLU:CD	1:E:149:GLU:H	2.29	0.41
1:A:59:GLY:O	1:A:316:GLN:HA	2.21	0.41
1:B:25:GLN:O	1:B:28:ARG:HB3	2.21	0.41
1:B:224:GLU:HG2	1:B:281:ARG:HH11	1.86	0.41
1:D:220:PRO:HA	1:D:278:ILE:CD1	2.51	0.41
1:E:153:ASP:O	1:E:157:ILE:HG13	2.21	0.41
1:A:223:SER:OG	1:A:226:GLU:HG3	2.20	0.40
1:A:87:VAL:HG23	1:A:117:ASN:HD22	1.86	0.40
1:A:132:TYR:CZ	1:A:134:GLY:HA3	2.56	0.40
1:B:279:ILE:HD12	1:B:307:LYS:CD	2.51	0.40
1:D:25:GLN:O	1:D:28:ARG:HB3	2.21	0.40
1:E:109:LEU:O	1:E:266:LEU:HD12	2.21	0.40
1:E:220:PRO:HA	1:E:278:ILE:CD1	2.51	0.40
1:A:13:LEU:HD13	1:A:17:ARG:HH11	1.86	0.40
1:B:105:ASP:HB2	1:B:257:MSE:HE2	2.02	0.40
1:B:257:MSE:HE2	5:B:1636:HOH:O	2.21	0.40
1:D:117:ASN:HD22	1:D:119:GLY:H	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:VAL:HG21	1:E:120:VAL:HA	2.03	0.40
1:B:220:PRO:HB3	1:B:245:THR:OG1	2.22	0.40
1:D:175:SER:HB3	1:D:181:LEU:CD2	2.50	0.40
1:E:279:ILE:CD1	1:E:307:LYS:HD2	2.52	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	336/336 (100%)	327 (97%)	9 (3%)	0	100	100
1	B	336/336 (100%)	326 (97%)	10 (3%)	0	100	100
1	D	334/336 (99%)	320 (96%)	13 (4%)	1 (0%)	36	55
1	E	337/336 (100%)	329 (98%)	8 (2%)	0	100	100
All	All	1343/1344 (100%)	1302 (97%)	40 (3%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	187	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	281/272 (103%)	263 (94%)	18 (6%)	16	33
1	B	281/272 (103%)	268 (95%)	13 (5%)	24	48
1	D	279/272 (103%)	265 (95%)	14 (5%)	22	44
1	E	282/272 (104%)	269 (95%)	13 (5%)	24	48
All	All	1123/1088 (103%)	1065 (95%)	58 (5%)	21	42

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	14	ASP
1	A	17	ARG
1	A	42	VAL
1	A	60	LEU
1	A	99	ARG
1	A	118	LEU
1	A	150	GLN
1	A	152	LYS
1	A	193	LEU
1	A	200	LYS
1	A	224	GLU
1	A	225	GLU
1	A	245	THR
1	A	271	LEU
1	A	282	LEU
1	A	318	TYR
1	A	328	LEU
1	B	14	ASP
1	B	42	VAL
1	B	55	LYS
1	B	56	ASN
1	B	60	LEU
1	B	99	ARG
1	B	118	LEU
1	B	152	LYS
1	B	193	LEU
1	B	200	LYS
1	B	282	LEU
1	B	318	TYR
1	B	328	LEU
1	D	14	ASP
1	D	56	ASN

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Mol	Chain	Res	Type
1	D	60	LEU
1	D	90	ARG
1	D	99	ARG
1	D	118	LEU
1	D	148	VAL
1	D	193	LEU
1	D	200	LYS
1	D	271	LEU
1	D	282	LEU
1	D	301	VAL
1	D	318	TYR
1	D	328	LEU
1	E	12	GLN
1	E	33	PRO
1	E	60	LEU
1	E	99	ARG
1	E	118	LEU
1	E	152	LYS
1	E	193	LEU
1	E	200	LYS
1	E	271	LEU
1	E	282	LEU
1	E	284	LEU
1	E	318	TYR
1	E	328	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	40	GLN
1	A	92	GLN
1	A	117	ASN
1	A	143	ASN
1	A	150	GLN
1	A	177	ASN
1	A	237	HIS
1	A	238	ASN
1	B	12	GLN
1	B	40	GLN
1	B	56	ASN
1	B	126	ASN

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Mol	Chain	Res	Type
1	B	150	GLN
1	B	177	ASN
1	B	201	GLN
1	B	259	ASN
1	D	12	GLN
1	D	40	GLN
1	D	56	ASN
1	D	117	ASN
1	D	126	ASN
1	D	185	GLN
1	D	201	GLN
1	D	262	GLN
1	E	12	GLN
1	E	19	HIS
1	E	40	GLN
1	E	117	ASN
1	E	126	ASN
1	E	150	GLN
1	E	185	GLN
1	E	201	GLN
1	E	205	GLN
1	E	229	GLN
1	E	237	HIS
1	E	238	ASN
1	E	259	ASN
1	E	287	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FMT	E	1638	-	2,2,2	0.47	0	1,1,1	0.15	0
4	FMT	E	1640	-	2,2,2	0.91	0	1,1,1	0.01	0
4	FMT	B	1438	-	2,2,2	0.35	0	1,1,1	0.07	0
2	FMN	B	1437	-	33,33,33	2.52	14 (42%)	48,50,50	2.30	19 (39%)
2	FMN	E	1637	-	33,33,33	2.57	11 (33%)	48,50,50	2.25	20 (41%)
2	FMN	D	1537	-	33,33,33	2.63	11 (33%)	48,50,50	2.29	20 (41%)
4	FMT	D	1539	-	2,2,2	0.42	0	1,1,1	0.16	0
3	ORO	D	1540	-	11,11,11	1.61	2 (18%)	14,15,15	0.98	0
4	FMT	D	1538	-	2,2,2	0.49	0	1,1,1	0.17	0
3	ORO	A	1338	-	11,11,11	1.48	1 (9%)	14,15,15	1.05	0
3	ORO	A	1339[A]	-	11,11,11	1.82	4 (36%)	14,15,15	1.47	3 (21%)
3	ORO	A	1339[B]	-	11,11,11	1.79	6 (54%)	14,15,15	1.11	1 (7%)
2	FMN	A	1337	-	33,33,33	2.91	13 (39%)	48,50,50	2.13	17 (35%)
4	FMT	E	1639	-	2,2,2	0.64	0	1,1,1	0.16	0
4	FMT	B	1440	-	2,2,2	0.43	0	1,1,1	0.15	0
4	FMT	B	1439	-	2,2,2	0.39	0	1,1,1	0.03	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	B	1437	-	-	5/18/18/18	0/3/3/3
2	FMN	E	1637	-	-	5/18/18/18	0/3/3/3
2	FMN	D	1537	-	-	5/18/18/18	0/3/3/3
3	ORO	D	1540	-	-	0/4/4/4	0/1/1/1
3	ORO	A	1338	-	-	4/4/4/4	0/1/1/1
3	ORO	A	1339[A]	-	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ORO	A	1339[B]	-	-	0/4/4/4	0/1/1/1
2	FMN	A	1337	-	-	5/18/18/18	0/3/3/3

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1337	FMN	C4A-N5	7.42	1.46	1.30
2	B	1437	FMN	C4'-C3'	6.41	1.64	1.53
2	D	1537	FMN	C4A-N5	6.30	1.44	1.30
2	E	1637	FMN	C4A-N5	6.20	1.44	1.30
2	A	1337	FMN	C5A-N5	-6.06	1.28	1.39
2	E	1637	FMN	C4'-C3'	5.96	1.63	1.53
2	D	1537	FMN	C4'-C3'	5.91	1.63	1.53
2	A	1337	FMN	C4'-C3'	5.78	1.63	1.53
2	D	1537	FMN	C9A-C5A	5.62	1.50	1.41
2	B	1437	FMN	C9A-C5A	5.47	1.50	1.41
2	A	1337	FMN	C9A-C5A	5.42	1.49	1.41
2	D	1537	FMN	C1'-C2'	5.01	1.59	1.52
2	E	1637	FMN	C9A-C5A	4.96	1.49	1.41
2	A	1337	FMN	C1'-C2'	4.92	1.59	1.52
2	B	1437	FMN	C4A-N5	4.63	1.40	1.30
2	E	1637	FMN	C1'-N10	-4.43	1.37	1.47
2	A	1337	FMN	C1'-N10	-4.41	1.37	1.47
2	B	1437	FMN	C1'-C2'	4.37	1.58	1.52
2	E	1637	FMN	C1'-C2'	4.33	1.58	1.52
2	D	1537	FMN	C1'-N10	-4.14	1.37	1.47
2	B	1437	FMN	C1'-N10	-3.96	1.38	1.47
2	A	1337	FMN	C7M-C7	3.76	1.58	1.51
2	D	1537	FMN	C7M-C7	3.70	1.57	1.51
2	E	1637	FMN	C7M-C7	3.65	1.57	1.51
2	B	1437	FMN	C7M-C7	3.54	1.57	1.51
3	A	1339[A]	ORO	O72-C7	-3.42	1.21	1.30
2	B	1437	FMN	C9A-N10	3.32	1.46	1.41
2	A	1337	FMN	C9A-N10	3.23	1.46	1.41
2	A	1337	FMN	C5'-C4'	-3.18	1.47	1.51
2	E	1637	FMN	C5A-N5	-3.18	1.33	1.39
2	E	1637	FMN	C9A-N10	3.01	1.46	1.41
3	A	1339[A]	ORO	O71-C7	2.97	1.29	1.22
2	D	1537	FMN	C9A-N10	2.92	1.46	1.41
2	A	1337	FMN	P-O2P	-2.68	1.44	1.54
2	D	1537	FMN	C5A-N5	-2.67	1.34	1.39
3	A	1339[B]	ORO	C4-N3	2.66	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1537	FMN	P-O2P	-2.57	1.45	1.54
2	B	1437	FMN	P-O2P	-2.56	1.45	1.54
2	E	1637	FMN	P-O2P	-2.51	1.45	1.54
2	D	1537	FMN	C5'-C4'	-2.32	1.48	1.51
2	D	1537	FMN	O2-C2	-2.29	1.19	1.24
3	A	1339[B]	ORO	O71-C7	2.28	1.28	1.22
3	A	1339[B]	ORO	C6-C7	2.28	1.54	1.48
2	B	1437	FMN	C5'-C4'	-2.27	1.48	1.51
3	D	1540	ORO	C2-N1	2.25	1.41	1.37
2	B	1437	FMN	C10-N1	2.23	1.37	1.33
3	A	1339[A]	ORO	C2-N3	2.22	1.41	1.37
2	E	1637	FMN	C5'-C4'	-2.20	1.48	1.51
3	D	1540	ORO	O72-C7	-2.15	1.24	1.30
2	B	1437	FMN	C10-N10	2.13	1.41	1.37
2	B	1437	FMN	C6-C7	2.13	1.42	1.39
2	E	1637	FMN	O2-C2	-2.12	1.20	1.24
2	A	1337	FMN	C8M-C8	2.12	1.55	1.51
3	A	1339[B]	ORO	C2-N1	2.08	1.40	1.37
2	B	1437	FMN	C2-N1	2.08	1.41	1.36
2	B	1437	FMN	C4-N3	2.07	1.42	1.38
3	A	1339[B]	ORO	O4-C4	-2.06	1.20	1.24
2	A	1337	FMN	O2-C2	-2.06	1.20	1.24
3	A	1339[A]	ORO	C4-N3	2.04	1.42	1.38
3	A	1338	ORO	C2-N1	2.04	1.40	1.37
2	A	1337	FMN	C2-N1	2.03	1.41	1.36
3	A	1339[B]	ORO	C2-N3	2.02	1.40	1.37

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1537	FMN	C5A-C9A-N10	5.79	123.20	117.97
2	E	1637	FMN	C5A-C9A-N10	5.44	122.89	117.97
2	B	1437	FMN	C5A-C9A-N10	5.34	122.80	117.97
2	E	1637	FMN	C10-N1-C2	4.71	127.06	116.85
2	B	1437	FMN	C10-N1-C2	4.70	127.03	116.85
2	D	1537	FMN	C10-N1-C2	4.68	126.98	116.85
2	B	1437	FMN	C9A-N10-C10	-4.65	113.67	120.75
2	A	1337	FMN	C10-N1-C2	4.59	126.80	116.85
2	E	1637	FMN	C9A-N10-C10	-4.49	113.90	120.75
2	D	1537	FMN	C9A-N10-C10	-4.44	113.98	120.75
2	A	1337	FMN	C9A-N10-C10	-4.40	114.04	120.75
2	B	1437	FMN	C4A-C10-N1	-4.16	114.39	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1337	FMN	C4A-C10-N1	-4.15	114.40	124.59
2	E	1637	FMN	C4A-C10-N1	-4.10	114.53	124.59
2	A	1337	FMN	C5A-C9A-N10	4.07	121.65	117.97
2	D	1537	FMN	C4A-C10-N1	-4.07	114.61	124.59
2	A	1337	FMN	C4-C4A-C10	3.84	123.52	116.93
2	E	1637	FMN	C4-C4A-C10	3.76	123.39	116.93
2	D	1537	FMN	C4A-C10-N10	3.64	121.69	116.48
2	B	1437	FMN	C4-C4A-C10	3.64	123.17	116.93
2	D	1537	FMN	C4-C4A-C10	3.61	123.12	116.93
2	E	1637	FMN	C4A-C10-N10	3.50	121.48	116.48
2	E	1637	FMN	O2-C2-N3	3.47	125.25	118.58
2	A	1337	FMN	C4A-C10-N10	3.46	121.43	116.48
2	B	1437	FMN	O2-C2-N3	3.45	125.21	118.58
2	D	1537	FMN	O2-C2-N3	3.44	125.19	118.58
2	B	1437	FMN	C4A-C10-N10	3.43	121.39	116.48
2	A	1337	FMN	O2-C2-N3	3.41	125.11	118.58
2	B	1437	FMN	C9A-C5A-N5	-3.40	118.84	122.45
2	D	1537	FMN	C9A-C5A-N5	-3.36	118.89	122.45
2	D	1537	FMN	C9-C9A-N10	-3.34	117.36	121.85
2	B	1437	FMN	C9-C9A-N10	-3.30	117.41	121.85
2	B	1437	FMN	C4-C4A-N5	-3.29	113.66	118.21
2	E	1637	FMN	C9-C9A-N10	-3.23	117.51	121.85
2	E	1637	FMN	C4-C4A-N5	-3.01	114.05	118.21
2	A	1337	FMN	C9-C9A-N10	-3.01	117.81	121.85
2	B	1437	FMN	O5'-C5'-C4'	2.96	117.28	109.36
2	E	1637	FMN	O5'-C5'-C4'	2.88	117.04	109.36
2	E	1637	FMN	C9A-C5A-N5	-2.85	119.43	122.45
2	D	1537	FMN	O5'-C5'-C4'	2.75	116.69	109.36
2	D	1537	FMN	C1'-N10-C9A	2.70	125.88	120.63
2	A	1337	FMN	C4-C4A-N5	-2.69	114.49	118.21
2	D	1537	FMN	C4-C4A-N5	-2.68	114.51	118.21
3	A	1339[A]	ORO	O4-C4-C5	-2.65	121.80	125.46
2	A	1337	FMN	O2-C2-N1	-2.64	117.42	121.80
2	D	1537	FMN	O2-C2-N1	-2.63	117.42	121.80
2	E	1637	FMN	O2-C2-N1	-2.61	117.46	121.80
2	B	1437	FMN	O2-C2-N1	-2.59	117.49	121.80
2	B	1437	FMN	C1'-N10-C9A	2.58	125.65	120.63
2	A	1337	FMN	O5'-C5'-C4'	2.57	116.21	109.36
2	B	1437	FMN	O2P-P-O1P	2.54	120.72	110.83
2	A	1337	FMN	C1'-N10-C9A	2.52	125.53	120.63
2	E	1637	FMN	O2P-P-O1P	2.52	120.65	110.83
2	A	1337	FMN	O2P-P-O1P	2.51	120.62	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1537	FMN	C5'-C4'-C3'	-2.51	107.49	112.22
2	A	1337	FMN	C5'-C4'-C3'	-2.44	107.61	112.22
2	D	1537	FMN	O2P-P-O1P	2.42	120.27	110.83
2	B	1437	FMN	C6-C5A-N5	2.42	122.46	118.44
2	E	1637	FMN	C1'-N10-C9A	2.39	125.28	120.63
3	A	1339[A]	ORO	O4-C4-N3	2.28	122.58	119.27
2	B	1437	FMN	C5'-C4'-C3'	-2.26	107.96	112.22
2	E	1637	FMN	C5'-C4'-C3'	-2.25	107.97	112.22
2	E	1637	FMN	O4'-C4'-C5'	2.15	114.74	109.99
2	E	1637	FMN	C4-N3-C2	-2.14	121.84	125.64
2	A	1337	FMN	O4'-C4'-C5'	2.13	114.68	109.99
2	D	1537	FMN	C4-N3-C2	-2.12	121.88	125.64
2	D	1537	FMN	C8M-C8-C9	-2.11	115.85	119.57
2	A	1337	FMN	C4-N3-C2	-2.11	121.89	125.64
3	A	1339[A]	ORO	O72-C7-O71	2.10	128.90	123.90
2	D	1537	FMN	O3'-C3'-C4'	2.10	113.69	108.93
3	A	1339[B]	ORO	O4-C4-C5	-2.09	122.57	125.46
2	E	1637	FMN	C8M-C8-C9	-2.08	115.90	119.57
2	D	1537	FMN	O3'-C3'-C2'	-2.07	104.22	108.93
2	A	1337	FMN	O3'-C3'-C4'	2.07	113.64	108.93
2	E	1637	FMN	O3'-C3'-C4'	2.06	113.61	108.93
2	B	1437	FMN	C4-N3-C2	-2.06	121.99	125.64
2	E	1637	FMN	O3'-C3'-C2'	-2.03	104.31	108.93
2	B	1437	FMN	C4'-C3'-C2'	2.01	116.92	113.57
2	D	1537	FMN	O4'-C4'-C5'	2.01	114.43	109.99
2	B	1437	FMN	O3'-C3'-C2'	-2.00	104.38	108.93

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1338	ORO	N1-C6-C7-O71
3	A	1338	ORO	N1-C6-C7-O72
3	A	1338	ORO	C5-C6-C7-O71
3	A	1338	ORO	C5-C6-C7-O72
2	B	1437	FMN	C2'-C3'-C4'-O4'
2	D	1537	FMN	C2'-C3'-C4'-O4'
2	E	1637	FMN	C2'-C3'-C4'-O4'
2	B	1437	FMN	O3'-C3'-C4'-O4'
2	D	1537	FMN	O3'-C3'-C4'-O4'
2	E	1637	FMN	O3'-C3'-C4'-O4'
2	B	1437	FMN	O3'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
2	D	1537	FMN	O3'-C3'-C4'-C5'
2	E	1637	FMN	O3'-C3'-C4'-C5'
2	B	1437	FMN	C2'-C3'-C4'-C5'
2	D	1537	FMN	C2'-C3'-C4'-C5'
2	A	1337	FMN	C2'-C3'-C4'-O4'
2	E	1637	FMN	C4'-C5'-O5'-P
2	A	1337	FMN	O3'-C3'-C4'-O4'
2	E	1637	FMN	C2'-C3'-C4'-C5'
2	B	1437	FMN	C4'-C5'-O5'-P
2	A	1337	FMN	C4'-C5'-O5'-P
2	D	1537	FMN	C4'-C5'-O5'-P
2	A	1337	FMN	O3'-C3'-C4'-C5'
2	A	1337	FMN	C2'-C3'-C4'-C5'

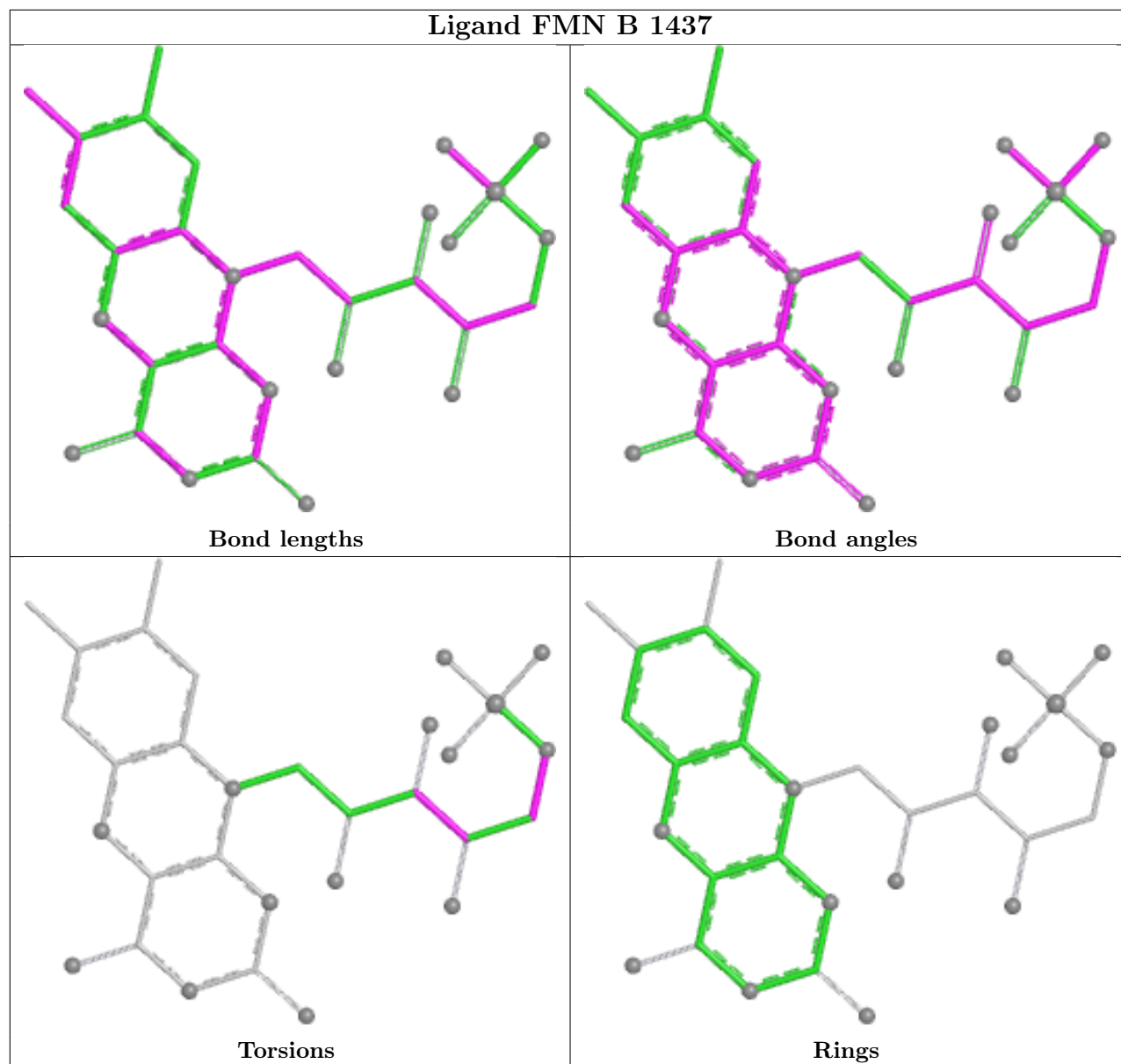
There are no ring outliers.

5 monomers are involved in 5 short contacts:

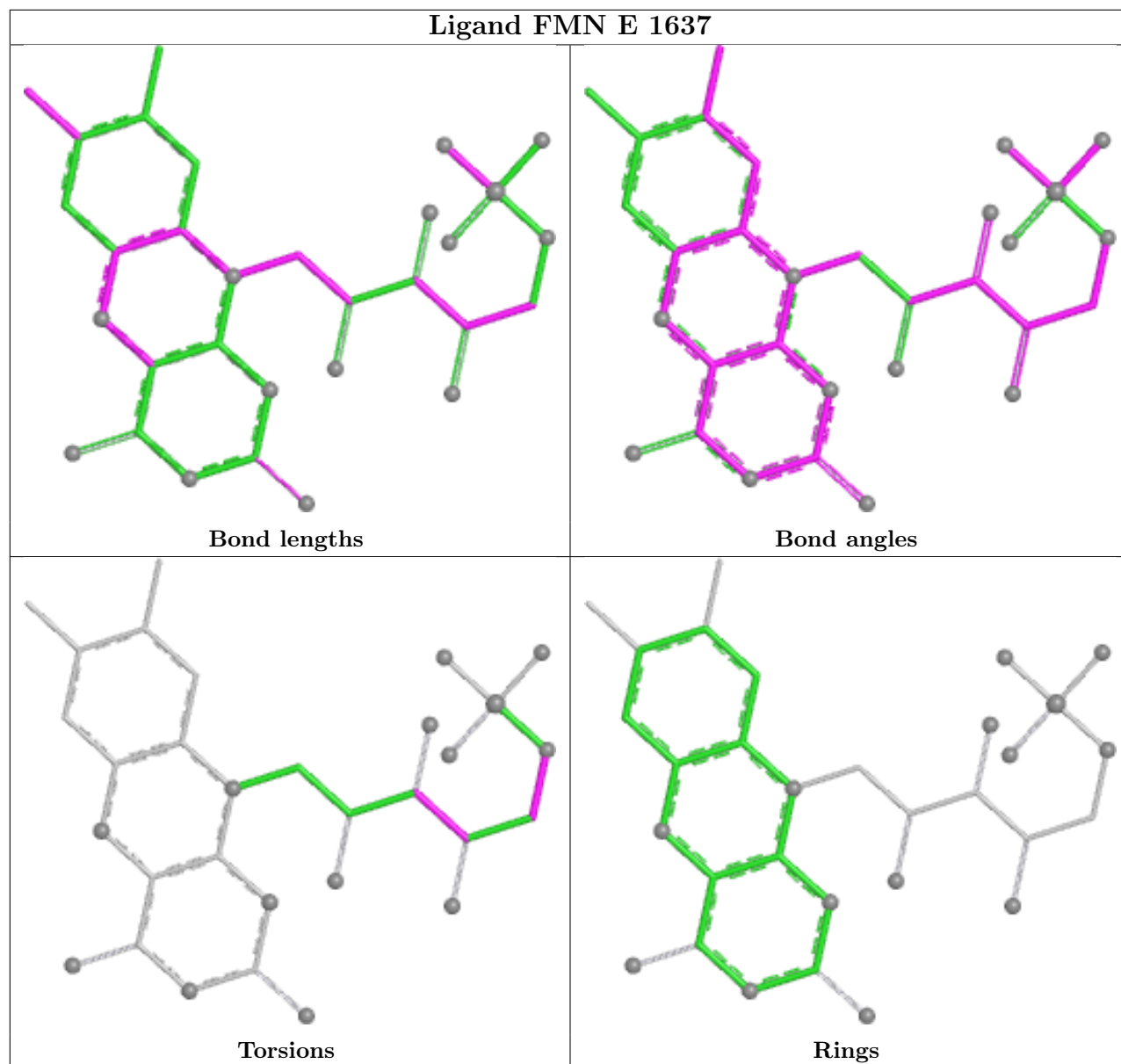
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1638	FMT	1	0
4	D	1539	FMT	1	0
3	A	1339[A]	ORO	1	0
4	E	1639	FMT	1	0
4	B	1440	FMT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

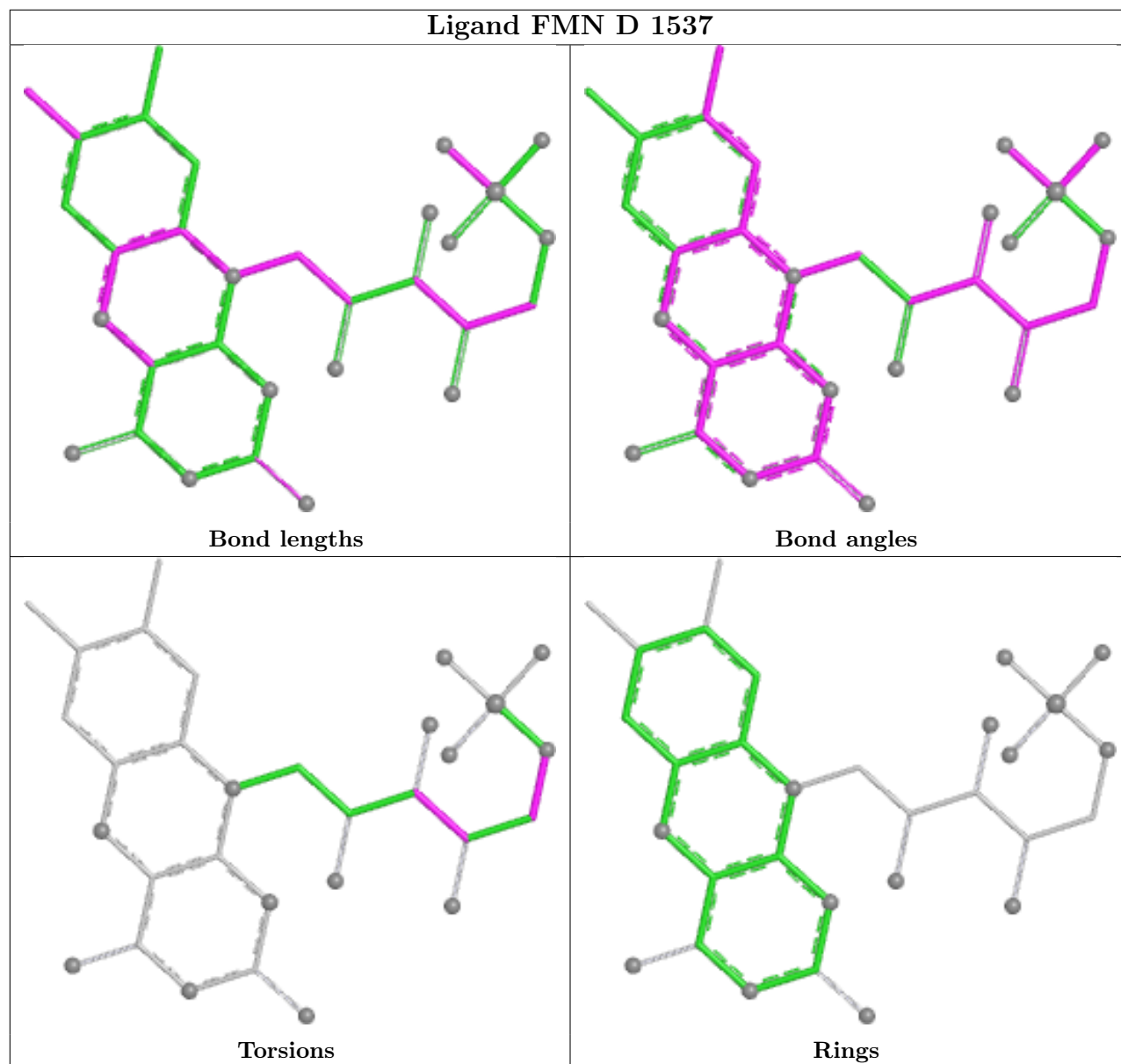
Ligand FMN B 1437

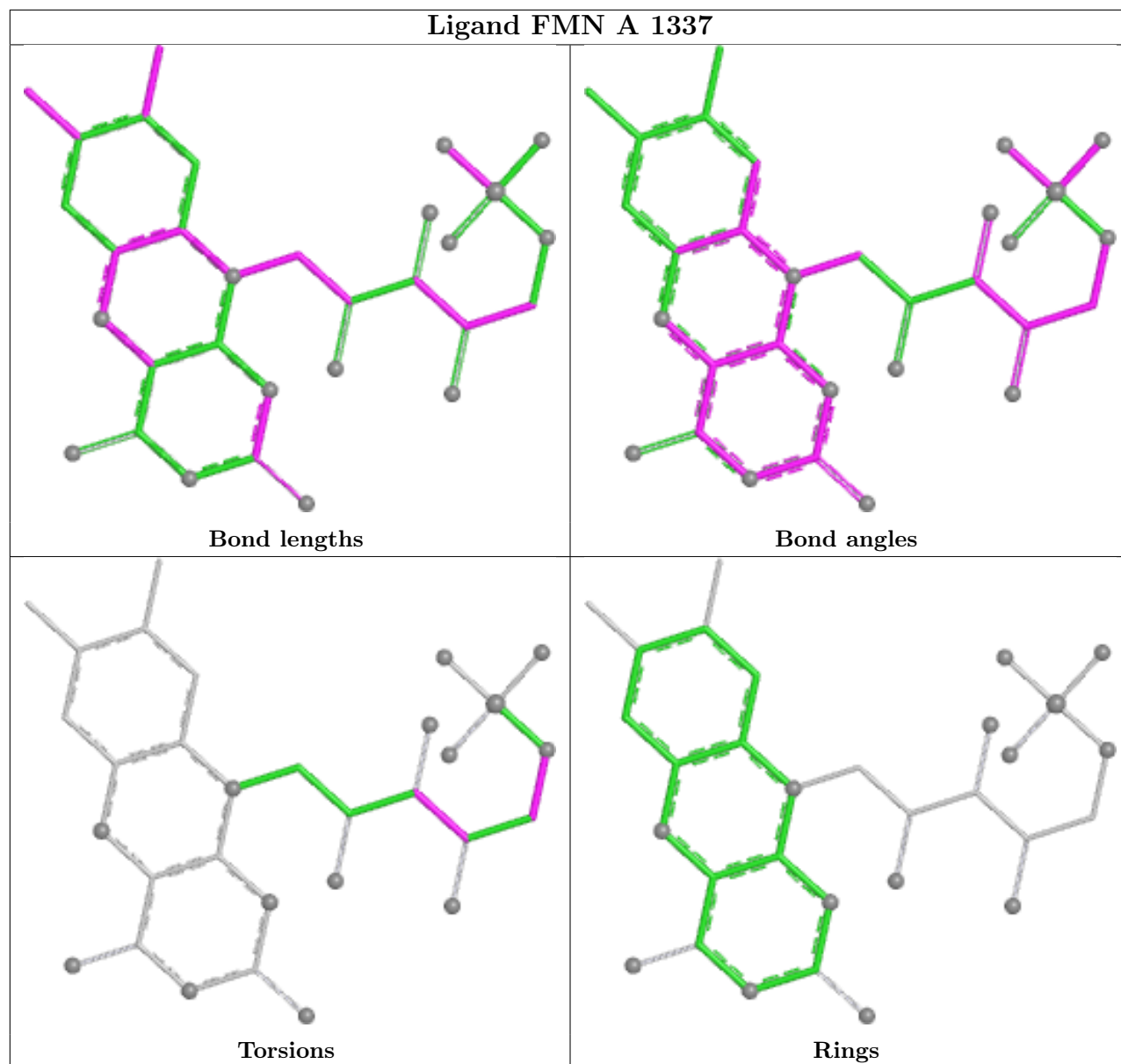


Ligand FMN E 1637



Ligand FMN D 1537





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	329/336 (97%)	-0.60	3 (0%) 81 78	10, 20, 35, 49	11 (3%)
1	B	329/336 (97%)	-0.30	9 (2%) 56 51	12, 26, 47, 68	17 (5%)
1	D	329/336 (97%)	-0.03	10 (3%) 52 48	20, 34, 58, 67	22 (6%)
1	E	329/336 (97%)	-0.40	9 (2%) 56 51	12, 24, 44, 63	18 (5%)
All	All	1316/1344 (97%)	-0.33	31 (2%) 59 55	10, 26, 49, 68	68 (5%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	TYR	6.7
1	E	199[A]	ASN	6.2
1	A	153[A]	ASP	5.6
1	B	34	PHE	5.1
1	B	5	PHE	5.0
1	A	12[A]	GLN	4.7
1	E	48[A]	ASN	4.6
1	B	205[A]	GLN	4.5
1	D	8	LYS	4.4
1	D	28	ARG	4.4
1	E	5	PHE	4.3
1	D	34	PHE	4.0
1	B	8	LYS	3.9
1	E	39[A]	ARG	3.9
1	D	2	TYR	3.2
1	D	225	GLU	2.9
1	E	3	TYR	2.7
1	D	41	LYS	2.6
1	B	3	TYR	2.6
1	D	258	LYS	2.4
1	E	2	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	34	PHE	2.3
1	E	8	LYS	2.3
1	D	148	VAL	2.3
1	D	5	PHE	2.2
1	B	41	LYS	2.1
1	E	41	LYS	2.1
1	B	131	HIS	2.1
1	A	2	TYR	2.1
1	D	133	ASP	2.1
1	B	33	PRO	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ORO	D	1540	11/11	0.73	0.13	75,76,77,78	0
3	ORO	A	1339[B]	11/11	0.77	0.23	66,67,68,68	11
3	ORO	A	1339[A]	11/11	0.77	0.23	68,68,69,69	11
4	FMT	B	1439	3/3	0.79	0.27	43,43,47,52	0
4	FMT	B	1438	3/3	0.84	0.25	63,63,64,64	0
4	FMT	D	1538	3/3	0.85	0.21	53,53,57,58	0
4	FMT	E	1639	3/3	0.92	0.21	59,59,61,63	0
4	FMT	E	1640	3/3	0.92	0.11	33,33,35,37	0
4	FMT	B	1440	3/3	0.95	0.07	40,40,40,40	0
4	FMT	D	1539	3/3	0.95	0.07	34,34,34,37	0
2	FMN	D	1537	31/31	0.96	0.07	23,29,33,34	0
4	FMT	E	1638	3/3	0.96	0.07	23,23,26,27	0
3	ORO	A	1338	11/11	0.97	0.08	17,21,23,23	0

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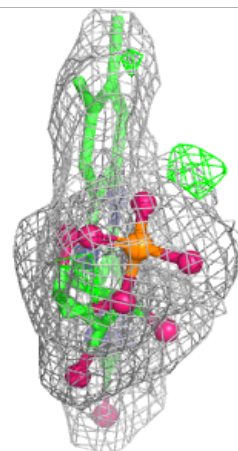
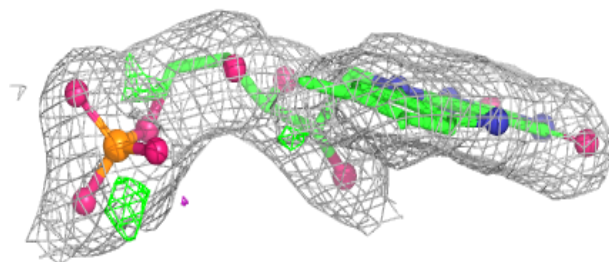
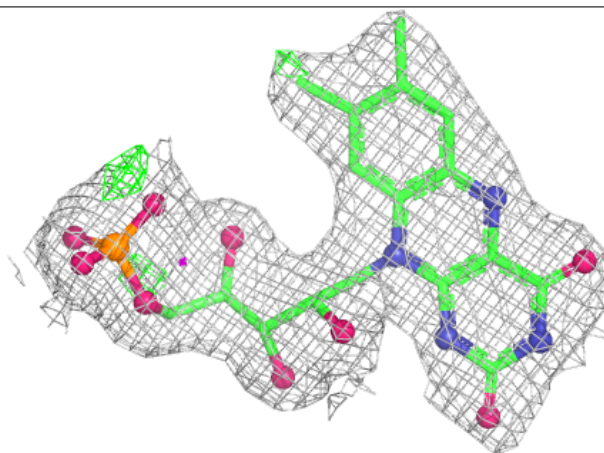
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMN	B	1437	31/31	0.97	0.06	15,19,23,25	0
2	FMN	A	1337	31/31	0.98	0.05	11,15,19,20	0
2	FMN	E	1637	31/31	0.98	0.06	12,19,22,23	0

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.

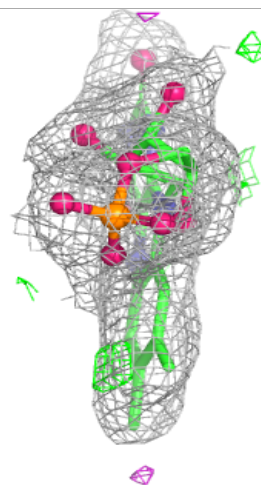
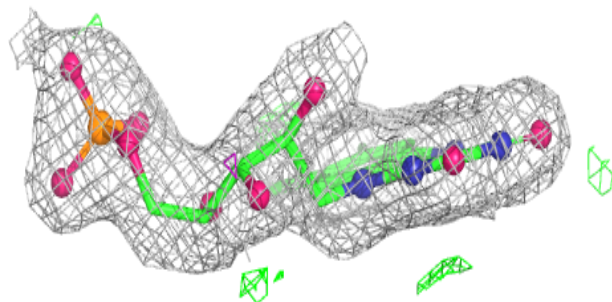
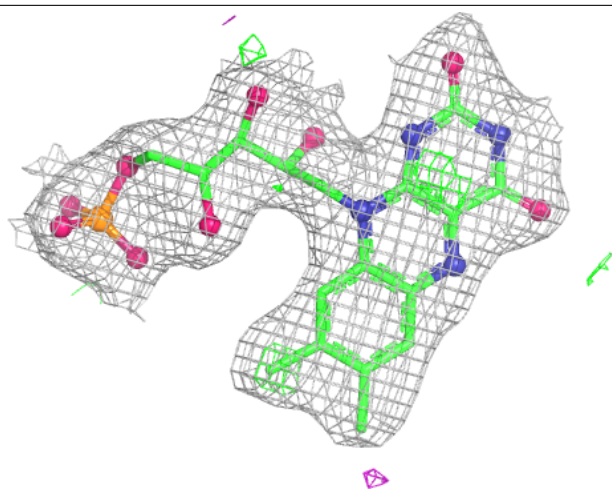
Electron density around FMN D 1537:

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



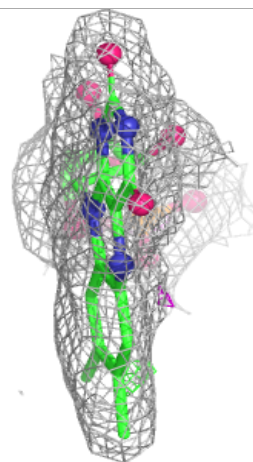
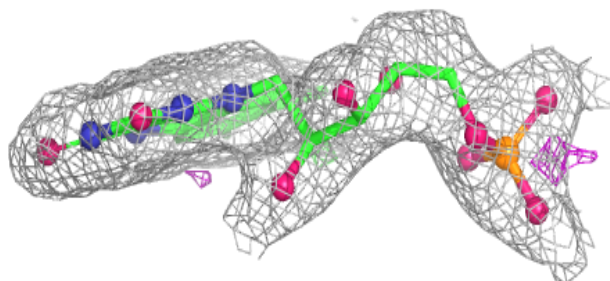
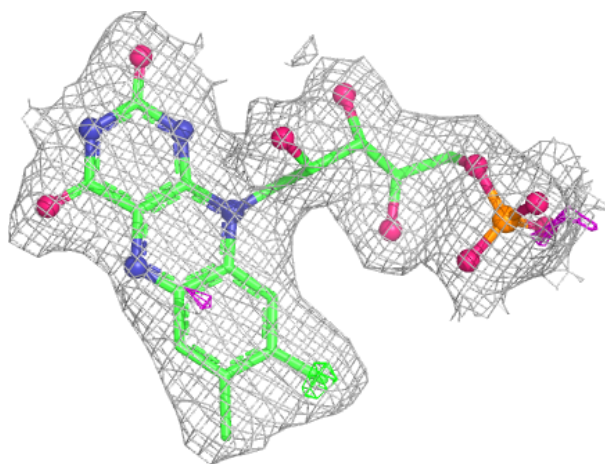
Electron density around FMN B 1437:

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



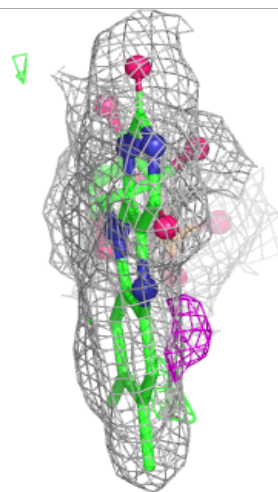
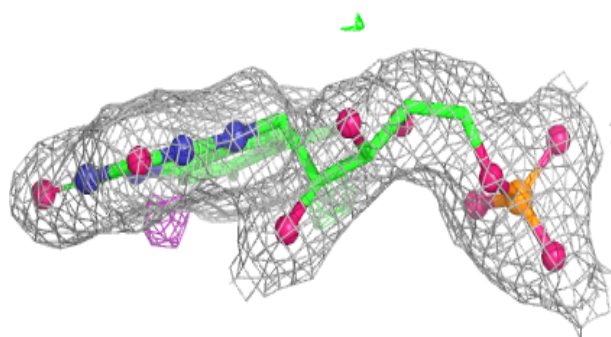
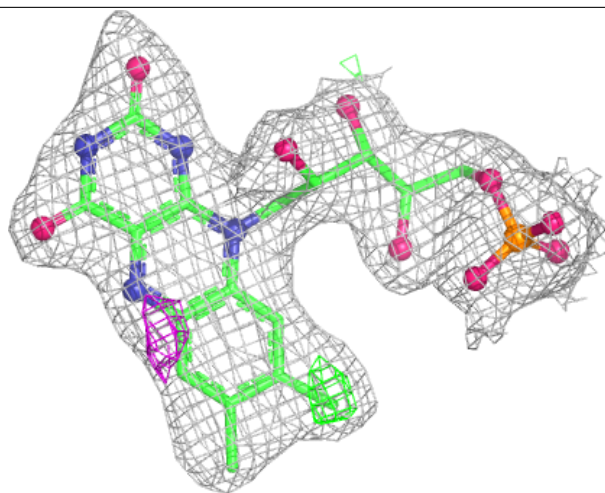
Electron density around FMN A 1337:

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



Electron density around FMN E 1637:

$2mF_o-DF_c$ (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.