



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:05 am BST

PDB ID : 2OHI
Title : Crystal Structure of coenzyme F420H2 oxidase (FprA), a diiron flavoprotein, reduced state
Authors : Seedorf, H.; Warkentin, E.; Ermler, U.
Deposited on : 2007-01-10
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

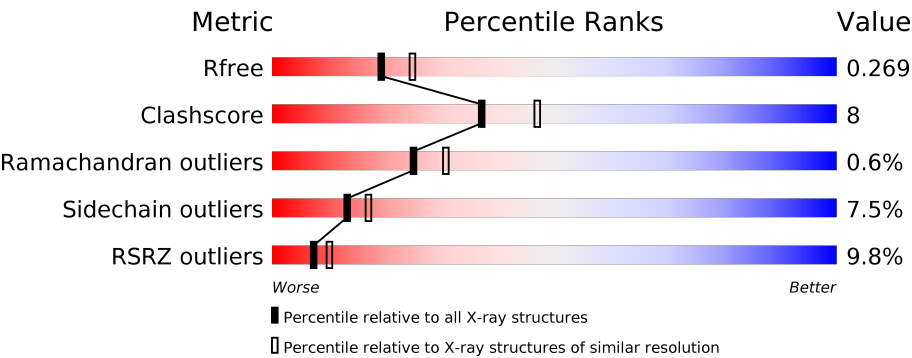
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	404	<div><div>11%</div><div><div></div><div>77%</div><div>22%</div></div><div></div></div>
1	B	404	<div><div>6%</div><div><div></div><div>80%</div><div>17%</div></div><div></div></div>
1	D	404	<div><div>8%</div><div><div></div><div>82%</div><div>15%</div></div><div></div></div>
1	E	404	<div><div>12%</div><div><div></div><div>73%</div><div>25%</div></div><div></div></div>
1	G	404	<div><div>10%</div><div><div></div><div>76%</div><div>21%</div></div><div></div></div>
1	H	404	<div><div>9%</div><div><div></div><div>76%</div><div>20%</div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	I	404	<div><div></div><div>14%</div><div></div><div>77%</div><div></div><div>21%</div><div></div></div>
1	J	404	<div><div></div><div>8%</div><div></div><div>80%</div><div></div><div>18%</div><div></div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 25966 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 Type A flavoprotein fprA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	1	0
			3166	2014	526	604	22			
1	B	403	Total	C	N	O	S	0	0	0
			3162	2012	525	603	22			
1	D	403	Total	C	N	O	S	0	3	0
			3178	2022	530	604	22			
1	E	403	Total	C	N	O	S	0	1	0
			3168	2016	527	603	22			
1	G	403	Total	C	N	O	S	0	1	0
			3166	2014	526	604	22			
1	H	403	Total	C	N	O	S	0	0	0
			3162	2012	525	603	22			
1	I	403	Total	C	N	O	S	0	0	0
			3162	2012	525	603	22			
1	J	403	Total	C	N	O	S	0	2	0
			3169	2016	527	604	22			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

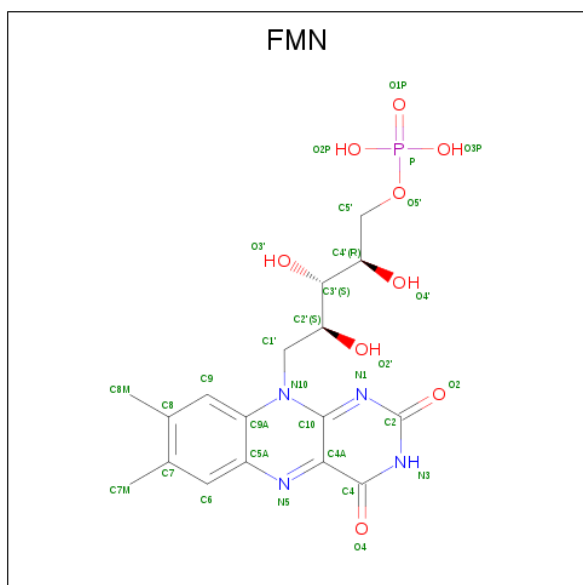
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Fe	0	0
			2	2		
2	J	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		
2	E	2	Total	Fe	0	0
			2	2		
2	H	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	I	2	Total	Fe	0	0
			2	2		
2	A	2	Total	Fe	0	0
			2	2		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total 1	Cl 1	0	0
4	J	2	Total 2	Cl 2	0	0
4	D	1	Total 1	Cl 1	0	0

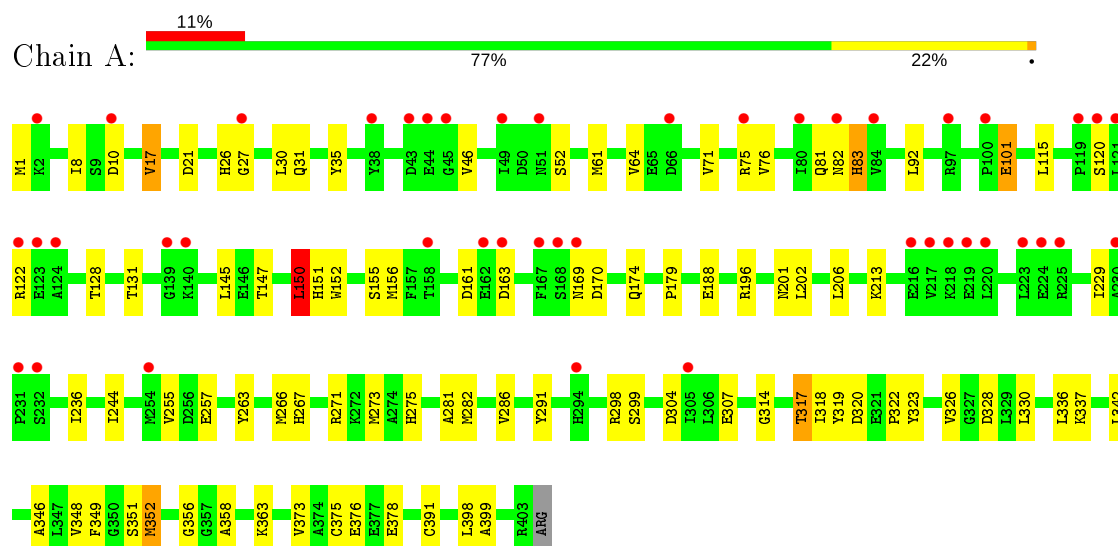
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total 46	O 46	0	0
5	B	47	Total 47	O 47	0	0
5	D	57	Total 57	O 57	0	0
5	E	42	Total 42	O 42	0	0
5	G	50	Total 50	O 50	0	0
5	H	45	Total 45	O 45	0	0
5	I	33	Total 33	O 33	0	0
5	J	45	Total 45	O 45	0	0

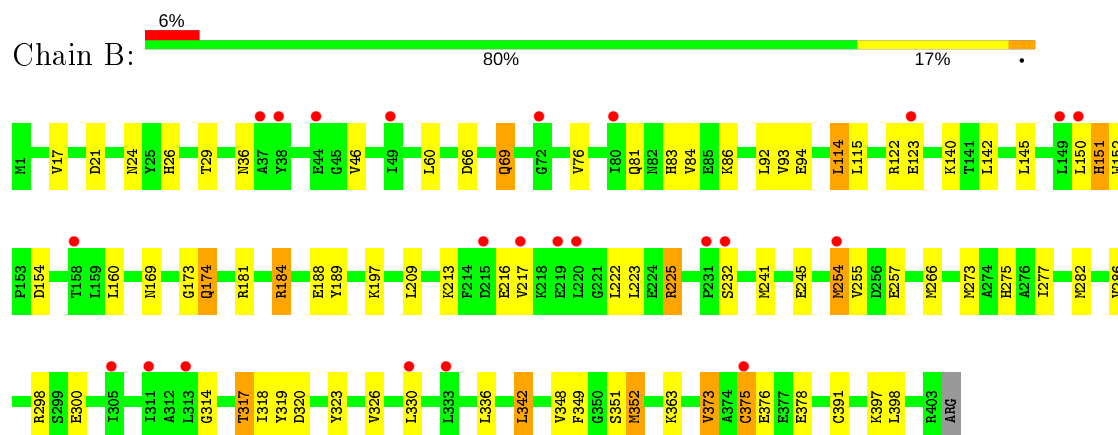
3 Residue-property plots [i](#)

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

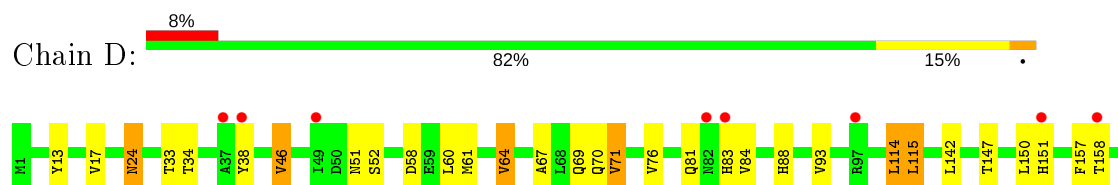
• Molecule 1: Type A flavoprotein fprA

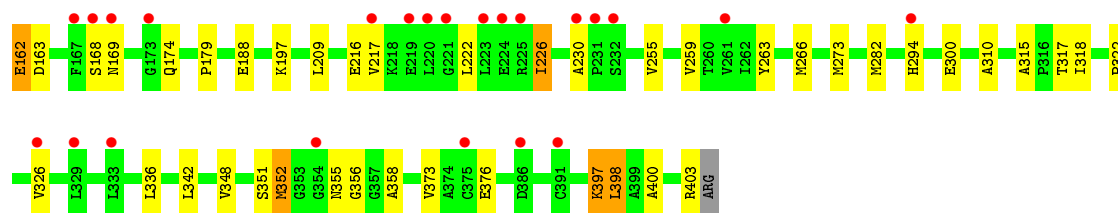


• Molecule 1: Type A flavoprotein fprA

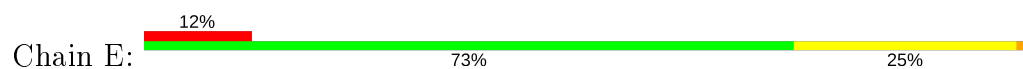


• Molecule 1: Type A flavoprotein fprA

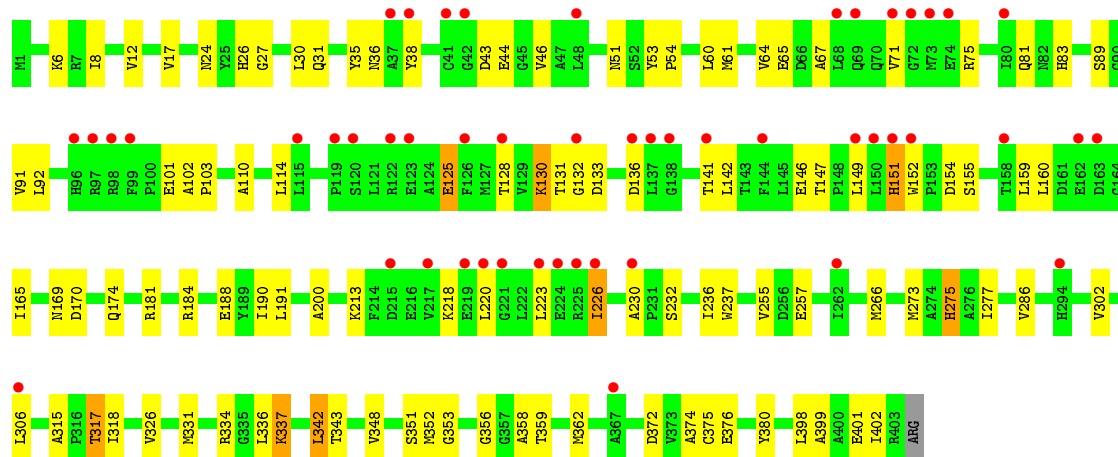




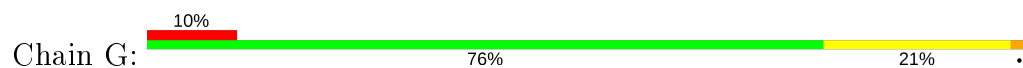
• Molecule 1: Type A flavoprotein fprA



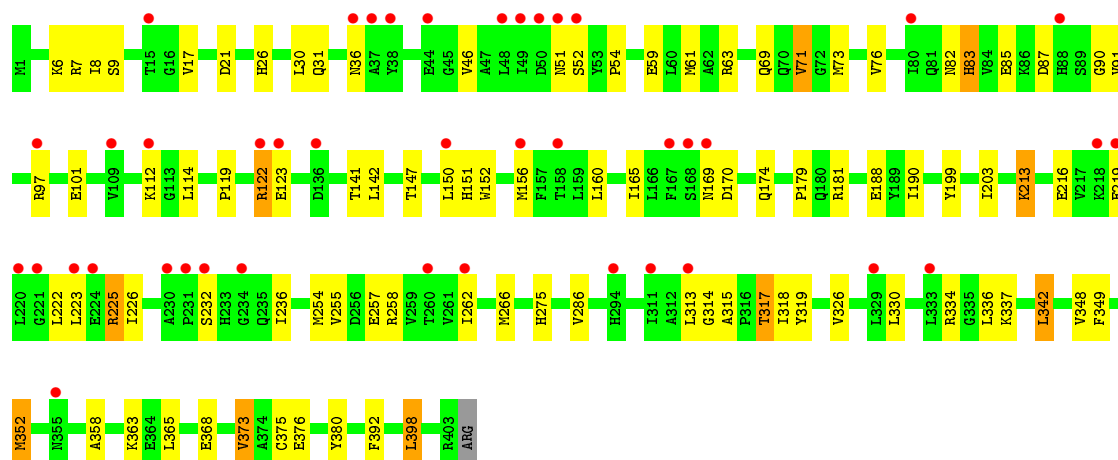
Chain E:



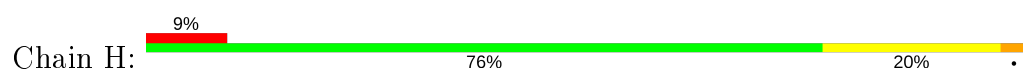
• Molecule 1: Type A flavoprotein fprA



Chain G:

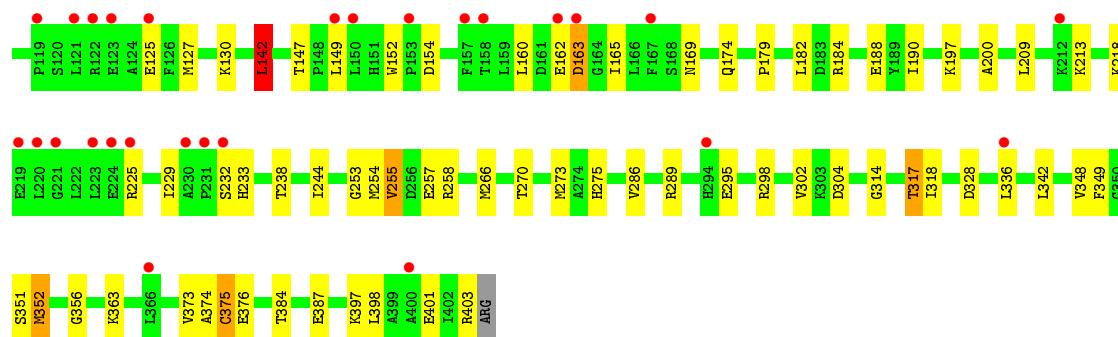


• Molecule 1: Type A flavoprotein fprA

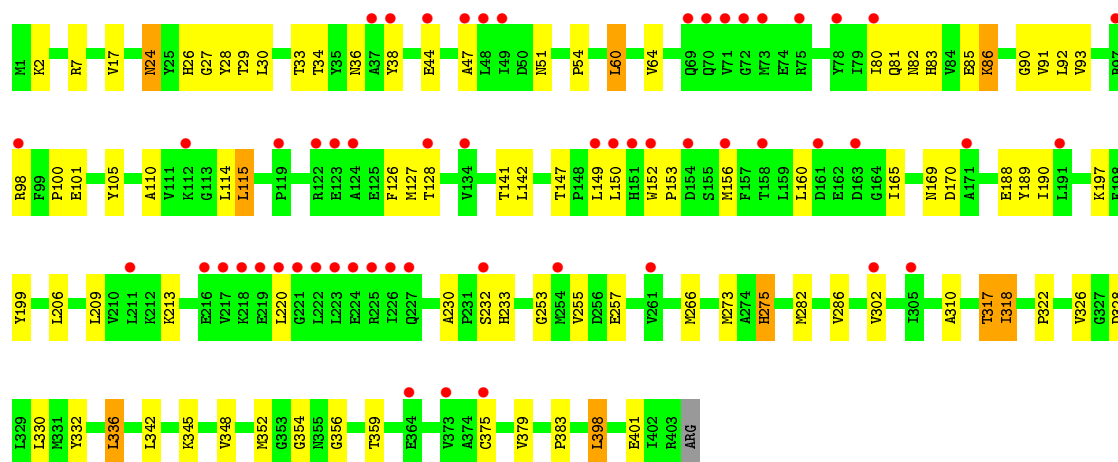
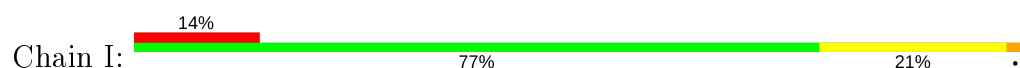


Chain H:

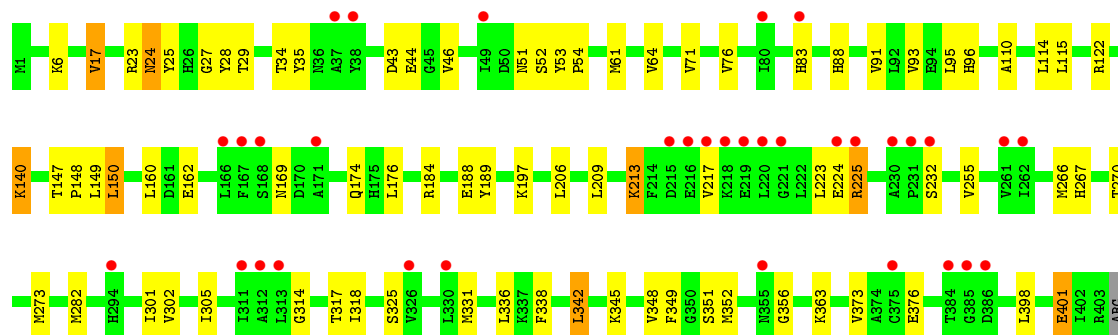
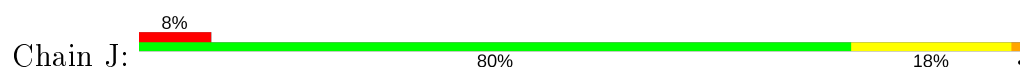




• Molecule 1: Type A flavoprotein fprA



• Molecule 1: Type A flavoprotein fprA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.80Å 123.11Å 135.86Å 90.00° 103.40° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 29.58 – 2.28	Depositor EDS
% Data completeness (in resolution range)	78.9 (20.00-2.30) 77.6 (29.58-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	6.60	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.269 0.203 , 0.269	Depositor DCC
R_{free} test set	6932 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25966	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.3444e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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, FE, CL

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	0.66	2/3237 (0.1%)	0.66	1/4386 (0.0%)
1	B	0.54	0/3229	0.69	2/4375 (0.0%)
1	D	0.52	0/3259	0.65	0/4416
1	E	0.92	9/3240 (0.3%)	0.73	8/4390 (0.2%)
1	G	0.52	0/3237	0.69	2/4386 (0.0%)
1	H	0.60	4/3229 (0.1%)	0.67	1/4375 (0.0%)
1	I	0.50	0/3229	0.63	0/4375
1	J	0.53	0/3246	0.68	1/4398 (0.0%)
All	All	0.61	15/25906 (0.1%)	0.67	15/35101 (0.0%)

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	A	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	125	GLU	CD-OE2	27.93	1.56	1.25
1	E	132	GLY	C-O	18.60	1.53	1.23
1	A	101	GLU	CD-OE1	17.32	1.44	1.25
1	A	101	GLU	CD-OE2	17.25	1.44	1.25
1	E	43	ASP	CG-OD2	11.48	1.51	1.25
1	H	125	GLU	CG-CD	10.27	1.67	1.51
1	E	130	LYS	CE-NZ	9.57	1.73	1.49
1	H	125	GLU	CD-OE1	7.08	1.33	1.25
1	E	44	GLU	CD-OE1	6.61	1.32	1.25
1	H	101	GLU	CD-OE2	5.96	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	125	GLU	CD-OE1	-5.80	1.19	1.25
1	E	44	GLU	CG-CD	5.71	1.60	1.51
1	E	133	ASP	CB-CG	5.20	1.62	1.51
1	E	132	GLY	CA-C	5.19	1.60	1.51
1	H	125	GLU	CB-CG	5.07	1.61	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	132	GLY	O-C-N	9.03	137.15	122.70
1	E	133	ASP	CB-CG-OD1	-8.86	110.33	118.30
1	E	43	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	J	342	LEU	CA-CB-CG	6.39	129.99	115.30
1	G	398	LEU	CA-CB-CG	6.06	129.24	115.30
1	G	342	LEU	CA-CB-CG	5.74	128.50	115.30
1	E	125	GLU	CG-CD-OE1	5.55	129.40	118.30
1	E	132	GLY	CA-C-N	-5.51	105.07	117.20
1	A	150	LEU	CA-CB-CG	5.43	127.79	115.30
1	B	342	LEU	CA-CB-CG	5.34	127.59	115.30
1	B	298	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	H	142	LEU	CA-CB-CG	5.17	127.19	115.30
1	E	75	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	E	43	ASP	CB-CG-OD1	5.08	122.87	118.30
1	E	342	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	GLU	Sidechain

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	3166	0	3113	54	0
1	B	3162	0	3111	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3178	0	3119	47	0
1	E	3168	0	3114	60	0
1	G	3166	0	3113	56	0
1	H	3162	0	3111	48	0
1	I	3162	0	3111	58	0
1	J	3169	0	3115	58	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
3	A	31	0	19	0	0
3	B	31	0	19	0	0
3	D	31	0	19	0	0
3	E	31	0	19	0	0
3	G	31	0	19	0	0
3	H	31	0	19	0	0
3	I	31	0	19	1	0
3	J	31	0	19	0	0
4	D	1	0	0	0	0
4	H	1	0	0	0	0
4	J	2	0	0	0	0
5	A	46	0	0	1	0
5	B	47	0	0	2	0
5	D	57	0	0	3	0
5	E	42	0	0	2	0
5	G	50	0	0	3	0
5	H	45	0	0	3	0
5	I	33	0	0	1	0
5	J	45	0	0	4	0
All	All	25966	0	25059	397	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (397) 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:E:130:LYS:CE	1:E:130:LYS:NZ	1.73	1.47
1:H:266:MET:SD	1:H:318:ILE:HD11	1.98	1.04
1:B:266:MET:SD	1:B:318:ILE:HD11	1.97	1.03
1:I:266:MET:SD	1:I:318:ILE:HD11	2.05	0.95
1:J:24:ASN:HD21	1:J:27:GLY:H	1.16	0.93
1:J:51:ASN:HD22	1:J:52:SER:H	1.24	0.85
1:G:71:VAL:HG12	1:G:73:MET:HG2	1.58	0.84
1:I:24:ASN:HD21	1:I:27:GLY:H	1.24	0.81
1:A:266:MET:SD	1:A:318:ILE:HD11	2.20	0.81
1:D:317:THR:HG22	1:D:352:MET:HB3	1.63	0.81
1:D:266:MET:SD	1:D:318:ILE:HD11	2.23	0.78
1:D:67:ALA:O	1:D:71:VAL:HG23	1.83	0.78
1:G:83:HIS:HD2	1:G:169[A]:ASN:HD21	1.33	0.76
1:E:147:THR:HG22	1:E:213:LYS:HE2	1.66	0.76
1:D:266:MET:HG2	1:E:26:HIS:HB2	1.65	0.76
1:E:81:GLN:HE21	1:E:92:LEU:HD13	1.52	0.75
1:G:85:GLU:HG2	1:G:87:ASP:OD1	1.87	0.74
1:G:83:HIS:CD2	1:G:169[A]:ASN:ND2	2.56	0.74
1:J:317:THR:HG21	1:J:356:GLY:HA2	1.70	0.74
1:I:82:ASN:HD22	1:I:156:MET:HG3	1.52	0.73
1:G:83:HIS:CD2	1:G:169[A]:ASN:HD21	2.07	0.73
1:G:51:ASN:HD22	1:G:52:SER:H	1.34	0.72
1:I:317:THR:HG21	1:I:356:GLY:HA2	1.72	0.72
1:A:317:THR:HG21	1:A:356:GLY:HA2	1.71	0.71
1:E:151[A]:HIS:CE1	1:E:169:ASN:HB3	2.24	0.71
1:I:147:THR:HG22	1:I:213:LYS:HE2	1.72	0.71
1:A:26:HIS:HB2	1:B:266:MET:HG2	1.72	0.71
1:H:182:LEU:HD13	1:H:238:THR:HG21	1.73	0.71
1:H:147:THR:HG22	1:H:213:LYS:HE2	1.72	0.71
1:I:83:HIS:HE1	1:I:152:TRP:HB2	1.57	0.70
1:G:257:GLU:HB3	1:G:286:VAL:HG22	1.74	0.69
1:H:289:ARG:HG3	1:H:304:ASP:OD1	1.92	0.69
1:A:317:THR:HG22	1:A:352:MET:HB3	1.74	0.69
1:G:83:HIS:HD2	1:G:169[A]:ASN:ND2	1.89	0.69
1:H:253:GLY:HA2	5:H:1745:HOH:O	1.92	0.68
1:E:223:LEU:HA	1:E:226:ILE:HD13	1.74	0.68
1:H:179:PRO:HB3	1:J:282:MET:HG2	1.76	0.67
1:B:46:VAL:HG22	1:B:76:VAL:HA	1.77	0.67
1:G:314:GLY:HA2	1:G:349:PHE:O	1.95	0.67
1:A:169[A]:ASN:HD22	1:A:170:ASP:H	1.43	0.67
1:G:71:VAL:CG1	1:G:73:MET:HG2	2.25	0.66
1:E:317:THR:HG21	1:E:356:GLY:HA2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ASN:HD22	1:A:156:MET:HG3	1.62	0.65
1:J:83[B]:HIS:CE1	1:J:169:ASN:HB2	2.31	0.65
1:H:190:ILE:HD11	1:J:189:TYR:CZ	2.31	0.65
1:G:169[B]:ASN:HD22	1:G:170:ASP:H	1.45	0.64
1:J:24:ASN:C	1:J:24:ASN:HD22	2.00	0.64
1:B:84:VAL:HG12	1:B:114:LEU:HD13	1.77	0.64
1:J:46:VAL:HG22	1:J:76:VAL:HA	1.79	0.64
1:D:162:GLU:HG2	1:D:163:ASP:OD1	1.97	0.64
1:H:142:LEU:HD12	1:H:160:LEU:HD13	1.79	0.64
1:E:266:MET:SD	1:E:318:ILE:HD11	2.38	0.63
1:A:273:MET:CE	1:A:351:SER:HB2	2.28	0.63
1:D:317:THR:HG21	1:D:356:GLY:HA2	1.81	0.63
1:I:142:LEU:HD12	1:I:160:LEU:HD13	1.81	0.62
1:A:257:GLU:HB3	1:A:286:VAL:HG22	1.82	0.62
1:I:81:GLN:HE21	1:I:92:LEU:HD13	1.65	0.61
1:G:348:VAL:O	1:G:376:GLU:HA	2.00	0.61
1:I:110:ALA:O	1:I:114:LEU:HB2	2.00	0.61
1:G:26:HIS:HB2	1:H:266:MET:HG2	1.80	0.61
1:J:267:HIS:HB3	5:J:3728:HOH:O	2.01	0.61
1:A:83:HIS:HE1	1:A:152:TRP:CG	2.19	0.60
1:I:332:TYR:O	1:I:336:LEU:HD22	2.01	0.60
1:J:150:LEU:HA	1:J:206:LEU:HD13	1.83	0.60
1:H:17:VAL:HG22	1:H:35:TYR:HD2	1.66	0.60
1:G:46:VAL:HG22	1:G:76:VAL:HA	1.83	0.60
1:B:352:MET:HG2	1:B:378:GLU:OE2	2.01	0.60
1:I:83:HIS:CE1	1:I:152:TRP:HB2	2.36	0.59
1:I:54:PRO:HD3	1:I:90:GLY:HA3	1.84	0.59
1:I:93:VAL:HG12	5:I:2724:HOH:O	2.02	0.59
1:G:254:MET:O	5:G:740:HOH:O	2.17	0.59
1:I:86:LYS:HD2	5:J:3728:HOH:O	2.01	0.59
1:J:17:VAL:HG22	1:J:35:TYR:HD2	1.67	0.59
1:B:189:TYR:CE2	1:E:190:ILE:HD11	2.37	0.59
1:A:273:MET:HE1	1:A:351:SER:HB2	1.84	0.59
1:E:151[A]:HIS:HE1	1:E:169:ASN:HB3	1.68	0.59
1:J:17:VAL:CG2	1:J:35:TYR:HD2	2.16	0.59
1:H:57:PHE:CZ	1:H:61:MET:HG2	2.38	0.59
1:B:36:ASN:HB2	1:B:232:SER:HA	1.83	0.58
1:D:83[B]:HIS:CE1	1:D:169[B]:ASN:HB2	2.38	0.58
1:E:81:GLN:HE22	1:E:89:SER:HA	1.67	0.58
1:J:162:GLU:CD	1:J:162:GLU:H	2.05	0.58
1:H:254:MET:O	1:H:255:VAL:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:163:ASP:HB3	1:H:165:ILE:HG13	1.85	0.57
1:B:318:ILE:CD1	1:B:323:TYR:HD1	2.17	0.57
1:H:273:MET:CE	1:H:351:SER:HB2	2.34	0.57
1:G:169[B]:ASN:HD22	1:G:170:ASP:N	2.02	0.57
1:H:273:MET:HE1	1:H:351:SER:HB2	1.86	0.57
1:G:122:ARG:HE	1:G:123:GLU:N	2.03	0.57
1:B:317:THR:HG23	1:B:352:MET:HB3	1.86	0.56
1:G:51:ASN:ND2	1:G:52:SER:H	2.03	0.56
1:A:317:THR:CG2	1:A:352:MET:HB3	2.36	0.56
1:A:179:PRO:HB3	1:D:282:MET:HG2	1.87	0.56
1:E:24:ASN:HD21	1:E:27:GLY:H	1.54	0.56
1:J:147:THR:HG22	1:J:213:LYS:HD3	1.87	0.56
1:G:315:ALA:HB2	1:G:326:VAL:HG21	1.88	0.56
1:D:317:THR:CG2	1:D:352:MET:HB3	2.36	0.56
1:I:326:VAL:HG12	1:I:330:LEU:HD12	1.87	0.56
1:E:317:THR:HG22	5:E:3717:HOH:O	2.05	0.56
1:B:348:VAL:O	1:B:376:GLU:HA	2.06	0.55
1:E:83:HIS:HE1	1:E:152:TRP:HB2	1.71	0.55
1:E:273:MET:CE	1:E:351:SER:HB2	2.37	0.55
1:J:110:ALA:O	1:J:114:LEU:HB2	2.06	0.55
1:G:317:THR:HG23	1:G:352:MET:HB3	1.88	0.55
1:D:397:LYS:HD3	1:D:398:LEU:N	2.21	0.55
1:E:257:GLU:O	1:E:286:VAL:HG13	2.06	0.55
1:H:317:THR:HG23	1:H:352:MET:HB3	1.89	0.55
1:D:83[B]:HIS:CE1	1:D:88:HIS:CD2	2.96	0.54
1:G:222:LEU:HA	1:G:225:ARG:HD2	1.89	0.54
1:A:319:TYR:O	1:A:320:ASP:HB2	2.07	0.54
1:B:222:LEU:HA	1:B:225:ARG:HD2	1.90	0.54
1:D:273:MET:CE	1:D:351:SER:HB2	2.38	0.54
1:E:110:ALA:HB2	1:E:154:ASP:HB2	1.89	0.54
1:E:130:LYS:CD	1:E:130:LYS:NZ	2.66	0.54
1:G:21:ASP:OD2	1:I:275:HIS:CE1	2.61	0.54
1:J:83[B]:HIS:ND1	1:J:169:ASN:HB2	2.23	0.54
1:A:46:VAL:HG23	1:A:76:VAL:HA	1.88	0.54
1:I:114:LEU:HD23	1:I:126:PHE:HE2	1.73	0.53
1:D:358:ALA:HB3	5:D:2715:HOH:O	2.07	0.53
1:D:93:VAL:HG12	5:D:2742:HOH:O	2.08	0.53
1:I:26:HIS:HB2	1:J:266:MET:HG2	1.90	0.53
1:J:51:ASN:HD22	1:J:52:SER:N	2.00	0.53
1:E:83:HIS:HE1	1:E:152:TRP:CG	2.27	0.53
1:E:273:MET:HE3	1:E:351:SER:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:GLU:HB3	1:B:286:VAL:HG22	1.90	0.53
1:J:96:HIS:HD2	5:J:3707:HOH:O	1.91	0.53
1:B:81:GLN:HG3	1:B:114:LEU:HD21	1.91	0.53
1:G:160:LEU:HD23	1:G:165:ILE:HD12	1.91	0.53
1:G:334:ARG:HH21	1:G:368:GLU:CD	2.12	0.53
1:B:273:MET:CE	1:B:351:SER:HB2	2.39	0.52
1:H:257:GLU:HB3	1:H:286:VAL:HG22	1.91	0.52
1:A:346:ALA:HB3	1:A:373:VAL:HB	1.90	0.52
1:I:273:MET:CE	1:I:379:VAL:HB	2.40	0.52
1:J:51:ASN:ND2	1:J:52:SER:H	2.02	0.52
1:E:348:VAL:HG12	1:E:359:THR:HG22	1.91	0.52
1:H:190:ILE:HD11	1:J:189:TYR:OH	2.08	0.52
1:E:83:HIS:CE1	1:E:152:TRP:HB2	2.45	0.52
1:I:322:PRO:HG2	1:J:331:MET:SD	2.50	0.52
1:D:217:VAL:HG13	1:D:222:LEU:HB2	1.91	0.52
1:A:348:VAL:O	1:A:376:GLU:HA	2.10	0.51
1:E:146:GLU:O	1:E:213:LYS:NZ	2.43	0.51
1:G:216:GLU:HA	1:G:219:GLU:OE1	2.10	0.51
1:J:24:ASN:HD21	1:J:27:GLY:N	1.96	0.51
1:I:160:LEU:HD23	1:I:165:ILE:HD12	1.92	0.51
1:D:60:LEU:O	1:D:64:VAL:HG13	2.11	0.51
1:G:21:ASP:OD2	1:I:275:HIS:HE1	1.94	0.51
1:E:147:THR:HG22	1:E:213:LYS:CE	2.40	0.51
1:A:61:MET:HA	1:A:64:VAL:HG22	1.93	0.51
1:B:66:ASP:O	1:B:69:GLN:HB2	2.11	0.51
1:I:149:LEU:O	1:I:206:LEU:HD22	2.11	0.51
1:I:24:ASN:C	1:I:24:ASN:HD22	2.14	0.51
1:G:119:PRO:O	1:G:122:ARG:HG3	2.11	0.51
1:J:224:GLU:HG2	1:J:225:ARG:HG3	1.93	0.51
1:B:241:MET:O	1:B:245:GLU:HG3	2.11	0.50
1:H:348:VAL:O	1:H:376:GLU:HA	2.11	0.50
1:E:169:ASN:HD22	1:E:170:ASP:H	1.59	0.50
1:D:142:LEU:HD23	1:D:158:THR:HG21	1.93	0.50
1:A:229:ILE:HD11	1:A:244:ILE:HD11	1.94	0.50
1:B:81:GLN:HE21	1:B:92:LEU:HD13	1.77	0.50
1:B:21:ASP:OD2	1:E:275:HIS:CE1	2.64	0.50
1:A:147:THR:HG22	1:A:213:LYS:HE2	1.94	0.50
1:B:319:TYR:O	1:B:320:ASP:HB2	2.12	0.50
1:D:13:TYR:HE1	1:D:70:GLN:NE2	2.09	0.50
1:E:315:ALA:HB2	1:E:326:VAL:HG21	1.94	0.50
1:B:266:MET:SD	1:B:318:ILE:CD1	2.87	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:MET:HG2	1:B:26:HIS:HB2	1.93	0.50
1:G:363:LYS:HE3	1:G:373:VAL:HG22	1.93	0.50
1:J:150:LEU:HG	1:J:150:LEU:O	2.12	0.50
1:H:317:THR:HG22	5:H:1713:HOH:O	2.11	0.50
1:E:24:ASN:ND2	1:E:27:GLY:H	2.10	0.49
1:G:151:HIS:HD2	5:G:709:HOH:O	1.95	0.49
1:G:61:MET:HA	1:G:61:MET:CE	2.42	0.49
1:J:88:HIS:CE1	1:J:232[B]:SER:HB3	2.46	0.49
1:A:83:HIS:HE1	1:A:152:TRP:CD2	2.30	0.49
1:G:330:LEU:HD13	1:G:365:LEU:HB2	1.95	0.49
1:D:273:MET:HE1	1:D:351:SER:HB2	1.93	0.49
1:A:202:LEU:O	1:B:319:TYR:OH	2.20	0.49
1:I:152:TRP:HB3	1:I:153:PRO:HD2	1.95	0.49
1:A:17:VAL:HG11	1:A:52:SER:HB2	1.94	0.49
1:E:273:MET:O	1:E:277:ILE:HG13	2.12	0.49
1:A:196:ARG:HD3	1:A:307:GLU:HG3	1.95	0.49
1:A:46:VAL:HG21	1:A:75:ARG:O	2.13	0.49
1:E:83:HIS:CE1	1:E:151[A]:HIS:HD2	2.31	0.49
1:B:84:VAL:HG13	1:B:154:ASP:OD2	2.13	0.49
1:B:314:GLY:HA2	1:B:349:PHE:O	2.13	0.49
1:E:38:TYR:CZ	1:E:230:ALA:HB1	2.48	0.49
1:H:84:VAL:HG12	1:H:114:LEU:HD22	1.95	0.48
1:I:273:MET:HE1	1:I:379:VAL:HB	1.94	0.48
1:J:266:MET:SD	1:J:318:ILE:HD11	2.52	0.48
1:A:169[A]:ASN:HD22	1:A:170:ASP:N	2.10	0.48
1:H:374:ALA:O	1:H:375:CYS:HB2	2.14	0.48
1:E:160:LEU:HD23	1:E:165:ILE:HD12	1.96	0.48
1:D:58:ASP:HB2	5:D:2705:HOH:O	2.13	0.48
1:E:61:MET:O	1:E:65:GLU:HG3	2.14	0.48
1:H:200:ALA:HB1	1:H:302:VAL:HG12	1.96	0.48
1:E:8:ILE:HG21	1:E:236:ILE:HD13	1.95	0.48
1:J:348:VAL:O	1:J:376:GLU:HA	2.12	0.48
1:B:152:TRP:HB3	1:B:154:ASP:OD1	2.14	0.47
1:E:200:ALA:HB2	1:E:306:LEU:HD22	1.95	0.47
1:A:326:VAL:HG12	1:A:330:LEU:HD12	1.96	0.47
1:A:273:MET:HE3	1:A:351:SER:HB2	1.95	0.47
1:H:83:HIS:CD2	1:H:169:ASN:HD21	2.32	0.47
1:G:6:LYS:HE3	1:G:181:ARG:HB2	1.96	0.47
1:E:334:ARG:O	1:E:337:LYS:NZ	2.47	0.47
1:J:53:TYR:CG	1:J:54:PRO:HD2	2.49	0.47
1:H:28:TYR:CE2	1:H:197:LYS:HE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:ALA:O	1:H:71:VAL:HG23	2.15	0.47
1:I:266:MET:SD	1:I:318:ILE:CD1	2.92	0.47
1:D:259:VAL:HG22	1:D:310:ALA:HB3	1.96	0.47
1:D:294:HIS:ND1	1:D:294:HIS:O	2.45	0.47
1:E:53:TYR:CG	1:E:54:PRO:HD2	2.50	0.47
1:J:345:LYS:HD2	1:J:401:GLU:OE2	2.15	0.47
1:B:181:ARG:NH2	5:B:1742:HOH:O	2.42	0.46
1:B:273:MET:HE3	1:B:351:SER:HB2	1.96	0.46
1:A:282:MET:HG2	1:D:179:PRO:HB3	1.96	0.46
1:A:83:HIS:CE1	1:A:152:TRP:HB2	2.50	0.46
1:H:363:LYS:O	1:H:373:VAL:HG11	2.15	0.46
1:J:301:ILE:O	1:J:305:ILE:HG13	2.15	0.46
1:I:38:TYR:CZ	1:I:230:ALA:HB1	2.50	0.46
1:H:88:HIS:CE1	1:H:232:SER:HB2	2.50	0.46
1:I:169:ASN:ND2	1:I:170:ASP:H	2.12	0.46
1:J:88:HIS:CE1	1:J:232[A]:SER:HB2	2.49	0.46
1:A:46:VAL:CG2	1:A:75:ARG:O	2.64	0.46
1:G:223:LEU:HA	1:G:226:ILE:HD12	1.97	0.46
1:J:34:THR:HG23	1:J:176:LEU:O	2.16	0.46
1:G:199:TYR:HA	1:G:203:ILE:HG12	1.96	0.46
1:B:363:LYS:HG2	1:B:373:VAL:HG21	1.98	0.46
1:G:71:VAL:CG1	1:G:73:MET:CG	2.93	0.46
1:G:179:PRO:HB3	1:I:282:MET:HG2	1.98	0.46
1:I:51:ASN:HD22	1:I:91:VAL:HG22	1.81	0.46
1:J:184:ARG:NH1	5:J:3722:HOH:O	2.30	0.46
1:D:317:THR:HG22	1:D:352:MET:CB	2.42	0.46
1:I:310:ALA:HB1	1:I:398:LEU:HD22	1.98	0.46
1:A:271:ARG:NH1	5:A:741:HOH:O	2.48	0.46
1:E:257:GLU:C	1:E:286:VAL:HG13	2.36	0.46
1:G:8:ILE:HG21	1:G:236:ILE:HD13	1.98	0.45
1:H:295:GLU:HB3	1:J:23:ARG:HG3	1.98	0.45
1:E:374:ALA:O	1:E:375:CYS:HB2	2.17	0.45
1:G:380:TYR:CD1	1:H:116:LYS:HG2	2.51	0.45
1:I:348:VAL:HG12	1:I:359:THR:HG22	1.99	0.45
1:D:310:ALA:HB1	1:D:398:LEU:HD22	1.98	0.45
1:D:61:MET:CE	1:D:61:MET:HA	2.46	0.45
1:I:36:ASN:HB2	1:I:232:SER:HA	1.99	0.45
1:I:60:LEU:O	1:I:64:VAL:HG13	2.17	0.45
1:H:105:TYR:CE1	1:H:127:MET:HG2	2.52	0.45
1:I:33:THR:OG1	1:I:34:THR:N	2.50	0.45
1:D:84:VAL:HG12	1:D:114:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:VAL:HG22	1:E:35:TYR:HD2	1.82	0.45
1:B:150:LEU:HA	1:B:151:HIS:HA	1.75	0.45
1:A:21:ASP:OD1	1:D:263:TYR:OH	2.29	0.44
1:H:317:THR:HG21	1:H:356:GLY:HA2	1.99	0.44
1:I:29:THR:O	1:I:197:LYS:NZ	2.49	0.44
1:J:169:ASN:HA	1:J:232[B]:SER:OG	2.17	0.44
1:J:273:MET:HE1	1:J:351:SER:HB2	1.99	0.44
1:B:184:ARG:NH1	5:B:1706:HOH:O	2.50	0.44
1:A:8:ILE:HG21	1:A:236:ILE:HD13	2.00	0.44
1:G:82:ASN:HD22	1:G:156:MET:HG3	1.81	0.44
1:E:348:VAL:O	1:E:376:GLU:HA	2.18	0.44
1:J:363:LYS:HG3	1:J:373:VAL:HG11	2.00	0.44
1:A:273:MET:HG2	1:A:391:CYS:SG	2.58	0.44
1:D:397:LYS:C	1:D:397:LYS:HD3	2.38	0.44
1:G:258:ARG:HB2	1:G:258:ARG:NH1	2.32	0.44
1:H:229:ILE:HD11	1:H:244:ILE:HD11	2.00	0.44
1:I:199:TYR:C	1:I:199:TYR:CD2	2.91	0.44
1:J:61:MET:HE3	1:J:95:LEU:HD23	1.98	0.44
1:B:83:HIS:HE1	1:B:152:TRP:CE3	2.35	0.44
1:H:81:GLN:HE21	1:H:92:LEU:HD13	1.83	0.44
1:A:150:LEU:HA	1:A:206:LEU:HD13	2.00	0.43
1:A:317:THR:HB	1:A:358:ALA:HB2	2.00	0.43
1:D:142:LEU:N	1:D:142:LEU:HD12	2.32	0.43
1:E:53:TYR:CD1	1:E:54:PRO:HD2	2.53	0.43
1:G:83:HIS:HE1	1:G:152:TRP:CD2	2.35	0.43
1:G:262:ILE:O	1:G:313:LEU:HA	2.18	0.43
1:H:83:HIS:HD2	1:H:169:ASN:HD21	1.66	0.43
1:I:34:THR:O	1:I:233:HIS:ND1	2.50	0.43
1:J:61:MET:CE	1:J:61:MET:HA	2.48	0.43
1:H:384:THR:HG23	1:H:387:GLU:OE1	2.18	0.43
1:B:140:LYS:HG2	1:B:160:LEU:HD11	2.00	0.43
1:G:54:PRO:HD3	1:G:90:GLY:HA3	2.00	0.43
1:G:51:ASN:ND2	1:G:91:VAL:H	2.16	0.43
1:H:51:ASN:HD22	1:H:52:SER:H	1.65	0.43
1:A:291:TYR:OH	1:A:304:ASP:OD1	2.23	0.43
1:D:38:TYR:CZ	1:D:230:ALA:HB1	2.54	0.43
1:I:85:GLU:OE2	1:J:267:HIS:NE2	2.51	0.43
1:A:267:HIS:HB3	1:B:86:LYS:HD2	2.01	0.43
1:D:348:VAL:O	1:D:376:GLU:HA	2.18	0.43
1:E:102:ALA:HA	1:E:103:PRO:HD2	1.94	0.43
1:E:83:HIS:HD1	1:E:155:SER:HG	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:ASN:HB2	1:G:232:SER:HA	1.99	0.43
1:A:314:GLY:HA2	1:A:349:PHE:O	2.18	0.43
1:B:254:MET:HA	1:B:254:MET:CE	2.48	0.43
1:D:226:ILE:HG23	1:D:226:ILE:O	2.18	0.43
1:H:298:ARG:NH1	1:H:328:ASP:OD1	2.51	0.43
1:H:83:HIS:HE1	1:H:152:TRP:CG	2.36	0.43
1:I:257:GLU:HB3	1:I:286:VAL:HG22	2.01	0.42
1:A:281:ALA:HA	1:A:399:ALA:HB2	2.02	0.42
1:B:213:LYS:O	1:B:217:VAL:HG23	2.19	0.42
1:E:131:THR:H	1:E:146:GLU:HG3	1.84	0.42
1:I:345:LYS:HD2	1:I:401:GLU:HG2	2.01	0.42
1:J:213:LYS:O	1:J:217:VAL:HG23	2.19	0.42
1:I:354:GLY:N	3:I:2702:FMN:O2	2.51	0.42
1:A:131:THR:HG23	1:A:145:LEU:HD12	2.01	0.42
1:G:8:ILE:HG21	1:G:236:ILE:CD1	2.50	0.42
1:H:403:ARG:HD2	5:H:1718:HOH:O	2.18	0.42
1:I:253:GLY:O	1:I:342:LEU:HD12	2.20	0.42
1:J:24:ASN:C	1:J:24:ASN:ND2	2.70	0.42
1:J:71:VAL:O	1:J:71:VAL:HG12	2.18	0.42
1:A:17:VAL:HG13	1:A:35:TYR:HB2	2.01	0.42
1:E:61:MET:HB3	5:E:3705:HOH:O	2.19	0.42
1:E:67:ALA:O	1:E:71:VAL:HG23	2.19	0.42
1:B:277:ILE:HG13	1:B:391:CYS:HB3	2.01	0.42
1:D:24:ASN:C	1:D:24:ASN:HD22	2.23	0.42
1:D:400:ALA:HA	1:D:403:ARG:HG3	2.01	0.42
1:H:363:LYS:HD3	1:H:376:GLU:OE2	2.20	0.42
1:I:47:ALA:HB1	1:I:80:ILE:HD12	2.02	0.42
1:I:83:HIS:HB2	1:I:169:ASN:OD1	2.19	0.42
1:J:270:THR:HA	1:J:273:MET:CE	2.49	0.42
1:E:343:THR:HG22	1:E:372:ASP:HB2	2.01	0.42
1:I:100:PRO:HG2	1:I:101:GLU:OE1	2.20	0.42
1:B:29:THR:O	1:B:197:LYS:NZ	2.51	0.42
1:E:358:ALA:O	1:E:362:MET:HG3	2.20	0.42
1:G:190:ILE:HD11	1:I:189:TYR:CE2	2.54	0.42
1:G:337:LYS:NZ	5:G:751:HOH:O	2.52	0.42
1:H:83:HIS:CD2	1:H:169:ASN:ND2	2.87	0.42
1:H:270:THR:HA	1:H:273:MET:HE3	2.01	0.42
1:I:328:ASP:OD1	1:J:325:SER:HA	2.20	0.42
1:E:61:MET:HA	1:E:64:VAL:HG22	2.01	0.41
1:H:314:GLY:HA2	1:H:349:PHE:O	2.20	0.41
1:A:147:THR:HB	1:A:150:LEU:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:ASN:OD1	1:D:81:GLN:NE2	2.54	0.41
1:G:317:THR:HG22	1:G:358:ALA:HB3	2.02	0.41
1:I:115:LEU:HA	1:I:115:LEU:HD13	1.85	0.41
1:J:29:THR:O	1:J:197:LYS:NZ	2.47	0.41
1:J:363:LYS:HG3	1:J:373:VAL:HG21	2.00	0.41
1:A:201:ASN:OD1	1:A:299:SER:HA	2.20	0.41
1:A:27:GLY:HA3	1:B:323:TYR:OH	2.21	0.41
1:D:115:LEU:HD12	1:D:115:LEU:HA	1.94	0.41
1:J:140:LYS:HG2	1:J:160:LEU:HD11	2.01	0.41
1:B:173:GLY:C	1:B:174:GLN:HG3	2.41	0.41
1:D:147:THR:HB	1:D:150:LEU:HB2	2.02	0.41
1:G:59:GLU:OE1	1:G:63:ARG:NH2	2.49	0.41
1:H:102:ALA:HA	1:H:103:PRO:HD3	1.95	0.41
1:H:258:ARG:HE	1:H:289:ARG:NH1	2.18	0.41
1:I:379:VAL:HG11	1:I:383:PRO:HB3	2.03	0.41
1:J:53:TYR:CD2	1:J:54:PRO:HD2	2.56	0.41
1:D:46:VAL:HG22	1:D:76:VAL:HA	2.01	0.41
1:E:26:HIS:O	1:E:26:HIS:CD2	2.74	0.41
1:H:16:GLY:HA3	1:H:35:TYR:O	2.21	0.41
1:D:197:LYS:NZ	1:D:300:GLU:OE1	2.51	0.41
1:J:25:TYR:O	1:J:28:TYR:HB3	2.21	0.41
1:E:136:ASP:HA	1:E:141:THR:HG22	2.03	0.41
1:E:36:ASN:HB2	1:E:232:SER:HA	2.03	0.41
1:G:317:THR:HG22	1:G:358:ALA:CB	2.51	0.41
1:I:114:LEU:HD12	1:I:114:LEU:HA	1.98	0.41
1:I:83:HIS:CD2	1:I:169:ASN:HD21	2.39	0.41
1:I:190:ILE:HD13	1:I:190:ILE:HA	1.86	0.41
1:A:298:ARG:NH1	1:A:328:ASP:OD1	2.53	0.41
1:B:326:VAL:HG13	1:B:330:LEU:HD12	2.03	0.41
1:E:51:ASN:ND2	1:E:91:VAL:H	2.18	0.41
1:G:69:GLN:HE21	1:G:69:GLN:HB2	1.63	0.41
1:I:152:TRP:HB3	1:I:153:PRO:CD	2.51	0.41
1:A:263:TYR:HA	1:A:314:GLY:O	2.21	0.41
1:A:81:GLN:HE21	1:A:92:LEU:HD13	1.85	0.41
1:B:145:LEU:HD11	1:B:216:GLU:OE2	2.21	0.41
1:B:83:HIS:CD2	1:B:169:ASN:ND2	2.89	0.41
1:D:51:ASN:HD22	1:D:52:SER:H	1.67	0.41
1:I:105:TYR:CE1	1:I:127:MET:HG2	2.56	0.41
1:J:189:TYR:CD2	1:J:189:TYR:C	2.94	0.41
1:J:51:ASN:ND2	1:J:91:VAL:H	2.19	0.41
1:B:83:HIS:HE1	1:B:152:TRP:CD2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:PHE:CD1	1:D:168:SER:HA	2.56	0.41
1:D:315:ALA:HB2	1:D:326:VAL:HG21	2.03	0.41
1:D:33:THR:OG1	1:D:34:THR:N	2.54	0.41
1:E:191:LEU:HD21	1:E:237:TRP:CZ3	2.55	0.41
1:J:148:PRO:O	1:J:149:LEU:C	2.60	0.41
1:A:161:ASP:C	1:A:163:ASP:H	2.23	0.40
1:J:302:VAL:HG13	1:J:338:PHE:HZ	1.86	0.40
1:G:266:MET:SD	1:G:318:ILE:HD11	2.61	0.40
1:G:392:PHE:CD1	1:I:2:LYS:HB3	2.56	0.40
1:H:34:THR:O	1:H:233:HIS:ND1	2.50	0.40
1:I:85:GLU:HG2	1:I:152:TRP:CH2	2.57	0.40
1:A:322:PRO:O	1:A:323:TYR:C	2.60	0.40
1:G:147:THR:HG22	1:G:213:LYS:HD3	2.02	0.40
1:J:314:GLY:HA2	1:J:349:PHE:O	2.22	0.40
1:A:363:LYS:NZ	1:A:373:VAL:O	2.55	0.40
1:D:322:PRO:HG2	1:E:331:MET:SD	2.61	0.40
1:E:399:ALA:O	1:E:402:ILE:HG13	2.21	0.40
1:J:273:MET:CE	1:J:351:SER:HB2	2.50	0.40
1:A:82:ASN:O	1:A:155:SER:HA	2.21	0.40
1:A:169[B]:ASN:OD1	1:A:170:ASP:N	2.55	0.40
1:B:189:TYR:CZ	1:E:190:ILE:HD11	2.57	0.40
1:E:12:VAL:HG21	1:E:165:ILE:CD1	2.52	0.40
1:E:353:GLY:O	1:E:380:TYR:HE2	2.05	0.40
1:G:318:ILE:O	1:G:319:TYR:C	2.59	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	402/404 (100%)	384 (96%)	16 (4%)	2 (0%)	29 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	401/404 (99%)	382 (95%)	16 (4%)	3 (1%)	22	26
1	D	404/404 (100%)	388 (96%)	14 (4%)	2 (0%)	29	35
1	E	402/404 (100%)	377 (94%)	22 (6%)	3 (1%)	22	26
1	G	402/404 (100%)	386 (96%)	14 (4%)	2 (0%)	29	35
1	H	401/404 (99%)	381 (95%)	17 (4%)	3 (1%)	22	26
1	I	401/404 (99%)	374 (93%)	24 (6%)	3 (1%)	22	26
1	J	403/404 (100%)	388 (96%)	13 (3%)	2 (0%)	29	35
All	All	3216/3232 (100%)	3060 (95%)	136 (4%)	20 (1%)	25	31

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	VAL
1	B	375	CYS
1	D	255	VAL
1	J	150	LEU
1	B	255	VAL
1	E	255	VAL
1	G	255	VAL
1	G	375	CYS
1	H	255	VAL
1	I	255	VAL
1	J	255	VAL
1	B	254	MET
1	E	149	LEU
1	H	26	HIS
1	A	375	CYS
1	D	226	ILE
1	H	375	CYS
1	I	86	LYS
1	I	375	CYS
1	E	226	ILE

5.3.2 Protein sidechains ⓘ

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	336/336 (100%)	313 (93%)	23 (7%)	16	21
1	B	335/336 (100%)	306 (91%)	29 (9%)	10	12
1	D	338/336 (101%)	318 (94%)	20 (6%)	19	27
1	E	336/336 (100%)	308 (92%)	28 (8%)	11	14
1	G	336/336 (100%)	310 (92%)	26 (8%)	13	16
1	H	335/336 (100%)	303 (90%)	32 (10%)	8	10
1	I	335/336 (100%)	313 (93%)	22 (7%)	16	22
1	J	337/336 (100%)	316 (94%)	21 (6%)	18	25
All	All	2688/2688 (100%)	2487 (92%)	201 (8%)	13	17

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	ASP
1	A	17	VAL
1	A	30	LEU
1	A	31	GLN
1	A	71	VAL
1	A	83	HIS
1	A	115	LEU
1	A	120	SER
1	A	122	ARG
1	A	128	THR
1	A	150	LEU
1	A	151	HIS
1	A	174	GLN
1	A	188	GLU
1	A	275	HIS
1	A	317	THR
1	A	336	LEU
1	A	337	LYS
1	A	342	LEU
1	A	352	MET
1	A	378	GLU
1	A	398	LEU
1	B	17	VAL
1	B	24	ASN

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Mol	Chain	Res	Type
1	B	60	LEU
1	B	69	GLN
1	B	93	VAL
1	B	94	GLU
1	B	114	LEU
1	B	115	LEU
1	B	122	ARG
1	B	123	GLU
1	B	142	LEU
1	B	151	HIS
1	B	174	GLN
1	B	184	ARG
1	B	188	GLU
1	B	209	LEU
1	B	223	LEU
1	B	225	ARG
1	B	275	HIS
1	B	282	MET
1	B	300	GLU
1	B	317	THR
1	B	336	LEU
1	B	342	LEU
1	B	352	MET
1	B	373	VAL
1	B	375	CYS
1	B	397	LYS
1	B	398	LEU
1	D	17	VAL
1	D	24	ASN
1	D	46	VAL
1	D	64	VAL
1	D	69	GLN
1	D	71	VAL
1	D	114	LEU
1	D	115	LEU
1	D	162	GLU
1	D	174	GLN
1	D	188	GLU
1	D	209	LEU
1	D	216	GLU
1	D	336	LEU
1	D	342	LEU

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Mol	Chain	Res	Type
1	D	352	MET
1	D	355	ASN
1	D	373	VAL
1	D	397	LYS
1	D	398	LEU
1	E	6	LYS
1	E	30	LEU
1	E	31	GLN
1	E	46	VAL
1	E	60	LEU
1	E	101	GLU
1	E	114	LEU
1	E	125	GLU
1	E	128	THR
1	E	142	LEU
1	E	151[A]	HIS
1	E	151[B]	HIS
1	E	159	LEU
1	E	174	GLN
1	E	181	ARG
1	E	184	ARG
1	E	188	GLU
1	E	218	LYS
1	E	220	LEU
1	E	275	HIS
1	E	302	VAL
1	E	317	THR
1	E	336	LEU
1	E	337	LYS
1	E	342	LEU
1	E	352	MET
1	E	398	LEU
1	E	401	GLU
1	G	7	ARG
1	G	9	SER
1	G	17	VAL
1	G	30	LEU
1	G	31	GLN
1	G	71	VAL
1	G	83	HIS
1	G	97	ARG
1	G	101	GLU

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Mol	Chain	Res	Type
1	G	112	LYS
1	G	114	LEU
1	G	122	ARG
1	G	141	THR
1	G	142	LEU
1	G	150	LEU
1	G	174	GLN
1	G	188	GLU
1	G	213	LYS
1	G	225	ARG
1	G	275	HIS
1	G	317	THR
1	G	336	LEU
1	G	342	LEU
1	G	352	MET
1	G	373	VAL
1	G	398	LEU
1	H	1	MET
1	H	17	VAL
1	H	28	TYR
1	H	46	VAL
1	H	51	ASN
1	H	52	SER
1	H	58	ASP
1	H	61	MET
1	H	95	LEU
1	H	101	GLU
1	H	114	LEU
1	H	115	LEU
1	H	130	LYS
1	H	142	LEU
1	H	149	LEU
1	H	154	ASP
1	H	162	GLU
1	H	163	ASP
1	H	174	GLN
1	H	184	ARG
1	H	188	GLU
1	H	209	LEU
1	H	218	LYS
1	H	225	ARG
1	H	275	HIS

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Mol	Chain	Res	Type
1	H	317	THR
1	H	336	LEU
1	H	342	LEU
1	H	352	MET
1	H	397	LYS
1	H	398	LEU
1	H	401	GLU
1	I	7	ARG
1	I	17	VAL
1	I	24	ASN
1	I	28	TYR
1	I	30	LEU
1	I	44	GLU
1	I	60	LEU
1	I	98	ARG
1	I	115	LEU
1	I	128	THR
1	I	141	THR
1	I	150	LEU
1	I	188	GLU
1	I	209	LEU
1	I	220	LEU
1	I	275	HIS
1	I	302	VAL
1	I	317	THR
1	I	318	ILE
1	I	336	LEU
1	I	352	MET
1	I	398	LEU
1	J	6	LYS
1	J	17	VAL
1	J	24	ASN
1	J	43	ASP
1	J	44	GLU
1	J	64	VAL
1	J	93	VAL
1	J	115	LEU
1	J	122	ARG
1	J	140	LYS
1	J	174	GLN
1	J	188	GLU
1	J	209	LEU

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Mol	Chain	Res	Type
1	J	213	LYS
1	J	223	LEU
1	J	225	ARG
1	J	336	LEU
1	J	342	LEU
1	J	352	MET
1	J	398	LEU
1	J	401	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	31	GLN
1	A	51	ASN
1	A	81	GLN
1	A	82	ASN
1	A	83	HIS
1	A	355	ASN
1	B	26	HIS
1	B	31	GLN
1	B	51	ASN
1	B	70	GLN
1	B	81	GLN
1	B	82	ASN
1	B	83	HIS
1	B	275	HIS
1	B	355	ASN
1	D	24	ASN
1	D	26	HIS
1	D	51	ASN
1	D	69	GLN
1	D	70	GLN
1	D	81	GLN
1	D	82	ASN
1	D	96	HIS
1	D	275	HIS
1	E	24	ASN
1	E	26	HIS
1	E	31	GLN
1	E	51	ASN
1	E	81	GLN

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Mol	Chain	Res	Type
1	E	82	ASN
1	E	169	ASN
1	E	275	HIS
1	G	26	HIS
1	G	51	ASN
1	G	69	GLN
1	G	81	GLN
1	G	82	ASN
1	G	83	HIS
1	G	151	HIS
1	G	267	HIS
1	G	275	HIS
1	G	355	ASN
1	H	26	HIS
1	H	51	ASN
1	H	70	GLN
1	H	81	GLN
1	H	82	ASN
1	H	83	HIS
1	H	275	HIS
1	I	24	ASN
1	I	26	HIS
1	I	31	GLN
1	I	51	ASN
1	I	81	GLN
1	I	82	ASN
1	I	83	HIS
1	I	169	ASN
1	I	275	HIS
1	J	24	ASN
1	J	31	GLN
1	J	51	ASN
1	J	81	GLN
1	J	275	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 20 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FMN	G	702	-	31,33,33	1.47	4 (12%)	40,50,50	1.76	7 (17%)
3	FMN	B	1701	-	31,33,33	1.52	5 (16%)	40,50,50	1.74	7 (17%)
3	FMN	J	3702	-	31,33,33	1.75	5 (16%)	40,50,50	1.68	6 (15%)
3	FMN	I	2702	-	31,33,33	1.56	4 (12%)	40,50,50	1.56	5 (12%)
3	FMN	D	2701	-	31,33,33	1.58	5 (16%)	40,50,50	1.64	7 (17%)
3	FMN	H	1702	-	31,33,33	1.57	6 (19%)	40,50,50	1.89	7 (17%)
3	FMN	A	701	-	31,33,33	1.53	5 (16%)	40,50,50	2.15	9 (22%)
3	FMN	E	3701	-	31,33,33	1.55	5 (16%)	40,50,50	2.02	8 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	G	702	-	-	0/18/18/18	0/3/3/3
3	FMN	B	1701	-	-	3/18/18/18	0/3/3/3
3	FMN	J	3702	-	-	3/18/18/18	0/3/3/3
3	FMN	I	2702	-	-	0/18/18/18	0/3/3/3
3	FMN	D	2701	-	-	3/18/18/18	0/3/3/3
3	FMN	H	1702	-	-	7/18/18/18	0/3/3/3
3	FMN	A	701	-	-	2/18/18/18	0/3/3/3
3	FMN	E	3701	-	-	5/18/18/18	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	3702	FMN	C10-N1	4.87	1.39	1.33
3	J	3702	FMN	C1'-N10	4.81	1.53	1.48
3	I	2702	FMN	C10-N1	4.74	1.39	1.33
3	D	2701	FMN	C4A-N5	4.71	1.40	1.33
3	A	701	FMN	C4A-N5	4.64	1.40	1.33
3	G	702	FMN	C4A-N5	4.53	1.39	1.33
3	E	3701	FMN	C4A-N5	4.46	1.39	1.33
3	D	2701	FMN	C10-N1	4.46	1.39	1.33
3	E	3701	FMN	C10-N1	4.45	1.39	1.33
3	H	1702	FMN	C4A-N5	4.38	1.39	1.33
3	B	1701	FMN	C4A-N5	4.34	1.39	1.33
3	H	1702	FMN	C10-N1	4.25	1.38	1.33
3	B	1701	FMN	C4-N3	4.07	1.40	1.33
3	J	3702	FMN	C4A-N5	3.85	1.38	1.33
3	G	702	FMN	C10-N1	3.73	1.38	1.33
3	A	701	FMN	C10-N1	3.73	1.38	1.33
3	B	1701	FMN	C10-N1	3.62	1.37	1.33
3	I	2702	FMN	C4A-N5	3.47	1.38	1.33
3	I	2702	FMN	C4-N3	3.37	1.38	1.33
3	G	702	FMN	C4-N3	3.14	1.38	1.33
3	E	3701	FMN	C4-N3	3.08	1.38	1.33
3	H	1702	FMN	C4-N3	3.06	1.38	1.33
3	J	3702	FMN	C4-N3	3.04	1.38	1.33
3	H	1702	FMN	C1'-N10	2.99	1.51	1.48
3	D	2701	FMN	C1'-N10	2.95	1.51	1.48
3	A	701	FMN	C5A-N5	2.76	1.39	1.35
3	D	2701	FMN	C4-N3	2.70	1.37	1.33
3	I	2702	FMN	C1'-N10	2.55	1.50	1.48
3	G	702	FMN	C1'-N10	2.53	1.50	1.48
3	D	2701	FMN	C5A-N5	2.52	1.39	1.35
3	A	701	FMN	C1'-N10	2.50	1.50	1.48
3	A	701	FMN	C4-N3	2.46	1.37	1.33
3	E	3701	FMN	C5A-N5	2.43	1.39	1.35
3	H	1702	FMN	C5A-N5	2.33	1.39	1.35
3	B	1701	FMN	C5A-N5	2.23	1.39	1.35
3	J	3702	FMN	C5A-N5	2.05	1.38	1.35
3	E	3701	FMN	C1'-N10	2.04	1.50	1.48
3	B	1701	FMN	C1'-N10	2.03	1.50	1.48
3	H	1702	FMN	C4A-C10	2.01	1.40	1.38

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	FMN	C4-N3-C2	8.89	122.64	115.14
3	E	3701	FMN	C4-N3-C2	7.40	121.39	115.14
3	H	1702	FMN	C4-N3-C2	7.13	121.16	115.14
3	J	3702	FMN	C4-N3-C2	5.87	120.10	115.14
3	I	2702	FMN	C4-N3-C2	5.85	120.08	115.14
3	G	702	FMN	C4-N3-C2	5.53	119.81	115.14
3	D	2701	FMN	C4-N3-C2	5.26	119.59	115.14
3	B	1701	FMN	C4-N3-C2	5.15	119.49	115.14
3	E	3701	FMN	C1'-N10-C9A	5.14	122.34	118.29
3	G	702	FMN	C5A-C9A-N10	4.51	120.98	117.72
3	H	1702	FMN	C5A-C9A-N10	4.35	120.87	117.72
3	B	1701	FMN	C4A-N5-C5A	4.18	120.95	116.77
3	G	702	FMN	C4A-N5-C5A	4.10	120.87	116.77
3	J	3702	FMN	C5A-C9A-N10	4.06	120.66	117.72
3	A	701	FMN	C10-C4A-N5	-4.00	118.49	121.26
3	A	701	FMN	C4-C4A-N5	3.95	123.12	118.60
3	J	3702	FMN	C1'-N10-C9A	3.87	121.34	118.29
3	B	1701	FMN	C10-C4A-N5	-3.87	118.58	121.26
3	B	1701	FMN	C5A-C9A-N10	3.79	120.46	117.72
3	I	2702	FMN	C4A-N5-C5A	3.73	120.50	116.77
3	E	3701	FMN	C4A-N5-C5A	3.68	120.45	116.77
3	I	2702	FMN	C1'-N10-C9A	3.55	121.09	118.29
3	D	2701	FMN	C5A-C9A-N10	3.52	120.27	117.72
3	A	701	FMN	C1'-N10-C9A	3.46	121.02	118.29
3	A	701	FMN	C4A-C4-N3	-3.46	118.70	123.43
3	H	1702	FMN	C4A-N5-C5A	3.38	120.15	116.77
3	J	3702	FMN	C4A-N5-C5A	3.35	120.12	116.77
3	E	3701	FMN	C4-C4A-N5	3.27	122.33	118.60
3	A	701	FMN	C4A-N5-C5A	3.25	120.02	116.77
3	D	2701	FMN	C1'-N10-C9A	3.16	120.78	118.29
3	G	702	FMN	C4A-C4-N3	-3.15	119.12	123.43
3	D	2701	FMN	C4A-N5-C5A	3.02	119.79	116.77
3	E	3701	FMN	C5A-C9A-N10	2.91	119.82	117.72
3	G	702	FMN	C10-C4A-N5	-2.88	119.26	121.26
3	H	1702	FMN	C1'-N10-C9A	2.88	120.56	118.29
3	E	3701	FMN	C4A-C4-N3	-2.87	119.51	123.43
3	E	3701	FMN	C10-C4A-N5	-2.73	119.37	121.26
3	H	1702	FMN	C4A-C4-N3	-2.69	119.75	123.43
3	D	2701	FMN	O5'-P-O1P	2.65	113.91	106.47
3	B	1701	FMN	C4-C4A-N5	2.64	121.62	118.60
3	B	1701	FMN	C4A-C4-N3	-2.63	119.83	123.43
3	D	2701	FMN	C4-C4A-N5	2.52	121.48	118.60
3	H	1702	FMN	C4-C4A-N5	2.51	121.46	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3701	FMN	C4-C4A-C10	-2.49	118.30	119.95
3	A	701	FMN	C5A-C9A-N10	2.39	119.45	117.72
3	G	702	FMN	O2P-P-O5'	2.39	113.09	106.73
3	A	701	FMN	C4-C4A-C10	-2.36	118.39	119.95
3	I	2702	FMN	C4A-C4-N3	-2.33	120.24	123.43
3	J	3702	FMN	C9A-N10-C10	-2.30	118.89	121.91
3	H	1702	FMN	C9A-N10-C10	-2.19	119.04	121.91
3	G	702	FMN	C9A-C5A-N5	-2.19	118.94	122.36
3	D	2701	FMN	C10-C4A-N5	-2.18	119.75	121.26
3	I	2702	FMN	C5A-C9A-N10	2.18	119.29	117.72
3	J	3702	FMN	C4A-C4-N3	-2.16	120.48	123.43
3	B	1701	FMN	C9A-N10-C10	-2.08	119.19	121.91
3	A	701	FMN	C5'-C4'-C3'	2.05	116.17	112.20

There are no chirality outliers.

All (23) torsion outliers are listed below:

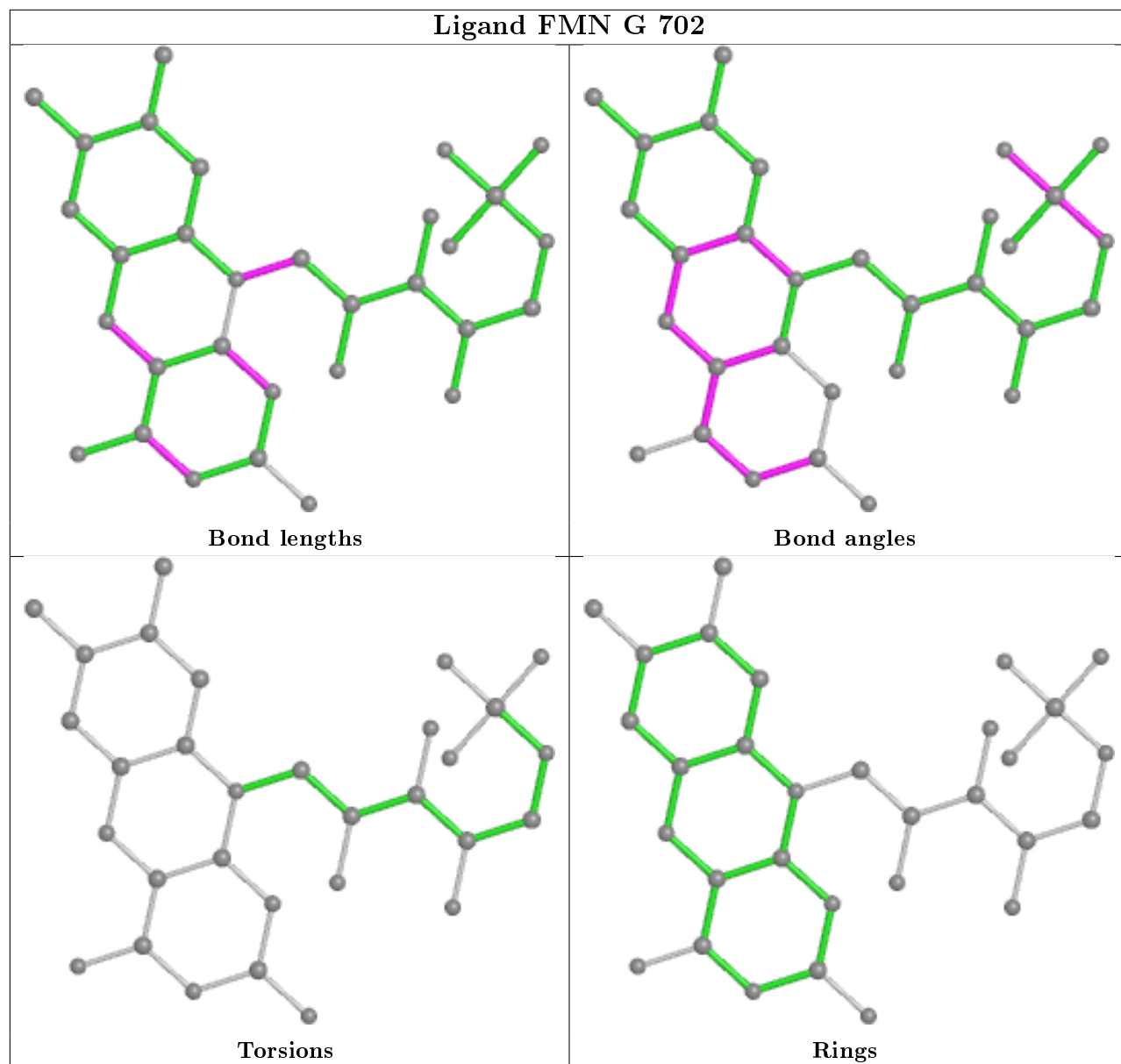
Mol	Chain	Res	Type	Atoms
3	J	3702	FMN	C5'-O5'-P-O1P
3	J	3702	FMN	C5'-O5'-P-O2P
3	A	701	FMN	C5'-O5'-P-O1P
3	B	1701	FMN	C5'-O5'-P-O1P
3	B	1701	FMN	C5'-O5'-P-O2P
3	H	1702	FMN	C5'-O5'-P-O2P
3	E	3701	FMN	C2'-C3'-C4'-O4'
3	E	3701	FMN	O3'-C3'-C4'-O4'
3	E	3701	FMN	C2'-C3'-C4'-C5'
3	H	1702	FMN	O2'-C2'-C3'-C4'
3	D	2701	FMN	C5'-O5'-P-O1P
3	H	1702	FMN	C5'-O5'-P-O1P
3	E	3701	FMN	O3'-C3'-C4'-C5'
3	H	1702	FMN	O2'-C2'-C3'-O3'
3	H	1702	FMN	C1'-C2'-C3'-O3'
3	E	3701	FMN	C5'-O5'-P-O1P
3	H	1702	FMN	C2'-C3'-C4'-O4'
3	J	3702	FMN	C5'-O5'-P-O3P
3	A	701	FMN	C5'-O5'-P-O2P
3	B	1701	FMN	C5'-O5'-P-O3P
3	D	2701	FMN	C5'-O5'-P-O2P
3	H	1702	FMN	C5'-O5'-P-O3P
3	D	2701	FMN	C2'-C3'-C4'-C5'

There are no ring outliers.

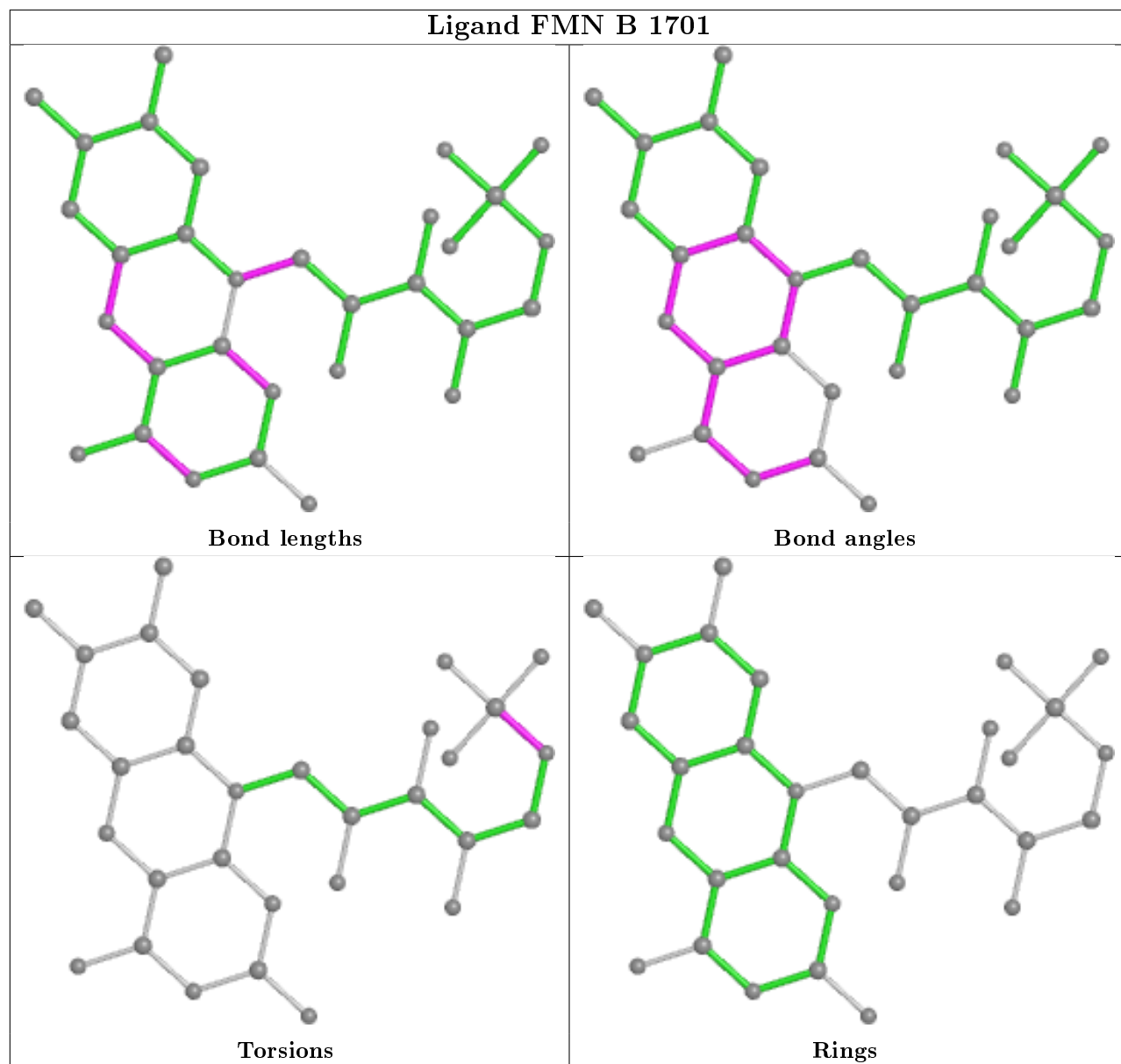
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	2702	FMN	1	0

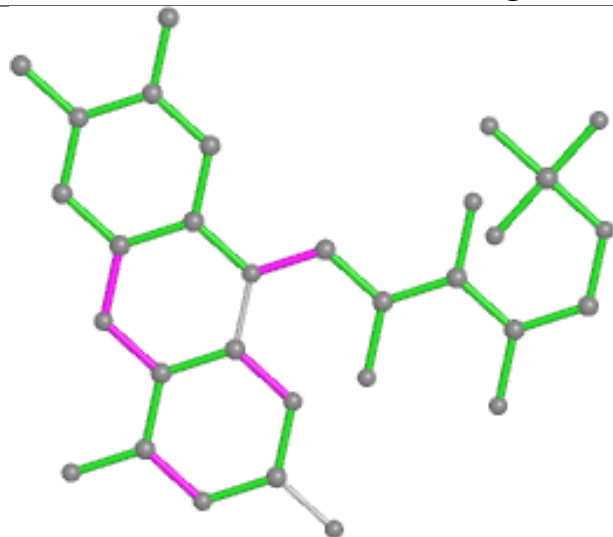
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



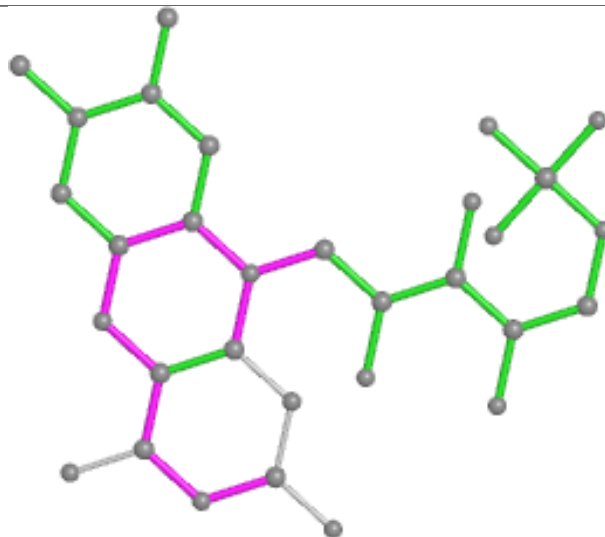
Ligand FMN B 1701



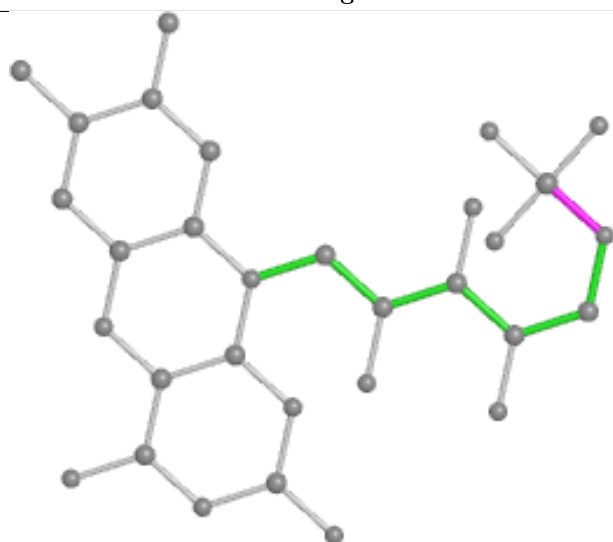
Ligand FMN J 3702



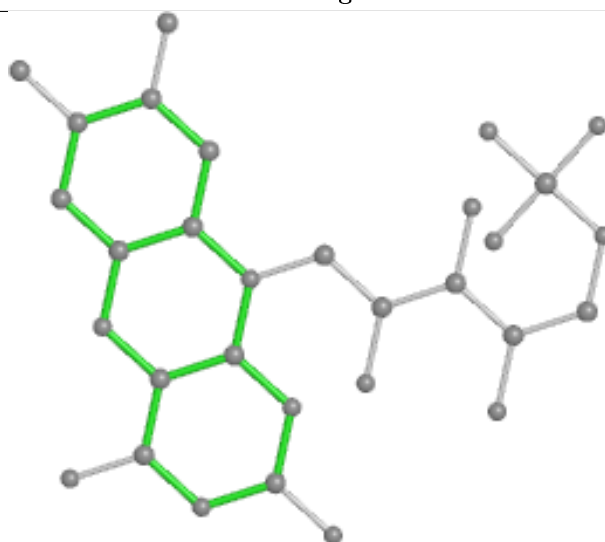
Bond lengths



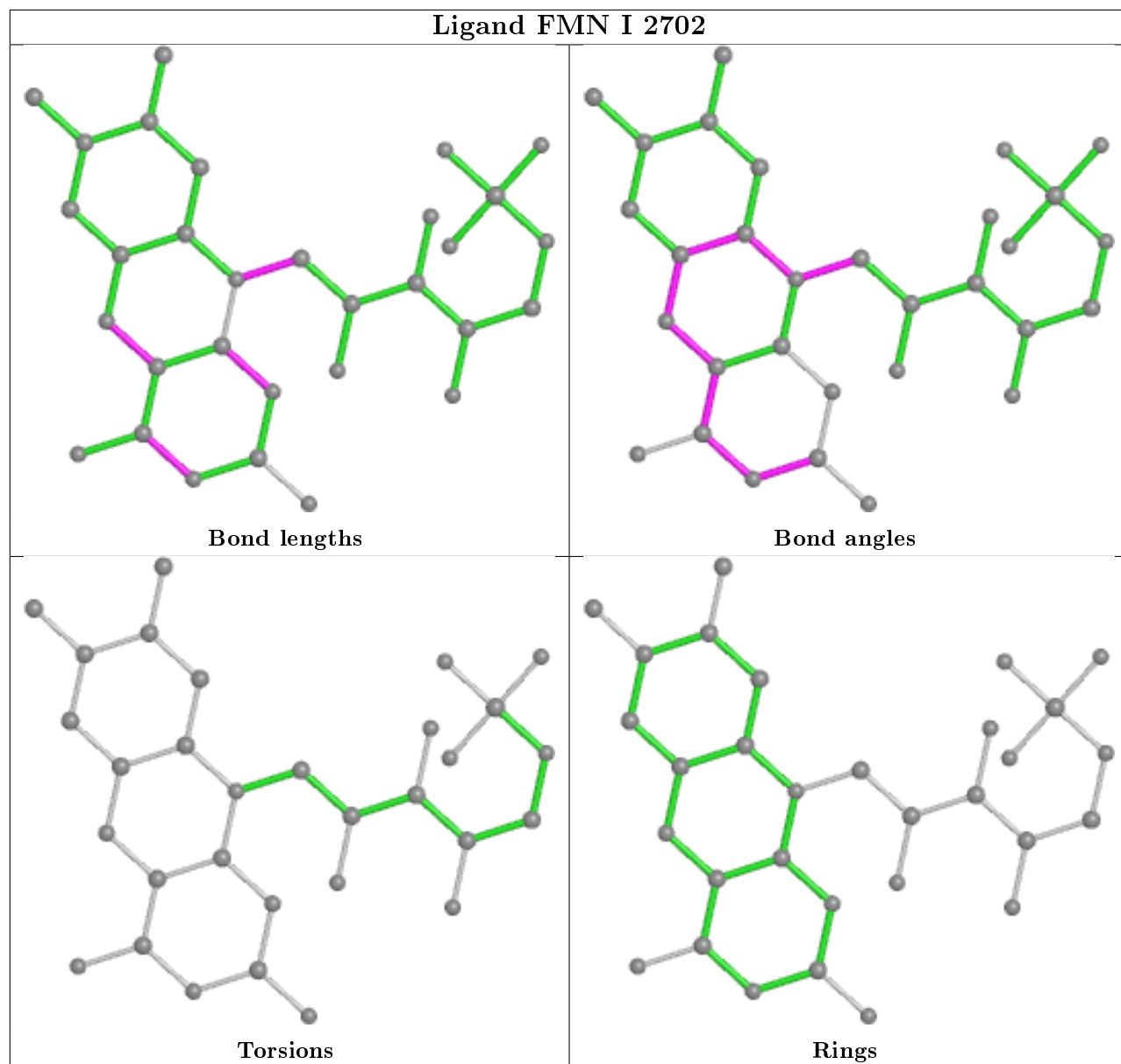
Bond angles



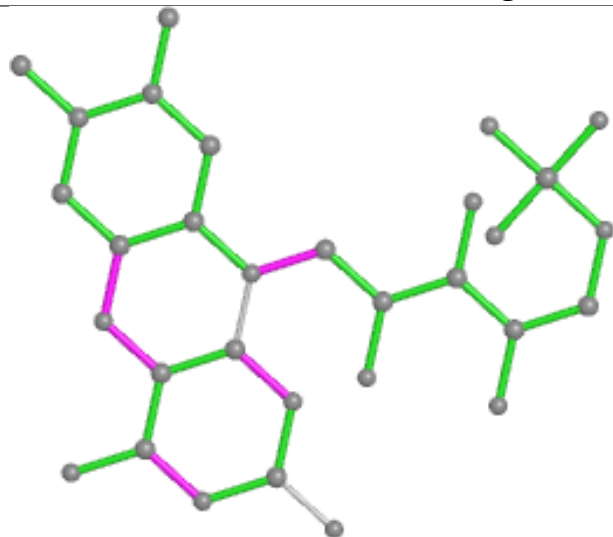
Torsions



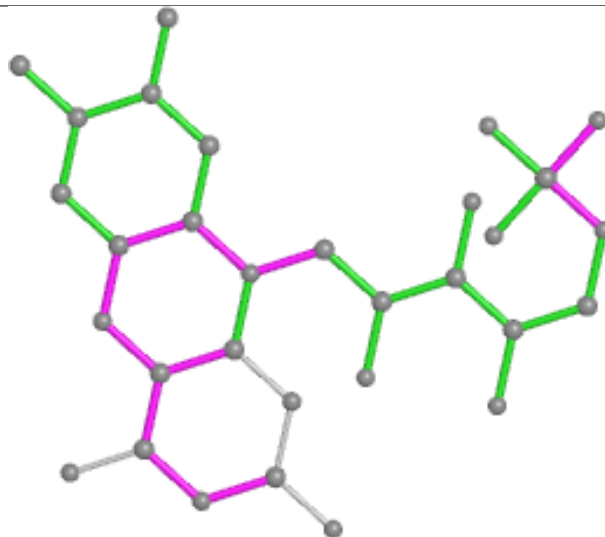
Rings



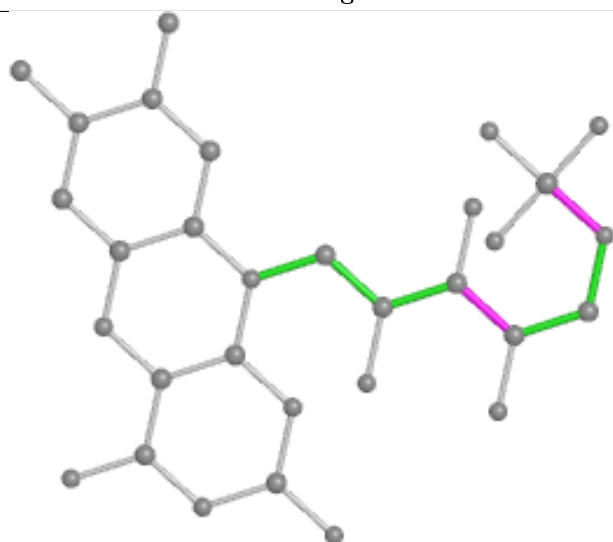
Ligand FMN D 2701



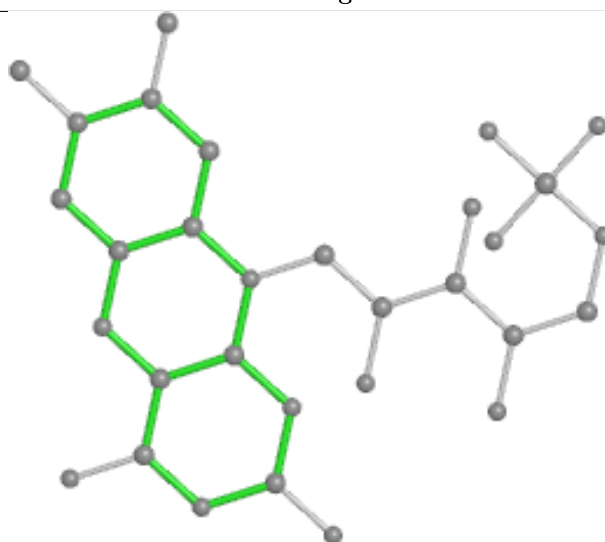
Bond lengths



Bond angles

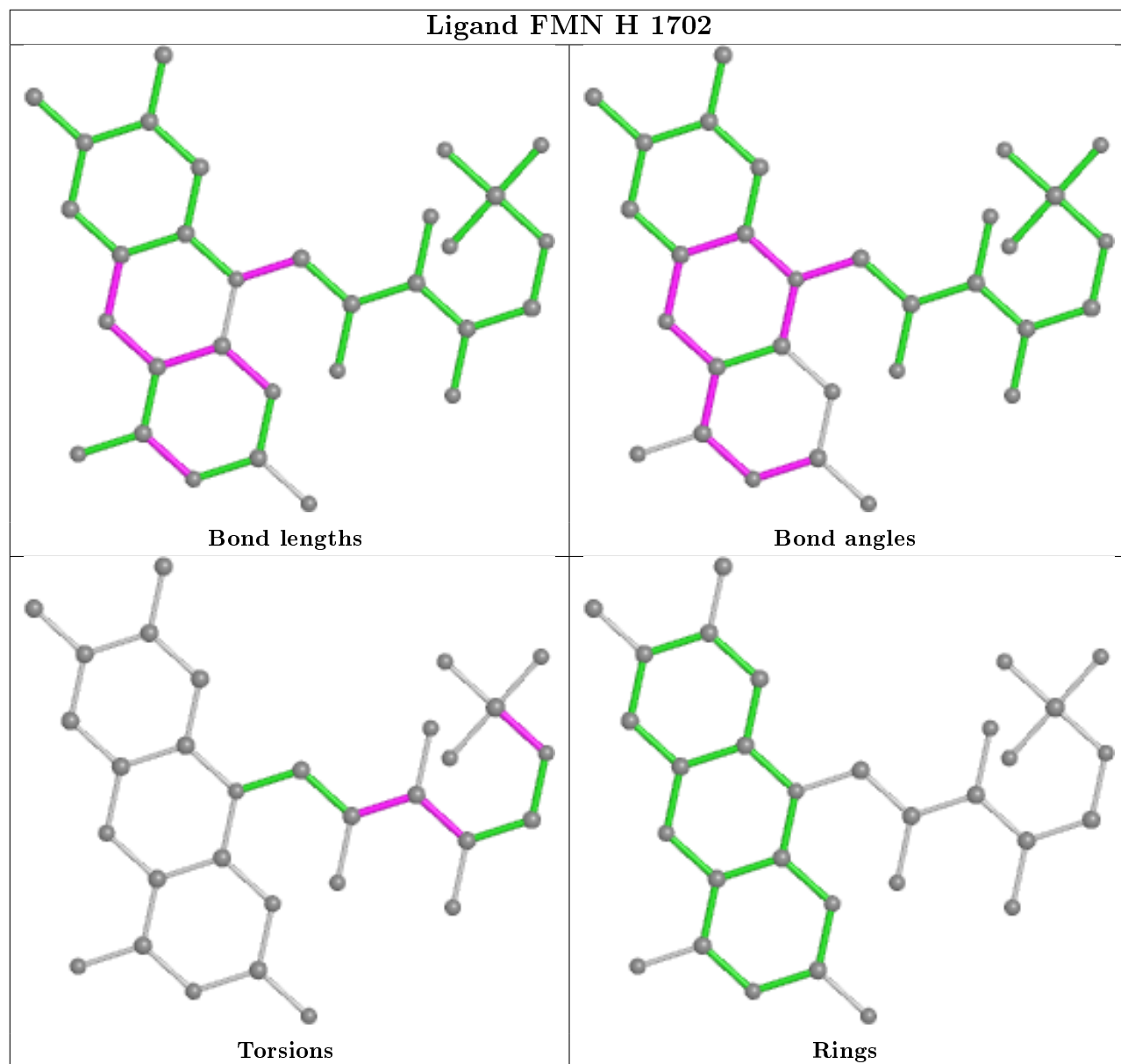


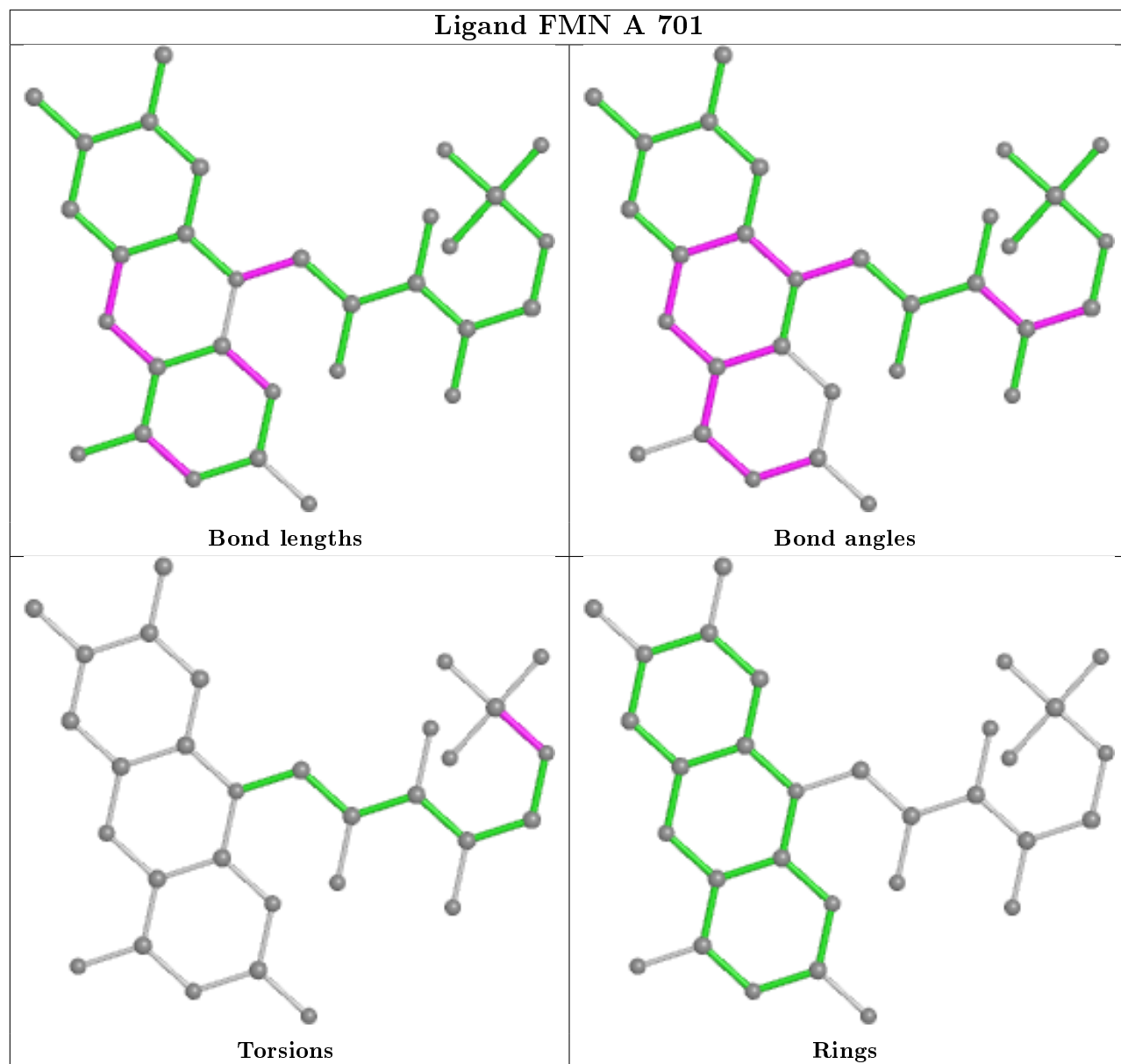
Torsions

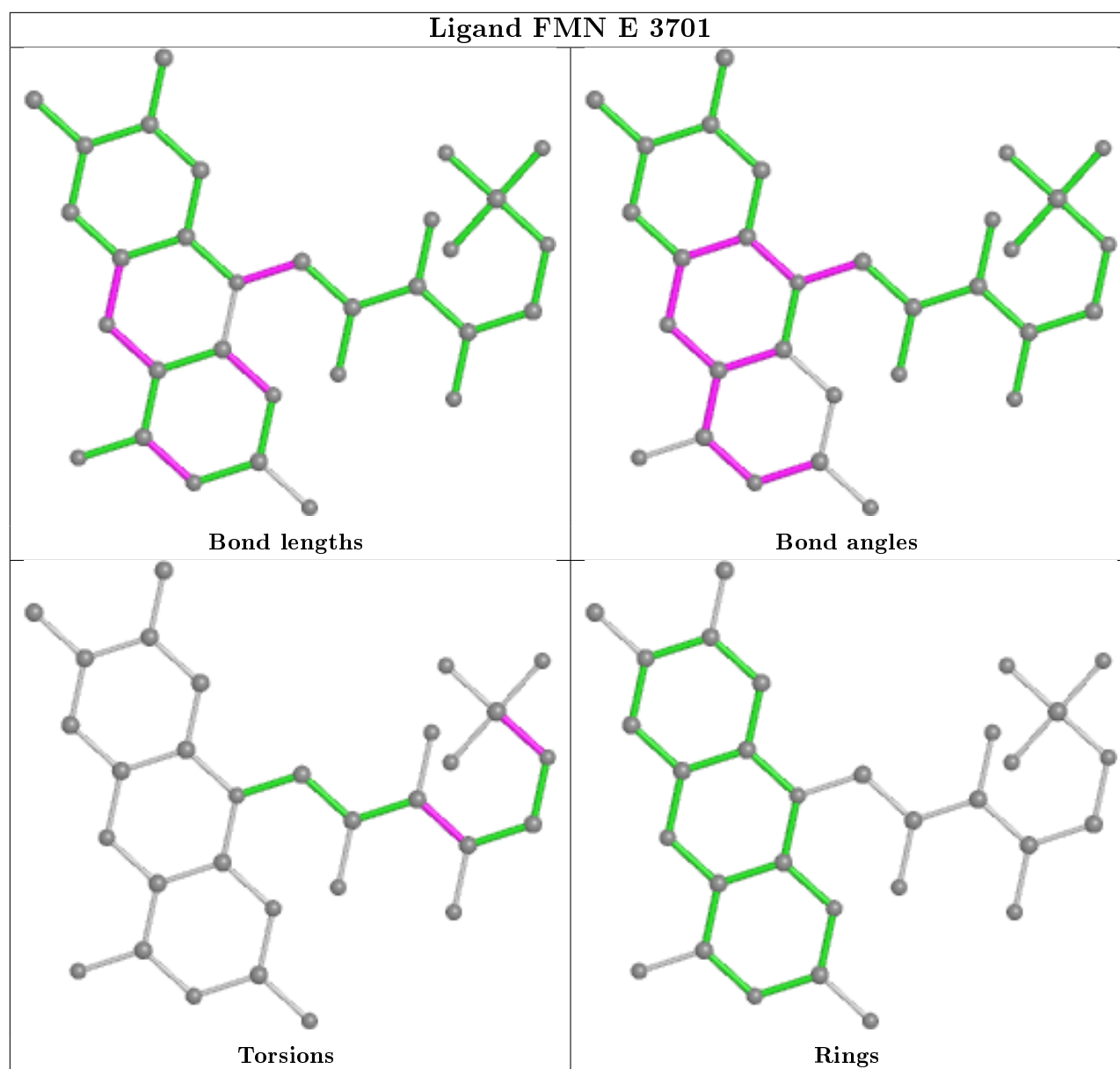


Rings

Ligand FMN H 1702







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	403/404 (99%)	0.79	44 (10%) 5 8	35, 43, 56, 64	0
1	B	403/404 (99%)	0.57	23 (5%) 23 30	35, 43, 56, 65	0
1	D	403/404 (99%)	0.60	31 (7%) 13 17	34, 43, 55, 64	0
1	E	403/404 (99%)	0.89	50 (12%) 4 5	35, 43, 55, 64	0
1	G	403/404 (99%)	0.67	42 (10%) 6 9	34, 42, 55, 65	0
1	H	403/404 (99%)	0.70	38 (9%) 8 11	35, 43, 55, 65	0
1	I	403/404 (99%)	0.85	55 (13%) 3 4	35, 43, 55, 63	0
1	J	403/404 (99%)	0.56	34 (8%) 11 15	34, 43, 56, 65	0
All	All	3224/3232 (99%)	0.70	317 (9%) 7 10	34, 43, 56, 65	0

All (317) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	LEU	7.5
1	E	151[A]	HIS	7.4
1	E	223	LEU	7.3
1	I	223	LEU	7.0
1	I	217	VAL	7.0
1	J	221	GLY	6.9
1	I	221	GLY	6.6
1	E	226	ILE	6.2
1	A	162	GLU	5.6
1	J	375	CYS	5.6
1	H	225	ARG	5.5
1	E	225	ARG	5.5
1	E	122	ARG	5.5
1	D	225	ARG	5.3
1	A	45	GLY	4.9
1	I	73	MET	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	169[A]	ASN	4.8
1	A	119	PRO	4.7
1	G	38	TYR	4.6
1	I	224	GLU	4.6
1	J	220	LEU	4.6
1	A	124	ALA	4.5
1	H	122	ARG	4.5
1	E	96	HIS	4.4
1	A	38	TYR	4.3
1	H	162	GLU	4.2
1	I	225	ARG	4.2
1	I	49	ILE	4.2
1	B	49	ILE	4.1
1	D	231	PRO	4.1
1	H	96	HIS	4.1
1	H	72	GLY	4.0
1	J	83[A]	HIS	4.0
1	J	225	ARG	3.9
1	A	224	GLU	3.9
1	I	80	ILE	3.9
1	E	73	MET	3.9
1	A	123	GLU	3.9
1	B	123	GLU	3.8
1	D	49	ILE	3.8
1	I	226	ILE	3.8
1	A	120	SER	3.8
1	H	123	GLU	3.7
1	J	219	GLU	3.7
1	I	69	GLN	3.7
1	A	294	HIS	3.7
1	H	38	TYR	3.7
1	E	80	ILE	3.6
1	J	49	ILE	3.6
1	I	220	LEU	3.6
1	E	41	CYS	3.6
1	E	119	PRO	3.6
1	D	220	LEU	3.6
1	J	232[A]	SER	3.6
1	E	136	ASP	3.5
1	H	97	ARG	3.5
1	G	311	ILE	3.5
1	E	150	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	42	GLY	3.5
1	E	224	GLU	3.5
1	J	385	GLY	3.5
1	G	80	ILE	3.4
1	G	224	GLU	3.4
1	E	132	GLY	3.4
1	A	80	ILE	3.4
1	A	231	PRO	3.4
1	D	151[A]	HIS	3.4
1	D	224	GLU	3.4
1	D	167	PHE	3.4
1	I	305	ILE	3.3
1	G	220	LEU	3.3
1	I	219	GLU	3.3
1	J	262	ILE	3.3
1	B	313	LEU	3.3
1	E	162	GLU	3.3
1	I	37	ALA	3.2
1	E	152	TRP	3.2
1	G	123	GLU	3.2
1	A	158	THR	3.2
1	G	169[A]	ASN	3.2
1	H	230	ALA	3.2
1	G	37	ALA	3.2
1	A	254	MET	3.2
1	E	74	GLU	3.2
1	A	49	ILE	3.2
1	H	149	LEU	3.2
1	E	221	GLY	3.2
1	E	294	HIS	3.1
1	D	223	LEU	3.1
1	G	167	PHE	3.1
1	D	375	CYS	3.1
1	G	122	ARG	3.1
1	I	122	ARG	3.1
1	H	224	GLU	3.1
1	H	43	ASP	3.1
1	G	221	GLY	3.1
1	B	217	VAL	3.1
1	I	171	ALA	3.1
1	H	44	GLU	3.0
1	B	231	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	50	ASP	3.0
1	H	294	HIS	3.0
1	E	69	GLN	3.0
1	A	218	LYS	3.0
1	E	97	ARG	3.0
1	E	367	ALA	3.0
1	G	219	GLU	3.0
1	D	169[A]	ASN	3.0
1	D	333	LEU	3.0
1	E	71	VAL	3.0
1	I	78	TYR	3.0
1	B	220	LEU	3.0
1	B	232	SER	3.0
1	D	219	GLU	2.9
1	E	149	LEU	2.9
1	E	138	GLY	2.9
1	A	100	PRO	2.9
1	E	219	GLU	2.9
1	H	121	LEU	2.9
1	E	72	GLY	2.9
1	I	163	ASP	2.9
1	D	294	HIS	2.9
1	G	294	HIS	2.9
1	G	44	GLU	2.9
1	I	123	GLU	2.9
1	A	122	ARG	2.9
1	G	49	ILE	2.9
1	A	97	ARG	2.9
1	A	168	SER	2.9
1	H	49	ILE	2.8
1	A	230	ALA	2.8
1	J	230	ALA	2.8
1	B	38	TYR	2.8
1	E	99	PHE	2.8
1	J	167	PHE	2.8
1	E	37	ALA	2.8
1	H	119	PRO	2.8
1	A	43	ASP	2.8
1	I	222	LEU	2.8
1	J	313	LEU	2.8
1	G	260	THR	2.8
1	A	10	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	163	ASP	2.7
1	I	218	LYS	2.7
1	J	38	TYR	2.7
1	D	37	ALA	2.7
1	D	326	VAL	2.7
1	E	123	GLU	2.7
1	H	158	THR	2.7
1	J	384	THR	2.7
1	D	83[A]	HIS	2.7
1	D	232	SER	2.7
1	A	220	LEU	2.7
1	B	72	GLY	2.7
1	G	158	THR	2.7
1	B	80	ILE	2.7
1	E	120	SER	2.7
1	E	158	THR	2.7
1	D	221	GLY	2.7
1	H	221	GLY	2.7
1	A	232	SER	2.6
1	D	217	VAL	2.6
1	I	97	ARG	2.6
1	I	44	GLU	2.6
1	I	112	LYS	2.6
1	I	38	TYR	2.6
1	I	227	GLN	2.6
1	G	97	ARG	2.6
1	J	294	HIS	2.6
1	A	219	GLU	2.6
1	A	167	PHE	2.6
1	G	36	ASN	2.6
1	A	84	VAL	2.6
1	I	71	VAL	2.6
1	A	2	LYS	2.6
1	A	44	GLU	2.6
1	E	220	LEU	2.6
1	H	167	PHE	2.6
1	J	312	ALA	2.6
1	H	232	SER	2.5
1	B	330	LEU	2.5
1	G	109	VAL	2.5
1	J	326	VAL	2.5
1	D	38	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	51	ASN	2.5
1	B	44	GLU	2.5
1	J	218	LYS	2.5
1	G	313	LEU	2.5
1	H	75	ARG	2.5
1	A	75	ARG	2.5
1	A	225	ARG	2.5
1	G	333	LEU	2.5
1	H	150	LEU	2.5
1	I	149	LEU	2.5
1	D	386	ASP	2.5
1	E	141	THR	2.5
1	B	305	ILE	2.5
1	E	48	LEU	2.5
1	G	150	LEU	2.5
1	I	254	MET	2.4
1	I	373	VAL	2.4
1	H	100	PRO	2.4
1	G	329	LEU	2.4
1	J	168	SER	2.4
1	H	212	LYS	2.4
1	D	329	LEU	2.4
1	E	230	ALA	2.4
1	E	98	ARG	2.4
1	I	154	ASP	2.4
1	A	305	ILE	2.4
1	A	121	LEU	2.4
1	E	68	LEU	2.4
1	D	158	THR	2.4
1	A	216	GLU	2.4
1	E	137	LEU	2.4
1	J	330	LEU	2.4
1	B	37	ALA	2.4
1	B	254	MET	2.4
1	I	119	PRO	2.4
1	E	262	ILE	2.4
1	G	234	GLY	2.4
1	E	128	THR	2.4
1	J	217	VAL	2.4
1	G	168	SER	2.4
1	B	149	LEU	2.3
1	H	336	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	38	TYR	2.3
1	D	261	VAL	2.3
1	D	82	ASN	2.3
1	J	37	ALA	2.3
1	I	261	VAL	2.3
1	B	311	ILE	2.3
1	B	219	GLU	2.3
1	D	230	ALA	2.3
1	E	306	LEU	2.3
1	G	48	LEU	2.3
1	G	232	SER	2.3
1	I	151	HIS	2.3
1	H	231	PRO	2.3
1	J	386	ASP	2.3
1	G	262	ILE	2.3
1	A	82	ASN	2.3
1	J	355	ASN	2.3
1	A	140	LYS	2.3
1	G	52	SER	2.3
1	I	47	ALA	2.3
1	I	124	ALA	2.3
1	H	125	GLU	2.2
1	G	88	HIS	2.2
1	J	224	GLU	2.2
1	B	150	LEU	2.2
1	B	333	LEU	2.2
1	I	48	LEU	2.2
1	E	163	ASP	2.2
1	I	156	MET	2.2
1	I	216	GLU	2.2
1	D	168	SER	2.2
1	B	215	ASP	2.2
1	D	97	ARG	2.2
1	E	126	PHE	2.2
1	H	157	PHE	2.2
1	H	220	LEU	2.2
1	H	223	LEU	2.2
1	H	25	TYR	2.2
1	I	72	GLY	2.2
1	B	375	CYS	2.2
1	D	391	CYS	2.2
1	G	231	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	27	GLY	2.2
1	G	15	THR	2.2
1	H	71	VAL	2.1
1	B	158	THR	2.1
1	I	150	LEU	2.1
1	I	375	CYS	2.1
1	E	144	PHE	2.1
1	G	156	MET	2.1
1	A	217	VAL	2.1
1	G	218	LYS	2.1
1	I	161	ASP	2.1
1	G	223	LEU	2.1
1	J	215	ASP	2.1
1	G	230	ALA	2.1
1	I	75	ARG	2.1
1	E	215	ASP	2.1
1	J	261	VAL	2.1
1	G	112	LYS	2.1
1	E	115	LEU	2.1
1	I	191	LEU	2.1
1	J	80	ILE	2.1
1	J	166	LEU	2.1
1	J	311	ILE	2.1
1	G	136	ASP	2.1
1	H	400	ALA	2.1
1	D	354	GLY	2.1
1	I	134	VAL	2.1
1	H	219	GLU	2.0
1	I	70	GLN	2.0
1	A	66	ASP	2.0
1	H	366	LEU	2.0
1	I	128	THR	2.0
1	I	158	THR	2.0
1	D	173	GLY	2.0
1	J	171	ALA	2.0
1	J	216	GLU	2.0
1	I	302	VAL	2.0
1	J	231	PRO	2.0
1	H	163	ASP	2.0
1	I	98	ARG	2.0
1	I	364	GLU	2.0
1	H	153	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	217	VAL	2.0
1	I	152	TRP	2.0
1	A	51	ASN	2.0
1	G	355	ASN	2.0
1	I	211	LEU	2.0
1	A	139	GLY	2.0
1	I	232	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	CL	J	3505	1/1	0.86	0.21	37,37,37,37	1
2	FE	I	2503	1/1	0.91	0.25	63,63,63,63	1
2	FE	B	1503	1/1	0.93	0.08	45,45,45,45	1
3	FMN	D	2701	31/31	0.93	0.13	37,40,43,44	0
2	FE	J	3503	1/1	0.93	0.19	48,48,48,48	1
2	FE	H	1503	1/1	0.95	0.08	44,44,44,44	1
3	FMN	J	3702	31/31	0.96	0.11	38,41,42,42	0
3	FMN	G	702	31/31	0.96	0.11	29,32,34,35	0
3	FMN	B	1701	31/31	0.96	0.10	33,35,39,40	0
4	CL	J	3504	1/1	0.96	0.06	36,36,36,36	1
3	FMN	I	2702	31/31	0.96	0.11	29,33,34,35	0
4	CL	D	2504	1/1	0.96	0.05	41,41,41,41	1
2	FE	E	3503	1/1	0.96	0.26	58,58,58,58	1
4	CL	H	1504	1/1	0.96	0.12	47,47,47,47	1
2	FE	D	2503	1/1	0.97	0.08	36,36,36,36	1
3	FMN	H	1702	31/31	0.97	0.11	28,35,36,36	0

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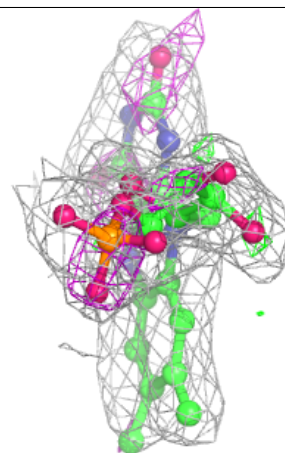
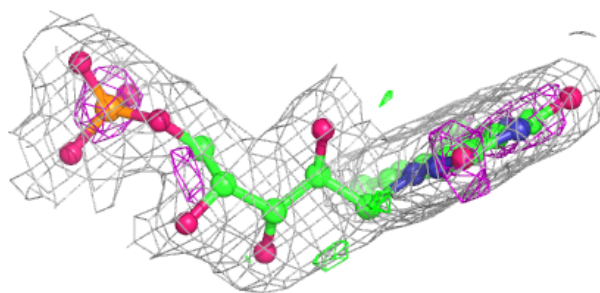
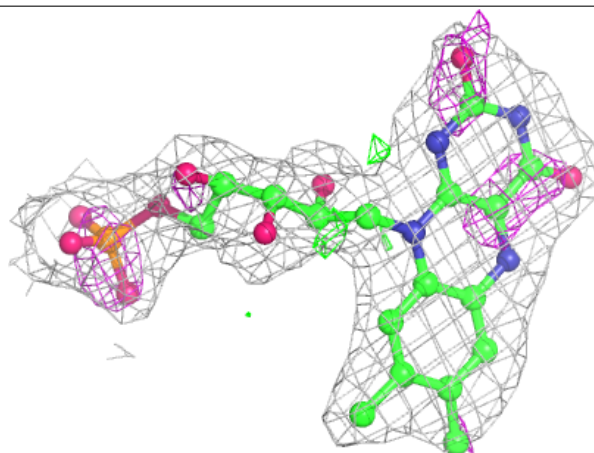
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FMN	A	701	31/31	0.97	0.10	24,33,34,35	0
3	FMN	E	3701	31/31	0.97	0.10	29,32,33,34	0
2	FE	A	503	1/1	0.97	0.07	47,47,47,47	1
2	FE	E	3501	1/1	0.98	0.05	44,44,44,44	0
2	FE	I	2501	1/1	0.98	0.05	48,48,48,48	0
2	FE	H	1501	1/1	0.98	0.05	47,47,47,47	0
2	FE	G	501	1/1	0.99	0.05	37,37,37,37	0
2	FE	J	3501	1/1	0.99	0.04	37,37,37,37	0
2	FE	G	503	1/1	0.99	0.07	32,32,32,32	1
2	FE	A	501	1/1	0.99	0.02	45,45,45,45	0
2	FE	B	1501	1/1	0.99	0.04	36,36,36,36	0
2	FE	D	2501	1/1	0.99	0.06	39,39,39,39	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.

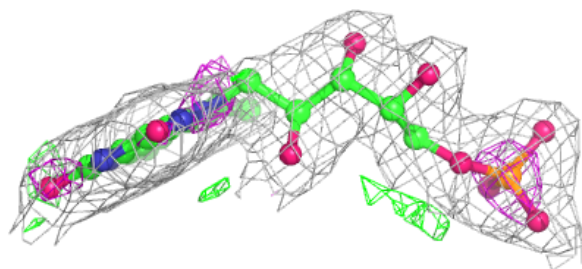
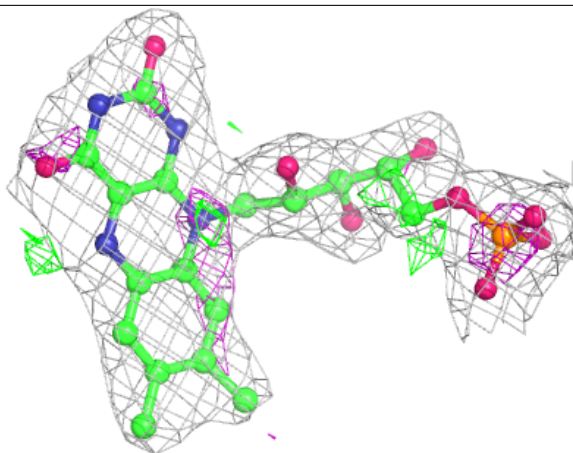
Electron density around FMN D 2701:

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



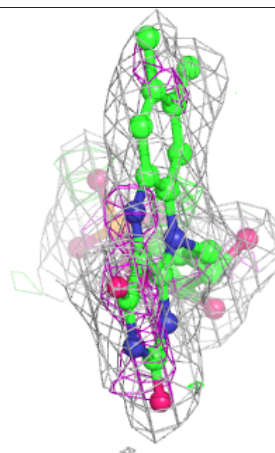
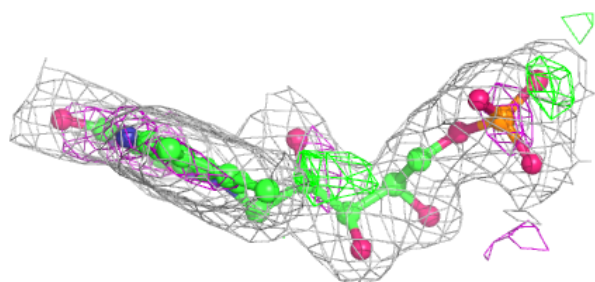
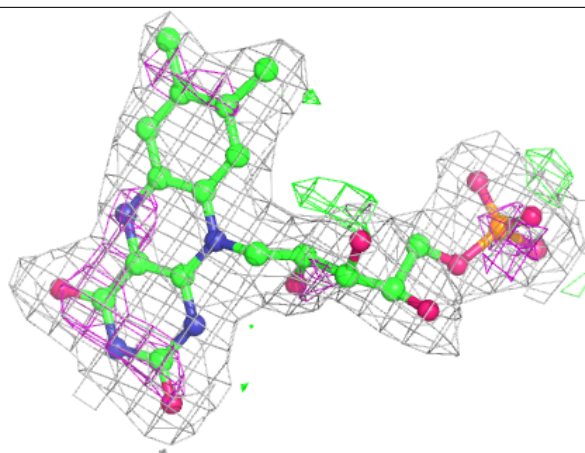
Electron density around FMN J 3702:

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



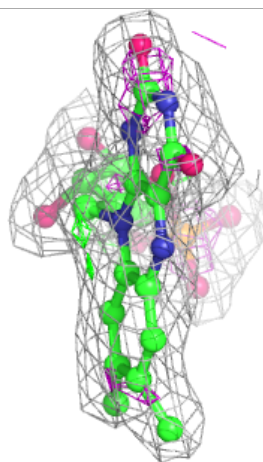
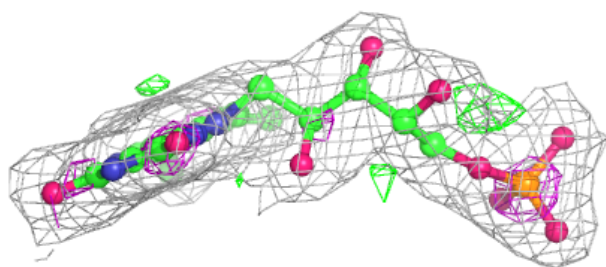
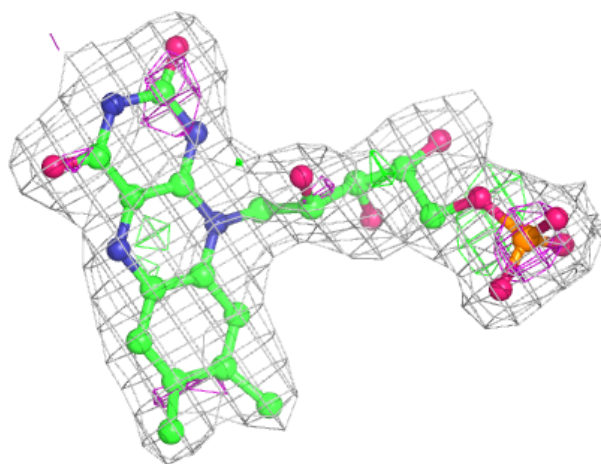
Electron density around FMN G 702:

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



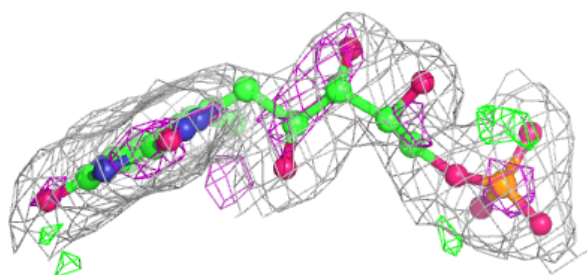
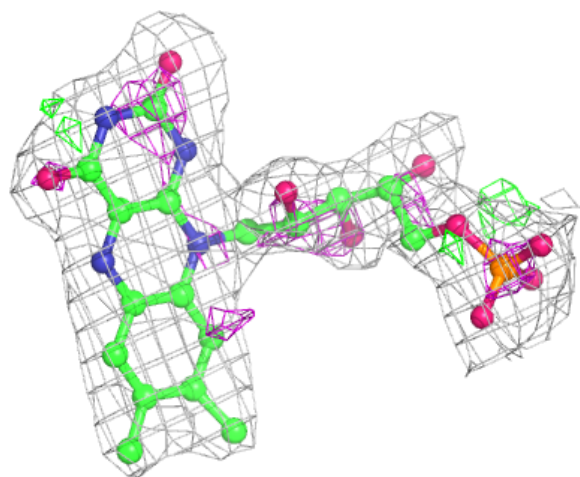
Electron density around FMN B 1701:

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



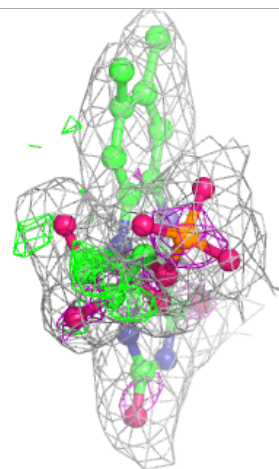
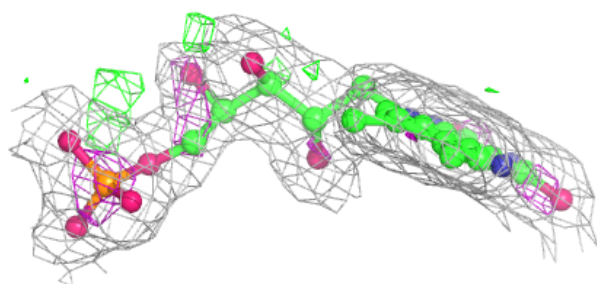
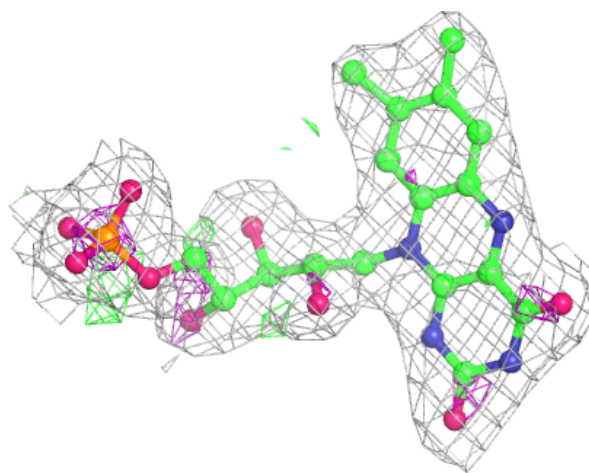
Electron density around FMN I 2702:

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



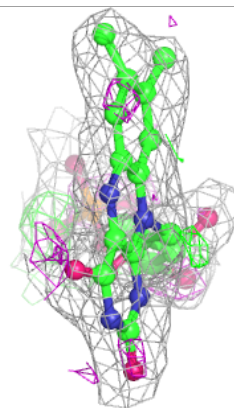
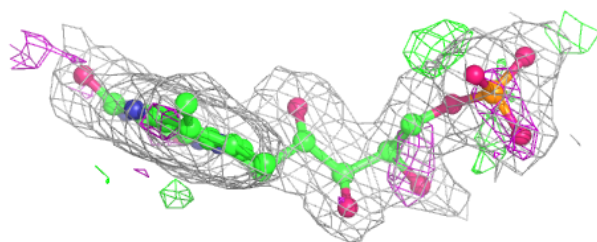
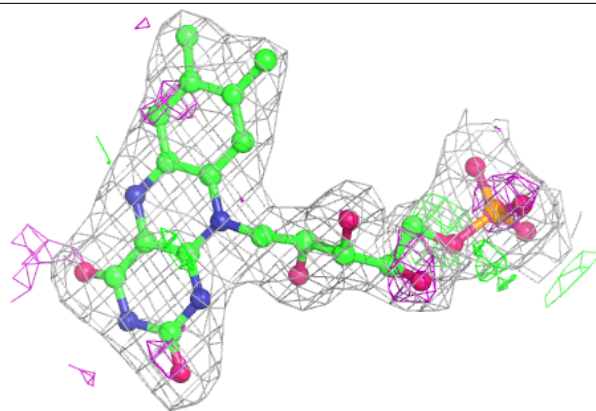
Electron density around FMN H 1702:

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



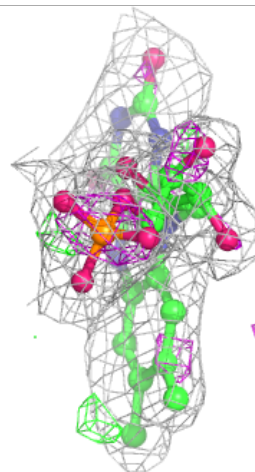
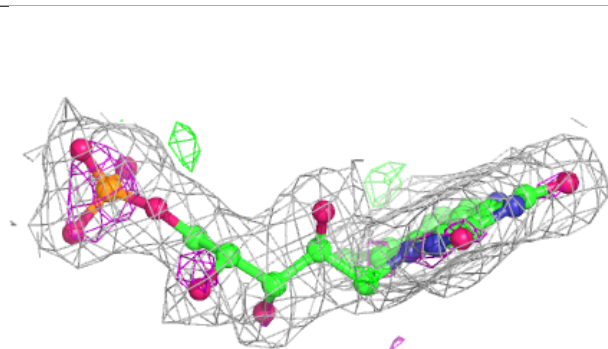
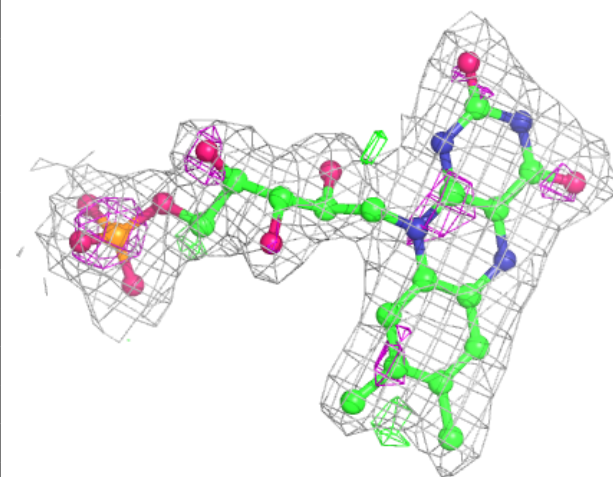
Electron density around FMN A 701:

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



Electron density around FMN E 3701:

$2mF_o-DF_c$ (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.