



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2021 – 10:08 PM JST

PDB ID : 7E1R
Title : Crystal structure of Dehydrogenase/isomerase FabX from *Helicobacter pylori* in complex with holo-ACP
Authors : Zhou, J.S.; Zhang, L.; Zhang, L.
Deposited on : 2021-02-03
Resolution : 2.79 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 : 2.23.2
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) : 2.23.2

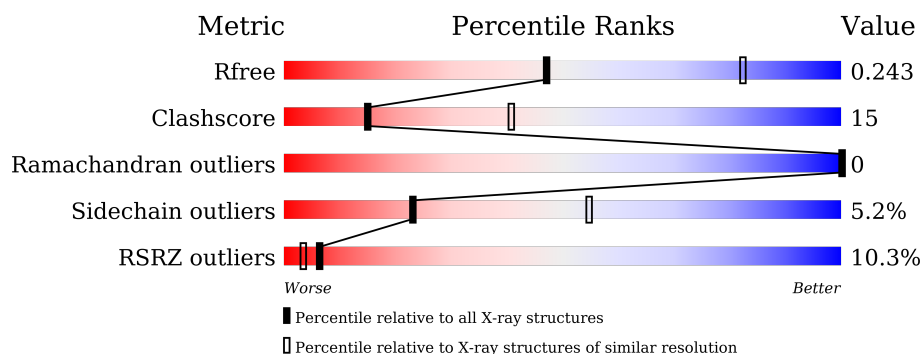
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	372	<div> <div>71%</div> <div>24%</div> <div>...</div> </div>
1	C	372	<div> <div>%</div> <div>72%</div> <div>22%</div> <div>..</div> </div>
2	B	86	<div> <div>52%</div> <div>42%</div> <div>37%</div> <div>..</div> <div>17%</div> </div>
2	D	86	<div> <div>49%</div> <div>45%</div> <div>36%</div> <div>.</div> <div>16%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6895 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 2-nitropropane dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2813	1799	487	512	15			
1	C	366	Total	C	N	O	S	0	0	0
			2812	1799	486	512	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP A0A0B2E3F3
A	-7	LYS	-	expression tag	UNP A0A0B2E3F3
A	-6	HIS	-	expression tag	UNP A0A0B2E3F3
A	-5	HIS	-	expression tag	UNP A0A0B2E3F3
A	-4	HIS	-	expression tag	UNP A0A0B2E3F3
A	-3	HIS	-	expression tag	UNP A0A0B2E3F3
A	-2	HIS	-	expression tag	UNP A0A0B2E3F3
A	-1	HIS	-	expression tag	UNP A0A0B2E3F3
A	0	HIS	-	expression tag	UNP A0A0B2E3F3
C	-8	MET	-	initiating methionine	UNP A0A0B2E3F3
C	-7	LYS	-	expression tag	UNP A0A0B2E3F3
C	-6	HIS	-	expression tag	UNP A0A0B2E3F3
C	-5	HIS	-	expression tag	UNP A0A0B2E3F3
C	-4	HIS	-	expression tag	UNP A0A0B2E3F3
C	-3	HIS	-	expression tag	UNP A0A0B2E3F3
C	-2	HIS	-	expression tag	UNP A0A0B2E3F3
C	-1	HIS	-	expression tag	UNP A0A0B2E3F3
C	0	HIS	-	expression tag	UNP A0A0B2E3F3

- Molecule 2 is a protein called Acyl carrier protein,Acyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	71	Total	C	N	O	S	0	0	0
			549	349	81	118	1			

Continued on next page...

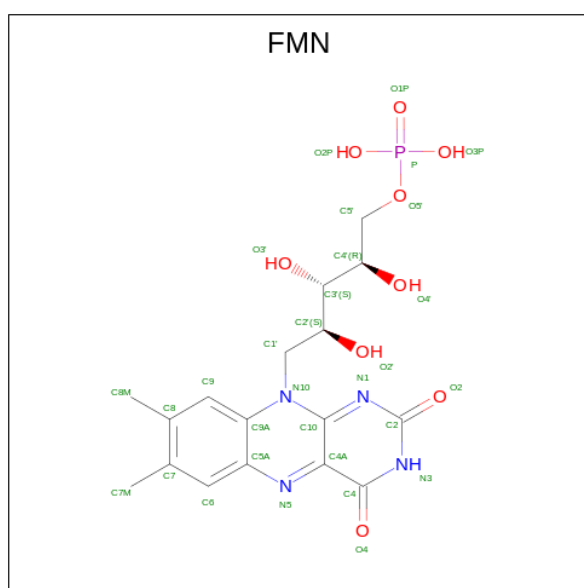
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	72	Total	C	N	O	S	0	0	0
			557	353	83	120	1			

There are 16 discrepancies between the modelled and reference sequences:

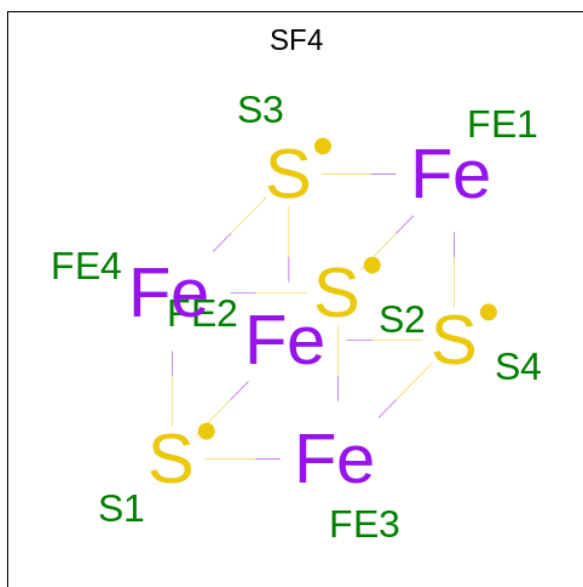
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLY	-	expression tag	UNP A0A0T6M3S8
B	-6	THR	-	expression tag	UNP A0A0T6M3S8
B	-5	SER	-	expression tag	UNP A0A0T6M3S8
B	-4	SER	-	expression tag	UNP A0A0T6M3S8
B	-3	MET	-	expression tag	UNP A0A0T6M3S8
B	-2	GLY	-	expression tag	UNP A0A0T6M3S8
B	-1	TYR	-	expression tag	UNP A0A0T6M3S8
B	0	LEU	-	expression tag	UNP A0A0T6M3S8
D	-7	GLY	-	expression tag	UNP A0A0T6M3S8
D	-6	THR	-	expression tag	UNP A0A0T6M3S8
D	-5	SER	-	expression tag	UNP A0A0T6M3S8
D	-4	SER	-	expression tag	UNP A0A0T6M3S8
D	-3	MET	-	expression tag	UNP A0A0T6M3S8
D	-2	GLY	-	expression tag	UNP A0A0T6M3S8
D	-1	TYR	-	expression tag	UNP A0A0T6M3S8
D	0	LEU	-	expression tag	UNP A0A0T6M3S8

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



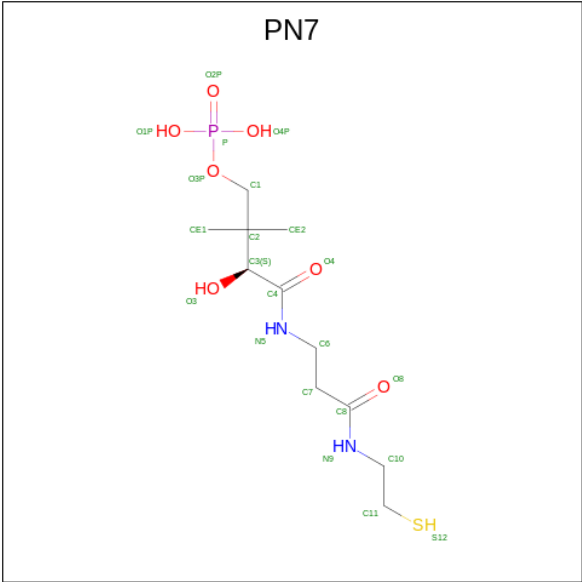
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is N 3 -[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-N-(2-sulfanylethyl)-beta-alaninamide (three-letter code: PN7) (formula: C₁₁H₂₃N₂O₇PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		
5	D	1	Total	C	N	O	P	S	0	0
			21	11	2	6	1	1		

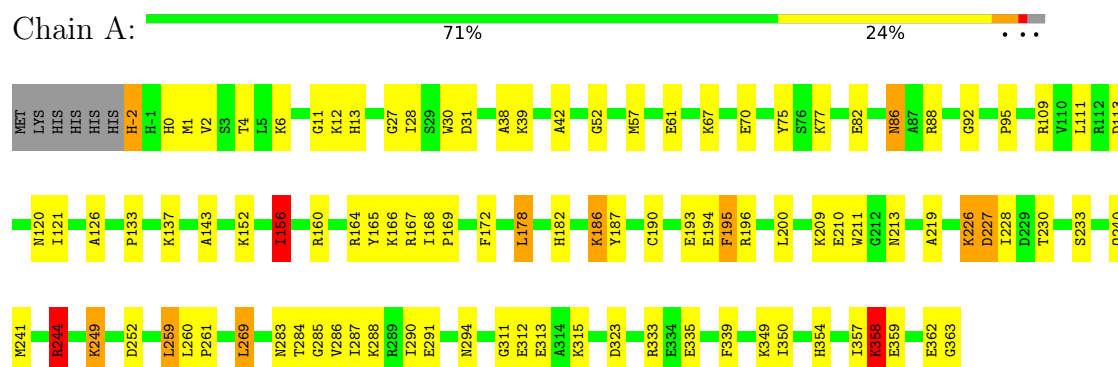
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	23	Total	O	0	0
			23	23		
6	B	1	Total	O	0	0
			1	1		
6	C	20	Total	O	0	0
			20	20		

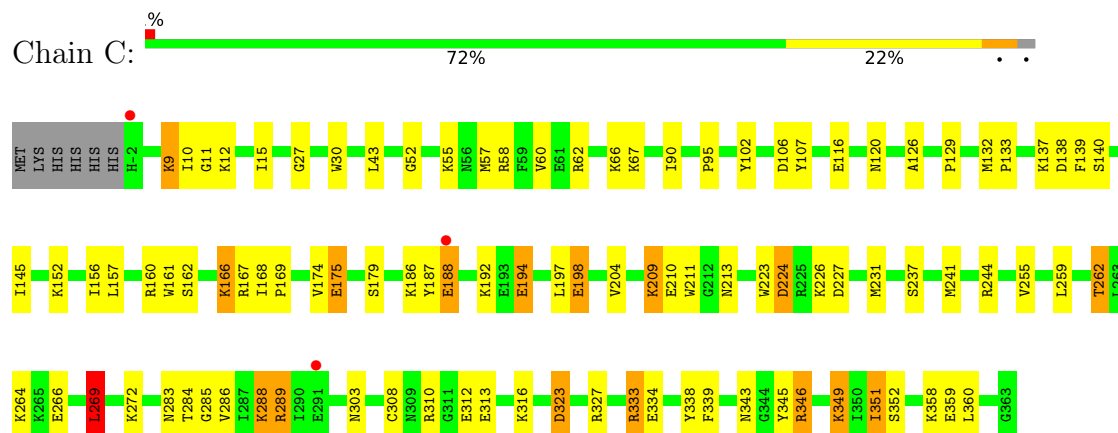
3 Residue-property plots [i](#)

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

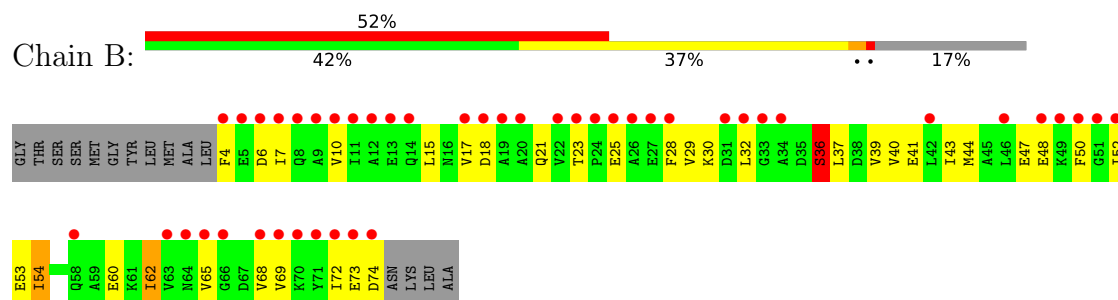
• Molecule 1: 2-nitropropane dioxygenase



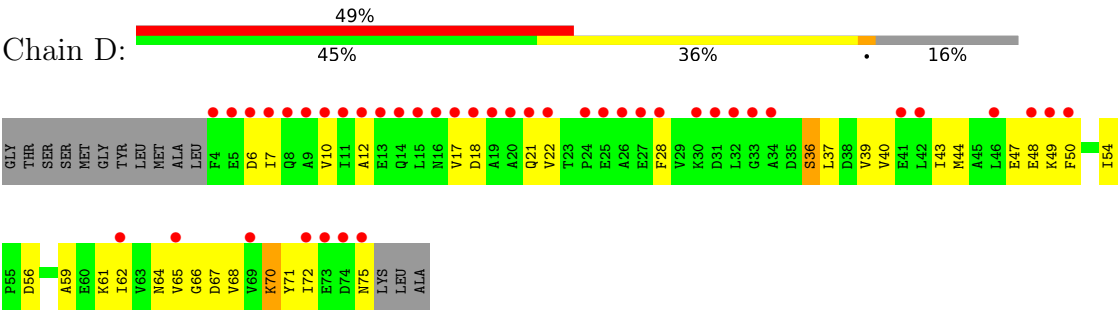
• Molecule 1: 2-nitropropane dioxygenase



• Molecule 2: Acyl carrier protein, Acyl carrier protein



● Molecule 2: Acyl carrier protein,Acyl carrier protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.79Å 104.44Å 99.58Å 90.00° 99.52° 90.00°	Depositor
Resolution (Å)	48.74 – 2.79 48.74 – 2.79	Depositor EDS
% Data completeness (in resolution range)	82.8 (48.74-2.79) 82.8 (48.74-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.206 , 0.243 0.206 , 0.243	Depositor DCC
R_{free} test set	1104 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.5	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	0.91	EDS
Total number of atoms	6895	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, PN7, SF4

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	1.06	15/2869 (0.5%)	0.90	17/3869 (0.4%)
1	C	1.08	18/2868 (0.6%)	0.89	7/3867 (0.2%)
2	B	0.85	0/554	0.81	2/752 (0.3%)
2	D	0.48	0/562	0.69	1/763 (0.1%)
All	All	1.01	33/6853 (0.5%)	0.87	27/9251 (0.3%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	116	GLU	CD-OE1	-8.89	1.15	1.25
1	A	313	GLU	CD-OE1	-7.99	1.16	1.25
1	A	313	GLU	CD-OE2	-7.09	1.17	1.25
1	A	244	ARG	CZ-NH1	-6.79	1.24	1.33
1	A	2	VAL	C-O	-6.79	1.10	1.23
1	C	358	LYS	C-O	-6.76	1.10	1.23
1	C	224	ASP	C-O	-6.69	1.10	1.23
1	C	327	ARG	C-O	-6.43	1.11	1.23
1	A	210	GLU	CD-OE1	-6.43	1.18	1.25
1	C	60	VAL	CB-CG2	6.33	1.66	1.52
1	A	312	GLU	C-O	-6.14	1.11	1.23
1	C	231	MET	C-O	-6.13	1.11	1.23
1	C	139	PHE	CB-CG	-5.98	1.41	1.51
1	A	354	HIS	C-O	-5.87	1.12	1.23
1	A	358	LYS	C-O	-5.83	1.12	1.23
1	C	323	ASP	C-O	-5.79	1.12	1.23
1	A	249	LYS	C-O	-5.76	1.12	1.23
1	C	327	ARG	CZ-NH1	-5.70	1.25	1.33
1	A	252	ASP	CG-OD2	-5.69	1.12	1.25
1	C	198	GLU	C-O	-5.67	1.12	1.23
1	C	349	LYS	N-CA	-5.62	1.35	1.46
1	C	166	LYS	C-O	-5.57	1.12	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	227	ASP	C-O	-5.53	1.12	1.23
1	C	227	ASP	C-O	-5.53	1.12	1.23
1	C	198	GLU	CD-OE1	-5.50	1.19	1.25
1	C	9	LYS	C-O	-5.50	1.12	1.23
1	A	244	ARG	C-O	-5.42	1.13	1.23
1	C	209	LYS	C-O	-5.39	1.13	1.23
1	A	0	HIS	C-O	-5.38	1.13	1.23
1	A	195	PHE	C-O	-5.32	1.13	1.23
1	A	-2	HIS	C-O	-5.22	1.13	1.23
1	C	345	TYR	CE1-CZ	-5.09	1.31	1.38
1	C	138	ASP	C-O	-5.02	1.13	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ILE	CG1-CB-CG2	-8.48	92.74	111.40
1	A	244	ARG	NE-CZ-NH2	8.47	124.54	120.30
2	D	22	VAL	C-N-CA	7.97	141.63	121.70
1	A	156	ILE	CG1-CB-CG2	-7.71	94.45	111.40
1	C	349	LYS	N-CA-CB	-7.27	97.52	110.60
1	C	269	LEU	CB-CG-CD2	7.19	123.22	111.00
1	A	252	ASP	CB-CG-OD1	6.83	124.45	118.30
1	C	116	GLU	OE1-CD-OE2	-6.63	115.34	123.30
1	A	244	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	A	11	GLY	N-CA-C	-6.34	97.25	113.10
1	C	269	LEU	CB-CA-C	-6.18	98.46	110.20
1	A	190	CYS	CA-CB-SG	6.16	125.08	114.00
1	A	39	LYS	CD-CE-NZ	-5.94	98.04	111.70
2	B	36	SER	CA-CB-OG	5.87	127.05	111.20
1	A	287	ILE	CG1-CB-CG2	-5.78	98.69	111.40
1	A	259	LEU	CA-CB-CG	5.68	128.36	115.30
1	A	6	LYS	CG-CD-CE	-5.65	94.95	111.90
2	B	54	ILE	CG1-CB-CG2	-5.63	99.02	111.40
1	A	210	GLU	OE1-CD-OE2	-5.51	116.68	123.30
1	A	269	LEU	CA-CB-CG	5.49	127.92	115.30
1	C	269	LEU	CB-CG-CD1	5.38	120.15	111.00
1	C	351	ILE	CG1-CB-CG2	-5.21	99.93	111.40
1	C	333	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	294	ASN	CB-CA-C	5.15	120.69	110.40
1	A	111	LEU	CB-CG-CD2	5.09	119.65	111.00
1	A	0	HIS	N-CA-CB	-5.04	101.54	110.60
1	A	200	LEU	CB-CG-CD2	-5.02	102.46	111.00

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	2813	0	2865	71	2
1	C	2812	0	2863	81	0
2	B	549	0	534	43	2
2	D	557	0	540	33	0
3	A	31	0	19	2	0
3	C	31	0	19	1	0
4	A	8	0	0	1	0
4	C	8	0	0	0	0
5	B	21	0	22	6	0
5	D	21	0	22	2	0
6	A	23	0	0	5	0
6	B	1	0	0	0	0
6	C	20	0	0	3	0
All	All	6895	0	6884	207	2

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 15.

All (207) 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:A:152:LYS:HE2	2:B:37:LEU:HB2	1.43	0.98
2:B:48:GLU:CD	1:C:213:ASN:ND2	2.19	0.96
1:C:55:LYS:HG3	1:C:58:ARG:HH11	1.33	0.90
1:A:152:LYS:HE2	2:B:37:LEU:CB	2.03	0.89
2:B:28:PHE:CE1	2:B:65:VAL:HG12	2.10	0.85
2:B:48:GLU:CD	1:C:213:ASN:HD22	1.79	0.82
2:B:37:LEU:O	2:B:41:GLU:HG3	1.80	0.80
2:B:48:GLU:CG	1:C:213:ASN:HD22	1.94	0.80
2:D:28:PHE:CE1	2:D:65:VAL:HG12	2.16	0.80
1:A:126:ALA:H	5:B:101:PN7:C7	1.96	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ALA:H	5:B:101:PN7:H15	1.46	0.79
1:C:269:LEU:HD21	1:C:283:ASN:HB2	1.65	0.76
2:B:48:GLU:CG	1:C:213:ASN:ND2	2.50	0.74
2:D:10:VAL:HG21	2:D:49:LYS:HD3	1.70	0.72
1:C:259:LEU:O	1:C:262:THR:HG23	1.89	0.71
2:D:10:VAL:HG21	2:D:49:LYS:CD	2.20	0.70
1:C:192:LYS:NZ	1:C:194:GLU:OE1	2.24	0.69
2:D:12:ALA:HA	2:D:17:VAL:HG23	1.76	0.67
1:A:288:LYS:O	1:A:291:GLU:HG2	1.95	0.67
1:A:121:ILE:HG12	1:A:143:ALA:HB3	1.77	0.66
2:B:48:GLU:HG3	1:C:213:ASN:HD22	1.59	0.66
1:A:260:LEU:N	1:A:261:PRO:HD2	2.11	0.66
2:B:68:VAL:O	2:B:72:ILE:HG13	1.97	0.65
1:A:260:LEU:HB2	1:A:261:PRO:HD3	1.79	0.65
2:B:28:PHE:CZ	2:B:65:VAL:HG12	2.33	0.64
1:C:55:LYS:CG	1:C:58:ARG:HH11	2.09	0.63
2:B:41:GLU:O	2:B:44:MET:HB2	1.98	0.63
1:C:67:LYS:HD3	1:C:323:ASP:OD2	1.98	0.63
2:D:28:PHE:CZ	2:D:65:VAL:HG12	2.34	0.62
1:A:126:ALA:N	5:B:101:PN7:H15	2.14	0.62
1:C:160:ARG:NH2	2:D:44:MET:HG2	2.15	0.62
2:B:18:ASP:HB2	2:B:21:GLN:OE1	2.01	0.61
1:A:260:LEU:N	1:A:261:PRO:CD	2.63	0.60
1:A:194:GLU:O	6:A:1101:HOH:O	2.17	0.60
2:D:36:SER:O	2:D:39:VAL:HG22	2.01	0.60
2:D:6:ASP:O	2:D:10:VAL:HG23	2.00	0.60
1:C:349:LYS:O	1:C:349:LYS:HG3	2.01	0.60
2:D:68:VAL:HG12	2:D:72:ILE:HD11	1.83	0.60
1:A:284:THR:HG22	1:A:285:GLY:N	2.17	0.60
1:C:12:LYS:HD2	1:C:12:LYS:O	2.02	0.60
1:C:186:LYS:HG3	1:C:188:GLU:HG3	1.83	0.60
2:B:43:ILE:HG23	2:B:54:ILE:HD12	1.83	0.59
1:C:255:VAL:HG11	1:C:338:TYR:HE2	1.67	0.59
2:B:43:ILE:O	2:B:47:GLU:HG2	2.03	0.59
1:A:286:VAL:O	1:A:290:ILE:HG23	2.04	0.58
1:C:241:MET:HE1	1:C:360:LEU:HD13	1.84	0.58
1:A:86:ASN:N	1:A:86:ASN:OD1	2.34	0.58
1:A:61:GLU:OE2	1:A:61:GLU:HA	2.04	0.57
1:A:209:LYS:HG2	1:A:213:ASN:ND2	2.19	0.57
2:B:65:VAL:O	2:B:68:VAL:HG12	2.05	0.57
1:A:27:GLY:HA2	1:A:30:TRP:CD2	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:LEU:O	2:B:41:GLU:CG	2.51	0.56
1:A:152:LYS:HG2	2:B:37:LEU:CD2	2.36	0.56
1:A:311:GLY:O	1:A:315:LYS:HG3	2.05	0.56
2:D:40:VAL:O	2:D:44:MET:HG3	2.06	0.56
1:C:351:ILE:HG22	1:C:352:SER:N	2.21	0.55
1:A:339:PHE:HB2	3:A:1001:FMN:HM72	1.88	0.55
1:A:178:LEU:H	1:A:178:LEU:HD12	1.70	0.55
1:A:284:THR:HG22	1:A:285:GLY:H	1.70	0.55
2:B:47:GLU:OE1	2:B:54:ILE:N	2.32	0.55
1:A:178:LEU:HD12	1:A:178:LEU:N	2.21	0.55
2:D:68:VAL:O	2:D:72:ILE:HD12	2.06	0.55
1:A:193:GLU:HG2	1:A:196:ARG:HD2	1.89	0.55
2:B:47:GLU:HB2	2:B:52:ILE:O	2.07	0.54
2:D:43:ILE:O	2:D:47:GLU:HG3	2.06	0.54
1:C:339:PHE:HB2	3:C:1001:FMN:HM72	1.90	0.54
2:D:70:LYS:O	2:D:70:LYS:HD3	2.06	0.54
1:C:272:LYS:NZ	6:C:1104:HOH:O	2.41	0.54
1:C:269:LEU:HD21	1:C:283:ASN:CB	2.36	0.54
2:D:36:SER:O	2:D:40:VAL:HG23	2.09	0.53
1:C:269:LEU:CD2	1:C:283:ASN:HB2	2.38	0.53
1:A:168:ILE:HG22	1:C:166:LYS:HB3	1.90	0.53
1:C:27:GLY:HA2	1:C:30:TRP:CD2	2.44	0.53
1:A:31:ASP:N	1:A:31:ASP:OD1	2.39	0.53
2:B:48:GLU:CD	1:C:213:ASN:HD21	2.07	0.53
1:A:228:ILE:HD11	1:A:241:MET:HE1	1.90	0.53
1:A:88:ARG:HD3	1:A:92:GLY:O	2.08	0.53
1:A:311:GLY:HA2	4:A:1002:SF4:S4	2.49	0.52
1:C:343:ASN:O	1:C:346:ARG:HG3	2.09	0.52
1:A:269:LEU:HD22	1:A:283:ASN:HB2	1.92	0.52
1:A:160:ARG:HE	1:A:164:ARG:NH2	2.08	0.52
1:A:209:LYS:HE2	2:D:48:GLU:HG3	1.91	0.52
1:C:52:GLY:O	1:C:57:MET:HA	2.09	0.52
1:C:55:LYS:HG3	1:C:58:ARG:NH1	2.15	0.52
2:B:29:VAL:HG23	2:B:30:LYS:HB2	1.93	0.51
1:A:260:LEU:H	1:A:261:PRO:HD2	1.75	0.51
1:C:9:LYS:HE2	1:C:11:GLY:O	2.10	0.51
1:A:169:PRO:HG2	1:A:172:PHE:CZ	2.45	0.51
1:C:266:GLU:OE1	1:C:266:GLU:N	2.44	0.51
1:A:95:PRO:HA	1:A:120:ASN:OD1	2.12	0.50
1:A:12:LYS:HZ2	1:A:13:HIS:CE1	2.29	0.50
1:A:160:ARG:HE	1:A:164:ARG:HH21	1.59	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:VAL:O	2:D:43:ILE:HD12	2.11	0.50
1:A:67:LYS:HD3	1:A:323:ASP:OD1	2.12	0.50
2:D:62:ILE:HG23	2:D:67:ASP:HB2	1.93	0.50
1:A:152:LYS:HE2	2:B:37:LEU:HB3	1.88	0.50
1:C:160:ARG:NH2	2:D:47:GLU:OE2	2.36	0.50
1:C:126:ALA:H	5:D:101:PN7:C7	2.24	0.50
1:C:192:LYS:CE	1:C:194:GLU:OE1	2.59	0.50
1:C:313:GLU:OE2	1:C:316:LYS:NZ	2.33	0.49
1:C:285:GLY:O	1:C:288:LYS:HB2	2.12	0.49
1:A:152:LYS:HG2	2:B:37:LEU:HD23	1.94	0.49
1:A:182:HIS:O	6:A:1102:HOH:O	2.20	0.49
1:A:219:ALA:HB2	1:A:240:GLN:HB3	1.95	0.49
1:C:15:ILE:HD13	1:C:43:LEU:HB2	1.94	0.49
1:C:160:ARG:HD3	2:D:44:MET:SD	2.52	0.48
2:B:37:LEU:HD11	5:B:101:PN7:H10	1.94	0.48
1:C:237:SER:N	6:C:1102:HOH:O	2.46	0.48
2:B:29:VAL:HG23	2:B:30:LYS:N	2.27	0.48
1:A:52:GLY:O	1:A:57:MET:HA	2.14	0.48
2:D:68:VAL:HG12	2:D:72:ILE:CD1	2.43	0.48
1:A:70:GLU:HG3	6:A:1118:HOH:O	2.14	0.47
6:A:1102:HOH:O	5:B:101:PN7:H21	2.13	0.47
1:C:10:ILE:HG21	1:C:145:ILE:HD11	1.97	0.47
1:C:161:TRP:HB3	1:C:167:ARG:O	2.15	0.47
1:A:156:ILE:HD11	2:B:41:GLU:HG2	1.96	0.47
2:B:4:PHE:HA	2:B:7:ILE:HD12	1.97	0.46
1:C:351:ILE:HD13	1:C:351:ILE:HG21	1.66	0.46
3:A:1001:FMN:C2	5:B:101:PN7:H20	2.45	0.46
1:C:259:LEU:O	1:C:262:THR:CG2	2.60	0.46
1:A:249:LYS:HG3	1:A:350:ILE:HG22	1.98	0.46
1:A:156:ILE:HG23	1:A:156:ILE:HD13	1.34	0.46
2:B:69:VAL:O	2:B:73:GLU:HG2	2.16	0.46
1:A:186:LYS:O	1:A:187:TYR:C	2.50	0.46
1:A:27:GLY:HA2	1:A:30:TRP:CE3	2.51	0.46
2:B:6:ASP:O	2:B:10:VAL:HG23	2.16	0.46
1:C:266:GLU:CD	1:C:266:GLU:H	2.19	0.45
1:A:160:ARG:NH2	2:B:47:GLU:OE2	2.50	0.45
1:C:175:GLU:OE2	1:C:179:SER:HB2	2.17	0.45
1:A:38:ALA:HA	1:A:42:ALA:O	2.17	0.45
1:A:358:LYS:O	1:A:362:GLU:HG3	2.16	0.45
1:C:168:ILE:HG23	1:C:169:PRO:HD2	1.99	0.45
2:D:28:PHE:HZ	2:D:68:VAL:HG21	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ILE:HD12	2:B:40:VAL:HB	1.98	0.45
1:C:284:THR:HA	1:C:288:LYS:HG3	1.99	0.45
1:A:82:GLU:O	1:A:86:ASN:OD1	2.34	0.44
1:A:156:ILE:HD12	1:A:156:ILE:HG21	1.43	0.44
1:C:66:LYS:HA	1:C:66:LYS:HD2	1.43	0.44
2:B:52:ILE:HG22	2:B:53:GLU:N	2.31	0.44
1:A:168:ILE:HD13	1:C:162:SER:OG	2.17	0.44
2:B:23:THR:OG1	2:B:25:GLU:OE1	2.27	0.44
1:C:95:PRO:HA	1:C:120:ASN:OD1	2.17	0.44
1:C:107:TYR:OH	1:C:132:MET:HG3	2.18	0.44
2:D:56:ASP:HA	2:D:59:ALA:HB3	2.00	0.44
1:A:75:TYR:HB2	1:A:109:ARG:HH22	1.82	0.44
1:A:133:PRO:HB2	1:A:165:TYR:CG	2.53	0.44
1:A:168:ILE:HD11	1:A:211:TRP:HB3	2.00	0.44
1:C:156:ILE:O	1:C:160:ARG:HG2	2.18	0.44
1:C:194:GLU:H	1:C:194:GLU:HG3	1.61	0.43
2:D:10:VAL:CG2	2:D:49:LYS:NZ	2.81	0.43
2:D:71:TYR:O	2:D:75:ASN:ND2	2.47	0.43
1:C:349:LYS:HB2	1:C:351:ILE:HD11	2.00	0.43
2:D:43:ILE:HG23	2:D:54:ILE:HD12	1.99	0.43
1:A:77:LYS:HE2	1:A:113:ASP:OD1	2.18	0.43
1:C:137:LYS:HD3	1:C:137:LYS:HA	1.62	0.43
2:B:65:VAL:O	2:B:69:VAL:HG23	2.19	0.43
1:C:132:MET:HB3	1:C:133:PRO:HD3	2.01	0.43
1:C:132:MET:HB3	1:C:161:TRP:CZ2	2.53	0.43
2:D:7:ILE:HG12	2:D:50:PHE:CE2	2.53	0.43
2:B:62:ILE:HD13	2:B:62:ILE:HG21	1.69	0.43
1:C:312:GLU:O	1:C:316:LYS:HG3	2.19	0.43
2:B:15:LEU:O	2:B:17:VAL:HG23	2.18	0.43
2:B:36:SER:O	2:B:39:VAL:HB	2.18	0.42
1:C:102:TYR:CZ	1:C:129:PRO:HA	2.54	0.42
2:D:10:VAL:CG2	2:D:49:LYS:HZ2	2.31	0.42
1:C:126:ALA:H	5:D:101:PN7:H15	1.83	0.42
1:C:197:LEU:HD12	1:C:197:LEU:O	2.18	0.42
1:C:152:LYS:HB3	2:D:37:LEU:HD12	2.02	0.42
2:D:65:VAL:HA	2:D:68:VAL:HG23	2.01	0.42
1:A:286:VAL:HG22	1:A:335:GLU:O	2.19	0.42
2:B:54:ILE:HG21	2:B:54:ILE:HD13	1.68	0.42
1:C:192:LYS:HE3	1:C:194:GLU:OE1	2.20	0.42
1:C:244:ARG:HA	1:C:244:ARG:HD2	1.79	0.42
1:A:166:LYS:NZ	1:C:140:SER:O	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:TRP:CZ3	1:C:211:TRP:CD1	3.08	0.42
1:C:129:PRO:HD2	1:C:157:LEU:HD11	2.01	0.42
1:A:333:ARG:HG2	6:A:1115:HOH:O	2.20	0.42
1:C:241:MET:HE2	1:C:241:MET:HB2	1.83	0.41
1:A:230:THR:O	1:A:233:SER:OG	2.34	0.41
1:C:223:TRP:CH2	1:C:346:ARG:HB2	2.55	0.41
2:D:18:ASP:HB2	2:D:21:GLN:OE1	2.20	0.41
1:A:196:ARG:H	1:A:196:ARG:HG3	1.69	0.41
1:C:289:ARG:HA	1:C:289:ARG:HD3	1.65	0.41
2:D:44:MET:HE2	2:D:44:MET:HB3	1.96	0.41
1:A:284:THR:CG2	1:A:285:GLY:N	2.83	0.41
1:C:264:LYS:HB3	1:C:264:LYS:HE2	1.85	0.41
1:C:308:CYS:HA	1:C:313:GLU:HB2	2.03	0.41
1:A:195:PHE:O	1:A:196:ARG:C	2.50	0.41
1:C:289:ARG:HH21	1:C:334:GLU:HA	1.85	0.41
1:A:244:ARG:HA	1:A:244:ARG:HD2	1.85	0.41
1:A:260:LEU:CB	1:A:261:PRO:HD3	2.46	0.41
2:B:25:GLU:H	2:B:25:GLU:HG3	1.70	0.41
2:B:62:ILE:O	2:B:62:ILE:CG1	2.69	0.41
1:C:209:LYS:O	1:C:210:GLU:C	2.53	0.41
1:C:272:LYS:HZ3	1:C:272:LYS:HB2	1.85	0.41
2:D:28:PHE:CZ	2:D:68:VAL:HG21	2.55	0.41
1:C:90:ILE:HD11	6:C:1109:HOH:O	2.21	0.41
1:C:174:VAL:HG11	1:C:204:VAL:HG21	2.03	0.41
2:B:50:PHE:O	2:B:52:ILE:HG12	2.22	0.40
1:C:286:VAL:O	1:C:289:ARG:HB2	2.21	0.40
1:C:303:ASN:OD1	1:C:310:ARG:HG2	2.21	0.40
2:D:64:ASN:HD22	2:D:66:GLY:H	1.69	0.40
1:A:4:THR:OG1	1:A:363:GLY:O	2.34	0.40
2:B:17:VAL:HG11	2:B:32:LEU:HD23	2.03	0.40
1:C:209:LYS:C	1:C:211:TRP:N	2.74	0.40
1:C:241:MET:HE1	1:C:360:LEU:CD1	2.49	0.40
1:C:224:ASP:OD1	1:C:226:LYS:HG2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LYS:NZ	2:B:25:GLU:OE2[2_555]	1.59	0.61
1:A:226:LYS:NZ	2:B:25:GLU:CD[2_555]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone

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	364/372 (98%)	352 (97%)	12 (3%)	0	100	100
1	C	364/372 (98%)	355 (98%)	9 (2%)	0	100	100
2	B	69/86 (80%)	66 (96%)	3 (4%)	0	100	100
2	D	70/86 (81%)	64 (91%)	6 (9%)	0	100	100
All	All	867/916 (95%)	837 (96%)	30 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	294/300 (98%)	278 (95%)	16 (5%)	22	53
1	C	293/300 (98%)	279 (95%)	14 (5%)	25	58
2	B	60/71 (84%)	56 (93%)	4 (7%)	16	43
2	D	61/71 (86%)	58 (95%)	3 (5%)	25	57
All	All	708/742 (95%)	671 (95%)	37 (5%)	23	55

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	86	ASN
1	A	137	LYS
1	A	156	ILE
1	A	167	ARG
1	A	178	LEU
1	A	186	LYS
1	A	226	LYS
1	A	227	ASP
1	A	244	ARG
1	A	259	LEU
1	A	349	LYS
1	A	357	ILE
1	A	358	LYS
1	A	359	GLU
2	B	36	SER
2	B	60	GLU
2	B	62	ILE
2	B	74	ASP
1	C	62	ARG
1	C	106	ASP
1	C	175	GLU
1	C	187	TYR
1	C	188	GLU
1	C	194	GLU
1	C	198	GLU
1	C	262	THR
1	C	269	LEU
1	C	288	LYS
1	C	289	ARG
1	C	333	ARG
1	C	346	ARG
1	C	359	GLU
2	D	36	SER
2	D	61	LYS
2	D	70	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
1	C	199	ASN
1	C	213	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PN7	D	101	2	13,20,21	1.14	0	18,26,29	3.66	11 (61%)
4	SF4	C	1002	1	0,12,12	-	-	-		
3	FMN	A	1001	-	31,33,33	2.09	4 (12%)	40,50,50	1.66	8 (20%)
5	PN7	B	101	2	13,20,21	1.09	0	18,26,29	3.69	10 (55%)
4	SF4	A	1002	1	0,12,12	-	-	-		
3	FMN	C	1001	-	31,33,33	2.12	7 (22%)	40,50,50	1.59	7 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PN7	D	101	2	-	11/24/26/27	-
4	SF4	C	1002	1	-	-	0/6/5/5
3	FMN	A	1001	-	-	5/18/18/18	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PN7	B	101	2	-	12/24/26/27	-
4	SF4	A	1002	1	-	-	0/6/5/5
3	FMN	C	1001	-	-	5/18/18/18	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	FMN	C10-N1	5.68	1.40	1.33
3	C	1001	FMN	C8M-C8	-5.68	1.39	1.51
3	A	1001	FMN	C8M-C8	-5.67	1.39	1.51
3	A	1001	FMN	C10-N1	5.57	1.40	1.33
3	A	1001	FMN	C7M-C7	-5.42	1.40	1.51
3	C	1001	FMN	C7M-C7	-5.13	1.40	1.51
3	A	1001	FMN	C4-N3	4.29	1.40	1.33
3	C	1001	FMN	C4-N3	4.24	1.40	1.33
3	C	1001	FMN	C9A-N10	-2.47	1.35	1.38
3	C	1001	FMN	P-O3P	-2.04	1.47	1.54
3	C	1001	FMN	P-O2P	-2.01	1.47	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	101	PN7	C10-N9-C8	9.93	141.28	122.84
5	D	101	PN7	C10-N9-C8	9.59	140.64	122.84
5	B	101	PN7	C7-C8-N9	7.35	128.79	116.42
5	D	101	PN7	C7-C8-N9	6.99	128.18	116.42
3	C	1001	FMN	C4-N3-C2	5.34	119.65	115.14
3	A	1001	FMN	C4-N3-C2	5.17	119.51	115.14
5	B	101	PN7	O8-C8-C7	-4.62	113.56	122.02
5	D	101	PN7	C11-C10-N9	-4.56	101.88	112.31
3	A	1001	FMN	C1'-N10-C9A	4.53	121.86	118.29
5	D	101	PN7	O8-C8-C7	-3.88	114.92	122.02
5	B	101	PN7	CE2-C2-C3	-3.66	102.47	108.82
5	D	101	PN7	O8-C8-N9	-3.24	116.90	123.01
5	B	101	PN7	C11-C10-N9	-3.24	104.90	112.31
5	D	101	PN7	CE2-C2-C3	-3.21	103.25	108.82
3	A	1001	FMN	C4A-N5-C5A	3.18	119.95	116.77
5	B	101	PN7	C7-C6-N5	3.11	118.17	111.90
3	C	1001	FMN	C4A-N5-C5A	3.10	119.87	116.77
3	C	1001	FMN	C5A-C9A-N10	3.10	119.96	117.72
3	C	1001	FMN	C1'-N10-C9A	2.99	120.65	118.29
3	A	1001	FMN	C10-C4A-N5	-2.86	119.28	121.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	101	PN7	O8-C8-N9	-2.85	117.64	123.01
5	D	101	PN7	O4-C4-N5	-2.70	117.20	122.99
5	B	101	PN7	C6-N5-C4	2.66	127.34	122.59
5	D	101	PN7	CE2-C2-CE1	-2.62	103.83	109.17
5	D	101	PN7	CE1-C2-C1	2.62	112.50	108.23
3	C	1001	FMN	C10-C4A-N5	-2.59	119.47	121.26
3	A	1001	FMN	C4A-C4-N3	-2.56	119.93	123.43
3	A	1001	FMN	C5A-C9A-N10	2.56	119.57	117.72
5	D	101	PN7	C3-C4-N5	2.55	121.66	116.58
3	C	1001	FMN	C4A-C4-N3	-2.54	119.95	123.43
3	A	1001	FMN	C9A-N10-C10	-2.35	118.83	121.91
3	C	1001	FMN	O3P-P-O2P	2.30	116.44	107.64
5	D	101	PN7	C6-C7-C8	-2.27	108.58	112.36
3	A	1001	FMN	O3P-P-O2P	2.15	115.87	107.64
5	B	101	PN7	C6-C7-C8	-2.08	108.89	112.36
5	B	101	PN7	C3-C4-N5	2.05	120.67	116.58

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	101	PN7	C1-C2-C3-O3
5	B	101	PN7	C1-C2-C3-C4
5	B	101	PN7	CE2-C2-C3-C4
5	B	101	PN7	N9-C10-C11-S12
5	D	101	PN7	C1-C2-C3-O3
5	D	101	PN7	C1-C2-C3-C4
5	D	101	PN7	CE1-C2-C3-O3
5	D	101	PN7	CE1-C2-C3-C4
5	D	101	PN7	CE2-C2-C3-O3
5	D	101	PN7	CE2-C2-C3-C4
5	B	101	PN7	C7-C8-N9-C10
5	D	101	PN7	C7-C8-N9-C10
5	B	101	PN7	O8-C8-N9-C10
5	D	101	PN7	O8-C8-N9-C10
3	A	1001	FMN	C2'-C3'-C4'-O4'
3	A	1001	FMN	O3'-C3'-C4'-C5'
3	C	1001	FMN	O3'-C3'-C4'-C5'
3	A	1001	FMN	C2'-C3'-C4'-C5'
3	C	1001	FMN	C2'-C3'-C4'-C5'
3	C	1001	FMN	C2'-C3'-C4'-O4'
3	A	1001	FMN	O3'-C3'-C4'-O4'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	1001	FMN	O3'-C3'-C4'-O4'
5	B	101	PN7	CE2-C2-C3-O3
5	D	101	PN7	C2-C3-C4-N5
5	B	101	PN7	CE1-C2-C3-C4
3	A	1001	FMN	C4'-C5'-O5'-P
3	C	1001	FMN	C4'-C5'-O5'-P
5	B	101	PN7	C2-C3-C4-O4
5	D	101	PN7	C2-C3-C4-O4
5	B	101	PN7	C11-C10-N9-C8
5	D	101	PN7	C11-C10-N9-C8
5	B	101	PN7	C2-C3-C4-N5
5	B	101	PN7	CE1-C2-C3-O3

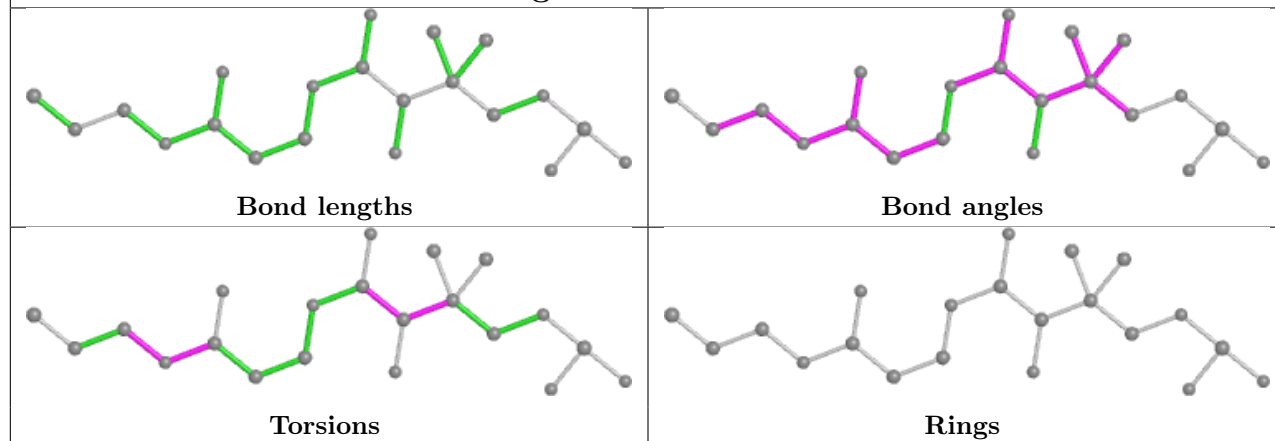
There are no ring outliers.

5 monomers are involved in 11 short contacts:

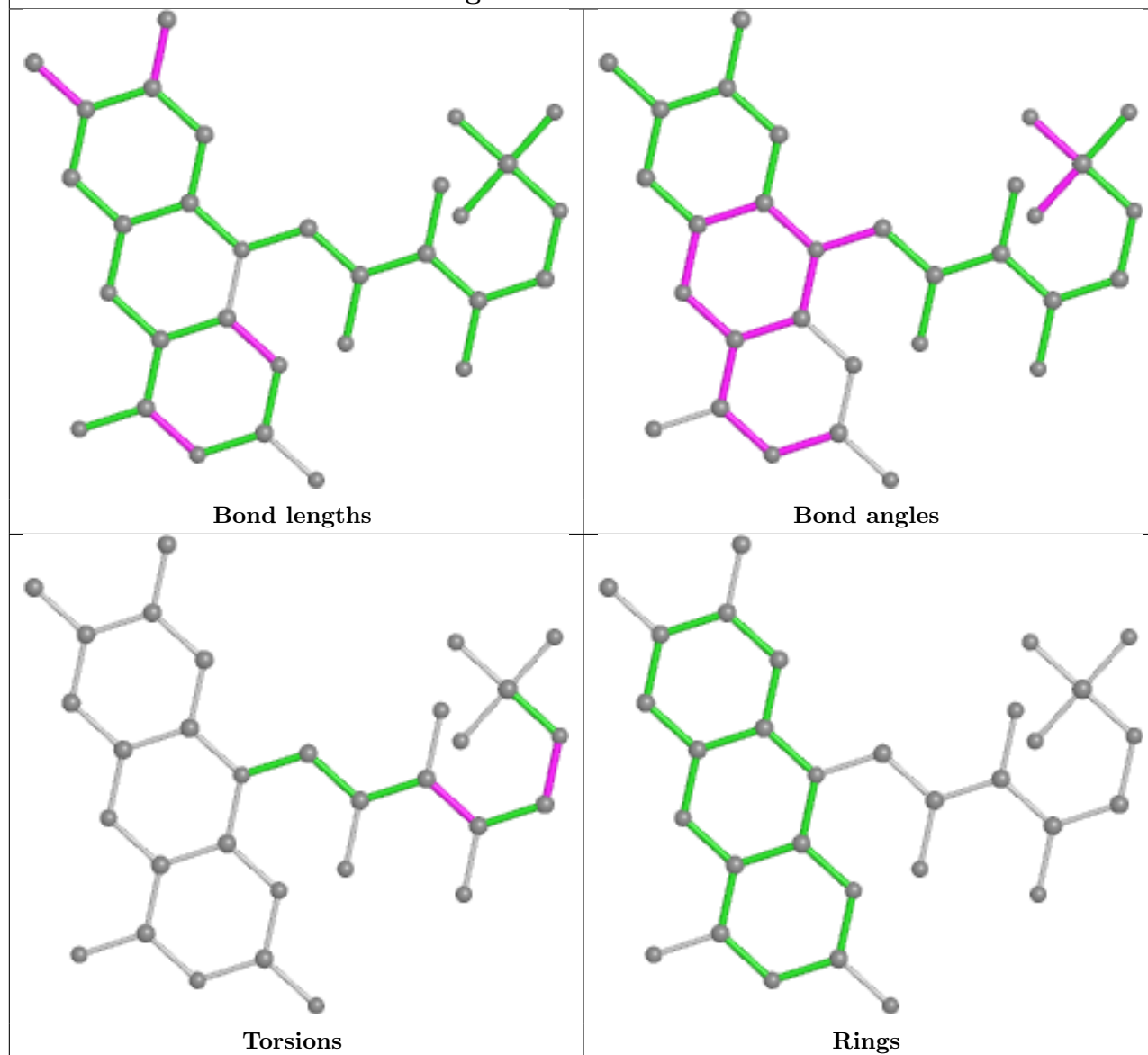
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	101	PN7	2	0
3	A	1001	FMN	2	0
5	B	101	PN7	6	0
4	A	1002	SF4	1	0
3	C	1001	FMN	1	0

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.

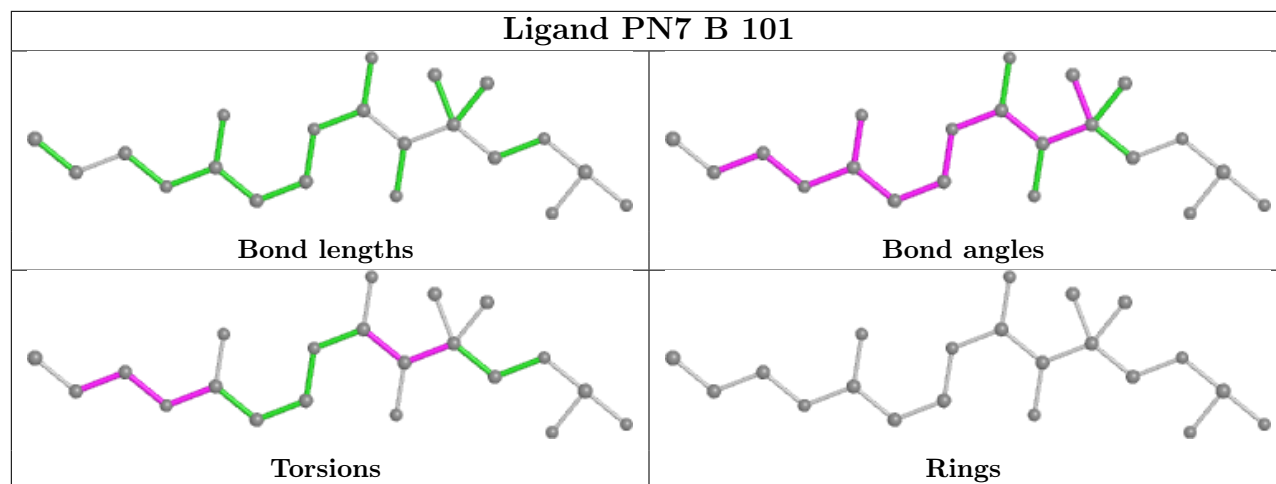
Ligand PN7 D 101



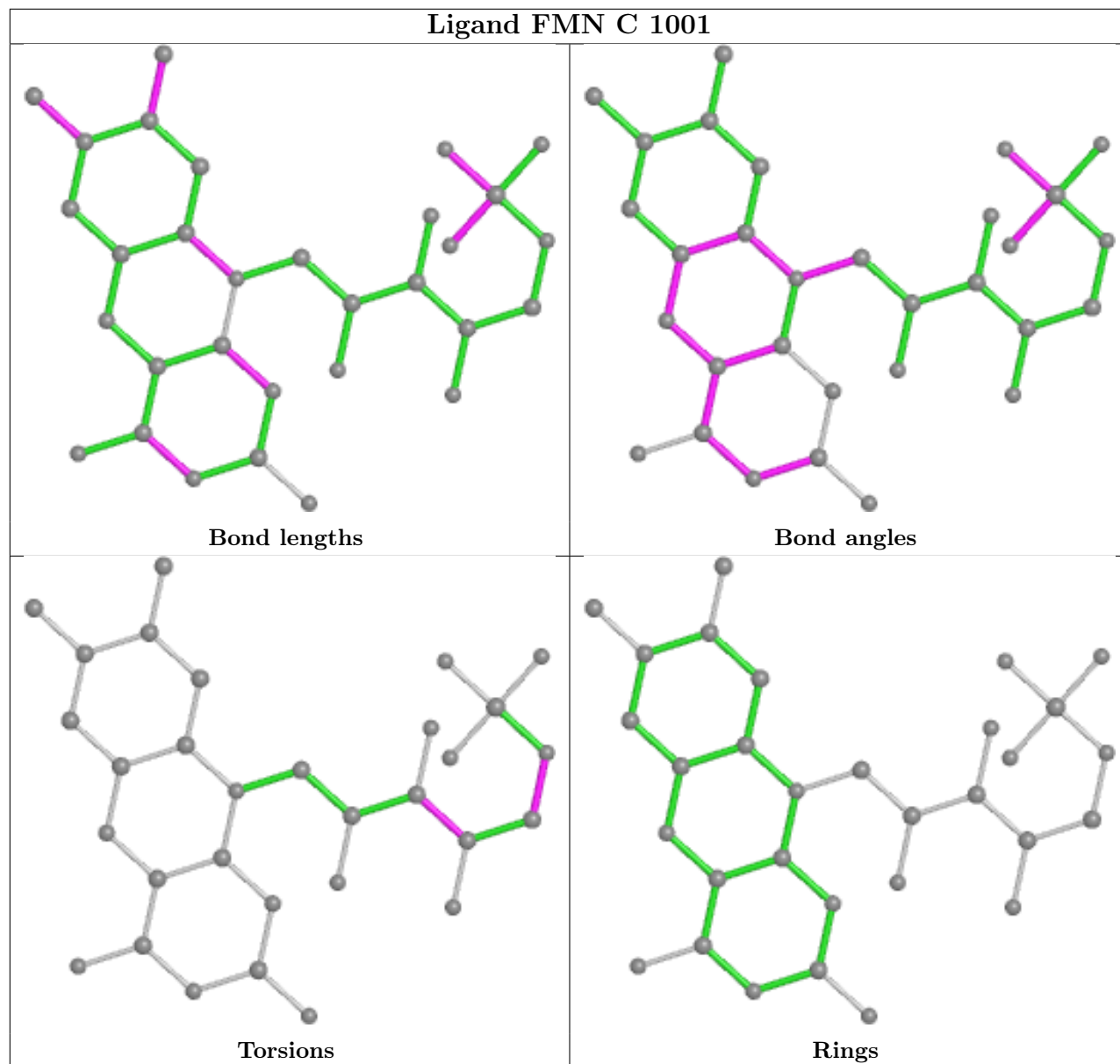
Ligand FMN A 1001



Ligand PN7 B 101



Ligand FMN C 1001



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	366/372 (98%)	-0.04	0 100 100	20, 36, 61, 75	0
1	C	366/372 (98%)	-0.01	3 (0%) 86 81	23, 39, 66, 95	0
2	B	71/86 (82%)	2.76	45 (63%) 0 0	74, 100, 120, 131	0
2	D	72/86 (83%)	2.77	42 (58%) 0 0	63, 91, 115, 120	0
All	All	875/916 (95%)	0.43	90 (10%) 6 3	20, 41, 106, 131	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	20	ALA	10.4
2	D	19	ALA	8.7
2	D	32	LEU	7.7
2	B	18	ASP	7.5
2	B	19	ALA	7.4
2	D	26	ALA	7.4
2	D	17	VAL	7.0
2	D	34	ALA	6.4
2	B	34	ALA	6.3
2	B	28	PHE	6.1
2	D	10	VAL	6.1
2	D	25	GLU	6.1
2	D	22	VAL	6.0
2	B	22	VAL	5.9
2	B	7	ILE	5.9
2	D	18	ASP	5.7
2	D	28	PHE	5.7
2	B	24	PRO	5.5
2	D	13	GLU	5.5
2	B	17	VAL	5.2
2	D	31	ASP	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	20	ALA	5.1
2	D	42	LEU	4.7
2	B	32	LEU	4.6
2	B	10	VAL	4.6
2	B	25	GLU	4.5
2	B	63	VAL	4.5
2	D	7	ILE	4.5
2	B	48	GLU	4.4
2	B	9	ALA	4.4
2	B	31	ASP	4.2
2	D	12	ALA	4.2
2	B	74	ASP	4.2
2	B	5	GLU	4.0
2	B	13	GLU	4.0
2	B	50	PHE	4.0
2	B	71	TYR	3.8
2	B	6	ASP	3.7
2	B	73	GLU	3.7
2	D	74	ASP	3.7
2	B	51	GLY	3.7
1	C	188	GLU	3.5
2	B	27	GLU	3.5
2	B	8	GLN	3.5
2	D	27	GLU	3.5
2	B	14	GLN	3.5
2	B	4	PHE	3.4
2	B	42	LEU	3.4
2	D	15	LEU	3.4
2	D	49	LYS	3.3
2	D	16	ASN	3.2
2	D	65	VAL	3.2
2	B	11	ILE	3.1
2	B	46	LEU	3.1
2	B	33	GLY	3.0
2	D	11	ILE	3.0
2	D	73	GLU	3.0
2	B	68	VAL	3.0
2	D	33	GLY	3.0
2	D	9	ALA	2.9
2	D	14	GLN	2.9
2	B	26	ALA	2.9
2	D	62	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	75	ASN	2.9
2	D	21	GLN	2.8
2	D	6	ASP	2.8
2	D	8	GLN	2.8
2	B	70	LYS	2.8
2	D	50	PHE	2.8
2	B	65	VAL	2.7
2	B	12	ALA	2.7
2	D	72	ILE	2.7
2	B	64	ASN	2.7
2	D	24	PRO	2.6
2	B	66	GLY	2.6
2	D	41	GLU	2.6
2	B	69	VAL	2.5
2	B	72	ILE	2.5
2	D	5	GLU	2.4
2	B	52	ILE	2.4
2	D	69	VAL	2.3
2	D	46	LEU	2.3
2	D	30	LYS	2.2
2	B	49	LYS	2.2
2	B	23	THR	2.2
2	D	4	PHE	2.2
1	C	-2	HIS	2.2
1	C	291	GLU	2.1
2	D	48	GLU	2.1
2	B	58	GLN	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 monosaccharides 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,

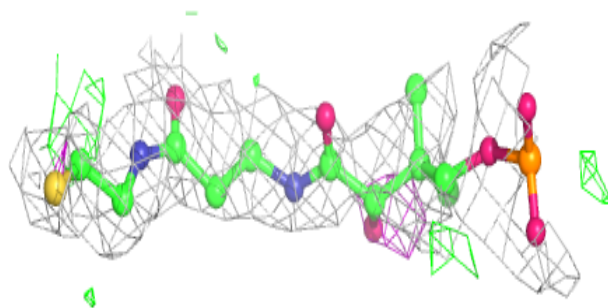
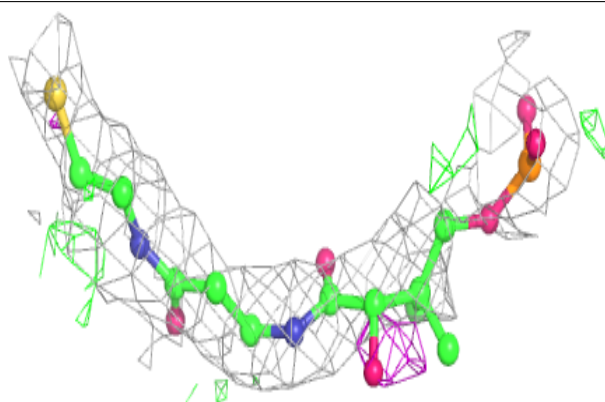
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PN7	D	101	21/22	0.72	0.33	52,69,84,99	0
5	PN7	B	101	21/22	0.81	0.26	49,59,89,105	0
3	FMN	A	1001	31/31	0.97	0.18	20,25,30,41	0
3	FMN	C	1001	31/31	0.97	0.17	25,31,36,42	0
4	SF4	A	1002	8/8	0.99	0.14	20,24,27,31	0
4	SF4	C	1002	8/8	0.99	0.12	21,27,32,39	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.

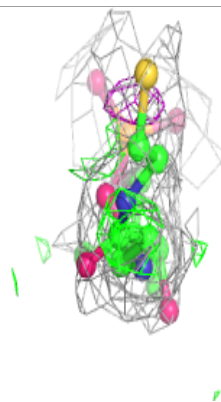
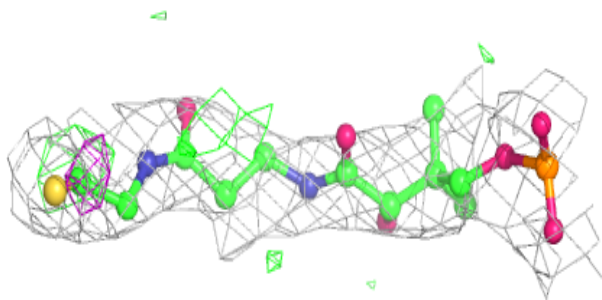
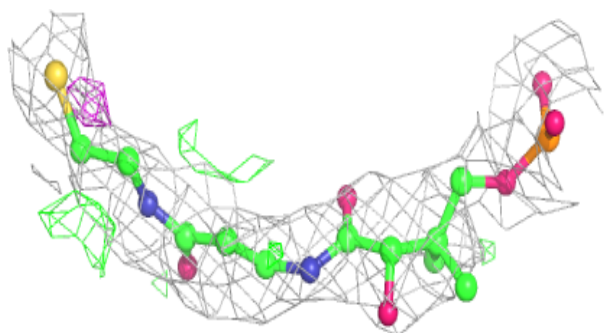
Electron density around PN7 D 101:

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

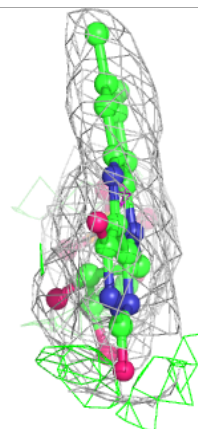
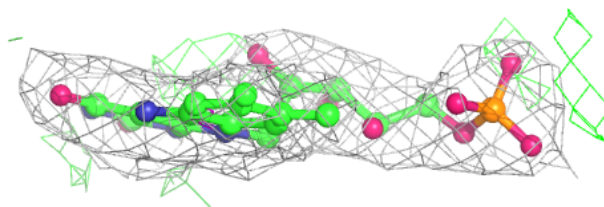
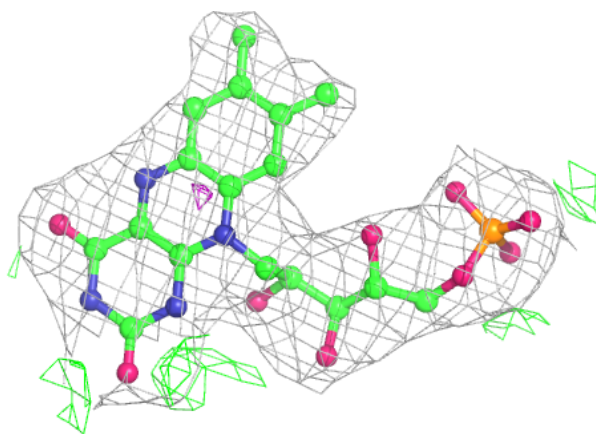


Electron density around PN7 B 101:

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

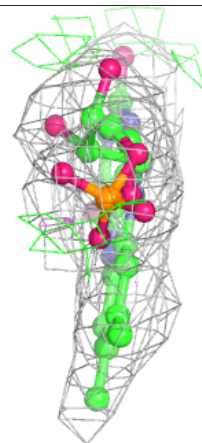
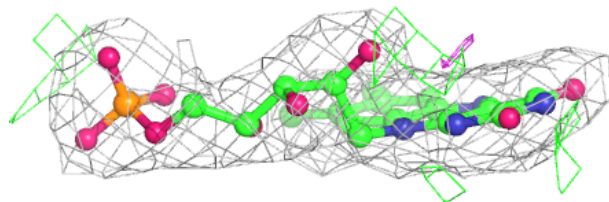
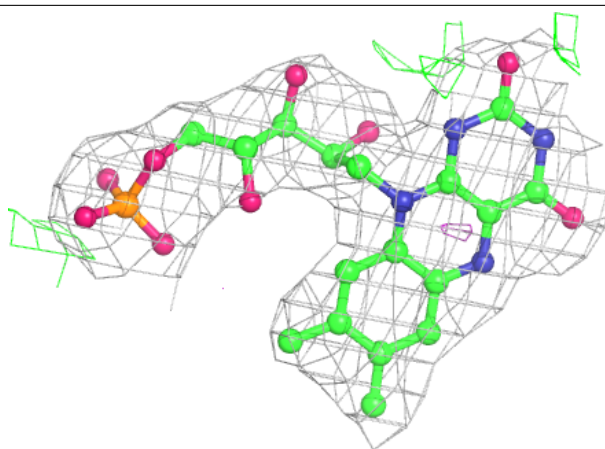
**Electron density around FMN A 1001:**

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



Electron density around FMN C 1001:

$2mF_o - DF_c$ (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.