



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:23 PM UTC

PDB ID : 7E1R / pdb_00007e1r
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 types of validation reports are described at

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

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

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

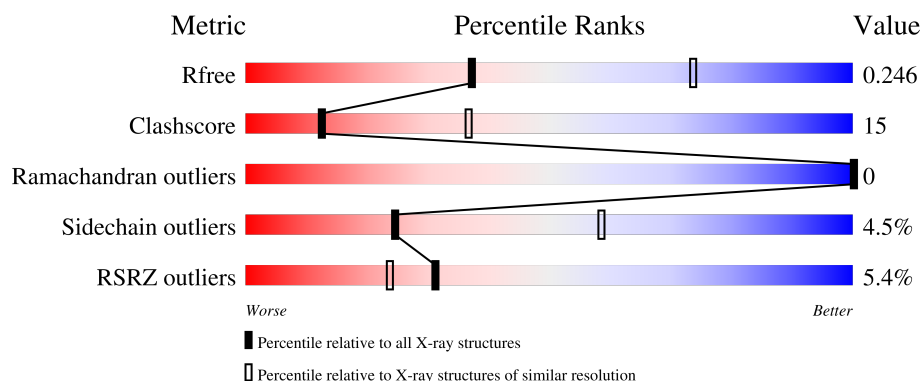
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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	
1	C	372	
2	B	86	
2	D	86	

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			

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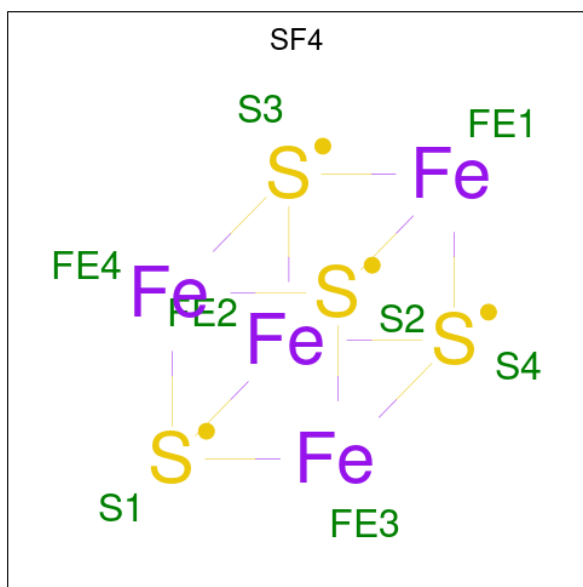
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	72	Total	C	N	O	S	0	0	0
			557	353	83	120	1			

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

-
- The chemical structure of FMN (Flavin Mononucleotide) is shown. It consists of an isoalloxazine ring system (a fused bicyclic system with two nitrogen atoms, N1 and N5, and two carbonyl groups, C2=O2 and C4=O4). The ring is substituted with a ribitol chain at the C10 position (N10). The ribitol chain is a five-carbon chain (C1' to C5') with hydroxyl groups at C1' (OH), C2' (OH), C3' (OH), and C4' (OH). The C5' carbon is attached to a phosphate group (O1P, O2P, O3P, O4P, O5P). The ribitol chain is shown in a chair conformation with the hydroxyl groups at C2', C3', and C4' in the endo position and the phosphate group at C5' in the exo position. The ribitol chain is labeled with C1', C2', C3', C4', and C5' for the carbons, and N10 for the nitrogen atom. The phosphate group is labeled with O1P, O2P, O3P, O4P, and O5P for the oxygens. The isoalloxazine ring is labeled with C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, N1, N5, N10, and O2, O4 for the atoms. The ribitol chain is shown in a chair conformation with the hydroxyl groups at C2', C3', and C4' in the endo position and the phosphate group at C5' in the exo position. The ribitol chain is labeled with C1', C2', C3', C4', and C5' for the carbons, and N10 for the nitrogen atom. The phosphate group is labeled with O1P, O2P, O3P, O4P, and O5P for the oxygens.

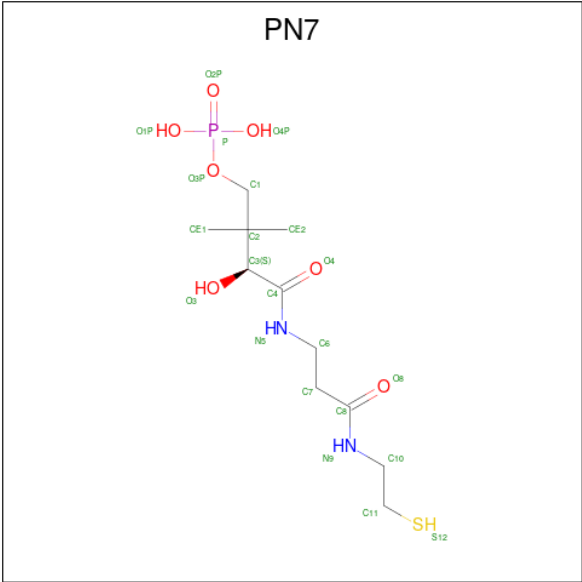
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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-sulfany ethyl)-beta-alaninamide (CCD ID: PN7) (formula: $\text{C}_{11}\text{H}_{23}\text{N}_2\text{O}_7\text{PS}$) (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		

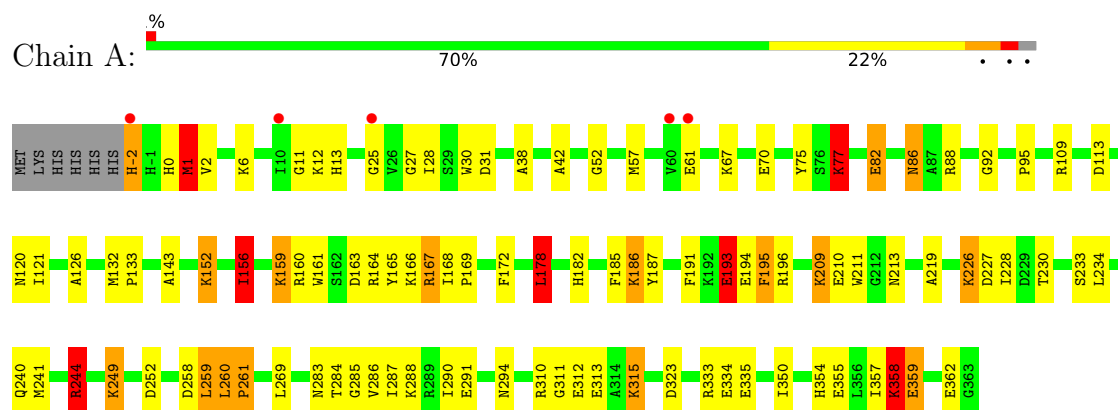
- Molecule 6 is water.

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		

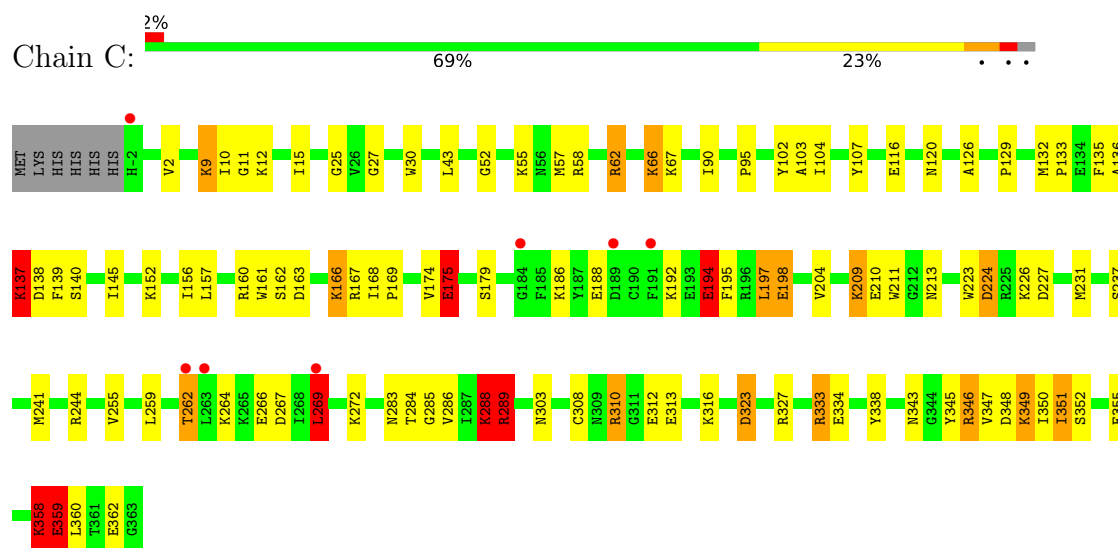
3 Residue-property plots [i](#)

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.

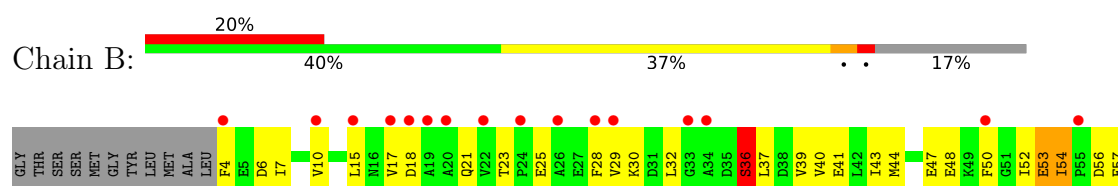
• Molecule 1: 2-nitropropane dioxygenase



• Molecule 1: 2-nitropropane dioxygenase

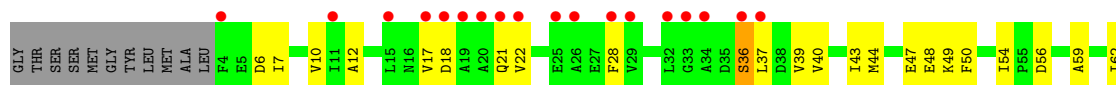


• Molecule 2: Acyl carrier protein, Acyl carrier protein





- 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 0.205 , 0.246	Depositor DCC
R_{free} test set	1104 reflections (4.25%)	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 , 42.5	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

5.1 Standard geometry

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	1.39	61/2869 (2.1%)	0.96	17/3869 (0.4%)
1	C	1.42	64/2868 (2.2%)	1.03	19/3867 (0.5%)
2	B	1.14	8/554 (1.4%)	0.96	3/752 (0.4%)
2	D	0.48	0/562	1.04	2/763 (0.3%)
All	All	1.33	133/6853 (1.9%)	1.00	41/9251 (0.4%)

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	358	LYS	C-O	-11.71	1.10	1.24
1	A	312	GLU	C-O	-10.72	1.11	1.24
1	C	231	MET	C-O	-10.43	1.11	1.24
1	C	224	ASP	C-O	-10.41	1.10	1.24
1	C	358	LYS	CA-C	-10.37	1.40	1.52
1	A	2	VAL	C-O	-10.35	1.10	1.24
1	C	327	ARG	C-O	-10.02	1.11	1.24
1	A	354	HIS	C-O	-10.01	1.12	1.24
1	C	323	ASP	C-O	-9.89	1.12	1.24
1	A	358	LYS	C-O	-9.67	1.12	1.24
1	A	244	ARG	C-O	-9.61	1.13	1.24
1	C	227	ASP	C-O	-9.46	1.12	1.24
1	C	9	LYS	C-O	-9.19	1.12	1.24
1	C	349	LYS	N-CA	-9.14	1.35	1.46
1	C	347	VAL	C-O	-9.03	1.14	1.24
1	A	249	LYS	C-O	-9.03	1.12	1.24
1	A	0	HIS	C-O	-8.90	1.13	1.24
1	C	198	GLU	C-O	-8.75	1.12	1.24
1	A	227	ASP	C-O	-8.74	1.12	1.24
1	C	209	LYS	C-O	-8.70	1.13	1.24
1	C	166	LYS	C-O	-8.58	1.12	1.23
1	A	1	MET	C-O	-8.27	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	163	ASP	C-O	-8.06	1.14	1.24
1	A	195	PHE	C-O	-8.00	1.13	1.24
1	C	175	GLU	C-O	-7.96	1.14	1.24
1	C	136	ALA	C-O	-7.69	1.14	1.24
1	A	0	HIS	CA-C	-7.65	1.43	1.52
1	C	138	ASP	C-O	-7.64	1.13	1.24
1	A	209	LYS	C-O	-7.56	1.14	1.24
1	C	345	TYR	C-O	-7.54	1.14	1.24
1	C	195	PHE	C-O	-7.48	1.14	1.24
1	C	350	ILE	CA-CB	-7.46	1.45	1.53
1	C	289	ARG	C-O	-7.38	1.15	1.24
1	A	258	ASP	C-O	-7.33	1.14	1.24
1	A	244	ARG	N-CA	-7.27	1.37	1.46
1	C	62	ARG	C-O	-7.21	1.15	1.23
1	A	261	PRO	C-O	-7.13	1.15	1.24
1	C	288	LYS	C-O	-7.12	1.15	1.24
1	C	333	ARG	N-CA	-7.09	1.36	1.46
1	A	315	LYS	CA-C	-7.05	1.43	1.52
1	A	259	LEU	C-O	-6.96	1.14	1.24
1	C	350	ILE	C-O	-6.94	1.16	1.24
1	C	135	PHE	CA-C	-6.94	1.43	1.52
1	C	197	LEU	C-O	-6.93	1.16	1.24
1	A	252	ASP	CG-OD2	-6.89	1.12	1.25
1	A	315	LYS	C-O	-6.89	1.15	1.24
1	C	333	ARG	CA-C	-6.83	1.43	1.52
1	C	359	GLU	C-O	-6.76	1.16	1.24
1	A	210	GLU	C-O	-6.75	1.15	1.24
1	A	226	LYS	C-O	-6.73	1.15	1.24
1	C	327	ARG	CA-C	-6.72	1.43	1.52
1	A	313	GLU	C-O	-6.69	1.15	1.24
1	A	163	ASP	C-O	-6.68	1.16	1.24
1	A	167	ARG	C-O	-6.67	1.15	1.23
1	C	175	GLU	CA-C	-6.67	1.44	1.52
1	A	334	GLU	C-O	-6.64	1.15	1.24
1	C	194	GLU	CA-C	-6.63	1.43	1.52
1	A	312	GLU	CA-C	-6.56	1.44	1.52
1	C	135	PHE	C-O	-6.56	1.14	1.23
1	C	345	TYR	CA-C	-6.53	1.43	1.52
1	C	104	ILE	C-O	-6.46	1.15	1.24
1	A	310	ARG	CA-C	-6.43	1.44	1.52
1	C	351	ILE	C-O	-6.43	1.16	1.23
1	A	313	GLU	CA-C	-6.38	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	LEU	C-O	-6.37	1.15	1.24
1	A	359	GLU	C-O	-6.37	1.16	1.24
1	C	137	LYS	N-CA	-6.36	1.38	1.46
1	C	116	GLU	C-O	-6.35	1.16	1.24
1	C	333	ARG	C-O	-6.30	1.15	1.24
1	A	358	LYS	CA-C	-6.28	1.44	1.52
1	C	209	LYS	CA-C	-6.21	1.44	1.52
1	A	355	GLU	C-O	-6.20	1.16	1.24
1	A	227	ASP	CA-C	-6.18	1.44	1.52
2	B	57	GLU	CA-C	-6.16	1.45	1.52
1	A	354	HIS	CA-C	-6.13	1.44	1.52
1	A	244	ARG	CZ-NH1	-6.10	1.24	1.32
1	C	362	GLU	CA-C	-6.08	1.44	1.52
2	B	57	GLU	C-O	-6.07	1.17	1.24
1	C	231	MET	CA-C	-6.06	1.45	1.52
1	A	310	ARG	N-CA	-6.06	1.38	1.46
1	A	260	LEU	C-O	-5.95	1.16	1.24
1	C	138	ASP	N-CA	-5.94	1.38	1.46
1	A	312	GLU	N-CA	-5.93	1.39	1.46
1	A	252	ASP	C-O	-5.92	1.16	1.24
1	C	103	ALA	C-N	-5.89	1.26	1.33
1	A	178	LEU	C-O	-5.86	1.16	1.24
2	B	56	ASP	C-O	-5.85	1.17	1.24
2	B	54	ILE	CA-C	-5.79	1.46	1.52
1	A	82	GLU	C-O	-5.74	1.17	1.24
1	C	138	ASP	CA-C	-5.72	1.43	1.52
1	A	193	GLU	CA-C	-5.72	1.44	1.52
1	A	287	ILE	CA-CB	-5.68	1.46	1.54
1	A	159	LYS	C-O	-5.67	1.17	1.24
1	C	348	ASP	C-O	-5.66	1.16	1.24
1	A	244	ARG	CA-CB	-5.66	1.44	1.53
1	A	193	GLU	C-N	-5.62	1.26	1.34
1	A	209	LYS	N-CA	-5.59	1.39	1.46
1	A	249	LYS	CA-C	-5.59	1.45	1.52
1	C	362	GLU	C-O	-5.58	1.17	1.23
1	A	191	PHE	C-O	-5.57	1.17	1.24
1	C	288	LYS	C-N	-5.57	1.26	1.33
2	B	54	ILE	C-O	-5.54	1.17	1.24
1	A	209	LYS	CA-C	-5.52	1.45	1.52
2	B	53	GLU	CA-C	-5.44	1.46	1.52
1	A	334	GLU	CA-C	-5.43	1.45	1.52
1	C	135	PHE	CA-CB	-5.42	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	310	ARG	CA-CB	-5.39	1.44	1.53
1	C	198	GLU	N-CA	-5.38	1.39	1.46
1	C	197	LEU	CA-C	-5.33	1.45	1.52
1	A	77	LYS	C-O	-5.33	1.17	1.24
1	C	137	LYS	CA-C	-5.31	1.45	1.52
1	A	193	GLU	C-O	-5.30	1.17	1.24
1	C	327	ARG	N-CA	-5.28	1.39	1.46
1	C	195	PHE	C-N	-5.28	1.26	1.33
2	B	60	GLU	C-O	-5.26	1.17	1.24
1	A	252	ASP	CG-OD1	-5.26	1.15	1.25
1	A	185	PHE	C-O	-5.23	1.17	1.23
1	A	152	LYS	C-O	-5.22	1.18	1.24
1	C	310	ARG	CA-C	-5.19	1.45	1.53
1	A	167	ARG	CA-C	-5.18	1.46	1.52
1	C	224	ASP	CA-C	-5.18	1.46	1.52
1	C	323	ASP	CA-C	-5.17	1.46	1.52
1	C	327	ARG	CZ-NH2	-5.17	1.26	1.33
1	A	315	LYS	C-N	-5.14	1.26	1.34
2	B	62	ILE	C-O	-5.12	1.18	1.24
1	C	333	ARG	CD-NE	-5.09	1.39	1.46
1	C	349	LYS	CA-C	-5.08	1.46	1.52
1	A	312	GLU	CA-CB	-5.08	1.45	1.53
1	C	327	ARG	CZ-NH1	-5.08	1.25	1.32
1	A	-2	HIS	C-O	-5.06	1.13	1.23
1	C	267	ASP	C-O	-5.06	1.17	1.24
1	C	139	PHE	C-O	-5.05	1.16	1.23
1	C	136	ALA	CA-C	-5.03	1.45	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	22	VAL	CA-C-N	15.64	141.63	120.67
2	D	22	VAL	C-N-CA	15.64	141.63	120.67
1	C	349	LYS	N-CA-CB	-8.61	97.52	110.35
1	A	259	LEU	N-CA-C	8.37	123.61	113.23
2	B	36	SER	CA-CB-OG	7.97	127.05	111.10
1	A	6	LYS	CG-CD-CE	-7.11	94.95	111.30
1	C	2	VAL	N-CA-C	7.06	119.80	109.63
1	C	348	ASP	CA-C-N	7.01	132.71	122.41
1	C	348	ASP	C-N-CA	7.01	132.71	122.41
1	C	310	ARG	N-CA-C	6.99	121.18	112.24
1	A	11	GLY	N-CA-C	-6.72	97.25	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62	ARG	N-CA-C	6.69	120.53	108.69
1	C	224	ASP	N-CA-C	6.61	118.18	108.86
1	C	25	GLY	N-CA-C	6.60	120.52	111.54
1	C	358	LYS	CB-CA-C	-6.46	100.93	110.95
1	C	197	LEU	N-CA-C	6.35	119.01	111.33
2	B	59	ALA	N-CA-C	6.26	120.18	112.54
1	A	244	ARG	CB-CA-C	-6.25	101.08	110.88
1	A	25	GLY	N-CA-C	6.22	120.00	111.54
1	A	193	GLU	N-CA-C	-6.10	105.67	113.23
1	A	310	ARG	N-CA-C	5.99	123.56	110.80
1	A	28	ILE	CG1-CB-CG2	-5.99	92.74	110.70
1	A	294	ASN	CB-CA-C	5.96	120.69	111.28
1	C	2	VAL	CA-C-N	5.95	129.21	120.82
1	C	2	VAL	C-N-CA	5.95	129.21	120.82
1	C	348	ASP	CA-C-O	5.93	125.35	118.77
1	A	244	ARG	NE-CZ-NH2	5.93	124.54	119.20
1	A	2	VAL	CA-C-N	5.87	129.89	121.50
1	A	2	VAL	C-N-CA	5.87	129.89	121.50
1	C	269	LEU	CB-CA-C	-5.77	98.46	109.66
1	C	351	ILE	N-CA-CB	-5.70	102.89	112.47
1	C	66	LYS	CG-CD-CE	5.53	124.01	111.30
1	A	156	ILE	CG1-CB-CG2	-5.42	94.45	110.70
1	C	104	ILE	N-CA-C	5.34	116.90	109.80
1	C	269	LEU	N-CA-CB	5.34	119.85	111.20
1	A	6	LYS	CB-CA-C	5.27	116.45	108.86
1	A	193	GLU	CA-C-O	5.26	125.42	119.27
1	A	0	HIS	N-CA-CB	-5.23	101.54	110.16
1	A	210	GLU	CB-CG-CD	5.21	121.47	112.60
2	B	62	ILE	N-CA-C	5.21	116.09	108.58
1	C	351	ILE	CB-CA-C	-5.07	103.60	110.90

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	73	2
1	C	2812	0	2863	83	0
2	B	549	0	534	43	2
2	D	557	0	540	33	0
3	A	31	0	19	1	0
3	C	31	0	19	0	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	4	0
All	All	6895	0	6884	210	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 (210) 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)
2:B:48:GLU:CD	1:C:213:ASN:ND2	2.19	1.01
1:A:152:LYS:HE2	2:B:37:LEU:HB2	1.43	0.98
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:48:GLU:CD	1:C:213:ASN:HD22	1.79	0.87
2:B:28:PHE:CE1	2:B:65:VAL:HG12	2.10	0.85
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:48:GLU:CD	1:C:213:ASN:HD21	2.07	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: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
1:C:57:MET:HE1	1:C:66:LYS:O	2.05	0.56
2:B:37:LEU:O	2:B:41:GLU:CG	2.51	0.56
1:A:132:MET:HE3	1:A:161:TRP:CZ2	2.41	0.56
1:A:152:LYS:HG2	2:B:37:LEU:CD2	2.36	0.56
1:C:241:MET:HE1	1:C:360:LEU:HD13	1.88	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:70:LYS:O	2:D:70:LYS:HD3	2.06	0.54
1:A:132:MET:HE3	1:A:161:TRP:HZ2	1.72	0.54
1:C:272:LYS:NZ	6:C:1104:HOH:O	2.41	0.54
1:C:241:MET:HE1	1:C:360:LEU:CD1	2.37	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
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:160:ARG:HE	1:A:164:ARG:HH21	1.59	0.50
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:266:GLU:CD	1:C:266:GLU:H	2.19	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:A:186:LYS:O	1:A:187:TYR:C	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:159:LYS:HB2	2:B:44:MET:HE1	1.94	0.48
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:C:313:GLU:OE2	1:C:316:LYS:NZ	2.33	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:27:GLY:HA2	1:A:30:TRP:CE3	2.51	0.46
1:A:195:PHE:O	1:A:196:ARG:C	2.50	0.46
2:B:6:ASP:O	2:B:10:VAL:HG23	2.16	0.46
1:C:209:LYS:O	1:C:210:GLU:C	2.53	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:PRO:HA	1:C:120:ASN:OD1	2.17	0.44
1:A:1:MET:HB3	1:A:1:MET:HE3	1.70	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:A:228:ILE:HD11	1:A:241:MET:HE1	2.00	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
1:A:12:LYS:HZ2	1:A:13:HIS:CE1	2.37	0.42
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:67:LYS:HD3	1:C:323:ASP:CG	2.44	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
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:C:358:LYS:NZ	6:C:1107:HOH:O	2.53	0.42
1:A:333:ARG:HG2	6:A:1115:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:209:LYS:C	1:C:211:TRP:N	2.74	0.41
1:C:308:CYS:HA	1:C:313:GLU:HB2	2.03	0.41
1:C:289:ARG:HH21	1:C:334:GLU:HA	1.85	0.41
1:C:358:LYS:O	1:C:359:GLU:C	2.62	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
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
2:B:17:VAL:HG11	2:B:32:LEU:HD23	2.03	0.40
1:C:224:ASP:OD1	1:C:226:LYS:HG2	2.21	0.40
2:D:70:LYS:HD3	2:D:70:LYS:C	2.47	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 [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	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%)	280 (95%)	14 (5%)	23	56
1	C	293/300 (98%)	279 (95%)	14 (5%)	23	56
2	B	60/71 (84%)	57 (95%)	3 (5%)	22	54
2	D	61/71 (86%)	60 (98%)	1 (2%)	55	83
All	All	708/742 (95%)	676 (96%)	32 (4%)	24	58

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	1	MET
1	A	77	LYS
1	A	86	ASN
1	A	156	ILE
1	A	167	ARG
1	A	178	LEU
1	A	186	LYS
1	A	193	GLU
1	A	244	ARG

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Mol	Chain	Res	Type
1	A	259	LEU
1	A	357	ILE
1	A	358	LYS
1	A	359	GLU
2	B	36	SER
2	B	60	GLU
2	B	62	ILE
1	C	62	ARG
1	C	137	LYS
1	C	175	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	355	GLU
1	C	358	LYS
1	C	359	GLU
2	D	36	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	213	ASN
1	A	240	GLN
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
4	SF4	A	1002	1	0,12,12	-	-	-		
3	FMN	A	1001	-	33,33,33	1.95	6 (18%)	48,50,50	1.34	7 (14%)
3	FMN	C	1001	-	33,33,33	2.00	8 (24%)	48,50,50	1.35	10 (20%)
5	PN7	B	101	2	14,20,21	1.18	1 (7%)	18,26,29	3.63	10 (55%)
4	SF4	C	1002	1	0,12,12	-	-	-		
5	PN7	D	101	2	14,20,21	1.47	1 (7%)	18,26,29	3.61	11 (61%)

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
4	SF4	A	1002	1	-	-	0/6/5/5
3	FMN	A	1001	-	-	5/18/18/18	0/3/3/3
3	FMN	C	1001	-	-	5/18/18/18	0/3/3/3
5	PN7	B	101	2	-	12/24/26/27	-
4	SF4	C	1002	1	-	-	0/6/5/5
5	PN7	D	101	2	-	12/24/26/27	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	FMN	C8M-C8	-6.06	1.39	1.51
3	A	1001	FMN	C8M-C8	-6.05	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	FMN	C7M-C7	-5.79	1.40	1.51
3	C	1001	FMN	C7M-C7	-5.48	1.40	1.51
5	D	101	PN7	C1-C2	3.72	1.58	1.52
3	C	1001	FMN	C10-N1	3.62	1.40	1.33
3	A	1001	FMN	C10-N1	3.55	1.40	1.33
3	C	1001	FMN	C9A-N10	-3.46	1.35	1.41
3	A	1001	FMN	C9A-N10	-2.97	1.36	1.41
3	C	1001	FMN	C1'-C2'	2.69	1.56	1.52
3	C	1001	FMN	C5A-N5	-2.51	1.34	1.39
3	A	1001	FMN	C5A-N5	-2.47	1.34	1.39
3	C	1001	FMN	P-O3P	-2.10	1.47	1.54
5	B	101	PN7	C1-C2	2.09	1.56	1.52
3	C	1001	FMN	P-O2P	-2.08	1.47	1.54
3	A	1001	FMN	P-O3P	-2.06	1.47	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	101	PN7	C10-N9-C8	9.91	141.28	122.82
5	D	101	PN7	C10-N9-C8	9.57	140.64	122.82
5	B	101	PN7	C7-C8-N9	6.83	128.79	116.34
5	D	101	PN7	C7-C8-N9	6.50	128.18	116.34
5	B	101	PN7	O8-C8-C7	-4.67	113.56	122.02
5	D	101	PN7	C11-C10-N9	-4.60	101.88	112.31
5	D	101	PN7	O8-C8-C7	-3.92	114.92	122.02
5	B	101	PN7	CE2-C2-C3	-3.69	102.47	108.77
3	A	1001	FMN	C4-N3-C2	-3.45	119.51	125.64
3	C	1001	FMN	C4-N3-C2	-3.37	119.65	125.64
5	B	101	PN7	C11-C10-N9	-3.27	104.90	112.31
5	D	101	PN7	CE2-C2-C3	-3.24	103.25	108.77
3	A	1001	FMN	C4A-C10-N10	3.17	121.02	116.48
5	D	101	PN7	O8-C8-N9	-3.13	116.90	123.03
5	B	101	PN7	C7-C6-N5	2.90	118.17	112.00
3	C	1001	FMN	C4A-C10-N10	2.77	120.44	116.48
5	B	101	PN7	O8-C8-N9	-2.75	117.64	123.03
5	D	101	PN7	O4-C4-N5	-2.73	117.20	122.98
5	D	101	PN7	C3-C4-N5	2.73	121.66	116.48
3	A	1001	FMN	C10-C4A-N5	-2.71	119.28	124.81
5	D	101	PN7	CE2-C2-CE1	-2.70	103.83	109.20
5	B	101	PN7	C6-N5-C4	2.67	127.34	122.55
3	C	1001	FMN	C4A-C4-N3	2.63	119.95	113.25
3	A	1001	FMN	C4A-C4-N3	2.62	119.93	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1001	FMN	C10-C4A-N5	-2.62	119.47	124.81
5	D	101	PN7	CE1-C2-C1	2.59	112.50	108.22
3	C	1001	FMN	O3P-P-O2P	2.30	116.44	107.80
5	D	101	PN7	C6-C7-C8	-2.29	108.58	112.39
3	C	1001	FMN	C9A-C5A-N5	-2.29	120.03	122.45
3	C	1001	FMN	C5A-C9A-N10	2.21	119.96	117.97
5	B	101	PN7	C3-C4-N5	2.21	120.67	116.48
3	A	1001	FMN	O3P-P-O2P	2.15	115.87	107.80
3	A	1001	FMN	C4-C4A-C10	2.13	120.59	116.93
5	B	101	PN7	C6-C7-C8	-2.10	108.89	112.39
3	C	1001	FMN	C4-C4A-C10	2.07	120.48	116.93
3	C	1001	FMN	O4-C4-C4A	-2.06	121.10	126.53
3	C	1001	FMN	C4A-C10-N1	-2.03	119.60	124.59
3	A	1001	FMN	C4A-C10-N1	-2.00	119.68	124.59

There are no chirality outliers.

All (34) 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'
3	C	1001	FMN	O3'-C3'-C4'-O4'
5	B	101	PN7	CE2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	D	101	PN7	C2-C3-C4-N5
5	B	101	PN7	CE1-C2-C3-C4
5	D	101	PN7	N9-C10-C11-S12
5	B	101	PN7	C2-C3-C4-O4
5	D	101	PN7	C2-C3-C4-O4
3	A	1001	FMN	C4'-C5'-O5'-P
3	C	1001	FMN	C4'-C5'-O5'-P
5	B	101	PN7	C2-C3-C4-N5
5	B	101	PN7	C11-C10-N9-C8
5	D	101	PN7	C11-C10-N9-C8
5	B	101	PN7	CE1-C2-C3-O3

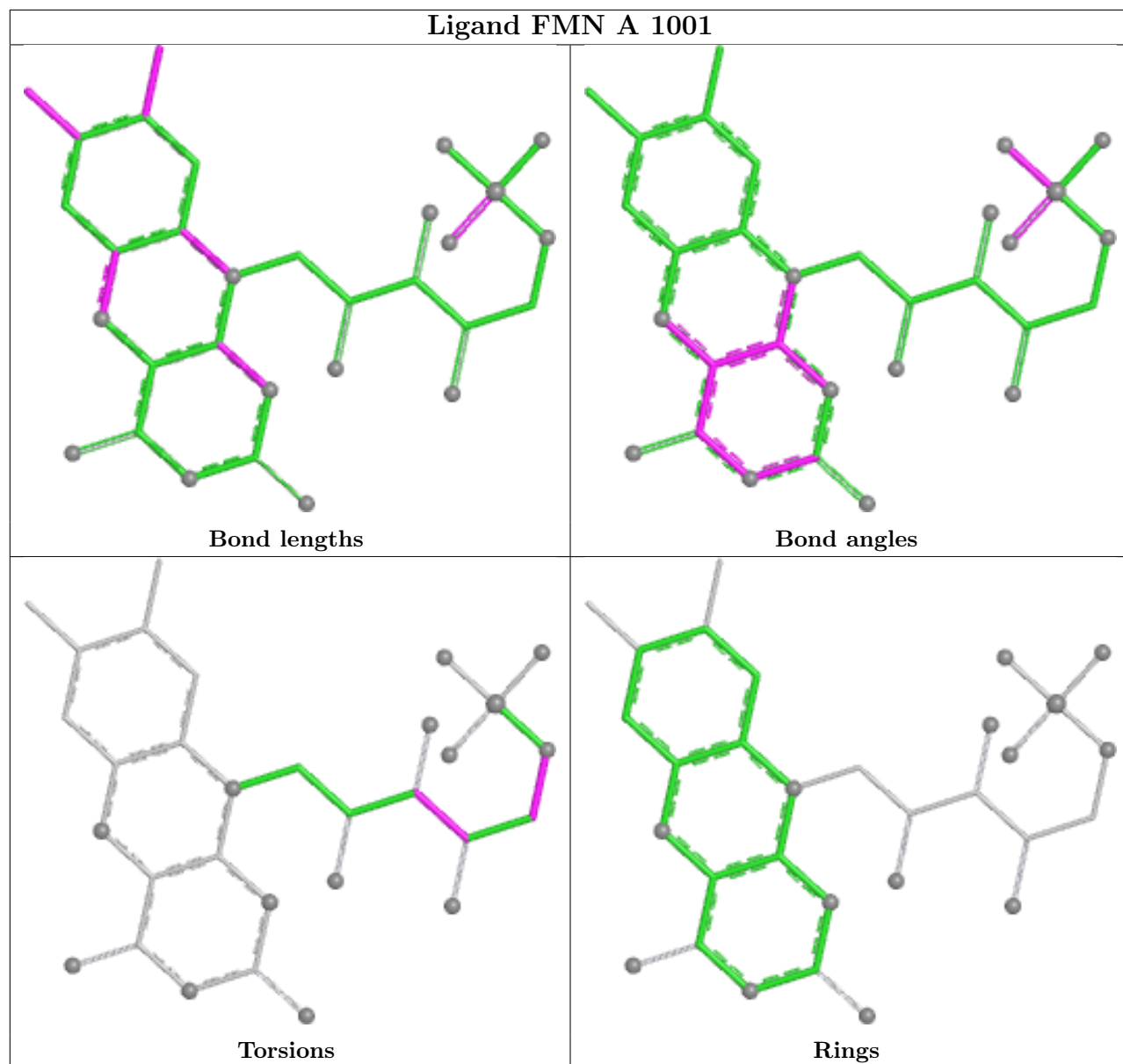
There are no ring outliers.

4 monomers are involved in 9 short contacts:

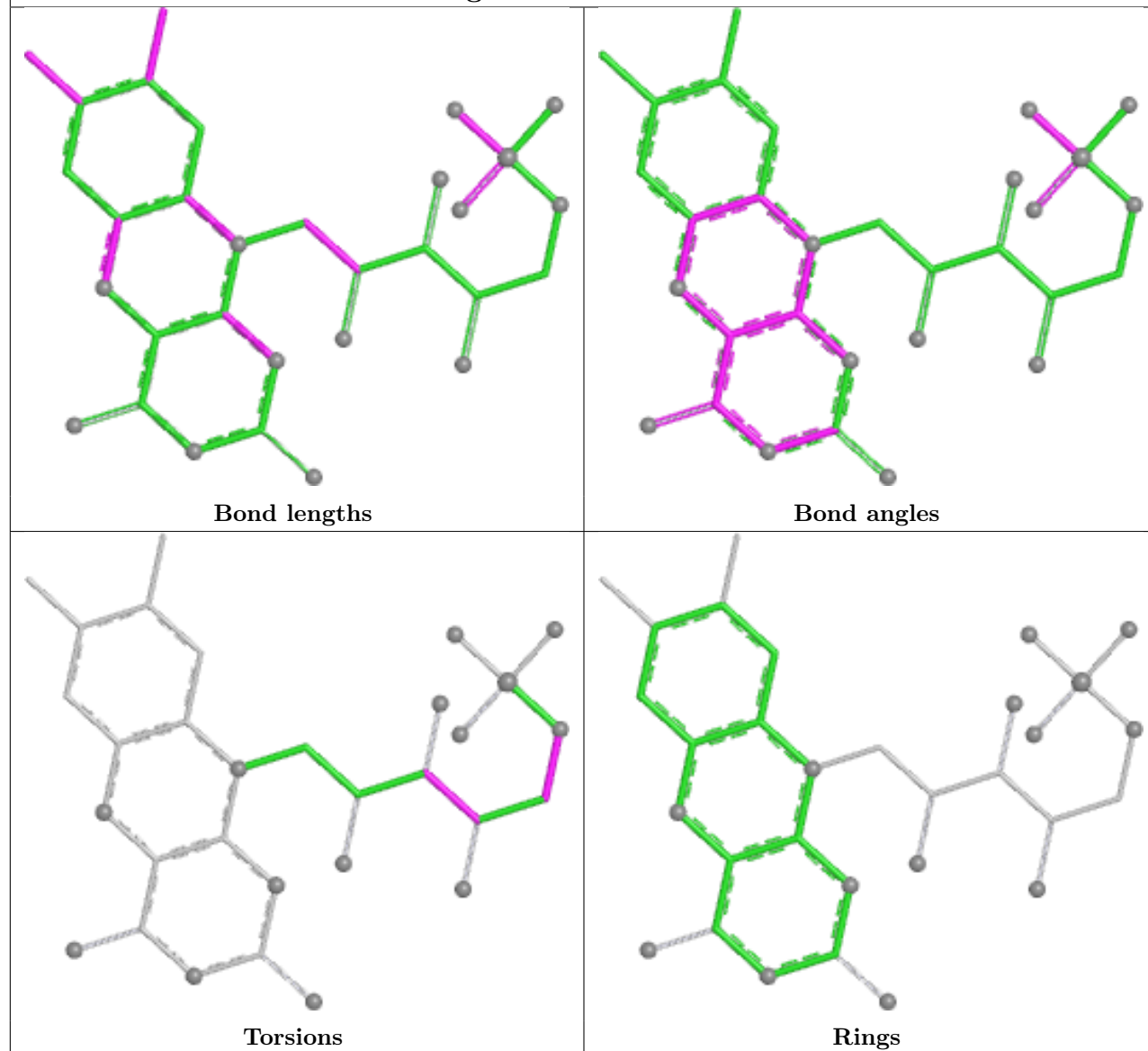
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	SF4	1	0
3	A	1001	FMN	1	0
5	B	101	PN7	6	0
5	D	101	PN7	2	0

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

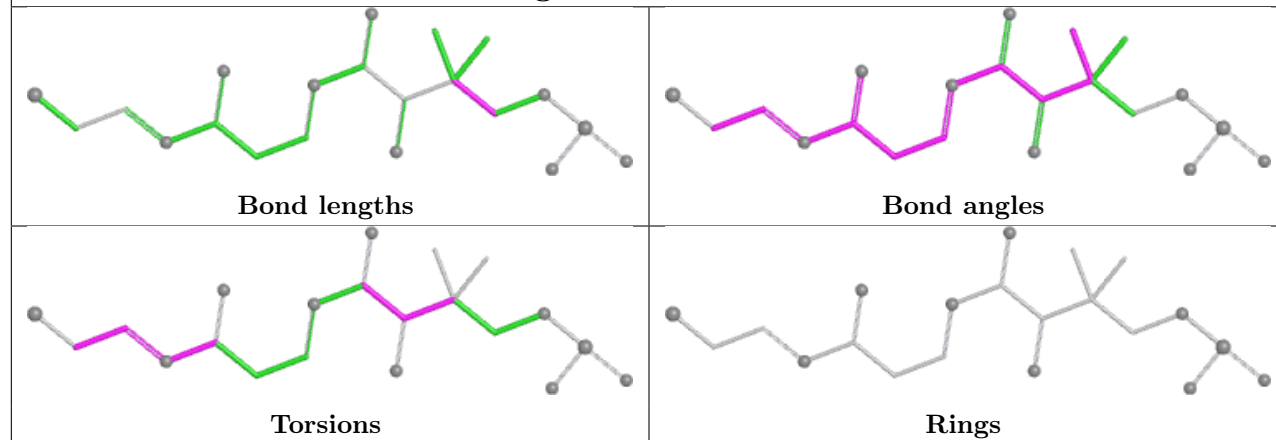
Ligand FMN A 1001

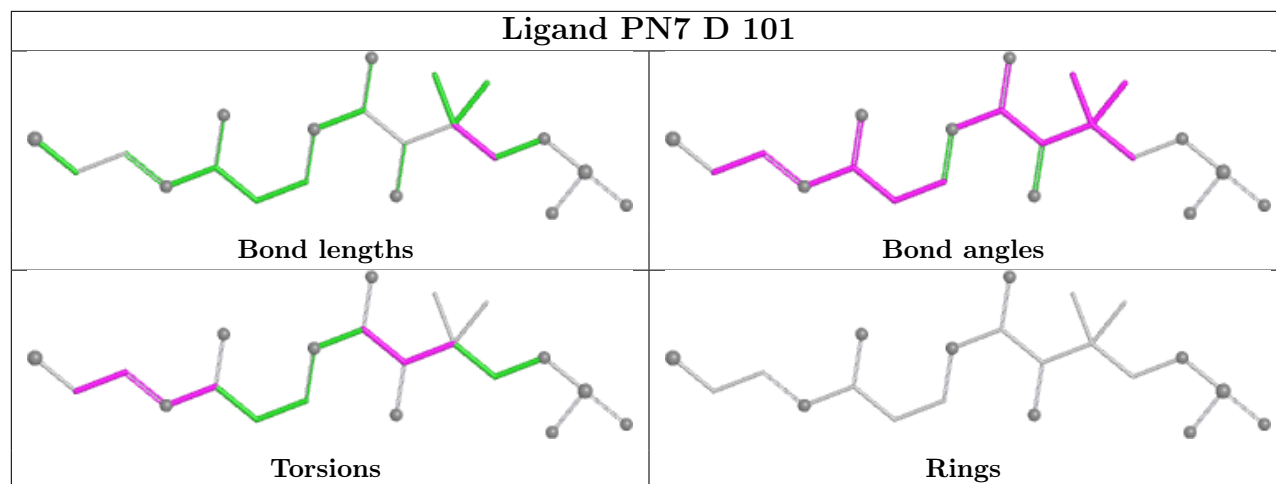


Ligand FMN C 1001



Ligand PN7 B 101





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%)	0.06	5 (1%) 73 64	20, 36, 61, 75	0
1	C	366/372 (98%)	0.13	7 (1%) 66 57	23, 39, 66, 95	0
2	B	71/86 (82%)	1.48	17 (23%) 2 1	74, 100, 120, 131	0
2	D	72/86 (83%)	1.45	18 (25%) 2 1	63, 91, 115, 120	0
All	All	875/916 (95%)	0.32	47 (5%) 31 24	20, 41, 106, 131	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	20	ALA	4.0
2	D	29	VAL	3.8
2	D	19	ALA	3.8
2	D	34	ALA	3.6
2	D	26	ALA	3.5
2	B	19	ALA	3.5
1	C	-2	HIS	3.5
2	D	15	LEU	3.3
2	B	33	GLY	3.1
2	B	17	VAL	3.1
2	B	22	VAL	3.1
2	D	36	SER	3.0
2	B	18	ASP	2.8
2	B	4	PHE	2.8
2	B	29	VAL	2.8
2	B	50	PHE	2.8
2	B	28	PHE	2.7
2	B	20	ALA	2.6
1	C	262	THR	2.5
2	D	33	GLY	2.5
2	B	15	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	-2	HIS	2.4
1	C	191	PHE	2.4
2	D	28	PHE	2.4
1	C	184	GLY	2.4
2	B	34	ALA	2.4
1	C	189	ASP	2.3
2	D	17	VAL	2.3
2	D	22	VAL	2.3
2	D	32	LEU	2.3
2	D	25	GLU	2.3
1	C	269	LEU	2.3
2	B	65	VAL	2.3
2	D	37	LEU	2.3
2	D	21	GLN	2.2
1	A	25	GLY	2.2
1	C	263	LEU	2.2
2	B	24	PRO	2.2
1	A	60	VAL	2.2
2	D	18	ASP	2.2
2	D	11	ILE	2.1
2	D	4	PHE	2.1
1	A	10	ILE	2.1
2	B	10	VAL	2.1
1	A	61	GLU	2.0
2	B	26	ALA	2.0
2	B	55	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

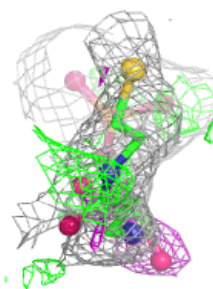
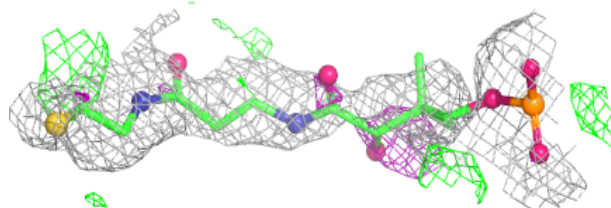
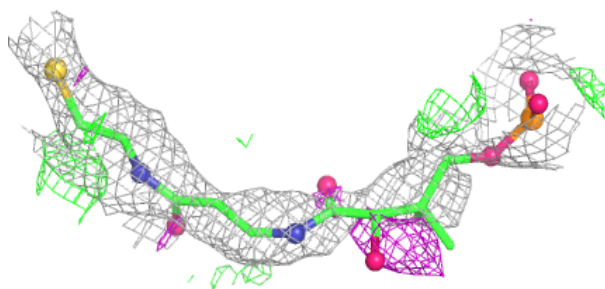
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PN7	D	101	21/22	0.73	0.21	52,69,84,99	0
5	PN7	B	101	21/22	0.74	0.19	49,59,89,105	0
3	FMN	A	1001	31/31	0.96	0.07	20,25,30,41	0
3	FMN	C	1001	31/31	0.96	0.07	25,31,36,42	0
4	SF4	A	1002	8/8	0.99	0.05	20,24,27,31	0
4	SF4	C	1002	8/8	0.99	0.03	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.

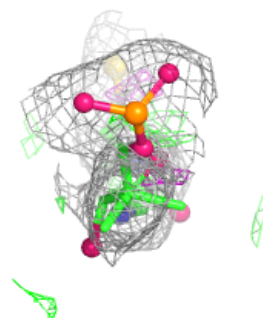
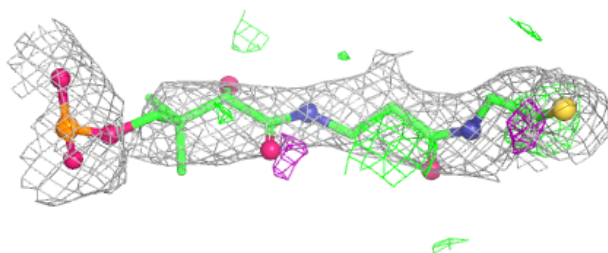
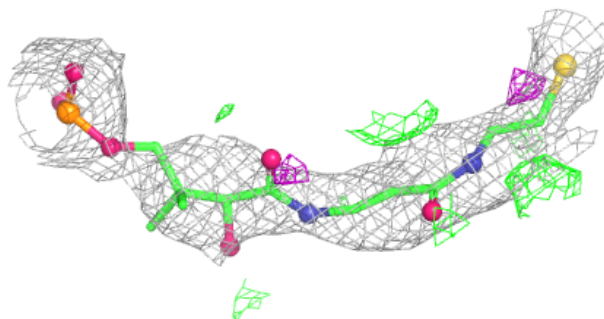
Electron density around PN7 D 101:

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

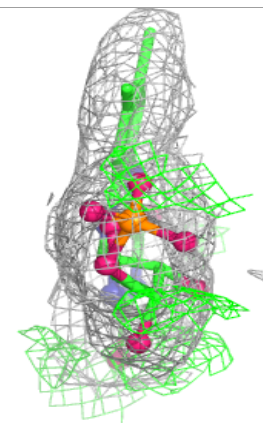
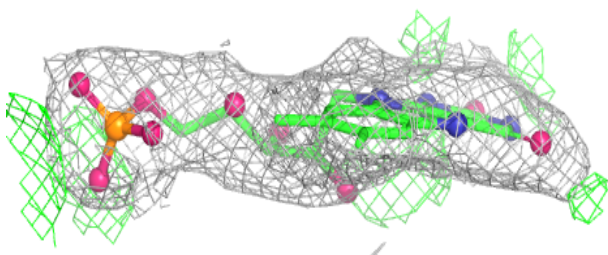
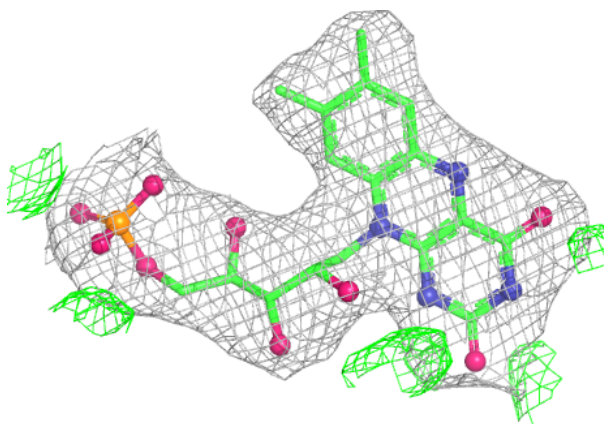


Electron density around PN7 B 101:

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

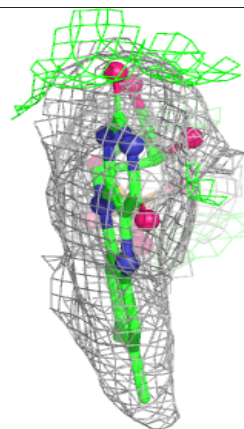
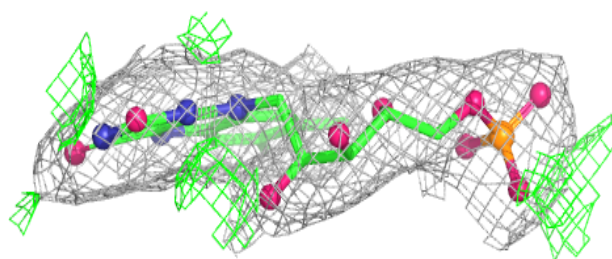
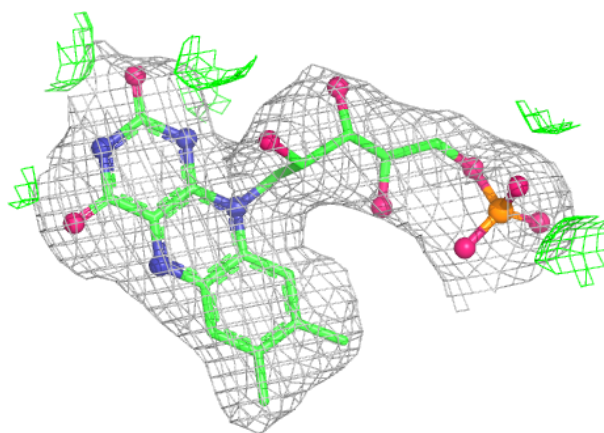
**Electron density around FMN A 1001:**

$2mF_o-DF_c$ (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.