



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:04 PM UTC

PDB ID : 4YX6 / pdb_00004yx6
Title : Architectural hierarchy of trans-acting enoyl reductases from polyunsaturated fatty acid and trans-AT polyketide synthases
Authors : Till, M.; Race, P.R.
Deposited on : 2015-03-22
Resolution : 1.86 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

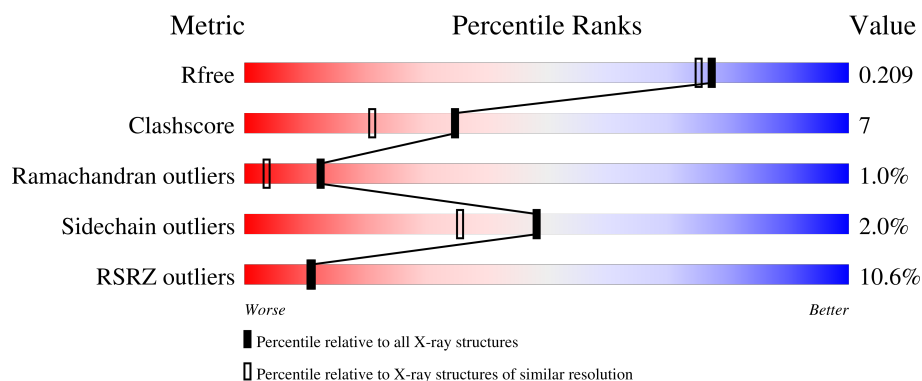
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	547	9% 52% 39% 5%
1	B	547	11% 53% 34% 5% 8%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8098 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 Omega-3 polyunsaturated fatty acid synthase subunit PfaD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			3880	2473	673	717	17			
1	B	502	Total	C	N	O	S	0	0	0
			3749	2390	647	696	16			

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



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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
3	B	1	Total 1	Ca 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	212	Total 212	O 212	0	0
4	B	193	Total 193	O 193	0	0

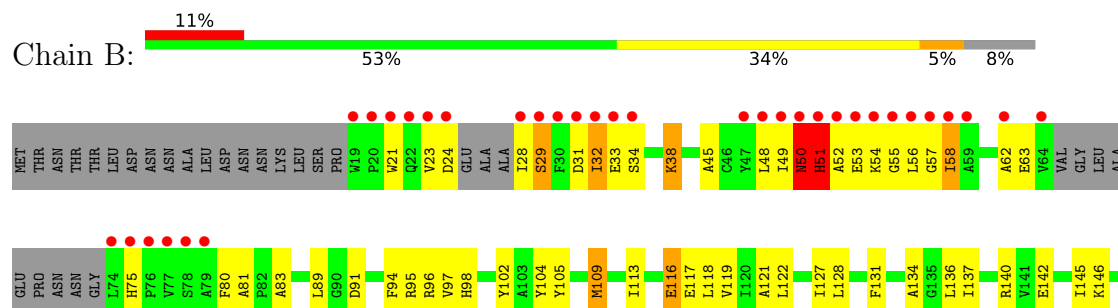
3 Residue-property plots

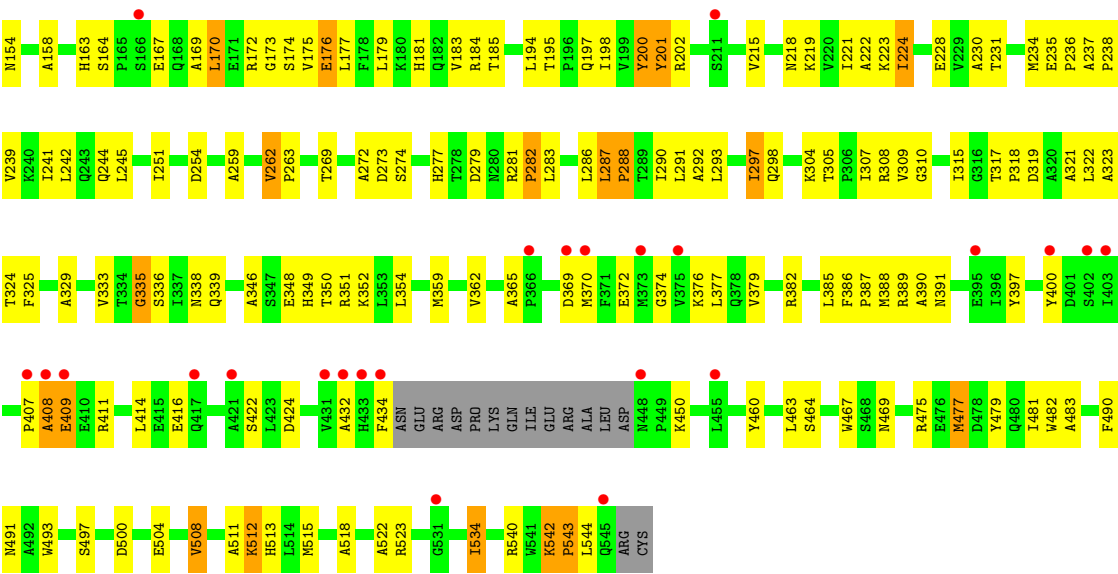
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Omega-3 polyunsaturated fatty acid synthase subunit Pfad



- Molecule 1: Omega-3 polyunsaturated fatty acid synthase subunit Pfad





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.57Å 105.57Å 214.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.41 – 1.86 47.41 – 1.86	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.41-1.86) 100.0 (47.41-1.86)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.21 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.7.009	Depositor
R, R_{free}	0.173 , 0.199 0.187 , 0.209	Depositor DCC
R_{free} test set	5107 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8098	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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, CA

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	2.09	192/3959 (4.8%)	1.05	12/5379 (0.2%)
1	B	2.04	168/3823 (4.4%)	1.10	9/5196 (0.2%)
All	All	2.07	360/7782 (4.6%)	1.07	21/10575 (0.2%)

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 (360) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	386	PHE	C-O	-9.53	1.15	1.24
1	A	412	GLN	C-N	-9.02	1.21	1.34
1	B	170	LEU	C-N	-8.88	1.22	1.33
1	B	463	LEU	C-N	-8.88	1.22	1.34
1	A	317	THR	C-O	-8.76	1.16	1.24
1	B	287	LEU	C-O	-8.22	1.16	1.24
1	A	520	TYR	C-O	-8.20	1.14	1.24
1	B	329	ALA	C-O	-8.20	1.14	1.23
1	B	291	LEU	C-O	-8.11	1.14	1.24
1	A	221	ILE	C-O	-8.08	1.15	1.24
1	A	254	ASP	C-O	-8.03	1.14	1.24
1	B	422	SER	C-N	-8.02	1.23	1.33
1	A	197	GLN	C-O	-7.73	1.15	1.24
1	B	202	ARG	C-O	-7.72	1.15	1.24
1	A	322	LEU	C-O	-7.71	1.15	1.24
1	A	220	VAL	C-O	-7.69	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	365	ALA	C-O	-7.63	1.17	1.24
1	B	338	ASN	C-O	-7.62	1.14	1.24
1	B	195	THR	C-O	-7.60	1.17	1.24
1	B	145	ILE	C-O	-7.57	1.15	1.24
1	A	502	TYR	C-O	-7.53	1.14	1.24
1	A	319	ASP	C-O	-7.49	1.15	1.24
1	A	365	ALA	C-O	-7.44	1.17	1.24
1	B	181	HIS	CD2-NE2	-7.41	1.29	1.37
1	A	225	SER	C-O	-7.40	1.14	1.24
1	A	514	LEU	C-O	-7.34	1.15	1.24
1	A	445	ALA	CA-C	-7.32	1.46	1.53
1	B	317	THR	C-O	-7.24	1.17	1.24
1	B	339	GLN	C-O	-7.10	1.15	1.24
1	A	486	ALA	C-O	-7.06	1.15	1.24
1	A	512	LYS	C-O	-7.05	1.15	1.24
1	A	283	LEU	C-O	-7.04	1.15	1.24
1	A	336	SER	C-O	-7.03	1.15	1.24
1	A	518	ALA	C-O	-7.01	1.16	1.24
1	A	294	LYS	C-O	-6.97	1.16	1.24
1	B	237	ALA	C-O	-6.95	1.15	1.23
1	A	522	ALA	C-O	-6.94	1.16	1.24
1	B	184	ARG	C-N	-6.91	1.25	1.33
1	B	97	VAL	C-O	-6.89	1.16	1.24
1	B	305	THR	C-O	-6.87	1.16	1.24
1	A	375	VAL	C-O	-6.86	1.16	1.24
1	B	169	ALA	C-N	-6.82	1.24	1.33
1	B	239	VAL	C-O	-6.80	1.16	1.24
1	B	534	ILE	C-O	-6.80	1.15	1.24
1	B	310	GLY	C-O	-6.77	1.17	1.23
1	B	277	HIS	C-O	-6.76	1.15	1.23
1	B	282	PRO	C-O	-6.76	1.16	1.23
1	A	277	HIS	CG-ND1	-6.76	1.30	1.38
1	A	298	GLN	C-O	-6.75	1.16	1.24
1	B	350	THR	C-O	-6.74	1.16	1.24
1	A	389	ARG	C-O	-6.71	1.16	1.24
1	B	469	ASN	C-O	-6.68	1.16	1.24
1	B	279	ASP	C-O	-6.65	1.15	1.24
1	A	380	VAL	C-O	-6.62	1.17	1.24
1	A	334	THR	C-O	-6.62	1.15	1.23
1	A	323	ALA	C-O	-6.61	1.16	1.24
1	A	131	PHE	C-O	-6.60	1.16	1.23
1	A	293	LEU	C-O	-6.60	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	319	ASP	C-O	-6.59	1.16	1.24
1	A	473	VAL	C-O	-6.57	1.17	1.24
1	B	51	HIS	CD2-NE2	-6.55	1.30	1.37
1	B	131	PHE	C-O	-6.54	1.16	1.23
1	B	221	ILE	C-O	-6.52	1.17	1.24
1	B	274	SER	C-O	-6.51	1.15	1.23
1	B	542	LYS	C-O	-6.50	1.16	1.24
1	A	332	ILE	C-O	-6.50	1.16	1.24
1	B	283	LEU	C-O	-6.49	1.16	1.24
1	B	98	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	344	ALA	C-O	-6.48	1.15	1.23
1	A	339	GLN	C-O	-6.48	1.15	1.24
1	A	95	ARG	C-O	-6.47	1.16	1.24
1	A	288	PRO	C-O	-6.45	1.16	1.24
1	B	323	ALA	C-O	-6.44	1.16	1.24
1	A	122	LEU	C-O	-6.44	1.16	1.24
1	B	158	ALA	C-O	-6.42	1.15	1.23
1	A	169	ALA	C-N	-6.42	1.25	1.33
1	B	183	VAL	C-O	-6.40	1.16	1.23
1	B	80	PHE	C-O	-6.39	1.16	1.23
1	A	324	THR	C-O	-6.38	1.16	1.24
1	B	116	GLU	C-O	-6.38	1.16	1.24
1	B	181	HIS	CG-ND1	-6.38	1.31	1.38
1	A	93	ASN	C-O	-6.37	1.16	1.24
1	B	222	ALA	C-O	-6.35	1.16	1.24
1	B	164	SER	C-O	-6.35	1.16	1.24
1	B	386	PHE	C-O	-6.35	1.18	1.24
1	A	325	PHE	C-O	-6.34	1.16	1.24
1	A	500	ASP	C-O	-6.33	1.16	1.24
1	B	321	ALA	C-O	-6.32	1.16	1.24
1	A	519	ALA	C-O	-6.29	1.16	1.24
1	B	318	PRO	C-O	-6.29	1.16	1.24
1	B	322	LEU	C-O	-6.29	1.16	1.24
1	A	291	LEU	C-O	-6.28	1.16	1.24
1	A	460	TYR	C-O	-6.27	1.16	1.24
1	A	180	LYS	C-O	-6.26	1.17	1.24
1	B	146	LYS	C-O	-6.25	1.17	1.24
1	B	134	ALA	C-O	-6.23	1.16	1.23
1	B	511	ALA	C-O	-6.22	1.17	1.24
1	A	377	LEU	C-O	-6.22	1.16	1.23
1	A	241	ILE	C-O	-6.22	1.16	1.24
1	A	163	HIS	CG-ND1	-6.21	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	415	GLU	C-O	-6.21	1.16	1.24
1	B	518	ALA	C-O	-6.21	1.17	1.24
1	A	388	MET	C-O	-6.20	1.16	1.24
1	B	297	ILE	C-O	-6.20	1.17	1.24
1	A	202	ARG	C-O	-6.19	1.17	1.24
1	A	363	THR	C-O	-6.19	1.16	1.23
1	B	273	ASP	C-O	-6.18	1.16	1.23
1	A	510	LEU	C-O	-6.18	1.17	1.24
1	B	38	LYS	C-O	-6.18	1.17	1.24
1	B	136	LEU	C-O	-6.18	1.16	1.23
1	B	508	VAL	C-O	-6.17	1.17	1.24
1	A	240	LYS	C-O	-6.16	1.17	1.24
1	A	521	GLN	C-O	-6.15	1.16	1.24
1	B	286	LEU	C-O	-6.15	1.17	1.24
1	A	150	ALA	C-O	-6.12	1.17	1.24
1	A	351	ARG	C-O	-6.12	1.17	1.24
1	B	288	PRO	C-O	-6.12	1.16	1.24
1	A	422	SER	C-O	-6.12	1.16	1.23
1	A	515	MET	C-O	-6.11	1.17	1.24
1	A	526	LEU	C-O	-6.11	1.16	1.24
1	A	509	ASP	C-O	-6.09	1.17	1.24
1	A	349	HIS	CG-ND1	-6.08	1.31	1.38
1	A	267	ASP	C-O	-6.08	1.16	1.23
1	A	128	LEU	C-O	-6.08	1.16	1.23
1	A	119	VAL	C-O	-6.07	1.17	1.24
1	A	230	ALA	C-O	-6.07	1.17	1.24
1	A	258	MET	C-O	-6.06	1.17	1.24
1	B	177	LEU	C-O	-6.06	1.17	1.24
1	A	91	ASP	C-O	-6.06	1.16	1.24
1	A	478	ASP	C-O	-6.04	1.15	1.24
1	A	151	ALA	C-O	-6.04	1.16	1.24
1	A	83	ALA	C-O	-6.04	1.17	1.24
1	B	513	HIS	CG-ND1	-6.04	1.31	1.38
1	A	466	ARG	C-O	-6.03	1.17	1.24
1	A	191	PHE	C-O	-6.03	1.16	1.23
1	A	487	LEU	C-O	-6.02	1.17	1.24
1	A	201	TYR	C-O	-6.01	1.17	1.24
1	B	336	SER	C-O	-6.01	1.17	1.24
1	B	198	ILE	C-O	-6.00	1.16	1.24
1	A	158	ALA	C-O	-6.00	1.16	1.23
1	B	163	HIS	CG-ND1	-6.00	1.31	1.38
1	B	259	ALA	C-O	-5.98	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	523	ARG	C-O	-5.97	1.17	1.24
1	B	96	ARG	C-O	-5.97	1.17	1.24
1	B	201	TYR	C-O	-5.97	1.17	1.24
1	A	206	LEU	C-O	-5.96	1.16	1.24
1	A	242	LEU	C-O	-5.96	1.17	1.24
1	B	176	GLU	C-O	-5.96	1.17	1.24
1	B	63	GLU	C-O	-5.95	1.17	1.24
1	A	402	SER	C-O	-5.95	1.17	1.23
1	A	256	MET	C-O	-5.94	1.17	1.24
1	B	348	GLU	C-O	-5.92	1.17	1.24
1	A	257	LEU	C-O	-5.91	1.17	1.24
1	A	229	VAL	C-O	-5.91	1.17	1.24
1	B	362	VAL	C-O	-5.90	1.18	1.24
1	B	104	TYR	C-O	-5.90	1.16	1.23
1	B	163	HIS	CD2-NE2	-5.89	1.31	1.37
1	A	456	ILE	C-O	-5.88	1.17	1.24
1	A	125	ALA	C-O	-5.87	1.16	1.24
1	B	176	GLU	C-N	-5.87	1.26	1.33
1	A	264	MET	C-O	-5.87	1.16	1.24
1	A	330	ALA	C-O	-5.87	1.16	1.24
1	A	286	LEU	C-O	-5.87	1.17	1.24
1	A	227	THR	C-O	-5.86	1.17	1.24
1	A	464	SER	C-O	-5.86	1.16	1.24
1	B	352	LYS	C-O	-5.86	1.17	1.24
1	B	543	PRO	C-O	-5.85	1.19	1.24
1	A	524	ILE	C-O	-5.84	1.17	1.24
1	A	129	CYS	C-O	-5.84	1.17	1.23
1	A	111	ASN	C-O	-5.83	1.16	1.23
1	B	414	LEU	C-O	-5.82	1.17	1.24
1	B	224	ILE	C-O	-5.82	1.16	1.23
1	A	176	GLU	C-O	-5.81	1.17	1.24
1	B	333	VAL	C-O	-5.81	1.18	1.24
1	A	157	TYR	C-O	-5.81	1.17	1.23
1	A	350	THR	C-O	-5.81	1.17	1.24
1	A	259	ALA	C-O	-5.80	1.16	1.24
1	A	461	LEU	C-O	-5.80	1.17	1.24
1	B	127	ILE	C-O	-5.80	1.18	1.24
1	A	348	GLU	C-O	-5.79	1.17	1.24
1	B	388	MET	C-O	-5.78	1.17	1.24
1	B	391	ASN	C-O	-5.78	1.17	1.24
1	B	262	VAL	C-O	-5.76	1.17	1.24
1	A	163	HIS	CD2-NE2	-5.76	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	VAL	C-O	-5.76	1.17	1.24
1	A	507	ALA	C-O	-5.76	1.17	1.24
1	B	215	VAL	C-O	-5.75	1.17	1.24
1	A	142	GLU	C-O	-5.75	1.17	1.24
1	B	117	GLU	C-O	-5.75	1.17	1.24
1	B	81	ALA	C-O	-5.72	1.18	1.25
1	B	170	LEU	C-O	-5.71	1.17	1.24
1	A	215	VAL	C-O	-5.70	1.18	1.24
1	A	98	HIS	CG-ND1	-5.69	1.31	1.38
1	B	113	ILE	C-O	-5.69	1.17	1.24
1	B	460	TYR	C-O	-5.69	1.17	1.24
1	A	306	PRO	C-O	-5.69	1.17	1.23
1	A	390	ALA	C-O	-5.68	1.17	1.24
1	A	361	ASP	C-O	-5.68	1.16	1.24
1	B	231	THR	C-O	-5.67	1.17	1.24
1	A	287	LEU	C-O	-5.67	1.19	1.24
1	B	481	ILE	C-O	-5.67	1.17	1.24
1	A	419	PHE	C-O	-5.65	1.16	1.24
1	B	98	HIS	CG-ND1	-5.65	1.32	1.38
1	A	106	ALA	C-O	-5.64	1.17	1.24
1	A	116	GLU	C-O	-5.64	1.17	1.24
1	A	147	ARG	C-O	-5.64	1.17	1.24
1	A	224	ILE	C-O	-5.62	1.17	1.23
1	A	534	ILE	C-O	-5.62	1.16	1.24
1	A	329	ALA	C-O	-5.61	1.17	1.23
1	B	245	LEU	C-O	-5.61	1.17	1.24
1	A	97	VAL	C-O	-5.61	1.17	1.24
1	B	515	MET	C-O	-5.61	1.17	1.24
1	A	105	TYR	C-O	-5.60	1.17	1.23
1	B	293	LEU	C-O	-5.59	1.17	1.24
1	A	200	TYR	C-O	-5.58	1.17	1.24
1	A	513	HIS	CD2-NE2	-5.57	1.31	1.37
1	A	266	ASP	C-O	-5.57	1.16	1.24
1	A	159	PHE	C-O	-5.56	1.16	1.24
1	A	289	THR	C-O	-5.56	1.17	1.24
1	B	75	HIS	CA-C	-5.55	1.46	1.52
1	B	335	GLY	C-O	-5.55	1.16	1.23
1	A	109	MET	C-O	-5.55	1.17	1.23
1	A	133	ALA	C-O	-5.55	1.16	1.24
1	A	222	ALA	C-O	-5.54	1.17	1.24
1	A	459	TRP	C-O	-5.54	1.17	1.24
1	B	95	ARG	C-O	-5.54	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	324	THR	C-O	-5.54	1.17	1.24
1	A	236	PRO	C-O	-5.54	1.17	1.23
1	A	47	TYR	C-O	-5.53	1.17	1.24
1	A	172	ARG	C-O	-5.52	1.17	1.24
1	B	197	GLN	C-O	-5.52	1.17	1.24
1	A	141	VAL	C-O	-5.51	1.17	1.24
1	B	349	HIS	CG-ND1	-5.51	1.32	1.38
1	A	474	GLY	C-O	-5.51	1.16	1.24
1	B	390	ALA	C-O	-5.51	1.17	1.24
1	A	89	LEU	C-O	-5.51	1.17	1.24
1	B	242	LEU	C-O	-5.50	1.17	1.24
1	A	219	LYS	C-O	-5.50	1.17	1.23
1	A	472	GLU	C-O	-5.50	1.17	1.24
1	B	219	LYS	C-O	-5.49	1.17	1.23
1	A	263	PRO	C-O	-5.49	1.17	1.23
1	B	174	SER	C-O	-5.47	1.17	1.24
1	B	500	ASP	C-O	-5.47	1.17	1.24
1	A	144	ALA	C-O	-5.45	1.17	1.24
1	A	452	LYS	C-O	-5.44	1.17	1.24
1	B	359	MET	C-O	-5.44	1.17	1.24
1	B	292	ALA	C-O	-5.44	1.17	1.24
1	B	513	HIS	CD2-NE2	-5.43	1.31	1.37
1	B	354	LEU	C-O	-5.43	1.17	1.24
1	A	85	GLY	C-O	-5.42	1.16	1.23
1	B	251	ILE	C-O	-5.42	1.17	1.23
1	A	110	ALA	C-O	-5.42	1.17	1.23
1	B	411	ARG	C-O	-5.42	1.17	1.24
1	A	321	ALA	C-O	-5.41	1.17	1.24
1	B	298	GLN	C-O	-5.41	1.17	1.24
1	B	200	TYR	C-O	-5.41	1.17	1.24
1	A	501	ASP	C-O	-5.40	1.17	1.24
1	B	83	ALA	C-O	-5.40	1.17	1.24
1	B	254	ASP	C-O	-5.40	1.17	1.24
1	A	462	GLY	C-O	-5.39	1.17	1.23
1	B	105	TYR	C-O	-5.39	1.17	1.23
1	B	523	ARG	C-O	-5.39	1.17	1.24
1	B	307	ILE	C-O	-5.38	1.18	1.24
1	A	56	LEU	C-O	-5.38	1.17	1.24
1	B	172	ARG	C-O	-5.38	1.17	1.24
1	A	265	ALA	C-O	-5.38	1.17	1.23
1	B	483	ALA	C-O	-5.37	1.17	1.23
1	B	102	TYR	C-O	-5.37	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	94	PHE	C-O	-5.36	1.18	1.24
1	A	277	HIS	CD2-NE2	-5.35	1.31	1.37
1	B	236	PRO	C-O	-5.35	1.17	1.23
1	A	311	ALA	C-O	-5.34	1.17	1.23
1	B	416	GLU	C-O	-5.34	1.17	1.24
1	B	119	VAL	C-O	-5.34	1.18	1.24
1	A	223	LYS	C-O	-5.34	1.17	1.24
1	B	175	VAL	C-O	-5.34	1.18	1.24
1	B	379	VAL	C-O	-5.34	1.18	1.23
1	B	179	LEU	C-O	-5.33	1.17	1.24
1	B	309	VAL	C-O	-5.33	1.18	1.24
1	A	234	MET	C-O	-5.32	1.17	1.24
1	A	164	SER	C-O	-5.31	1.18	1.24
1	A	314	GLY	C-O	-5.31	1.16	1.24
1	A	490	PHE	C-O	-5.31	1.18	1.24
1	B	308	ARG	C-O	-5.31	1.17	1.23
1	A	527	LEU	C-O	-5.30	1.18	1.24
1	A	320	ALA	C-O	-5.30	1.18	1.24
1	A	78	SER	C-O	-5.28	1.17	1.24
1	A	337	ILE	C-O	-5.28	1.17	1.24
1	B	185	THR	C-O	-5.27	1.18	1.23
1	B	522	ALA	C-O	-5.27	1.18	1.24
1	B	325	PHE	C-O	-5.26	1.18	1.24
1	A	84	LEU	C-O	-5.26	1.17	1.23
1	B	121	ALA	C-O	-5.26	1.18	1.24
1	B	244	GLN	C-O	-5.25	1.18	1.24
1	A	77	VAL	C-O	-5.25	1.17	1.24
1	B	118	LEU	C-O	-5.24	1.18	1.24
1	B	281	ARG	C-O	-5.24	1.17	1.23
1	B	463	LEU	C-O	-5.24	1.17	1.24
1	A	338	ASN	C-O	-5.23	1.17	1.24
1	A	414	LEU	C-O	-5.23	1.18	1.24
1	B	45	ALA	C-O	-5.23	1.16	1.23
1	B	272	ALA	C-O	-5.23	1.18	1.23
1	B	91	ASP	C-O	-5.23	1.17	1.24
1	B	228	GLU	C-O	-5.23	1.18	1.24
1	A	516	GLN	C-O	-5.22	1.18	1.24
1	B	387	PRO	C-O	-5.22	1.17	1.24
1	B	269	THR	C-O	-5.22	1.17	1.24
1	A	118	LEU	C-O	-5.22	1.18	1.24
1	B	304	LYS	C-O	-5.21	1.18	1.24
1	A	203	ALA	C-O	-5.21	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	373	MET	C-O	-5.21	1.17	1.24
1	B	163	HIS	C-O	-5.21	1.17	1.23
1	A	393	LEU	C-O	-5.20	1.18	1.24
1	A	198	ILE	C-O	-5.20	1.17	1.24
1	B	128	LEU	C-O	-5.19	1.17	1.23
1	A	481	ILE	C-O	-5.18	1.18	1.24
1	A	517	GLY	C-O	-5.18	1.17	1.23
1	A	185	THR	C-O	-5.17	1.18	1.23
1	A	463	LEU	C-O	-5.16	1.17	1.24
1	A	186	VAL	C-O	-5.16	1.18	1.24
1	B	382	ARG	C-O	-5.15	1.17	1.24
1	B	109	MET	C-O	-5.15	1.18	1.23
1	A	148	ILE	C-O	-5.14	1.18	1.24
1	A	398	THR	C-O	-5.14	1.17	1.24
1	A	540	ARG	C-O	-5.13	1.17	1.23
1	A	179	LEU	C-O	-5.12	1.18	1.24
1	A	416	GLU	C-O	-5.12	1.18	1.24
1	B	315	ILE	C-O	-5.12	1.17	1.23
1	B	290	ILE	C-O	-5.12	1.17	1.24
1	B	137	ILE	C-O	-5.11	1.18	1.24
1	B	173	GLY	C-O	-5.11	1.17	1.23
1	B	346	ALA	C-O	-5.11	1.17	1.23
1	B	424	ASP	C-O	-5.11	1.18	1.24
1	A	39	LEU	C-O	-5.10	1.18	1.24
1	A	379	VAL	C-O	-5.10	1.18	1.23
1	B	235	GLU	C-O	-5.10	1.18	1.23
1	A	160	ASN	C-O	-5.10	1.17	1.24
1	B	490	PHE	C-O	-5.09	1.18	1.24
1	B	389	ARG	C-O	-5.09	1.18	1.24
1	B	122	LEU	C-O	-5.08	1.18	1.24
1	B	223	LYS	C-O	-5.08	1.17	1.24
1	B	477	MET	C-O	-5.08	1.17	1.24
1	A	354	LEU	C-O	-5.08	1.17	1.24
1	B	497	SER	C-O	-5.07	1.17	1.23
1	A	352	LYS	C-O	-5.07	1.18	1.24
1	A	195	THR	C-O	-5.07	1.19	1.24
1	A	362	VAL	C-O	-5.06	1.19	1.24
1	B	365	ALA	CA-CB	-5.06	1.47	1.53
1	A	174	SER	C-O	-5.06	1.18	1.24
1	B	142	GLU	C-O	-5.06	1.18	1.24
1	A	181	HIS	CG-ND1	-5.05	1.32	1.38
1	A	192	LEU	C-O	-5.05	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	504	GLU	C-O	-5.05	1.17	1.24
1	A	175	VAL	C-O	-5.04	1.18	1.24
1	B	512	LYS	C-O	-5.02	1.18	1.24
1	A	123	GLY	C-O	-5.01	1.17	1.23
1	A	438	ASP	C-O	-5.01	1.18	1.24
1	B	491	ASN	C-O	-5.01	1.18	1.24
1	A	196	PRO	C-O	-5.00	1.18	1.24
1	B	89	LEU	C-O	-5.00	1.18	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	GLY	N-CA-C	14.75	134.39	115.21
1	B	50	ASN	N-CA-C	9.91	129.78	110.56
1	B	50	ASN	CB-CA-C	-8.31	97.13	112.00
1	B	544	LEU	N-CA-C	-8.03	104.00	113.88
1	A	448	ASN	CA-C-N	7.96	128.04	119.28
1	A	448	ASN	C-N-CA	7.96	128.04	119.28
1	A	110	ALA	N-CA-C	7.08	119.44	110.24
1	B	422	SER	O-C-N	6.58	131.24	122.82
1	A	30	PHE	CA-C-N	6.36	130.15	121.05
1	A	30	PHE	C-N-CA	6.36	130.15	121.05
1	A	23	VAL	N-CA-C	6.28	117.75	108.45
1	B	97	VAL	N-CA-C	6.07	116.24	110.42
1	B	55	GLY	CA-C-N	5.82	131.06	121.86
1	B	55	GLY	C-N-CA	5.82	131.06	121.86
1	A	64	VAL	CB-CA-C	-5.37	102.48	111.29
1	A	381	LYS	CA-C-N	5.35	130.54	123.05
1	A	381	LYS	C-N-CA	5.35	130.54	123.05
1	B	194	LEU	CA-C-O	-5.33	115.52	121.81
1	A	183	VAL	CA-C-N	5.25	131.83	122.06
1	A	183	VAL	C-N-CA	5.25	131.83	122.06
1	A	31	ASP	N-CA-CB	-5.05	101.65	109.48

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	526	LEU	Mainchain

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	3880	0	3840	45	0
1	B	3749	0	3697	72	0
2	A	31	0	19	4	0
2	B	31	0	19	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	212	0	0	1	0
4	B	193	0	0	6	0
All	All	8098	0	7575	114	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 7.

All (114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:PRO:O	1:B:409:GLU:N	1.68	1.27
1:A:63:GLU:O	1:A:64:VAL:HG23	1.43	1.14
1:B:53:GLU:CB	1:B:54:LYS:HA	1.76	1.09
1:B:241:ILE:HD12	4:B:868:HOH:O	1.57	1.02
1:B:28:ILE:HG22	1:B:28:ILE:O	1.55	1.01
1:A:446:LEU:HA	1:A:448:ASN:N	1.80	0.97
1:A:64:VAL:O	1:A:64:VAL:HG12	1.61	0.96
1:B:28:ILE:HA	1:B:29:SER:HB2	1.48	0.92
1:A:446:LEU:HA	1:A:448:ASN:H	1.35	0.86
1:B:407:PRO:C	1:B:409:GLU:H	1.85	0.84
1:B:49:ILE:O	1:B:57:GLY:N	2.11	0.83
1:B:31:ASP:HB3	1:B:34:SER:OG	1.80	0.81
1:A:64:VAL:O	1:A:64:VAL:CG1	2.29	0.80
1:B:407:PRO:C	1:B:409:GLU:N	2.37	0.80
1:B:53:GLU:CB	1:B:54:LYS:CA	2.60	0.79
1:A:63:GLU:O	1:A:64:VAL:CG2	2.29	0.77
1:B:28:ILE:CA	1:B:29:SER:HB2	2.13	0.77
1:B:28:ILE:O	1:B:28:ILE:CG2	2.30	0.76
1:B:400:TYR:O	1:B:450:LYS:NZ	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ARG:HD2	4:B:766:HOH:O	1.87	0.74
1:B:407:PRO:O	1:B:408:ALA:C	2.30	0.74
1:B:238:PRO:HG2	1:B:241:ILE:HG22	1.69	0.73
1:B:109:MET:HA	2:B:601:FMN:N5	2.07	0.70
1:A:445:ALA:O	1:A:446:LEU:CB	2.41	0.69
1:B:109:MET:HA	2:B:601:FMN:C5A	2.22	0.69
1:B:241:ILE:CD1	4:B:868:HOH:O	2.25	0.69
1:B:287:LEU:HB3	1:B:288:PRO:HD3	1.74	0.69
1:B:238:PRO:HG2	1:B:241:ILE:CG2	2.22	0.68
1:A:20:PRO:HD3	1:B:21:TRP:CZ2	2.29	0.68
1:A:25:GLU:O	1:A:26:ALA:HB3	1.93	0.67
1:A:109:MET:HA	2:A:601:FMN:N5	2.11	0.66
1:B:508:VAL:HG12	1:B:512:LYS:HE3	1.78	0.66
1:B:29:SER:O	1:B:57:GLY:HA2	1.96	0.65
1:A:449:PRO:HD2	4:A:739:HOH:O	1.96	0.65
1:B:28:ILE:HA	1:B:29:SER:CB	2.26	0.65
1:B:51:HIS:ND1	1:B:52:ALA:N	2.44	0.64
1:A:166:SER:C	1:A:167:GLU:HG2	2.22	0.64
1:A:53:GLU:CB	1:A:54:LYS:HA	2.28	0.64
1:B:21:TRP:HB3	1:B:62:ALA:HB1	1.81	0.60
1:A:109:MET:HA	2:A:601:FMN:C5A	2.32	0.60
1:B:38:LYS:CD	1:B:58:ILE:HG23	2.34	0.58
1:A:287:LEU:HB3	1:A:288:PRO:HD3	1.84	0.58
1:B:508:VAL:CG1	1:B:512:LYS:HE3	2.33	0.58
1:A:446:LEU:HA	1:A:447:ASP:C	2.23	0.57
1:B:432:ALA:C	1:B:434:PHE:H	2.13	0.57
1:B:369:ASP:O	1:B:370:MET:HB2	2.02	0.57
1:A:464:SER:HA	1:A:467:TRP:CE3	2.40	0.56
1:A:20:PRO:HD3	1:B:21:TRP:HZ2	1.71	0.55
1:A:75:HIS:N	1:A:75:HIS:ND1	2.54	0.55
1:A:224:ILE:C	1:A:224:ILE:HD12	2.31	0.55
1:B:51:HIS:CG	1:B:52:ALA:H	2.25	0.55
1:B:374:GLY:HA2	4:B:837:HOH:O	2.07	0.54
1:A:21:TRP:HA	1:A:64:VAL:HA	1.88	0.54
1:B:32:ILE:CG2	1:B:33:GLU:N	2.69	0.53
1:A:431:VAL:HG12	1:A:432:ALA:N	2.24	0.53
1:A:447:ASP:O	1:A:448:ASN:HB2	2.07	0.53
1:A:526:LEU:O	1:A:526:LEU:HD12	2.10	0.52
1:B:116:GLU:OE2	1:B:140:ARG:NH1	2.43	0.52
1:B:224:ILE:HD12	1:B:224:ILE:C	2.34	0.52
1:A:25:GLU:C	1:A:27:ALA:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LYS:HD3	1:B:58:ILE:HG23	1.91	0.51
1:B:372:GLU:HG2	1:B:397:TYR:OH	2.09	0.51
1:B:31:ASP:O	1:B:32:ILE:C	2.54	0.49
1:A:459:TRP:CE2	1:A:463:LEU:HD12	2.48	0.49
1:B:50:ASN:O	1:B:51:HIS:O	2.31	0.48
1:A:167:GLU:HB3	1:A:170:LEU:HD12	1.95	0.48
1:B:50:ASN:ND2	1:B:50:ASN:H	2.11	0.48
1:B:31:ASP:HB3	1:B:34:SER:HG	1.73	0.48
1:A:64:VAL:O	1:A:65:VAL:O	2.31	0.48
1:B:28:ILE:N	1:B:29:SER:HB2	2.29	0.48
1:B:167:GLU:CB	1:B:170:LEU:HD12	2.45	0.47
1:B:493:TRP:CZ2	1:B:543:PRO:HD3	2.50	0.47
1:A:377:LEU:C	1:A:377:LEU:HD12	2.40	0.47
1:A:475:ARG:O	1:A:479:TYR:CD1	2.68	0.46
1:A:482:TRP:HB2	2:A:601:FMN:C7M	2.46	0.46
1:B:385:LEU:HG	1:B:477:MET:HE3	1.97	0.46
1:B:464:SER:HA	1:B:467:TRP:CE3	2.51	0.46
1:B:482:TRP:HB2	2:B:601:FMN:C7M	2.46	0.45
1:A:485:PRO:HG2	1:B:282:PRO:HG2	1.99	0.45
1:A:33:GLU:O	1:A:37:LYS:HG3	2.17	0.45
1:B:38:LYS:HD2	1:B:58:ILE:HG23	1.98	0.45
1:B:477:MET:HB2	4:B:859:HOH:O	2.16	0.45
1:B:58:ILE:HG23	1:B:58:ILE:O	2.17	0.45
1:B:238:PRO:HG2	1:B:241:ILE:HG21	1.98	0.45
1:B:262:VAL:HB	1:B:263:PRO:HD2	1.99	0.45
1:B:140:ARG:HG3	1:B:140:ARG:HH11	1.82	0.45
1:B:32:ILE:HG22	1:B:33:GLU:N	2.31	0.44
1:A:268:ILE:HD12	1:A:268:ILE:N	2.32	0.44
1:A:25:GLU:O	1:A:26:ALA:CB	2.59	0.44
1:A:209:ASP:OD1	1:A:209:ASP:C	2.60	0.44
1:B:48:LEU:HD23	1:B:56:LEU:HD11	2.00	0.44
1:B:176:GLU:OE2	1:B:200:TYR:HE2	2.00	0.44
1:B:201:TYR:CE1	1:B:218:ASN:HB3	2.53	0.44
1:A:377:LEU:HD12	1:A:377:LEU:O	2.18	0.43
1:A:448:ASN:HA	1:A:449:PRO:HD3	1.71	0.43
1:B:51:HIS:CG	1:B:52:ALA:N	2.82	0.43
1:A:353:LEU:HD12	1:A:353:LEU:O	2.19	0.43
1:B:23:VAL:HG12	1:B:24:ASP:N	2.33	0.43
1:A:412:GLN:O	1:A:416:GLU:HG3	2.19	0.42
1:A:482:TRP:HB2	2:A:601:FMN:HM73	2.00	0.42
1:B:475:ARG:O	1:B:479:TYR:CD1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ASN:O	1:B:51:HIS:C	2.58	0.42
1:B:482:TRP:HB2	2:B:601:FMN:HM73	2.02	0.42
1:B:230:ALA:O	1:B:234:MET:HG3	2.20	0.42
1:B:351:ARG:NH1	4:B:701:HOH:O	2.18	0.42
1:B:50:ASN:HB2	1:B:51:HIS:H	1.58	0.41
1:A:272:ALA:O	1:A:273:ASP:C	2.64	0.41
1:B:38:LYS:HD2	1:B:58:ILE:CG2	2.50	0.41
1:B:52:ALA:HA	1:B:53:GLU:HA	1.64	0.41
1:A:224:ILE:HD12	1:A:224:ILE:O	2.21	0.41
1:A:267:ASP:C	1:A:268:ILE:HD12	2.46	0.41
1:B:31:ASP:O	1:B:34:SER:N	2.50	0.41
1:A:164:SER:HA	1:A:165:PRO:HD2	1.89	0.40
1:B:542:LYS:HE3	1:B:543:PRO:HD2	2.04	0.40

There are no symmetry-related clashes.

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	514/547 (94%)	494 (96%)	15 (3%)	5 (1%)	12	4
1	B	494/547 (90%)	473 (96%)	16 (3%)	5 (1%)	12	4
All	All	1008/1094 (92%)	967 (96%)	31 (3%)	10 (1%)	12	4

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	VAL
1	A	446	LEU
1	B	408	ALA
1	A	335	GLY
1	B	335	GLY

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Mol	Chain	Res	Type
1	B	51	HIS
1	B	409	GLU
1	A	61	SER
1	A	63	GLU
1	B	29	SER

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	384/433 (89%)	378 (98%)	6 (2%)	55	44
1	B	371/433 (86%)	362 (98%)	9 (2%)	43	28
All	All	755/866 (87%)	740 (98%)	15 (2%)	48	36

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ILE
1	A	75	HIS
1	A	319	ASP
1	A	409	GLU
1	A	495	LYS
1	A	526	LEU
1	B	32	ILE
1	B	50	ASN
1	B	58	ILE
1	B	154	ASN
1	B	297	ILE
1	B	376	LYS
1	B	377	LEU
1	B	534	ILE
1	B	540	ARG

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	277	HIS
1	B	50	ASN
1	B	516	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
2	FMN	A	601	-	33,33,33	1.45	4 (12%)	48,50,50	1.21	6 (12%)
2	FMN	B	601	-	33,33,33	1.46	5 (15%)	48,50,50	1.21	6 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	A	601	-	-	6/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	B	601	-	-	6/18/18/18	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FMN	C9A-C5A	5.28	1.49	1.41
2	A	601	FMN	C9A-C5A	5.24	1.49	1.41
2	B	601	FMN	C8-C7	3.43	1.49	1.40
2	A	601	FMN	C8-C7	3.39	1.49	1.40
2	A	601	FMN	C4-N3	-2.45	1.34	1.38
2	B	601	FMN	C4-N3	-2.41	1.34	1.38
2	A	601	FMN	C4A-N5	2.23	1.35	1.30
2	B	601	FMN	C4A-N5	2.23	1.35	1.30
2	B	601	FMN	C5A-N5	-2.01	1.35	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FMN	C4-C4A-N5	2.86	122.16	118.21
2	A	601	FMN	C4-C4A-N5	2.83	122.11	118.21
2	A	601	FMN	C4A-C10-N1	-2.44	118.61	124.59
2	B	601	FMN	C4A-C10-N1	-2.43	118.63	124.59
2	B	601	FMN	O4-C4-C4A	-2.19	120.76	126.53
2	A	601	FMN	O4-C4-C4A	-2.18	120.78	126.53
2	B	601	FMN	C10-N1-C2	2.09	121.38	116.85
2	A	601	FMN	C4A-C10-N10	2.08	119.47	116.48
2	A	601	FMN	C10-N1-C2	2.08	121.34	116.85
2	B	601	FMN	C4A-C10-N10	2.05	119.42	116.48
2	B	601	FMN	C4A-C4-N3	2.05	118.48	113.25
2	A	601	FMN	C4A-C4-N3	2.04	118.44	113.25

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FMN	C5'-O5'-P-O3P
2	A	601	FMN	C2'-C3'-C4'-O4'
2	B	601	FMN	C2'-C3'-C4'-O4'
2	A	601	FMN	O3'-C3'-C4'-C5'
2	B	601	FMN	O3'-C3'-C4'-C5'
2	A	601	FMN	C2'-C3'-C4'-C5'

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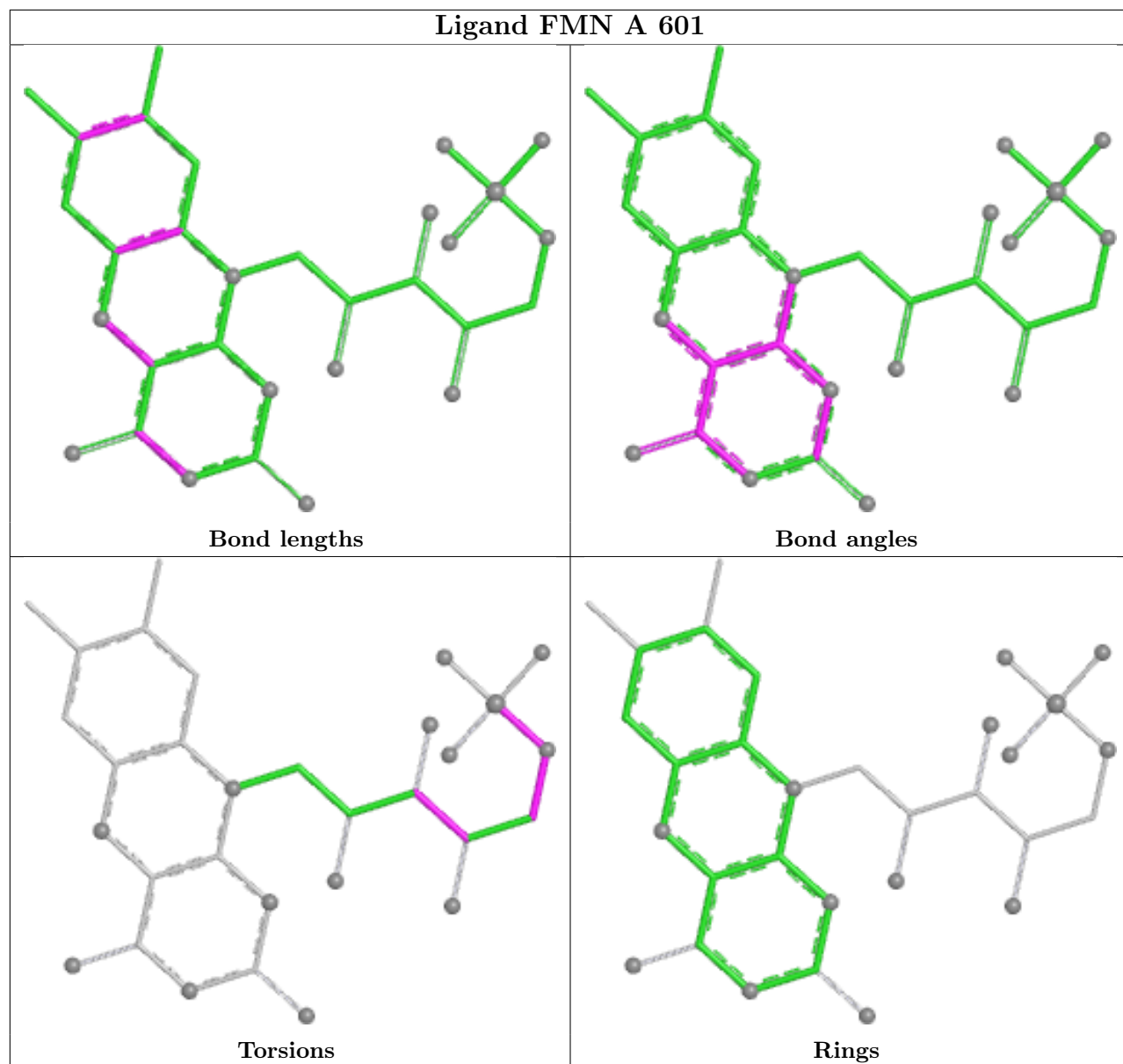
Mol	Chain	Res	Type	Atoms
2	B	601	FMN	C2'-C3'-C4'-C5'
2	A	601	FMN	O3'-C3'-C4'-O4'
2	B	601	FMN	O3'-C3'-C4'-O4'
2	A	601	FMN	C4'-C5'-O5'-P
2	B	601	FMN	C4'-C5'-O5'-P
2	B	601	FMN	C5'-O5'-P-O2P

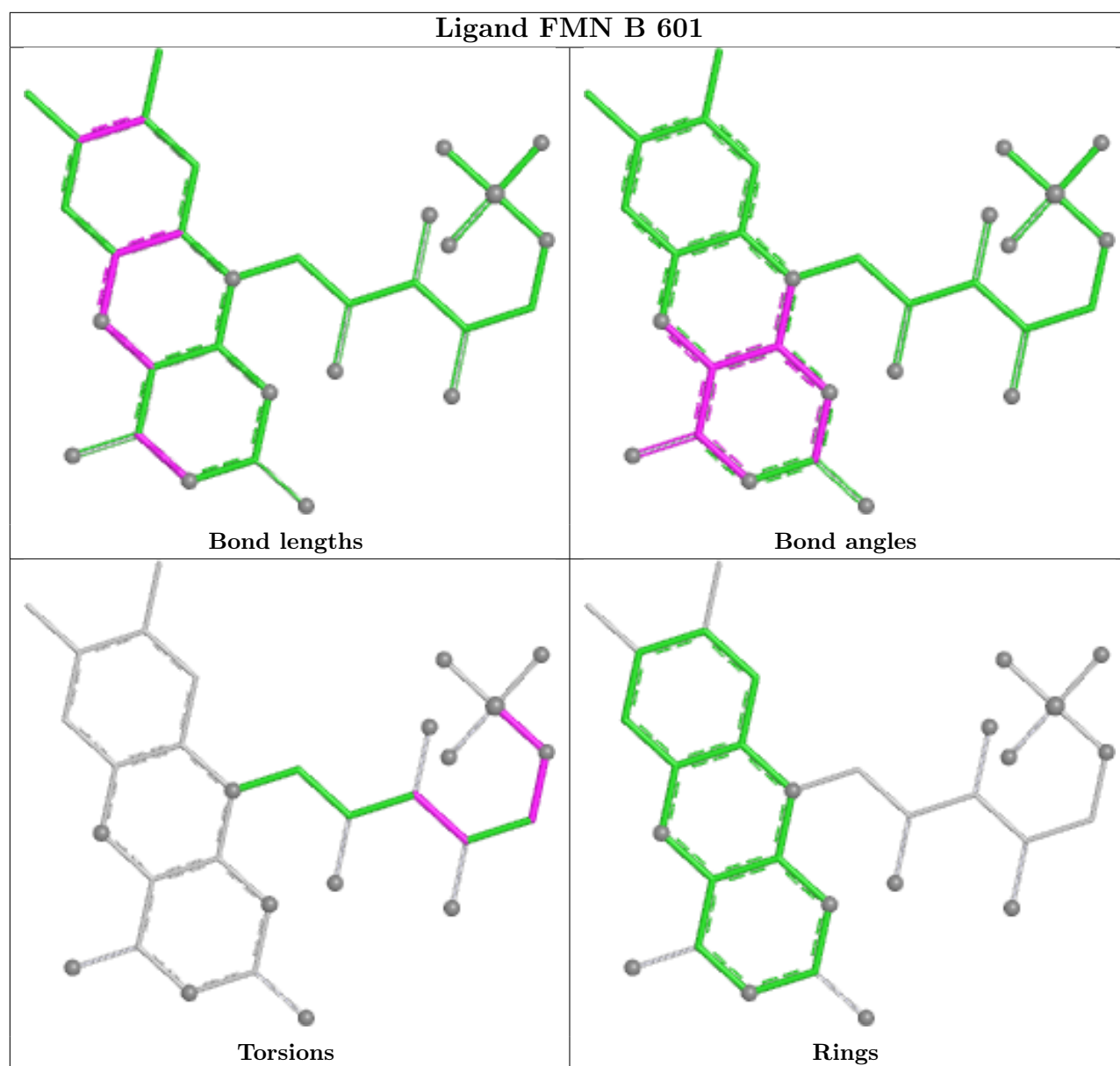
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FMN	4	0
2	B	601	FMN	4	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.





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	518/547 (94%)	0.19	50 (9%)	13 13	6, 14, 49, 68	0
1	B	502/547 (91%)	0.30	58 (11%)	9 9	6, 14, 47, 78	0
All	All	1020/1094 (93%)	0.24	108 (10%)	11 11	6, 14, 48, 78	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	VAL	6.6
1	A	74	LEU	5.7
1	A	447	ASP	5.7
1	B	49	ILE	5.6
1	B	74	LEU	5.6
1	B	75	HIS	5.5
1	B	434	PHE	5.4
1	A	446	LEU	5.3
1	B	28	ILE	5.1
1	B	64	VAL	4.9
1	A	52	ALA	4.9
1	A	64	VAL	4.7
1	B	50	ASN	4.7
1	B	54	LYS	4.7
1	B	448	ASN	4.6
1	B	55	GLY	4.6
1	B	52	ALA	4.5
1	B	24	ASP	4.5
1	B	51	HIS	4.4
1	B	29	SER	4.3
1	A	76	PRO	4.3
1	B	19	TRP	4.3
1	B	76	PRO	4.2
1	B	77	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	30	PHE	4.1
1	A	445	ALA	3.9
1	A	63	GLU	3.8
1	A	438	ASP	3.8
1	A	23	VAL	3.8
1	B	421	ALA	3.7
1	A	441	GLN	3.7
1	A	26	ALA	3.6
1	A	434	PHE	3.6
1	B	373	MET	3.6
1	B	23	VAL	3.6
1	B	409	GLU	3.5
1	B	433	HIS	3.5
1	B	31	ASP	3.5
1	B	53	GLU	3.5
1	A	27	ALA	3.5
1	B	33	GLU	3.5
1	B	370	MET	3.5
1	A	53	GLU	3.4
1	B	21	TRP	3.4
1	A	28	ILE	3.4
1	A	18	PRO	3.4
1	A	436	GLU	3.3
1	B	408	ALA	3.3
1	B	48	LEU	3.3
1	B	22	GLN	3.2
1	B	56	LEU	3.2
1	A	46	CYS	3.2
1	A	455	LEU	3.2
1	A	54	LYS	3.0
1	B	32	ILE	3.0
1	A	431	VAL	3.0
1	B	59	ALA	3.0
1	B	407	PRO	2.9
1	A	21	TRP	2.9
1	A	437	ARG	2.9
1	B	545	GLN	2.8
1	B	20	PRO	2.8
1	B	58	ILE	2.8
1	B	78	SER	2.8
1	A	49	ILE	2.7
1	A	24	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	402	SER	2.7
1	A	60	GLN	2.6
1	A	412	GLN	2.6
1	B	79	ALA	2.6
1	A	50	ASN	2.6
1	A	31	ASP	2.6
1	A	55	GLY	2.4
1	A	75	HIS	2.4
1	B	211	SER	2.4
1	A	442	ILE	2.4
1	A	408	ALA	2.4
1	A	448	ASN	2.4
1	A	51	HIS	2.4
1	B	395	GLU	2.4
1	A	62	ALA	2.4
1	B	400	TYR	2.3
1	A	20	PRO	2.3
1	B	531	GLY	2.3
1	A	25	GLU	2.3
1	A	440	LYS	2.3
1	B	57	GLY	2.3
1	B	166	SER	2.3
1	B	369	ASP	2.3
1	B	375	VAL	2.3
1	A	444	ARG	2.2
1	A	543	PRO	2.2
1	B	432	ALA	2.2
1	A	30	PHE	2.1
1	A	409	GLU	2.1
1	B	403	ILE	2.1
1	B	34	SER	2.1
1	B	417	GLN	2.1
1	A	369	ASP	2.1
1	A	533	SER	2.1
1	B	366	PRO	2.1
1	A	48	LEU	2.1
1	B	62	ALA	2.1
1	B	47	TYR	2.0
1	B	431	VAL	2.0
1	B	455	LEU	2.0
1	A	22	GLN	2.0
1	A	435	ASN	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](#)

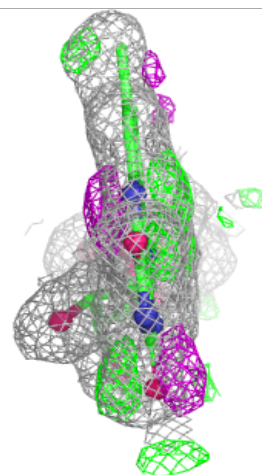
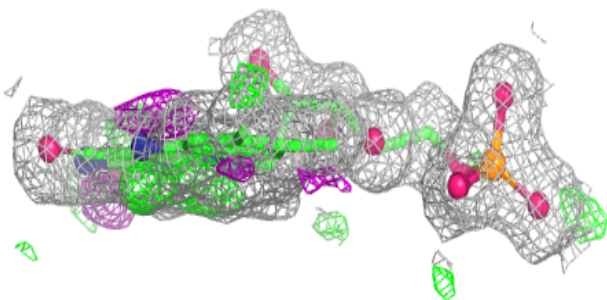
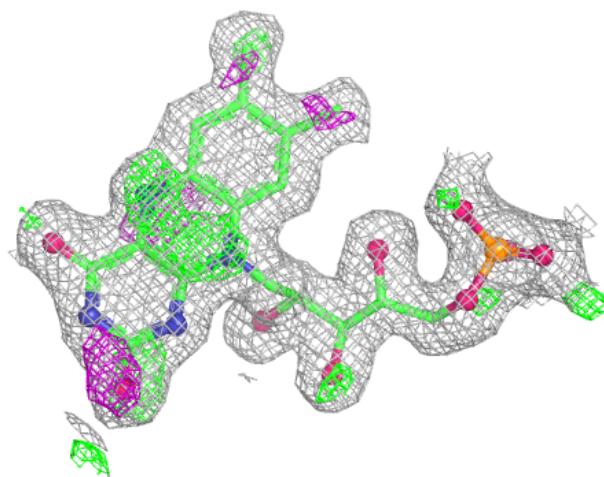
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

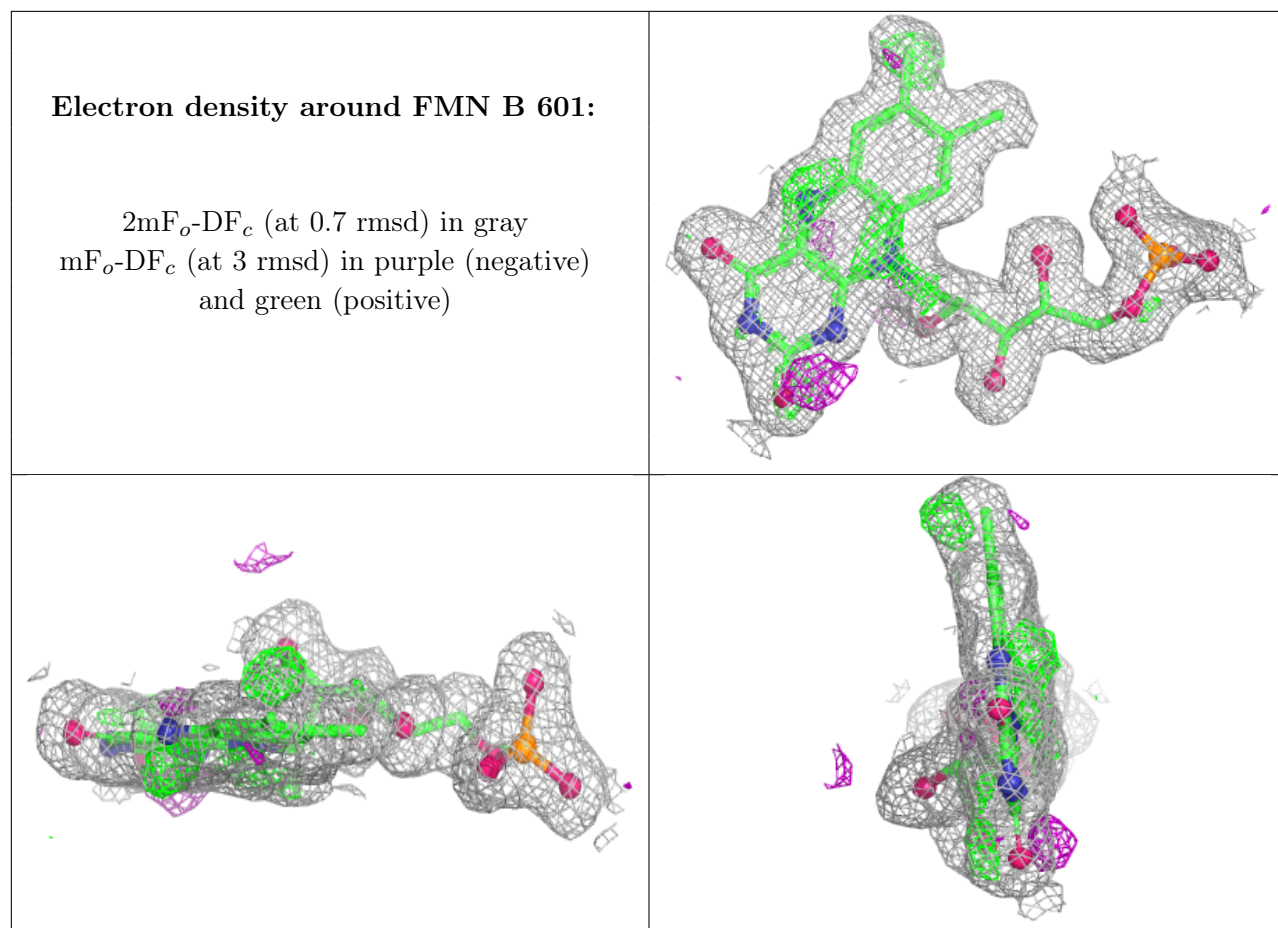
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FMN	A	601	31/31	0.94	0.08	6,8,10,13	0
2	FMN	B	601	31/31	0.95	0.07	7,9,10,11	0
3	CA	A	602	1/1	0.99	0.04	20,20,20,20	0
3	CA	B	602	1/1	0.99	0.03	15,15,15,15	0

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 A 601:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.