



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 11:23 PM UTC

PDB ID : 9TLZ / pdb_00009tlz
Title : Plasmodium falciparum dihydroorotate dehydrogenase in complex with 3-hydroxy-1-methyl pyrazole derivatives
Authors : Alberti, M.; Miggiano, R.
Deposited on : 2025-12-11
Resolution : 2.95 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

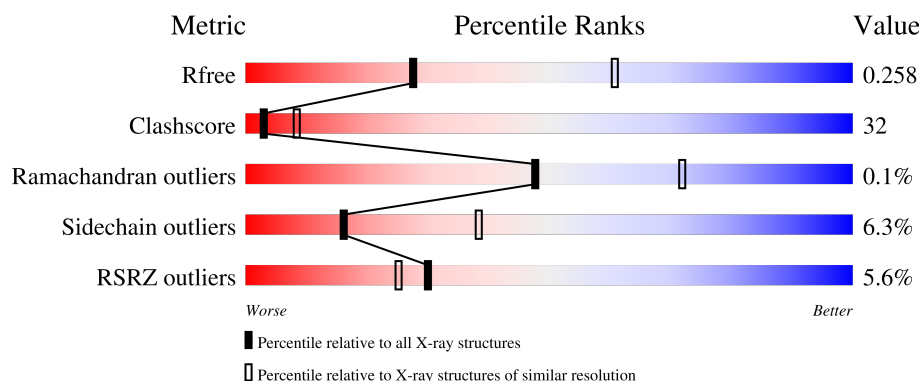
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	405	
1	B	405	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	A1JWR	B	603	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6144 atoms, of which 22 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dihydroorotate dehydrogenase (quinone), mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			3005	1919	503	568	15			
1	B	374	Total	C	N	O	S	0	0	0
			2964	1895	497	558	14			

There are 106 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	MET	-	initiating methionine	UNP Q08210
A	136	HIS	-	expression tag	UNP Q08210
A	137	HIS	-	expression tag	UNP Q08210
A	138	HIS	-	expression tag	UNP Q08210
A	139	HIS	-	expression tag	UNP Q08210
A	140	HIS	-	expression tag	UNP Q08210
A	141	HIS	-	expression tag	UNP Q08210
A	142	SER	-	expression tag	UNP Q08210
A	143	SER	-	expression tag	UNP Q08210
A	144	GLY	-	expression tag	UNP Q08210
A	145	VAL	-	expression tag	UNP Q08210
A	146	ASP	-	expression tag	UNP Q08210
A	147	LEU	-	expression tag	UNP Q08210
A	148	GLY	-	expression tag	UNP Q08210
A	149	THR	-	expression tag	UNP Q08210
A	150	GLU	-	expression tag	UNP Q08210
A	151	ASN	-	expression tag	UNP Q08210
A	152	LEU	-	expression tag	UNP Q08210
A	153	TYR	-	expression tag	UNP Q08210
A	154	PHE	-	expression tag	UNP Q08210
A	155	GLN	-	expression tag	UNP Q08210
A	156	SER	-	expression tag	UNP Q08210
A	157	MET	-	expression tag	UNP Q08210
A	?	-	SER	deletion	UNP Q08210
A	?	-	THR	deletion	UNP Q08210

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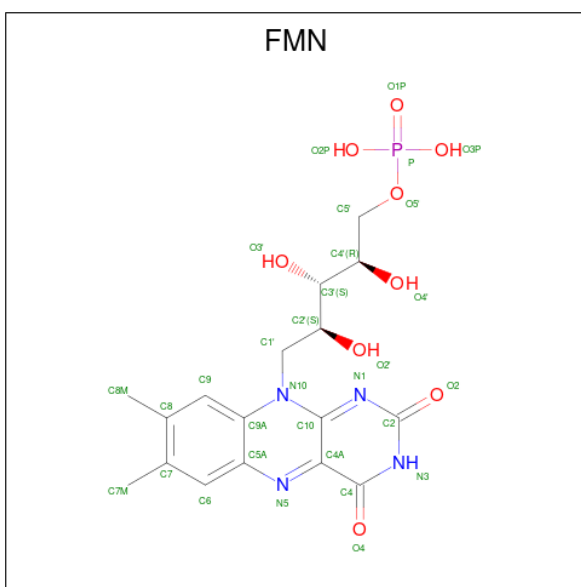
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	GLU	deletion	UNP Q08210
A	?	-	ASP	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ILE	deletion	UNP Q08210
A	?	-	VAL	deletion	UNP Q08210
A	?	-	GLU	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	PHE	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
A	?	-	SER	deletion	UNP Q08210
A	?	-	HIS	deletion	UNP Q08210
A	?	-	MET	deletion	UNP Q08210
A	?	-	MET	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASP	deletion	UNP Q08210
A	?	-	ALA	deletion	UNP Q08210
A	?	-	LYS	deletion	UNP Q08210
A	?	-	ASP	deletion	UNP Q08210
A	?	-	ASN	deletion	UNP Q08210
B	135	MET	-	initiating methionine	UNP Q08210
B	136	HIS	-	expression tag	UNP Q08210
B	137	HIS	-	expression tag	UNP Q08210
B	138	HIS	-	expression tag	UNP Q08210
B	139	HIS	-	expression tag	UNP Q08210
B	140	HIS	-	expression tag	UNP Q08210
B	141	HIS	-	expression tag	UNP Q08210
B	142	SER	-	expression tag	UNP Q08210
B	143	SER	-	expression tag	UNP Q08210
B	144	GLY	-	expression tag	UNP Q08210
B	145	VAL	-	expression tag	UNP Q08210
B	146	ASP	-	expression tag	UNP Q08210
B	147	LEU	-	expression tag	UNP Q08210
B	148	GLY	-	expression tag	UNP Q08210

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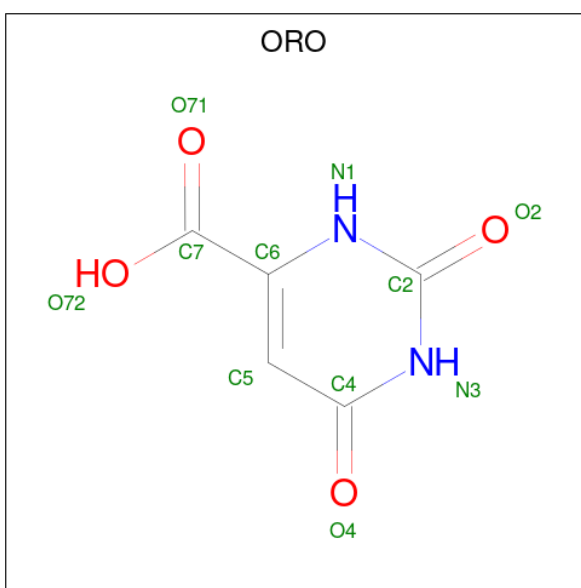
Chain	Residue	Modelled	Actual	Comment	Reference
B	149	THR	-	expression tag	UNP Q08210
B	150	GLU	-	expression tag	UNP Q08210
B	151	ASN	-	expression tag	UNP Q08210
B	152	LEU	-	expression tag	UNP Q08210
B	153	TYR	-	expression tag	UNP Q08210
B	154	PHE	-	expression tag	UNP Q08210
B	155	GLN	-	expression tag	UNP Q08210
B	156	SER	-	expression tag	UNP Q08210
B	157	MET	-	expression tag	UNP Q08210
B	?	-	SER	deletion	UNP Q08210
B	?	-	THR	deletion	UNP Q08210
B	?	-	TYR	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	GLU	deletion	UNP Q08210
B	?	-	ASP	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ILE	deletion	UNP Q08210
B	?	-	VAL	deletion	UNP Q08210
B	?	-	GLU	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	PHE	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210
B	?	-	SER	deletion	UNP Q08210
B	?	-	HIS	deletion	UNP Q08210
B	?	-	MET	deletion	UNP Q08210
B	?	-	MET	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASP	deletion	UNP Q08210
B	?	-	ALA	deletion	UNP Q08210
B	?	-	LYS	deletion	UNP Q08210
B	?	-	ASP	deletion	UNP Q08210
B	?	-	ASN	deletion	UNP Q08210

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



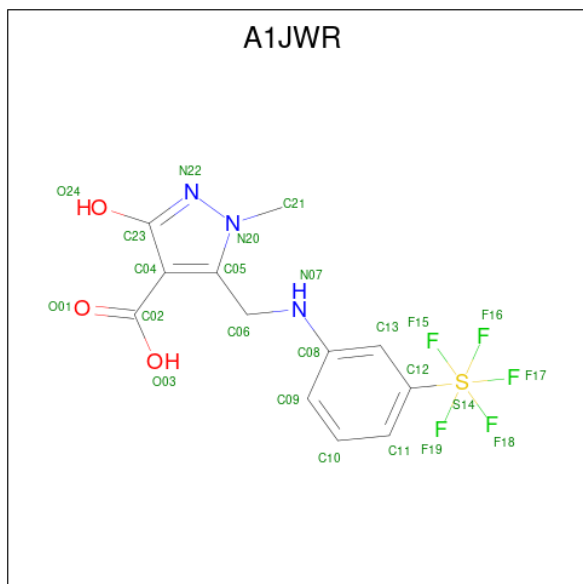
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	5	2	4		
3	B	1	Total	C	N	O	0	0
			11	5	2	4		

- Molecule 4 is 1-methyl-3-oxidanyl-5-[[[3-[pentakis(fluoranyl)- $\text{S}^{\wedge}\{6\}$ -sulfanyl]phenyl]amino]methyl]pyrazole-4-carboxylic acid (CCD ID: A1JWR) (formula: $\text{C}_{12}\text{H}_{12}\text{F}_5\text{N}_3\text{O}_3\text{S}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	F	H	N	O	S	0	0
			35	12	5	11	3	3	1		
4	B	1	Total	C	F	H	N	O	S	0	0
			35	12	5	11	3	3	1		

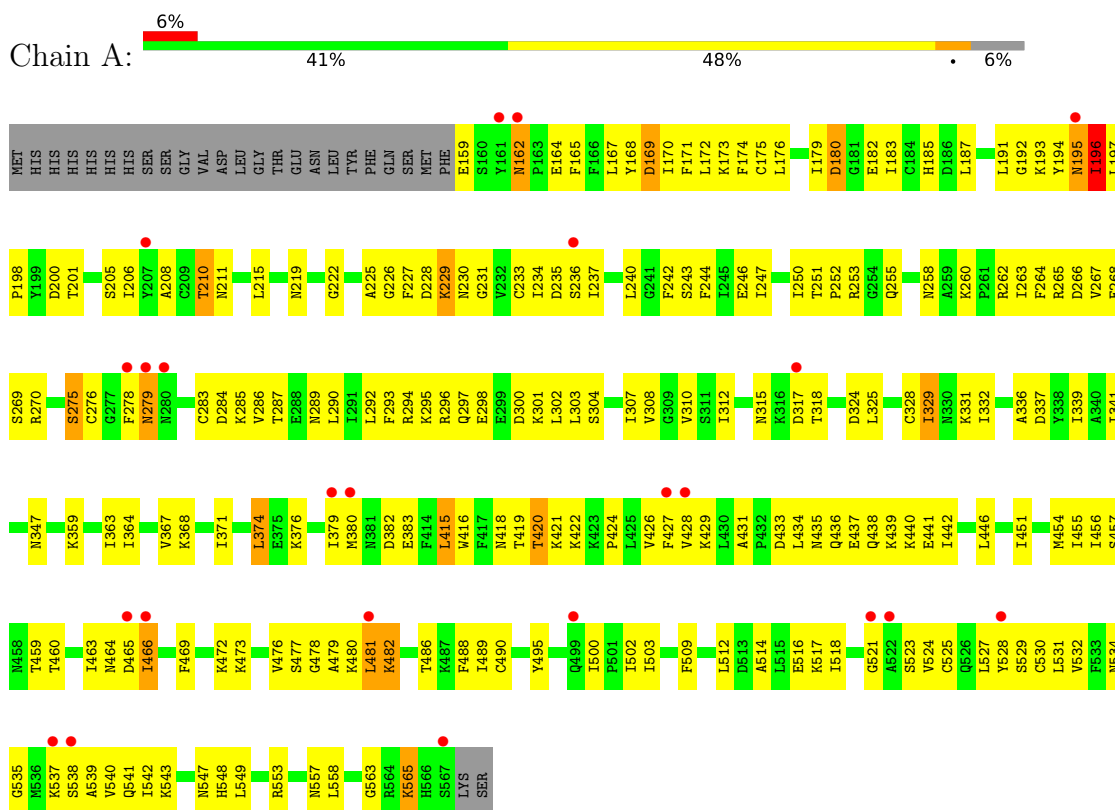
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	O	0	0
			12	12		
5	B	9	Total	O	0	0
			9	9		

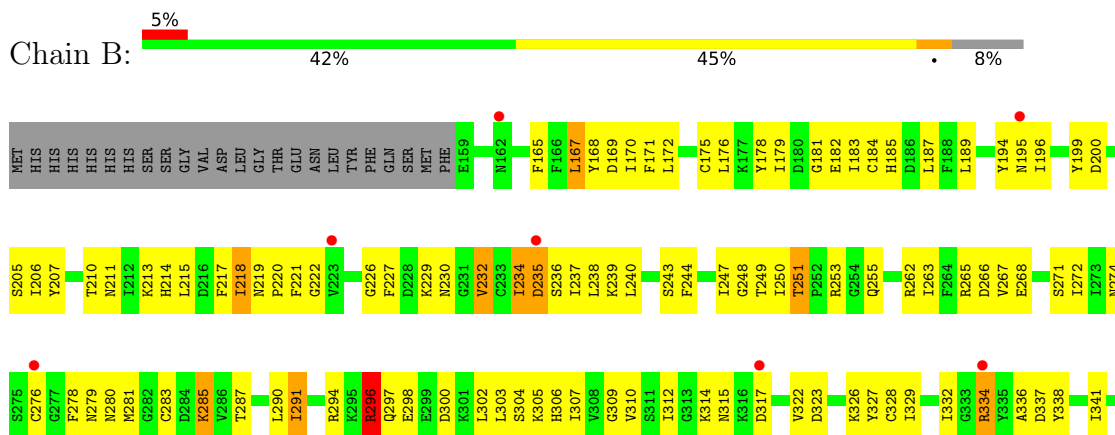
3 Residue-property plots [i](#)

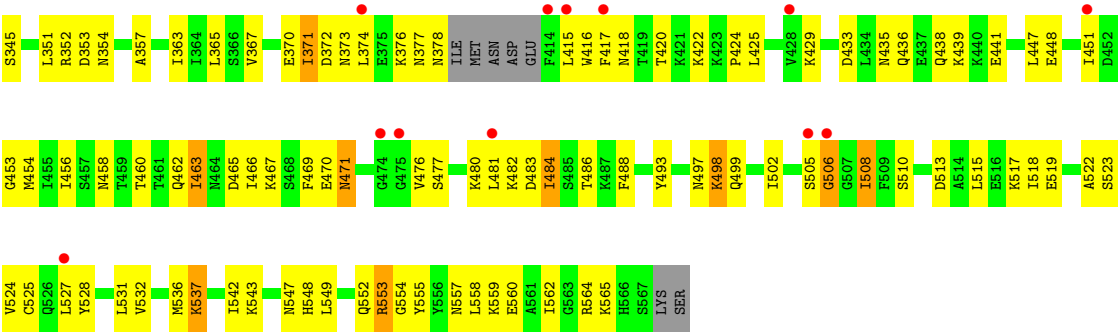
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dihydroorotate dehydrogenase (quinone), mitochondrial



- Molecule 1: Dihydroorotate dehydrogenase (quinone), mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.36Å 163.13Å 62.66Å 90.00° 107.91° 90.00°	Depositor
Resolution (Å)	48.13 – 2.95 48.13 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.13-2.95) 97.8 (48.13-2.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: v1.0)	Depositor
R, R_{free}	0.190 , 0.261 0.201 , 0.258	Depositor DCC
R_{free} test set	1005 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	1.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 66.9	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	0.93	EDS
Total number of atoms	6144	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, ORO, A1JWR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/3056	0.89	6/4115 (0.1%)
1	B	0.54	0/3014	0.87	4/4057 (0.1%)
All	All	0.53	0/6070	0.88	10/8172 (0.1%)

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
1	B	0	3
All	All	0	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	196	ILE	N-CA-C	-8.87	102.31	113.22
1	A	481	LEU	CB-CA-C	-8.40	97.09	111.46
1	A	482	LYS	N-CA-C	-6.75	96.43	110.80
1	B	537	LYS	N-CA-C	6.74	120.11	112.97
1	A	547	ASN	N-CA-C	-6.50	104.11	111.07
1	B	508	ILE	N-CA-C	6.39	117.90	109.21
1	B	236	SER	N-CA-CB	-5.68	101.55	110.30
1	B	234	ILE	CB-CA-C	-5.63	104.45	112.22
1	A	420	THR	N-CA-C	-5.35	105.85	112.38
1	A	464	ASN	N-CA-C	-5.03	108.41	114.75

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	553	ARG	Sidechain
1	B	296	ARG	Sidechain
1	B	334	ARG	Sidechain
1	B	553	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3005	0	3042	207	0
1	B	2964	0	3005	182	0
2	A	31	0	19	3	0
2	B	31	0	19	2	0
3	A	11	0	3	1	0
3	B	11	0	3	1	0
4	A	24	11	0	3	0
4	B	24	11	0	7	0
5	A	12	0	0	1	0
5	B	9	0	0	0	0
All	All	6122	22	6091	389	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 32.

All (389) 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:334:ARG:HH21	1:B:417:PHE:HB2	1.27	0.96
1:A:379:ILE:CG2	1:A:380:MET:CE	2.46	0.94
1:A:379:ILE:HG22	1:A:380:MET:CE	2.02	0.89
1:A:265:ARG:HH11	1:A:265:ARG:HG2	1.38	0.88
1:A:379:ILE:HG22	1:A:380:MET:HE2	1.58	0.86
1:A:379:ILE:CG2	1:A:380:MET:HE1	2.05	0.86
1:B:266:ASP:CG	1:B:466:ILE:HD11	2.06	0.80
1:A:431:ALA:O	1:A:434:LEU:HD12	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HG	1:A:171:PHE:CE2	2.17	0.79
1:A:364:ILE:HD12	1:A:451:ILE:HD13	1.64	0.78
1:B:559:LYS:HA	1:B:562:ILE:HD12	1.65	0.77
1:A:262:ARG:HD2	1:A:276:CYS:HA	1.67	0.77
1:A:162:ASN:HD21	1:A:164:GLU:HG3	1.50	0.77
1:B:199:TYR:CE1	1:B:239:LYS:HD2	2.20	0.77
1:A:222:GLY:HA2	1:A:242:PHE:HB3	1.67	0.77
1:B:481:LEU:O	1:B:481:LEU:HG	1.84	0.76
1:A:258:ASN:O	1:A:262:ARG:HD3	1.86	0.76
1:B:519:GLU:HG2	1:B:564:ARG:HB3	1.67	0.76
1:B:253:ARG:HG3	1:B:253:ARG:HH11	1.51	0.76
1:B:329:ILE:HG21	1:B:370:GLU:HB3	1.68	0.76
1:B:226:GLY:HA2	1:B:229:LYS:HG2	1.68	0.75
1:A:379:ILE:HG23	1:A:380:MET:CE	2.15	0.75
1:B:337:ASP:OD1	1:B:418:ASN:HB2	1.87	0.75
1:A:267:VAL:HG12	1:A:267:VAL:O	1.88	0.74
1:B:262:ARG:HD2	1:B:276:CYS:HA	1.69	0.74
1:A:302:LEU:O	1:A:303:LEU:HD23	1.87	0.74
1:A:435:ASN:OD1	1:A:438:GLN:HG3	1.88	0.73
1:A:512:LEU:HD12	1:A:512:LEU:O	1.88	0.73
1:A:514:ALA:O	1:A:518:ILE:HD12	1.88	0.73
1:A:182:GLU:HB2	1:A:263:ILE:HD12	1.71	0.72
1:A:379:ILE:HG23	1:A:380:MET:SD	2.29	0.72
1:A:512:LEU:O	1:A:516:GLU:HG3	1.89	0.72
1:B:300:ASP:OD1	1:B:302:LEU:HB2	1.89	0.72
1:A:300:ASP:OD1	1:A:302:LEU:HB2	1.90	0.72
1:A:481:LEU:O	1:A:481:LEU:HG	1.88	0.71
1:A:359:LYS:O	1:A:363:ILE:HD13	1.91	0.71
1:A:382:ASP:OD1	1:A:383:GLU:N	2.24	0.70
1:B:206:ILE:HD12	1:B:206:ILE:H	1.57	0.70
1:B:363:ILE:O	1:B:367:VAL:HG23	1.92	0.69
1:A:429:LYS:NZ	2:A:601:FMN:O3'	2.25	0.69
1:A:415:LEU:HD12	1:A:415:LEU:O	1.92	0.69
1:B:253:ARG:NH2	1:B:317:ASP:OD2	2.26	0.69
1:B:484:ILE:HD12	1:B:484:ILE:H	1.58	0.68
1:A:180:ASP:HB3	1:A:183:ILE:CG1	2.23	0.67
1:A:229:LYS:HD2	1:A:279:ASN:O	1.94	0.67
1:B:420:THR:O	1:B:422:LYS:HG3	1.94	0.67
1:B:439:LYS:HE2	1:B:488:PHE:CE1	2.30	0.67
1:B:497:ASN:O	1:B:499:GLN:HG2	1.95	0.67
1:B:237:ILE:HA	1:B:240:LEU:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:ASN:OD1	1:B:438:GLN:HG3	1.94	0.66
1:A:187:LEU:HD11	1:A:191:LEU:HD11	1.76	0.66
1:B:206:ILE:HD12	1:B:206:ILE:N	2.10	0.66
1:B:328:CYS:O	1:B:332:ILE:HG22	1.96	0.66
1:A:262:ARG:C	1:A:263:ILE:HG13	2.20	0.65
1:A:215:LEU:HD22	1:A:307:ILE:HD13	1.77	0.65
1:B:314:LYS:HG2	1:B:315:ASN:O	1.97	0.65
1:B:287:THR:O	1:B:291:ILE:HG13	1.97	0.64
1:A:180:ASP:OD2	1:A:183:ILE:HG12	1.98	0.64
1:A:276:CYS:HB3	1:A:279:ASN:OD1	1.97	0.64
1:A:172:LEU:HD22	1:A:535:GLY:HA3	1.80	0.64
1:B:493:TYR:CE2	1:B:498:LYS:HG2	2.32	0.64
1:A:439:LYS:HD3	1:A:488:PHE:CE1	2.33	0.63
1:A:187:LEU:HD13	1:A:187:LEU:C	2.23	0.63
1:B:463:ILE:HG23	1:B:476:VAL:HG21	1.80	0.63
1:A:428:VAL:HG12	1:A:451:ILE:HG12	1.81	0.63
1:A:329:ILE:HD11	1:A:339:ILE:HG12	1.81	0.62
1:B:219:ASN:HB2	1:B:220:PRO:HD2	1.80	0.62
1:A:180:ASP:HB3	1:A:183:ILE:HG13	1.82	0.62
1:A:187:LEU:HD12	4:A:603:A1JWR:F17	1.89	0.62
1:A:260:LYS:HA	1:A:262:ARG:HG3	1.81	0.61
1:B:251:THR:HG22	1:B:314:LYS:C	2.24	0.61
1:A:234:ILE:HD11	1:A:247:ILE:HG21	1.81	0.61
1:B:222:GLY:HA3	1:B:244:PHE:CE1	2.36	0.61
1:B:367:VAL:O	1:B:371:ILE:HG13	2.00	0.61
1:B:167:LEU:HD22	1:B:171:PHE:CZ	2.36	0.60
1:A:275:SER:HA	1:A:347:ASN:ND2	2.17	0.60
1:B:302:LEU:O	1:B:303:LEU:HD23	2.01	0.60
1:B:341:ILE:CD1	1:B:367:VAL:HG21	2.31	0.60
1:B:510:SER:N	1:B:513:ASP:OD2	2.33	0.60
1:A:530:CYS:O	1:A:534:ASN:HB2	2.01	0.60
1:B:294:ARG:NE	1:B:418:ASN:HA	2.16	0.60
1:A:284:ASP:OD1	1:A:331:LYS:HD3	2.01	0.59
1:B:255:GLN:OE1	1:B:315:ASN:ND2	2.31	0.59
1:A:174:PHE:HE1	1:A:179:ILE:HD11	1.66	0.59
5:A:710:HOH:O	1:B:213:LYS:HA	2.02	0.59
1:B:484:ILE:HD12	1:B:484:ILE:N	2.17	0.59
1:A:219:ASN:ND2	1:A:243:SER:HB3	2.17	0.59
1:A:226:GLY:HA2	1:A:229:LYS:HG2	1.84	0.59
1:A:300:ASP:OD1	1:A:302:LEU:N	2.35	0.59
1:B:484:ILE:H	1:B:484:ILE:CD1	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:GLU:CD	1:B:268:GLU:H	2.11	0.59
1:A:341:ILE:CD1	1:A:367:VAL:HG21	2.33	0.59
1:A:268:GLU:OE2	1:A:268:GLU:HA	2.03	0.59
1:A:337:ASP:OD1	1:A:418:ASN:HB2	2.01	0.59
1:A:233:CYS:HB3	1:A:237:ILE:HD11	1.85	0.58
1:B:230:ASN:HB2	1:B:232:VAL:HG13	1.85	0.58
1:B:253:ARG:HG3	1:B:253:ARG:NH1	2.18	0.58
1:A:172:LEU:O	1:A:176:LEU:HD12	2.03	0.58
1:B:194:TYR:O	1:B:196:ILE:HG13	2.03	0.58
1:A:524:VAL:HG12	1:A:525:CYS:N	2.18	0.58
1:A:420:THR:C	1:A:422:LYS:H	2.11	0.58
1:A:172:LEU:CD1	1:A:176:LEU:HD11	2.34	0.57
1:A:341:ILE:HD11	1:A:367:VAL:HG21	1.86	0.57
1:B:451:ILE:HG23	1:B:453:GLY:H	1.69	0.57
1:B:210:THR:HB	1:B:558:LEU:HD22	1.86	0.57
1:B:182:GLU:HB2	1:B:263:ILE:HD12	1.86	0.57
1:A:265:ARG:HH11	1:A:265:ARG:CG	2.16	0.56
1:A:429:LYS:HG3	1:A:455:ILE:HB	1.87	0.56
1:A:226:GLY:HA3	2:A:601:FMN:N5	2.20	0.56
1:A:172:LEU:HG	1:A:176:LEU:HD11	1.88	0.56
1:A:310:VAL:HG11	1:A:332:ILE:HD13	1.87	0.56
1:B:168:TYR:CD1	1:B:536:MET:HG3	2.40	0.56
1:A:329:ILE:CD1	1:A:339:ILE:HG12	2.35	0.56
1:A:200:ASP:OD1	1:A:201:THR:N	2.39	0.56
1:A:265:ARG:HG2	1:A:265:ARG:NH1	2.17	0.56
1:B:181:GLY:HA2	1:B:265:ARG:NH1	2.21	0.56
1:B:336:ALA:O	1:B:424:PRO:HB3	2.05	0.56
1:A:285:LYS:HE3	1:B:448:GLU:OE1	2.06	0.56
1:A:180:ASP:HB3	1:A:183:ILE:HG12	1.87	0.55
1:B:290:LEU:HD22	1:B:332:ILE:HD11	1.88	0.55
1:B:508:ILE:HG22	1:B:527:LEU:HD21	1.88	0.55
1:A:420:THR:C	1:A:422:LYS:N	2.64	0.55
1:A:565:LYS:O	1:A:565:LYS:HG2	2.07	0.55
1:B:206:ILE:H	1:B:206:ILE:CD1	2.19	0.55
1:A:459:THR:HG22	1:A:477:SER:HB2	1.88	0.55
1:B:207:TYR:N	1:B:207:TYR:CD1	2.73	0.55
1:A:292:LEU:HB3	1:A:296:ARG:HH12	1.70	0.55
1:A:472:LYS:C	1:A:473:LYS:HD3	2.31	0.55
1:A:528:TYR:O	1:A:531:LEU:HB2	2.06	0.55
1:A:194:TYR:O	1:A:195:ASN:C	2.50	0.54
1:A:230:ASN:HA	1:A:286:VAL:CG2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:GLN:NE2	1:A:495:TYR:OH	2.41	0.54
1:B:466:ILE:HG23	1:B:469:PHE:HB2	1.89	0.54
1:B:205:SER:HB3	1:B:547:ASN:HD21	1.73	0.54
1:B:312:ILE:HG13	1:B:312:ILE:O	2.07	0.54
1:A:191:LEU:HA	1:A:196:ILE:HD12	1.90	0.54
1:A:210:THR:OG1	1:A:211:ASN:N	2.40	0.54
1:A:267:VAL:O	1:A:267:VAL:CG1	2.56	0.54
1:B:351:LEU:O	1:B:354:ASN:HB2	2.07	0.54
1:B:373:ASN:O	1:B:377:ASN:CG	2.50	0.53
1:A:416:TRP:HB3	1:A:418:ASN:HD21	1.73	0.53
1:B:373:ASN:HA	1:B:376:LYS:HB3	1.90	0.53
1:A:225:ALA:HA	1:A:246:GLU:O	2.08	0.53
1:A:415:LEU:HD12	1:A:415:LEU:C	2.34	0.53
1:A:539:ALA:O	1:A:540:VAL:C	2.51	0.53
1:B:205:SER:HB3	1:B:547:ASN:ND2	2.24	0.53
1:B:219:ASN:HB2	1:B:220:PRO:CD	2.39	0.53
1:B:178:TYR:C	1:B:179:ILE:HD12	2.35	0.52
1:A:227:PHE:HD2	1:A:528:TYR:CE1	2.27	0.52
1:B:249:THR:HG22	1:B:250:ILE:N	2.24	0.52
1:B:341:ILE:HD11	1:B:367:VAL:HG21	1.90	0.52
1:B:175:CYS:HB3	1:B:184:CYS:SG	2.49	0.52
1:B:462:GLN:O	1:B:462:GLN:HG3	2.10	0.52
1:A:294:ARG:HH11	1:A:297:GLN:NE2	2.07	0.52
1:B:196:ILE:HG22	1:B:196:ILE:O	2.08	0.52
1:A:262:ARG:O	1:A:263:ILE:HG13	2.10	0.52
1:A:456:ILE:HG22	1:A:489:ILE:HG13	1.91	0.52
1:B:185:HIS:HD1	4:B:603:A1JWR:C02	2.23	0.52
1:A:297:GLN:HG3	1:A:298:GLU:N	2.25	0.51
1:B:185:HIS:ND1	4:B:603:A1JWR:O03	2.41	0.51
1:B:518:ILE:HA	1:B:522:ALA:O	2.10	0.51
1:A:456:ILE:CG2	1:A:489:ILE:HG13	2.41	0.51
1:B:536:MET:HE2	4:B:603:A1JWR:C11	2.41	0.51
1:A:524:VAL:CG1	1:A:525:CYS:N	2.75	0.50
1:B:548:HIS:O	1:B:552:GLN:HG2	2.12	0.50
1:B:454:MET:HE3	1:B:502:ILE:HG12	1.93	0.50
1:B:194:TYR:O	1:B:195:ASN:C	2.54	0.50
1:B:227:PHE:HD1	1:B:528:TYR:CE1	2.29	0.50
1:A:185:HIS:HD1	4:A:603:A1JWR:C02	2.24	0.50
1:A:219:ASN:CG	1:A:243:SER:HB3	2.37	0.50
1:B:227:PHE:CZ	1:B:531:LEU:HD13	2.47	0.50
1:A:159:GLU:N	1:A:159:GLU:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:LYS:HD2	1:A:541:GLN:OE1	2.12	0.50
1:B:172:LEU:HD11	1:B:176:LEU:CD1	2.41	0.50
1:B:482:LYS:HA	1:B:506:GLY:O	2.12	0.49
1:B:532:VAL:HG13	4:B:603:A1JWR:C23	2.42	0.49
1:A:182:GLU:OE2	1:A:262:ARG:NH2	2.31	0.49
1:A:429:LYS:CE	2:A:601:FMN:O3'	2.61	0.49
1:B:249:THR:HG22	1:B:250:ILE:H	1.77	0.49
1:A:253:ARG:NH1	1:A:317:ASP:OD2	2.45	0.49
1:A:264:PHE:CD2	1:A:472:LYS:HE2	2.48	0.49
1:A:427:PHE:CE2	1:A:503:ILE:HD11	2.46	0.49
1:B:199:TYR:CZ	1:B:239:LYS:HD2	2.47	0.49
1:B:278:PHE:CE1	3:B:602:ORO:H5	2.46	0.49
1:B:523:SER:HA	1:B:562:ILE:HG12	1.94	0.49
1:A:230:ASN:HA	1:A:286:VAL:HG22	1.94	0.49
1:A:278:PHE:CE1	3:A:602:ORO:H5	2.47	0.49
1:B:187:LEU:HD23	4:B:603:A1JWR:F17	2.03	0.49
1:A:228:ASP:OD1	1:A:230:ASN:O	2.30	0.49
1:A:317:ASP:HB2	1:B:213:LYS:HD3	1.93	0.49
1:A:509:PHE:O	1:A:542:ILE:HD12	2.13	0.49
1:B:220:PRO:HG2	1:B:221:PHE:CE2	2.48	0.49
1:B:234:ILE:O	1:B:235:ASP:C	2.57	0.48
1:A:266:ASP:OD1	1:A:268:GLU:HB3	2.13	0.48
1:B:376:LYS:O	1:B:376:LYS:HG2	2.13	0.48
1:B:433:ASP:OD1	1:B:460:THR:OG1	2.16	0.48
1:B:271:SER:C	1:B:272:ILE:HG13	2.38	0.48
1:B:238:LEU:HD13	1:B:306:HIS:HB3	1.95	0.48
1:A:512:LEU:HD12	1:A:512:LEU:C	2.37	0.48
1:B:565:LYS:O	1:B:565:LYS:HG2	2.13	0.48
1:A:208:ALA:O	1:A:558:LEU:HD13	2.13	0.48
1:A:328:CYS:O	1:A:332:ILE:HG22	2.14	0.48
4:A:603:A1JWR:C21	4:A:603:A1JWR:N07	2.77	0.48
1:B:466:ILE:HG23	1:B:466:ILE:O	2.13	0.48
1:B:471:ASN:OD1	1:B:471:ASN:N	2.46	0.48
1:B:436:GLN:HA	1:B:439:LYS:HG3	1.96	0.48
1:A:252:PRO:HG2	1:A:324:ASP:OD1	2.14	0.48
1:B:215:LEU:HD22	1:B:307:ILE:HD13	1.96	0.48
1:B:532:VAL:HG13	4:B:603:A1JWR:N22	2.29	0.48
1:B:557:ASN:OD1	1:B:560:GLU:HG3	2.14	0.48
1:A:478:GLY:O	1:A:479:ALA:C	2.56	0.47
1:B:279:ASN:OD1	1:B:279:ASN:N	2.39	0.47
1:B:378:ASN:HD22	1:B:415:LEU:HD21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LEU:HD23	1:A:416:TRP:CH2	2.49	0.47
1:B:309:GLY:HA3	1:B:338:TYR:CZ	2.49	0.47
1:B:460:THR:O	1:B:460:THR:HG23	2.14	0.47
1:A:292:LEU:HB3	1:A:296:ARG:NH1	2.28	0.47
1:A:509:PHE:CE1	1:A:530:CYS:HA	2.48	0.47
1:B:218:ILE:HD11	1:B:305:LYS:HD3	1.96	0.47
1:A:168:TYR:CE2	1:A:198:PRO:HG3	2.49	0.47
1:A:180:ASP:O	1:A:183:ILE:HB	2.14	0.47
1:A:463:ILE:HB	1:A:476:VAL:HG21	1.96	0.47
1:B:170:ILE:HG22	1:B:171:PHE:N	2.29	0.47
1:A:503:ILE:H	1:A:503:ILE:HD12	1.80	0.47
1:B:267:VAL:O	1:B:268:GLU:C	2.57	0.47
1:A:264:PHE:CE2	1:A:472:LYS:HE2	2.50	0.47
1:B:179:ILE:HD12	1:B:179:ILE:N	2.28	0.47
1:B:334:ARG:NH2	1:B:417:PHE:HB2	2.10	0.47
1:B:420:THR:C	1:B:422:LYS:N	2.71	0.47
1:A:244:PHE:HA	1:A:307:ILE:O	2.15	0.47
1:B:169:ASP:OD2	1:B:537:LYS:HD3	2.15	0.47
1:B:221:PHE:CZ	1:B:542:ILE:HG12	2.49	0.47
1:B:172:LEU:HD11	1:B:176:LEU:HD11	1.97	0.47
1:B:219:ASN:ND2	1:B:243:SER:HB3	2.30	0.47
1:B:357:ALA:HB2	1:B:441:GLU:HB3	1.96	0.47
1:A:173:LYS:HD3	1:A:173:LYS:N	2.30	0.46
1:A:192:GLY:HA2	1:A:197:LEU:HG	1.97	0.46
1:A:529:SER:O	1:A:532:VAL:N	2.48	0.46
1:A:537:LYS:O	1:A:541:GLN:HB3	2.15	0.46
1:B:218:ILE:HD11	1:B:305:LYS:HB3	1.96	0.46
1:A:162:ASN:O	1:A:165:PHE:HB2	2.16	0.46
1:A:548:HIS:O	1:A:549:LEU:C	2.54	0.46
1:B:183:ILE:HD13	1:B:183:ILE:HA	1.73	0.46
1:A:173:LYS:N	1:A:173:LYS:CD	2.79	0.46
1:B:542:ILE:O	1:B:543:LYS:C	2.59	0.46
1:A:300:ASP:CG	1:A:302:LEU:HB2	2.40	0.46
1:A:231:GLY:O	1:A:289:ASN:HB3	2.16	0.46
1:B:179:ILE:N	1:B:179:ILE:CD1	2.78	0.46
1:A:304:SER:H	1:A:304:SER:HG	1.51	0.45
1:B:463:ILE:CG2	1:B:476:VAL:HG21	2.45	0.45
1:B:165:PHE:CE2	1:B:167:LEU:HB2	2.52	0.45
1:A:371:ILE:O	1:A:374:LEU:HB3	2.16	0.45
1:A:514:ALA:C	1:A:518:ILE:HD12	2.41	0.45
1:B:196:ILE:O	1:B:196:ILE:CG2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ASN:HB2	1:A:275:SER:O	2.16	0.45
1:A:312:ILE:HD12	1:A:325:LEU:HD22	1.98	0.45
1:A:380:MET:SD	1:A:380:MET:N	2.89	0.45
1:A:172:LEU:C	1:A:176:LEU:HD12	2.42	0.45
1:A:211:ASN:HA	1:A:215:LEU:O	2.16	0.45
1:B:552:GLN:C	1:B:554:GLY:H	2.25	0.45
1:A:558:LEU:O	1:A:558:LEU:HD23	2.16	0.45
1:B:467:LYS:O	1:B:470:GLU:HB2	2.16	0.45
1:A:446:LEU:HD13	1:A:454:MET:HG2	1.99	0.45
1:B:549:LEU:O	1:B:553:ARG:HG2	2.17	0.45
1:A:169:ASP:O	1:A:172:LEU:HB3	2.17	0.45
1:A:294:ARG:HH11	1:A:297:GLN:HE22	1.65	0.45
1:B:189:LEU:HA	1:B:189:LEU:HD23	1.63	0.45
1:B:508:ILE:HD11	1:B:517:LYS:HG3	1.98	0.45
1:A:175:CYS:O	1:A:265:ARG:NH2	2.51	0.44
1:A:279:ASN:OD1	1:A:279:ASN:N	2.45	0.44
1:B:466:ILE:CG2	1:B:469:PHE:HB2	2.47	0.44
1:B:176:LEU:CD2	1:B:265:ARG:HD2	2.46	0.44
1:B:482:LYS:O	1:B:483:ASP:C	2.60	0.44
1:A:332:ILE:HG12	1:A:332:ILE:O	2.18	0.44
1:A:364:ILE:O	1:A:368:LYS:HG3	2.18	0.44
1:B:214:HIS:CE1	1:B:425:LEU:HD21	2.52	0.44
1:B:255:GLN:HE21	1:B:255:GLN:HB3	1.46	0.44
1:B:283:CYS:SG	1:B:328:CYS:HA	2.57	0.44
1:B:528:TYR:O	1:B:531:LEU:HB2	2.18	0.44
1:B:226:GLY:N	1:B:248:GLY:O	2.51	0.44
1:B:460:THR:HG23	1:B:463:ILE:HG22	1.99	0.44
1:A:429:LYS:HB2	1:A:455:ILE:HD12	2.00	0.44
1:B:297:GLN:O	1:B:298:GLU:C	2.60	0.44
1:A:426:VAL:O	1:A:427:PHE:HD1	2.01	0.44
1:A:266:ASP:H	1:A:469:PHE:HZ	1.66	0.43
1:B:247:ILE:HD13	1:B:290:LEU:HD13	2.00	0.43
4:B:603:A1JWR:C21	4:B:603:A1JWR:N07	2.80	0.43
1:A:269:SER:O	1:A:270:ARG:C	2.60	0.43
1:B:251:THR:HG21	1:B:315:ASN:HA	2.00	0.43
1:A:315:ASN:HB2	1:A:318:THR:OG1	2.19	0.43
1:A:197:LEU:HD12	1:A:236:SER:HB2	2.01	0.43
1:A:466:ILE:HG23	1:A:469:PHE:HB2	2.00	0.43
1:B:255:GLN:HG3	1:B:315:ASN:HD21	1.82	0.43
1:B:524:VAL:HG22	1:B:525:CYS:H	1.84	0.43
1:A:250:ILE:HD12	1:A:283:CYS:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:THR:HG21	1:A:331:LYS:O	2.18	0.43
1:A:419:THR:C	1:A:421:LYS:N	2.75	0.43
1:A:521:GLY:HA2	1:A:563:GLY:HA2	2.01	0.43
1:B:247:ILE:HG12	1:B:310:VAL:HG22	2.01	0.43
1:B:493:TYR:CZ	1:B:498:LYS:HG2	2.53	0.43
1:A:240:LEU:HD23	1:A:240:LEU:HA	1.60	0.43
1:B:230:ASN:OD1	1:B:281:MET:HG3	2.18	0.43
1:B:352:ARG:C	1:B:354:ASN:H	2.27	0.43
1:B:484:ILE:N	1:B:484:ILE:CD1	2.80	0.43
1:A:301:LYS:HA	1:A:304:SER:OG	2.19	0.43
1:B:215:LEU:HD23	1:B:215:LEU:HA	1.72	0.43
1:A:250:ILE:CG1	1:A:312:ILE:HG22	2.49	0.43
1:A:172:LEU:HD22	1:A:535:GLY:CA	2.48	0.43
1:B:266:ASP:CB	1:B:466:ILE:HD11	2.49	0.43
1:B:515:LEU:HD23	1:B:549:LEU:HD21	2.01	0.43
1:A:211:ASN:HB2	1:A:215:LEU:O	2.19	0.42
1:A:235:ASP:OD1	1:A:293:PHE:CD1	2.72	0.42
1:A:290:LEU:HD23	1:A:332:ILE:HD11	2.01	0.42
1:A:301:LYS:O	1:A:304:SER:OG	2.32	0.42
1:A:379:ILE:CG2	1:A:380:MET:HE2	2.27	0.42
1:A:418:ASN:OD1	1:A:421:LYS:N	2.52	0.42
1:B:218:ILE:HD11	1:B:305:LYS:CB	2.49	0.42
1:B:222:GLY:HA3	1:B:244:PHE:CD1	2.54	0.42
1:A:489:ILE:O	1:A:490:CYS:C	2.61	0.42
1:A:565:LYS:O	1:A:565:LYS:CG	2.68	0.42
1:A:266:ASP:CB	1:A:466:ILE:HD11	2.49	0.42
1:A:557:ASN:OD1	1:A:557:ASN:C	2.62	0.42
1:B:559:LYS:HA	1:B:562:ILE:CD1	2.43	0.42
1:A:179:ILE:HG22	1:A:183:ILE:HB	2.01	0.42
1:A:558:LEU:HD23	1:A:558:LEU:C	2.45	0.42
1:B:337:ASP:HB3	1:B:420:THR:HG23	2.00	0.42
1:B:200:ASP:N	1:B:239:LYS:O	2.48	0.42
1:B:371:ILE:HG21	1:B:424:PRO:HG2	2.01	0.42
1:B:486:THR:OG1	1:B:517:LYS:HE2	2.19	0.42
1:A:193:LYS:HE3	1:A:194:TYR:CZ	2.55	0.42
1:A:534:ASN:O	1:A:537:LYS:HG2	2.20	0.42
1:B:210:THR:OG1	1:B:211:ASN:N	2.52	0.42
1:A:170:ILE:O	1:A:171:PHE:C	2.63	0.42
1:A:287:THR:HG23	1:A:332:ILE:HG13	2.02	0.42
1:B:456:ILE:HG23	1:B:488:PHE:CD2	2.55	0.42
1:B:542:ILE:HG23	1:B:543:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.80	0.42
1:A:433:ASP:OD1	1:A:460:THR:OG1	2.32	0.42
1:B:235:ASP:HB3	1:B:296:ARG:NH1	2.35	0.42
1:A:466:ILE:HG23	1:A:466:ILE:O	2.20	0.41
1:A:486:THR:OG1	1:A:517:LYS:HE2	2.20	0.41
1:B:181:GLY:HA2	1:B:265:ARG:HH11	1.84	0.41
1:B:285:LYS:HD2	1:B:285:LYS:HA	1.64	0.41
1:B:309:GLY:HA3	1:B:338:TYR:CE2	2.56	0.41
1:B:365:LEU:HD23	1:B:365:LEU:HA	1.81	0.41
1:B:542:ILE:CG2	1:B:543:LYS:N	2.82	0.41
1:A:565:LYS:HB2	1:A:565:LYS:HE3	1.77	0.41
1:B:372:ASP:C	1:B:374:LEU:N	2.78	0.41
1:A:206:ILE:O	1:A:206:ILE:HG22	2.20	0.41
1:A:473:LYS:HD3	1:A:473:LYS:N	2.34	0.41
1:A:521:GLY:HA2	1:A:563:GLY:CA	2.50	0.41
1:B:168:TYR:CG	1:B:536:MET:HG3	2.55	0.41
1:A:255:GLN:HG3	1:A:315:ASN:ND2	2.35	0.41
1:A:376:LYS:H	1:A:376:LYS:HG2	1.53	0.41
1:A:442:ILE:O	1:A:446:LEU:HG	2.21	0.41
1:B:219:ASN:CB	1:B:220:PRO:CD	2.98	0.41
1:B:341:ILE:HD13	1:B:367:VAL:HG21	2.03	0.41
1:A:336:ALA:O	1:A:424:PRO:HB3	2.20	0.41
1:A:456:ILE:HA	1:A:457:SER:HA	1.61	0.41
1:A:237:ILE:O	1:A:240:LEU:HB2	2.20	0.41
1:A:460:THR:O	1:A:476:VAL:HG23	2.20	0.41
1:B:465:ASP:O	1:B:465:ASP:CG	2.63	0.41
1:B:555:TYR:OH	1:B:564:ARG:HG2	2.20	0.41
1:A:172:LEU:CG	1:A:176:LEU:HD11	2.50	0.41
1:A:187:LEU:O	1:A:187:LEU:HD22	2.21	0.41
1:A:275:SER:HA	1:A:347:ASN:CG	2.46	0.41
1:A:307:ILE:HG22	1:A:308:VAL:N	2.35	0.41
1:A:503:ILE:HD12	1:A:503:ILE:N	2.35	0.41
1:B:220:PRO:HG2	1:B:221:PHE:CD2	2.56	0.41
1:B:322:VAL:O	1:B:323:ASP:C	2.62	0.41
1:A:294:ARG:CZ	1:A:418:ASN:HA	2.50	0.41
1:B:429:LYS:NZ	2:B:601:FMN:O2'	2.48	0.40
1:A:440:LYS:HG2	1:A:495:TYR:CD1	2.56	0.40
1:A:465:ASP:O	1:A:465:ASP:CG	2.63	0.40
1:B:326:LYS:HB3	1:B:326:LYS:HE2	1.88	0.40
1:B:338:TYR:CD1	1:B:338:TYR:C	2.99	0.40
1:B:477:SER:HA	1:B:481:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HD11	1:A:191:LEU:CD1	2.47	0.40
1:A:367:VAL:O	1:A:371:ILE:HG13	2.21	0.40
1:A:437:GLU:O	1:A:441:GLU:HG3	2.20	0.40
1:B:345:SER:HA	1:B:458:ASN:ND2	2.37	0.40
1:A:454:MET:HG3	1:A:500:ILE:CG2	2.51	0.40
1:A:472:LYS:HD2	1:A:472:LYS:HA	1.82	0.40
1:A:542:ILE:O	1:A:543:LYS:C	2.64	0.40
1:B:415:LEU:O	1:B:416:TRP:C	2.64	0.40
1:B:505:SER:OG	2:B:601:FMN:H5'1	2.21	0.40
1:A:173:LYS:HD3	1:A:173:LYS:H	1.85	0.40
1:B:217:PHE:O	1:B:218:ILE:C	2.64	0.40
1:B:327:TYR:O	1:B:328:CYS:C	2.64	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	377/405 (93%)	338 (90%)	39 (10%)	0	100	100
1	B	370/405 (91%)	321 (87%)	48 (13%)	1 (0%)	36	59
All	All	747/810 (92%)	659 (88%)	87 (12%)	1 (0%)	48	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	506	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/360 (93%)	313 (93%)	23 (7%)	14	35
1	B	331/360 (92%)	312 (94%)	19 (6%)	18	42
All	All	667/720 (93%)	625 (94%)	42 (6%)	16	38

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	169	ASP
1	A	180	ASP
1	A	195	ASN
1	A	196	ILE
1	A	205	SER
1	A	210	THR
1	A	229	LYS
1	A	251	THR
1	A	275	SER
1	A	279	ASN
1	A	295	LYS
1	A	329	ILE
1	A	374	LEU
1	A	415	LEU
1	A	466	ILE
1	A	480	LYS
1	A	482	LYS
1	A	502	ILE
1	A	523	SER
1	A	527	LEU
1	A	538	SER
1	A	565	LYS
1	B	167	LEU
1	B	218	ILE
1	B	232	VAL
1	B	235	ASP

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Mol	Chain	Res	Type
1	B	251	THR
1	B	274	ASN
1	B	280	ASN
1	B	285	LYS
1	B	291	ILE
1	B	296	ARG
1	B	304	SER
1	B	353	ASP
1	B	371	ILE
1	B	447	LEU
1	B	463	ILE
1	B	471	ASN
1	B	480	LYS
1	B	484	ILE
1	B	498	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	A	330	ASN
1	A	436	GLN
1	A	526	GLN
1	B	214	HIS
1	B	499	GLN
1	B	547	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
2	FMN	A	601	-	33,33,33	1.02	1 (3%)	48,50,50	1.51	12 (25%)
4	A1JWR	B	603	-	24,25,25	2.06	10 (41%)	34,43,43	1.13	3 (8%)
4	A1JWR	A	603	-	24,25,25	2.01	8 (33%)	34,43,43	1.16	3 (8%)
3	ORO	B	602	-	11,11,11	1.05	1 (9%)	14,15,15	0.77	1 (7%)
3	ORO	A	602	-	11,11,11	1.05	1 (9%)	14,15,15	0.77	0
2	FMN	B	601	-	33,33,33	1.09	1 (3%)	48,50,50	1.57	9 (18%)

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	-	-	4/18/18/18	0/3/3/3
4	A1JWR	B	603	-	-	12/19/19/19	0/2/2/2
4	A1JWR	A	603	-	-	12/19/19/19	0/2/2/2
3	ORO	B	602	-	-	4/4/4/4	0/1/1/1
3	ORO	A	602	-	-	4/4/4/4	0/1/1/1
2	FMN	B	601	-	-	6/18/18/18	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	A1JWR	F15-S14	4.01	1.63	1.58
4	A	603	A1JWR	C08-N07	3.61	1.48	1.38
4	B	603	A1JWR	C08-N07	3.53	1.48	1.38
4	B	603	A1JWR	F15-S14	3.47	1.62	1.58
4	A	603	A1JWR	F16-S14	3.43	1.62	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FMN	C4A-N5	3.35	1.38	1.30
4	A	603	A1JWR	F17-S14	3.29	1.62	1.58
4	B	603	A1JWR	F17-S14	3.29	1.62	1.58
2	A	601	FMN	C4A-N5	3.27	1.37	1.30
4	B	603	A1JWR	F16-S14	3.19	1.62	1.58
4	B	603	A1JWR	C04-C02	3.05	1.54	1.48
3	B	602	ORO	O72-C7	-3.00	1.22	1.30
3	A	602	ORO	O72-C7	-3.00	1.22	1.30
4	B	603	A1JWR	F18-S14	2.95	1.62	1.58
4	A	603	A1JWR	F18-S14	2.93	1.62	1.58
4	A	603	A1JWR	F19-S14	2.86	1.61	1.58
4	B	603	A1JWR	C12-S14	2.82	1.84	1.80
4	B	603	A1JWR	F19-S14	2.76	1.61	1.58
4	A	603	A1JWR	C04-C02	2.76	1.54	1.48
4	B	603	A1JWR	C04-C23	-2.23	1.38	1.45
4	A	603	A1JWR	O24-C23	2.19	1.40	1.33
4	B	603	A1JWR	C06-N07	2.14	1.48	1.45

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FMN	C5'-C4'-C3'	-5.07	102.65	112.22
2	B	601	FMN	O2'-C2'-C3'	-3.78	100.39	109.25
2	A	601	FMN	C4-N3-C2	-3.73	119.01	125.64
2	B	601	FMN	C4-N3-C2	-3.60	119.26	125.64
4	A	603	A1JWR	O03-C02-C04	3.37	125.18	116.58
4	A	603	A1JWR	C02-C04-C23	3.04	127.39	121.80
2	A	601	FMN	C4A-C10-N10	2.90	120.63	116.48
2	B	601	FMN	C5A-C9A-N10	2.87	120.56	117.97
2	A	601	FMN	C5A-C9A-N10	2.85	120.54	117.97
4	A	603	A1JWR	O01-C02-C04	-2.72	115.46	121.64
2	A	601	FMN	O3'-C3'-C2'	2.69	115.05	108.93
2	B	601	FMN	O4-C4-C4A	-2.67	119.47	126.53
2	B	601	FMN	C4A-C10-N10	2.63	120.25	116.48
4	B	603	A1JWR	C21-N20-N22	2.60	123.17	119.29
2	A	601	FMN	O5'-C5'-C4'	-2.57	102.51	109.36
2	A	601	FMN	C4-C4A-C10	2.51	121.24	116.93
2	A	601	FMN	C4A-C10-N1	-2.42	118.64	124.59
2	B	601	FMN	C4-C4A-C10	2.41	121.06	116.93
2	A	601	FMN	C1'-C2'-C3'	2.33	115.98	109.66
2	A	601	FMN	O4-C4-C4A	-2.32	120.41	126.53
2	A	601	FMN	C4A-C4-N3	2.31	119.12	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FMN	C4A-C4-N3	2.30	119.10	113.25
4	B	603	A1JWR	O03-C02-O01	-2.20	118.66	123.90
2	A	601	FMN	C10-C4A-N5	-2.16	120.40	124.81
4	B	603	A1JWR	C13-C12-S14	2.15	120.67	119.07
2	A	601	FMN	O3P-P-O2P	2.10	115.68	107.80
2	B	601	FMN	C4A-C10-N1	-2.06	119.53	124.59
3	B	602	ORO	O71-C7-C6	-2.02	116.92	121.01

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FMN	C5'-O5'-P-O2P
2	B	601	FMN	O4'-C4'-C5'-O5'
2	B	601	FMN	C5'-O5'-P-O2P
2	B	601	FMN	C5'-O5'-P-O3P
3	A	602	ORO	N1-C6-C7-O71
3	A	602	ORO	N1-C6-C7-O72
3	A	602	ORO	C5-C6-C7-O71
3	A	602	ORO	C5-C6-C7-O72
3	B	602	ORO	N1-C6-C7-O71
3	B	602	ORO	N1-C6-C7-O72
3	B	602	ORO	C5-C6-C7-O71
3	B	602	ORO	C5-C6-C7-O72
4	A	603	A1JWR	C13-C12-S14-F17
4	A	603	A1JWR	C11-C12-S14-F15
4	A	603	A1JWR	C11-C12-S14-F17
4	B	603	A1JWR	C13-C12-S14-F18
4	B	603	A1JWR	C11-C12-S14-F18
4	A	603	A1JWR	C11-C12-S14-F16
4	A	603	A1JWR	C13-C12-S14-F15
4	A	603	A1JWR	C13-C12-S14-F16
4	B	603	A1JWR	C13-C12-S14-F15
4	B	603	A1JWR	C13-C12-S14-F16
4	B	603	A1JWR	C11-C12-S14-F15
4	B	603	A1JWR	C11-C12-S14-F16
4	A	603	A1JWR	C13-C08-N07-C06
4	A	603	A1JWR	C09-C08-N07-C06
4	B	603	A1JWR	C09-C08-N07-C06
4	B	603	A1JWR	C13-C08-N07-C06
2	A	601	FMN	C3'-C4'-C5'-O5'
2	B	601	FMN	C3'-C4'-C5'-O5'

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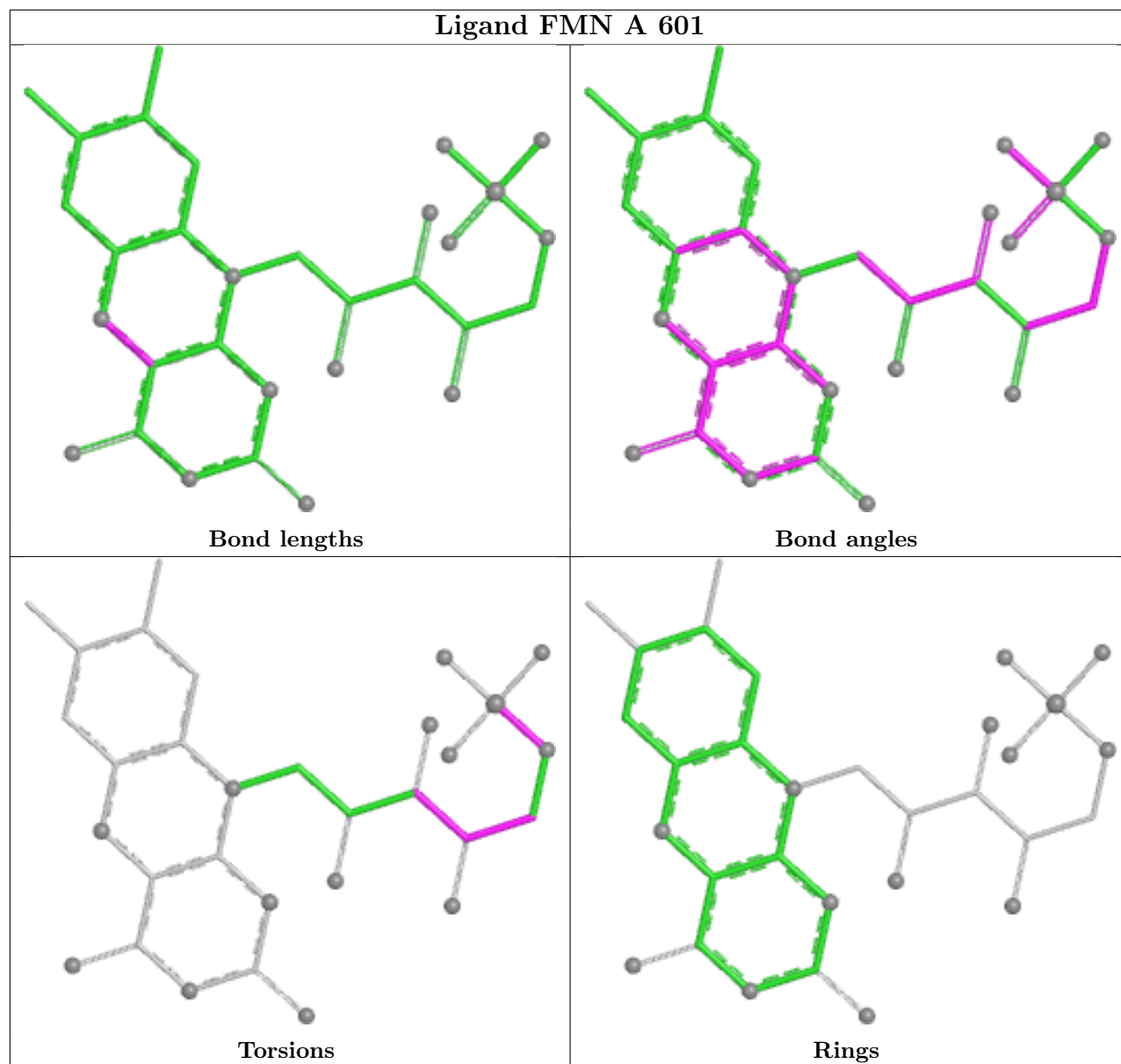
Mol	Chain	Res	Type	Atoms
4	A	603	A1JWR	C13-C12-S14-F19
2	B	601	FMN	C5'-O5'-P-O1P
2	A	601	FMN	O4'-C4'-C5'-O5'
4	A	603	A1JWR	C11-C12-S14-F19
4	B	603	A1JWR	C11-C12-S14-F19
2	A	601	FMN	C2'-C3'-C4'-C5'
4	B	603	A1JWR	C13-C12-S14-F19
2	B	601	FMN	C4'-C5'-O5'-P
4	B	603	A1JWR	C05-C06-N07-C08
4	A	603	A1JWR	C04-C05-C06-N07
4	B	603	A1JWR	C04-C05-C06-N07
4	A	603	A1JWR	N20-C05-C06-N07

There are no ring outliers.

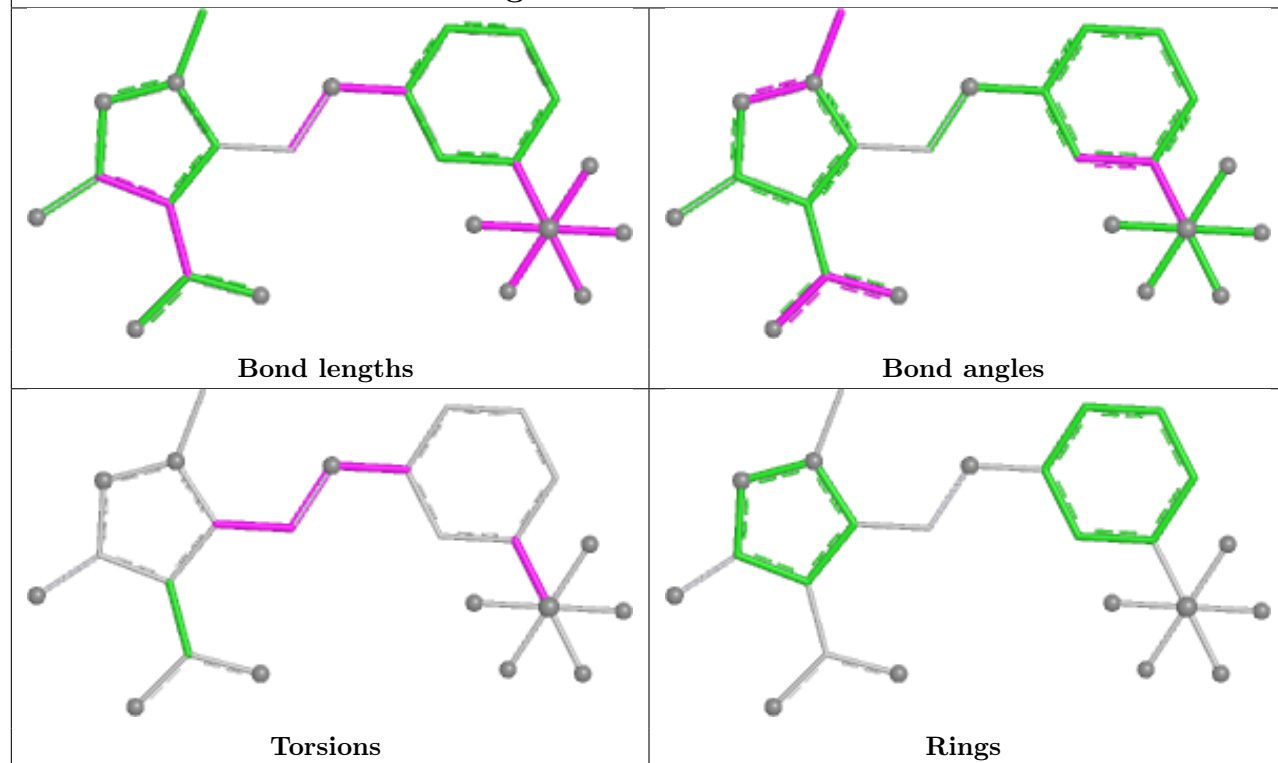
6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FMN	3	0
4	B	603	A1JWR	7	0
4	A	603	A1JWR	3	0
3	B	602	ORO	1	0
3	A	602	ORO	1	0
2	B	601	FMN	2	0

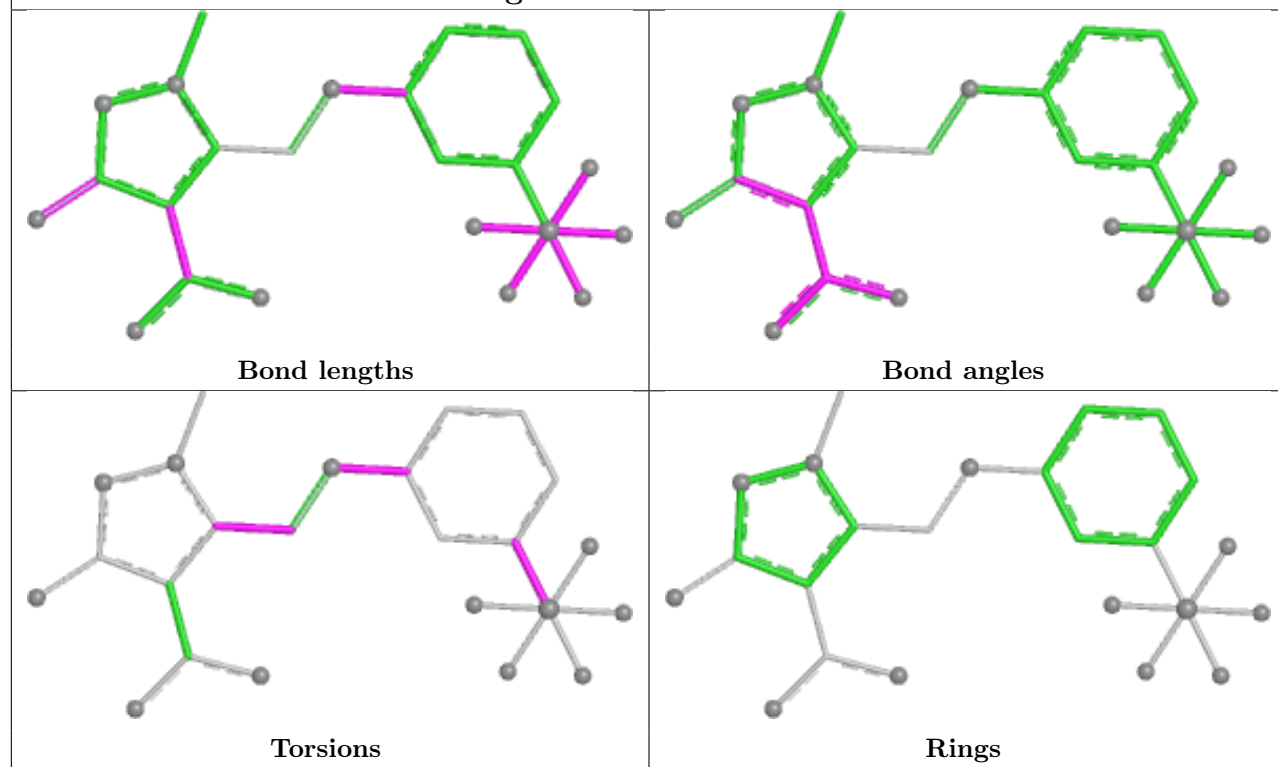
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

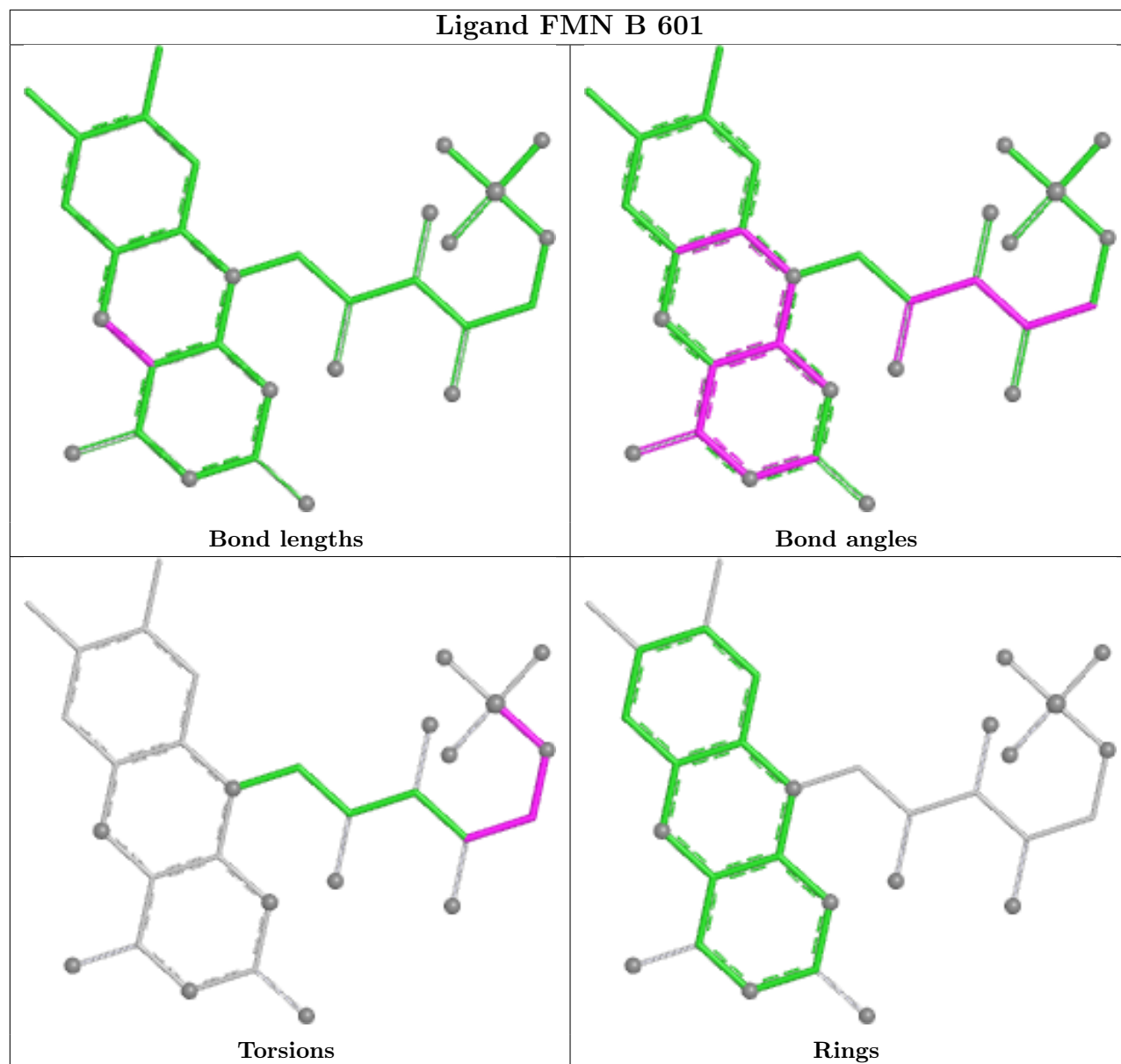


Ligand A1JWR B 603



Ligand A1JWR A 603





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	379/405 (93%)	0.55	23 (6%) 27 22	38, 56, 87, 119	0
1	B	374/405 (92%)	0.54	19 (5%) 33 28	37, 54, 84, 117	0
All	All	753/810 (92%)	0.55	42 (5%) 30 25	37, 55, 86, 119	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	527	LEU	4.0
1	A	521	GLY	3.6
1	A	161	TYR	3.4
1	A	538	SER	3.3
1	A	522	ALA	3.3
1	A	162	ASN	3.1
1	A	236	SER	3.1
1	B	414	PHE	3.1
1	A	279	ASN	3.0
1	B	415	LEU	2.9
1	B	235	ASP	2.9
1	B	417	PHE	2.9
1	B	276	CYS	2.9
1	A	481	LEU	2.8
1	B	374	LEU	2.8
1	B	475	GLY	2.8
1	B	474	GLY	2.7
1	B	162	ASN	2.7
1	A	317	ASP	2.7
1	B	317	ASP	2.7
1	A	195	ASN	2.6
1	A	379	ILE	2.5
1	A	280	ASN	2.5
1	B	195	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	334	ARG	2.4
1	A	528	TYR	2.4
1	A	278	PHE	2.4
1	A	567	SER	2.4
1	A	207	TYR	2.4
1	A	428	VAL	2.4
1	B	506	GLY	2.4
1	A	466	ILE	2.4
1	A	499	GLN	2.2
1	A	427	PHE	2.2
1	B	481	LEU	2.2
1	B	223	VAL	2.2
1	A	465	ASP	2.2
1	A	537	LYS	2.2
1	B	428	VAL	2.1
1	A	380	MET	2.1
1	B	505	SER	2.1
1	B	451	ILE	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

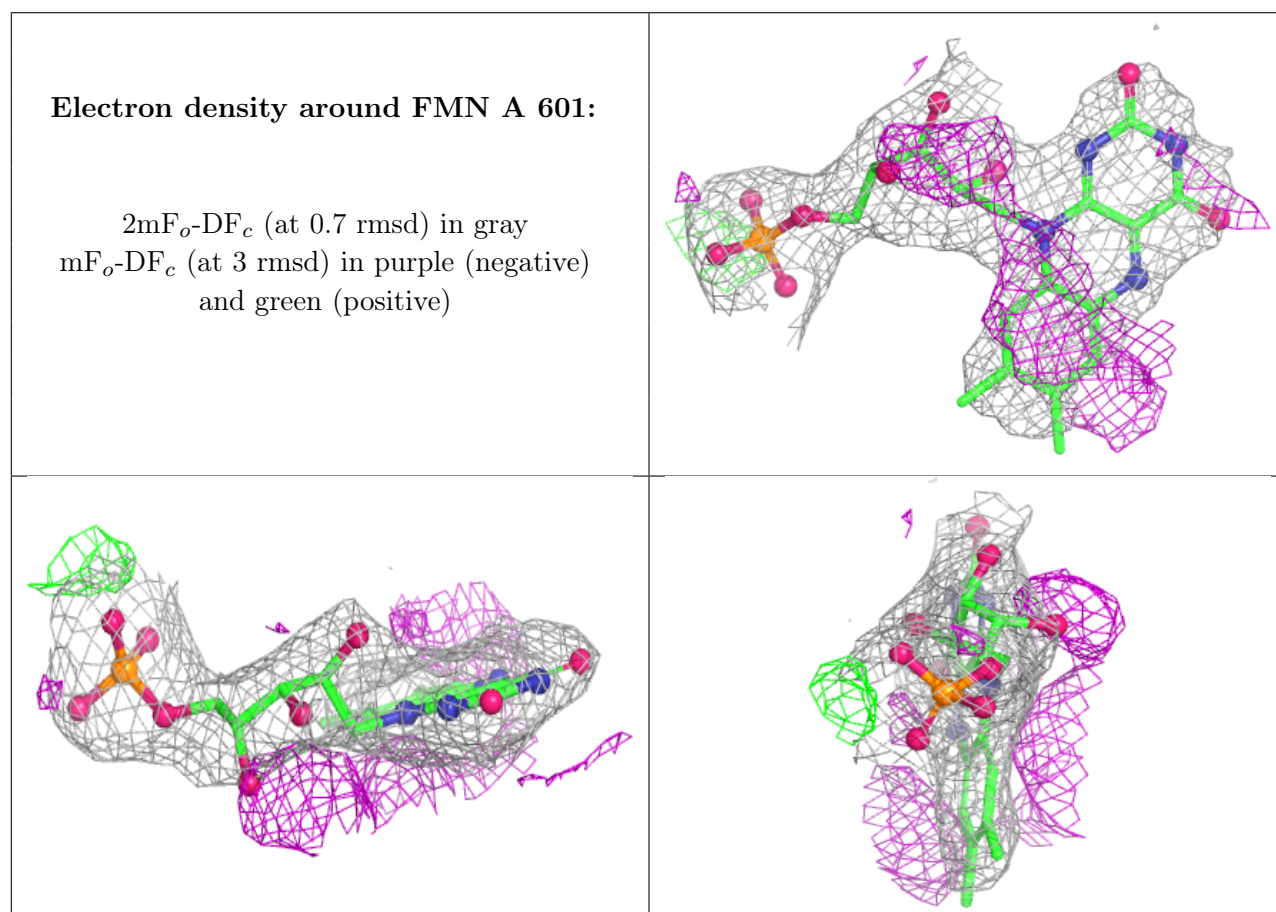
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ORO	B	602	11/11	0.83	0.21	48,51,55,56	0
3	ORO	A	602	11/11	0.86	0.26	49,52,54,55	0
2	FMN	A	601	31/31	0.88	0.13	46,52,58,64	0
4	A1JWR	A	603	24/24	0.92	0.12	42,74,96,97	0
4	A1JWR	B	603	24/24	0.93	0.10	48,78,94,98	0

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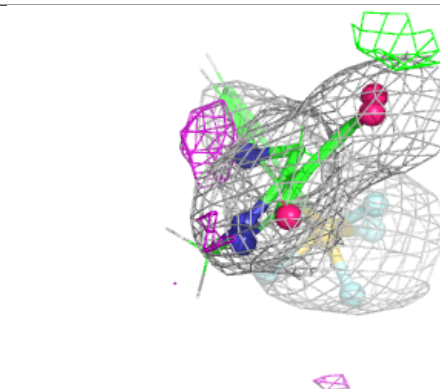
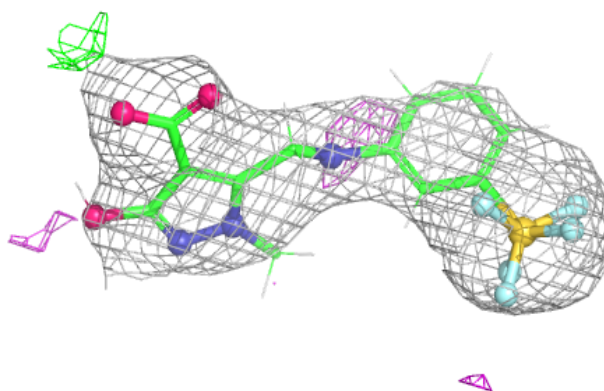
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FMN	B	601	31/31	0.94	0.10	45,52,59,65	0

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.

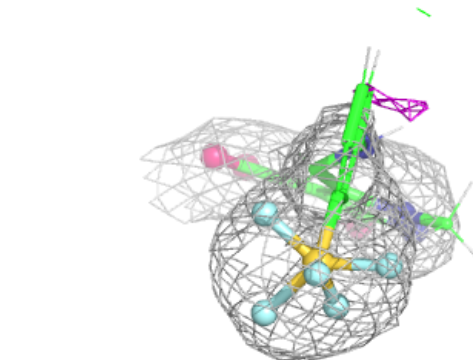
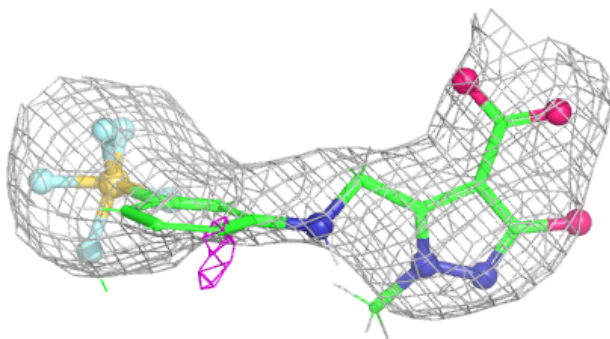
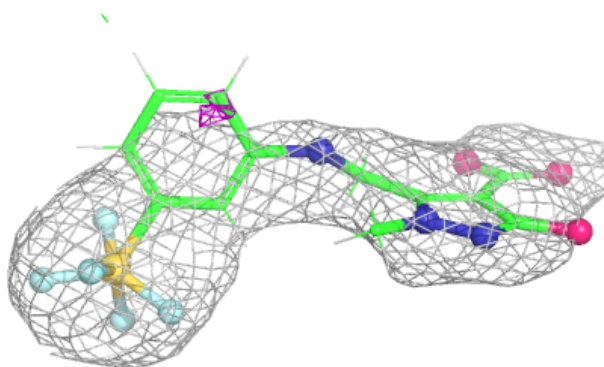


Electron density around A1JWR A 603:

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

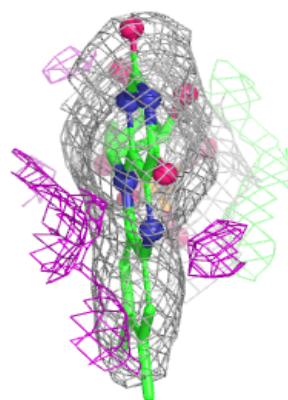
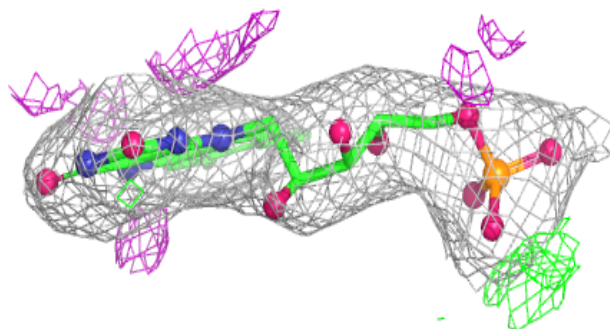
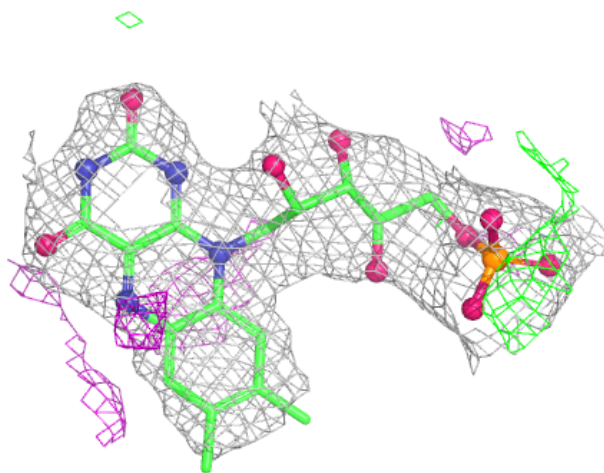
**Electron density around A1JWR B 603:**

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



Electron density around FMN B 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 [i](#)

There are no such residues in this entry.