



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:58 AM UTC

PDB ID : 6THQ / pdb_00006thq
Title : Crystal structure of branched-chain aminotransferase from thermophilic archaea *Thermoproteus uzoniensis* with norvaline
Authors : Boyko, K.M.; Nikolaeva, A.Y.; Bezsudnova, E.Y.; Popov, V.O.
Deposited on : 2019-11-21
Resolution : 2.15 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

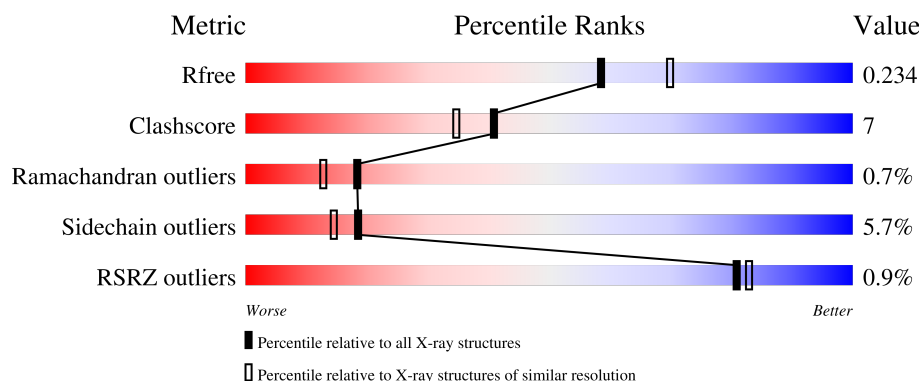
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	307	% 80% 14% ...
1	B	307	% 82% 14% ..
1	C	307	% 81% 13% ..

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
3	PY5	A	302[A]	-	-	X	-
3	PY5	B	302[A]	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7304 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 Branched-chain-amino-acid aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	3	0
			2326	1494	398	425	9			
1	B	301	Total	C	N	O	S	0	3	0
			2358	1518	402	430	8			
1	C	296	Total	C	N	O	S	0	5	0
			2327	1496	397	426	8			

There are 36 discrepancies between the modelled and reference sequences:

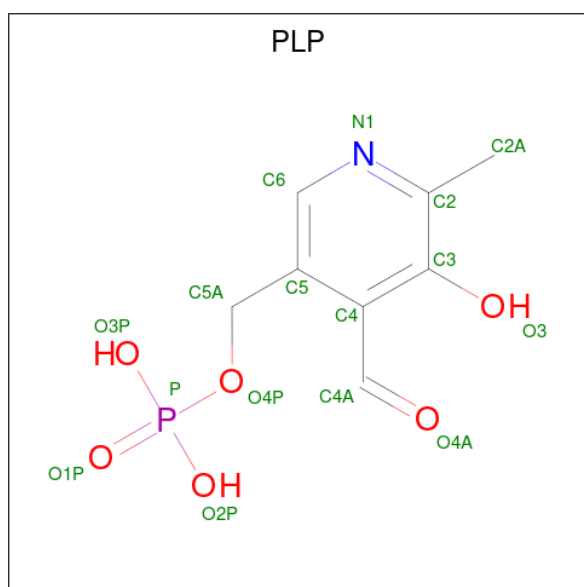
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP F2L0W0
A	-10	ARG	-	expression tag	UNP F2L0W0
A	-9	GLY	-	expression tag	UNP F2L0W0
A	-8	SER	-	expression tag	UNP F2L0W0
A	-7	HIS	-	expression tag	UNP F2L0W0
A	-6	HIS	-	expression tag	UNP F2L0W0
A	-5	HIS	-	expression tag	UNP F2L0W0
A	-4	HIS	-	expression tag	UNP F2L0W0
A	-3	HIS	-	expression tag	UNP F2L0W0
A	-2	HIS	-	expression tag	UNP F2L0W0
A	-1	GLY	-	expression tag	UNP F2L0W0
A	0	SER	-	expression tag	UNP F2L0W0
B	-11	MET	-	initiating methionine	UNP F2L0W0
B	-10	ARG	-	expression tag	UNP F2L0W0
B	-9	GLY	-	expression tag	UNP F2L0W0
B	-8	SER	-	expression tag	UNP F2L0W0
B	-7	HIS	-	expression tag	UNP F2L0W0
B	-6	HIS	-	expression tag	UNP F2L0W0
B	-5	HIS	-	expression tag	UNP F2L0W0
B	-4	HIS	-	expression tag	UNP F2L0W0
B	-3	HIS	-	expression tag	UNP F2L0W0
B	-2	HIS	-	expression tag	UNP F2L0W0
B	-1	GLY	-	expression tag	UNP F2L0W0

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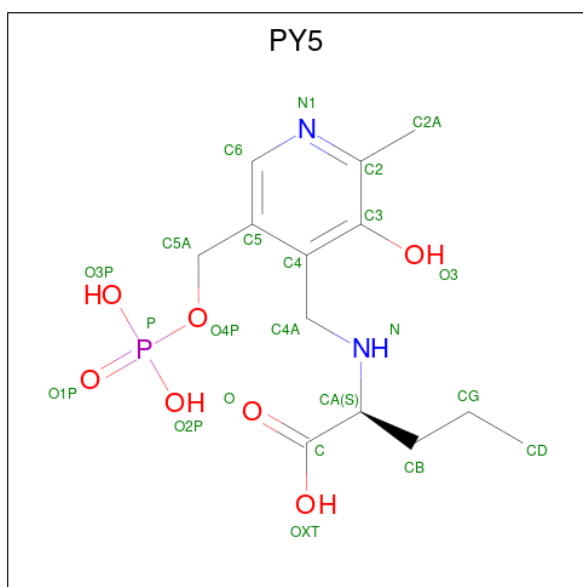
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP F2L0W0
C	-11	MET	-	initiating methionine	UNP F2L0W0
C	-10	ARG	-	expression tag	UNP F2L0W0
C	-9	GLY	-	expression tag	UNP F2L0W0
C	-8	SER	-	expression tag	UNP F2L0W0
C	-7	HIS	-	expression tag	UNP F2L0W0
C	-6	HIS	-	expression tag	UNP F2L0W0
C	-5	HIS	-	expression tag	UNP F2L0W0
C	-4	HIS	-	expression tag	UNP F2L0W0
C	-3	HIS	-	expression tag	UNP F2L0W0
C	-2	HIS	-	expression tag	UNP F2L0W0
C	-1	GLY	-	expression tag	UNP F2L0W0
C	0	SER	-	expression tag	UNP F2L0W0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	1
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	1
			15	8	1	5	1		

- Molecule 3 is 2-[O-PHOSPHONOPYRIDOXYL]-AMINO-PENTANOIC ACID (CCD ID: PY5) (formula: $C_{13}H_{21}N_2O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			23	13	2	7	1		
3	B	1	Total	C	N	O	P	0	1
			23	13	2	7	1		
3	C	1	Total	C	N	O	P	0	1
			23	13	2	7	1		

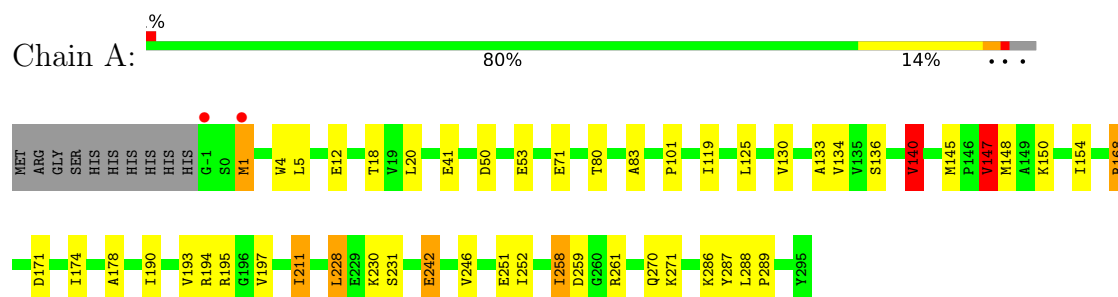
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	54	Total	O	0	0
			54	54		
4	C	54	Total	O	0	0
			54	54		

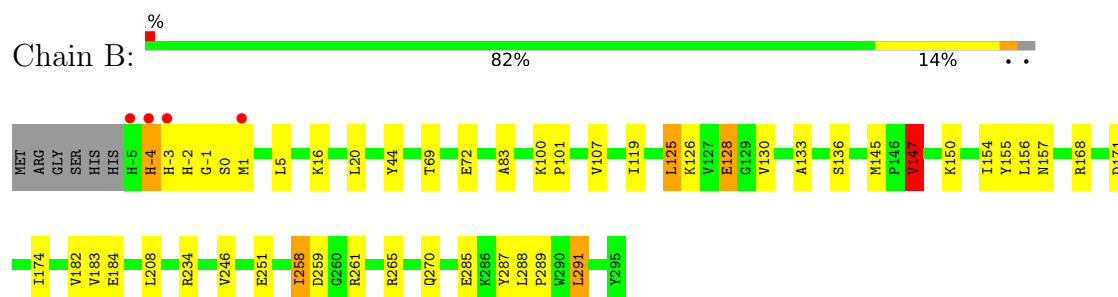
3 Residue-property plots [i](#)

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.

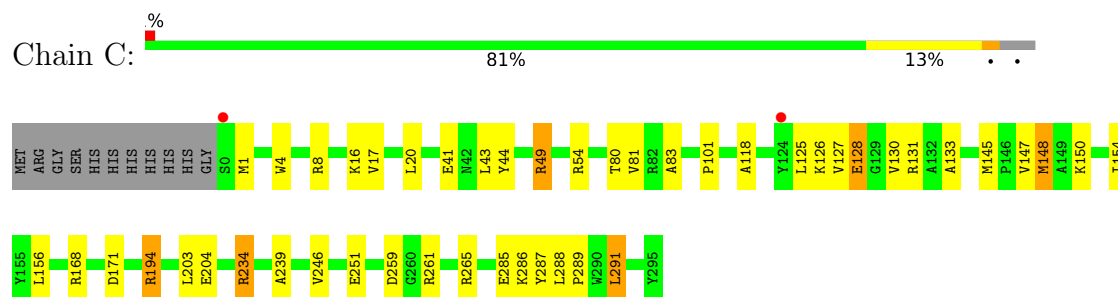
- Molecule 1: Branched-chain-amino-acid aminotransferase



- Molecule 1: Branched-chain-amino-acid aminotransferase



- Molecule 1: Branched-chain-amino-acid aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	93.46Å 93.46Å 213.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.94 – 2.15 80.94 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (80.94-2.15) 99.6 (80.94-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.187 , 0.234 0.187 , 0.234	Depositor DCC
R_{free} test set	2979 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7304	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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: PLP, PY5

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	1.25	6/2386 (0.3%)	1.20	2/3231 (0.1%)
1	B	1.27	7/2417 (0.3%)	1.23	10/3276 (0.3%)
1	C	1.23	1/2398 (0.0%)	1.18	4/3247 (0.1%)
All	All	1.25	14/7201 (0.2%)	1.20	16/9754 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	-4	HIS	CA-C	7.12	1.62	1.52
1	B	-3	HIS	N-CA	6.63	1.54	1.45
1	B	-3	HIS	CA-C	6.62	1.60	1.52
1	B	-2	HIS	N-CA	6.43	1.54	1.45
1	B	234	ARG	CD-NE	-6.20	1.37	1.46
1	A	252	ILE	C-O	-5.76	1.18	1.24
1	A	145	MET	C-O	-5.53	1.18	1.24
1	A	168	ARG	CZ-NH2	5.46	1.40	1.33
1	C	265	ARG	C-O	-5.41	1.17	1.24
1	B	-4	HIS	N-CA	5.17	1.52	1.46
1	A	178	ALA	C-O	-5.16	1.17	1.24
1	A	148[A]	MET	CA-C	5.09	1.59	1.52
1	A	148[B]	MET	CA-C	5.09	1.59	1.52
1	B	100	LYS	CA-C	5.04	1.58	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	ARG	NE-CZ-NH2	-9.45	110.69	119.20
1	B	-2	HIS	N-CA-C	9.33	122.85	110.53
1	A	140	VAL	CB-CA-C	-7.63	99.86	111.08
1	A	147	VAL	CB-CA-C	-7.05	95.76	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	ARG	CB-CG-CD	-6.82	95.61	111.30
1	B	147	VAL	CB-CA-C	-6.44	97.15	111.77
1	B	183	VAL	N-CA-C	6.43	117.52	112.12
1	C	168	ARG	CG-CD-NE	6.31	125.88	112.00
1	C	148	MET	CG-SD-CE	6.20	114.53	100.90
1	C	234	ARG	NE-CZ-NH2	-6.11	113.71	119.20
1	C	168	ARG	CA-CB-CG	6.00	126.09	114.10
1	B	-3	HIS	N-CA-C	5.94	117.81	108.96
1	B	182	VAL	CA-C-N	-5.92	116.55	122.77
1	B	182	VAL	C-N-CA	-5.92	116.55	122.77
1	B	-4	HIS	N-CA-C	5.82	123.20	110.80
1	B	147	VAL	CG1-CB-CG2	5.15	122.12	110.80

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	2326	0	2378	32	0
1	B	2358	0	2400	33	0
1	C	2327	0	2370	32	0
2	A	15	0	7	0	0
2	B	15	0	6	4	0
2	C	15	0	7	1	0
3	A	23	0	18	10	0
3	B	23	0	18	11	0
3	C	23	0	18	4	0
4	A	71	0	0	1	0
4	B	54	0	0	0	0
4	C	54	0	0	1	0
All	All	7304	0	7222	94	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 (94) 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)
3:B:302[A]:PY5:HB2	3:B:302[A]:PY5:O3	1.62	0.99
1:B:150[A]:LYS:NZ	3:B:302[A]:PY5:HN2	1.60	0.99
1:A:168:ARG:HD3	1:B:168:ARG:HD3	1.46	0.96
1:B:145:MET:HE2	1:C:156:LEU:HB3	1.46	0.96
1:B:156:LEU:HB3	1:C:145:MET:HE2	1.48	0.93
1:B:150[A]:LYS:NZ	3:B:302[A]:PY5:N	2.29	0.81
1:B:155:TYR:OH	2:B:301[B]:PLP:O3	2.01	0.78
1:C:150[B]:LYS:NZ	3:C:302[B]:PY5:HN2	1.81	0.77
1:B:150[A]:LYS:HZ1	3:B:302[A]:PY5:HN2	1.36	0.73
1:A:195:ARG:HH11	1:A:195:ARG:HG2	1.54	0.72
1:C:150[B]:LYS:NZ	3:C:302[B]:PY5:N	2.39	0.69
1:B:156:LEU:HB3	1:C:145:MET:CE	2.21	0.69
3:A:302[A]:PY5:HB2	3:A:302[A]:PY5:O3	1.94	0.68
1:C:150[B]:LYS:HZ3	3:C:302[B]:PY5:HN2	1.43	0.66
1:A:150[A]:LYS:NZ	3:A:302[A]:PY5:N	2.46	0.64
1:B:145:MET:CE	1:C:156:LEU:HB3	2.25	0.64
1:B:150[A]:LYS:CE	3:B:302[A]:PY5:HN2	2.10	0.64
1:B:174:ILE:HD12	1:B:258:ILE:HD13	1.80	0.63
1:A:1:MET:HE3	1:A:12:GLU:CD	2.26	0.61
1:A:150[A]:LYS:NZ	3:A:302[A]:PY5:HN2	2.01	0.59
3:B:302[A]:PY5:O3	3:B:302[A]:PY5:CB	2.45	0.59
1:A:174:ILE:HD12	1:A:258:ILE:HD13	1.85	0.58
1:C:44:TYR:HB3	1:C:291:LEU:HB3	1.86	0.58
1:C:126:LYS:NZ	1:C:131[B]:ARG:HH12	2.03	0.55
1:A:150[A]:LYS:NZ	3:A:302[A]:PY5:CA	2.70	0.55
1:B:287:TYR:C	1:B:289:PRO:HD2	2.31	0.55
1:B:125:LEU:HG	1:B:130:VAL:HG11	1.89	0.54
1:B:16:LYS:HB3	1:C:16:LYS:HB3	1.89	0.54
1:A:195:ARG:HG2	1:A:195:ARG:NH1	2.19	0.54
1:A:150[A]:LYS:CE	3:A:302[A]:PY5:HN2	2.21	0.53
1:B:44:TYR:HB3	1:B:291:LEU:HB3	1.90	0.53
1:A:231:SER:HB2	1:C:204:GLU:HG3	1.91	0.52
1:A:53:GLU:HG2	4:A:469:HOH:O	2.09	0.52
1:A:287:TYR:C	1:A:289:PRO:HD2	2.35	0.52
1:B:69:THR:OG1	1:B:72:GLU:HG3	2.09	0.51
1:A:150[A]:LYS:HZ3	3:A:302[A]:PY5:CA	2.24	0.51
1:B:16:LYS:HA	1:C:17:VAL:O	2.11	0.51
1:A:197:VAL:HG11	1:A:228:LEU:HD22	1.93	0.50
1:C:286:LYS:HD3	1:C:287:TYR:CZ	2.47	0.50
3:C:302[B]:PY5:O	3:C:302[B]:PY5:H4A2	2.08	0.50
1:B:133:ALA:HA	1:B:259:ASP:OD1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LEU:N	1:B:289:PRO:CD	2.75	0.49
1:C:49:ARG:CG	1:C:49:ARG:HH11	2.26	0.48
1:C:133:ALA:HA	1:C:259:ASP:OD1	2.14	0.48
1:C:288:LEU:N	1:C:289:PRO:CD	2.77	0.48
1:A:288:LEU:N	1:A:289:PRO:CD	2.76	0.48
3:B:302[A]:PY5:HB2	3:B:302[A]:PY5:C3	2.43	0.48
3:A:302[A]:PY5:O3	3:A:302[A]:PY5:N	2.47	0.47
1:B:20:LEU:HB2	1:B:101:PRO:HB3	1.95	0.47
1:B:150[A]:LYS:NZ	3:B:302[A]:PY5:CA	2.78	0.47
3:B:302[A]:PY5:O4P	3:B:302[A]:PY5:H4A1	2.14	0.47
1:A:230:LYS:HE3	1:C:204:GLU:OE1	2.14	0.47
1:B:184:GLU:OE1	2:B:301[B]:PLP:N1	2.48	0.47
1:B:288:LEU:N	1:B:289:PRO:HD2	2.30	0.46
1:B:130:VAL:HB	1:B:171:ASP:HB2	1.97	0.46
1:A:150[A]:LYS:HZ3	3:A:302[A]:PY5:HA	1.81	0.46
1:B:246:VAL:HA	1:B:251:GLU:O	2.15	0.46
1:C:246:VAL:HA	1:C:251:GLU:O	2.15	0.46
1:A:130:VAL:HB	1:A:171:ASP:HB2	1.97	0.46
1:A:246:VAL:HA	1:A:251:GLU:O	2.16	0.46
1:A:150[A]:LYS:HZ3	3:A:302[A]:PY5:HN2	1.64	0.45
1:B:147:VAL:HA	1:B:154:ILE:HD13	1.98	0.44
1:A:150[A]:LYS:NZ	3:A:302[A]:PY5:HA	2.32	0.44
1:A:20:LEU:HB2	1:A:101:PRO:HB3	1.99	0.43
1:A:134:VAL:HG23	1:A:258:ILE:HD11	1.99	0.43
1:C:128:GLU:H	1:C:128:GLU:CD	2.26	0.43
1:A:193:VAL:HB	1:A:242:GLU:HG3	2.00	0.43
1:B:128:GLU:H	1:B:128:GLU:CD	2.27	0.43
1:C:130:VAL:HB	1:C:171:ASP:HB2	2.00	0.43
1:A:147:VAL:HA	1:A:154:ILE:HD13	2.01	0.42
1:B:150[A]:LYS:HZ1	3:B:302[A]:PY5:CA	2.32	0.42
1:C:1:MET:HE1	1:C:118:ALA:H	1.83	0.42
1:A:133:ALA:HA	1:A:259:ASP:OD1	2.18	0.42
1:B:157:ASN:H	1:C:145:MET:HE3	1.84	0.42
1:C:287:TYR:C	1:C:289:PRO:HD2	2.43	0.42
1:A:50:ASP:HB3	1:A:211:ILE:HD12	2.01	0.42
1:C:125:LEU:HB3	1:C:130:VAL:HG11	2.01	0.42
1:C:194[A]:ARG:HH22	1:C:239:ALA:HB3	1.84	0.42
1:C:4:TRP:HB2	1:C:80:THR:OG1	2.20	0.41
1:B:208:LEU:HD22	2:B:301[B]:PLP:C4	2.50	0.41
1:C:49:ARG:CG	1:C:49:ARG:NH1	2.83	0.41
1:C:54:ARG:NH2	2:C:301[A]:PLP:O3P	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ARG:HH11	1:B:261:ARG:HD2	1.71	0.41
1:A:125:LEU:HB3	1:A:130:VAL:HG11	2.02	0.41
1:C:20:LEU:HB2	1:C:101:PRO:HB3	2.03	0.41
1:C:43:LEU:HD23	1:C:81:VAL:HG11	2.03	0.41
1:C:147:VAL:HA	1:C:154:ILE:HD13	2.03	0.41
1:A:140:VAL:HG21	1:A:154:ILE:HG23	2.02	0.40
1:A:136:SER:HA	1:B:136:SER:HA	2.03	0.40
3:B:302[A]:PY5:O	3:B:302[A]:PY5:H4A2	2.20	0.40
1:A:4:TRP:HB2	1:A:80:THR:OG1	2.21	0.40
1:C:234:ARG:HD2	4:C:441:HOH:O	2.21	0.40
1:A:261:ARG:HH11	1:A:261:ARG:HD2	1.66	0.40
1:B:208:LEU:HD22	2:B:301[B]:PLP:C3	2.52	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	298/307 (97%)	285 (96%)	12 (4%)	1 (0%)	36	34
1	B	302/307 (98%)	285 (94%)	13 (4%)	4 (1%)	9	5
1	C	299/307 (97%)	289 (97%)	9 (3%)	1 (0%)	36	34
All	All	899/921 (98%)	859 (96%)	34 (4%)	6 (1%)	18	13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	0	SER
1	B	83	ALA
1	A	83	ALA
1	C	83	ALA
1	B	-4	HIS

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Mol	Chain	Res	Type
1	B	-1	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	243/253 (96%)	226 (93%)	17 (7%)	14	9
1	B	244/253 (96%)	231 (95%)	13 (5%)	20	17
1	C	243/253 (96%)	231 (95%)	12 (5%)	22	19
All	All	730/759 (96%)	688 (94%)	42 (6%)	18	14

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LEU
1	A	18	THR
1	A	41	GLU
1	A	71	GLU
1	A	119	ILE
1	A	140	VAL
1	A	147	VAL
1	A	190	ILE
1	A	194	ARG
1	A	211	ILE
1	A	228	LEU
1	A	242	GLU
1	A	258	ILE
1	A	270	GLN
1	A	271	LYS
1	A	286	LYS
1	B	1	MET
1	B	5	LEU
1	B	107	VAL
1	B	119	ILE

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Mol	Chain	Res	Type
1	B	125	LEU
1	B	126	LYS
1	B	128	GLU
1	B	147	VAL
1	B	258	ILE
1	B	265	ARG
1	B	270	GLN
1	B	285	GLU
1	B	291	LEU
1	C	8	ARG
1	C	41	GLU
1	C	49	ARG
1	C	127	VAL
1	C	128	GLU
1	C	148	MET
1	C	194[A]	ARG
1	C	194[B]	ARG
1	C	203	LEU
1	C	261	ARG
1	C	285	GLU
1	C	291	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	PLP	B	301[B]	1	15,15,16	2.96	3 (20%)	21,22,23	1.71	6 (28%)
3	PY5	B	302[A]	-	23,23,23	2.77	4 (17%)	28,32,32	1.99	12 (42%)
3	PY5	C	302[B]	-	23,23,23	3.29	6 (26%)	28,32,32	2.00	8 (28%)
2	PLP	A	301[B]	1	15,15,16	3.46	3 (20%)	21,22,23	1.80	7 (33%)
3	PY5	A	302[A]	-	23,23,23	2.90	3 (13%)	28,32,32	2.16	6 (21%)
2	PLP	C	301[A]	1	15,15,16	3.73	4 (26%)	21,22,23	1.73	6 (28%)

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	PLP	B	301[B]	1	-	0/6/6/8	0/1/1/1
3	PY5	B	302[A]	-	-	12/18/18/18	0/1/1/1
3	PY5	C	302[B]	-	-	12/18/18/18	0/1/1/1
2	PLP	A	301[B]	1	-	0/6/6/8	0/1/1/1
3	PY5	A	302[A]	-	-	12/18/18/18	0/1/1/1
2	PLP	C	301[A]	1	-	0/6/6/8	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302[B]	PY5	C3-C2	10.26	1.51	1.41
3	A	302[A]	PY5	C3-C2	9.54	1.50	1.41
2	C	301[A]	PLP	C3-C2	9.48	1.50	1.41
2	C	301[A]	PLP	C5-C4	9.16	1.50	1.40
2	A	301[B]	PLP	C3-C2	8.89	1.50	1.41
2	A	301[B]	PLP	C5-C4	8.27	1.49	1.40
3	B	302[A]	PY5	C3-C2	8.27	1.49	1.41
3	C	302[B]	PY5	C5-C4	7.48	1.51	1.40
3	A	302[A]	PY5	C3-C4	7.42	1.50	1.40
2	B	301[B]	PLP	C3-C2	7.33	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301[B]	PLP	C5-C4	7.31	1.48	1.40
3	C	302[B]	PY5	C3-C4	6.86	1.50	1.40
3	B	302[A]	PY5	C3-C4	6.68	1.49	1.40
3	B	302[A]	PY5	C5-C4	6.09	1.49	1.40
3	A	302[A]	PY5	C5-C4	6.07	1.49	1.40
2	A	301[B]	PLP	C3-C4	5.08	1.49	1.40
2	C	301[A]	PLP	C3-C4	4.51	1.48	1.40
3	C	302[B]	PY5	OXT-C	-4.20	1.17	1.30
2	B	301[B]	PLP	C3-C4	3.77	1.47	1.40
3	B	302[A]	PY5	OXT-C	-3.08	1.20	1.30
2	C	301[A]	PLP	C2-N1	2.34	1.38	1.33
3	C	302[B]	PY5	CB-CA	2.29	1.58	1.53
3	C	302[B]	PY5	C2-N1	2.21	1.37	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302[A]	PY5	CB-CA-C	5.33	123.01	110.35
3	A	302[A]	PY5	O-C-CA	-5.26	105.30	122.26
3	C	302[B]	PY5	C3-C4-C5	-4.95	114.24	118.73
3	A	302[A]	PY5	OXT-C-CA	4.94	130.24	113.51
3	C	302[B]	PY5	C6-C5-C4	4.83	121.72	118.06
3	B	302[A]	PY5	CB-CA-C	4.28	120.51	110.35
3	C	302[B]	PY5	C4A-C4-C3	3.82	125.05	119.98
2	C	301[A]	PLP	C4A-C4-C5	3.79	124.85	120.94
3	B	302[A]	PY5	O2P-P-O4P	-3.55	97.41	106.67
2	C	301[A]	PLP	O3-C3-C2	3.30	124.42	117.58
2	A	301[B]	PLP	C4A-C4-C5	3.26	124.30	120.94
3	B	302[A]	PY5	O4P-C5A-C5	-3.23	103.30	109.36
2	B	301[B]	PLP	O3P-P-O4P	-3.21	98.30	106.67
2	A	301[B]	PLP	O3-C3-C2	3.20	124.22	117.58
2	C	301[A]	PLP	C6-C5-C4	2.99	120.55	118.10
2	B	301[B]	PLP	C4A-C4-C5	2.96	123.99	120.94
3	C	302[B]	PY5	O-C-CA	2.90	131.60	122.26
2	A	301[B]	PLP	C6-C5-C4	2.85	120.44	118.10
2	B	301[B]	PLP	O3P-P-O2P	2.77	118.19	107.80
3	B	302[A]	PY5	C4-C3-C2	-2.75	115.75	119.91
3	C	302[B]	PY5	O3P-P-O2P	2.75	118.10	107.80
2	C	301[A]	PLP	O3P-P-O4P	-2.73	99.54	106.67
2	B	301[B]	PLP	O2P-P-O4P	-2.68	99.69	106.67
2	B	301[B]	PLP	O4P-C5A-C5	2.67	114.35	109.36
3	C	302[B]	PY5	O3-C3-C2	2.59	122.96	117.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302[A]	PY5	C5A-C5-C6	2.56	123.53	119.36
3	B	302[A]	PY5	C5A-C5-C4	-2.53	117.34	122.67
3	A	302[A]	PY5	C6-N1-C2	2.49	123.71	119.20
3	B	302[A]	PY5	C4A-C4-C3	2.47	123.26	119.98
2	A	301[B]	PLP	C6-N1-C2	2.47	123.68	119.20
3	B	302[A]	PY5	O3P-P-O1P	2.47	120.45	110.83
2	C	301[A]	PLP	O3P-P-O2P	2.45	117.00	107.80
3	A	302[A]	PY5	O3P-P-O2P	2.43	116.92	107.80
3	C	302[B]	PY5	CB-CA-C	2.43	116.11	110.35
2	A	301[B]	PLP	C2A-C2-C3	2.41	123.62	120.80
3	B	302[A]	PY5	O3P-P-O2P	2.39	116.78	107.80
2	A	301[B]	PLP	C3-C4-C5	-2.35	115.77	118.59
3	B	302[A]	PY5	C6-N1-C2	2.32	123.40	119.20
2	C	301[A]	PLP	C3-C4-C5	-2.31	115.81	118.59
3	A	302[A]	PY5	O3-C3-C2	2.27	122.29	117.58
2	B	301[B]	PLP	O3P-P-O1P	2.20	119.41	110.83
3	B	302[A]	PY5	O-C-CA	2.15	129.18	122.26
2	A	301[B]	PLP	O3P-P-O2P	2.07	115.57	107.80
3	B	302[A]	PY5	O3-C3-C2	2.06	121.85	117.58
3	C	302[B]	PY5	OXT-C-CA	-2.04	106.60	113.51

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302[A]	PY5	C5A-O4P-P-O1P
3	A	302[A]	PY5	C5A-O4P-P-O3P
3	C	302[B]	PY5	C5-C4-C4A-N
3	C	302[B]	PY5	C-CA-N-C4A
3	A	302[A]	PY5	N-CA-CB-CG
3	B	302[A]	PY5	N-CA-CB-CG
3	A	302[A]	PY5	C5-C4-C4A-N
3	B	302[A]	PY5	C5-C4-C4A-N
3	B	302[A]	PY5	C4-C4A-N-CA
3	C	302[B]	PY5	CA-CB-CG-CD
3	C	302[B]	PY5	N-CA-CB-CG
3	A	302[A]	PY5	C-CA-CB-CG
3	B	302[A]	PY5	C-CA-CB-CG
3	C	302[B]	PY5	C-CA-CB-CG
3	A	302[A]	PY5	C4-C4A-N-CA
3	C	302[B]	PY5	C4-C4A-N-CA
3	C	302[B]	PY5	C3-C4-C4A-N

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Mol	Chain	Res	Type	Atoms
3	A	302[A]	PY5	O-C-CA-N
3	A	302[A]	PY5	OXT-C-CA-N
3	C	302[B]	PY5	OXT-C-CA-N
3	B	302[A]	PY5	OXT-C-CA-N
3	C	302[B]	PY5	O-C-CA-N
3	B	302[A]	PY5	O-C-CA-N
3	A	302[A]	PY5	C3-C4-C4A-N
3	B	302[A]	PY5	C3-C4-C4A-N
3	A	302[A]	PY5	CA-CB-CG-CD
3	B	302[A]	PY5	CA-CB-CG-CD
3	A	302[A]	PY5	C5A-O4P-P-O2P
3	A	302[A]	PY5	CB-CA-N-C4A
3	C	302[B]	PY5	CB-CA-N-C4A
3	B	302[A]	PY5	OXT-C-CA-CB
3	C	302[B]	PY5	OXT-C-CA-CB
3	C	302[B]	PY5	O-C-CA-CB
3	B	302[A]	PY5	O-C-CA-CB
3	B	302[A]	PY5	C5A-O4P-P-O3P
3	B	302[A]	PY5	CB-CA-N-C4A

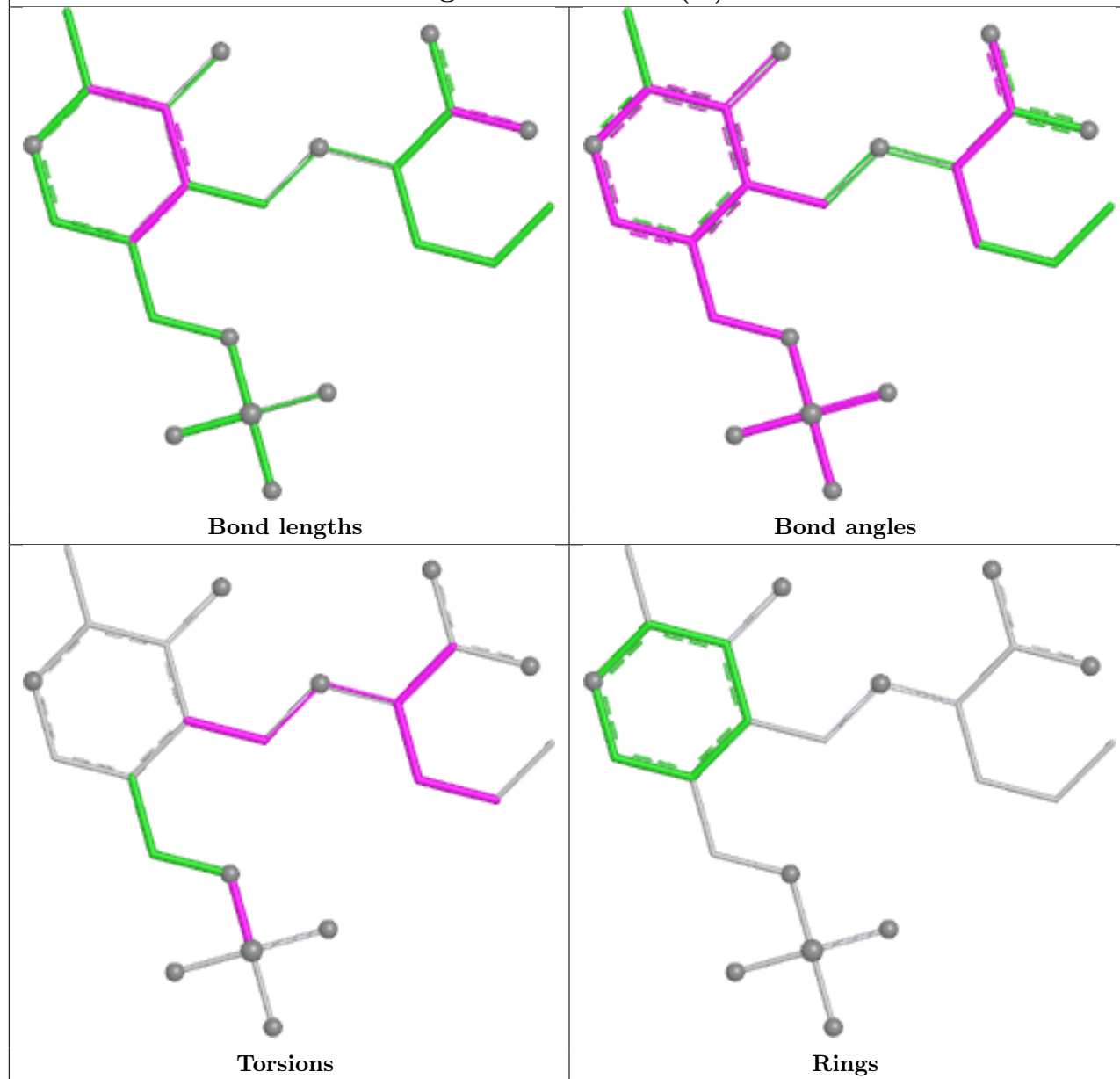
There are no ring outliers.

5 monomers are involved in 30 short contacts:

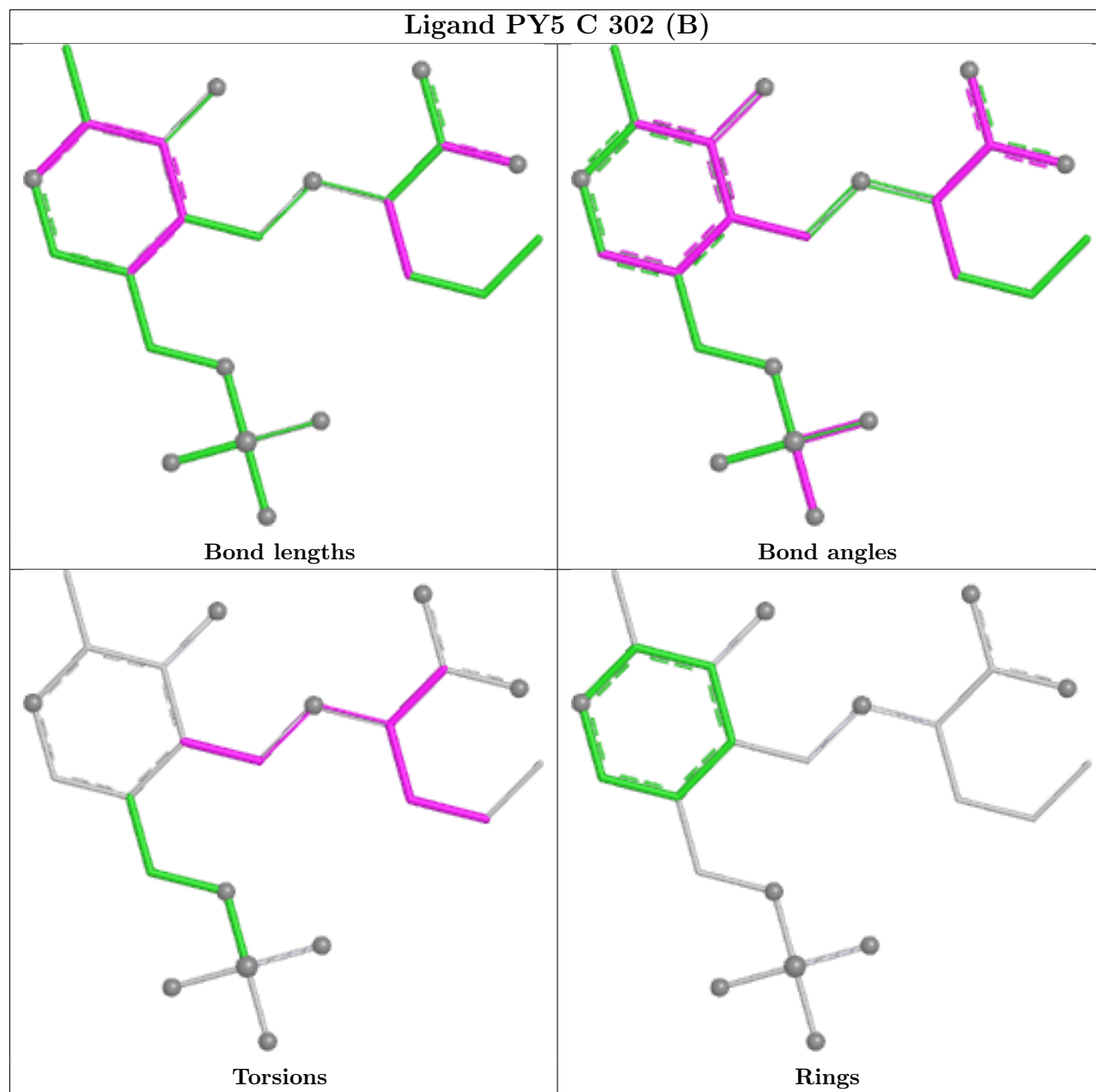
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301[B]	PLP	4	0
3	B	302[A]	PY5	11	0
3	C	302[B]	PY5	4	0
3	A	302[A]	PY5	10	0
2	C	301[A]	PLP	1	0

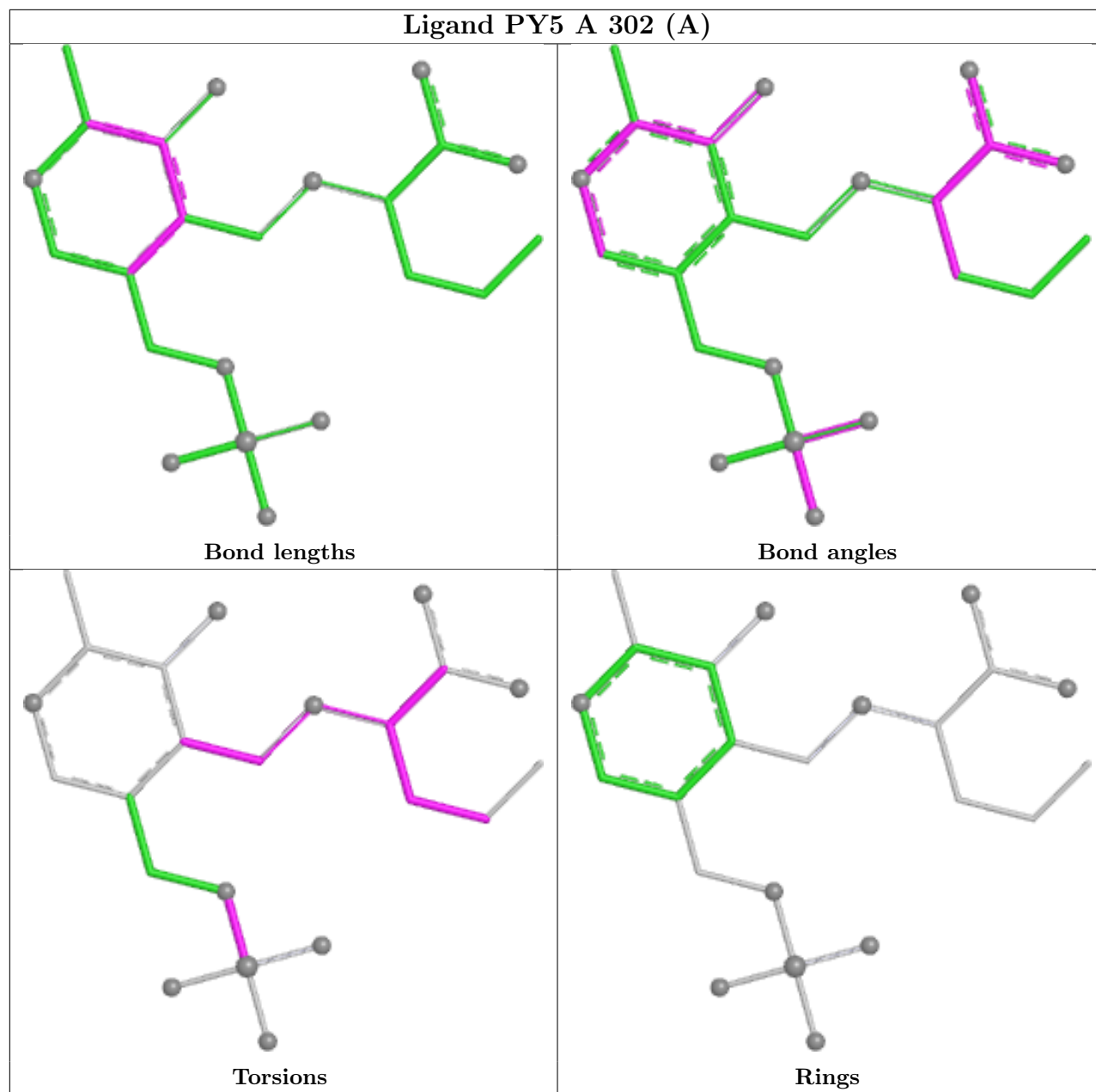
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PY5 B 302 (A)



Ligand PY5 C 302 (B)





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	297/307 (96%)	-0.43	2 (0%) 84 85	24, 41, 64, 105	3 (1%)
1	B	301/307 (98%)	-0.19	4 (1%) 75 78	24, 45, 74, 144	3 (0%)
1	C	296/307 (96%)	-0.11	2 (0%) 84 85	27, 47, 74, 100	5 (1%)
All	All	894/921 (97%)	-0.25	8 (0%) 81 83	24, 45, 73, 144	11 (1%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-5	HIS	4.4
1	B	-4	HIS	4.2
1	B	-3	HIS	3.7
1	C	0	SER	2.9
1	A	1	MET	2.7
1	B	1	MET	2.7
1	A	-1	GLY	2.2
1	C	124	TYR	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,

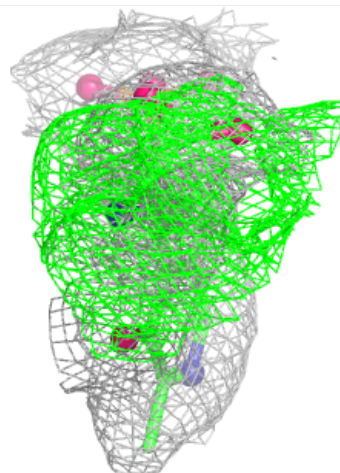
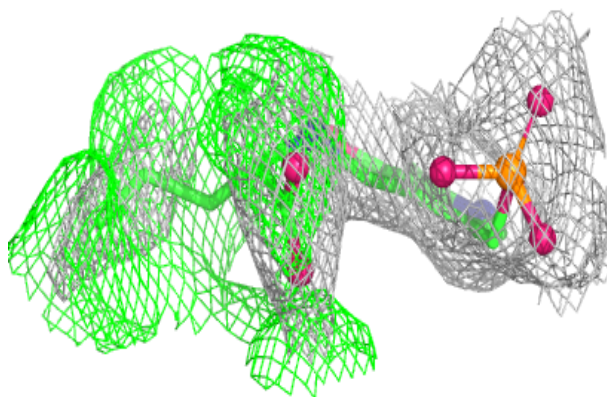
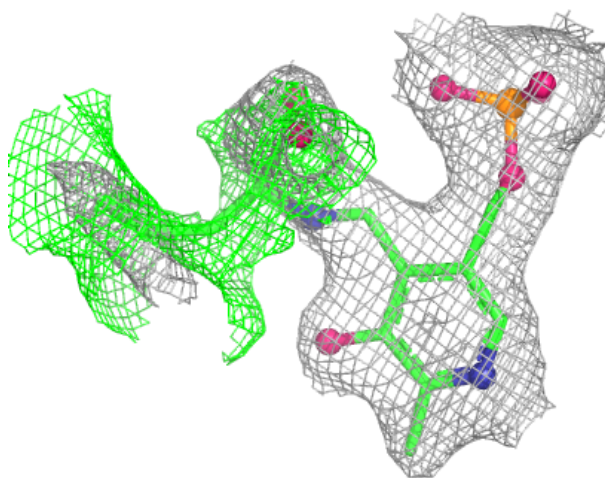
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PY5	C	302[B]	23/23	0.86	0.18	30,39,50,59	23
3	PY5	A	302[A]	23/23	0.87	0.14	28,33,43,44	23
3	PY5	B	302[A]	23/23	0.90	0.15	28,46,52,55	23
2	PLP	C	301[A]	15/16	0.97	0.06	35,45,47,48	15
2	PLP	A	301[B]	15/16	0.98	0.05	34,38,41,41	15
2	PLP	B	301[B]	15/16	0.98	0.06	37,40,43,43	15

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.

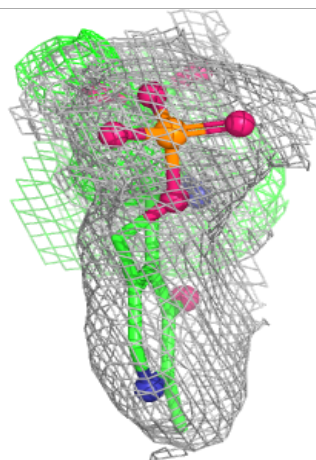
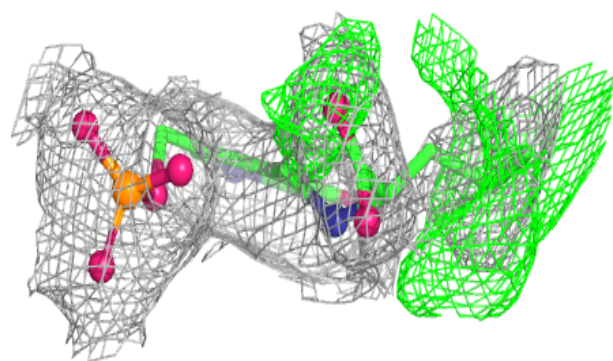
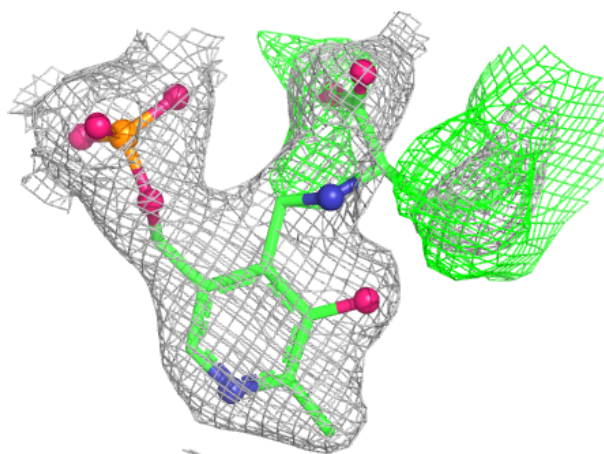
Electron density around PY5 C 302 (B):

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



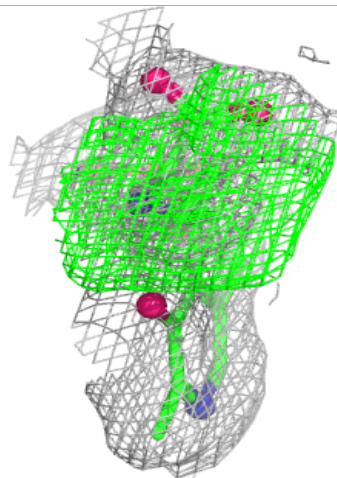
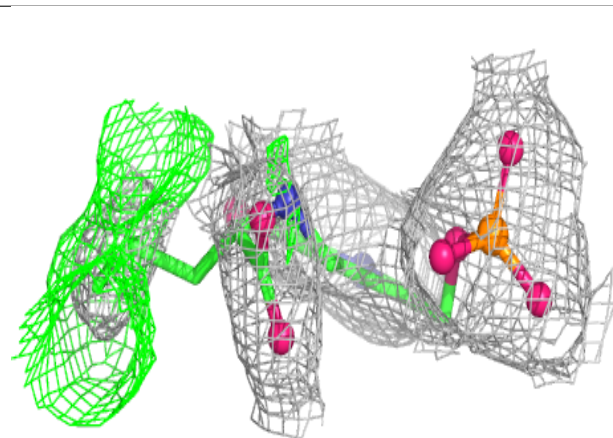
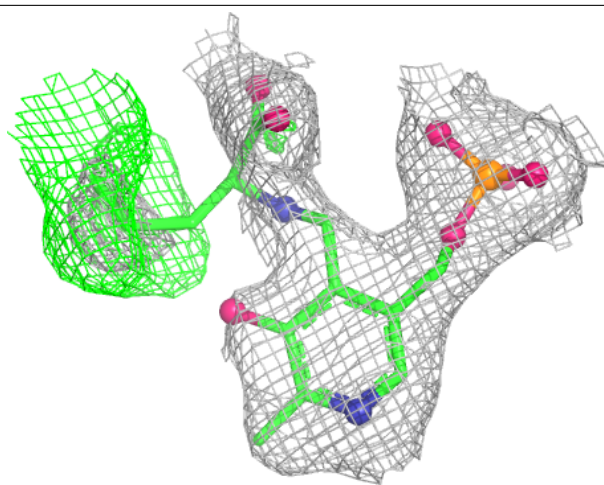
Electron density around PY5 A 302 (A):

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



Electron density around PY5 B 302 (A):

$2mF_o-DF_c$ (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.