



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:39 PM UTC

PDB ID : 1JU6 / pdb_00001ju6
Title : Human Thymidylate Synthase Complex with dUMP and LY231514, A Pyrrolo(2,3-d)pyrimidine-based Antifolate
Authors : Sayre, P.H.; Finer-Moore, J.S.; Fritz, T.A.; Biermann, D.; Gates, S.B.; MacKellar, W.C.; Patel, V.F.; Stroud, R.M.
Deposited on : 2001-08-23
Resolution : 2.89 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

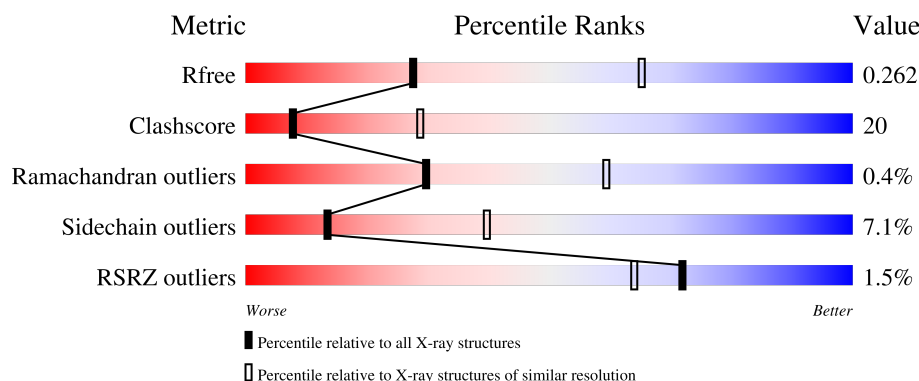
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	313	
1	B	313	
1	C	313	
1	D	313	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9493 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.

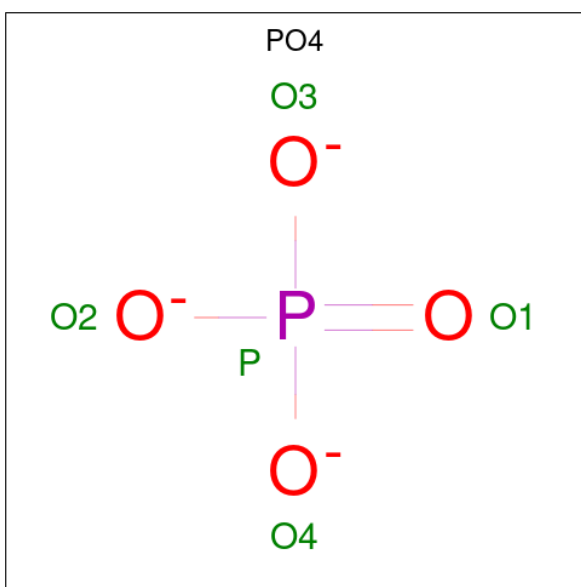
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2309	1475	400	421	13			
1	B	286	Total	C	N	O	S	0	0	0
			2309	1475	400	421	13			
1	C	286	Total	C	N	O	S	0	0	0
			2309	1475	400	421	13			
1	D	286	Total	C	N	O	S	0	0	0
			2309	1475	400	421	13			

There are 4 discrepancies between the modelled and reference sequences:

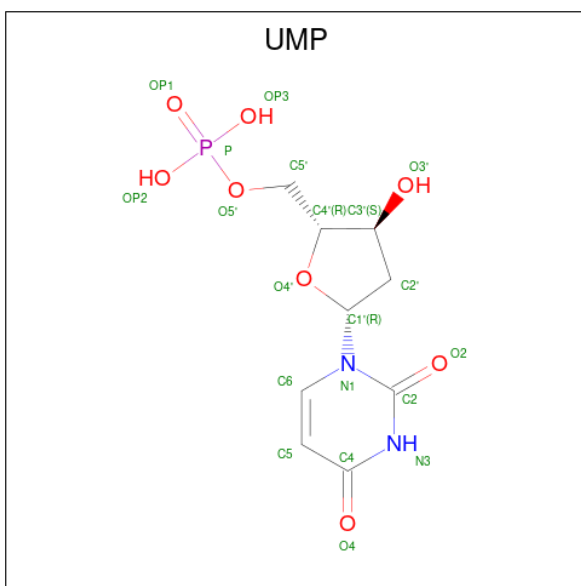
Chain	Residue	Modelled	Actual	Comment	Reference
A	46	GLU	ARG	engineered mutation	UNP P04818
B	46	GLU	ARG	engineered mutation	UNP P04818
C	46	GLU	ARG	engineered mutation	UNP P04818
D	46	GLU	ARG	engineered mutation	UNP P04818

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: $C_9H_{13}N_2O_8P$).



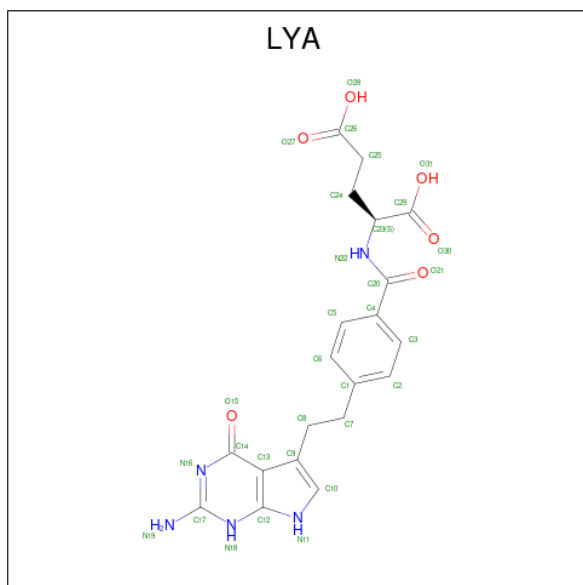
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
3	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 4 is 2-{4-[2-(2-AMINO-4-OXO-4,7-DIHYDRO-3H-PYRROLO[2,3-D]PYRIMIDIN-5-YL)-ETHYL]-BENZOYLAMINO}-PENTANEDIOIC ACID (CCD ID: LYA) (formula: $C_{20}H_{21}N_5O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 31	C 20	N 5	O 6	0	0
4	B	1	Total 31	C 20	N 5	O 6	0	0
4	C	1	Total 31	C 20	N 5	O 6	0	0
4	D	1	Total 31	C 20	N 5	O 6	0	0

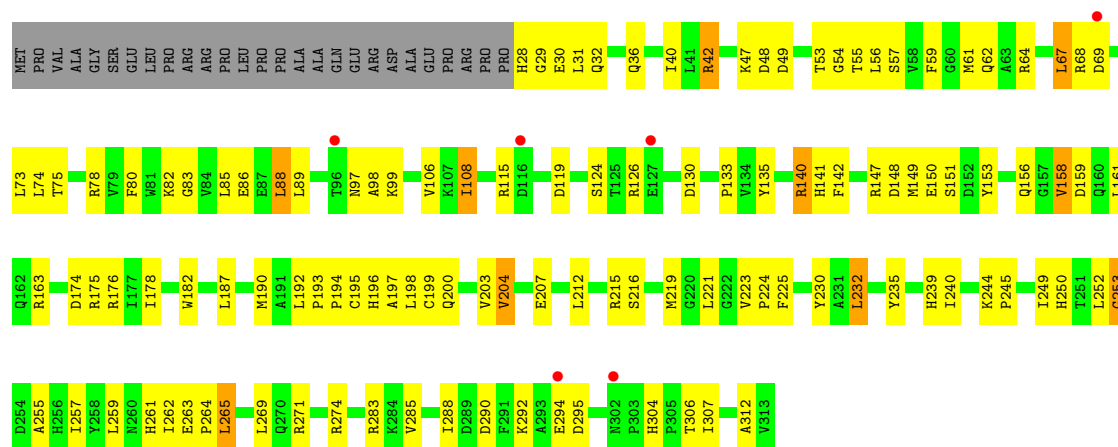
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	12	Total O 12 12	0	0
5	B	12	Total O 12 12	0	0
5	C	13	Total O 13 13	0	0

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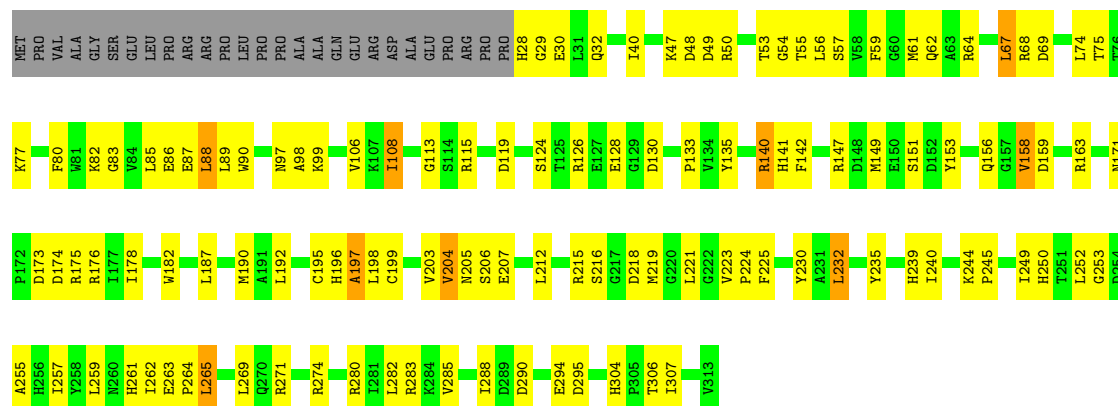
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	11	Total	O	0	0
			11	11		



• Molecule 1: THYMIDYLATE SYNTHASE

Chain D: 53% 35% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.14Å 69.63Å 73.96Å 71.67° 85.72° 75.11°	Depositor
Resolution (Å)	22.95 – 2.89 22.95 – 2.89	Depositor EDS
% Data completeness (in resolution range)	83.8 (22.95-2.89) 83.7 (22.95-2.89)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.89Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.264 0.236 , 0.262	Depositor DCC
R_{free} test set	2443 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9493	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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: UMP, LYA, PO4

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	0.47	0/2367	0.94	8/3199 (0.3%)
1	B	0.48	0/2367	0.94	9/3199 (0.3%)
1	C	0.48	0/2367	0.93	7/3199 (0.2%)
1	D	0.48	0/2367	0.94	9/3199 (0.3%)
All	All	0.48	0/9468	0.94	33/12796 (0.3%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	ILE	N-CA-C	6.35	116.52	110.42
1	A	178	ILE	N-CA-C	6.25	117.48	108.48
1	D	195	CYS	N-CA-C	-6.22	103.81	112.45
1	B	178	ILE	N-CA-C	6.13	117.31	108.48
1	C	262	ILE	N-CA-C	6.09	116.27	110.42
1	D	262	ILE	N-CA-C	5.95	116.14	110.42
1	B	56	LEU	N-CA-C	-5.95	98.72	108.41
1	B	195	CYS	N-CA-C	-5.91	104.23	112.45
1	C	195	CYS	N-CA-C	-5.85	104.31	112.45
1	C	178	ILE	N-CA-C	5.82	116.86	108.48
1	A	262	ILE	N-CA-C	5.78	115.96	110.42
1	D	56	LEU	N-CA-C	-5.77	99.00	108.41
1	D	57	SER	N-CA-C	5.72	117.88	109.24
1	A	56	LEU	N-CA-C	-5.66	99.18	108.41
1	D	178	ILE	N-CA-C	5.61	117.49	108.85
1	A	253	GLY	N-CA-C	-5.56	105.15	110.21
1	A	195	CYS	N-CA-C	-5.52	104.78	112.45
1	C	253	GLY	N-CA-C	-5.51	105.19	110.21
1	D	171	ASN	CA-C-N	5.39	125.11	119.82
1	D	171	ASN	C-N-CA	5.39	125.11	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	ILE	N-CA-C	5.33	120.43	109.34
1	C	56	LEU	N-CA-C	-5.32	99.73	108.41
1	B	171	ASN	CA-C-N	5.29	125.01	119.82
1	B	171	ASN	C-N-CA	5.29	125.01	119.82
1	C	57	SER	N-CA-C	5.26	117.67	109.52
1	C	108	ILE	N-CA-C	5.13	120.01	109.34
1	A	57	SER	N-CA-C	5.10	117.43	109.52
1	A	108	ILE	N-CA-C	5.08	119.91	109.34
1	D	108	ILE	N-CA-C	5.02	119.78	109.34
1	D	197	ALA	N-CA-C	5.01	119.45	113.23
1	A	197	ALA	N-CA-C	5.01	119.44	113.23
1	B	57	SER	N-CA-C	5.01	117.28	109.52
1	B	180	CYS	N-CA-C	5.01	116.57	108.41

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	2309	0	2274	106	0
1	B	2309	0	2274	99	0
1	C	2309	0	2274	97	0
1	D	2309	0	2274	95	0
2	A	5	0	0	0	0
3	A	20	0	10	4	0
3	B	20	0	10	4	0
3	C	20	0	10	1	0
3	D	20	0	10	3	0
4	A	31	0	19	0	0
4	B	31	0	19	0	0
4	C	31	0	19	1	0
4	D	31	0	19	0	0
5	A	12	0	0	1	0
5	B	12	0	0	0	0
5	C	13	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	11	0	0	0	0
All	All	9493	0	9212	371	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 20.

All (371) 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:D:280:ARG:HH12	1:D:282:LEU:HA	1.01	1.14
1:C:130:ASP:HB2	1:C:149:MET:HE2	1.38	1.05
1:A:130:ASP:HB2	1:A:149:MET:HE2	1.38	1.00
1:D:130:ASP:HB2	1:D:149:MET:HE2	1.43	1.00
1:B:130:ASP:HB2	1:B:149:MET:HE2	1.41	0.98
1:D:280:ARG:NH1	1:D:282:LEU:HA	1.77	0.98
1:C:88:LEU:HD12	1:C:232:LEU:HD13	1.52	0.92
1:D:280:ARG:HH11	1:D:282:LEU:HD23	1.34	0.91
1:A:88:LEU:HD12	1:A:232:LEU:HD13	1.52	0.90
1:A:47:LYS:HE2	1:B:173:ASP:HA	1.57	0.86
1:D:88:LEU:HD12	1:D:232:LEU:HD13	1.58	0.86
1:D:280:ARG:NH1	1:D:282:LEU:HD23	1.90	0.84
1:A:32:GLN:HE22	1:A:64:ARG:H	1.28	0.81
1:B:88:LEU:HD12	1:B:232:LEU:HD13	1.60	0.81
1:A:143:GLY:HA3	1:B:185:ARG:CZ	2.12	0.79
1:C:32:GLN:HE22	1:C:64:ARG:H	1.31	0.78
1:B:32:GLN:HE22	1:B:64:ARG:H	1.32	0.78
1:D:32:GLN:HE22	1:D:64:ARG:H	1.33	0.76
1:C:196:HIS:HB2	1:C:212:LEU:HD11	1.70	0.74
1:A:175:ARG:HH11	3:B:314:UMP:P	2.11	0.73
1:B:42:ARG:HH11	1:B:42:ARG:HG2	1.52	0.73
1:C:175:ARG:NH1	3:D:314:UMP:P	2.62	0.72
1:C:175:ARG:HH11	3:D:314:UMP:P	2.13	0.70
1:C:49:ASP:HB2	1:D:175:ARG:NH2	2.07	0.70
1:A:30:GLU:HG3	1:A:74:LEU:HD22	1.72	0.70
1:B:196:HIS:HB2	1:B:212:LEU:HD11	1.74	0.70
1:A:196:HIS:HB2	1:A:212:LEU:HD11	1.73	0.69
1:C:175:ARG:NH1	3:D:314:UMP:OP1	2.25	0.69
1:D:239:HIS:HE1	1:D:285:VAL:H	1.41	0.69
1:A:271:ARG:HH11	1:A:304:HIS:HB3	1.58	0.68
1:C:73:LEU:HA	5:C:434:HOH:O	1.92	0.68
1:A:239:HIS:HE1	1:A:285:VAL:H	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:GLU:HG3	1:B:74:LEU:HD22	1.75	0.68
1:C:271:ARG:HH11	1:C:304:HIS:HB3	1.60	0.67
1:D:30:GLU:HG3	1:D:74:LEU:HD22	1.75	0.67
1:C:30:GLU:HG3	1:C:74:LEU:HD22	1.76	0.66
1:C:239:HIS:CE1	1:C:285:VAL:H	2.13	0.66
1:C:47:LYS:HE2	1:D:173:ASP:HA	1.78	0.66
1:D:271:ARG:HH11	1:D:304:HIS:HB3	1.61	0.66
1:A:49:ASP:HB2	1:B:175:ARG:NH2	2.11	0.66
1:D:196:HIS:HB2	1:D:212:LEU:HD11	1.76	0.65
1:A:239:HIS:CE1	1:A:285:VAL:H	2.14	0.65
1:A:78:ARG:NH1	5:A:409:HOH:O	2.29	0.65
1:A:175:ARG:NH1	3:B:314:UMP:P	2.69	0.65
1:C:239:HIS:HE1	1:C:285:VAL:H	1.43	0.65
1:D:239:HIS:CE1	1:D:285:VAL:H	2.15	0.63
1:D:257:ILE:HD13	1:D:265:LEU:HD23	1.80	0.63
1:A:54:GLY:C	1:A:259:LEU:HG	2.24	0.63
1:B:239:HIS:CE1	1:B:285:VAL:H	2.16	0.63
1:C:54:GLY:C	1:C:259:LEU:HG	2.24	0.62
1:C:61:MET:HE2	1:C:255:ALA:CB	2.30	0.61
1:D:28:HIS:ND1	1:D:29:GLY:N	2.48	0.61
1:C:221:LEU:O	1:C:224:PRO:HD2	2.01	0.61
1:A:53:THR:HG22	1:A:54:GLY:H	1.65	0.61
1:A:184:PRO:HD2	1:B:142:PHE:CE1	2.35	0.61
1:A:215:ARG:HG3	1:A:216:SER:N	2.14	0.61
1:D:53:THR:HG22	1:D:54:GLY:H	1.65	0.61
1:A:157:GLY:HA2	1:B:185:ARG:NH2	2.14	0.61
1:B:249:ILE:N	1:B:249:ILE:HD12	2.16	0.61
1:C:42:ARG:HG2	1:C:42:ARG:HH11	1.66	0.61
1:D:61:MET:HE2	1:D:255:ALA:CB	2.30	0.61
1:B:271:ARG:HH11	1:B:304:HIS:HB3	1.65	0.61
1:C:28:HIS:ND1	1:C:29:GLY:N	2.49	0.61
1:B:28:HIS:ND1	1:B:29:GLY:N	2.48	0.61
1:A:28:HIS:ND1	1:A:29:GLY:N	2.49	0.60
1:B:239:HIS:HE1	1:B:285:VAL:H	1.46	0.60
1:C:215:ARG:HG3	1:C:216:SER:N	2.16	0.60
1:C:80:PHE:CE2	1:C:82:LYS:HB3	2.36	0.60
1:B:53:THR:HG22	1:B:54:GLY:H	1.66	0.60
1:A:175:ARG:O	1:B:215:ARG:NH1	2.34	0.60
1:A:184:PRO:HD2	1:B:142:PHE:CZ	2.36	0.60
1:D:80:PHE:CE2	1:D:82:LYS:HB3	2.37	0.60
1:A:257:ILE:HD13	1:A:265:LEU:HD23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ILE:HD13	1:B:265:LEU:HD23	1.83	0.59
1:D:54:GLY:C	1:D:259:LEU:HG	2.27	0.59
1:B:54:GLY:C	1:B:259:LEU:HG	2.28	0.59
1:C:78:ARG:NH1	5:C:433:HOH:O	2.36	0.59
3:C:314:UMP:OP1	1:D:175:ARG:NH1	2.36	0.59
1:A:54:GLY:HA3	1:A:259:LEU:CD1	2.33	0.58
1:A:221:LEU:O	1:A:224:PRO:HD2	2.03	0.58
1:C:257:ILE:HD13	1:C:265:LEU:HD23	1.85	0.58
1:A:61:MET:HE2	1:A:255:ALA:CB	2.33	0.58
1:A:126:ARG:HD3	1:A:130:ASP:O	2.03	0.58
1:C:126:ARG:HD3	1:C:130:ASP:O	2.03	0.58
1:C:53:THR:HG22	1:C:54:GLY:H	1.68	0.58
1:C:215:ARG:NH1	1:C:216:SER:HB2	2.18	0.58
1:B:61:MET:HE2	1:B:255:ALA:CB	2.33	0.57
1:B:126:ARG:HD3	1:B:130:ASP:O	2.04	0.57
1:C:54:GLY:HA3	1:C:259:LEU:CD1	2.34	0.57
1:A:249:ILE:HD12	1:A:249:ILE:N	2.19	0.57
1:A:80:PHE:CE2	1:A:82:LYS:HB3	2.39	0.57
1:B:133:PRO:O	1:B:190:MET:HE2	2.04	0.57
1:B:80:PHE:CE2	1:B:82:LYS:HB3	2.40	0.57
1:C:249:ILE:HD12	1:C:249:ILE:N	2.20	0.57
1:A:215:ARG:NH1	1:A:216:SER:HB2	2.20	0.56
1:B:163:ARG:HH11	1:B:163:ARG:HG2	1.70	0.56
1:B:215:ARG:HG3	1:B:216:SER:N	2.21	0.56
1:D:53:THR:HG22	1:D:54:GLY:N	2.19	0.56
1:A:271:ARG:NH1	1:A:304:HIS:HB3	2.21	0.56
1:D:126:ARG:HD3	1:D:130:ASP:O	2.06	0.56
1:B:53:THR:HG22	1:B:54:GLY:N	2.21	0.56
1:D:54:GLY:HA3	1:D:259:LEU:CD1	2.36	0.56
1:D:182:TRP:CZ2	1:D:187:LEU:HD21	2.40	0.56
1:A:53:THR:HG22	1:A:54:GLY:N	2.21	0.55
1:B:198:LEU:HD23	1:B:198:LEU:C	2.31	0.55
1:B:221:LEU:O	1:B:224:PRO:HD2	2.06	0.55
1:D:306:THR:HG22	1:D:307:ILE:N	2.21	0.55
1:A:49:ASP:CB	1:B:175:ARG:NH2	2.69	0.55
1:A:133:PRO:O	1:A:190:MET:HE2	2.07	0.55
1:A:244:LYS:HD2	1:A:245:PRO:O	2.06	0.55
1:A:175:ARG:NH1	3:B:314:UMP:OP1	2.39	0.55
1:A:198:LEU:C	1:A:198:LEU:HD23	2.32	0.55
1:B:306:THR:HG22	1:B:307:ILE:N	2.21	0.55
1:C:200:GLN:HE22	1:D:215:ARG:HB2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ARG:HG2	1:B:42:ARG:NH1	2.21	0.55
1:D:198:LEU:C	1:D:198:LEU:HD23	2.32	0.55
1:D:133:PRO:O	1:D:190:MET:HE2	2.07	0.54
1:D:223:VAL:HB	1:D:224:PRO:HD3	1.89	0.54
1:D:151:SER:HB2	1:D:153:TYR:CZ	2.43	0.54
1:B:244:LYS:HD2	1:B:245:PRO:O	2.08	0.54
1:D:249:ILE:N	1:D:249:ILE:HD12	2.22	0.54
1:A:163:ARG:HG2	1:A:163:ARG:HH11	1.73	0.54
1:B:54:GLY:HA3	1:B:259:LEU:CD1	2.38	0.54
1:C:271:ARG:NH1	1:C:304:HIS:HB3	2.23	0.54
1:B:106:VAL:HG12	1:B:108:ILE:HG12	1.90	0.53
1:B:151:SER:HB2	1:B:153:TYR:CZ	2.43	0.53
1:C:223:VAL:HB	1:C:224:PRO:HD3	1.91	0.53
1:B:294:GLU:CD	1:B:294:GLU:H	2.16	0.53
1:C:200:GLN:NE2	1:D:215:ARG:HB2	2.24	0.53
1:C:244:LYS:HD2	1:C:245:PRO:O	2.08	0.53
1:D:221:LEU:O	1:D:224:PRO:HD2	2.08	0.53
1:C:119:ASP:OD1	1:C:124:SER:HA	2.09	0.53
1:D:215:ARG:HG3	1:D:216:SER:N	2.23	0.53
1:D:30:GLU:CD	1:D:75:THR:H	2.17	0.53
1:D:106:VAL:HG12	1:D:108:ILE:HG12	1.90	0.53
1:D:163:ARG:HG2	1:D:163:ARG:HH11	1.74	0.53
1:D:271:ARG:NH1	1:D:304:HIS:HB3	2.23	0.53
1:A:30:GLU:CD	1:A:75:THR:H	2.17	0.53
1:B:30:GLU:CD	1:B:75:THR:H	2.17	0.53
1:B:182:TRP:CZ2	1:B:187:LEU:HD21	2.44	0.53
1:C:163:ARG:HG2	1:C:163:ARG:HH11	1.72	0.53
1:D:294:GLU:CD	1:D:294:GLU:H	2.16	0.53
1:A:200:GLN:NE2	1:B:215:ARG:HB2	2.24	0.52
1:A:97:ASN:HD22	1:A:97:ASN:C	2.16	0.52
1:A:203:VAL:O	1:A:204:VAL:HG23	2.09	0.52
1:B:97:ASN:ND2	1:B:99:LYS:H	2.08	0.52
1:D:280:ARG:NH1	1:D:282:LEU:CA	2.64	0.52
1:A:294:GLU:CD	1:A:294:GLU:H	2.17	0.52
1:C:133:PRO:O	1:C:190:MET:HE2	2.10	0.52
1:C:142:PHE:HB3	1:C:158:VAL:HG13	1.91	0.52
1:D:97:ASN:ND2	1:D:99:LYS:H	2.07	0.52
1:D:142:PHE:HB3	1:D:158:VAL:HG13	1.91	0.52
1:B:142:PHE:HB3	1:B:158:VAL:HG13	1.92	0.52
1:C:294:GLU:H	1:C:294:GLU:CD	2.16	0.52
1:A:306:THR:HG22	1:A:307:ILE:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ASN:C	1:D:97:ASN:HD22	2.18	0.52
1:D:215:ARG:NH1	1:D:216:SER:HB2	2.24	0.52
1:A:106:VAL:HG12	1:A:108:ILE:HG12	1.92	0.52
1:C:151:SER:HB2	1:C:153:TYR:CZ	2.45	0.52
1:C:97:ASN:CG	1:C:149:MET:SD	2.93	0.52
1:A:223:VAL:HB	1:A:224:PRO:HD3	1.92	0.52
1:B:97:ASN:C	1:B:97:ASN:HD22	2.18	0.52
1:B:215:ARG:NH1	1:B:216:SER:HB2	2.25	0.52
1:C:97:ASN:C	1:C:97:ASN:HD22	2.17	0.52
1:C:30:GLU:CD	1:C:75:THR:H	2.18	0.51
1:B:223:VAL:HB	1:B:224:PRO:HD3	1.91	0.51
1:D:203:VAL:O	1:D:204:VAL:HG23	2.11	0.51
1:A:97:ASN:ND2	1:A:99:LYS:H	2.08	0.51
1:A:119:ASP:OD1	1:A:124:SER:HA	2.11	0.51
1:C:198:LEU:C	1:C:198:LEU:HD23	2.35	0.51
1:D:244:LYS:HD2	1:D:245:PRO:O	2.10	0.51
1:A:142:PHE:HB3	1:A:158:VAL:HG13	1.92	0.51
1:C:32:GLN:NE2	1:C:64:ARG:H	2.05	0.51
1:C:182:TRP:CZ2	1:C:187:LEU:HD21	2.46	0.51
1:A:151:SER:HB2	1:A:153:TYR:CZ	2.46	0.51
1:C:42:ARG:HG2	1:C:42:ARG:NH1	2.25	0.51
1:C:306:THR:HG22	1:C:307:ILE:N	2.26	0.51
1:B:271:ARG:NH1	1:B:304:HIS:HB3	2.26	0.50
1:C:53:THR:HG22	1:C:54:GLY:N	2.25	0.50
1:C:97:ASN:HD22	1:C:98:ALA:N	2.10	0.50
1:C:312:ALA:O	4:C:315:LYA:N19	2.44	0.50
1:C:106:VAL:HG12	1:C:108:ILE:HG12	1.94	0.50
1:B:203:VAL:O	1:B:204:VAL:HG23	2.12	0.49
1:D:280:ARG:HH11	1:D:280:ARG:HG2	1.77	0.49
1:A:97:ASN:CG	1:A:149:MET:SD	2.96	0.49
1:C:97:ASN:ND2	1:C:99:LYS:H	2.10	0.49
1:A:97:ASN:HD22	1:A:98:ALA:N	2.11	0.49
1:C:49:ASP:CB	1:D:175:ARG:NH2	2.76	0.49
1:A:32:GLN:NE2	1:A:64:ARG:H	2.03	0.48
3:A:314:UMP:P	1:B:176:ARG:HH21	2.36	0.48
1:C:212:LEU:HD22	1:C:230:TYR:CD2	2.48	0.48
1:C:175:ARG:HG3	5:C:440:HOH:O	2.12	0.48
1:C:175:ARG:NH2	1:D:49:ASP:HB2	2.28	0.48
1:D:147:ARG:NH1	1:D:156:GLN:HE22	2.12	0.48
1:D:67:LEU:HB3	1:D:235:TYR:CE1	2.49	0.48
1:A:182:TRP:CZ2	1:A:187:LEU:HD21	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ASP:HB2	1:B:149:MET:CE	2.29	0.48
1:C:147:ARG:NH1	1:C:156:GLN:HE22	2.11	0.48
1:C:203:VAL:O	1:C:204:VAL:HG23	2.14	0.48
1:A:54:GLY:CA	1:A:259:LEU:HG	2.44	0.47
1:C:240:ILE:HD11	1:C:288:ILE:HA	1.95	0.47
1:B:83:GLY:HA2	1:B:106:VAL:CG2	2.44	0.47
1:B:174:ASP:OD1	1:B:176:ARG:N	2.45	0.47
1:C:182:TRP:HB2	1:C:197:ALA:HB1	1.96	0.47
1:C:198:LEU:HD23	1:C:199:CYS:N	2.29	0.47
1:D:97:ASN:HD22	1:D:98:ALA:N	2.11	0.47
1:D:83:GLY:HA2	1:D:106:VAL:CG2	2.44	0.47
1:D:40:ILE:HD12	1:D:219:MET:HG3	1.97	0.47
1:B:59:PHE:HA	1:B:253:GLY:O	2.15	0.47
1:B:306:THR:HG22	1:B:307:ILE:H	1.80	0.47
1:C:68:ARG:NH1	1:C:68:ARG:HG3	2.30	0.47
1:D:119:ASP:OD1	1:D:124:SER:HA	2.13	0.47
1:D:198:LEU:HD23	1:D:199:CYS:N	2.30	0.47
1:A:47:LYS:CE	1:B:173:ASP:HA	2.39	0.47
1:D:240:ILE:HD11	1:D:288:ILE:HA	1.95	0.47
1:B:97:ASN:HD22	1:B:98:ALA:N	2.13	0.47
1:C:40:ILE:HD12	1:C:219:MET:HG3	1.97	0.47
1:B:119:ASP:OD1	1:B:124:SER:HA	2.15	0.47
1:A:50:ARG:HD3	1:B:176:ARG:NH2	2.30	0.46
1:C:54:GLY:CA	1:C:259:LEU:HG	2.45	0.46
1:D:212:LEU:HD22	1:D:230:TYR:CD2	2.50	0.46
1:A:203:VAL:O	1:B:47:LYS:HE3	2.15	0.46
1:D:97:ASN:CG	1:D:149:MET:SD	2.98	0.46
1:D:283:ARG:HD3	1:D:295:ASP:OD1	2.15	0.46
1:D:67:LEU:HB3	1:D:235:TYR:HE1	1.80	0.46
1:D:141:HIS:O	1:D:142:PHE:C	2.58	0.46
1:D:306:THR:HG22	1:D:307:ILE:H	1.80	0.46
1:A:68:ARG:NH1	1:A:68:ARG:HG3	2.30	0.46
1:B:285:VAL:HG13	1:B:290:ASP:HB2	1.96	0.46
1:D:59:PHE:HA	1:D:253:GLY:O	2.14	0.46
1:A:175:ARG:NH2	1:B:49:ASP:HB2	2.31	0.46
1:C:62:GLN:HA	1:C:250:HIS:O	2.15	0.46
1:A:97:ASN:C	1:A:97:ASN:ND2	2.74	0.46
1:A:175:ARG:HB2	3:B:314:UMP:OP2	2.14	0.46
1:A:240:ILE:HD11	1:A:288:ILE:HA	1.98	0.46
1:B:212:LEU:HD22	1:B:230:TYR:CD2	2.50	0.46
1:B:130:ASP:CG	1:B:149:MET:HB3	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LEU:HB3	1:B:235:TYR:CE1	2.51	0.46
1:B:240:ILE:HD11	1:B:288:ILE:HA	1.96	0.46
1:D:182:TRP:HB2	1:D:197:ALA:HB1	1.98	0.46
1:A:130:ASP:HB2	1:A:149:MET:CE	2.28	0.45
1:A:141:HIS:O	1:A:142:PHE:C	2.59	0.45
1:A:283:ARG:HD3	1:A:295:ASP:OD1	2.15	0.45
1:B:86:GLU:HB2	1:B:106:VAL:HG21	1.97	0.45
1:D:32:GLN:NE2	1:D:64:ARG:H	2.08	0.45
1:D:83:GLY:HA2	1:D:106:VAL:HG21	1.98	0.45
1:A:182:TRP:HB2	1:A:197:ALA:HB1	1.99	0.45
1:A:67:LEU:HB3	1:A:235:TYR:CE1	2.51	0.45
1:A:130:ASP:CG	1:A:149:MET:HB3	2.42	0.45
1:A:207:GLU:HA	1:A:244:LYS:O	2.17	0.45
1:D:285:VAL:HG13	1:D:290:ASP:HB2	1.97	0.45
1:A:83:GLY:HA2	1:A:106:VAL:CG2	2.46	0.45
1:D:54:GLY:CA	1:D:259:LEU:HG	2.47	0.45
1:A:147:ARG:NH1	1:A:156:GLN:HE22	2.14	0.45
1:A:175:ARG:NH2	1:B:258:TYR:OH	2.50	0.45
1:A:200:GLN:HE22	1:B:215:ARG:HB2	1.81	0.45
1:A:198:LEU:HD23	1:A:199:CYS:N	2.31	0.45
1:B:147:ARG:NH1	1:B:156:GLN:HE22	2.13	0.45
1:C:83:GLY:HA2	1:C:106:VAL:CG2	2.47	0.45
1:C:97:ASN:C	1:C:97:ASN:ND2	2.75	0.45
1:C:141:HIS:O	1:C:142:PHE:C	2.59	0.45
1:D:140:ARG:HH21	1:D:159:ASP:CG	2.25	0.45
3:A:314:UMP:OP3	1:B:176:ARG:NH2	2.49	0.45
1:C:161:LEU:HD21	1:C:288:ILE:HD13	1.98	0.45
1:B:141:HIS:O	1:B:142:PHE:C	2.60	0.45
1:D:86:GLU:HB2	1:D:106:VAL:HG21	1.99	0.45
1:B:163:ARG:HG2	1:B:163:ARG:NH1	2.31	0.44
1:C:274:ARG:HG3	1:C:274:ARG:HH11	1.82	0.44
1:A:43:CYS:O	1:A:44:GLY:C	2.60	0.44
1:B:54:GLY:CA	1:B:259:LEU:HG	2.48	0.44
1:B:68:ARG:HG3	1:B:68:ARG:NH1	2.31	0.44
1:C:59:PHE:HA	1:C:253:GLY:O	2.17	0.44
1:A:40:ILE:HD12	1:A:219:MET:HG3	1.99	0.44
1:A:215:ARG:CG	1:A:216:SER:N	2.79	0.44
1:A:174:ASP:OD1	1:A:176:ARG:N	2.46	0.44
1:A:212:LEU:HD22	1:A:230:TYR:CD2	2.52	0.44
1:A:215:ARG:CB	1:B:178:ILE:HD11	2.47	0.44
1:B:182:TRP:HB2	1:B:197:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:GLY:HA2	1:C:106:VAL:HG21	1.99	0.44
1:C:163:ARG:HG2	1:C:163:ARG:NH1	2.33	0.44
1:D:207:GLU:HA	1:D:244:LYS:O	2.18	0.44
1:A:62:GLN:HA	1:A:250:HIS:O	2.18	0.44
1:B:62:GLN:HA	1:B:250:HIS:O	2.17	0.44
1:B:75:THR:C	1:B:77:LYS:H	2.26	0.44
1:B:261:HIS:C	1:B:264:PRO:HD2	2.43	0.44
1:C:67:LEU:HB3	1:C:235:TYR:CE1	2.53	0.44
1:B:40:ILE:HD12	1:B:219:MET:HG3	1.99	0.44
1:B:97:ASN:ND2	1:B:97:ASN:C	2.76	0.44
1:C:86:GLU:HB2	1:C:106:VAL:HG21	2.00	0.43
1:C:175:ARG:O	1:D:215:ARG:NH1	2.50	0.43
1:C:207:GLU:HA	1:C:244:LYS:O	2.17	0.43
1:D:97:ASN:ND2	1:D:97:ASN:C	2.76	0.43
1:A:32:GLN:O	1:A:36:GLN:HG3	2.18	0.43
1:A:68:ARG:HG3	1:A:68:ARG:HH11	1.83	0.43
3:A:314:UMP:OP3	1:B:176:ARG:NE	2.51	0.43
1:B:198:LEU:HD23	1:B:199:CYS:N	2.34	0.43
1:D:62:GLN:HA	1:D:250:HIS:O	2.18	0.43
1:C:292:LYS:HE2	1:C:294:GLU:OE1	2.18	0.43
1:C:215:ARG:CG	1:C:216:SER:N	2.81	0.43
1:D:163:ARG:HG2	1:D:163:ARG:NH1	2.33	0.43
1:A:83:GLY:HA2	1:A:106:VAL:HG21	2.00	0.43
1:B:207:GLU:HA	1:B:244:LYS:O	2.18	0.43
1:C:31:LEU:HD23	1:C:31:LEU:HA	1.87	0.43
1:C:32:GLN:O	1:C:36:GLN:HG3	2.18	0.43
1:C:68:ARG:HG3	1:C:68:ARG:HH11	1.83	0.43
1:C:140:ARG:HH21	1:C:159:ASP:CG	2.27	0.43
1:A:86:GLU:HB2	1:A:106:VAL:HG21	1.99	0.43
1:B:67:LEU:HB3	1:B:235:TYR:HE1	1.84	0.43
1:B:139:TRP:CE2	1:B:179:MET:HE3	2.53	0.43
1:D:87:GLU:O	1:D:90:TRP:HB3	2.19	0.43
1:D:285:VAL:CG1	1:D:290:ASP:HB2	2.48	0.43
1:A:140:ARG:HH21	1:A:159:ASP:CG	2.26	0.43
1:C:40:ILE:CD1	1:C:219:MET:HG3	2.49	0.43
1:C:130:ASP:CG	1:C:149:MET:HB3	2.43	0.43
1:D:140:ARG:NH2	1:D:159:ASP:OD1	2.51	0.43
1:A:67:LEU:HB3	1:A:235:TYR:HE1	1.84	0.43
1:A:163:ARG:HG2	1:A:163:ARG:NH1	2.33	0.43
1:A:205:ASN:O	1:A:206:SER:HB2	2.19	0.42
1:A:274:ARG:HG3	1:A:274:ARG:HH11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ASN:O	1:B:206:SER:HB2	2.19	0.42
1:B:83:GLY:HA2	1:B:106:VAL:HG21	2.00	0.42
1:D:205:ASN:O	1:D:206:SER:HB2	2.19	0.42
1:D:50:ARG:HG2	1:D:50:ARG:HH11	1.84	0.42
1:D:61:MET:HE2	1:D:255:ALA:HB3	1.98	0.42
1:D:75:THR:C	1:D:77:LYS:H	2.27	0.42
1:B:140:ARG:HH21	1:B:159:ASP:CG	2.27	0.42
1:A:306:THR:HG22	1:A:307:ILE:H	1.83	0.42
1:C:28:HIS:CE1	1:C:30:GLU:H	2.37	0.42
1:C:285:VAL:HG13	1:C:290:ASP:HB2	2.02	0.42
1:D:130:ASP:CG	1:D:149:MET:HB3	2.45	0.42
1:B:283:ARG:HD3	1:B:295:ASP:OD1	2.18	0.42
1:C:174:ASP:OD1	1:C:176:ARG:N	2.47	0.42
1:C:204:VAL:HG23	1:D:47:LYS:HE3	2.01	0.42
1:C:283:ARG:HD3	1:C:295:ASP:OD1	2.19	0.42
1:B:28:HIS:CE1	1:B:30:GLU:H	2.37	0.42
1:D:218:ASP:OD2	1:D:218:ASP:C	2.63	0.42
1:A:47:LYS:HE2	1:B:173:ASP:CA	2.41	0.42
1:D:113:GLY:O	1:D:128:GLU:HG3	2.20	0.42
1:B:68:ARG:HG3	1:B:68:ARG:HH11	1.85	0.42
1:B:285:VAL:CG1	1:B:290:ASP:HB2	2.50	0.42
1:C:148:ASP:C	1:C:150:GLU:H	2.28	0.42
1:D:174:ASP:OD1	1:D:176:ARG:N	2.47	0.42
1:A:285:VAL:HG13	1:A:290:ASP:HB2	2.01	0.42
1:C:261:HIS:C	1:C:264:PRO:HD2	2.45	0.42
1:A:28:HIS:CE1	1:A:30:GLU:H	2.38	0.41
1:A:75:THR:C	1:A:77:LYS:H	2.28	0.41
1:C:193:PRO:HA	1:C:194:PRO:HD3	1.95	0.41
1:A:28:HIS:HE1	1:A:30:GLU:HB2	1.85	0.41
1:D:68:ARG:HG3	1:D:68:ARG:NH1	2.35	0.41
1:A:195:CYS:HB2	3:A:314:UMP:C4	2.54	0.41
1:D:261:HIS:C	1:D:264:PRO:HD2	2.45	0.41
1:A:59:PHE:HA	1:A:253:GLY:O	2.20	0.41
1:C:263:GLU:HB2	1:C:264:PRO:HD3	2.03	0.41
1:A:54:GLY:HA3	1:A:259:LEU:HG	2.02	0.41
1:A:81:TRP:O	1:A:84:VAL:HB	2.21	0.41
1:A:148:ASP:C	1:A:150:GLU:H	2.29	0.41
1:A:161:LEU:HD21	1:A:288:ILE:HD13	2.03	0.41
1:B:46:GLU:HA	1:B:55:THR:O	2.21	0.41
1:B:97:ASN:CG	1:B:149:MET:SD	3.04	0.41
1:D:28:HIS:CE1	1:D:30:GLU:H	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:HIS:NE2	1:A:309:MET:HB3	2.36	0.41
1:D:40:ILE:CD1	1:D:219:MET:HG3	2.51	0.41
1:C:306:THR:HG22	1:C:307:ILE:H	1.84	0.41
1:D:263:GLU:HB2	1:D:264:PRO:HD3	2.02	0.40
1:C:140:ARG:NH2	1:C:159:ASP:OD1	2.55	0.40
1:A:140:ARG:HD2	1:A:159:ASP:OD2	2.20	0.40
1:C:61:MET:HE2	1:C:255:ALA:HB3	2.03	0.40
1:A:143:GLY:HA3	1:B:185:ARG:NH2	2.36	0.40
1:B:140:ARG:HD2	1:B:159:ASP:OD2	2.22	0.40
1:D:274:ARG:HH11	1:D:274:ARG:HG3	1.86	0.40
1:B:274:ARG:HH11	1:B:274:ARG:HG3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	284/313 (91%)	256 (90%)	26 (9%)	2 (1%)	18	48
1	B	284/313 (91%)	258 (91%)	25 (9%)	1 (0%)	30	59
1	C	284/313 (91%)	258 (91%)	25 (9%)	1 (0%)	30	59
1	D	284/313 (91%)	258 (91%)	25 (9%)	1 (0%)	30	59
All	All	1136/1252 (91%)	1030 (91%)	101 (9%)	5 (0%)	30	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	TYR
1	B	135	TYR
1	C	135	TYR
1	D	135	TYR

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Mol	Chain	Res	Type
1	A	149	MET

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	249/271 (92%)	231 (93%)	18 (7%)	13	39
1	B	249/271 (92%)	231 (93%)	18 (7%)	13	39
1	C	249/271 (92%)	231 (93%)	18 (7%)	13	39
1	D	249/271 (92%)	232 (93%)	17 (7%)	14	42
All	All	996/1084 (92%)	925 (93%)	71 (7%)	13	40

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	CYS
1	A	48	ASP
1	A	55	THR
1	A	67	LEU
1	A	69	ASP
1	A	85	LEU
1	A	88	LEU
1	A	89	LEU
1	A	115	ARG
1	A	140	ARG
1	A	158	VAL
1	A	192	LEU
1	A	204	VAL
1	A	225	PHE
1	A	232	LEU
1	A	252	LEU
1	A	265	LEU
1	A	269	LEU
1	B	48	ASP
1	B	55	THR

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Mol	Chain	Res	Type
1	B	67	LEU
1	B	69	ASP
1	B	85	LEU
1	B	88	LEU
1	B	89	LEU
1	B	115	ARG
1	B	140	ARG
1	B	158	VAL
1	B	163	ARG
1	B	192	LEU
1	B	204	VAL
1	B	225	PHE
1	B	232	LEU
1	B	252	LEU
1	B	265	LEU
1	B	269	LEU
1	C	42	ARG
1	C	48	ASP
1	C	55	THR
1	C	67	LEU
1	C	69	ASP
1	C	85	LEU
1	C	88	LEU
1	C	89	LEU
1	C	115	ARG
1	C	140	ARG
1	C	158	VAL
1	C	192	LEU
1	C	204	VAL
1	C	225	PHE
1	C	232	LEU
1	C	252	LEU
1	C	265	LEU
1	C	269	LEU
1	D	48	ASP
1	D	55	THR
1	D	67	LEU
1	D	69	ASP
1	D	85	LEU
1	D	88	LEU
1	D	89	LEU
1	D	115	ARG

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Mol	Chain	Res	Type
1	D	140	ARG
1	D	158	VAL
1	D	192	LEU
1	D	204	VAL
1	D	225	PHE
1	D	232	LEU
1	D	252	LEU
1	D	265	LEU
1	D	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	62	GLN
1	A	97	ASN
1	A	156	GLN
1	A	162	GLN
1	A	205	ASN
1	A	239	HIS
1	A	268	GLN
1	A	302	ASN
1	B	32	GLN
1	B	62	GLN
1	B	97	ASN
1	B	156	GLN
1	B	171	ASN
1	B	205	ASN
1	B	239	HIS
1	B	268	GLN
1	B	302	ASN
1	C	32	GLN
1	C	62	GLN
1	C	97	ASN
1	C	156	GLN
1	C	162	GLN
1	C	205	ASN
1	C	239	HIS
1	C	268	GLN
1	C	302	ASN
1	D	32	GLN
1	D	62	GLN

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Mol	Chain	Res	Type
1	D	97	ASN
1	D	156	GLN
1	D	162	GLN
1	D	205	ASN
1	D	211	GLN
1	D	239	HIS
1	D	268	GLN
1	D	302	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
3	UMP	C	314	1	21,21,21	2.71	5 (23%)	30,31,31	2.13	11 (36%)
3	UMP	B	314	1	21,21,21	2.62	6 (28%)	30,31,31	2.08	10 (33%)
3	UMP	A	314	1	21,21,21	2.59	6 (28%)	30,31,31	2.18	12 (40%)
3	UMP	D	314	1	21,21,21	2.53	4 (19%)	30,31,31	2.66	11 (36%)
4	LYA	C	315	-	32,33,33	2.21	9 (28%)	41,46,46	1.43	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LYA	D	315	-	32,33,33	2.14	10 (31%)	41,46,46	1.48	4 (9%)
4	LYA	A	317	-	32,33,33	2.13	8 (25%)	41,46,46	1.55	4 (9%)
4	LYA	B	315	-	32,33,33	2.13	10 (31%)	41,46,46	1.48	5 (12%)
2	PO4	A	316	-	4,4,4	1.53	0	6,6,6	0.43	0

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
3	UMP	C	314	1	-	1/10/22/22	0/2/2/2
3	UMP	B	314	1	-	0/10/22/22	0/2/2/2
3	UMP	A	314	1	-	1/10/22/22	0/2/2/2
3	UMP	D	314	1	-	1/10/22/22	0/2/2/2
4	LYA	C	315	-	-	9/22/22/22	0/3/3/3
4	LYA	D	315	-	-	3/22/22/22	0/3/3/3
4	LYA	A	317	-	-	4/22/22/22	0/3/3/3
4	LYA	B	315	-	-	4/22/22/22	0/3/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	314	UMP	C6-C5	8.25	1.54	1.35
3	B	314	UMP	C6-C5	8.22	1.54	1.35
3	C	314	UMP	C6-C5	8.09	1.53	1.35
3	A	314	UMP	C6-C5	8.06	1.53	1.35
3	C	314	UMP	C6-N1	6.72	1.54	1.38
3	B	314	UMP	C6-N1	5.86	1.52	1.38
4	C	315	LYA	C17-N16	5.70	1.47	1.33
3	A	314	UMP	C6-N1	5.65	1.51	1.38
4	D	315	LYA	C17-N16	5.50	1.46	1.33
4	A	317	LYA	C12-N18	5.48	1.45	1.37
4	C	315	LYA	C12-N18	5.38	1.45	1.37
4	D	315	LYA	C12-N18	5.28	1.45	1.37
4	B	315	LYA	C12-N18	5.14	1.44	1.37
4	A	317	LYA	C17-N16	5.02	1.45	1.33
4	B	315	LYA	C17-N16	4.92	1.45	1.33
3	D	314	UMP	C6-N1	4.46	1.48	1.38
3	D	314	UMP	C5-C4	4.45	1.53	1.43
3	B	314	UMP	C5-C4	3.95	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	314	UMP	C5-C4	3.76	1.51	1.43
4	A	317	LYA	C3-C4	3.64	1.44	1.39
3	D	314	UMP	O4'-C1'	3.57	1.50	1.42
3	A	314	UMP	O4'-C1'	3.56	1.50	1.42
3	A	314	UMP	C5-C4	3.54	1.51	1.43
4	C	315	LYA	C3-C4	3.51	1.44	1.39
3	C	314	UMP	O4'-C4'	3.45	1.52	1.45
4	C	315	LYA	C13-C12	3.24	1.43	1.37
4	B	315	LYA	C17-N18	-3.21	1.29	1.37
4	A	317	LYA	C13-C12	3.04	1.43	1.37
4	B	315	LYA	C5-C4	3.01	1.44	1.39
4	D	315	LYA	C5-C4	3.00	1.44	1.39
4	C	315	LYA	C17-N18	-2.98	1.30	1.37
4	D	315	LYA	C17-N18	-2.95	1.30	1.37
4	A	317	LYA	C10-N11	2.91	1.42	1.36
4	D	315	LYA	C3-C4	2.86	1.43	1.39
3	B	314	UMP	O4'-C1'	2.80	1.48	1.42
4	C	315	LYA	C10-N11	2.80	1.41	1.36
4	B	315	LYA	C23-N22	2.77	1.51	1.45
4	B	315	LYA	C3-C2	2.73	1.43	1.38
4	C	315	LYA	C3-C2	2.70	1.43	1.38
4	D	315	LYA	C13-C12	2.63	1.42	1.37
4	A	317	LYA	C17-N18	-2.61	1.31	1.37
4	A	317	LYA	C3-C2	2.60	1.43	1.38
4	D	315	LYA	C3-C2	2.58	1.43	1.38
4	B	315	LYA	C13-C12	2.53	1.42	1.37
3	C	314	UMP	O4'-C1'	2.51	1.48	1.42
4	B	315	LYA	C3-C4	2.50	1.43	1.39
4	C	315	LYA	C23-N22	2.37	1.50	1.45
4	C	315	LYA	C5-C4	2.33	1.43	1.39
4	D	315	LYA	C6-C5	2.33	1.42	1.38
3	A	314	UMP	O4'-C4'	2.31	1.50	1.45
3	B	314	UMP	O3'-C3'	-2.31	1.38	1.43
4	B	315	LYA	C6-C5	2.28	1.42	1.38
4	A	317	LYA	C2-C1	2.27	1.43	1.38
3	A	314	UMP	P-OP3	-2.23	1.46	1.54
4	B	315	LYA	C10-N11	2.22	1.40	1.36
4	D	315	LYA	C4-C20	2.15	1.54	1.50
4	D	315	LYA	C10-N11	2.04	1.40	1.36
3	B	314	UMP	P-OP3	-2.02	1.47	1.54

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	317	LYA	C13-C12-N18	-6.08	118.55	123.46
3	D	314	UMP	C5-C6-N1	-6.07	111.97	121.84
3	D	314	UMP	O4'-C1'-N1	6.00	118.51	107.86
4	D	315	LYA	C13-C12-N18	-5.66	118.89	123.46
4	B	315	LYA	C13-C12-N18	-5.61	118.92	123.46
4	C	315	LYA	C13-C12-N18	-5.52	119.00	123.46
3	C	314	UMP	C5-C6-N1	-5.48	112.94	121.84
3	B	314	UMP	C6-C5-C4	-5.31	112.74	119.53
3	A	314	UMP	C6-C5-C4	-5.31	112.76	119.53
3	D	314	UMP	C5-C4-N3	5.20	122.08	114.80
3	C	314	UMP	C6-C5-C4	-5.08	113.05	119.53
3	D	314	UMP	C6-C5-C4	-5.04	113.10	119.53
3	B	314	UMP	C5-C6-N1	-4.92	113.84	121.84
3	A	314	UMP	C5-C6-N1	-4.56	114.42	121.84
3	D	314	UMP	C6-N1-C2	4.18	126.08	121.00
3	D	314	UMP	O5'-P-OP1	4.12	117.56	106.44
3	B	314	UMP	C5-C4-N3	4.02	120.44	114.80
3	A	314	UMP	C5-C4-N3	3.89	120.25	114.80
3	A	314	UMP	O5'-C5'-C4'	-3.49	97.12	108.99
3	C	314	UMP	C6-N1-C2	3.17	124.86	121.00
3	B	314	UMP	O4'-C1'-N1	3.14	113.43	107.86
4	D	315	LYA	C24-C25-C26	3.01	120.51	112.49
3	C	314	UMP	C5-C4-N3	3.00	119.00	114.80
3	A	314	UMP	O4'-C4'-C3'	-2.89	99.07	105.65
3	C	314	UMP	O4-C4-C5	-2.87	120.22	125.16
4	A	317	LYA	C7-C8-C9	2.78	116.25	112.61
3	C	314	UMP	OP3-P-O5'	2.76	113.86	106.67
3	C	314	UMP	C2'-C1'-N1	-2.75	106.94	113.81
3	A	314	UMP	O4-C4-C5	-2.72	120.48	125.16
3	D	314	UMP	O3'-C3'-C2'	-2.66	101.62	110.88
4	B	315	LYA	C24-C25-C26	2.63	119.51	112.49
4	A	317	LYA	N11-C12-N18	2.62	133.94	128.34
3	C	314	UMP	O4'-C4'-C3'	-2.62	99.67	105.65
3	A	314	UMP	O4'-C1'-C2'	-2.57	101.44	106.25
3	D	314	UMP	O4-C4-C5	-2.54	120.78	125.16
3	B	314	UMP	O3'-C3'-C2'	-2.49	102.23	110.88
3	B	314	UMP	O4'-C4'-C3'	-2.48	99.98	105.65
3	B	314	UMP	O4-C4-C5	-2.48	120.89	125.16
3	A	314	UMP	O3'-C3'-C4'	-2.47	100.70	110.07
3	A	314	UMP	C1'-N1-C6	-2.43	116.76	121.53
4	B	315	LYA	N11-C12-N18	2.41	133.48	128.34
3	D	314	UMP	C2'-C1'-N1	-2.36	107.91	113.81
4	D	315	LYA	N11-C12-N18	2.35	133.36	128.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	314	UMP	OP3-P-O5'	2.34	112.76	106.67
3	D	314	UMP	OP3-P-OP2	2.33	116.55	107.80
3	B	314	UMP	C6-N1-C2	2.33	123.83	121.00
4	C	315	LYA	N11-C12-N18	2.32	133.28	128.34
3	C	314	UMP	O4'-C1'-N1	2.23	111.82	107.86
3	D	314	UMP	O4'-C4'-C3'	-2.22	100.58	105.65
4	D	315	LYA	C24-C23-C29	2.20	115.58	110.35
3	A	314	UMP	C4-N3-C2	-2.20	123.89	126.61
4	B	315	LYA	C23-N22-C20	2.17	126.76	121.56
3	B	314	UMP	O4'-C1'-C2'	-2.17	102.20	106.25
4	A	317	LYA	C24-C25-C26	2.14	118.20	112.49
3	C	314	UMP	O4'-C1'-C2'	-2.11	102.30	106.25
4	B	315	LYA	C24-C23-N22	2.06	114.99	110.91
3	A	314	UMP	C4'-O4'-C1'	2.06	114.41	109.51
4	C	315	LYA	C24-C25-C26	2.06	117.98	112.49
3	C	314	UMP	O2-C2-N3	2.03	125.23	121.49
3	B	314	UMP	OP3-P-O5'	2.02	111.94	106.67

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	317	LYA	N22-C23-C24-C25
4	B	315	LYA	N22-C23-C24-C25
4	A	317	LYA	C29-C23-C24-C25
4	C	315	LYA	C24-C23-N22-C20
4	D	315	LYA	C1-C7-C8-C9
4	C	315	LYA	C7-C8-C9-C10
4	D	315	LYA	C7-C8-C9-C10
4	C	315	LYA	C29-C23-N22-C20
4	B	315	LYA	C1-C7-C8-C9
4	C	315	LYA	C24-C23-C29-O30
4	C	315	LYA	C24-C23-C29-O31
4	C	315	LYA	C24-C25-C26-O28
4	C	315	LYA	C7-C8-C9-C13
4	C	315	LYA	C1-C7-C8-C9
4	A	317	LYA	C24-C25-C26-O27
4	A	317	LYA	C24-C25-C26-O28
4	C	315	LYA	C24-C25-C26-O27
4	B	315	LYA	C29-C23-C24-C25
4	D	315	LYA	C7-C8-C9-C13
3	A	314	UMP	O4'-C4'-C5'-O5'

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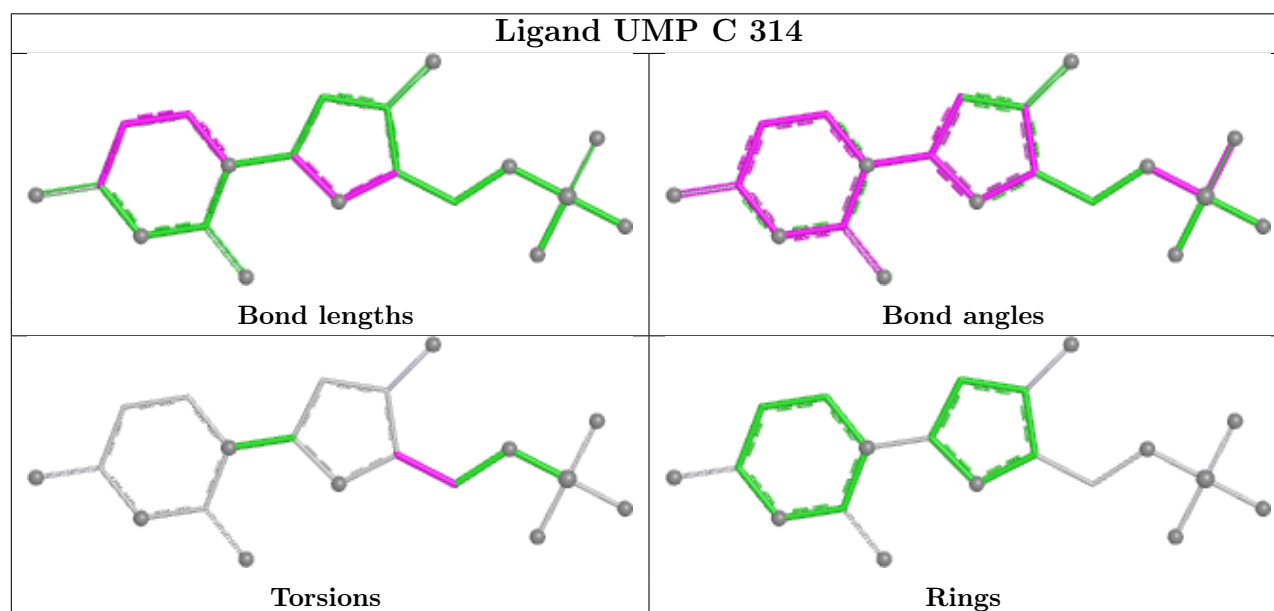
Mol	Chain	Res	Type	Atoms
3	D	314	UMP	O4'-C4'-C5'-O5'
4	B	315	LYA	C24-C25-C26-O28
3	C	314	UMP	O4'-C4'-C5'-O5'

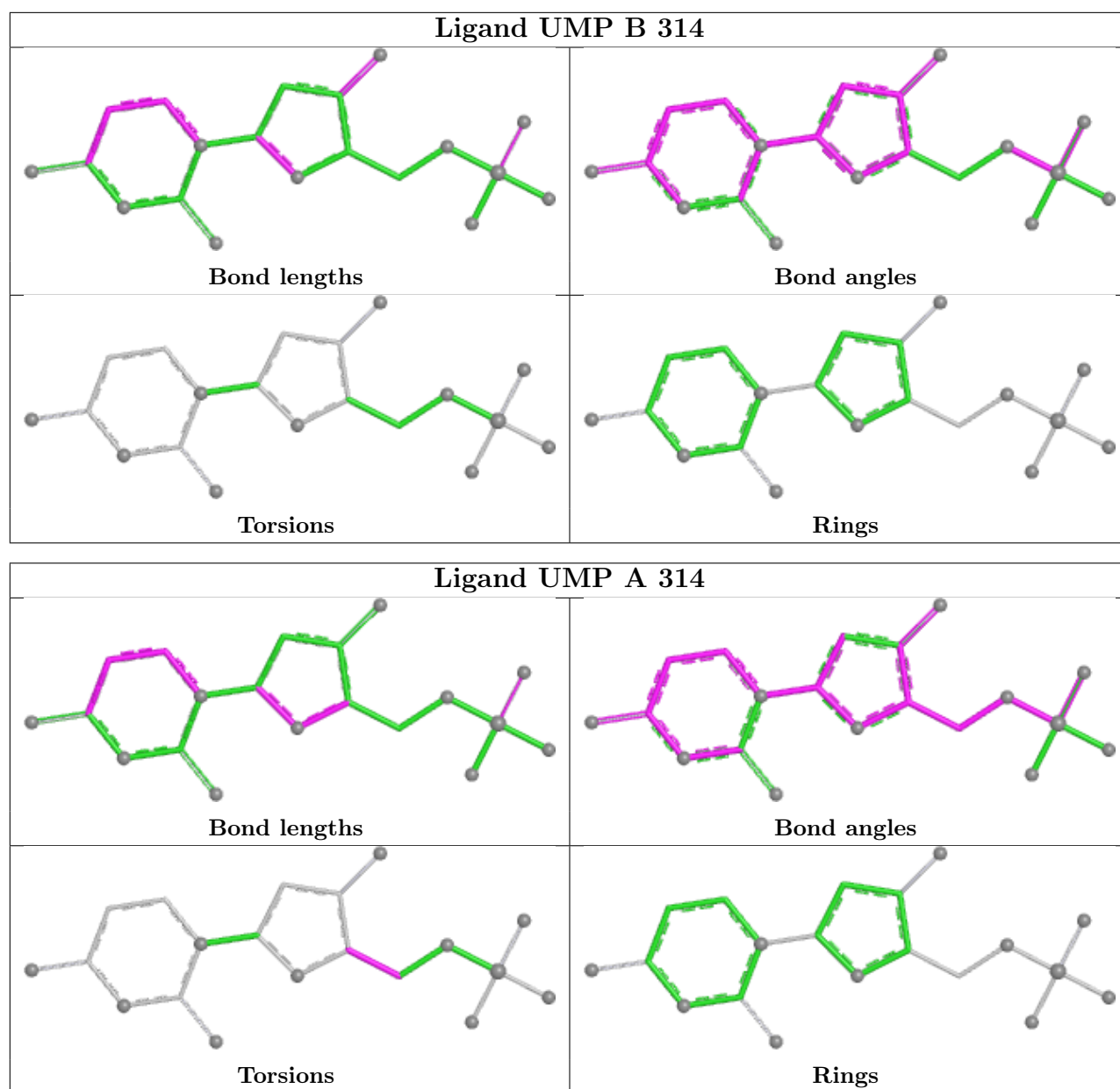
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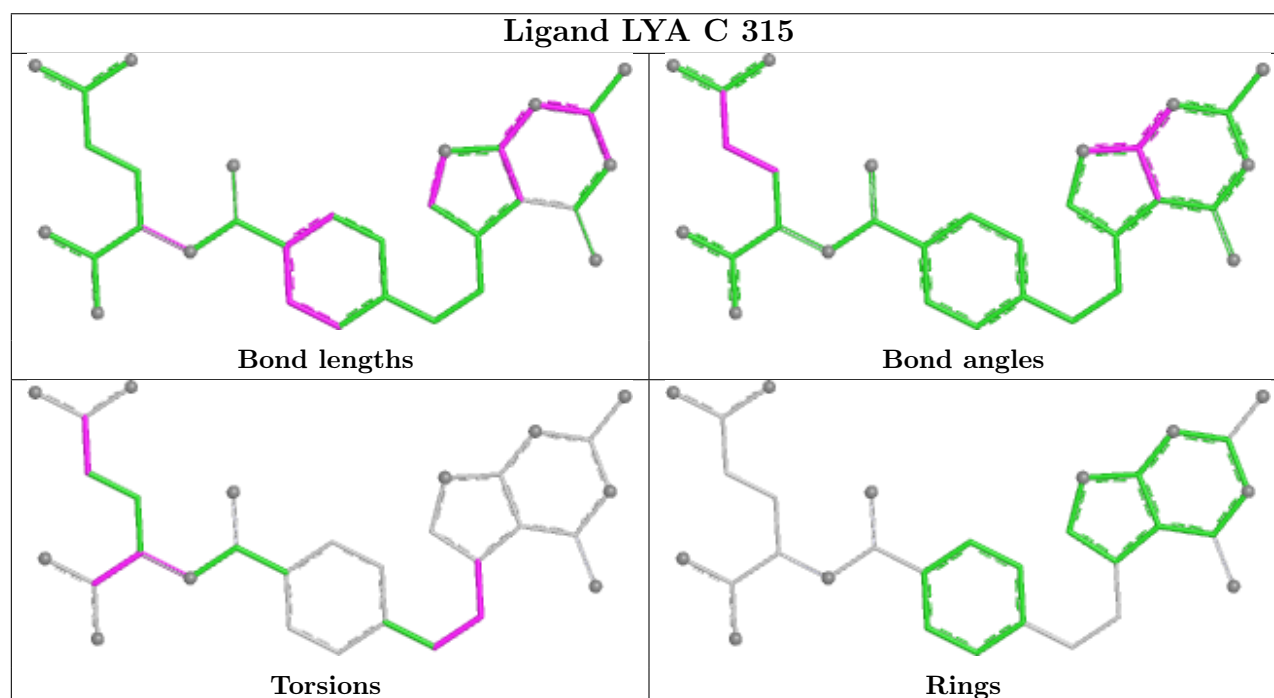
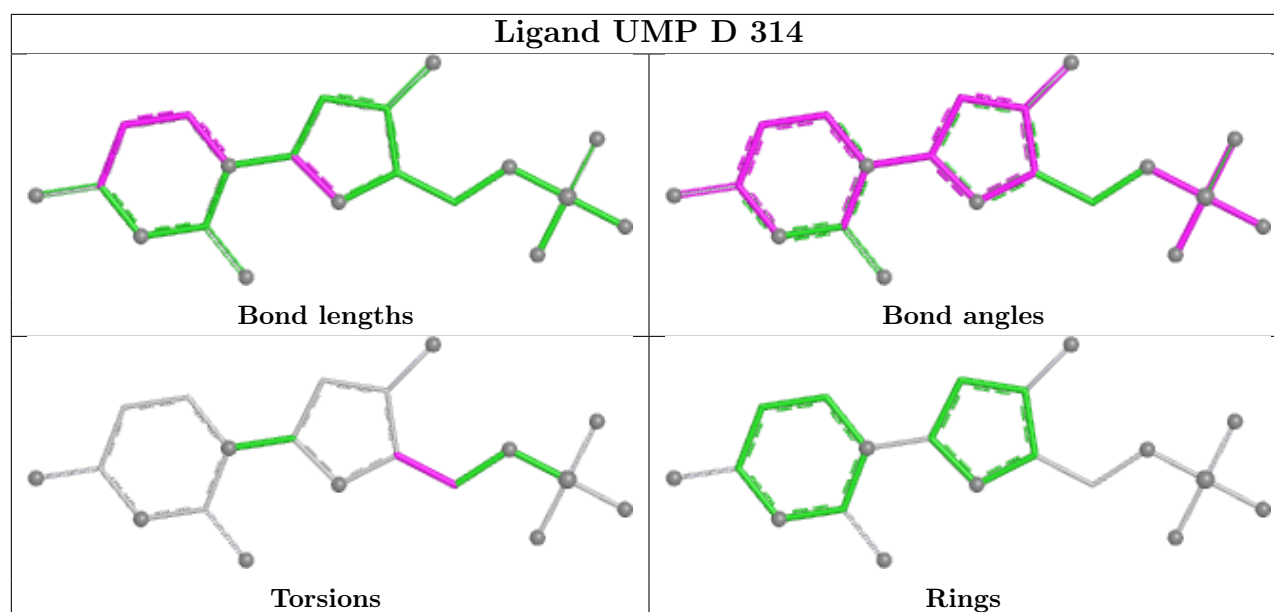
5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	314	UMP	1	0
3	B	314	UMP	4	0
3	A	314	UMP	4	0
3	D	314	UMP	3	0
4	C	315	LYA	1	0

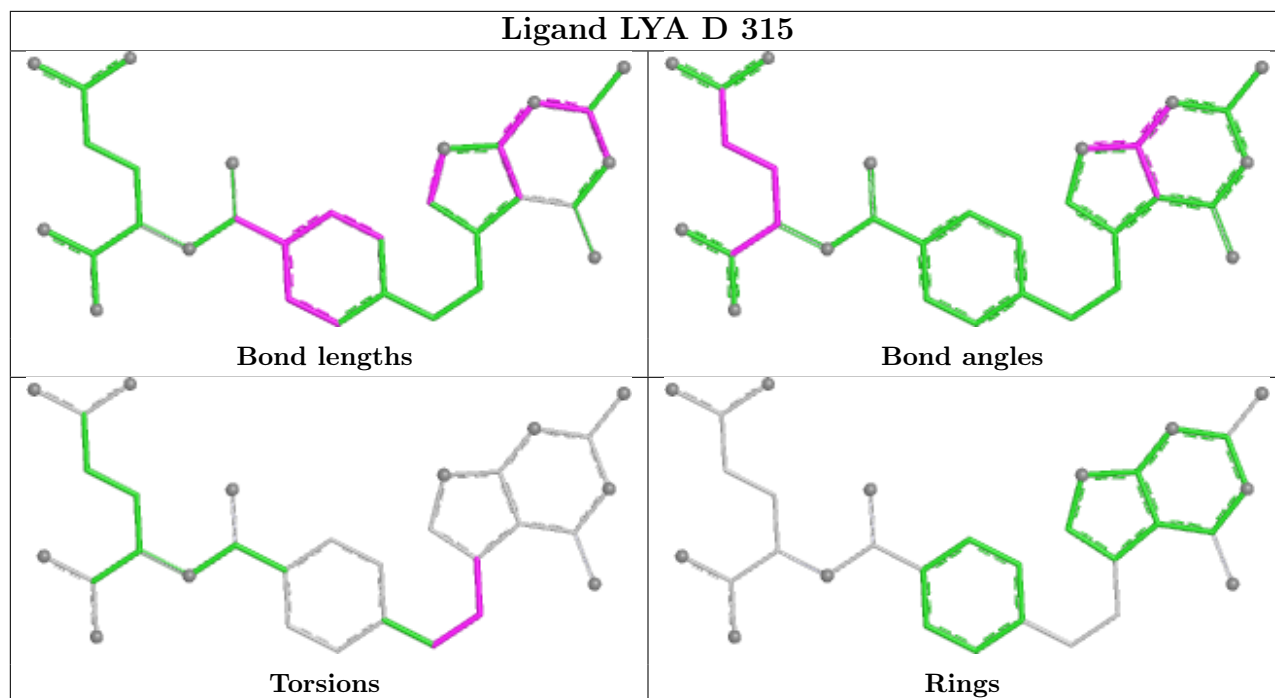
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



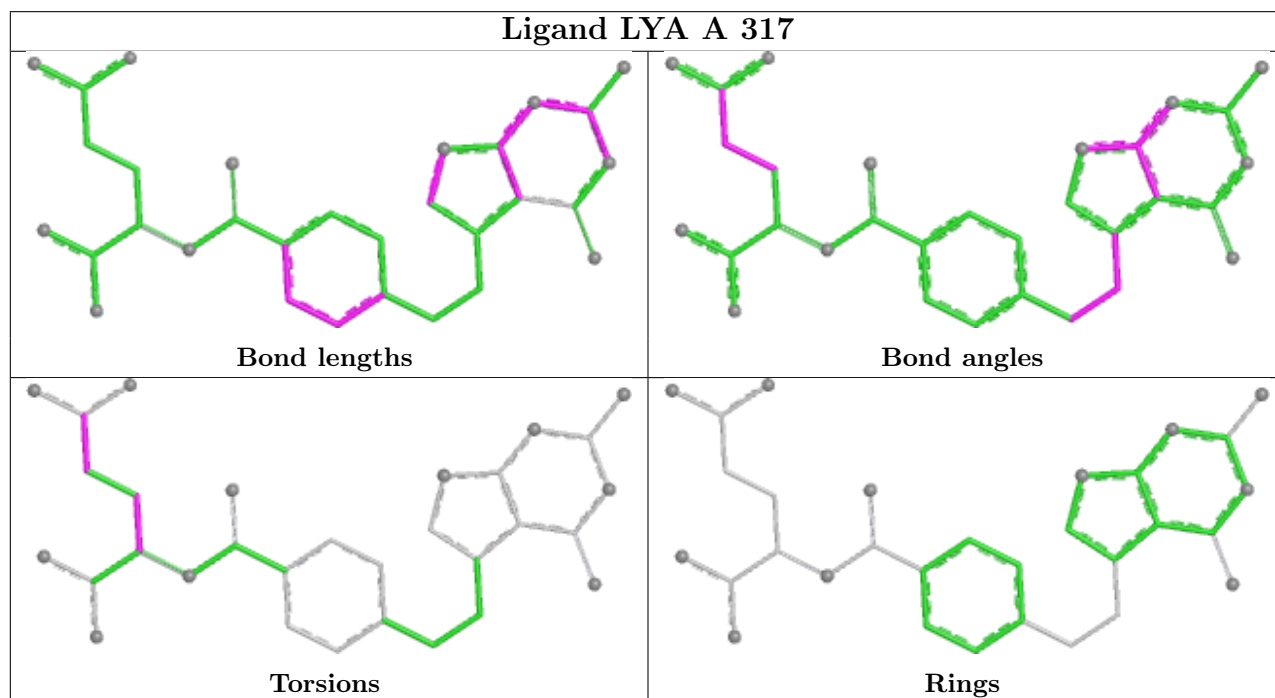


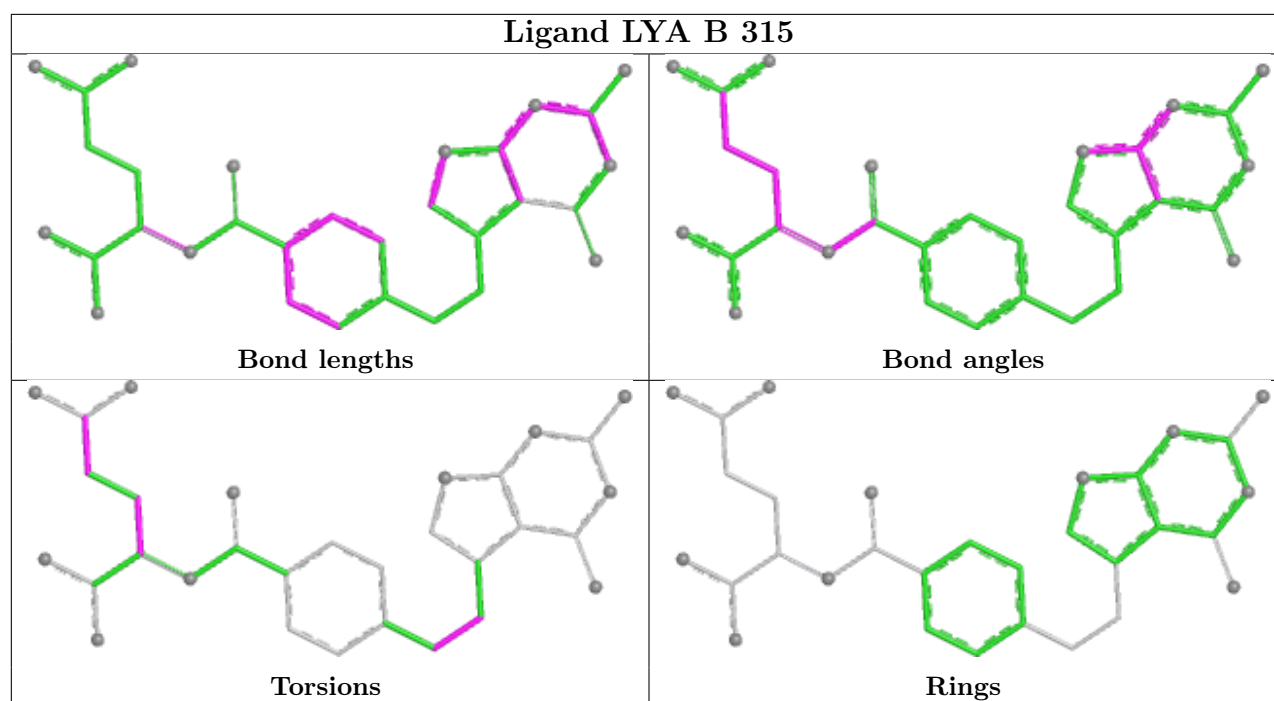


Ligand LYA D 315



Ligand LYA A 317





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	286/313 (91%)	0.37	5 (1%) 69 61	7, 23, 37, 47	0
1	B	286/313 (91%)	0.45	6 (2%) 63 54	7, 23, 37, 47	0
1	C	286/313 (91%)	0.49	6 (2%) 63 54	7, 23, 37, 47	0
1	D	286/313 (91%)	0.36	0 100 100	7, 23, 37, 47	0
All	All	1144/1252 (91%)	0.42	17 (1%) 72 64	7, 23, 38, 47	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	127	GLU	3.3
1	A	47	LYS	2.8
1	B	48	ASP	2.6
1	A	267	ILE	2.6
1	C	302	ASN	2.3
1	C	116	ASP	2.3
1	B	41	LEU	2.3
1	A	282	LEU	2.2
1	B	55	THR	2.2
1	B	100	GLU	2.2
1	A	127	GLU	2.2
1	A	116	ASP	2.2
1	B	116	ASP	2.2
1	C	96	THR	2.2
1	C	69	ASP	2.1
1	C	294	GLU	2.1
1	B	124	SER	2.0

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

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](#)

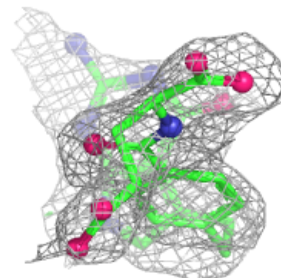
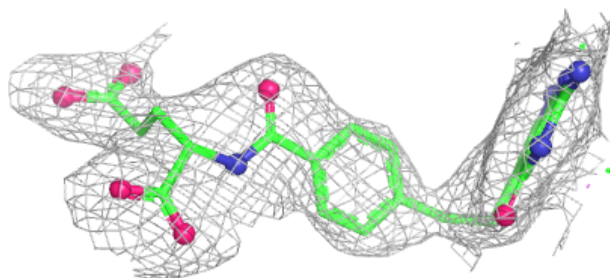
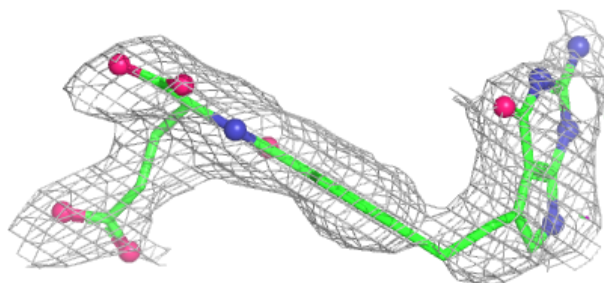
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	LYA	C	315	31/31	0.85	0.14	30,36,55,56	0
4	LYA	D	315	31/31	0.87	0.16	30,36,55,56	0
4	LYA	A	317	31/31	0.88	0.13	30,36,55,56	0
4	LYA	B	315	31/31	0.90	0.15	30,36,55,56	0
2	PO4	A	316	5/5	0.96	0.10	22,23,24,24	0
3	UMP	A	314	20/20	0.96	0.07	11,14,16,16	0
3	UMP	C	314	20/20	0.96	0.07	11,14,16,16	0
3	UMP	D	314	20/20	0.96	0.08	11,14,16,16	0
3	UMP	B	314	20/20	0.97	0.07	11,14,16,16	0

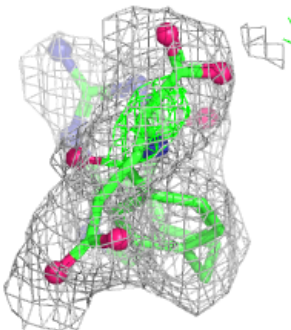
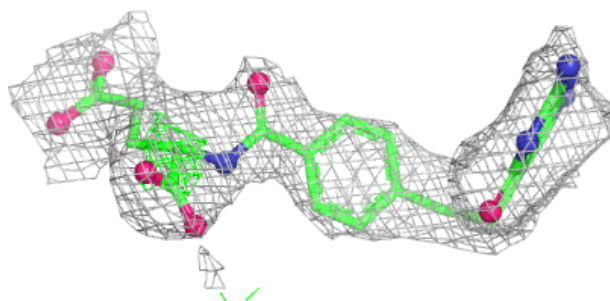
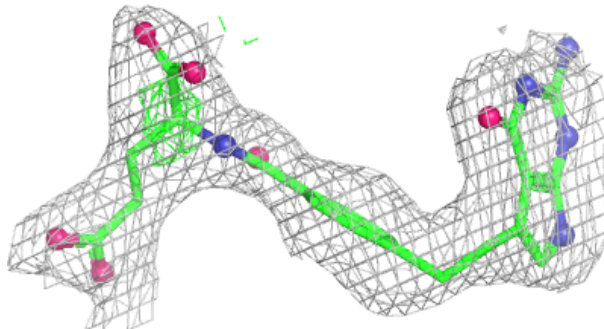
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LYA C 315:

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

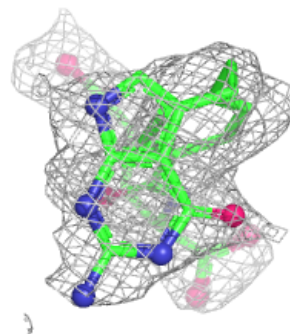
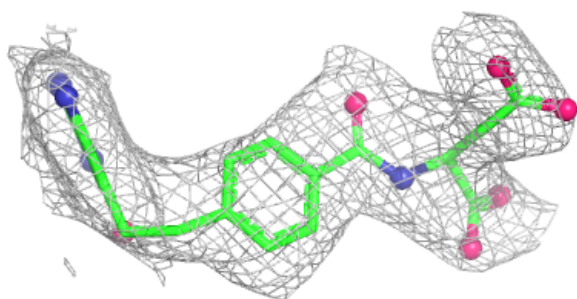
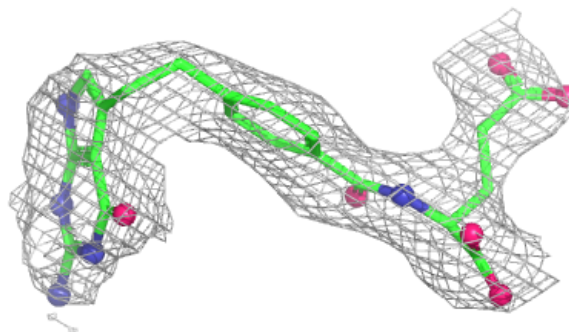
**Electron density around LYA D 315:**

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

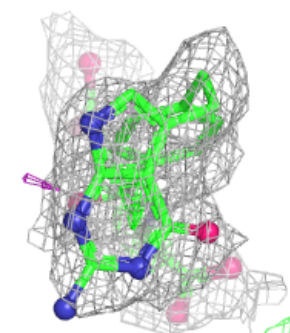
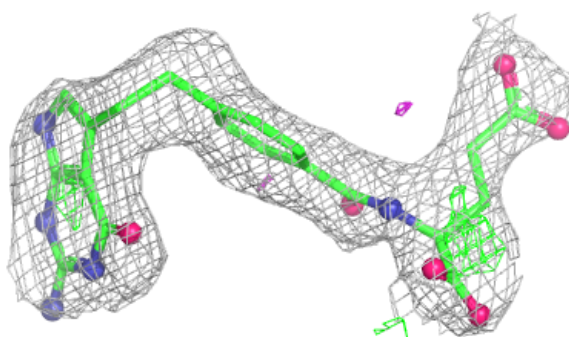


Electron density around LYA A 317:

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

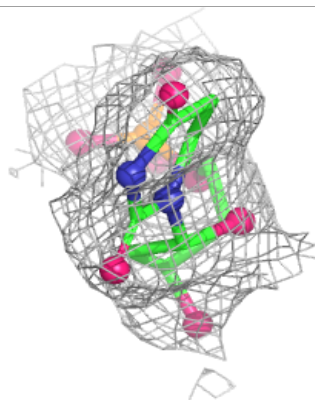
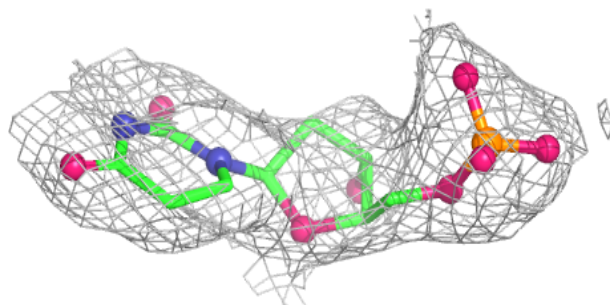
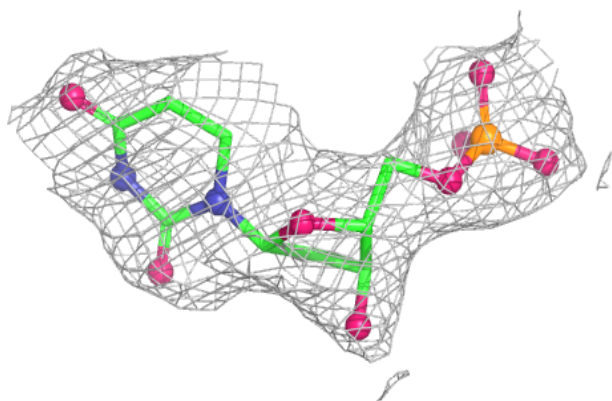
**Electron density around LYA B 315:**

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

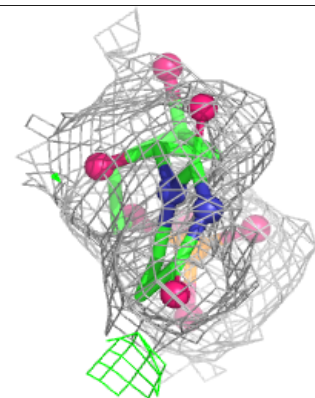
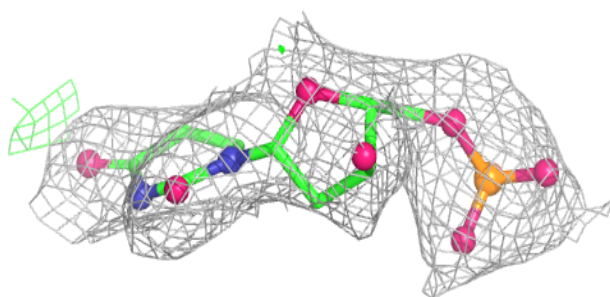
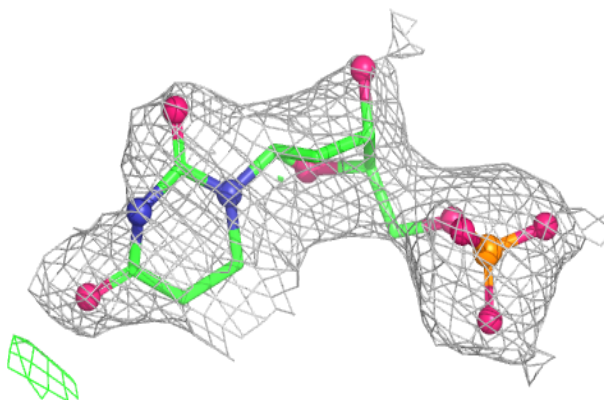


Electron density around UMP A 314:

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

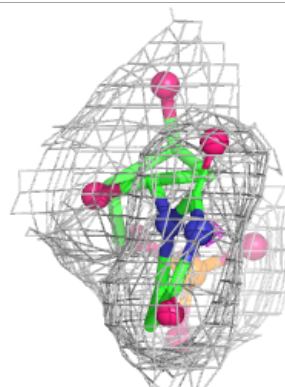
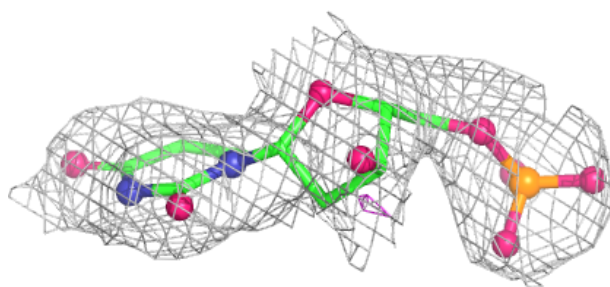
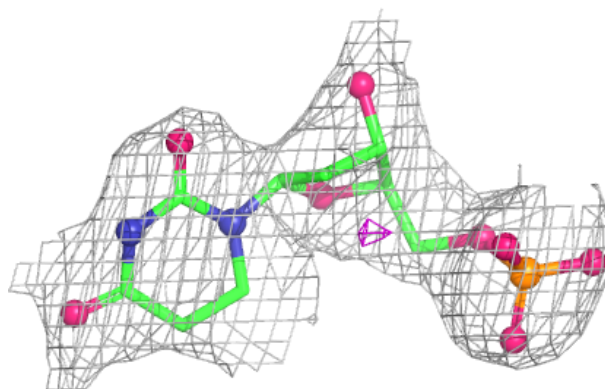
**Electron density around UMP C 314:**

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

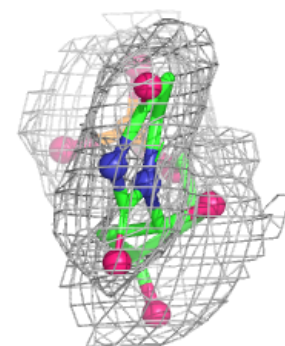
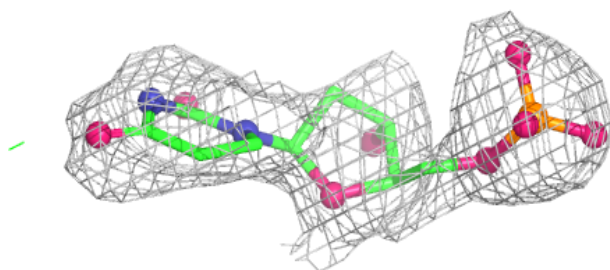
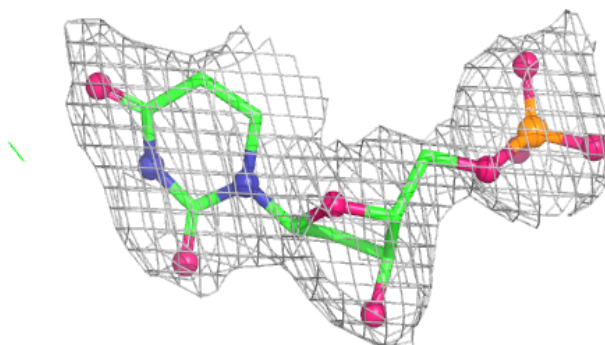


Electron density around UMP D 314:

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

**Electron density around UMP B 314:**

$2mF_o-DF_c$ (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.