



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:13 PM UTC

PDB ID : 3JSU / pdb_00003jsu
Title : Quadruple mutant(N51I+C59R+S108N+I164L) plasmodium falciparum dihydrofolate reductase-thymidylate synthase(PFDHFR-TS) complexed with QN254, NADPH, and dUMP
Authors : Chitnumsub, P.; Maneeruttanarungroj, C.; Kamchonwongpaisan, S.; Yuthavong, Y.; Diagana, T.T.
Deposited on : 2009-09-11
Resolution : 2.70 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](#) ①) 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

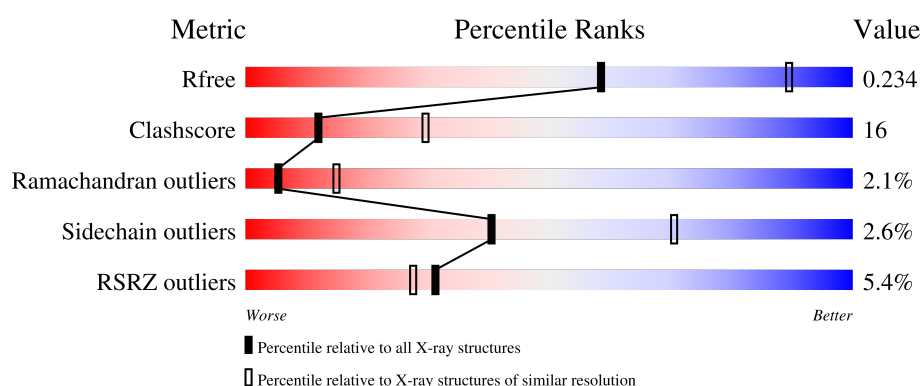
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	608	4% 59% 27% • 10%
1	B	608	6% 60% 26% • 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9487 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.

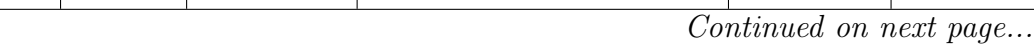
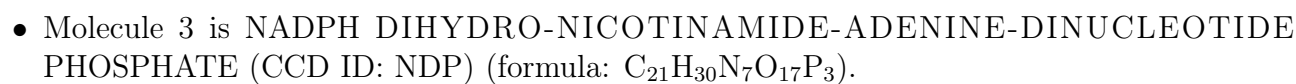
- Molecule 1 is a protein called Dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	545	Total	C	N	O	S	0	0	0
			4539	2931	751	830	27			
1	B	542	Total	C	N	O	S	0	0	0
			4511	2914	747	825	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ILE	ASN	engineered mutation	UNP A7UD79
A	59	ARG	TYR	engineered mutation	UNP A7UD79
A	108	ASN	SER	engineered mutation	UNP A7UD79
A	164	LEU	ILE	engineered mutation	UNP A7UD79
B	51	ILE	ASN	engineered mutation	UNP A7UD79
B	59	ARG	TYR	engineered mutation	UNP A7UD79
B	108	ASN	SER	engineered mutation	UNP A7UD79
B	164	LEU	ILE	engineered mutation	UNP A7UD79

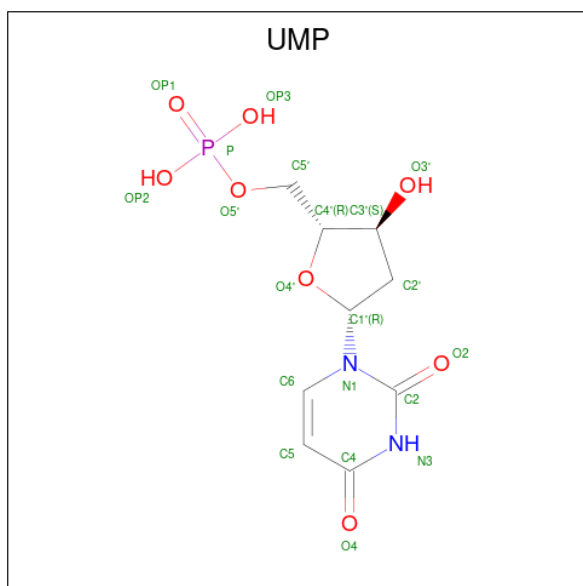
- Molecule 2 is 5-chloro-N 6 -(2,5-dimethoxybenzyl)quinazoline-2,4,6-triamine (CCD ID: KA5) (formula: C₁₇H₁₈ClN₅O₂).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: $C_9H_{13}N_2O_8P$).



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

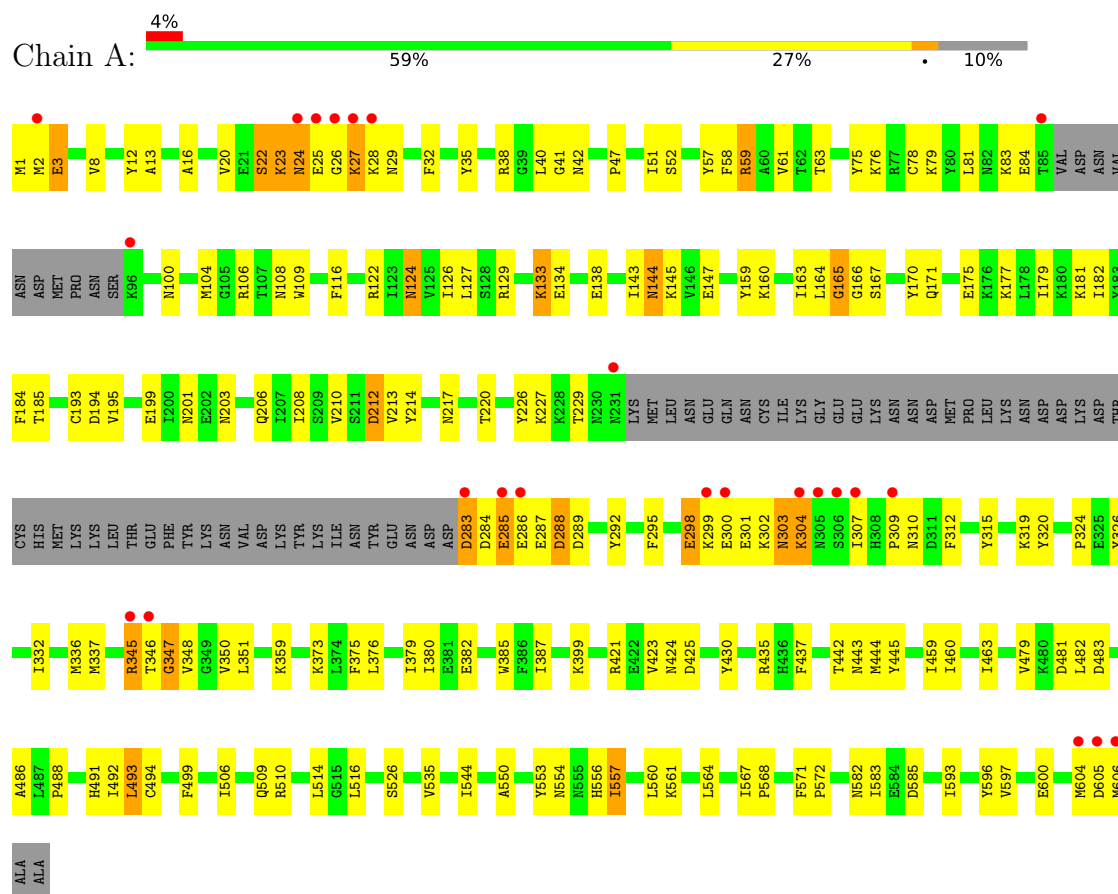
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	124	Total	O	0	0
			124	124		
5	B	127	Total	O	0	0
			127	127		

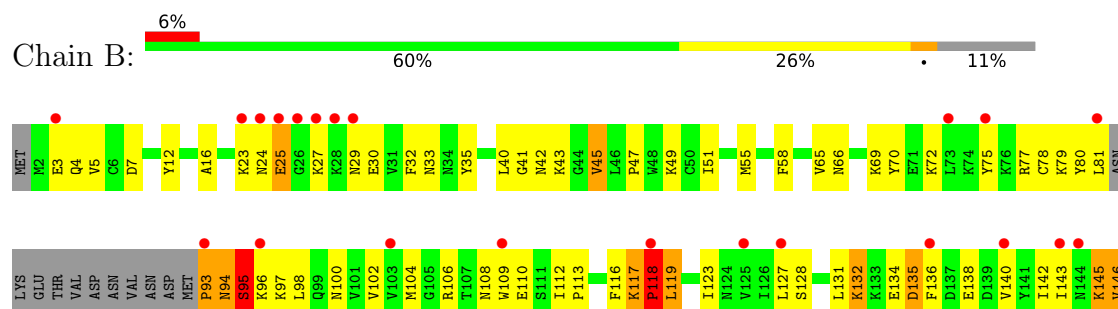
3 Residue-property plots

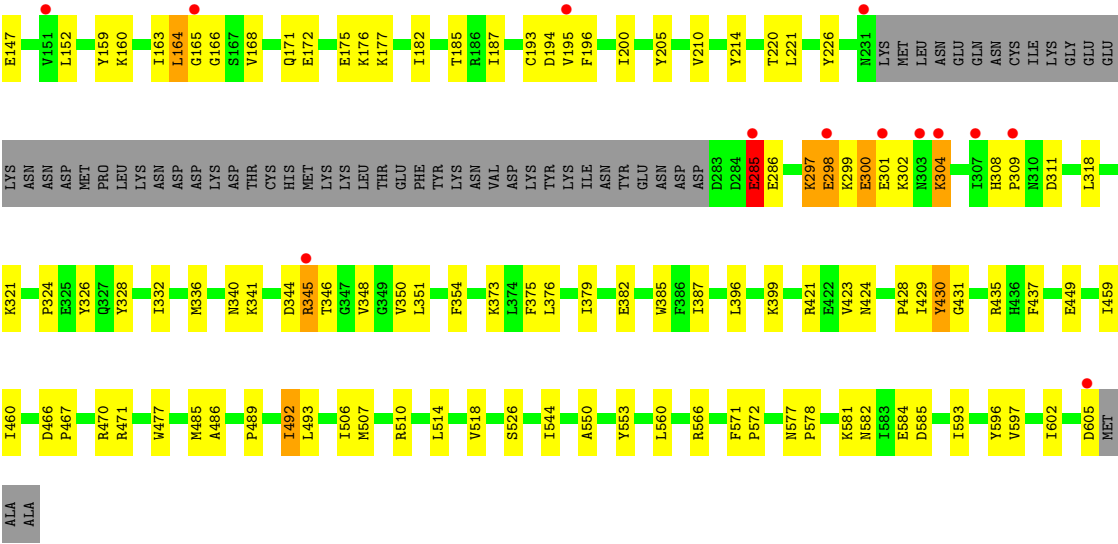
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Dihydrofolate reductase-thymidylate synthase



• Molecule 1: Dihydrofolate reductase-thymidylate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.99Å 157.38Å 165.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.50 – 2.70 29.50 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.50-2.70) 99.6 (29.50-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.69Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.206 , 0.233 0.206 , 0.234	Depositor DCC
R_{free} test set	2169 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9487	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: UMP, KA5, NDP

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	0.40	0/4644	0.93	16/6267 (0.3%)
1	B	0.41	0/4617	0.96	20/6233 (0.3%)
All	All	0.41	0/9261	0.95	36/12500 (0.3%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	GLU	N-CA-C	-11.47	96.76	112.94
1	A	27	LYS	N-CA-C	-9.57	101.80	113.19
1	B	117	LYS	CA-CB-CG	-8.23	97.64	114.10
1	B	118	PRO	CA-N-CD	-7.66	101.27	112.00
1	B	166	GLY	N-CA-C	-7.48	99.31	110.38
1	A	165	GLY	N-CA-C	6.80	124.88	112.37
1	B	118	PRO	N-CA-C	-6.58	98.92	112.47
1	B	117	LYS	C-N-CD	-6.42	98.69	125.00
1	B	351	LEU	N-CA-C	-6.41	98.46	108.90
1	A	129	ARG	N-CA-C	-6.23	103.59	112.13
1	B	526	SER	N-CA-C	-6.19	104.46	111.14
1	B	297	LYS	N-CA-C	6.04	118.30	108.63
1	A	166	GLY	N-CA-C	-5.94	93.07	111.07
1	B	30	GLU	N-CA-C	5.89	118.78	110.23
1	A	399	LYS	N-CA-C	-5.81	105.39	112.88
1	A	286	GLU	N-CA-C	-5.80	106.25	113.15
1	B	77	ARG	N-CA-C	5.80	117.47	111.03
1	B	164	LEU	N-CA-C	-5.70	105.59	112.54
1	B	492	ILE	N-CA-C	5.65	116.10	110.23
1	B	96	LYS	N-CA-C	-5.56	106.19	112.87
1	A	138	GLU	N-CA-C	5.42	117.86	110.55
1	B	93	PRO	CA-C-N	5.39	131.83	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	PRO	C-N-CA	5.39	131.83	121.54
1	B	486	ALA	N-CA-C	-5.38	104.86	111.75
1	A	351	LEU	N-CA-C	-5.33	100.48	109.07
1	B	138	GLU	N-CA-C	-5.33	105.52	112.23
1	B	285	GLU	N-CA-C	5.30	118.90	112.23
1	A	493	LEU	N-CA-C	5.21	115.41	108.38
1	A	212	ASP	N-CA-C	-5.20	103.62	110.33
1	B	3	GLU	N-CA-C	5.15	117.69	110.23
1	A	52	SER	N-CA-C	5.08	117.48	111.33
1	A	184	PHE	N-CA-C	5.08	116.79	108.52
1	B	399	LYS	N-CA-C	-5.07	106.34	112.88
1	A	486	ALA	N-CA-C	-5.04	105.23	111.33
1	A	557	ILE	N-CA-C	5.01	116.33	110.62
1	A	526	SER	N-CA-C	-5.00	105.54	111.69

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	4539	0	4501	150	0
1	B	4511	0	4467	144	0
2	A	25	0	18	1	0
2	B	25	0	18	1	0
3	A	48	0	26	2	0
3	B	48	0	26	4	0
4	A	20	0	11	0	0
4	B	20	0	11	1	0
5	A	124	0	0	6	0
5	B	127	0	0	4	0
All	All	9487	0	9078	287	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 16.

All (287) 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:117:LYS:HB3	1:B:118:PRO:HD2	1.21	1.16
1:B:376:LEU:HD22	1:B:379:ILE:HD11	1.36	1.08
1:A:1:MET:HG3	1:A:2:MET:H	1.18	1.06
1:B:346:THR:HG22	1:B:348:VAL:HG23	1.39	1.03
1:A:376:LEU:HD22	1:A:379:ILE:HD11	1.45	0.99
1:B:117:LYS:CB	1:B:118:PRO:HD2	1.95	0.91
1:A:127:LEU:HD23	1:A:143:ILE:HG13	1.55	0.88
1:B:104:MET:HB2	1:B:108:ASN:HD22	1.38	0.87
1:A:167:SER:HB2	1:A:195:VAL:CG1	2.05	0.87
1:A:8:VAL:HA	1:A:76:LYS:HD3	1.62	0.81
1:B:605:ASP:HB2	5:B:1221:HOH:O	1.80	0.80
1:A:346:THR:HG22	1:A:347:GLY:N	1.95	0.79
1:A:59:ARG:HG2	1:A:59:ARG:HH21	1.47	0.79
1:A:26:GLY:C	1:A:28:LYS:H	1.89	0.77
1:B:117:LYS:HB3	1:B:118:PRO:CD	2.11	0.75
1:B:300:GLU:HG3	1:B:301:GLU:H	1.51	0.75
1:B:136:PHE:CD2	1:B:142:ILE:HD11	2.22	0.74
1:B:97:LYS:NZ	1:B:97:LYS:HB3	2.03	0.73
1:A:1:MET:HG3	1:A:2:MET:N	1.97	0.73
1:A:13:ALA:HB2	1:A:179:ILE:HD12	1.72	0.71
1:A:23:LYS:O	1:A:24:ASN:HB3	1.91	0.70
1:A:307:ILE:HG21	1:A:312:PHE:HE2	1.58	0.69
1:A:375:PHE:HB3	5:A:1071:HOH:O	1.93	0.69
1:A:298:GLU:HG2	1:A:302:LYS:NZ	2.08	0.68
1:B:29:ASN:HD21	1:B:373:LYS:HZ1	1.42	0.68
1:A:41:GLY:HA2	1:A:47:PRO:HD3	1.77	0.67
1:A:298:GLU:HB3	1:A:302:LYS:HD2	1.76	0.67
1:B:318:LEU:HB2	1:B:321:LYS:HD2	1.76	0.67
1:B:29:ASN:HD21	1:B:373:LYS:NZ	1.93	0.66
1:B:376:LEU:CD2	1:B:379:ILE:HD11	2.22	0.66
1:B:514:LEU:HD21	1:B:550:ALA:HB1	1.77	0.66
1:A:421:ARG:HG2	1:A:421:ARG:HH11	1.61	0.66
1:B:4:GLN:HB2	1:B:7:ASP:OD2	1.94	0.66
1:B:336:MET:HE1	1:B:560:LEU:HB2	1.78	0.65
1:A:20:VAL:HG21	1:A:38:ARG:NH2	2.10	0.65
1:A:346:THR:HG21	1:A:348:VAL:HG23	1.78	0.64
1:B:117:LYS:CB	1:B:118:PRO:CD	2.73	0.64
1:A:376:LEU:HD22	1:A:379:ILE:CD1	2.26	0.64
1:A:26:GLY:C	1:A:28:LYS:N	2.50	0.63
1:B:493:LEU:HD12	1:B:493:LEU:C	2.24	0.63
1:A:124:ASN:N	1:A:124:ASN:HD22	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:TYR:HB2	1:A:564:LEU:O	1.99	0.62
1:B:346:THR:CG2	1:B:348:VAL:HG23	2.23	0.62
1:B:298:GLU:O	1:B:299:LYS:C	2.42	0.61
1:A:133:LYS:HG3	1:A:134:GLU:OE2	2.00	0.61
1:B:285:GLU:OE1	1:B:285:GLU:HA	2.00	0.61
1:A:299:LYS:H	1:A:299:LYS:HD3	1.65	0.61
1:B:104:MET:HE1	1:B:119:LEU:HD12	1.81	0.61
1:B:341:LYS:HG3	5:B:1107:HOH:O	1.99	0.61
1:B:324:PRO:HB2	1:B:571:PHE:HE2	1.66	0.61
1:B:58:PHE:HE1	1:B:164:LEU:HD22	1.67	0.60
1:A:442:THR:OG1	1:A:443:ASN:N	2.34	0.60
1:A:104:MET:HB2	1:A:108:ASN:HD22	1.67	0.59
1:B:131:LEU:HD22	1:B:136:PHE:HE2	1.67	0.59
1:B:297:LYS:O	1:B:299:LYS:N	2.36	0.59
1:B:32:PHE:CD1	1:B:597:VAL:HG13	2.38	0.59
1:A:12:TYR:HD1	1:A:181:LYS:HB2	1.68	0.58
1:A:289:ASP:HA	1:A:292:TYR:CD2	2.39	0.58
1:B:134:GLU:C	1:B:136:PHE:H	2.11	0.58
1:A:100:ASN:OD1	1:A:159:TYR:HB3	2.04	0.58
1:A:194:ASP:OD1	1:A:195:VAL:HG23	2.04	0.57
1:B:51:ILE:HD13	1:B:187:ILE:HD12	1.86	0.57
1:B:100:ASN:OD1	1:B:159:TYR:HB3	2.04	0.57
1:B:344:ASP:C	1:B:346:THR:H	2.13	0.57
1:A:572:PRO:HB3	1:A:596:TYR:HA	1.86	0.57
1:A:285:GLU:C	1:A:287:GLU:H	2.11	0.57
1:A:324:PRO:HB2	1:A:571:PHE:HE2	1.68	0.57
1:B:584:GLU:HG3	5:B:1136:HOH:O	2.05	0.57
1:B:97:LYS:HB3	1:B:97:LYS:HZ2	1.70	0.57
1:A:133:LYS:HB2	1:A:133:LYS:NZ	2.20	0.57
1:A:22:SER:HB3	5:A:1181:HOH:O	2.04	0.56
1:B:66:ASN:CG	1:B:69:LYS:HD3	2.30	0.56
1:B:376:LEU:HD12	1:B:593:ILE:HG13	1.86	0.56
1:B:506:ILE:HG12	1:B:544:ILE:HB	1.87	0.56
1:B:41:GLY:HA2	1:B:47:PRO:HD3	1.87	0.56
1:B:58:PHE:CE1	1:B:164:LEU:HD22	2.41	0.56
1:A:499:PHE:CE1	1:B:340:ASN:HB3	2.41	0.56
1:A:208:ILE:HD13	1:A:227:LYS:HD2	1.88	0.55
1:A:303:ASN:OD1	1:A:337:MET:HE3	2.06	0.55
1:B:75:TYR:O	1:B:79:LYS:HB2	2.05	0.55
1:A:165:GLY:HA3	1:A:170:TYR:CZ	2.42	0.55
1:A:289:ASP:HA	1:A:292:TYR:HD2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:HD13	1:B:560:LEU:HD22	1.88	0.54
1:A:459:ILE:O	1:A:463:ILE:HG13	2.08	0.54
1:B:131:LEU:HD22	1:B:136:PHE:CE2	2.42	0.54
1:B:134:GLU:O	1:B:136:PHE:N	2.41	0.54
1:B:459:ILE:HG13	1:B:460:ILE:N	2.21	0.54
1:A:40:LEU:O	3:A:610:NDP:H2N	2.09	0.53
1:A:298:GLU:HG2	1:A:302:LYS:HZ3	1.71	0.53
1:A:22:SER:O	1:A:23:LYS:C	2.50	0.53
1:A:59:ARG:HH21	1:A:59:ARG:CG	2.20	0.53
1:B:168:VAL:HG23	3:B:610:NDP:O2N	2.07	0.53
1:A:493:LEU:C	1:A:493:LEU:HD12	2.34	0.53
1:A:206:GLN:HG2	1:A:229:THR:CG2	2.39	0.53
1:A:283:ASP:CG	1:A:284:ASP:N	2.66	0.53
1:B:106:ARG:HG2	1:B:110:GLU:OE2	2.09	0.53
1:B:421:ARG:HH11	1:B:421:ARG:HG2	1.74	0.52
1:A:421:ARG:HD2	1:A:425:ASP:CG	2.33	0.52
1:A:319:LYS:HG2	1:B:286:GLU:HG2	1.91	0.52
1:A:332:ILE:CD1	1:A:514:LEU:HB3	2.40	0.52
1:B:55:MET:HE1	2:B:609:KA5:H8	1.90	0.52
1:B:78:CYS:C	1:B:80:TYR:H	2.16	0.52
1:B:423:VAL:O	1:B:424:ASN:HB2	2.09	0.52
1:A:492:ILE:HD11	1:A:510:ARG:HD3	1.90	0.52
1:A:582:ASN:HB2	1:A:585:ASP:OD2	2.10	0.52
1:A:346:THR:CG2	1:A:348:VAL:HG23	2.39	0.51
1:B:387:ILE:O	1:B:435:ARG:NH1	2.44	0.51
1:B:477:TRP:HE3	1:B:489:PRO:HG2	1.75	0.51
1:A:605:ASP:O	1:A:606:MET:HB3	2.11	0.51
1:B:109:TRP:CZ2	1:B:117:LYS:HD2	2.45	0.51
1:B:301:GLU:HA	1:B:301:GLU:OE1	2.11	0.51
1:B:108:ASN:O	1:B:112:ILE:HG13	2.10	0.51
1:A:421:ARG:HG2	1:A:421:ARG:NH1	2.24	0.51
1:A:116:PHE:HB3	2:A:609:KA5:H25B	1.93	0.51
1:A:214:TYR:O	1:A:220:THR:HA	2.11	0.51
1:B:12:TYR:O	1:B:163:ILE:HG12	2.11	0.51
1:B:145:LYS:HZ3	1:B:146:VAL:N	2.09	0.51
1:A:298:GLU:HG2	1:A:302:LYS:HZ2	1.74	0.51
1:B:308:HIS:HB2	1:B:311:ASP:OD2	2.11	0.51
1:B:132:LYS:HG3	1:B:135:ASP:OD2	2.11	0.51
1:B:302:LYS:NZ	1:B:302:LYS:HB2	2.26	0.51
1:B:578:PRO:O	1:B:581:LYS:HE3	2.12	0.51
1:A:23:LYS:O	1:A:24:ASN:CB	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ILE:HB	1:A:226:TYR:HB2	1.92	0.50
1:A:488:PRO:HG2	1:B:471:ARG:HD3	1.92	0.50
1:B:428:PRO:O	1:B:485:MET:HE2	2.11	0.50
1:A:133:LYS:HG2	5:A:1088:HOH:O	2.12	0.50
1:B:514:LEU:HD13	1:B:518:VAL:HG21	1.95	0.49
1:A:59:ARG:NH2	1:A:63:THR:HG21	2.27	0.49
1:A:382:GLU:O	1:A:385:TRP:HB3	2.11	0.49
1:B:582:ASN:HB2	1:B:585:ASP:OD2	2.13	0.49
1:B:33:ASN:OD1	1:B:35:TYR:HB3	2.13	0.49
1:A:124:ASN:HD22	1:A:124:ASN:H	1.61	0.49
1:A:144:ASN:H	1:A:144:ASN:HD22	1.59	0.49
1:A:346:THR:HG22	1:A:347:GLY:H	1.77	0.49
1:B:132:LYS:HE2	1:B:134:GLU:OE2	2.13	0.49
1:A:78:CYS:HB3	1:A:83:LYS:O	2.11	0.49
1:B:336:MET:CE	1:B:560:LEU:HB2	2.43	0.49
1:A:106:ARG:HE	3:A:610:NDP:P2B	2.36	0.48
1:B:25:GLU:HA	1:B:25:GLU:OE1	2.12	0.48
1:B:344:ASP:O	1:B:346:THR:N	2.46	0.48
1:A:16:ALA:HA	1:A:185:THR:HB	1.96	0.48
1:B:136:PHE:HD2	1:B:142:ILE:HD11	1.72	0.48
1:A:292:TYR:O	1:A:295:PHE:HB3	2.13	0.48
1:B:72:LYS:NZ	1:B:72:LYS:HB3	2.28	0.48
1:B:214:TYR:O	1:B:220:THR:HA	2.14	0.48
1:A:212:ASP:OD1	1:A:213:VAL:N	2.47	0.47
1:B:145:LYS:HA	3:B:610:NDP:N1A	2.29	0.47
1:A:387:ILE:O	1:A:435:ARG:NH1	2.47	0.47
1:A:459:ILE:HG13	1:A:460:ILE:N	2.29	0.47
1:A:506:ILE:HG12	1:A:544:ILE:HB	1.95	0.47
1:B:42:ASN:O	1:B:45:VAL:HG23	2.14	0.47
1:B:106:ARG:HE	3:B:610:NDP:P2B	2.37	0.47
1:B:297:LYS:C	1:B:299:LYS:H	2.22	0.47
1:A:58:PHE:HE1	1:A:164:LEU:HD22	1.79	0.47
1:A:144:ASN:ND2	1:A:145:LYS:HG3	2.30	0.47
1:A:210:VAL:HG21	1:A:326:TYR:HE2	1.80	0.47
1:A:481:ASP:O	1:A:482:LEU:C	2.58	0.47
1:B:12:TYR:HE2	1:B:160:LYS:HD3	1.80	0.47
1:B:117:LYS:O	1:B:118:PRO:C	2.58	0.47
1:A:307:ILE:CG2	1:A:312:PHE:HE2	2.27	0.47
1:A:605:ASP:O	1:A:606:MET:CB	2.63	0.47
1:B:43:LYS:O	1:B:45:VAL:HG22	2.15	0.47
1:B:145:LYS:NZ	1:B:145:LYS:HB3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:VAL:HG11	1:A:583:ILE:N	2.30	0.46
1:B:373:LYS:HE2	1:B:375:PHE:CE1	2.49	0.46
1:B:300:GLU:HG3	1:B:301:GLU:N	2.25	0.46
1:A:3:GLU:H	1:A:3:GLU:HG3	1.58	0.46
1:A:483:ASP:HB2	5:A:1246:HOH:O	2.16	0.46
1:B:350:VAL:HG12	1:B:553:TYR:CD1	2.50	0.46
5:A:1142:HOH:O	1:B:470:ARG:HD3	2.16	0.46
1:A:163:ILE:C	1:A:165:GLY:H	2.23	0.46
1:A:201:ASN:OD1	1:A:203:ASN:HB2	2.16	0.46
1:B:566:ARG:NH1	1:B:602:ILE:HD11	2.30	0.46
1:A:345:ARG:HG2	1:A:345:ARG:HH11	1.81	0.46
1:A:12:TYR:CD1	1:A:181:LYS:HB2	2.50	0.45
1:A:376:LEU:O	1:A:380:ILE:HG13	2.16	0.45
1:B:182:ILE:HB	1:B:226:TYR:HB2	1.98	0.45
1:A:159:TYR:CD2	1:A:160:LYS:HG3	2.52	0.45
1:B:300:GLU:CG	1:B:301:GLU:H	2.17	0.45
1:A:35:TYR:O	1:A:38:ARG:NH1	2.49	0.45
1:A:285:GLU:C	1:A:287:GLU:N	2.75	0.45
1:A:175:GLU:C	1:A:177:LYS:H	2.25	0.45
1:B:127:LEU:HD11	1:B:143:ILE:HD11	1.97	0.45
1:A:167:SER:HB2	1:A:195:VAL:HG13	1.93	0.45
1:A:350:VAL:HG12	1:A:553:TYR:CD1	2.51	0.45
1:A:57:TYR:O	1:A:61:VAL:HG23	2.17	0.45
1:B:345:ARG:HG2	1:B:345:ARG:HH11	1.81	0.45
1:A:376:LEU:HD12	1:A:593:ILE:HG13	1.99	0.45
1:A:35:TYR:CE1	1:A:199:GLU:HB2	2.51	0.44
1:A:300:GLU:O	1:A:301:GLU:HB3	2.17	0.44
1:B:134:GLU:C	1:B:136:PHE:N	2.75	0.44
1:B:304:LYS:H	1:B:304:LYS:HD2	1.83	0.44
1:B:421:ARG:HG2	1:B:421:ARG:NH1	2.32	0.44
1:A:58:PHE:HZ	1:A:164:LEU:HD13	1.82	0.44
1:A:506:ILE:HG13	1:B:354:PHE:CE2	2.51	0.44
1:A:104:MET:HB2	1:A:108:ASN:ND2	2.32	0.44
1:A:124:ASN:N	1:A:124:ASN:ND2	2.65	0.44
1:B:65:VAL:HA	1:B:159:TYR:CD2	2.51	0.44
1:A:63:THR:HG22	1:A:122:ARG:CD	2.48	0.44
1:A:516:LEU:CD2	1:A:604:MET:HG3	2.47	0.44
1:B:106:ARG:HD3	1:B:128:SER:OG	2.18	0.44
1:B:145:LYS:NZ	1:B:147:GLU:OE1	2.51	0.44
1:B:382:GLU:O	1:B:385:TRP:HB3	2.18	0.44
1:A:63:THR:HG22	1:A:122:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:VAL:O	1:A:424:ASN:HB2	2.18	0.43
1:A:29:ASN:ND2	1:A:373:LYS:NZ	2.67	0.43
1:B:430:TYR:O	1:B:431:GLY:C	2.62	0.43
1:B:321:LYS:HB3	1:B:326:TYR:CD2	2.52	0.43
1:B:324:PRO:HB2	1:B:571:PHE:CE2	2.49	0.43
1:B:328:TYR:CZ	1:B:332:ILE:HD11	2.53	0.43
1:A:133:LYS:HG3	1:A:134:GLU:CD	2.43	0.43
1:A:210:VAL:O	1:A:210:VAL:HG23	2.18	0.43
1:A:554:ASN:C	1:A:556:HIS:H	2.27	0.43
1:A:147:GLU:H	1:A:147:GLU:CD	2.26	0.43
1:A:479:VAL:HB	1:B:437:PHE:CD1	2.53	0.43
1:A:32:PHE:CD1	1:A:597:VAL:HG13	2.54	0.43
1:A:171:GLN:HG2	1:A:175:GLU:OE2	2.19	0.43
1:A:299:LYS:HE2	1:A:302:LYS:HB2	1.99	0.43
1:A:359:LYS:HG2	1:A:544:ILE:HG12	2.01	0.43
1:B:492:ILE:HD11	1:B:510:ARG:HD3	2.00	0.43
1:A:75:TYR:CZ	1:A:79:LYS:HD2	2.53	0.43
1:A:144:ASN:HD22	1:A:144:ASN:N	2.16	0.43
1:A:284:ASP:O	1:A:285:GLU:HG3	2.19	0.42
1:B:210:VAL:HG21	1:B:326:TYR:HE2	1.84	0.42
1:B:171:GLN:O	1:B:175:GLU:HG3	2.19	0.42
1:A:284:ASP:HA	1:A:287:GLU:HG3	2.00	0.42
1:A:23:LYS:NZ	1:A:23:LYS:HB3	2.34	0.42
1:A:163:ILE:C	1:A:165:GLY:N	2.77	0.42
1:B:40:LEU:O	3:B:610:NDP:H2N	2.19	0.42
1:B:42:ASN:HA	1:B:194:ASP:OD2	2.19	0.42
1:B:566:ARG:CZ	1:B:602:ILE:HD11	2.50	0.42
1:A:319:LYS:HG3	1:A:320:TYR:CD2	2.54	0.42
1:B:95:SER:C	1:B:97:LYS:N	2.77	0.42
1:A:51:ILE:HA	1:A:217:ASN:OD1	2.20	0.42
1:A:288:ASP:OD1	1:B:69:LYS:NZ	2.52	0.42
1:B:429:ILE:O	1:B:430:TYR:C	2.62	0.42
1:A:42:ASN:HB2	1:A:193:CYS:HA	2.01	0.42
1:A:59:ARG:HG2	1:A:59:ARG:NH2	2.24	0.42
1:A:167:SER:CB	1:A:195:VAL:CG1	2.90	0.42
1:A:437:PHE:CD1	1:A:437:PHE:C	2.98	0.42
1:B:104:MET:HE1	1:B:119:LEU:CD1	2.47	0.42
1:B:466:ASP:N	1:B:467:PRO:CD	2.82	0.42
1:A:81:LEU:HB2	1:A:83:LYS:HG2	2.01	0.42
1:A:144:ASN:H	1:A:144:ASN:ND2	2.18	0.42
1:A:144:ASN:HD22	1:A:144:ASN:C	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:TRP:CE3	1:B:396:LEU:HD11	2.55	0.42
1:A:514:LEU:HD21	1:A:550:ALA:HB1	2.02	0.42
1:A:557:ILE:O	1:A:561:LYS:HG3	2.20	0.41
1:B:143:ILE:HD12	1:B:145:LYS:O	2.19	0.41
1:B:152:LEU:HD12	1:B:152:LEU:O	2.20	0.41
1:B:345:ARG:HH21	4:B:611:UMP:P	2.43	0.41
1:A:493:LEU:CD2	1:B:492:ILE:HG21	2.49	0.41
1:B:42:ASN:HB2	1:B:193:CYS:HA	2.03	0.41
1:B:23:LYS:C	1:B:25:GLU:H	2.27	0.41
1:B:572:PRO:HB3	1:B:596:TYR:HA	2.01	0.41
1:A:567:ILE:HA	1:A:568:PRO:HD3	1.91	0.41
1:B:97:LYS:HB3	1:B:97:LYS:HZ3	1.80	0.41
1:B:168:VAL:O	1:B:172:GLU:HG2	2.20	0.41
1:B:113:PRO:HB2	1:B:116:PHE:CD2	2.55	0.41
1:B:70:TYR:HB2	1:B:98:LEU:CD2	2.49	0.41
1:B:132:LYS:HB2	1:B:134:GLU:CD	2.45	0.41
1:B:200:ILE:CG2	1:B:205:TYR:HB2	2.51	0.41
1:A:332:ILE:HD13	1:A:514:LEU:HB3	2.03	0.41
1:A:336:MET:HE1	1:A:560:LEU:HB2	2.03	0.41
1:A:553:TYR:O	1:A:556:HIS:HB2	2.21	0.41
1:B:102:VAL:HG23	1:B:102:VAL:O	2.20	0.41
1:B:194:ASP:OD1	1:B:195:VAL:HG22	2.20	0.41
1:B:493:LEU:O	1:B:507:MET:HA	2.21	0.41
1:A:375:PHE:N	1:A:375:PHE:CD1	2.88	0.40
1:A:491:HIS:HD2	1:A:509:GLN:HG3	1.86	0.40
1:A:600:GLU:HB2	5:A:1092:HOH:O	2.21	0.40
1:A:444:MET:HE3	1:A:445:TYR:CZ	2.55	0.40
1:B:16:ALA:HA	1:B:185:THR:HB	2.03	0.40
1:B:78:CYS:C	1:B:80:TYR:N	2.74	0.40
1:B:94:ASN:OD1	1:B:94:ASN:O	2.39	0.40
1:B:176:LYS:O	1:B:177:LYS:C	2.65	0.40
1:A:494:CYS:HA	1:A:506:ILE:O	2.21	0.40
1:B:221:LEU:HD23	1:B:221:LEU:N	2.36	0.40
1:B:300:GLU:CG	1:B:301:GLU:N	2.83	0.40
1:B:577:ASN:HA	1:B:578:PRO:HD2	1.96	0.40
1:B:297:LYS:HD3	1:B:297:LYS:HA	1.73	0.40
1:B:449:GLU:HG3	5:B:1169:HOH:O	2.20	0.40
1:A:41:GLY:HA2	1:A:47:PRO:CD	2.50	0.40
1:A:109:TRP:CE3	1:A:126:ILE:HD11	2.56	0.40
1:A:167:SER:HB2	1:A:195:VAL:HG11	1.95	0.40
1:B:27:LYS:HD3	1:B:27:LYS:HA	1.80	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	539/608 (89%)	486 (90%)	45 (8%)	8 (2%)	8	22
1	B	536/608 (88%)	475 (89%)	46 (9%)	15 (3%)	4	9
All	All	1075/1216 (88%)	961 (89%)	91 (8%)	23 (2%)	5	15

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	B	118	PRO
1	B	135	ASP
1	B	298	GLU
1	B	345	ARG
1	A	285	GLU
1	A	304	LYS
1	A	430	TYR
1	B	24	ASN
1	B	94	ASN
1	B	95	SER
1	B	300	GLU
1	B	430	TYR
1	B	119	LEU
1	B	140	VAL
1	A	310	ASN
1	B	165	GLY
1	B	146	VAL
1	A	345	ARG
1	A	309	PRO
1	B	123	ILE
1	A	347	GLY

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Mol	Chain	Res	Type
1	B	309	PRO

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	510/570 (90%)	496 (97%)	14 (3%)	39	69
1	B	507/570 (89%)	495 (98%)	12 (2%)	43	72
All	All	1017/1140 (89%)	991 (97%)	26 (3%)	40	70

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	22	SER
1	A	23	LYS
1	A	27	LYS
1	A	59	ARG
1	A	84	GLU
1	A	124	ASN
1	A	133	LYS
1	A	144	ASN
1	A	283	ASP
1	A	288	ASP
1	A	298	GLU
1	A	303	ASN
1	A	304	LYS
1	B	5	VAL
1	B	25	GLU
1	B	45	VAL
1	B	49	LYS
1	B	81	LEU
1	B	93	PRO
1	B	95	SER
1	B	132	LYS

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Mol	Chain	Res	Type
1	B	145	LYS
1	B	196	PHE
1	B	285	GLU
1	B	304	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	42	ASN
1	A	99	GLN
1	A	108	ASN
1	A	121	ASN
1	A	144	ASN
1	A	171	GLN
1	A	296	ASN
1	A	303	ASN
1	A	310	ASN
1	A	338	ASN
1	A	394	ASN
1	A	415	ASN
1	A	424	ASN
1	A	491	HIS
1	A	554	ASN
1	B	29	ASN
1	B	99	GLN
1	B	108	ASN
1	B	121	ASN
1	B	206	GLN
1	B	217	ASN
1	B	310	ASN
1	B	338	ASN
1	B	340	ASN
1	B	394	ASN
1	B	407	ASN
1	B	424	ASN
1	B	465	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	KA5	A	609	-	27,27,27	1.45	4 (14%)	35,38,38	2.01	8 (22%)
4	UMP	A	611	-	21,21,21	2.02	7 (33%)	30,31,31	2.00	9 (30%)
3	NDP	A	610	-	51,52,52	1.62	9 (17%)	71,80,80	1.61	15 (21%)
4	UMP	B	611	-	21,21,21	2.05	8 (38%)	30,31,31	2.07	9 (30%)
2	KA5	B	609	-	27,27,27	1.53	4 (14%)	35,38,38	1.93	8 (22%)
3	NDP	B	610	-	51,52,52	1.65	11 (21%)	71,80,80	1.57	12 (16%)

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	KA5	A	609	-	-	2/9/9/9	0/3/3/3
4	UMP	A	611	-	-	0/10/22/22	0/2/2/2
3	NDP	A	610	-	-	3/34/77/77	0/5/5/5
4	UMP	B	611	-	-	1/10/22/22	0/2/2/2
2	KA5	B	609	-	-	4/9/9/9	0/3/3/3
3	NDP	B	610	-	-	3/34/77/77	0/5/5/5

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	609	KA5	C6-N1	-5.06	1.29	1.37
2	A	609	KA5	C6-N1	-4.75	1.30	1.37
3	B	610	NDP	C4N-C3N	-4.55	1.41	1.50
4	A	611	UMP	O4'-C1'	4.35	1.52	1.42
4	B	611	UMP	O4'-C1'	4.32	1.52	1.42
3	A	610	NDP	C4N-C3N	-4.25	1.42	1.50
3	B	610	NDP	C2N-C3N	4.20	1.46	1.35
3	B	610	NDP	C4N-C5N	-4.11	1.38	1.49
4	B	611	UMP	C2-N1	4.02	1.44	1.38
3	A	610	NDP	C4N-C5N	-4.01	1.38	1.49
4	A	611	UMP	C2-N1	3.92	1.44	1.38
3	A	610	NDP	C2N-C3N	3.91	1.45	1.35
2	A	609	KA5	C2-N3	-3.57	1.29	1.35
2	B	609	KA5	C2-N3	-3.47	1.29	1.35
2	B	609	KA5	C7-C6	-2.92	1.37	1.41
3	A	610	NDP	PA-O3	-2.88	1.56	1.59
3	B	610	NDP	P2B-O2B	-2.87	1.54	1.59
3	A	610	NDP	P2B-O2B	-2.85	1.54	1.59
4	B	611	UMP	C4-N3	2.83	1.43	1.38
3	B	610	NDP	C4A-N3A	2.82	1.39	1.34
3	B	610	NDP	C8A-N9A	2.79	1.42	1.37
3	A	610	NDP	C4A-N3A	2.72	1.39	1.34
4	B	611	UMP	P-OP3	-2.72	1.44	1.54
4	A	611	UMP	P-OP2	-2.70	1.44	1.54
3	A	610	NDP	C8A-N9A	2.70	1.42	1.37
4	B	611	UMP	C6-C5	2.62	1.41	1.35
4	A	611	UMP	P-OP3	-2.61	1.45	1.54
2	A	609	KA5	C7-C6	-2.58	1.37	1.41
4	A	611	UMP	C6-C5	2.55	1.41	1.35
4	A	611	UMP	O4'-C4'	2.54	1.50	1.45
3	B	610	NDP	C3B-C2B	-2.52	1.47	1.53
4	B	611	UMP	C2-N3	2.30	1.42	1.38
4	B	611	UMP	O4'-C4'	2.29	1.50	1.45
2	A	609	KA5	C4-N3	-2.22	1.29	1.33
3	B	610	NDP	C6N-N1N	2.21	1.42	1.37
4	A	611	UMP	C4-N3	2.20	1.42	1.38
4	B	611	UMP	P-OP2	-2.19	1.46	1.54
3	A	610	NDP	C3B-C2B	-2.17	1.48	1.53
3	A	610	NDP	C6N-C5N	2.10	1.39	1.33
3	B	610	NDP	C6N-C5N	2.08	1.39	1.33
2	B	609	KA5	C4-N3	-2.08	1.30	1.33
3	B	610	NDP	C5D-C4D	2.04	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	610	NDP	C2D-C1D	2.03	1.59	1.53

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	611	UMP	O4'-C1'-N1	5.69	117.96	107.86
4	B	611	UMP	O4'-C1'-N1	5.37	117.39	107.86
2	A	609	KA5	O22-C21-C16	5.01	123.42	115.96
2	A	609	KA5	N1-C2-N3	-4.98	120.87	127.21
2	B	609	KA5	N1-C2-N3	-4.91	120.97	127.21
3	B	610	NDP	C3N-C2N-N1N	-4.33	116.85	123.20
3	B	610	NDP	O4B-C1B-N9A	4.22	116.19	108.09
3	A	610	NDP	C1D-N1N-C2N	-4.20	114.21	121.14
4	B	611	UMP	C1'-N1-C6	-4.16	113.36	121.53
3	A	610	NDP	C3N-C2N-N1N	-4.12	117.16	123.20
3	A	610	NDP	C3B-C2B-C1B	-4.07	95.01	102.81
4	A	611	UMP	C1'-N1-C6	-3.92	113.83	121.53
2	B	609	KA5	C4-C5-C6	-3.78	112.24	114.90
2	B	609	KA5	O22-C21-C16	3.76	121.55	115.96
4	B	611	UMP	O4'-C1'-C2'	-3.71	99.32	106.25
3	B	610	NDP	C1D-N1N-C2N	-3.71	115.03	121.14
3	A	610	NDP	O4B-C1B-N9A	3.62	115.04	108.09
2	A	609	KA5	C4-C5-C6	-3.58	112.38	114.90
4	A	611	UMP	O4'-C1'-C2'	-3.51	99.68	106.25
2	B	609	KA5	C19-C18-C17	-3.39	115.94	120.50
2	A	609	KA5	C19-C18-C17	-3.35	116.00	120.50
4	B	611	UMP	C2'-C1'-N1	3.28	122.01	113.81
3	B	610	NDP	C3B-C2B-C1B	-3.21	96.65	102.81
3	A	610	NDP	O7N-C7N-N7N	-3.04	116.07	122.89
2	A	609	KA5	C9-C10-CL13	-3.01	115.73	119.44
4	B	611	UMP	C1'-N1-C2	2.99	123.51	117.66
3	B	610	NDP	O3B-C3B-C4B	2.97	119.63	111.08
4	A	611	UMP	C2'-C1'-N1	2.97	121.23	113.81
3	B	610	NDP	O7N-C7N-N7N	-2.96	116.25	122.89
3	A	610	NDP	C3D-C2D-C1D	-2.86	96.06	101.46
2	A	609	KA5	O22-C21-C20	-2.82	119.55	124.30
4	B	611	UMP	O4'-C4'-C3'	-2.81	99.24	105.65
3	A	610	NDP	C2B-C1B-N9A	2.79	118.34	113.75
2	B	609	KA5	C18-C17-C16	2.76	124.20	120.46
4	A	611	UMP	O4'-C4'-C3'	-2.74	99.40	105.65
2	B	609	KA5	C8-C9-N14	-2.73	117.24	121.75
4	A	611	UMP	C1'-N1-C2	2.64	122.83	117.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	609	KA5	C18-C17-C16	2.64	124.03	120.46
3	B	610	NDP	O3B-C3B-C2B	2.56	118.35	111.19
3	A	610	NDP	C6N-N1N-C2N	2.55	122.05	119.32
4	B	611	UMP	C4'-O4'-C1'	2.53	115.52	109.51
4	B	611	UMP	O2-C2-N1	2.48	126.03	122.80
3	A	610	NDP	O3B-C3B-C2B	2.45	118.04	111.19
4	A	611	UMP	O2-C2-N1	2.43	125.96	122.80
3	B	610	NDP	C6N-N1N-C2N	2.40	121.88	119.32
3	B	610	NDP	N3A-C2A-N1A	-2.39	124.96	128.58
3	A	610	NDP	C2D-C3D-C4D	2.35	107.15	102.61
4	A	611	UMP	C4'-O4'-C1'	2.30	114.98	109.51
3	A	610	NDP	O3B-C3B-C4B	2.30	117.68	111.08
4	B	611	UMP	O4-C4-N3	2.30	122.61	119.27
3	A	610	NDP	C4B-O4B-C1B	-2.20	104.62	109.47
3	A	610	NDP	N3A-C2A-N1A	-2.19	125.27	128.58
4	A	611	UMP	O5'-P-OP1	2.16	112.28	106.44
3	B	610	NDP	C4B-O4B-C1B	-2.16	104.70	109.47
3	B	610	NDP	O2A-PA-O1A	2.15	122.46	112.44
3	A	610	NDP	O2N-PN-O1N	2.12	122.32	112.44
2	A	609	KA5	C25-O24-C18	2.12	122.04	117.50
3	A	610	NDP	O2A-PA-O1A	2.10	122.20	112.44
2	B	609	KA5	C7-C6-N1	-2.03	115.73	118.69
2	B	609	KA5	C25-O24-C18	2.03	121.84	117.50
3	B	610	NDP	N9A-C8A-N7A	-2.00	111.09	113.94

There are no chirality outliers.

All (13) torsion outliers are listed below:

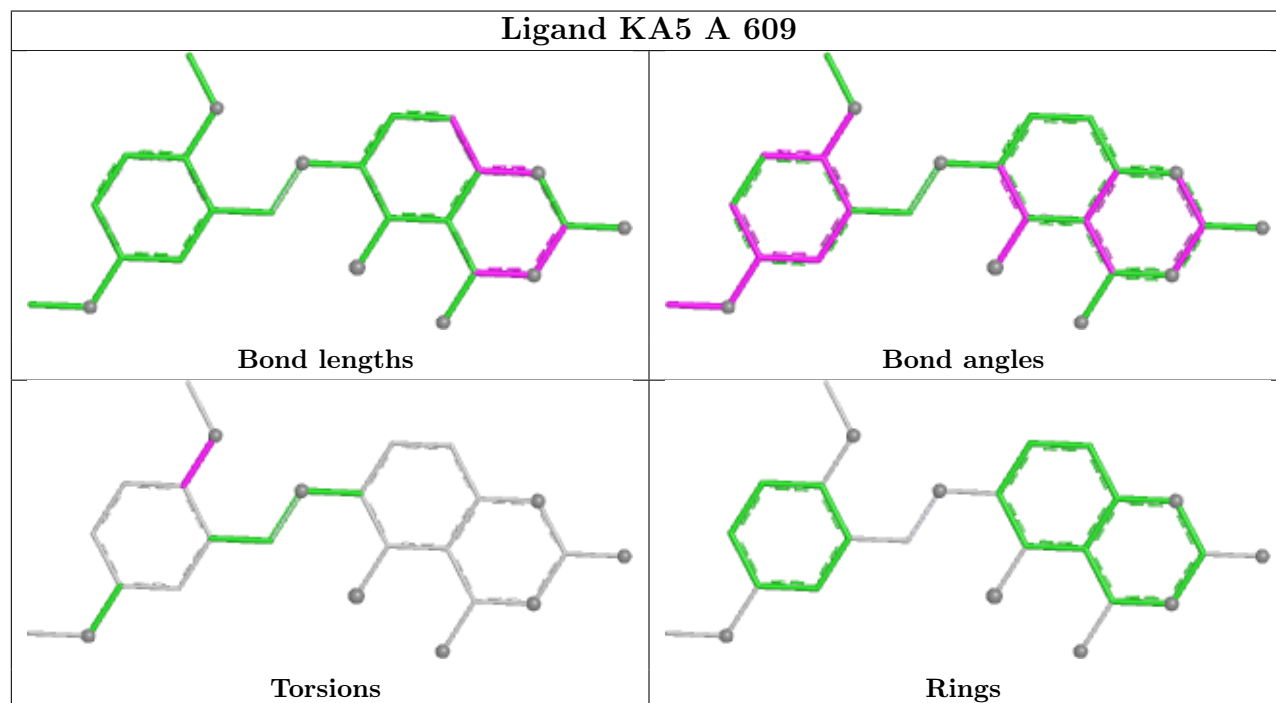
Mol	Chain	Res	Type	Atoms
2	B	609	KA5	C8-C9-N14-C15
2	A	609	KA5	C16-C21-O22-C23
2	B	609	KA5	C10-C9-N14-C15
2	B	609	KA5	C20-C21-O22-C23
2	A	609	KA5	C20-C21-O22-C23
2	B	609	KA5	C16-C21-O22-C23
3	A	610	NDP	O4D-C1D-N1N-C2N
3	B	610	NDP	O4D-C1D-N1N-C2N
3	A	610	NDP	C2N-C3N-C7N-N7N
3	B	610	NDP	C2N-C3N-C7N-N7N
3	B	610	NDP	C2B-O2B-P2B-O1X
4	B	611	UMP	C3'-C4'-C5'-O5'
3	A	610	NDP	C2B-O2B-P2B-O3X

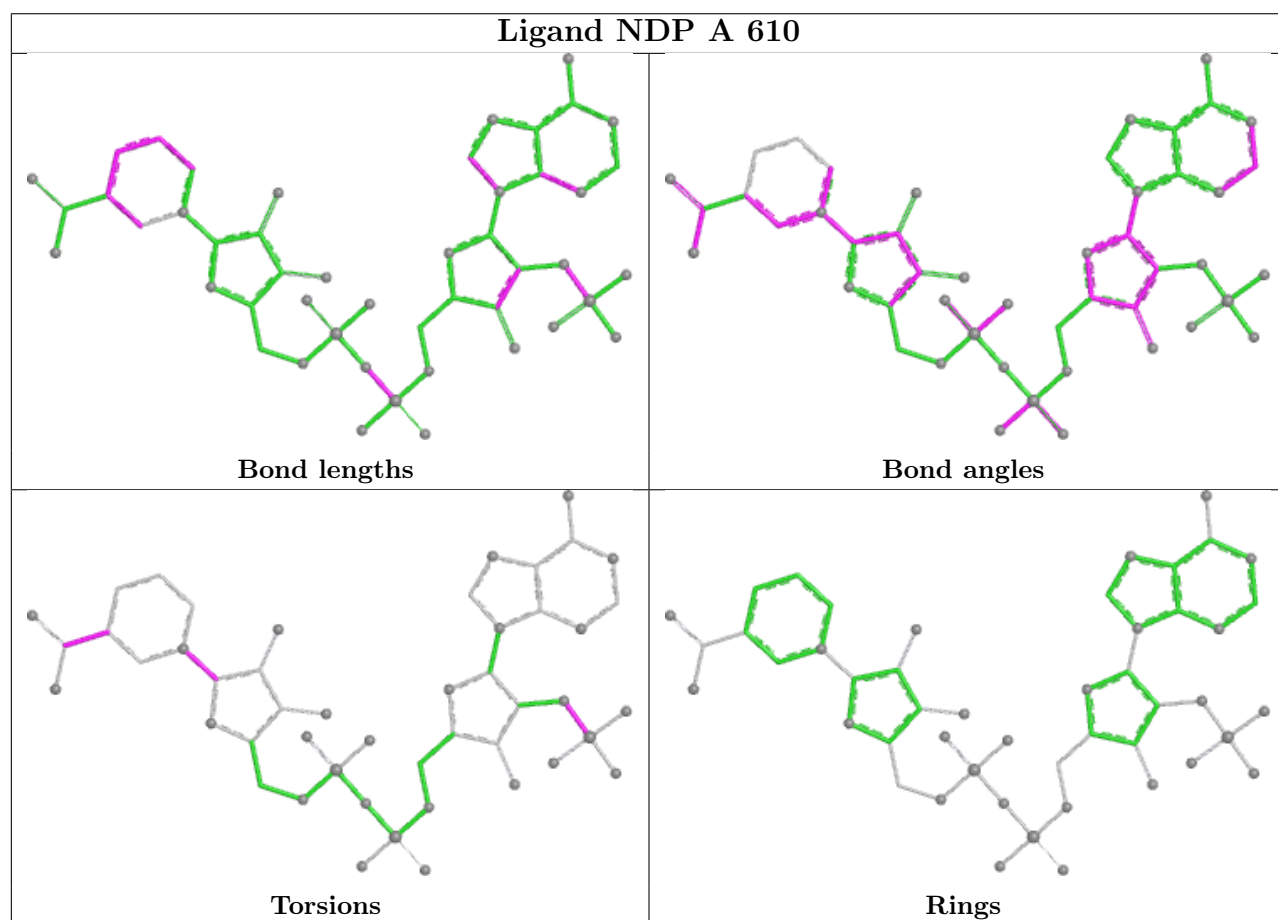
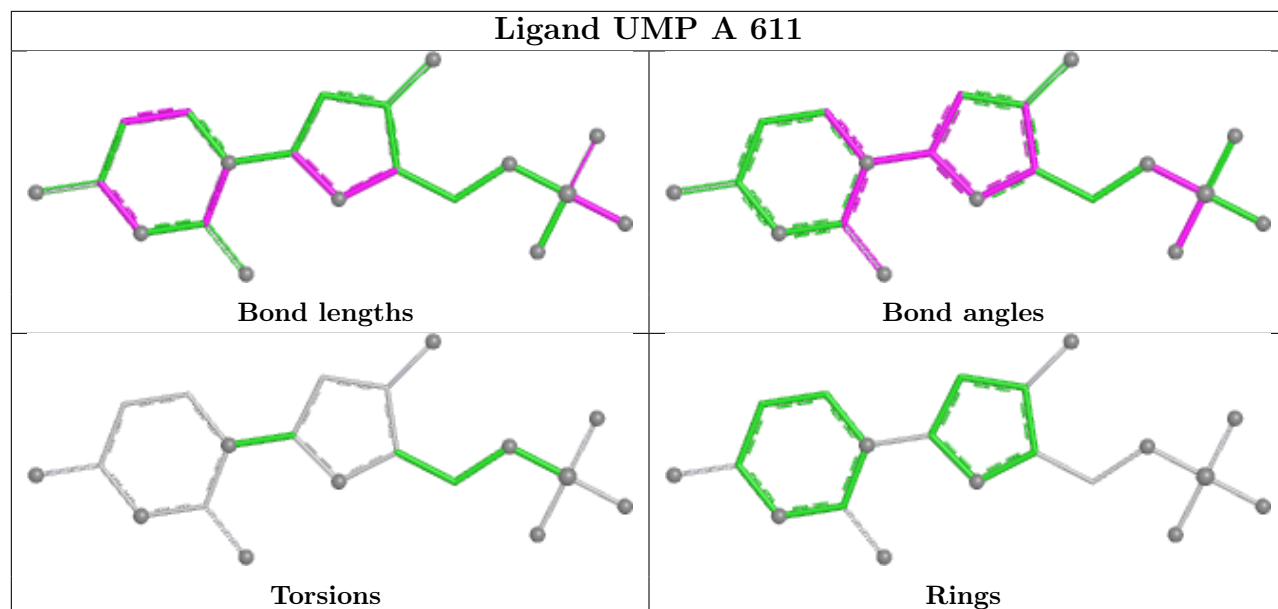
There are no ring outliers.

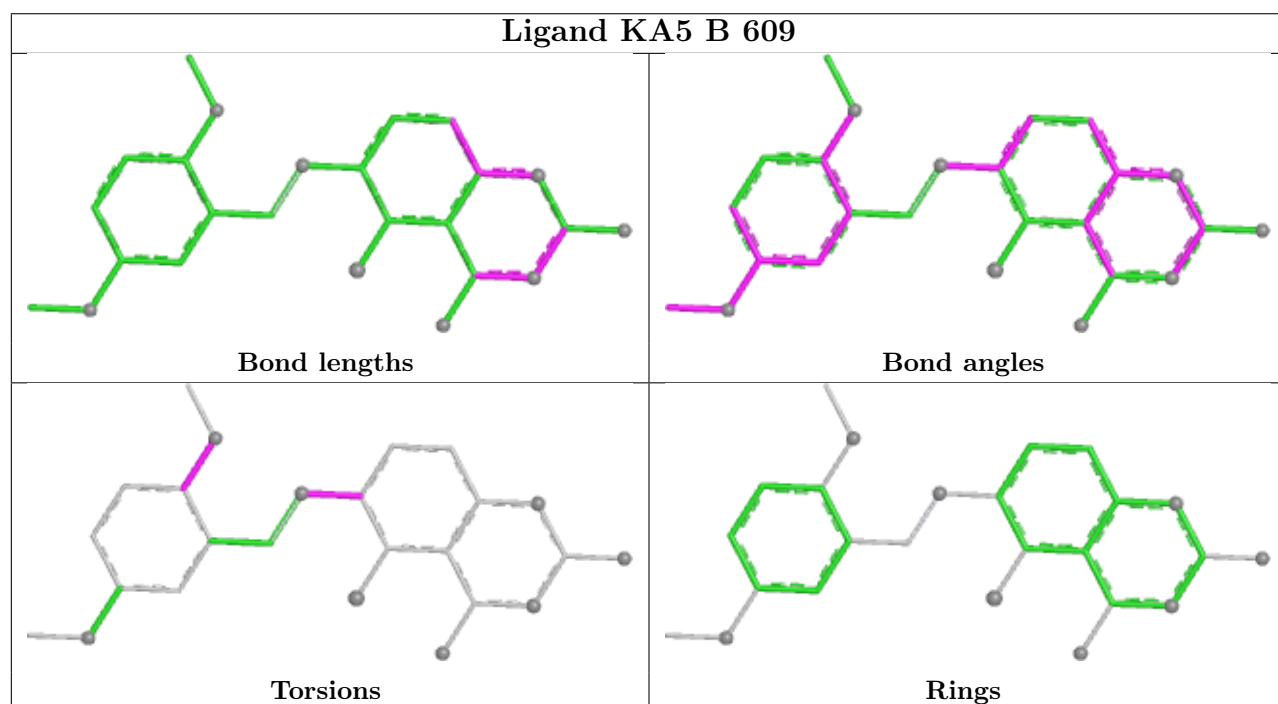
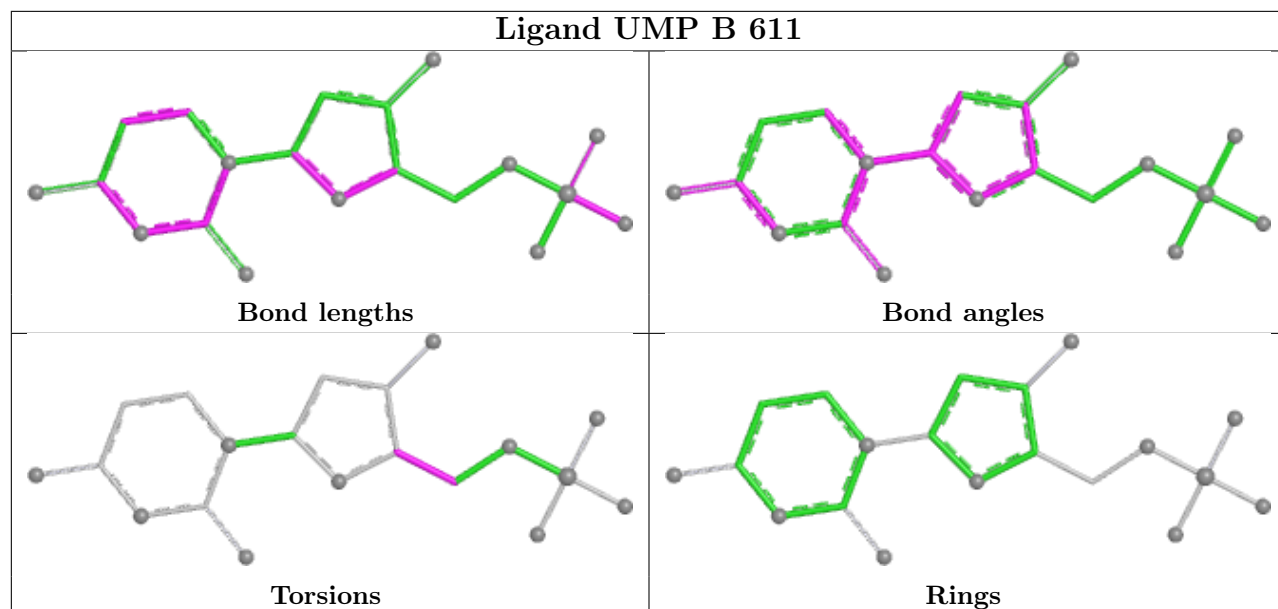
5 monomers are involved in 9 short contacts:

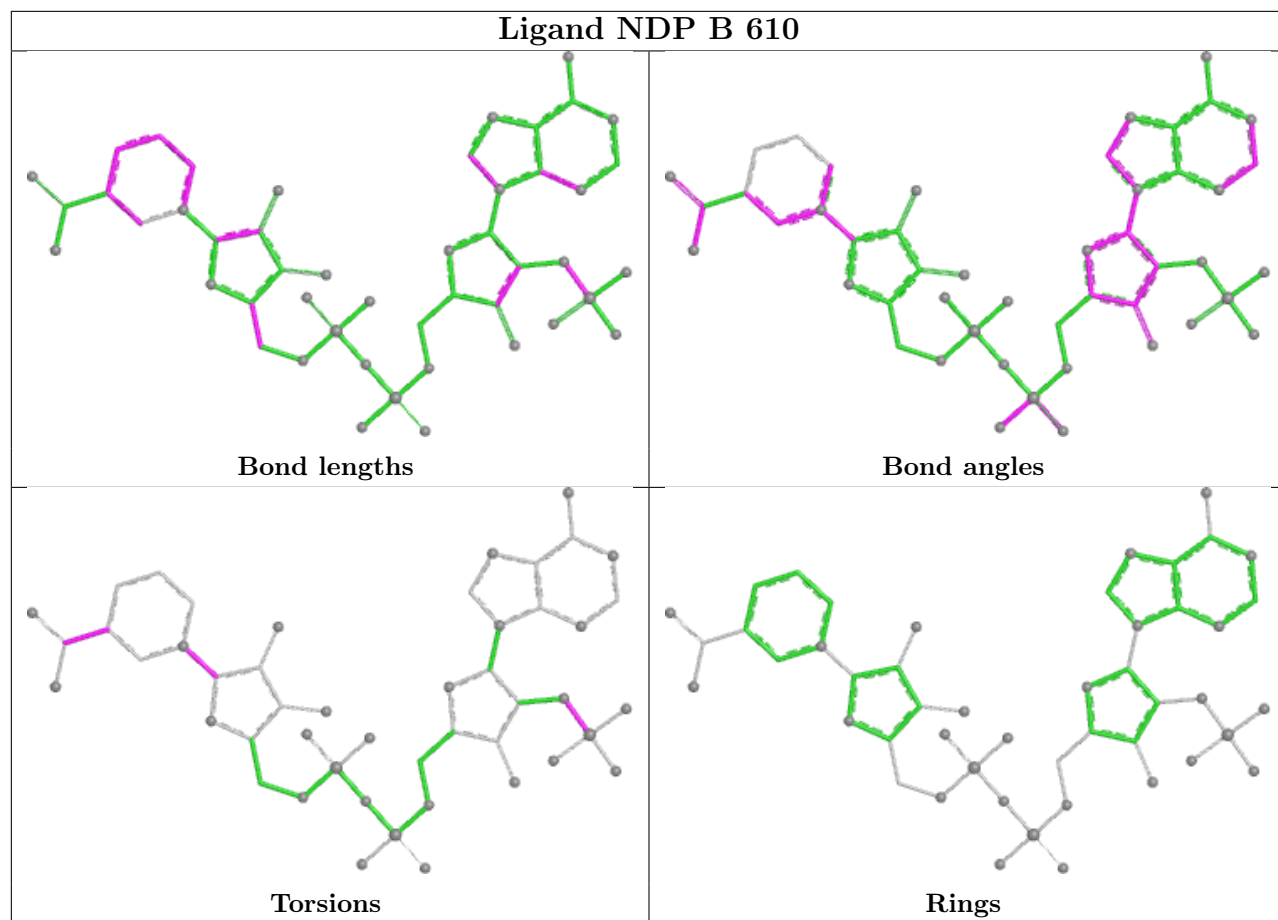
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	609	KA5	1	0
3	A	610	NDP	2	0
4	B	611	UMP	1	0
2	B	609	KA5	1	0
3	B	610	NDP	4	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	545/608 (89%)	-0.12	24 (4%)	39 35	22, 40, 89, 91	0
1	B	542/608 (89%)	0.15	35 (6%)	25 22	22, 44, 90, 91	0
All	All	1087/1216 (89%)	0.02	59 (5%)	31 27	22, 41, 90, 91	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	ILE	4.6
1	B	81	LEU	4.2
1	B	165	GLY	4.1
1	A	605	ASP	4.1
1	B	25	GLU	4.0
1	A	2	MET	3.8
1	A	85	THR	3.6
1	B	93	PRO	3.4
1	B	303	ASN	3.3
1	B	307	ILE	3.3
1	A	27	LYS	3.3
1	B	298	GLU	3.1
1	A	286	GLU	3.0
1	B	605	ASP	3.0
1	B	24	ASN	3.0
1	A	606	MET	2.9
1	B	23	LYS	2.9
1	B	125	VAL	2.9
1	A	26	GLY	2.8
1	B	3	GLU	2.7
1	A	304	LYS	2.7
1	B	304	LYS	2.7
1	A	25	GLU	2.6
1	A	346	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	103	VAL	2.6
1	B	118	PRO	2.6
1	B	29	ASN	2.6
1	B	301	GLU	2.5
1	B	75	TYR	2.5
1	B	140	VAL	2.4
1	B	28	LYS	2.4
1	A	231	ASN	2.3
1	B	309	PRO	2.3
1	B	144	ASN	2.3
1	A	306	SER	2.3
1	B	127	LEU	2.3
1	B	26	GLY	2.2
1	B	136	PHE	2.2
1	A	305	ASN	2.2
1	B	27	LYS	2.2
1	B	96	LYS	2.2
1	A	604	MET	2.2
1	B	143	ILE	2.2
1	A	24	ASN	2.2
1	B	73	LEU	2.2
1	B	195	VAL	2.2
1	B	285	GLU	2.1
1	A	309	PRO	2.1
1	A	299	LYS	2.1
1	B	109	TRP	2.1
1	A	28	LYS	2.1
1	A	283	ASP	2.1
1	B	345	ARG	2.1
1	B	231	ASN	2.1
1	B	151	VAL	2.1
1	A	300	GLU	2.0
1	A	345	ARG	2.0
1	A	96	LYS	2.0
1	A	285	GLU	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](#)

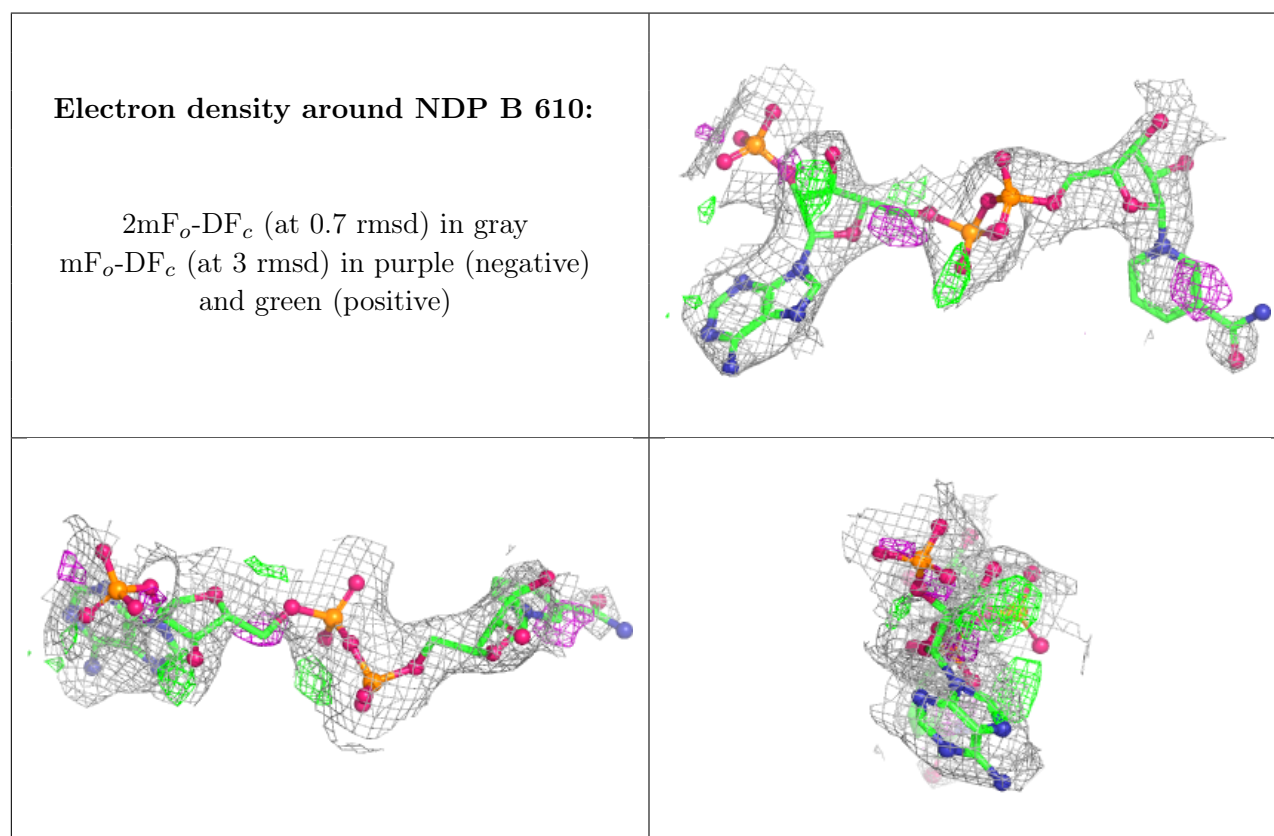
There are no oligosaccharides in this entry.

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.

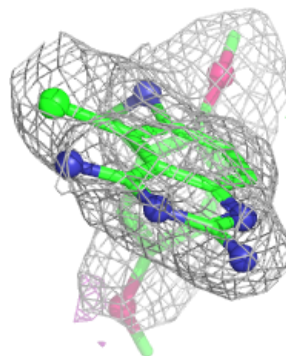
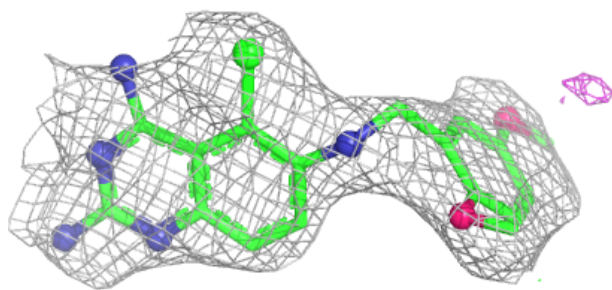
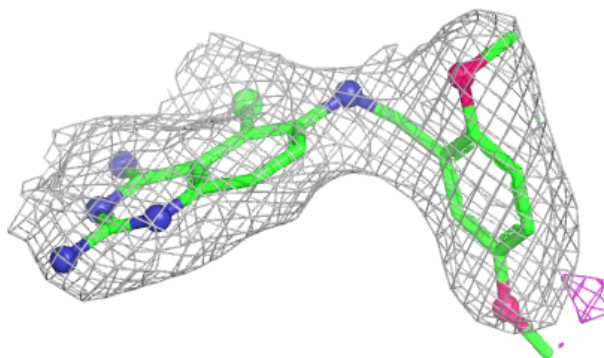
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NDP	B	610	48/48	0.81	0.14	88,90,90,90	0
2	KA5	B	609	25/25	0.85	0.17	67,74,77,79	0
4	UMP	B	611	20/20	0.92	0.14	44,63,71,72	0
4	UMP	A	611	20/20	0.93	0.14	49,72,80,82	0
2	KA5	A	609	25/25	0.93	0.10	39,44,49,55	0
3	NDP	A	610	48/48	0.95	0.09	51,60,63,63	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.

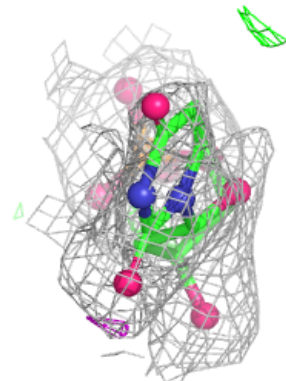
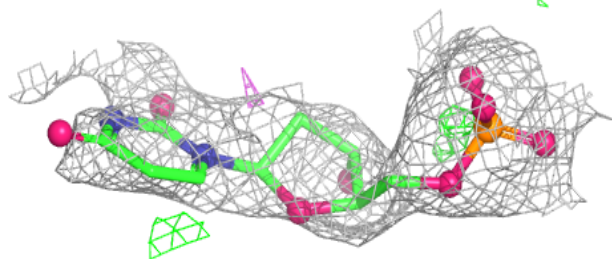
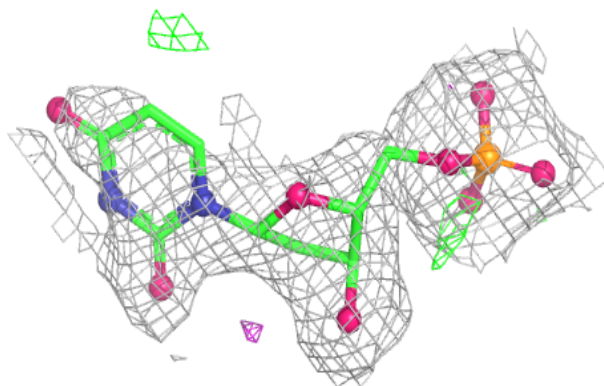


Electron density around KA5 B 609:

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

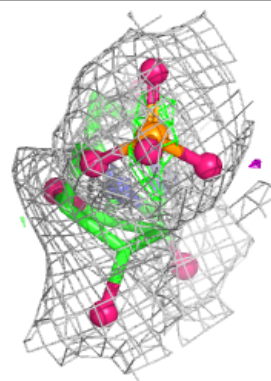
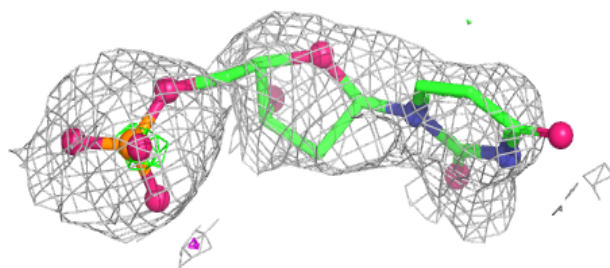
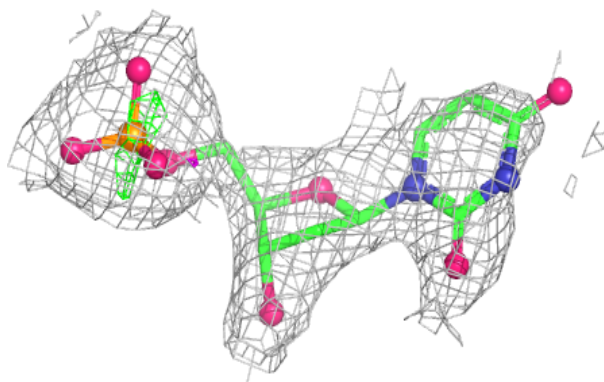
**Electron density around UMP B 611:**

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



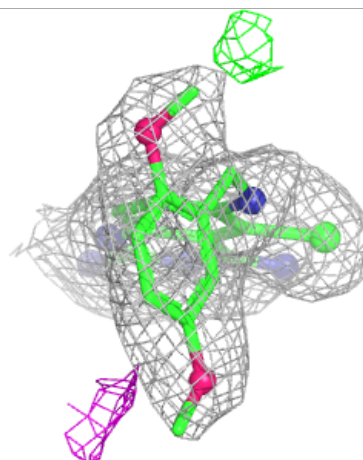
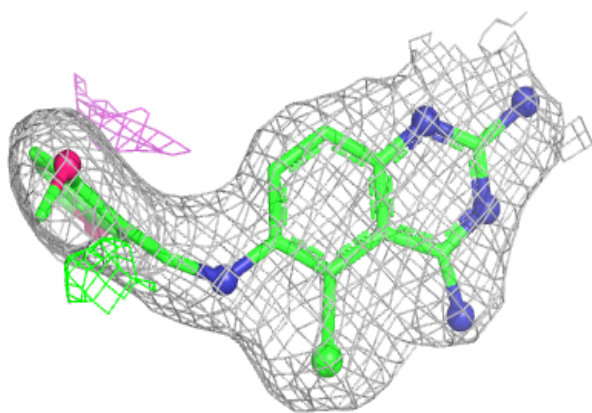
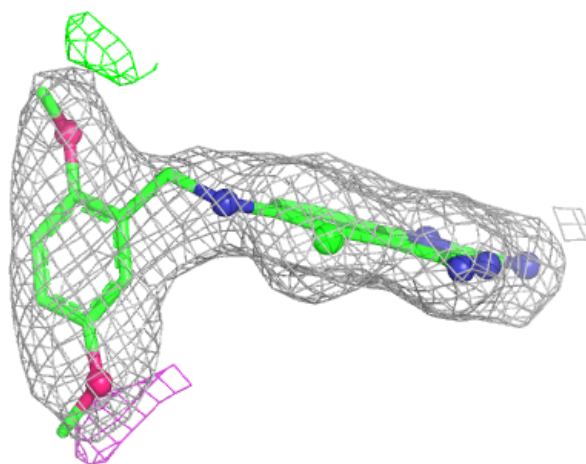
Electron density around UMP A 611:

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



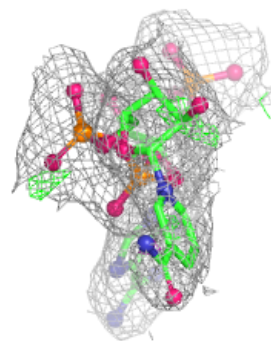
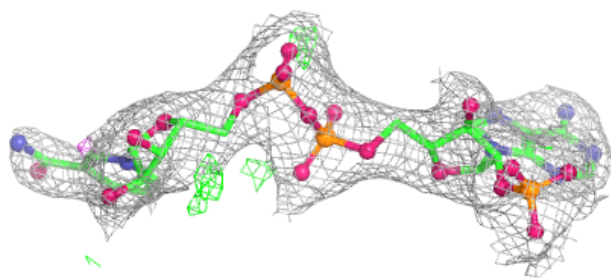
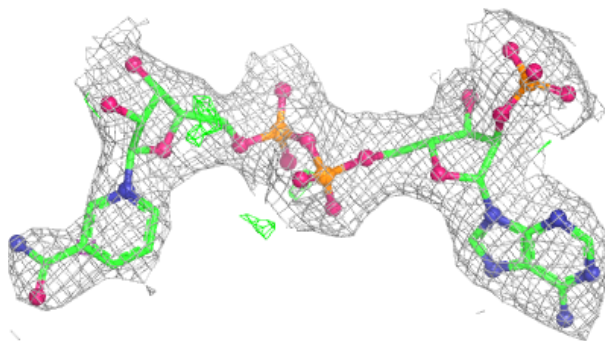
Electron density around KA5 A 609:

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



Electron density around NDP A 610:

$2mF_o-DF_c$ (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.