



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:25 PM UTC

PDB ID : 1J3K / pdb_00001j3k
Title : Quadruple mutant (N51I+C59R+S108N+I164L) Plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with WR99210, NADPH, and dUMP
Authors : Yuvaniyama, J.; Chitnumsub, P.; Kamchonwongpaisan, S.; Vanichtanankul, J.; Sirawaraporn, W.; Taylor, P.; Walkinshaw, M.; Yuthavong, Y.
Deposited on : 2003-02-03
Resolution : 2.10 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

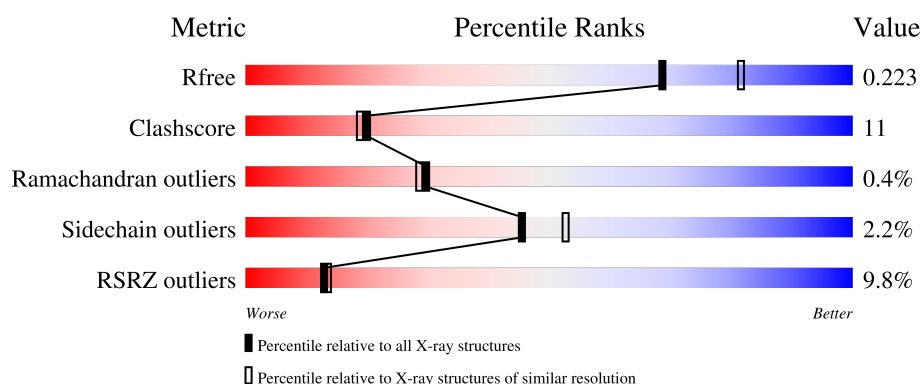
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	280	5% 57% 20% • 21%
1	B	280	23% 44% 30% • • 21%
2	C	328	4% 83% 15% ••
2	D	328	5% 78% 20% ••

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10528 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 Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1837	1190	297	338	12			
1	B	221	Total	C	N	O	S	0	0	0
			1834	1189	297	336	12			

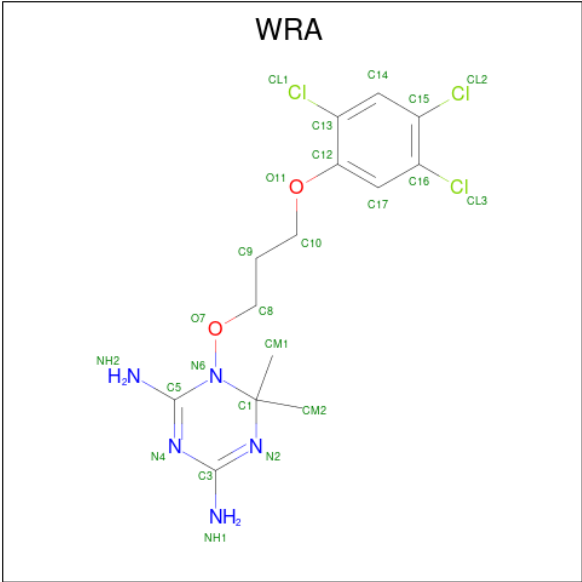
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ILE	ASN	engineered mutation	UNP P13922
A	59	ARG	CYS	engineered mutation	UNP P13922
A	108	ASN	SER	engineered mutation	UNP P13922
A	164	LEU	ILE	engineered mutation	UNP P13922
B	51	ILE	ASN	engineered mutation	UNP P13922
B	59	ARG	CYS	engineered mutation	UNP P13922
B	108	ASN	SER	engineered mutation	UNP P13922
B	164	LEU	ILE	engineered mutation	UNP P13922

- Molecule 2 is a protein called Bifunctional dihydrofolate reductase-thymidylate synthase.

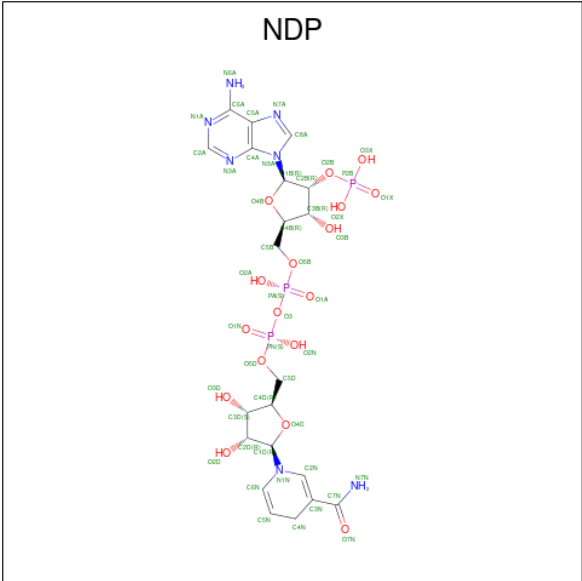
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	326	Total	C	N	O	S	0	0	0
			2713	1747	456	495	15			
2	D	326	Total	C	N	O	S	0	0	0
			2713	1747	456	495	15			

- Molecule 3 is 6,6-DIMETHYL-1-[3-(2,4,5-TRICHLOROPHENOXY)PROPOXY]-1,6-DIHYDRO-1,3,5-TRIAZINE-2,4-DIAMINE (CCD ID: WRA) (formula: C₁₄H₁₈Cl₃N₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			24	14	3	5	2		
3	B	1	Total	C	Cl	N	O	0	0
			24	14	3	5	2		

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



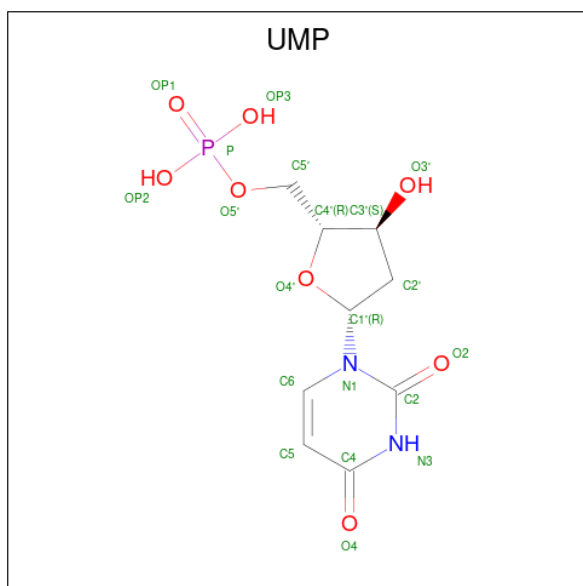
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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

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



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

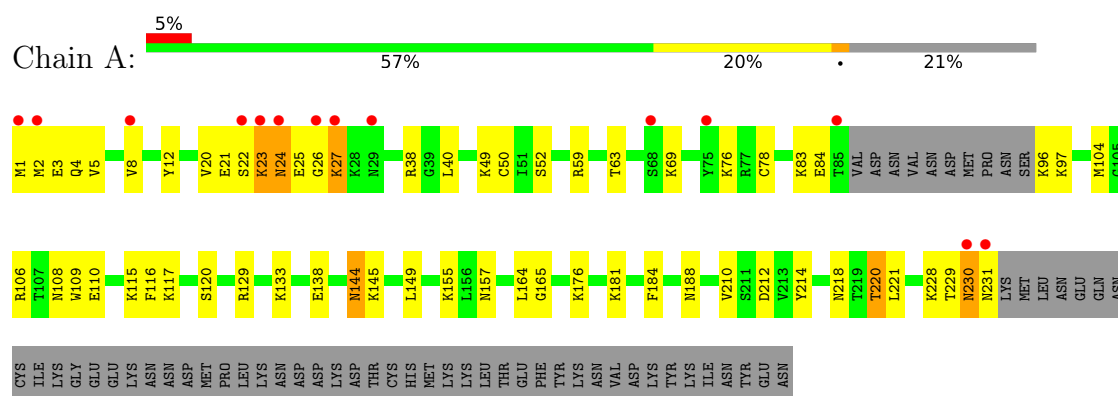
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	238	Total	O	0	0
			238	238		
6	B	102	Total	O	0	0
			102	102		
6	C	428	Total	O	0	0
			428	428		
6	D	479	Total	O	0	0
			479	479		

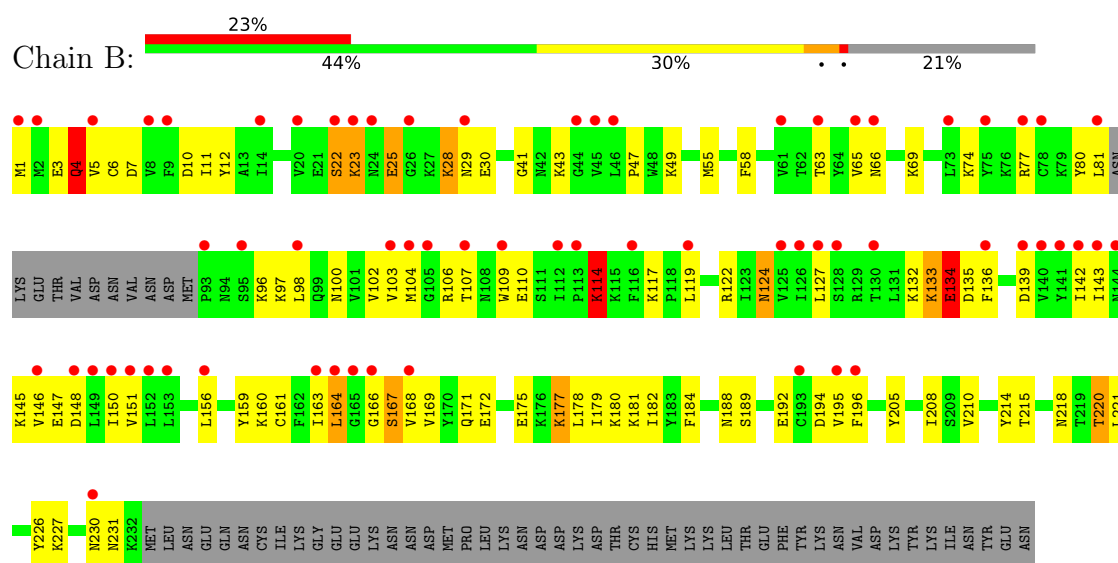
3 Residue-property plots [i](#)

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.

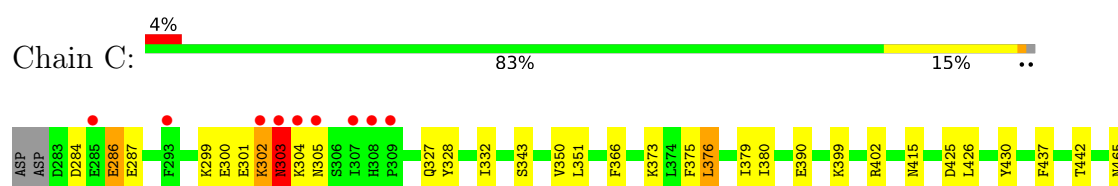
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

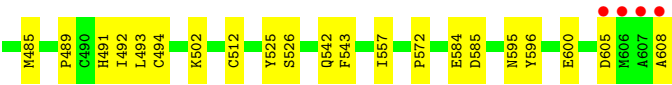


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

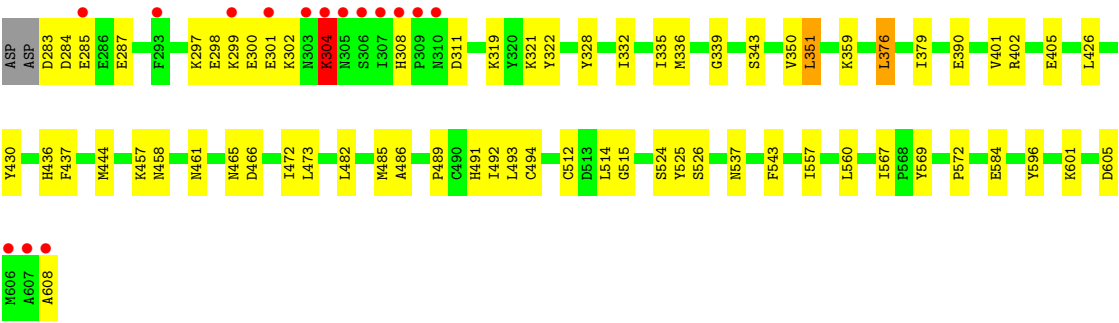
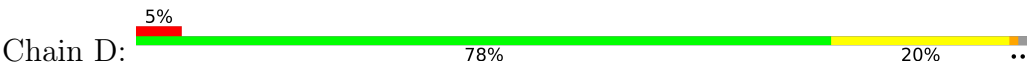


- Molecule 2: Bifunctional dihydrofolate reductase-thymidylate synthase





● Molecule 2: Bifunctional 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	59.68Å 158.09Å 165.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.98 – 2.10 28.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.8 (28.98-2.10) 97.3 (28.98-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.182 , 0.222 0.183 , 0.223	Depositor DCC
R_{free} test set	4523 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 64.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10528	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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, NDP, WRA

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	0.72	0/1871	1.27	23/2515 (0.9%)
1	B	0.50	0/1869	1.14	16/2512 (0.6%)
2	C	0.86	0/2784	1.20	27/3766 (0.7%)
2	D	0.84	1/2784 (0.0%)	1.17	23/3766 (0.6%)
All	All	0.77	1/9308 (0.0%)	1.19	89/12559 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	350	VAL	CA-CB	5.14	1.61	1.54

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	SER	N-CA-C	-14.29	87.17	110.17
2	C	304	LYS	N-CA-C	13.67	129.22	112.54
1	B	134	GLU	N-CA-C	12.35	124.43	110.97
1	B	30	GLU	N-CA-C	11.74	126.79	110.24
1	A	24	ASN	N-CA-C	11.71	125.25	110.61
1	A	3	GLU	N-CA-C	11.00	124.54	110.24
1	A	27	LYS	N-CA-C	10.62	125.83	113.19
1	A	25	GLU	N-CA-C	9.35	124.81	113.12
2	C	351	LEU	N-CA-C	-9.03	94.19	108.90
2	D	351	LEU	N-CA-C	-9.00	94.23	108.90
1	A	229	THR	N-CA-C	8.62	123.10	110.59
1	A	83	LYS	N-CA-C	-8.50	97.94	110.52
2	D	486	ALA	N-CA-C	-8.24	101.35	111.33
2	C	302	LYS	N-CA-C	-8.10	103.53	113.50
2	C	492	ILE	N-CA-C	8.03	118.13	110.42
1	A	23	LYS	N-CA-C	7.71	124.36	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	465	ASN	N-CA-C	7.66	122.92	113.50
1	A	212	ASP	N-CA-C	-7.62	101.03	110.41
1	A	129	ARG	N-CA-C	-7.56	103.91	113.43
1	B	156	LEU	N-CA-C	7.29	119.98	110.43
2	D	557	ILE	N-CA-C	7.09	117.81	110.36
2	D	402	ARG	N-CA-C	7.05	121.19	112.59
1	B	74	LYS	N-CA-C	-6.73	103.63	110.97
2	D	543	PHE	N-CA-C	-6.67	97.65	108.52
1	A	218	ASN	N-CA-C	6.59	121.28	113.23
2	C	303	ASN	N-CA-C	-6.59	100.55	110.24
1	B	4	GLN	N-CA-C	6.57	119.31	109.25
2	D	465	ASN	N-CA-C	6.56	121.57	113.50
1	A	52	SER	N-CA-C	6.56	118.43	111.28
1	A	138	GLU	N-CA-C	6.44	119.03	110.53
1	A	164	LEU	N-CA-C	6.39	121.09	113.16
2	C	543	PHE	N-CA-C	-6.35	98.17	108.52
1	B	167	SER	N-CA-C	6.34	118.72	111.11
1	A	188	ASN	N-CA-C	6.34	120.52	110.70
2	C	557	ILE	N-CA-C	6.26	117.75	110.62
2	C	526	SER	N-CA-C	-6.24	104.55	111.36
2	D	567	ILE	N-CA-C	6.14	113.96	107.76
1	B	114	LYS	N-CA-C	6.14	117.84	111.03
1	B	218	ASN	N-CA-C	6.05	119.99	112.24
2	C	542	GLN	N-CA-C	6.03	119.54	109.95
2	C	399	LYS	N-CA-C	-6.00	105.14	112.88
2	D	343	SER	N-CA-C	-5.97	101.10	110.36
2	D	512	CYS	N-CA-C	5.91	118.03	108.34
2	D	390	GLU	N-CA-C	5.88	118.78	110.50
2	D	444	MET	N-CA-C	5.83	119.86	112.87
1	B	28	LYS	N-CA-C	5.82	123.20	110.80
2	D	492	ILE	N-CA-C	5.73	115.92	110.42
1	B	220	THR	N-CA-C	-5.69	101.61	110.42
1	A	184	PHE	N-CA-C	5.65	117.72	108.52
1	B	177	LYS	N-CA-C	5.59	119.11	111.39
2	C	595	ASN	N-CA-C	5.57	119.25	111.74
2	D	482	LEU	N-CA-C	5.54	117.76	111.11
2	C	366	PHE	N-CA-C	-5.53	99.92	109.15
1	A	165	GLY	N-CA-C	-5.48	103.52	112.83
1	A	220	THR	N-CA-C	-5.45	101.97	110.42
2	C	600	GLU	N-CA-C	5.40	117.69	110.35
2	D	515	GLY	N-CA-C	5.40	119.21	112.73
2	C	402	ARG	N-CA-C	5.39	119.16	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	376	LEU	N-CA-C	5.37	120.70	113.72
2	D	350	VAL	CB-CA-C	-5.36	102.50	111.29
2	D	526	SER	N-CA-C	-5.36	105.52	111.36
2	C	380	ILE	N-CA-C	-5.35	105.32	110.72
1	B	184	PHE	N-CA-C	5.35	117.44	108.73
1	B	164	LEU	N-CA-C	5.34	119.42	113.02
2	D	401	VAL	N-CA-C	-5.33	99.48	107.37
1	B	77	ARG	N-CA-C	5.29	116.73	111.07
1	A	5	VAL	N-CA-C	5.28	115.90	110.36
1	B	188	ASN	N-CA-C	5.27	118.87	110.70
2	C	343	SER	N-CA-C	-5.26	102.97	110.59
2	C	585	ASP	N-CA-C	5.25	119.67	113.16
2	D	426	LEU	N-CA-C	5.25	119.31	113.01
2	D	569	TYR	N-CA-C	-5.24	102.53	110.50
1	A	120	SER	N-CA-C	5.22	117.80	110.23
2	C	426	LEU	N-CA-C	5.18	119.22	113.01
2	C	376	LEU	N-CA-C	5.15	120.21	113.30
1	B	133	LYS	N-CA-C	5.13	118.31	111.75
2	C	305	ASN	N-CA-C	5.11	117.66	110.14
2	C	442	THR	N-CA-C	-5.11	103.72	111.34
2	D	524	SER	CB-CA-C	-5.11	102.86	110.88
2	C	327	GLN	N-CA-C	-5.10	105.72	111.28
1	A	184	PHE	N-CA-CB	-5.10	102.55	110.55
2	C	512	CYS	N-CA-C	5.10	116.70	108.34
2	D	304	LYS	N-CA-C	5.08	117.10	109.23
1	A	157	ASN	N-CA-C	-5.06	99.03	107.99
2	C	390	GLU	N-CA-C	5.05	117.62	110.50
2	C	425	ASP	N-CA-C	-5.05	99.11	107.99
1	A	149	LEU	N-CA-C	-5.04	105.70	111.14
2	D	405	GLU	N-CA-C	5.03	116.45	111.07
2	C	350	VAL	CB-CA-C	-5.01	103.08	111.29

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	1837	0	1873	43	0
1	B	1834	0	1873	91	0
2	C	2713	0	2638	24	0
2	D	2713	0	2638	51	0
3	A	24	0	18	1	0
3	B	24	0	18	0	0
4	A	48	0	26	4	0
4	B	48	0	26	6	0
5	C	20	0	11	1	0
5	D	20	0	11	0	0
6	A	238	0	0	12	1
6	B	102	0	0	12	0
6	C	428	0	0	5	1
6	D	479	0	0	14	0
All	All	10528	0	9132	209	1

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 11.

All (209) 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:A:1:MET:HG3	1:A:2:MET:H	0.97	1.11
1:A:1:MET:HG3	1:A:2:MET:N	1.78	0.98
2:D:300:GLU:HG3	2:D:304:LYS:NZ	1.78	0.98
2:D:605:ASP:HB3	2:D:608:ALA:HB2	1.46	0.98
1:B:210:VAL:HB	6:B:2028:HOH:O	1.64	0.95
1:A:210:VAL:HB	6:A:2086:HOH:O	1.66	0.95
2:D:461:ASN:HB3	6:D:1537:HOH:O	1.68	0.93
1:B:114:LYS:H	1:B:114:LYS:HD2	1.37	0.89
1:A:1:MET:CG	1:A:2:MET:H	1.84	0.88
2:C:415:ASN:HB2	6:C:1911:HOH:O	1.73	0.88
1:B:142:ILE:HG22	6:B:1389:HOH:O	1.75	0.87
1:A:50:CYS:SG	6:A:1300:HOH:O	2.33	0.85
2:D:376:LEU:HD22	2:D:379:ILE:HD11	1.57	0.84
1:B:145:LYS:HE3	1:B:147:GLU:HB2	1.58	0.83
2:D:584:GLU:HB2	6:D:1723:HOH:O	1.79	0.81
1:B:171:GLN:O	1:B:175:GLU:HG3	1.81	0.80
1:A:133:LYS:HE3	6:A:1232:HOH:O	1.82	0.79
2:C:286:GLU:HG2	2:D:319:LYS:HG2	1.65	0.78
1:B:106:ARG:HB3	4:B:710:NDP:O3B	1.85	0.77
2:D:300:GLU:O	2:D:300:GLU:HG2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:302:LYS:HE3	6:D:1790:HOH:O	1.86	0.75
2:D:332:ILE:CG2	2:D:336:MET:HE3	2.16	0.75
2:D:300:GLU:HG3	2:D:304:LYS:HZ1	1.49	0.73
1:B:41:GLY:HA2	1:B:47:PRO:HD3	1.69	0.73
2:C:375:PHE:HD1	6:C:1945:HOH:O	1.70	0.73
2:C:605:ASP:HB3	2:C:608:ALA:HB2	1.71	0.73
1:A:96:LYS:HE2	6:A:1129:HOH:O	1.89	0.72
2:D:300:GLU:HG3	2:D:304:LYS:HZ2	1.54	0.70
1:B:134:GLU:C	1:B:136:PHE:H	1.99	0.70
2:D:605:ASP:HB3	2:D:608:ALA:CB	2.21	0.69
1:B:25:GLU:HA	1:B:25:GLU:OE1	1.93	0.69
1:B:124:ASN:N	1:B:124:ASN:HD22	1.89	0.68
1:B:145:LYS:HG2	1:B:146:VAL:N	2.08	0.68
1:A:78:CYS:SG	6:A:1201:HOH:O	2.51	0.68
1:B:23:LYS:HA	1:B:23:LYS:CE	2.22	0.68
1:B:114:LYS:H	1:B:114:LYS:CD	1.99	0.67
1:A:230:ASN:O	1:A:230:ASN:CG	2.38	0.66
1:A:21:GLU:CD	1:A:23:LYS:HE2	2.21	0.65
2:D:458:ASN:HB3	6:D:1541:HOH:O	1.94	0.65
1:B:161:CYS:SG	6:B:2219:HOH:O	2.54	0.65
2:D:301:GLU:HA	2:D:301:GLU:OE1	1.96	0.64
1:B:11:ILE:HG12	6:B:2219:HOH:O	1.97	0.64
2:C:605:ASP:HB3	2:C:608:ALA:CB	2.27	0.64
1:B:103:VAL:HB	1:B:163:ILE:HD13	1.80	0.64
1:B:11:ILE:HG23	6:B:2219:HOH:O	1.97	0.63
2:D:300:GLU:C	2:D:302:LYS:N	2.55	0.63
1:B:23:LYS:HA	1:B:23:LYS:HE3	1.81	0.63
1:A:96:LYS:HG3	1:A:97:LYS:N	2.15	0.62
1:B:127:LEU:HB3	4:B:710:NDP:N3A	2.15	0.62
1:B:3:GLU:HG3	1:B:80:TYR:HE1	1.66	0.61
1:B:161:CYS:HB3	6:B:2219:HOH:O	2.01	0.61
1:B:80:TYR:O	1:B:81:LEU:C	2.44	0.61
2:D:322:TYR:OH	6:D:1347:HOH:O	2.16	0.61
1:A:69:LYS:HE2	2:D:284:ASP:OD2	2.01	0.60
2:D:457:LYS:NZ	6:D:1696:HOH:O	2.35	0.60
2:C:502:LYS:NZ	6:C:1797:HOH:O	2.33	0.59
1:B:97:LYS:NZ	1:B:97:LYS:HB3	2.18	0.59
1:B:124:ASN:HD22	1:B:124:ASN:H	1.50	0.59
1:A:21:GLU:HG2	1:A:23:LYS:HE2	1.84	0.58
2:D:493:LEU:C	2:D:493:LEU:HD12	2.27	0.58
1:A:96:LYS:HG3	1:A:97:LYS:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LYS:HD2	6:B:1383:HOH:O	2.05	0.56
1:B:107:THR:OG1	4:B:710:NDP:H51A	2.03	0.56
2:D:300:GLU:C	2:D:302:LYS:H	2.11	0.56
1:A:115:LYS:HE3	1:A:116:PHE:CZ	2.39	0.56
2:C:494:CYS:SG	2:C:525:TYR:CE2	2.99	0.56
1:B:1:MET:O	1:B:1:MET:HG3	2.06	0.55
1:A:176:LYS:HD3	6:A:1165:HOH:O	2.06	0.55
2:C:584:GLU:HB2	6:C:2237:HOH:O	2.07	0.55
2:C:491:HIS:ND1	6:C:2176:HOH:O	2.24	0.55
2:D:537:ASN:HB3	6:D:2230:HOH:O	2.07	0.55
2:D:321:LYS:HE3	6:D:1342:HOH:O	2.05	0.55
2:C:493:LEU:HD12	2:C:493:LEU:C	2.31	0.54
2:D:332:ILE:HG22	2:D:336:MET:HE3	1.90	0.54
1:B:12:TYR:HE2	1:B:160:LYS:HD3	1.72	0.54
1:B:168:VAL:O	1:B:172:GLU:HG2	2.07	0.54
2:D:332:ILE:HD13	2:D:560:LEU:HD22	1.89	0.54
1:B:58:PHE:HZ	1:B:164:LEU:HD13	1.73	0.54
1:B:132:LYS:NZ	1:B:135:ASP:OD2	2.41	0.54
1:B:109:TRP:CZ2	1:B:117:LYS:HD2	2.43	0.53
1:B:22:SER:O	1:B:23:LYS:HB2	2.07	0.53
1:B:133:LYS:O	1:B:136:PHE:HB2	2.09	0.53
1:B:106:ARG:NH1	1:B:110:GLU:OE1	2.42	0.52
1:B:145:LYS:HE3	1:B:147:GLU:CB	2.34	0.52
1:A:20:VAL:HG21	1:A:38:ARG:NH2	2.24	0.52
1:B:3:GLU:CG	1:B:80:TYR:HE1	2.21	0.52
2:D:336:MET:HE1	2:D:560:LEU:HB3	1.92	0.52
2:D:336:MET:HE1	2:D:560:LEU:CB	2.40	0.52
1:A:21:GLU:CG	1:A:23:LYS:HE2	2.39	0.51
1:B:124:ASN:N	1:B:124:ASN:ND2	2.59	0.51
2:D:491:HIS:ND1	6:D:1876:HOH:O	2.29	0.51
1:B:11:ILE:HB	1:B:178:LEU:O	2.10	0.51
1:A:214:TYR:O	1:A:220:THR:HA	2.11	0.50
2:D:601:LYS:HG2	6:D:1429:HOH:O	2.11	0.50
4:A:610:NDP:H52A	4:A:610:NDP:H8A	1.94	0.50
1:B:196:PHE:CD1	1:B:196:PHE:N	2.79	0.50
2:C:299:LYS:HE3	2:C:302:LYS:HB2	1.93	0.50
1:B:41:GLY:N	1:B:195:VAL:HG23	2.27	0.50
2:C:376:LEU:HD22	2:C:379:ILE:HD11	1.93	0.50
1:A:50:CYS:HB2	6:A:2115:HOH:O	2.11	0.50
1:B:167:SER:HB3	4:B:710:NDP:O2N	2.12	0.50
2:C:494:CYS:SG	2:C:525:TYR:HE2	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:GLU:HG3	6:B:1449:HOH:O	2.11	0.50
2:D:494:CYS:SG	2:D:525:TYR:CE2	3.05	0.50
1:B:12:TYR:CE2	1:B:160:LYS:HD3	2.47	0.49
1:A:109:TRP:CE2	1:A:117:LYS:HD2	2.48	0.49
2:C:373:LYS:HE2	2:C:375:PHE:CE2	2.47	0.49
2:C:300:GLU:HG3	2:C:301:GLU:HG3	1.95	0.49
1:A:230:ASN:O	1:A:230:ASN:OD1	2.30	0.49
2:D:494:CYS:SG	2:D:525:TYR:HE2	2.36	0.49
2:D:308:HIS:O	2:D:311:ASP:HB2	2.12	0.49
1:A:4:GLN:NE2	1:A:228:LYS:NZ	2.61	0.49
2:D:332:ILE:HG23	2:D:336:MET:HE3	1.94	0.49
1:B:80:TYR:HA	6:B:2213:HOH:O	2.14	0.48
1:B:114:LYS:HD2	1:B:114:LYS:N	2.16	0.48
1:A:20:VAL:CG2	1:A:38:ARG:NH2	2.77	0.48
1:B:66:ASN:ND2	1:B:69:LYS:HD2	2.29	0.48
1:B:119:LEU:HB3	1:B:122:ARG:CZ	2.44	0.48
1:B:134:GLU:C	1:B:136:PHE:N	2.65	0.48
1:A:109:TRP:CZ2	1:A:117:LYS:HD2	2.49	0.48
1:A:230:ASN:O	1:A:231:ASN:ND2	2.46	0.47
2:C:373:LYS:HE2	2:C:375:PHE:CZ	2.49	0.47
2:D:466:ASP:OD2	6:D:1534:HOH:O	2.20	0.47
2:D:572:PRO:HB3	2:D:596:TYR:HA	1.96	0.47
1:B:7:ASP:OD1	1:B:180:LYS:HE3	2.15	0.47
1:B:43:LYS:N	1:B:194:ASP:OD2	2.36	0.47
2:C:572:PRO:HB3	2:C:596:TYR:HA	1.95	0.47
1:B:3:GLU:HG3	1:B:80:TYR:CE1	2.48	0.47
2:C:328:TYR:CZ	2:C:332:ILE:HD11	2.50	0.47
1:B:55:MET:HE2	6:B:2031:HOH:O	2.14	0.47
1:B:136:PHE:CD2	1:B:142:ILE:HD11	2.50	0.47
2:C:299:LYS:CE	2:C:302:LYS:HB2	2.44	0.47
1:A:4:GLN:NE2	1:A:228:LYS:HZ3	2.13	0.47
1:B:175:GLU:C	1:B:177:LYS:H	2.23	0.47
2:D:584:GLU:HG2	6:D:1724:HOH:O	2.14	0.47
1:B:106:ARG:O	1:B:110:GLU:HG3	2.15	0.46
1:B:182:ILE:HB	1:B:226:TYR:HB2	1.97	0.46
1:A:40:LEU:O	4:A:610:NDP:H2N	2.16	0.46
2:D:297:LYS:HD3	2:D:297:LYS:HA	1.59	0.46
2:D:328:TYR:CZ	2:D:332:ILE:HD11	2.50	0.46
2:D:284:ASP:O	2:D:287:GLU:HB2	2.16	0.46
1:A:144:ASN:H	1:A:144:ASN:HD22	1.63	0.46
1:A:96:LYS:HA	6:A:1209:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:GLN:OE1	1:B:5:VAL:HG23	2.14	0.45
1:B:12:TYR:CD1	1:B:181:LYS:HB2	2.52	0.45
1:A:84:GLU:HB3	6:A:1199:HOH:O	2.16	0.45
1:B:214:TYR:O	1:B:220:THR:HA	2.16	0.45
1:B:104:MET:HE1	1:B:119:LEU:CD1	2.47	0.45
1:A:8:VAL:HA	1:A:76:LYS:HD3	1.99	0.45
1:B:145:LYS:HB3	1:B:145:LYS:HE2	1.51	0.45
4:A:610:NDP:H3B	6:A:1171:HOH:O	2.17	0.45
2:C:491:HIS:CE1	5:C:611:UMP:O4	2.69	0.45
2:D:284:ASP:O	2:D:285:GLU:C	2.60	0.45
1:B:23:LYS:HE3	1:B:23:LYS:CA	2.45	0.44
1:B:102:VAL:HG23	1:B:102:VAL:O	2.16	0.44
1:A:106:ARG:HE	4:A:610:NDP:P2B	2.41	0.44
1:B:139:ASP:O	1:B:139:ASP:OD1	2.36	0.44
1:B:171:GLN:HG3	1:B:175:GLU:OE2	2.18	0.44
1:B:221:LEU:N	1:B:221:LEU:HD23	2.33	0.44
1:B:107:THR:HB	4:B:710:NDP:O2A	2.18	0.44
2:C:284:ASP:O	2:C:287:GLU:HB2	2.18	0.44
1:A:96:LYS:CG	1:A:97:LYS:H	2.29	0.43
1:B:41:GLY:HA2	1:B:47:PRO:CD	2.43	0.43
1:B:145:LYS:CG	1:B:146:VAL:N	2.78	0.43
1:B:179:ILE:HB	1:B:205:TYR:OH	2.18	0.43
2:C:437:PHE:C	2:C:437:PHE:CD1	2.97	0.43
1:A:155:LYS:NZ	6:A:1153:HOH:O	2.50	0.43
1:B:65:VAL:HG11	1:B:98:LEU:HG	2.00	0.43
1:B:166:GLY:O	1:B:169:VAL:HB	2.19	0.43
1:A:228:LYS:HE3	6:A:1190:HOH:O	2.18	0.43
1:B:166:GLY:N	4:B:710:NDP:O1A	2.51	0.43
1:A:108:ASN:HD21	3:A:609:WRA:H91	1.83	0.43
1:A:221:LEU:HD23	1:A:221:LEU:N	2.33	0.42
2:C:300:GLU:O	2:C:303:ASN:HB2	2.19	0.42
1:B:63:THR:HG22	1:B:122:ARG:NE	2.34	0.42
1:B:161:CYS:CB	6:B:2219:HOH:O	2.61	0.42
2:D:351:LEU:HD23	2:D:351:LEU:HA	1.92	0.42
1:B:132:LYS:NZ	1:B:135:ASP:CG	2.78	0.42
2:D:321:LYS:CE	6:D:1342:HOH:O	2.65	0.42
1:B:100:ASN:OD1	1:B:159:TYR:HB3	2.18	0.42
1:B:106:ARG:HH11	1:B:110:GLU:CD	2.27	0.42
2:D:359:LYS:NZ	6:D:1474:HOH:O	2.53	0.42
2:D:472:ILE:C	2:D:473:LEU:HD12	2.45	0.42
1:A:59:ARG:O	1:A:63:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLU:CG	1:B:3:GLU:O	2.68	0.42
2:D:436:HIS:O	2:D:437:PHE:C	2.63	0.42
1:B:58:PHE:HE1	1:B:164:LEU:HD22	1.84	0.42
1:B:41:GLY:H	1:B:195:VAL:HG23	1.83	0.41
2:D:284:ASP:N	2:D:284:ASP:OD1	2.53	0.41
1:B:148:ASP:O	1:B:151:VAL:HB	2.20	0.41
1:B:127:LEU:HD12	1:B:127:LEU:N	2.35	0.41
2:D:299:LYS:HG2	2:D:301:GLU:HB2	2.02	0.41
1:B:1:MET:O	1:B:1:MET:CG	2.68	0.41
2:D:283:ASP:C	2:D:285:GLU:H	2.27	0.41
1:B:6:CYS:O	1:B:10:ASP:HA	2.20	0.41
2:D:335:ILE:O	2:D:339:GLY:N	2.50	0.41
2:D:376:LEU:HD22	2:D:379:ILE:CD1	2.39	0.41
1:A:106:ARG:NH1	1:A:110:GLU:OE1	2.54	0.41
1:B:208:ILE:HD13	1:B:227:LYS:HB2	2.02	0.41
1:A:144:ASN:ND2	1:A:145:LYS:HG3	2.36	0.41
1:B:96:LYS:HA	1:B:96:LYS:HD3	1.84	0.41
2:C:485:MET:SD	2:C:489:PRO:HD3	2.60	0.41
1:B:230:ASN:C	1:B:231:ASN:HD22	2.29	0.41
1:A:12:TYR:CD1	1:A:181:LYS:HB2	2.56	0.40
1:B:5:VAL:HG11	1:B:150:ILE:HD12	2.03	0.40
2:D:437:PHE:C	2:D:437:PHE:CD1	2.99	0.40
1:A:21:GLU:HG2	1:A:23:LYS:HG2	2.04	0.40
1:B:143:ILE:C	6:B:1389:HOH:O	2.63	0.40
2:D:485:MET:SD	2:D:489:PRO:HD3	2.61	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1592:HOH:O	6:C:1593:HOH:O[3_645]	2.18	0.02

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	217/280 (78%)	208 (96%)	8 (4%)	1 (0%)	24	22
1	B	217/280 (78%)	198 (91%)	18 (8%)	1 (0%)	24	22
2	C	324/328 (99%)	312 (96%)	11 (3%)	1 (0%)	36	36
2	D	324/328 (99%)	307 (95%)	16 (5%)	1 (0%)	36	36
All	All	1082/1216 (89%)	1025 (95%)	53 (5%)	4 (0%)	30	28

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	430	TYR
1	A	26	GLY
1	B	28	LYS
2	D	430	TYR

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	210/268 (78%)	204 (97%)	6 (3%)	37	42
1	B	210/268 (78%)	199 (95%)	11 (5%)	21	20
2	C	300/302 (99%)	298 (99%)	2 (1%)	76	83
2	D	300/302 (99%)	297 (99%)	3 (1%)	68	76
All	All	1020/1140 (90%)	998 (98%)	22 (2%)	45	53

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	27	LYS
1	A	49	LYS
1	A	104	MET

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Mol	Chain	Res	Type
1	A	144	ASN
1	A	230	ASN
1	B	4	GLN
1	B	22	SER
1	B	23	LYS
1	B	25	GLU
1	B	29	ASN
1	B	49	LYS
1	B	114	LYS
1	B	124	ASN
1	B	134	GLU
1	B	189	SER
1	B	215	THR
2	C	286	GLU
2	C	303	ASN
2	D	298	GLU
2	D	304	LYS
2	D	514	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	24	ASN
1	A	99	GLN
1	A	121	ASN
1	A	144	ASN
1	A	171	GLN
1	A	231	ASN
1	B	42	ASN
1	B	121	ASN
1	B	157	ASN
1	B	171	GLN
1	B	231	ASN
2	C	294	ASN
2	C	303	ASN
2	C	338	ASN
2	C	394	ASN
2	C	400	ASN
2	C	407	ASN
2	C	424	ASN
2	C	433	GLN

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Mol	Chain	Res	Type
2	C	478	ASN
2	C	534	GLN
2	C	537	ASN
2	C	542	GLN
2	C	563	GLN
2	D	310	ASN
2	D	338	ASN
2	D	340	ASN
2	D	394	ASN
2	D	424	ASN
2	D	450	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	$\# Z > 2$
3	WRA	B	709	-	22,25,25	3.34	13 (59%)	27,36,36	1.65	4 (14%)
4	NDP	A	610	-	51,52,52	2.48	23 (45%)	71,80,80	1.96	22 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	UMP	C	611	-	21,21,21	1.72	6 (28%)	30,31,31	1.60	7 (23%)
3	WRA	A	609	-	22,25,25	3.05	14 (63%)	27,36,36	1.51	4 (14%)
4	NDP	B	710	-	51,52,52	2.74	23 (45%)	71,80,80	1.82	17 (23%)
5	UMP	D	711	-	21,21,21	1.65	4 (19%)	30,31,31	1.73	9 (30%)

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	WRA	B	709	-	-	2/8/27/27	0/2/2/2
4	NDP	A	610	-	-	5/34/77/77	0/5/5/5
5	UMP	C	611	-	-	0/10/22/22	0/2/2/2
3	WRA	A	609	-	-	2/8/27/27	0/2/2/2
4	NDP	B	710	-	-	10/34/77/77	0/5/5/5
5	UMP	D	711	-	-	1/10/22/22	0/2/2/2

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	710	NDP	PN-O3	7.15	1.67	1.59
3	B	709	WRA	C17-C12	6.52	1.49	1.38
4	B	710	NDP	C5D-C4D	6.06	1.69	1.51
3	B	709	WRA	C17-C16	5.34	1.47	1.38
3	A	609	WRA	C14-C15	5.22	1.47	1.38
3	B	709	WRA	C16-C15	5.18	1.50	1.39
3	A	609	WRA	C14-C13	5.16	1.47	1.38
3	A	609	WRA	O7-N6	5.12	1.46	1.40
3	B	709	WRA	O7-N6	5.10	1.46	1.40
4	A	610	NDP	O4B-C4B	5.06	1.56	1.45
4	A	610	NDP	O4B-C1B	5.03	1.53	1.42
4	A	610	NDP	C4A-N3A	5.01	1.43	1.34
3	B	709	WRA	C12-C13	4.84	1.48	1.39
4	B	710	NDP	O3B-C3B	4.81	1.54	1.43
3	A	609	WRA	O7-C8	4.75	1.54	1.45
4	A	610	NDP	PN-O3	4.71	1.64	1.59
4	B	710	NDP	C3B-C2B	-4.65	1.42	1.53
4	B	710	NDP	C2N-C3N	4.60	1.47	1.35
4	A	610	NDP	PA-O3	-4.57	1.54	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	710	NDP	O4D-C1D	4.52	1.52	1.42
4	B	710	NDP	PN-O1N	4.51	1.66	1.50
4	B	710	NDP	C6N-N1N	4.46	1.48	1.37
4	B	710	NDP	C4A-N3A	4.34	1.42	1.34
4	A	610	NDP	O4D-C1D	4.18	1.51	1.42
4	B	710	NDP	PA-O3	4.16	1.64	1.59
4	B	710	NDP	PA-O2A	-4.14	1.36	1.55
3	B	709	WRA	C14-C15	4.08	1.45	1.38
3	B	709	WRA	O11-C12	4.00	1.45	1.37
4	B	710	NDP	C3B-C4B	-3.92	1.43	1.53
3	A	609	WRA	C17-C12	3.73	1.45	1.38
3	A	609	WRA	O11-C12	3.70	1.44	1.37
3	A	609	WRA	C17-C16	3.67	1.44	1.38
4	A	610	NDP	P2B-O2X	-3.65	1.41	1.54
5	D	711	UMP	O4'-C1'	3.49	1.50	1.42
4	A	610	NDP	C4N-C3N	-3.48	1.43	1.50
4	A	610	NDP	PA-O5B	3.46	1.72	1.59
5	C	611	UMP	C5-C4	3.43	1.51	1.43
4	A	610	NDP	C5D-C4D	3.40	1.61	1.51
3	A	609	WRA	C12-C13	3.34	1.45	1.39
3	A	609	WRA	C5-N4	3.34	1.39	1.33
3	B	709	WRA	O11-C10	3.25	1.54	1.43
4	A	610	NDP	C2D-C3D	-3.24	1.44	1.53
3	B	709	WRA	C5-N4	3.24	1.38	1.33
5	D	711	UMP	P-O5'	-3.23	1.50	1.60
3	B	709	WRA	C14-C13	3.20	1.43	1.38
4	B	710	NDP	PA-O1A	-3.11	1.40	1.50
4	A	610	NDP	C2B-C1B	-3.06	1.45	1.53
4	B	710	NDP	C4N-C5N	-3.04	1.41	1.49
4	A	610	NDP	C5A-N7A	-3.02	1.33	1.39
3	B	709	WRA	C9-C10	3.02	1.63	1.51
4	A	610	NDP	C2N-C3N	2.98	1.43	1.35
4	B	710	NDP	C2D-C3D	-2.95	1.45	1.53
5	D	711	UMP	C6-C5	2.91	1.41	1.35
4	A	610	NDP	C6N-C5N	2.87	1.41	1.33
3	A	609	WRA	O11-C10	2.85	1.53	1.43
3	B	709	WRA	C15-CL2	2.83	1.80	1.73
5	C	611	UMP	O4'-C1'	2.82	1.48	1.42
3	A	609	WRA	C16-C15	2.81	1.45	1.39
4	A	610	NDP	C6N-N1N	2.80	1.44	1.37
4	A	610	NDP	C8A-N9A	2.75	1.42	1.37
4	A	610	NDP	C2A-N1A	2.71	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	611	UMP	O3'-C3'	2.68	1.48	1.43
3	A	609	WRA	C16-CL3	2.64	1.79	1.73
3	A	609	WRA	C9-C10	2.61	1.61	1.51
4	B	710	NDP	C6N-C5N	2.59	1.41	1.33
4	A	610	NDP	C1B-N9A	2.51	1.53	1.46
4	B	710	NDP	C2B-C1B	2.51	1.59	1.53
4	B	710	NDP	O4B-C1B	-2.48	1.36	1.42
5	D	711	UMP	O3'-C3'	2.44	1.48	1.43
4	B	710	NDP	C2A-N1A	2.43	1.38	1.33
4	A	610	NDP	C4N-C5N	-2.39	1.42	1.49
4	A	610	NDP	C7N-C3N	2.38	1.53	1.48
4	B	710	NDP	PN-O2N	-2.32	1.44	1.55
4	B	710	NDP	C8A-N9A	2.31	1.41	1.37
5	C	611	UMP	C6-C5	2.30	1.40	1.35
3	A	609	WRA	C15-CL2	2.30	1.79	1.73
4	B	710	NDP	C2D-C1D	2.27	1.60	1.53
4	A	610	NDP	O3D-C3D	2.27	1.48	1.43
5	C	611	UMP	C2-N1	2.25	1.42	1.38
4	A	610	NDP	P2B-O2B	-2.22	1.55	1.59
4	B	710	NDP	C4N-C3N	-2.15	1.45	1.50
3	B	709	WRA	O7-C8	2.14	1.49	1.45
5	C	611	UMP	P-O5'	-2.10	1.53	1.60

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	709	WRA	NH2-C5-N6	5.34	121.84	117.46
4	A	610	NDP	C1D-N1N-C2N	-5.26	112.47	121.14
4	A	610	NDP	O4B-C1B-N9A	4.70	117.11	108.09
4	B	710	NDP	O2X-P2B-O1X	4.60	128.76	110.83
4	B	710	NDP	O3X-P2B-O1X	-4.21	94.44	110.83
4	A	610	NDP	P2B-O2B-C2B	4.20	134.65	123.43
4	B	710	NDP	C1D-N1N-C2N	-4.18	114.25	121.14
4	B	710	NDP	C3N-C2N-N1N	-4.08	117.22	123.20
4	A	610	NDP	O2X-P2B-O1X	4.01	126.46	110.83
4	B	710	NDP	C2B-C3B-C4B	4.01	110.62	101.99
5	D	711	UMP	C1'-N1-C6	-3.83	113.99	121.53
4	B	710	NDP	C2B-C1B-N9A	3.76	119.93	113.75
3	A	609	WRA	NH2-C5-N6	3.75	120.54	117.46
4	A	610	NDP	C3N-C2N-N1N	-3.61	117.90	123.20
4	B	710	NDP	O2A-PA-O1A	3.55	128.97	112.44
5	C	611	UMP	C1'-N1-C6	-3.50	114.64	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	609	WRA	N4-C3-N2	-3.47	120.75	126.48
4	A	610	NDP	C6N-N1N-C2N	3.47	123.03	119.32
4	B	710	NDP	C2D-C3D-C4D	3.37	109.12	102.61
4	A	610	NDP	O4B-C4B-C5B	-3.33	98.67	109.33
5	C	611	UMP	O4'-C1'-N1	3.28	113.69	107.86
3	B	709	WRA	N6-C5-N4	-3.22	119.45	121.53
3	B	709	WRA	N4-C3-N2	-3.21	121.18	126.48
4	A	610	NDP	O5D-C5D-C4D	-3.16	98.23	108.99
5	D	711	UMP	O4'-C1'-N1	3.03	113.23	107.86
4	A	610	NDP	O3X-P2B-O1X	-3.01	99.11	110.83
5	C	611	UMP	C6-N1-C2	2.95	124.59	121.00
3	A	609	WRA	O11-C12-C13	2.90	119.84	116.39
5	D	711	UMP	C4'-O4'-C1'	2.89	116.37	109.51
4	B	710	NDP	O5B-PA-O1A	-2.81	97.79	108.94
4	A	610	NDP	C5A-N7A-C8A	2.81	107.86	103.45
4	B	710	NDP	O7N-C7N-N7N	-2.76	116.71	122.89
4	A	610	NDP	C2D-C3D-C4D	2.64	107.72	102.61
4	B	710	NDP	C2D-C1D-N1N	-2.62	106.87	113.31
5	D	711	UMP	O4'-C4'-C3'	-2.59	99.74	105.65
4	B	710	NDP	C6N-N1N-C2N	2.57	122.07	119.32
3	B	709	WRA	O11-C12-C13	2.56	119.44	116.39
4	A	610	NDP	O5B-C5B-C4B	-2.55	100.32	108.99
4	A	610	NDP	C4A-N9A-C8A	-2.51	103.10	105.74
4	A	610	NDP	O7N-C7N-N7N	-2.51	117.26	122.89
5	C	611	UMP	C2'-C1'-N1	2.51	120.08	113.81
5	C	611	UMP	C4'-O4'-C1'	2.50	115.46	109.51
5	D	711	UMP	C2'-C3'-C4'	2.47	107.82	102.80
4	A	610	NDP	O3X-P2B-O2B	-2.47	96.23	105.85
4	A	610	NDP	O3B-C3B-C4B	-2.46	104.03	111.08
4	A	610	NDP	C4B-O4B-C1B	-2.41	104.16	109.47
4	B	710	NDP	O4D-C1D-N1N	2.39	112.65	108.08
5	D	711	UMP	C2'-C1'-N1	2.39	119.78	113.81
5	D	711	UMP	C1'-N1-C2	2.38	122.32	117.66
5	D	711	UMP	O4'-C1'-C2'	-2.37	101.81	106.25
4	A	610	NDP	O2X-P2B-O2B	2.30	114.81	105.85
4	B	710	NDP	O3D-C3D-C4D	-2.28	104.53	111.08
4	A	610	NDP	O3D-C3D-C4D	-2.28	104.54	111.08
3	A	609	WRA	N6-C5-N4	-2.26	120.07	121.53
5	C	611	UMP	O4'-C1'-C2'	-2.24	102.07	106.25
4	B	710	NDP	N3A-C2A-N1A	-2.22	125.22	128.58
4	B	710	NDP	O2X-P2B-O2B	2.22	114.49	105.85
5	D	711	UMP	C6-N1-C2	2.21	123.69	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	611	UMP	C2'-C3'-C4'	2.14	107.14	102.80
4	B	710	NDP	O3X-P2B-O2X	-2.13	99.81	107.80
4	A	610	NDP	O2A-PA-O1A	2.10	122.22	112.44
4	A	610	NDP	C5B-C4B-C3B	2.09	122.72	115.21
4	A	610	NDP	O2N-PN-O1N	2.04	121.94	112.44

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	609	WRA	C5-N6-O7-C8
3	B	709	WRA	C1-N6-O7-C8
3	B	709	WRA	C5-N6-O7-C8
4	A	610	NDP	PA-O3-PN-O5D
4	A	610	NDP	C5D-O5D-PN-O1N
4	B	710	NDP	C5D-O5D-PN-O1N
4	B	710	NDP	C3B-C2B-O2B-P2B
4	B	710	NDP	PA-O3-PN-O5D
4	B	710	NDP	O4B-C4B-C5B-O5B
3	A	609	WRA	C1-N6-O7-C8
4	A	610	NDP	O4D-C1D-N1N-C2N
4	B	710	NDP	O4D-C1D-N1N-C2N
4	A	610	NDP	C2N-C3N-C7N-N7N
4	B	710	NDP	C2N-C3N-C7N-N7N
4	B	710	NDP	C2D-C1D-N1N-C2N
4	A	610	NDP	C2D-C1D-N1N-C2N
4	B	710	NDP	C3B-C4B-C5B-O5B
4	B	710	NDP	C1B-C2B-O2B-P2B
4	B	710	NDP	C2B-O2B-P2B-O1X
5	D	711	UMP	O4'-C4'-C5'-O5'

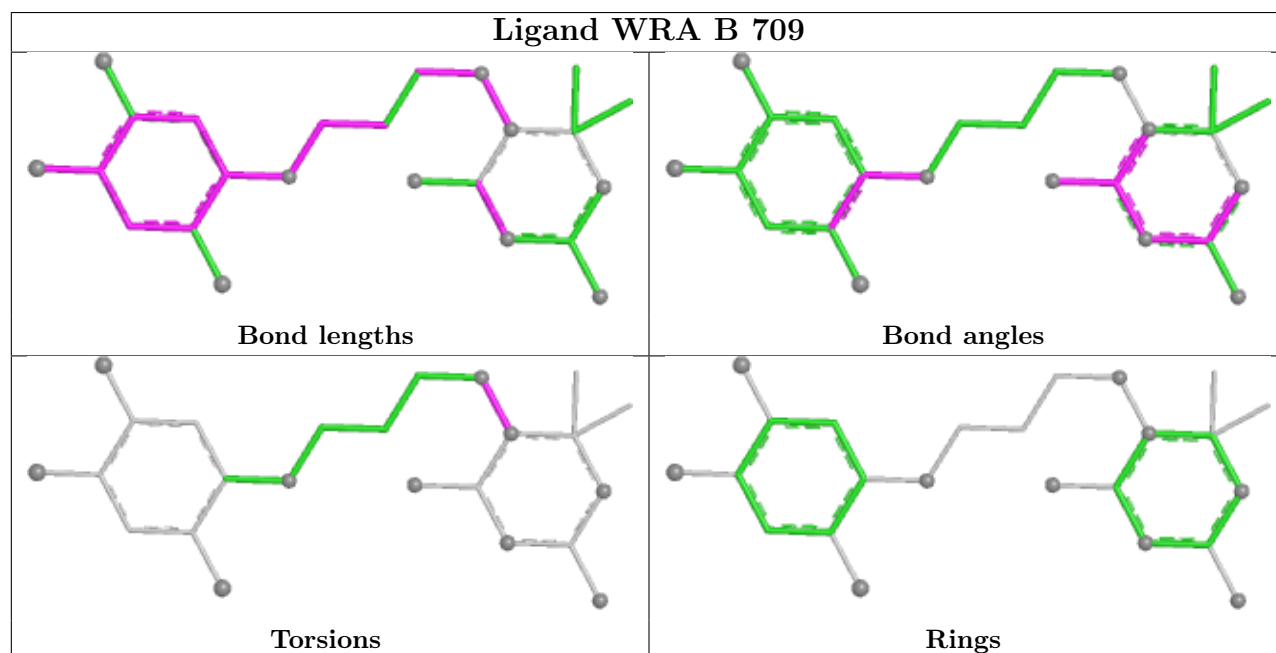
There are no ring outliers.

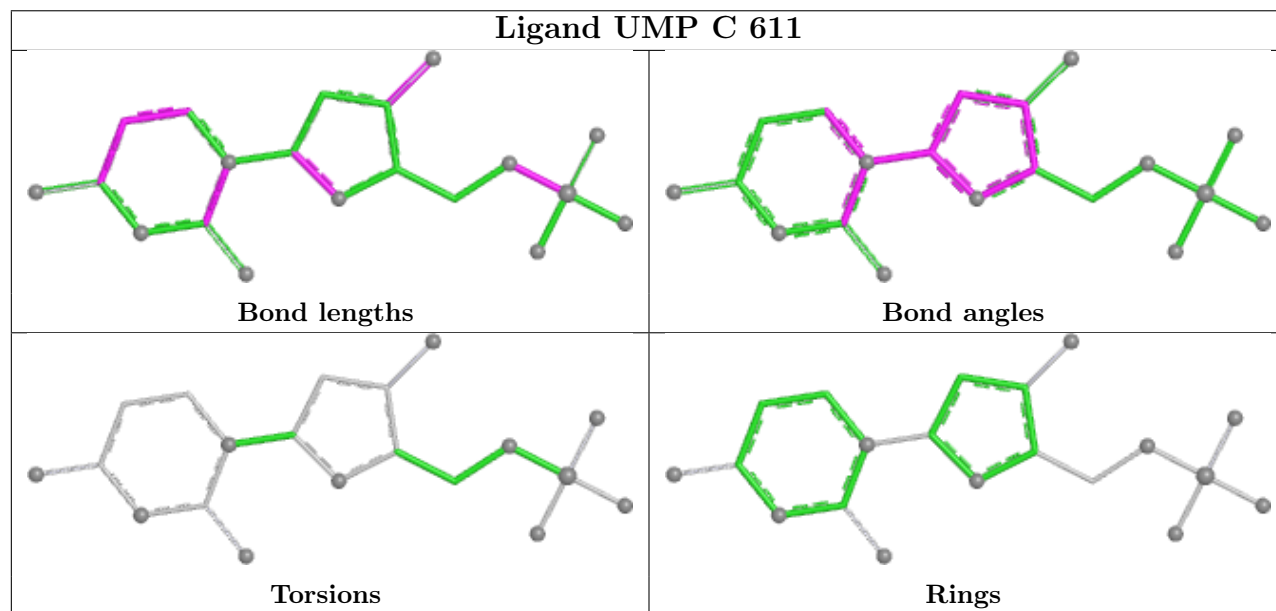
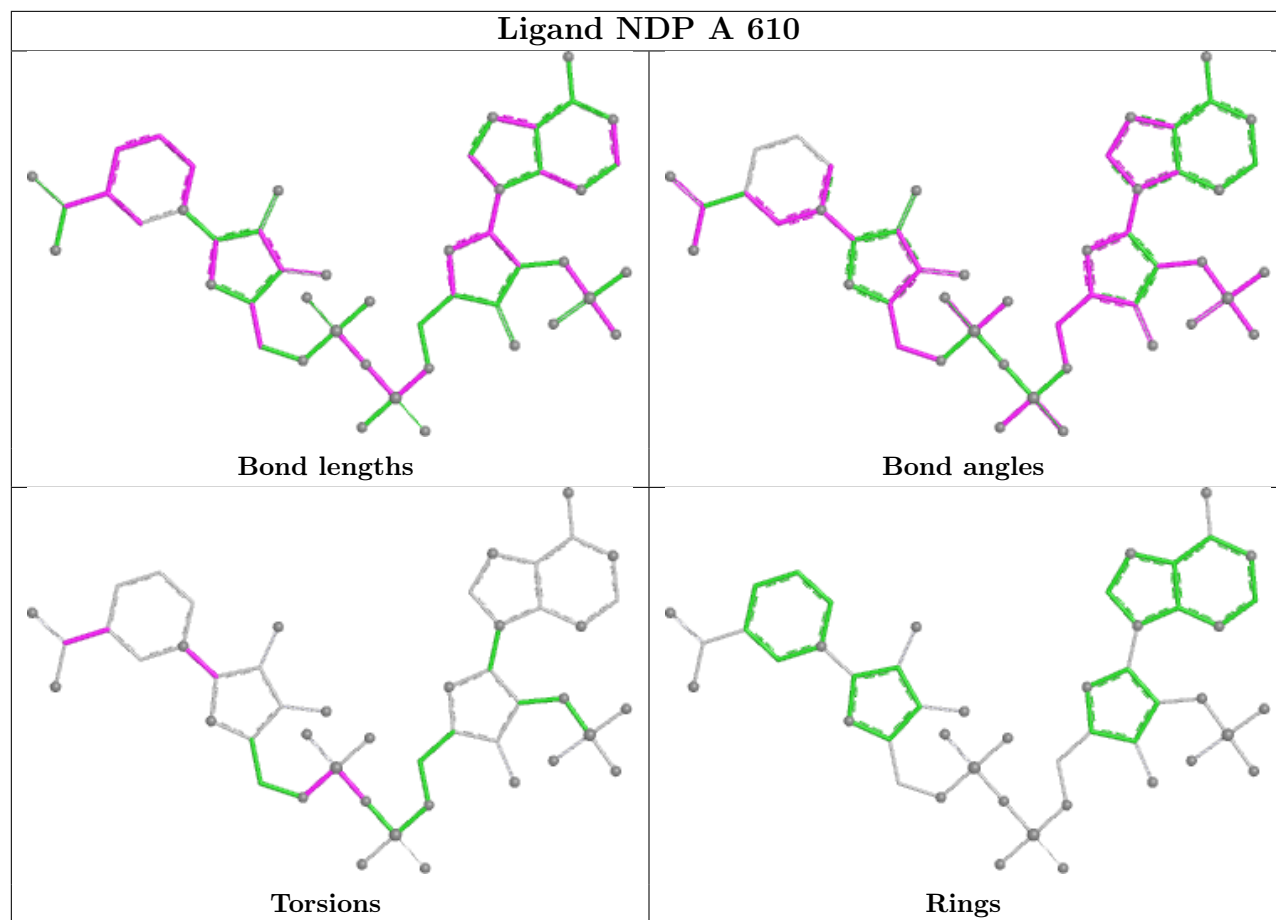
4 monomers are involved in 12 short contacts:

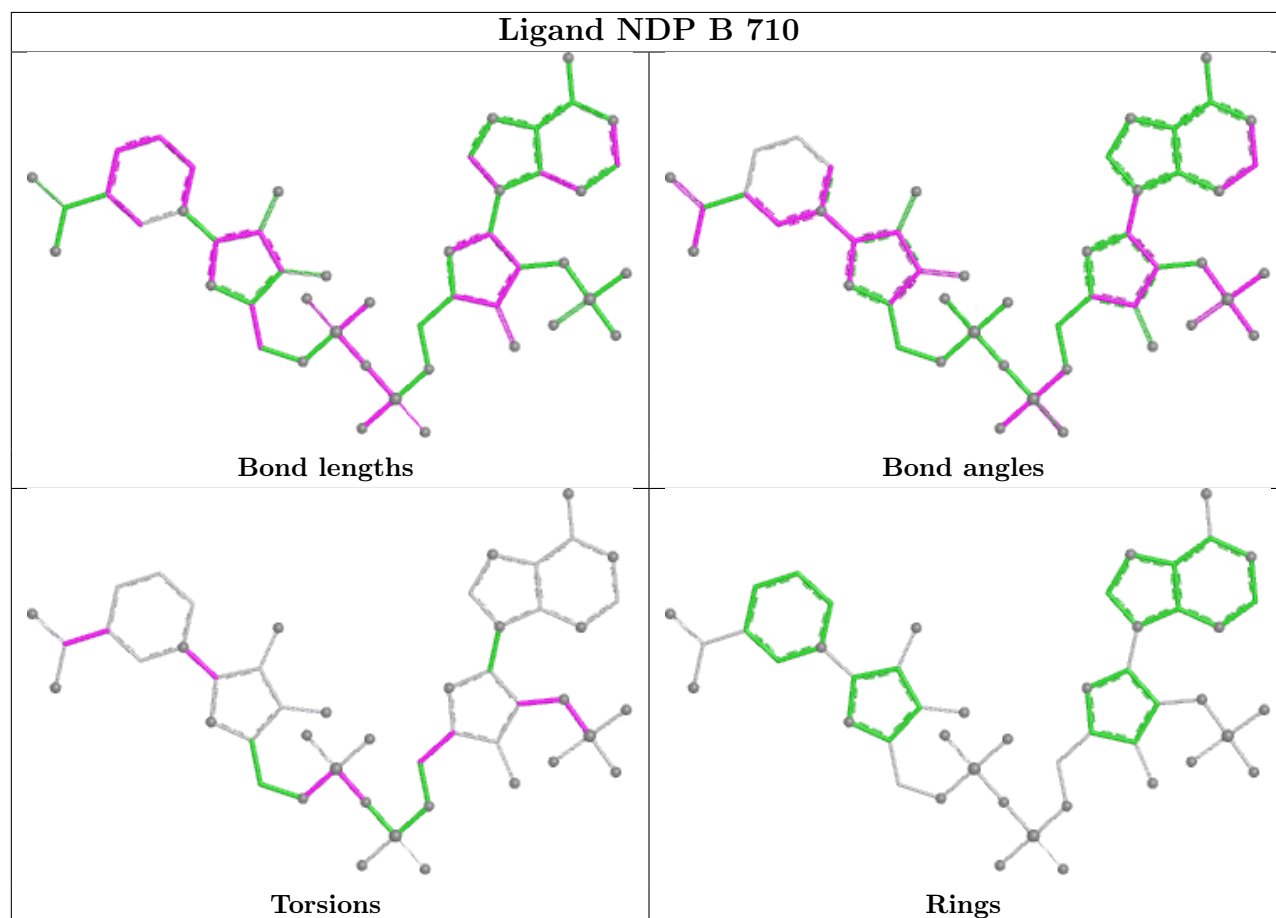
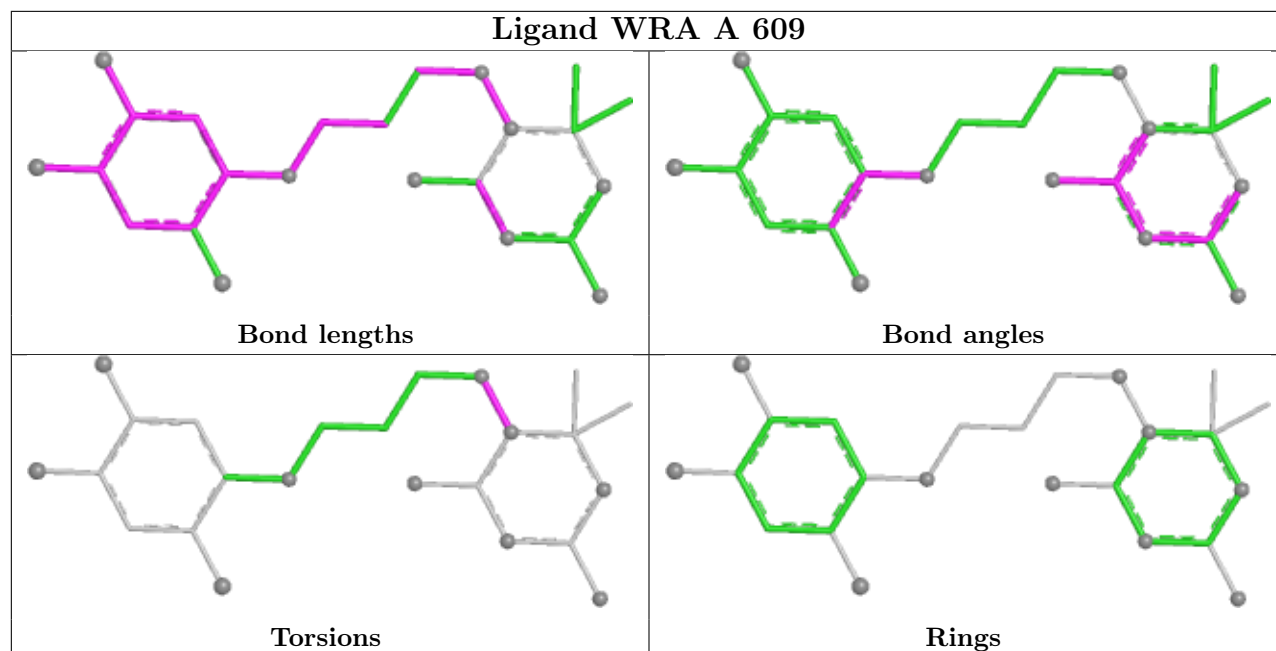
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	610	NDP	4	0
5	C	611	UMP	1	0
3	A	609	WRA	1	0
4	B	710	NDP	6	0

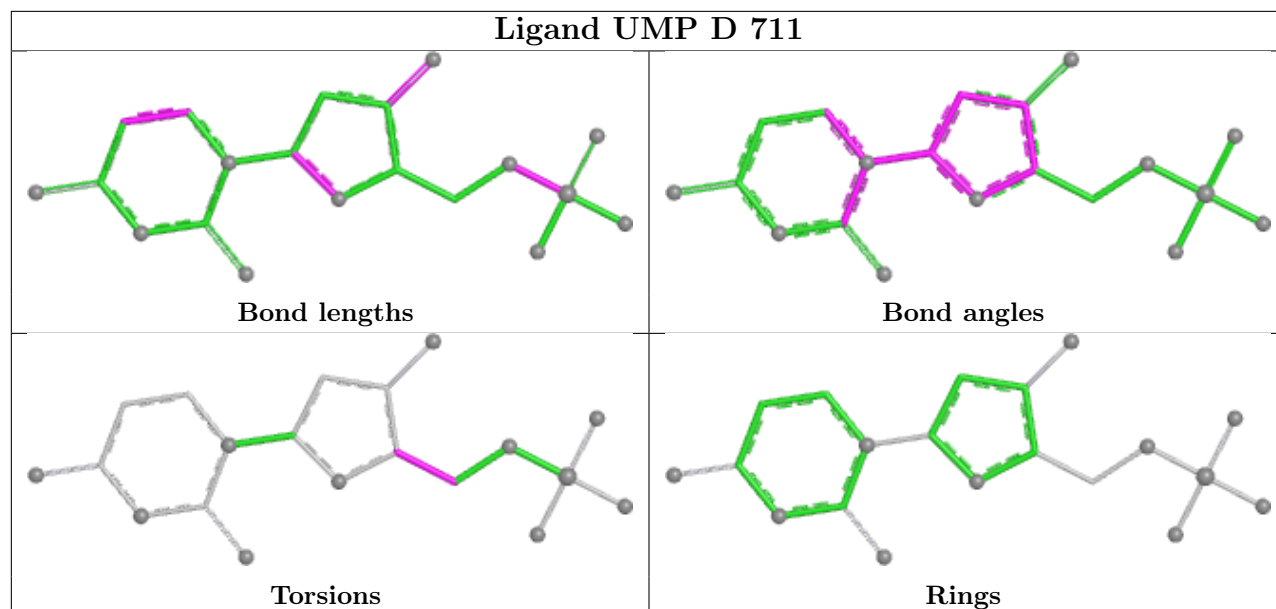
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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	221/280 (78%)	0.29	14 (6%) 26 27	23, 41, 87, 95	0
1	B	221/280 (78%)	1.52	65 (29%) 1 1	29, 73, 95, 95	0
2	C	326/328 (99%)	-0.19	13 (3%) 42 44	21, 31, 90, 95	0
2	D	326/328 (99%)	-0.15	15 (4%) 37 39	19, 32, 86, 95	0
All	All	1094/1216 (89%)	0.26	107 (9%) 13 13	19, 37, 94, 95	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	607	ALA	6.6
1	B	75	TYR	5.3
1	B	165	GLY	4.9
1	B	126	ILE	4.5
1	A	230	ASN	4.3
2	C	607	ALA	4.0
2	C	307	ILE	4.0
1	B	127	LEU	3.9
1	B	150	ILE	3.7
1	B	151	VAL	3.6
2	D	608	ALA	3.6
2	C	305	ASN	3.6
1	B	141	TYR	3.5
2	C	303	ASN	3.4
1	B	112	ILE	3.4
1	A	27	LYS	3.4
1	B	128	SER	3.3
2	D	305	ASN	3.3
1	B	22	SER	3.3
1	B	26	GLY	3.2
1	B	125	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	231	ASN	3.2
1	B	139	ASP	3.2
2	C	304	LYS	3.2
2	D	304	LYS	3.2
2	C	608	ALA	3.1
1	B	98	LEU	3.1
1	B	142	ILE	3.1
1	B	9	PHE	3.1
1	B	113	PRO	3.1
1	A	1	MET	3.1
1	B	105	GLY	3.0
1	B	146	VAL	3.0
1	B	66	ASN	3.0
1	B	107	THR	3.0
1	B	93	PRO	3.0
1	B	116	PHE	3.0
1	B	78	CYS	2.9
1	B	140	VAL	2.9
2	C	302	LYS	2.9
1	A	2	MET	2.9
2	C	606	MET	2.9
1	B	81	LEU	2.9
1	B	166	GLY	2.9
1	B	168	VAL	2.8
2	D	303	ASN	2.8
2	D	606	MET	2.8
1	B	149	LEU	2.8
1	B	5	VAL	2.8
2	D	307	ILE	2.8
1	B	104	MET	2.8
1	B	73	LEU	2.8
2	D	285	GLU	2.7
2	D	306	SER	2.7
1	B	153	LEU	2.6
1	A	24	ASN	2.6
1	B	119	LEU	2.6
1	B	2	MET	2.6
2	D	308	HIS	2.6
1	B	23	LYS	2.6
1	B	156	LEU	2.6
2	C	285	GLU	2.6
1	B	20	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	65	VAL	2.5
2	D	301	GLU	2.5
1	B	144	ASN	2.5
1	A	26	GLY	2.5
1	B	143	ILE	2.5
1	B	29	ASN	2.5
1	B	63	THR	2.4
1	B	130	THR	2.4
2	D	309	PRO	2.4
1	A	23	LYS	2.4
1	B	45	VAL	2.4
1	B	193	CYS	2.4
1	B	152	LEU	2.4
1	A	22	SER	2.4
2	C	308	HIS	2.4
1	B	44	GLY	2.4
2	C	605	ASP	2.4
1	B	14	ILE	2.4
1	B	24	ASN	2.3
1	B	230	ASN	2.3
1	B	148	ASP	2.3
1	B	196	PHE	2.3
1	B	95	SER	2.3
1	A	68	SER	2.3
1	B	136	PHE	2.3
1	B	46	LEU	2.3
1	B	8	VAL	2.2
1	B	61	VAL	2.2
2	C	309	PRO	2.2
1	A	29	ASN	2.2
2	D	310	ASN	2.2
1	B	1	MET	2.2
1	B	164	LEU	2.2
1	B	109	TRP	2.2
2	D	293	PHE	2.1
1	A	75	TYR	2.1
1	A	85	THR	2.1
1	B	77	ARG	2.1
1	B	195	VAL	2.1
2	D	299	LYS	2.1
1	B	103	VAL	2.1
2	C	293	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	163	ILE	2.0
1	A	8	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

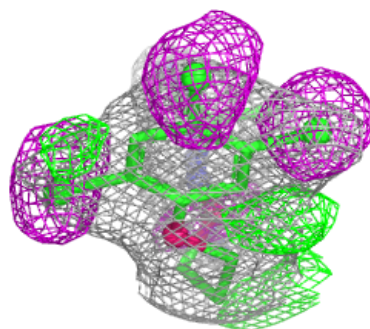
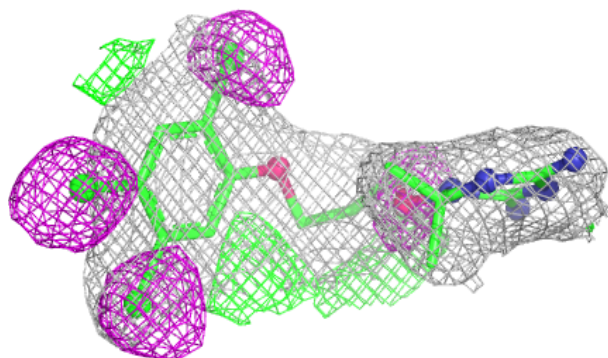
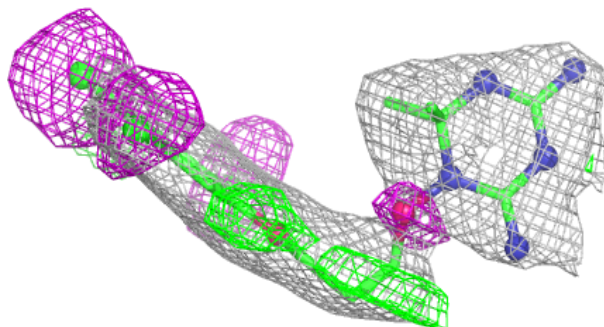
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	WRA	B	709	24/24	0.63	0.18	57,64,65,67	0
3	WRA	A	609	24/24	0.67	0.18	29,41,47,49	0
4	NDP	B	710	48/48	0.78	0.16	76,85,95,95	0
4	NDP	A	610	48/48	0.95	0.09	32,40,49,50	0
5	UMP	C	611	20/20	0.98	0.06	23,27,32,32	0
5	UMP	D	711	20/20	0.98	0.05	27,31,36,37	0

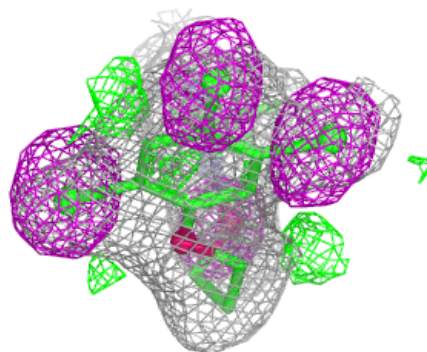
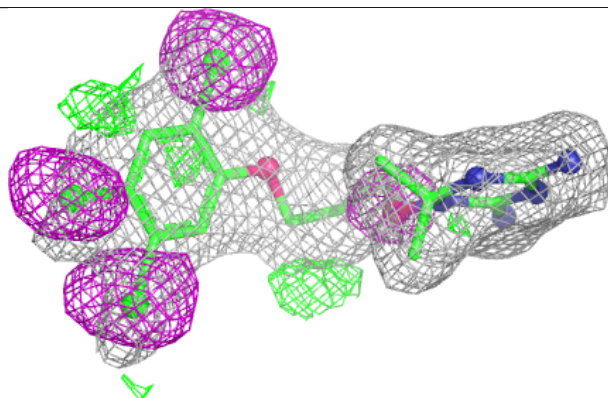
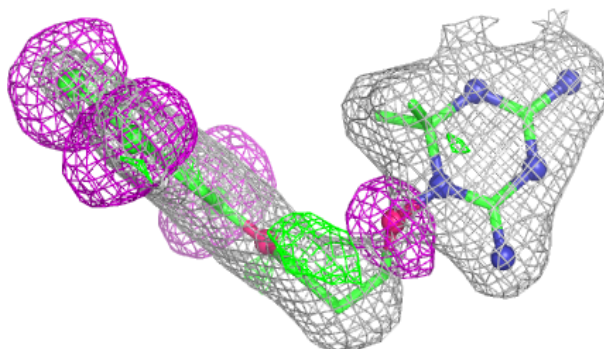
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around WRA B 709:

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

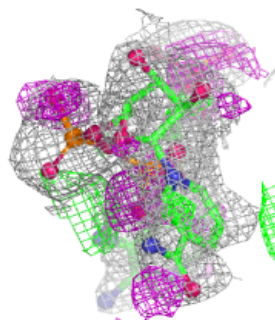
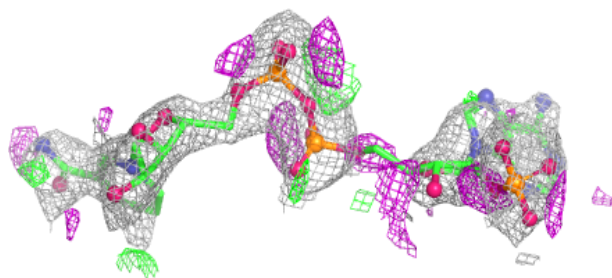
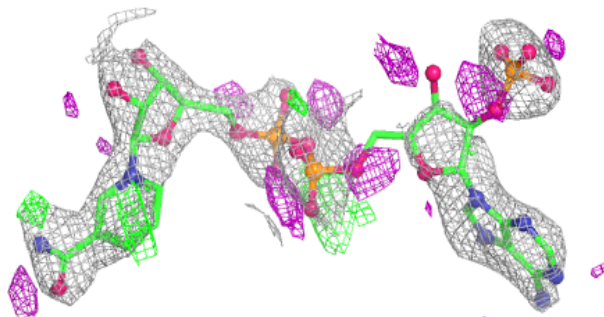
**Electron density around WRA A 609:**

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

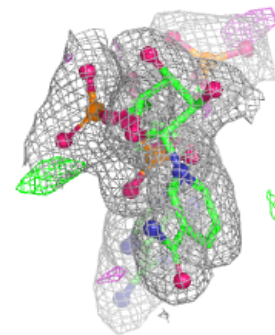
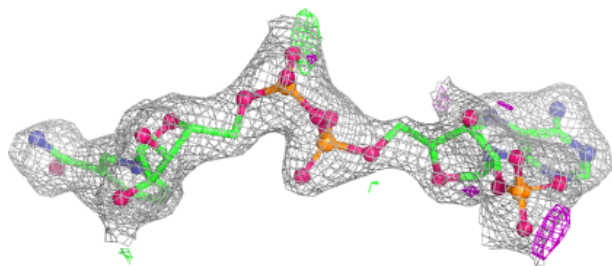
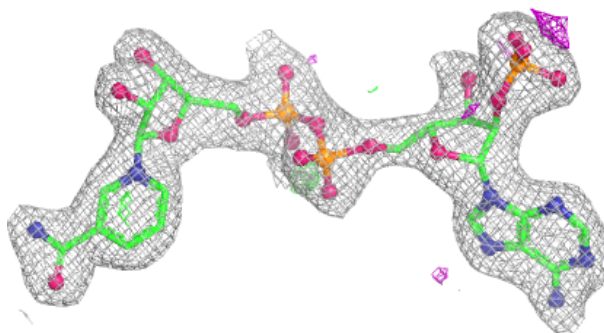


Electron density around NDP B 710:

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

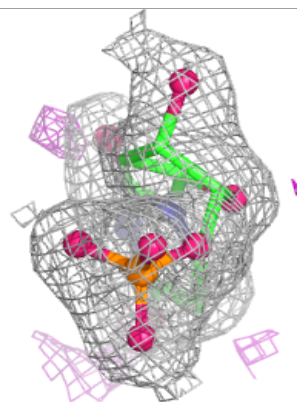
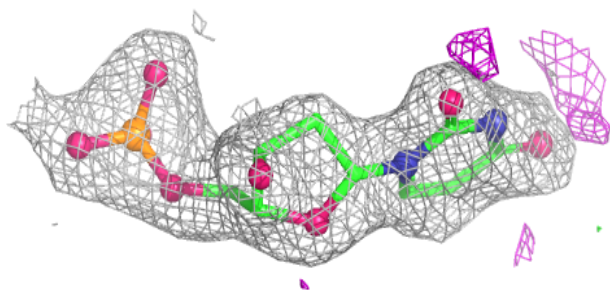
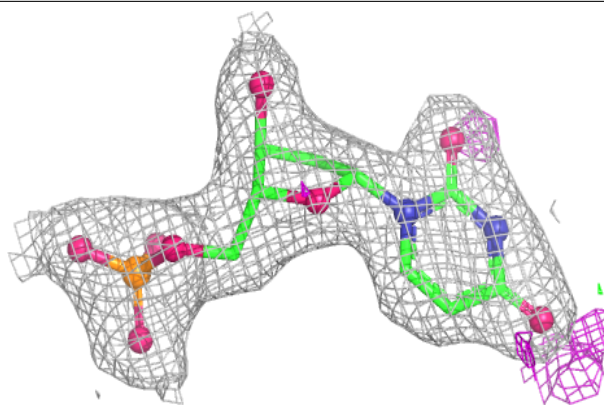
**Electron density around NDP A 610:**

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

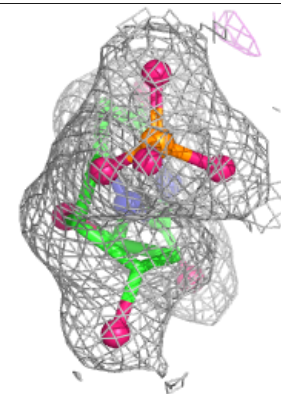
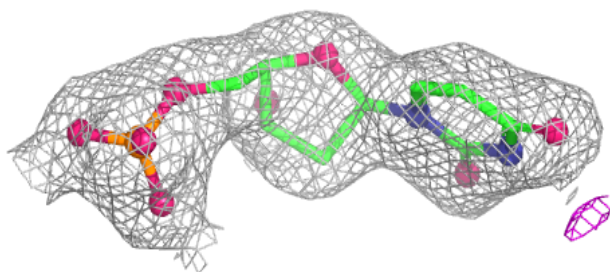
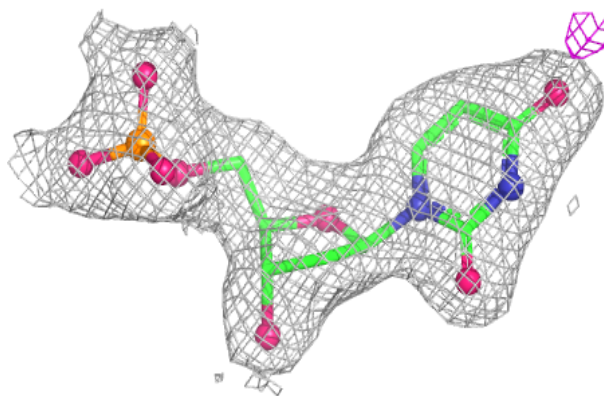


Electron density around UMP C 611:

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

**Electron density around UMP D 711:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.