



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:53 PM UTC

PDB ID : 1J3J / pdb_00001j3j
Title : Double mutant (C59R+S108N) Plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with pyrimethamine, 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 : 2.30 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

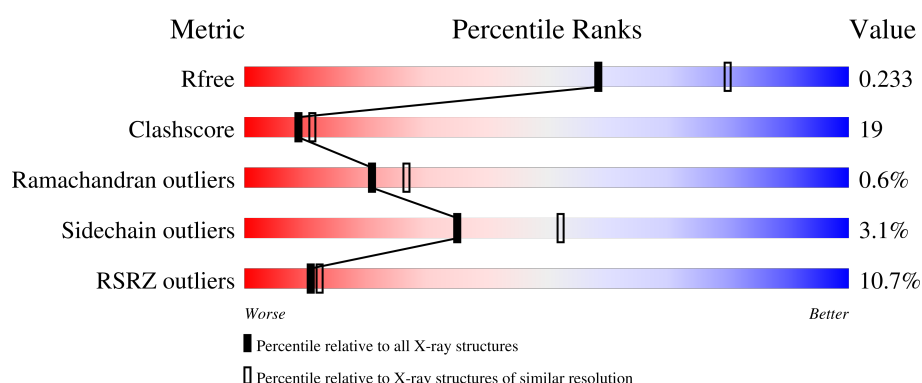
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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% 56% 20% •• 21%
1	B	280	22% 37% 33% 6% • 23%
2	C	328	6% 68% 26% 5% ••
2	D	328	6% 72% 24% •••

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9961 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	1188	298	339	12			
1	B	216	Total	C	N	O	S	0	0	0
			1795	1163	290	330	12			

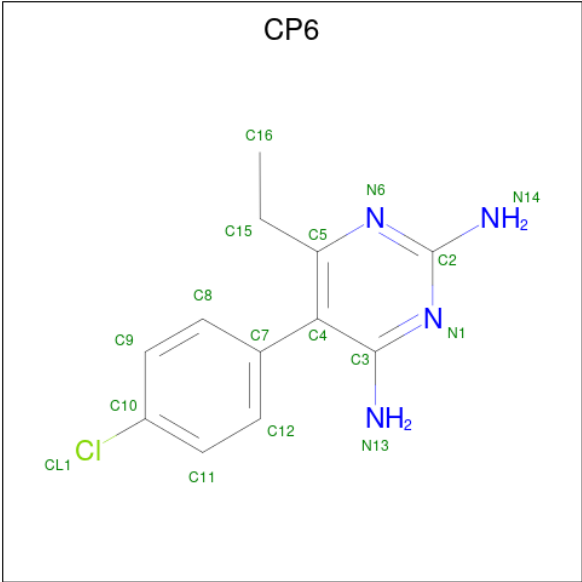
There are 4 discrepancies between the modelled and reference sequences:

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

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

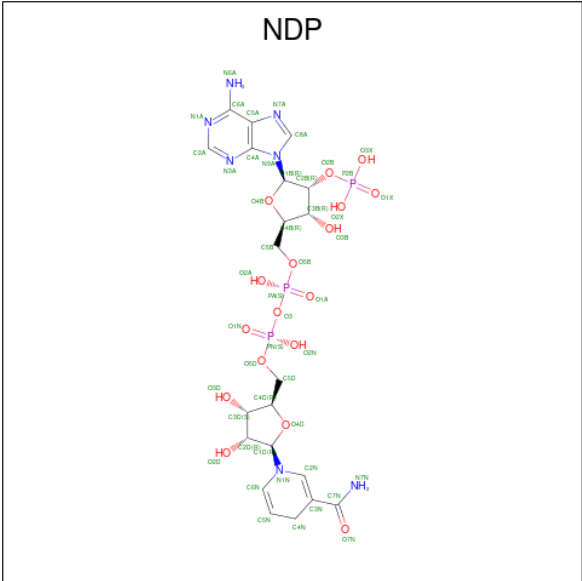
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	326	Total	C	N	O	S	0	0	0
			2713	1747	456	495	15			
2	D	326	Total	C	N	O	S	0	0	0
			2713	1747	456	495	15			

- Molecule 3 is 5-(4-CHLORO-PHENYL)-6-ETHYL-PYRIMIDINE-2,4-DIAMINE (CCD ID: CP6) (formula: C₁₂H₁₃ClN₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			17	12	1	4		
3	B	1	Total	C	Cl	N	0	0
			17	12	1	4		

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



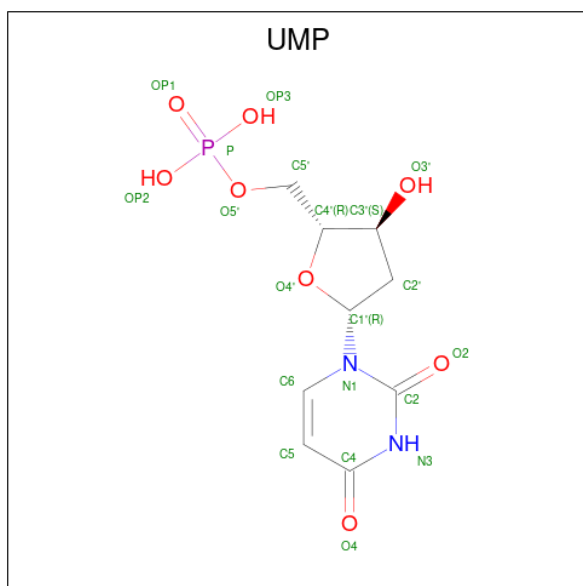
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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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		

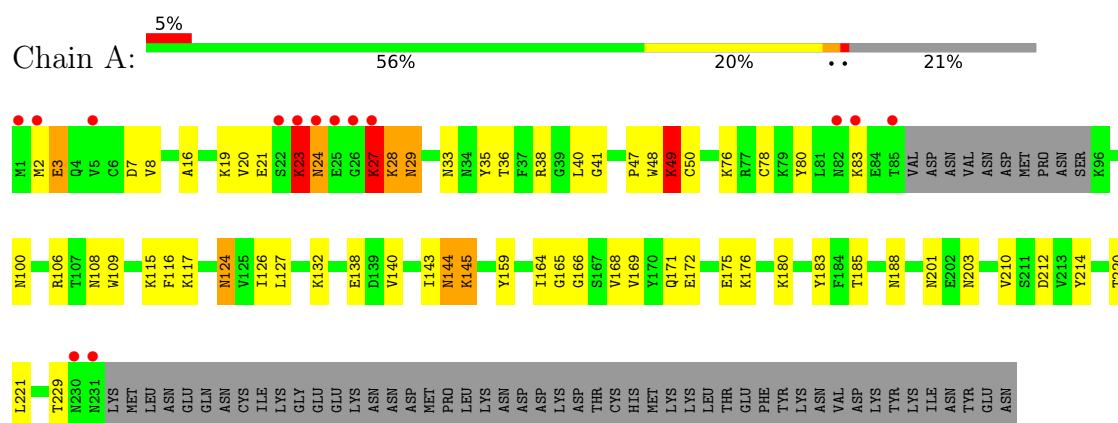
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	125	Total	O	0	0
			125	125		
6	B	60	Total	O	0	0
			60	60		
6	C	265	Total	O	0	0
			265	265		
6	D	283	Total	O	0	0
			283	283		

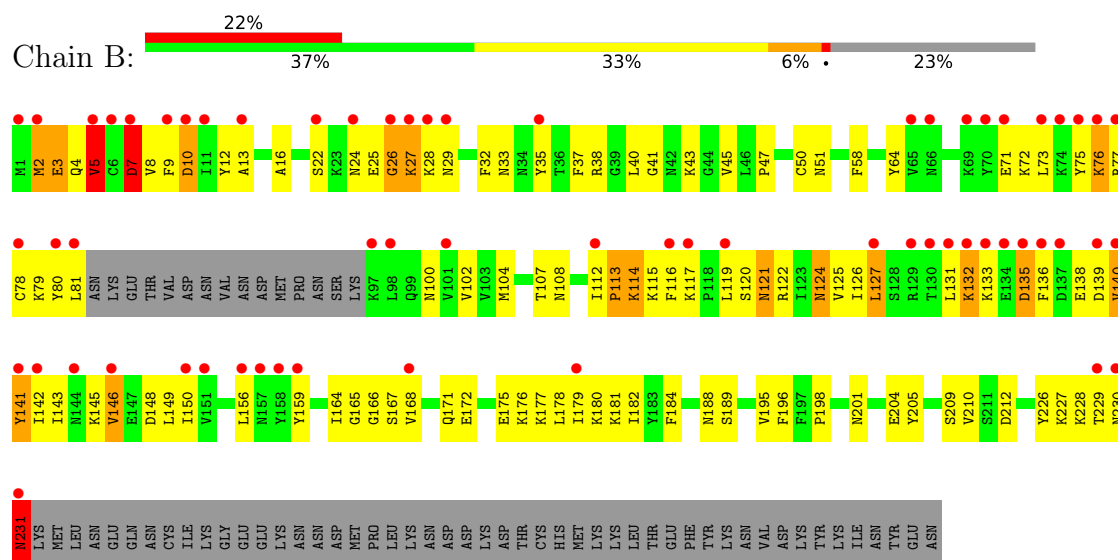
3 Residue-property plots

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.

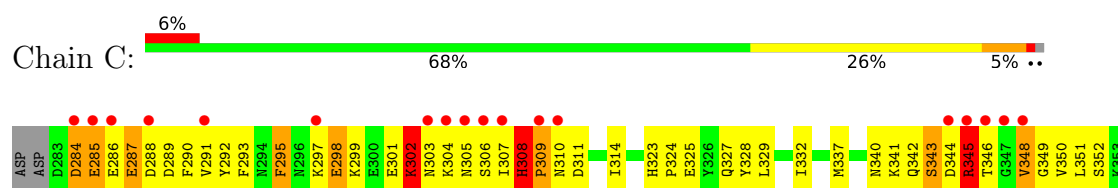
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

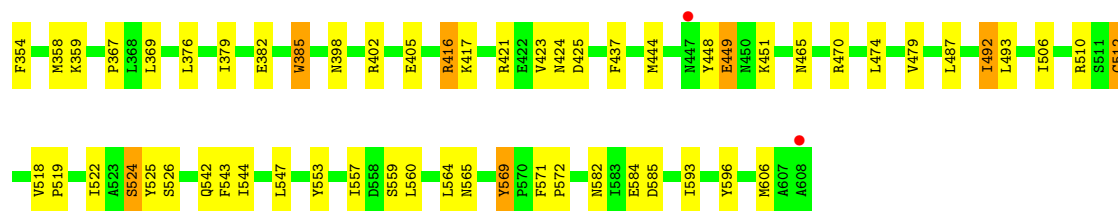


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

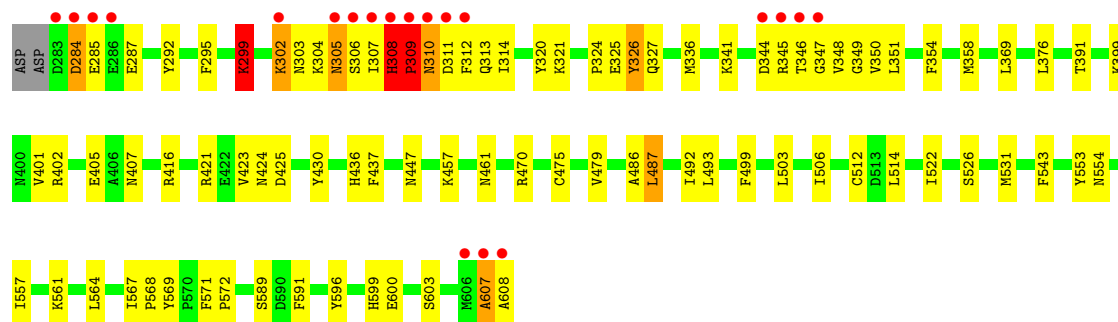


- Molecule 2: Bifunctional dihydrofolate reductase-thymidylate synthase





● 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	56.34Å 155.00Å 164.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.83 – 2.30 23.83 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.3 (23.83-2.30) 94.3 (23.83-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.231 0.198 , 0.233	Depositor DCC
R_{free} test set	3087 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9961	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: CP6, UMP, 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	0.64	0/1871	1.17	12/2515 (0.5%)
1	B	0.72	4/1829 (0.2%)	1.27	20/2460 (0.8%)
2	C	0.69	0/2784	1.28	37/3766 (1.0%)
2	D	0.67	0/2784	1.26	36/3766 (1.0%)
All	All	0.68	4/9268 (0.0%)	1.25	105/12507 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	VAL	N-CA	7.71	1.55	1.46
1	B	140	VAL	CA-C	7.16	1.61	1.52
1	B	3	GLU	CA-C	6.38	1.61	1.52
1	B	140	VAL	CA-CB	6.08	1.62	1.54

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	MET	N-CA-C	16.46	135.56	109.39
2	C	298	GLU	N-CA-C	-14.35	87.40	109.94
1	B	135	ASP	N-CA-C	13.35	127.06	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	310	ASN	N-CA-C	-12.32	98.23	113.01
1	A	23	LYS	N-CA-C	-12.09	91.49	109.62
1	A	229	THR	N-CA-C	10.62	125.00	110.35
2	C	348	VAL	N-CA-C	10.47	120.46	110.30
1	B	72	LYS	N-CA-C	-10.30	99.98	112.54
2	D	310	ASN	N-CA-C	-10.26	99.92	111.71
2	D	308	HIS	CA-C-N	10.23	131.34	119.47
2	D	308	HIS	C-N-CA	10.23	131.34	119.47
2	D	314	ILE	N-CA-C	-10.06	103.16	111.81
2	C	299	LYS	N-CA-C	-9.78	102.14	114.56
2	C	286	GLU	N-CA-C	-9.75	101.58	113.19
2	C	345	ARG	N-CA-C	-9.53	92.85	109.06
1	B	3	GLU	N-CA-C	9.27	124.46	112.41
2	C	307	ILE	N-CA-C	9.18	121.31	111.58
2	D	284	ASP	N-CA-C	-8.56	102.84	113.28
1	A	138	GLU	N-CA-C	8.48	121.73	110.53
2	D	309	PRO	N-CA-C	8.34	125.91	113.81
2	D	543	PHE	N-CA-C	-8.16	95.22	108.52
1	A	29	ASN	N-CA-C	-7.91	98.74	110.06
2	D	308	HIS	N-CA-C	7.80	127.04	109.81
2	D	347	GLY	N-CA-C	-7.79	104.80	114.92
2	C	492	ILE	N-CA-C	7.71	117.82	110.42
2	C	351	LEU	N-CA-C	-7.64	96.44	108.90
1	B	27	LYS	N-CA-C	7.57	119.93	109.18
2	D	492	ILE	N-CA-C	7.39	117.51	110.42
1	B	141	TYR	N-CA-C	7.38	126.52	110.80
2	D	302	LYS	N-CA-C	7.38	123.47	111.37
1	A	164	ILE	N-CA-C	7.31	119.16	112.29
2	D	486	ALA	N-CA-C	-7.26	102.55	111.33
1	A	27	LYS	CA-C-N	-6.99	111.86	122.21
1	A	27	LYS	C-N-CA	-6.99	111.86	122.21
2	D	526	SER	N-CA-C	-6.98	103.10	111.69
2	D	401	VAL	N-CA-C	-6.97	96.20	107.28
2	C	416	ARG	N-CA-C	-6.91	104.46	113.17
2	C	309	PRO	N-CA-C	6.88	122.46	113.86
2	D	607	ALA	N-CA-C	6.85	118.82	111.36
2	D	416	ARG	N-CA-C	-6.83	104.57	113.17
2	C	512	CYS	N-CA-C	6.80	119.50	108.34
2	C	298	GLU	N-CA-CB	-6.71	97.92	110.07
1	A	188	ASN	N-CA-C	6.69	121.07	110.70
2	C	302	LYS	N-CA-C	6.68	125.03	110.80
2	C	367	PRO	N-CA-C	6.64	121.44	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	VAL	N-CA-C	6.61	123.09	109.34
1	B	212	ASP	N-CA-C	-6.57	102.06	110.53
1	B	140	VAL	N-CA-C	6.55	122.96	109.34
1	B	230	ASN	N-CA-C	-6.54	103.84	112.34
2	C	449	GLU	N-CA-C	6.54	120.32	110.64
2	C	308	HIS	CA-C-N	6.54	126.16	119.56
2	C	308	HIS	C-N-CA	6.54	126.16	119.56
2	D	351	LEU	N-CA-C	-6.51	98.29	108.90
2	C	543	PHE	N-CA-C	-6.51	97.80	108.41
2	D	603	SER	N-CA-C	-6.40	98.30	108.73
1	B	10	ASP	N-CA-C	6.34	119.84	111.28
2	D	514	LEU	N-CA-C	6.34	117.85	111.07
1	B	188	ASN	N-CA-C	6.28	119.04	109.62
2	C	557	ILE	N-CA-C	6.22	116.70	110.23
2	D	503	LEU	N-CA-C	6.19	119.04	109.07
2	C	425	ASP	N-CA-C	-6.12	97.23	107.99
1	B	139	ASP	N-CA-C	-6.11	105.92	113.19
2	D	327	GLN	N-CA-C	-6.10	104.64	111.28
2	C	343	SER	CA-C-N	6.08	129.95	120.82
2	C	343	SER	C-N-CA	6.08	129.95	120.82
1	B	133	LYS	N-CA-C	-6.02	104.72	111.28
2	D	299	LYS	N-CA-C	6.00	117.82	111.28
1	B	26	GLY	N-CA-C	5.97	122.82	113.86
2	D	436	HIS	N-CA-C	5.90	119.61	111.71
2	D	304	LYS	N-CA-C	-5.85	104.90	111.28
1	B	120	SER	N-CA-C	5.74	118.55	110.23
2	D	569	TYR	N-CA-C	-5.71	102.92	110.40
2	D	512	CYS	N-CA-C	5.70	117.68	108.34
1	B	2	MET	CB-CA-C	-5.64	102.91	112.00
2	D	391	THR	N-CA-C	-5.64	104.28	113.19
1	B	7	ASP	N-CA-C	-5.56	105.14	111.14
2	C	352	SER	N-CA-C	5.50	117.55	109.24
1	A	183	TYR	N-CA-C	-5.50	99.55	108.41
2	D	425	ASP	N-CA-C	-5.46	98.38	107.99
2	C	298	GLU	CA-CB-CG	-5.45	103.19	114.10
1	A	24	ASN	N-CA-C	-5.44	102.14	110.30
2	D	475	CYS	N-CA-C	5.41	117.78	109.07
2	D	405	GLU	N-CA-C	5.41	117.60	111.11
2	C	444	MET	N-CA-C	5.41	119.36	112.87
2	C	298	GLU	CA-C-N	-5.38	113.85	122.08
2	C	298	GLU	C-N-CA	-5.38	113.85	122.08
2	C	526	SER	N-CA-C	-5.37	105.51	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	487	LEU	CA-C-N	5.35	123.56	119.66
2	D	487	LEU	C-N-CA	5.35	123.56	119.66
2	D	399	LYS	N-CA-C	-5.31	106.03	112.88
1	B	45	VAL	N-CA-C	5.23	115.19	108.82
2	C	295	PHE	N-CA-C	5.22	118.75	112.38
2	D	599	HIS	N-CA-C	-5.22	103.80	110.53
2	C	385	TRP	N-CA-C	-5.20	105.51	111.07
1	A	27	LYS	N-CA-C	5.15	118.55	107.67
1	B	231	ASN	N-CA-CB	-5.15	101.75	110.50
1	A	212	ASP	N-CA-C	-5.14	103.74	110.53
2	C	474	LEU	N-CA-C	-5.12	99.06	108.02
2	C	585	ASP	N-CA-C	5.12	119.51	113.16
2	C	327	GLN	N-CA-C	-5.11	105.89	111.82
2	C	285	GLU	N-CA-C	-5.11	106.90	113.23
2	C	593	ILE	N-CA-C	-5.06	101.12	108.36
2	D	376	LEU	N-CA-C	5.05	121.14	114.12
2	C	569	TYR	N-CA-C	-5.03	103.20	110.40
2	D	402	ARG	N-CA-C	5.01	118.43	112.72

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	525	TYR	Sidechain
2	D	326	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	1868	61	0
1	B	1795	0	1823	138	0
2	C	2713	0	2638	82	0
2	D	2713	0	2638	69	0
3	A	17	0	13	0	0
3	B	17	0	13	2	0
4	A	48	0	26	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	48	0	26	12	0
5	C	20	0	11	0	0
5	D	20	0	11	0	0
6	A	125	0	0	5	0
6	B	60	0	0	39	0
6	C	265	0	0	12	0
6	D	283	0	0	24	0
All	All	9961	0	9067	339	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 19.

All (339) 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:78:CYS:HA	6:B:1635:HOH:O	1.40	1.20
1:B:178:LEU:HG	6:B:1639:HOH:O	1.43	1.19
1:B:2:MET:HE2	1:B:2:MET:HA	1.22	1.14
2:C:346:THR:HA	6:C:1377:HOH:O	1.48	1.12
1:A:165:GLY:HA3	4:A:610:NDP:H5N	1.31	1.11
2:D:309:PRO:HA	6:D:1684:HOH:O	1.49	1.09
1:A:140:VAL:HB	6:A:1679:HOH:O	1.55	1.06
1:B:131:LEU:HB3	6:B:1628:HOH:O	1.56	1.05
1:B:4:GLN:O	1:B:8:VAL:HG23	1.57	1.03
1:B:114:LYS:HD2	1:B:114:LYS:H	1.24	0.98
1:B:179:ILE:HG23	6:B:1640:HOH:O	1.68	0.94
1:B:140:VAL:HG12	1:B:140:VAL:O	1.67	0.93
1:B:4:GLN:HG3	1:B:7:ASP:OD2	1.69	0.93
1:B:210:VAL:HB	6:B:1645:HOH:O	1.69	0.91
1:B:24:ASN:HB3	6:B:1001:HOH:O	1.69	0.91
1:A:3:GLU:OE1	1:A:80:TYR:HD1	1.51	0.91
2:C:344:ASP:HB2	2:D:470:ARG:NH1	1.87	0.88
1:B:12:TYR:HA	6:B:1640:HOH:O	1.73	0.88
2:C:344:ASP:HB2	2:D:470:ARG:HH12	1.39	0.88
1:B:176:LYS:C	6:B:1639:HOH:O	2.17	0.87
1:B:136:PHE:CE2	6:B:1628:HOH:O	2.28	0.86
1:B:138:GLU:O	1:B:141:TYR:CE1	2.30	0.84
2:C:345:ARG:HE	2:C:348:VAL:HG21	1.41	0.83
1:B:136:PHE:HE2	6:B:1628:HOH:O	1.60	0.83
1:B:2:MET:HE2	1:B:2:MET:CA	2.07	0.82
2:C:332:ILE:HD13	2:C:560:LEU:HD22	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:MET:HA	1:B:2:MET:CE	2.10	0.81
2:D:348:VAL:HA	6:D:1314:HOH:O	1.79	0.81
1:B:165:GLY:HA3	4:B:710:NDP:H5N	1.61	0.81
2:C:376:LEU:HD22	2:C:379:ILE:HD11	1.63	0.80
1:B:81:LEU:HD12	6:B:1635:HOH:O	1.80	0.80
1:A:78:CYS:HB3	1:A:83:LYS:O	1.84	0.78
4:B:710:NDP:H52N	6:B:1627:HOH:O	1.82	0.77
2:C:303:ASN:HB3	2:C:306:SER:OG	1.85	0.76
1:B:124:ASN:H	1:B:124:ASN:HD22	1.30	0.76
1:B:124:ASN:HD22	1:B:124:ASN:N	1.84	0.75
1:B:29:ASN:HB2	1:B:32:PHE:CE1	2.22	0.75
1:B:177:LYS:HD3	6:B:1638:HOH:O	1.87	0.73
4:A:610:NDP:H8A	4:A:610:NDP:H52A	1.71	0.73
1:B:4:GLN:C	1:B:8:VAL:HG23	2.14	0.73
2:C:285:GLU:C	2:C:287:GLU:H	1.94	0.73
1:A:126:ILE:HG13	6:A:1679:HOH:O	1.90	0.72
1:B:41:GLY:HA2	1:B:47:PRO:HD3	1.73	0.71
1:B:182:ILE:HB	1:B:226:TYR:HB2	1.72	0.71
1:B:9:PHE:HE2	1:B:80:TYR:HE2	1.38	0.71
1:B:107:THR:HB	4:B:710:NDP:O2A	1.91	0.71
1:B:8:VAL:HG22	6:B:1636:HOH:O	1.90	0.70
1:B:81:LEU:CD1	6:B:1635:HOH:O	2.38	0.70
1:B:112:ILE:HB	1:B:117:LYS:HD3	1.74	0.69
2:D:457:LYS:HE2	6:D:1229:HOH:O	1.93	0.69
1:A:171:GLN:HG3	1:A:175:GLU:OE2	1.93	0.68
1:B:3:GLU:HG2	1:B:80:TYR:HE1	1.59	0.68
2:C:284:ASP:O	2:C:287:GLU:HB3	1.93	0.68
2:C:309:PRO:C	2:C:311:ASP:H	2.00	0.68
1:A:210:VAL:HG12	6:A:1665:HOH:O	1.93	0.68
2:D:447:ASN:HA	6:D:1220:HOH:O	1.94	0.68
2:D:308:HIS:O	2:D:311:ASP:HB2	1.94	0.68
1:B:40:LEU:O	4:B:710:NDP:H2N	1.94	0.67
1:B:171:GLN:HG3	1:B:175:GLU:OE2	1.95	0.67
1:B:71:GLU:O	1:B:75:TYR:HB2	1.95	0.67
1:A:48:TRP:O	1:A:49:LYS:HB2	1.95	0.67
2:C:309:PRO:C	2:C:311:ASP:N	2.49	0.67
1:B:171:GLN:O	1:B:175:GLU:HG3	1.95	0.67
2:C:285:GLU:C	2:C:287:GLU:N	2.51	0.66
1:A:24:ASN:HB2	1:A:28:LYS:HE2	1.77	0.66
2:C:376:LEU:HD22	2:C:379:ILE:CD1	2.26	0.66
4:B:710:NDP:H6N	6:B:1627:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:VAL:O	1:B:140:VAL:CG1	2.42	0.65
2:C:344:ASP:CG	2:C:345:ARG:HG2	2.22	0.65
2:C:344:ASP:OD1	2:C:345:ARG:N	2.31	0.64
1:B:114:LYS:H	1:B:114:LYS:CD	1.99	0.64
1:B:229:THR:C	1:B:231:ASN:N	2.52	0.64
2:C:493:LEU:C	2:C:493:LEU:HD12	2.22	0.63
1:B:13:ALA:N	6:B:1640:HOH:O	2.31	0.63
1:A:106:ARG:HE	4:A:610:NDP:P2B	2.22	0.63
2:C:344:ASP:O	6:C:1185:HOH:O	2.15	0.63
1:B:176:LYS:O	6:B:1639:HOH:O	2.15	0.62
2:D:421:ARG:NE	6:D:1206:HOH:O	2.20	0.62
1:B:76:LYS:HA	1:B:79:LYS:HB3	1.81	0.62
1:B:121:ASN:N	1:B:121:ASN:HD22	1.97	0.62
2:C:341:LYS:HE3	6:C:1362:HOH:O	2.00	0.62
1:A:127:LEU:HD23	1:A:143:ILE:HG13	1.81	0.61
1:B:104:MET:HB2	1:B:108:ASN:HD22	1.65	0.61
1:A:41:GLY:HA2	1:A:47:PRO:HD3	1.81	0.61
1:B:127:LEU:HD12	1:B:143:ILE:HD11	1.81	0.61
1:B:9:PHE:CE2	1:B:80:TYR:HE2	2.18	0.61
1:B:229:THR:C	1:B:231:ASN:H	2.08	0.61
2:D:310:ASN:O	2:D:313:GLN:HB2	2.00	0.61
1:A:27:LYS:HD2	1:A:27:LYS:O	2.01	0.60
1:A:108:ASN:OD1	4:A:610:NDP:H2D	2.01	0.60
1:B:8:VAL:CG2	6:B:1636:HOH:O	2.47	0.60
2:C:287:GLU:O	2:C:290:PHE:HB3	2.02	0.60
2:D:421:ARG:NH2	6:D:1206:HOH:O	2.22	0.60
2:D:493:LEU:HD12	2:D:493:LEU:C	2.27	0.60
1:B:29:ASN:HD22	1:B:32:PHE:HE1	1.49	0.59
2:C:542:GLN:NE2	6:C:1046:HOH:O	2.30	0.59
1:A:2:MET:O	1:A:2:MET:HG3	2.03	0.59
1:A:210:VAL:CG1	6:A:1665:HOH:O	2.49	0.59
1:B:9:PHE:HE2	1:B:80:TYR:CE2	2.19	0.59
1:B:166:GLY:HA2	4:B:710:NDP:C5N	2.33	0.59
1:A:27:LYS:C	1:A:29:ASN:H	2.11	0.58
1:B:171:GLN:HE21	1:B:175:GLU:CG	2.16	0.58
2:C:301:GLU:O	2:C:304:LYS:HG3	2.02	0.58
2:D:457:LYS:HG2	6:D:1229:HOH:O	2.03	0.58
1:B:9:PHE:HZ	1:B:81:LEU:HD23	1.69	0.58
1:B:25:GLU:HA	1:B:25:GLU:OE1	2.03	0.58
2:C:344:ASP:OD2	2:C:345:ARG:HG2	2.04	0.58
2:D:303:ASN:HB3	2:D:306:SER:OG	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:301:GLU:OE1	2:C:337:MET:HE3	2.03	0.58
1:A:40:LEU:O	4:A:610:NDP:H2N	2.02	0.58
1:B:5:VAL:HA	1:B:8:VAL:HB	1.86	0.58
1:A:109:TRP:CE2	1:A:117:LYS:HD2	2.39	0.58
1:B:3:GLU:N	6:B:1636:HOH:O	2.37	0.57
2:C:301:GLU:OE1	2:C:337:MET:CE	2.52	0.57
2:D:346:THR:CG2	2:D:348:VAL:HG23	2.34	0.57
1:A:109:TRP:CZ2	1:A:117:LYS:HD2	2.39	0.57
1:B:210:VAL:HG23	1:B:210:VAL:O	2.05	0.57
2:C:465:ASN:O	2:D:345:ARG:NH2	2.38	0.57
2:C:284:ASP:OD1	2:C:284:ASP:N	2.38	0.56
2:D:344:ASP:C	2:D:346:THR:H	2.13	0.56
1:A:3:GLU:OE1	1:A:80:TYR:CD1	2.44	0.56
1:B:115:LYS:C	6:B:1631:HOH:O	2.49	0.56
1:B:131:LEU:HD22	6:B:1628:HOH:O	2.04	0.56
2:D:561:LYS:NZ	6:D:1606:HOH:O	2.37	0.56
2:C:344:ASP:OD2	2:C:553:TYR:HE1	1.88	0.55
2:D:421:ARG:CZ	6:D:1206:HOH:O	2.53	0.55
1:B:121:ASN:N	1:B:121:ASN:ND2	2.52	0.55
2:D:336:MET:HE2	2:D:557:ILE:HG23	1.89	0.55
1:A:124:ASN:N	1:A:124:ASN:HD22	2.05	0.55
1:B:168:VAL:HG11	4:B:710:NDP:H8A	1.88	0.55
2:C:301:GLU:CG	2:C:304:LYS:HE2	2.37	0.55
1:A:172:GLU:OE2	4:A:610:NDP:N7A	2.40	0.54
1:B:9:PHE:CE2	1:B:80:TYR:CE2	2.95	0.54
2:C:340:ASN:HB3	2:D:499:PHE:CE1	2.42	0.54
1:A:24:ASN:HB2	1:A:28:LYS:CE	2.38	0.54
1:A:169:VAL:HG23	4:A:610:NDP:O1A	2.08	0.54
2:C:344:ASP:CB	2:D:470:ARG:HH12	2.18	0.54
2:D:358:MET:HE1	2:D:522:ILE:HD11	1.90	0.54
1:B:9:PHE:CZ	1:B:81:LEU:HD23	2.42	0.54
1:B:142:ILE:HG22	1:B:143:ILE:N	2.23	0.54
2:C:350:VAL:HG12	2:C:553:TYR:CD1	2.43	0.54
1:B:12:TYR:CD1	1:B:181:LYS:HB2	2.43	0.53
1:B:167:SER:HB3	4:B:710:NDP:O2N	2.08	0.53
1:A:166:GLY:HA2	4:A:610:NDP:C5N	2.39	0.53
1:B:5:VAL:HG11	1:B:150:ILE:HD12	1.91	0.53
2:D:309:PRO:N	6:D:1683:HOH:O	2.41	0.53
1:B:12:TYR:CE1	1:B:180:LYS:HD3	2.44	0.53
1:B:131:LEU:HD13	6:B:1628:HOH:O	2.07	0.53
1:B:12:TYR:CA	6:B:1640:HOH:O	2.45	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LEU:O	4:A:610:NDP:H1B	2.09	0.53
2:C:288:ASP:HA	2:C:291:VAL:HG23	1.91	0.53
2:C:402:ARG:HG2	2:C:402:ARG:HH11	1.73	0.53
2:D:309:PRO:C	2:D:311:ASP:N	2.62	0.53
2:D:344:ASP:HA	6:D:1328:HOH:O	2.07	0.53
2:D:572:PRO:HB3	2:D:596:TYR:HA	1.90	0.53
1:B:3:GLU:HG2	1:B:80:TYR:CE1	2.42	0.53
1:B:119:LEU:HB3	1:B:122:ARG:CZ	2.39	0.53
1:B:4:GLN:C	1:B:8:VAL:CG2	2.82	0.52
2:C:448:TYR:O	2:C:451:LYS:HB2	2.09	0.52
2:D:607:ALA:O	2:D:608:ALA:CB	2.56	0.52
1:B:9:PHE:HZ	1:B:81:LEU:CD2	2.23	0.52
1:B:124:ASN:N	1:B:124:ASN:ND2	2.51	0.52
1:A:8:VAL:HA	1:A:76:LYS:HD3	1.90	0.52
2:C:572:PRO:HB3	2:C:596:TYR:HA	1.91	0.52
1:B:76:LYS:O	1:B:80:TYR:N	2.43	0.52
1:B:113:PRO:O	1:B:117:LYS:HG3	2.09	0.52
1:A:20:VAL:HG12	1:A:21:GLU:N	2.24	0.51
4:B:710:NDP:H2D	6:B:1627:HOH:O	2.10	0.51
1:B:132:LYS:HE2	1:B:135:ASP:OD2	2.10	0.51
2:C:421:ARG:NH2	6:C:1119:HOH:O	2.40	0.51
1:B:131:LEU:CB	6:B:1628:HOH:O	2.32	0.51
2:C:421:ARG:NE	6:C:1119:HOH:O	2.25	0.51
2:D:346:THR:HB	2:D:348:VAL:HG23	1.93	0.51
1:A:166:GLY:HA2	4:A:610:NDP:C6N	2.41	0.51
1:B:26:GLY:C	1:B:27:LYS:HG2	2.36	0.51
2:C:343:SER:CB	6:C:1378:HOH:O	2.58	0.51
2:C:398:ASN:ND2	6:C:1517:HOH:O	2.22	0.50
1:B:29:ASN:HB2	1:B:32:PHE:CZ	2.46	0.50
1:B:138:GLU:C	1:B:140:VAL:H	2.19	0.50
1:B:2:MET:CA	1:B:2:MET:CE	2.80	0.50
1:B:80:TYR:O	1:B:81:LEU:C	2.55	0.50
2:D:309:PRO:O	2:D:310:ASN:C	2.48	0.50
1:A:100:ASN:OD1	1:A:159:TYR:HB3	2.12	0.50
2:C:301:GLU:HG3	2:C:304:LYS:HE2	1.92	0.50
2:C:584:GLU:HB2	6:C:1061:HOH:O	2.10	0.50
1:B:166:GLY:HA2	4:B:710:NDP:H5N	1.94	0.50
1:A:168:VAL:HB	4:A:610:NDP:H51A	1.94	0.49
2:C:329:LEU:HD22	2:C:564:LEU:HD12	1.94	0.49
1:B:29:ASN:ND2	1:B:32:PHE:CE1	2.78	0.49
2:C:290:PHE:HB2	2:D:320:TYR:OH	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:342:GLN:O	2:C:349:GLY:HA2	2.11	0.49
1:B:145:LYS:O	1:B:148:ASP:HB2	2.12	0.49
1:B:171:GLN:HE21	1:B:175:GLU:HG3	1.77	0.49
2:D:461:ASN:ND2	6:D:1229:HOH:O	2.44	0.49
2:D:321:LYS:HB3	2:D:326:TYR:CD2	2.48	0.49
2:D:312:PHE:HE1	2:D:561:LYS:HA	1.77	0.49
2:C:292:TYR:O	2:C:295:PHE:HB3	2.13	0.49
2:C:512:CYS:SG	2:C:547:LEU:HD22	2.53	0.49
2:C:382:GLU:O	2:C:385:TRP:HB3	2.12	0.49
1:B:35:TYR:CZ	1:B:38:ARG:HD3	2.48	0.48
1:B:125:VAL:HG12	1:B:126:ILE:N	2.28	0.48
2:C:302:LYS:HB2	6:C:1359:HOH:O	2.13	0.48
1:A:35:TYR:CZ	1:A:38:ARG:HD3	2.48	0.48
1:B:4:GLN:N	6:B:1636:HOH:O	2.24	0.48
2:C:359:LYS:HG2	2:C:544:ILE:HG12	1.95	0.48
1:A:24:ASN:CB	1:A:28:LYS:NZ	2.76	0.48
1:B:210:VAL:HG21	2:D:326:TYR:HE2	1.76	0.48
2:C:305:ASN:O	2:C:308:HIS:NE2	2.47	0.48
2:C:402:ARG:HD3	2:C:405:GLU:OE1	2.14	0.48
1:B:104:MET:HE2	1:B:164:ILE:HD11	1.95	0.48
1:B:131:LEU:CG	6:B:1628:HOH:O	2.60	0.48
1:B:41:GLY:H	1:B:195:VAL:HG23	1.79	0.48
2:C:344:ASP:OD2	2:C:553:TYR:CE1	2.67	0.48
1:B:138:GLU:C	1:B:140:VAL:N	2.71	0.47
2:D:302:LYS:O	2:D:305:ASN:ND2	2.46	0.47
1:B:75:TYR:O	1:B:79:LYS:HB2	2.15	0.47
2:C:344:ASP:CG	2:C:345:ARG:N	2.72	0.47
2:D:447:ASN:CG	6:D:1220:HOH:O	2.57	0.47
1:A:20:VAL:CG1	1:A:21:GLU:N	2.77	0.47
1:B:77:ARG:O	1:B:81:LEU:HG	2.15	0.47
1:B:166:GLY:N	4:B:710:NDP:O1A	2.41	0.47
1:B:176:LYS:CB	6:B:1639:HOH:O	2.63	0.47
1:B:205:TYR:HA	1:B:227:LYS:O	2.14	0.47
2:C:324:PRO:HB2	2:C:571:PHE:HE2	1.79	0.47
1:A:214:TYR:O	1:A:220:THR:HA	2.15	0.47
2:C:416:ARG:O	2:C:417:LYS:HB2	2.13	0.47
1:B:29:ASN:ND2	1:B:32:PHE:HE1	2.12	0.47
1:B:168:VAL:O	1:B:172:GLU:HG2	2.15	0.47
1:A:115:LYS:HE3	1:A:116:PHE:CE2	2.49	0.47
2:D:303:ASN:O	2:D:307:ILE:HG12	2.15	0.47
2:C:524:SER:OG	6:C:1523:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:H	1:A:3:GLU:HG3	1.42	0.46
1:A:24:ASN:HB2	1:A:28:LYS:NZ	2.31	0.46
1:B:10:ASP:OD2	1:B:73:LEU:HD22	2.15	0.46
2:C:354:PHE:CE2	2:D:506:ILE:HG13	2.51	0.46
2:D:423:VAL:O	2:D:424:ASN:HB2	2.15	0.46
1:A:201:ASN:OD1	1:A:203:ASN:HB2	2.16	0.46
2:C:582:ASN:HB3	6:C:1061:HOH:O	2.15	0.46
2:D:307:ILE:HG22	2:D:312:PHE:CE2	2.51	0.46
2:D:600:GLU:HG3	6:D:1691:HOH:O	2.16	0.46
1:A:23:LYS:O	1:A:24:ASN:C	2.58	0.46
1:A:27:LYS:C	1:A:29:ASN:N	2.73	0.46
1:A:109:TRP:CE3	1:A:126:ILE:HD11	2.51	0.45
1:B:58:PHE:CZ	3:B:709:CP6:H12	2.51	0.45
1:B:177:LYS:CD	6:B:1638:HOH:O	2.55	0.45
2:C:328:TYR:CZ	2:C:332:ILE:HD11	2.52	0.45
1:B:100:ASN:OD1	1:B:159:TYR:HB3	2.16	0.45
1:B:12:TYR:C	6:B:1640:HOH:O	2.56	0.45
1:B:41:GLY:N	1:B:195:VAL:HG23	2.32	0.45
2:D:344:ASP:CA	6:D:1328:HOH:O	2.64	0.45
1:A:166:GLY:HA2	4:A:610:NDP:H5N	1.99	0.45
1:A:221:LEU:N	1:A:221:LEU:HD23	2.32	0.45
2:C:559:SER:OG	2:C:606:MET:HE2	2.16	0.45
1:A:23:LYS:H	1:A:23:LYS:HG2	1.49	0.45
2:C:437:PHE:CD1	2:D:479:VAL:HB	2.51	0.45
2:D:607:ALA:O	2:D:608:ALA:HB3	2.16	0.45
1:A:35:TYR:CE2	1:A:38:ARG:HD3	2.51	0.45
2:D:292:TYR:O	2:D:295:PHE:HB3	2.16	0.45
2:C:297:LYS:HA	2:C:297:LYS:HD3	1.61	0.44
1:B:201:ASN:HB3	1:B:204:GLU:HG3	1.98	0.44
1:B:51:ASN:HB2	6:B:1008:HOH:O	2.17	0.44
2:C:305:ASN:O	2:C:308:HIS:CE1	2.71	0.44
2:D:344:ASP:N	6:D:1328:HOH:O	2.49	0.44
2:D:344:ASP:OD1	6:D:1328:HOH:O	2.21	0.44
1:A:132:LYS:HB3	6:A:1481:HOH:O	2.18	0.44
1:B:22:SER:HB3	6:B:1001:HOH:O	2.18	0.44
1:B:122:ARG:O	1:B:124:ASN:ND2	2.51	0.44
2:D:407:ASN:ND2	6:D:1569:HOH:O	2.49	0.44
1:B:64:TYR:HB3	6:B:1642:HOH:O	2.17	0.44
2:D:324:PRO:HB2	2:D:571:PHE:HE2	1.82	0.44
2:D:346:THR:HG22	2:D:348:VAL:HG23	1.99	0.44
1:A:27:LYS:O	1:A:29:ASN:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:470:ARG:HD3	6:D:1329:HOH:O	2.17	0.44
2:D:308:HIS:O	2:D:311:ASP:CB	2.65	0.44
1:B:9:PHE:CZ	1:B:81:LEU:CD2	3.00	0.44
1:B:43:LYS:N	6:B:1626:HOH:O	2.49	0.44
2:C:314:ILE:HD12	2:C:565:ASN:HB3	1.98	0.44
1:A:7:ASP:OD1	1:A:180:LYS:HE3	2.18	0.43
1:B:227:LYS:HG2	1:B:228:LYS:N	2.33	0.43
2:D:312:PHE:CE1	2:D:561:LYS:HG2	2.53	0.43
2:D:344:ASP:C	2:D:346:THR:N	2.75	0.43
2:D:349:GLY:HA3	2:D:554:ASN:ND2	2.34	0.43
1:A:108:ASN:OD1	4:A:610:NDP:H6N	2.18	0.43
2:D:350:VAL:HG12	2:D:553:TYR:CD1	2.53	0.43
1:B:41:GLY:HA3	4:B:710:NDP:H1D	2.00	0.43
1:A:109:TRP:CD2	1:A:126:ILE:HD11	2.54	0.43
1:B:196:PHE:HB2	6:B:1620:HOH:O	2.18	0.43
2:C:423:VAL:O	2:C:424:ASN:HB2	2.19	0.43
1:B:28:LYS:HA	6:B:1703:HOH:O	2.19	0.42
1:B:114:LYS:HD2	1:B:114:LYS:N	2.08	0.42
2:C:325:GLU:HG3	2:C:369:LEU:HD22	2.00	0.42
2:C:449:GLU:HG3	2:C:449:GLU:O	2.20	0.42
1:A:23:LYS:HE2	1:A:23:LYS:HB3	1.53	0.42
1:A:144:ASN:ND2	1:A:145:LYS:HG2	2.34	0.42
1:A:210:VAL:HG12	2:C:323:HIS:HB2	2.00	0.42
1:A:40:LEU:HD22	4:A:610:NDP:C3N	2.50	0.42
1:B:102:VAL:HG23	1:B:102:VAL:O	2.20	0.42
2:C:506:ILE:HG13	2:D:354:PHE:CE2	2.54	0.42
2:D:341:LYS:HE2	6:D:1316:HOH:O	2.18	0.42
2:D:457:LYS:NZ	6:D:1228:HOH:O	2.53	0.42
1:B:178:LEU:CD2	6:B:1639:HOH:O	2.60	0.42
2:C:289:ASP:HA	2:C:292:TYR:CD2	2.54	0.42
1:A:172:GLU:O	1:A:176:LYS:HG3	2.19	0.42
2:C:493:LEU:C	2:C:493:LEU:CD1	2.91	0.42
2:D:421:ARG:HH11	2:D:421:ARG:HG2	1.84	0.42
2:D:567:ILE:HA	2:D:568:PRO:HD3	1.90	0.42
1:B:209:SER:HB3	2:C:293:PHE:CE2	2.55	0.42
2:C:297:LYS:HB3	2:C:298:GLU:O	2.20	0.42
1:B:2:MET:C	6:B:1636:HOH:O	2.62	0.42
1:B:171:GLN:OE1	1:B:198:PRO:HB3	2.19	0.42
1:B:209:SER:HB3	2:C:293:PHE:HE2	1.85	0.42
1:A:19:LYS:HG2	1:A:36:THR:HG22	2.00	0.42
2:D:341:LYS:HG3	6:D:1316:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:VAL:HG11	1:B:80:TYR:CD2	2.55	0.41
2:D:531:MET:HE3	2:D:591:PHE:HZ	1.85	0.41
2:C:518:VAL:O	2:C:519:PRO:C	2.62	0.41
2:D:589:SER:HB3	6:D:1270:HOH:O	2.20	0.41
1:B:16:ALA:HB2	3:B:709:CP6:N14	2.34	0.41
2:C:479:VAL:HB	2:D:437:PHE:CD1	2.54	0.41
1:A:16:ALA:HA	1:A:185:THR:HB	2.01	0.41
2:C:421:ARG:HH11	2:C:421:ARG:HG2	1.85	0.41
2:D:312:PHE:HB2	6:D:1684:HOH:O	2.21	0.41
1:A:171:GLN:OE1	1:A:171:GLN:HA	2.21	0.41
1:B:126:ILE:O	1:B:143:ILE:HG12	2.21	0.41
1:B:141:TYR:CE2	1:B:156:LEU:HD11	2.55	0.41
1:A:33:ASN:HA	2:C:569:TYR:OH	2.21	0.41
1:B:33:ASN:OD1	1:B:35:TYR:N	2.53	0.41
1:B:37:PHE:O	1:B:184:PHE:HZ	2.04	0.41
2:C:343:SER:HA	2:C:349:GLY:HA2	2.03	0.40
1:B:145:LYS:HG2	1:B:146:VAL:N	2.35	0.40
1:B:149:LEU:O	1:B:150:ILE:C	2.63	0.40
2:D:325:GLU:HG3	2:D:369:LEU:HD22	2.03	0.40
1:B:113:PRO:HB2	1:B:116:PHE:CD2	2.56	0.40
2:C:358:MET:HE1	2:C:522:ILE:HD11	2.03	0.40
2:D:346:THR:CB	2:D:348:VAL:HG23	2.51	0.40
2:D:284:ASP:O	2:D:287:GLU:HB3	2.22	0.40
1:B:113:PRO:HB2	1:B:116:PHE:HD2	1.87	0.40
2:C:492:ILE:HD11	2:C:510:ARG:HD3	2.03	0.40
2:D:299:LYS:HA	2:D:299:LYS:HD3	1.21	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	217/280 (78%)	208 (96%)	8 (4%)	1 (0%)	24	31
1	B	212/280 (76%)	193 (91%)	16 (8%)	3 (1%)	9	9
2	C	324/328 (99%)	303 (94%)	20 (6%)	1 (0%)	36	46
2	D	324/328 (99%)	309 (95%)	13 (4%)	2 (1%)	21	27
All	All	1077/1216 (89%)	1013 (94%)	57 (5%)	7 (1%)	21	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	5	VAL
2	C	308	HIS
2	D	430	TYR
1	A	49	LYS
2	D	308	HIS
1	B	113	PRO
1	B	146	VAL

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%)	201 (96%)	9 (4%)	26	39
1	B	205/268 (76%)	195 (95%)	10 (5%)	22	34
2	C	300/302 (99%)	294 (98%)	6 (2%)	48	67
2	D	300/302 (99%)	294 (98%)	6 (2%)	48	67
All	All	1015/1140 (89%)	984 (97%)	31 (3%)	35	52

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	23	LYS
1	A	27	LYS
1	A	28	LYS

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Mol	Chain	Res	Type
1	A	49	LYS
1	A	50	CYS
1	A	124	ASN
1	A	144	ASN
1	A	145	LYS
1	B	7	ASP
1	B	50	CYS
1	B	76	LYS
1	B	114	LYS
1	B	121	ASN
1	B	124	ASN
1	B	127	LEU
1	B	132	LYS
1	B	189	SER
1	B	231	ASN
2	C	284	ASP
2	C	287	GLU
2	C	302	LYS
2	C	345	ARG
2	C	487	LEU
2	C	524	SER
2	D	285	GLU
2	D	299	LYS
2	D	305	ASN
2	D	309	PRO
2	D	487	LEU
2	D	564	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	121	ASN
1	A	144	ASN
1	B	42	ASN
1	B	99	GLN
1	B	121	ASN
1	B	171	GLN
2	C	294	ASN
2	C	310	ASN
2	C	338	ASN
2	C	394	ASN

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Mol	Chain	Res	Type
2	C	407	ASN
2	C	424	ASN
2	C	542	GLN
2	D	394	ASN
2	D	407	ASN
2	D	424	ASN
2	D	534	GLN
2	D	539	GLN
2	D	554	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](#)

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	$\# Z > 2$
5	UMP	C	611	-	21,21,21	2.13	7 (33%)	30,31,31	2.13	11 (36%)
3	CP6	B	709	-	18,18,18	2.75	10 (55%)	25,25,25	2.32	10 (40%)
5	UMP	D	711	-	21,21,21	2.21	8 (38%)	30,31,31	2.16	11 (36%)
3	CP6	A	609	-	18,18,18	2.66	11 (61%)	25,25,25	2.23	8 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NDP	A	610	-	51,52,52	3.05	26 (50%)	71,80,80	2.17	26 (36%)
4	NDP	B	710	-	51,52,52	2.36	18 (35%)	71,80,80	1.56	13 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	UMP	C	611	-	-	0/10/22/22	0/2/2/2
3	CP6	B	709	-	-	0/6/6/6	0/2/2/2
5	UMP	D	711	-	-	2/10/22/22	0/2/2/2
3	CP6	A	609	-	-	1/6/6/6	0/2/2/2
4	NDP	A	610	-	-	3/34/77/77	0/5/5/5
4	NDP	B	710	-	-	7/34/77/77	0/5/5/5

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	610	NDP	PA-O3	7.82	1.67	1.59
4	A	610	NDP	C2B-C1B	-6.20	1.37	1.53
4	A	610	NDP	C2N-C3N	6.15	1.52	1.35
4	B	710	NDP	C2N-C3N	5.94	1.51	1.35
4	B	710	NDP	PN-O3	5.58	1.65	1.59
3	B	709	CP6	C4-C5	5.31	1.52	1.40
4	A	610	NDP	O4B-C1B	5.21	1.54	1.42
4	A	610	NDP	O4B-C4B	5.19	1.56	1.45
4	A	610	NDP	C1B-N9A	5.04	1.60	1.46
4	A	610	NDP	O4D-C1D	4.99	1.53	1.42
4	B	710	NDP	C5D-C4D	4.83	1.66	1.51
4	A	610	NDP	C4A-N3A	4.70	1.43	1.34
5	C	611	UMP	O4'-C1'	4.51	1.52	1.42
3	A	609	CP6	C4-C5	4.50	1.50	1.40
5	D	711	UMP	C2-N1	4.49	1.45	1.38
5	C	611	UMP	C2-N1	4.45	1.45	1.38
5	D	711	UMP	O4'-C1'	4.43	1.52	1.42
3	B	709	CP6	C9-C10	4.40	1.46	1.38
4	A	610	NDP	C4N-C5N	-4.37	1.37	1.49
4	A	610	NDP	C8A-N9A	4.26	1.44	1.37
4	B	710	NDP	C4A-N3A	4.18	1.42	1.34
4	B	710	NDP	C4N-C5N	-4.17	1.38	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	710	NDP	PA-O3	4.14	1.64	1.59
4	A	610	NDP	P2B-O2B	-4.11	1.52	1.59
4	A	610	NDP	C2A-N1A	4.00	1.41	1.33
3	A	609	CP6	C9-C10	3.90	1.45	1.38
4	A	610	NDP	C2D-C3D	-3.85	1.42	1.53
4	B	710	NDP	C8A-N9A	3.84	1.44	1.37
3	A	609	CP6	C12-C7	3.76	1.46	1.39
3	B	709	CP6	C2-N14	3.60	1.41	1.33
3	B	709	CP6	C4-C3	3.59	1.50	1.43
4	A	610	NDP	C6N-C5N	3.55	1.44	1.33
3	B	709	CP6	C12-C7	3.45	1.46	1.39
3	A	609	CP6	C2-N14	3.42	1.40	1.33
3	B	709	CP6	C3-N1	3.42	1.39	1.35
4	B	710	NDP	C2A-N1A	3.41	1.40	1.33
3	A	609	CP6	C10-CL1	-3.32	1.66	1.74
4	A	610	NDP	P2B-O2X	-3.31	1.42	1.54
5	D	711	UMP	C4-N3	3.30	1.44	1.38
4	B	710	NDP	O4D-C1D	3.27	1.49	1.42
3	A	609	CP6	C4-C3	3.25	1.49	1.43
4	A	610	NDP	C5A-C6A	3.23	1.50	1.41
4	B	710	NDP	PA-O1A	-3.20	1.39	1.50
3	B	709	CP6	C10-CL1	-3.18	1.67	1.74
4	B	710	NDP	C6N-N1N	3.14	1.44	1.37
4	A	610	NDP	C2A-N3A	3.08	1.39	1.33
4	A	610	NDP	C5D-C4D	3.03	1.60	1.51
5	D	711	UMP	C2-N3	2.93	1.43	1.38
4	B	710	NDP	C4N-C3N	-2.91	1.44	1.50
3	A	609	CP6	C2-N6	2.88	1.40	1.35
3	A	609	CP6	C4-C7	-2.81	1.45	1.50
4	A	610	NDP	C6N-N1N	2.80	1.44	1.37
3	B	709	CP6	C2-N6	2.78	1.40	1.35
5	C	611	UMP	C4-N3	2.77	1.43	1.38
5	D	711	UMP	C6-C5	2.76	1.41	1.35
3	A	609	CP6	C12-C11	2.74	1.43	1.38
4	B	710	NDP	C6N-C5N	2.71	1.41	1.33
3	A	609	CP6	C2-N1	2.67	1.40	1.35
5	C	611	UMP	P-OP3	-2.67	1.44	1.54
4	B	710	NDP	C1B-N9A	2.67	1.53	1.46
4	A	610	NDP	PA-O5B	2.60	1.69	1.59
5	C	611	UMP	C2-N3	2.58	1.42	1.38
3	B	709	CP6	C12-C11	2.47	1.42	1.38
5	C	611	UMP	C6-C5	2.47	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	610	NDP	PA-O1A	-2.47	1.42	1.50
5	C	611	UMP	P-OP2	-2.46	1.45	1.54
3	A	609	CP6	C3-N1	2.45	1.38	1.35
4	A	610	NDP	C1D-N1N	2.43	1.53	1.46
4	A	610	NDP	PN-O3	2.42	1.62	1.59
4	B	710	NDP	C2D-C1D	2.36	1.60	1.53
4	A	610	NDP	C3B-C4B	2.29	1.58	1.53
4	A	610	NDP	C5A-N7A	-2.29	1.34	1.39
5	D	711	UMP	P-OP3	-2.28	1.46	1.54
5	D	711	UMP	O4'-C4'	2.23	1.49	1.45
5	D	711	UMP	O3'-C3'	2.22	1.48	1.43
4	B	710	NDP	C1D-N1N	2.17	1.52	1.46
3	B	709	CP6	C2-N1	2.11	1.39	1.35
4	B	710	NDP	C2A-N3A	2.02	1.37	1.33
4	B	710	NDP	PA-O5B	2.01	1.67	1.59
4	A	610	NDP	C4N-C3N	-2.01	1.46	1.50

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	609	CP6	C15-C5-C4	-6.72	117.99	122.47
4	A	610	NDP	O4B-C1B-N9A	6.37	120.32	108.09
4	A	610	NDP	O4B-C4B-C5B	-6.36	88.96	109.33
3	B	709	CP6	C15-C5-C4	-5.93	118.52	122.47
5	C	611	UMP	O4'-C1'-N1	5.11	116.93	107.86
5	D	711	UMP	C1'-N1-C6	-4.62	112.43	121.53
5	C	611	UMP	C1'-N1-C6	-4.50	112.68	121.53
4	B	710	NDP	C3N-C2N-N1N	-4.48	116.62	123.20
4	A	610	NDP	C3N-C2N-N1N	-4.42	116.72	123.20
5	D	711	UMP	O4'-C1'-N1	4.35	115.59	107.86
4	A	610	NDP	O4D-C1D-N1N	4.09	115.88	108.08
3	B	709	CP6	C2-N6-C5	4.03	119.20	116.26
4	A	610	NDP	O2X-P2B-O1X	3.86	125.88	110.83
4	B	710	NDP	O2X-P2B-O1X	3.84	125.81	110.83
5	D	711	UMP	C1'-N1-C2	3.68	124.85	117.66
5	D	711	UMP	C2'-C1'-N1	3.67	123.00	113.81
5	C	611	UMP	C2'-C1'-N1	3.66	122.97	113.81
4	B	710	NDP	O3X-P2B-O1X	-3.59	96.84	110.83
4	A	610	NDP	C1D-N1N-C2N	-3.59	115.23	121.14
5	D	711	UMP	O4'-C1'-C2'	-3.53	99.64	106.25
5	C	611	UMP	O4'-C1'-C2'	-3.47	99.75	106.25
4	A	610	NDP	C5B-C4B-C3B	3.42	127.54	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	710	NDP	O2X-P2B-O2B	3.40	119.09	105.85
3	A	609	CP6	C11-C10-CL1	3.39	124.36	119.36
4	A	610	NDP	C2D-C1D-N1N	-3.34	105.09	113.31
5	C	611	UMP	C1'-N1-C2	3.25	124.01	117.66
4	A	610	NDP	O2X-P2B-O2B	3.23	118.45	105.85
3	B	709	CP6	C7-C4-C3	3.18	124.41	120.33
4	A	610	NDP	O5D-C5D-C4D	-3.17	98.19	108.99
3	B	709	CP6	C3-C4-C5	-3.14	113.70	115.97
4	B	710	NDP	C1D-N1N-C2N	-3.13	115.99	121.14
5	D	711	UMP	C4'-O4'-C1'	3.12	116.93	109.51
3	B	709	CP6	N13-C3-N1	3.12	121.23	117.03
5	D	711	UMP	O4'-C4'-C3'	-3.10	98.57	105.65
3	A	609	CP6	C4-C3-N1	-3.02	120.80	122.55
3	B	709	CP6	C11-C10-CL1	2.95	123.71	119.36
4	A	610	NDP	C4A-N9A-C8A	-2.94	102.66	105.74
4	B	710	NDP	O3X-P2B-O2X	-2.93	96.80	107.80
3	B	709	CP6	C4-C3-N1	-2.93	120.85	122.55
4	A	610	NDP	P2B-O2B-C2B	2.93	131.25	123.43
3	A	609	CP6	N13-C3-N1	2.91	120.95	117.03
4	A	610	NDP	O5B-C5B-C4B	-2.89	99.14	108.99
4	A	610	NDP	O3X-P2B-O2X	-2.84	97.16	107.80
5	C	611	UMP	O2-C2-N1	2.79	126.42	122.80
4	A	610	NDP	O4B-C4B-C3B	-2.73	99.73	105.15
3	A	609	CP6	C7-C4-C3	2.73	123.83	120.33
5	D	711	UMP	O2-C2-N1	2.71	126.32	122.80
4	A	610	NDP	C5A-N7A-C8A	2.69	107.67	103.45
5	D	711	UMP	O4-C4-N3	2.69	123.17	119.27
5	C	611	UMP	O4'-C4'-C3'	-2.68	99.53	105.65
4	B	710	NDP	O7N-C7N-N7N	-2.68	116.88	122.89
3	A	609	CP6	C9-C10-CL1	-2.67	115.42	119.36
3	B	709	CP6	C4-C3-N13	-2.62	117.50	120.82
3	A	609	CP6	C2-N6-C5	2.61	118.16	116.26
5	C	611	UMP	O4-C4-N3	2.61	123.06	119.27
5	C	611	UMP	C4'-O4'-C1'	2.59	115.66	109.51
4	A	610	NDP	O4B-C1B-C2B	-2.50	102.28	106.59
4	B	710	NDP	C4B-O4B-C1B	-2.46	104.03	109.47
4	A	610	NDP	C2D-C3D-C4D	2.41	107.27	102.61
4	B	710	NDP	O4B-C1B-N9A	2.39	112.68	108.09
4	A	610	NDP	O3D-C3D-C4D	-2.39	104.22	111.08
3	B	709	CP6	C9-C10-CL1	-2.38	115.85	119.36
4	A	610	NDP	O3X-P2B-O1X	-2.37	101.61	110.83
4	B	710	NDP	O3X-P2B-O2B	-2.37	96.63	105.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	610	NDP	O2B-C2B-C3B	2.35	120.09	111.68
4	A	610	NDP	O2A-PA-O1A	2.30	123.13	112.44
3	B	709	CP6	C12-C7-C4	2.21	124.59	120.80
4	B	710	NDP	C2D-C3D-C4D	2.17	106.79	102.61
5	D	711	UMP	C2'-C3'-C4'	2.16	107.18	102.80
4	A	610	NDP	O7N-C7N-N7N	-2.15	118.07	122.89
4	B	710	NDP	N3A-C2A-N1A	-2.14	125.34	128.58
3	A	609	CP6	C4-C3-N13	-2.13	118.12	120.82
5	D	711	UMP	O4-C4-C5	-2.12	121.51	125.16
4	A	610	NDP	C1B-N9A-C8A	2.10	131.75	127.09
5	C	611	UMP	O4-C4-C5	-2.10	121.55	125.16
4	A	610	NDP	C5D-C4D-C3D	2.09	122.73	115.21
5	C	611	UMP	C2'-C3'-C4'	2.04	106.95	102.80
4	B	710	NDP	O2B-C2B-C3B	2.03	118.95	111.68
4	A	610	NDP	O5B-PA-O1A	-2.01	100.95	108.94

There are no chirality outliers.

All (13) torsion outliers are listed below:

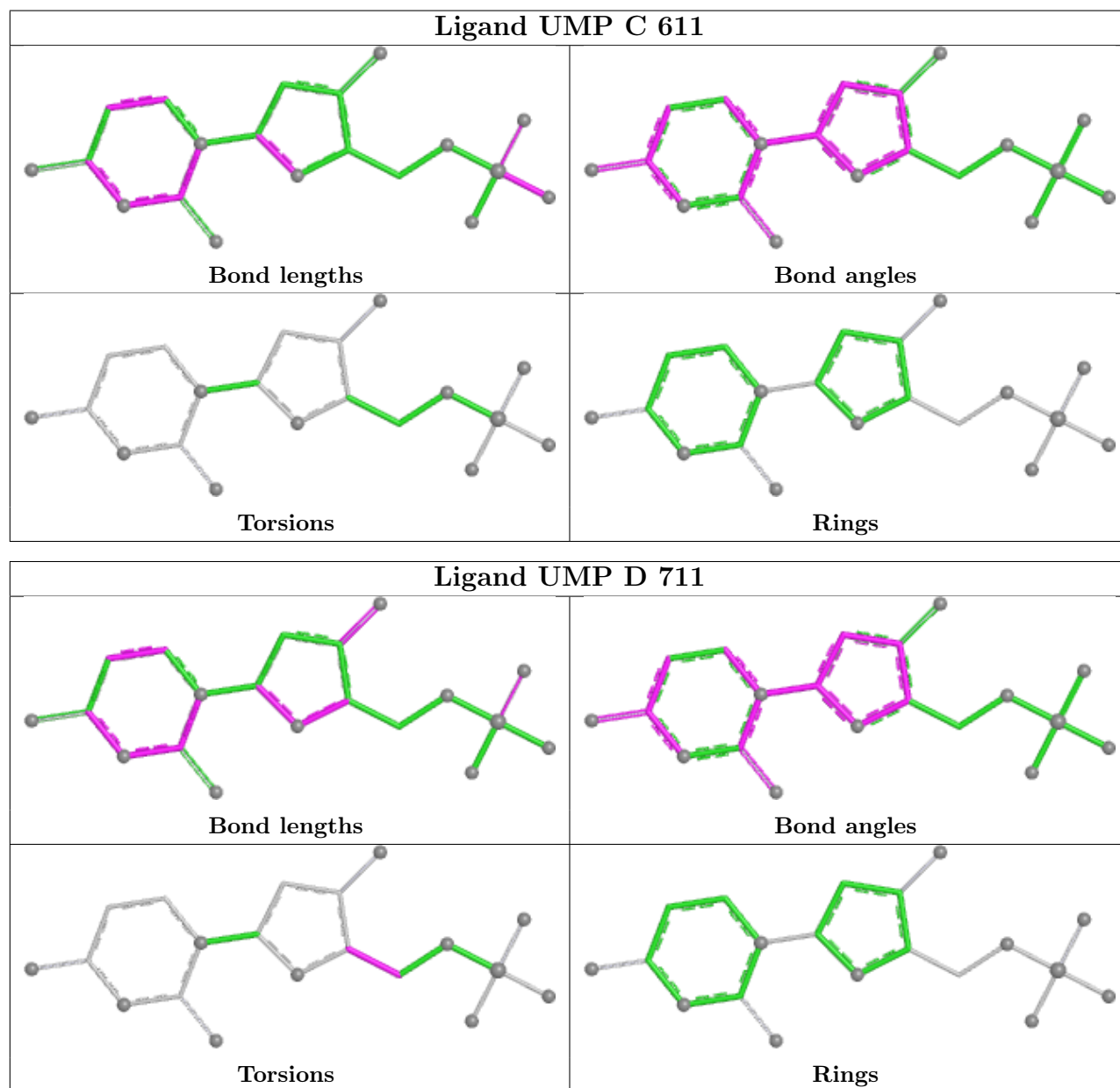
Mol	Chain	Res	Type	Atoms
4	A	610	NDP	C5D-O5D-PN-O1N
4	B	710	NDP	C5D-O5D-PN-O1N
4	A	610	NDP	O4D-C1D-N1N-C2N
5	D	711	UMP	C3'-C4'-C5'-O5'
4	B	710	NDP	PA-O3-PN-O5D
4	B	710	NDP	O4D-C1D-N1N-C2N
4	B	710	NDP	C3B-C4B-C5B-O5B
4	A	610	NDP	C2N-C3N-C7N-N7N
4	B	710	NDP	O4B-C4B-C5B-O5B
4	B	710	NDP	C2N-C3N-C7N-N7N
3	A	609	CP6	C16-C15-C5-N6
5	D	711	UMP	O4'-C4'-C5'-O5'
4	B	710	NDP	C3B-C2B-O2B-P2B

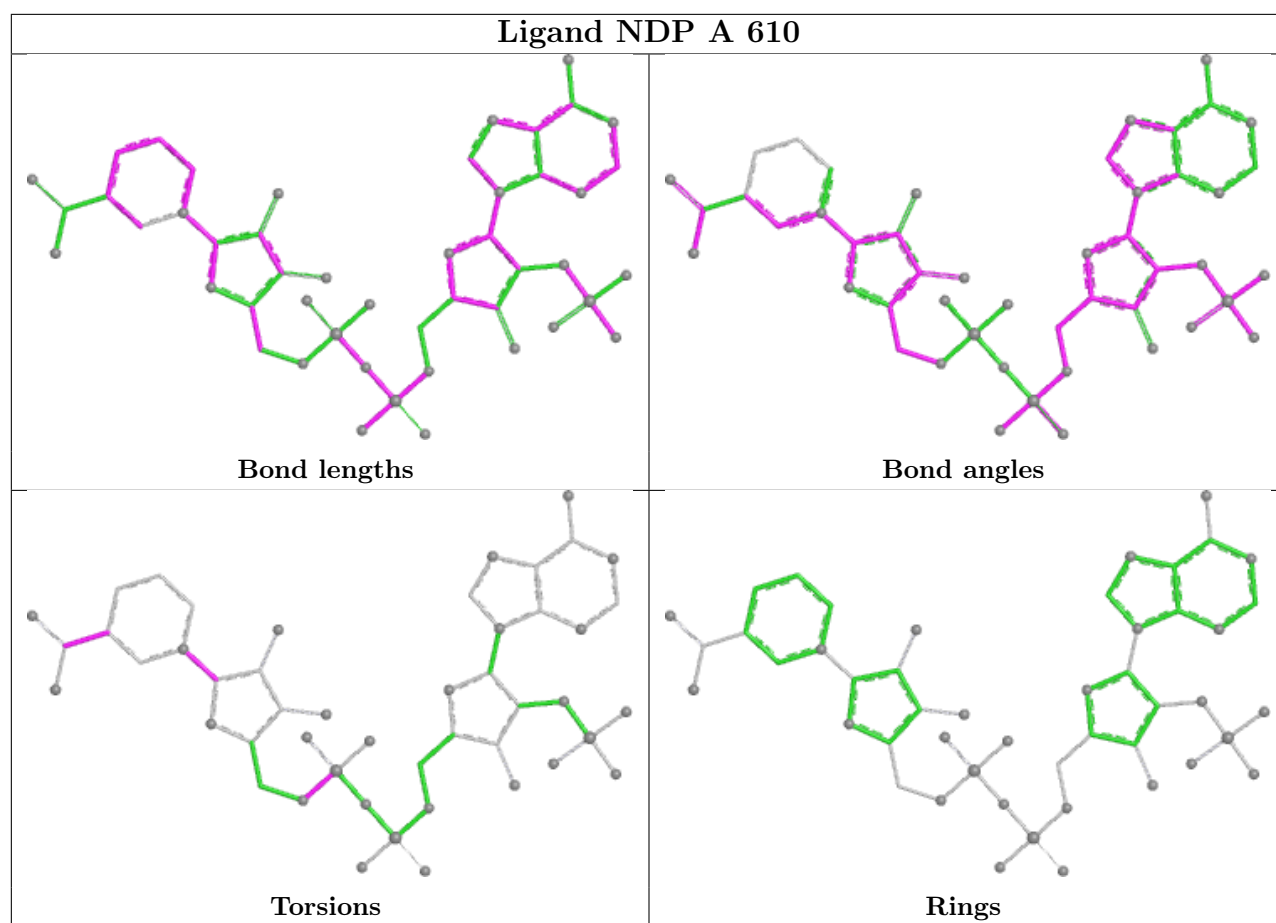
There are no ring outliers.

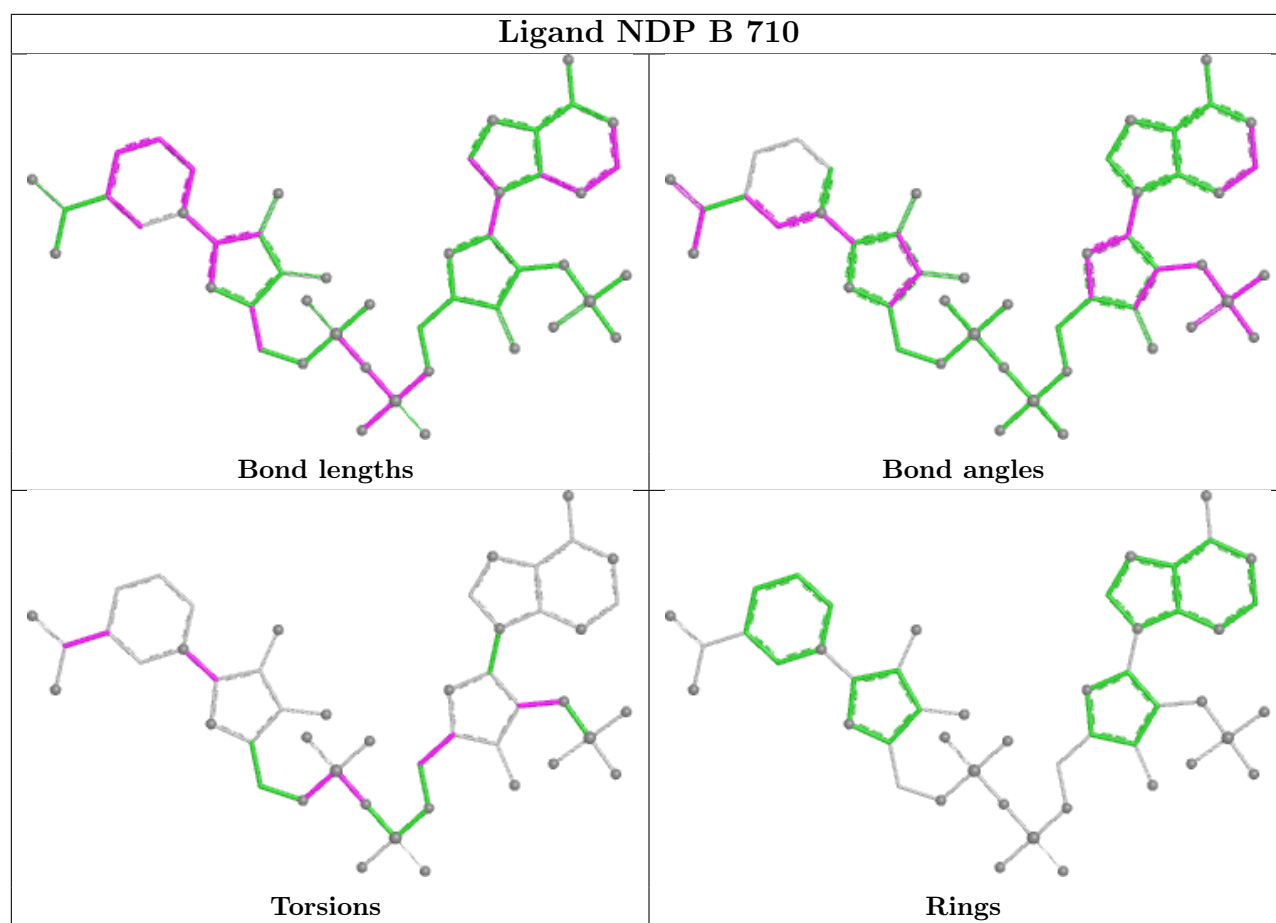
3 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	709	CP6	2	0
4	A	610	NDP	14	0
4	B	710	NDP	12	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%)	0.14	14 (6%) 26 28	16, 34, 86, 94	0
1	B	216/280 (77%)	1.48	63 (29%) 1 1	23, 73, 94, 94	0
2	C	326/328 (99%)	-0.27	20 (6%) 27 29	14, 23, 77, 94	0
2	D	326/328 (99%)	-0.39	20 (6%) 27 29	14, 22, 71, 94	0
All	All	1089/1216 (89%)	0.12	117 (10%) 11 12	14, 28, 93, 94	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	344	ASP	6.4
1	B	70	TYR	5.1
2	D	608	ALA	5.0
1	B	80	TYR	4.9
1	B	29	ASN	4.7
2	C	307	ILE	4.7
1	A	1	MET	4.7
1	B	75	TYR	4.7
2	C	309	PRO	4.5
1	B	6	CYS	4.2
2	D	309	PRO	4.2
1	A	2	MET	4.1
1	B	2	MET	4.1
1	B	130	THR	4.1
1	B	73	LEU	4.0
1	B	9	PHE	4.0
1	A	24	ASN	4.0
1	B	135	ASP	4.0
1	A	85	THR	3.9
1	B	136	PHE	3.9
2	C	285	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	179	ILE	3.8
1	B	5	VAL	3.7
2	C	608	ALA	3.7
2	C	347	GLY	3.7
1	B	1	MET	3.6
1	B	26	GLY	3.6
1	B	151	VAL	3.5
1	A	26	GLY	3.5
2	C	348	VAL	3.4
2	D	306	SER	3.4
1	B	78	CYS	3.4
2	D	284	ASP	3.4
1	B	28	LYS	3.4
2	D	305	ASN	3.4
1	B	81	LEU	3.3
2	D	312	PHE	3.3
2	D	285	GLU	3.3
1	B	131	LEU	3.3
2	D	344	ASP	3.3
1	B	11	ILE	3.2
2	D	286	GLU	3.2
2	D	310	ASN	3.1
1	B	137	ASP	3.1
2	D	307	ILE	3.1
1	B	133	LYS	3.1
1	B	98	LEU	3.0
1	B	74	LYS	3.0
1	B	66	ASN	3.0
1	A	25	GLU	3.0
1	B	144	ASN	3.0
2	C	306	SER	3.0
1	B	112	ILE	2.9
1	B	134	GLU	2.9
1	B	159	TYR	2.9
2	C	345	ARG	2.8
2	D	283	ASP	2.8
2	D	311	ASP	2.8
1	B	139	ASP	2.7
1	B	27	LYS	2.7
2	C	304	LYS	2.7
1	B	101	VAL	2.7
1	B	142	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	116	PHE	2.7
1	B	24	ASN	2.7
1	B	146	VAL	2.6
2	C	346	THR	2.6
1	B	141	TYR	2.6
2	C	310	ASN	2.6
2	C	297	LYS	2.6
1	A	230	ASN	2.6
1	B	231	ASN	2.6
1	B	65	VAL	2.6
2	D	345	ARG	2.6
1	B	129	ARG	2.5
1	A	5	VAL	2.5
1	B	157	ASN	2.5
1	B	230	ASN	2.5
2	C	284	ASP	2.5
2	C	303	ASN	2.5
2	C	305	ASN	2.5
1	B	150	ILE	2.5
1	B	156	LEU	2.4
1	A	231	ASN	2.4
2	C	447	ASN	2.4
1	B	229	THR	2.4
2	D	346	THR	2.4
1	B	76	LYS	2.4
1	B	168	VAL	2.4
1	B	119	LEU	2.4
1	B	158	TYR	2.4
1	B	13	ALA	2.4
1	B	140	VAL	2.4
2	C	286	GLU	2.4
1	A	22	SER	2.3
1	B	77	ARG	2.3
1	B	10	ASP	2.3
1	A	83	LYS	2.3
1	B	132	LYS	2.3
2	C	291	VAL	2.3
1	B	97	LYS	2.3
2	D	347	GLY	2.3
2	D	308	HIS	2.2
1	B	7	ASP	2.2
2	C	288	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	606	MET	2.2
2	D	302	LYS	2.2
1	A	23	LYS	2.1
1	B	22	SER	2.1
2	D	607	ALA	2.1
1	B	127	LEU	2.1
1	A	82	ASN	2.1
1	B	35	TYR	2.1
1	B	71	GLU	2.0
1	B	69	LYS	2.0
1	B	117	LYS	2.0
1	A	27	LYS	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](#)

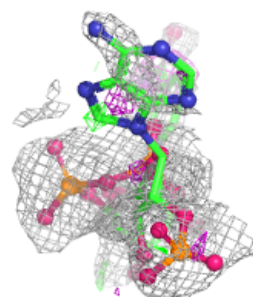
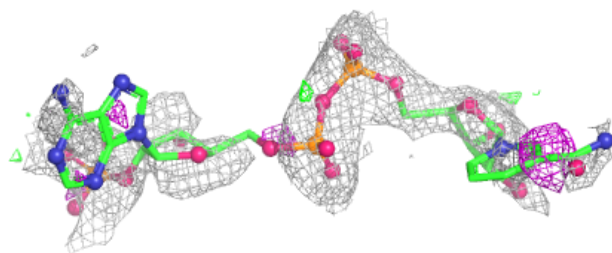
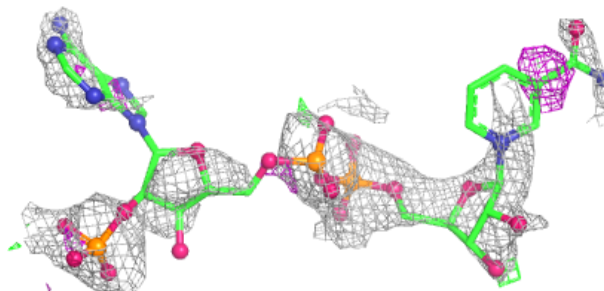
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	NDP	B	710	48/48	0.67	0.18	93,93,93,93	0
3	CP6	B	709	17/17	0.81	0.13	44,49,50,52	0
5	UMP	D	711	20/20	0.85	0.17	49,65,74,74	0
3	CP6	A	609	17/17	0.86	0.10	5,17,19,20	0
5	UMP	C	611	20/20	0.89	0.15	42,56,66,67	0
4	NDP	A	610	48/48	0.90	0.14	48,53,68,70	0

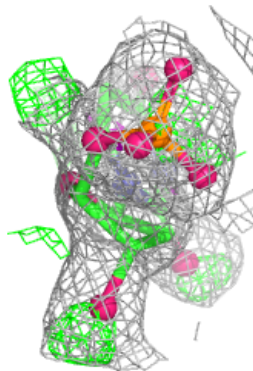
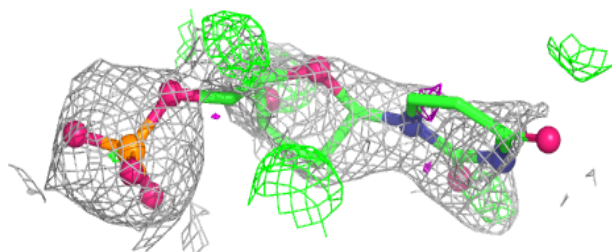
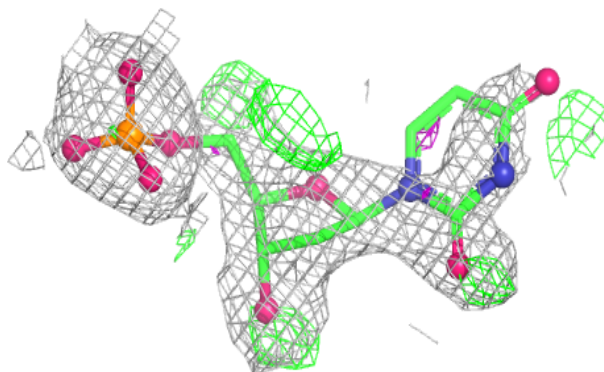
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

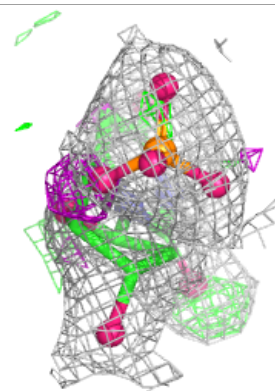
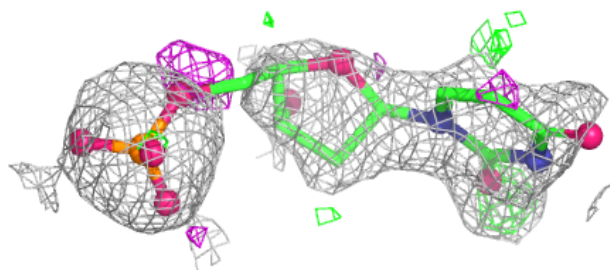
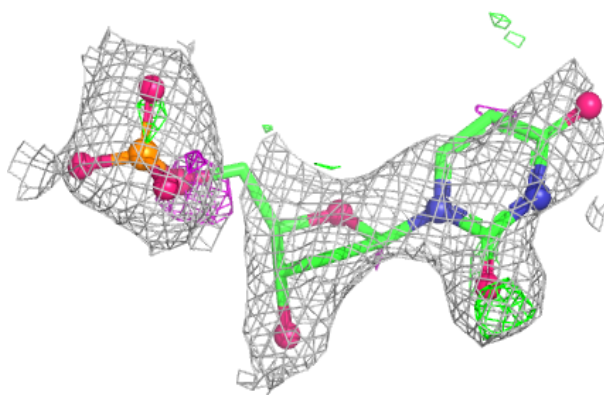
**Electron density around UMP D 711:**

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

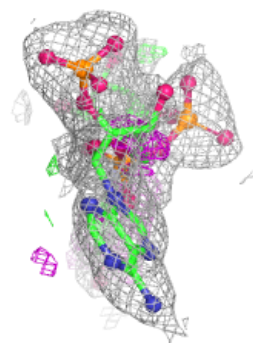
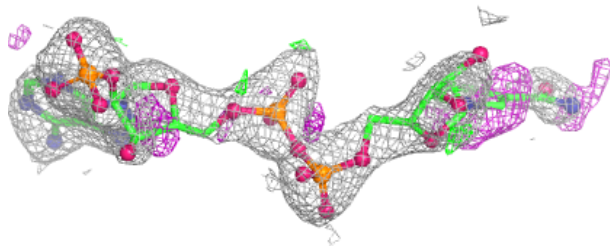
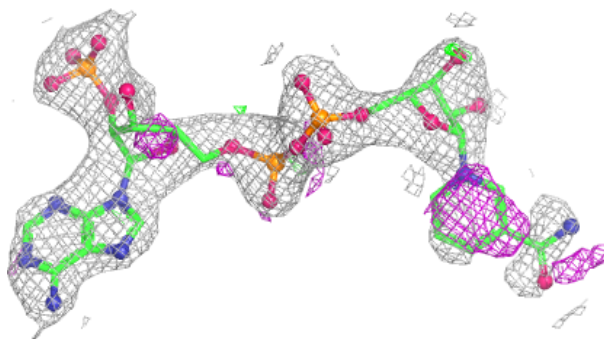


Electron density around UMP C 611:

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

**Electron density around 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.