



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:07 PM UTC

PDB ID : 7CTZ / pdb_00007ctz
Title : Wild-type plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with fragment 148, NADPH, and dUMP
Authors : Vitsupakorn, D.
Deposited on : 2020-08-20
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

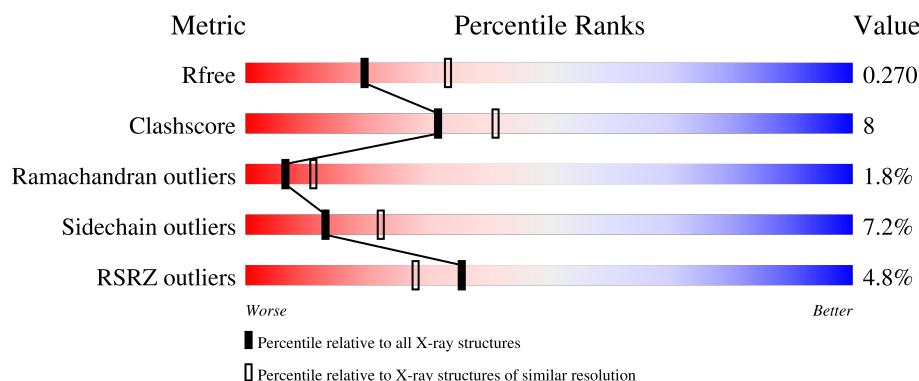
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	608	3% 65% 18% • 12%
1	B	608	5% 63% 22% • 12%

2 Entry composition [i](#)

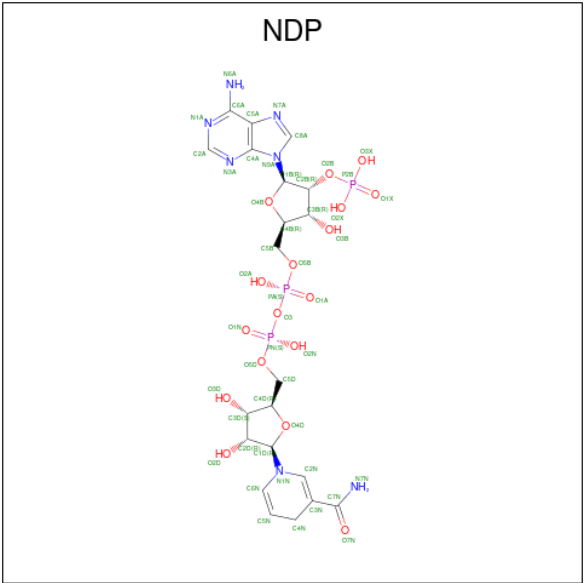
There are 5 unique types of molecules in this entry. The entry contains 17985 atoms, of which 8888 are hydrogens and 0 are deuteriums.

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.

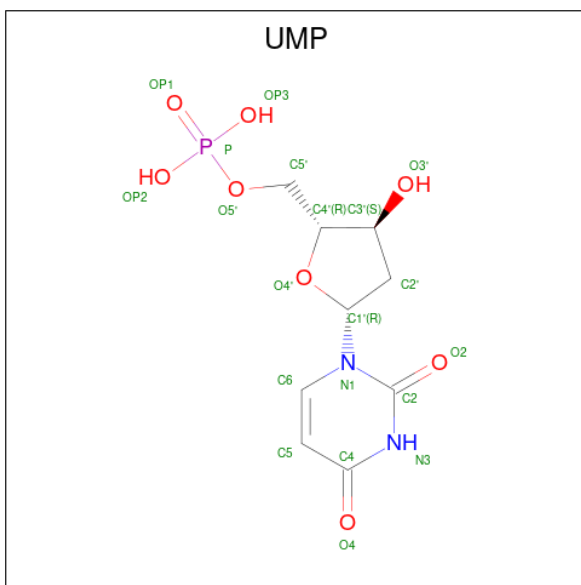
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	534	Total	C	H	N	O	S	253	0	0
			8858	2876	4411	731	813	27			
1	B	532	Total	C	H	N	O	S	257	0	0
			8817	2863	4389	730	809	26			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



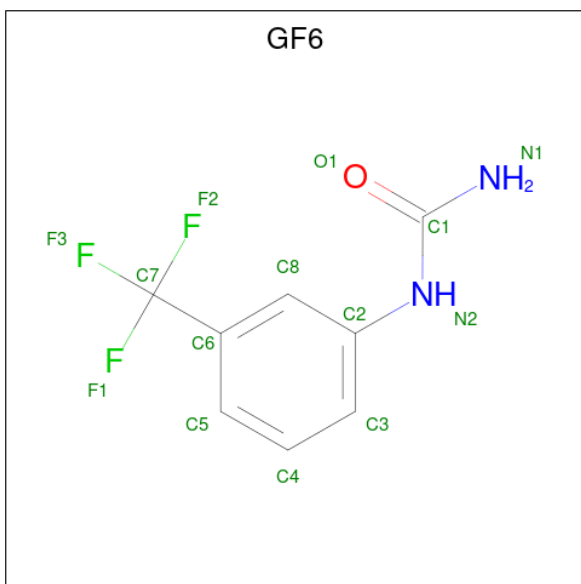
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	7	0
			74	21	26	7	17	3		
2	B	1	Total	C	H	N	O	P	7	0
			74	21	26	7	17	3		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	1	0
			31	9	11	2	8	1		
3	B	1	Total	C	H	N	O	P	1	0
			31	9	11	2	8	1		

- Molecule 4 is 1-[3-(trifluoromethyl)phenyl]urea (CCD ID: GF6) (formula: $C_8H_7F_3N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	H	N	O	4	1
			42	16	6	14	4	2		

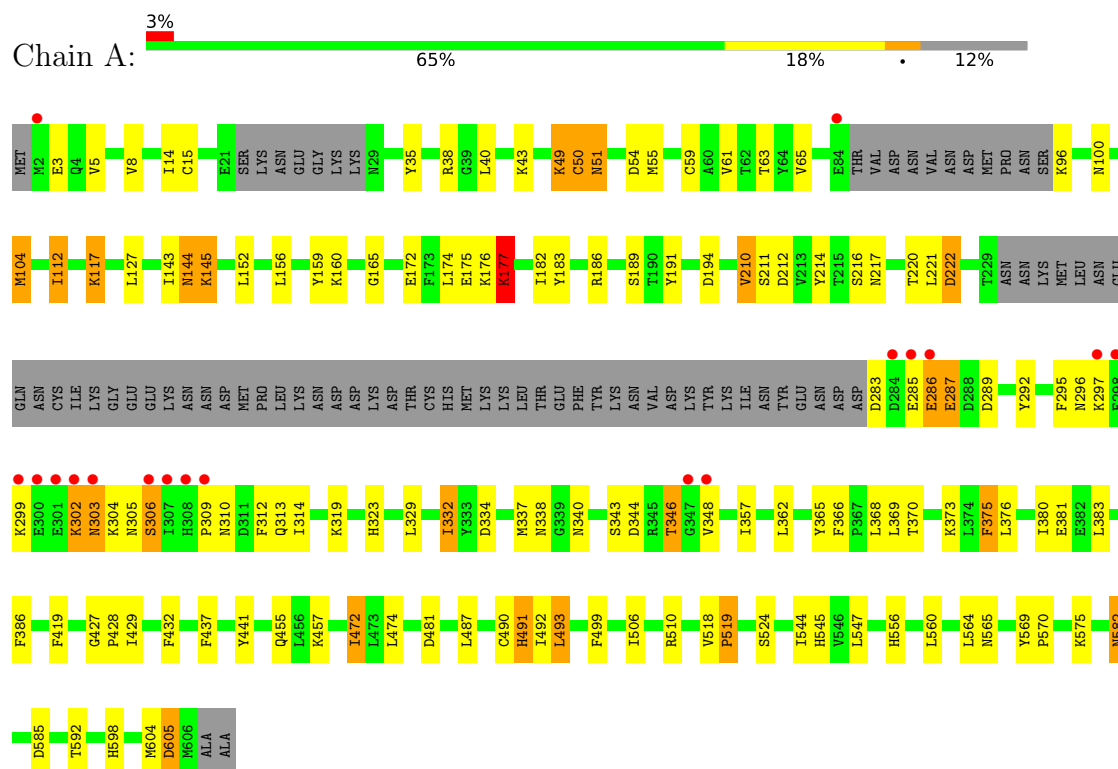
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	24	Total 24	O 24	0	0
5	B	34	Total 34	O 34	0	0

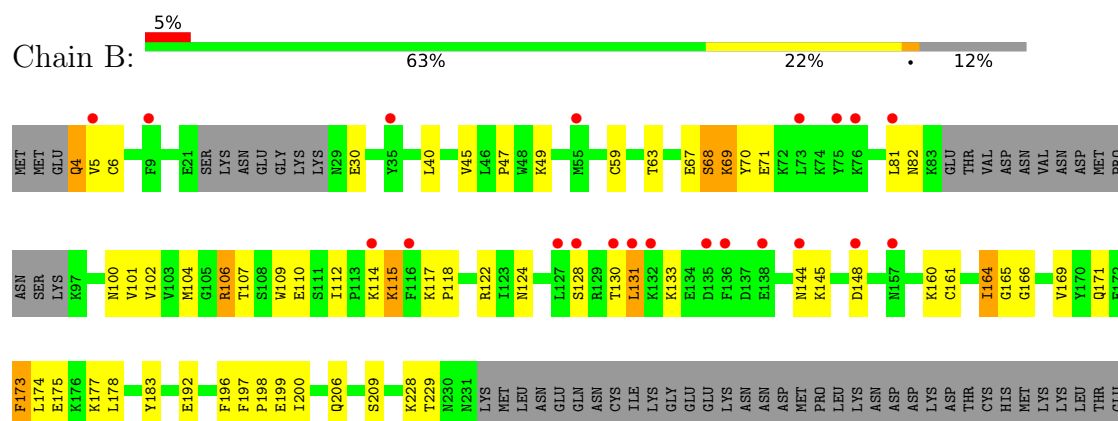
3 Residue-property plots

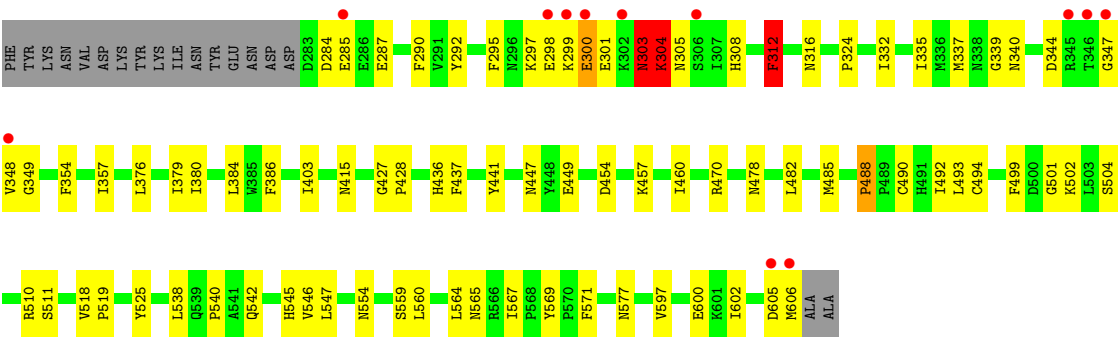
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.64Å 155.64Å 164.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.83 – 2.65 24.83 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.8 (24.83-2.65) 92.2 (24.83-2.65)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.255 , 0.325 0.198 , 0.270	Depositor DCC
R_{free} test set	2095 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17985	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: GF6, NDP, UMP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.10	4/4551 (0.1%)	1.51	20/6144 (0.3%)
1	B	1.13	3/4531 (0.1%)	1.48	9/6118 (0.1%)
All	All	1.12	7/9082 (0.1%)	1.50	29/12262 (0.2%)

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
1	A	0	2
1	B	0	4
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	519	PRO	C-O	-7.31	1.14	1.24
1	B	511	SER	C-O	5.79	1.30	1.23
1	A	544	ILE	C-O	-5.52	1.18	1.24
1	B	403	ILE	C-O	-5.41	1.18	1.24
1	A	491	HIS	CE1-NE2	5.24	1.37	1.32
1	B	540	PRO	C-O	-5.10	1.18	1.23
1	A	419	PHE	C-O	5.00	1.30	1.24

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	HIS	CA-C-N	6.26	128.57	120.56
1	A	491	HIS	C-N-CA	6.26	128.57	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	415	ASN	CB-CA-C	6.17	122.04	110.63
1	B	470	ARG	N-CA-C	-6.01	105.25	112.59
1	A	3	GLU	CA-C-N	5.96	129.58	120.82
1	A	3	GLU	C-N-CA	5.96	129.58	120.82
1	B	384	LEU	CA-C-N	5.96	128.19	120.44
1	B	384	LEU	C-N-CA	5.96	128.19	120.44
1	A	222	ASP	CA-CB-CG	5.91	118.51	112.60
1	B	344	ASP	CA-C-N	5.91	128.20	120.28
1	B	344	ASP	C-N-CA	5.91	128.20	120.28
1	A	605	ASP	CA-CB-CG	5.89	118.49	112.60
1	A	303	ASN	CA-C-N	5.76	132.54	121.54
1	A	303	ASN	C-N-CA	5.76	132.54	121.54
1	A	104	MET	CA-C-N	5.65	125.47	120.10
1	A	104	MET	C-N-CA	5.65	125.47	120.10
1	B	312	PHE	CA-CB-CG	5.56	119.36	113.80
1	A	582	ASN	CA-C-N	5.55	128.35	120.53
1	A	582	ASN	C-N-CA	5.55	128.35	120.53
1	B	488	PRO	N-CA-CB	5.55	106.30	103.19
1	A	493	LEU	CA-C-N	5.33	130.36	123.00
1	A	493	LEU	C-N-CA	5.33	130.36	123.00
1	A	8	VAL	O-C-N	5.27	127.38	121.90
1	A	381	GLU	CB-CG-CD	5.20	121.45	112.60
1	B	386	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	370	THR	N-CA-C	-5.10	107.73	114.31
1	A	306	SER	CA-C-N	5.05	127.37	120.35
1	A	306	SER	C-N-CA	5.05	127.37	120.35
1	A	472	ILE	O-C-N	5.04	126.20	121.96

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	302	LYS	Peptide
1	A	306	SER	Peptide
1	B	164	ILE	Peptide
1	B	165	GLY	Peptide
1	B	297	LYS	Peptide
1	B	347	GLY	Peptide

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	4447	4411	4396	74	0
1	B	4428	4389	4373	76	0
2	A	48	26	26	2	0
2	B	48	26	26	2	0
3	A	20	11	11	1	0
3	B	20	11	11	1	0
4	A	28	14	0	1	0
5	A	24	0	0	0	0
5	B	34	0	0	1	0
All	All	9097	8888	8843	144	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 8.

All (144) 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:312:PHE:HA	1:B:565:ASN:HD21	1.32	0.92
1:A:376:LEU:O	1:A:380:ILE:HG13	1.76	0.85
1:B:171:GLN:NE2	1:B:175:GLU:OE2	2.11	0.83
1:B:605:ASP:O	1:B:606:MET:N	2.12	0.82
1:A:334:ASP:OD1	1:A:338:ASN:ND2	2.22	0.72
1:B:312:PHE:HA	1:B:565:ASN:ND2	2.03	0.71
1:B:376:LEU:O	1:B:380:ILE:HG13	1.92	0.70
1:A:144:ASN:HD22	1:A:145:LYS:HB2	1.58	0.69
1:B:312:PHE:CA	1:B:565:ASN:HD21	2.07	0.64
1:A:492:ILE:HD11	1:A:510:ARG:HD3	1.80	0.64
1:A:211:SER:OG	1:A:212:ASP:O	2.15	0.63
1:A:15:CYS:C	4:A:703[A]:GF6:F2	2.31	0.63
1:B:303:ASN:O	1:B:305:ASN:N	2.32	0.62
1:A:332:ILE:HD12	1:A:560:LEU:HD22	1.82	0.62
1:B:428:PRO:O	1:B:485:MET:HE2	2.00	0.61
1:A:312:PHE:HA	1:A:565:ASN:HD21	1.66	0.61
1:A:332:ILE:CD1	1:A:560:LEU:HD22	2.32	0.59
1:A:210:VAL:HG22	1:A:323:HIS:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:HIS:HA	1:A:604:MET:O	2.03	0.59
1:B:100:ASN:OD1	1:B:160:LYS:N	2.35	0.58
1:A:144:ASN:HD22	1:A:144:ASN:C	2.10	0.58
1:A:455:GLN:HB3	1:A:474:LEU:HD12	1.87	0.57
1:A:493:LEU:C	1:A:493:LEU:HD12	2.30	0.57
1:A:65:VAL:HA	1:A:159:TYR:CD2	2.40	0.57
1:B:70:TYR:O	1:B:71:GLU:C	2.48	0.56
1:B:303:ASN:O	1:B:305:ASN:O	2.24	0.56
1:B:501:GLY:HA2	1:B:538:LEU:HD22	1.89	0.55
1:A:59:CYS:O	1:A:63:THR:HG23	2.07	0.55
1:A:506:ILE:HD12	1:B:354:PHE:CZ	2.42	0.55
1:B:494:CYS:SG	1:B:525:TYR:CE2	3.00	0.55
1:B:518:VAL:N	1:B:519:PRO:CD	2.70	0.54
1:A:302:LYS:HG2	1:A:302:LYS:O	2.07	0.54
1:B:379:ILE:HD12	1:B:379:ILE:C	2.32	0.54
1:A:295:PHE:CG	1:A:296:ASN:N	2.76	0.54
1:B:106:ARG:HD2	1:B:110:GLU:OE2	2.08	0.54
1:A:329:LEU:HD22	1:A:564:LEU:HD12	1.90	0.54
1:A:289:ASP:OD1	1:B:183:TYR:OH	2.25	0.54
1:A:346:THR:HB	1:A:348:VAL:HG23	1.90	0.53
1:A:43:LYS:N	1:A:194:ASP:OD2	2.39	0.53
1:B:197:PHE:CD1	1:B:198:PRO:HD2	2.44	0.53
1:A:493:LEU:HD22	1:B:492:ILE:HG21	1.90	0.53
1:B:169:VAL:O	1:B:173:PHE:HB2	2.09	0.53
1:B:501:GLY:HA2	1:B:538:LEU:CD2	2.39	0.53
1:A:427:GLY:HA2	1:A:441:TYR:CE2	2.43	0.53
1:B:312:PHE:HB3	1:B:565:ASN:ND2	2.24	0.52
1:A:292:TYR:O	1:A:295:PHE:HB3	2.10	0.52
1:A:14:ILE:HA	1:A:183:TYR:O	2.10	0.51
1:A:100:ASN:OD1	1:A:159:TYR:HB3	2.11	0.50
1:A:186:ARG:NH2	1:A:222:ASP:OD2	2.43	0.50
1:B:304:LYS:HB2	1:B:337:MET:O	2.10	0.50
1:A:499:PHE:CE1	1:B:340:ASN:HB3	2.47	0.50
1:B:312:PHE:HD2	1:B:316:ASN:HD21	1.58	0.50
1:A:176:LYS:O	1:A:177:LYS:C	2.55	0.49
1:A:373:LYS:HG3	1:A:598:HIS:CE1	2.48	0.49
1:B:482:LEU:HD22	1:B:488:PRO:HB3	1.95	0.49
1:B:166:GLY:HA3	2:B:702:NDP:O1A	2.13	0.49
1:B:112:ILE:HB	1:B:117:LYS:HD3	1.95	0.49
1:A:490:CYS:SG	3:A:702:UMP:C6	3.06	0.49
1:B:101:VAL:HB	1:B:161:CYS:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LEU:HD23	1:A:143:ILE:HG13	1.95	0.48
1:B:102:VAL:HG11	1:B:122:ARG:HD2	1.94	0.48
1:B:102:VAL:HG23	1:B:102:VAL:O	2.12	0.48
1:B:493:LEU:HD12	1:B:493:LEU:C	2.37	0.48
1:A:189:SER:HG	1:A:191:TYR:HE2	1.60	0.48
1:A:40:LEU:O	2:A:701:NDP:H2N	2.14	0.47
1:B:4:GLN:HE21	1:B:5:VAL:H	1.61	0.47
1:B:292:TYR:O	1:B:295:PHE:HB3	2.13	0.47
1:B:324:PRO:HB2	1:B:571:PHE:HE2	1.79	0.47
1:A:174:LEU:HD21	1:A:182:ILE:HD11	1.96	0.47
1:B:447:ASN:OD1	1:B:449:GLU:HB2	2.14	0.47
1:A:152:LEU:HG	1:A:156:LEU:HD12	1.95	0.47
1:A:569:TYR:HB3	1:A:570:PRO:HD2	1.97	0.47
1:A:189:SER:OG	1:A:191:TYR:CE2	2.68	0.47
1:B:171:GLN:O	1:B:175:GLU:HG2	2.14	0.47
1:B:427:GLY:HA2	1:B:441:TYR:CE2	2.49	0.47
1:A:144:ASN:ND2	1:A:145:LYS:HB2	2.29	0.47
1:A:437:PHE:C	1:A:437:PHE:CD1	2.93	0.47
1:B:349:GLY:C	1:B:554:ASN:ND2	2.73	0.47
1:A:545:HIS:CD2	1:A:547:LEU:CD2	2.98	0.46
1:B:40:LEU:O	1:B:47:PRO:HD3	2.14	0.46
1:A:303:ASN:OD1	1:A:337:MET:HE3	2.15	0.46
1:A:582:ASN:HB3	1:A:585:ASP:OD2	2.15	0.46
1:B:197:PHE:CG	1:B:198:PRO:HD2	2.49	0.46
1:A:428:PRO:HG2	1:A:481:ASP:HB3	1.97	0.46
1:B:128:SER:OG	1:B:131:LEU:HB2	2.14	0.46
1:B:335:ILE:O	1:B:339:GLY:N	2.48	0.46
1:A:518:VAL:N	1:A:519:PRO:HD2	2.31	0.46
1:A:61:VAL:HG22	1:B:292:TYR:CG	2.51	0.46
1:B:494:CYS:SG	1:B:525:TYR:HE2	2.39	0.45
1:A:340:ASN:HB3	1:B:499:PHE:CE1	2.51	0.45
1:B:67:GLU:C	1:B:69:LYS:H	2.22	0.45
1:B:106:ARG:HD2	1:B:110:GLU:CD	2.41	0.45
1:A:362:LEU:HA	1:A:365:TYR:O	2.16	0.45
1:A:375:PHE:CD1	1:A:375:PHE:N	2.84	0.45
1:A:144:ASN:ND2	1:A:145:LYS:HE3	2.31	0.45
1:B:332:ILE:HG23	1:B:560:LEU:HD13	1.98	0.45
1:B:436:HIS:O	1:B:437:PHE:C	2.58	0.45
1:A:189:SER:OG	1:A:191:TYR:HE2	2.00	0.44
1:A:51:ASN:C	1:A:51:ASN:HD22	2.24	0.44
1:A:214:TYR:O	1:A:220:THR:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:SER:HA	1:B:542:GLN:O	2.17	0.44
1:A:127:LEU:O	2:A:701:NDP:H1B	2.17	0.44
1:A:428:PRO:CB	1:A:432:PHE:CD2	3.00	0.44
1:B:287:GLU:O	1:B:290:PHE:HB3	2.17	0.44
1:B:299:LYS:HG2	1:B:301:GLU:H	1.82	0.44
1:B:122:ARG:O	1:B:124:ASN:ND2	2.48	0.44
1:B:454:ASP:CG	1:B:457:LYS:HB2	2.43	0.44
1:A:186:ARG:O	1:A:221:LEU:HA	2.18	0.44
1:B:499:PHE:O	1:B:502:LYS:HB2	2.17	0.43
1:B:109:TRP:CZ2	1:B:117:LYS:HD2	2.53	0.43
1:B:117:LYS:HA	1:B:118:PRO:C	2.43	0.43
1:B:357:ILE:HD12	1:B:546:VAL:HG22	2.01	0.43
1:A:35:TYR:CZ	1:A:38:ARG:HD3	2.54	0.43
1:A:49:LYS:HD2	1:A:50:CYS:H	1.84	0.43
1:A:51:ASN:C	1:A:51:ASN:ND2	2.76	0.43
1:A:518:VAL:O	1:A:519:PRO:C	2.62	0.43
2:B:702:NDP:O1A	2:B:702:NDP:O2N	2.35	0.43
1:A:545:HIS:CD2	1:A:547:LEU:HD23	2.54	0.43
1:B:545:HIS:CD2	1:B:547:LEU:CD2	3.01	0.43
1:A:506:ILE:HD12	1:B:354:PHE:CE1	2.54	0.43
1:B:6:CYS:HB3	1:B:178:LEU:C	2.44	0.42
1:A:216:SER:O	1:A:217:ASN:C	2.61	0.42
1:B:492:ILE:HD11	1:B:510:ARG:HD3	2.00	0.42
1:B:460:ILE:HD13	5:B:817:HOH:O	2.19	0.42
1:A:159:TYR:CD2	1:A:160:LYS:HG3	2.54	0.42
1:B:40:LEU:HD12	1:B:196:PHE:O	2.19	0.42
1:B:198:PRO:O	1:B:200:ILE:N	2.52	0.42
1:A:172:GLU:HA	1:A:175:GLU:HB2	2.00	0.42
1:A:303:ASN:HD22	1:A:303:ASN:HA	1.77	0.42
1:A:112:ILE:HB	1:A:117:LYS:HD3	2.01	0.42
1:A:144:ASN:HD21	1:A:145:LYS:HE3	1.85	0.41
1:B:577:ASN:OD1	1:B:577:ASN:C	2.62	0.41
1:B:299:LYS:HG2	1:B:300:GLU:N	2.35	0.41
1:B:312:PHE:HB3	1:B:565:ASN:HD21	1.83	0.41
1:B:109:TRP:CH2	1:B:117:LYS:HB3	2.55	0.41
1:B:59:CYS:O	1:B:63:THR:OG1	2.20	0.41
1:B:312:PHE:CB	1:B:565:ASN:HD21	2.33	0.41
1:A:383:LEU:O	1:A:386:PHE:HB2	2.21	0.41
1:A:366:PHE:CE2	1:A:368:LEU:HB2	2.57	0.40
1:B:569:TYR:CG	1:B:597:VAL:HG12	2.56	0.40
1:A:51:ASN:HD22	1:A:54:ASP:H	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:PHE:CE2	1:B:478:ASN:HB2	2.57	0.40
1:A:104:MET:HA	1:A:165:GLY:O	2.21	0.40
1:B:490:CYS:SG	3:B:703:UMP:C6	3.15	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	526/608 (86%)	478 (91%)	39 (7%)	9 (2%)	7	12
1	B	523/608 (86%)	470 (90%)	43 (8%)	10 (2%)	6	10
All	All	1049/1216 (86%)	948 (90%)	82 (8%)	19 (2%)	6	11

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	LYS
1	A	310	ASN
1	B	68	SER
1	B	82	ASN
1	B	199	GLU
1	B	303	ASN
1	B	304	LYS
1	A	286	GLU
1	A	287	GLU
1	B	115	LYS
1	A	177	LYS
1	B	49	LYS
1	A	297	LYS
1	A	285	GLU
1	A	309	PRO

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Mol	Chain	Res	Type
1	B	69	LYS
1	B	148	ASP
1	B	308	HIS
1	A	429	ILE

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	500/570 (88%)	465 (93%)	35 (7%)	14	24
1	B	498/570 (87%)	461 (93%)	37 (7%)	13	21
All	All	998/1140 (88%)	926 (93%)	72 (7%)	13	22

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	49	LYS
1	A	50	CYS
1	A	51	ASN
1	A	55	MET
1	A	96	LYS
1	A	112	ILE
1	A	117	LYS
1	A	144	ASN
1	A	145	LYS
1	A	177	LYS
1	A	210	VAL
1	A	283	ASP
1	A	286	GLU
1	A	287	GLU
1	A	299	LYS
1	A	305	ASN
1	A	313	GLN
1	A	314	ILE

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Mol	Chain	Res	Type
1	A	319	LYS
1	A	332	ILE
1	A	343	SER
1	A	344	ASP
1	A	346	THR
1	A	357	ILE
1	A	369	LEU
1	A	375	PHE
1	A	457	LYS
1	A	472	ILE
1	A	487	LEU
1	A	491	HIS
1	A	524	SER
1	A	575	LYS
1	A	592	THR
1	A	605	ASP
1	B	4	GLN
1	B	30	GLU
1	B	45	VAL
1	B	68	SER
1	B	81	LEU
1	B	104	MET
1	B	106	ARG
1	B	107	THR
1	B	114	LYS
1	B	115	LYS
1	B	130	THR
1	B	131	LEU
1	B	133	LYS
1	B	144	ASN
1	B	145	LYS
1	B	164	ILE
1	B	173	PHE
1	B	174	LEU
1	B	177	LYS
1	B	192	GLU
1	B	206	GLN
1	B	209	SER
1	B	228	LYS
1	B	229	THR
1	B	284	ASP
1	B	285	GLU

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Mol	Chain	Res	Type
1	B	298	GLU
1	B	300	GLU
1	B	303	ASN
1	B	304	LYS
1	B	312	PHE
1	B	348	VAL
1	B	559	SER
1	B	564	LEU
1	B	567	ILE
1	B	600	GLU
1	B	602	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	51	ASN
1	A	99	GLN
1	A	144	ASN
1	A	206	GLN
1	A	313	GLN
1	A	394	ASN
1	A	407	ASN
1	A	415	ASN
1	A	424	ASN
1	A	530	HIS
1	A	556	HIS
1	A	594	GLN
1	B	4	GLN
1	B	82	ASN
1	B	99	GLN
1	B	144	ASN
1	B	231	ASN
1	B	303	ASN
1	B	316	ASN
1	B	394	ASN
1	B	424	ASN
1	B	554	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	UMP	A	702	-	21,21,21	0.58	0	30,31,31	0.74	0
2	NDP	A	701	-	51,52,52	2.03	16 (31%)	71,80,80	2.05	17 (23%)
4	GF6	A	703[A]	-	14,14,14	0.51	0	20,20,20	1.19	1 (5%)
2	NDP	B	702	-	51,52,52	2.26	16 (31%)	71,80,80	2.18	21 (29%)
4	GF6	A	703[B]	-	14,14,14	0.29	0	20,20,20	0.77	0
3	UMP	B	703	-	21,21,21	0.59	0	30,31,31	0.77	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UMP	A	702	-	-	0/10/22/22	0/2/2/2
2	NDP	A	701	-	-	12/34/77/77	0/5/5/5
4	GF6	A	703[A]	-	-	2/10/10/10	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	B	702	-	-	14/34/77/77	0/5/5/5
4	GF6	A	703[B]	-	-	4/10/10/10	0/1/1/1
3	UMP	B	703	-	-	3/10/22/22	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	NDP	PN-O3	9.30	1.69	1.59
2	A	701	NDP	C4N-C3N	-5.98	1.38	1.50
2	A	701	NDP	PN-O3	5.10	1.65	1.59
2	B	702	NDP	PA-O3	4.02	1.63	1.59
2	A	701	NDP	C2A-N3A	3.94	1.40	1.33
2	B	702	NDP	P2B-O2B	3.78	1.66	1.59
2	B	702	NDP	C4N-C3N	-3.69	1.43	1.50
2	B	702	NDP	C4N-C5N	-3.67	1.39	1.49
2	B	702	NDP	C7N-C3N	-3.56	1.41	1.48
2	A	701	NDP	C7N-C3N	-3.52	1.41	1.48
2	A	701	NDP	O3B-C3B	3.45	1.51	1.43
2	B	702	NDP	C2A-N1A	3.20	1.39	1.33
2	B	702	NDP	O4B-C1B	3.08	1.49	1.42
2	A	701	NDP	PA-O3	2.95	1.62	1.59
2	A	701	NDP	C4N-C5N	-2.91	1.41	1.49
2	B	702	NDP	O2B-C2B	2.87	1.53	1.44
2	A	701	NDP	O4D-C1D	2.86	1.48	1.42
2	A	701	NDP	C2A-N1A	2.85	1.39	1.33
2	A	701	NDP	O2D-C2D	2.81	1.49	1.43
2	B	702	NDP	C5A-C4A	-2.76	1.34	1.39
2	B	702	NDP	C5A-N7A	-2.66	1.34	1.39
2	A	701	NDP	C4A-N9A	-2.61	1.32	1.37
2	B	702	NDP	C1B-N9A	2.60	1.53	1.46
2	B	702	NDP	C5A-C6A	-2.57	1.33	1.41
2	A	701	NDP	P2B-O2X	-2.41	1.45	1.54
2	A	701	NDP	C4A-N3A	-2.40	1.29	1.34
2	B	702	NDP	C2A-N3A	2.33	1.38	1.33
2	B	702	NDP	PN-O5D	2.29	1.68	1.59
2	A	701	NDP	C5A-C4A	-2.28	1.35	1.39
2	B	702	NDP	C4A-N9A	-2.28	1.32	1.37
2	A	701	NDP	O4B-C1B	2.25	1.47	1.42
2	A	701	NDP	C1D-N1N	2.24	1.52	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	702	NDP	N3A-C2A-N1A	-7.55	117.15	128.58
2	A	701	NDP	O3-PN-O1N	-7.48	88.19	110.70
2	B	702	NDP	O3-PN-O1N	-6.96	89.77	110.70
2	A	701	NDP	O2N-PN-O3	-6.78	88.95	107.27
2	B	702	NDP	O2N-PN-O3	-5.94	91.21	107.27
2	A	701	NDP	N9A-C8A-N7A	-4.46	107.61	113.94
2	A	701	NDP	C4A-C5A-N7A	-4.16	105.83	110.58
2	A	701	NDP	C5A-C4A-N3A	-4.13	121.02	126.72
2	B	702	NDP	C3B-C2B-C1B	-3.76	95.61	102.81
2	B	702	NDP	N9A-C8A-N7A	-3.73	108.65	113.94
2	A	701	NDP	N3A-C2A-N1A	-3.58	123.16	128.58
2	B	702	NDP	O2N-PN-O5D	3.52	123.54	107.57
2	B	702	NDP	C5A-C4A-N3A	-3.49	121.91	126.72
2	B	702	NDP	C2A-N3A-C4A	3.36	120.04	111.83
2	A	701	NDP	C5A-N7A-C8A	3.34	108.69	103.45
2	A	701	NDP	C5A-C4A-N9A	3.27	109.38	105.81
2	B	702	NDP	C4A-N9A-C1B	-3.18	119.19	126.63
2	B	702	NDP	O2B-P2B-O1X	-3.13	98.17	109.33
2	B	702	NDP	O4D-C1D-N1N	-2.86	102.63	108.08
2	A	701	NDP	C2A-N3A-C4A	2.83	118.73	111.83
2	A	701	NDP	O3X-P2B-O2X	2.80	118.29	107.80
2	B	702	NDP	C1B-N9A-C8A	2.67	133.03	127.09
2	A	701	NDP	O2N-PN-O5D	2.63	119.48	107.57
2	A	701	NDP	C4A-N9A-C8A	2.62	108.49	105.74
2	B	702	NDP	C5A-C6A-N6A	-2.60	116.85	123.29
2	A	701	NDP	C4A-N9A-C1B	-2.51	120.77	126.63
2	A	701	NDP	O2N-PN-O1N	2.49	124.05	112.44
2	A	701	NDP	C2A-N1A-C6A	-2.41	114.77	118.73
2	A	701	NDP	O4D-C1D-N1N	2.40	112.66	108.08
2	B	702	NDP	C5A-N7A-C8A	2.39	107.20	103.45
2	B	702	NDP	O2N-PN-O1N	2.38	123.52	112.44
2	B	702	NDP	C1D-N1N-C2N	-2.28	117.38	121.14
2	A	701	NDP	C6A-C5A-C4A	2.27	120.28	117.18
2	B	702	NDP	C2B-C1B-N9A	2.17	117.32	113.75
2	B	702	NDP	O2A-PA-O1A	2.11	122.27	112.44
2	B	702	NDP	O3X-P2B-O2X	2.10	115.66	107.80
2	B	702	NDP	C5A-C4A-N9A	2.07	108.07	105.81
2	B	702	NDP	C3N-C2N-N1N	-2.06	120.18	123.20
4	A	703[A]	GF6	C8-C2-N2	2.04	126.76	120.13
3	B	703	UMP	C2'-C3'-C4'	-2.02	98.71	102.80

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	NDP	C5B-O5B-PA-O1A
2	A	701	NDP	C5B-O5B-PA-O2A
2	A	701	NDP	C5B-O5B-PA-O3
2	A	701	NDP	C5D-O5D-PN-O1N
2	B	702	NDP	C5B-O5B-PA-O1A
2	B	702	NDP	C5B-O5B-PA-O3
2	B	702	NDP	C5D-O5D-PN-O1N
4	A	703[B]	GF6	N1-C1-N2-C2
4	A	703[B]	GF6	O1-C1-N2-C2
2	A	701	NDP	C3B-C4B-C5B-O5B
2	A	701	NDP	O4B-C4B-C5B-O5B
4	A	703[A]	GF6	N1-C1-N2-C2
4	A	703[A]	GF6	O1-C1-N2-C2
4	A	703[B]	GF6	C3-C2-N2-C1
4	A	703[B]	GF6	C8-C2-N2-C1
2	B	702	NDP	PN-O3-PA-O1A
2	B	702	NDP	PA-O3-PN-O1N
2	B	702	NDP	C2D-C1D-N1N-C2N
2	A	701	NDP	C5D-O5D-PN-O3
2	B	702	NDP	C5B-O5B-PA-O2A
2	A	701	NDP	C4D-C5D-O5D-PN
3	B	703	UMP	C5'-O5'-P-OP1
2	B	702	NDP	O4D-C1D-N1N-C2N
2	B	702	NDP	C2D-C1D-N1N-C6N
2	A	701	NDP	O4D-C1D-N1N-C2N
2	A	701	NDP	C2N-C3N-C7N-N7N
2	B	702	NDP	C2N-C3N-C7N-N7N
2	B	702	NDP	C2B-O2B-P2B-O1X
2	B	702	NDP	PA-O3-PN-O2N
2	A	701	NDP	C2D-C1D-N1N-C2N
2	A	701	NDP	C3D-C4D-C5D-O5D
3	B	703	UMP	O4'-C4'-C5'-O5'
2	B	702	NDP	PN-O3-PA-O2A
2	B	702	NDP	C2B-O2B-P2B-O2X
3	B	703	UMP	C4'-C5'-O5'-P

There are no ring outliers.

5 monomers are involved in 7 short contacts:

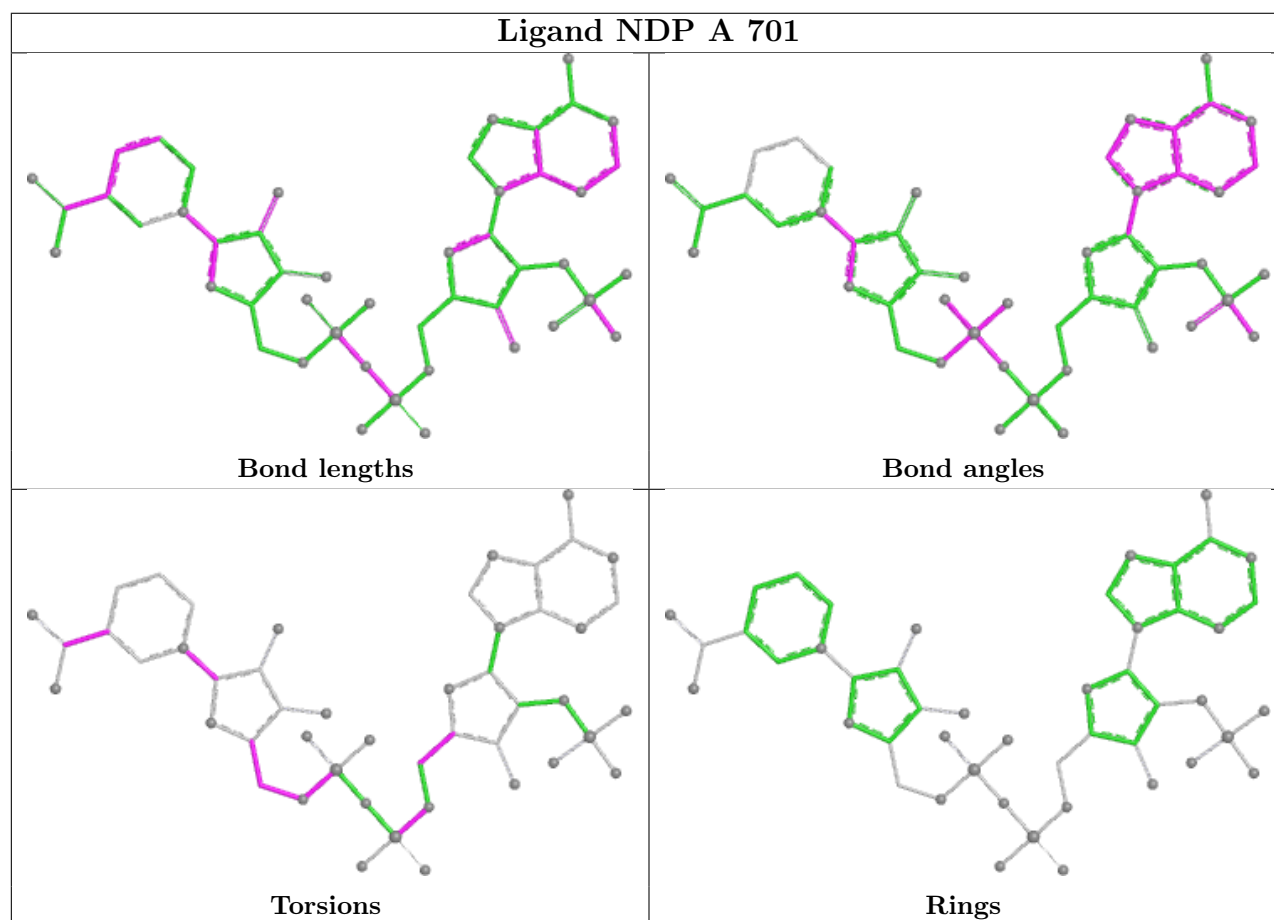
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	UMP	1	0
2	A	701	NDP	2	0
4	A	703[A]	GF6	1	0

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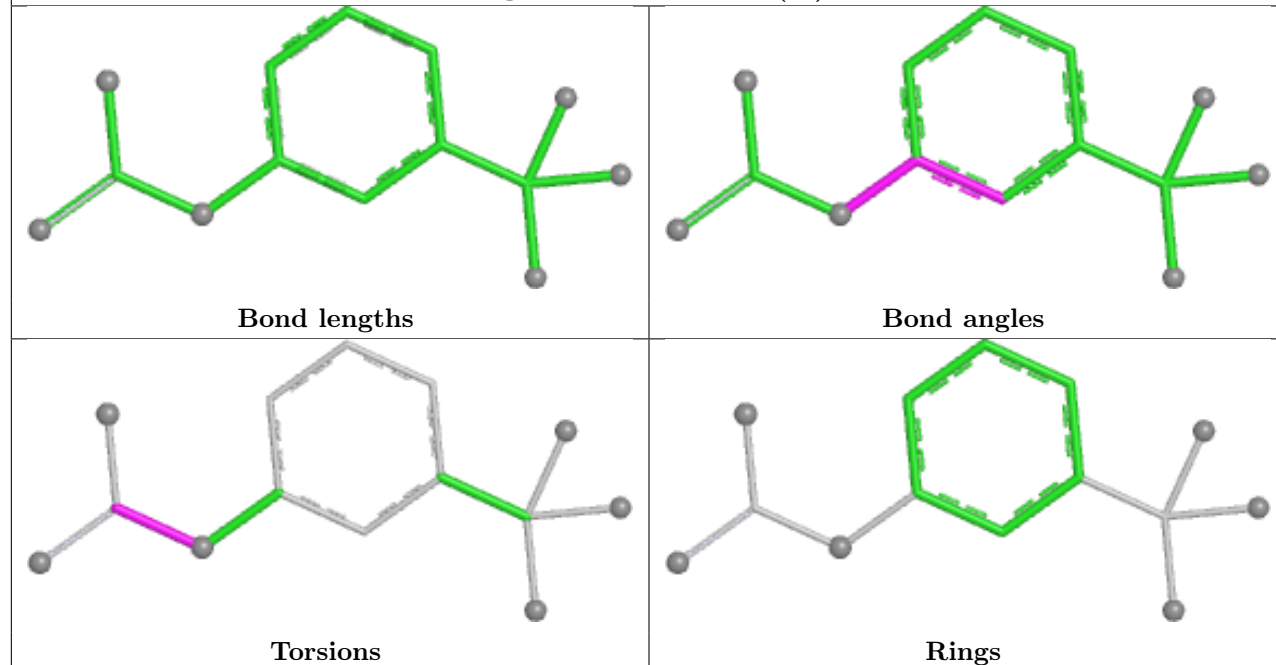
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	702	NDP	2	0
3	B	703	UMP	1	0

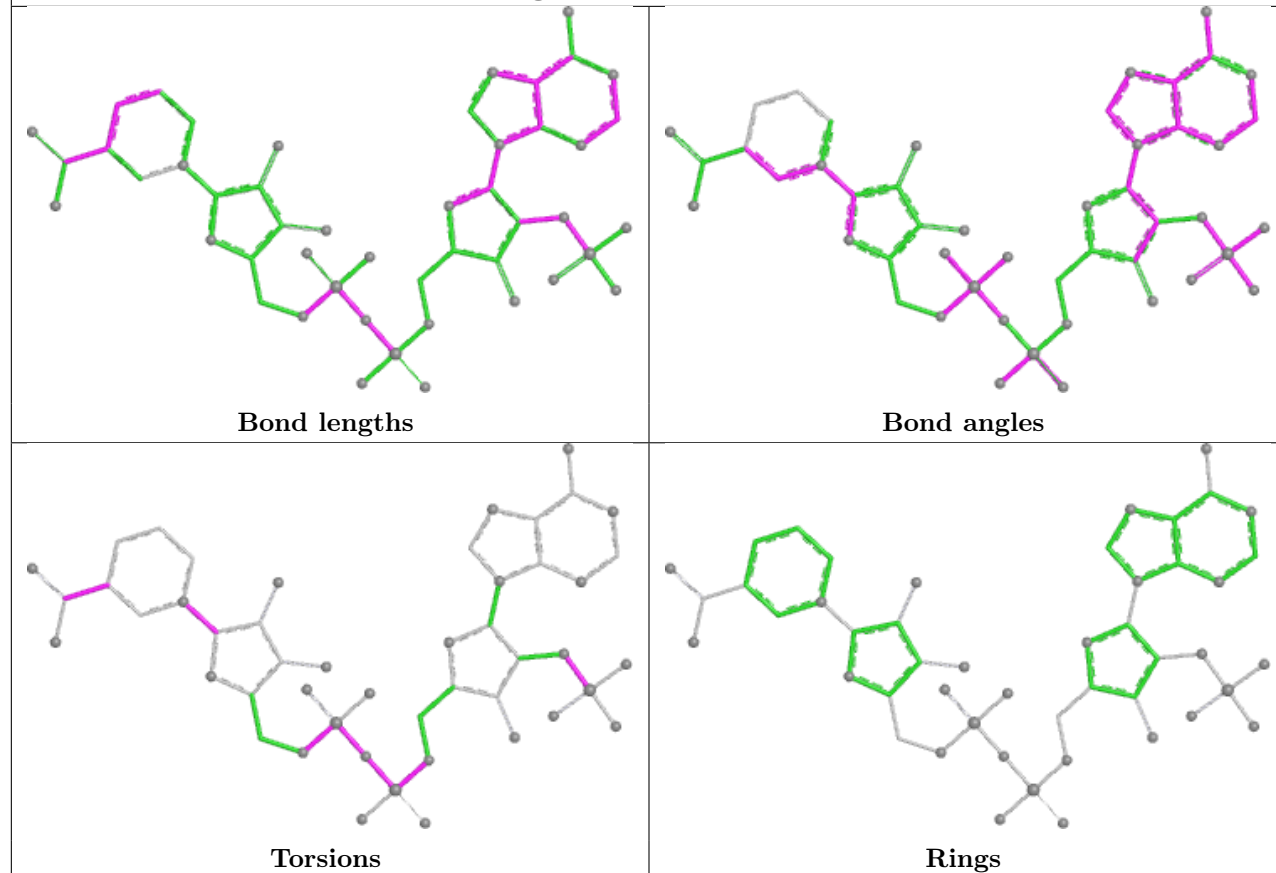
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

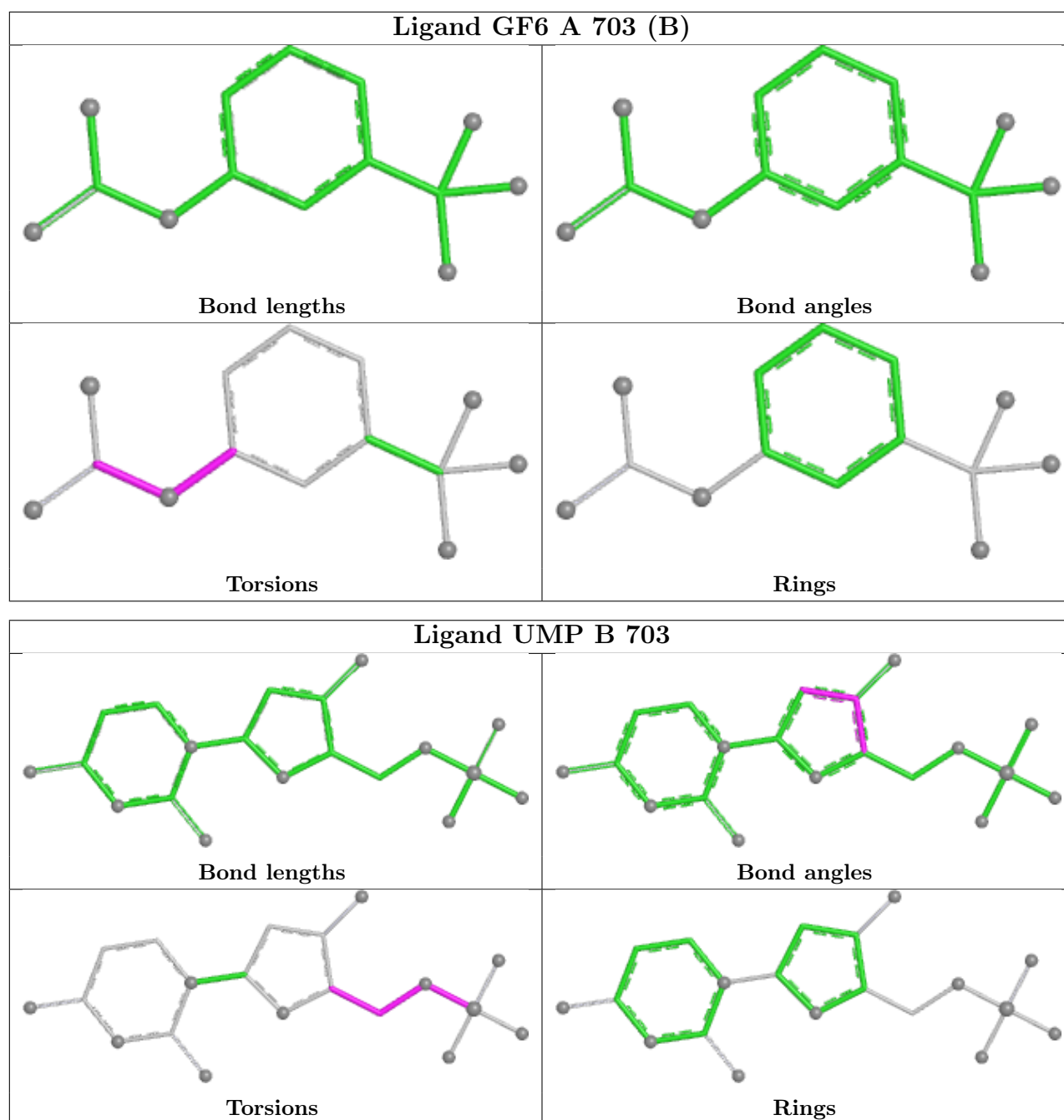


Ligand GF6 A 703 (A)



Ligand NDP B 702





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	605:ASP	C	606:MET	N	3.30

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	534/608 (87%)	-0.37	18 (3%)	48 40	9, 22, 63, 115	0
1	B	532/608 (87%)	0.02	33 (6%)	26 20	9, 28, 85, 153	0
All	All	1066/1216 (87%)	-0.18	51 (4%)	35 28	9, 24, 79, 153	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	136	PHE	6.4
1	A	348	VAL	4.7
1	A	347	GLY	4.3
1	B	116	PHE	3.9
1	B	144	ASN	3.8
1	B	130	THR	3.8
1	B	302	LYS	3.7
1	B	299	LYS	3.6
1	A	84	GLU	3.4
1	B	9	PHE	3.0
1	A	286	GLU	3.0
1	B	138	GLU	2.8
1	B	300	GLU	2.8
1	A	285	GLU	2.7
1	B	306	SER	2.7
1	A	298	GLU	2.7
1	A	300	GLU	2.7
1	B	76	LYS	2.7
1	B	75	TYR	2.7
1	B	55	MET	2.7
1	B	131	LEU	2.7
1	A	2	MET	2.6
1	B	157	ASN	2.6
1	B	128	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	302	LYS	2.5
1	A	297	LYS	2.5
1	B	347	GLY	2.4
1	A	299	LYS	2.4
1	B	346	THR	2.4
1	A	307	ILE	2.4
1	A	306	SER	2.4
1	B	81	LEU	2.4
1	A	284	ASP	2.4
1	B	148	ASP	2.4
1	B	285	GLU	2.3
1	A	303	ASN	2.3
1	B	127	LEU	2.3
1	B	114	LYS	2.2
1	B	605	ASP	2.2
1	B	135	ASP	2.2
1	A	309	PRO	2.1
1	B	606	MET	2.1
1	A	301	GLU	2.1
1	B	132	LYS	2.1
1	B	73	LEU	2.1
1	A	308	HIS	2.1
1	B	35	TYR	2.1
1	B	348	VAL	2.0
1	B	298	GLU	2.0
1	B	5	VAL	2.0
1	B	345	ARG	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,

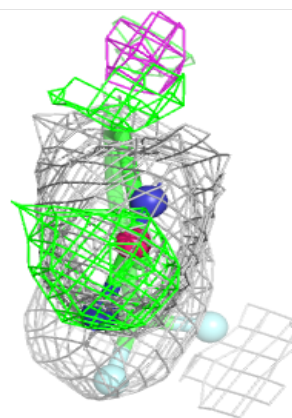
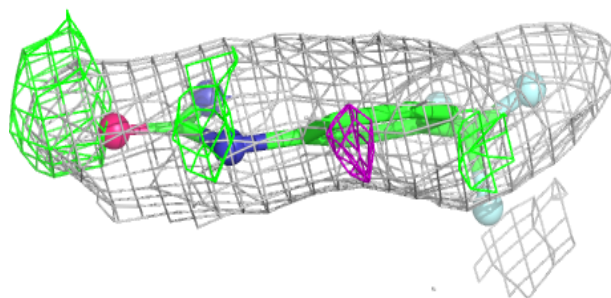
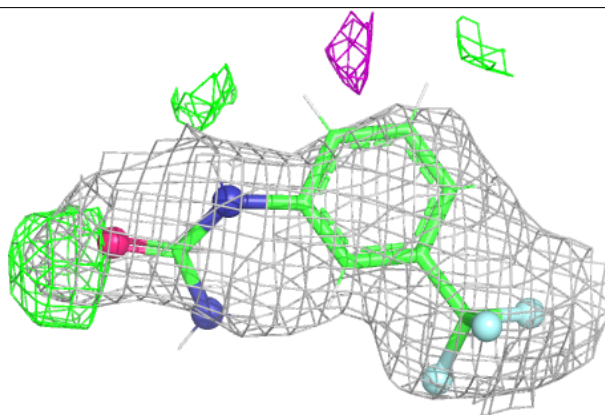
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GF6	A	703[A]	14/14	0.85	0.15	29,32,38,38	21
4	GF6	A	703[B]	14/14	0.85	0.15	24,34,46,52	21
2	NDP	B	702	48/48	0.91	0.12	40,57,89,93	7
3	UMP	B	703	20/20	0.96	0.09	23,29,35,35	1
3	UMP	A	702	20/20	0.98	0.07	19,27,33,40	1
2	NDP	A	701	48/48	0.98	0.05	15,19,24,27	7

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.

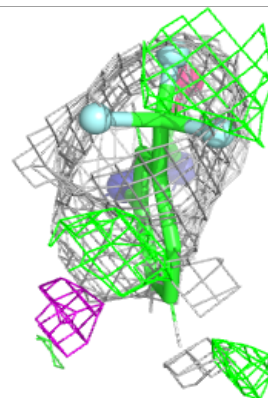
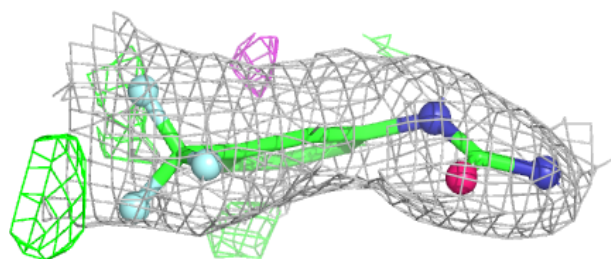
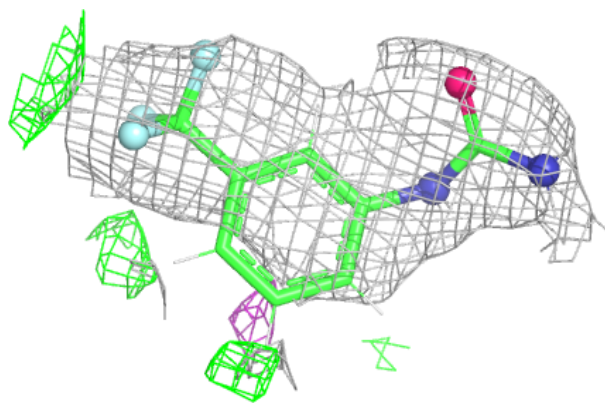
Electron density around GF6 A 703 (A):

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

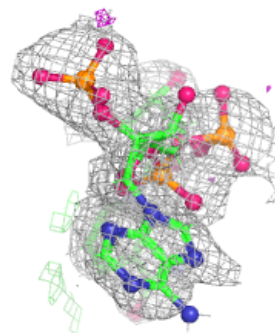
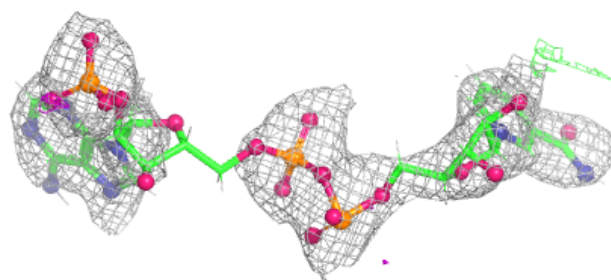
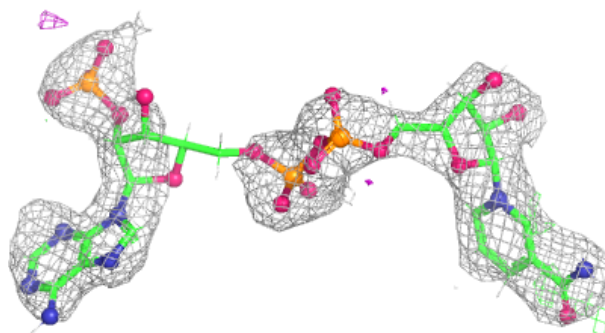


Electron density around GF6 A 703 (B):

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

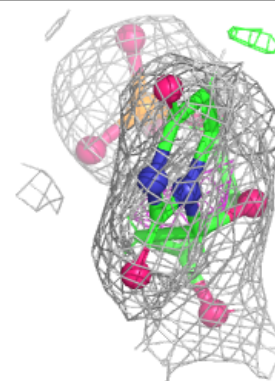
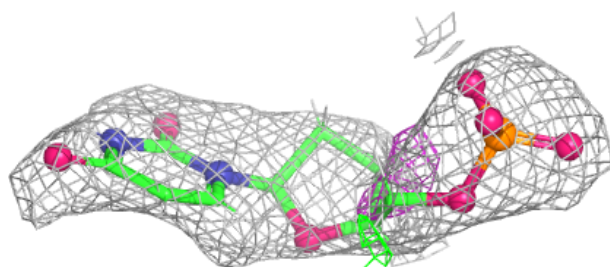
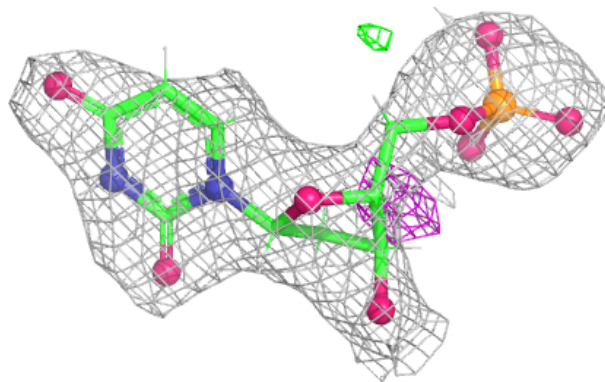
**Electron density around NDP B 702:**

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

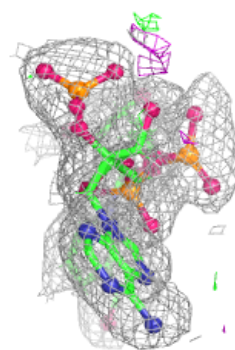
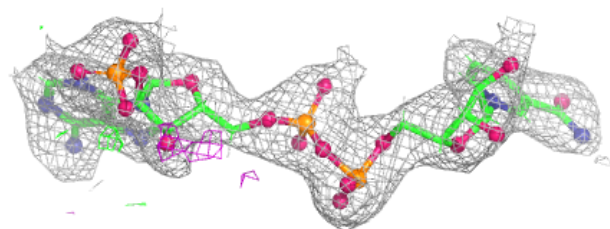
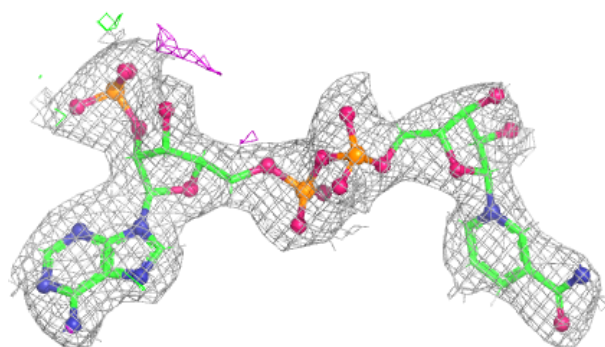


Electron density around UMP B 703:

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

**Electron density around NDP A 701:**

$2mF_o-DF_c$ (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.