



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:56 PM UTC

PDB ID : 6KOT / pdb_00006kot
Title : Quadruple mutant (N51I+C59R+S108N+I164L) plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with B12128 and NADPH
Authors : Vanichtanankul, J.; Vitsupakorn, D.
Deposited on : 2019-08-13
Resolution : 2.15 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

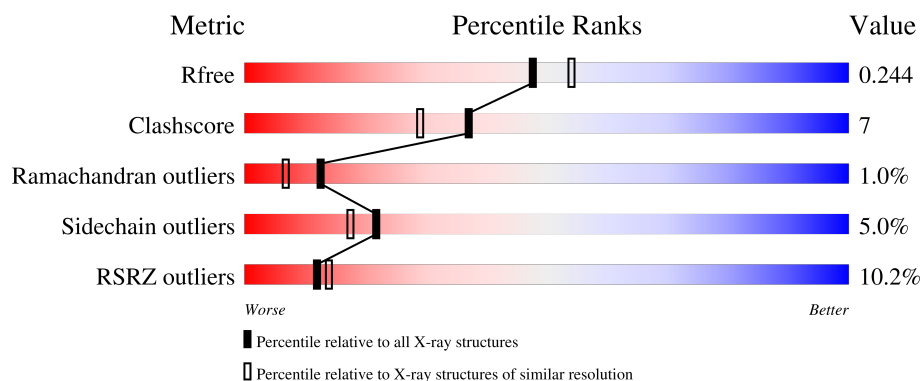
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	6% 71% 14% • 13%
1	B	608	12% 70% 13% • 14%

2 Entry composition [i](#)

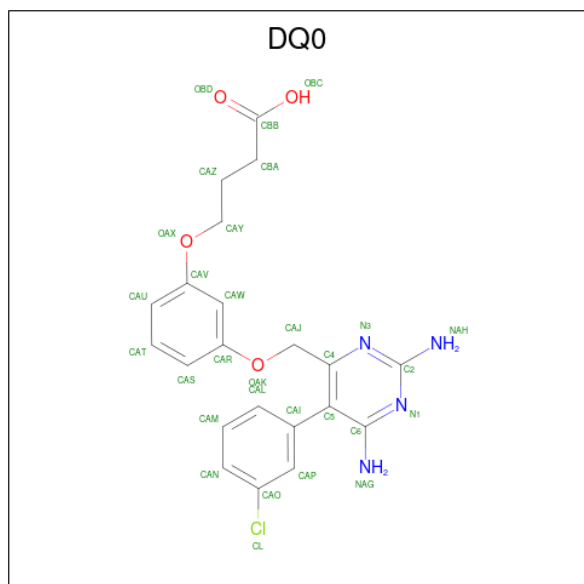
There are 5 unique types of molecules in this entry. The entry contains 9234 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	526	Total	C	N	O	S	0	0	0
			4383	2842	724	792	25			
1	B	522	Total	C	N	O	S	0	0	0
			4339	2809	718	788	24			

- Molecule 2 is 4-[3-[[2,6-bis(azanyl)-5-(3-chlorophenyl)pyrimidin-4-yl]methoxy]phenoxy]butanoic acid (CCD ID: DQ0) (formula: C₂₁H₂₁ClN₄O₄) (labeled as "Ligand of Interest" by depositor).



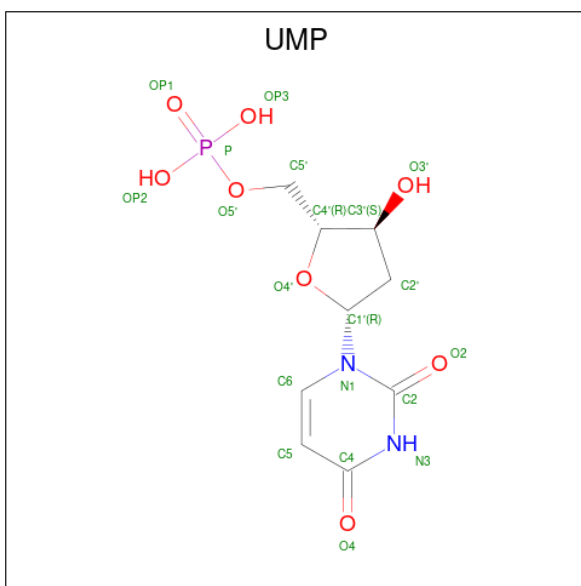
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			30	21	1	4	4		
2	B	1	Total	C	Cl	N	O	0	0
			30	21	1	4	4		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

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



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

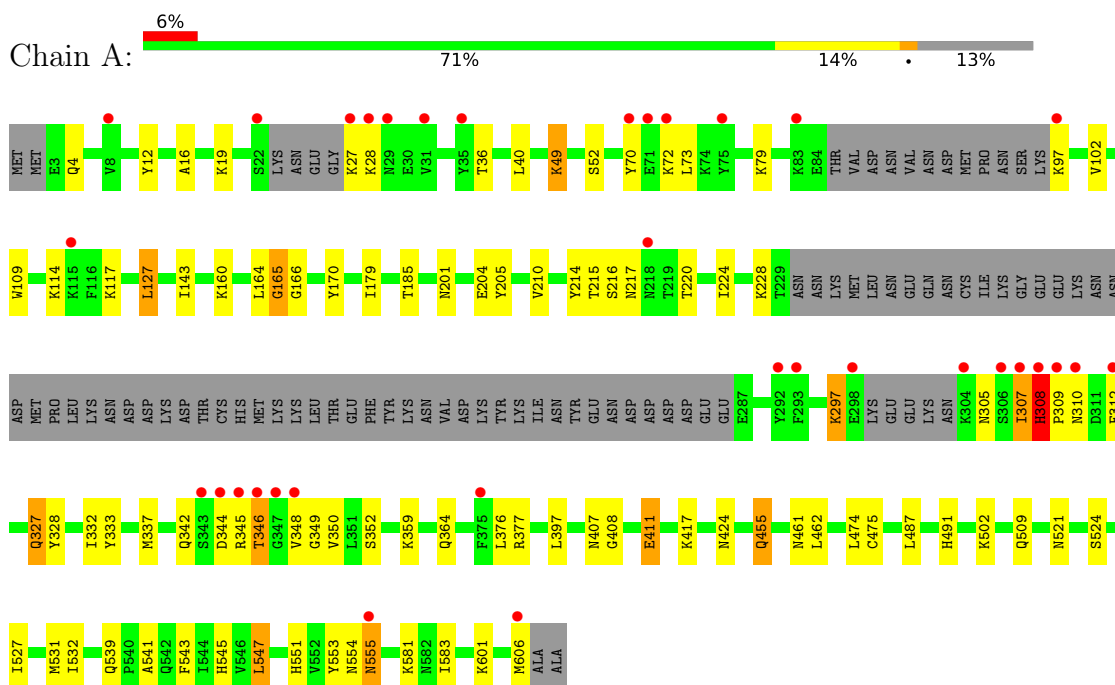
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	165	Total 165	O 165	0	0
5	B	151	Total 151	O 151	0	0

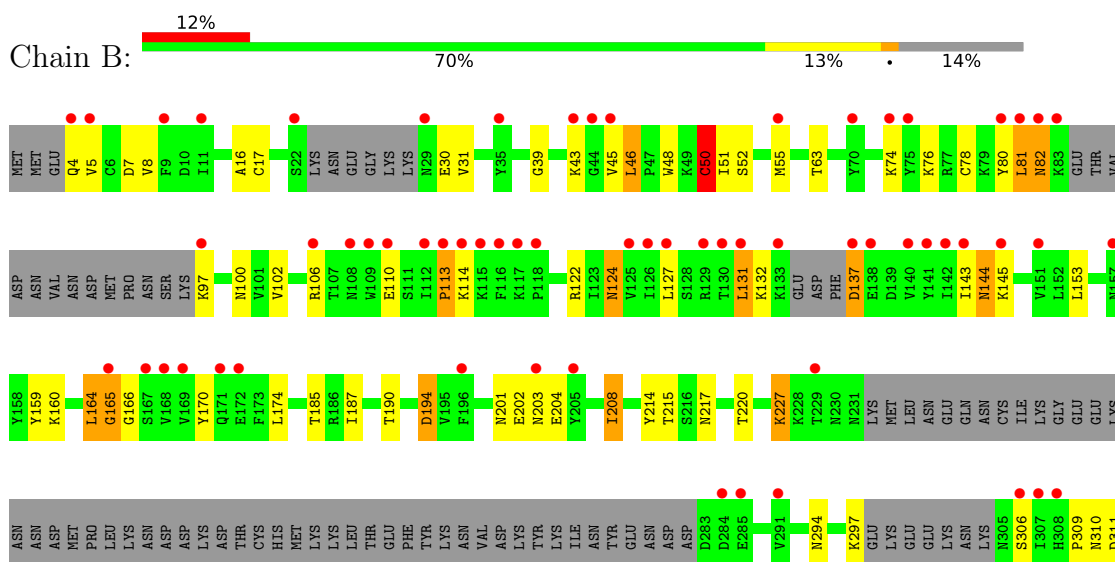
3 Residue-property plots

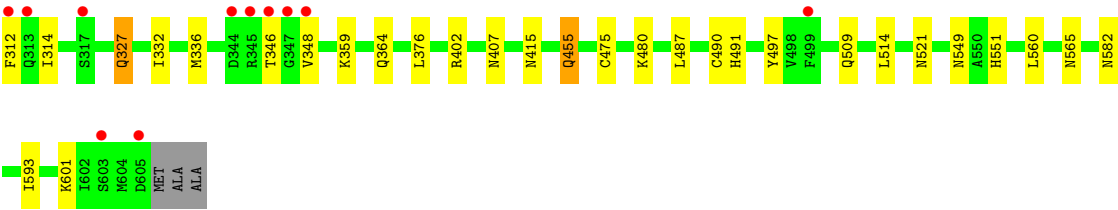
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	57.18Å 156.18Å 165.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.05 – 2.15 45.05 – 2.15	Depositor EDS
% Data completeness (in resolution range)	82.2 (45.05-2.15) 82.2 (45.05-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.194 , 0.249 (Not available) , 0.244	Depositor DCC
R_{free} test set	3355 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9234	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 3.51% 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: NDP, UMP, DQ0

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	1.04	2/4486 (0.0%)	1.34	4/6056 (0.1%)
1	B	1.06	0/4440	1.36	9/5999 (0.2%)
All	All	1.05	2/8926 (0.0%)	1.35	13/12055 (0.1%)

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	3
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	541	ALA	CA-C	6.28	1.55	1.52
1	A	543	PHE	C-O	5.13	1.30	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	ARG	CA-C-N	6.45	127.09	119.94
1	A	377	ARG	C-N-CA	6.45	127.09	119.94
1	A	455	GLN	CB-CA-C	-6.14	100.60	110.79
1	B	194	ASP	CB-CA-C	-5.93	98.91	110.11
1	B	402	ARG	CA-C-N	5.23	127.63	120.46
1	B	402	ARG	C-N-CA	5.23	127.63	120.46
1	B	327	GLN	CB-CG-CD	-5.22	103.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	455	GLN	CB-CA-C	-5.15	102.23	110.79
1	B	48	TRP	CA-C-N	5.10	127.42	120.54
1	B	48	TRP	C-N-CA	5.10	127.42	120.54
1	B	137	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	327	GLN	CB-CG-CD	-5.04	104.04	112.60
1	B	190	THR	CA-CB-OG1	-5.02	102.07	109.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	GLY	Peptide
1	A	310	ASN	Peptide
1	B	113	PRO	Peptide
1	B	131	LEU	Peptide
1	B	165	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	4383	0	4354	58	0
1	B	4339	0	4289	66	0
2	A	30	0	0	1	0
2	B	30	0	0	1	0
3	A	48	0	26	6	0
3	B	48	0	26	2	0
4	A	20	0	11	3	0
4	B	20	0	11	5	0
5	A	165	0	0	3	0
5	B	151	0	0	8	0
All	All	9234	0	8717	125	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 7.

All (125) 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:114:LYS:HB3	5:A:945:HOH:O	1.62	0.97
1:B:137:ASP:HB2	5:B:929:HOH:O	1.69	0.92
1:B:327:GLN:HE22	1:B:359:LYS:H	1.22	0.84
1:B:415:ASN:HB2	5:B:809:HOH:O	1.78	0.83
1:A:327:GLN:HE22	1:A:359:LYS:H	1.30	0.79
1:B:100:ASN:HD22	1:B:160:LYS:H	1.29	0.79
1:A:127:LEU:HD13	1:A:143:ILE:HG13	1.63	0.78
1:A:333:TYR:CE1	1:A:337:MET:HE3	2.19	0.76
1:B:201:ASN:HD21	1:B:203:ASN:HB2	1.50	0.75
1:A:461:ASN:HB3	5:A:940:HOH:O	1.86	0.75
1:B:312:PHE:HA	1:B:565:ASN:HD21	1.53	0.74
1:B:455:GLN:HE22	1:B:475:CYS:H	1.33	0.73
1:A:455:GLN:HE22	1:A:475:CYS:H	1.33	0.73
1:B:491:HIS:CE1	4:B:703:UMP:O4	2.42	0.73
1:B:215:THR:H	1:B:364:GLN:NE2	1.92	0.67
1:B:132:LYS:NZ	1:B:144:ASN:HD21	1.95	0.64
1:A:553:TYR:HB3	1:A:555:ASN:ND2	2.13	0.62
1:A:328:TYR:CZ	1:A:332:ILE:HD11	2.35	0.62
1:A:166:GLY:HA3	3:A:702:NDP:O1A	2.00	0.61
1:A:166:GLY:HA3	3:A:702:NDP:PA	2.42	0.59
1:B:491:HIS:HE1	4:B:703:UMP:O4	1.85	0.59
1:A:491:HIS:CE1	4:A:703:UMP:O4	2.57	0.58
1:A:4:GLN:OE1	1:A:228:LYS:NZ	2.36	0.58
1:A:127:LEU:CD1	1:A:143:ILE:HG13	2.33	0.57
1:B:311:ASP:O	1:B:565:ASN:ND2	2.37	0.57
1:A:102:VAL:HB	1:A:164:LEU:HD11	1.87	0.57
1:B:165:GLY:HA3	1:B:170:TYR:CZ	2.39	0.57
1:A:312:PHE:CE2	1:A:337:MET:HE1	2.39	0.56
1:A:352:SER:OG	1:B:497:TYR:OH	2.25	0.54
1:B:201:ASN:ND2	1:B:203:ASN:HB2	2.22	0.54
1:B:314:ILE:HD12	5:B:932:HOH:O	2.08	0.53
1:A:509:GLN:HE22	1:A:521:ASN:ND2	2.07	0.52
2:B:701:DQ0:CAL	3:B:702:NDP:H42N	2.39	0.52
1:B:8:VAL:HA	1:B:76:LYS:HD2	1.91	0.52
1:B:122:ARG:O	1:B:124:ASN:ND2	2.42	0.52
1:B:509:GLN:HE22	1:B:521:ASN:ND2	2.08	0.52
1:B:100:ASN:ND2	1:B:159:TYR:HB3	2.25	0.52
1:B:201:ASN:HD21	1:B:203:ASN:CB	2.21	0.51
1:A:521:ASN:HD21	4:A:703:UMP:HN3	1.57	0.51
1:A:346:THR:HB	1:A:348:VAL:HG13	1.91	0.51
1:B:43:LYS:N	1:B:194:ASP:OD2	2.32	0.51
1:B:415:ASN:CB	5:B:809:HOH:O	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:PHE:HA	1:B:565:ASN:ND2	2.25	0.51
1:B:78:CYS:O	1:B:82:ASN:N	2.44	0.50
1:A:308:HIS:H	1:A:309:PRO:HD3	1.75	0.50
1:B:582:ASN:HB3	5:B:910:HOH:O	2.12	0.50
1:A:166:GLY:H	3:A:702:NDP:C5N	2.26	0.49
1:B:336:MET:HE1	1:B:560:LEU:HB2	1.94	0.49
1:B:521:ASN:HD21	4:B:703:UMP:HN3	1.59	0.49
1:A:52:SER:H	1:A:217:ASN:ND2	2.09	0.49
1:B:106:ARG:O	1:B:110:GLU:HG2	2.13	0.49
1:B:490:CYS:SG	4:B:703:UMP:C6	3.05	0.49
1:A:532:ILE:HD13	1:A:583:ILE:HD13	1.95	0.48
1:B:336:MET:HE1	1:B:560:LEU:CB	2.43	0.48
1:A:545:HIS:CD2	1:A:547:LEU:CD1	2.97	0.48
1:B:127:LEU:HD12	1:B:143:ILE:HG13	1.95	0.48
1:A:179:ILE:O	1:A:205:TYR:OH	2.20	0.47
1:B:144:ASN:N	1:B:144:ASN:HD22	2.12	0.47
1:B:50:CYS:O	1:B:50:CYS:SG	2.71	0.47
1:A:201:ASN:HD22	1:A:204:GLU:HG3	1.80	0.47
1:A:551:HIS:HE1	4:A:703:UMP:O3'	1.97	0.47
1:A:555:ASN:HD22	1:A:555:ASN:H	1.61	0.47
1:B:80:TYR:HD2	1:B:81:LEU:HD13	1.79	0.47
1:A:12:TYR:CE2	1:A:160:LYS:HD3	2.50	0.46
1:B:102:VAL:HB	1:B:164:LEU:HD22	1.97	0.46
1:A:165:GLY:HA3	1:A:170:TYR:CZ	2.50	0.46
1:A:40:LEU:O	3:A:702:NDP:H2N	2.16	0.46
1:B:376:LEU:HD12	1:B:593:ILE:HG13	1.98	0.46
1:B:455:GLN:NE2	1:B:475:CYS:H	2.06	0.46
1:A:308:HIS:N	1:A:309:PRO:HD3	2.31	0.45
1:A:455:GLN:NE2	1:A:475:CYS:H	2.07	0.45
2:A:701:DQ0:CAI	2:A:701:DQ0:OAK	2.62	0.45
1:B:549:ASN:OD1	1:B:551:HIS:HD2	1.99	0.45
1:A:350:VAL:HG12	1:A:553:TYR:CD1	2.50	0.45
1:B:45:VAL:HG22	1:B:46:LEU:H	1.81	0.45
1:A:411:GLU:H	1:A:411:GLU:CD	2.23	0.45
1:B:480:LYS:HD3	5:B:816:HOH:O	2.17	0.44
1:A:349:GLY:C	1:A:554:ASN:OD1	2.61	0.44
1:B:214:TYR:O	1:B:220:THR:HA	2.18	0.44
1:A:305:ASN:HB3	1:A:307:ILE:HG22	1.99	0.44
1:A:417:LYS:N	1:A:417:LYS:HD3	2.33	0.44
1:B:208:ILE:HG21	1:B:227:LYS:HD3	1.99	0.43
1:A:215:THR:H	1:A:364:GLN:NE2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ASN:ND2	5:A:816:HOH:O	2.50	0.43
1:A:555:ASN:HD22	1:A:555:ASN:N	2.17	0.43
1:B:102:VAL:HB	1:B:164:LEU:CD2	2.48	0.43
1:A:166:GLY:H	3:A:702:NDP:H5N	1.84	0.43
1:A:342:GLN:NE2	1:A:352:SER:OG	2.52	0.43
1:B:132:LYS:NZ	1:B:144:ASN:ND2	2.65	0.42
1:B:100:ASN:HD22	1:B:160:LYS:N	2.05	0.42
1:A:16:ALA:HA	1:A:185:THR:HB	2.02	0.42
1:A:216:SER:OG	1:A:217:ASN:ND2	2.52	0.42
1:B:4:GLN:HB2	1:B:7:ASP:OD1	2.19	0.42
1:B:166:GLY:HA3	3:B:702:NDP:PA	2.59	0.42
1:B:208:ILE:CG2	1:B:227:LYS:HD3	2.50	0.42
1:A:109:TRP:CE2	1:A:117:LYS:HD2	2.54	0.42
1:A:210:VAL:HG12	1:A:224:ILE:HG22	2.00	0.42
1:B:336:MET:CE	1:B:560:LEU:HB2	2.49	0.42
1:B:165:GLY:HA3	1:B:170:TYR:CE1	2.55	0.42
1:A:109:TRP:CZ2	1:A:117:LYS:HD2	2.55	0.42
1:B:100:ASN:ND2	1:B:160:LYS:H	2.06	0.42
1:B:551:HIS:HE1	4:B:703:UMP:O3'	2.03	0.42
1:A:19:LYS:HG2	1:A:36:THR:HG22	2.01	0.42
1:B:214:TYR:HA	1:B:364:GLN:HE21	1.83	0.41
1:A:127:LEU:HD13	1:A:143:ILE:CG1	2.43	0.41
1:A:70:TYR:O	1:A:73:LEU:N	2.53	0.41
1:B:332:ILE:CD1	1:B:514:LEU:HB3	2.50	0.41
1:A:527:ILE:O	1:A:531:MET:HG3	2.20	0.41
1:B:81:LEU:O	1:B:82:ASN:CG	2.63	0.41
1:B:407:ASN:ND2	5:B:820:HOH:O	2.54	0.41
1:B:16:ALA:HA	1:B:185:THR:HB	2.03	0.41
1:B:17:CYS:HA	1:B:39:GLY:O	2.20	0.41
1:A:166:GLY:CA	3:A:702:NDP:PA	3.09	0.41
1:A:214:TYR:O	1:A:220:THR:HA	2.21	0.41
1:A:408:GLY:HA3	1:A:424:ASN:HD22	1.86	0.41
1:A:502:LYS:HA	1:A:539:GLN:O	2.21	0.41
1:B:124:ASN:HD22	1:B:124:ASN:N	2.18	0.41
1:A:455:GLN:HB2	1:A:474:LEU:HD12	2.02	0.41
1:B:52:SER:H	1:B:217:ASN:HD21	1.69	0.41
1:B:201:ASN:HD22	1:B:204:GLU:HG3	1.86	0.40
1:B:52:SER:H	1:B:217:ASN:ND2	2.19	0.40
1:B:51:ILE:HD13	1:B:187:ILE:HD12	2.03	0.40
1:B:314:ILE:CD1	5:B:932:HOH:O	2.67	0.40
1:A:553:TYR:HB3	1:A:555:ASN:HD21	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:PRO:HA	1:B:312:PHE:CD2	2.56	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	516/608 (85%)	482 (93%)	29 (6%)	5 (1%)	12	7
1	B	510/608 (84%)	478 (94%)	27 (5%)	5 (1%)	12	7
All	All	1026/1216 (84%)	960 (94%)	56 (6%)	10 (1%)	12	7

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	308	HIS
1	B	50	CYS
1	B	82	ASN
1	B	113	PRO
1	A	297	LYS
1	A	601	LYS
1	A	345	ARG
1	B	30	GLU
1	B	306	SER

5.3.2 Protein sidechains [i](#)

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	492/570 (86%)	470 (96%)	22 (4%)	24	21
1	B	487/570 (85%)	460 (94%)	27 (6%)	19	15
All	All	979/1140 (86%)	930 (95%)	49 (5%)	22	17

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LYS
1	A	28	LYS
1	A	49	LYS
1	A	72	LYS
1	A	79	LYS
1	A	97	LYS
1	A	127	LEU
1	A	297	LYS
1	A	307	ILE
1	A	308	HIS
1	A	344	ASP
1	A	346	THR
1	A	376	LEU
1	A	397	LEU
1	A	411	GLU
1	A	462	LEU
1	A	487	LEU
1	A	524	SER
1	A	547	LEU
1	A	555	ASN
1	A	581	LYS
1	A	606	MET
1	B	5	VAL
1	B	31	VAL
1	B	46	LEU
1	B	50	CYS
1	B	55	MET
1	B	63	THR
1	B	74	LYS
1	B	81	LEU
1	B	97	LYS
1	B	114	LYS
1	B	124	ASN

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Mol	Chain	Res	Type
1	B	131	LEU
1	B	144	ASN
1	B	145	LYS
1	B	153	LEU
1	B	164	LEU
1	B	174	LEU
1	B	202	GLU
1	B	208	ILE
1	B	227	LYS
1	B	294	ASN
1	B	297	LYS
1	B	310	ASN
1	B	346	THR
1	B	348	VAL
1	B	487	LEU
1	B	601	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	171	GLN
1	A	201	ASN
1	A	217	ASN
1	A	218	ASN
1	A	327	GLN
1	A	338	ASN
1	A	342	GLN
1	A	364	GLN
1	A	394	ASN
1	A	407	ASN
1	A	424	ASN
1	A	455	GLN
1	A	461	ASN
1	A	521	ASN
1	A	530	HIS
1	A	551	HIS
1	A	555	ASN
1	B	29	ASN
1	B	100	ASN
1	B	144	ASN
1	B	201	ASN

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Mol	Chain	Res	Type
1	B	217	ASN
1	B	231	ASN
1	B	294	ASN
1	B	305	ASN
1	B	316	ASN
1	B	327	GLN
1	B	338	ASN
1	B	364	GLN
1	B	407	ASN
1	B	415	ASN
1	B	424	ASN
1	B	455	GLN
1	B	461	ASN
1	B	521	ASN
1	B	551	HIS
1	B	555	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
2	DQ0	B	701	-	32,32,32	1.46	3 (9%)	40,43,43	2.71	11 (27%)
2	DQ0	A	701	-	32,32,32	2.21	3 (9%)	40,43,43	2.23	10 (25%)
4	UMP	A	703	-	21,21,21	0.47	0	30,31,31	1.22	3 (10%)
3	NDP	B	702	-	51,52,52	2.47	14 (27%)	71,80,80	2.09	18 (25%)
4	UMP	B	703	-	21,21,21	0.49	0	30,31,31	0.84	0
3	NDP	A	702	-	51,52,52	2.29	14 (27%)	71,80,80	2.03	19 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DQ0	B	701	-	-	5/16/16/16	0/3/3/3
2	DQ0	A	701	-	-	9/16/16/16	0/3/3/3
4	UMP	A	703	-	-	6/10/22/22	0/2/2/2
3	NDP	B	702	-	-	6/34/77/77	0/5/5/5
4	UMP	B	703	-	-	3/10/22/22	0/2/2/2
3	NDP	A	702	-	-	5/34/77/77	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	DQ0	CAJ-C4	-9.29	1.41	1.50
3	B	702	NDP	PA-O3	9.25	1.69	1.59
3	B	702	NDP	PN-O3	8.91	1.69	1.59
3	A	702	NDP	PA-O3	7.69	1.67	1.59
3	A	702	NDP	PN-O3	6.56	1.66	1.59
2	A	701	DQ0	C5-CAI	-5.62	1.40	1.50
2	B	701	DQ0	C5-CAI	-5.30	1.40	1.50
3	A	702	NDP	C2A-N1A	4.80	1.42	1.33
3	B	702	NDP	C4N-C3N	-4.79	1.41	1.50
2	A	701	DQ0	CAO-CL	4.40	1.84	1.74
3	B	702	NDP	C2A-N1A	4.09	1.41	1.33
3	A	702	NDP	C2A-N3A	3.67	1.40	1.33
3	A	702	NDP	C4N-C3N	-3.60	1.43	1.50
3	A	702	NDP	O4B-C1B	3.55	1.50	1.42
3	B	702	NDP	C2A-N3A	3.22	1.39	1.33
3	B	702	NDP	C5A-N7A	-3.10	1.33	1.39
3	B	702	NDP	C4N-C5N	-3.09	1.41	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NDP	C4N-C5N	-2.90	1.41	1.49
3	A	702	NDP	O2D-C2D	2.89	1.50	1.43
3	A	702	NDP	C2B-C1B	-2.88	1.46	1.53
3	A	702	NDP	C5A-N7A	-2.65	1.34	1.39
3	B	702	NDP	C5A-C6A	-2.60	1.33	1.41
3	A	702	NDP	C6N-C5N	2.59	1.41	1.33
3	A	702	NDP	C2N-C3N	2.59	1.42	1.35
3	B	702	NDP	C5A-C4A	-2.52	1.34	1.39
3	A	702	NDP	O4D-C1D	2.51	1.47	1.42
2	B	701	DQ0	OAK-CAR	2.44	1.43	1.37
3	B	702	NDP	C8A-N9A	-2.42	1.33	1.37
2	B	701	DQ0	CAW-CAV	2.41	1.43	1.39
3	B	702	NDP	O4B-C1B	2.24	1.47	1.42
3	B	702	NDP	C7N-C3N	-2.20	1.44	1.48
3	B	702	NDP	C2N-C3N	2.08	1.40	1.35
3	A	702	NDP	O3D-C3D	2.08	1.48	1.43
3	B	702	NDP	C6N-C5N	2.03	1.39	1.33

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	DQ0	C2-N3-C4	10.94	124.24	116.26
2	A	701	DQ0	C2-N3-C4	7.97	122.07	116.26
3	B	702	NDP	O3-PN-O1N	-7.76	87.37	110.70
2	B	701	DQ0	C5-C4-N3	-7.36	115.04	123.47
3	B	702	NDP	N3A-C2A-N1A	-6.30	119.05	128.58
3	A	702	NDP	O2N-PN-O3	-6.04	90.94	107.27
2	A	701	DQ0	CAZ-CBA-CBB	-6.04	98.75	114.51
3	B	702	NDP	O2N-PN-O3	-5.64	92.04	107.27
3	A	702	NDP	N3A-C2A-N1A	-5.48	120.28	128.58
3	A	702	NDP	O3-PN-O1N	-5.14	95.25	110.70
3	A	702	NDP	C5A-C4A-N3A	-4.62	120.36	126.72
2	B	701	DQ0	CAS-CAR-CAW	-4.36	114.64	120.50
3	B	702	NDP	C5A-C4A-N3A	-4.29	120.81	126.72
3	B	702	NDP	N9A-C8A-N7A	-4.16	108.03	113.94
2	B	701	DQ0	CAY-OAX-CAV	4.04	128.42	117.93
3	A	702	NDP	O2N-PN-O1N	4.01	131.11	112.44
2	B	701	DQ0	C6-C5-C4	3.90	118.78	115.97
3	A	702	NDP	N9A-C8A-N7A	-3.66	108.74	113.94
2	A	701	DQ0	CBA-CAZ-CAY	-3.54	105.21	112.33
3	A	702	NDP	C4A-C5A-N7A	-3.53	106.54	110.58
2	A	701	DQ0	C5-C4-N3	-3.53	119.43	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	UMP	OP2-P-O5'	-3.48	97.59	106.67
3	B	702	NDP	O4B-C1B-N9A	3.43	114.67	108.09
3	A	702	NDP	C5A-N7A-C8A	3.34	108.70	103.45
2	B	701	DQ0	CBA-CAZ-CAY	-3.29	105.73	112.33
3	B	702	NDP	C5A-N7A-C8A	3.23	108.53	103.45
3	A	702	NDP	O4B-C1B-N9A	3.19	114.21	108.09
2	B	701	DQ0	CAT-CAS-CAR	3.16	123.75	118.98
3	A	702	NDP	O2A-PA-O3	3.11	115.67	107.27
4	A	703	UMP	OP3-P-O5'	3.10	114.76	106.67
3	B	702	NDP	C5A-C6A-N6A	-3.07	115.69	123.29
2	A	701	DQ0	N3-C2-N1	-3.04	120.82	125.48
2	B	701	DQ0	N3-C2-N1	-3.04	120.82	125.48
2	A	701	DQ0	C5-C6-N1	-3.00	120.81	122.55
3	B	702	NDP	C2A-N3A-C4A	2.98	119.12	111.83
2	A	701	DQ0	NAG-C6-N1	2.97	121.04	117.03
3	A	702	NDP	C5A-C4A-N9A	2.97	109.05	105.81
3	B	702	NDP	O2N-PN-O5D	2.94	120.88	107.57
3	A	702	NDP	C2A-N3A-C4A	2.91	118.93	111.83
3	A	702	NDP	C6A-C5A-C4A	2.85	121.06	117.18
3	B	702	NDP	C6A-C5A-C4A	2.84	121.05	117.18
3	B	702	NDP	C4A-C5A-N7A	-2.67	107.53	110.58
3	B	702	NDP	O2N-PN-O1N	2.62	124.63	112.44
2	B	701	DQ0	NAH-C2-N3	2.58	121.09	117.22
3	A	702	NDP	C2D-C1D-N1N	2.50	119.45	113.31
3	B	702	NDP	N3A-C4A-N9A	2.40	131.25	127.17
2	B	701	DQ0	CAR-CAW-CAV	2.40	121.94	118.48
3	B	702	NDP	O3X-P2B-O2X	2.38	116.71	107.80
3	B	702	NDP	O2B-P2B-O1X	-2.37	100.90	109.33
2	A	701	DQ0	C6-C5-C4	2.36	117.67	115.97
3	A	702	NDP	O3X-P2B-O2B	-2.34	96.72	105.85
3	A	702	NDP	O2N-PN-O5D	2.31	118.02	107.57
3	A	702	NDP	O3X-P2B-O2X	2.28	116.34	107.80
2	A	701	DQ0	NAH-C2-N1	2.28	120.64	117.22
3	A	702	NDP	C5A-C6A-N6A	-2.26	117.70	123.29
3	B	702	NDP	O2A-PA-O1A	2.16	122.50	112.44
3	B	702	NDP	C4A-N9A-C8A	2.13	107.98	105.74
2	A	701	DQ0	C5-C6-NAG	-2.12	118.14	120.82
4	A	703	UMP	C1'-N1-C6	-2.03	117.54	121.53
2	B	701	DQ0	CAJ-OAK-CAR	2.02	122.44	117.62
3	A	702	NDP	N3A-C4A-N9A	2.01	130.59	127.17

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	NDP	C5D-O5D-PN-O1N
3	B	702	NDP	C5D-O5D-PN-O1N
4	A	703	UMP	C5'-O5'-P-OP1
4	A	703	UMP	C5'-O5'-P-OP2
4	A	703	UMP	C5'-O5'-P-OP3
2	B	701	DQ0	CAW-CAV-OAX-CAY
2	B	701	DQ0	CAU-CAV-OAX-CAY
2	A	701	DQ0	CAU-CAV-OAX-CAY
2	B	701	DQ0	OAX-CAY-CAZ-CBA
2	A	701	DQ0	CAW-CAV-OAX-CAY
4	B	703	UMP	C3'-C4'-C5'-O5'
4	B	703	UMP	O4'-C4'-C5'-O5'
2	A	701	DQ0	CAW-CAR-OAK-CAJ
2	A	701	DQ0	CAS-CAR-OAK-CAJ
2	A	701	DQ0	CAY-CAZ-CBA-CBB
4	A	703	UMP	O4'-C4'-C5'-O5'
2	B	701	DQ0	C4-CAJ-OAK-CAR
3	B	702	NDP	C4D-C5D-O5D-PN
2	A	701	DQ0	C5-C4-CAJ-OAK
3	A	702	NDP	PA-O3-PN-O5D
3	B	702	NDP	C2B-O2B-P2B-O1X
4	B	703	UMP	C5'-O5'-P-OP1
2	A	701	DQ0	OAX-CAY-CAZ-CBA
4	A	703	UMP	C2'-C1'-N1-C2
3	A	702	NDP	O4D-C1D-N1N-C2N
3	A	702	NDP	C4D-C5D-O5D-PN
3	A	702	NDP	C2N-C3N-C7N-N7N
3	B	702	NDP	O4D-C1D-N1N-C2N
3	B	702	NDP	C2N-C3N-C7N-N7N
2	A	701	DQ0	CAZ-CBA-CBB-OB
3	B	702	NDP	C2D-C1D-N1N-C2N
2	A	701	DQ0	CAZ-CBA-CBB-OB
2	B	701	DQ0	CAZ-CAY-OAX-CAV
4	A	703	UMP	C2'-C1'-N1-C6

There are no ring outliers.

6 monomers are involved in 17 short contacts:

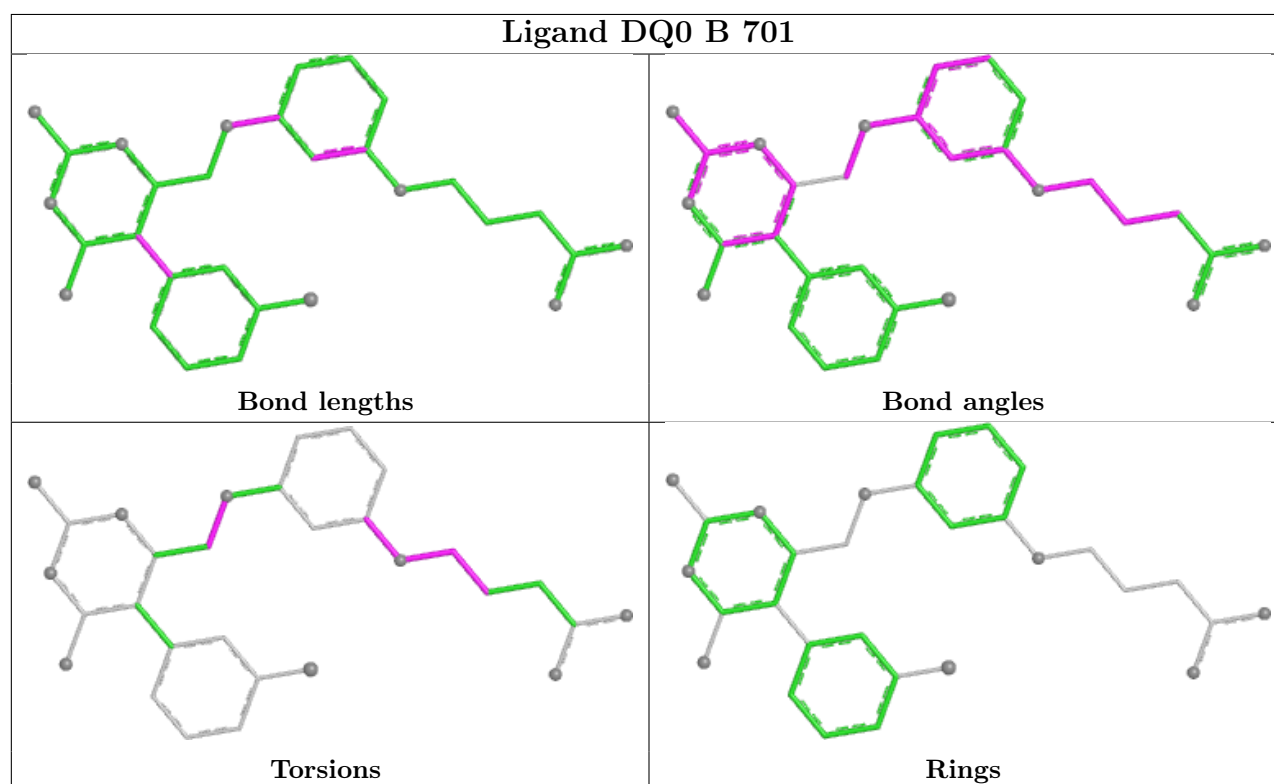
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	DQ0	1	0
2	A	701	DQ0	1	0

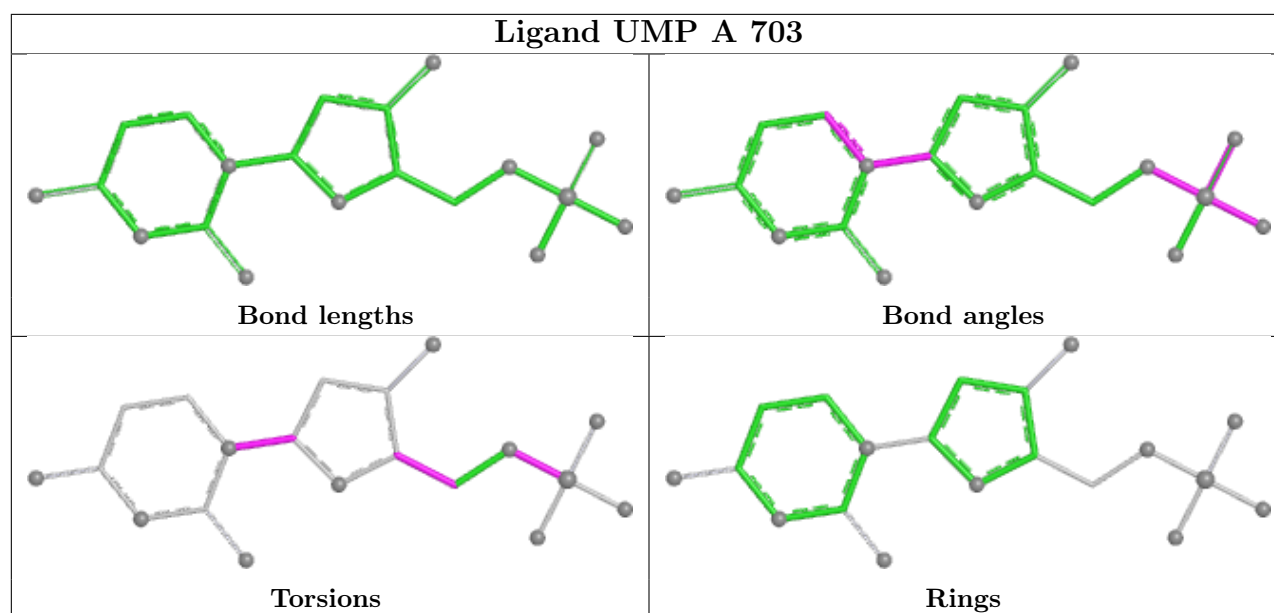
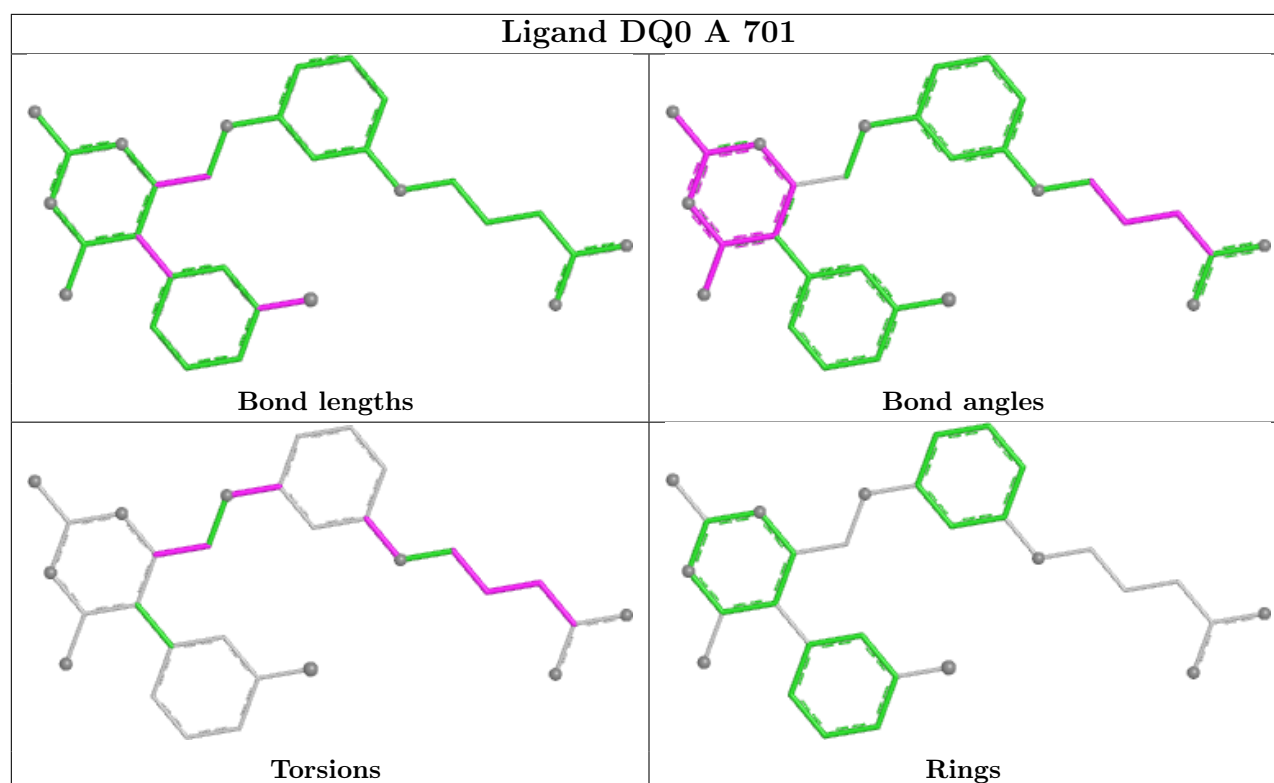
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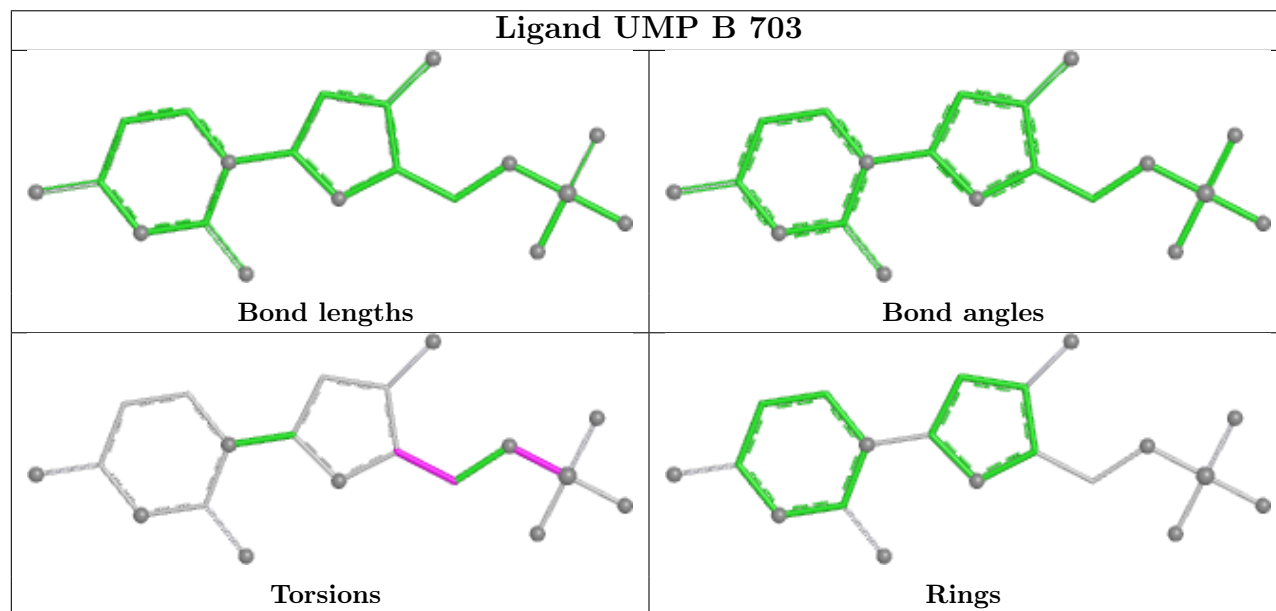
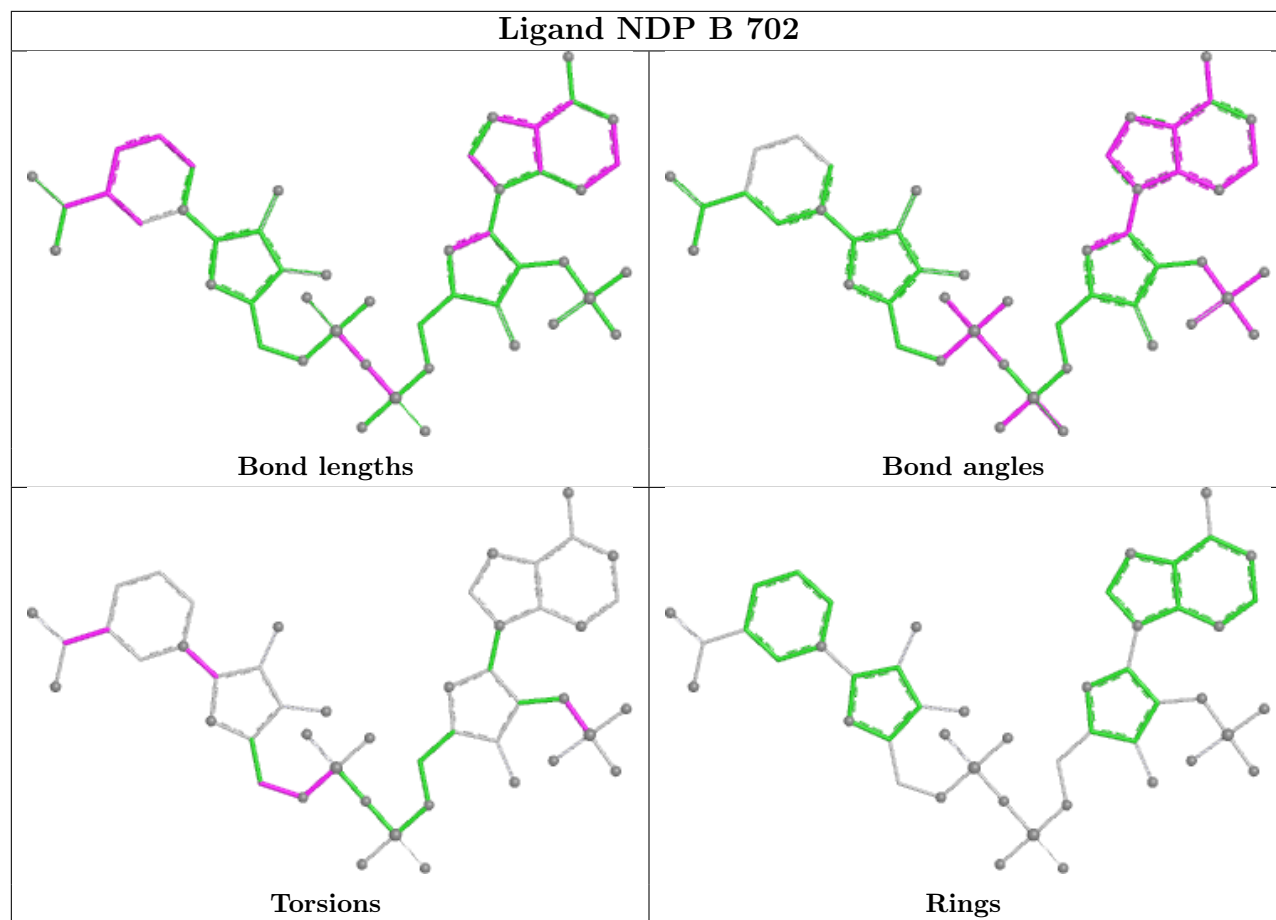
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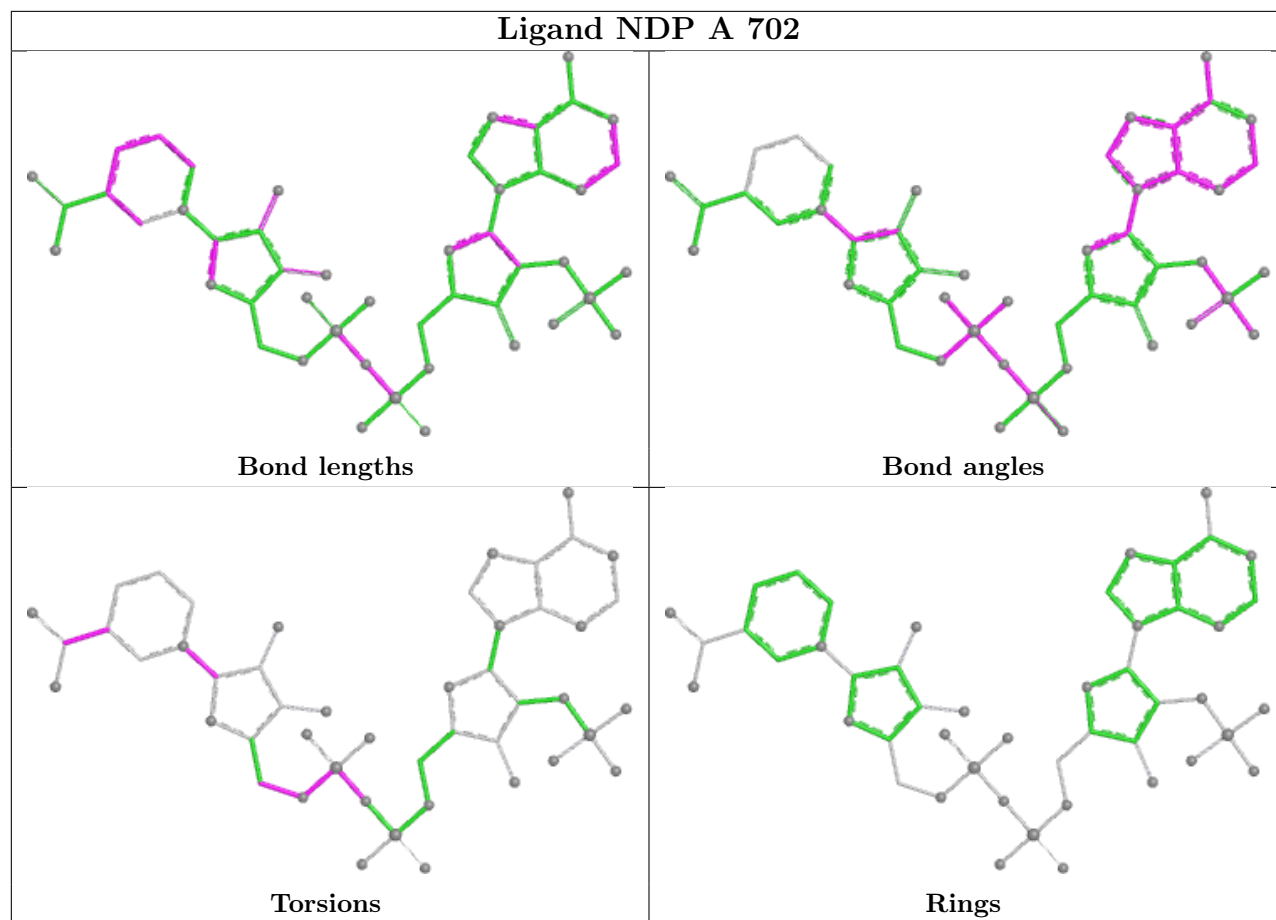
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	UMP	3	0
3	B	702	NDP	2	0
4	B	703	UMP	5	0
3	A	702	NDP	6	0

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	526/608 (86%)	0.30	34 (6%) 25 29	14, 27, 62, 105	0
1	B	522/608 (85%)	0.59	73 (13%) 6 8	12, 30, 72, 118	0
All	All	1048/1216 (86%)	0.44	107 (10%) 12 14	12, 28, 70, 118	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	PHE	6.5
1	A	606	MET	5.7
1	A	308	HIS	5.0
1	B	347	GLY	4.7
1	B	131	LEU	4.7
1	B	45	VAL	4.7
1	A	346	THR	4.7
1	B	35	TYR	4.1
1	B	348	VAL	4.1
1	B	346	THR	4.1
1	B	168	VAL	4.0
1	B	157	ASN	4.0
1	B	151	VAL	3.9
1	A	348	VAL	3.8
1	A	292	TYR	3.6
1	A	310	ASN	3.6
1	A	345	ARG	3.6
1	B	112	ILE	3.5
1	B	118	PRO	3.5
1	B	75	TYR	3.4
1	A	309	PRO	3.4
1	A	28	LYS	3.3
1	B	306	SER	3.3
1	B	11	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	9	PHE	3.3
1	A	343	SER	3.2
1	B	113	PRO	3.2
1	B	5	VAL	3.2
1	B	142	ILE	3.2
1	B	115	LYS	3.1
1	B	110	GLU	3.1
1	A	344	ASP	3.1
1	A	347	GLY	3.1
1	B	312	PHE	3.1
1	B	140	VAL	3.1
1	A	307	ILE	3.1
1	B	108	ASN	3.0
1	B	114	LYS	3.0
1	B	285	GLU	3.0
1	B	605	ASP	3.0
1	A	75	TYR	3.0
1	B	55	MET	3.0
1	A	27	LYS	2.9
1	B	117	LYS	2.9
1	B	137	ASP	2.9
1	B	229	THR	2.9
1	B	43	LYS	2.9
1	B	97	LYS	2.8
1	A	218	ASN	2.8
1	A	375	PHE	2.8
1	A	293	PHE	2.8
1	A	8	VAL	2.8
1	B	291	VAL	2.8
1	B	345	ARG	2.7
1	B	127	LEU	2.7
1	B	143	ILE	2.7
1	B	44	GLY	2.7
1	B	313	GLN	2.6
1	A	312	PHE	2.6
1	B	603	SER	2.6
1	B	169	VAL	2.6
1	B	307	ILE	2.5
1	B	205	TYR	2.5
1	A	83	LYS	2.5
1	B	172	GLU	2.5
1	B	196	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	555	ASN	2.4
1	B	29	ASN	2.4
1	B	4	GLN	2.4
1	A	22	SER	2.4
1	B	109	TRP	2.4
1	B	74	LYS	2.3
1	B	22	SER	2.3
1	B	167	SER	2.3
1	B	126	ILE	2.3
1	B	130	THR	2.3
1	B	82	ASN	2.3
1	B	106	ARG	2.3
1	B	344	ASP	2.3
1	B	133	LYS	2.3
1	A	31	VAL	2.3
1	B	284	ASP	2.3
1	B	317	SER	2.2
1	B	499	PHE	2.2
1	A	71	GLU	2.2
1	A	306	SER	2.2
1	B	129	ARG	2.2
1	A	304	LYS	2.2
1	B	138	GLU	2.2
1	B	141	TYR	2.2
1	B	81	LEU	2.2
1	B	70	TYR	2.2
1	B	80	TYR	2.2
1	B	145	LYS	2.2
1	B	203	ASN	2.2
1	A	97	LYS	2.1
1	B	83	LYS	2.1
1	A	29	ASN	2.1
1	A	72	LYS	2.1
1	B	308	HIS	2.1
1	A	298	GLU	2.1
1	A	35	TYR	2.1
1	B	125	VAL	2.1
1	A	70	TYR	2.0
1	A	115	LYS	2.0
1	B	165	GLY	2.0
1	B	171	GLN	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](#)

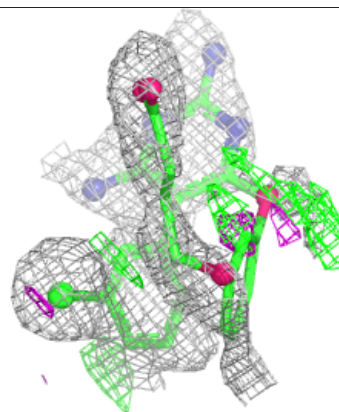
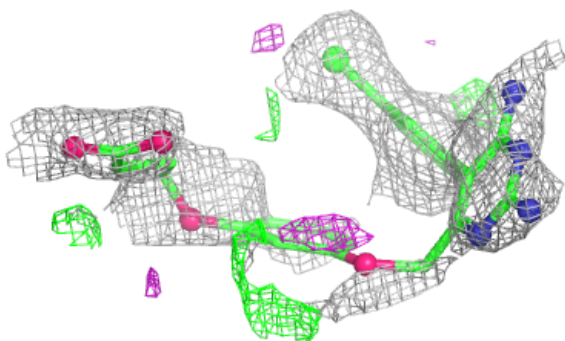
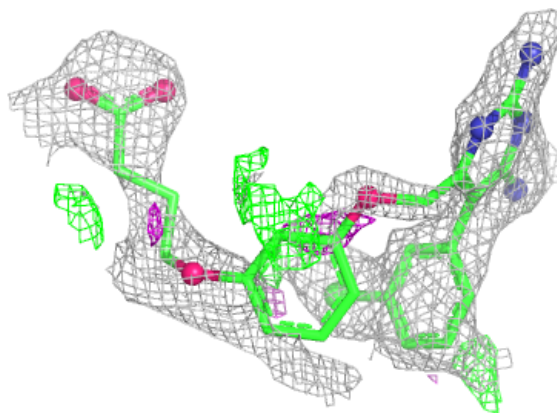
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	DQ0	B	701	30/30	0.78	0.21	39,63,94,96	0
3	NDP	B	702	48/48	0.84	0.15	42,64,94,98	0
4	UMP	B	703	20/20	0.87	0.17	41,57,68,70	0
4	UMP	A	703	20/20	0.91	0.12	35,49,59,60	0
2	DQ0	A	701	30/30	0.94	0.12	17,33,70,73	0
3	NDP	A	702	48/48	0.96	0.07	23,30,38,40	0

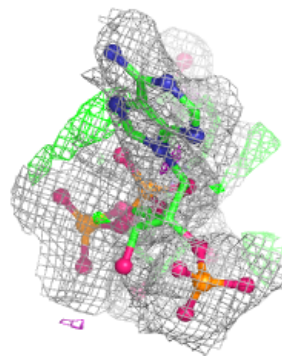
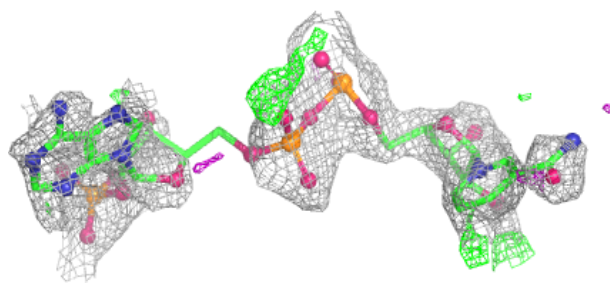
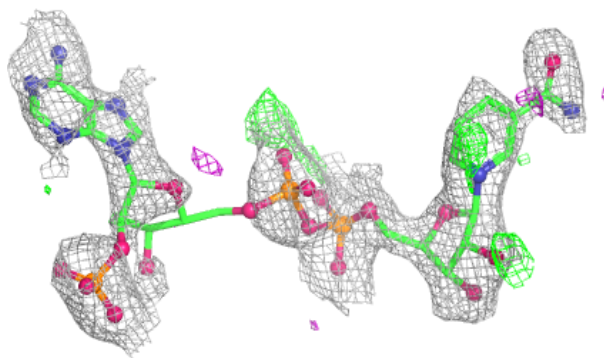
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DQ0 B 701:

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

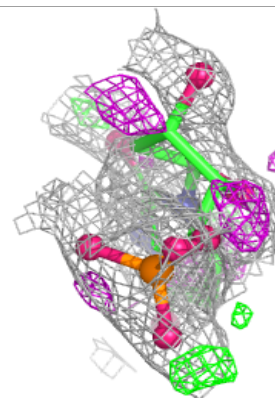
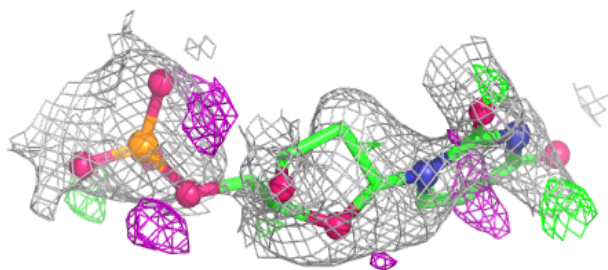
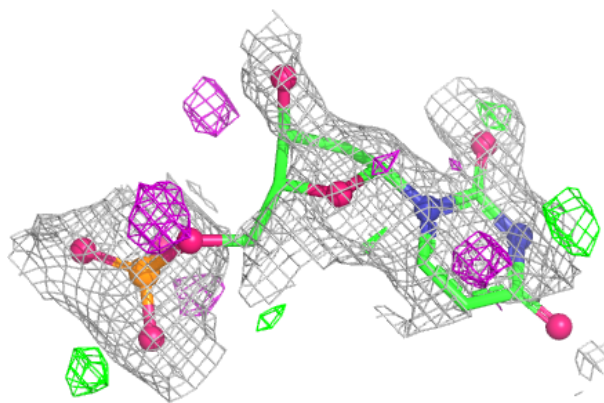
**Electron density around NDP B 702:**

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

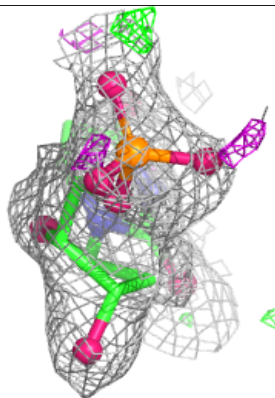
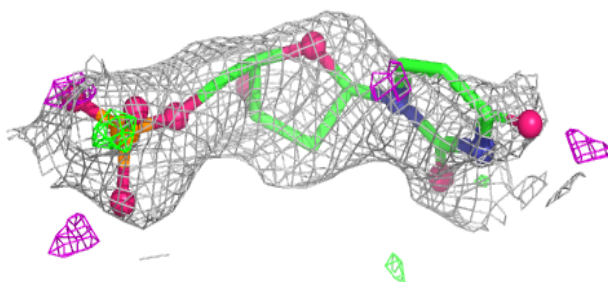
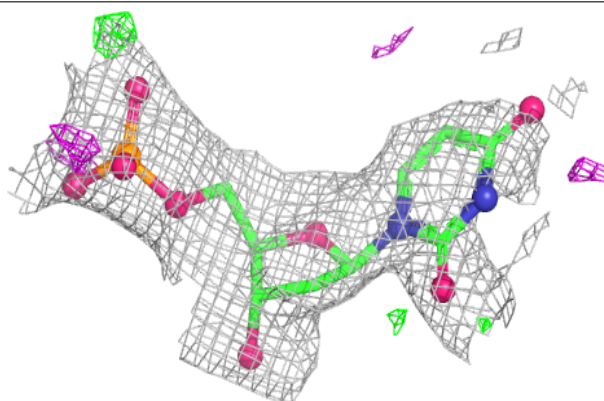


Electron density around UMP B 703:

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

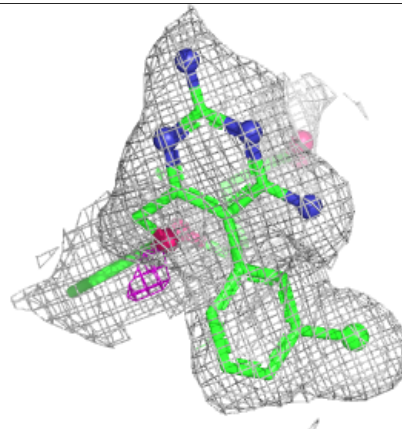
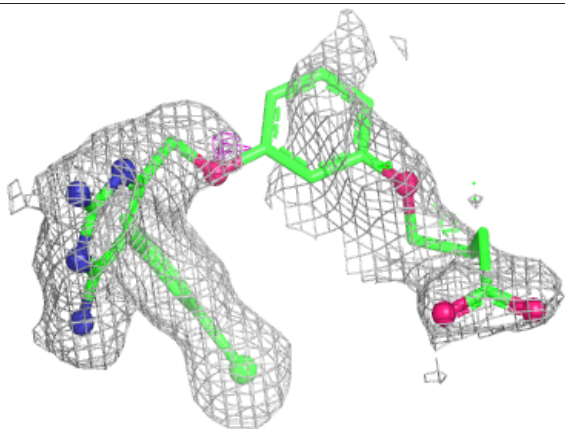
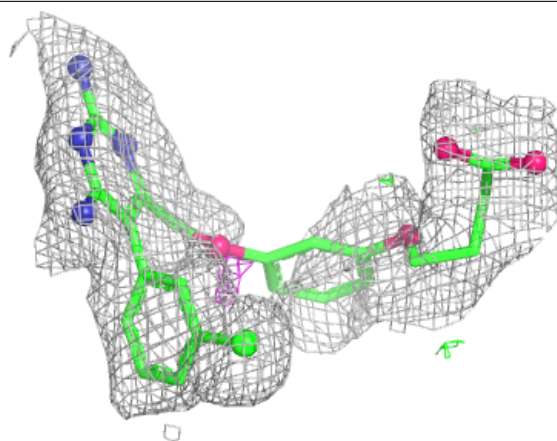
**Electron density around UMP A 703:**

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

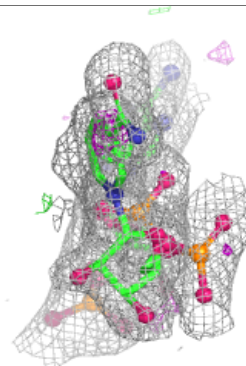
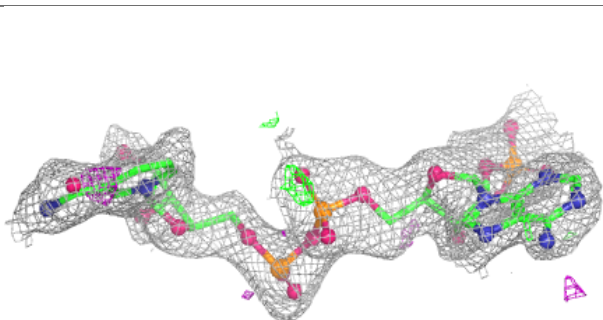
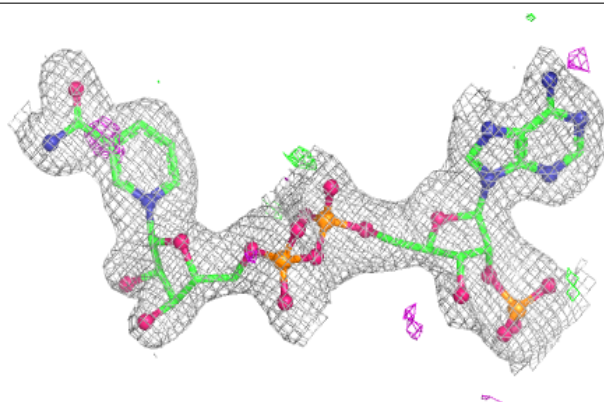


Electron density around DQ0 A 701:

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

**Electron density around NDP A 702:**

$2mF_o-DF_c$ (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.