Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:32 PM UTC

PDB ID	:	6LEU / pdb_00006leu
Title	:	Quadruple mutant (N51I+C59R+S108N+I164L) plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with compound 42 and NADPH
Authors	:	Vanichtanankul, J.; Vitsupakorn, D.
Deposited on	:	2019-11-27
Resolution	:	2.59 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:

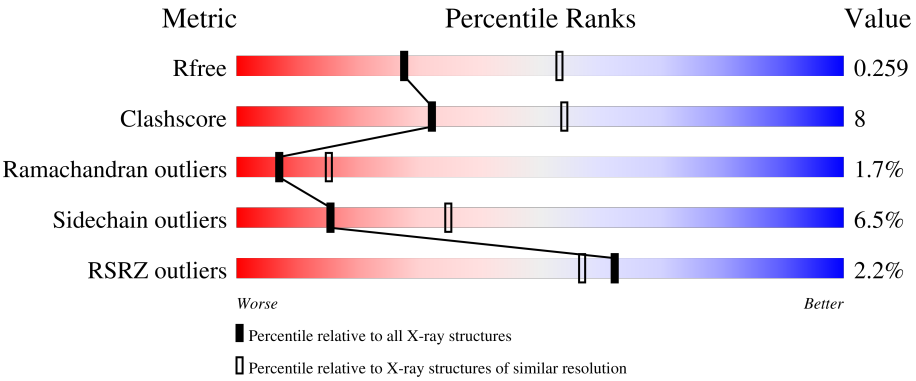
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

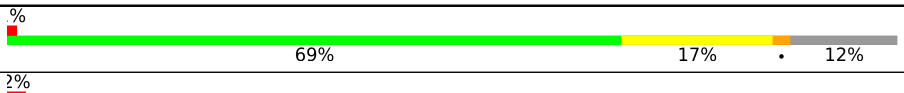
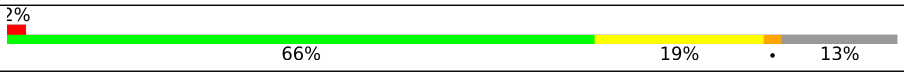
The reported resolution of this entry is 2.59 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 <=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	
1	B	608	

2 Entry composition

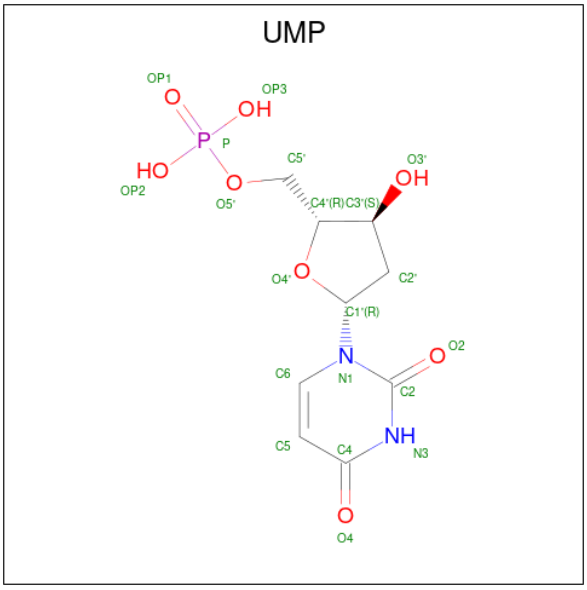
There are 5 unique types of molecules in this entry. The entry contains 9192 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

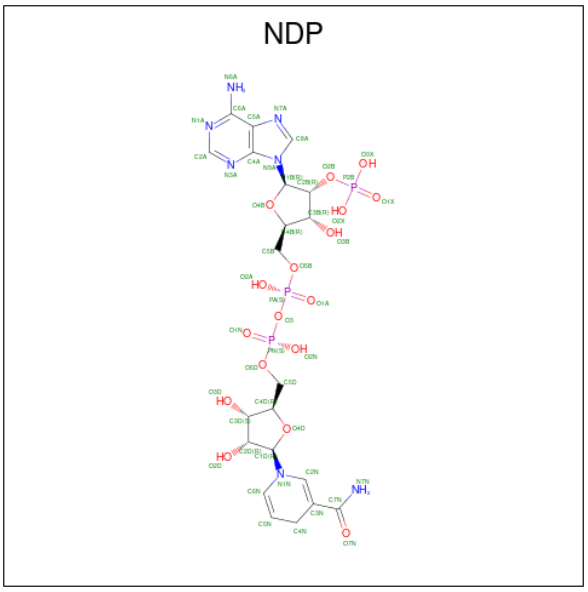
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4465	2885	739	817	24			
1	B	529	Total	C	N	O	S	0	0	0
			4410	2855	727	803	25			

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



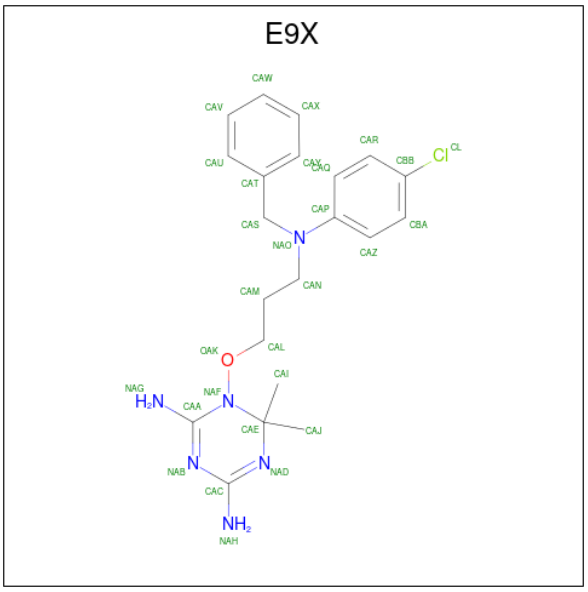
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 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
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is 1-[3-[(4-chlorophenyl)-(phenylmethyl)amino]propoxy]-6,6-dimethyl-1,3,5-triazine-2,4-diamine (CCD ID: E9X) (formula: $C_{21}H_{27}ClN_6O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			29	21	1	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	0	0
			29	21	1	6	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total	O	0	0
			61	61		
5	B	62	Total	O	0	0
			62	62		

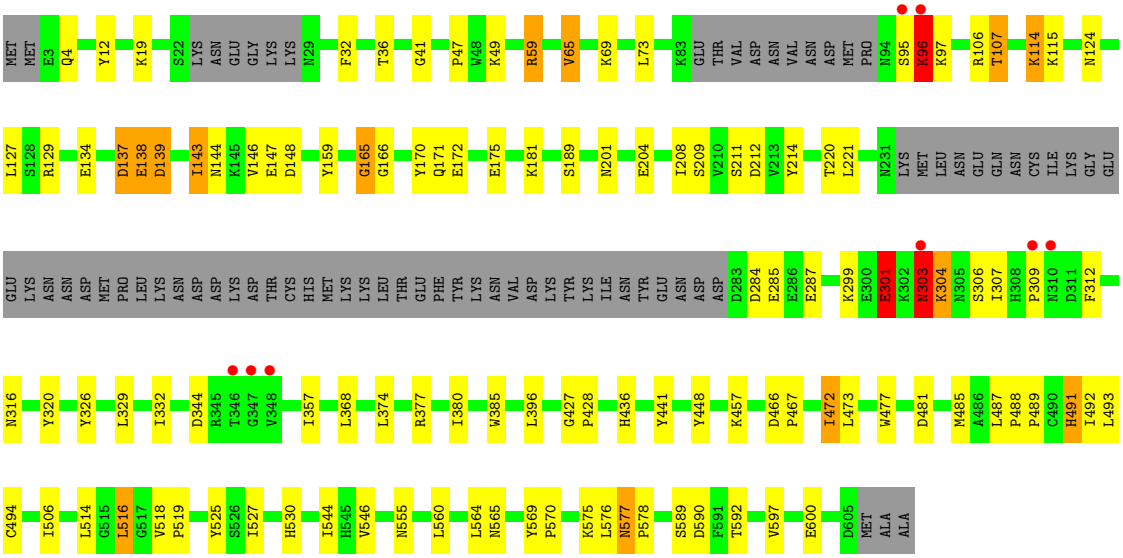
3 Residue-property plots (i)

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

• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain A:

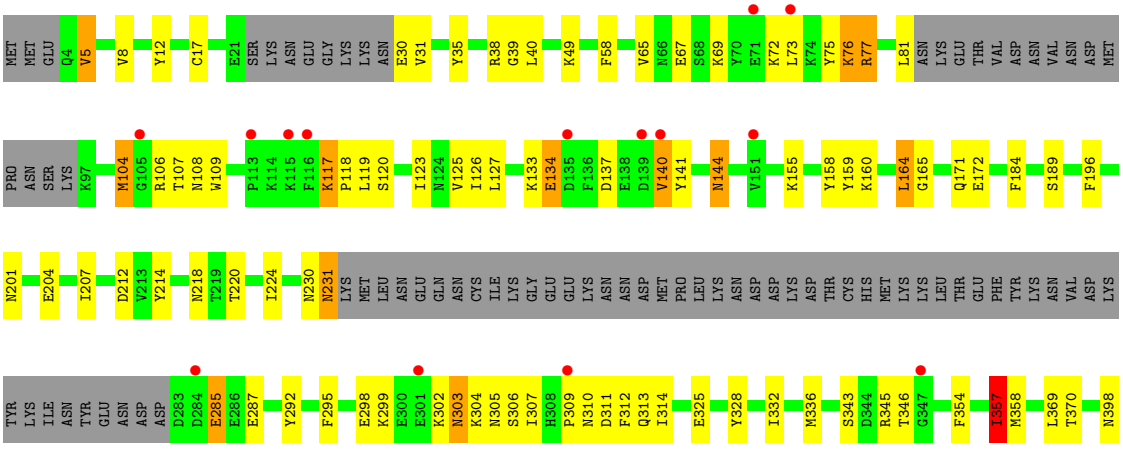




• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain B:






R402
R416
P428
I429
Y430
N447
N450
K457
R471
L482
M485
P488
P489
C490
H491
I492
L493
C494
Y508
Q509
R510
S511
C512
L516
G517
V518
P519
I522
A523
S524
Y525
A541
I544
A550
Y553
L560
L564
N565
R566
I567
P568

Y569
E584
H599
D605
M606
ALA
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.31Å 154.49Å 163.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.59 10.00 – 2.59	Depositor EDS
% Data completeness (in resolution range)	88.4 (10.00-2.59) 88.4 (10.00-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.189 , 0.261 0.194 , 0.259	Depositor DCC
R_{free} test set	2053 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9192	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UMP, E9X, 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	1.05	3/4569 (0.1%)	1.45	16/6170 (0.3%)
1	B	1.07	1/4514 (0.0%)	1.44	11/6097 (0.2%)
All	All	1.06	4/9083 (0.0%)	1.45	27/12267 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	GLU	C-O	5.81	1.31	1.24
1	B	541	ALA	CA-C	5.25	1.55	1.52
1	A	208	ILE	N-CA	5.13	1.50	1.46
1	A	491	HIS	CE1-NE2	5.02	1.37	1.32

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	472	ILE	CA-C-O	-7.19	116.37	122.63
1	A	144	ASN	CB-CA-C	-7.06	97.12	110.67
1	B	357	ILE	CB-CA-C	6.05	117.31	110.41
1	B	212	ASP	CA-CB-CG	6.04	118.64	112.60
1	B	553	TYR	CB-CA-C	6.02	119.71	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	125	VAL	CA-C-O	-6.01	116.63	120.66
1	A	377	ARG	CA-C-N	5.86	126.45	119.94
1	A	377	ARG	C-N-CA	5.86	126.45	119.94
1	A	107	THR	N-CA-C	-5.79	105.05	111.36
1	A	137	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	402	ARG	CA-C-N	5.78	128.67	120.53
1	B	402	ARG	C-N-CA	5.78	128.67	120.53
1	A	525	TYR	CB-CA-C	5.67	121.57	110.67
1	B	398	ASN	CA-CB-CG	5.58	118.18	112.60
1	A	344	ASP	CA-C-N	5.47	127.87	120.38
1	A	344	ASP	C-N-CA	5.47	127.87	120.38
1	A	284	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	305	ASN	CA-C-N	5.23	131.02	122.65
1	B	305	ASN	C-N-CA	5.23	131.02	122.65
1	A	578	PRO	N-CA-C	5.11	120.32	114.03
1	A	143	ILE	CA-C-N	5.10	128.06	120.31
1	A	143	ILE	C-N-CA	5.10	128.06	120.31
1	A	4	GLN	CA-C-N	5.09	128.96	120.62
1	A	4	GLN	C-N-CA	5.09	128.96	120.62
1	B	488	PRO	N-CA-CB	5.07	106.03	103.19
1	A	303	ASN	CA-CB-CG	5.01	117.61	112.60
1	B	605	ASP	CA-CB-CG	5.00	117.61	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ASP	Peptide
1	A	165	GLY	Peptide
1	B	117	LYS	Peptide
1	B	165	GLY	Peptide
1	B	303	ASN	Peptide
1	B	304	LYS	Peptide

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	4465	0	4414	73	0
1	B	4410	0	4363	71	0
2	A	20	0	11	0	0
2	B	20	0	11	2	0
3	A	48	0	26	6	0
3	B	48	0	26	6	0
4	A	29	0	0	2	0
4	B	29	0	0	3	0
5	A	61	0	0	2	0
5	B	62	0	0	1	0
All	All	9192	0	8851	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)
4:B:703:E9X:OAK	4:B:703:E9X:NAF	1.71	1.19
1:B:312:PHE:HA	1:B:565:ASN:HD21	1.19	1.05
1:B:312:PHE:HA	1:B:565:ASN:ND2	1.93	0.83
1:A:506:ILE:HD12	1:B:354:PHE:CZ	2.18	0.78
1:A:312:PHE:HA	1:A:565:ASN:HD21	1.48	0.77
1:B:328:TYR:CZ	1:B:332:ILE:HD11	2.23	0.74
1:A:166:GLY:HA3	3:A:702:NDP:O1A	1.93	0.69
1:A:201:ASN:HD22	1:A:204:GLU:HG3	1.57	0.69
1:B:73:LEU:O	1:B:77:ARG:HG3	1.93	0.68
1:B:40:LEU:HD12	1:B:196:PHE:C	2.19	0.67
1:A:127:LEU:HD23	1:A:143:ILE:HG13	1.76	0.66
1:A:166:GLY:HA3	3:A:702:NDP:PA	2.37	0.65
1:B:109:TRP:CZ2	1:B:117:LYS:HD2	2.35	0.62
1:A:107:THR:HG21	5:A:839:HOH:O	1.99	0.61
1:B:490:CYS:SG	2:B:701:UMP:C6	2.93	0.61
1:A:493:LEU:C	1:A:493:LEU:HD12	2.26	0.60
1:B:207:ILE:HB	1:B:567:ILE:HD13	1.84	0.60
1:B:306:SER:HA	5:B:844:HOH:O	2.02	0.60
1:B:35:TYR:O	1:B:38:ARG:NH1	2.35	0.59
1:A:303:ASN:O	1:A:303:ASN:ND2	2.35	0.58
4:B:703:E9X:OAK	4:B:703:E9X:CAA	2.49	0.58
1:B:8:VAL:O	1:B:76:LYS:NZ	2.36	0.58
1:A:506:ILE:HD12	1:B:354:PHE:CE1	2.38	0.57
1:B:428:PRO:O	1:B:485:MET:HE2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:O	1:A:139:ASP:CB	2.53	0.57
4:A:703:E9X:CAU	4:A:703:E9X:CAZ	2.82	0.56
1:B:332:ILE:HD13	1:B:560:LEU:HD22	1.86	0.56
1:B:490:CYS:SG	2:B:701:UMP:C5	2.98	0.56
1:B:492:ILE:HD11	1:B:510:ARG:HD3	1.86	0.56
1:B:58:PHE:HZ	1:B:164:LEU:HD13	1.70	0.55
1:A:493:LEU:CD2	1:B:492:ILE:HG21	2.37	0.55
1:B:17:CYS:HB2	1:B:184:PHE:CZ	2.42	0.55
1:B:493:LEU:HD12	1:B:493:LEU:C	2.31	0.55
1:B:140:VAL:C	1:B:141:TYR:HD2	2.15	0.54
1:A:32:PHE:CD1	1:A:597:VAL:HG13	2.43	0.54
1:A:69:LYS:O	1:A:73:LEU:HG	2.07	0.54
1:A:19:LYS:HG2	1:A:36:THR:HG22	1.90	0.54
1:A:332:ILE:HD13	1:A:560:LEU:HD22	1.89	0.54
1:B:303:ASN:C	1:B:303:ASN:HD22	2.14	0.54
1:A:436:HIS:CE1	1:A:448:TYR:O	2.61	0.53
1:A:114:LYS:N	1:A:114:LYS:HD2	2.23	0.53
1:B:312:PHE:CA	1:B:565:ASN:HD21	2.07	0.53
1:A:95:SER:O	1:A:96:LYS:HB3	2.07	0.53
1:A:487:LEU:HD12	1:A:488:PRO:O	2.09	0.53
1:A:357:ILE:HD12	1:A:546:VAL:HG22	1.91	0.52
1:A:138:GLU:O	1:A:139:ASP:HB3	2.10	0.52
1:A:129:ARG:HD2	5:A:805:HOH:O	2.08	0.52
1:A:326:TYR:HA	1:A:329:LEU:HB2	1.92	0.52
1:B:606:MET:SD	1:B:606:MET:N	2.83	0.51
1:A:312:PHE:HA	1:A:565:ASN:ND2	2.22	0.51
1:A:301:GLU:O	1:A:301:GLU:HG3	2.10	0.51
1:A:96:LYS:HG2	1:A:96:LYS:O	2.10	0.51
3:A:702:NDP:O1X	3:A:702:NDP:O3B	2.25	0.51
1:A:65:VAL:HG22	1:A:159:TYR:CB	2.41	0.50
1:A:427:GLY:HA2	1:A:441:TYR:CE2	2.47	0.50
1:A:472:ILE:C	1:A:473:LEU:HD12	2.37	0.50
1:B:201:ASN:HB3	1:B:204:GLU:HB3	1.94	0.50
1:A:473:LEU:HD12	1:A:473:LEU:N	2.27	0.49
1:B:17:CYS:HA	1:B:39:GLY:O	2.12	0.49
1:A:41:GLY:HA2	1:A:47:PRO:HD3	1.95	0.49
1:A:577:ASN:ND2	1:A:590:ASP:OD1	2.38	0.49
4:A:703:E9X:CAZ	4:A:703:E9X:CAT	2.90	0.49
1:B:77:ARG:NH1	1:B:158:TYR:CZ	2.81	0.49
1:A:368:LEU:HD11	1:A:374:LEU:HB2	1.95	0.49
1:A:12:TYR:HD1	1:A:181:LYS:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:MET:SD	1:A:489:PRO:HD3	2.53	0.48
1:A:172:GLU:OE2	3:A:702:NDP:N7A	2.46	0.48
3:B:702:NDP:O1A	3:B:702:NDP:O2N	2.30	0.48
1:A:312:PHE:HB2	1:A:316:ASN:ND2	2.29	0.48
1:A:106:ARG:NE	3:A:702:NDP:O2X	2.42	0.48
1:A:492:ILE:HG21	1:B:493:LEU:CD2	2.44	0.48
1:A:106:ARG:HE	3:A:702:NDP:P2B	2.38	0.47
1:B:457:LYS:NZ	1:B:584:GLU:OE1	2.47	0.47
1:A:488:PRO:HG3	1:B:471:ARG:HD3	1.97	0.47
1:A:530:HIS:HB3	1:A:576:LEU:HD11	1.97	0.47
1:A:114:LYS:H	1:A:114:LYS:CD	2.27	0.47
1:A:165:GLY:HA3	1:A:170:TYR:CZ	2.50	0.47
1:B:303:ASN:C	1:B:303:ASN:ND2	2.72	0.47
1:B:358:MET:HE1	1:B:522:ILE:HD11	1.97	0.46
1:B:518:VAL:N	1:B:519:PRO:CD	2.78	0.46
1:A:493:LEU:HD12	1:A:493:LEU:O	2.15	0.46
1:A:385:TRP:CE3	1:A:396:LEU:HD11	2.50	0.46
1:A:221:LEU:HD23	1:A:221:LEU:N	2.31	0.46
1:B:325:GLU:HG3	1:B:369:LEU:HD22	1.97	0.46
1:B:77:ARG:NH1	1:B:158:TYR:OH	2.49	0.45
1:B:311:ASP:O	1:B:565:ASN:ND2	2.50	0.45
1:A:12:TYR:OH	1:B:285:GLU:OE1	2.27	0.45
1:B:214:TYR:O	1:B:220:THR:HA	2.16	0.45
1:B:108:ASN:N	3:B:702:NDP:O2A	2.42	0.45
1:B:109:TRP:CZ2	1:B:117:LYS:CD	3.00	0.45
1:A:357:ILE:CD1	1:A:546:VAL:HG22	2.46	0.45
1:A:516:LEU:HD23	1:A:516:LEU:HA	1.83	0.45
1:B:325:GLU:CD	1:B:370:THR:H	2.25	0.45
1:B:482:LEU:HD22	1:B:488:PRO:HB3	1.98	0.44
1:A:171:GLN:NE2	1:A:175:GLU:OE1	2.38	0.44
1:B:118:PRO:O	1:B:119:LEU:C	2.59	0.44
1:A:487:LEU:HB2	1:A:488:PRO:HD2	1.98	0.44
1:B:605:ASP:HB2	1:B:606:MET:SD	2.57	0.44
1:A:209:SER:HB3	1:A:320:TYR:HB2	1.99	0.44
1:B:292:TYR:O	1:B:295:PHE:HB3	2.18	0.44
1:A:506:ILE:HA	1:A:544:ILE:O	2.17	0.44
1:B:127:LEU:HD22	3:B:702:NDP:C2A	2.47	0.44
1:B:144:ASN:O	3:B:702:NDP:H2A	2.18	0.44
1:B:164:LEU:HD23	1:B:164:LEU:N	2.33	0.44
1:A:211:SER:OG	1:A:212:ASP:O	2.33	0.44
1:B:508:TYR:C	1:B:508:TYR:CD1	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ILE:HB	1:B:565:ASN:OD1	2.18	0.43
1:A:477:TRP:CE3	1:A:492:ILE:CD1	3.01	0.43
1:A:59:ARG:CA	1:A:59:ARG:HE	2.31	0.43
1:A:114:LYS:HD2	1:A:114:LYS:H	1.83	0.43
1:B:140:VAL:C	1:B:141:TYR:CD2	2.94	0.43
1:B:569:TYR:CE2	1:B:599:HIS:CD2	3.07	0.43
1:B:285:GLU:C	1:B:287:GLU:H	2.26	0.43
1:A:577:ASN:OD1	1:A:577:ASN:C	2.61	0.42
1:B:357:ILE:HD11	1:B:544:ILE:HG23	2.01	0.42
1:B:493:LEU:HD12	1:B:493:LEU:O	2.18	0.42
1:B:134:GLU:H	1:B:134:GLU:HG3	1.68	0.42
1:A:214:TYR:O	1:A:220:THR:HA	2.19	0.42
1:B:40:LEU:HD23	3:B:702:NDP:N7N	2.35	0.42
1:B:104:MET:O	1:B:126:ILE:HA	2.20	0.42
1:A:569:TYR:O	1:A:570:PRO:C	2.63	0.42
1:B:494:CYS:SG	1:B:525:TYR:CE2	3.12	0.42
1:A:493:LEU:C	1:A:493:LEU:CD1	2.93	0.41
4:B:703:E9X:NAF	4:B:703:E9X:CAL	2.78	0.41
1:B:336:MET:HE1	1:B:560:LEU:HB2	2.03	0.41
1:A:287:GLU:OE1	1:B:69:LYS:HE2	2.21	0.41
1:A:304:LYS:H	1:A:304:LYS:CD	2.33	0.41
1:A:466:ASP:N	1:A:467:PRO:CD	2.84	0.41
1:B:447:ASN:OD1	1:B:447:ASN:C	2.63	0.41
1:A:312:PHE:HB2	1:A:316:ASN:HD21	1.86	0.41
1:B:141:TYR:CD2	1:B:141:TYR:N	2.89	0.41
1:B:231:ASN:N	1:B:231:ASN:ND2	2.68	0.41
1:B:12:TYR:HE2	1:B:160:LYS:HD3	1.86	0.41
1:B:605:ASP:CB	1:B:606:MET:SD	3.09	0.41
1:A:380:ILE:HG12	1:A:527:ILE:HD13	2.03	0.40
1:A:473:LEU:HA	1:A:494:CYS:O	2.21	0.40
1:B:429:ILE:O	1:B:430:TYR:C	2.64	0.40
1:A:428:PRO:HG2	1:A:481:ASP:HB3	2.03	0.40
1:B:65:VAL:HG12	1:B:159:TYR:HB3	2.02	0.40
1:A:146:VAL:C	1:A:148:ASP:N	2.79	0.40
1:A:518:VAL:N	1:A:519:PRO:CD	2.85	0.40
1:A:560:LEU:HD23	1:A:560:LEU:HA	1.97	0.40
1:B:172:GLU:OE2	3:B:702:NDP:N6A	2.54	0.40
1:B:512:CYS:HB2	1:B:550:ALA:HA	2.03	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	528/608 (87%)	493 (93%)	28 (5%)	7 (1%)	9	21
1	B	521/608 (86%)	470 (90%)	40 (8%)	11 (2%)	5	11
All	All	1049/1216 (86%)	963 (92%)	68 (6%)	18 (2%)	7	15

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	96	LYS
1	A	139	ASP
1	A	301	GLU
1	B	310	ASN
1	B	345	ARG
1	A	299	LYS
1	B	49	LYS
1	B	67	GLU
1	B	140	VAL
1	B	75	TYR
1	B	309	PRO
1	B	430	TYR
1	A	303	ASN
1	B	5	VAL
1	B	137	ASP
1	A	309	PRO
1	B	123	ILE

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	502/570 (88%)	475 (95%)	27 (5%)	20 42
1	B	495/570 (87%)	457 (92%)	38 (8%)	12 27
All	All	997/1140 (88%)	932 (94%)	65 (6%)	15 35

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	65	VAL
1	A	96	LYS
1	A	97	LYS
1	A	114	LYS
1	A	115	LYS
1	A	124	ASN
1	A	134	GLU
1	A	147	GLU
1	A	189	SER
1	A	285	GLU
1	A	301	GLU
1	A	303	ASN
1	A	304	LYS
1	A	306	SER
1	A	307	ILE
1	A	457	LYS
1	A	491	HIS
1	A	514	LEU
1	A	516	LEU
1	A	555	ASN
1	A	564	LEU
1	A	575	LYS
1	A	577	ASN
1	A	589	SER
1	A	592	THR
1	A	600	GLU
1	B	5	VAL
1	B	30	GLU
1	B	31	VAL
1	B	72	LYS
1	B	76	LYS
1	B	77	ARG

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Mol	Chain	Res	Type
1	B	81	LEU
1	B	104	MET
1	B	106	ARG
1	B	107	THR
1	B	120	SER
1	B	133	LYS
1	B	134	GLU
1	B	144	ASN
1	B	155	LYS
1	B	164	LEU
1	B	171	GLN
1	B	189	SER
1	B	218	ASN
1	B	224	ILE
1	B	230	ASN
1	B	231	ASN
1	B	285	GLU
1	B	298	GLU
1	B	299	LYS
1	B	302	LYS
1	B	307	ILE
1	B	313	GLN
1	B	343	SER
1	B	346	THR
1	B	357	ILE
1	B	416	ARG
1	B	450	ASN
1	B	516	LEU
1	B	524	SER
1	B	564	LEU
1	B	605	ASP
1	B	606	MET

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	29	ASN
1	A	99	GLN
1	A	201	ASN
1	A	316	ASN
1	A	415	ASN
1	A	555	ASN

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Mol	Chain	Res	Type
1	A	556	HIS
1	A	563	GLN
1	B	108	ASN
1	B	171	GLN
1	B	231	ASN
1	B	303	ASN
1	B	338	ASN
1	B	394	ASN
1	B	398	ASN
1	B	400	ASN
1	B	424	ASN
1	B	530	HIS
1	B	554	ASN
1	B	556	HIS

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	$\#\|Z\|>2$
4	E9X	A	703	-	28,31,31	1.91	4 (14%)	34,43,43	2.32	13 (38%)
3	NDP	A	702	-	51,52,52	2.49	14 (27%)	71,80,80	2.17	19 (26%)
3	NDP	B	702	-	51,52,52	2.41	17 (33%)	71,80,80	2.22	20 (28%)
2	UMP	A	701	-	21,21,21	0.52	0	30,31,31	0.71	1 (3%)
4	E9X	B	703	-	28,31,31	5.02	4 (14%)	34,43,43	2.05	7 (20%)
2	UMP	B	701	-	21,21,21	0.46	0	30,31,31	0.95	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
4	E9X	A	703	-	-	7/15/34/34	0/2/3/3
3	NDP	A	702	-	-	6/34/77/77	0/5/5/5
3	NDP	B	702	-	-	7/34/77/77	0/5/5/5
2	UMP	A	701	-	-	2/10/22/22	0/2/2/2
4	E9X	B	703	-	-	8/15/34/34	0/2/3/3
2	UMP	B	701	-	-	2/10/22/22	0/2/2/2

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	E9X	OAK-NAF	25.30	1.71	1.40
3	B	702	NDP	PA-O3	9.82	1.70	1.59
3	A	702	NDP	PA-O3	9.32	1.69	1.59
3	B	702	NDP	PN-O3	6.44	1.66	1.59
4	A	703	E9X	OAK-NAF	-6.35	1.32	1.40
4	A	703	E9X	CAS-CAT	-6.18	1.40	1.51
3	A	702	NDP	PN-O3	6.14	1.66	1.59
3	A	702	NDP	C4N-C3N	-5.74	1.39	1.50
3	A	702	NDP	C2A-N1A	5.08	1.43	1.33
3	B	702	NDP	C4N-C3N	-5.06	1.40	1.50
4	B	703	E9X	CBB-CL	-4.58	1.63	1.74
3	A	702	NDP	C4A-N9A	-3.80	1.29	1.37
3	B	702	NDP	C2A-N1A	3.79	1.40	1.33
4	B	703	E9X	CAS-NAO	3.51	1.51	1.46
4	B	703	E9X	CAS-CAT	-3.40	1.45	1.51
3	B	702	NDP	C2A-N3A	3.31	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NDP	C2B-C1B	-3.29	1.45	1.53
3	A	702	NDP	C5A-N7A	-3.17	1.33	1.39
3	A	702	NDP	C7N-C3N	-3.16	1.41	1.48
3	B	702	NDP	C7N-C3N	-3.13	1.42	1.48
3	B	702	NDP	C4N-C5N	-3.10	1.41	1.49
3	B	702	NDP	C5A-N7A	-3.07	1.33	1.39
4	A	703	E9X	CAP-NAO	-2.83	1.31	1.38
3	A	702	NDP	C2A-N3A	2.80	1.38	1.33
3	B	702	NDP	C5A-C4A	-2.71	1.34	1.39
3	A	702	NDP	PA-O2A	-2.65	1.43	1.55
3	B	702	NDP	O4D-C1D	2.64	1.48	1.42
3	B	702	NDP	O4B-C1B	2.62	1.48	1.42
3	A	702	NDP	C8A-N9A	-2.57	1.33	1.37
4	A	703	E9X	CBB-CL	-2.50	1.68	1.74
3	B	702	NDP	C5A-C6A	-2.50	1.34	1.41
3	B	702	NDP	C8A-N9A	-2.31	1.33	1.37
3	B	702	NDP	C6N-C5N	2.25	1.39	1.33
3	A	702	NDP	C5A-C4A	-2.23	1.35	1.39
3	B	702	NDP	C4A-N9A	-2.19	1.33	1.37
3	A	702	NDP	C6N-C5N	2.12	1.39	1.33
3	A	702	NDP	C4N-C5N	-2.12	1.43	1.49
3	B	702	NDP	C1B-N9A	2.09	1.52	1.46
3	B	702	NDP	C2N-C3N	2.01	1.40	1.35

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	NDP	O2N-PN-O3	-9.06	82.77	107.27
4	A	703	E9X	CAT-CAS-NAO	7.40	126.11	114.13
3	B	702	NDP	N3A-C2A-N1A	-6.77	118.33	128.58
3	A	702	NDP	O2N-PN-O3	-6.39	89.99	107.27
4	B	703	E9X	CAT-CAS-NAO	6.06	123.94	114.13
4	B	703	E9X	NAF-CAA-NAB	5.83	125.30	121.53
3	A	702	NDP	O3-PN-O1N	-5.43	94.37	110.70
3	A	702	NDP	O4D-C1D-N1N	-5.15	98.27	108.08
3	A	702	NDP	N3A-C2A-N1A	-5.01	121.00	128.58
4	B	703	E9X	NAB-CAC-NAD	-4.79	118.57	126.48
3	A	702	NDP	C4A-C5A-N7A	-4.45	105.50	110.58
3	A	702	NDP	C5A-C4A-N9A	4.43	110.64	105.81
4	A	703	E9X	CAJ-CAE-CAI	-4.42	103.35	110.68
3	B	702	NDP	O4B-C1B-N9A	4.34	116.43	108.09
3	B	702	NDP	O3-PN-O1N	-4.26	97.88	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	703	E9X	NAB-CAC-NAD	-4.23	119.50	126.48
3	B	702	NDP	C5A-C4A-N3A	-4.22	120.91	126.72
4	A	703	E9X	NAF-CAA-NAB	4.13	124.21	121.53
3	A	702	NDP	N9A-C8A-N7A	-3.93	108.36	113.94
3	A	702	NDP	C5A-C4A-N3A	-3.81	121.47	126.72
4	A	703	E9X	NAG-CAA-NAF	3.59	120.41	117.46
3	B	702	NDP	N9A-C8A-N7A	-3.57	108.87	113.94
3	A	702	NDP	O2B-P2B-O1X	-3.56	96.64	109.33
3	B	702	NDP	O2N-PN-O5D	3.40	123.00	107.57
3	B	702	NDP	C2A-N3A-C4A	3.28	119.84	111.83
3	A	702	NDP	C5A-N7A-C8A	3.11	108.34	103.45
3	B	702	NDP	C5A-C6A-N6A	-2.91	116.07	123.29
3	B	702	NDP	O2B-P2B-O1X	-2.88	99.07	109.33
4	A	703	E9X	CAS-NAO-CAP	2.84	125.65	120.72
4	B	703	E9X	NAH-CAC-NAB	2.83	121.06	116.57
3	A	702	NDP	O2N-PN-O5D	2.82	120.34	107.57
3	A	702	NDP	O2A-PA-O3	2.79	114.81	107.27
3	A	702	NDP	O2N-PN-O1N	2.74	125.19	112.44
3	A	702	NDP	C2A-N3A-C4A	2.64	118.27	111.83
3	A	702	NDP	C6A-C5A-C4A	2.63	120.77	117.18
3	A	702	NDP	C4A-N9A-C1B	-2.60	120.55	126.63
3	B	702	NDP	C5A-N7A-C8A	2.60	107.53	103.45
3	B	702	NDP	C5A-C4A-N9A	2.58	108.62	105.81
3	B	702	NDP	C4A-C5A-N7A	-2.46	107.76	110.58
4	B	703	E9X	CBA-CBB-CL	2.44	122.95	119.36
3	B	702	NDP	O4D-C1D-N1N	2.43	112.73	108.08
3	B	702	NDP	O3X-P2B-O2X	2.40	116.79	107.80
4	A	703	E9X	CBA-CBB-CL	-2.38	115.85	119.36
3	B	702	NDP	C6A-C5A-C4A	2.30	120.32	117.18
4	A	703	E9X	CAI-CAE-NAF	2.30	113.33	109.02
4	B	703	E9X	CAR-CBB-CL	-2.29	115.97	119.36
3	A	702	NDP	O5D-C5D-C4D	-2.25	101.34	108.99
3	A	702	NDP	C1D-N1N-C2N	-2.23	117.47	121.14
4	A	703	E9X	NAH-CAC-NAB	2.23	120.11	116.57
3	A	702	NDP	C1B-N9A-C8A	2.21	131.99	127.09
3	B	702	NDP	C2B-C3B-C4B	-2.19	97.29	101.99
4	A	703	E9X	CAS-CAT-CAU	2.16	124.72	120.75
2	A	701	UMP	OP3-P-OP2	2.15	115.87	107.80
2	B	701	UMP	C2'-C3'-C4'	-2.15	98.44	102.80
4	A	703	E9X	NAH-CAC-NAD	2.13	120.39	117.09
4	B	703	E9X	NAH-CAC-NAD	2.12	120.36	117.09
4	A	703	E9X	CAR-CBB-CL	2.11	122.48	119.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	702	NDP	O4D-C4D-C5D	2.07	115.95	109.33
4	A	703	E9X	NAG-CAA-NAB	-2.02	115.13	119.75
3	B	702	NDP	O4B-C1B-C2B	-2.02	103.11	106.59
3	B	702	NDP	C4A-N9A-C1B	-2.00	121.95	126.63

There are no chirality outliers.

All (32) 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	E9X	OAK-CAL-CAM-CAN
4	A	703	E9X	CAT-CAS-NAO-CAP
4	B	703	E9X	CAE-NAF-OAK-CAL
4	B	703	E9X	CAA-NAF-OAK-CAL
4	B	703	E9X	OAK-CAL-CAM-CAN
4	B	703	E9X	CAQ-CAP-NAO-CAS
4	B	703	E9X	CAZ-CAP-NAO-CAS
4	B	703	E9X	CAZ-CAP-NAO-CAN
4	B	703	E9X	CAQ-CAP-NAO-CAN
4	A	703	E9X	CAZ-CAP-NAO-CAN
3	B	702	NDP	O4D-C4D-C5D-O5D
3	B	702	NDP	C3D-C4D-C5D-O5D
4	A	703	E9X	CAQ-CAP-NAO-CAN
4	A	703	E9X	CAZ-CAP-NAO-CAS
2	B	701	UMP	C3'-C4'-C5'-O5'
2	B	701	UMP	O4'-C4'-C5'-O5'
4	A	703	E9X	CAQ-CAP-NAO-CAS
4	B	703	E9X	CAL-CAM-CAN-NAO
3	A	702	NDP	PA-O3-PN-O5D
2	A	701	UMP	O4'-C4'-C5'-O5'
2	A	701	UMP	C3'-C4'-C5'-O5'
3	A	702	NDP	O4D-C1D-N1N-C2N
3	B	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	C2N-C3N-C7N-N7N
3	B	702	NDP	C2D-C1D-N1N-C2N
3	B	702	NDP	C4D-C5D-O5D-PN
4	A	703	E9X	CAT-CAS-NAO-CAN
3	A	702	NDP	C2D-C1D-N1N-C2N

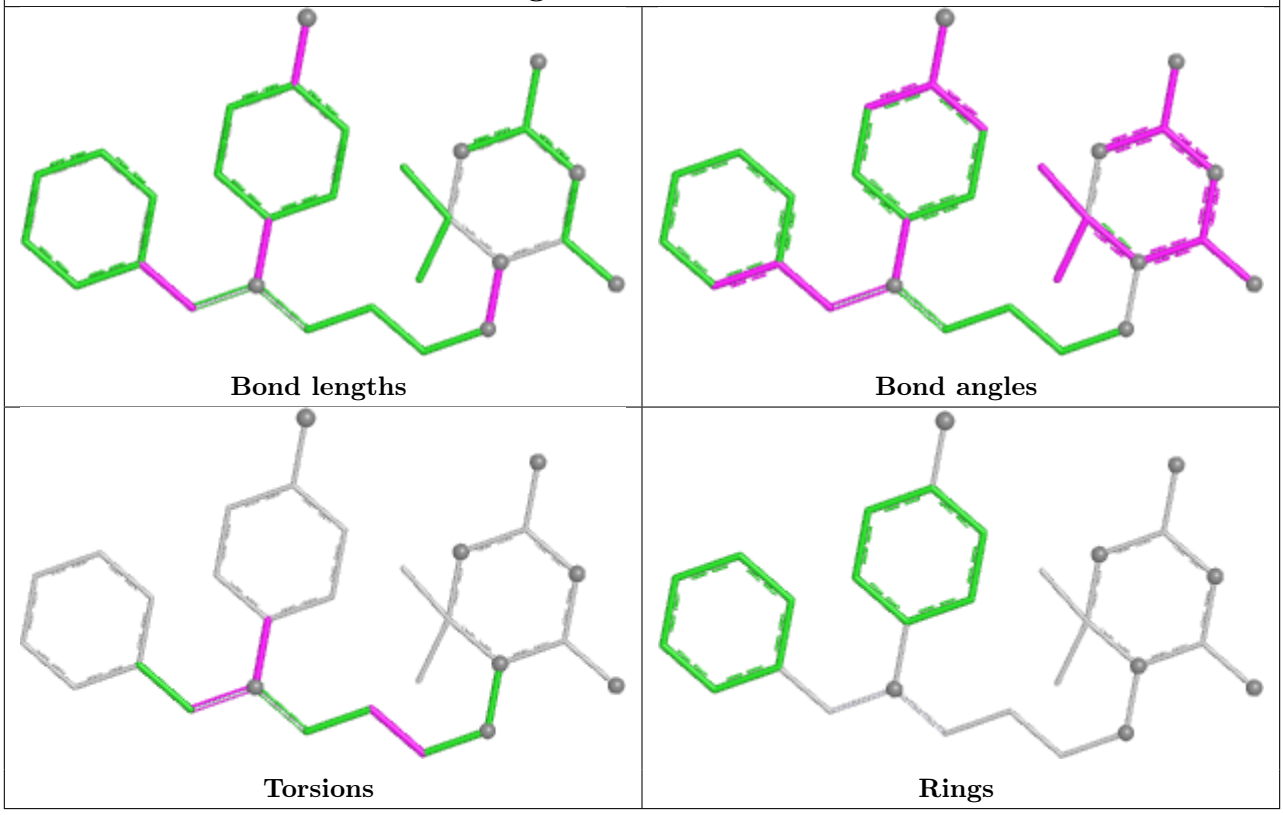
There are no ring outliers.

5 monomers are involved in 19 short contacts:

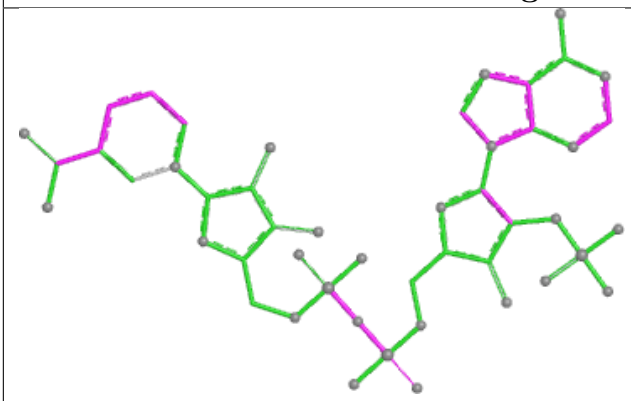
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	E9X	2	0
3	A	702	NDP	6	0
3	B	702	NDP	6	0
4	B	703	E9X	3	0
2	B	701	UMP	2	0

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 then 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.

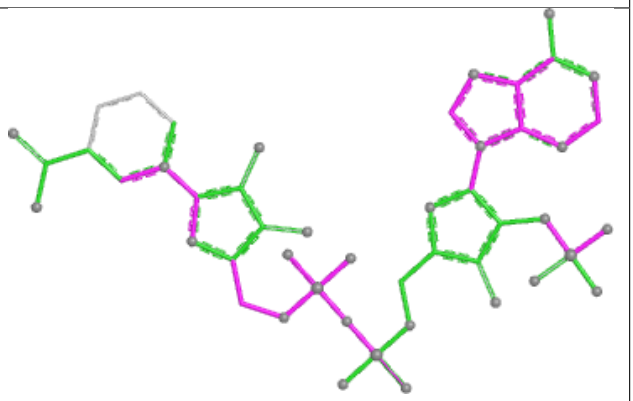
Ligand E9X A 703



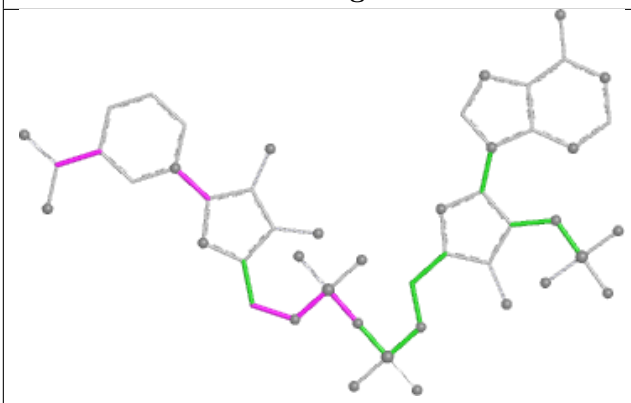
Ligand NDP A 702



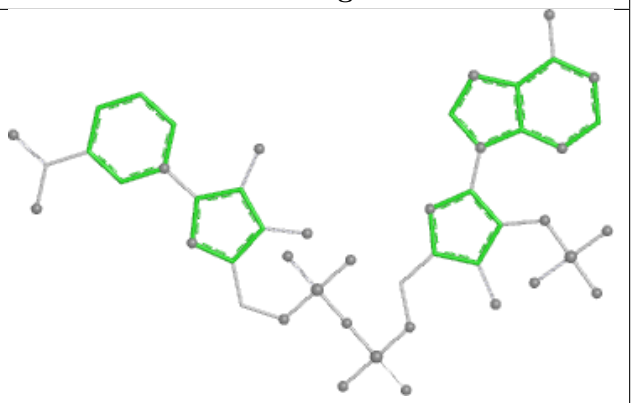
Bond lengths



Bond angles

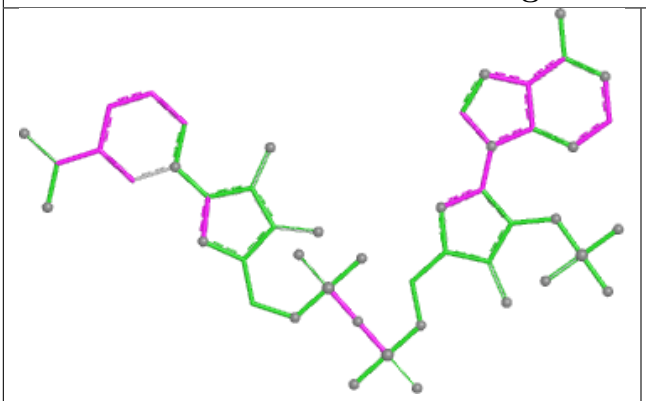


Torsions

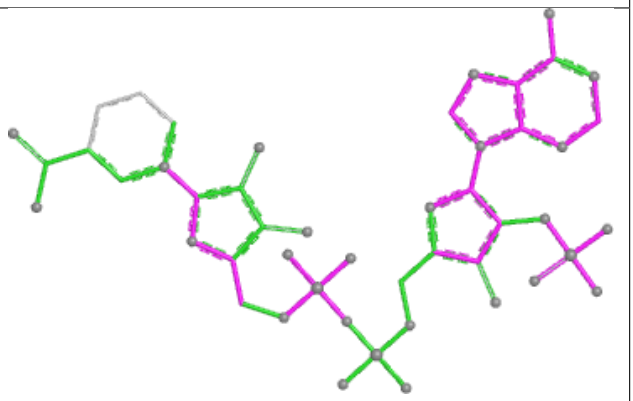


Rings

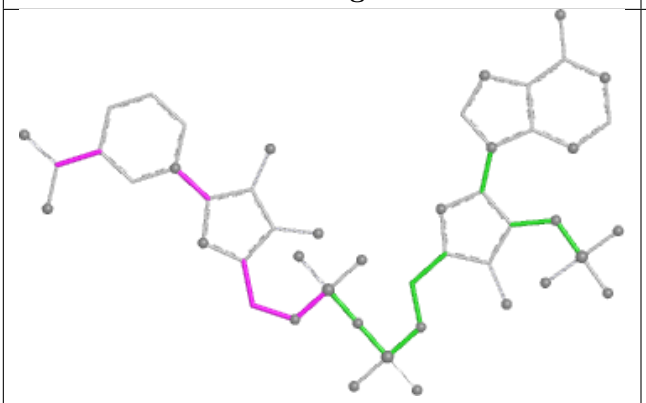
Ligand NDP B 702



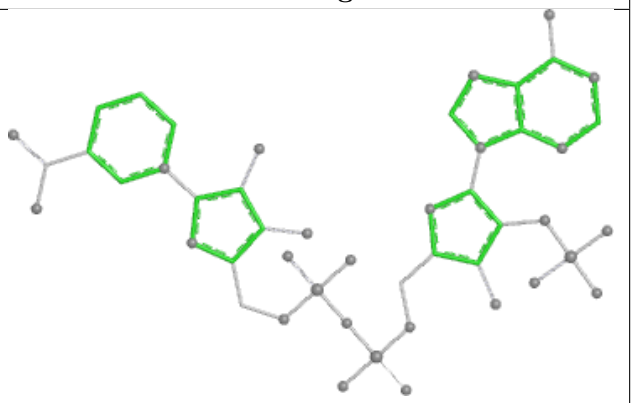
Bond lengths



Bond angles

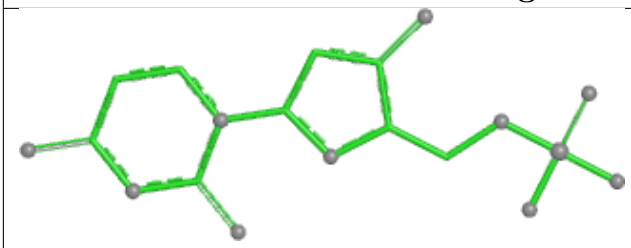


Torsions

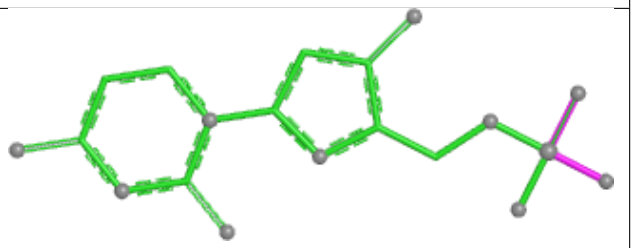


Rings

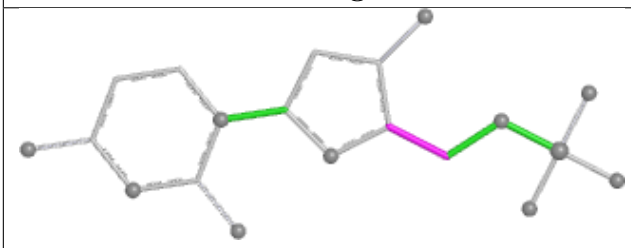
Ligand UMP A 701



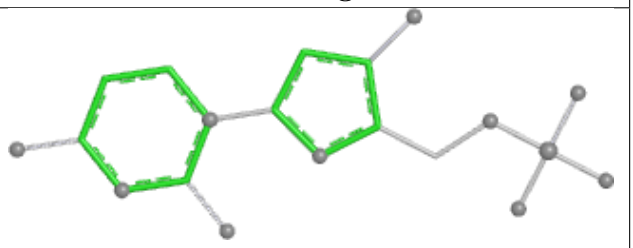
Bond lengths



Bond angles

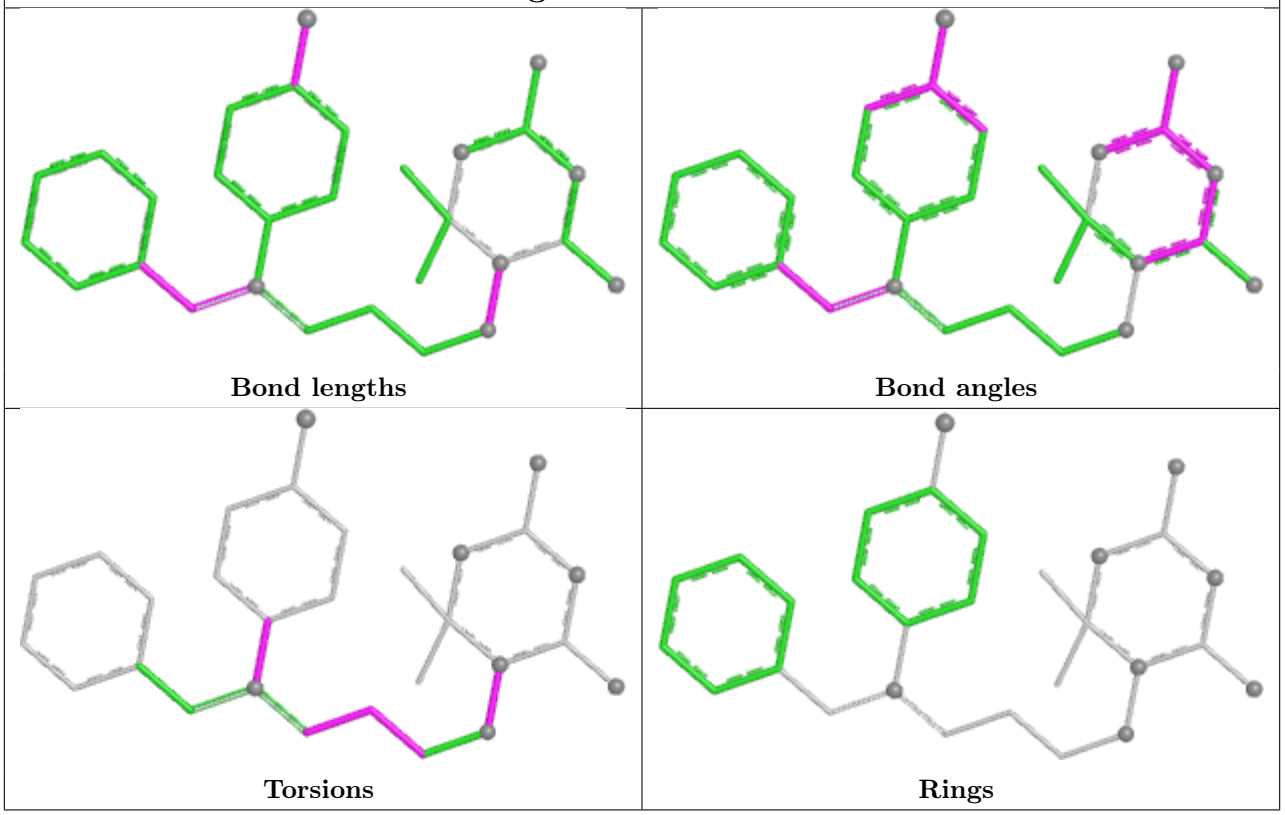


Torsions

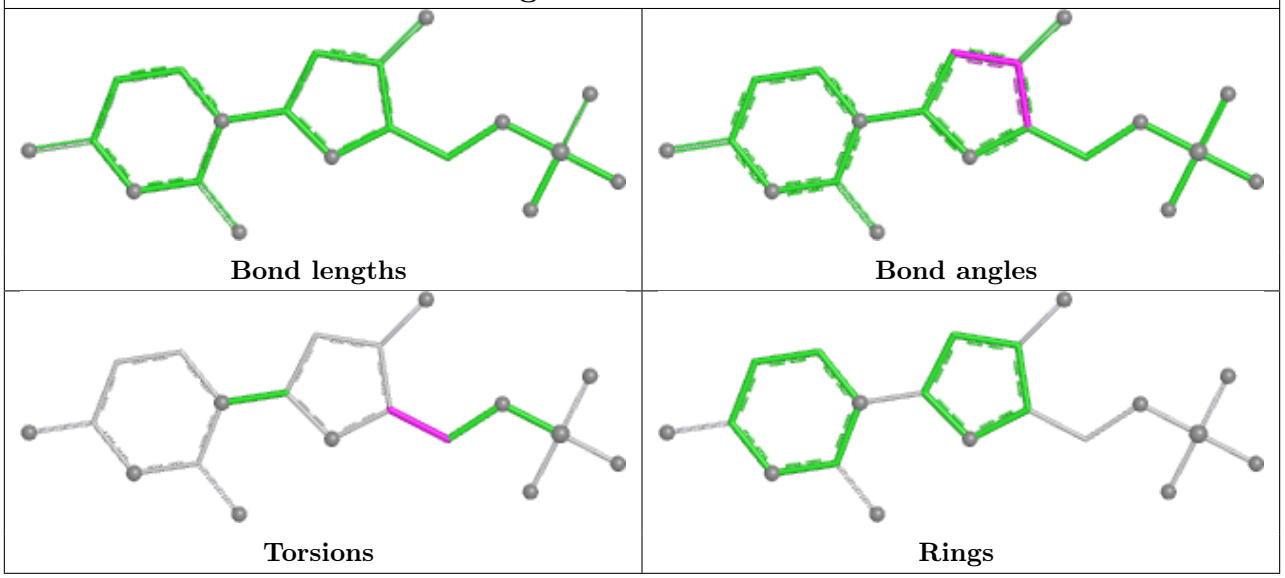


Rings

Ligand E9X B 703



Ligand UMP B 701



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	536/608 (88%)	-0.51	8 (1%)	72	68	16, 29, 77, 151	0
1	B	529/608 (87%)	-0.22	15 (2%)	55	49	16, 33, 111, 134	0
All	All	1065/1216 (87%)	-0.36	23 (2%)	62	57	16, 30, 105, 151	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	SER	4.4
1	B	140	VAL	3.9
1	A	303	ASN	3.7
1	B	309	PRO	3.2
1	A	346	THR	3.1
1	B	151	VAL	3.0
1	B	347	GLY	3.0
1	B	606	MET	2.9
1	B	116	PHE	2.8
1	A	96	LYS	2.8
1	B	113	PRO	2.7
1	B	105	GLY	2.5
1	A	309	PRO	2.4
1	B	115	LYS	2.3
1	B	301	GLU	2.3
1	A	348	VAL	2.3
1	B	71	GLU	2.2
1	B	284	ASP	2.2
1	A	347	GLY	2.2
1	B	135	ASP	2.2
1	A	310	ASN	2.1
1	B	139	ASP	2.1
1	B	73	LEU	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)

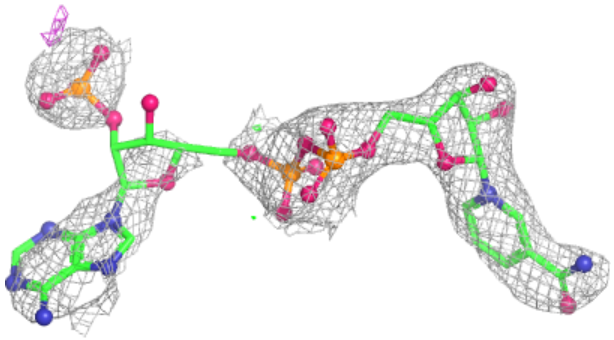
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

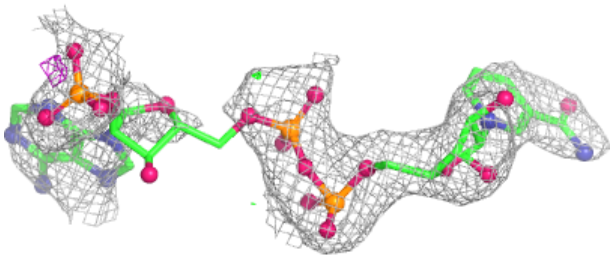
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NDP	B	702	48/48	0.86	0.11	61,84,121,126	0
4	E9X	B	703	29/29	0.86	0.09	62,73,81,86	0
4	E9X	A	703	29/29	0.95	0.07	22,34,56,63	0
2	UMP	B	701	20/20	0.96	0.08	28,37,44,46	0
3	NDP	A	702	48/48	0.98	0.04	21,25,27,28	0
2	UMP	A	701	20/20	0.98	0.06	24,35,43,46	0

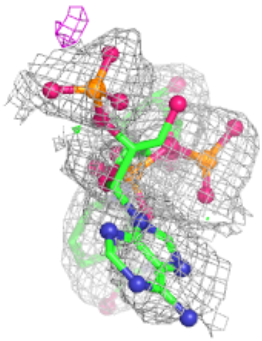
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP B 702:

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

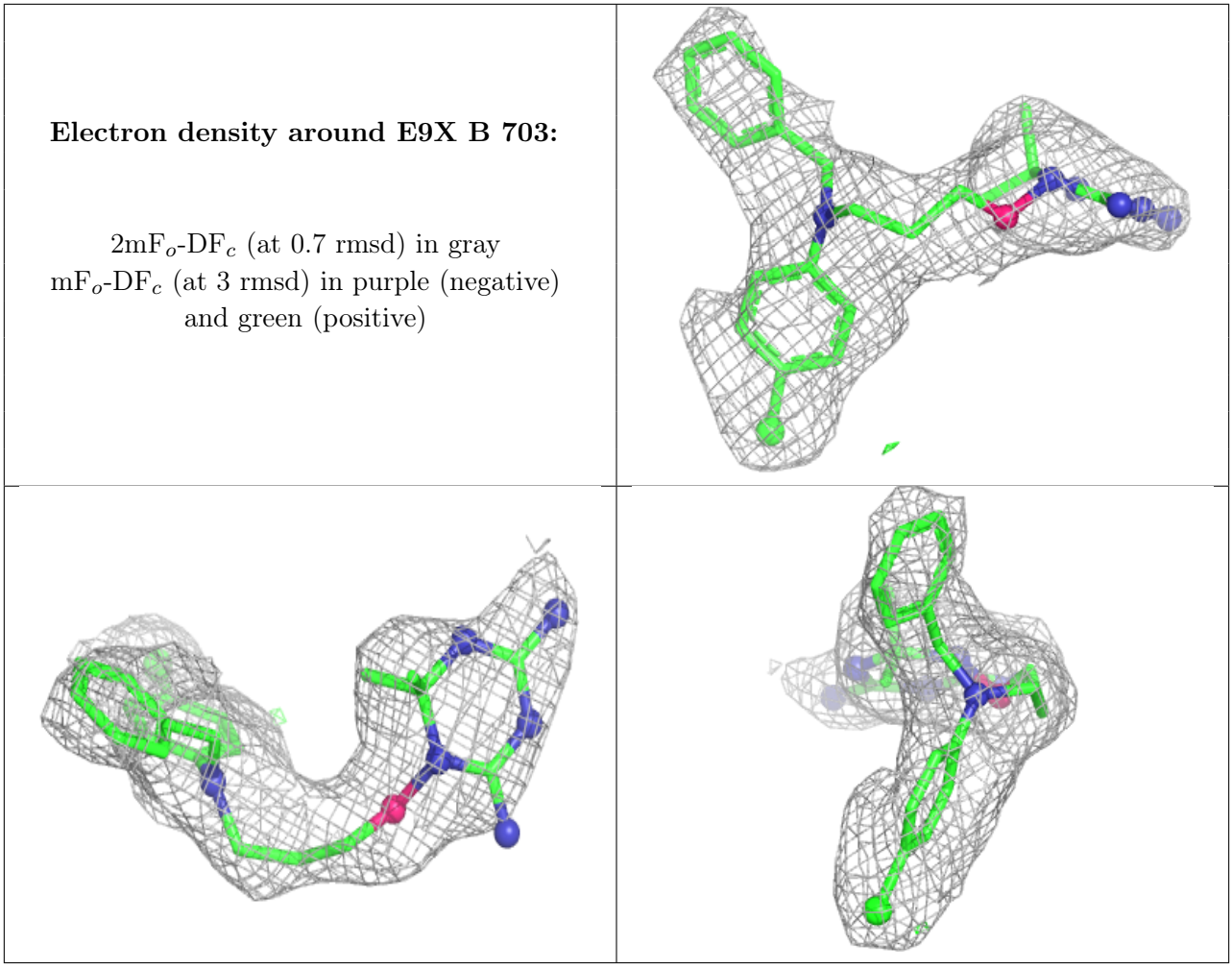






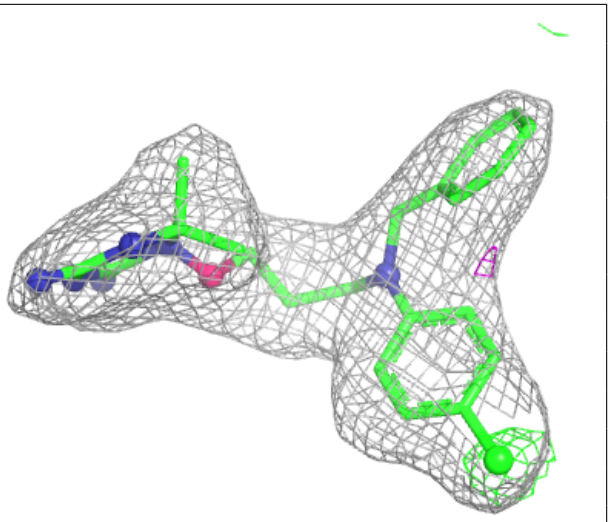
Electron density around E9X B 703:

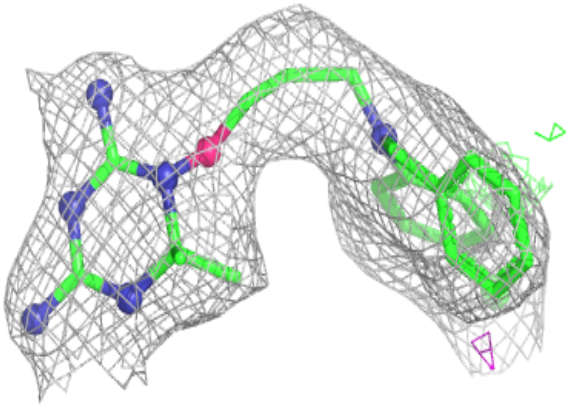
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

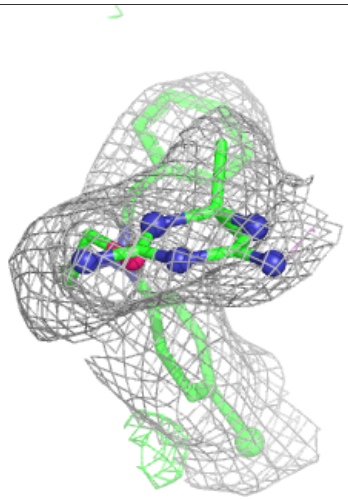


Electron density around E9X A 703:

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

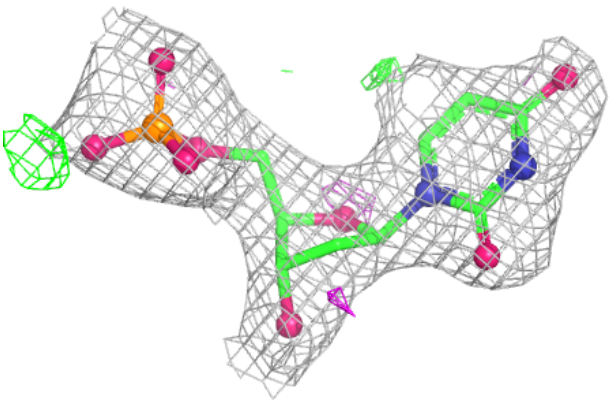


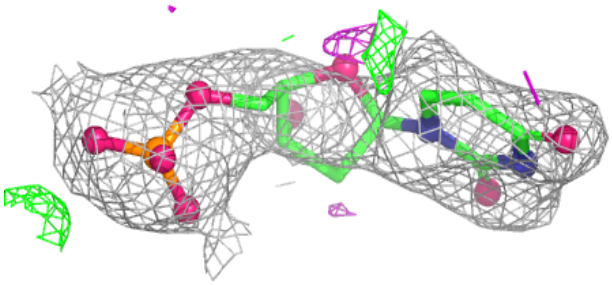


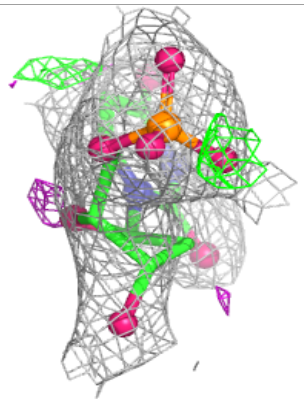


Electron density around UMP B 701:

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

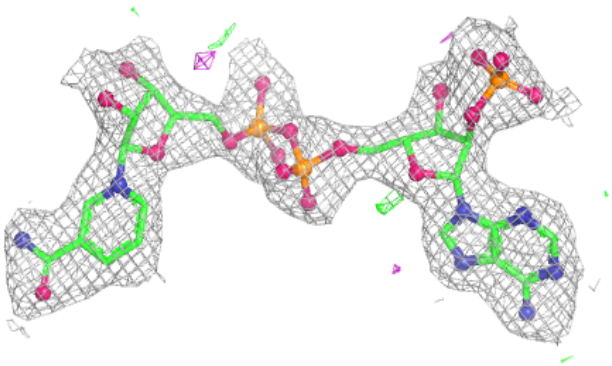


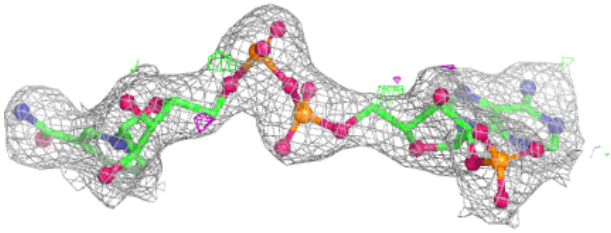


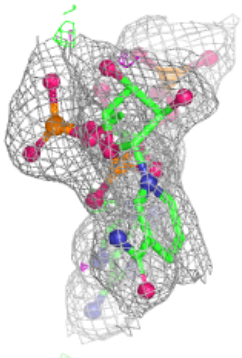


Electron density around NDP A 702:

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

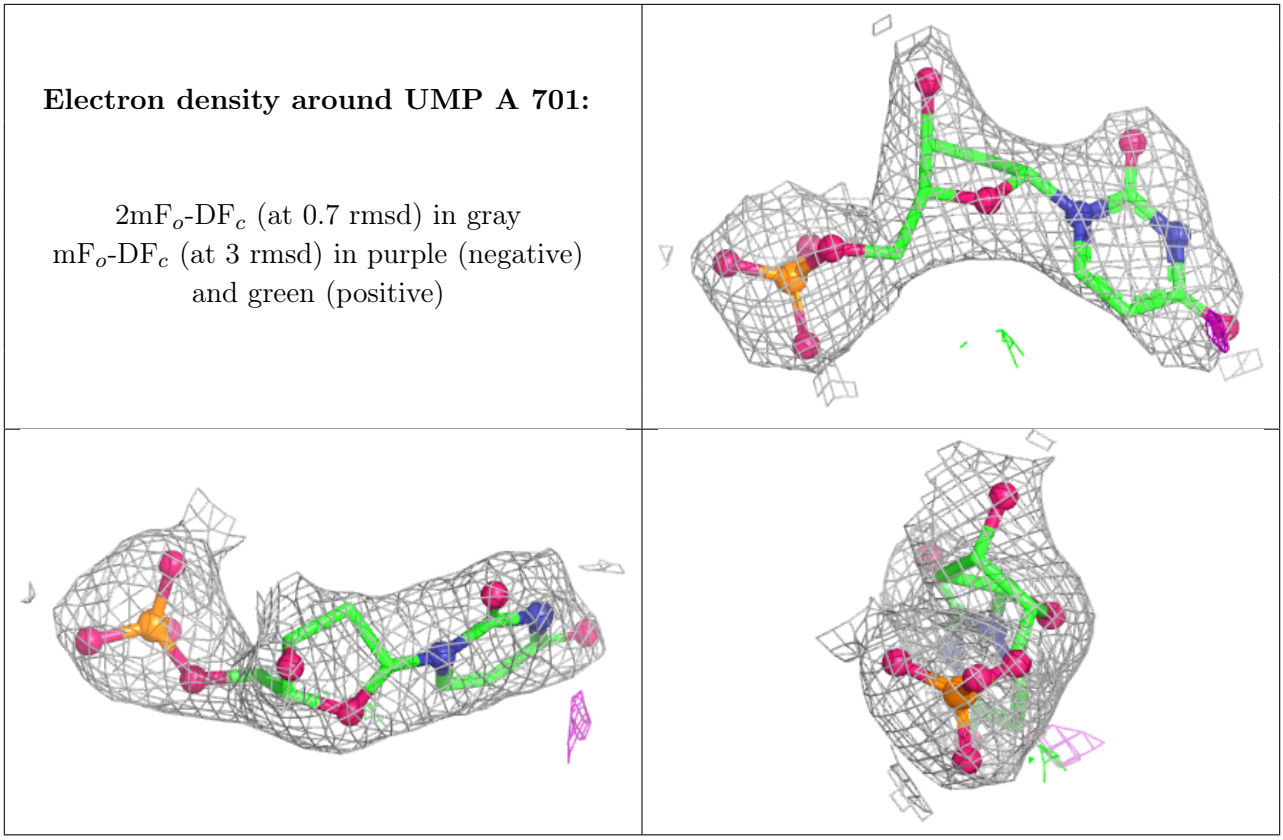






Electron density around UMP A 701:

$2mF_o$-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.