



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 02:55 PM BST

PDB ID : 4ECK
Title : Crystal Structure of the Toxoplasma gondii TS-DHFR
Authors : Sharma, H.; Anderson, K.S.
Deposited on : 2012-03-26
Resolution : 3.52 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

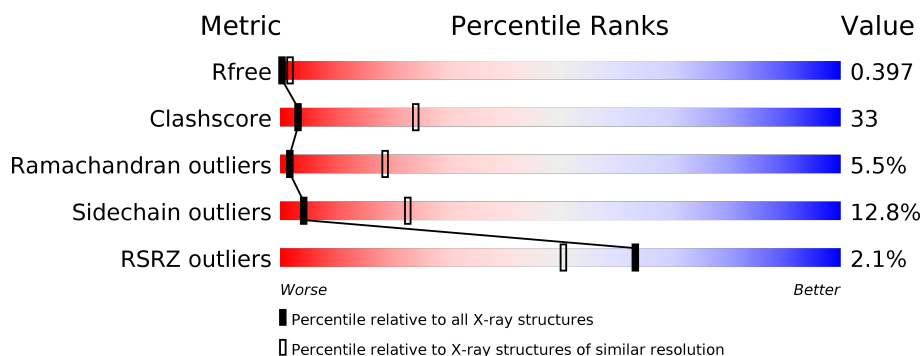
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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 on 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	610	<div> <div> <div></div> <div>37%</div> <div>36%</div> <div>8%</div> <div>18%</div> </div> </div>
1	B	610	<div> <div> <div>2%</div> <div>36%</div> <div>37%</div> <div>9%</div> <div>18%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UMP	A	701	-	-	X	-
2	UMP	B	701	-	-	X	-
3	CB3	A	702	-	-	X	X
3	CB3	B	702	-	-	X	X
4	FOL	A	703	-	-	X	X
4	FOL	B	703	-	-	X	X

2 Entry composition [i](#)

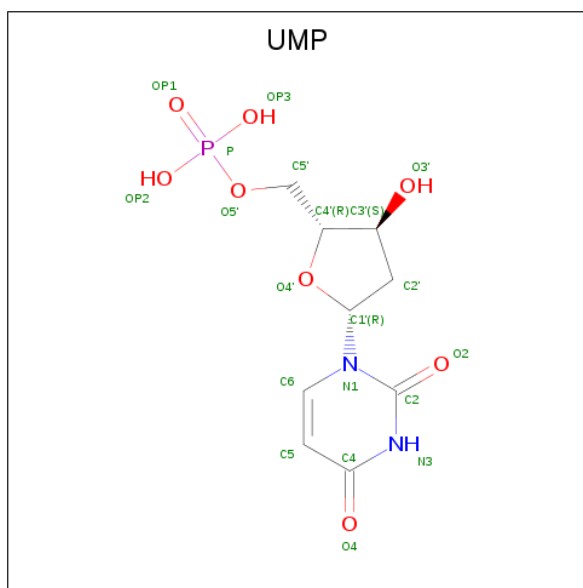
There are 5 unique types of molecules in this entry. The entry contains 8248 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

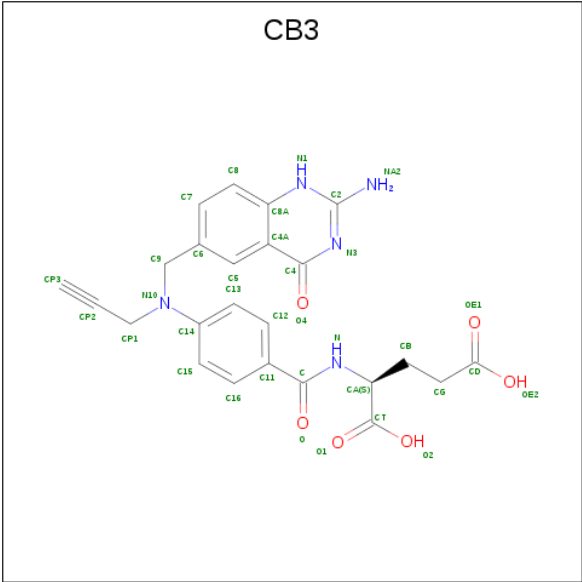
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	0	0
			3989	2550	697	717	25			
1	B	498	Total	C	N	O	S	0	0	0
			3989	2550	697	717	25			

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



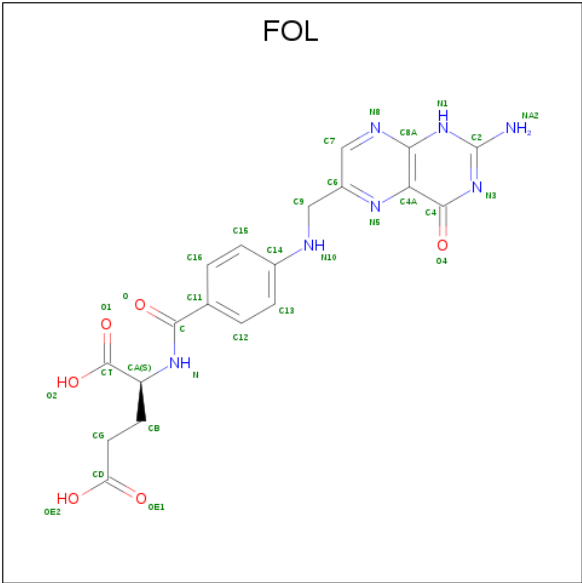
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3) (formula: $C_{24}H_{23}N_5O_6$).



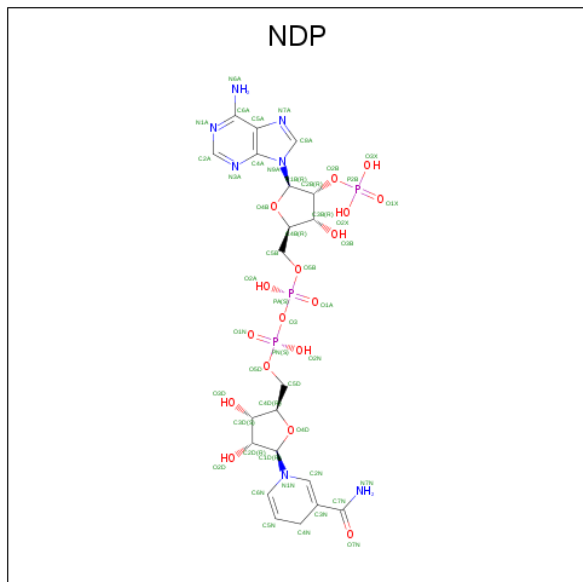
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			35	24	5	6		
3	B	1	Total	C	N	O	0	0
			35	24	5	6		

- Molecule 4 is FOLIC ACID (three-letter code: FOL) (formula: C₁₉H₁₉N₇O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			32	19	7	6		
4	B	1	Total	C	N	O	0	0
			32	19	7	6		

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

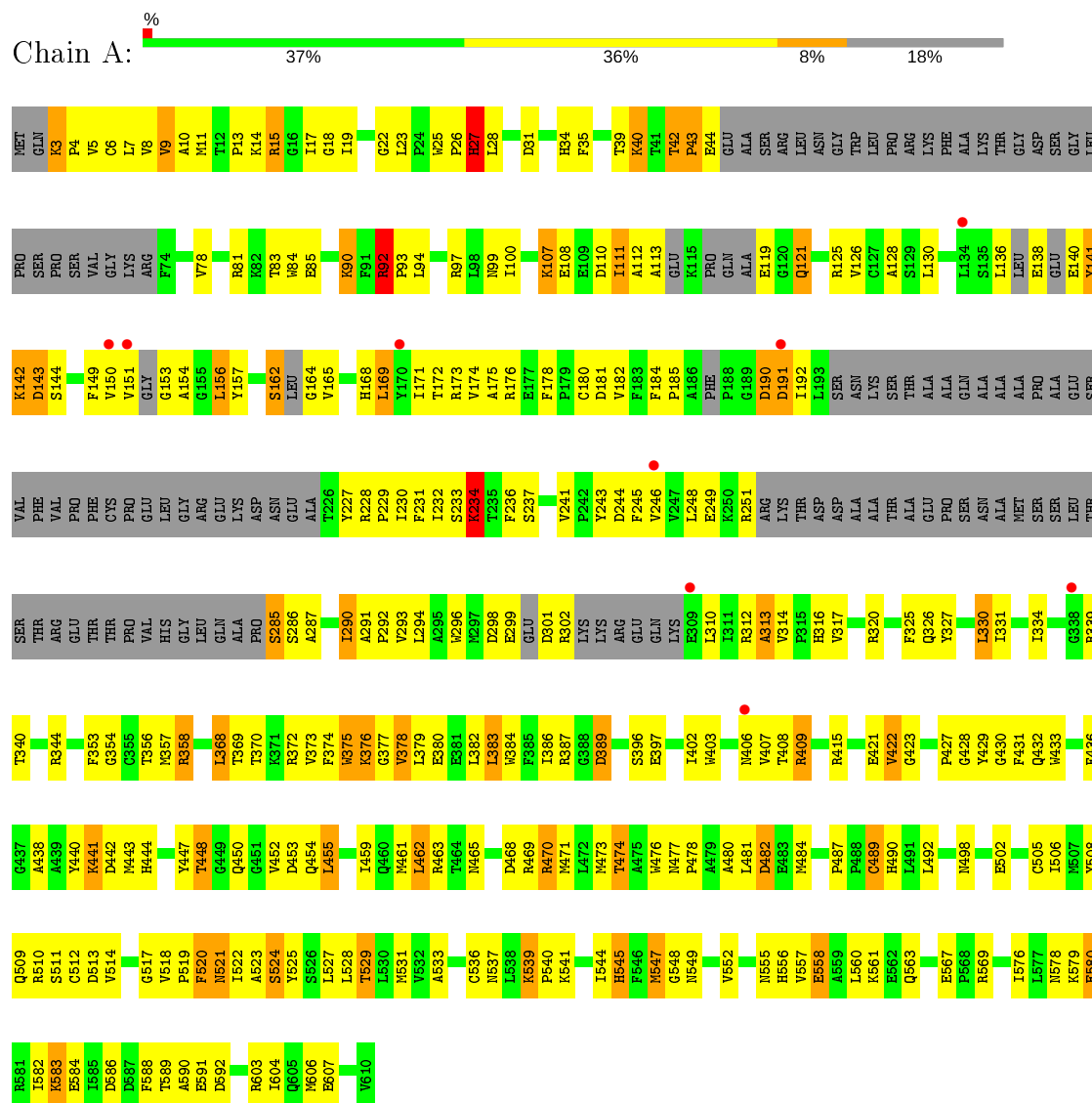


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
5	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

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	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.94Å 143.01Å 59.84Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	46.18 – 3.52 46.18 – 3.52	Depositor EDS
% Data completeness (in resolution range)	95.9 (46.18-3.52) 95.9 (46.18-3.52)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.332 , 0.395 0.328 , 0.397	Depositor DCC
R_{free} test set	982 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	70.5	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.387 for -h,-k,l	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	8248	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.87 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2797e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: FOL, CB3, UMP, NDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.58	1/4078 (0.0%)	0.73	0/5510
1	B	0.59	3/4078 (0.1%)	0.73	0/5510
All	All	0.59	4/8156 (0.0%)	0.73	0/11020

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	403	TRP	CD2-CE2	5.34	1.47	1.41
1	B	25	TRP	CD2-CE2	5.26	1.47	1.41
1	B	433	TRP	CD2-CE2	5.02	1.47	1.41
1	A	403	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	42	THR	Peptide
1	A	92	ARG	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	3989	0	3939	267	0
1	B	3989	0	3940	295	0
2	A	20	0	11	25	0
2	B	20	0	11	15	0
3	A	35	0	21	15	0
3	B	35	0	21	18	0
4	A	32	0	17	10	0
4	B	32	0	17	26	0
5	A	48	0	26	8	0
5	B	48	0	26	16	0
All	All	8248	0	8029	543	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 33.

All (543) 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:402:ILE:HG22	3:B:702:CB3:C16	1.09	1.56
1:B:402:ILE:CG2	3:B:702:CB3:C16	1.91	1.46
1:B:510:ARG:HH12	2:B:701:UMP:P	1.40	1.41
1:A:489:CYS:SG	2:A:701:UMP:C6	2.28	1.25
1:A:344:ARG:NH2	2:A:701:UMP:OP3	1.72	1.21
1:B:23:LEU:CD2	5:B:704:NDP:H2N	1.74	1.17
1:A:151:VAL:HG12	4:A:703:FOL:H7	1.22	1.16
1:B:402:ILE:CG2	3:B:702:CB3:C11	2.24	1.16
1:A:83:THR:OG1	5:A:704:NDP:O2A	1.66	1.12
1:B:510:ARG:NH1	2:B:701:UMP:OP2	1.82	1.11
1:B:156:LEU:HD12	5:B:704:NDP:N7A	1.65	1.10
1:B:35:PHE:CE2	4:B:703:FOL:H12	1.86	1.09
1:B:402:ILE:HG22	3:B:702:CB3:H16	1.31	1.09
1:B:91:PHE:CD1	4:B:703:FOL:O	2.05	1.09
1:B:23:LEU:HD21	5:B:704:NDP:H2N	1.30	1.09
1:B:402:ILE:CG2	3:B:702:CB3:C15	2.31	1.09
1:B:510:ARG:NH1	2:B:701:UMP:P	2.25	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ILE:HG22	3:B:702:CB3:C11	1.82	1.07
1:A:344:ARG:HH21	2:A:701:UMP:P	1.81	1.04
1:B:402:ILE:HG22	3:B:702:CB3:C15	1.89	1.03
1:B:35:PHE:HE2	4:B:703:FOL:H12	1.27	0.99
1:A:433:TRP:HZ2	1:A:525:TYR:HH	1.04	0.98
1:A:521:ASN:ND2	3:A:702:CB3:CP3	2.27	0.98
1:A:94:LEU:HB2	1:A:99:ASN:HD21	1.22	0.98
1:A:151:VAL:CG1	4:A:703:FOL:H7	1.94	0.97
1:A:558:GLU:H	1:A:558:GLU:CD	1.63	0.94
1:A:8:VAL:HG22	4:A:703:FOL:HN1	1.30	0.94
2:A:701:UMP:OP3	1:B:470:ARG:NH2	2.01	0.93
1:A:470:ARG:NH2	2:B:701:UMP:OP2	2.03	0.91
1:A:136:LEU:O	1:A:141:TYR:HB2	1.69	0.91
1:A:151:VAL:CG1	4:A:703:FOL:C7	2.48	0.91
1:B:81:ARG:NE	5:B:704:NDP:O1X	2.04	0.91
1:A:402:ILE:HB	3:A:702:CB3:C15	2.01	0.90
1:B:402:ILE:HG21	3:B:702:CB3:C11	2.02	0.89
1:B:89:ARG:HA	1:B:92:ARG:HG3	1.56	0.88
1:A:489:CYS:SG	2:A:701:UMP:C5	2.68	0.87
1:B:156:LEU:HD12	5:B:704:NDP:C8A	2.03	0.87
1:A:40:LYS:HG2	1:A:97:ARG:HD3	1.57	0.86
1:B:23:LEU:HD21	5:B:704:NDP:C2N	2.05	0.86
1:A:470:ARG:HH21	2:B:701:UMP:P	1.98	0.85
2:A:701:UMP:P	1:B:470:ARG:NH2	2.49	0.85
1:A:27:HIS:CG	1:A:27:HIS:O	2.30	0.84
1:A:151:VAL:HG12	4:A:703:FOL:C7	2.03	0.84
1:A:9:VAL:HG23	1:A:171:ILE:HG12	1.60	0.83
1:A:344:ARG:NH2	2:A:701:UMP:P	2.47	0.83
1:B:427:PRO:HD2	1:B:484:MET:HG2	1.59	0.82
1:B:229:PRO:O	1:B:230:ILE:HB	1.78	0.82
1:B:244:ASP:HB2	1:B:570:PRO:HG3	1.62	0.81
1:A:344:ARG:NH2	2:A:701:UMP:C5'	2.44	0.81
1:B:344:ARG:HG3	1:B:345:THR:N	1.97	0.80
1:B:156:LEU:CD1	5:B:704:NDP:C8A	2.59	0.80
1:B:402:ILE:HB	3:B:702:CB3:C15	2.12	0.80
1:B:402:ILE:HG21	3:B:702:CB3:C12	2.11	0.80
1:B:138:GLU:HA	1:B:142:LYS:HB2	1.64	0.80
1:B:76:ALA:HB3	1:B:148:ILE:HG22	1.64	0.80
1:A:375:TRP:CH2	1:A:379:LEU:HD22	2.17	0.79
1:B:87:MET:CE	4:B:703:FOL:C16	2.60	0.79
1:A:344:ARG:HH22	2:A:701:UMP:H5''	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:VAL:HG12	4:B:703:FOL:HN1	1.45	0.78
1:A:233:SER:O	1:A:234:LYS:HB3	1.84	0.78
1:A:521:ASN:OD1	2:A:701:UMP:N3	2.16	0.77
1:A:22:GLY:O	5:A:704:NDP:O2D	2.02	0.77
1:B:87:MET:HE1	4:B:703:FOL:C11	2.14	0.77
1:B:87:MET:CE	4:B:703:FOL:C11	2.61	0.77
1:B:227:TYR:HB3	1:B:248:LEU:HB3	1.67	0.77
1:A:8:VAL:HG22	4:A:703:FOL:N1	2.00	0.76
1:B:489:CYS:SG	2:B:701:UMP:C6	2.79	0.76
1:A:489:CYS:SG	2:A:701:UMP:N1	2.58	0.76
1:B:510:ARG:NH2	2:B:701:UMP:OP1	2.20	0.74
1:B:402:ILE:CB	3:B:702:CB3:C15	2.65	0.74
1:B:560:LEU:O	1:B:561:LYS:HB3	1.87	0.74
1:A:344:ARG:HH22	2:A:701:UMP:C5'	2.02	0.73
1:B:322:HIS:O	1:B:323:GLU:HB2	1.87	0.73
1:A:84:TRP:CH2	1:A:92:ARG:O	2.42	0.72
1:B:81:ARG:HE	5:B:704:NDP:P2B	2.11	0.72
1:A:558:GLU:N	1:A:558:GLU:CD	2.42	0.72
2:A:701:UMP:P	1:B:470:ARG:HH22	2.12	0.72
1:B:510:ARG:NH1	2:B:701:UMP:OP1	2.19	0.72
1:B:140:GLU:O	1:B:141:TYR:HB2	1.89	0.71
1:B:8:VAL:HG12	4:B:703:FOL:N1	2.05	0.71
1:B:402:ILE:HG21	3:B:702:CB3:C16	2.09	0.70
1:B:94:LEU:HB2	1:B:99:ASN:HD21	1.55	0.70
1:B:87:MET:HE3	4:B:703:FOL:C15	2.21	0.70
1:B:193:LEU:HD11	1:B:601:HIS:HA	1.72	0.70
1:A:580:GLU:CD	1:A:580:GLU:H	1.95	0.69
1:A:533:ALA:HB1	1:A:540:PRO:HD3	1.74	0.69
1:B:233:SER:O	1:B:234:LYS:HB3	1.92	0.69
1:B:87:MET:HE3	4:B:703:FOL:C14	2.23	0.69
1:A:469:ARG:HB2	1:B:510:ARG:NH2	2.07	0.69
1:A:436:PHE:CZ	1:A:477:ASN:HB2	2.28	0.69
1:B:9:VAL:CG2	1:B:171:ILE:HG12	2.22	0.68
1:B:9:VAL:HG23	1:B:171:ILE:HG12	1.76	0.68
1:A:344:ARG:CZ	2:A:701:UMP:OP3	2.41	0.68
1:B:507:MET:HB2	1:B:525:TYR:CD2	2.29	0.68
1:B:91:PHE:CE1	4:B:703:FOL:O	2.47	0.68
1:A:151:VAL:HG13	4:A:703:FOL:C7	2.23	0.68
1:A:107:LYS:HD2	1:A:108:GLU:HG3	1.74	0.68
1:A:402:ILE:HG22	3:A:702:CB3:C16	2.23	0.68
1:B:381:GLU:OE1	1:B:520:PHE:HE1	1.77	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ARG:HD3	1:A:244:ASP:OD1	1.95	0.67
1:B:10:ALA:O	1:B:25:TRP:HZ2	1.76	0.67
1:B:389:ASP:OD2	1:B:394:HIS:ND1	2.26	0.67
1:A:190:ASP:O	1:A:191:ASP:HB2	1.95	0.67
1:B:344:ARG:HG3	1:B:345:THR:H	1.58	0.67
1:A:296:TRP:CZ2	1:B:34:HIS:HB2	2.29	0.67
1:A:505:CYS:SG	1:A:506:ILE:N	2.68	0.67
1:B:94:LEU:HB2	1:B:99:ASN:ND2	2.10	0.67
1:A:589:THR:O	1:A:591:GLU:N	2.28	0.66
1:B:589:THR:O	1:B:591:GLU:N	2.28	0.66
1:A:107:LYS:HG2	1:A:126:VAL:HB	1.78	0.66
1:B:510:ARG:HG3	1:B:511:SER:N	2.10	0.66
1:A:84:TRP:HH2	1:A:92:ARG:O	1.78	0.66
1:B:313:ALA:O	1:B:320:ARG:NH1	2.28	0.66
1:A:18:GLY:HA3	5:A:704:NDP:H1D	1.75	0.66
1:B:151:VAL:HB	4:B:703:FOL:H7	1.78	0.66
1:B:23:LEU:HD13	1:B:25:TRP:CZ3	2.30	0.66
1:A:287:ALA:O	1:A:290:ILE:HD13	1.94	0.66
1:A:427:PRO:HD2	1:A:484:MET:HG2	1.78	0.66
1:A:502:GLU:HB3	1:A:541:LYS:HB2	1.78	0.66
1:A:528:LEU:O	1:A:531:MET:HB2	1.94	0.66
1:A:138:GLU:HA	1:A:142:LYS:HG2	1.78	0.65
1:B:89:ARG:HA	1:B:92:ARG:CG	2.24	0.65
1:B:35:PHE:CE2	4:B:703:FOL:C12	2.74	0.65
1:A:382:LEU:HD11	1:A:528:LEU:HD13	1.79	0.65
1:B:6:CYS:SG	1:B:168:HIS:HB2	2.36	0.65
1:B:433:TRP:HZ2	1:B:525:TYR:HH	1.44	0.65
1:B:402:ILE:HG21	3:B:702:CB3:C13	2.26	0.65
1:B:5:VAL:CG2	1:B:6:CYS:N	2.60	0.65
1:A:358:ARG:HB2	1:A:544:ILE:HG12	1.80	0.64
1:B:42:THR:O	1:B:43:PRO:C	2.35	0.64
1:A:233:SER:OG	1:A:244:ASP:HB2	1.98	0.64
1:B:19:ILE:HG13	1:B:181:ASP:OD2	1.96	0.64
1:A:162:SER:O	1:A:164:GLY:N	2.30	0.64
1:A:181:ASP:OD1	1:A:182:VAL:HG23	1.98	0.64
1:B:166:ALA:O	1:B:167:SER:HB3	1.98	0.64
1:A:9:VAL:CG2	1:A:171:ILE:HG12	2.27	0.64
1:B:371:LYS:HG2	1:B:563:GLN:NE2	2.14	0.63
1:A:521:ASN:CG	3:A:702:CB3:CP3	2.67	0.63
1:B:358:ARG:HB2	1:B:544:ILE:HG12	1.79	0.63
1:B:154:ALA:O	5:B:704:NDP:O1A	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:SER:OG	1:B:469:ARG:HD2	1.98	0.63
1:A:94:LEU:HB2	1:A:99:ASN:ND2	2.06	0.63
1:B:397:GLU:O	1:B:397:GLU:CD	2.36	0.62
1:A:470:ARG:NH2	2:B:701:UMP:P	2.69	0.62
1:B:8:VAL:HG11	1:B:35:PHE:HD1	1.63	0.62
1:B:531:MET:HB3	1:B:588:PHE:CE2	2.34	0.62
1:B:167:SER:O	1:B:249:GLU:HA	1.99	0.62
1:A:508:TYR:HD2	1:B:508:TYR:HD2	1.48	0.62
1:A:368:LEU:HD22	1:A:368:LEU:H	1.64	0.61
1:A:438:ALA:HB1	1:A:450:GLN:HE21	1.64	0.61
1:A:455:LEU:HD22	1:A:473:MET:SD	2.40	0.61
1:A:489:CYS:HB3	1:A:509:GLN:HE21	1.65	0.61
1:A:291:ALA:HA	1:A:294:LEU:HD12	1.82	0.61
1:B:233:SER:O	1:B:234:LYS:CB	2.49	0.61
1:B:391:ASN:HB2	1:B:443:MET:HB2	1.82	0.61
1:B:5:VAL:HG23	1:B:6:CYS:H	1.65	0.61
1:A:13:PRO:HG3	1:A:175:ALA:HA	1.82	0.61
1:A:290:ILE:O	1:A:290:ILE:HG12	2.01	0.61
1:A:536:CYS:O	1:A:537:ASN:HB3	2.01	0.60
1:B:91:PHE:CE1	4:B:703:FOL:HA	2.36	0.60
1:A:228:ARG:HG3	1:A:251:ARG:HG3	1.83	0.60
1:B:14:LYS:O	1:B:15:ARG:HB2	2.01	0.60
1:B:368:LEU:HD22	1:B:368:LEU:H	1.65	0.60
1:B:514:VAL:HB	1:B:552:VAL:HG23	1.82	0.60
1:B:402:ILE:HG21	3:B:702:CB3:C15	2.26	0.60
1:B:138:GLU:CA	1:B:142:LYS:HB2	2.32	0.60
1:B:166:ALA:O	1:B:167:SER:CB	2.50	0.60
1:A:331:ILE:HD13	1:A:560:LEU:HD22	1.82	0.60
1:A:34:HIS:HB2	1:B:296:TRP:CZ2	2.37	0.59
1:A:384:TRP:NE1	1:A:389:ASP:HB3	2.16	0.59
1:B:140:GLU:N	1:B:140:GLU:OE1	2.35	0.59
1:B:509:GLN:NE2	1:B:512:CYS:SG	2.75	0.59
1:A:431:PHE:CE2	1:A:440:TYR:HD2	2.19	0.59
1:B:154:ALA:HB3	5:B:704:NDP:O1N	2.03	0.59
1:B:505:CYS:SG	1:B:506:ILE:N	2.75	0.59
1:B:39:THR:O	1:B:75:ASN:HB2	2.03	0.59
1:B:493:CYS:HB3	1:B:525:TYR:HE2	1.68	0.59
1:A:402:ILE:CG2	3:A:702:CB3:C16	2.81	0.58
1:B:560:LEU:O	1:B:561:LYS:CB	2.50	0.58
1:A:233:SER:O	1:A:234:LYS:CB	2.51	0.58
1:A:27:HIS:CD2	1:A:27:HIS:O	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LYS:N	1:A:4:PRO:HD3	2.18	0.58
1:A:287:ALA:O	1:A:290:ILE:CD1	2.52	0.57
1:A:525:TYR:O	1:A:529:THR:OG1	2.21	0.57
1:A:154:ALA:HB3	5:A:704:NDP:O1N	2.04	0.57
1:A:402:ILE:HG22	3:A:702:CB3:C11	2.34	0.57
1:B:531:MET:O	1:B:535:VAL:HG22	2.04	0.57
1:B:334:ILE:O	1:B:350:ILE:HG22	2.05	0.57
1:B:510:ARG:CZ	2:B:701:UMP:OP1	2.52	0.57
1:A:521:ASN:HD21	3:A:702:CB3:CP3	2.12	0.57
1:B:131:PRO:HA	1:B:134:LEU:HD12	1.86	0.57
1:A:17:ILE:HD11	1:A:154:ALA:HB2	1.86	0.57
1:A:517:GLY:O	1:A:520:PHE:HB3	2.04	0.57
1:A:330:LEU:O	1:A:334:ILE:HG13	2.04	0.57
1:B:344:ARG:HD3	2:B:701:UMP:OP3	2.05	0.57
1:B:433:TRP:HZ2	1:B:525:TYR:OH	1.87	0.57
1:B:508:TYR:C	1:B:508:TYR:CD1	2.79	0.57
1:B:10:ALA:O	1:B:25:TRP:CZ2	2.57	0.56
1:B:15:ARG:HD2	1:B:184:PHE:HB3	1.87	0.56
1:B:421:GLU:O	1:B:422:VAL:C	2.43	0.56
1:B:402:ILE:HG21	3:B:702:CB3:C14	2.35	0.56
1:A:241:VAL:HG12	1:A:243:TYR:HD2	1.69	0.56
1:B:15:ARG:HB3	1:B:184:PHE:HB3	1.87	0.56
1:B:81:ARG:CD	5:B:704:NDP:O1X	2.52	0.56
1:A:138:GLU:HA	1:A:142:LYS:CG	2.35	0.56
1:B:330:LEU:O	1:B:334:ILE:HD12	2.05	0.56
1:B:384:TRP:NE1	1:B:389:ASP:HB3	2.20	0.56
1:A:556:HIS:CD2	1:A:606:MET:HB3	2.40	0.56
1:A:370:THR:HG23	1:A:563:GLN:NE2	2.20	0.56
1:A:474:THR:HG21	1:B:476:TRP:O	2.06	0.56
1:B:136:LEU:O	1:B:141:TYR:HB2	2.06	0.56
1:B:322:HIS:O	1:B:323:GLU:CB	2.52	0.56
1:B:461:MET:SD	1:B:468:ASP:OD2	2.63	0.56
1:B:381:GLU:OE1	1:B:520:PHE:CE1	2.59	0.56
1:B:241:VAL:HG12	1:B:243:TYR:HD2	1.71	0.56
1:A:11:MET:SD	1:A:15:ARG:HG2	2.46	0.56
1:A:407:VAL:O	1:A:422:VAL:HG13	2.06	0.55
1:A:90:LYS:NZ	1:A:90:LYS:H	2.04	0.55
1:B:491:LEU:HD21	1:B:510:ARG:HB3	1.87	0.55
1:A:356:THR:HA	1:A:545:HIS:O	2.07	0.55
1:A:370:THR:HG23	1:A:563:GLN:HE21	1.72	0.55
1:B:390:THR:HG21	1:B:440:TYR:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:PRO:O	1:A:28:LEU:HD23	2.07	0.55
1:A:312:ARG:HG2	1:A:313:ALA:H	1.71	0.55
1:A:463:ARG:HH12	1:A:584:GLU:CD	2.09	0.55
1:B:454:GLN:NE2	1:B:474:THR:O	2.37	0.55
1:A:229:PRO:HB2	1:A:317:VAL:HG22	1.89	0.55
1:A:34:HIS:HA	1:B:296:TRP:NE1	2.21	0.55
1:A:107:LYS:HD2	1:A:108:GLU:CG	2.36	0.55
1:A:35:PHE:CE2	4:A:703:FOL:H12	2.42	0.55
1:B:390:THR:HG21	1:B:440:TYR:HE2	1.72	0.55
1:B:556:HIS:CD2	1:B:606:MET:HB3	2.42	0.55
1:A:111:ILE:O	1:A:112:ALA:HB3	2.08	0.54
1:B:458:VAL:HG11	1:B:495:PHE:CE2	2.43	0.54
1:B:455:LEU:HD21	1:B:585:ILE:HG21	1.88	0.54
1:B:87:MET:HE2	4:B:703:FOL:C16	2.38	0.54
1:A:90:LYS:HZ1	1:A:90:LYS:H	1.54	0.54
1:B:531:MET:HB3	1:B:588:PHE:HE2	1.71	0.54
1:A:384:TRP:CE2	1:A:389:ASP:HB3	2.43	0.54
1:B:491:LEU:CD2	1:B:510:ARG:HB3	2.38	0.54
1:A:110:ASP:O	1:A:113:ALA:HB3	2.08	0.53
1:A:9:VAL:HG11	1:A:184:PHE:CE2	2.43	0.53
1:B:11:MET:SD	1:B:15:ARG:HA	2.49	0.53
1:B:119:GLU:HG3	1:B:121:GLN:HG3	1.90	0.53
1:B:3:LYS:N	1:B:4:PRO:HD3	2.24	0.53
1:A:11:MET:O	1:A:174:VAL:HB	2.08	0.53
1:A:169:LEU:HD12	1:A:248:LEU:HD12	1.90	0.53
1:A:415:ARG:HH11	1:A:487:PRO:HD3	1.74	0.53
1:B:510:ARG:HG3	1:B:511:SER:H	1.72	0.53
1:A:138:GLU:HA	1:A:142:LYS:CB	2.39	0.53
1:A:521:ASN:CG	3:A:702:CB3:HP3	2.28	0.53
1:B:156:LEU:HD12	5:B:704:NDP:C5A	2.36	0.53
1:A:521:ASN:OD1	2:A:701:UMP:C4	2.61	0.53
1:B:335:ILE:HA	1:B:350:ILE:HG21	1.91	0.53
1:A:558:GLU:N	1:A:558:GLU:OE2	2.41	0.52
1:A:374:PHE:O	1:A:378:VAL:CG1	2.57	0.52
1:A:461:MET:SD	1:A:468:ASP:OD2	2.66	0.52
1:A:521:ASN:ND2	3:A:702:CB3:CP2	2.70	0.52
1:A:514:VAL:HB	1:A:552:VAL:HG12	1.92	0.52
1:B:22:GLY:O	5:B:704:NDP:O2D	2.19	0.52
1:A:10:ALA:HA	1:A:172:THR:HB	1.91	0.52
1:B:507:MET:HB2	1:B:525:TYR:HD2	1.71	0.52
1:B:156:LEU:HD13	5:B:704:NDP:C8A	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:VAL:CG2	1:B:6:CYS:H	2.23	0.52
1:B:87:MET:HE3	4:B:703:FOL:C13	2.39	0.52
1:A:433:TRP:CD1	1:A:473:MET:HG2	2.45	0.51
1:B:497:VAL:HG12	1:B:498:ASN:O	2.10	0.51
1:B:569:ARG:HD2	1:B:599:VAL:O	2.09	0.51
1:B:165:VAL:O	1:B:166:ALA:HB2	2.10	0.51
1:A:521:ASN:HD21	3:A:702:CB3:CP2	2.23	0.51
1:B:525:TYR:O	1:B:529:THR:OG1	2.29	0.51
1:A:227:TYR:HB3	1:A:248:LEU:HB3	1.92	0.51
1:B:168:HIS:O	1:B:169:LEU:HD23	2.10	0.51
1:B:326:GLN:O	1:B:330:LEU:HB2	2.11	0.51
1:B:8:VAL:HB	1:B:151:VAL:HG12	1.92	0.51
1:A:107:LYS:HD2	1:A:108:GLU:CD	2.30	0.51
1:A:430:GLY:HA2	1:A:433:TRP:HB2	1.93	0.51
1:A:508:TYR:CD2	1:B:508:TYR:HD2	2.28	0.51
1:B:533:ALA:HB1	1:B:540:PRO:HD3	1.91	0.51
1:B:87:MET:HE3	4:B:703:FOL:C16	2.37	0.51
1:A:249:GLU:OE2	1:A:251:ARG:HD3	2.11	0.51
1:B:158:GLU:HB3	1:B:185:PRO:HG3	1.93	0.51
1:B:28:LEU:O	1:B:32:PHE:HD1	1.93	0.51
1:A:427:PRO:O	1:A:432:GLN:HG2	2.10	0.51
1:B:559:ALA:HB1	1:B:604:ILE:HG21	1.93	0.51
1:B:472:LEU:HG	1:B:494:GLN:HG3	1.92	0.50
1:B:543:PHE:C	1:B:543:PHE:CD1	2.85	0.50
1:B:87:MET:HE1	4:B:703:FOL:C12	2.41	0.50
1:B:402:ILE:CG2	3:B:702:CB3:C14	2.89	0.50
1:B:505:CYS:O	1:B:544:ILE:N	2.45	0.50
1:B:578:ASN:O	1:B:582:ILE:HD12	2.12	0.50
1:A:474:THR:HB	1:B:476:TRP:CD1	2.47	0.50
1:A:589:THR:C	1:A:591:GLU:H	2.14	0.50
1:B:9:VAL:HG21	1:B:171:ILE:HG12	1.93	0.50
1:A:173:ARG:HD2	1:A:246:VAL:CG1	2.42	0.49
1:A:344:ARG:NH2	2:A:701:UMP:O5'	2.44	0.49
1:A:375:TRP:O	1:A:378:VAL:HG13	2.12	0.49
1:A:344:ARG:NH2	2:A:701:UMP:H5''	2.13	0.49
1:B:7:LEU:HD13	1:B:157:TYR:HD1	1.77	0.49
2:A:701:UMP:P	1:B:469:ARG:HH21	2.34	0.49
1:B:87:MET:CE	4:B:703:FOL:C12	2.90	0.49
1:A:232:ILE:HD12	1:A:325:PHE:HZ	1.77	0.49
1:A:580:GLU:O	1:A:583:LYS:NZ	2.44	0.49
1:A:344:ARG:NE	2:A:701:UMP:OP3	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:PHE:HE2	4:B:703:FOL:HN	1.61	0.49
1:B:508:TYR:C	1:B:508:TYR:HD1	2.16	0.49
1:A:402:ILE:CG2	3:A:702:CB3:C11	2.91	0.49
1:B:561:LYS:HA	1:B:564:LEU:HG	1.94	0.49
1:A:330:LEU:O	1:A:330:LEU:HD22	2.12	0.49
1:B:374:PHE:O	1:B:378:VAL:HG23	2.13	0.49
1:A:441:LYS:N	1:A:447:TYR:OH	2.46	0.49
1:A:455:LEU:HD13	1:A:473:MET:SD	2.53	0.48
1:B:527:LEU:O	1:B:531:MET:HG3	2.12	0.48
1:A:604:ILE:HG22	1:A:606:MET:HG3	1.94	0.48
1:B:512:CYS:O	1:B:551:HIS:CE1	2.66	0.48
1:B:331:ILE:HD13	1:B:560:LEU:HD22	1.94	0.48
1:A:22:GLY:C	5:A:704:NDP:HO2N	2.11	0.48
1:A:490:HIS:HD2	2:A:701:UMP:O4	1.96	0.48
1:B:409:ARG:HD2	1:B:422:VAL:HG22	1.95	0.48
1:A:291:ALA:N	1:A:292:PRO:HD2	2.28	0.48
1:B:91:PHE:HE1	4:B:703:FOL:HA	1.78	0.48
1:A:313:ALA:HB3	1:A:320:ARG:HH22	1.78	0.48
1:A:517:GLY:O	1:A:521:ASN:N	2.44	0.48
1:B:34:HIS:O	1:B:38:VAL:HG23	2.13	0.48
1:A:474:THR:HB	1:B:476:TRP:HD1	1.77	0.48
1:A:229:PRO:HG2	1:A:316:HIS:CD2	2.49	0.48
1:B:15:ARG:HH21	1:B:15:ARG:CB	2.25	0.48
1:B:514:VAL:HB	1:B:552:VAL:CG2	2.42	0.48
1:B:10:ALA:HA	1:B:172:THR:HB	1.96	0.48
1:B:102:VAL:HA	1:B:127:CYS:HB3	1.94	0.48
1:B:10:ALA:HB2	4:B:703:FOL:C2	2.44	0.48
1:A:480:ALA:O	1:A:482:ASP:N	2.47	0.48
1:B:361:LEU:HD23	1:B:366:PRO:HD3	1.95	0.48
1:B:40:LYS:O	1:B:41:THR:HG23	2.13	0.48
1:B:91:PHE:CD1	4:B:703:FOL:HA	2.49	0.48
1:A:31:ASP:OD2	4:A:703:FOL:N3	2.47	0.47
1:A:11:MET:SD	1:A:15:ARG:HA	2.54	0.47
1:A:312:ARG:HG2	1:A:313:ALA:N	2.29	0.47
2:A:701:UMP:OP3	1:B:469:ARG:NH2	2.33	0.47
1:B:75:ASN:HA	1:B:145:VAL:HG23	1.95	0.47
1:B:13:PRO:HD3	1:B:174:VAL:O	2.15	0.47
1:B:296:TRP:O	1:B:299:GLU:HB2	2.14	0.47
1:B:7:LEU:HD13	1:B:157:TYR:CD1	2.50	0.47
1:B:192:ILE:HD12	1:B:193:LEU:H	1.80	0.47
1:B:26:PRO:O	1:B:27:HIS:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:LEU:H	1:B:368:LEU:CD2	2.26	0.47
1:A:459:ILE:HG22	1:A:463:ARG:NE	2.29	0.47
1:B:518:VAL:O	1:B:522:ILE:HG13	2.15	0.47
1:A:469:ARG:HB2	1:B:510:ARG:HH22	1.76	0.47
1:A:5:VAL:HG22	1:A:6:CYS:N	2.29	0.47
1:B:409:ARG:HH11	1:B:422:VAL:HG22	1.80	0.47
1:A:327:TYR:CZ	1:A:331:ILE:HD11	2.49	0.47
1:A:22:GLY:N	5:A:704:NDP:O3D	2.46	0.47
1:B:234:LYS:O	1:B:236:PHE:CE1	2.68	0.47
1:B:441:LYS:N	1:B:447:TYR:OH	2.47	0.47
1:A:407:VAL:HG21	1:A:423:GLY:HA2	1.96	0.47
1:A:107:LYS:HA	1:A:126:VAL:HG21	1.97	0.47
1:A:354:GLY:HA2	1:A:547:MET:O	2.15	0.46
1:A:421:GLU:O	1:A:422:VAL:C	2.52	0.46
1:B:3:LYS:HG2	1:B:142:LYS:NZ	2.30	0.46
1:B:589:THR:C	1:B:591:GLU:H	2.18	0.46
1:A:231:PHE:HD2	1:B:290:ILE:HG23	1.81	0.46
1:A:326:GLN:OE1	1:A:357:MET:HB3	2.15	0.46
1:B:81:ARG:NH2	1:B:82:LYS:HD2	2.31	0.46
1:A:353:PHE:HB2	1:B:496:TYR:CE2	2.50	0.46
1:A:39:THR:HA	1:A:149:PHE:CE2	2.51	0.46
1:B:385:PHE:HB3	1:B:433:TRP:CZ3	2.50	0.46
1:B:88:PRO:HG2	1:B:91:PHE:HB2	1.97	0.46
1:A:237:SER:HA	1:A:241:VAL:O	2.14	0.46
1:B:151:VAL:HB	4:B:703:FOL:C7	2.43	0.46
1:B:299:GLU:O	1:B:301:ASP:HA	2.15	0.46
1:B:370:THR:O	1:B:566:ARG:HD3	2.16	0.46
1:B:232:ILE:HD12	1:B:325:PHE:HZ	1.81	0.46
1:B:474:THR:HA	1:B:492:LEU:HG	1.98	0.46
1:B:87:MET:CE	4:B:703:FOL:C15	2.88	0.46
1:A:14:LYS:O	1:A:15:ARG:HB2	2.15	0.46
1:A:544:ILE:HG22	1:A:545:HIS:N	2.30	0.46
1:B:489:CYS:SG	2:B:701:UMP:C5	3.08	0.46
1:A:299:GLU:O	1:A:301:ASP:HA	2.16	0.45
1:A:428:GLY:HA2	1:A:484:MET:SD	2.56	0.45
1:A:520:PHE:CD1	3:A:702:CB3:CP2	2.99	0.45
1:A:489:CYS:CB	2:A:701:UMP:C5	2.99	0.45
1:B:19:ILE:HB	1:B:180:CYS:HA	1.98	0.45
1:B:230:ILE:O	1:B:247:VAL:HB	2.16	0.45
1:B:356:THR:O	1:B:357:MET:HG2	2.16	0.45
1:A:19:ILE:HG13	1:A:181:ASP:OD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:PHE:HB3	1:A:452:VAL:HB	1.97	0.45
1:A:462:LEU:HG	1:A:471:MET:SD	2.56	0.45
1:B:586:ASP:C	1:B:588:PHE:H	2.19	0.45
1:A:294:LEU:O	1:A:298:ASP:HB2	2.15	0.45
1:A:407:VAL:HG11	1:A:423:GLY:O	2.17	0.45
1:B:356:THR:CG2	1:B:357:MET:N	2.80	0.45
1:B:380:GLU:HA	1:B:383:LEU:HD12	1.99	0.45
1:B:81:ARG:HD3	5:B:704:NDP:O1X	2.16	0.45
1:A:520:PHE:CE1	3:A:702:CB3:HP12	2.51	0.45
1:A:78:VAL:HG22	1:A:100:ILE:HB	1.99	0.45
1:B:188:PRO:O	1:B:190:ASP:N	2.50	0.45
1:A:344:ARG:HE	1:B:470:ARG:NH2	2.15	0.45
1:A:153:GLY:O	1:A:157:TYR:N	2.47	0.45
1:A:293:VAL:HA	1:A:296:TRP:CD1	2.52	0.45
1:A:40:LYS:HG2	1:A:97:ARG:CD	2.38	0.45
1:A:518:VAL:HB	1:A:519:PRO:HD3	1.99	0.45
1:A:344:ARG:HE	1:B:470:ARG:HH22	1.64	0.45
1:B:461:MET:HG2	1:B:471:MET:HG2	1.99	0.45
1:B:516:LEU:HD13	1:B:606:MET:HB2	1.99	0.45
1:A:26:PRO:O	1:A:27:HIS:C	2.55	0.45
4:A:703:FOL:C7	5:A:704:NDP:H42N	2.47	0.45
1:A:513:ASP:HB2	2:A:701:UMP:H2"	1.99	0.45
1:B:136:LEU:HD22	1:B:141:TYR:CD2	2.52	0.45
1:B:39:THR:OG1	1:B:97:ARG:NH1	2.48	0.45
1:A:454:GLN:NE2	1:A:474:THR:O	2.45	0.44
1:B:461:MET:O	1:B:465:ASN:N	2.50	0.44
1:A:518:VAL:O	1:A:522:ILE:HG13	2.16	0.44
1:B:356:THR:O	1:B:357:MET:CG	2.65	0.44
1:B:442:ASP:OD1	1:B:445:THR:N	2.48	0.44
1:A:3:LYS:N	1:A:4:PRO:CD	2.81	0.44
1:B:102:VAL:HG21	1:B:129:SER:HA	1.99	0.44
1:B:384:TRP:CD1	1:B:389:ASP:HB3	2.53	0.44
1:A:478:PRO:HD2	1:B:436:PHE:CE1	2.52	0.44
1:B:5:VAL:HG22	1:B:6:CYS:N	2.30	0.44
1:A:234:LYS:HD2	1:A:236:PHE:CE1	2.52	0.44
1:A:42:THR:C	1:A:43:PRO:O	2.56	0.44
1:A:469:ARG:NH1	2:B:701:UMP:OP3	2.51	0.44
1:A:375:TRP:O	1:A:376:LYS:C	2.56	0.44
1:B:138:GLU:O	1:B:140:GLU:N	2.50	0.44
1:B:173:ARG:HD2	1:B:246:VAL:CG1	2.48	0.44
1:A:5:VAL:HG22	1:A:6:CYS:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:HG21	1:A:35:PHE:HD1	1.83	0.44
1:A:111:ILE:O	1:A:112:ALA:CB	2.66	0.44
1:A:22:GLY:H	5:A:704:NDP:HO3N	1.65	0.44
1:A:558:GLU:O	1:A:561:LYS:HB2	2.18	0.44
1:B:453:ASP:O	1:B:454:GLN:C	2.56	0.44
1:A:580:GLU:CD	1:A:580:GLU:N	2.68	0.44
1:A:168:HIS:HA	1:A:248:LEU:O	2.18	0.43
1:B:136:LEU:HD22	1:B:141:TYR:HD2	1.82	0.43
1:B:40:LYS:HB3	1:B:97:ARG:HG3	1.98	0.43
1:A:130:LEU:HD22	1:A:156:LEU:HD22	2.00	0.43
1:A:462:LEU:HA	1:A:471:MET:HE1	1.99	0.43
1:A:78:VAL:HG22	1:A:100:ILE:HD12	1.98	0.43
1:B:526:SER:O	1:B:530:LEU:HD13	2.19	0.43
1:A:168:HIS:NE2	1:A:249:GLU:HG3	2.33	0.43
1:A:296:TRP:HB2	1:B:37:ARG:CZ	2.48	0.43
1:B:344:ARG:HG3	1:B:345:THR:HG23	2.00	0.43
1:A:539:LYS:HA	1:A:540:PRO:HD2	1.76	0.43
1:A:586:ASP:C	1:A:588:PHE:H	2.22	0.43
1:B:79:MET:HG2	1:B:101:VAL:HG22	2.00	0.43
1:B:78:VAL:HB	1:B:150:VAL:HG22	1.99	0.43
1:B:167:SER:HA	1:B:250:LYS:HB2	2.00	0.43
1:B:534:HIS:NE2	1:B:579:LYS:HB3	2.33	0.43
1:B:27:HIS:HE1	1:B:29:THR:HG23	1.83	0.43
1:A:141:TYR:O	1:A:144:SER:OG	2.27	0.43
1:A:373:VAL:HG12	1:A:374:PHE:N	2.33	0.43
1:B:5:VAL:N	1:B:166:ALA:O	2.43	0.43
1:B:293:VAL:HG12	1:B:297:MET:SD	2.59	0.43
1:B:91:PHE:CG	4:B:703:FOL:O	2.67	0.43
1:B:490:HIS:HD2	2:B:701:UMP:O4	2.02	0.43
1:A:375:TRP:O	1:A:377:GLY:N	2.52	0.42
1:A:233:SER:HB3	1:A:245:PHE:O	2.18	0.42
1:A:291:ALA:N	1:A:292:PRO:CD	2.83	0.42
1:B:462:LEU:CB	1:B:536:CYS:SG	3.07	0.42
1:A:374:PHE:CE1	1:A:376:LYS:HB3	2.54	0.42
1:A:523:ALA:O	1:A:524:SER:C	2.56	0.42
1:A:548:GLY:O	1:A:549:ASN:C	2.57	0.42
1:A:296:TRP:HB2	1:B:37:ARG:NH1	2.33	0.42
1:A:173:ARG:HD2	1:A:246:VAL:HG13	2.01	0.42
1:A:374:PHE:O	1:A:378:VAL:HG12	2.18	0.42
1:B:586:ASP:C	1:B:588:PHE:N	2.72	0.42
1:B:586:ASP:O	1:B:588:PHE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:PRO:O	1:A:28:LEU:N	2.52	0.42
1:B:168:HIS:HA	1:B:248:LEU:O	2.19	0.42
1:A:154:ALA:HB3	1:A:182:VAL:HG13	2.02	0.42
1:B:391:ASN:OD1	1:B:393:ASN:HB2	2.19	0.42
1:B:517:GLY:O	1:B:520:PHE:HB3	2.19	0.42
1:B:122:GLN:O	1:B:123:ARG:HB2	2.19	0.42
1:B:19:ILE:O	1:B:20:ASN:C	2.58	0.42
1:B:374:PHE:HD1	1:B:603:ARG:NH1	2.18	0.42
1:B:511:SER:OG	1:B:551:HIS:HE1	2.03	0.42
1:A:339:ARG:HH12	1:B:500:GLN:HG2	1.84	0.42
1:B:442:ASP:OD2	1:B:444:HIS:HD2	2.02	0.42
1:A:314:VAL:H	1:A:320:ARG:NH2	2.17	0.42
1:A:578:ASN:O	1:A:582:ILE:HD12	2.20	0.42
1:B:102:VAL:CG2	1:B:129:SER:HA	2.50	0.42
1:B:23:LEU:HD22	5:B:704:NDP:H2N	1.85	0.42
1:A:142:LYS:O	1:A:143:ASP:CG	2.59	0.41
1:A:382:LEU:HD23	1:A:527:LEU:HG	2.02	0.41
1:A:490:HIS:CD2	2:A:701:UMP:O4	2.73	0.41
1:A:81:ARG:HB3	1:A:81:ARG:HE	1.71	0.41
1:B:229:PRO:HB2	1:B:317:VAL:HG22	2.01	0.41
1:A:382:LEU:O	1:A:386:ILE:N	2.40	0.41
1:B:242:PRO:HB3	1:B:573:ILE:HG23	2.02	0.41
1:B:372:ARG:HD2	1:B:603:ARG:HG2	2.02	0.41
1:A:7:LEU:HG	1:A:150:VAL:HB	2.02	0.41
1:A:509:GLN:O	1:A:548:GLY:N	2.44	0.41
1:B:237:SER:HA	1:B:241:VAL:O	2.20	0.41
1:B:486:LEU:HA	1:B:487:PRO:HD3	1.90	0.41
1:A:586:ASP:C	1:A:588:PHE:N	2.74	0.41
1:B:78:VAL:HA	1:B:100:ILE:O	2.21	0.41
1:B:368:LEU:HD22	1:B:368:LEU:N	2.33	0.41
1:B:374:PHE:CE1	3:B:702:CB3:OE2	2.73	0.41
1:A:138:GLU:O	1:A:140:GLU:N	2.53	0.41
1:A:498:ASN:HB2	1:B:339:ARG:HG3	2.01	0.41
1:A:603:ARG:NH1	3:A:702:CB3:O2	2.53	0.41
1:A:81:ARG:HD2	1:A:85:GLU:OE2	2.21	0.41
1:B:382:LEU:O	1:B:386:ILE:N	2.48	0.41
1:B:433:TRP:CZ2	1:B:525:TYR:OH	2.63	0.41
1:B:378:VAL:HG11	1:B:523:ALA:HB3	2.01	0.41
1:A:138:GLU:HA	1:A:142:LYS:HB2	2.02	0.41
1:B:15:ARG:NH2	1:B:15:ARG:HB2	2.36	0.41
1:A:285:SER:OG	1:A:286:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:THR:HG21	1:A:569:ARG:O	2.21	0.41
1:A:555:ASN:HD21	1:A:607:GLU:HB2	1.85	0.41
1:B:481:LEU:H	1:B:481:LEU:HG	1.69	0.41
1:B:462:LEU:HB3	1:B:536:CYS:SG	2.60	0.41
1:A:327:TYR:CE2	1:A:331:ILE:HD11	2.55	0.41
1:A:372:ARG:HB3	1:A:603:ARG:HG2	2.03	0.41
1:A:539:LYS:C	1:A:539:LYS:HD2	2.41	0.41
1:A:576:ILE:HB	1:A:579:LYS:HE2	2.02	0.41
1:A:119:GLU:O	1:A:121:GLN:N	2.53	0.41
1:A:176:ARG:NH1	1:A:178:PHE:HE1	2.18	0.41
1:A:453:ASP:O	1:A:454:GLN:C	2.58	0.41
1:B:3:LYS:N	1:B:4:PRO:CD	2.84	0.41
1:B:74:PHE:O	1:B:145:VAL:HA	2.21	0.41
1:B:520:PHE:CG	3:B:702:CB3:H13	2.56	0.40
3:A:702:CB3:H15	3:A:702:CB3:C6	2.51	0.40
1:B:173:ARG:NH1	1:B:570:PRO:HD3	2.37	0.40
1:A:19:ILE:HA	1:A:181:ASP:OD2	2.22	0.40
1:A:327:TYR:O	1:A:330:LEU:HB3	2.21	0.40
1:A:442:ASP:C	1:A:444:HIS:H	2.25	0.40
1:A:520:PHE:O	1:A:522:ILE:N	2.54	0.40
1:B:521:ASN:HD22	1:B:521:ASN:HA	1.76	0.40
1:A:190:ASP:O	1:A:191:ASP:CB	2.67	0.40
1:A:19:ILE:HB	1:A:180:CYS:HA	2.02	0.40
1:A:293:VAL:HA	1:A:296:TRP:HD1	1.87	0.40
1:A:469:ARG:HH11	2:B:701:UMP:P	2.44	0.40
1:A:489:CYS:HB2	2:A:701:UMP:C5	2.57	0.40
1:B:96:ASP:H	1:B:122:GLN:HE21	1.70	0.40
1:B:499:ASP:N	1:B:499:ASP:OD1	2.53	0.40
1:A:383:LEU:O	1:A:387:ARG:N	2.39	0.40
1:A:408:THR:O	1:A:409:ARG:C	2.59	0.40
1:A:459:ILE:HG22	1:A:463:ARG:CZ	2.51	0.40
1:A:432:GLN:HE22	1:A:477:ASN:HD22	1.70	0.40
1:B:403:TRP:C	1:B:405:LYS:H	2.24	0.40
1:A:476:TRP:O	1:B:474:THR:HG21	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	474/610 (78%)	379 (80%)	68 (14%)	27 (6%)	1	18
1	B	474/610 (78%)	385 (81%)	64 (14%)	25 (5%)	2	19
All	All	948/1220 (78%)	764 (81%)	132 (14%)	52 (6%)	2	19

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	PRO
1	A	92	ARG
1	A	128	ALA
1	A	165	VAL
1	A	313	ALA
1	A	376	LYS
1	A	481	LEU
1	A	524	SER
1	A	590	ALA
1	B	43	PRO
1	B	166	ALA
1	B	167	SER
1	B	189	GLY
1	B	229	PRO
1	B	234	LYS
1	B	422	VAL
1	B	590	ALA
1	A	27	HIS
1	A	93	PRO
1	A	191	ASP
1	A	422	VAL
1	A	429	TYR
1	A	443	MET
1	B	41	THR
1	B	141	TYR

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Mol	Chain	Res	Type
1	B	144	SER
1	B	287	ALA
1	B	323	GLU
1	B	561	LYS
1	A	121	GLN
1	A	375	TRP
1	A	489	CYS
1	A	592	ASP
1	B	424	ASP
1	B	587	ASP
1	A	234	LYS
1	A	396	SER
1	A	520	PHE
1	A	521	ASN
1	B	15	ARG
1	B	123	ARG
1	B	230	ILE
1	B	353	PHE
1	B	592	ASP
1	A	448	THR
1	B	231	PHE
1	B	314	VAL
1	B	605	GLN
1	A	15	ARG
1	A	185	PRO
1	B	489	CYS
1	A	557	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	433/525 (82%)	378 (87%)	55 (13%)	4	23
1	B	433/525 (82%)	377 (87%)	56 (13%)	4	22
All	All	866/1050 (82%)	755 (87%)	111 (13%)	4	23

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	9	VAL
1	A	23	LEU
1	A	25	TRP
1	A	27	HIS
1	A	40	LYS
1	A	44	GLU
1	A	90	LYS
1	A	107	LYS
1	A	111	ILE
1	A	125	ARG
1	A	141	TYR
1	A	142	LYS
1	A	143	ASP
1	A	156	LEU
1	A	162	SER
1	A	169	LEU
1	A	190	ASP
1	A	192	ILE
1	A	230	ILE
1	A	234	LYS
1	A	285	SER
1	A	290	ILE
1	A	302	ARG
1	A	310	LEU
1	A	330	LEU
1	A	340	THR
1	A	358	ARG
1	A	368	LEU
1	A	378	VAL
1	A	380	GLU
1	A	383	LEU
1	A	389	ASP
1	A	397	GLU
1	A	406	ASN
1	A	409	ARG
1	A	441	LYS
1	A	448	THR
1	A	455	LEU
1	A	462	LEU
1	A	465	ASN
1	A	470	ARG

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Mol	Chain	Res	Type
1	A	474	THR
1	A	482	ASP
1	A	492	LEU
1	A	510	ARG
1	A	512	CYS
1	A	529	THR
1	A	539	LYS
1	A	545	HIS
1	A	547	MET
1	A	558	GLU
1	A	567	GLU
1	A	580	GLU
1	A	583	LYS
1	B	5	VAL
1	B	9	VAL
1	B	25	TRP
1	B	29	THR
1	B	37	ARG
1	B	41	THR
1	B	44	GLU
1	B	82	LYS
1	B	87	MET
1	B	89	ARG
1	B	98	LEU
1	B	102	VAL
1	B	107	LYS
1	B	108	GLU
1	B	109	GLU
1	B	110	ASP
1	B	111	ILE
1	B	156	LEU
1	B	162	SER
1	B	181	ASP
1	B	192	ILE
1	B	193	LEU
1	B	249	GLU
1	B	302	ARG
1	B	318	HIS
1	B	320	ARG
1	B	344	ARG
1	B	368	LEU
1	B	376	LYS

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Mol	Chain	Res	Type
1	B	386	ILE
1	B	395	LEU
1	B	402	ILE
1	B	404	ASP
1	B	409	ARG
1	B	441	LYS
1	B	456	LYS
1	B	470	ARG
1	B	474	THR
1	B	491	LEU
1	B	492	LEU
1	B	493	CYS
1	B	505	CYS
1	B	508	TYR
1	B	526	SER
1	B	529	THR
1	B	535	VAL
1	B	539	LYS
1	B	543	PHE
1	B	545	HIS
1	B	547	MET
1	B	564	LEU
1	B	579	LYS
1	B	587	ASP
1	B	589	THR
1	B	599	VAL
1	B	603	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	406	ASN
1	A	450	GLN
1	A	465	ASN
1	A	490	HIS
1	A	545	HIS
1	B	27	HIS
1	B	99	ASN
1	B	168	HIS
1	B	406	ASN
1	B	444	HIS

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Mol	Chain	Res	Type
1	B	490	HIS
1	B	509	GLN
1	B	545	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	FOL	A	703	-	28,34,34	1.38	3 (10%)	36,47,47	2.06	8 (22%)
4	FOL	B	703	-	28,34,34	1.35	4 (14%)	36,47,47	2.25	7 (19%)
3	CB3	A	702	-	30,37,37	1.32	3 (10%)	38,51,51	2.68	8 (21%)
2	UMP	B	701	-	18,21,21	0.79	1 (5%)	21,31,31	1.26	3 (14%)
5	NDP	A	704	-	45,52,52	2.05	8 (17%)	53,80,80	2.28	6 (11%)
5	NDP	B	704	-	45,52,52	2.05	8 (17%)	53,80,80	2.22	7 (13%)
2	UMP	A	701	-	18,21,21	0.77	1 (5%)	21,31,31	1.16	2 (9%)
3	CB3	B	702	-	30,37,37	1.33	3 (10%)	38,51,51	2.59	11 (28%)

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	FOL	A	703	-	-	3/16/22/22	0/3/3/3
4	FOL	B	703	-	-	4/16/22/22	0/3/3/3
3	CB3	A	702	-	-	6/21/28/28	0/3/3/3
2	UMP	B	701	-	-	3/7/22/22	0/2/2/2
5	NDP	A	704	-	-	3/30/77/77	0/5/5/5
5	NDP	B	704	-	-	3/30/77/77	0/5/5/5
2	UMP	A	701	-	-	3/7/22/22	0/2/2/2
3	CB3	B	702	-	-	5/21/28/28	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	NDP	C6N-C5N	8.29	1.48	1.33
5	A	704	NDP	C6N-C5N	8.15	1.47	1.33
5	A	704	NDP	C2N-C3N	4.93	1.48	1.34
5	B	704	NDP	C2N-C3N	4.89	1.48	1.34
4	A	703	FOL	C4A-C8A	4.69	1.49	1.40
5	A	704	NDP	C7N-N7N	4.08	1.44	1.33
5	B	704	NDP	C3B-C2B	-4.07	1.43	1.52
4	B	703	FOL	C4A-C8A	4.02	1.48	1.40
5	A	704	NDP	C3B-C2B	-3.93	1.44	1.52
5	B	704	NDP	C7N-N7N	3.92	1.43	1.33
5	B	704	NDP	C6A-N6A	3.85	1.48	1.34
3	A	702	CB3	C4A-C8A	3.81	1.48	1.41
3	B	702	CB3	C4A-C8A	3.80	1.48	1.41
5	A	704	NDP	C6A-N6A	3.72	1.47	1.34
5	A	704	NDP	C2D-C3D	-3.24	1.44	1.53
5	B	704	NDP	C2D-C3D	-3.13	1.44	1.53
3	A	702	CB3	CP2-CP3	3.11	1.27	1.18
4	A	703	FOL	C7-N8	2.90	1.36	1.31
5	B	704	NDP	C6N-N1N	2.89	1.44	1.37
3	B	702	CB3	CP2-CP3	2.82	1.26	1.18
5	A	704	NDP	C6N-N1N	2.78	1.44	1.37
4	A	703	FOL	C4-C4A	2.75	1.46	1.41
4	B	703	FOL	C4-C4A	2.74	1.46	1.41
4	B	703	FOL	C7-N8	2.63	1.36	1.31
5	A	704	NDP	C2A-N3A	2.34	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	NDP	C2A-N3A	2.33	1.35	1.32
2	B	701	UMP	C2-N3	-2.31	1.33	1.38
2	A	701	UMP	C2-N3	-2.22	1.33	1.38
4	B	703	FOL	C7-C6	2.15	1.43	1.39
3	B	702	CB3	C8A-N1	-2.13	1.34	1.37
3	A	702	CB3	C8A-N1	-2.10	1.34	1.37

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	CB3	C4A-C4-N3	-10.43	117.13	124.40
3	A	702	CB3	C4A-C4-N3	-10.34	117.19	124.40
5	A	704	NDP	C1D-N1N-C2N	10.13	137.99	121.11
5	B	704	NDP	C1D-N1N-C2N	9.64	137.16	121.11
3	A	702	CB3	C4A-C8A-N1	-9.58	118.40	123.60
3	B	702	CB3	C4A-C8A-N1	-8.31	119.09	123.60
5	A	704	NDP	C1D-N1N-C6N	-7.92	103.77	120.83
4	B	703	FOL	N8-C8A-N1	7.45	124.33	115.82
5	B	704	NDP	C1D-N1N-C6N	-7.29	105.12	120.83
4	A	703	FOL	N8-C8A-N1	7.02	123.83	115.82
5	B	704	NDP	O4D-C1D-N1N	6.31	120.39	108.06
5	A	704	NDP	O4D-C1D-N1N	5.96	119.71	108.06
4	B	703	FOL	C2-N1-C8A	4.93	120.99	115.36
4	B	703	FOL	C4A-C4-N3	-4.77	116.91	123.43
5	A	704	NDP	N3A-C2A-N1A	-4.69	121.35	128.68
4	A	703	FOL	C4A-C4-N3	-4.66	117.06	123.43
5	B	704	NDP	N3A-C2A-N1A	-4.53	121.60	128.68
4	A	703	FOL	C2-N1-C8A	4.21	120.16	115.36
4	B	703	FOL	C4-N3-C2	3.98	122.25	115.93
4	A	703	FOL	C4-N3-C2	3.96	122.22	115.93
4	B	703	FOL	CA-N-C	3.81	127.26	122.34
3	A	702	CB3	C4-N3-C2	3.49	121.48	115.93
3	B	702	CB3	C4-N3-C2	3.36	121.27	115.93
5	A	704	NDP	C3N-C2N-N1N	-3.35	118.31	123.10
4	B	703	FOL	N1-C2-N3	-3.26	122.88	127.22
5	B	704	NDP	C3N-C2N-N1N	-3.06	118.73	123.10
3	A	702	CB3	C11-C-N	2.82	122.47	117.06
4	A	703	FOL	N1-C2-N3	-2.81	123.48	127.22
3	A	702	CB3	O-C-C11	-2.70	116.13	120.94
3	A	702	CB3	N1-C2-N3	-2.65	123.68	127.22
3	B	702	CB3	CP1-N10-C9	-2.63	114.60	117.10
3	B	702	CB3	C6-C5-C4A	-2.52	118.88	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	CB3	O-C-C11	-2.47	116.53	120.94
3	A	702	CB3	C6-C5-C4A	-2.44	119.00	122.65
3	B	702	CB3	N1-C2-N3	-2.44	123.97	127.22
3	B	702	CB3	CB-CA-N	2.43	113.73	110.19
4	B	703	FOL	C4A-C8A-N1	-2.43	117.73	121.80
2	B	701	UMP	O5'-C5'-C4'	2.36	117.12	108.99
4	A	703	FOL	CB-CG-CD	-2.33	108.58	113.59
4	A	703	FOL	CA-N-C	2.29	125.30	122.34
3	A	702	CB3	C8-C8A-N1	2.29	122.18	118.69
2	A	701	UMP	O5'-C5'-C4'	2.24	116.72	108.99
3	B	702	CB3	C11-C-N	2.24	121.36	117.06
3	B	702	CB3	CB-CG-CD	-2.24	108.78	113.59
5	A	704	NDP	PN-O3-PA	-2.19	125.32	132.83
2	A	701	UMP	O4'-C4'-C5'	2.10	116.27	109.37
2	B	701	UMP	O4'-C4'-C5'	2.07	116.19	109.37
5	B	704	NDP	PN-O3-PA	-2.04	125.83	132.83
2	B	701	UMP	OP3-P-OP2	2.02	115.37	107.64
3	B	702	CB3	C7-C8-C8A	-2.02	118.29	120.84
4	A	703	FOL	C4-C4A-C8A	-2.01	118.62	119.95
5	B	704	NDP	C4A-C5A-N7A	-2.01	107.31	109.40

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	703	FOL	N-CA-CB-CG
4	A	703	FOL	CT-CA-CB-CG
4	A	703	FOL	CA-CB-CG-CD
4	B	703	FOL	N-CA-CB-CG
4	B	703	FOL	CT-CA-CB-CG
4	B	703	FOL	CA-CB-CG-CD
3	A	702	CB3	CB-CA-N-C
3	A	702	CB3	CT-CA-N-C
3	A	702	CB3	CT-CA-CB-CG
2	B	701	UMP	C5'-O5'-P-OP1
2	A	701	UMP	C5'-O5'-P-OP1
2	A	701	UMP	C5'-O5'-P-OP2
3	B	702	CB3	CB-CA-N-C
3	B	702	CB3	CT-CA-N-C
3	B	702	CB3	CT-CA-CB-CG
3	B	702	CB3	N-CA-CB-CG
3	A	702	CB3	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
3	B	702	CB3	CA-CB-CG-CD
5	A	704	NDP	O4D-C4D-C5D-O5D
5	A	704	NDP	C3D-C4D-C5D-O5D
3	A	702	CB3	N-CA-CB-CG
2	B	701	UMP	C5'-O5'-P-OP2
5	B	704	NDP	O4D-C4D-C5D-O5D
5	B	704	NDP	C3D-C4D-C5D-O5D
5	B	704	NDP	O4D-C1D-N1N-C2N
5	A	704	NDP	O4D-C1D-N1N-C2N
2	B	701	UMP	C5'-O5'-P-OP3
2	A	701	UMP	C5'-O5'-P-OP3
3	A	702	CB3	C6-C9-N10-C14
4	B	703	FOL	CT-CA-N-C

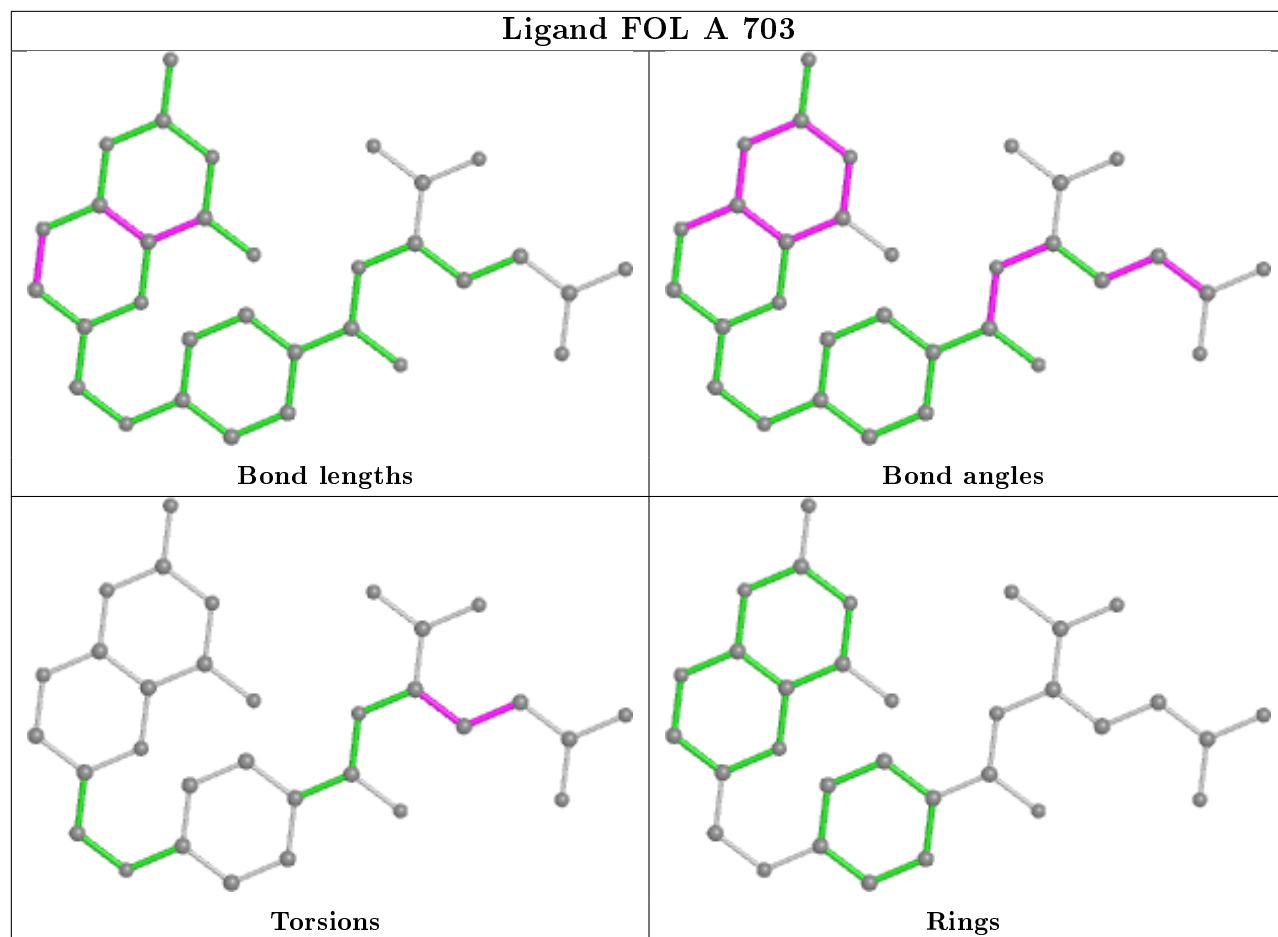
There are no ring outliers.

8 monomers are involved in 132 short contacts:

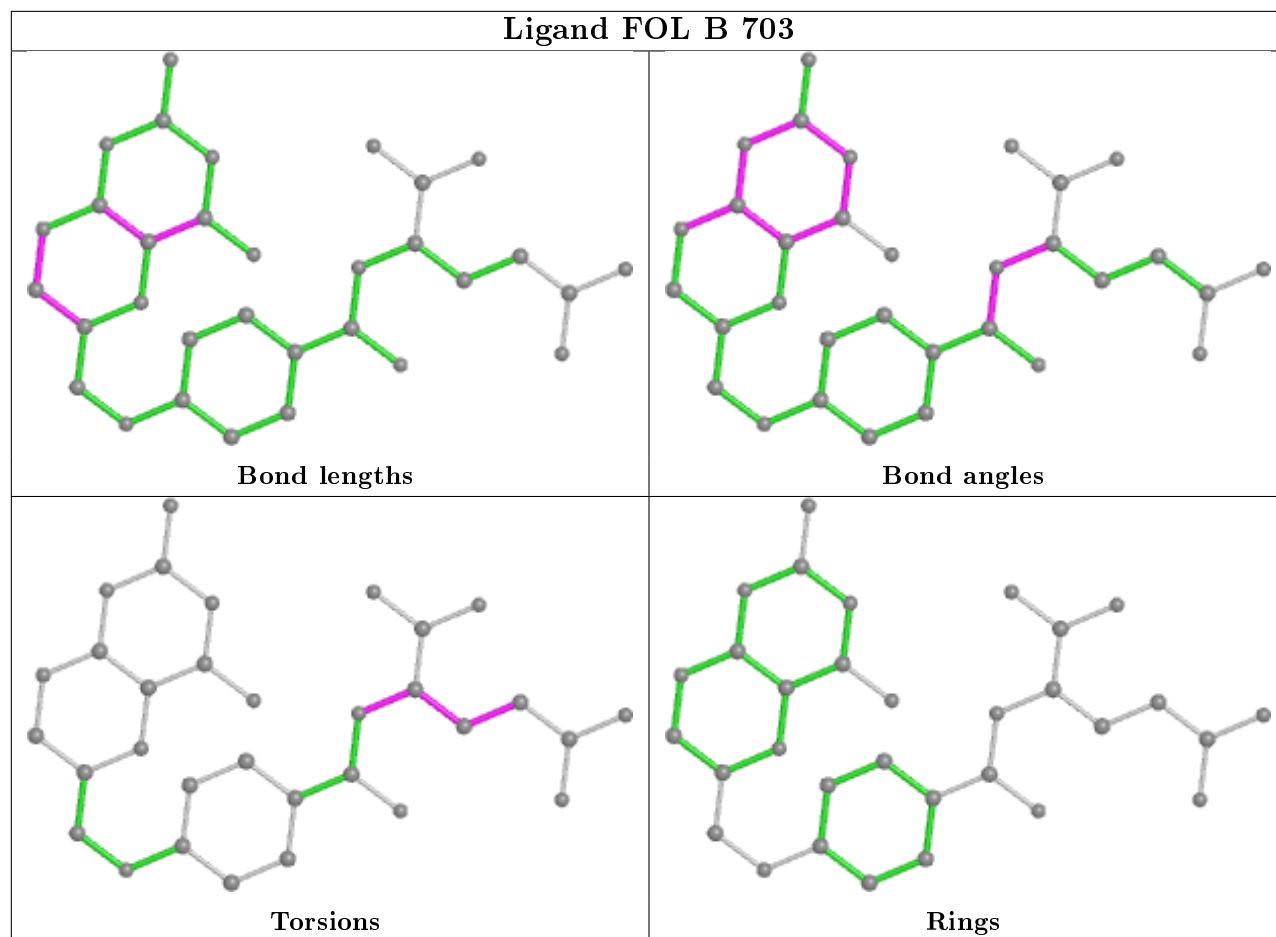
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	FOL	10	0
4	B	703	FOL	26	0
3	A	702	CB3	15	0
2	B	701	UMP	15	0
5	A	704	NDP	8	0
5	B	704	NDP	16	0
2	A	701	UMP	25	0
3	B	702	CB3	18	0

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.

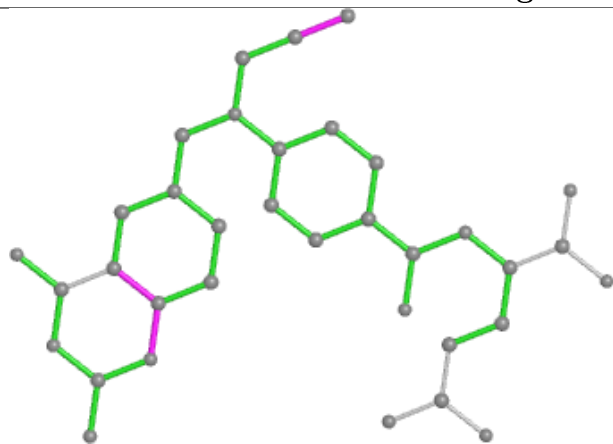
Ligand FOL A 703



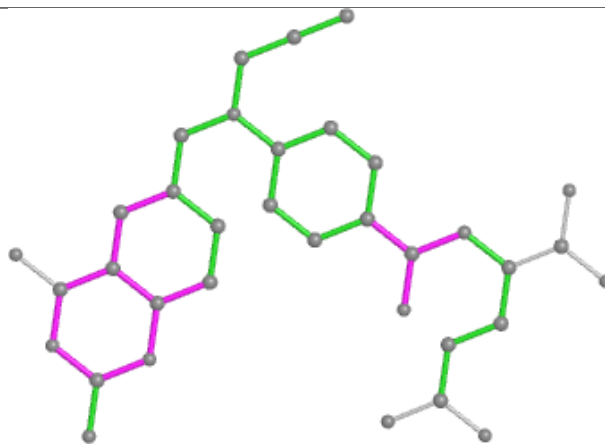
Ligand FOL B 703



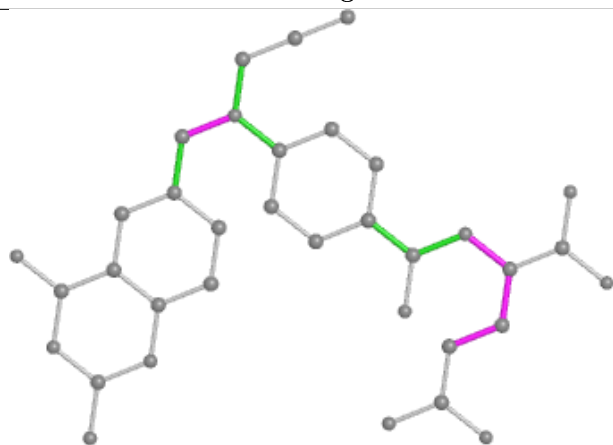
Ligand CB3 A 702



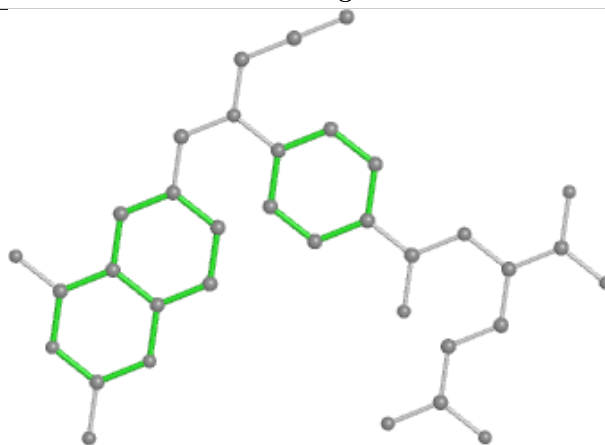
Bond lengths



Bond angles

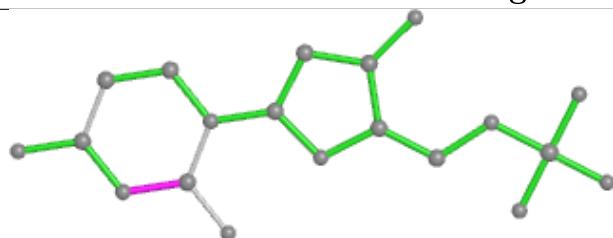


Torsions

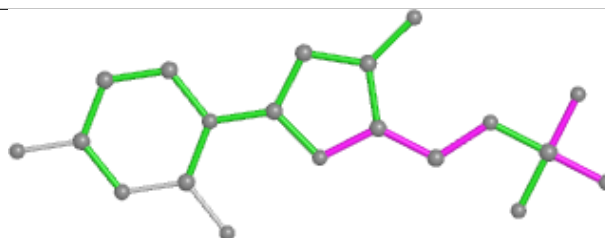


Rings

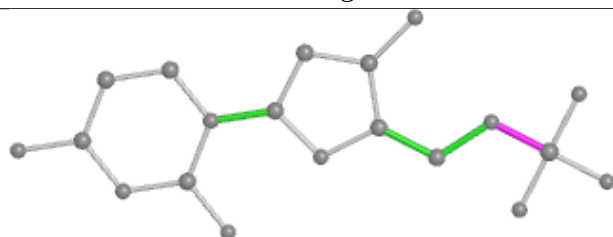
Ligand UMP B 701



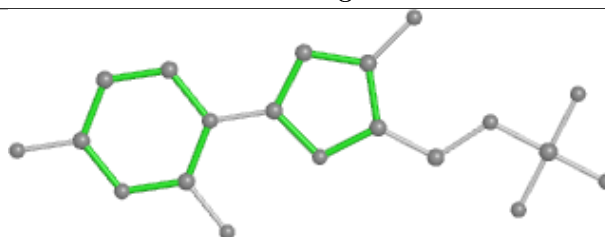
Bond lengths



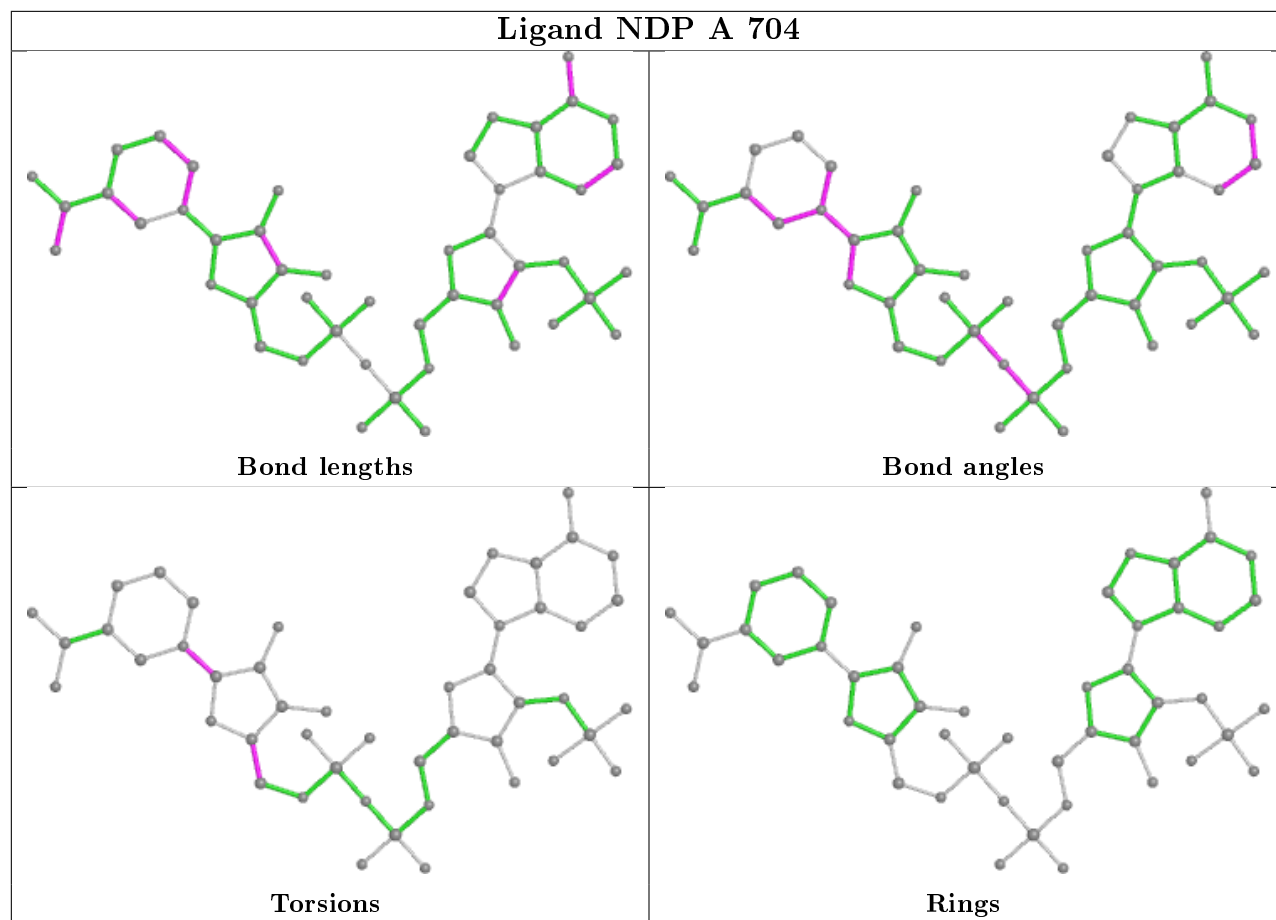
Bond angles

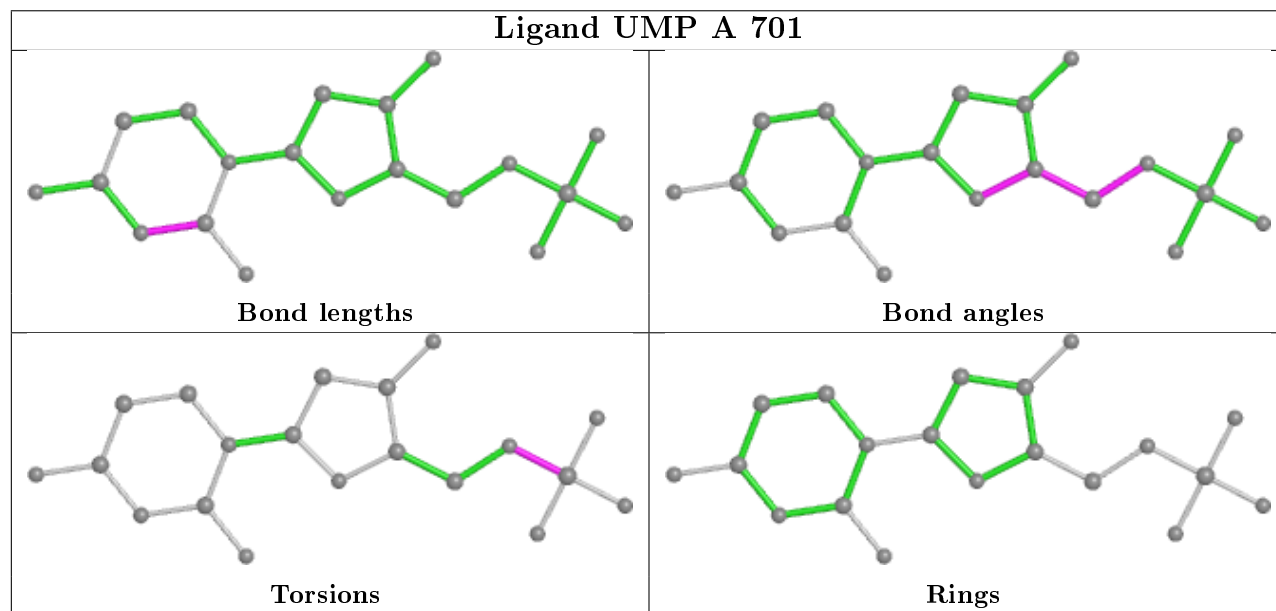
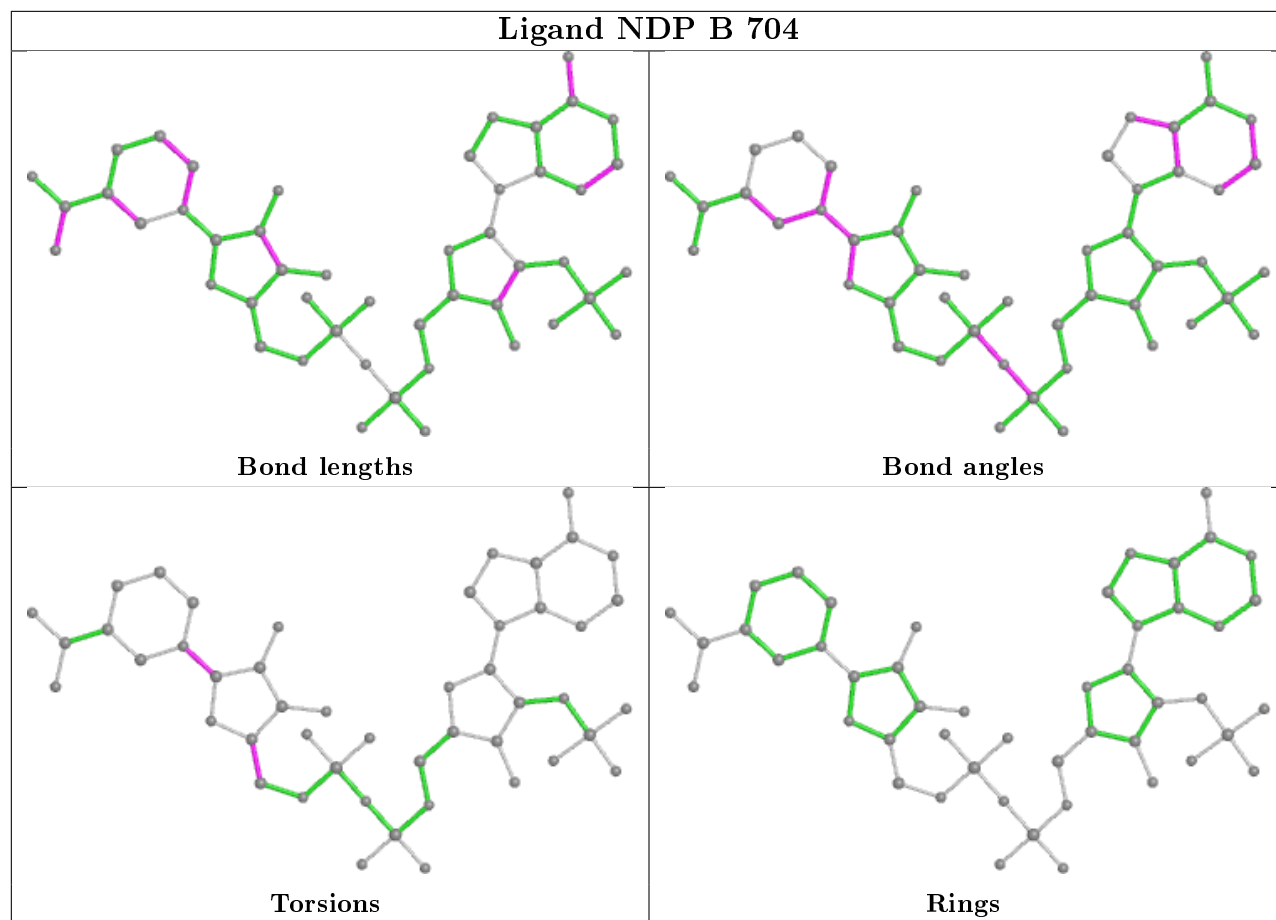


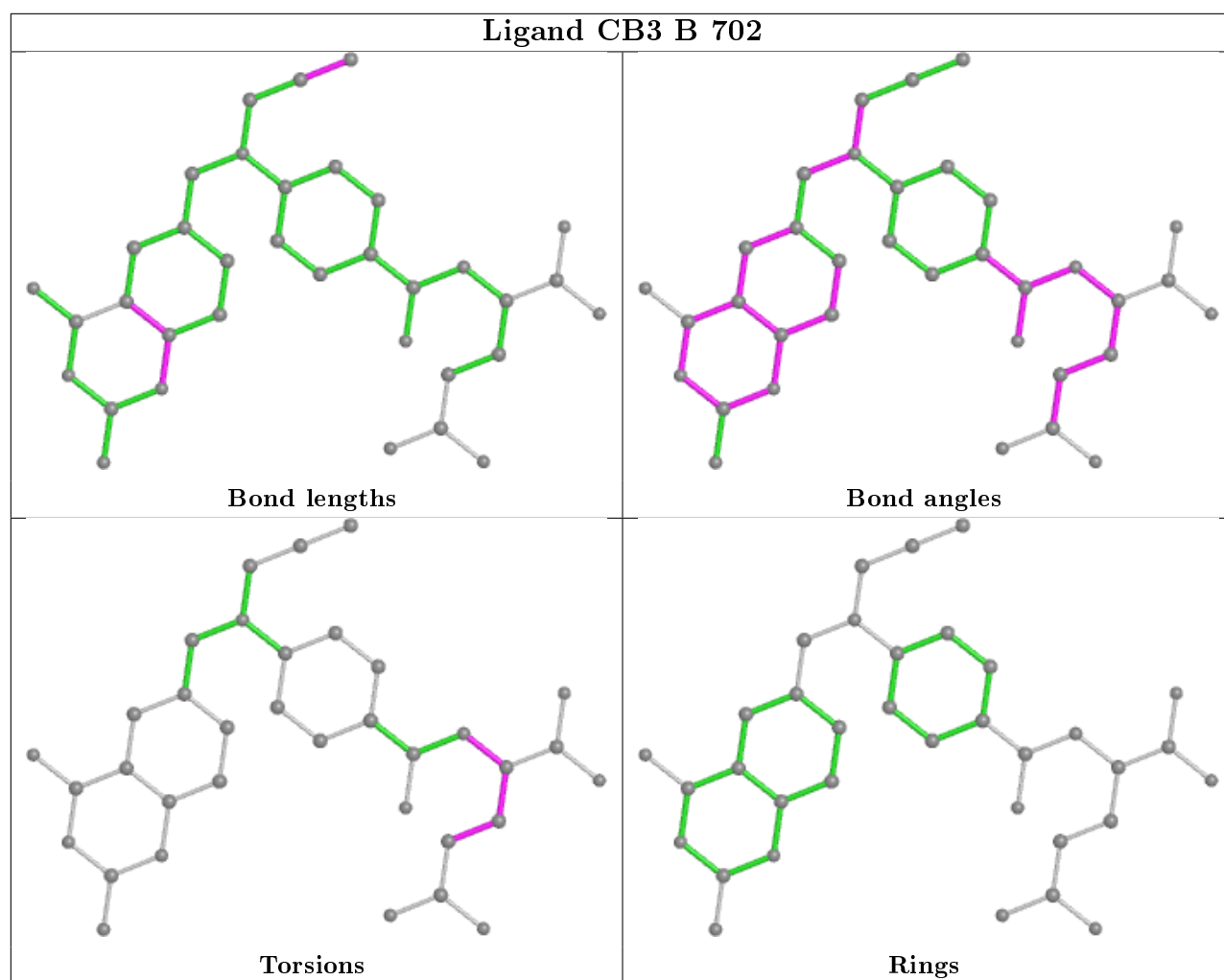
Torsions



Rings







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	498/610 (81%)	0.08	9 (1%) 68 55	39, 57, 83, 115	2 (0%)
1	B	498/610 (81%)	0.05	12 (2%) 59 45	39, 58, 79, 103	2 (0%)
All	All	996/1220 (81%)	0.07	21 (2%) 63 50	39, 57, 81, 115	4 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	150	VAL	3.7
1	A	151	VAL	3.0
1	A	338	GLY	3.0
1	A	309	GLU	2.9
1	A	406	ASN	2.9
1	B	150	VAL	2.9
1	B	609	ALA	2.9
1	A	170	TYR	2.6
1	B	191	ASP	2.5
1	A	134	LEU	2.4
1	A	191	ASP	2.4
1	B	406	ASN	2.4
1	B	170	TYR	2.3
1	B	246	VAL	2.2
1	B	610	VAL	2.2
1	A	246	VAL	2.2
1	B	367	LEU	2.2
1	B	387	ARG	2.1
1	B	354	GLY	2.1
1	B	596	VAL	2.1
1	B	605	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

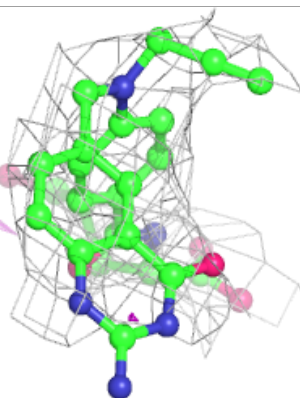
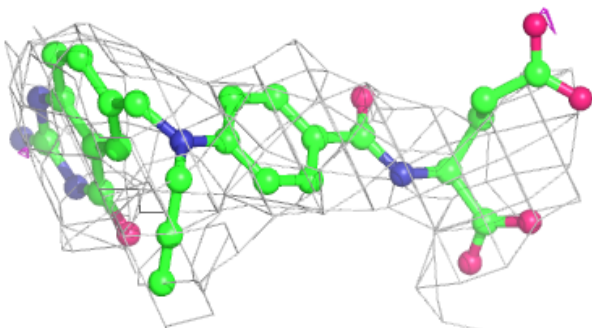
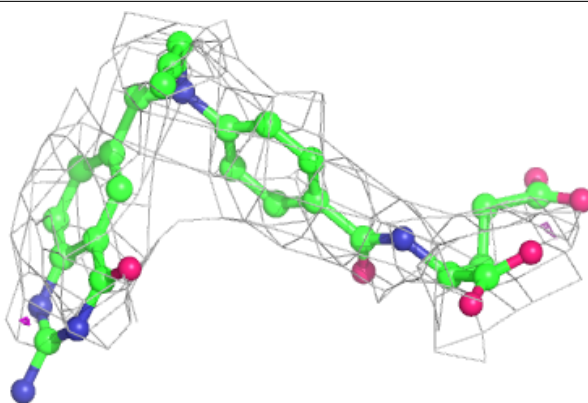
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CB3	A	702	35/35	0.74	0.48	80,90,105,105	0
3	CB3	B	702	35/35	0.74	0.53	72,92,110,116	0
4	FOL	A	703	32/32	0.77	0.47	72,86,94,98	0
4	FOL	B	703	32/32	0.78	0.49	72,82,105,110	0
5	NDP	B	704	48/48	0.86	0.32	75,84,99,102	0
5	NDP	A	704	48/48	0.88	0.31	75,83,100,104	0
2	UMP	B	701	20/20	0.93	0.28	68,79,103,105	0
2	UMP	A	701	20/20	0.94	0.25	71,78,95,97	0

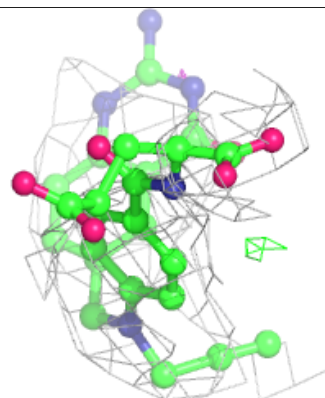
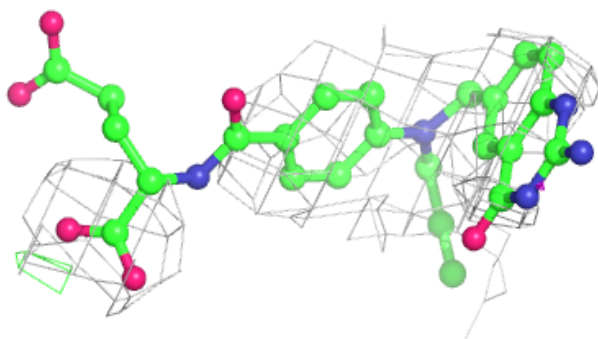
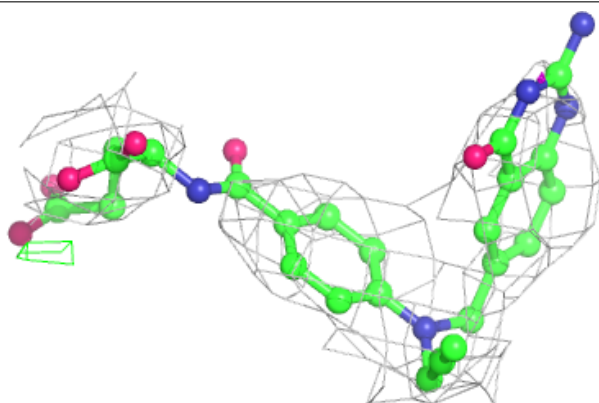
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CB3 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)

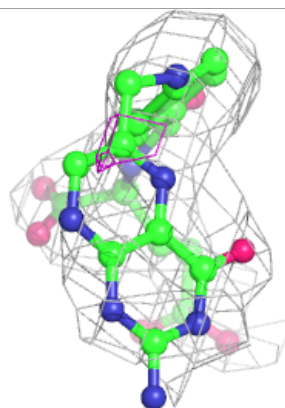
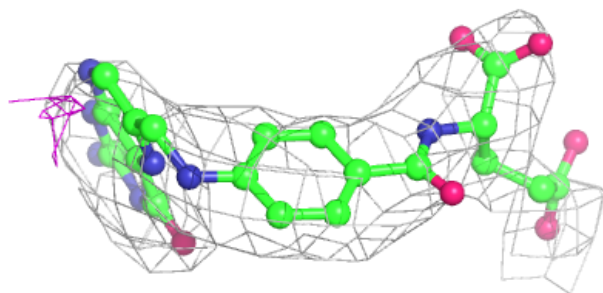
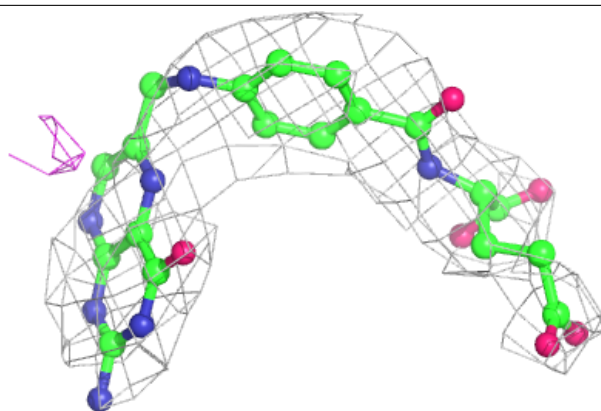
**Electron density around CB3 B 702:**

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



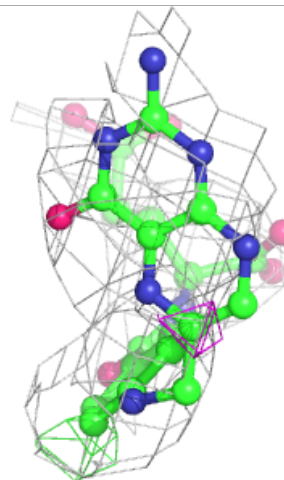
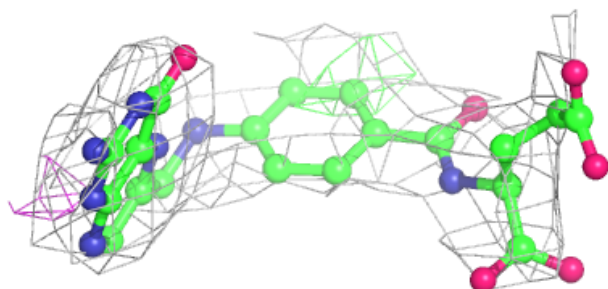
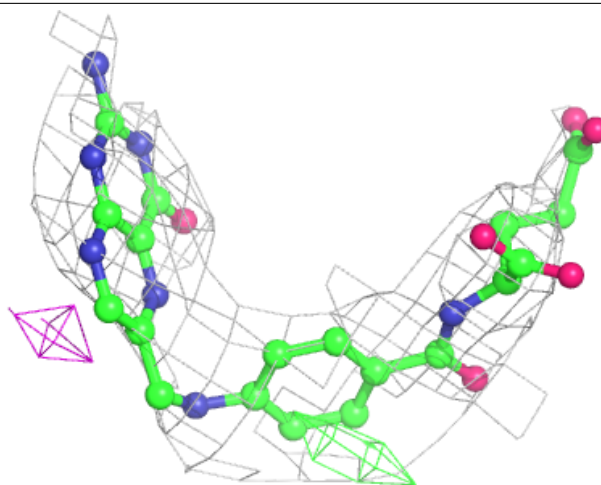
Electron density around FOL A 703:

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



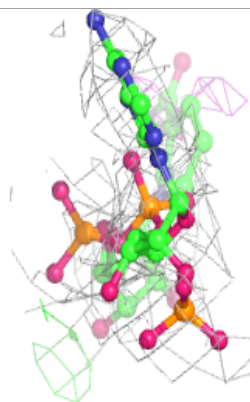
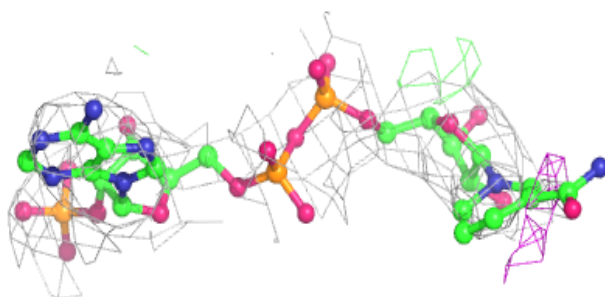
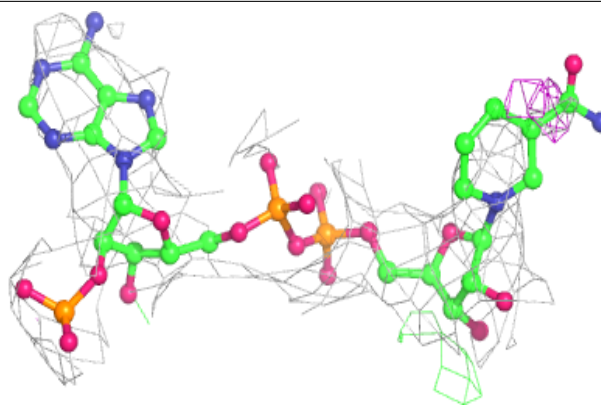
Electron density around FOL B 703:

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

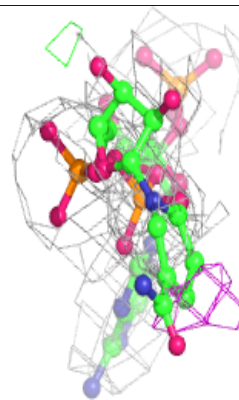
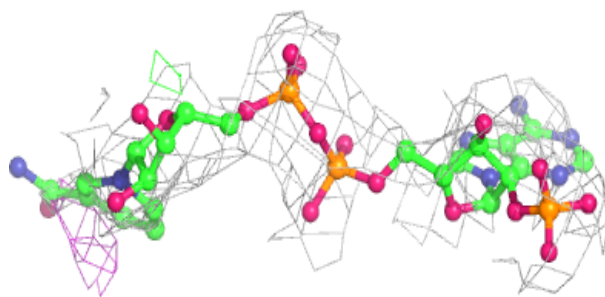
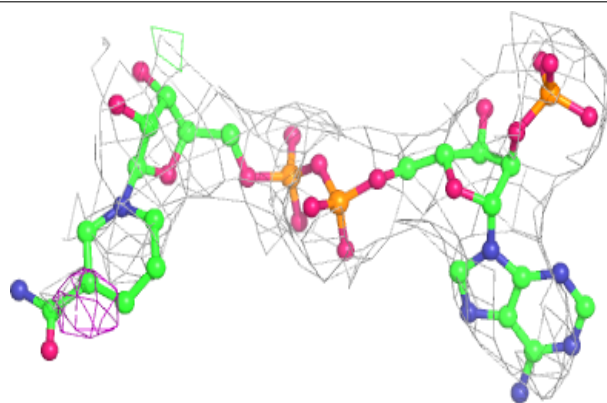


Electron density around NDP B 704:

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

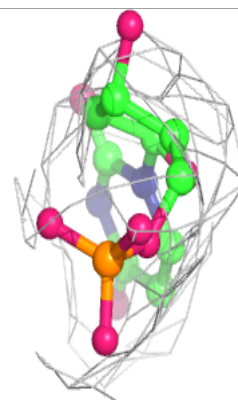
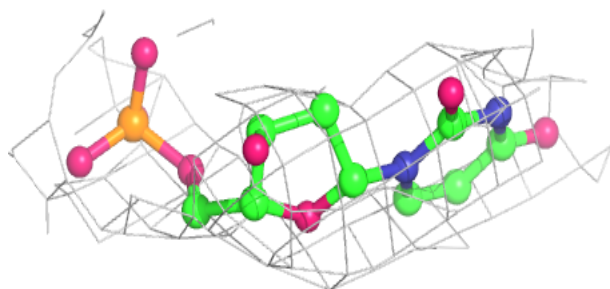
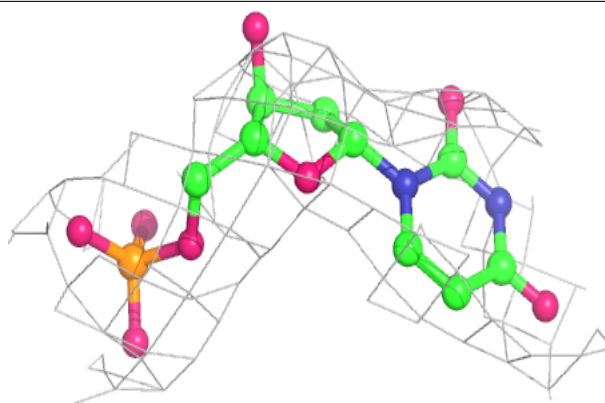
**Electron density around NDP A 704:**

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

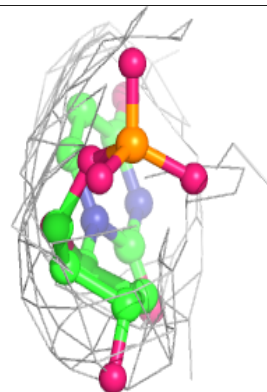
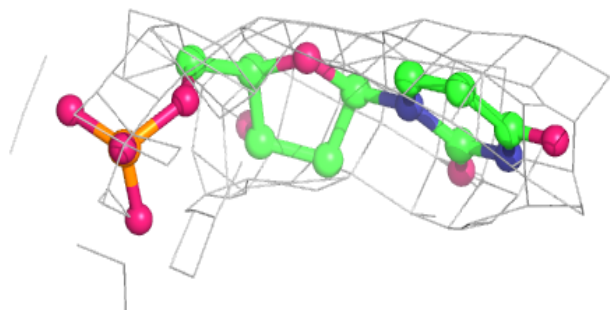
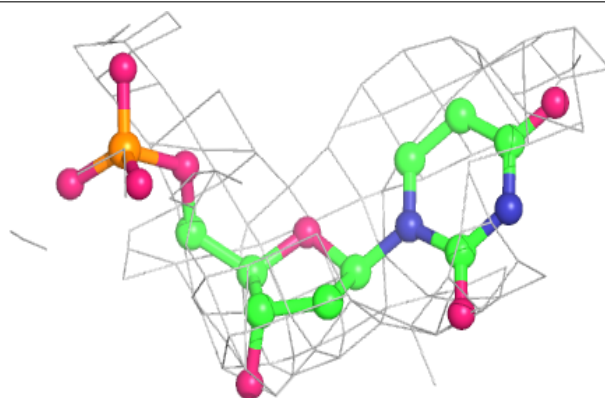


Electron density around UMP B 701:

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

**Electron density around 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.