



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:43 PM UTC

PDB ID : 5T7O / pdb_00005t7o
Title : Crystal structure of Trypanosoma cruzi Dihydrofolate Reductase-Thymidylate Synthase in complex with (6S)-5,6,7,8-TETRAHYDROFOLATE
Authors : Di Pisa, F.; Dello Iacono, L.; Bonucci, A.; Mangani, S.
Deposited on : 2016-09-05
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

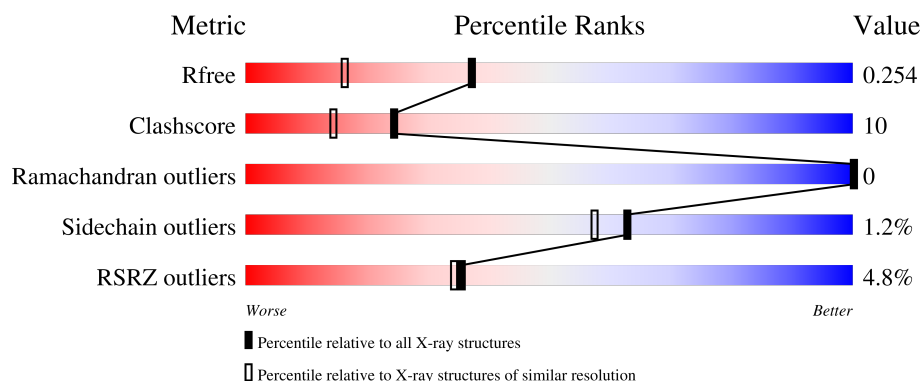
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

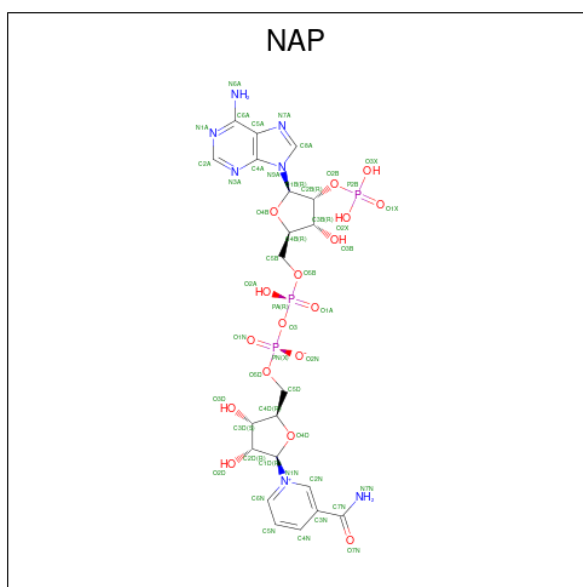
Mol	Chain	Length	Quality of chain
1	A	521	5% 78% 15% • 5%
1	B	521	5% 71% 22% • 5%
1	C	521	3% 77% 15% • 7%
1	D	521	5% 70% 22% • 6%

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	494	Total 4003	C 2563	N 698	O 720	S 22	0	25	0
1	B	495	Total 4017	C 2572	N 701	O 722	S 22	0	21	0
1	C	487	Total 3947	C 2531	N 689	O 707	S 20	0	23	0
1	D	489	Total 3909	C 2501	N 684	O 707	S 17	0	13	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



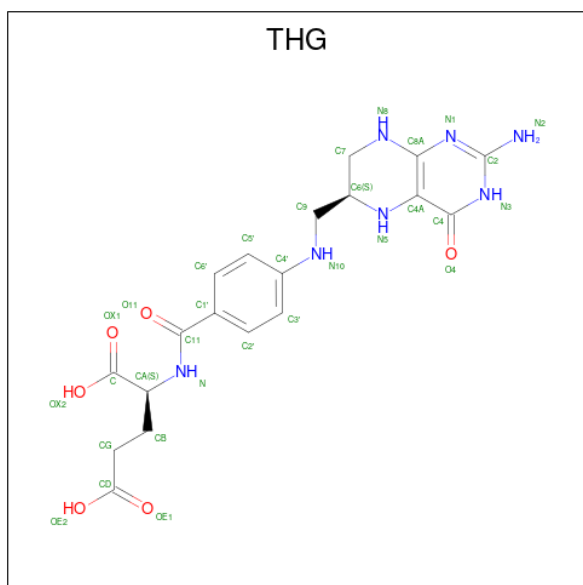
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

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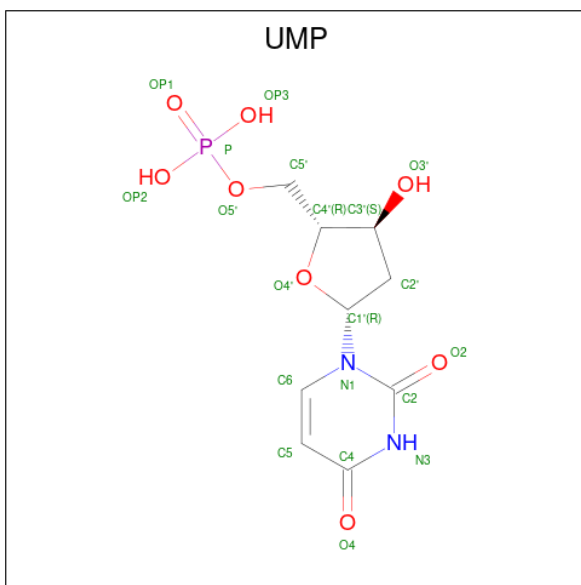
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			48	21	7	17		
2	D	1	Total	C	N	O	0	0
			48	21	7	17		

- Molecule 3 is (6S)-5,6,7,8-TETRAHYDROFOLATE (CCD ID: THG) (formula: C₁₉H₂₃N₇O₆).



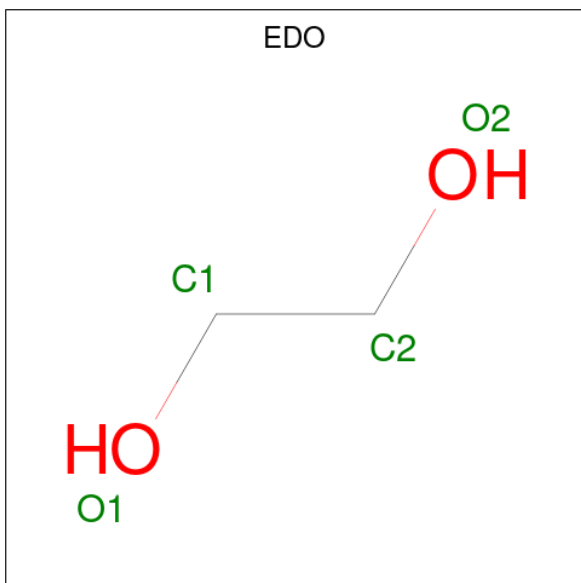
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	19	7	6		
3	B	1	Total	C	N	O	0	0
			32	19	7	6		
3	C	1	Total	C	N	O	0	0
			32	19	7	6		
3	D	1	Total	C	N	O	0	0
			32	19	7	6		

- Molecule 4 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (CCD ID: UMP) (formula: C₉H₁₃N₂O₈P).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

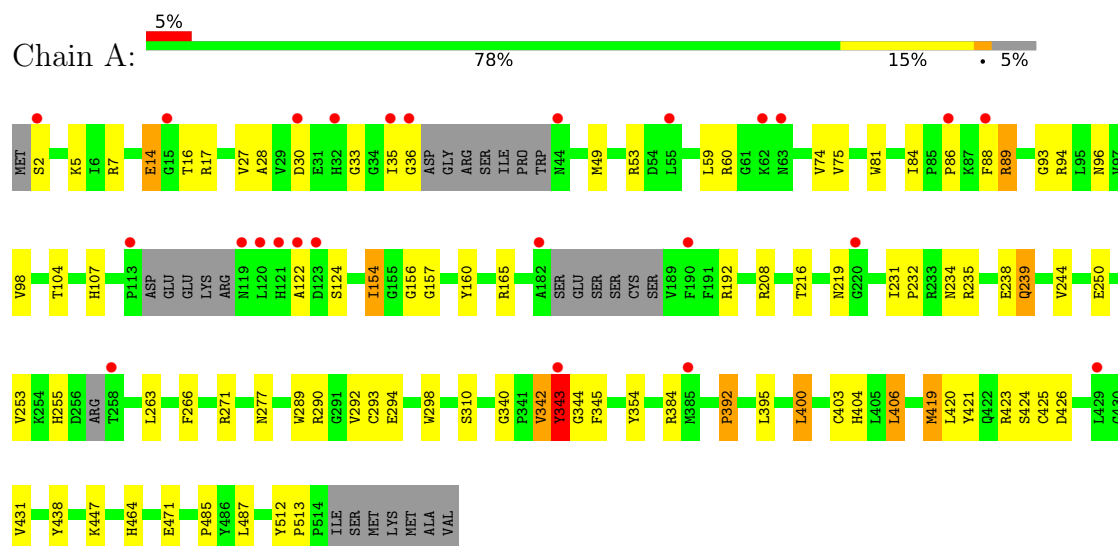
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	527	Total O 527 527	0	0
6	B	514	Total O 514 514	0	4
6	C	518	Total O 518 518	0	1
6	D	465	Total O 465 465	0	0

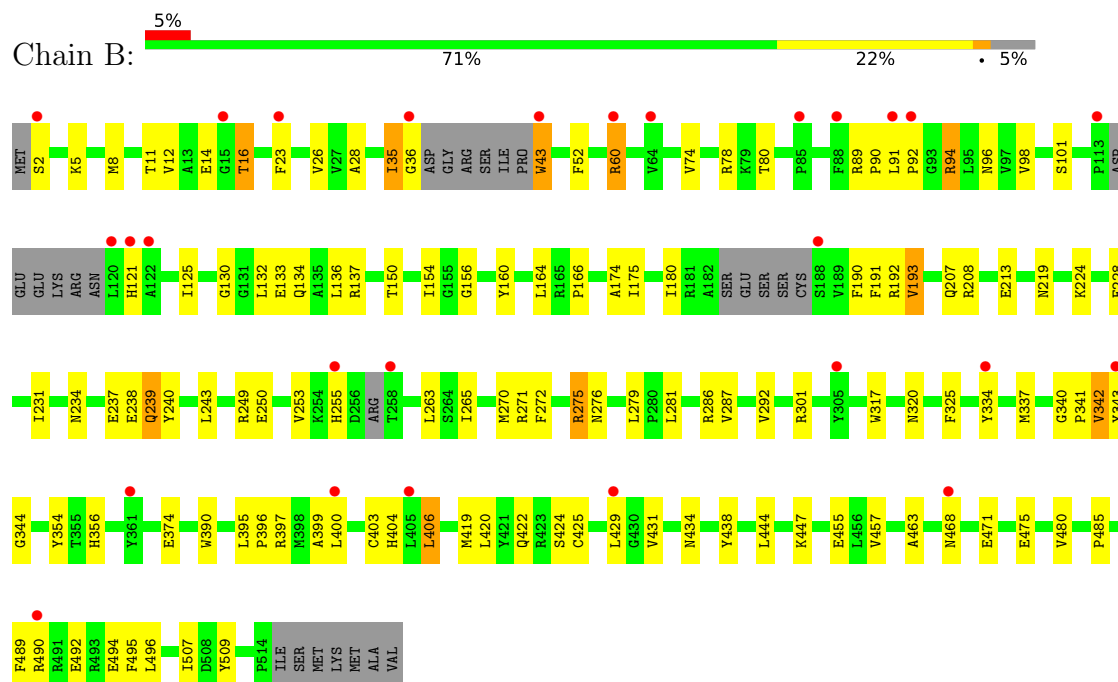
3 Residue-property plots [i](#)

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.

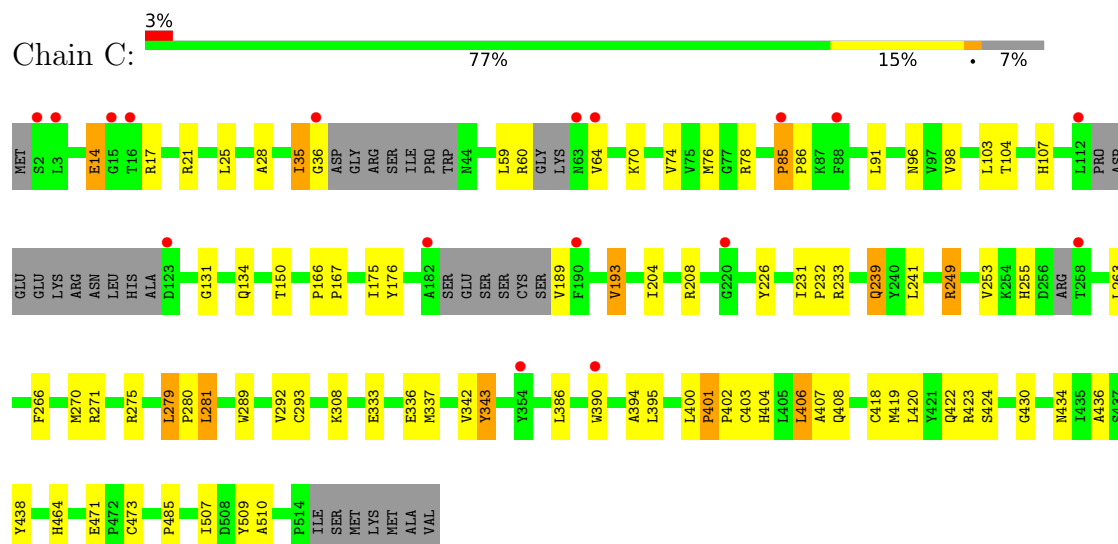
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



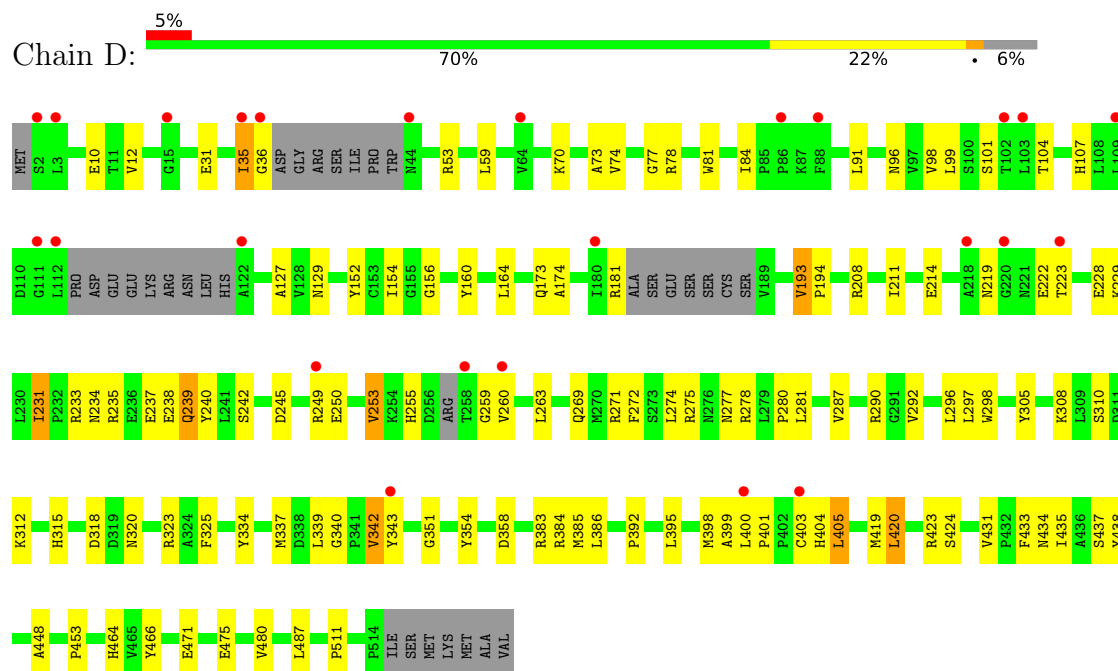
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.55Å 173.54Å 174.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.77 – 1.80 86.77 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (86.77-1.80) 99.2 (86.77-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.177 , 0.220 (Not available) , 0.254	Depositor DCC
R_{free} test set	10547 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18488	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 48.86 % 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 8.0996e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: THG, NAP, EDO, UMP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.58	35/4161 (0.8%)	1.30	21/5648 (0.4%)
1	B	1.57	35/4169 (0.8%)	1.30	21/5659 (0.4%)
1	C	1.56	29/4092 (0.7%)	1.32	13/5550 (0.2%)
1	D	1.57	43/4027 (1.1%)	1.29	18/5467 (0.3%)
All	All	1.57	142/16449 (0.9%)	1.30	73/22324 (0.3%)

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	1

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	385	MET	C-N	-14.35	1.15	1.33
1	C	343	TYR	CB-CG	12.97	1.80	1.51
1	A	487	LEU	N-CA	8.32	1.56	1.46
1	D	419	MET	SD-CE	-8.14	1.59	1.79
1	B	166	PRO	CA-C	8.05	1.57	1.52
1	B	406	LEU	C-O	-7.71	1.14	1.23
1	D	98	VAL	CA-CB	7.68	1.64	1.54
1	C	231	ILE	C-O	7.61	1.29	1.24
1	B	431	VAL	CA-CB	7.61	1.57	1.54
1	A	431	VAL	C-O	-7.49	1.18	1.24
1	C	280	PRO	CA-CB	7.35	1.62	1.53
1	D	174	ALA	N-CA	7.35	1.55	1.46
1	A	419	MET	SD-CE	-7.35	1.61	1.79
1	A	235	ARG	N-CA	7.28	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	GLY	N-CA	7.23	1.51	1.45
1	C	406	LEU	C-O	-7.16	1.15	1.23
1	A	406	LEU	C-N	-7.09	1.24	1.33
1	C	175	ILE	N-CA	7.05	1.55	1.46
1	C	406	LEU	C-N	-6.94	1.24	1.33
1	D	448	ALA	N-CA	6.93	1.55	1.46
1	A	344	GLY	N-CA	6.92	1.55	1.45
1	D	277	ASN	CA-CB	6.79	1.63	1.53
1	A	5	LYS	N-CA	6.72	1.54	1.45
1	C	394	ALA	C-N	6.72	1.42	1.33
1	A	344	GLY	CA-C	-6.71	1.43	1.51
1	A	98	VAL	CA-CB	6.67	1.62	1.54
1	B	507	ILE	N-CA	6.63	1.53	1.46
1	D	211	ILE	CA-C	6.62	1.61	1.52
1	D	308	LYS	N-CA	6.56	1.54	1.46
1	D	487	LEU	N-CA	6.47	1.53	1.46
1	C	96	ASN	CA-CB	6.40	1.61	1.53
1	D	229	LYS	CA-C	6.37	1.60	1.52
1	C	343	TYR	C-O	-6.36	1.16	1.24
1	C	279	LEU	CA-C	-6.35	1.47	1.52
1	C	85	PRO	CA-C	6.34	1.58	1.52
1	C	204	ILE	CA-CB	6.33	1.62	1.54
1	A	154	ILE	N-CA	6.30	1.52	1.46
1	A	94	ARG	N-CA	6.29	1.53	1.45
1	C	418	CYS	CA-C	-6.21	1.45	1.52
1	A	406	LEU	C-O	-6.19	1.16	1.23
1	B	406	LEU	C-N	-6.19	1.25	1.33
1	D	431	VAL	CA-CB	6.18	1.58	1.53
1	C	507	ILE	N-CA	6.15	1.53	1.46
1	A	342	VAL	CA-C	-6.13	1.45	1.53
1	B	174	ALA	N-CA	6.12	1.53	1.46
1	B	272	PHE	N-CA	6.12	1.53	1.46
1	A	471	GLU	C-O	-6.11	1.18	1.24
1	B	224	LYS	C-N	-6.10	1.25	1.33
1	D	237	GLU	C-O	-6.07	1.16	1.24
1	C	266	PHE	C-O	6.06	1.30	1.24
1	A	426	ASP	N-CA	6.06	1.53	1.46
1	D	405	LEU	N-CA	6.03	1.53	1.45
1	D	242	SER	N-CA	6.02	1.53	1.46
1	B	98	VAL	CA-CB	6.00	1.61	1.54
1	D	152	TYR	CA-C	-5.96	1.45	1.52
1	D	292	VAL	CA-CB	5.95	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	298	TRP	C-O	-5.93	1.17	1.24
1	C	402	PRO	C-O	5.89	1.30	1.23
1	D	453	PRO	C-O	5.89	1.30	1.23
1	B	492	GLU	CA-CB	-5.86	1.45	1.53
1	B	240	TYR	N-CA	-5.81	1.39	1.46
1	A	216	THR	N-CA	5.80	1.53	1.46
1	A	27	VAL	N-CA	5.79	1.53	1.46
1	D	239	GLN	N-CA	5.77	1.53	1.46
1	C	292	VAL	CA-CB	5.76	1.61	1.54
1	B	133	GLU	N-CA	5.74	1.53	1.46
1	C	510	ALA	N-CA	5.73	1.53	1.46
1	A	294	GLU	N-CA	5.71	1.53	1.46
1	C	150	THR	N-CA	5.70	1.53	1.46
1	A	219	ASN	C-N	-5.62	1.24	1.33
1	D	228	GLU	N-CA	5.56	1.52	1.45
1	A	423	ARG	N-CA	5.56	1.53	1.46
1	D	280	PRO	CA-CB	5.55	1.60	1.53
1	D	466	TYR	N-CA	5.51	1.52	1.46
1	D	231	ILE	N-CA	5.50	1.51	1.46
1	B	94	ARG	N-CA	5.47	1.52	1.45
1	B	494	GLU	CA-C	5.46	1.60	1.52
1	B	390	TRP	C-O	-5.44	1.16	1.23
1	A	400	LEU	C-O	-5.42	1.17	1.24
1	D	435	ILE	CA-CB	5.42	1.60	1.54
1	A	425	CYS	N-CA	-5.42	1.40	1.46
1	B	279	LEU	CA-C	-5.42	1.48	1.52
1	C	104	THR	N-CA	5.41	1.52	1.45
1	D	297	LEU	CA-CB	5.41	1.62	1.53
1	C	308	LYS	N-CA	5.38	1.53	1.46
1	D	290	ARG	N-CA	5.38	1.52	1.46
1	B	276	ASN	N-CA	5.37	1.54	1.46
1	A	310	SER	N-CA	5.36	1.53	1.46
1	A	81	TRP	CA-C	5.36	1.59	1.52
1	A	431	VAL	CA-CB	5.36	1.57	1.54
1	D	298	TRP	C-O	-5.34	1.18	1.24
1	D	127	ALA	CA-C	-5.34	1.46	1.52
1	B	447	LYS	N-CA	5.33	1.53	1.46
1	B	228	GLU	N-CA	5.31	1.52	1.45
1	C	342	VAL	C-N	-5.31	1.26	1.33
1	D	272	PHE	N-CA	5.30	1.52	1.46
1	D	339	LEU	N-CA	5.29	1.53	1.46
1	B	219	ASN	C-N	-5.28	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	98	VAL	CA-CB	5.27	1.60	1.54
1	D	96	ASN	CA-CB	5.27	1.60	1.53
1	C	21	ARG	CA-CB	5.25	1.61	1.53
1	C	76	MET	N-CA	5.24	1.52	1.45
1	B	444	LEU	CA-CB	5.24	1.61	1.53
1	C	270	MET	N-CA	5.24	1.52	1.45
1	D	305	TYR	CA-CB	5.23	1.59	1.53
1	D	269	GLN	N-CA	5.22	1.52	1.46
1	D	471	GLU	CA-C	5.22	1.59	1.52
1	A	244	VAL	CA-C	5.21	1.59	1.52
1	B	150	THR	N-CA	5.20	1.52	1.46
1	D	401	PRO	CA-CB	5.20	1.61	1.54
1	B	80	THR	CA-CB	5.19	1.61	1.53
1	C	239	GLN	C-O	-5.19	1.18	1.24
1	C	208	ARG	C-O	-5.18	1.17	1.24
1	D	511	PRO	N-CA	-5.18	1.41	1.47
1	A	277	ASN	CA-CB	5.17	1.61	1.53
1	D	77	GLY	CA-C	5.16	1.58	1.52
1	B	121	HIS	CA-C	5.15	1.59	1.52
1	B	231	ILE	C-N	5.14	1.38	1.33
1	B	237	GLU	CA-CB	5.14	1.61	1.53
1	B	356	HIS	N-CA	-5.13	1.39	1.45
1	A	292	VAL	CA-CB	5.11	1.60	1.54
1	A	485	PRO	CA-CB	5.11	1.61	1.53
1	B	96	ASN	CA-CB	5.11	1.60	1.53
1	D	10	GLU	C-O	-5.11	1.17	1.24
1	A	7	ARG	N-CA	5.10	1.52	1.46
1	B	52	PHE	N-CA	-5.08	1.40	1.46
1	B	270	MET	N-CA	5.08	1.52	1.45
1	A	471	GLU	CA-C	5.07	1.58	1.52
1	A	471	GLU	N-CA	5.07	1.51	1.46
1	D	480	VAL	CA-C	5.05	1.58	1.52
1	D	73	ALA	N-CA	-5.05	1.39	1.45
1	D	81	TRP	CA-C	5.04	1.59	1.52
1	B	207	GLN	C-O	5.03	1.29	1.23
1	C	471	GLU	CA-C	5.03	1.59	1.52
1	B	286	ARG	N-CA	5.03	1.52	1.46
1	B	26	VAL	C-O	5.02	1.29	1.24
1	D	310	SER	N-CA	5.02	1.52	1.46
1	D	433	PHE	N-CA	5.02	1.52	1.46
1	A	94	ARG	CD-NE	5.01	1.53	1.46
1	D	240	TYR	N-CA	-5.01	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	VAL	CA-CB	5.00	1.60	1.54
1	B	175	ILE	N-CA	5.00	1.52	1.46

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	471	GLU	CA-C-N	-9.21	110.26	119.56
1	B	471	GLU	C-N-CA	-9.21	110.26	119.56
1	D	342	VAL	N-CA-C	8.85	119.69	110.05
1	C	343	TYR	CA-CB-CG	-7.30	100.75	113.90
1	C	14	GLU	N-CA-C	7.28	118.86	111.07
1	B	12	VAL	N-CA-C	7.07	118.68	110.62
1	B	342	VAL	CB-CA-C	-6.95	103.94	111.59
1	D	12	VAL	N-CA-C	6.67	117.36	110.36
1	D	395	LEU	CA-C-N	-6.64	112.96	119.87
1	D	395	LEU	C-N-CA	-6.64	112.96	119.87
1	C	400	LEU	CA-C-N	6.53	124.36	119.66
1	C	400	LEU	C-N-CA	6.53	124.36	119.66
1	B	490	ARG	N-CA-C	-6.41	104.22	111.14
1	D	84	ILE	N-CA-CB	6.39	116.03	110.08
1	B	239	GLN	CB-CA-C	-6.31	100.98	110.88
1	A	84	ILE	N-CA-CB	6.20	115.85	110.08
1	D	274	LEU	N-CA-C	-6.13	105.11	112.59
1	C	275	ARG	N-CA-C	6.01	119.17	110.28
1	A	239	GLN	CB-CA-C	-6.00	101.47	110.88
1	D	275	ARG	N-CA-C	5.97	118.92	109.96
1	A	165	ARG	CA-C-N	-5.93	114.27	120.38
1	A	165	ARG	C-N-CA	-5.93	114.27	120.38
1	B	475	GLU	N-CA-C	-5.91	104.92	111.36
1	B	14	GLU	N-CA-C	5.90	117.39	111.07
1	D	260	VAL	CB-CA-C	-5.87	102.58	111.33
1	C	85	PRO	CA-C-N	5.84	127.14	119.84
1	C	85	PRO	C-N-CA	5.84	127.14	119.84
1	C	342	VAL	CB-CA-C	-5.83	105.18	111.59
1	B	275	ARG	N-CA-C	5.81	118.68	109.96
1	A	157	GLY	N-CA-C	5.78	119.66	112.73
1	C	401	PRO	O-C-N	5.73	123.84	121.15
1	B	35[A]	ILE	N-CA-C	-5.71	100.20	108.71
1	B	35[B]	ILE	N-CA-C	-5.71	100.20	108.71
1	D	211	ILE	N-CA-C	-5.69	100.48	108.27
1	B	164	LEU	N-CA-C	5.62	119.76	113.02
1	D	239	GLN	CB-CA-C	-5.62	101.82	110.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	239	GLN	CB-CA-C	-5.61	102.08	110.88
1	D	208	ARG	CB-CA-C	-5.61	100.70	109.84
1	B	101	SER	N-CA-C	-5.60	106.45	113.28
1	A	290	ARG	CA-C-N	5.55	125.99	119.94
1	A	290	ARG	C-N-CA	5.55	125.99	119.94
1	A	343	TYR	N-CA-CB	5.54	119.85	110.49
1	B	121	HIS	N-CA-C	5.51	120.12	113.17
1	A	14	GLU	N-CA-C	5.45	117.02	111.14
1	A	208	ARG	N-CA-C	5.40	117.53	109.59
1	A	232	PRO	CB-CA-C	5.40	116.31	111.40
1	D	214	GLU	N-CA-C	-5.34	102.97	110.50
1	B	60	ARG	N-CA-C	5.34	119.51	112.89
1	B	208	ARG	CB-CA-C	-5.32	101.56	110.29
1	B	292	VAL	N-CA-C	5.31	115.94	110.36
1	C	249	ARG	CA-CB-CG	-5.31	103.48	114.10
1	D	475	GLU	N-CA-C	-5.30	105.42	111.14
1	D	259	GLY	N-CA-C	5.29	122.62	115.32
1	C	343	TYR	N-CA-CB	5.27	119.40	110.49
1	D	253	VAL	N-CA-CB	5.27	116.46	110.72
1	B	480	VAL	CB-CA-C	-5.21	105.14	110.71
1	C	208	ARG	CB-CA-C	-5.21	101.35	109.84
1	A	122	ALA	N-CA-C	5.20	117.63	111.33
1	A	208	ARG	CB-CA-C	-5.20	102.45	110.26
1	A	84	ILE	N-CA-C	-5.15	103.90	108.95
1	A	392	PRO	CB-CA-C	-5.15	104.17	112.21
1	A	342	VAL	N-CA-C	5.14	116.02	110.21
1	B	265	ILE	CA-C-N	-5.14	115.52	122.77
1	B	265	ILE	C-N-CA	-5.14	115.52	122.77
1	D	164	LEU	N-CA-C	5.13	119.17	113.02
1	B	26	VAL	N-CA-C	-5.07	100.83	108.12
1	A	342	VAL	O-C-N	5.06	127.75	122.54
1	D	385	MET	CA-C-N	5.03	130.64	121.89
1	D	385	MET	C-N-CA	5.03	130.64	121.89
1	A	89[A]	ARG	CA-C-N	5.02	128.50	123.42
1	A	89[A]	ARG	C-N-CA	5.02	128.50	123.42
1	A	89[B]	ARG	CA-C-N	5.02	128.50	123.42
1	A	89[B]	ARG	C-N-CA	5.02	128.50	123.42

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	343	TYR	Mainchain

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	4003	0	3985	66	0
1	B	4017	0	3996	104	0
1	C	3947	0	3957	73	0
1	D	3909	0	3857	83	0
2	A	48	0	25	5	0
2	B	48	0	25	11	0
2	C	48	0	25	3	0
2	D	48	0	25	8	0
3	A	32	0	21	3	0
3	B	32	0	21	2	0
3	C	32	0	21	1	0
3	D	32	0	21	3	0
4	A	20	0	11	5	0
4	B	20	0	11	3	0
4	C	20	0	11	4	0
4	D	20	0	11	2	0
5	A	56	0	84	5	0
5	B	48	0	72	8	0
5	C	44	0	66	9	0
5	D	40	0	60	3	0
6	A	527	0	0	13	0
6	B	514	0	0	20	0
6	C	518	0	0	9	0
6	D	465	0	0	15	0
All	All	18488	0	16305	326	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 10.

All (326) 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:C:343:TYR:CG	1:C:343:TYR:CB	1.80	1.64
1:B:8[B]:MET:HE1	1:B:496:LEU:N	1.42	1.34
1:B:337:MET:HG3	6:B:1142:HOH:O	1.42	1.19
1:B:8[B]:MET:CE	1:B:496:LEU:N	2.07	1.15
1:D:337:MET:HG3	6:D:1228:HOH:O	1.47	1.15
6:C:1040:HOH:O	1:D:400:LEU:HD23	1.50	1.11
1:A:253[B]:VAL:HG22	6:A:968:HOH:O	1.53	1.05
1:D:238:GLU:OE1	6:D:801:HOH:O	1.78	1.01
1:A:238:GLU:OE1	6:A:801:HOH:O	1.81	0.98
1:A:403[C]:CYS:SG	4:A:703:UMP:C5	2.57	0.97
1:C:35[A]:ILE:HG13	1:C:36[A]:GLY:N	1.78	0.96
1:B:320:ASN:CG	1:B:400:LEU:HD11	1.91	0.96
1:B:334:TYR:OH	1:B:397[B]:ARG:NH2	1.99	0.95
1:A:403[C]:CYS:SG	4:A:703:UMP:C4	2.60	0.94
1:B:8[B]:MET:HE1	1:B:496:LEU:H	1.23	0.93
1:A:253[B]:VAL:HG21	6:D:919:HOH:O	1.70	0.92
1:C:390:TRP:CE2	1:D:386:LEU:HD22	2.05	0.90
1:C:289:TRP:CZ2	1:C:293[B]:CYS:SG	2.64	0.90
1:D:343:TYR:OH	6:D:802:HOH:O	1.90	0.89
1:B:8[B]:MET:HE1	1:B:496:LEU:CA	2.03	0.89
1:D:222:GLU:HG3	6:D:1014:HOH:O	1.73	0.88
1:B:403[C]:CYS:SG	4:B:602:UMP:C4	2.68	0.86
1:B:8[B]:MET:HE3	1:B:495:PHE:C	2.01	0.86
1:C:343:TYR:CG	1:C:343:TYR:CA	2.60	0.85
1:C:289:TRP:CE2	1:C:293[B]:CYS:SG	2.69	0.85
1:B:35[A]:ILE:HD12	2:B:603:NAP:C5N	2.07	0.84
1:C:166:PRO:HB2	5:C:610:EDO:H22	1.58	0.84
1:B:43:TRP:HZ3	2:B:603:NAP:H71N	1.26	0.83
1:B:320:ASN:ND2	1:B:400:LEU:HD11	1.95	0.82
1:D:239:GLN:HE22	1:D:271:ARG:H	1.28	0.82
5:A:714:EDO:H11	6:A:811:HOH:O	1.82	0.79
1:D:403:CYS:SG	1:D:424:SER:O	2.40	0.79
1:B:8[B]:MET:CE	1:B:495:PHE:C	2.56	0.79
1:A:104:THR:H	1:A:107[B]:HIS:HD2	1.26	0.78
1:B:334:TYR:OH	1:B:397[B]:ARG:CZ	2.31	0.78
1:C:434[A]:ASN:HD21	4:C:603:UMP:HN3	1.32	0.78
1:A:35[A]:ILE:HG13	1:A:36[A]:GLY:N	1.98	0.77
1:A:35[A]:ILE:CG1	1:A:36[A]:GLY:N	2.47	0.77
1:C:28:ALA:O	2:C:602:NAP:N7N	2.17	0.77
1:B:400:LEU:HD23	6:B:1063:HOH:O	1.84	0.77
1:C:78:ARG:HD3	2:C:602:NAP:O2X	1.85	0.77
1:D:253:VAL:HG22	1:D:263[A]:LEU:CD2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ARG:HD2	6:A:1025:HOH:O	1.86	0.75
1:B:43:TRP:HZ3	2:B:603:NAP:N7N	1.84	0.74
1:C:390:TRP:NE1	1:D:386:LEU:HD22	2.02	0.74
1:B:74:VAL:HG21	1:B:91:LEU:HD12	1.70	0.74
1:D:400:LEU:O	6:D:803:HOH:O	2.05	0.73
1:D:315:HIS:HE1	6:D:1135:HOH:O	1.72	0.72
1:B:400:LEU:O	6:B:701:HOH:O	2.06	0.72
1:A:156:GLY:HA2	2:A:701:NAP:H5N	1.72	0.72
1:C:253:VAL:HG22	1:C:263[A]:LEU:CD2	2.20	0.72
1:A:234:ASN:O	1:A:238:GLU:HG3	1.90	0.71
1:B:320:ASN:CG	1:B:400:LEU:CD1	2.64	0.71
1:B:255:HIS:HD2	6:C:1068:HOH:O	1.73	0.71
1:A:192:ARG:H	5:A:713:EDO:H22	1.54	0.71
1:A:404:HIS:HD2	1:A:438:TYR:OH	1.74	0.70
1:C:166:PRO:CB	5:C:610:EDO:H22	2.22	0.70
1:D:323:ARG:NH2	1:D:334:TYR:O	2.16	0.70
1:D:253:VAL:HG22	1:D:263[A]:LEU:HD21	1.73	0.70
1:A:406:LEU:HD21	1:B:406:LEU:CD2	2.23	0.69
1:B:403[C]:CYS:SG	4:B:602:UMP:C5	2.86	0.69
1:A:49[B]:MET:HE2	1:A:49[B]:MET:HA	1.76	0.68
1:D:233:ARG:NH2	1:D:235:ARG:NH1	2.41	0.68
1:D:233:ARG:HH21	1:D:235:ARG:NH1	1.92	0.68
1:B:374:GLU:HG3	6:B:1076:HOH:O	1.94	0.67
1:B:78:ARG:HD3	2:B:603:NAP:O2X	1.94	0.67
1:A:104:THR:H	1:A:107[B]:HIS:CD2	2.11	0.67
2:B:603:NAP:H52N	2:B:603:NAP:H6N	1.77	0.67
1:C:14:GLU:OE1	1:C:17:ARG:NH1	2.26	0.67
1:D:233:ARG:NE	1:D:235:ARG:CZ	2.58	0.67
1:A:404:HIS:HB2	1:A:420[A]:LEU:HD11	1.76	0.67
1:C:343:TYR:CB	1:C:343:TYR:CD2	2.72	0.66
1:C:386[B]:LEU:CD2	1:C:408:GLN:HB2	2.25	0.66
1:D:249:ARG:O	1:D:250:GLU:HG3	1.94	0.66
1:A:160:TYR:HE2	2:A:701:NAP:H4N	1.61	0.66
1:A:93:GLY:HA2	5:A:717:EDO:H22	1.77	0.66
1:B:422[B]:GLN:HE22	1:B:434[B]:ASN:CG	2.04	0.66
1:C:239:GLN:HE22	1:C:271:ARG:H	1.42	0.66
1:C:509:TYR:HD2	5:C:614:EDO:H21	1.61	0.66
1:A:255:HIS:HD2	6:A:1197:HOH:O	1.80	0.65
1:A:406:LEU:HD21	1:B:406:LEU:HD21	1.78	0.65
1:B:253:VAL:HG22	1:B:263[B]:LEU:CD2	2.26	0.65
1:D:320:ASN:ND2	1:D:400:LEU:HD11	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:TRP:CZ3	2:B:603:NAP:N7N	2.65	0.64
1:D:384:ARG:HD2	6:D:966:HOH:O	1.96	0.64
1:C:509:TYR:CD2	5:C:614:EDO:H21	2.32	0.64
1:C:253:VAL:HG22	1:C:263[A]:LEU:HD21	1.79	0.64
1:A:53:ARG:NH2	3:A:702:THG:OE2	2.30	0.64
1:D:281[A]:LEU:HD22	1:D:287:VAL:HB	1.78	0.64
6:A:1136:HOH:O	1:D:255:HIS:HD2	1.80	0.63
1:D:78:ARG:HD3	2:D:701:NAP:O2X	1.98	0.63
1:A:49[B]:MET:HE2	1:A:49[B]:MET:CA	2.28	0.63
1:B:419[B]:MET:HG2	1:B:457:VAL:HB	1.80	0.63
1:A:239:GLN:HE22	1:A:271:ARG:H	1.47	0.63
1:B:404:HIS:HB2	1:B:420:LEU:HD11	1.81	0.63
1:B:92:PRO:HD2	1:B:94:ARG:NH2	2.14	0.62
1:B:134[B]:GLN:NE2	1:B:137:ARG:HH11	1.98	0.62
1:B:403[A]:CYS:SG	1:B:424:SER:O	2.57	0.62
1:C:404:HIS:HD2	1:C:438:TYR:OH	1.82	0.62
1:D:234:ASN:O	1:D:238:GLU:HG3	1.99	0.62
1:B:404:HIS:HD2	1:B:438:TYR:OH	1.81	0.62
1:C:35[A]:ILE:HG13	1:C:36[A]:GLY:H	1.62	0.61
1:B:134[B]:GLN:NE2	1:B:137:ARG:NH1	2.49	0.61
1:D:405:LEU:HD23	1:D:423:ARG:HG2	1.83	0.61
1:B:239:GLN:HE22	1:B:271:ARG:H	1.47	0.61
1:D:343:TYR:CE1	1:D:404:HIS:CE1	2.88	0.61
1:C:390:TRP:NE1	1:D:386:LEU:CD2	2.62	0.61
1:D:74[A]:VAL:HG11	1:D:91:LEU:HD12	1.81	0.61
1:A:403[B]:CYS:SG	4:A:703:UMP:C6	2.94	0.60
1:A:403[A]:CYS:SG	1:A:424:SER:O	2.59	0.60
1:D:59[B]:LEU:HD21	1:D:70:LYS:HG3	1.84	0.60
1:D:404:HIS:HD2	1:D:438:TYR:OH	1.85	0.60
1:D:59[B]:LEU:CD2	1:D:70:LYS:HG3	2.31	0.60
1:B:35[A]:ILE:HG13	1:B:36[A]:GLY:N	2.16	0.59
1:B:92:PRO:HD2	1:B:94:ARG:HH21	1.66	0.59
1:C:249:ARG:NH1	5:C:607:EDO:H12	2.17	0.59
4:B:602:UMP:O4	5:B:611:EDO:H11	2.02	0.59
1:C:279:LEU:HG	1:C:281[C]:LEU:HD13	1.84	0.59
1:C:403[A]:CYS:SG	1:C:424:SER:O	2.61	0.58
1:B:253:VAL:HG22	1:B:263[B]:LEU:HD21	1.84	0.58
1:A:342:VAL:O	1:A:343:TYR:C	2.45	0.57
1:A:156:GLY:CA	2:A:701:NAP:H5N	2.34	0.57
1:A:16[B]:THR:HG21	1:A:447:LYS:NZ	2.19	0.57
1:D:358:ASP:H	5:D:708:EDO:C1	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35[A]:ILE:CG1	1:D:36[A]:GLY:N	2.68	0.57
1:A:35[A]:ILE:CG1	1:A:36[A]:GLY:H	2.16	0.56
1:A:35[A]:ILE:HG12	1:A:36[A]:GLY:H	1.71	0.56
1:B:160:TYR:HE2	2:B:603:NAP:H4N	1.69	0.56
1:D:104:THR:H	1:D:107[B]:HIS:HD2	1.53	0.56
1:A:406:LEU:CD2	1:B:406:LEU:CD2	2.84	0.56
1:D:315:HIS:HD2	1:D:318:ASP:OD2	1.89	0.56
1:B:16[A]:THR:HG22	6:B:756:HOH:O	2.05	0.56
1:B:154:ILE:O	3:B:601:THG:HC72	2.05	0.55
1:C:176:TYR:HE2	5:C:611:EDO:H21	1.71	0.55
1:A:406:LEU:CD2	1:B:406:LEU:HD23	2.36	0.55
2:A:701:NAP:H52N	2:A:701:NAP:H6N	1.89	0.55
1:C:464:HIS:NE2	4:C:603:UMP:O3'	2.34	0.55
1:A:271:ARG:HD2	6:A:980:HOH:O	2.06	0.55
1:C:386[B]:LEU:HD11	1:D:423:ARG:HD3	1.89	0.55
1:C:386[B]:LEU:HD21	1:C:408:GLN:HB2	1.88	0.55
2:D:701:NAP:C7N	6:D:813:HOH:O	2.54	0.55
1:C:253:VAL:HG22	1:C:263[A]:LEU:HD23	1.88	0.55
6:B:898:HOH:O	1:C:193[B]:VAL:HG22	2.07	0.55
1:D:233:ARG:NH2	1:D:235:ARG:HH12	2.04	0.55
1:D:358:ASP:H	5:D:708:EDO:H12	1.73	0.54
1:C:473:CYS:SG	6:C:1116:HOH:O	2.58	0.54
1:D:320:ASN:CG	1:D:400:LEU:CD1	2.81	0.54
1:B:8[B]:MET:CE	1:B:496:LEU:CA	2.74	0.54
1:B:374:GLU:CG	6:B:1076:HOH:O	2.52	0.54
1:C:422:GLN:HE22	1:C:434[A]:ASN:ND2	2.04	0.54
1:B:325:PHE:HZ	1:B:400:LEU:HD21	1.72	0.54
1:B:395:LEU:HB2	1:B:396:PRO:HD3	1.90	0.54
1:C:404:HIS:HB2	1:C:420[A]:LEU:HD11	1.88	0.54
1:B:249:ARG:NH1	5:B:606:EDO:H11	2.23	0.54
1:D:156:GLY:HA2	2:D:701:NAP:H5N	1.90	0.54
1:D:245:ASP:O	1:D:249:ARG:HG2	2.08	0.54
1:D:253:VAL:HG22	1:D:263[A]:LEU:HD23	1.91	0.54
1:A:266:PHE:CZ	1:B:419[B]:MET:HB2	2.43	0.53
1:A:60[A]:ARG:NH1	6:A:810:HOH:O	2.42	0.53
1:D:343:TYR:CE1	1:D:404:HIS:NE2	2.75	0.53
1:A:404:HIS:CD2	1:A:438:TYR:OH	2.58	0.53
1:A:343:TYR:CE1	1:A:404:HIS:CE1	2.97	0.53
1:D:315:HIS:CD2	1:D:318:ASP:OD2	2.61	0.53
1:C:404:HIS:CD2	1:C:438:TYR:OH	2.61	0.53
1:A:406:LEU:HD21	1:B:406:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:LEU:HD12	1:C:406:LEU:C	2.34	0.53
1:D:74[B]:VAL:HG11	1:D:154:ILE:HD13	1.91	0.53
1:D:231:ILE:HG13	6:D:858:HOH:O	2.09	0.52
1:D:253:VAL:HG22	1:D:263[B]:LEU:HD22	1.91	0.52
1:B:340:GLY:HA2	1:B:354:TYR:CE2	2.44	0.52
1:C:386[B]:LEU:HD23	1:C:408:GLN:CB	2.39	0.52
6:B:898:HOH:O	1:C:193[B]:VAL:CG2	2.57	0.52
1:B:35[A]:ILE:HD12	2:B:603:NAP:H5N	1.87	0.52
1:B:406:LEU:C	1:B:406:LEU:HD12	2.34	0.52
1:A:16[B]:THR:HG21	1:A:447:LYS:HG2	1.92	0.52
1:B:281[A]:LEU:HD22	1:B:287:VAL:HB	1.92	0.52
1:B:404:HIS:CD2	1:B:438:TYR:OH	2.62	0.52
1:D:399:ALA:O	1:D:400:LEU:HG	2.10	0.52
1:A:253[B]:VAL:CG2	6:D:919:HOH:O	2.43	0.52
5:A:714:EDO:C1	6:A:811:HOH:O	2.51	0.52
1:D:383:ARG:NH2	6:D:804:HOH:O	2.26	0.51
1:D:101:SER:HA	1:D:129:ASN:ND2	2.26	0.51
1:A:421:TYR:CE2	1:B:419[A]:MET:HE3	2.46	0.51
1:B:253:VAL:HG22	1:B:263[B]:LEU:HD23	1.91	0.51
1:B:250:GLU:HA	5:B:612:EDO:H21	1.93	0.51
1:A:340:GLY:HA2	1:A:354:TYR:CE2	2.45	0.51
1:C:35[A]:ILE:HD12	2:C:602:NAP:H2N	1.92	0.51
1:C:131:GLY:H	1:C:134:GLN:HE21	1.59	0.51
1:D:312:LYS:HE2	6:D:843:HOH:O	2.11	0.51
1:D:173:GLN:HE22	1:D:278:ARG:HH12	1.59	0.50
6:B:1070:HOH:O	1:C:255:HIS:HD2	1.93	0.50
1:B:156:GLY:HA2	2:B:603:NAP:H5N	1.93	0.50
5:C:604:EDO:H22	5:C:611:EDO:O1	2.11	0.50
1:B:2:SER:CB	6:B:1096:HOH:O	2.60	0.50
1:D:160:TYR:HE2	2:D:701:NAP:H4N	1.76	0.50
1:B:43:TRP:CD1	1:B:180:ILE:HG21	2.47	0.50
1:D:35[A]:ILE:HG12	1:D:36[A]:GLY:N	2.27	0.49
1:C:395:LEU:HD22	1:C:401:PRO:HB3	1.93	0.49
1:B:213:GLU:HG2	5:B:614:EDO:O2	2.13	0.49
1:B:8[B]:MET:HE1	1:B:496:LEU:CB	2.42	0.49
1:C:386[B]:LEU:CD2	1:C:408:GLN:CB	2.91	0.49
1:D:104:THR:O	1:D:107[B]:HIS:HB2	2.11	0.49
1:D:104:THR:H	1:D:107[B]:HIS:CD2	2.30	0.49
1:A:250:GLU:HA	5:A:708:EDO:H11	1.93	0.49
5:B:609:EDO:H11	6:B:871:HOH:O	2.12	0.49
1:C:343:TYR:CG	1:C:343:TYR:HA	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:PRO:HG3	1:B:125:ILE:HD11	1.95	0.49
1:C:386[B]:LEU:HD23	1:C:408:GLN:HB2	1.93	0.49
1:C:60:ARG:HD3	6:C:704:HOH:O	2.13	0.48
1:D:404:HIS:CD2	1:D:438:TYR:OH	2.66	0.48
1:C:59:LEU:HD12	1:C:64:VAL:HB	1.96	0.48
1:D:156:GLY:HA3	2:D:701:NAP:O1N	2.13	0.48
1:D:219:ASN:HD21	1:D:223:THR:HG23	1.79	0.48
1:A:403[B]:CYS:SG	6:A:1202:HOH:O	2.59	0.48
1:D:342:VAL:O	1:D:343:TYR:C	2.56	0.48
1:A:30:ASP:OD1	1:A:30:ASP:C	2.57	0.48
1:B:325:PHE:CZ	1:B:400:LEU:HD21	2.49	0.48
1:D:320:ASN:CG	1:D:400:LEU:HD12	2.39	0.47
1:B:341:PRO:HD2	1:B:397[B]:ARG:O	2.15	0.47
1:D:434[B]:ASN:HA	1:D:437[B]:SER:HB2	1.94	0.47
1:D:404:HIS:HB2	1:D:420:LEU:HD11	1.95	0.47
1:C:386[B]:LEU:CD1	1:D:423:ARG:HD3	2.45	0.47
1:D:154:ILE:O	3:D:703:THG:HC72	2.14	0.47
1:B:425[A]:CYS:HB2	1:B:463:ALA:HA	1.96	0.47
1:D:323:ARG:O	1:D:323:ARG:HD3	2.14	0.47
1:B:23:PHE:CE1	1:B:136:LEU:HD11	2.50	0.47
1:A:154:ILE:O	3:A:702:THG:HC72	2.15	0.47
1:A:464:HIS:NE2	4:A:703:UMP:O3'	2.36	0.47
1:C:107:HIS:HB2	6:C:1042:HOH:O	2.15	0.46
1:D:342:VAL:HG12	1:D:398:MET:HB3	1.97	0.46
1:C:167:PRO:N	5:C:610:EDO:H21	2.29	0.46
1:B:399:ALA:C	1:B:400:LEU:HG	2.41	0.46
1:A:512:TYR:HB3	1:A:513:PRO:HD2	1.98	0.46
1:B:317:TRP:CZ2	1:B:343:TYR:HE2	2.34	0.46
1:B:317:TRP:HZ2	1:B:343:TYR:CE2	2.33	0.46
1:B:399:ALA:O	1:B:400:LEU:HG	2.15	0.46
1:D:464:HIS:NE2	4:D:702:UMP:O3'	2.40	0.46
1:B:243[B]:LEU:HG	6:B:791:HOH:O	2.15	0.45
1:C:333:GLU:HB2	6:C:1009:HOH:O	2.16	0.45
2:B:603:NAP:H2N	6:B:714:HOH:O	2.15	0.45
1:C:134:GLN:HG3	6:C:1114:HOH:O	2.16	0.45
1:B:234:ASN:O	1:B:238:GLU:HG3	2.16	0.45
1:B:275:ARG:HH22	1:B:455[B]:GLU:HG3	1.81	0.45
1:B:28:ALA:HB3	2:B:603:NAP:H72N	1.82	0.45
1:A:392:PRO:HA	1:A:395:LEU:HG	1.98	0.45
1:D:343:TYR:HE1	1:D:404:HIS:CE1	2.33	0.45
1:D:343:TYR:HE1	1:D:404:HIS:NE2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ARG:NH2	1:B:455[B]:GLU:HG3	2.32	0.45
1:B:420:LEU:HD22	1:B:438:TYR:CD1	2.51	0.45
1:B:23:PHE:CZ	1:B:132:LEU:HD21	2.52	0.44
1:A:16[B]:THR:HG21	1:A:447:LYS:HZ3	1.81	0.44
1:C:386[B]:LEU:HD23	1:C:408:GLN:CA	2.47	0.44
1:B:406:LEU:HD12	1:B:406:LEU:O	2.17	0.44
1:D:320:ASN:CG	1:D:400:LEU:HD11	2.42	0.44
3:B:601:THG:HC92	3:B:601:THG:HC5	1.66	0.44
1:A:74[B]:VAL:HG11	1:A:154:ILE:HD13	2.00	0.44
1:A:345:PHE:CZ	1:A:354:TYR:HD1	2.35	0.44
1:B:11:THR:HA	6:B:1084:HOH:O	2.16	0.44
1:D:351:GLY:HA2	5:D:710:EDO:H12	1.99	0.44
1:C:59:LEU:HD13	1:C:70:LYS:HG3	2.00	0.43
1:D:233:ARG:HE	1:D:235:ARG:CZ	2.30	0.43
1:B:60:ARG:NH2	6:B:702:HOH:O	2.29	0.43
1:C:74:VAL:HG21	1:C:91:LEU:HD12	1.99	0.43
1:C:176:TYR:CE2	5:C:611:EDO:H21	2.52	0.43
1:C:279:LEU:CG	1:C:281[C]:LEU:HD13	2.48	0.43
1:C:281[A]:LEU:HD23	1:C:436:ALA:HB2	1.99	0.43
1:B:253:VAL:HG11	1:C:226:TYR:OH	2.19	0.43
1:A:30:ASP:OD1	1:A:33:GLY:N	2.51	0.43
1:A:86:PRO:HD3	1:A:89[A]:ARG:HH21	1.83	0.43
1:A:107[B]:HIS:CD2	6:A:888:HOH:O	2.71	0.43
1:D:53:ARG:NH1	3:D:703:THG:OE1	2.51	0.43
1:C:232:PRO:O	1:C:233:ARG:C	2.58	0.43
1:D:340:GLY:HA2	1:D:354:TYR:CE2	2.53	0.43
1:B:8[B]:MET:CE	1:B:496:LEU:H	2.02	0.43
1:B:317:TRP:CZ2	1:B:343:TYR:CE2	3.07	0.43
1:B:485:PRO:HB3	1:B:509:TYR:HA	2.00	0.43
1:B:91:LEU:HB3	1:B:94:ARG:CZ	2.48	0.43
1:A:14:GLU:OE1	1:A:17:ARG:NH1	2.51	0.43
1:B:343:TYR:HB3	1:B:344:GLY:H	1.55	0.43
1:B:5:LYS:NZ	6:B:723:HOH:O	2.52	0.43
1:B:191:PHE:HA	5:B:613:EDO:H22	2.00	0.43
1:C:485:PRO:HB3	1:C:509:TYR:HA	2.00	0.43
1:A:28:ALA:O	2:A:701:NAP:N7N	2.52	0.42
1:C:406:LEU:HD12	1:C:406:LEU:O	2.19	0.42
1:D:31:GLU:HG3	1:D:181:ARG:HA	2.02	0.42
1:A:289:TRP:CZ2	1:A:293[B]:CYS:SG	3.12	0.42
2:D:701:NAP:O7N	3:D:703:THG:HC71	2.20	0.42
1:A:2:SER:CB	6:A:1233:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403[B]:CYS:SG	4:A:703:UMP:C5	3.13	0.42
1:C:134:GLN:H	1:C:134:GLN:NE2	2.18	0.42
1:C:407:ALA:HA	1:C:419:MET:O	2.19	0.42
1:A:88:PHE:CE2	3:A:702:THG:HCG2	2.54	0.42
1:B:89:ARG:HA	1:B:90:PRO:HA	1.91	0.42
1:C:103:LEU:HD22	1:C:107:HIS:CD2	2.55	0.42
1:C:336:GLU:O	1:C:337[B]:MET:HB2	2.19	0.42
1:D:99:LEU:O	2:D:701:NAP:H1B	2.20	0.42
4:D:702:UMP:H5	6:D:802:HOH:O	2.01	0.42
1:C:430:GLY:HA3	4:C:603:UMP:O2	2.20	0.42
1:B:193[B]:VAL:HG22	6:B:1066:HOH:O	2.20	0.42
1:B:16[A]:THR:HG21	1:B:489:PHE:CD1	2.54	0.42
1:B:60:ARG:HD3	6:B:1152[A]:HOH:O	2.18	0.42
1:B:193[B]:VAL:CG2	6:B:1066:HOH:O	2.68	0.42
1:B:343:TYR:CE1	1:B:404:HIS:CE1	3.08	0.42
1:D:325:PHE:HZ	1:D:400:LEU:HD21	1.84	0.42
1:B:342:VAL:O	1:B:343:TYR:C	2.63	0.42
1:B:301:ARG:NH2	6:B:717:HOH:O	2.51	0.41
6:C:1183:HOH:O	1:D:392:PRO:HB3	2.19	0.41
1:B:190:PHE:O	5:B:613:EDO:H22	2.20	0.41
1:D:193:VAL:HA	1:D:194:PRO:HD3	1.77	0.41
1:D:315:HIS:CE1	6:D:1135:HOH:O	2.57	0.41
1:C:434[B]:ASN:ND2	4:C:603:UMP:O4	2.48	0.41
1:A:35[B]:ILE:H	1:A:35[B]:ILE:HG12	1.68	0.41
1:C:85:PRO:HA	1:C:86:PRO:HD2	1.77	0.41
1:C:386[B]:LEU:HD23	1:C:408:GLN:HA	2.02	0.41
1:C:423:ARG:NH1	1:D:383:ARG:O	2.48	0.41
2:D:701:NAP:H6N	2:D:701:NAP:H52N	2.03	0.41
1:B:249:ARG:HH12	5:B:606:EDO:H11	1.86	0.41
1:A:231:ILE:HG13	6:A:869:HOH:O	2.21	0.40
3:C:601:THG:HC5	3:C:601:THG:HC92	1.56	0.40
1:B:334:TYR:HH	1:B:397[B]:ARG:CZ	2.34	0.40
1:A:403[C]:CYS:SG	1:A:404:HIS:N	2.90	0.40
6:C:1040:HOH:O	1:D:400:LEU:CD2	2.31	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	508/521 (98%)	494 (97%)	14 (3%)	0	100	100
1	B	506/521 (97%)	495 (98%)	11 (2%)	0	100	100
1	C	497/521 (95%)	485 (98%)	12 (2%)	0	100	100
1	D	491/521 (94%)	474 (96%)	17 (4%)	0	100	100
All	All	2002/2084 (96%)	1948 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	429/446 (96%)	423 (99%)	6 (1%)	59	52
1	B	431/446 (97%)	423 (98%)	8 (2%)	50	41
1	C	424/446 (95%)	415 (98%)	9 (2%)	47	36
1	D	413/446 (93%)	408 (99%)	5 (1%)	63	57
All	All	1697/1784 (95%)	1669 (98%)	28 (2%)	63	47

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	96	ASN

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Mol	Chain	Res	Type
1	A	124[A]	SER
1	A	124[B]	SER
1	A	400	LEU
1	A	419	MET
1	B	16[A]	THR
1	B	16[B]	THR
1	B	43	TRP
1	B	192	ARG
1	B	193[A]	VAL
1	B	193[B]	VAL
1	B	429	LEU
1	B	468	ASN
1	C	35[A]	ILE
1	C	35[B]	ILE
1	C	189	VAL
1	C	193[A]	VAL
1	C	193[B]	VAL
1	C	241[A]	LEU
1	C	241[B]	LEU
1	C	281[A]	LEU
1	C	281[C]	LEU
1	D	35[A]	ILE
1	D	35[B]	ILE
1	D	193	VAL
1	D	296	LEU
1	D	420	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	GLN
1	A	252	ASN
1	A	277	ASN
1	A	404	HIS
1	A	476	GLN
1	B	121	HIS
1	B	129	ASN
1	B	143	ASN
1	B	239	GLN
1	B	255	HIS
1	B	404	HIS
1	B	469	HIS

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Mol	Chain	Res	Type
1	C	107	HIS
1	C	129	ASN
1	C	134	GLN
1	C	143	ASN
1	C	239	GLN
1	C	255	HIS
1	C	356	HIS
1	C	379	ASN
1	C	404	HIS
1	C	469	HIS
1	D	129	ASN
1	D	143	ASN
1	D	173	GLN
1	D	239	GLN
1	D	255	HIS
1	D	315	HIS
1	D	404	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](#)

59 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	711	-	3,3,3	0.42	0	2,2,2	0.38	0
5	EDO	D	706	-	3,3,3	0.43	0	2,2,2	0.38	0
5	EDO	A	716	-	3,3,3	0.45	0	2,2,2	1.18	0
5	EDO	A	704	-	3,3,3	0.42	0	2,2,2	0.38	0
5	EDO	D	707	-	3,3,3	0.40	0	2,2,2	0.64	0
5	EDO	D	708	-	3,3,3	0.43	0	2,2,2	0.38	0
5	EDO	D	712	-	3,3,3	0.38	0	2,2,2	0.22	0
5	EDO	C	612	-	3,3,3	0.83	0	2,2,2	0.71	0
5	EDO	A	708	-	3,3,3	0.38	0	2,2,2	0.41	0
5	EDO	C	606	-	3,3,3	0.42	0	2,2,2	0.38	0
5	EDO	D	709	-	3,3,3	0.89	0	2,2,2	0.75	0
5	EDO	D	713	-	3,3,3	0.42	0	2,2,2	0.38	0
5	EDO	A	706	-	3,3,3	0.61	0	2,2,2	0.80	0
5	EDO	D	704	-	3,3,3	0.43	0	2,2,2	0.88	0
5	EDO	B	604	-	3,3,3	0.42	0	2,2,2	0.38	0
5	EDO	B	612	-	3,3,3	0.43	0	2,2,2	0.38	0
5	EDO	C	605	-	3,3,3	0.33	0	2,2,2	0.82	0
5	EDO	C	607	-	3,3,3	0.43	0	2,2,2	0.38	0
5	EDO	C	610	-	3,3,3	0.42	0	2,2,2	0.38	0
2	NAP	C	602	-	50,52,52	1.80	9 (18%)	71,80,80	2.25	29 (40%)
5	EDO	A	713	-	3,3,3	0.96	0	2,2,2	0.46	0
3	THG	A	702	-	32,34,34	1.80	7 (21%)	39,47,47	1.74	8 (20%)
2	NAP	B	603	-	50,52,52	1.84	11 (22%)	71,80,80	1.86	20 (28%)
5	EDO	C	613	-	3,3,3	0.43	0	2,2,2	0.38	0
4	UMP	D	702	-	21,21,21	0.53	0	30,31,31	0.53	1 (3%)
5	EDO	A	715	-	3,3,3	0.47	0	2,2,2	0.73	0
5	EDO	B	606	-	3,3,3	0.42	0	2,2,2	0.38	0
3	THG	B	601	-	32,34,34	2.06	7 (21%)	39,47,47	1.54	6 (15%)
5	EDO	A	717	-	3,3,3	0.45	0	2,2,2	0.80	0
5	EDO	B	607	-	3,3,3	0.43	0	2,2,2	0.38	0
5	EDO	A	709	-	3,3,3	0.42	0	2,2,2	0.38	0
5	EDO	C	608	-	3,3,3	0.43	0	2,2,2	0.38	0
5	EDO	B	614	-	3,3,3	0.31	0	2,2,2	0.99	0
5	EDO	A	710	-	3,3,3	0.53	0	2,2,2	0.75	0
5	EDO	C	604	-	3,3,3	0.63	0	2,2,2	0.40	0
5	EDO	B	613	-	3,3,3	0.43	0	2,2,2	0.38	0
3	THG	D	703	-	32,34,34	1.36	3 (9%)	39,47,47	1.27	4 (10%)
5	EDO	A	707	-	3,3,3	0.47	0	2,2,2	0.78	0
2	NAP	A	701	-	50,52,52	1.73	9 (18%)	71,80,80	1.99	18 (25%)
2	NAP	D	701	-	50,52,52	1.46	8 (16%)	71,80,80	1.74	17 (23%)
5	EDO	C	609	-	3,3,3	0.43	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	608	-	3,3,3	0.42	0	2,2,2	0.38	0
5	EDO	D	710	-	3,3,3	0.43	0	2,2,2	0.38	0
5	EDO	D	711	-	3,3,3	0.41	0	2,2,2	0.75	0
5	EDO	A	714	-	3,3,3	0.43	0	2,2,2	0.38	0
5	EDO	A	705	-	3,3,3	0.56	0	2,2,2	0.79	0
4	UMP	B	602	-	21,21,21	0.85	2 (9%)	30,31,31	0.82	2 (6%)
5	EDO	C	614	-	3,3,3	0.43	0	2,2,2	0.38	0
5	EDO	A	712	-	3,3,3	0.41	0	2,2,2	0.42	0
5	EDO	B	609	-	3,3,3	0.43	0	2,2,2	0.38	0
4	UMP	A	703	-	21,21,21	0.54	0	30,31,31	0.55	1 (3%)
5	EDO	B	615	-	3,3,3	0.75	0	2,2,2	0.43	0
5	EDO	C	611	-	3,3,3	0.43	0	2,2,2	0.38	0
5	EDO	D	705	-	3,3,3	0.43	0	2,2,2	0.38	0
3	THG	C	601	-	32,34,34	1.67	6 (18%)	39,47,47	2.04	12 (30%)
4	UMP	C	603	-	21,21,21	0.54	0	30,31,31	0.54	1 (3%)
5	EDO	B	605	-	3,3,3	0.67	0	2,2,2	0.74	0
5	EDO	B	610	-	3,3,3	0.49	0	2,2,2	0.63	0
5	EDO	B	611	-	3,3,3	0.43	0	2,2,2	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	711	-	-	1/1/1/1	-
5	EDO	D	706	-	-	1/1/1/1	-
5	EDO	A	716	-	-	0/1/1/1	-
5	EDO	A	704	-	-	1/1/1/1	-
5	EDO	D	707	-	-	1/1/1/1	-
5	EDO	D	708	-	-	1/1/1/1	-
5	EDO	D	712	-	-	1/1/1/1	-
5	EDO	C	612	-	-	0/1/1/1	-
5	EDO	A	708	-	-	1/1/1/1	-
5	EDO	C	606	-	-	1/1/1/1	-
5	EDO	D	709	-	-	0/1/1/1	-
5	EDO	D	713	-	-	0/1/1/1	-
5	EDO	A	706	-	-	0/1/1/1	-
5	EDO	D	704	-	-	0/1/1/1	-
5	EDO	B	604	-	-	1/1/1/1	-
5	EDO	B	612	-	-	0/1/1/1	-
5	EDO	C	605	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	607	-	-	1/1/1/1	-
5	EDO	C	610	-	-	1/1/1/1	-
2	NAP	C	602	-	-	4/35/67/67	0/5/5/5
5	EDO	A	713	-	-	1/1/1/1	-
3	THG	A	702	-	-	2/22/31/31	0/3/3/3
2	NAP	B	603	-	-	3/35/67/67	0/5/5/5
5	EDO	C	613	-	-	1/1/1/1	-
4	UMP	D	702	-	-	1/10/22/22	0/2/2/2
5	EDO	A	715	-	-	1/1/1/1	-
5	EDO	B	606	-	-	0/1/1/1	-
3	THG	B	601	-	-	1/22/31/31	0/3/3/3
5	EDO	A	717	-	-	0/1/1/1	-
5	EDO	B	607	-	-	1/1/1/1	-
5	EDO	A	709	-	-	0/1/1/1	-
5	EDO	C	608	-	-	1/1/1/1	-
5	EDO	B	614	-	-	1/1/1/1	-
5	EDO	A	710	-	-	0/1/1/1	-
5	EDO	C	604	-	-	0/1/1/1	-
5	EDO	B	613	-	-	1/1/1/1	-
3	THG	D	703	-	-	5/22/31/31	0/3/3/3
5	EDO	A	707	-	-	1/1/1/1	-
2	NAP	A	701	-	-	5/35/67/67	0/5/5/5
2	NAP	D	701	-	-	2/35/67/67	0/5/5/5
5	EDO	C	609	-	-	1/1/1/1	-
5	EDO	B	608	-	-	1/1/1/1	-
5	EDO	D	710	-	-	1/1/1/1	-
5	EDO	D	711	-	-	0/1/1/1	-
5	EDO	A	714	-	-	0/1/1/1	-
5	EDO	A	705	-	-	0/1/1/1	-
4	UMP	B	602	-	-	1/10/22/22	0/2/2/2
5	EDO	C	614	-	-	0/1/1/1	-
5	EDO	A	712	-	-	0/1/1/1	-
5	EDO	B	609	-	-	1/1/1/1	-
4	UMP	A	703	-	-	1/10/22/22	0/2/2/2
5	EDO	B	615	-	-	0/1/1/1	-
5	EDO	C	611	-	-	1/1/1/1	-
5	EDO	D	705	-	-	0/1/1/1	-
3	THG	C	601	-	-	5/22/31/31	0/3/3/3
4	UMP	C	603	-	-	1/10/22/22	0/2/2/2
5	EDO	B	605	-	-	0/1/1/1	-
5	EDO	B	610	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	611	-	-	1/1/1/1	-

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	THG	C4A-C8A	8.01	1.52	1.38
3	A	702	THG	C4A-C8A	7.07	1.50	1.38
2	A	701	NAP	PA-O3	6.44	1.66	1.59
2	C	602	NAP	PA-O3	6.31	1.66	1.59
2	B	603	NAP	PN-O3	5.87	1.65	1.59
2	B	603	NAP	PA-O3	5.63	1.65	1.59
3	D	703	THG	C4A-C8A	5.57	1.48	1.38
3	C	601	THG	C4A-C8A	5.49	1.48	1.38
2	D	701	NAP	C5A-C4A	5.24	1.48	1.39
2	B	603	NAP	C5A-C4A	4.37	1.46	1.39
2	C	602	NAP	C8A-N7A	4.10	1.39	1.31
2	A	701	NAP	C5A-C4A	4.03	1.46	1.39
2	C	602	NAP	C5A-N7A	-3.96	1.31	1.39
2	A	701	NAP	PN-O3	3.78	1.63	1.59
2	C	602	NAP	C5A-C4A	3.77	1.45	1.39
2	C	602	NAP	PN-O3	3.56	1.63	1.59
2	D	701	NAP	C8A-N7A	3.50	1.38	1.31
3	B	601	THG	O4-C4	3.43	1.30	1.23
2	D	701	NAP	C5A-C6A	3.34	1.50	1.41
2	A	701	NAP	C8A-N7A	3.26	1.37	1.31
2	B	603	NAP	C8A-N7A	3.25	1.37	1.31
2	D	701	NAP	O4D-C1D	3.25	1.45	1.40
3	B	601	THG	C4A-C4	3.22	1.51	1.41
2	B	603	NAP	P2B-O2B	3.05	1.64	1.59
2	A	701	NAP	P2B-O2B	3.03	1.64	1.59
3	C	601	THG	C2'-C1'	3.01	1.44	1.39
2	C	602	NAP	O4D-C1D	2.88	1.44	1.40
2	D	701	NAP	PA-O3	2.77	1.62	1.59
2	C	602	NAP	P2B-O2B	2.71	1.64	1.59
2	B	603	NAP	O4D-C1D	2.69	1.44	1.40
2	A	701	NAP	C4A-N9A	-2.68	1.32	1.37
3	A	702	THG	C9-N10	2.66	1.50	1.45
2	A	701	NAP	C5A-N7A	-2.64	1.34	1.39
3	C	601	THG	O4-C4	2.63	1.28	1.23
3	A	702	THG	C4A-C4	2.56	1.49	1.41
2	C	602	NAP	C5A-C6A	2.53	1.48	1.41
4	B	602	UMP	P-OP2	-2.50	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	NAP	C4A-N3A	2.48	1.39	1.34
2	D	701	NAP	C4A-N9A	-2.46	1.32	1.37
3	C	601	THG	C4A-C4	2.45	1.49	1.41
2	B	603	NAP	C4A-N3A	2.45	1.39	1.34
2	A	701	NAP	O4D-C1D	2.45	1.44	1.40
2	B	603	NAP	C5A-N7A	-2.44	1.34	1.39
3	D	703	THG	C4-N3	-2.44	1.34	1.38
3	A	702	THG	OX1-C	2.35	1.29	1.22
2	B	603	NAP	C4A-N9A	-2.32	1.32	1.37
2	D	701	NAP	P2B-O2B	2.30	1.63	1.59
3	C	601	THG	C7-N8	-2.29	1.44	1.46
4	B	602	UMP	P-OP3	-2.19	1.46	1.54
3	D	703	THG	C4A-C4	2.19	1.48	1.41
3	B	601	THG	C2-N1	2.19	1.38	1.33
3	B	601	THG	C9-N10	2.18	1.49	1.45
3	C	601	THG	OX1-C	2.16	1.28	1.22
3	A	702	THG	C3'-C4'	2.15	1.42	1.39
2	B	603	NAP	C5A-C6A	2.14	1.46	1.41
3	A	702	THG	C6'-C1'	2.12	1.42	1.39
3	B	601	THG	C2'-C1'	2.12	1.42	1.39
2	D	701	NAP	C4A-N3A	2.10	1.38	1.34
2	B	603	NAP	P2B-O3X	-2.10	1.47	1.54
2	C	602	NAP	P2B-O2X	-2.04	1.47	1.54
3	B	601	THG	C5'-C4'	2.04	1.42	1.39
3	A	702	THG	O4-C4	2.02	1.27	1.23

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	THG	C2-N1-C8A	5.91	123.80	113.36
3	A	702	THG	C2-N1-C8A	5.75	123.51	113.36
2	C	602	NAP	N9A-C8A-N7A	-5.34	106.36	113.94
2	A	701	NAP	N3A-C2A-N1A	-5.25	120.63	128.58
2	A	701	NAP	C4A-N9A-C8A	5.19	111.19	105.74
3	C	601	THG	C7-C6-C9	-5.04	102.63	112.96
2	C	602	NAP	C5A-C4A-N3A	-4.85	120.04	126.72
2	A	701	NAP	N9A-C8A-N7A	-4.77	107.16	113.94
2	C	602	NAP	N3A-C2A-N1A	-4.62	121.59	128.58
3	B	601	THG	C2-N1-C8A	4.59	121.45	113.36
3	D	703	THG	C2-N1-C8A	4.44	121.20	113.36
2	C	602	NAP	C4A-N9A-C8A	4.24	110.19	105.74
2	D	701	NAP	C2B-C1B-N9A	-4.13	106.96	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	602	NAP	C5A-N7A-C8A	4.08	109.86	103.45
2	A	701	NAP	N3A-C4A-N9A	4.08	134.10	127.17
2	D	701	NAP	C5A-C4A-N3A	-4.05	121.13	126.72
2	A	701	NAP	C2B-C1B-N9A	-4.04	107.11	113.75
2	C	602	NAP	N3A-C4A-N9A	3.97	133.91	127.17
2	B	603	NAP	C5A-C4A-N3A	-3.96	121.27	126.72
2	A	701	NAP	C5A-C4A-N3A	-3.93	121.31	126.72
3	C	601	THG	C4-C4A-N5	3.86	126.80	116.27
2	C	602	NAP	C4D-O4D-C1D	-3.85	106.40	109.92
2	B	603	NAP	N3A-C4A-N9A	3.80	133.63	127.17
2	B	603	NAP	C4A-N9A-C8A	3.80	109.73	105.74
2	B	603	NAP	N3A-C2A-N1A	-3.75	122.91	128.58
2	D	701	NAP	C4A-C5A-N7A	-3.75	106.30	110.58
2	A	701	NAP	C2A-N1A-C6A	3.73	124.86	118.73
2	D	701	NAP	N3A-C2A-N1A	-3.71	122.97	128.58
2	C	602	NAP	C2A-N3A-C4A	3.66	120.76	111.83
2	C	602	NAP	C4A-N9A-C1B	-3.64	118.11	126.63
3	A	702	THG	O4-C4-C4A	-3.51	118.79	127.26
2	B	603	NAP	C4D-O4D-C1D	3.49	113.12	109.92
3	B	601	THG	CB-CA-C	-3.47	102.13	110.35
2	C	602	NAP	O7N-C7N-C3N	3.42	123.78	119.60
2	A	701	NAP	O2A-PA-O1A	3.40	128.26	112.44
2	B	603	NAP	O2A-PA-O1A	3.33	127.93	112.44
2	D	701	NAP	C2A-N1A-C6A	3.33	124.19	118.73
2	C	602	NAP	C3N-C7N-N7N	-3.28	113.69	117.74
2	B	603	NAP	C2B-C1B-N9A	-3.26	108.39	113.75
2	D	701	NAP	C6A-C5A-N7A	3.23	138.32	132.09
3	C	601	THG	O4-C4-C4A	-3.21	119.51	127.26
3	B	601	THG	O4-C4-C4A	-3.18	119.59	127.26
2	C	602	NAP	C2N-C3N-C4N	3.17	121.95	118.26
2	A	701	NAP	C2A-N3A-C4A	3.15	119.52	111.83
2	D	701	NAP	C4A-N9A-C8A	3.13	109.02	105.74
4	B	602	UMP	OP3-P-OP2	3.07	119.31	107.80
2	D	701	NAP	C4D-O4D-C1D	3.07	112.73	109.92
2	C	602	NAP	C5N-C6N-N1N	3.03	124.51	120.38
2	B	603	NAP	N9A-C8A-N7A	-3.02	109.65	113.94
2	C	602	NAP	C2N-N1N-C1D	3.00	125.77	119.13
2	B	603	NAP	C2A-N1A-C6A	3.00	123.66	118.73
2	B	603	NAP	O3-PN-O1N	3.00	119.72	110.70
2	D	701	NAP	O2N-PN-O3	-2.99	99.19	107.27
3	C	601	THG	C9-C6-N5	2.97	115.22	108.90
2	C	602	NAP	O5D-C5D-C4D	2.96	119.07	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	NAP	C2A-N3A-C4A	2.94	119.01	111.83
2	B	603	NAP	C2A-N3A-C4A	2.94	119.00	111.83
2	C	602	NAP	C6N-N1N-C1D	-2.92	113.99	119.73
3	C	601	THG	C9-N10-C4'	-2.88	114.66	122.00
2	C	602	NAP	C2B-C1B-N9A	-2.86	109.05	113.75
2	B	603	NAP	O3X-P2B-O2X	2.84	118.44	107.80
2	D	701	NAP	O2A-PA-O1A	2.82	125.56	112.44
3	A	702	THG	CA-N-C11	2.81	128.30	121.56
2	C	602	NAP	C4N-C3N-C7N	-2.81	113.41	121.06
2	C	602	NAP	O2B-P2B-O1X	-2.77	99.45	109.33
2	D	701	NAP	O2N-PN-O1N	2.76	125.27	112.44
2	A	701	NAP	C5A-N7A-C8A	2.75	107.78	103.45
3	A	702	THG	C4-C4A-N5	2.74	123.74	116.27
3	A	702	THG	OE1-CD-CG	-2.74	114.41	123.09
2	B	603	NAP	C4N-C3N-C7N	-2.72	113.66	121.06
2	B	603	NAP	O2B-P2B-O1X	-2.71	99.67	109.33
2	A	701	NAP	O2A-PA-O3	-2.66	100.08	107.27
2	C	602	NAP	C4A-C5A-N7A	-2.65	107.55	110.58
3	D	703	THG	O4-C4-C4A	-2.65	120.87	127.26
2	C	602	NAP	C2A-N1A-C6A	2.64	123.08	118.73
2	D	701	NAP	N3A-C4A-N9A	2.64	131.65	127.17
2	B	603	NAP	C2N-C3N-C7N	2.61	127.01	119.46
3	D	703	THG	C4-C4A-N5	2.57	123.27	116.27
3	B	601	THG	O4-C4-N3	2.55	124.92	120.11
3	C	601	THG	N3-C2-N1	-2.55	118.66	123.32
2	B	603	NAP	O2N-PN-O1N	2.51	124.13	112.44
2	A	701	NAP	O7N-C7N-C3N	2.51	122.66	119.60
3	A	702	THG	CB-CA-C	-2.50	104.43	110.35
2	D	701	NAP	N9A-C8A-N7A	-2.49	110.40	113.94
2	D	701	NAP	O3X-P2B-O2X	2.46	117.01	107.80
4	B	602	UMP	OP2-P-O5'	-2.45	100.27	106.67
2	A	701	NAP	C4A-N9A-C1B	-2.44	120.92	126.63
2	B	603	NAP	C2N-N1N-C1D	2.38	124.40	119.13
2	B	603	NAP	O3D-C3D-C4D	-2.38	104.23	111.08
2	C	602	NAP	O2N-PN-O3	-2.35	100.92	107.27
2	A	701	NAP	O2N-PN-O5D	-2.34	96.97	107.57
3	A	702	THG	C4A-C4-N3	2.33	118.52	112.13
2	C	602	NAP	C6A-C5A-N7A	2.32	136.56	132.09
3	A	702	THG	OX2-C-CA	2.30	121.28	113.51
3	B	601	THG	CA-N-C11	2.29	127.05	121.56
2	C	602	NAP	C6N-C5N-C4N	-2.28	116.16	119.45
2	D	701	NAP	C4A-N9A-C1B	-2.27	121.33	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	NAP	C5A-N7A-C8A	2.26	107.00	103.45
4	A	703	UMP	OP2-P-OP1	2.26	119.63	110.83
4	D	702	UMP	OP2-P-OP1	2.25	119.60	110.83
3	C	601	THG	O11-C11-C1'	-2.24	116.45	120.90
2	B	603	NAP	C6N-N1N-C1D	-2.24	115.33	119.73
4	C	603	UMP	OP2-P-OP1	2.24	119.57	110.83
3	C	601	THG	C4A-C4-N3	2.22	118.22	112.13
3	D	703	THG	C4A-C4-N3	2.22	118.22	112.13
2	C	602	NAP	O3X-P2B-O2X	2.22	116.11	107.80
2	C	602	NAP	C5D-C4D-C3D	-2.21	107.27	115.21
2	A	701	NAP	O4B-C4B-C5B	-2.20	102.30	109.33
2	C	602	NAP	O3-PN-O1N	-2.19	104.12	110.70
2	A	701	NAP	O2N-PN-O1N	2.17	122.56	112.44
2	A	701	NAP	O3-PN-O1N	2.16	117.19	110.70
2	C	602	NAP	O2A-PA-O1A	2.09	122.18	112.44
2	A	701	NAP	O2N-PN-O3	-2.09	101.62	107.27
3	B	601	THG	C4-C4A-N5	2.08	121.95	116.27
2	B	603	NAP	C4A-N9A-C1B	-2.06	121.82	126.63
2	C	602	NAP	C1B-N9A-C8A	2.01	131.56	127.09
3	C	601	THG	N2-C2-N3	2.01	121.00	116.76
3	C	601	THG	CB-CA-N	2.01	114.88	110.91
3	C	601	THG	C-CA-N	2.01	115.23	110.57

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	602	NAP	C2N-C3N-C7N-O7N
2	C	602	NAP	C2N-C3N-C7N-N7N
2	C	602	NAP	C4N-C3N-C7N-N7N
3	C	601	THG	C7-C6-C9-N10
3	C	601	THG	N5-C6-C9-N10
3	C	601	THG	C6-C9-N10-C4'
2	C	602	NAP	C4N-C3N-C7N-O7N
2	B	603	NAP	C3D-C4D-C5D-O5D
2	B	603	NAP	O4D-C4D-C5D-O5D
2	A	701	NAP	C4N-C3N-C7N-N7N
5	A	704	EDO	O1-C1-C2-O2
5	A	715	EDO	O1-C1-C2-O2
5	C	608	EDO	O1-C1-C2-O2
5	C	609	EDO	O1-C1-C2-O2
5	D	708	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	D	710	EDO	O1-C1-C2-O2
2	D	701	NAP	C3D-C4D-C5D-O5D
2	A	701	NAP	C4N-C3N-C7N-O7N
3	D	703	THG	C-CA-CB-CG
5	B	608	EDO	O1-C1-C2-O2
5	B	613	EDO	O1-C1-C2-O2
5	C	605	EDO	O1-C1-C2-O2
5	C	606	EDO	O1-C1-C2-O2
5	C	610	EDO	O1-C1-C2-O2
3	A	702	THG	C6-C9-N10-C4'
3	B	601	THG	C6-C9-N10-C4'
3	D	703	THG	C6-C9-N10-C4'
5	B	604	EDO	O1-C1-C2-O2
5	B	614	EDO	O1-C1-C2-O2
2	A	701	NAP	C3D-C4D-C5D-O5D
2	A	701	NAP	C2N-C3N-C7N-N7N
5	B	611	EDO	O1-C1-C2-O2
5	D	707	EDO	O1-C1-C2-O2
5	A	713	EDO	O1-C1-C2-O2
5	B	607	EDO	O1-C1-C2-O2
5	C	613	EDO	O1-C1-C2-O2
5	D	712	EDO	O1-C1-C2-O2
2	A	701	NAP	C2N-C3N-C7N-O7N
3	D	703	THG	C5'-C4'-N10-C9
5	A	707	EDO	O1-C1-C2-O2
5	B	609	EDO	O1-C1-C2-O2
2	B	603	NAP	PA-O3-PN-O1N
3	C	601	THG	OE2-CD-CG-CB
4	C	603	UMP	O4'-C4'-C5'-O5'
3	C	601	THG	OE1-CD-CG-CB
5	A	708	EDO	O1-C1-C2-O2
5	A	711	EDO	O1-C1-C2-O2
5	C	607	EDO	O1-C1-C2-O2
5	D	706	EDO	O1-C1-C2-O2
3	D	703	THG	C3'-C4'-N10-C9
3	D	703	THG	N-CA-CB-CG
4	B	602	UMP	O4'-C4'-C5'-O5'
2	D	701	NAP	PA-O3-PN-O1N
4	A	703	UMP	O4'-C4'-C5'-O5'
5	C	611	EDO	O1-C1-C2-O2
4	D	702	UMP	O4'-C4'-C5'-O5'
3	A	702	THG	OE1-CD-CG-CB

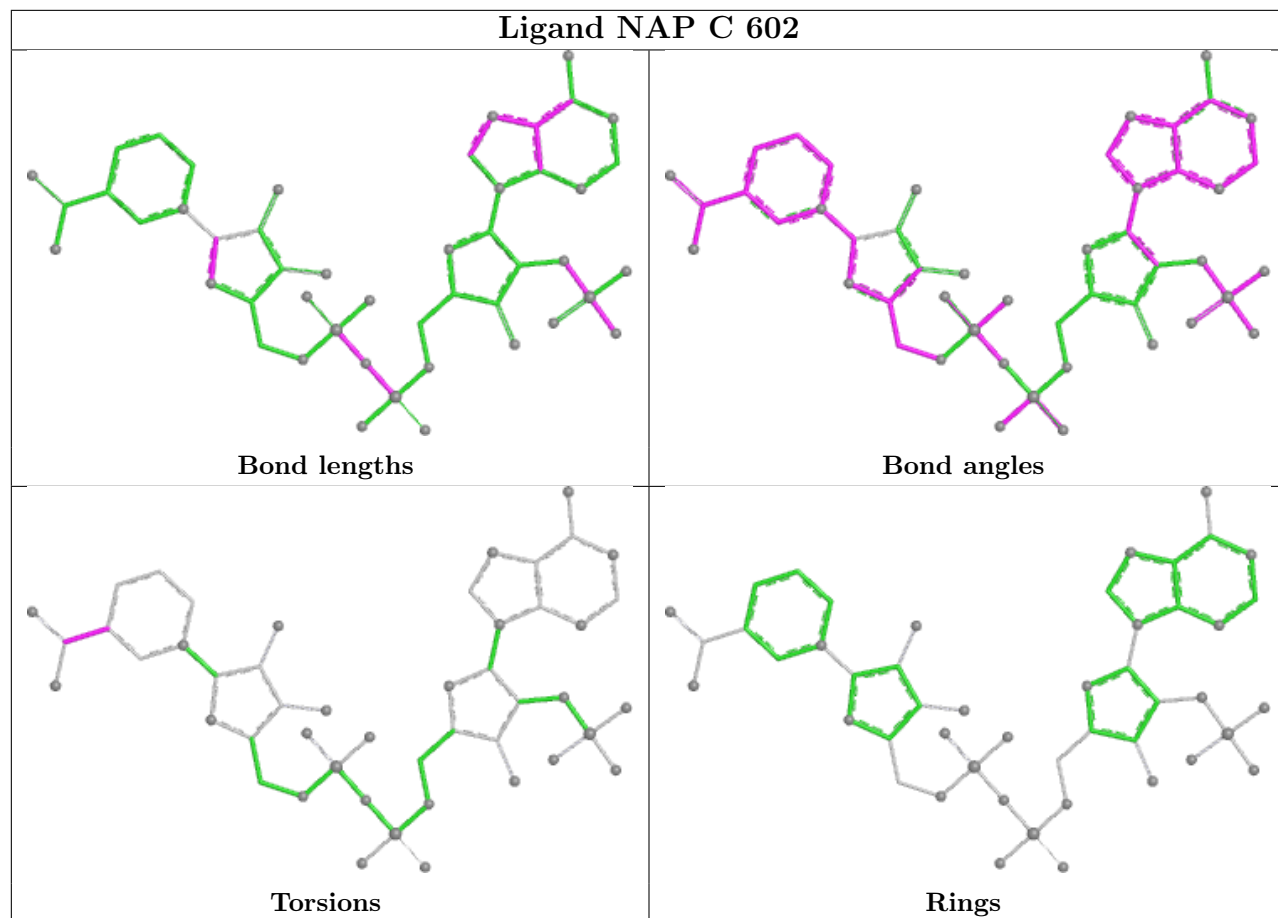
There are no ring outliers.

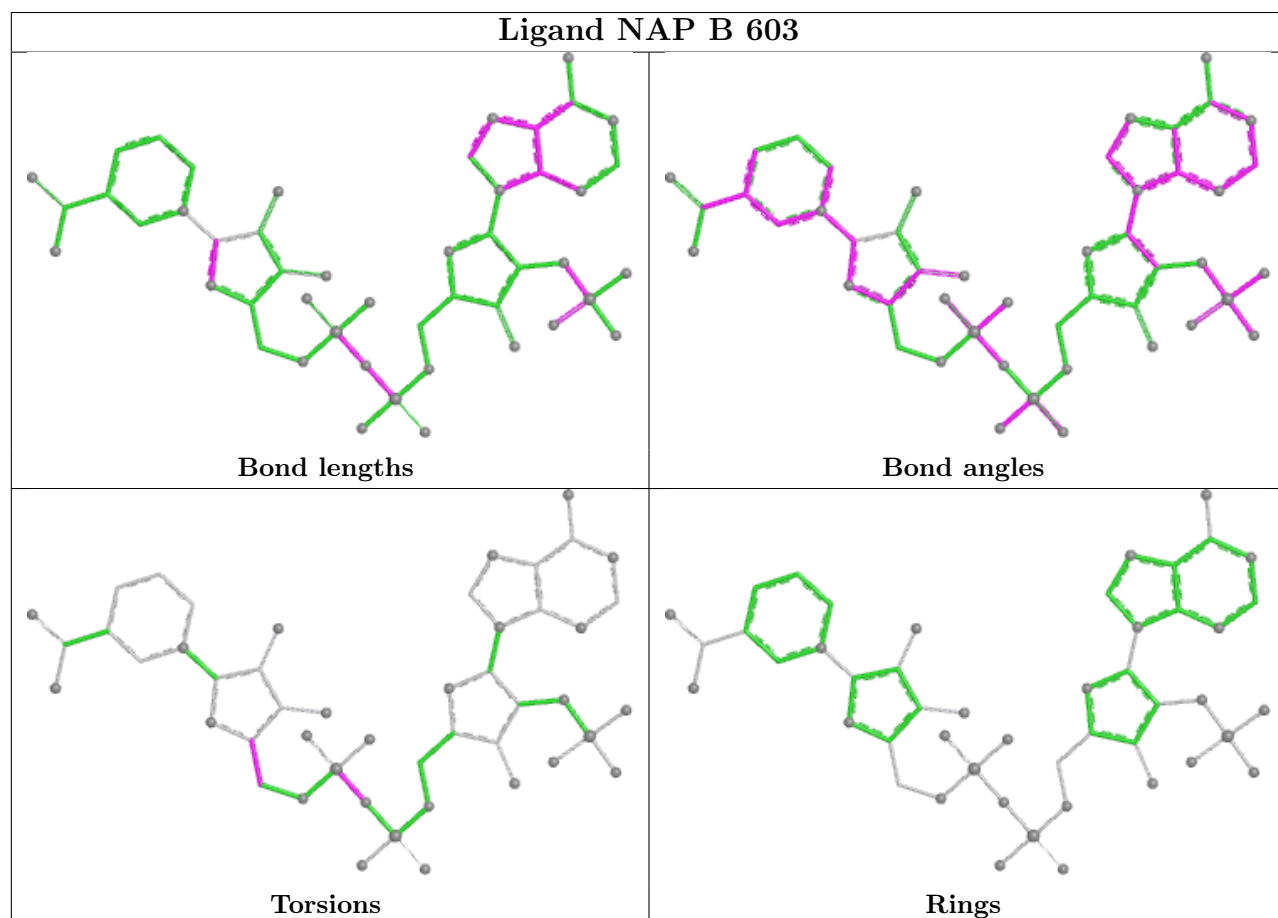
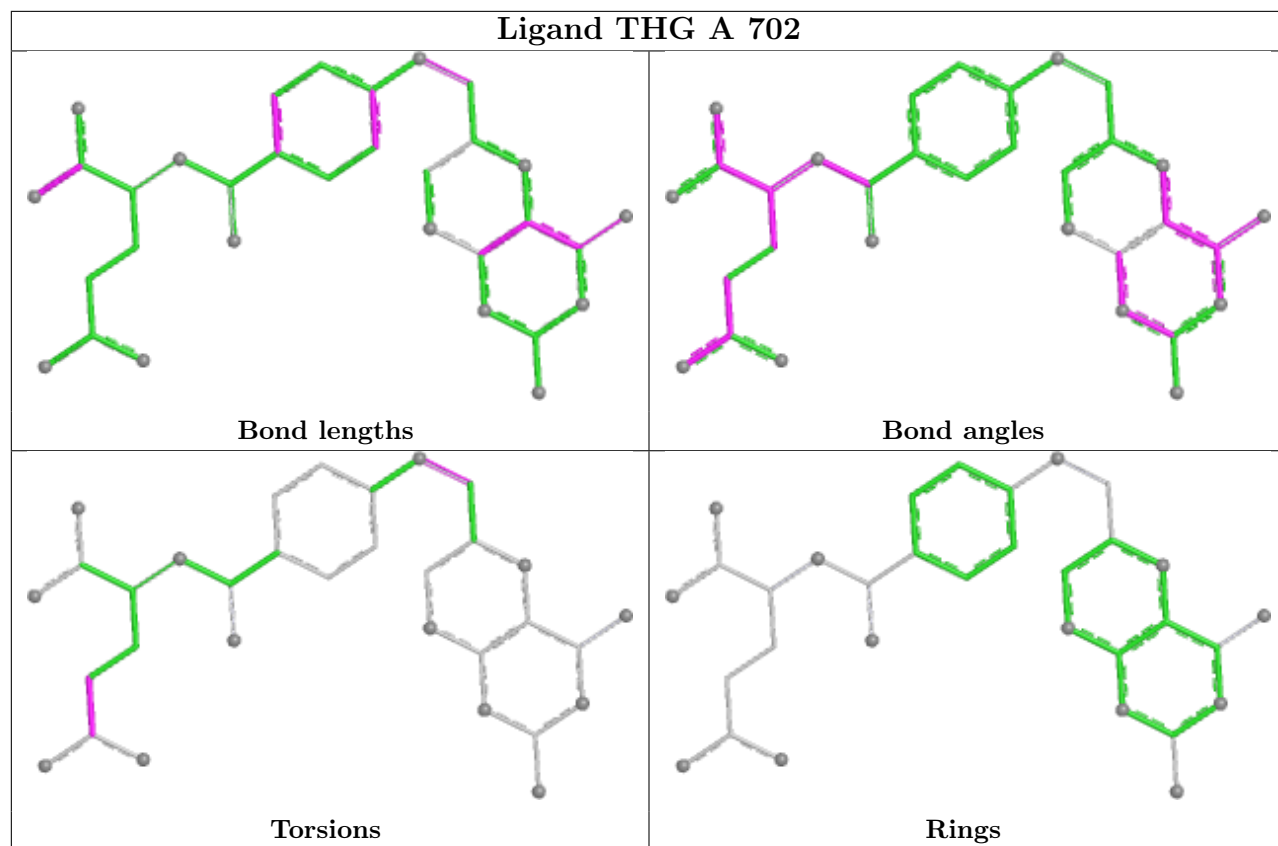
29 monomers are involved in 73 short contacts:

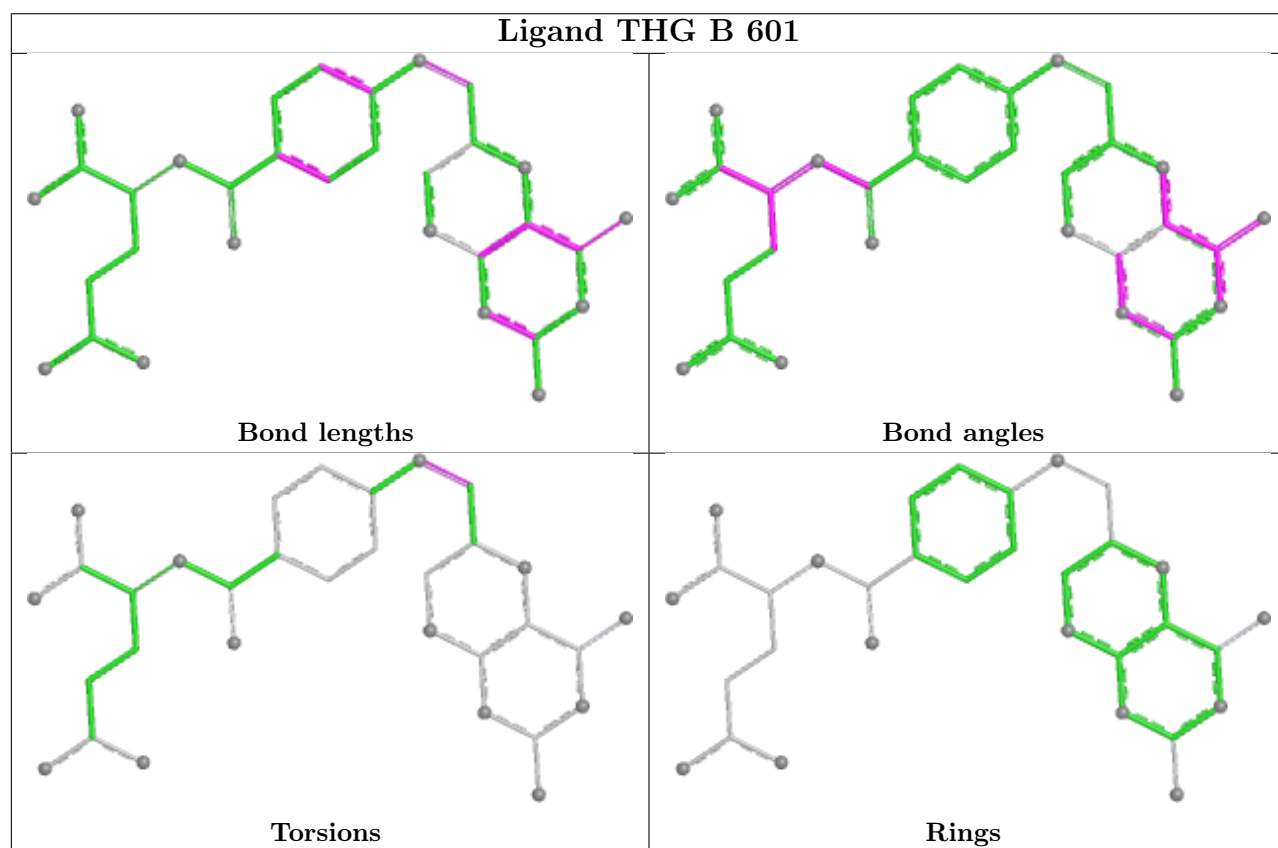
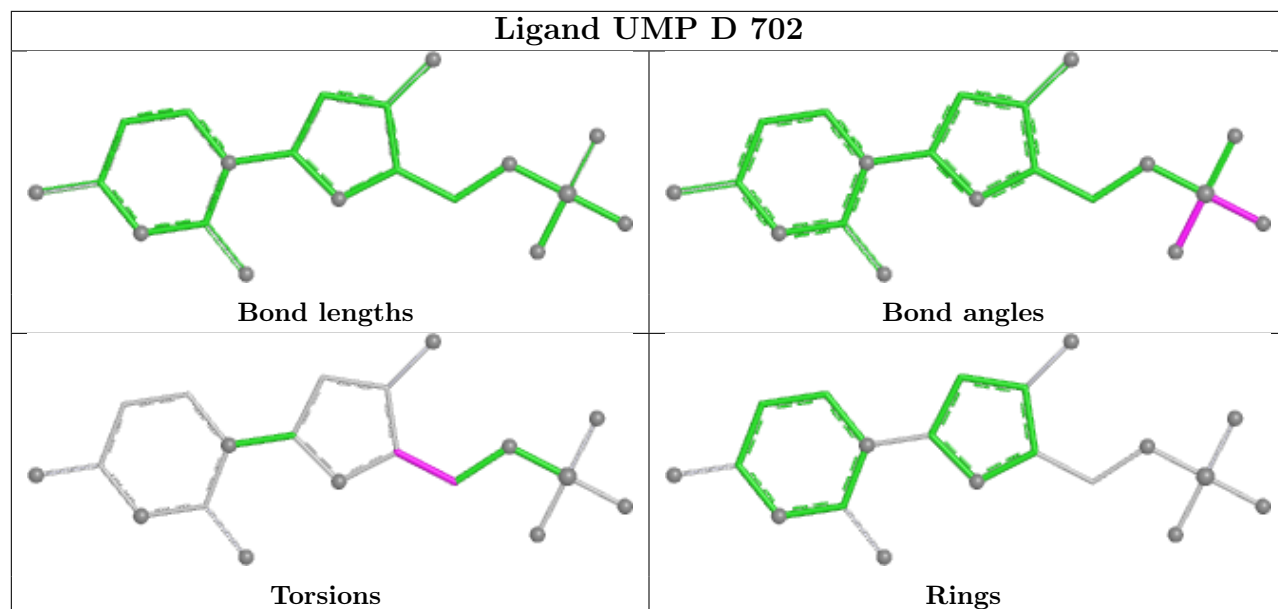
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	708	EDO	2	0
5	A	708	EDO	1	0
5	B	612	EDO	1	0
5	C	607	EDO	1	0
5	C	610	EDO	3	0
2	C	602	NAP	3	0
5	A	713	EDO	1	0
3	A	702	THG	3	0
2	B	603	NAP	11	0
4	D	702	UMP	2	0
5	B	606	EDO	2	0
3	B	601	THG	2	0
5	A	717	EDO	1	0
5	B	614	EDO	1	0
5	C	604	EDO	1	0
5	B	613	EDO	2	0
3	D	703	THG	3	0
2	A	701	NAP	5	0
2	D	701	NAP	8	0
5	D	710	EDO	1	0
5	A	714	EDO	2	0
4	B	602	UMP	3	0
5	C	614	EDO	2	0
5	B	609	EDO	1	0
4	A	703	UMP	5	0
5	C	611	EDO	3	0
3	C	601	THG	1	0
4	C	603	UMP	4	0
5	B	611	EDO	1	0

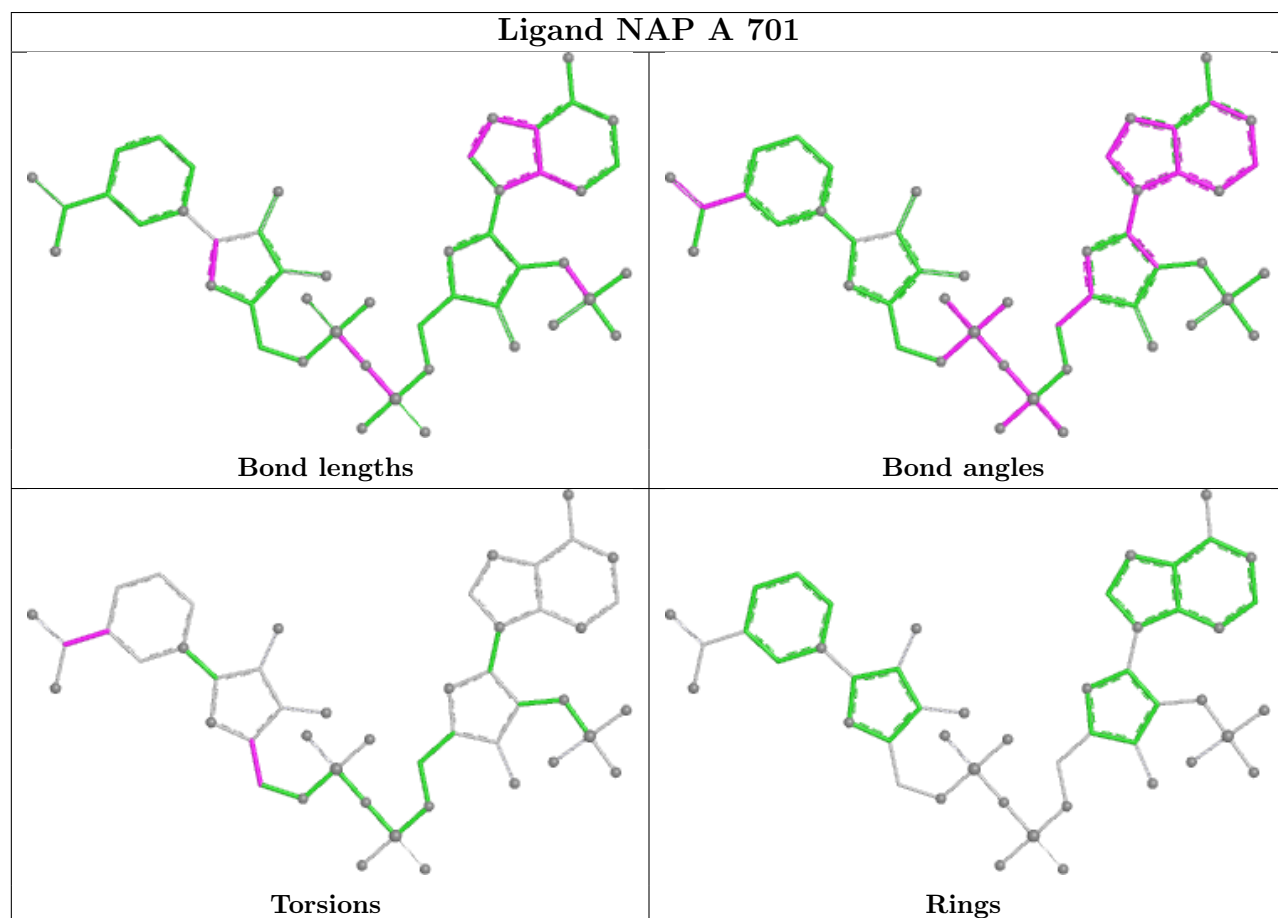
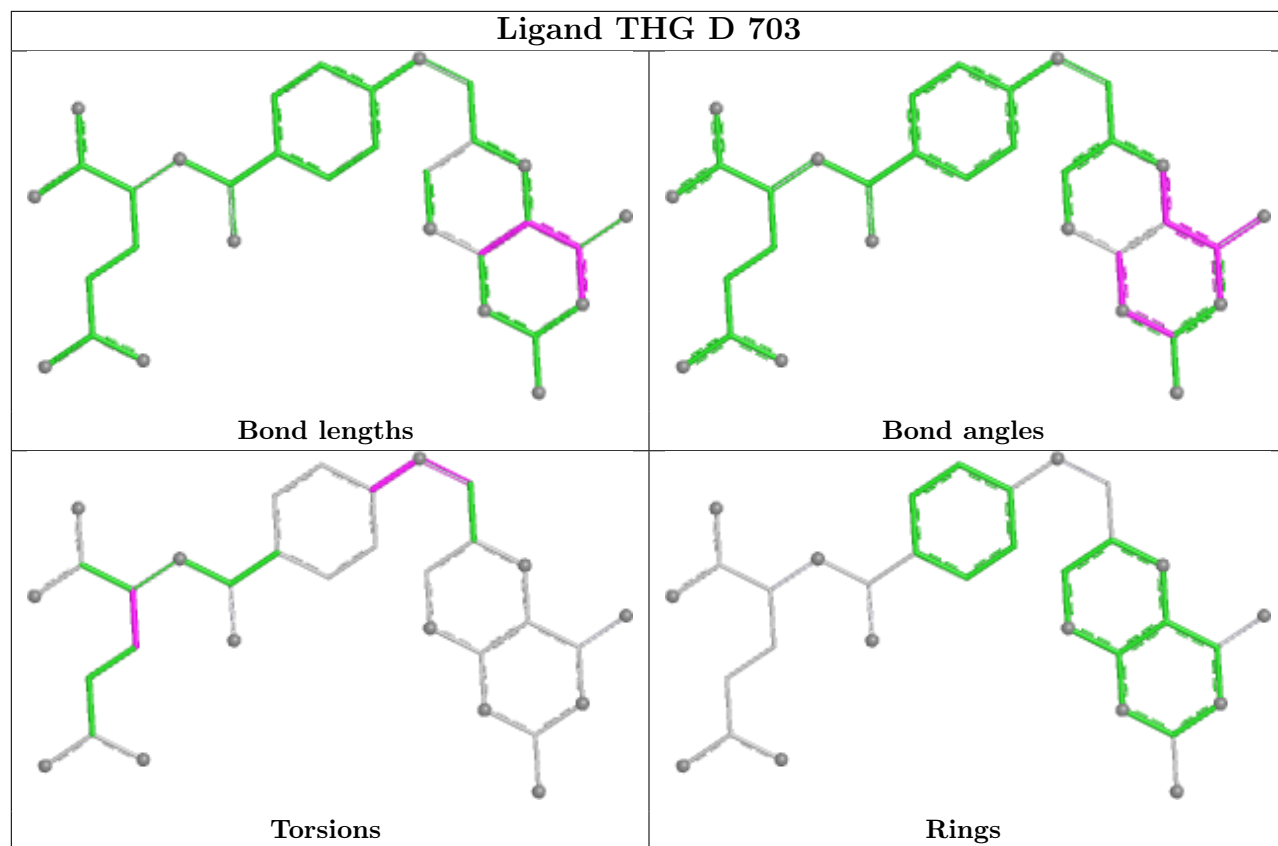
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

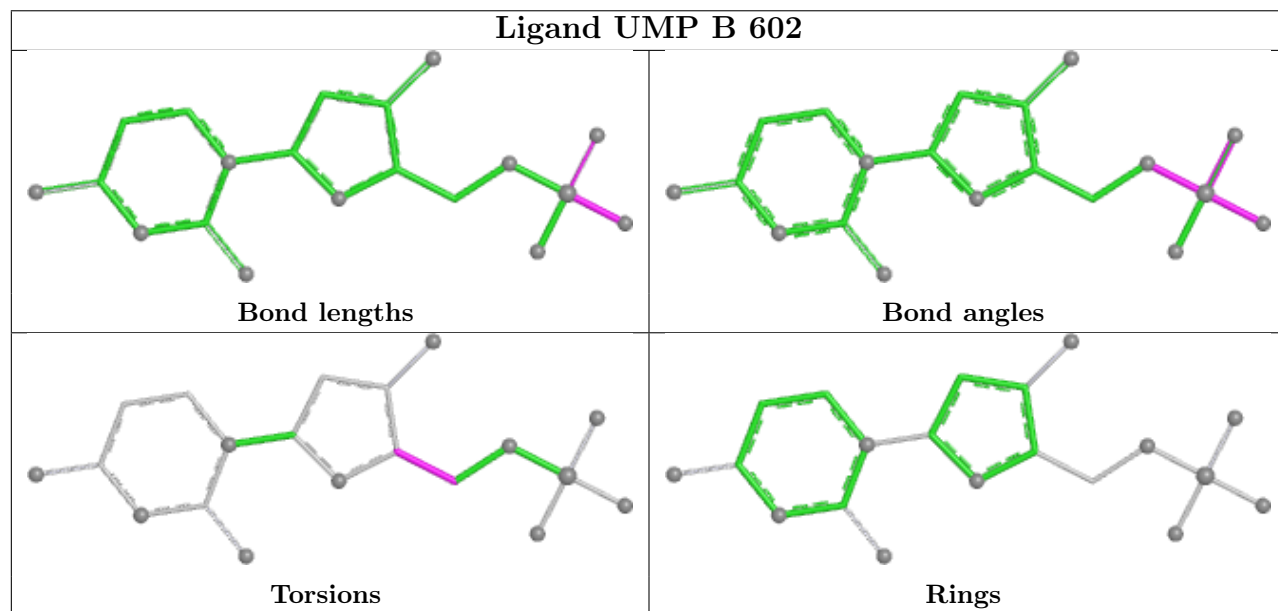
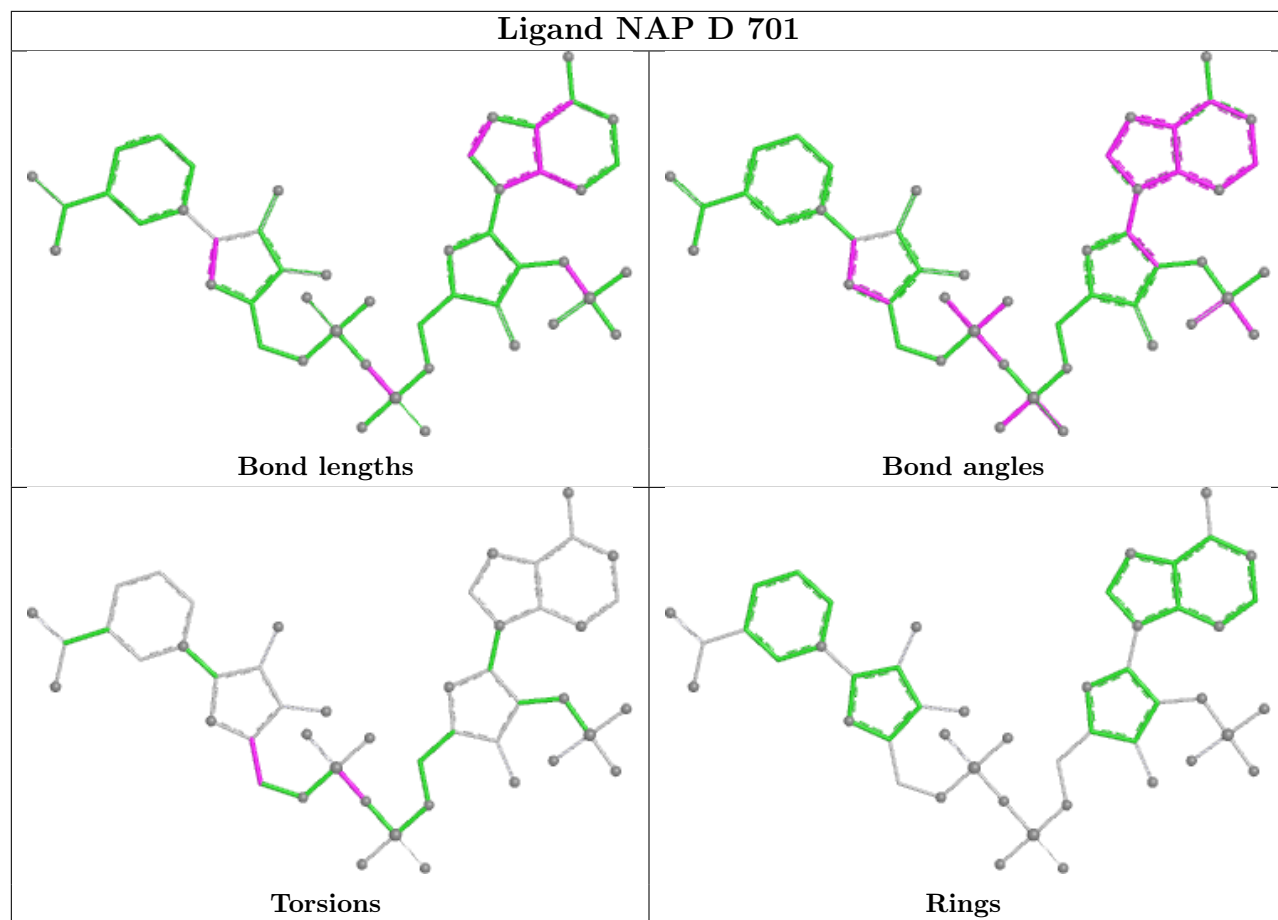
equivalents in the CSD to analyse the geometry.

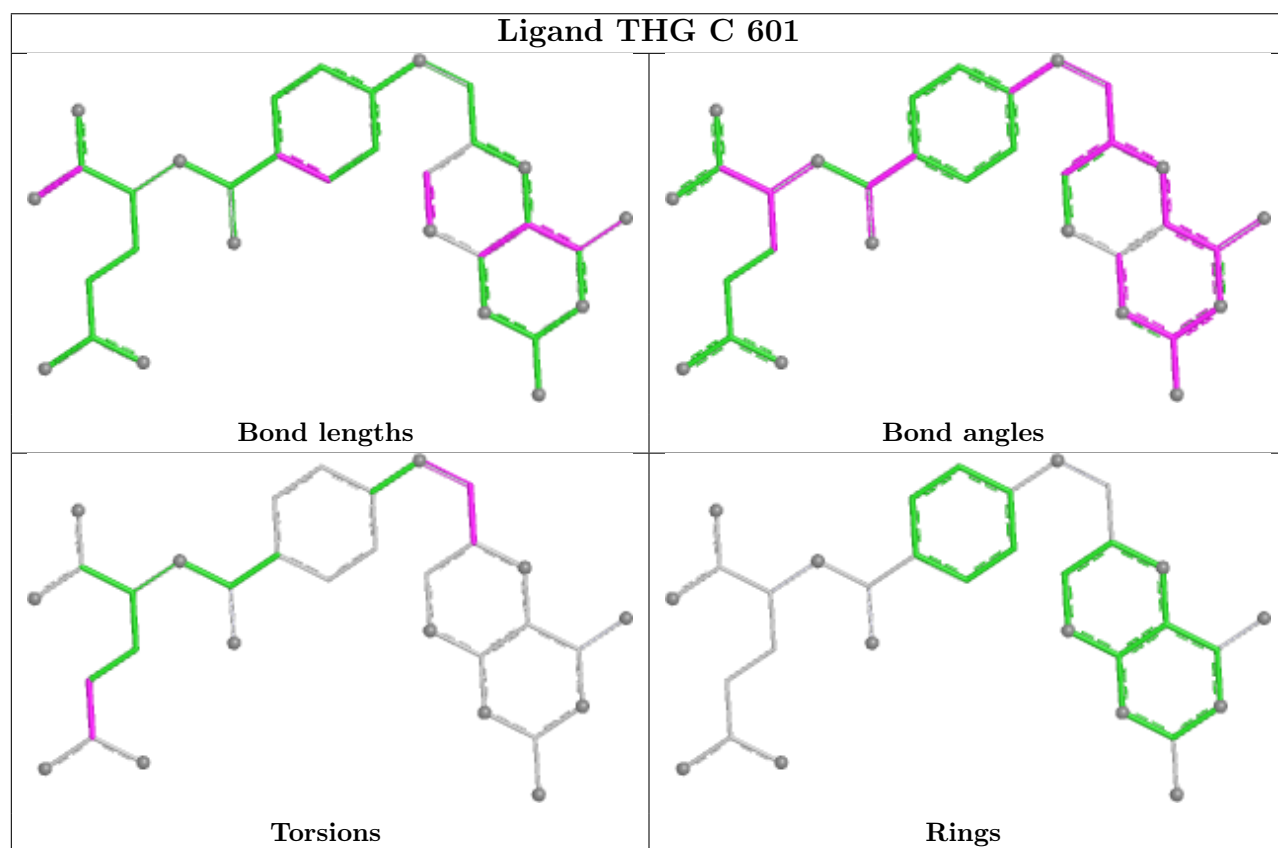
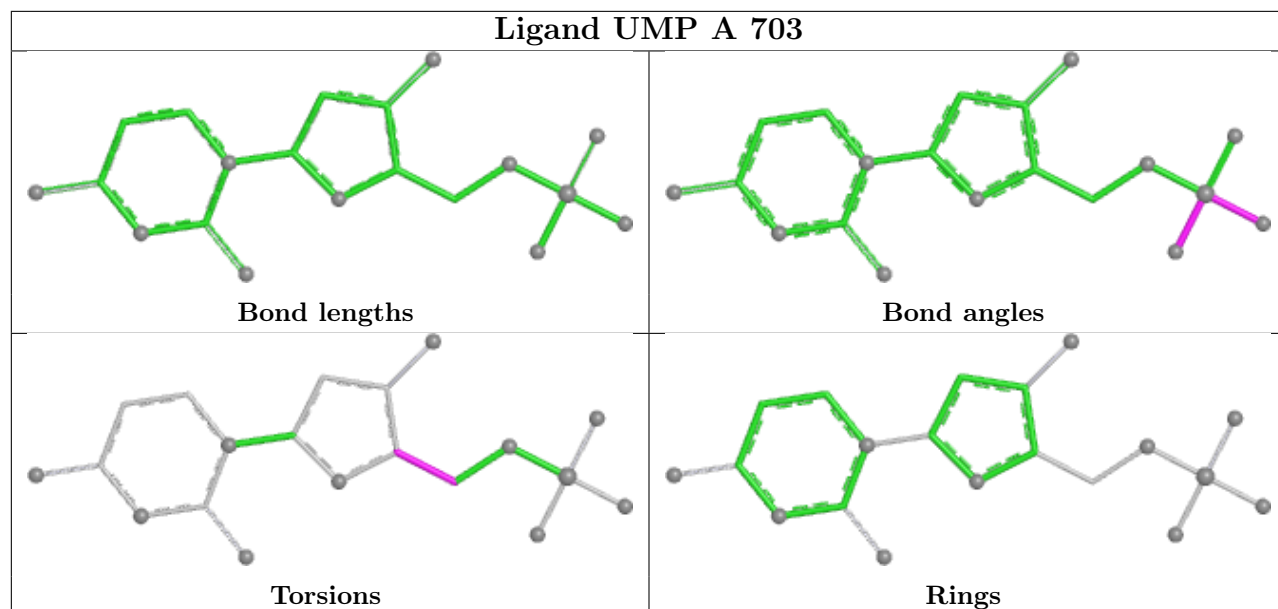


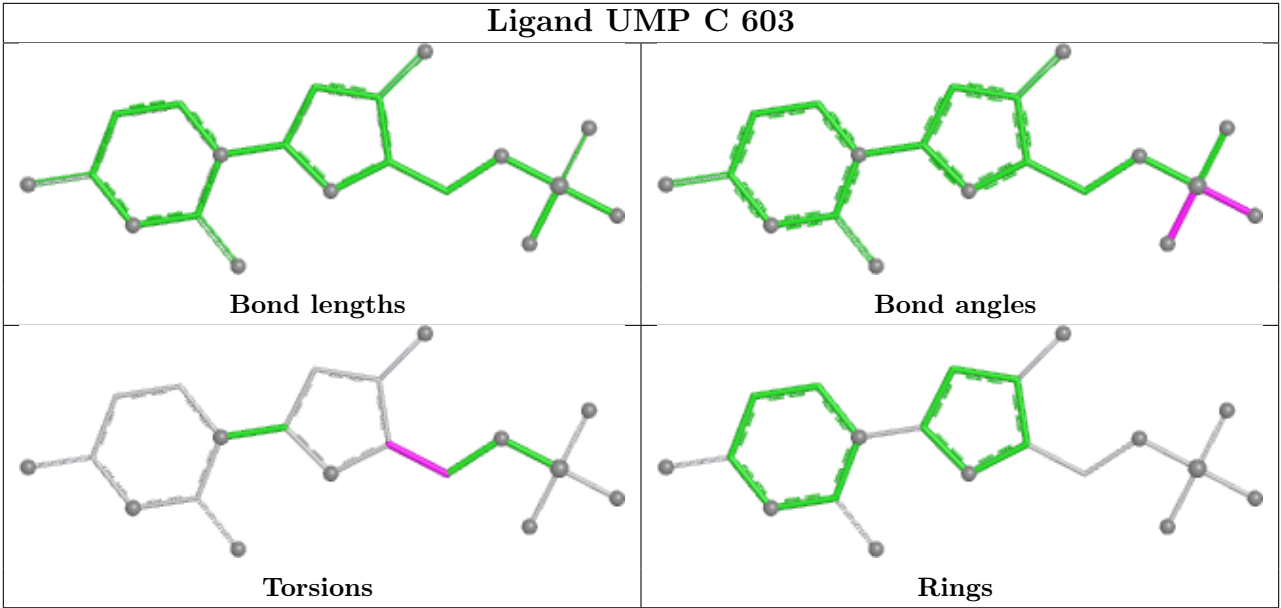












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	385:MET	C	386:LEU	N	1.14

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	494/521 (94%)	-0.05	25 (5%) 33 32	8, 21, 45, 66	24 (4%)
1	B	495/521 (95%)	-0.04	27 (5%) 30 29	9, 21, 44, 69	22 (4%)
1	C	487/521 (93%)	-0.08	17 (3%) 47 47	8, 21, 42, 65	23 (4%)
1	D	489/521 (93%)	0.07	25 (5%) 33 32	7, 23, 48, 69	13 (2%)
All	All	1965/2084 (94%)	-0.02	94 (4%) 35 34	7, 22, 45, 69	82 (4%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	36[A]	GLY	6.4
1	B	343	TYR	5.9
1	A	258	THR	5.8
1	B	400	LEU	5.8
1	D	400	LEU	5.5
1	D	343	TYR	5.1
1	B	334	TYR	5.0
1	D	36[A]	GLY	4.6
1	D	403	CYS	4.5
1	B	188	SER	4.5
1	B	43	TRP	4.4
1	B	36[A]	GLY	4.3
1	A	36[A]	GLY	4.1
1	B	91	LEU	4.0
1	D	112	LEU	4.0
1	D	88	PHE	4.0
1	D	249	ARG	3.8
1	C	63	ASN	3.7
1	D	44	ASN	3.7
1	B	122	ALA	3.6
1	B	64	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	258	THR	3.6
1	C	15	GLY	3.6
1	B	121	HIS	3.5
1	A	119	ASN	3.4
1	A	113	PRO	3.3
1	D	15	GLY	3.3
1	C	390	TRP	3.3
1	D	109	LEU	3.1
1	A	121	HIS	3.1
1	B	113	PRO	3.1
1	B	23	PHE	3.0
1	D	2	SER	3.0
1	C	85	PRO	2.9
1	B	120	LEU	2.8
1	C	88	PHE	2.8
1	A	120	LEU	2.8
1	B	305	TYR	2.8
1	A	429	LEU	2.7
1	A	190	PHE	2.7
1	D	35[A]	ILE	2.7
1	D	122	ALA	2.7
1	A	343	TYR	2.7
1	A	2	SER	2.6
1	C	64	VAL	2.6
1	B	92	PRO	2.6
1	A	15	GLY	2.6
1	A	62	LYS	2.6
1	B	60	ARG	2.5
1	A	55	LEU	2.5
1	C	182	ALA	2.5
1	C	354	TYR	2.5
1	B	2	SER	2.5
1	A	123	ASP	2.5
1	B	490	ARG	2.4
1	A	385	MET	2.4
1	B	258	THR	2.4
1	C	190	PHE	2.4
1	B	85	PRO	2.4
1	C	220	GLY	2.4
1	D	260	VAL	2.4
1	D	3	LEU	2.3
1	D	180	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	255	HIS	2.3
1	A	220	GLY	2.3
1	D	220	GLY	2.3
1	C	258	THR	2.3
1	D	102	THR	2.3
1	D	218	ALA	2.3
1	C	2	SER	2.3
1	A	182	ALA	2.2
1	D	111	GLY	2.2
1	B	15	GLY	2.2
1	D	86	PRO	2.2
1	A	122	ALA	2.2
1	B	361	TYR	2.2
1	A	44	ASN	2.2
1	A	63	ASN	2.2
1	A	30	ASP	2.2
1	B	429	LEU	2.2
1	D	223	THR	2.1
1	C	3	LEU	2.1
1	C	112	LEU	2.1
1	D	103	LEU	2.1
1	A	88	PHE	2.1
1	B	88	PHE	2.1
1	A	35[A]	ILE	2.1
1	B	468	ASN	2.1
1	C	123	ASP	2.1
1	C	16	THR	2.0
1	A	32	HIS	2.0
1	A	86	PRO	2.0
1	D	64	VAL	2.0
1	B	405	LEU	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 oligosaccharides 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(Å ²)	Q<0.9
5	EDO	A	714	4/4	0.75	0.20	38,39,49,51	0
3	THG	D	703	32/32	0.76	0.15	30,46,64,65	0
4	UMP	D	702	20/20	0.77	0.16	32,48,62,62	0
4	UMP	C	603	20/20	0.77	0.15	27,46,54,54	0
5	EDO	A	715	4/4	0.78	0.15	52,55,57,58	0
5	EDO	C	608	4/4	0.78	0.22	35,47,49,71	0
5	EDO	D	710	4/4	0.78	0.19	40,41,45,47	0
4	UMP	A	703	20/20	0.79	0.16	25,39,48,50	15
5	EDO	C	610	4/4	0.79	0.26	32,37,46,47	0
5	EDO	B	607	4/4	0.79	0.20	33,36,48,63	0
5	EDO	B	611	4/4	0.80	0.20	30,39,43,47	0
5	EDO	C	613	4/4	0.81	0.16	38,39,40,41	0
5	EDO	A	713	4/4	0.81	0.15	42,42,42,57	0
5	EDO	D	706	4/4	0.82	0.16	39,42,44,45	0
5	EDO	C	606	4/4	0.84	0.15	34,36,38,43	0
5	EDO	D	707	4/4	0.84	0.14	49,49,52,54	0
5	EDO	A	711	4/4	0.84	0.17	38,39,44,47	0
5	EDO	C	611	4/4	0.85	0.18	22,24,26,31	4
4	UMP	B	602	20/20	0.85	0.11	27,42,48,49	0
5	EDO	C	614	4/4	0.85	0.16	38,39,49,53	0
5	EDO	B	608	4/4	0.85	0.14	39,39,41,48	0
5	EDO	C	609	4/4	0.85	0.13	32,34,39,39	0
5	EDO	A	717	4/4	0.85	0.12	46,46,47,54	0
5	EDO	C	607	4/4	0.86	0.16	36,38,40,42	0
5	EDO	B	606	4/4	0.86	0.14	37,38,39,42	0
5	EDO	D	711	4/4	0.86	0.14	49,52,52,62	0
5	EDO	B	610	4/4	0.87	0.13	47,51,54,56	0
5	EDO	D	708	4/4	0.87	0.18	29,32,35,38	0
5	EDO	B	614	4/4	0.88	0.10	41,42,45,54	0
5	EDO	B	604	4/4	0.88	0.12	33,36,36,37	0
5	EDO	B	612	4/4	0.89	0.18	34,39,40,41	0
5	EDO	B	613	4/4	0.89	0.13	38,45,48,52	0
5	EDO	A	716	4/4	0.89	0.12	34,40,42,43	0
3	THG	A	702	32/32	0.89	0.10	24,38,50,55	0
3	THG	B	601	32/32	0.90	0.09	24,36,44,54	0
5	EDO	A	709	4/4	0.90	0.13	30,31,43,55	0
5	EDO	B	609	4/4	0.90	0.14	34,47,48,49	0

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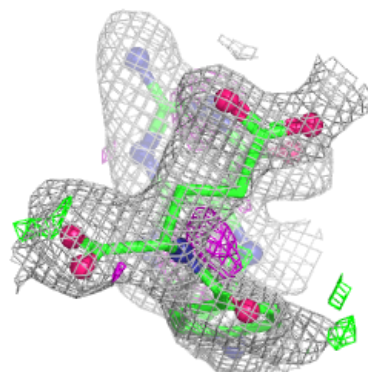
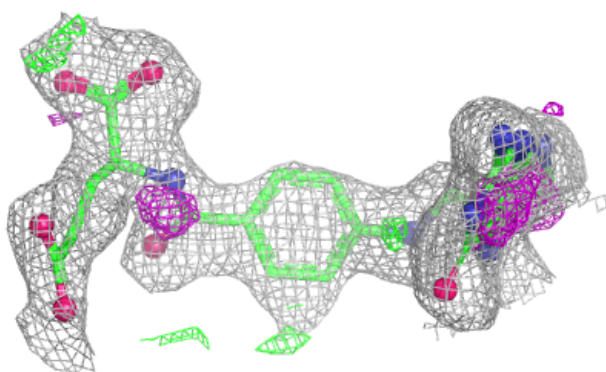
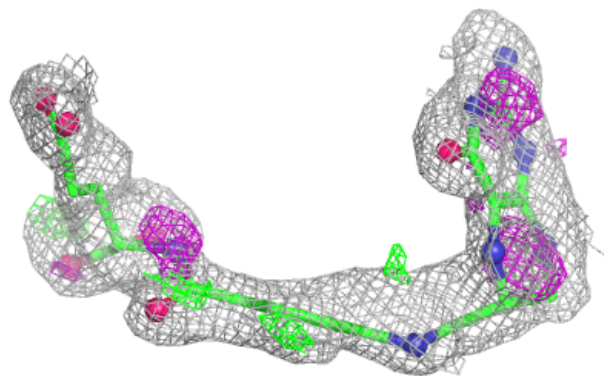
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	D	713	4/4	0.90	0.12	30,35,36,38	0
3	THG	C	601	32/32	0.91	0.10	27,44,53,55	0
5	EDO	A	704	4/4	0.91	0.10	27,30,30,34	0
5	EDO	C	605	4/4	0.91	0.10	36,38,43,51	0
5	EDO	D	705	4/4	0.91	0.14	31,43,43,51	0
5	EDO	A	708	4/4	0.91	0.12	37,41,43,54	0
5	EDO	D	712	4/4	0.92	0.10	27,32,33,42	0
2	NAP	D	701	48/48	0.92	0.12	31,37,112,117	0
5	EDO	B	605	4/4	0.93	0.08	23,23,24,25	0
5	EDO	A	710	4/4	0.93	0.10	28,29,36,44	0
5	EDO	A	712	4/4	0.93	0.09	35,43,46,54	0
5	EDO	C	604	4/4	0.94	0.07	21,21,22,22	0
5	EDO	A	707	4/4	0.94	0.10	31,32,32,45	0
5	EDO	D	709	4/4	0.95	0.08	24,25,28,29	0
2	NAP	A	701	48/48	0.96	0.10	25,31,88,97	0
5	EDO	A	706	4/4	0.96	0.06	22,23,23,26	0
5	EDO	D	704	4/4	0.96	0.07	21,22,23,25	0
2	NAP	B	603	48/48	0.96	0.10	23,30,95,101	0
2	NAP	C	602	48/48	0.96	0.10	25,32,101,111	0
5	EDO	C	612	4/4	0.96	0.07	23,24,25,27	0
5	EDO	B	615	4/4	0.97	0.06	26,26,27,29	0
5	EDO	A	705	4/4	0.97	0.06	20,22,22,23	0

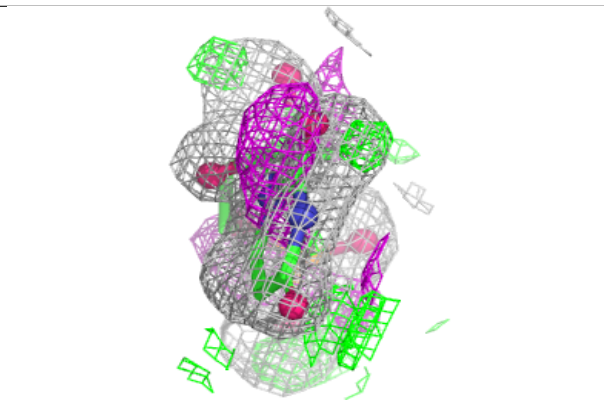
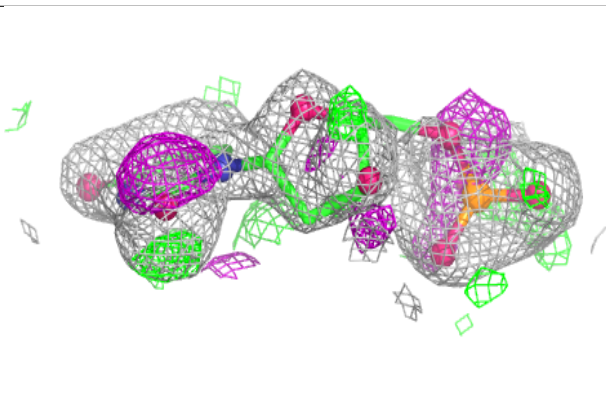
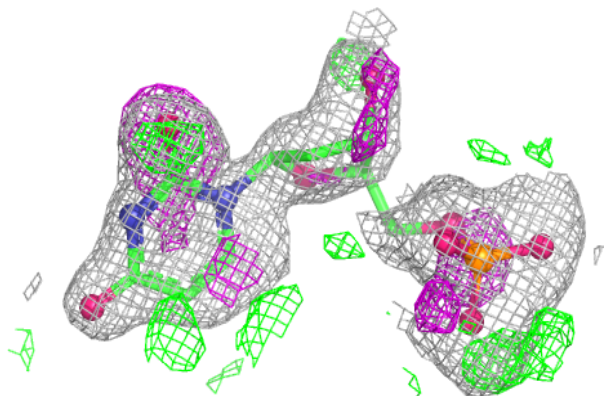
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around THG D 703:

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

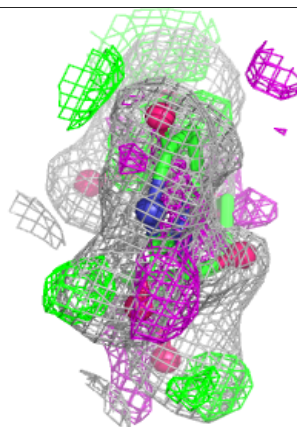
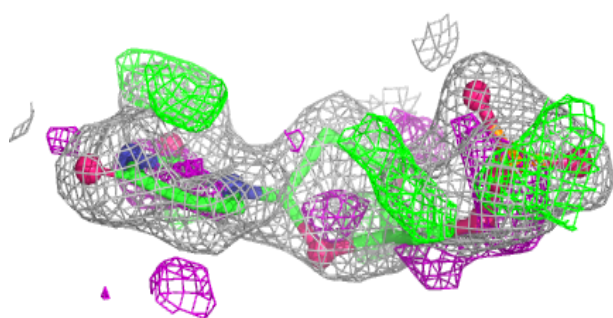
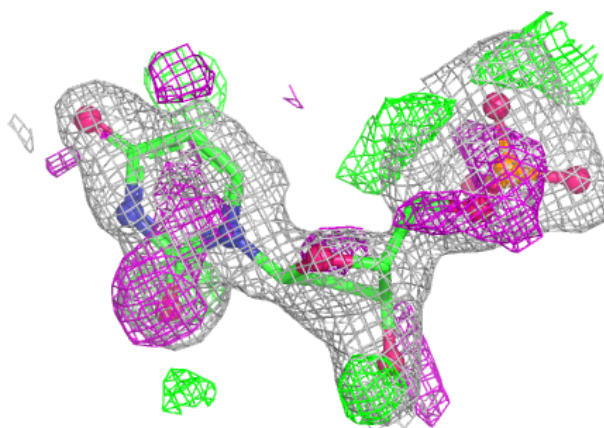
**Electron density around UMP D 702:**

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

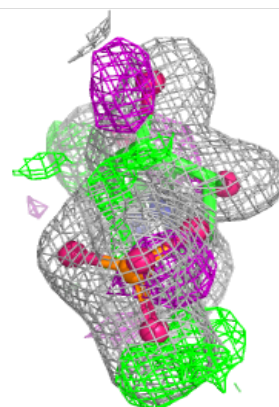
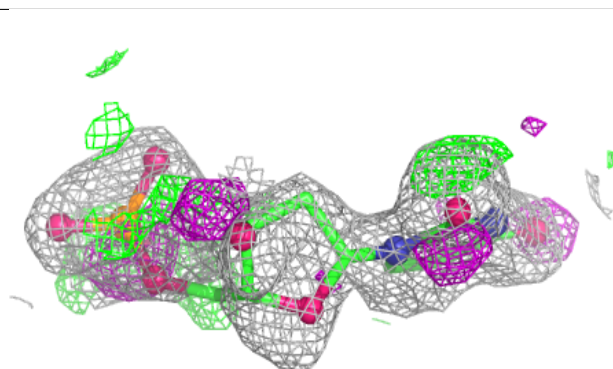
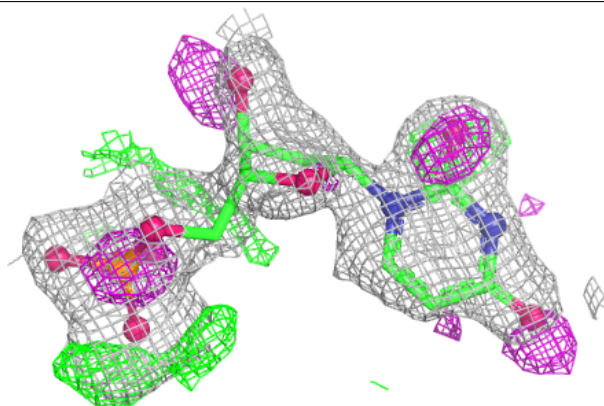


Electron density around UMP C 603:

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

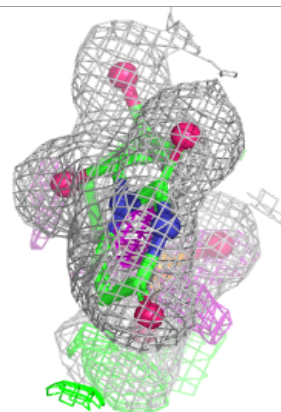
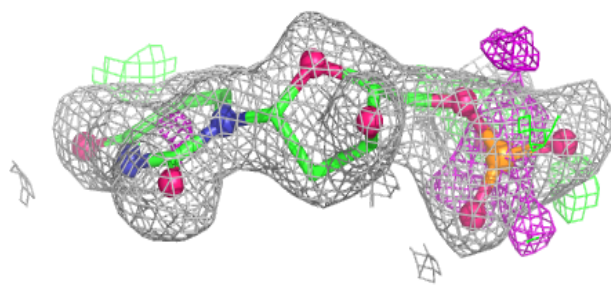
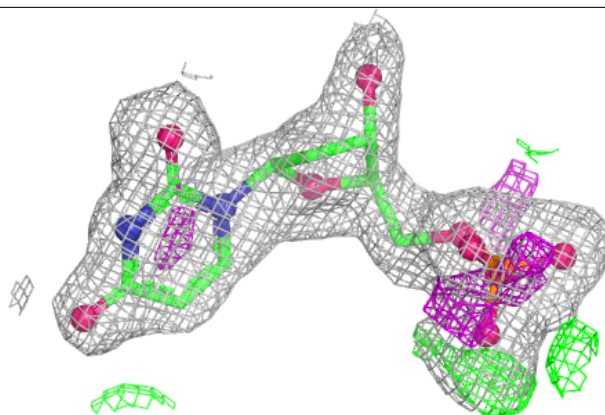
**Electron density around UMP A 703:**

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

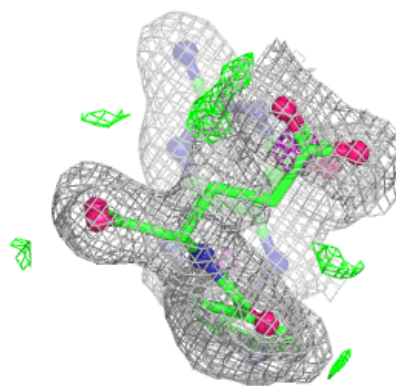
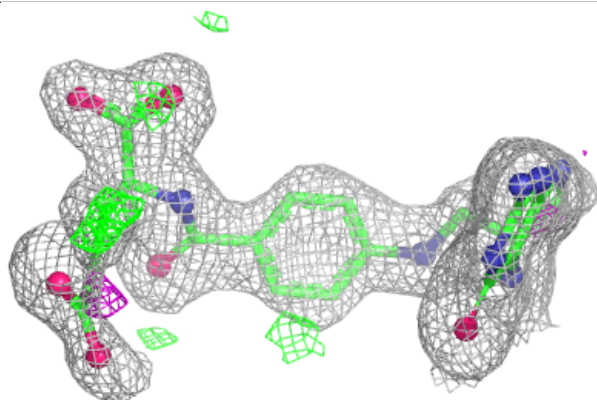
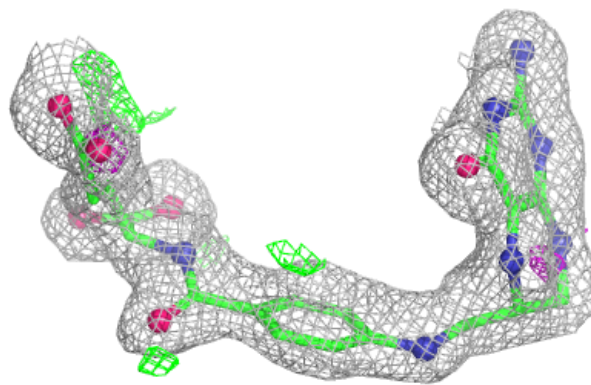


Electron density around UMP B 602:

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

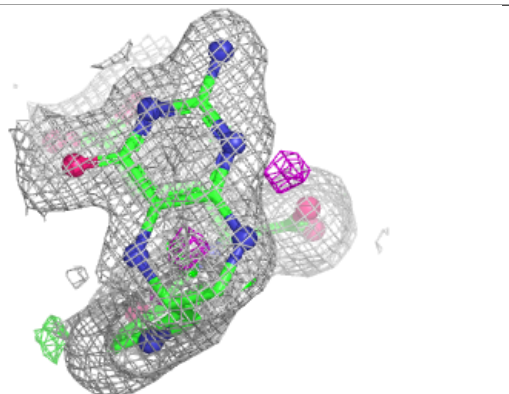
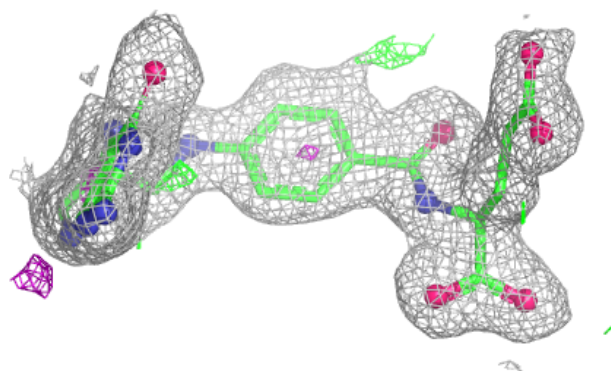
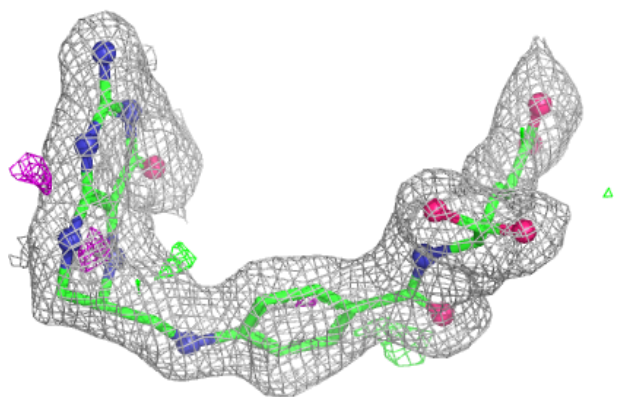
**Electron density around THG A 702:**

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

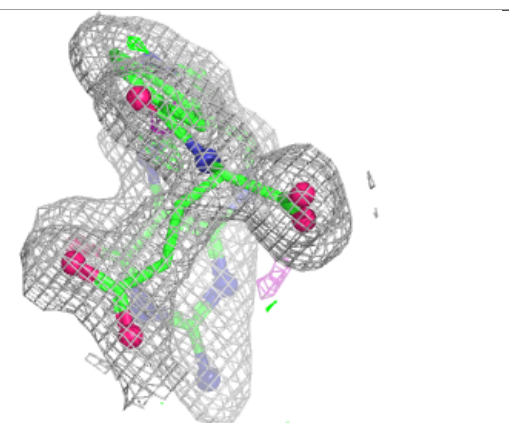
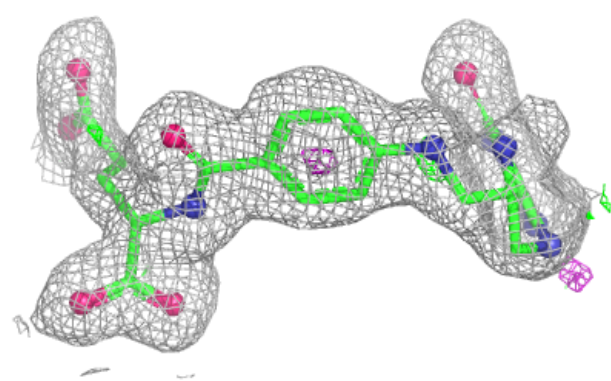
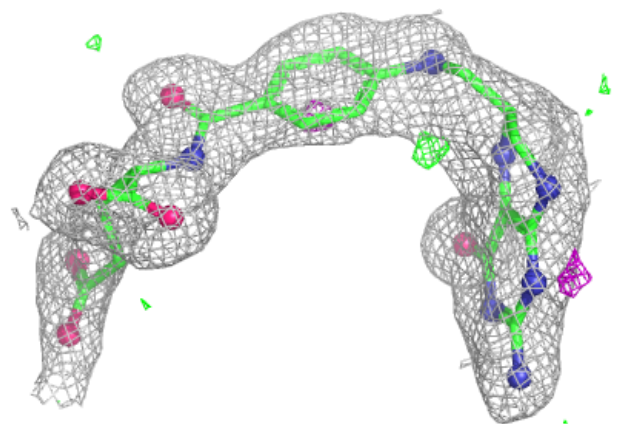


Electron density around THG B 601:

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

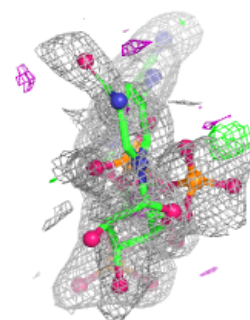
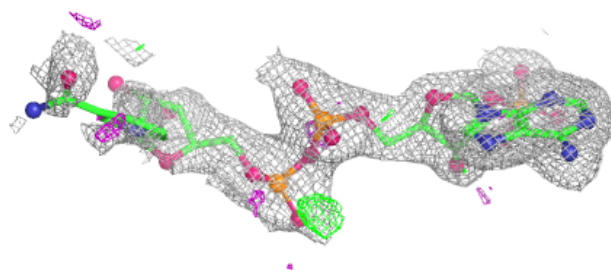
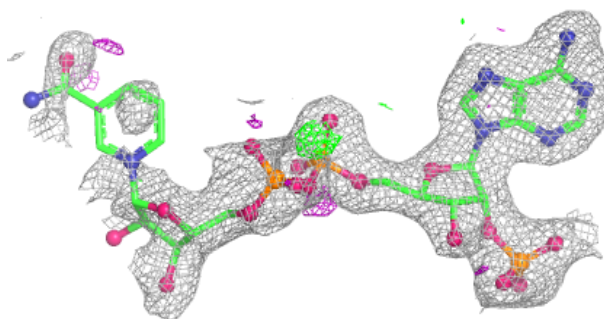
**Electron density around THG C 601:**

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

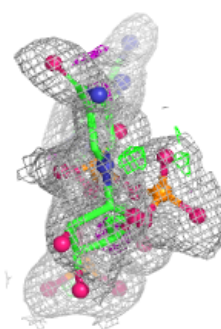
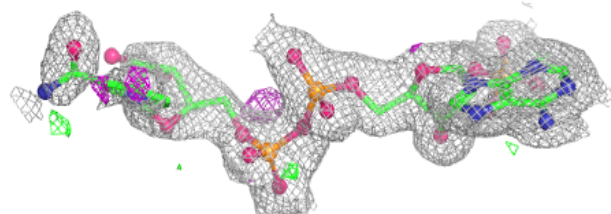
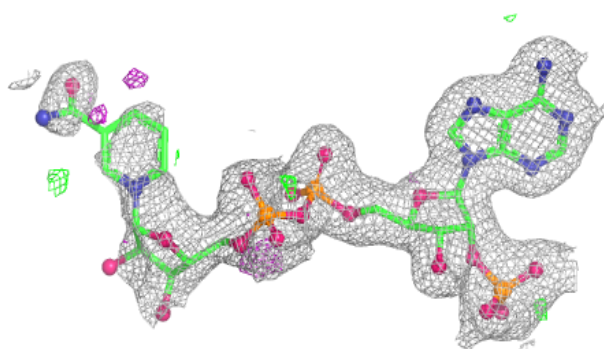


Electron density around NAP D 701:

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

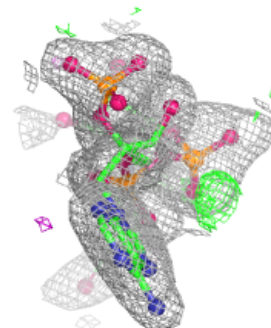
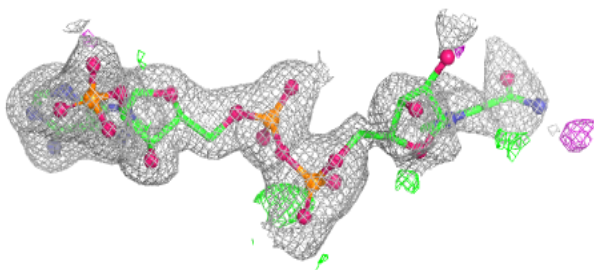
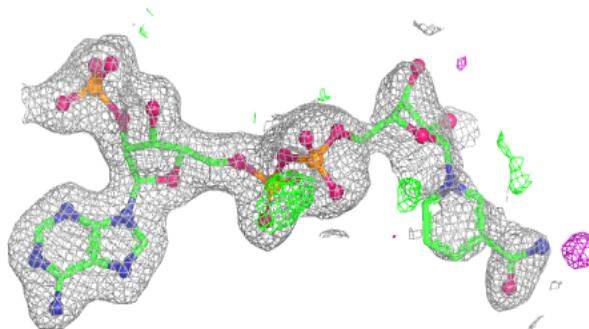
**Electron density around NAP A 701:**

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

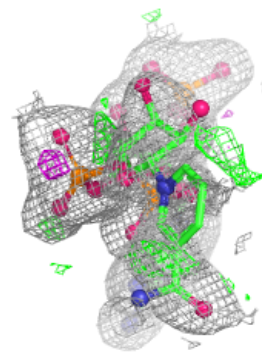
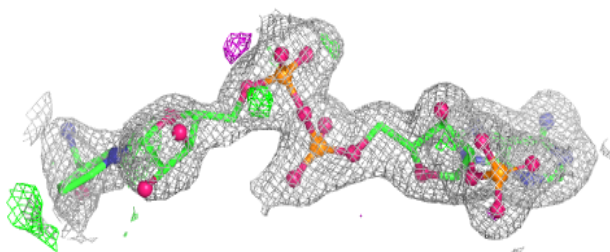
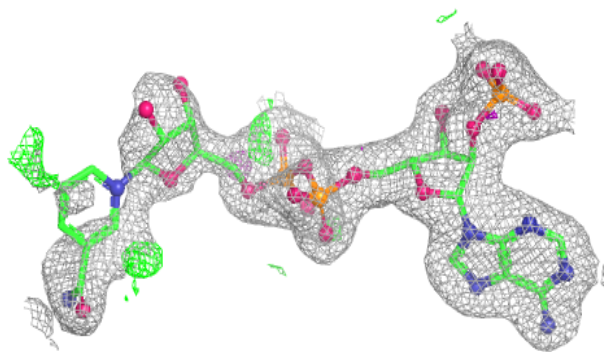


Electron density around NAP B 603:

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

**Electron density around NAP C 602:**

$2mF_o-DF_c$ (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.