



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 06:38 AM EDT

PDB ID : 3CLB / pdb\_00003clb  
Title : Structure of bifunctional TcDHFR-TS in complex with TMQ  
Authors : Schormann, N.; Senkovich, O.; Chattopadhyay, D.  
Deposited on : 2008-03-18  
Resolution : 3.00 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

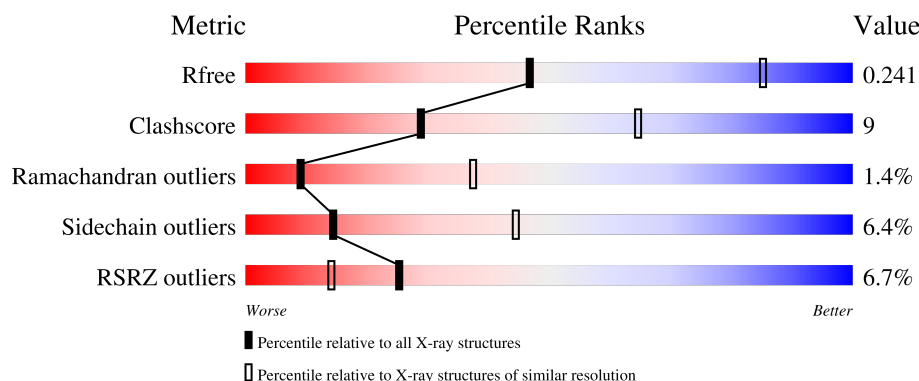
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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  $\geq 3$ , 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	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 83%, yellow 83%, yellow 96%, orange 96%, orange 99%, grey 99%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>83%</span> <span>13%</span> <span>..</span> </div> </div>
1	B	521	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 20%, green 20%, green 78%, yellow 78%, yellow 93%, orange 93%, orange 96%, grey 96%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>20%</span> <span>78%</span> <span>15%</span> <span>..</span> </div> </div>
1	C	521	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, green 4%, green 82%, yellow 82%, yellow 95%, orange 95%, orange 98%, grey 98%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>82%</span> <span>13%</span> <span>..</span> </div> </div>
1	D	521	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, green 2%, green 81%, yellow 81%, yellow 95%, orange 95%, orange 98%, grey 98%, grey 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>81%</span> <span>14%</span> <span>..</span> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16618 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.

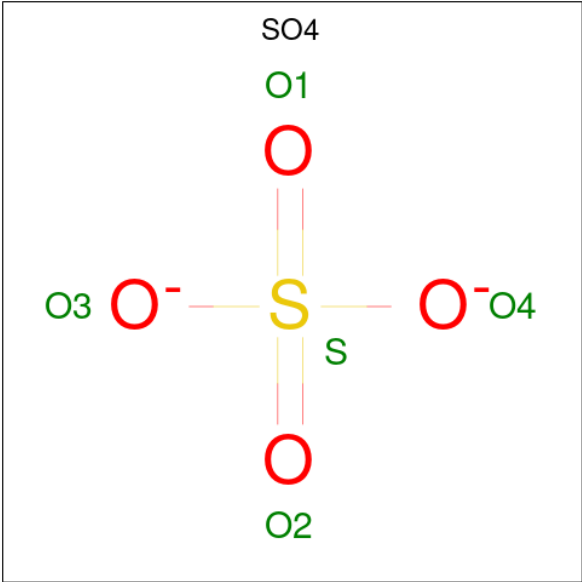
- Molecule 1 is a protein called DHFR-TS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4052	2571	714	749	18			
1	B	508	Total	C	N	O	S	0	0	0
			4036	2562	710	746	18			
1	C	510	Total	C	N	O	S	0	0	0
			4054	2573	714	748	19			
1	D	509	Total	C	N	O	S	0	0	0
			4038	2562	713	745	18			

There are 12 discrepancies between the modelled and reference sequences:

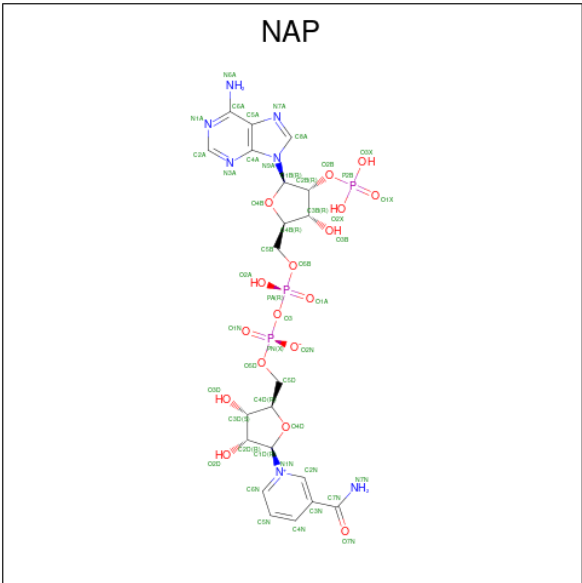
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ARG	HIS	SEE REMARK 999	UNP Q27793
A	55	VAL	LEU	SEE REMARK 999	UNP Q27793
A	137	GLN	ARG	SEE REMARK 999	UNP Q27793
B	32	ARG	HIS	SEE REMARK 999	UNP Q27793
B	55	VAL	LEU	SEE REMARK 999	UNP Q27793
B	137	GLN	ARG	SEE REMARK 999	UNP Q27793
C	32	ARG	HIS	SEE REMARK 999	UNP Q27793
C	55	VAL	LEU	SEE REMARK 999	UNP Q27793
C	137	GLN	ARG	SEE REMARK 999	UNP Q27793
D	32	ARG	HIS	SEE REMARK 999	UNP Q27793
D	55	VAL	LEU	SEE REMARK 999	UNP Q27793
D	137	GLN	ARG	SEE REMARK 999	UNP Q27793

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



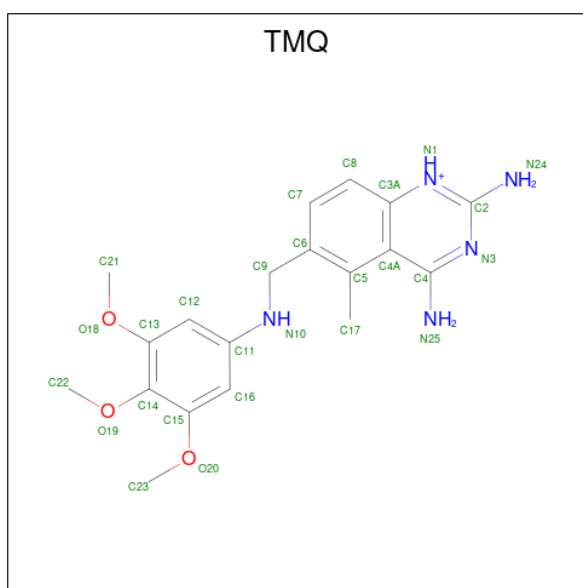
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

- Molecule 4 is TRIMETREXATE (CCD ID: TMQ) (formula:  $C_{19}H_{24}N_5O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			27	19	5	3		
4	B	1	Total	C	N	O	0	0
			27	19	5	3		
4	C	1	Total	C	N	O	0	0
			27	19	5	3		
4	D	1	Total	C	N	O	0	0
			27	19	5	3		

- 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	0	0
			4	2	2		
5	A	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	D	1	Total	C	O	0	0
			4	2	2		

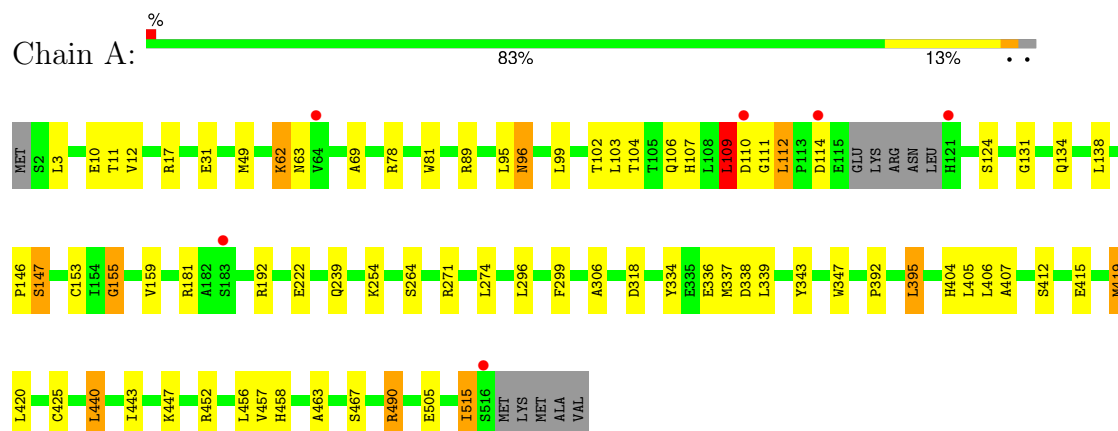
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total	O	0	0
			19	19		
6	B	21	Total	O	0	0
			21	21		
6	C	30	Total	O	0	0
			30	30		
6	D	24	Total	O	0	0
			24	24		

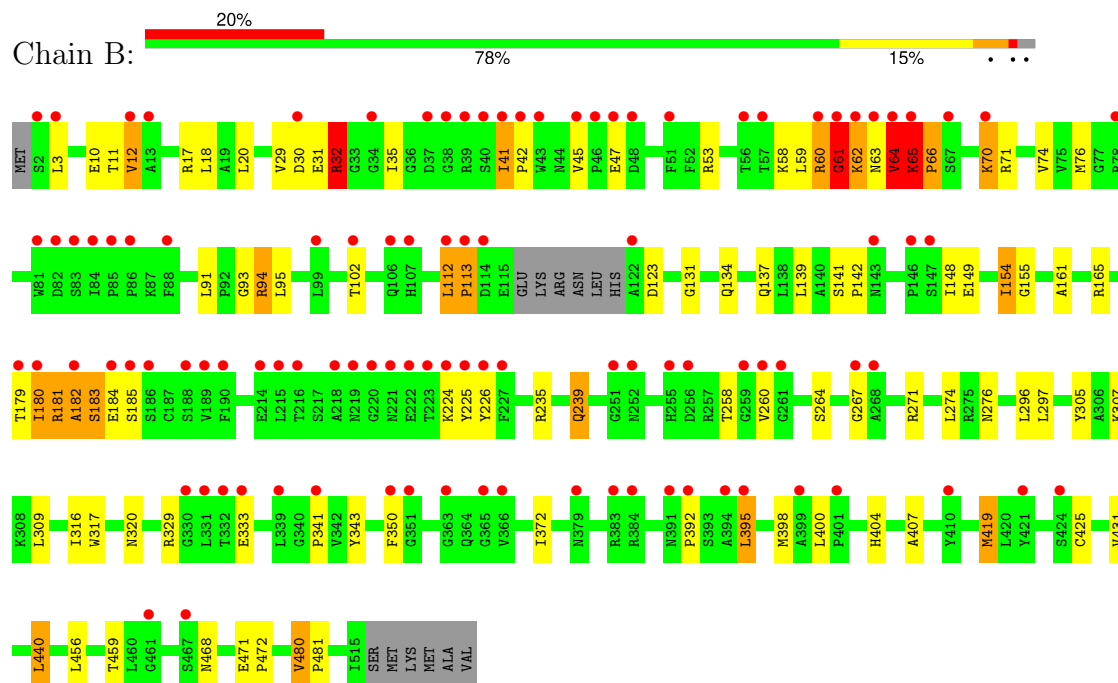
### 3 Residue-property plots

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.

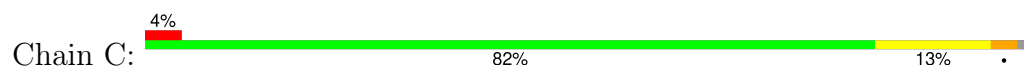
#### • Molecule 1: DHFR-TS

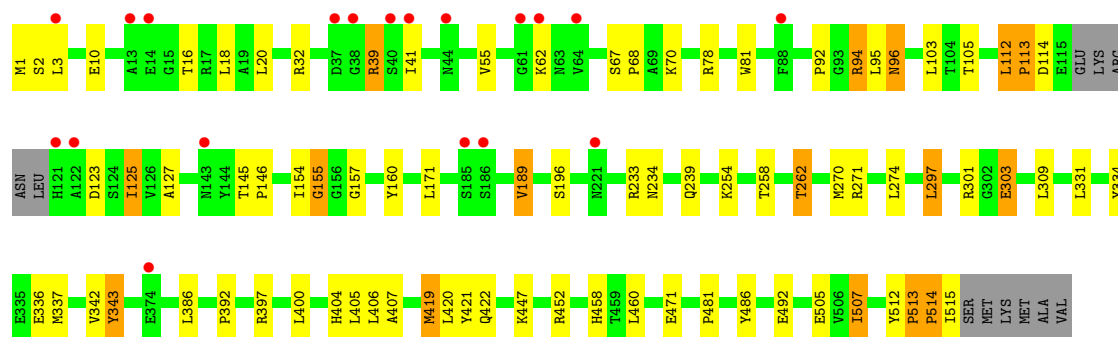


#### • Molecule 1: DHFR-TS

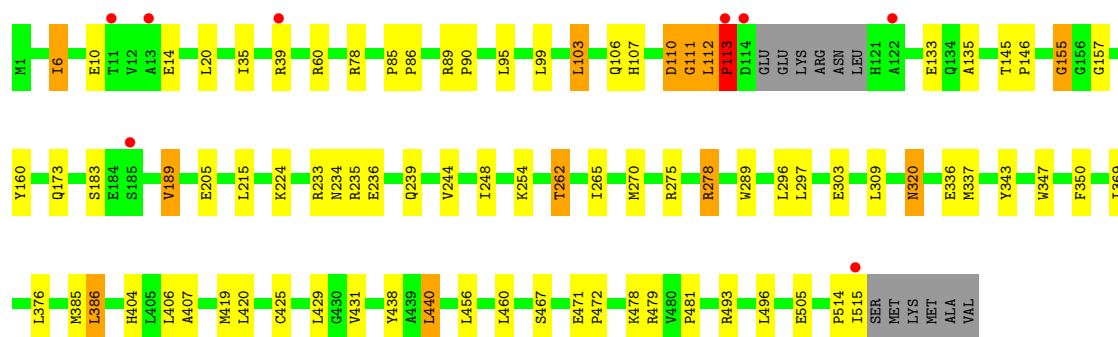
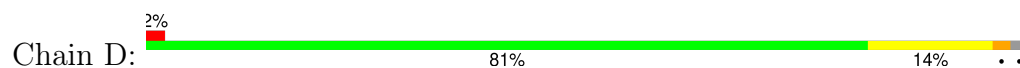


#### • Molecule 1: DHFR-TS





● Molecule 1: DHFR-TS





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.57Å 176.57Å 251.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 3.00 19.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (19.94-3.00) 96.7 (19.94-3.00)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.207 , 0.245 0.206 , 0.241	Depositor DCC
$R_{free}$ test set	3898 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.9	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	16618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: NAP, EDO, SO4, TMQ

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	0.48	0/4150	0.82	1/5632 (0.0%)
1	B	0.53	1/4133 (0.0%)	0.82	1/5609 (0.0%)
1	C	0.50	0/4152	0.82	1/5634 (0.0%)
1	D	0.50	2/4136 (0.0%)	0.80	2/5613 (0.0%)
All	All	0.50	3/16571 (0.0%)	0.81	5/22488 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	5
1	C	0	3
1	D	0	3
All	All	0	13

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	106	GLN	CD-NE2	7.71	1.49	1.33
1	D	106	GLN	CD-OE1	7.47	1.37	1.23
1	B	71	ARG	NE-CZ	6.33	1.40	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	GLY	N-CA-C	7.26	122.06	111.24
1	D	155	GLY	N-CA-C	7.20	121.97	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	106	GLN	OE1-CD-NE2	6.49	129.09	122.60
1	C	123	ASP	N-CA-C	6.05	119.59	110.64
1	B	71	ARG	NE-CZ-NH2	-5.73	114.05	119.20

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	LEU	Peptide
1	A	155	GLY	Peptide
1	B	180	ILE	Peptide
1	B	61	GLY	Peptide
1	B	62	LYS	Peptide
1	B	64	VAL	Peptide
1	B	65	LYS	Peptide
1	C	154	ILE	Peptide
1	C	155	GLY	Peptide
1	C	514	PRO	Peptide
1	D	110	ASP	Peptide
1	D	111	GLY	Peptide
1	D	113	PRO	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	4052	0	4000	49	0
1	B	4036	0	3988	135	0
1	C	4054	0	4007	45	0
1	D	4038	0	3984	48	0
2	A	5	0	0	0	0
2	C	10	0	0	0	0
2	D	5	0	0	0	0
3	A	48	0	25	2	0
3	B	48	0	25	1	0
3	C	48	0	25	3	0
3	D	48	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	27	0	24	5	0
4	B	27	0	24	1	0
4	C	27	0	24	3	0
4	D	27	0	24	4	0
5	A	8	0	12	0	0
5	B	4	0	6	1	0
5	C	8	0	12	1	0
5	D	4	0	6	1	0
6	A	19	0	0	0	0
6	B	21	0	0	0	0
6	C	30	0	0	1	0
6	D	24	0	0	0	0
All	All	16618	0	16211	282	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 9.

All (282) 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:59:LEU:CD1	1:B:65:LYS:HD2	1.00	1.46
1:B:59:LEU:CD1	1:B:65:LYS:CD	1.95	1.41
1:B:59:LEU:HD13	1:B:65:LYS:CD	1.60	1.27
1:B:65:LYS:CE	1:B:70:LYS:HG2	1.68	1.21
1:D:112:LEU:N	1:D:113:PRO:HD2	1.60	1.13
1:B:59:LEU:HD11	1:B:65:LYS:HD2	1.14	1.12
1:B:62:LYS:HB2	1:B:63:ASN:HA	1.15	1.11
1:C:112:LEU:HB2	1:C:113:PRO:HA	1.10	1.09
1:C:112:LEU:HB2	1:C:113:PRO:CA	1.82	1.07
1:B:65:LYS:HE2	1:B:70:LYS:HG2	1.08	1.06
1:B:180:ILE:HA	1:B:181:ARG:HG2	1.33	1.05
1:B:63:ASN:C	1:B:64:VAL:HG23	1.81	1.04
1:B:59:LEU:HD12	1:B:65:LYS:HD2	1.40	1.01
1:D:111:GLY:C	1:D:113:PRO:HD2	1.84	1.01
1:B:65:LYS:HE2	1:B:70:LYS:CG	1.90	1.00
4:D:614:TMQ:H171	4:D:614:TMQ:HN52	1.26	0.99
1:B:62:LYS:HD2	1:B:63:ASN:ND2	1.78	0.99
1:B:30:ASP:HA	1:B:180:ILE:O	1.60	0.99
4:A:611:TMQ:HN52	4:A:611:TMQ:H171	1.26	0.98
4:C:613:TMQ:H171	4:C:613:TMQ:HN52	1.31	0.94
1:A:112:LEU:N	1:A:112:LEU:HD23	1.81	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:THR:HG21	1:B:226:TYR:OH	1.68	0.93
1:C:112:LEU:CB	1:C:113:PRO:HA	1.91	0.91
1:B:31:GLU:O	1:B:32:ARG:HB2	1.68	0.91
1:B:180:ILE:CG2	1:B:225:TYR:HA	2.00	0.91
1:B:63:ASN:C	1:B:64:VAL:CG2	2.44	0.91
1:B:65:LYS:CE	1:B:70:LYS:CG	2.46	0.90
1:B:62:LYS:HD2	1:B:63:ASN:HD22	1.33	0.90
1:B:155:GLY:HA2	3:B:602:NAP:H5N	1.52	0.89
1:B:63:ASN:O	1:B:64:VAL:HG23	1.72	0.89
1:B:30:ASP:CA	1:B:180:ILE:O	2.19	0.88
1:B:179:THR:O	1:B:180:ILE:HG23	1.72	0.88
1:B:59:LEU:HD13	1:B:65:LYS:HD2	0.88	0.87
1:B:59:LEU:HD13	1:B:65:LYS:CE	2.05	0.87
1:B:65:LYS:NZ	1:B:70:LYS:HG2	1.89	0.87
1:C:515:ILE:O	1:C:515:ILE:HG22	1.75	0.86
1:B:62:LYS:HB2	1:B:63:ASN:CA	2.04	0.86
1:A:106:GLN:HA	1:A:109:LEU:HD21	1.57	0.85
1:B:45:VAL:HG21	1:B:180:ILE:HD11	1.59	0.84
1:B:180:ILE:HA	1:B:181:ARG:CG	2.07	0.84
1:B:65:LYS:NZ	1:B:70:LYS:CG	2.42	0.83
1:A:419:MET:HG2	1:A:457:VAL:HB	1.62	0.81
1:B:131:GLY:H	1:B:134:GLN:HE21	1.27	0.81
1:B:180:ILE:HG22	1:B:225:TYR:HA	1.63	0.81
1:B:62:LYS:CB	1:B:63:ASN:HA	2.04	0.80
1:D:112:LEU:N	1:D:113:PRO:CD	2.45	0.79
1:D:78:ARG:HD2	1:D:103:LEU:HD23	1.65	0.78
1:B:45:VAL:HG21	1:B:180:ILE:CD1	2.14	0.77
1:B:65:LYS:HD3	1:B:70:LYS:HB3	1.67	0.77
1:C:112:LEU:CB	1:C:113:PRO:CA	2.53	0.76
4:A:611:TMQ:HN52	4:A:611:TMQ:C17	1.99	0.76
1:B:179:THR:O	1:B:180:ILE:CG2	2.34	0.76
4:D:614:TMQ:HN52	4:D:614:TMQ:C17	1.98	0.76
4:D:614:TMQ:H171	4:D:614:TMQ:N25	2.01	0.75
1:A:109:LEU:HD23	1:A:109:LEU:O	1.86	0.75
1:B:181:ARG:O	1:B:183:SER:N	2.20	0.74
1:B:65:LYS:CD	1:B:70:LYS:HB3	2.18	0.73
1:B:180:ILE:HB	1:B:181:ARG:HB2	1.71	0.73
1:D:514:PRO:O	1:D:515:ILE:HB	1.90	0.70
4:C:613:TMQ:HN52	4:C:613:TMQ:C17	2.04	0.69
1:C:233:ARG:HH22	5:C:806:EDO:H21	1.56	0.68
1:B:225:TYR:CD1	1:B:225:TYR:C	2.70	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:611:TMQ:H171	4:A:611:TMQ:N25	2.01	0.68
1:A:110:ASP:O	1:A:112:LEU:CD2	2.43	0.67
1:A:112:LEU:N	1:A:112:LEU:CD2	2.55	0.67
1:D:146:PRO:HG3	1:D:505:GLU:HG2	1.77	0.67
1:B:179:THR:HG21	1:B:226:TYR:CZ	2.30	0.66
1:B:59:LEU:HD11	1:B:65:LYS:CD	1.94	0.66
1:B:47:GLU:HG2	1:B:225:TYR:HE2	1.61	0.65
1:D:111:GLY:O	1:D:113:PRO:HD2	1.97	0.65
1:B:181:ARG:O	1:B:183:SER:HB2	1.95	0.65
1:A:111:GLY:C	1:A:112:LEU:HD23	2.21	0.65
1:D:471:GLU:HB3	1:D:472:PRO:HD3	1.78	0.65
1:A:104:THR:H	1:A:107:HIS:HB2	1.63	0.64
1:B:64:VAL:C	1:B:65:LYS:HG3	2.23	0.64
1:B:59:LEU:HD12	1:B:65:LYS:CD	2.07	0.64
1:A:10:GLU:CD	1:A:10:GLU:H	2.06	0.63
1:A:110:ASP:O	1:A:112:LEU:HD23	1.98	0.63
1:A:31:GLU:OE2	1:A:181:ARG:HD2	1.99	0.63
1:B:181:ARG:C	1:B:183:SER:N	2.56	0.62
1:B:180:ILE:HG22	1:B:224:LYS:O	1.98	0.62
1:D:78:ARG:HD3	3:D:604:NAP:O1X	1.98	0.62
1:B:59:LEU:CD1	1:B:65:LYS:CG	2.75	0.62
1:B:60:ARG:O	1:B:61:GLY:C	2.42	0.62
1:B:65:LYS:NZ	1:B:70:LYS:HG3	2.13	0.62
1:A:110:ASP:O	1:A:112:LEU:N	2.30	0.62
1:A:420:LEU:HD23	1:A:458:HIS:CD2	2.35	0.62
1:C:155:GLY:HA3	1:C:160:TYR:CZ	2.35	0.61
1:B:112:LEU:HB3	1:B:113:PRO:HD3	1.83	0.60
1:B:30:ASP:HA	1:B:180:ILE:C	2.27	0.60
1:A:106:GLN:CA	1:A:109:LEU:HD21	2.30	0.60
1:B:65:LYS:HZ1	1:B:70:LYS:HG2	1.66	0.60
1:B:47:GLU:HG2	1:B:225:TYR:CE2	2.37	0.60
1:B:66:PRO:HB3	1:B:93:GLY:O	2.01	0.60
1:C:78:ARG:HD3	3:C:603:NAP:O1X	2.02	0.59
4:C:613:TMQ:H171	4:C:613:TMQ:N25	2.06	0.59
1:B:131:GLY:N	1:B:134:GLN:HE21	2.01	0.59
1:C:447:LYS:HZ1	1:C:492:GLU:CD	2.12	0.58
1:C:112:LEU:HB2	1:C:113:PRO:C	2.26	0.58
1:A:407:ALA:HA	1:A:419:MET:O	2.05	0.57
1:B:329:ARG:NH1	1:B:398:MET:O	2.37	0.57
1:A:49:MET:HE2	4:A:611:TMQ:H222	1.85	0.57
1:D:111:GLY:O	1:D:113:PRO:CD	2.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:O	3:A:601:NAP:H1B	2.04	0.57
1:B:180:ILE:CG2	1:B:225:TYR:CA	2.80	0.57
1:B:65:LYS:HZ1	1:B:70:LYS:CG	2.15	0.57
1:A:78:ARG:HD2	1:A:103:LEU:HD23	1.87	0.56
1:B:59:LEU:HD12	1:B:65:LYS:CG	2.34	0.56
1:C:20:LEU:HB2	1:C:171:LEU:HD13	1.88	0.56
1:B:59:LEU:O	1:B:60:ARG:C	2.48	0.56
1:D:347:TRP:HB3	1:D:369:ILE:HD13	1.88	0.55
1:B:58:LYS:O	1:B:59:LEU:HD23	2.05	0.55
1:C:105:THR:HB	1:C:127:ALA:H	1.72	0.55
1:B:154:ILE:O	4:B:612:TMQ:N25	2.40	0.55
1:B:179:THR:C	1:B:180:ILE:HG23	2.32	0.54
1:C:297:LEU:HB3	1:C:301:ARG:HH21	1.72	0.54
1:A:192:ARG:HH21	1:C:452:ARG:HH22	1.56	0.54
1:D:296:LEU:HD22	1:D:440:LEU:HB3	1.88	0.54
1:B:131:GLY:H	1:B:134:GLN:NE2	2.01	0.53
1:B:65:LYS:HE2	1:B:70:LYS:CB	2.38	0.53
1:B:76:MET:HB3	1:B:154:ILE:HD11	1.90	0.53
1:B:179:THR:HB	1:B:226:TYR:CZ	2.44	0.53
1:A:306:ALA:HB2	1:A:339:LEU:HD11	1.90	0.53
1:A:110:ASP:C	1:A:112:LEU:H	2.16	0.53
1:A:110:ASP:O	1:A:112:LEU:HG	2.09	0.53
1:B:225:TYR:C	1:B:225:TYR:HD1	2.17	0.53
1:C:78:ARG:HD2	1:C:103:LEU:HD23	1.91	0.53
1:A:334:TYR:HB3	1:A:338:ASP:HB3	1.89	0.52
1:B:180:ILE:CG2	1:B:224:LYS:O	2.56	0.52
1:B:30:ASP:CB	1:B:180:ILE:O	2.57	0.52
1:C:303:GLU:HG3	6:C:821:HOH:O	2.09	0.52
1:C:422:GLN:NE2	1:C:458:HIS:NE2	2.57	0.52
1:D:404:HIS:HB2	1:D:420:LEU:HD11	1.91	0.52
1:B:179:THR:CG2	1:B:226:TYR:CZ	2.92	0.52
1:B:20:LEU:HD23	1:B:137:GLN:HG3	1.91	0.51
1:B:74:VAL:HB	1:B:154:ILE:HD12	1.93	0.51
1:C:157:GLY:HA3	1:C:189:VAL:HG11	1.92	0.51
1:B:63:ASN:ND2	1:B:64:VAL:CG2	2.74	0.51
1:B:29:VAL:O	1:B:180:ILE:O	2.28	0.51
1:C:404:HIS:HB2	1:C:420:LEU:HD11	1.93	0.50
1:C:515:ILE:O	1:C:515:ILE:CG2	2.48	0.50
1:B:392:PRO:HA	1:B:395:LEU:HD22	1.94	0.50
1:C:512:TYR:O	1:C:513:PRO:O	2.30	0.50
1:A:69:ALA:O	1:A:147:SER:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:VAL:HG12	1:B:66:PRO:HD3	1.93	0.50
1:C:67:SER:HB2	1:C:68:PRO:HD2	1.94	0.50
1:B:59:LEU:HD13	1:B:65:LYS:NZ	2.26	0.49
1:C:10:GLU:CD	1:C:10:GLU:H	2.19	0.49
1:D:111:GLY:C	1:D:113:PRO:CD	2.73	0.49
1:C:234:ASN:HB3	1:C:481:PRO:HB2	1.94	0.49
1:C:270:MET:HE2	1:C:460:LEU:HD11	1.94	0.49
1:D:336:GLU:O	1:D:337:MET:HB2	2.13	0.49
1:B:471:GLU:HB2	1:B:472:PRO:HD3	1.94	0.48
1:C:146:PRO:HG3	1:C:505:GLU:HG2	1.95	0.48
1:A:239:GLN:HE22	1:A:271:ARG:H	1.61	0.48
1:B:65:LYS:HD3	1:B:70:LYS:CB	2.43	0.48
1:B:181:ARG:O	1:B:182:ALA:C	2.57	0.47
1:D:275:ARG:O	1:D:278:ARG:HB2	2.14	0.47
1:B:182:ALA:O	1:B:183:SER:O	2.31	0.47
1:B:179:THR:CB	1:B:226:TYR:CZ	2.97	0.47
1:C:405:LEU:HD12	1:C:406:LEU:HB2	1.97	0.47
1:D:111:GLY:O	1:D:112:LEU:CB	2.62	0.47
1:B:341:PRO:O	1:B:398:MET:HE2	2.14	0.47
1:B:419:MET:HG2	1:C:421:TYR:OH	2.14	0.47
1:D:471:GLU:OE1	1:D:471:GLU:HA	2.15	0.47
1:B:224:LYS:H	1:B:224:LYS:HD2	1.80	0.47
1:D:270:MET:HE2	1:D:460:LEU:HD11	1.97	0.47
1:B:180:ILE:HG21	1:B:225:TYR:CB	2.45	0.46
1:B:225:TYR:HD1	1:B:226:TYR:N	2.13	0.46
1:D:289:TRP:HH2	1:D:440:LEU:HG	1.81	0.46
1:B:141:SER:HB2	1:B:142:PRO:HD2	1.97	0.46
1:D:479:ARG:NH2	1:D:515:ILE:HG22	2.30	0.46
1:C:331:LEU:HD22	1:C:334:TYR:CE2	2.50	0.46
1:A:299:PHE:HB3	1:A:347:TRP:CZ3	2.51	0.46
1:B:161:ALA:O	1:B:165:ARG:HG2	2.16	0.46
1:C:20:LEU:HB2	1:C:171:LEU:CD1	2.45	0.46
1:A:131:GLY:H	1:A:134:GLN:HE21	1.62	0.46
1:B:17:ARG:HD2	1:B:276:ASN:HB3	1.97	0.46
1:B:419:MET:HE1	1:B:459:THR:OG1	2.15	0.46
1:D:320:ASN:N	1:D:320:ASN:HD22	2.13	0.46
1:B:60:ARG:O	1:B:61:GLY:O	2.34	0.46
1:A:490:ARG:HD2	1:A:505:GLU:OE1	2.17	0.45
1:A:515:ILE:C	1:A:515:ILE:HD13	2.41	0.45
1:B:59:LEU:HD22	1:B:149:GLU:OE1	2.17	0.45
1:B:91:LEU:HB3	1:B:94:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:LYS:HB2	1:D:262:THR:HG22	1.98	0.45
1:B:404:HIS:H	1:B:404:HIS:CD2	2.34	0.45
1:B:407:ALA:HA	1:B:419:MET:O	2.17	0.45
1:A:109:LEU:HD23	1:A:109:LEU:C	2.42	0.45
1:B:139:LEU:HD22	1:B:148:ILE:HG21	1.99	0.45
1:B:235:ARG:HH22	5:B:805:EDO:H12	1.82	0.45
1:C:336:GLU:O	1:C:337:MET:HB2	2.16	0.45
1:C:81:TRP:CH2	1:C:125:ILE:HD12	2.52	0.45
1:C:407:ALA:HA	1:C:419:MET:O	2.17	0.45
1:A:110:ASP:O	1:A:112:LEU:CG	2.65	0.45
1:A:392:PRO:HA	1:A:395:LEU:HD22	1.98	0.45
1:D:6:ILE:HG13	1:D:496:LEU:HD23	1.99	0.45
1:C:512:TYR:C	1:C:513:PRO:O	2.59	0.44
1:D:244:VAL:O	1:D:248:ILE:HG12	2.18	0.44
1:C:92:PRO:O	1:C:94:ARG:NH1	2.42	0.44
1:A:81:TRP:CE2	1:A:89:ARG:HD3	2.53	0.44
1:A:336:GLU:O	1:A:337:MET:HB2	2.16	0.44
1:A:425:CYS:HB2	1:A:463:ALA:HA	2.00	0.44
1:B:63:ASN:ND2	1:B:64:VAL:HG22	2.33	0.44
1:B:30:ASP:HB3	1:B:180:ILE:O	2.18	0.44
1:B:65:LYS:CE	1:B:70:LYS:CB	2.95	0.44
1:A:62:LYS:HB2	1:A:63:ASN:H	1.69	0.44
1:D:157:GLY:HA3	1:D:189:VAL:HG11	2.00	0.44
1:D:376:LEU:HD23	1:D:385:MET:SD	2.57	0.44
1:D:478:LYS:HA	1:D:478:LYS:HD3	1.85	0.44
1:D:20:LEU:HD21	1:D:133:GLU:HG2	2.00	0.44
1:D:155:GLY:HA3	1:D:160:TYR:CZ	2.52	0.44
1:B:239:GLN:HE22	1:B:271:ARG:H	1.66	0.44
1:A:404:HIS:HB2	1:A:420:LEU:HD11	2.00	0.43
1:B:65:LYS:CE	1:B:70:LYS:HB3	2.47	0.43
1:D:404:HIS:CB	1:D:420:LEU:HD11	2.48	0.43
1:B:76:MET:HB3	1:B:154:ILE:CD1	2.48	0.43
1:B:181:ARG:C	1:B:183:SER:H	2.25	0.43
1:C:239:GLN:HE22	1:C:271:ARG:H	1.67	0.43
4:D:614:TMQ:H92	4:D:614:TMQ:H173	1.82	0.43
1:B:62:LYS:CB	1:B:63:ASN:CA	2.79	0.43
1:B:180:ILE:HA	1:B:181:ARG:CB	2.49	0.43
1:B:31:GLU:CD	1:B:181:ARG:HD3	2.44	0.43
1:B:41:ILE:HA	1:B:42:PRO:HD3	1.85	0.43
1:B:296:LEU:HD22	1:B:440:LEU:HB3	2.00	0.43
1:C:486:TYR:HB2	1:C:507:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ARG:HH22	5:D:804:EDO:H22	1.83	0.43
1:B:59:LEU:HD12	1:B:64:VAL:HA	2.01	0.43
1:B:65:LYS:HZ3	1:B:70:LYS:HG3	1.82	0.43
1:D:234:ASN:HB3	1:D:481:PRO:HB2	2.00	0.43
4:A:611:TMQ:C17	4:A:611:TMQ:N25	2.68	0.43
1:B:62:LYS:CD	1:B:63:ASN:ND2	2.67	0.43
1:A:415:GLU:HA	1:A:452:ARG:O	2.19	0.43
1:B:258:THR:OG1	1:B:260:VAL:HG23	2.19	0.43
1:C:39:ARG:HA	3:C:603:NAP:H3D	2.01	0.43
1:D:425:CYS:HB3	1:D:431:VAL:HG22	2.01	0.43
1:C:254:LYS:HB2	1:C:262:THR:HG22	2.00	0.42
1:A:78:ARG:HD3	3:A:601:NAP:O1X	2.19	0.42
1:B:425:CYS:HB3	1:B:431:VAL:CG2	2.49	0.42
1:B:64:VAL:C	1:B:65:LYS:CG	2.90	0.42
1:A:318:ASP:HA	1:A:337:MET:HE1	1.99	0.42
1:B:112:LEU:N	1:B:113:PRO:CD	2.83	0.42
1:D:145:THR:HA	1:D:146:PRO:HA	1.81	0.42
1:A:405:LEU:HD11	1:D:406:LEU:HD11	2.01	0.42
1:B:419:MET:CE	1:B:459:THR:OG1	2.67	0.42
1:B:11:THR:HB	1:B:12:VAL:H	1.64	0.42
1:D:471:GLU:HB3	1:D:472:PRO:CD	2.49	0.42
1:B:305:TYR:CE2	1:B:307:LYS:HB3	2.55	0.42
1:B:59:LEU:O	1:B:60:ARG:O	2.38	0.42
1:B:316:ILE:HG13	1:B:317:TRP:CD1	2.54	0.42
1:C:78:ARG:HH11	3:C:603:NAP:P2B	2.43	0.42
1:D:205:GLU:CD	1:D:235:ARG:HH21	2.28	0.42
1:A:392:PRO:HD2	1:D:350:PHE:CZ	2.55	0.42
1:B:350:PHE:CZ	1:C:392:PRO:HD2	2.55	0.42
1:B:58:LYS:HG2	1:B:59:LEU:H	1.85	0.42
1:B:267:GLY:HA2	1:C:419:MET:HE2	2.02	0.42
1:C:145:THR:HA	1:C:146:PRO:HA	1.89	0.42
1:A:96:ASN:N	1:A:96:ASN:HD22	2.18	0.41
1:A:296:LEU:HD22	1:A:440:LEU:HB3	2.02	0.41
1:B:480:VAL:HA	1:B:481:PRO:HD3	1.92	0.41
1:A:131:GLY:N	1:A:134:GLN:HE21	2.18	0.41
1:A:81:TRP:CH2	1:A:89:ARG:HB3	2.55	0.41
1:B:65:LYS:HD3	1:B:70:LYS:O	2.20	0.41
1:D:85:PRO:HA	1:D:86:PRO:HD2	1.92	0.41
1:B:65:LYS:HD3	1:B:70:LYS:C	2.46	0.41
1:A:443:ILE:O	1:A:447:LYS:HG3	2.21	0.41
1:B:112:LEU:H	1:B:113:PRO:HD2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ASN:N	1:C:96:ASN:HD22	2.19	0.41
1:D:99:LEU:HD21	1:D:135:ALA:HB2	2.02	0.41
1:D:404:HIS:CD2	1:D:404:HIS:H	2.38	0.41
1:D:407:ALA:HA	1:D:419:MET:O	2.21	0.41
1:B:30:ASP:N	1:B:180:ILE:O	2.53	0.41
1:B:179:THR:HB	1:B:226:TYR:CE1	2.56	0.41
1:C:342:VAL:O	1:C:343:TYR:C	2.64	0.41
1:D:420:LEU:HD13	1:D:438:TYR:CZ	2.57	0.40
1:D:236:GLU:O	1:D:239:GLN:HB2	2.20	0.40
1:D:386:LEU:HB2	1:D:407:ALA:O	2.21	0.40
1:B:62:LYS:HG3	1:B:63:ASN:HB2	2.04	0.40
1:D:406:LEU:HD23	1:D:406:LEU:C	2.46	0.40
1:A:103:LEU:HD12	1:A:107:HIS:HB3	2.04	0.40
1:A:153:CYS:SG	1:A:159:VAL:HG12	2.61	0.40
1:D:89:ARG:HA	1:D:90:PRO:C	2.47	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	506/521 (97%)	483 (96%)	18 (4%)	5 (1%)	13	46
1	B	504/521 (97%)	471 (94%)	21 (4%)	12 (2%)	5	25
1	C	506/521 (97%)	475 (94%)	23 (4%)	8 (2%)	8	34
1	D	505/521 (97%)	487 (96%)	15 (3%)	3 (1%)	22	57
All	All	2021/2084 (97%)	1916 (95%)	77 (4%)	28 (1%)	9	37

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	343	TYR
1	B	60	ARG
1	B	61	GLY
1	B	64	VAL
1	B	65	LYS
1	B	66	PRO
1	B	182	ALA
1	B	185	SER
1	C	112	LEU
1	C	113	PRO
1	C	513	PRO
1	D	112	LEU
1	B	32	ARG
1	B	113	PRO
1	B	183	SER
1	B	343	TYR
1	C	2	SER
1	C	343	TYR
1	D	343	TYR
1	A	114	ASP
1	D	113	PRO
1	A	3	LEU
1	A	62	LYS
1	C	62	LYS
1	C	114	ASP
1	B	53	ARG
1	A	146	PRO
1	C	514	PRO

### 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	436/446 (98%)	412 (94%)	24 (6%)	18	50
1	B	434/446 (97%)	402 (93%)	32 (7%)	11	38
1	C	436/446 (98%)	409 (94%)	27 (6%)	15	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	433/446 (97%)	405 (94%)	28 (6%)	14	43
All	All	1739/1784 (98%)	1628 (94%)	111 (6%)	14	44

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

Mol	Chain	Res	Type
1	A	11	THR
1	A	12	VAL
1	A	17	ARG
1	A	95	LEU
1	A	96	ASN
1	A	102	THR
1	A	109	LEU
1	A	112	LEU
1	A	124	SER
1	A	138	LEU
1	A	147	SER
1	A	222	GLU
1	A	254	LYS
1	A	264	SER
1	A	274	LEU
1	A	395	LEU
1	A	406	LEU
1	A	412	SER
1	A	419	MET
1	A	440	LEU
1	A	456	LEU
1	A	467	SER
1	A	490	ARG
1	A	515	ILE
1	B	3	LEU
1	B	10	GLU
1	B	12	VAL
1	B	18	LEU
1	B	32	ARG
1	B	35	ILE
1	B	41	ILE
1	B	64	VAL
1	B	70	LYS
1	B	94	ARG
1	B	95	LEU
1	B	102	THR

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Mol	Chain	Res	Type
1	B	112	LEU
1	B	123	ASP
1	B	154	ILE
1	B	181	ARG
1	B	184	GLU
1	B	239	GLN
1	B	264	SER
1	B	274	LEU
1	B	297	LEU
1	B	309	LEU
1	B	320	ASN
1	B	333	GLU
1	B	372	ILE
1	B	395	LEU
1	B	400	LEU
1	B	419	MET
1	B	440	LEU
1	B	456	LEU
1	B	468	ASN
1	B	480	VAL
1	C	1	MET
1	C	3	LEU
1	C	16	THR
1	C	18	LEU
1	C	32	ARG
1	C	39	ARG
1	C	41	ILE
1	C	55	VAL
1	C	70	LYS
1	C	94	ARG
1	C	95	LEU
1	C	96	ASN
1	C	125	ILE
1	C	189	VAL
1	C	196	SER
1	C	258	THR
1	C	262	THR
1	C	274	LEU
1	C	297	LEU
1	C	303	GLU
1	C	309	LEU
1	C	386	LEU

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Mol	Chain	Res	Type
1	C	397	ARG
1	C	400	LEU
1	C	419	MET
1	C	471	GLU
1	C	507	ILE
1	D	6	ILE
1	D	10	GLU
1	D	14	GLU
1	D	35	ILE
1	D	39	ARG
1	D	60	ARG
1	D	95	LEU
1	D	103	LEU
1	D	107	HIS
1	D	110	ASP
1	D	173	GLN
1	D	183	SER
1	D	189	VAL
1	D	215	LEU
1	D	224	LYS
1	D	262	THR
1	D	265	ILE
1	D	278	ARG
1	D	297	LEU
1	D	303	GLU
1	D	309	LEU
1	D	320	ASN
1	D	386	LEU
1	D	429	LEU
1	D	440	LEU
1	D	456	LEU
1	D	467	SER
1	D	493	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	134	GLN
1	A	143	ASN
1	A	170	HIS
1	A	239	GLN

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Mol	Chain	Res	Type
1	A	320	ASN
1	A	364	GLN
1	A	422	GLN
1	B	63	ASN
1	B	106	GLN
1	B	134	GLN
1	B	170	HIS
1	B	173	GLN
1	B	207	GLN
1	B	239	GLN
1	B	469	HIS
1	C	107	HIS
1	C	137	GLN
1	C	170	HIS
1	C	173	GLN
1	C	207	GLN
1	C	239	GLN
1	C	255	HIS
1	C	320	ASN
1	C	422	GLN
1	C	434	ASN
1	C	464	HIS
1	D	173	GLN
1	D	255	HIS
1	D	320	ASN
1	D	346	GLN
1	D	360	ASN
1	D	364	GLN
1	D	422	GLN
1	D	434	ASN
1	D	464	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 oligosaccharides in this entry.

## 5.6 Ligand geometry

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	C	702	-	4,4,4	0.28	0	6,6,6	0.36	0
2	SO4	D	704	-	4,4,4	0.21	0	6,6,6	0.17	0
5	EDO	A	801	-	3,3,3	0.45	0	2,2,2	0.42	0
5	EDO	B	805	-	3,3,3	0.42	0	2,2,2	0.44	0
5	EDO	D	804	-	3,3,3	0.43	0	2,2,2	0.45	0
5	EDO	C	806	-	3,3,3	0.41	0	2,2,2	0.54	0
3	NAP	B	602	-	46,52,52	1.84	4 (8%)	61,80,80	1.09	1 (1%)
4	TMQ	B	612	-	29,29,29	1.31	2 (6%)	39,41,41	1.48	5 (12%)
5	EDO	C	803	-	3,3,3	0.39	0	2,2,2	0.55	0
2	SO4	A	701	-	4,4,4	0.25	0	6,6,6	0.24	0
3	NAP	C	603	-	46,52,52	1.77	3 (6%)	61,80,80	1.05	1 (1%)
4	TMQ	C	613	-	29,29,29	1.37	2 (6%)	39,41,41	1.50	6 (15%)
4	TMQ	D	614	-	29,29,29	1.33	2 (6%)	39,41,41	1.38	4 (10%)
4	TMQ	A	611	-	29,29,29	1.36	3 (10%)	39,41,41	1.54	6 (15%)
2	SO4	C	703	-	4,4,4	0.29	0	6,6,6	0.30	0
3	NAP	A	601	-	46,52,52	1.73	3 (6%)	61,80,80	1.25	4 (6%)
3	NAP	D	604	-	46,52,52	1.78	4 (8%)	61,80,80	1.14	2 (3%)
5	EDO	A	802	-	3,3,3	0.44	0	2,2,2	0.36	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	801	-	-	1/1/1/1	-
5	EDO	D	804	-	-	1/1/1/1	-
5	EDO	B	805	-	-	1/1/1/1	-
5	EDO	C	806	-	-	1/1/1/1	-
3	NAP	B	602	-	-	10/31/67/67	0/5/5/5
4	TMQ	B	612	-	-	6/11/11/11	0/3/3/3
5	EDO	C	803	-	-	1/1/1/1	-
3	NAP	C	603	-	-	5/31/67/67	0/5/5/5
4	TMQ	C	613	-	-	2/11/11/11	0/3/3/3
4	TMQ	D	614	-	-	7/11/11/11	0/3/3/3
4	TMQ	A	611	-	-	4/11/11/11	0/3/3/3
3	NAP	A	601	-	-	8/31/67/67	0/5/5/5
3	NAP	D	604	-	-	5/31/67/67	0/5/5/5
5	EDO	A	802	-	-	0/1/1/1	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	NAP	O7N-C7N	9.49	1.41	1.24
3	D	604	NAP	O7N-C7N	9.07	1.41	1.24
3	C	603	NAP	O7N-C7N	9.02	1.40	1.24
3	A	601	NAP	O7N-C7N	8.87	1.40	1.24
4	C	613	TMQ	C17-C5	-4.87	1.39	1.51
4	A	611	TMQ	C17-C5	-4.87	1.39	1.51
4	D	614	TMQ	C17-C5	-4.75	1.40	1.51
3	C	603	NAP	C2A-N3A	4.74	1.39	1.32
4	B	612	TMQ	C17-C5	-4.66	1.40	1.51
3	D	604	NAP	C2A-N3A	4.53	1.39	1.32
3	B	602	NAP	C2A-N3A	4.42	1.38	1.32
3	A	601	NAP	C2A-N3A	4.34	1.38	1.32
4	C	613	TMQ	C9-C6	-3.40	1.40	1.51
4	B	612	TMQ	C9-C6	-3.25	1.41	1.51
4	D	614	TMQ	C9-C6	-3.16	1.41	1.51
4	A	611	TMQ	C9-C6	-3.11	1.41	1.51
3	C	603	NAP	C2A-N1A	3.07	1.39	1.33
3	D	604	NAP	C2A-N1A	2.94	1.39	1.33
3	B	602	NAP	C2A-N1A	2.91	1.39	1.33
3	A	601	NAP	C2A-N1A	2.82	1.38	1.33
3	B	602	NAP	C2N-N1N	2.59	1.37	1.35
4	A	611	TMQ	C3A-N1	-2.08	1.34	1.37
3	D	604	NAP	C2N-N1N	2.02	1.37	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	604	NAP	N3A-C2A-N1A	-6.64	119.66	128.67
3	B	602	NAP	N3A-C2A-N1A	-6.49	119.87	128.67
3	A	601	NAP	N3A-C2A-N1A	-6.46	119.90	128.67
3	C	603	NAP	N3A-C2A-N1A	-6.13	120.35	128.67
4	A	611	TMQ	N1-C2-N3	-5.47	120.25	127.21
4	B	612	TMQ	N1-C2-N3	-5.46	120.26	127.21
4	C	613	TMQ	N1-C2-N3	-5.42	120.31	127.21
4	D	614	TMQ	N1-C2-N3	-5.32	120.45	127.21
4	C	613	TMQ	C21-O18-C13	-3.95	111.72	117.51
4	B	612	TMQ	C23-O20-C15	-3.19	112.84	117.51
4	A	611	TMQ	N24-C2-N3	2.89	121.56	117.22
3	A	601	NAP	O4B-C1B-N9A	2.89	112.58	108.75
4	A	611	TMQ	C23-O20-C15	-2.72	113.52	117.51
4	A	611	TMQ	C21-O18-C13	-2.69	113.57	117.51
4	B	612	TMQ	C21-O18-C13	-2.68	113.58	117.51
4	A	611	TMQ	C9-C6-C7	-2.60	115.23	120.98
3	A	601	NAP	C2B-C1B-N9A	-2.42	107.19	112.56
4	C	613	TMQ	N24-C2-N3	2.39	120.81	117.22
4	D	614	TMQ	C23-O20-C15	-2.37	114.04	117.51
4	B	612	TMQ	C4A-C4-N25	-2.30	118.61	122.70
4	B	612	TMQ	C2-N1-C3A	2.25	121.66	116.35
3	A	601	NAP	O2A-PA-O3	2.23	113.31	107.27
4	A	611	TMQ	C2-N1-C3A	2.22	121.60	116.35
3	D	604	NAP	O4B-C1B-N9A	2.14	111.58	108.75
4	C	613	TMQ	C17-C5-C6	-2.13	118.39	120.81
4	C	613	TMQ	C9-C6-C7	-2.13	116.28	120.98
4	C	613	TMQ	C2-N1-C3A	2.12	121.35	116.35
4	D	614	TMQ	C2-N1-C3A	2.08	121.27	116.35
4	D	614	TMQ	N24-C2-N3	2.08	120.34	117.22

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	NAP	O4D-C1D-N1N-C2N
3	A	601	NAP	O4D-C1D-N1N-C6N
3	B	602	NAP	O4D-C1D-N1N-C6N
3	C	603	NAP	O4D-C1D-N1N-C6N
3	D	604	NAP	O4D-C1D-N1N-C6N
4	A	611	TMQ	C16-C11-N10-C9
4	D	614	TMQ	C14-C15-O20-C23

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Mol	Chain	Res	Type	Atoms
4	B	612	TMQ	C14-C13-O18-C21
4	B	612	TMQ	C14-C15-O20-C23
4	A	611	TMQ	C12-C11-N10-C9
4	B	612	TMQ	C12-C11-N10-C9
4	A	611	TMQ	C14-C15-O20-C23
4	D	614	TMQ	C14-C13-O18-C21
4	B	612	TMQ	C16-C11-N10-C9
4	D	614	TMQ	C16-C15-O20-C23
4	B	612	TMQ	C12-C13-O18-C21
4	D	614	TMQ	C12-C13-O18-C21
4	A	611	TMQ	C16-C15-O20-C23
4	B	612	TMQ	C16-C15-O20-C23
3	B	602	NAP	C3D-C4D-C5D-O5D
4	C	613	TMQ	C12-C11-N10-C9
4	C	613	TMQ	C16-C11-N10-C9
4	D	614	TMQ	C12-C11-N10-C9
4	D	614	TMQ	C16-C11-N10-C9
3	B	602	NAP	O4D-C4D-C5D-O5D
3	A	601	NAP	C2B-O2B-P2B-O3X
3	D	604	NAP	C3B-C4B-C5B-O5B
3	A	601	NAP	C5D-O5D-PN-O1N
3	B	602	NAP	C5D-O5D-PN-O3
3	B	602	NAP	C5D-O5D-PN-O1N
3	B	602	NAP	C5D-O5D-PN-O2N
3	C	603	NAP	C5D-O5D-PN-O1N
3	D	604	NAP	C5D-O5D-PN-O1N
3	B	602	NAP	PN-O3-PA-O2A
3	B	602	NAP	C3B-C4B-C5B-O5B
5	C	803	EDO	O1-C1-C2-O2
3	B	602	NAP	O4D-C1D-N1N-C2N
3	C	603	NAP	O4D-C1D-N1N-C2N
3	D	604	NAP	O4D-C1D-N1N-C2N
3	A	601	NAP	C2B-O2B-P2B-O1X
3	B	602	NAP	C2B-O2B-P2B-O1X
3	A	601	NAP	PN-O3-PA-O2A
5	C	806	EDO	O1-C1-C2-O2
5	D	804	EDO	O1-C1-C2-O2
5	B	805	EDO	O1-C1-C2-O2
4	D	614	TMQ	C6-C9-N10-C11
3	A	601	NAP	PN-O3-PA-O1A
3	C	603	NAP	PN-O3-PA-O1A
3	C	603	NAP	PN-O3-PA-O2A

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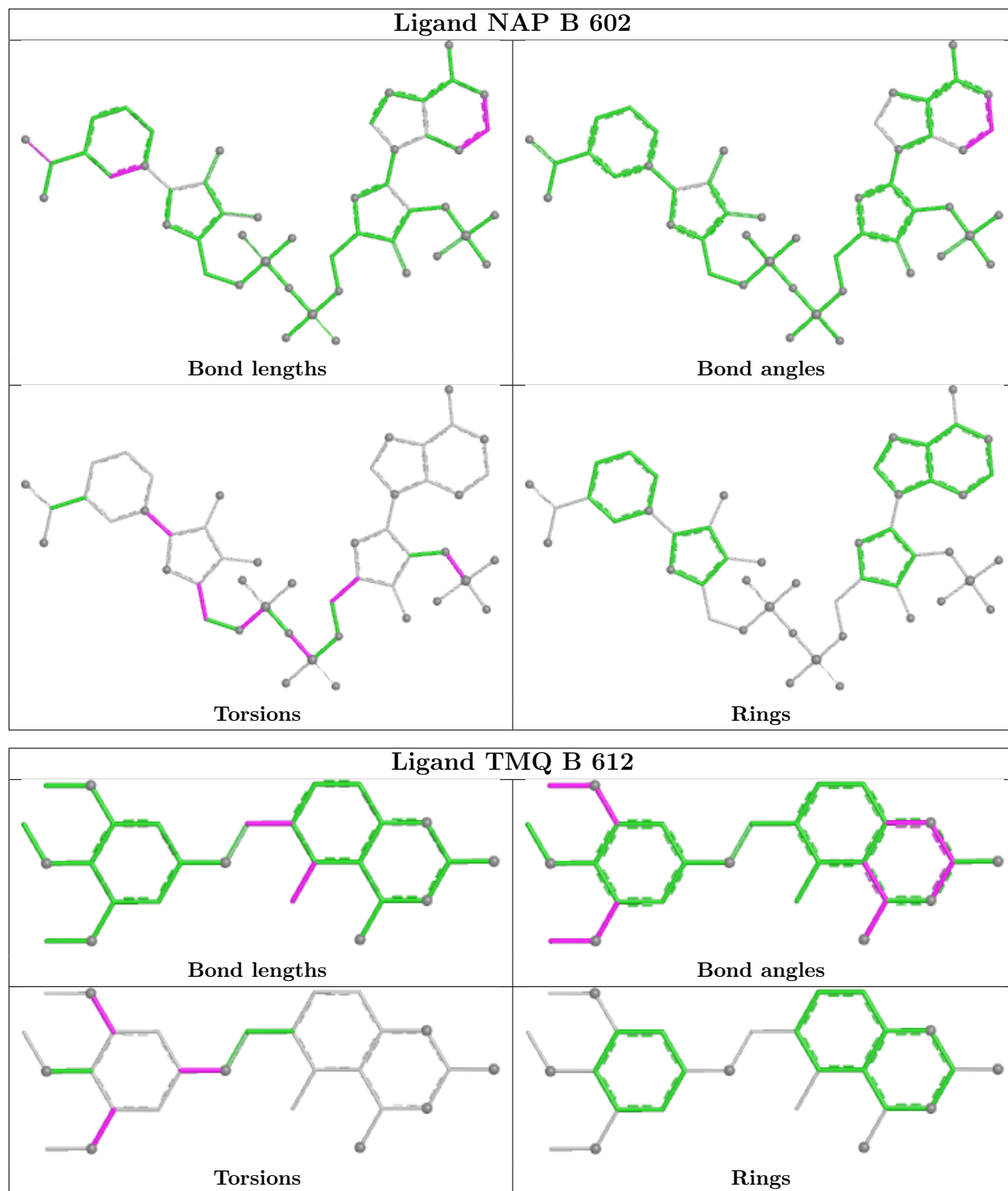
Mol	Chain	Res	Type	Atoms
3	D	604	NAP	PN-O3-PA-O2A
3	A	601	NAP	C2B-O2B-P2B-O2X
5	A	801	EDO	O1-C1-C2-O2

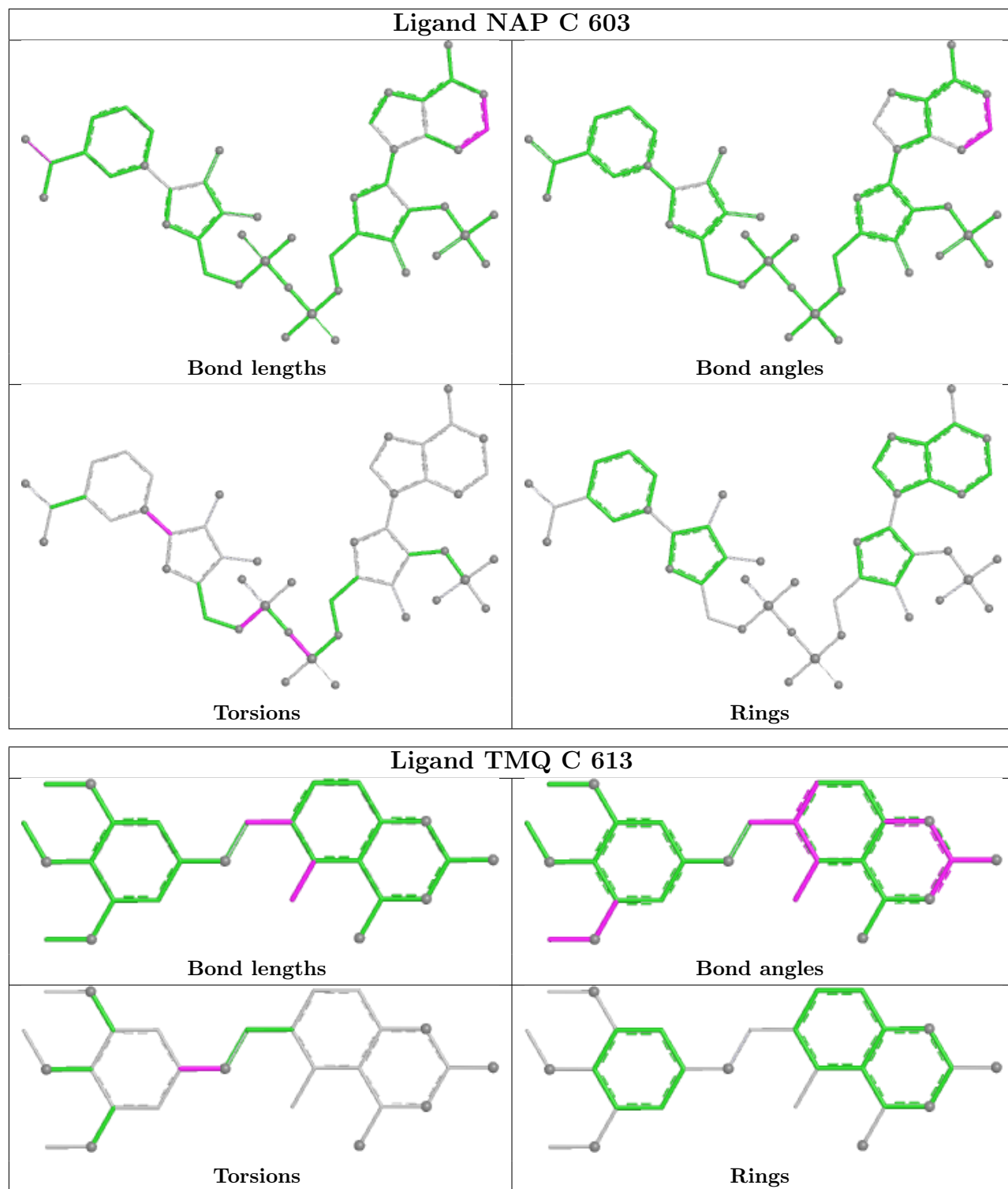
There are no ring outliers.

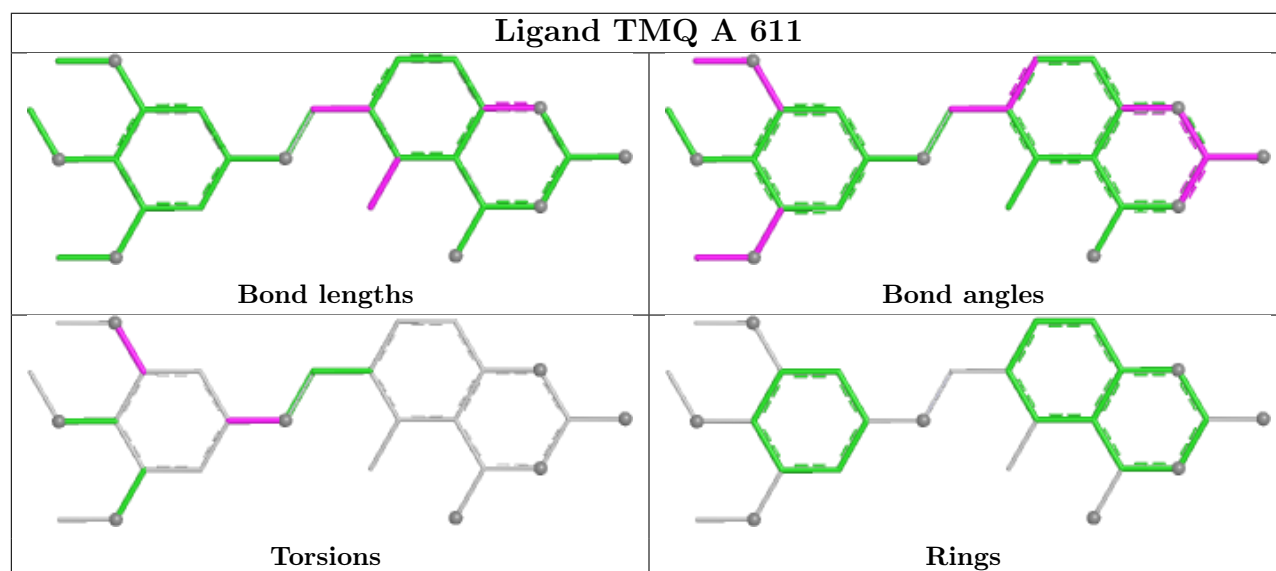
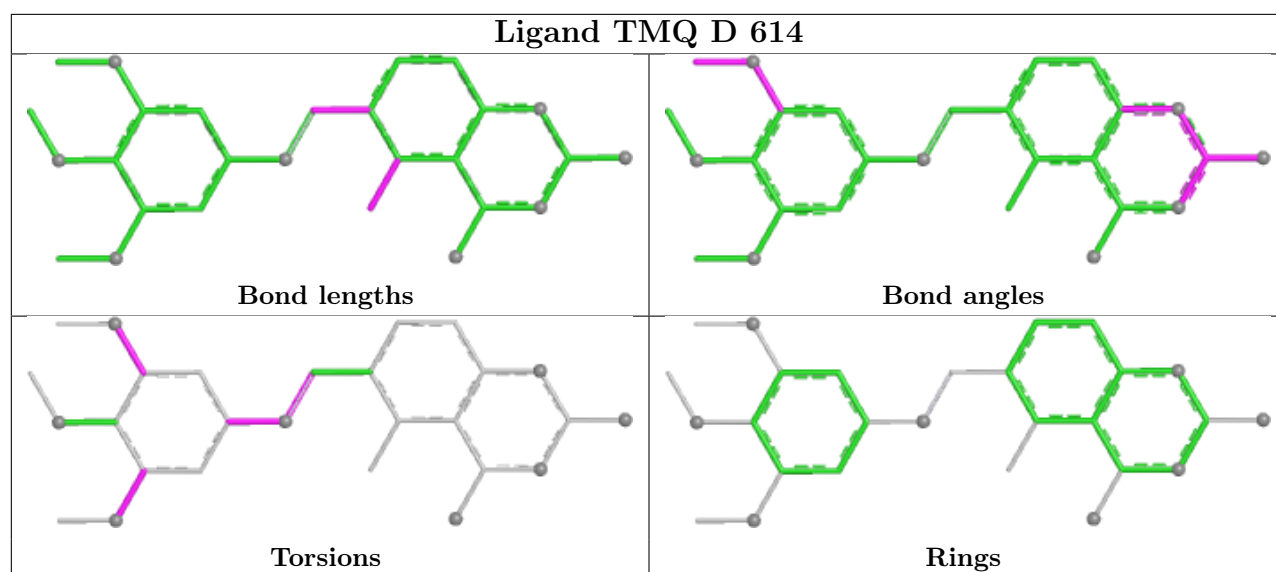
11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	805	EDO	1	0
5	D	804	EDO	1	0
5	C	806	EDO	1	0
3	B	602	NAP	1	0
4	B	612	TMQ	1	0
3	C	603	NAP	3	0
4	C	613	TMQ	3	0
4	D	614	TMQ	4	0
4	A	611	TMQ	5	0
3	A	601	NAP	2	0
3	D	604	NAP	1	0

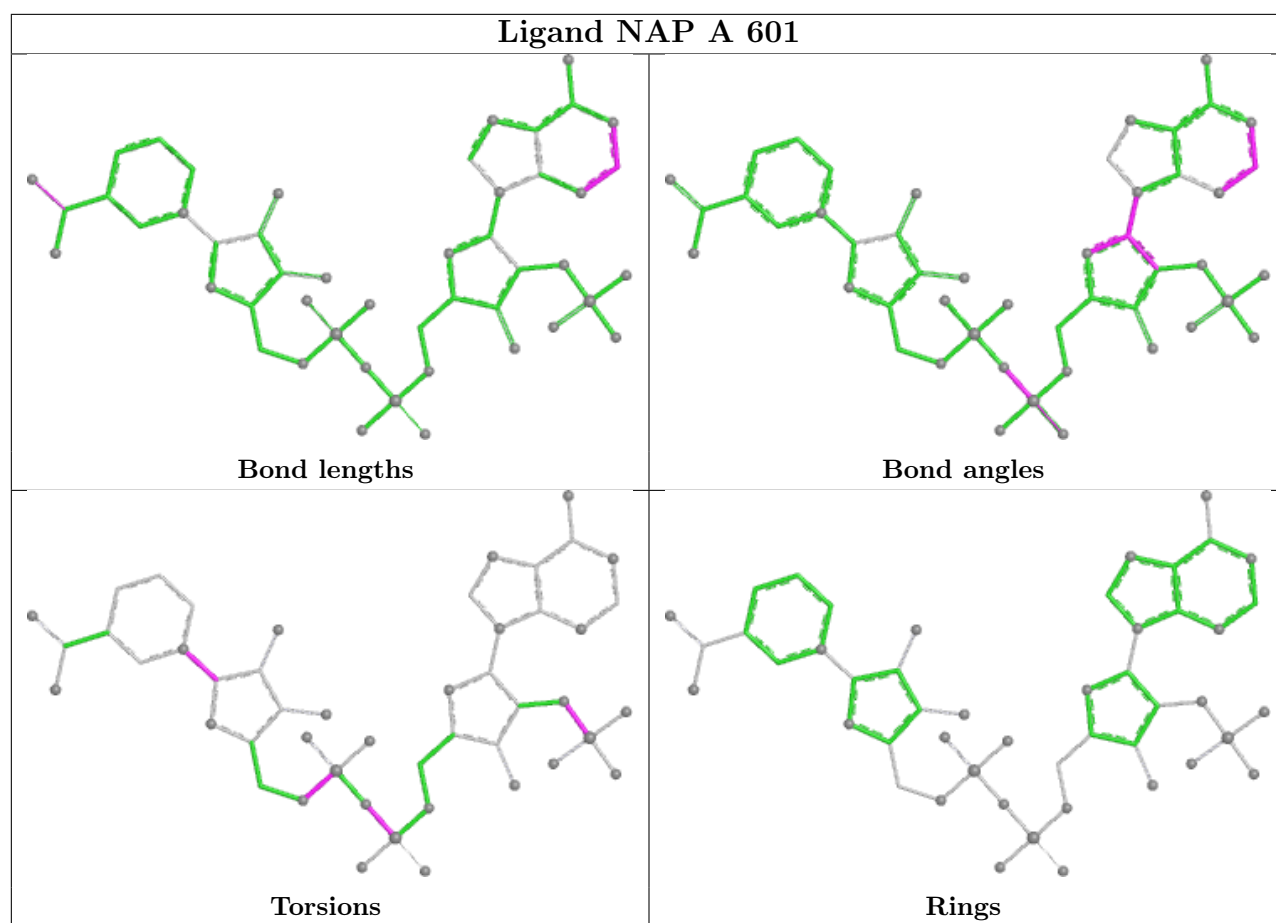
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

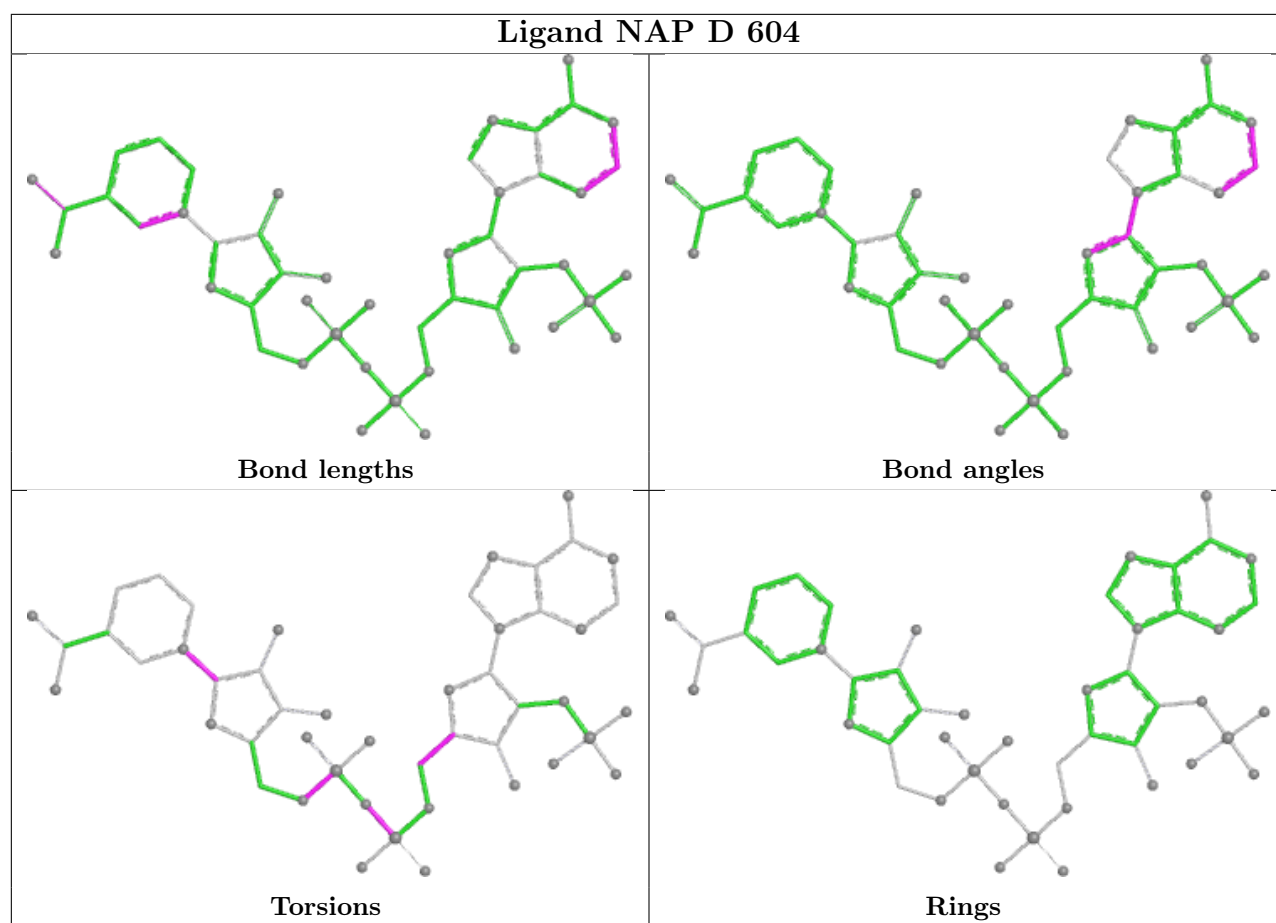












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	510/521 (97%)	-0.07	6 (1%) 76 56	44, 56, 69, 78	0
1	B	508/521 (97%)	1.04	103 (20%) 3 2	46, 56, 72, 81	0
1	C	510/521 (97%)	0.20	19 (3%) 45 27	43, 56, 71, 78	0
1	D	509/521 (97%)	-0.01	8 (1%) 70 49	45, 56, 71, 77	0
All	All	2037/2084 (97%)	0.29	136 (6%) 25 14	43, 56, 71, 81	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65	LYS	6.7
1	C	40	SER	6.0
1	B	112	LEU	5.4
1	B	41	ILE	4.8
1	B	114	ASP	4.1
1	B	83	SER	4.1
1	B	219	ASN	4.0
1	B	47	GLU	4.0
1	B	185	SER	3.9
1	D	515	ILE	3.9
1	B	38	GLY	3.9
1	C	185	SER	3.8
1	B	122	ALA	3.8
1	C	121	HIS	3.8
1	B	102	THR	3.8
1	D	39	ARG	3.7
1	B	39	ARG	3.7
1	B	188	SER	3.6
1	D	113	PRO	3.6
1	B	391	ASN	3.6
1	B	107	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	218	ALA	3.4
1	B	186	SER	3.4
1	B	179	THR	3.4
1	B	225	TYR	3.3
1	C	374	GLU	3.3
1	B	57	THR	3.3
1	B	216	THR	3.2
1	B	392	PRO	3.2
1	B	81	TRP	3.2
1	A	516	SER	3.1
1	B	384	ARG	3.1
1	B	113	PRO	3.1
1	B	85	PRO	3.1
1	B	222	GLU	3.0
1	D	114	ASP	3.0
1	B	40	SER	3.0
1	C	186	SER	3.0
1	B	350	PHE	3.0
1	B	184	GLU	3.0
1	B	261	GLY	3.0
1	B	467	SER	3.0
1	B	99	LEU	3.0
1	C	41	ILE	3.0
1	B	227	PHE	3.0
1	C	64	VAL	3.0
1	B	51	PHE	3.0
1	B	366	VAL	2.9
1	D	11	THR	2.9
1	B	189	VAL	2.9
1	B	330	GLY	2.9
1	B	86	PRO	2.8
1	B	61	GLY	2.8
1	B	255	HIS	2.8
1	B	190	PHE	2.8
1	B	379	ASN	2.7
1	B	383	ARG	2.7
1	D	13	ALA	2.7
1	A	110	ASP	2.7
1	B	60	ARG	2.7
1	B	182	ALA	2.7
1	B	424	SER	2.7
1	B	259	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	267	GLY	2.6
1	B	421	TYR	2.6
1	B	45	VAL	2.5
1	B	143	ASN	2.5
1	B	180	ILE	2.5
1	D	122	ALA	2.5
1	C	62	LYS	2.5
1	B	82	ASP	2.5
1	B	46	PRO	2.5
1	B	62	LYS	2.5
1	B	394	ALA	2.5
1	B	363	GLY	2.4
1	B	268	ALA	2.4
1	B	63	ASN	2.4
1	B	256	ASP	2.4
1	D	185	SER	2.4
1	B	331	LEU	2.4
1	B	223	THR	2.4
1	B	12	VAL	2.4
1	C	3	LEU	2.4
1	B	84	ILE	2.4
1	B	341	PRO	2.4
1	B	3	LEU	2.3
1	B	64	VAL	2.3
1	B	88	PHE	2.3
1	B	34	GLY	2.3
1	A	121	HIS	2.3
1	B	43	TRP	2.3
1	B	106	GLN	2.3
1	B	251	GLY	2.3
1	B	333	GLU	2.3
1	B	30	ASP	2.2
1	C	143	ASN	2.2
1	B	410	TYR	2.2
1	B	215	LEU	2.2
1	C	61	GLY	2.2
1	B	2	SER	2.2
1	B	146	PRO	2.2
1	A	64	VAL	2.2
1	B	260	VAL	2.2
1	B	395	LEU	2.2
1	C	37	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	122	ALA	2.2
1	C	38	GLY	2.2
1	B	67	SER	2.2
1	B	78	ARG	2.2
1	C	88	PHE	2.2
1	C	221	ASN	2.2
1	A	114	ASP	2.2
1	B	13	ALA	2.1
1	B	37	ASP	2.1
1	B	226	TYR	2.1
1	B	399	ALA	2.1
1	B	461	GLY	2.1
1	B	221	ASN	2.1
1	C	44	ASN	2.1
1	B	42	PRO	2.1
1	B	339	LEU	2.1
1	B	401	PRO	2.1
1	C	13	ALA	2.1
1	B	147	SER	2.1
1	B	224	LYS	2.1
1	B	214	GLU	2.1
1	C	14	GLU	2.1
1	B	56	THR	2.1
1	B	365	GLY	2.1
1	B	48	ASP	2.1
1	B	70	LYS	2.0
1	B	351	GLY	2.0
1	B	332	THR	2.0
1	B	252	ASN	2.0
1	B	220	GLY	2.0
1	A	183	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

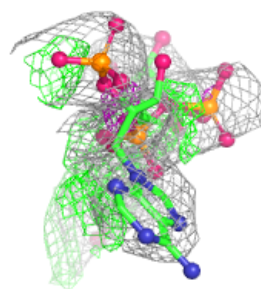
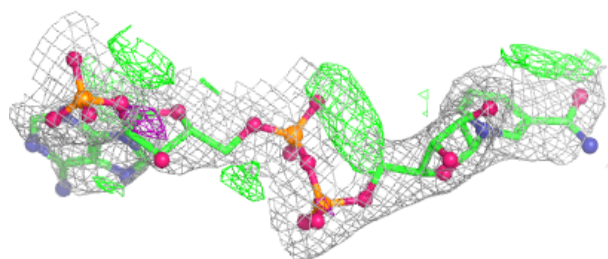
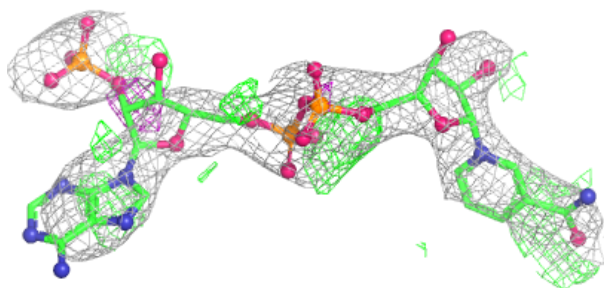
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAP	B	602	48/48	0.76	0.22	78,79,80,80	48
4	TMQ	B	612	27/27	0.76	0.34	73,73,74,74	27
4	TMQ	D	614	27/27	0.78	0.17	72,72,77,77	0
5	EDO	B	805	4/4	0.80	0.11	70,71,71,71	0
5	EDO	C	806	4/4	0.80	0.12	53,53,53,53	0
5	EDO	D	804	4/4	0.83	0.12	54,55,55,56	0
3	NAP	C	603	48/48	0.86	0.16	71,75,80,81	0
3	NAP	D	604	48/48	0.87	0.13	87,89,94,94	0
4	TMQ	C	613	27/27	0.87	0.15	56,56,61,62	0
4	TMQ	A	611	27/27	0.88	0.14	55,55,60,61	0
5	EDO	A	801	4/4	0.89	0.10	59,59,59,59	0
5	EDO	C	803	4/4	0.89	0.23	47,48,48,49	0
3	NAP	A	601	48/48	0.90	0.13	67,69,72,72	0
2	SO4	C	703	5/5	0.93	0.20	56,57,58,58	0
2	SO4	D	704	5/5	0.94	0.17	64,65,65,66	0
5	EDO	A	802	4/4	0.94	0.12	62,63,64,65	0
2	SO4	A	701	5/5	0.97	0.13	59,60,61,61	0
2	SO4	C	702	5/5	0.97	0.14	50,52,52,53	0

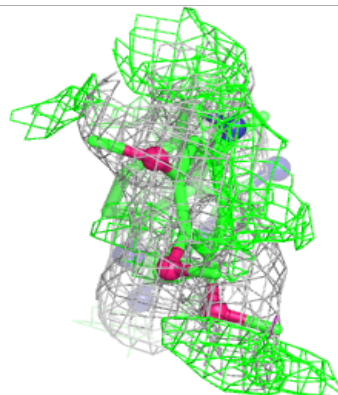
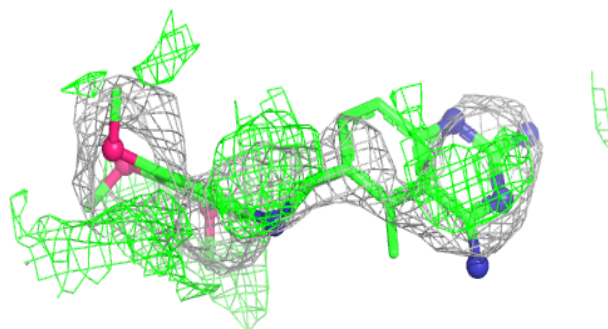
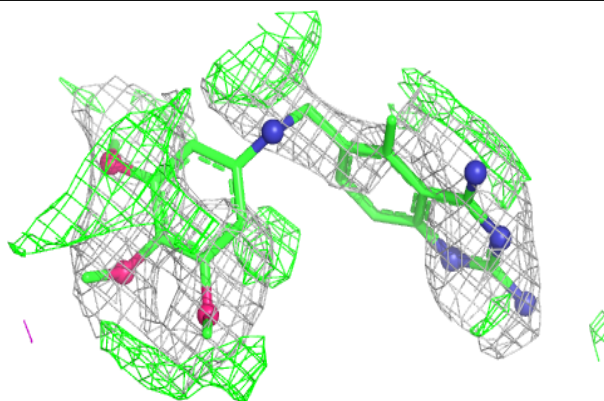
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NAP 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 TMQ B 612:**

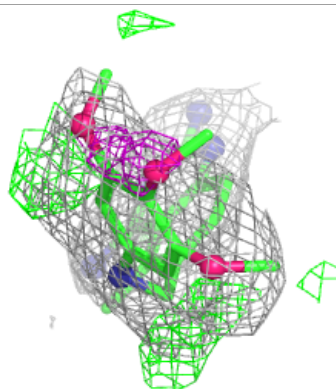
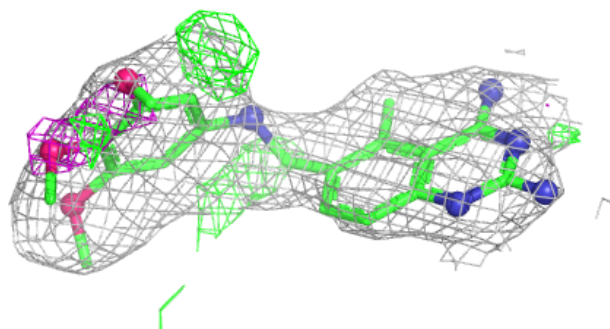
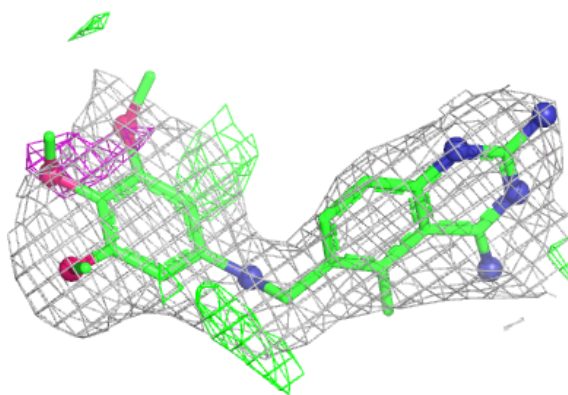
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



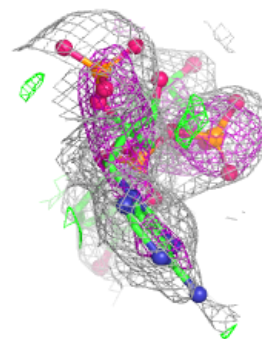
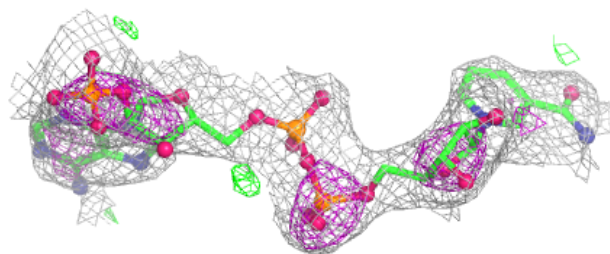
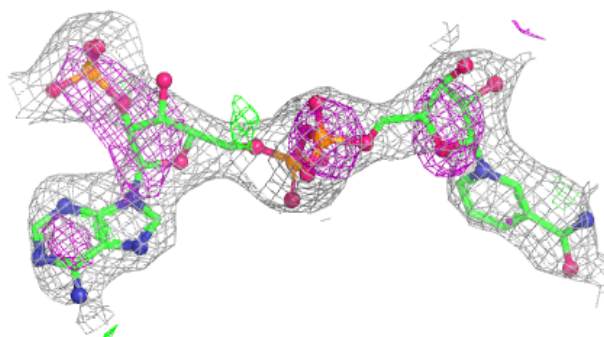


**Electron density around TMQ D 614:**

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

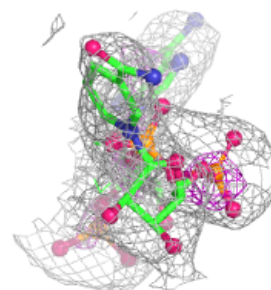
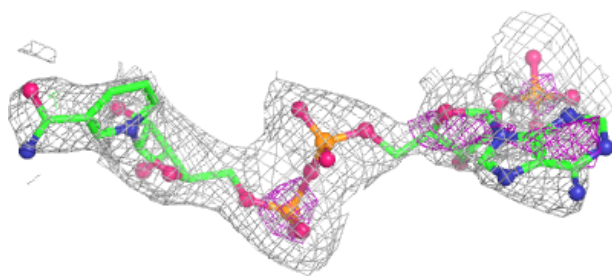
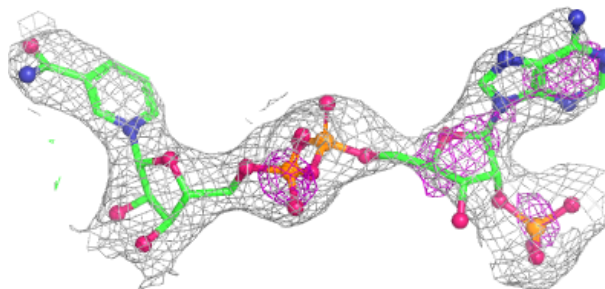
**Electron density around NAP C 603:**

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

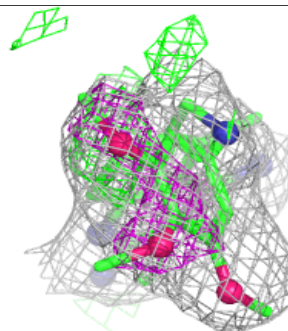
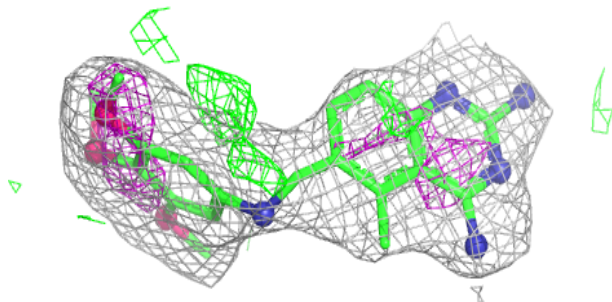
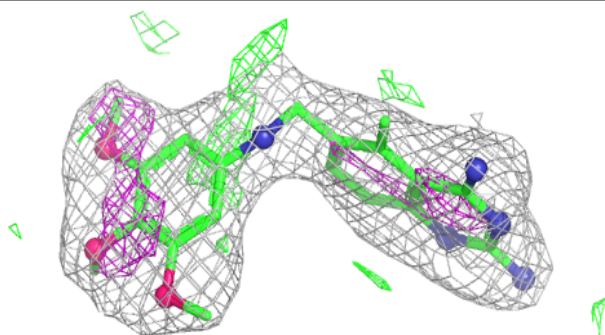


**Electron density around NAP D 604:**

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

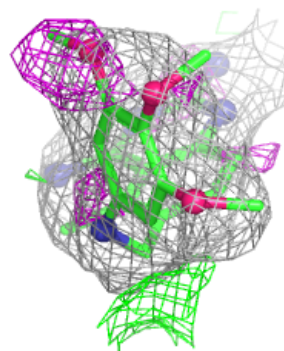
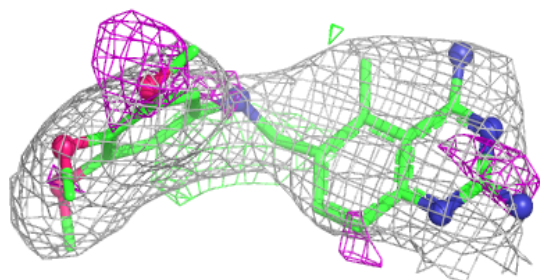
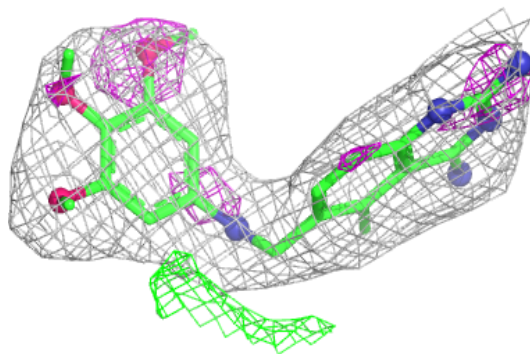
**Electron density around TMQ C 613:**

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

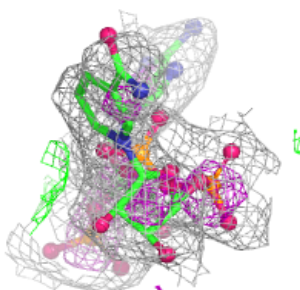
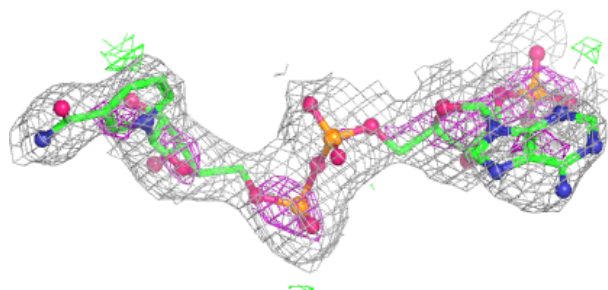
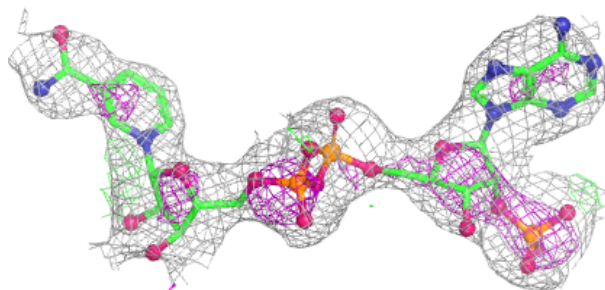


**Electron density around TMQ A 611:**

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

**Electron density around NAP A 601:**

$2mF_o-DF_c$  (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.