



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:00 pm BST

PDB ID : 3CLB
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

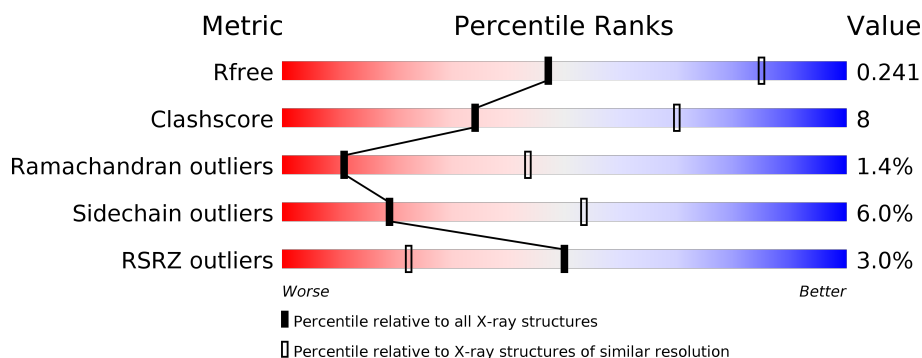
1 Overall quality at a glance

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	521	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>••</div> </div> </div>
1	B	521	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>•••</div> </div> </div>
1	C	521	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>••</div> </div> </div>
1	D	521	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>••</div> </div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TMQ	B	612	-	-	-	X

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.

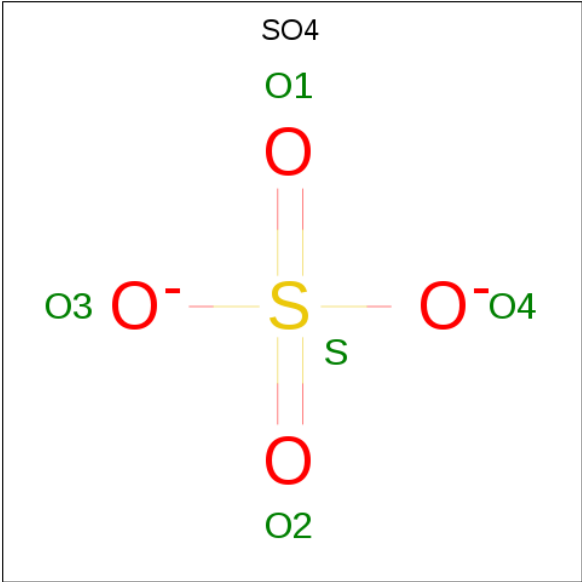
- Molecule 1 is a protein called DHFR-TS.

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:

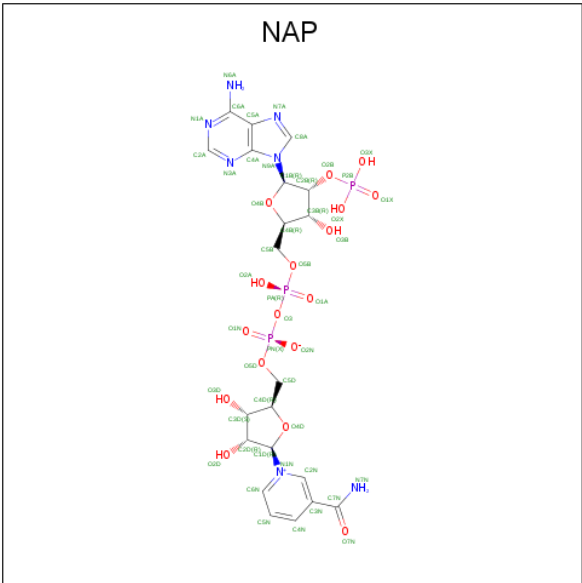
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ARG	HIS	SEE REMARK 999	UNP Q27793
A	55	VAL	LEU	SEE REMARK 999	UNP Q27793
A	137	GLN	ARG	SEE REMARK 999	UNP Q27793
B	32	ARG	HIS	SEE REMARK 999	UNP Q27793
B	55	VAL	LEU	SEE REMARK 999	UNP Q27793
B	137	GLN	ARG	SEE REMARK 999	UNP Q27793
C	32	ARG	HIS	SEE 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 (three-letter code: SO4) (formula: O₄S).



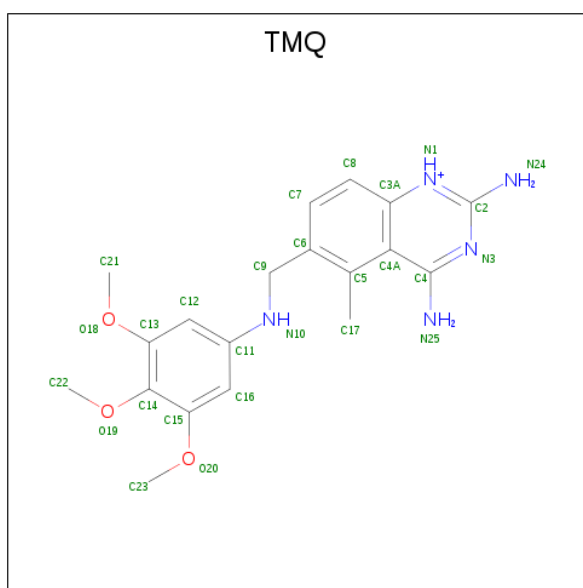
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 4 is TRIMETREXATE (three-letter code: TMQ) (formula: $C_{19}H_{24}N_5O_3$).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: 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		

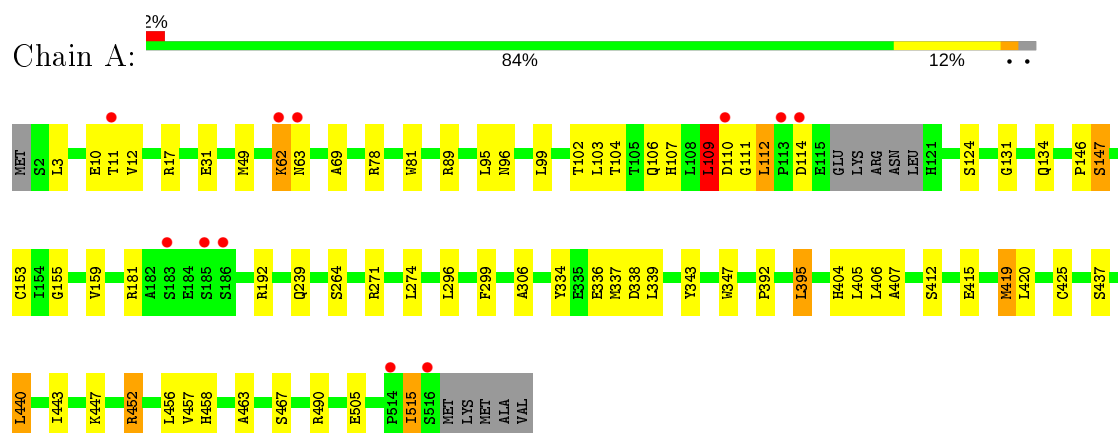
- Molecule 6 is water.

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		

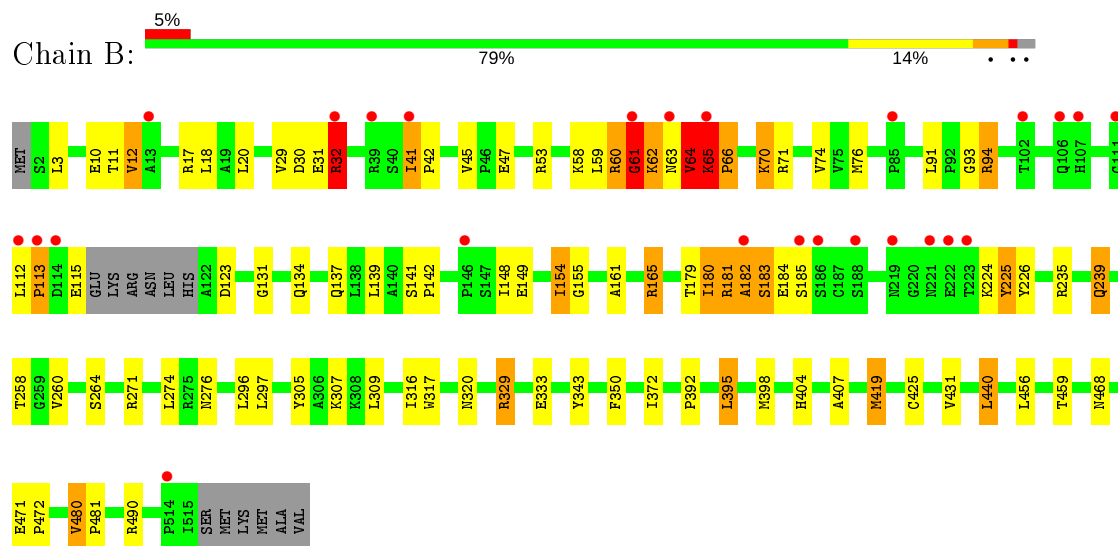
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

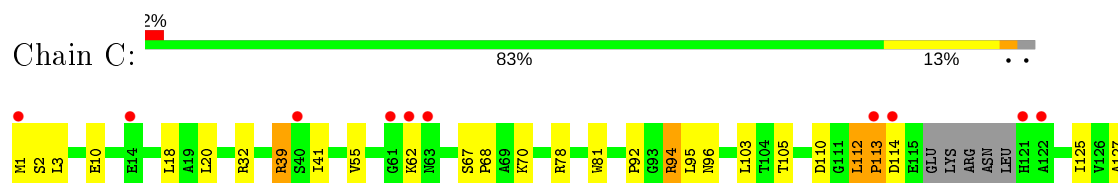
• Molecule 1: DHFR-TS

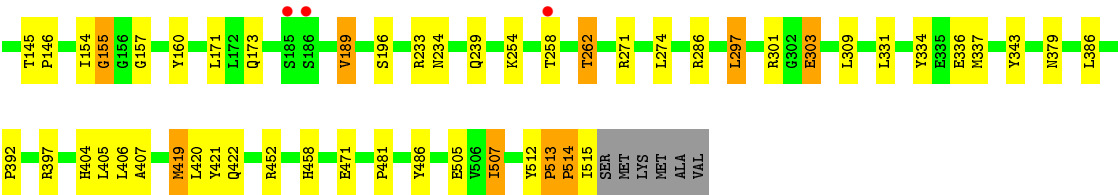


• Molecule 1: DHFR-TS

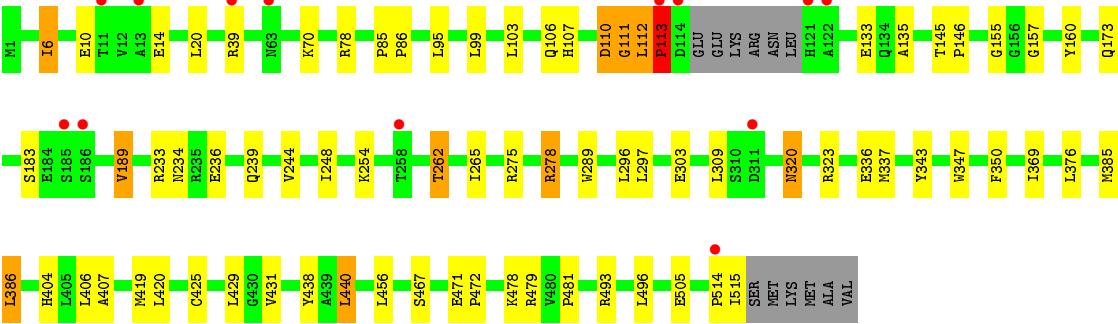
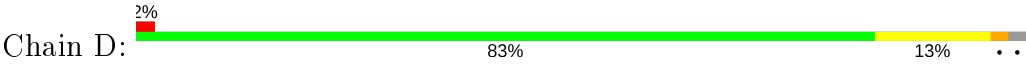


• Molecule 1: DHFR-TS





• Molecule 1: DHFR-TS



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	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) 97.1 (19.94-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	60.9	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16618	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: TMQ, NAP, SO4, EDO

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	0.39	0/4150	0.55	0/5632
1	B	0.43	1/4133 (0.0%)	0.59	2/5609 (0.0%)
1	C	0.40	0/4152	0.56	0/5634
1	D	0.40	2/4136 (0.0%)	0.54	0/5613
All	All	0.41	3/16571 (0.0%)	0.56	2/22488 (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	6.64	1.49	1.32
1	D	106	GLN	CD-OE1	6.27	1.37	1.24
1	B	71	ARG	NE-CZ	5.36	1.40	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	ARG	NE-CZ-NH2	-12.51	114.05	120.30
1	B	71	ARG	NE-CZ-NH1	11.06	125.83	120.30

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	48	0
1	B	4036	0	3988	129	0
1	C	4054	0	4007	40	0
1	D	4038	0	3984	43	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	5	0
3	B	48	0	25	3	0
3	C	48	0	25	4	0
3	D	48	0	25	1	0
4	A	27	0	24	8	0
4	B	27	0	24	6	0
4	C	27	0	24	4	0
4	D	27	0	24	4	0
5	A	8	0	12	0	0
5	B	4	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	275	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (275) 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:59:LEU:HD12	1:B:65:LYS:HD2	1.40	1.01
1:B:65:LYS:HE2	1:B:70:LYS:CG	1.90	1.00
1:B:63:ASN:C	1:B:64:VAL:HG23	1.81	1.00
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
1:D:111:GLY:C	1:D:113:PRO:HD2	1.84	0.96
1:A:112:LEU:N	1:A:112:LEU:HD23	1.81	0.93
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:180:ILE:CG2	1:B:225:TYR:HA	2.00	0.91
1:B:31:GLU:O	1:B:32:ARG:HB2	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:63:ASN:C	1:B:64:VAL:CG2	2.44	0.86
1:C:515:ILE:HG22	1:C:515:ILE:O	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
4:B:612:TMQ:C17	4:B:612:TMQ:HN52	1.93	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:C17	4:A:611:TMQ:HN52	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
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:A:110:ASP:O	1:A:112:LEU:CD2	2.43	0.67
1:A:112:LEU:CD2	1:A:112:LEU:N	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
3:A:601:NAP:C4N	4:A:611:TMQ:H172	2.26	0.65
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:D:471:GLU:HB3	1:D:472:PRO:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:THR:H	1:A:107:HIS:HB2	1.63	0.64
1:B:225:TYR:C	1:B:225:TYR:CD1	2.70	0.64
1:B:59:LEU:HD12	1:B:65:LYS:CD	2.07	0.64
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: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: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:A:111:GLY:C	1:A:112:LEU:HD23	2.21	0.60
4:B:612:TMQ:HN52	4:B:612:TMQ:H172	1.65	0.60
1:A:106:GLN:CA	1:A:109:LEU:HD21	2.30	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
1:B:64:VAL:C	1:B:65:LYS:HG3	2.23	0.59
1:B:131:GLY:N	1:B:134:GLN:HE21	2.01	0.59
4:B:612:TMQ:HN52	4:B:612:TMQ:H173	1.67	0.58
1:A:10:GLU:CD	1:A:10:GLU:H	2.06	0.58
1:B:181:ARG:C	1:B:183:SER:N	2.56	0.58
1:A:407:ALA:HA	1:A:419:MET:O	2.05	0.57
1:B:60:ARG:O	1:B:61:GLY:C	2.42	0.57
1:B:329:ARG:NH1	1:B:398:MET:O	2.37	0.57
1:D:111:GLY:O	1:D:113:PRO:CD	2.53	0.57
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
4:A:611:TMQ:H172	4:A:611:TMQ:HN52	1.70	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:65:LYS:HZ1	1:B:70:LYS:HG2	1.69	0.56
1:B:30:ASP:HA	1:B:180:ILE:C	2.27	0.56
4:D:614:TMQ:HN52	4:D:614:TMQ:H173	1.71	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
4:D:614:TMQ:HN52	4:D:614:TMQ:H172	1.70	0.55
1:C:105:THR:HB	1:C:127:ALA:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ILE:O	4:B:612:TMQ:N25	2.40	0.55
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
3:A:601:NAP:H4N	4:A:611:TMQ:H172	1.90	0.54
4:A:611:TMQ:H173	4:A:611:TMQ:HN52	1.73	0.53
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:C:112:LEU:HB2	1:C:113:PRO:C	2.26	0.53
1:A:110:ASP:O	1:A:112:LEU:HG	2.09	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:65:LYS:HZ1	1:B:70:LYS:CG	2.20	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
4:C:613:TMQ:HN52	4:C:613:TMQ:H172	1.75	0.51
1:B:59:LEU:O	1:B:60:ARG:C	2.48	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
3:B:602:NAP:C4N	4:B:612:TMQ:H172	2.41	0.51
1:A:49:MET:HE1	4:A:611:TMQ:C13	2.41	0.50
1:C:404:HIS:HB2	1:C:420:LEU:HD11	1.93	0.50
1:C:515:ILE:CG2	1:C:515:ILE:O	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
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:179:THR:C	1:B:180:ILE:HG23	2.32	0.49
1:B:59:LEU:HD13	1:B:65:LYS:NZ	2.26	0.49
1:C:234:ASN:HB3	1:C:481:PRO:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LYS:HZ3	1:B:70:LYS:HG3	1.76	0.49
1:D:336:GLU:O	1:D:337:MET:HB2	2.13	0.49
1:A:110:ASP:C	1:A:112:LEU:H	2.16	0.48
3:B:602:NAP:C5N	4:B:612:TMQ:H172	2.44	0.48
4:C:613:TMQ:HN52	4:C:613:TMQ:H173	1.77	0.48
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: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
3:A:601:NAP:C5N	4:A:611:TMQ:H172	2.44	0.47
1:B:179:THR:CB	1:B:226:TYR:CZ	2.97	0.47
1:B:225:TYR:C	1:B:225:TYR:HD1	2.17	0.47
1:C:405:LEU:HD12	1:C:406:LEU:HB2	1.97	0.47
1:B:179:THR:HG21	1:B:226:TYR:HH	1.78	0.47
1:D:111:GLY:O	1:D:112:LEU:CB	2.62	0.47
1:B:419:MET:HG2	1:C:421:TYR:OH	2.14	0.47
1:D:471:GLU:HA	1:D:471:GLU:OE1	2.15	0.47
1:B:224:LYS:H	1:B:224:LYS:HD2	1.80	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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:GLU:O	1:C:337:MET:HB2	2.16	0.45
1:C:407:ALA:HA	1:C:419:MET:O	2.17	0.45
1:C:81:TRP:CH2	1:C:125:ILE:HD12	2.52	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:10:GLU:CD	1:C:10:GLU:H	2.19	0.45
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:155:GLY:HA3	1:D:160:TYR:CZ	2.52	0.44
1:D:20:LEU:HD21	1:D:133:GLU:HG2	2.00	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:C:239:GLN:HE22	1:C:271:ARG:H	1.67	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: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
1:D:233:ARG:HH22	5:D:804:EDO:H22	1.83	0.43
1:B:181:ARG:O	1:B:182:ALA:C	2.57	0.43
1:B:59:LEU:HD12	1:B:64:VAL:HA	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:316:ILE:HG13	1:B:317:TRP:CD1	2.54	0.42
1:B:59:LEU:O	1:B:60:ARG:O	2.38	0.42
1:C:78:ARG:HH11	3:C:603:NAP:P2B	2.43	0.42
1:B:350:PHE:CZ	1:C:392:PRO:HD2	2.55	0.42
1:A:392:PRO:HD2	1:D:350:PHE:CZ	2.55	0.42
1:B:58:LYS:HG2	1:B:59:LEU:H	1.85	0.42
1:C:145:THR:HA	1:C:146:PRO:HA	1.89	0.42
3:C:603:NAP:C4N	4:C:613:TMQ:H172	2.50	0.42
1:A:296:LEU:HD22	1:A:440:LEU:HB3	2.02	0.41
1:A:96:ASN:HD22	1:A:96:ASN:N	2.18	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:A:443:ILE:O	1:A:447:LYS:HG3	2.21	0.41
1:D:404:HIS:H	1:D:404:HIS:CD2	2.38	0.41
1:B:112:LEU:H	1:B:113:PRO:HD2	1.84	0.41
1:C:96:ASN:N	1:C:96:ASN:HD22	2.19	0.41
1:D:407:ALA:HA	1:D:419:MET:O	2.21	0.41
1:D:99:LEU:HD21	1:D:135:ALA:HB2	2.02	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: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:A:109:LEU:HD23	1:A:109:LEU:C	2.42	0.40
1:A:515:ILE:HD13	1:A:515:ILE:C	2.41	0.40
1:B:62:LYS:HG3	1:B:63:ASN:HB2	2.04	0.40
1:A:103:LEU:HD12	1:A:107:HIS:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:CYS:SG	1:A:159:VAL:HG12	2.61	0.40
4:D:614:TMQ:C17	4:D:614:TMQ:N25	2.67	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%)	15	53
1	B	504/521 (97%)	471 (94%)	21 (4%)	12 (2%)	6	29
1	C	506/521 (97%)	475 (94%)	23 (4%)	8 (2%)	9	40
1	D	505/521 (97%)	487 (96%)	15 (3%)	3 (1%)	25	64
All	All	2021/2084 (97%)	1916 (95%)	77 (4%)	28 (1%)	11	43

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

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Mol	Chain	Res	Type
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%)	415 (95%)	21 (5%)	25	62
1	B	434/446 (97%)	402 (93%)	32 (7%)	13	44
1	C	436/446 (98%)	409 (94%)	27 (6%)	18	52
1	D	433/446 (97%)	408 (94%)	25 (6%)	20	55
All	All	1739/1784 (98%)	1634 (94%)	105 (6%)	19	53

All (105) 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	102	THR
1	A	109	LEU

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Mol	Chain	Res	Type
1	A	112	LEU
1	A	124	SER
1	A	147	SER
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	437	SER
1	A	440	LEU
1	A	452	ARG
1	A	456	LEU
1	A	467	SER
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	41	ILE
1	B	64	VAL
1	B	70	LYS
1	B	94	ARG
1	B	115	GLU
1	B	123	ASP
1	B	154	ILE
1	B	165	ARG
1	B	181	ARG
1	B	184	GLU
1	B	225	TYR
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	329	ARG
1	B	333	GLU
1	B	372	ILE
1	B	395	LEU
1	B	419	MET

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Mol	Chain	Res	Type
1	B	440	LEU
1	B	456	LEU
1	B	468	ASN
1	B	480	VAL
1	B	490	ARG
1	C	1	MET
1	C	3	LEU
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	110	ASP
1	C	173	GLN
1	C	189	VAL
1	C	196	SER
1	C	258	THR
1	C	262	THR
1	C	274	LEU
1	C	286	ARG
1	C	297	LEU
1	C	303	GLU
1	C	309	LEU
1	C	379	ASN
1	C	386	LEU
1	C	397	ARG
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	39	ARG
1	D	70	LYS
1	D	95	LEU
1	D	107	HIS
1	D	110	ASP
1	D	173	GLN
1	D	183	SER

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Mol	Chain	Res	Type
1	D	189	VAL
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	323	ARG
1	D	386	LEU
1	D	429	LEU
1	D	440	LEU
1	D	456	LEU
1	D	467	SER
1	D	493	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	107	HIS
1	A	134	GLN
1	A	143	ASN
1	A	239	GLN
1	A	422	GLN
1	B	63	ASN
1	B	106	GLN
1	B	134	GLN
1	B	173	GLN
1	B	239	GLN
1	B	320	ASN
1	B	379	ASN
1	B	468	ASN
1	B	469	HIS
1	C	107	HIS
1	C	207	GLN
1	C	239	GLN
1	C	255	HIS
1	C	320	ASN
1	C	360	ASN
1	C	422	GLN
1	C	434	ASN

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Mol	Chain	Res	Type
1	C	464	HIS
1	D	320	ASN
1	D	360	ASN
1	D	422	GLN
1	D	434	ASN

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 carbohydrates 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	$\# Z > 2$
4	TMQ	A	611	-	29,29,29	1.33	2 (6%)	39,41,41	1.50	6 (15%)
3	NAP	D	604	-	45,52,52	1.71	3 (6%)	56,80,80	0.99	1 (1%)
5	EDO	D	804	-	3,3,3	0.47	0	2,2,2	0.41	0
4	TMQ	B	612	-	29,29,29	1.29	2 (6%)	39,41,41	1.45	5 (12%)
3	NAP	C	603	-	45,52,52	1.72	3 (6%)	56,80,80	0.94	1 (1%)
2	SO4	C	703	-	4,4,4	0.19	0	6,6,6	0.26	0
5	EDO	C	803	-	3,3,3	0.41	0	2,2,2	0.51	0
4	TMQ	C	613	-	29,29,29	1.35	2 (6%)	39,41,41	1.46	6 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	C	806	-	3,3,3	0.45	0	2,2,2	0.50	0
3	NAP	B	602	-	45,52,52	1.76	4 (8%)	56,80,80	0.98	1 (1%)
5	EDO	B	805	-	3,3,3	0.45	0	2,2,2	0.40	0
2	SO4	D	704	-	4,4,4	0.12	0	6,6,6	0.17	0
4	TMQ	D	614	-	29,29,29	1.30	2 (6%)	39,41,41	1.35	2 (5%)
2	SO4	C	702	-	4,4,4	0.18	0	6,6,6	0.34	0
3	NAP	A	601	-	45,52,52	1.67	3 (6%)	56,80,80	1.05	1 (1%)
5	EDO	A	802	-	3,3,3	0.48	0	2,2,2	0.31	0
2	SO4	A	701	-	4,4,4	0.14	0	6,6,6	0.24	0
5	EDO	A	801	-	3,3,3	0.48	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
4	TMQ	A	611	-	-	4/11/11/11	0/3/3/3
3	NAP	D	604	-	-	5/31/67/67	0/5/5/5
5	EDO	D	804	-	-	1/1/1/1	-
4	TMQ	B	612	-	-	6/11/11/11	0/3/3/3
3	NAP	C	603	-	-	5/31/67/67	0/5/5/5
5	EDO	C	803	-	-	1/1/1/1	-
4	TMQ	C	613	-	-	2/11/11/11	0/3/3/3
5	EDO	C	806	-	-	1/1/1/1	-
3	NAP	B	602	-	-	9/31/67/67	0/5/5/5
4	TMQ	D	614	-	-	7/11/11/11	0/3/3/3
3	NAP	A	601	-	-	7/31/67/67	0/5/5/5
5	EDO	A	802	-	-	0/1/1/1	-
5	EDO	B	805	-	-	1/1/1/1	-
5	EDO	A	801	-	-	1/1/1/1	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	NAP	O7N-C7N	9.22	1.41	1.24
3	D	604	NAP	O7N-C7N	8.81	1.41	1.24
3	C	603	NAP	O7N-C7N	8.76	1.40	1.24
3	A	601	NAP	O7N-C7N	8.61	1.40	1.24
4	C	613	TMQ	C17-C5	-4.89	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	611	TMQ	C17-C5	-4.88	1.39	1.51
4	D	614	TMQ	C17-C5	-4.77	1.40	1.51
4	B	612	TMQ	C17-C5	-4.68	1.40	1.51
3	C	603	NAP	C2A-N3A	4.56	1.39	1.32
3	D	604	NAP	C2A-N3A	4.35	1.39	1.32
3	B	602	NAP	C2A-N3A	4.24	1.38	1.32
3	A	601	NAP	C2A-N3A	4.17	1.38	1.32
4	C	613	TMQ	C9-C6	-3.18	1.40	1.50
4	B	612	TMQ	C9-C6	-3.04	1.41	1.50
4	D	614	TMQ	C9-C6	-2.95	1.41	1.50
3	C	603	NAP	C2A-N1A	2.94	1.39	1.33
4	A	611	TMQ	C9-C6	-2.91	1.41	1.50
3	D	604	NAP	C2A-N1A	2.82	1.39	1.33
3	B	602	NAP	C2A-N1A	2.79	1.39	1.33
3	A	601	NAP	C2A-N1A	2.71	1.38	1.33
3	B	602	NAP	C2N-N1N	2.36	1.37	1.35

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	604	NAP	N3A-C2A-N1A	-5.77	119.66	128.68
3	B	602	NAP	N3A-C2A-N1A	-5.64	119.87	128.68
3	A	601	NAP	N3A-C2A-N1A	-5.62	119.90	128.68
3	C	603	NAP	N3A-C2A-N1A	-5.33	120.35	128.68
4	A	611	TMQ	N1-C2-N3	-5.23	120.25	127.22
4	B	612	TMQ	N1-C2-N3	-5.22	120.26	127.22
4	C	613	TMQ	N1-C2-N3	-5.18	120.31	127.22
4	D	614	TMQ	N1-C2-N3	-5.08	120.45	127.22
4	C	613	TMQ	C21-O18-C13	-3.85	111.72	117.53
4	B	612	TMQ	C23-O20-C15	-3.11	112.84	117.53
4	A	611	TMQ	N24-C2-N3	2.77	121.56	117.25
4	A	611	TMQ	C23-O20-C15	-2.66	113.52	117.53
4	A	611	TMQ	C21-O18-C13	-2.62	113.57	117.53
4	B	612	TMQ	C21-O18-C13	-2.62	113.58	117.53
4	A	611	TMQ	C9-C6-C7	-2.53	115.23	121.00
4	D	614	TMQ	C23-O20-C15	-2.31	114.04	117.53
4	C	613	TMQ	N24-C2-N3	2.29	120.81	117.25
4	B	612	TMQ	C4A-C4-N25	-2.25	118.61	122.67
4	B	612	TMQ	C2-N1-C3A	2.15	121.66	116.33
4	A	611	TMQ	C2-N1-C3A	2.13	121.60	116.33
4	C	613	TMQ	C17-C5-C6	-2.11	118.39	120.80
4	C	613	TMQ	C9-C6-C7	-2.07	116.28	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	613	TMQ	C2-N1-C3A	2.03	121.35	116.33

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	604	NAP	O4D-C1D-N1N-C6N
3	C	603	NAP	O4D-C1D-N1N-C6N
3	B	602	NAP	C2B-O2B-P2B-O1X
3	B	602	NAP	C5D-O5D-PN-O3
3	B	602	NAP	O4D-C1D-N1N-C6N
3	A	601	NAP	C2B-O2B-P2B-O1X
3	A	601	NAP	C2B-O2B-P2B-O3X
3	A	601	NAP	O4D-C1D-N1N-C2N
3	A	601	NAP	O4D-C1D-N1N-C6N
4	A	611	TMQ	C16-C11-N10-C9
4	D	614	TMQ	C14-C15-O20-C23
4	B	612	TMQ	C14-C15-O20-C23
4	B	612	TMQ	C14-C13-O18-C21
4	A	611	TMQ	C14-C15-O20-C23
4	A	611	TMQ	C12-C11-N10-C9
4	B	612	TMQ	C12-C11-N10-C9
4	D	614	TMQ	C14-C13-O18-C21
3	B	602	NAP	C3D-C4D-C5D-O5D
4	B	612	TMQ	C16-C15-O20-C23
4	B	612	TMQ	C16-C11-N10-C9
4	A	611	TMQ	C16-C15-O20-C23
4	B	612	TMQ	C12-C13-O18-C21
4	D	614	TMQ	C12-C13-O18-C21
4	D	614	TMQ	C16-C15-O20-C23
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	C	603	NAP	C5D-O5D-PN-O3
3	D	604	NAP	C3B-C4B-C5B-O5B
3	B	602	NAP	C5D-O5D-PN-O1N
3	B	602	NAP	C5D-O5D-PN-O2N
5	C	803	EDO	O1-C1-C2-O2
3	B	602	NAP	PN-O3-PA-O2A
3	B	602	NAP	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	A	601	NAP	PN-O3-PA-O2A
5	D	804	EDO	O1-C1-C2-O2
5	C	806	EDO	O1-C1-C2-O2
5	A	801	EDO	O1-C1-C2-O2
3	D	604	NAP	C2B-O2B-P2B-O3X
3	D	604	NAP	PN-O3-PA-O2A
3	C	603	NAP	PN-O3-PA-O1A
3	C	603	NAP	PN-O3-PA-O2A
3	A	601	NAP	PN-O3-PA-O1A
3	D	604	NAP	C5D-O5D-PN-O1N
3	C	603	NAP	C5D-O5D-PN-O1N
3	A	601	NAP	C5D-O5D-PN-O1N
5	B	805	EDO	O1-C1-C2-O2
4	D	614	TMQ	C6-C9-N10-C11

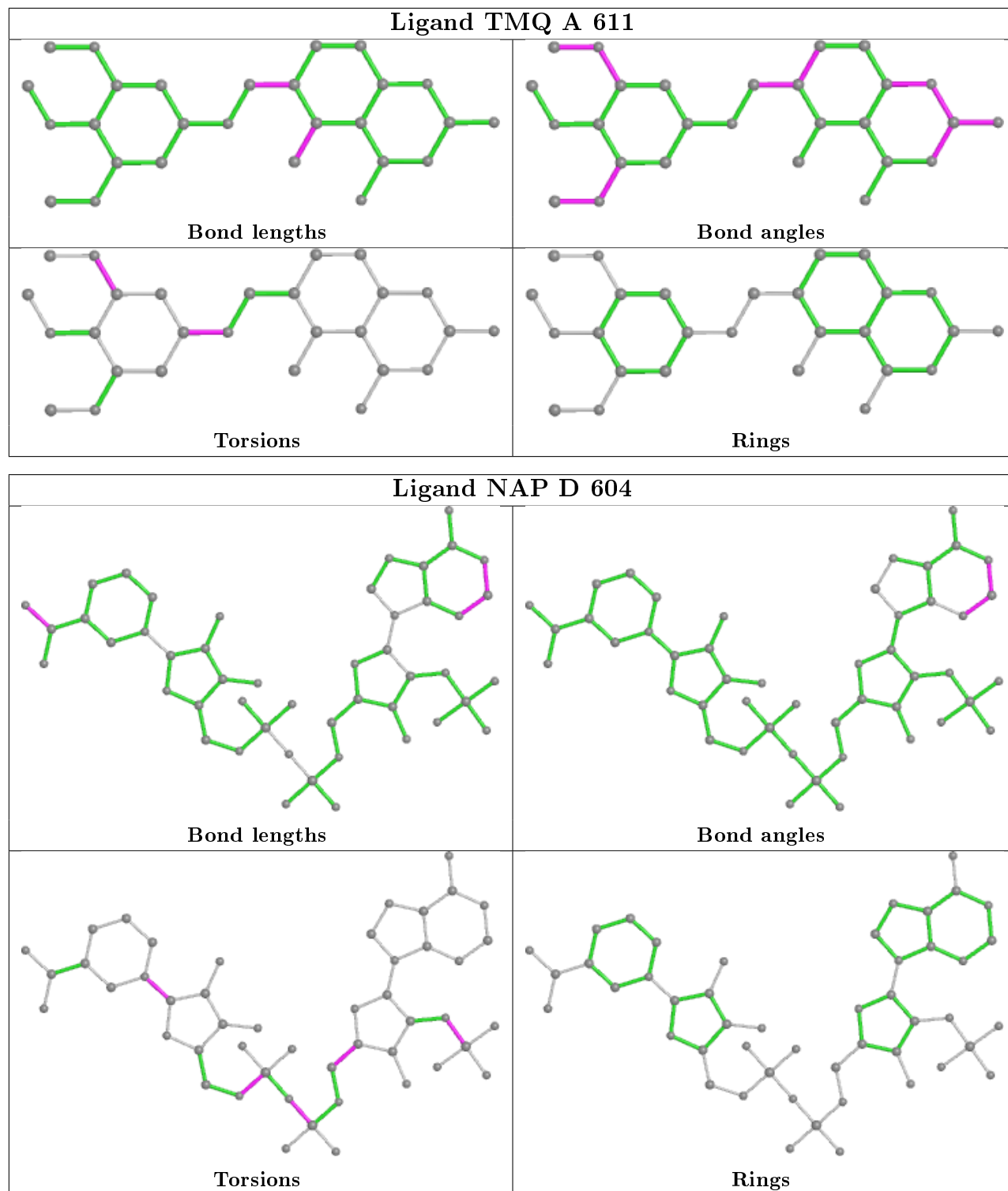
There are no ring outliers.

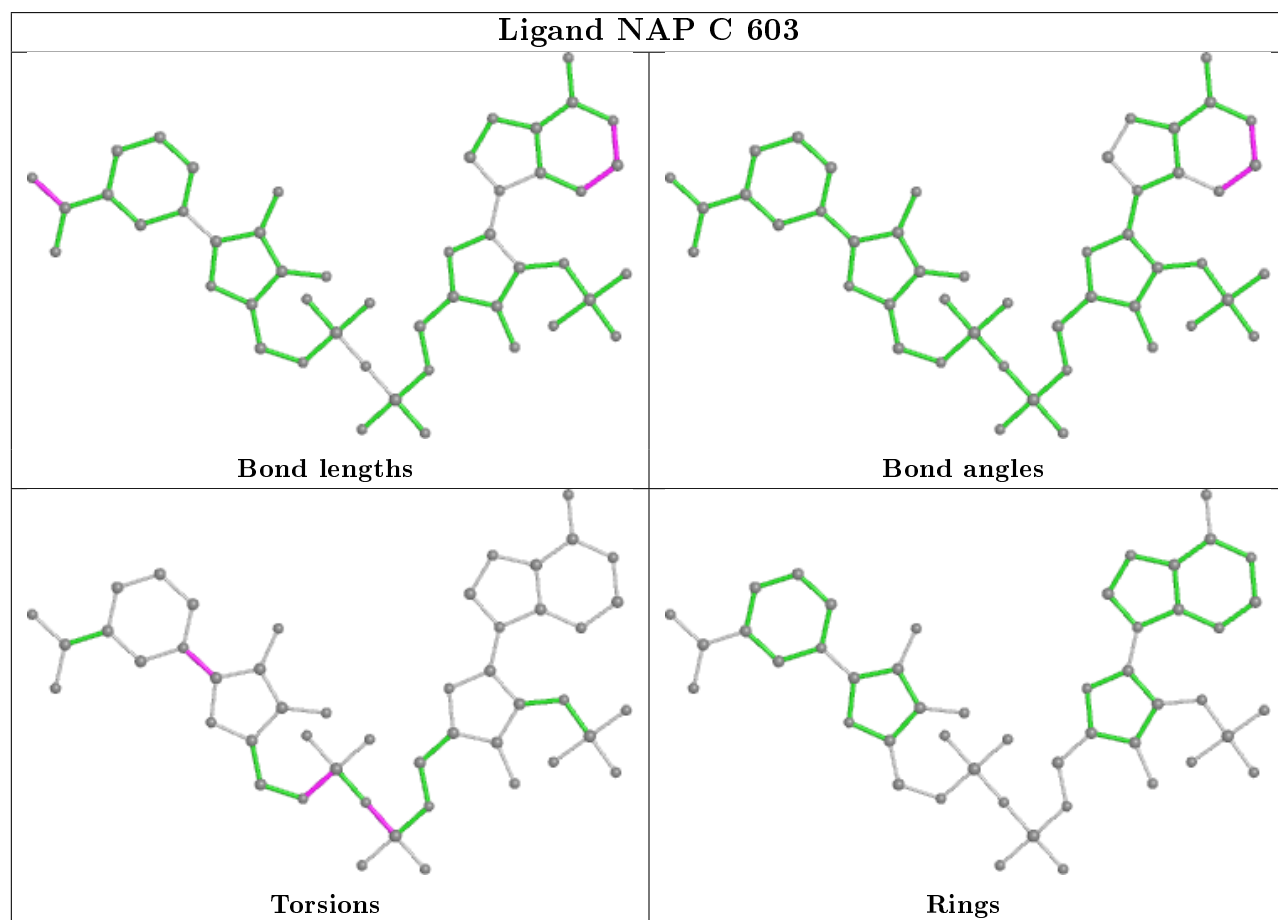
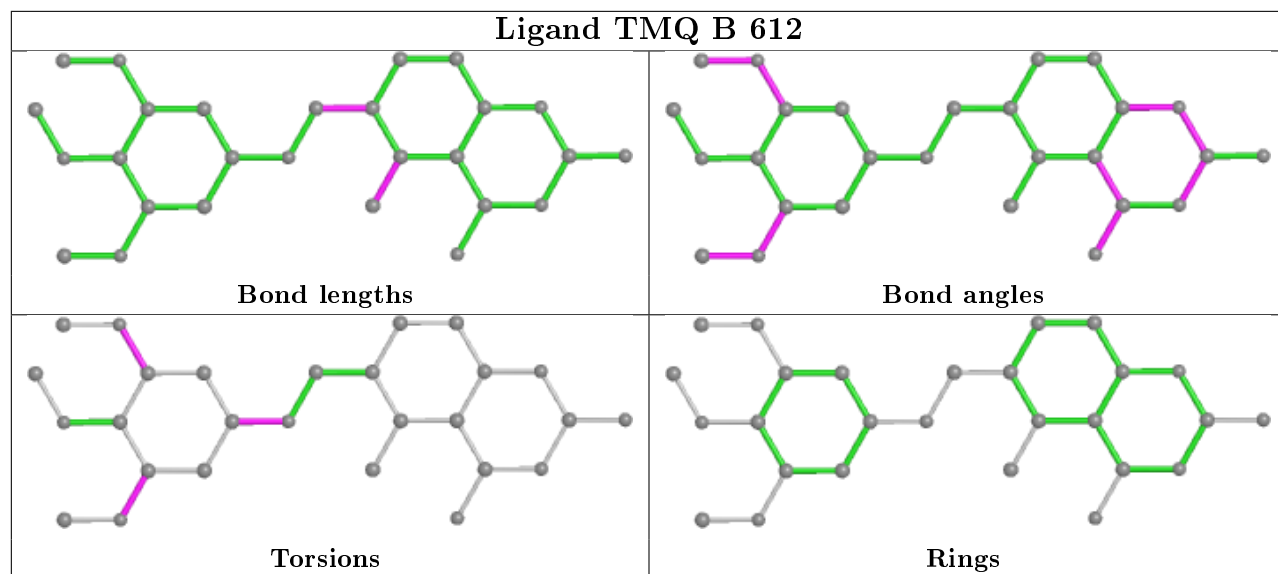
11 monomers are involved in 32 short contacts:

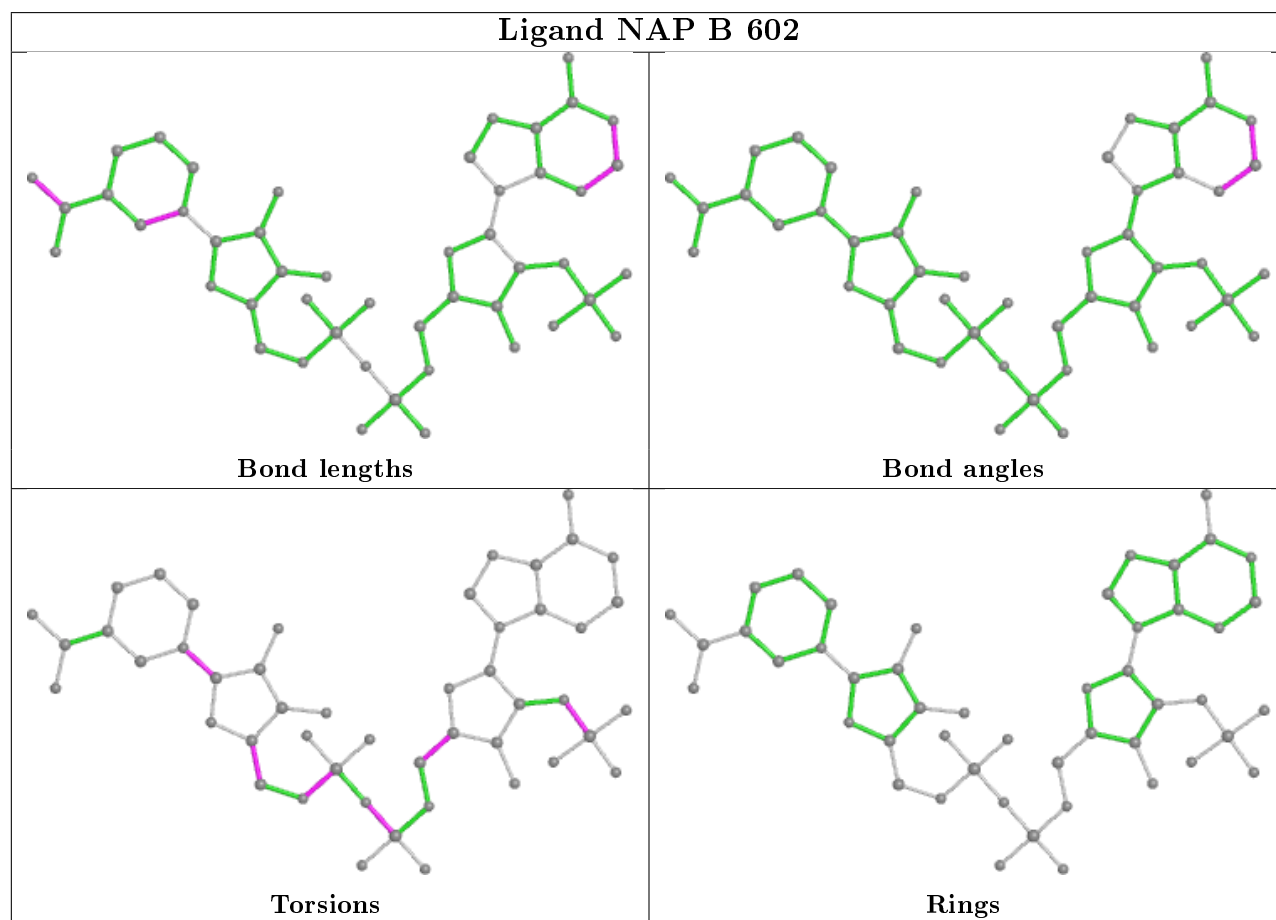
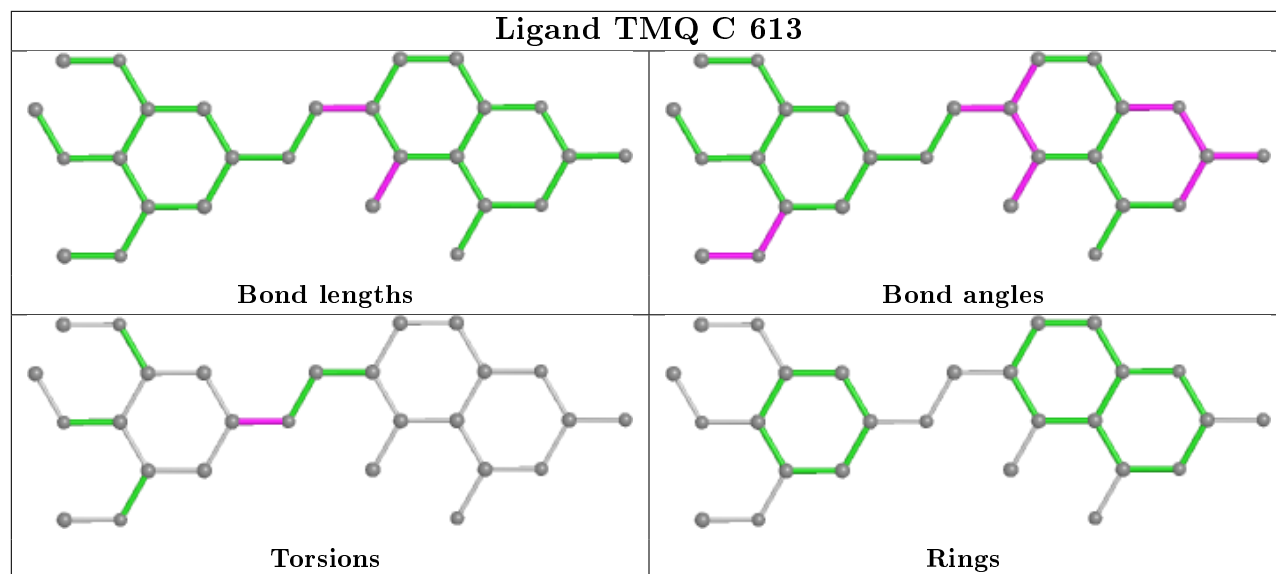
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	611	TMQ	8	0
3	D	604	NAP	1	0
5	D	804	EDO	1	0
4	B	612	TMQ	6	0
3	C	603	NAP	4	0
4	C	613	TMQ	4	0
5	C	806	EDO	1	0
3	B	602	NAP	3	0
5	B	805	EDO	1	0
4	D	614	TMQ	4	0
3	A	601	NAP	5	0

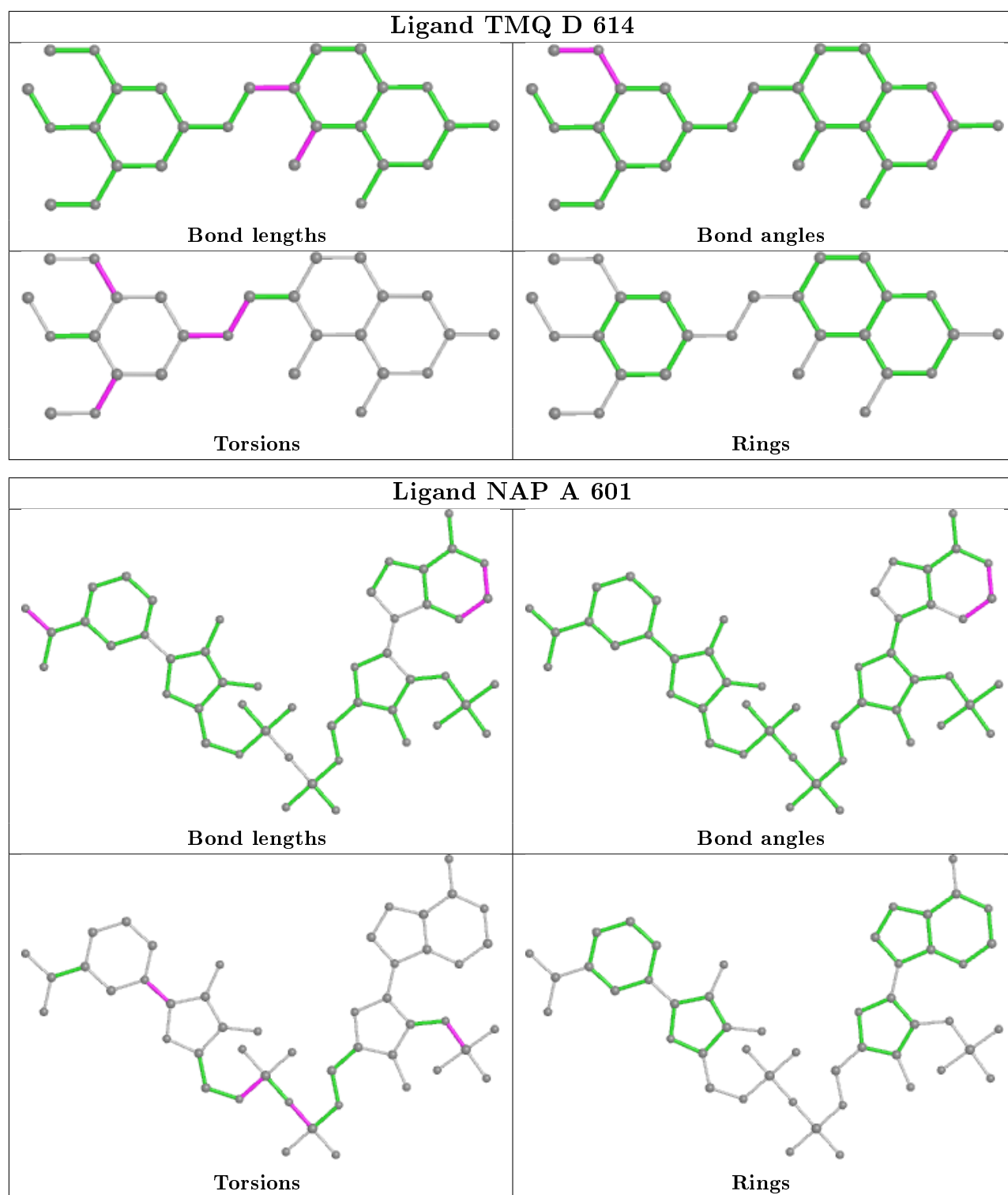
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	510/521 (97%)	-0.27	11 (2%) 62 33	44, 56, 69, 78	0
1	B	508/521 (97%)	-0.09	25 (4%) 29 11	46, 56, 72, 81	0
1	C	510/521 (97%)	-0.29	13 (2%) 57 29	43, 56, 71, 78	0
1	D	509/521 (97%)	-0.27	13 (2%) 56 27	45, 56, 71, 77	0
All	All	2037/2084 (97%)	-0.23	62 (3%) 50 22	43, 56, 71, 81	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	114	ASP	4.6
1	C	185	SER	4.3
1	B	114	ASP	4.3
1	B	186	SER	4.3
1	D	185	SER	4.1
1	A	185	SER	4.0
1	C	121	HIS	4.0
1	B	185	SER	3.8
1	B	188	SER	3.8
1	B	102	THR	3.7
1	B	111	GLY	3.3
1	B	85	PRO	3.3
1	B	61	GLY	3.3
1	A	62	LYS	3.1
1	D	11	THR	3.1
1	A	186	SER	3.1
1	C	14	GLU	3.0
1	B	221	ASN	2.9
1	A	516	SER	2.9
1	D	39	ARG	2.9
1	D	186	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	113	PRO	2.9
1	C	1	MET	2.8
1	C	62	LYS	2.7
1	A	11	THR	2.7
1	D	121	HIS	2.7
1	B	65	LYS	2.6
1	B	514	PRO	2.6
1	A	114	ASP	2.6
1	A	63	ASN	2.6
1	D	514	PRO	2.6
1	C	114	ASP	2.6
1	C	186	SER	2.6
1	C	258	THR	2.5
1	A	514	PRO	2.5
1	D	13	ALA	2.5
1	B	182	ALA	2.5
1	B	146	PRO	2.5
1	B	107	HIS	2.5
1	A	183	SER	2.4
1	B	39	ARG	2.4
1	D	311	ASP	2.4
1	D	122	ALA	2.4
1	D	63	ASN	2.3
1	B	112	LEU	2.3
1	C	63	ASN	2.3
1	D	258	THR	2.3
1	B	63	ASN	2.2
1	B	219	ASN	2.2
1	C	40	SER	2.2
1	B	41	ILE	2.2
1	A	113	PRO	2.1
1	B	13	ALA	2.1
1	B	222	GLU	2.1
1	C	122	ALA	2.1
1	C	61	GLY	2.1
1	A	110	ASP	2.1
1	B	106	GLN	2.1
1	B	113	PRO	2.0
1	C	113	PRO	2.0
1	B	32	ARG	2.0
1	B	223	THR	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 carbohydrates in this entry.

6.4 Ligands [i](#)

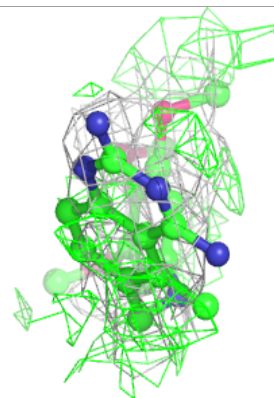
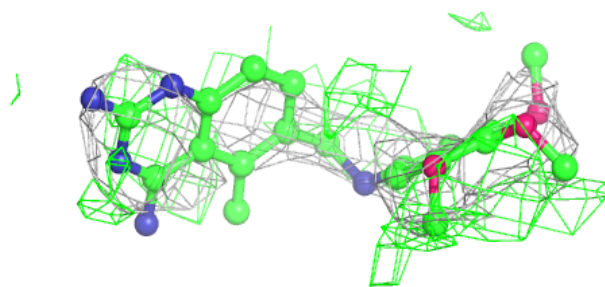
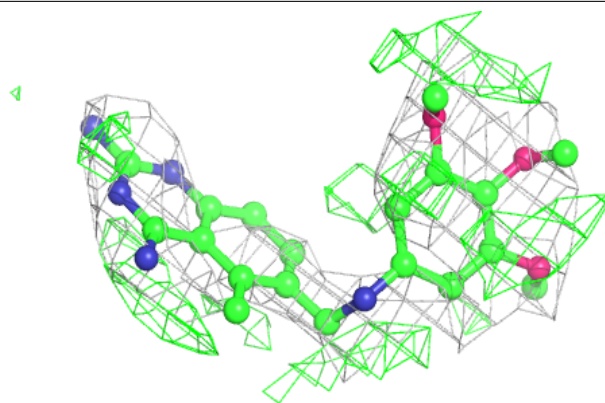
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	TMQ	B	612	27/27	0.59	0.48	73,73,74,74	27
3	NAP	B	602	48/48	0.78	0.31	78,79,80,80	48
4	TMQ	D	614	27/27	0.88	0.20	72,72,77,77	0
3	NAP	C	603	48/48	0.90	0.26	71,75,80,81	0
3	NAP	D	604	48/48	0.90	0.27	87,89,94,94	0
4	TMQ	A	611	27/27	0.90	0.21	55,55,60,61	0
5	EDO	B	805	4/4	0.91	0.35	70,71,71,71	0
5	EDO	A	801	4/4	0.91	0.28	59,59,59,59	0
4	TMQ	C	613	27/27	0.92	0.18	56,56,61,62	0
3	NAP	A	601	48/48	0.94	0.21	67,69,72,72	0
5	EDO	C	806	4/4	0.94	0.26	53,53,53,53	0
2	SO4	D	704	5/5	0.95	0.21	64,65,65,66	0
5	EDO	A	802	4/4	0.95	0.16	62,63,64,65	0
5	EDO	D	804	4/4	0.95	0.21	54,55,55,56	0
5	EDO	C	803	4/4	0.96	0.19	47,48,48,49	0
2	SO4	C	702	5/5	0.98	0.12	50,52,52,53	0
2	SO4	A	701	5/5	0.98	0.14	59,60,61,61	0
2	SO4	C	703	5/5	0.98	0.18	56,57,58,58	0

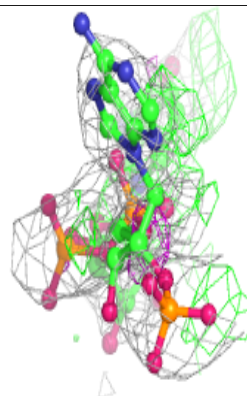
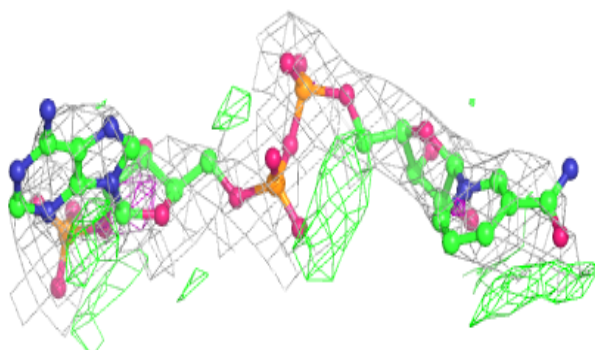
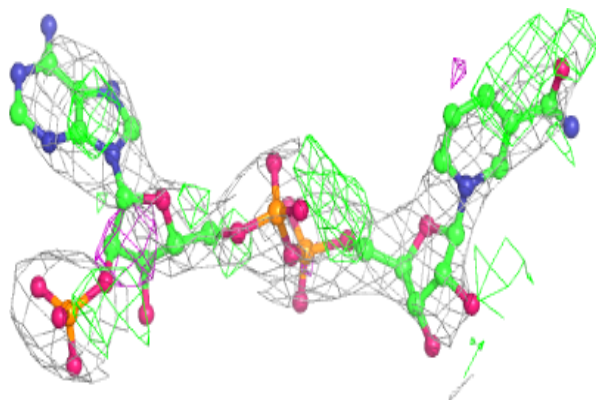
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

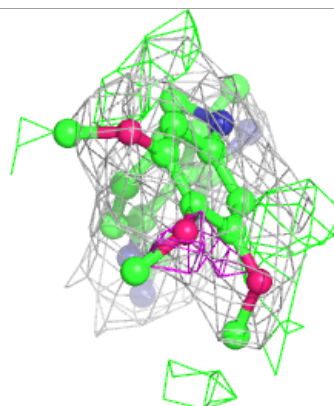
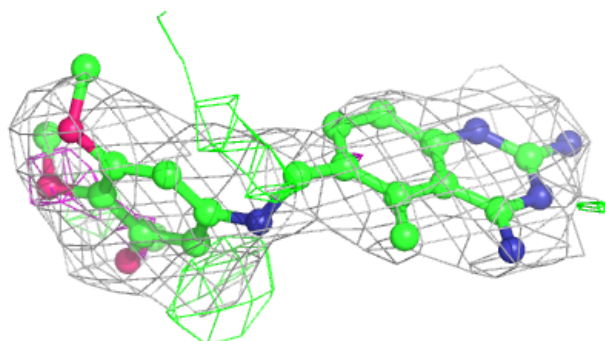
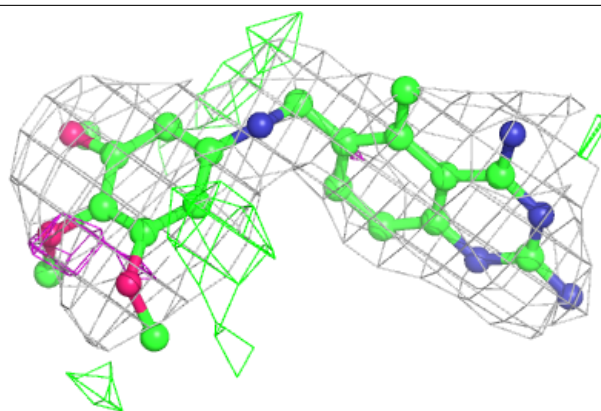
**Electron density around NAP B 602:**

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

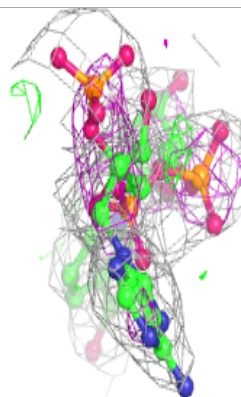
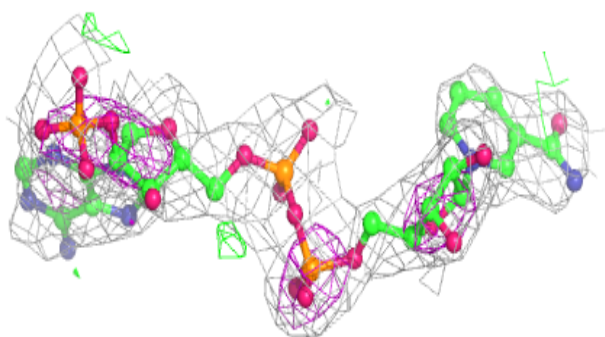
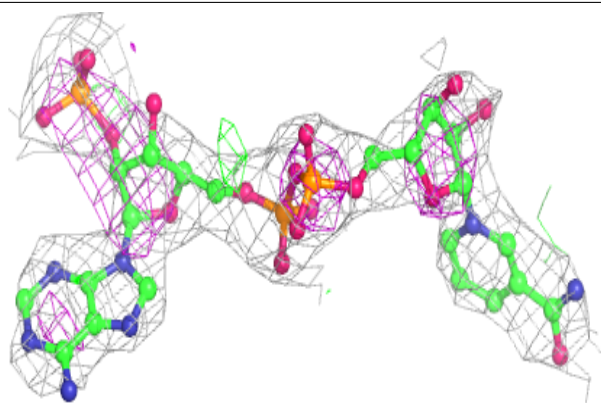


Electron density around TMQ D 614:

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

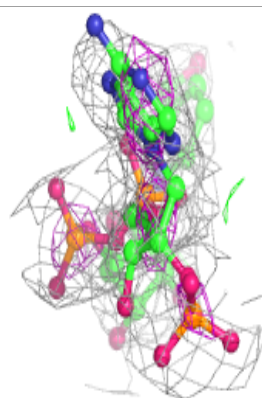
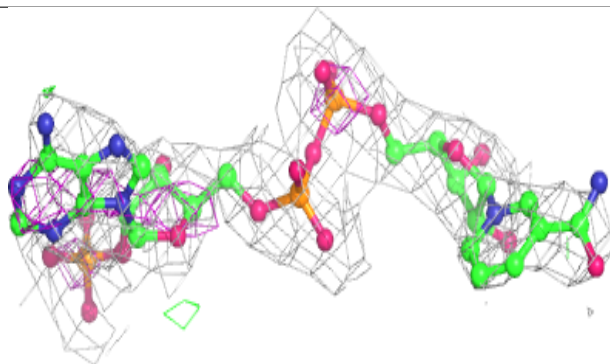
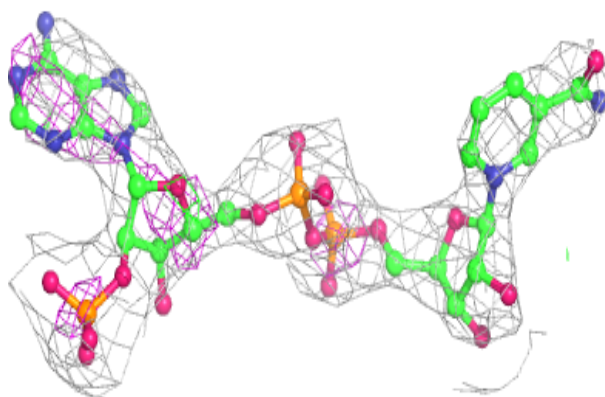
**Electron density around NAP C 603:**

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

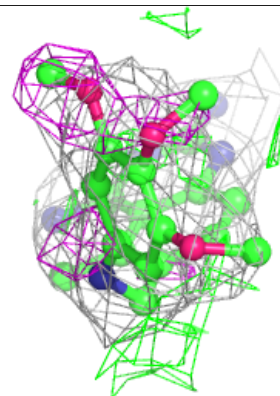
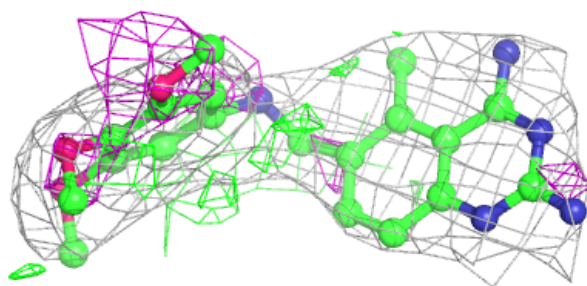
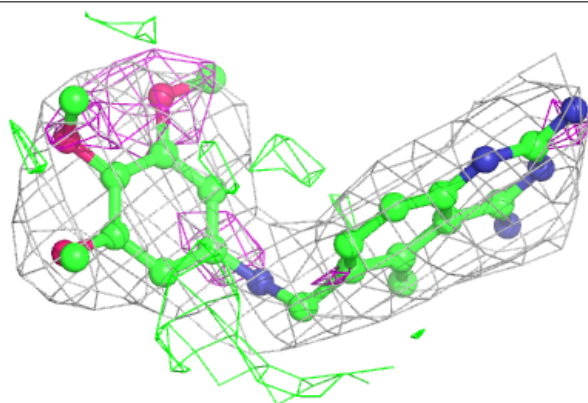


Electron density around NAP D 604:

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

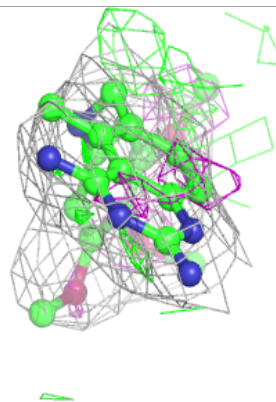
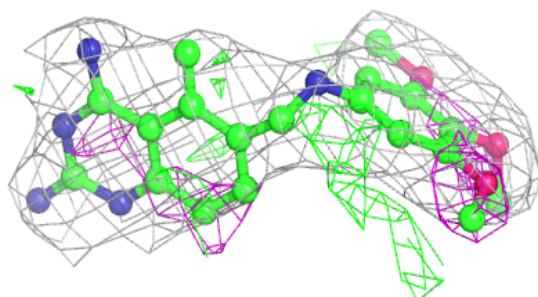
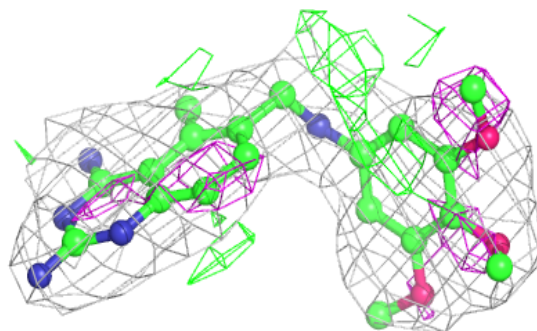
**Electron density around TMQ A 611:**

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

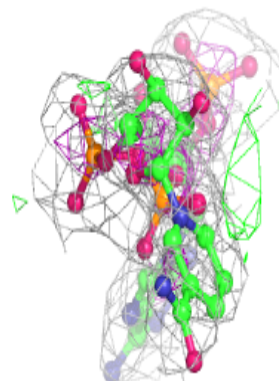
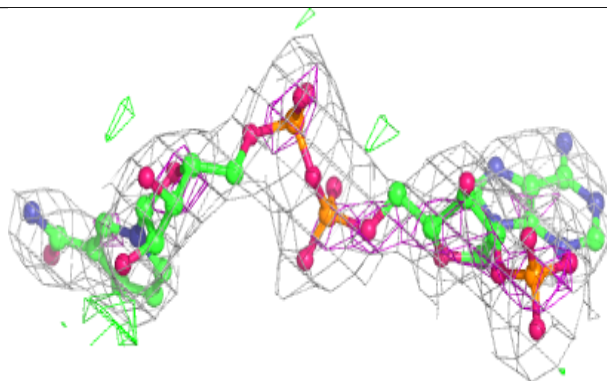
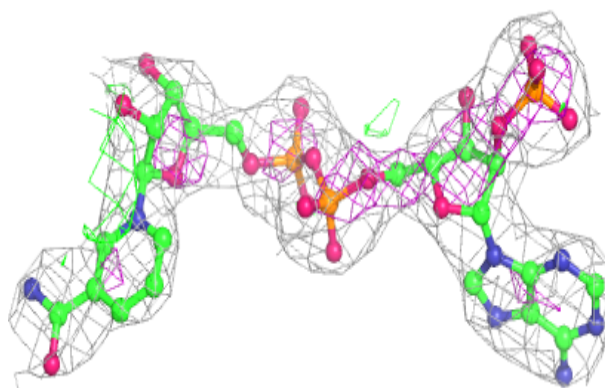


Electron density around TMQ C 613:

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

**Electron density around 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

There are no such residues in this entry.