



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 11:32 PM EDT

PDB ID : 7B0H
Title : TgoT_6G12 Ternary complex
Authors : Samson, C.; Legrand, P.; Tekpinar, M.; Rozenski, J.; Abramov, M.; Holliger, P.; Pinheiro, V.; Herdewijn, P.; Delarue, M.
Deposited on : 2020-11-19
Resolution : 3.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

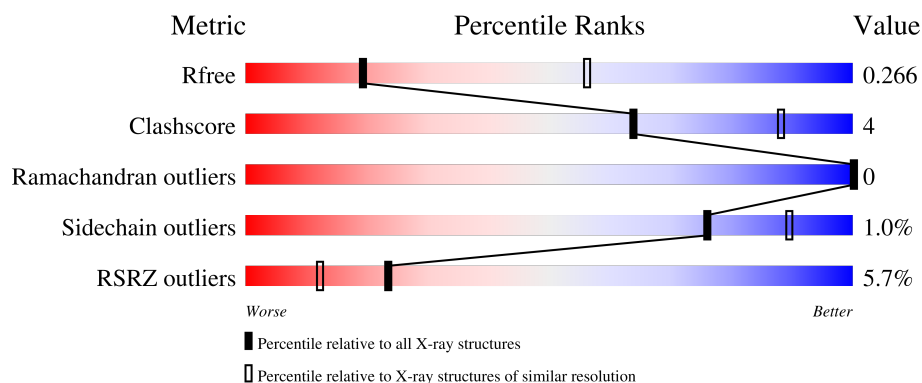
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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.



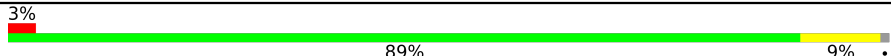
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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

Mol	Chain	Length	Quality of chain
1	A	13	<div> <div>15%</div> <div>69%</div> <div>31%</div> </div>
1	C	13	<div> <div>31%</div> <div>69%</div> <div>31%</div> </div>
2	D	6	<div> <div>83%</div> <div>17%</div> </div>
2	G	6	<div> <div>67%</div> <div>33%</div> </div>
3	E	773	<div> <div>7%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	773	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	F	803	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12977 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 DNA chain called DNA (5'-D(P*AP*AP*CP*GP*GP*CP*AP*AP*AP*TP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	13	Total	C	N	O	P	0	0	0
			267	127	56	72	12			
1	C	13	Total	C	N	O	P	0	0	0
			270	127	56	74	13			

- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*GP*CP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	6	Total	C	N	O	P	0	0	0
			121	58	20	37	6			
2	G	6	Total	C	N	O	P	0	0	0
			121	58	20	37	6			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	713	Total	C	N	O	S	0	0	0
			5870	3794	976	1086	14			
3	F	762	Total	C	N	O	S	0	0	0
			6264	4039	1062	1149	14			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	93	GLN	VAL	engineered mutation	UNP P56689
E	141	ALA	ASP	engineered mutation	UNP P56689
E	143	ALA	GLU	engineered mutation	UNP P56689
E	485	LEU	ALA	engineered mutation	UNP P56689
E	589	ALA	VAL	engineered mutation	UNP P56689
E	609	LYS	GLU	engineered mutation	UNP P56689
E	610	MET	ILE	engineered mutation	UNP P56689

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Chain	Residue	Modelled	Actual	Comment	Reference
E	659	GLN	LYS	engineered mutation	UNP P56689
E	664	GLN	GLU	engineered mutation	UNP P56689
E	665	PRO	GLN	engineered mutation	UNP P56689
E	668	LYS	ARG	engineered mutation	UNP P56689
E	669	GLN	ASP	engineered mutation	UNP P56689
E	671	HIS	LYS	engineered mutation	UNP P56689
E	674	ARG	LYS	engineered mutation	UNP P56689
E	676	ARG	THR	engineered mutation	UNP P56689
E	681	SER	ALA	engineered mutation	UNP P56689
E	704	PRO	LEU	engineered mutation	UNP P56689
E	730	GLY	GLU	engineered mutation	UNP P56689
F	93	GLN	VAL	engineered mutation	UNP P56689
F	141	ALA	ASP	engineered mutation	UNP P56689
F	143	ALA	GLU	engineered mutation	UNP P56689
F	485	LEU	ALA	engineered mutation	UNP P56689
F	589	ALA	VAL	engineered mutation	UNP P56689
F	609	LYS	GLU	engineered mutation	UNP P56689
F	610	MET	ILE	engineered mutation	UNP P56689
F	659	GLN	LYS	engineered mutation	UNP P56689
F	664	GLN	GLU	engineered mutation	UNP P56689
F	665	PRO	GLN	engineered mutation	UNP P56689
F	668	LYS	ARG	engineered mutation	UNP P56689
F	669	GLN	ASP	engineered mutation	UNP P56689
F	671	HIS	LYS	engineered mutation	UNP P56689
F	674	ARG	LYS	engineered mutation	UNP P56689
F	676	ARG	THR	engineered mutation	UNP P56689
F	681	SER	ALA	engineered mutation	UNP P56689
F	704	PRO	LEU	engineered mutation	UNP P56689
F	730	GLY	GLU	engineered mutation	UNP P56689

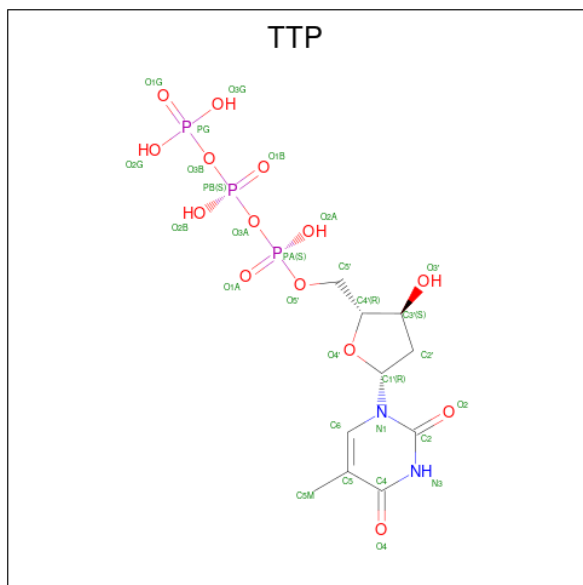
- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	2	Total Mn 2 2	0	0
4	F	2	Total Mn 2 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0

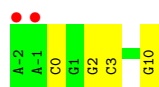
- Molecule 6 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



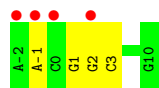
3 Residue-property plots [i](#)

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

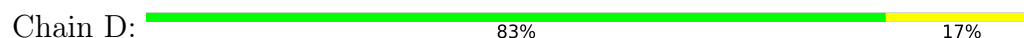
- Molecule 1: DNA (5'-D(P*AP*AP*CP*GP*GP*CP*AP*AP*AP*TP*GP*CP*G)-3')



- Molecule 1: DNA (5'-D(P*AP*AP*CP*GP*GP*CP*AP*AP*AP*TP*GP*CP*G)-3')



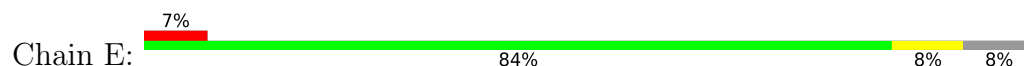
- Molecule 2: DNA (5'-D(P*CP*GP*CP*AP*TP*T)-3')

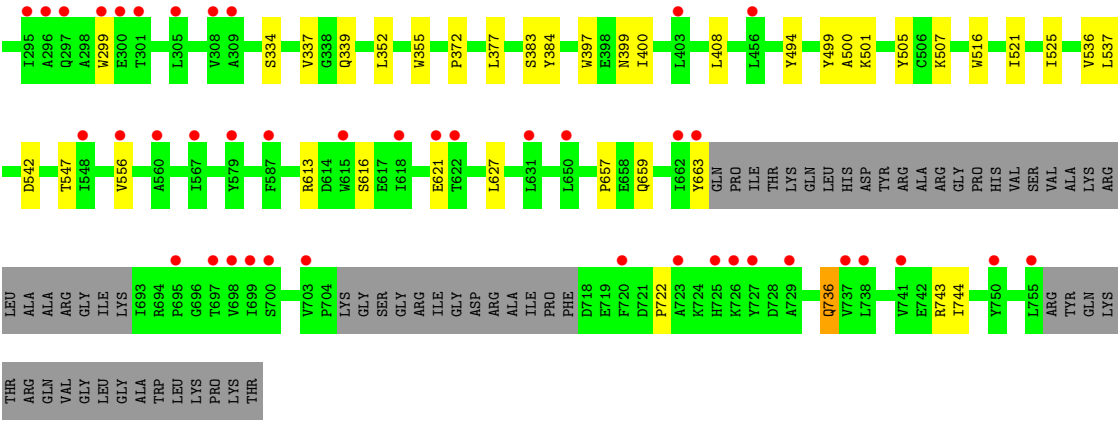


- Molecule 2: DNA (5'-D(P*CP*GP*CP*AP*TP*T)-3')

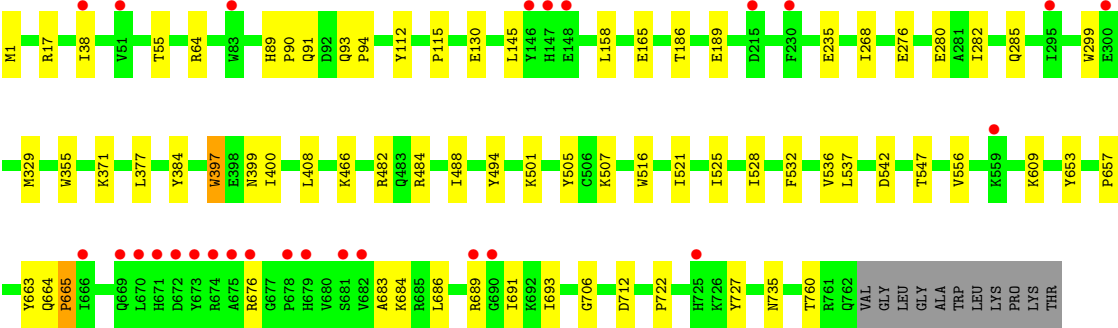
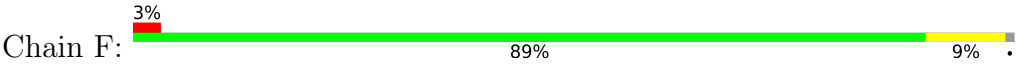


- Molecule 3: DNA polymerase





● Molecule 3: DNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.82Å 112.33Å 186.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.92 – 3.15 48.92 – 3.15	Depositor EDS
% Data completeness (in resolution range)	80.5 (48.92-3.15) 80.5 (48.92-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.232 , 0.247 0.256 , 0.266	Depositor DCC
R_{free} test set	1648 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	88.7	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12977	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TTP, MN

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	0.70	0/301	0.86	0/463
1	C	0.71	0/304	0.79	0/467
2	D	0.64	0/134	0.82	0/204
2	G	0.68	0/134	0.87	0/204
3	E	0.27	0/6004	0.50	0/8098
3	F	0.27	0/6408	0.51	2/8641 (0.0%)
All	All	0.32	0/13285	0.53	2/18077 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	665	PRO	N-CA-CB	-5.46	96.60	102.60
3	F	665	PRO	CA-N-CD	-5.45	103.88	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	267	0	146	7	0
1	C	270	0	145	3	0
2	D	121	0	69	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	121	0	69	3	0
3	E	5870	0	5883	39	0
3	F	6264	0	6304	67	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	E	29	0	13	0	0
6	F	29	0	13	0	0
All	All	12977	0	12642	108	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 4.

All (108) 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)
3:F:676:ARG:NE	3:F:684:LYS:NZ	2.02	1.06
3:F:676:ARG:NE	3:F:684:LYS:HZ2	1.62	0.94
3:F:689:ARG:NH2	3:F:691:ILE:HD11	1.87	0.90
3:F:683:ALA:O	3:F:693:ILE:CD1	2.24	0.85
3:F:676:ARG:CD	3:F:684:LYS:HZ2	1.93	0.82
3:F:686:LEU:HD22	3:F:691:ILE:CD1	2.11	0.80
3:F:683:ALA:HB1	3:F:693:ILE:HD13	1.67	0.76
3:F:676:ARG:HE	3:F:684:LYS:NZ	1.83	0.73
3:F:657:PRO:HG3	3:F:722:PRO:HG3	1.69	0.73
3:F:676:ARG:NE	3:F:684:LYS:HZ3	1.87	0.72
3:F:683:ALA:O	3:F:693:ILE:HD12	1.90	0.70
1:A:2:DG:H5'	3:E:245:GLY:HA3	1.75	0.69
3:F:686:LEU:HD22	3:F:691:ILE:HD12	1.73	0.69
3:E:616:SER:OG	3:E:736:GLN:HG2	1.97	0.65
3:F:686:LEU:CD2	3:F:691:ILE:HD12	2.28	0.63
3:F:676:ARG:CD	3:F:684:LYS:NZ	2.58	0.61
3:F:38:ILE:HG22	3:F:112:TYR:HA	1.83	0.61
3:F:665:PRO:HD2	3:F:665:PRO:O	1.98	0.60
3:F:686:LEU:HD22	3:F:691:ILE:HD13	1.83	0.59
3:F:115:PRO:HD2	3:F:355:TRP:HH2	1.68	0.59
3:F:89:HIS:HD1	3:F:91:GLN:H	1.53	0.57
3:E:38:ILE:HG22	3:E:112:TYR:HA	1.85	0.57
3:F:528:ILE:O	3:F:532:PHE:O	2.23	0.57
3:F:158:LEU:HD22	3:F:299:TRP:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:158:LEU:HD22	3:E:299:TRP:CE2	2.40	0.56
3:F:676:ARG:HE	3:F:684:LYS:HZ3	1.48	0.56
1:A:2:DG:H5'	3:E:245:GLY:CA	2.37	0.55
3:F:676:ARG:HD3	3:F:684:LYS:HZ2	1.72	0.54
3:F:689:ARG:HH21	3:F:691:ILE:HD11	1.74	0.52
3:E:408:LEU:HD22	3:E:542:ASP:HB3	1.92	0.52
3:F:38:ILE:CG2	3:F:112:TYR:HA	2.40	0.52
3:E:377:LEU:HD21	3:E:501:LYS:HG2	1.92	0.51
3:F:400:ILE:HG22	3:F:547:THR:HB	1.91	0.51
3:F:1:MET:HB3	3:F:130:GLU:O	2.11	0.51
3:E:397:TRP:CE2	3:E:537:LEU:HD22	2.46	0.51
3:E:400:ILE:HG22	3:E:547:THR:HB	1.92	0.50
3:E:172:THR:HG21	3:E:176:ILE:HD12	1.93	0.50
3:F:408:LEU:HD22	3:F:542:ASP:HB3	1.92	0.50
3:E:399:ASN:HB3	3:E:556:VAL:HG21	1.93	0.50
3:E:38:ILE:CG2	3:E:112:TYR:HA	2.42	0.50
3:F:484:ARG:O	3:F:488:ILE:HG12	2.11	0.50
3:F:683:ALA:CB	3:F:693:ILE:HD13	2.39	0.50
1:A:0:DC:OP2	3:E:97:ARG:NH2	2.39	0.49
3:F:399:ASN:HB3	3:F:556:VAL:HG21	1.93	0.49
3:F:676:ARG:CZ	3:F:684:LYS:NZ	2.75	0.49
3:F:235:GLU:HG2	3:F:235:GLU:O	2.11	0.48
1:C:-1:DA:H2	3:F:90:PRO:HB2	1.79	0.48
3:E:627:LEU:HD11	3:E:744:ILE:HD13	1.94	0.48
3:E:383:SER:HB2	3:F:706:GLY:HA2	1.95	0.48
3:F:115:PRO:HD2	3:F:355:TRP:CH2	2.47	0.48
3:E:397:TRP:CD2	3:E:537:LEU:HD22	2.49	0.47
3:F:276:GLU:O	3:F:280:GLU:HG3	2.14	0.47
3:E:276:GLU:O	3:E:280:GLU:HG3	2.13	0.47
3:E:337:VAL:HG21	3:E:352:LEU:HD22	1.96	0.47
3:E:408:LEU:HD22	3:E:542:ASP:CB	2.45	0.47
3:F:676:ARG:HG2	3:F:684:LYS:HZ1	1.80	0.46
2:D:11:DT:OP1	3:F:609:LYS:NZ	2.29	0.46
3:F:663:TYR:O	3:F:664:GLN:OE1	2.33	0.46
3:F:377:LEU:HD21	3:F:501:LYS:HG2	1.97	0.46
3:E:158:LEU:HD22	3:E:299:TRP:CD2	2.51	0.46
3:F:408:LEU:HD22	3:F:542:ASP:CB	2.45	0.46
1:A:2:DG:N2	3:F:712:ASP:OD2	2.37	0.46
3:E:627:LEU:CD1	3:E:744:ILE:HD13	2.46	0.46
3:E:657:PRO:HG3	3:E:722:PRO:HG3	1.98	0.46
3:E:115:PRO:HD2	3:E:355:TRP:HH2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:145:LEU:HB2	3:E:158:LEU:HD21	1.98	0.46
3:F:158:LEU:HD22	3:F:299:TRP:CD2	2.51	0.45
3:F:329:MET:HG3	3:F:482:ARG:HG2	1.98	0.45
3:F:145:LEU:HB2	3:F:158:LEU:HD21	1.98	0.45
3:E:521:ILE:O	3:E:525:ILE:HG12	2.17	0.45
3:E:525:ILE:HG23	3:E:536:VAL:HG21	2.00	0.44
3:E:93:GLN:HB2	3:E:94:PRO:HD3	2.00	0.44
3:F:686:LEU:CD2	3:F:691:ILE:CD1	2.88	0.44
2:G:7:DC:O5'	2:G:8:DG:OP2	2.36	0.44
3:F:186:THR:HG23	3:F:189:GLU:H	1.83	0.44
3:F:397:TRP:CD2	3:F:537:LEU:HD22	2.53	0.43
3:E:55:THR:HG22	3:E:64:ARG:HG2	1.99	0.43
3:E:384:TYR:CD1	3:E:507:LYS:HD2	2.53	0.43
3:F:93:GLN:HB2	3:F:94:PRO:HD3	1.99	0.43
3:F:525:ILE:HG23	3:F:536:VAL:HG21	2.00	0.43
3:F:55:THR:HG22	3:F:64:ARG:HG2	1.99	0.43
3:F:525:ILE:HD12	3:F:536:VAL:HG11	2.01	0.43
3:F:521:ILE:O	3:F:525:ILE:HG12	2.17	0.43
3:F:657:PRO:HG3	3:F:722:PRO:CG	2.43	0.43
1:C:2:DG:H2'	1:C:3:DC:C4'	2.48	0.43
3:E:186:THR:HG23	3:E:189:GLU:H	1.83	0.43
3:E:334:SER:OG	3:E:339:GLN:O	2.25	0.43
3:F:397:TRP:CD1	3:F:547:THR:HG21	2.53	0.43
3:F:165:GLU:H	3:F:165:GLU:CD	2.21	0.42
1:A:2:DG:OP2	3:E:245:GLY:HA2	2.18	0.42
3:F:665:PRO:O	3:F:665:PRO:CD	2.67	0.42
1:A:10:DG:N2	2:G:8:DG:C2	2.88	0.42
3:F:17:ARG:HH12	3:F:235:GLU:HG3	1.83	0.42
3:E:505:TYR:OH	3:E:507:LYS:HE2	2.20	0.42
3:E:525:ILE:HD12	3:E:536:VAL:HG11	2.01	0.42
1:C:1:DG:OP1	3:F:371:LYS:NZ	2.37	0.42
3:F:280:GLU:HG2	3:F:285:GLN:O	2.20	0.41
3:E:372:PRO:HG3	3:E:500:ALA:O	2.21	0.41
3:F:384:TYR:CD1	3:F:507:LYS:HD2	2.56	0.41
3:E:264:ILE:HG23	3:E:268:ILE:HD12	2.01	0.41
3:F:505:TYR:OH	3:F:507:LYS:HE2	2.19	0.41
3:E:280:GLU:HG2	3:E:285:GLN:O	2.20	0.41
3:E:621:GLU:OE2	3:E:659:GLN:OE1	2.39	0.40
1:A:3:DC:H2'	3:E:499:TYR:CE1	2.56	0.40
3:F:268:ILE:HD11	3:F:282:ILE:HD11	2.02	0.40
3:F:683:ALA:O	3:F:693:ILE:HD11	2.17	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:653:TYR:HA	3:F:727:TYR:OH	2.22	0.40
3:F:735:ASN:HD21	2:G:7:DC:H4'	1.87	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	
3	E	707/773 (92%)	685 (97%)	22 (3%)	0	100	100
3	F	760/773 (98%)	735 (97%)	25 (3%)	0	100	100
All	All	1467/1546 (95%)	1420 (97%)	47 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	621/668 (93%)	613 (99%)	8 (1%)	69	86
3	F	660/668 (99%)	655 (99%)	5 (1%)	81	92
All	All	1281/1336 (96%)	1268 (99%)	13 (1%)	76	89

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	175	ASN
3	E	229	LYS
3	E	494	TYR
3	E	516	TRP
3	E	613	ARG
3	E	663	TYR
3	E	736	GLN
3	E	743	ARG
3	F	397	TRP
3	F	466	LYS
3	F	494	TYR
3	F	516	TRP
3	F	760	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	436	GLN
3	F	491	ASN
3	F	664	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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
6	TTP	E	804	5,4	26,30,30	0.24	0	39,47,47	0.50	0
6	TTP	F	804	5,4	26,30,30	0.29	0	39,47,47	0.53	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
6	TTP	E	804	5,4	-	3/22/34/34	0/2/2/2
6	TTP	F	804	5,4	-	3/22/34/34	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

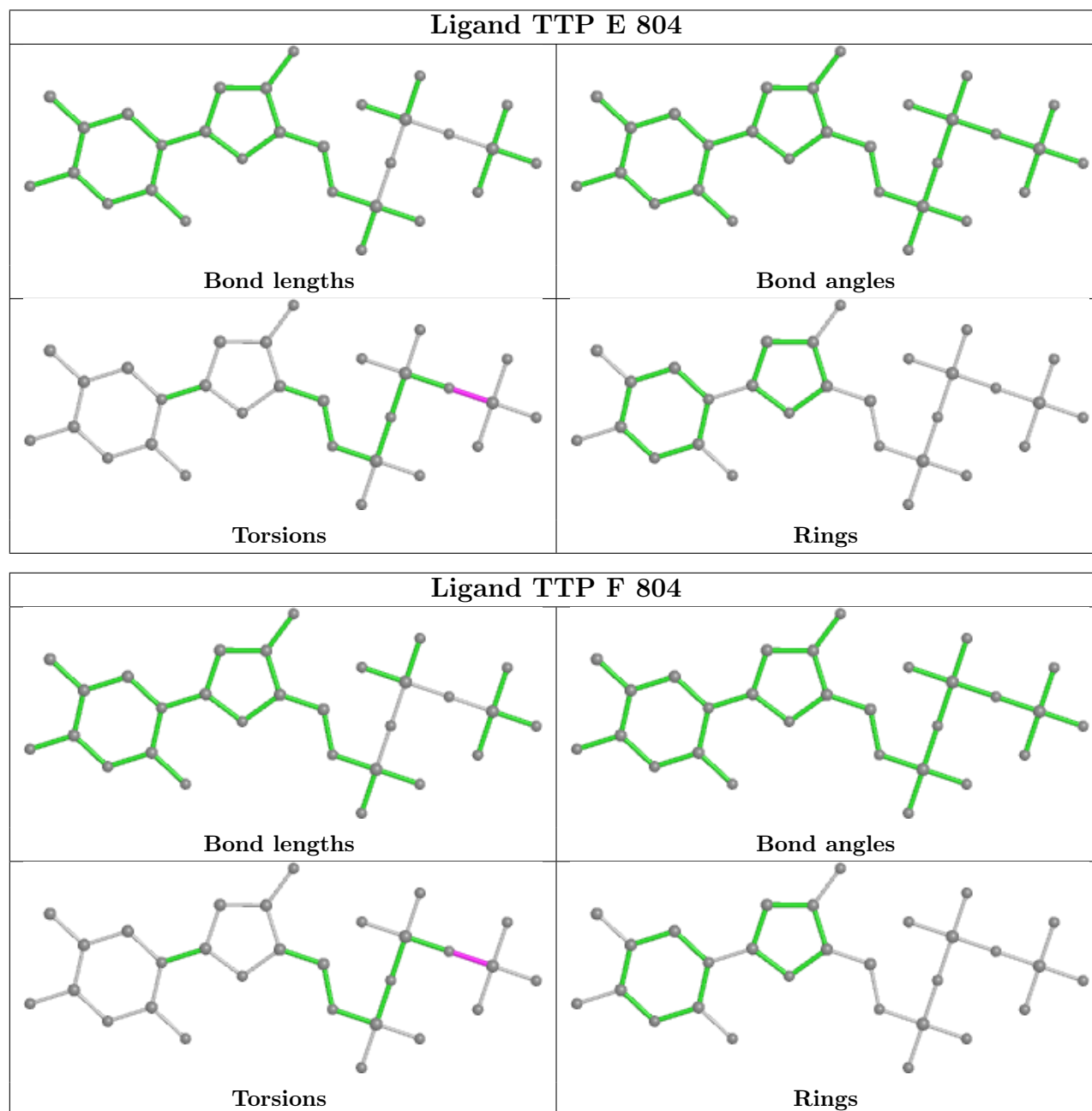
Mol	Chain	Res	Type	Atoms
6	E	804	TTP	PB-O3B-PG-O2G
6	F	804	TTP	PB-O3B-PG-O2G
6	F	804	TTP	PB-O3B-PG-O3G
6	E	804	TTP	PB-O3B-PG-O3G
6	E	804	TTP	PB-O3B-PG-O1G
6	F	804	TTP	PB-O3B-PG-O1G

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	13/13 (100%)	0.99	2 (15%) 2 1	60, 81, 153, 157	0
1	C	13/13 (100%)	1.87	4 (30%) 0 0	86, 108, 204, 208	0
2	D	6/6 (100%)	0.07	0 100 100	95, 102, 124, 131	0
2	G	6/6 (100%)	0.67	0 100 100	87, 97, 115, 119	0
3	E	713/773 (92%)	0.51	53 (7%) 14 8	50, 103, 166, 184	0
3	F	762/773 (98%)	0.38	27 (3%) 44 27	70, 100, 129, 171	0
All	All	1513/1584 (95%)	0.46	86 (5%) 23 12	50, 101, 153, 208	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	673	TYR	9.4
3	F	670	LEU	8.8
3	E	295	ILE	8.1
1	C	-2	DA	7.9
3	E	305	LEU	6.0
1	C	-1	DA	5.7
3	E	308	VAL	5.1
3	F	666	ILE	5.0
3	F	675	ALA	5.0
3	E	699	ILE	4.8
3	E	703	VAL	4.5
3	E	663	TYR	4.5
3	F	674	ARG	4.4
3	E	147	HIS	4.2
3	E	698	VAL	4.1
3	E	700	SER	4.1
3	E	618	ILE	3.9
3	F	679	HIS	3.9
3	E	153	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
3	F	672	ASP	3.7
3	E	695	PRO	3.7
3	E	299	TRP	3.7
3	E	615	TRP	3.6
3	E	650	LEU	3.6
3	F	51	VAL	3.4
3	F	146	TYR	3.4
3	E	309	ALA	3.4
3	E	755	LEU	3.3
3	F	669	GLN	3.3
3	F	689	ARG	3.3
3	F	230	PHE	3.2
3	E	579	TYR	3.1
3	F	690	GLY	3.0
3	E	290	VAL	3.0
3	E	183	VAL	3.0
3	E	621	GLU	2.9
3	F	678	PRO	2.9
3	E	631	LEU	2.9
3	F	671	HIS	2.9
3	F	681	SER	2.8
1	C	2	DG	2.8
3	F	295	ILE	2.7
3	F	676	ARG	2.7
3	E	662	ILE	2.7
3	F	559	LYS	2.6
3	E	697	THR	2.6
3	E	738	LEU	2.6
3	E	296	ALA	2.5
3	E	300	GLU	2.5
3	E	174	LYS	2.5
3	F	682	VAL	2.5
3	E	548	ILE	2.5
3	E	160	ILE	2.4
3	E	456	LEU	2.4
3	E	297	GLN	2.4
3	E	622	THR	2.4
3	E	720	PHE	2.4
3	E	750	TYR	2.4
1	A	-1	DA	2.3
3	E	723	ALA	2.3
3	F	148	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	E	567	ILE	2.3
3	E	587	PHE	2.3
3	E	159	MET	2.2
3	F	215	ASP	2.2
1	A	-2	DA	2.2
3	E	560	ALA	2.2
3	E	741	VAL	2.2
1	C	0	DC	2.2
3	E	726	LYS	2.2
3	F	83	TRP	2.2
3	F	147	HIS	2.2
3	E	180	TYR	2.2
3	E	230	PHE	2.1
3	F	300	GLU	2.1
3	E	737	VAL	2.1
3	E	152	PHE	2.1
3	F	38	ILE	2.1
3	F	725	HIS	2.1
3	E	556	VAL	2.1
3	E	725	HIS	2.1
3	E	162	TYR	2.1
3	E	727	TYR	2.0
3	E	301	THR	2.0
3	E	729	ALA	2.0
3	E	403	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

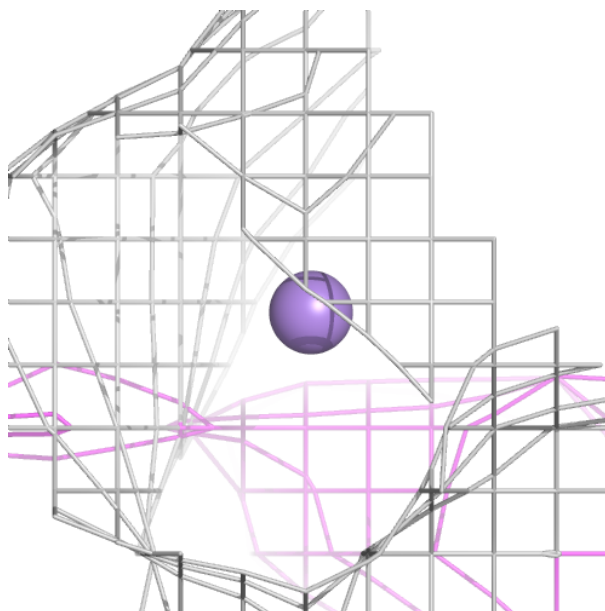
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MN	E	801	1/1	0.75	0.13	165,165,165,165	0
5	MG	F	803	1/1	0.78	0.41	96,96,96,96	0
5	MG	E	803	1/1	0.89	0.26	80,80,80,80	0
6	TTP	E	804	29/29	0.92	0.24	93,94,96,96	0
4	MN	F	801	1/1	0.94	0.26	118,118,118,118	0
4	MN	E	802	1/1	0.95	0.09	100,100,100,100	0
6	TTP	F	804	29/29	0.95	0.28	67,69,69,69	0
4	MN	F	802	1/1	0.98	0.16	71,71,71,71	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.

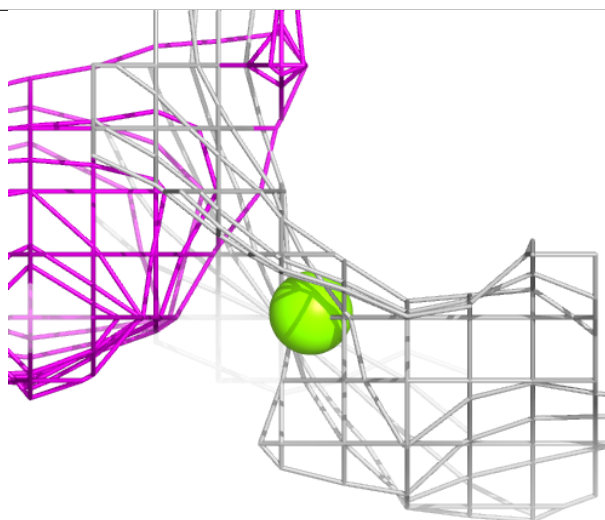
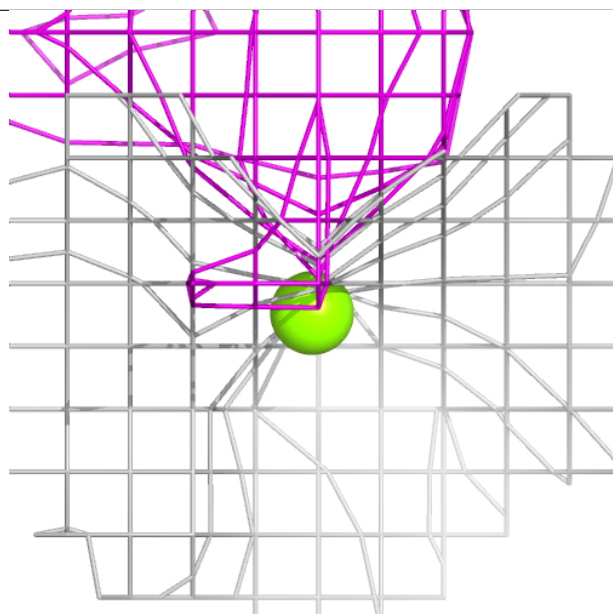
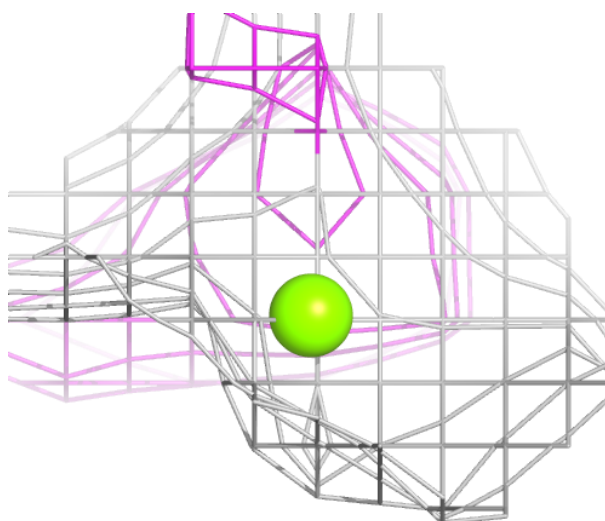
Electron density around MN E 801:

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



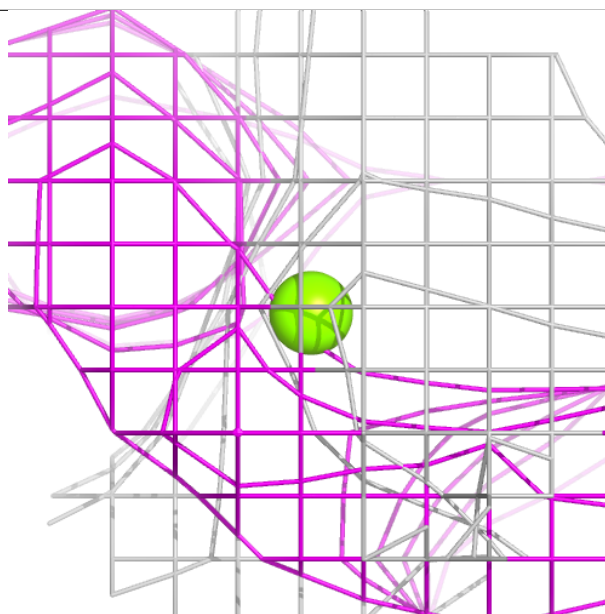
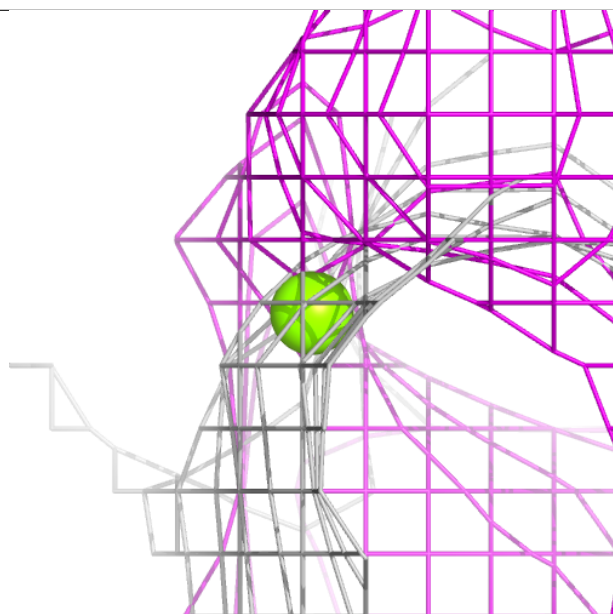
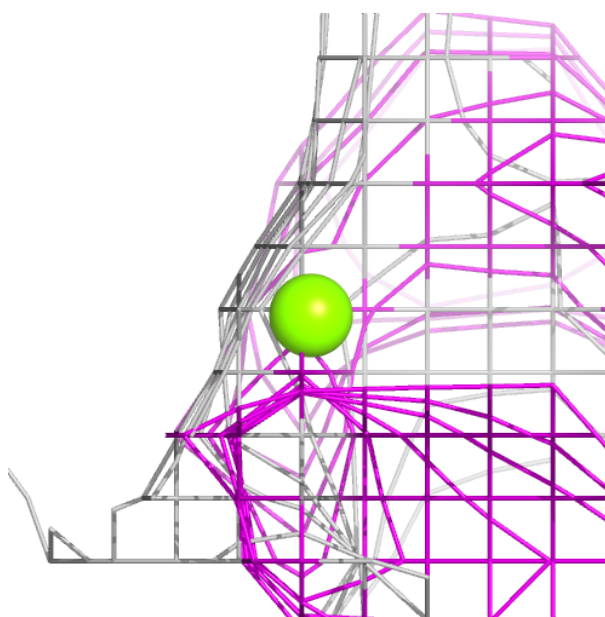
Electron density around MG F 803:

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



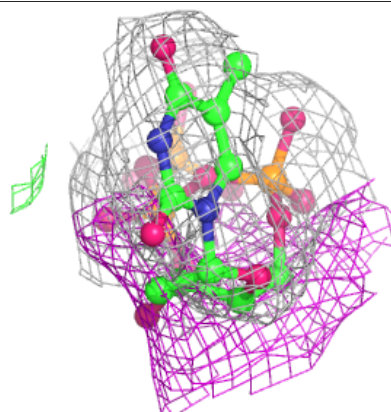
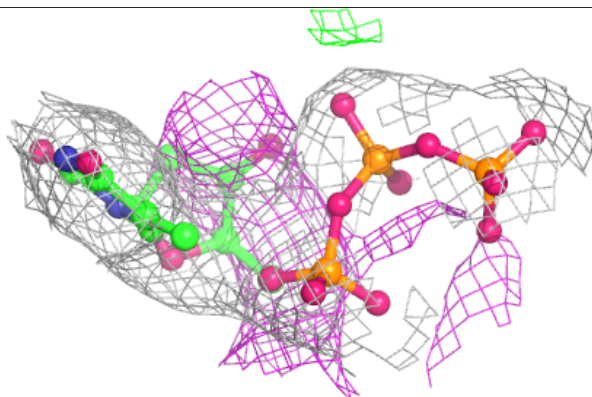
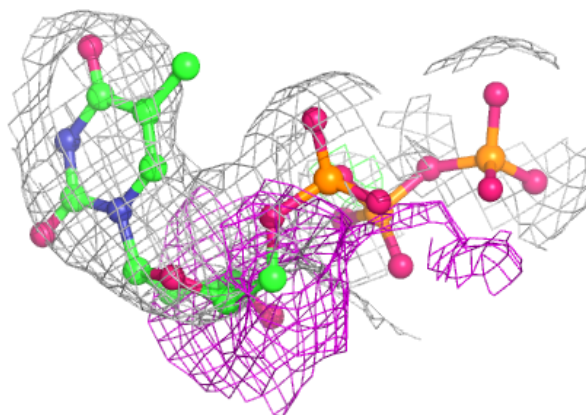
Electron density around MG E 803:

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and green (positive)



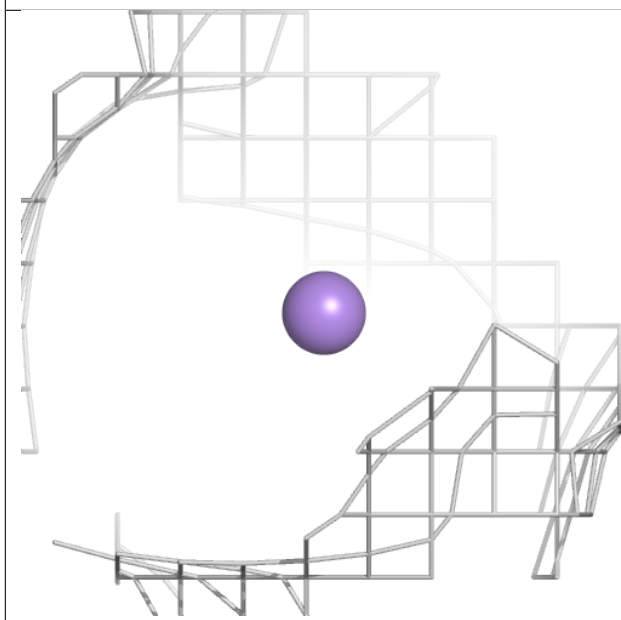
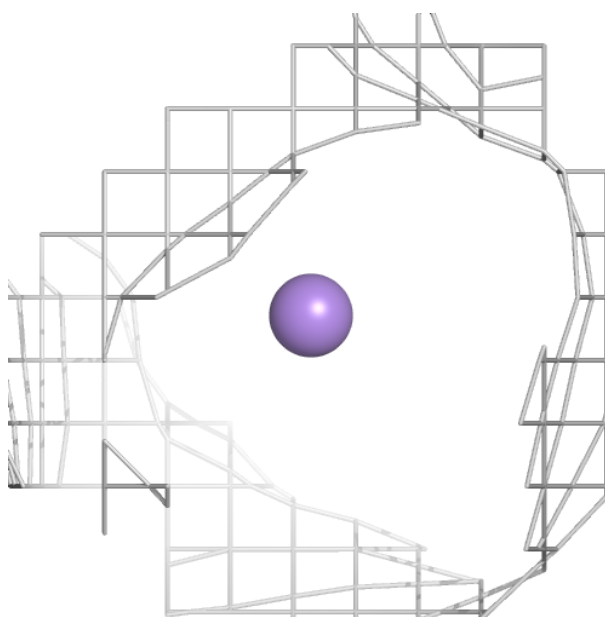
Electron density around TTP E 804:

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



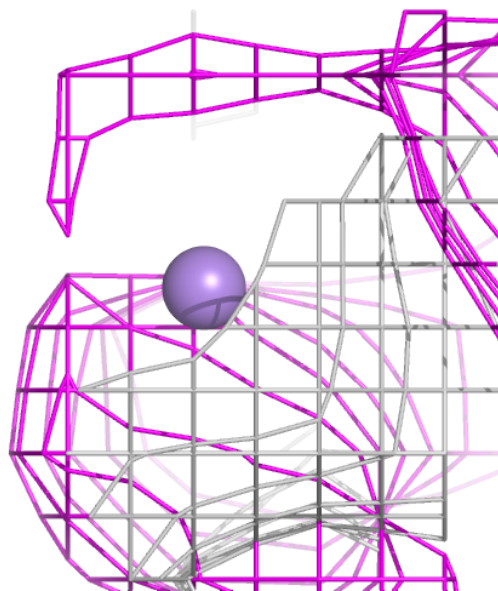
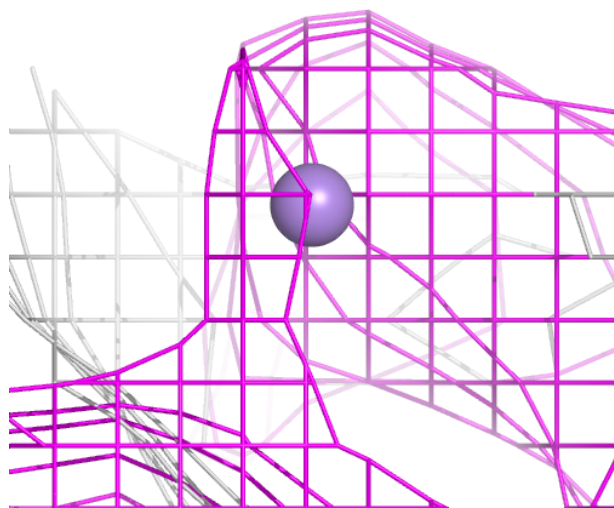
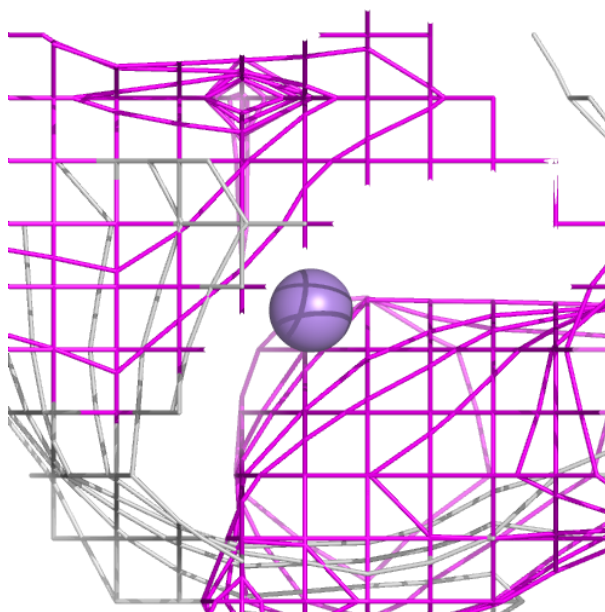
Electron density around MN F 801:

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



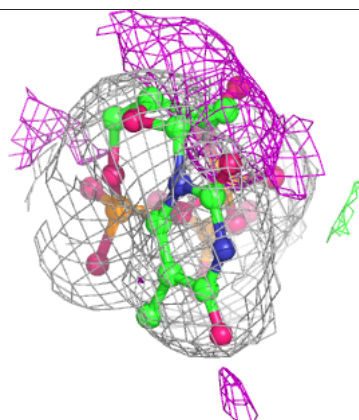
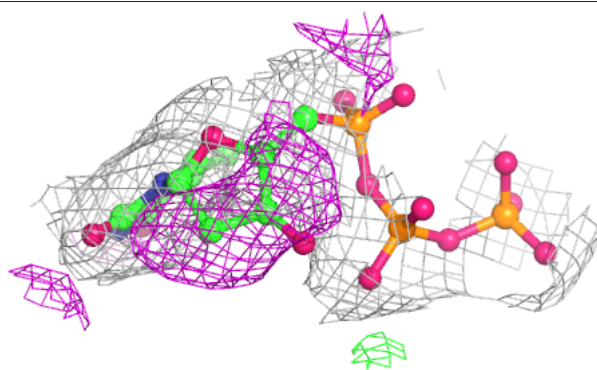
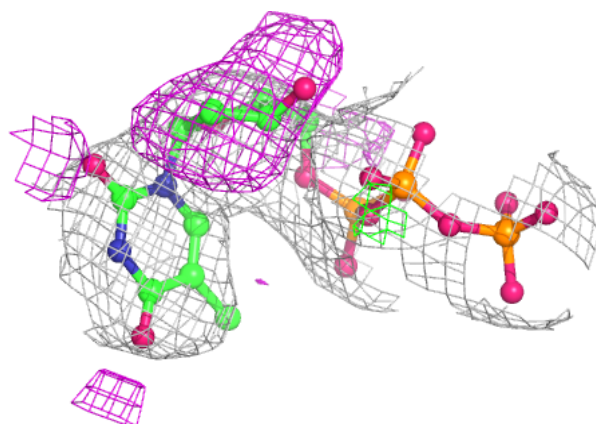
Electron density around MN E 802:

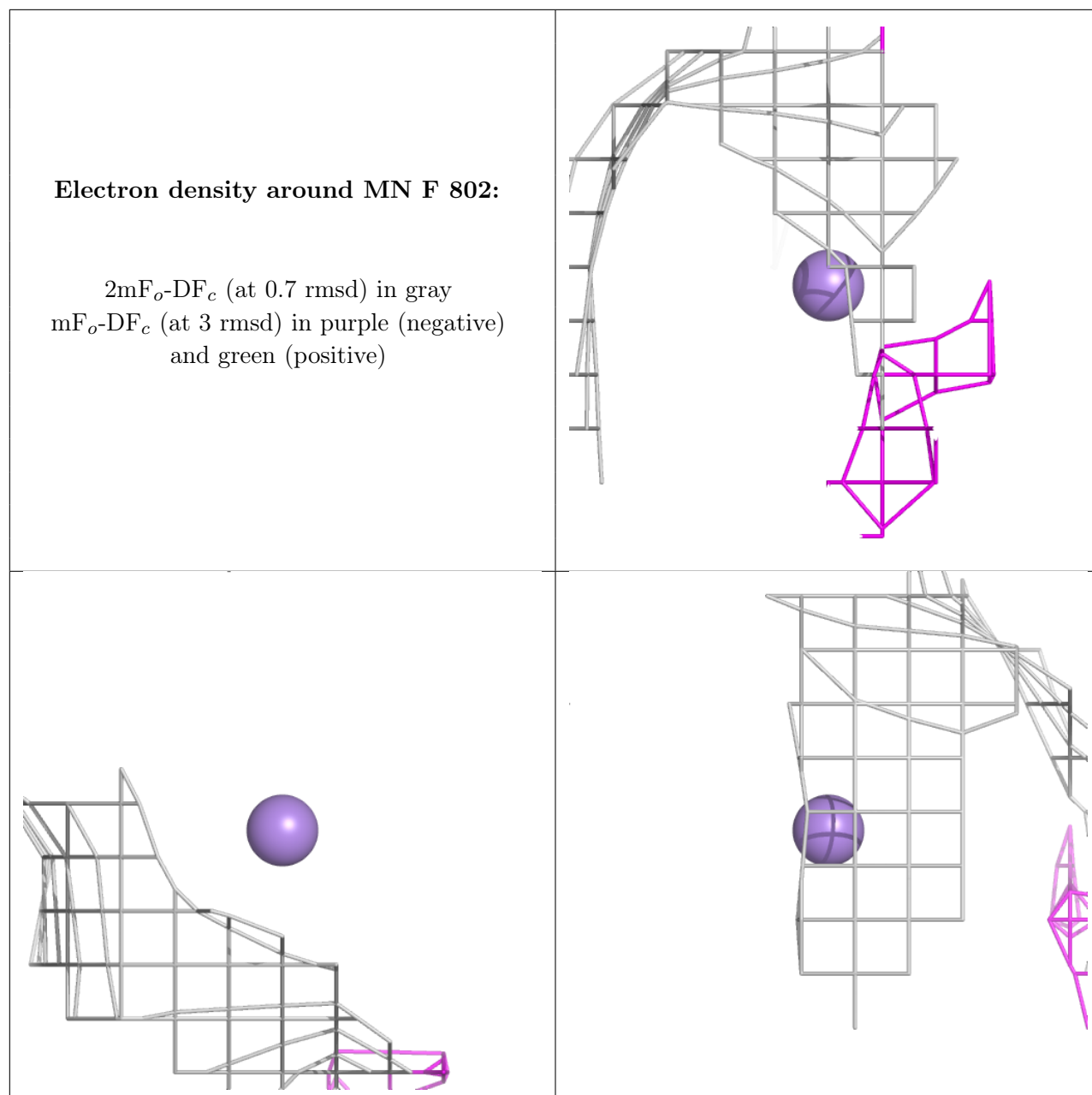
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TTP F 804:

$2mF_o-DF_c$ (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.