



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:08 PM UTC

PDB ID : 3HW4 / pdb_00003hw4
Title : Crystal structure of avian influenza A virus in complex with TMP
Authors : Zhao, C.; Lou, Z.; Guo, Y.; Ma, M.; Chen, Y.; Rao, Z.
Deposited on : 2009-06-17
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

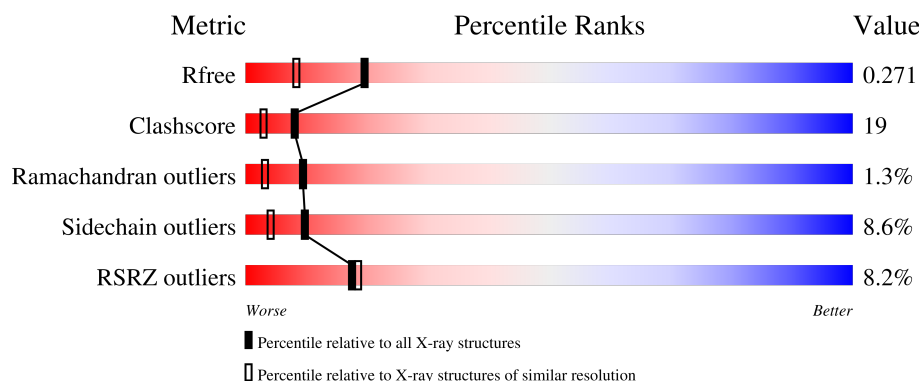
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	261	
1	B	261	
1	C	261	
1	D	261	

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
3	TMP	A	257	-	-	X	-
3	TMP	B	257	-	-	X	-
3	TMP	D	257	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6359 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1470	928	252	279	11			
1	B	180	Total	C	N	O	S	0	0	0
			1496	948	258	279	11			
1	C	177	Total	C	N	O	S	0	0	0
			1463	925	253	274	11			
1	D	176	Total	C	N	O	S	0	0	0
			1453	919	250	273	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q9Q0U9
A	-3	PRO	-	expression tag	UNP Q9Q0U9
A	-2	LEU	-	expression tag	UNP Q9Q0U9
A	-1	GLY	-	expression tag	UNP Q9Q0U9
A	0	SER	-	expression tag	UNP Q9Q0U9
A	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9
B	-4	GLY	-	expression tag	UNP Q9Q0U9
B	-3	PRO	-	expression tag	UNP Q9Q0U9
B	-2	LEU	-	expression tag	UNP Q9Q0U9
B	-1	GLY	-	expression tag	UNP Q9Q0U9
B	0	SER	-	expression tag	UNP Q9Q0U9
B	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9
C	-4	GLY	-	expression tag	UNP Q9Q0U9
C	-3	PRO	-	expression tag	UNP Q9Q0U9
C	-2	LEU	-	expression tag	UNP Q9Q0U9
C	-1	GLY	-	expression tag	UNP Q9Q0U9
C	0	SER	-	expression tag	UNP Q9Q0U9
C	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9
D	-4	GLY	-	expression tag	UNP Q9Q0U9
D	-3	PRO	-	expression tag	UNP Q9Q0U9
D	-2	LEU	-	expression tag	UNP Q9Q0U9

Continued on next page...

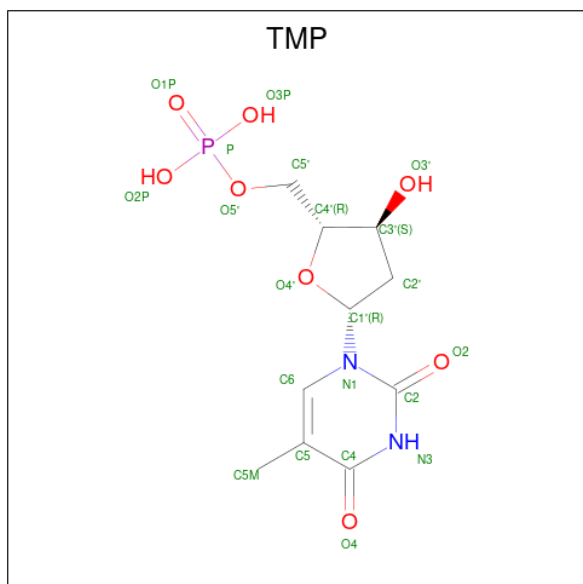
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP Q9Q0U9
D	0	SER	-	expression tag	UNP Q9Q0U9
D	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THYMIDINE-5'-PHOSPHATE (CCD ID: TMP) (formula: C₁₀H₁₅N₂O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
3	B	1	Total	C	N	O	P	0	0
			21	10	2	8	1		
3	D	1	Total	C	N	O	P	0	0
			21	10	2	8	1		

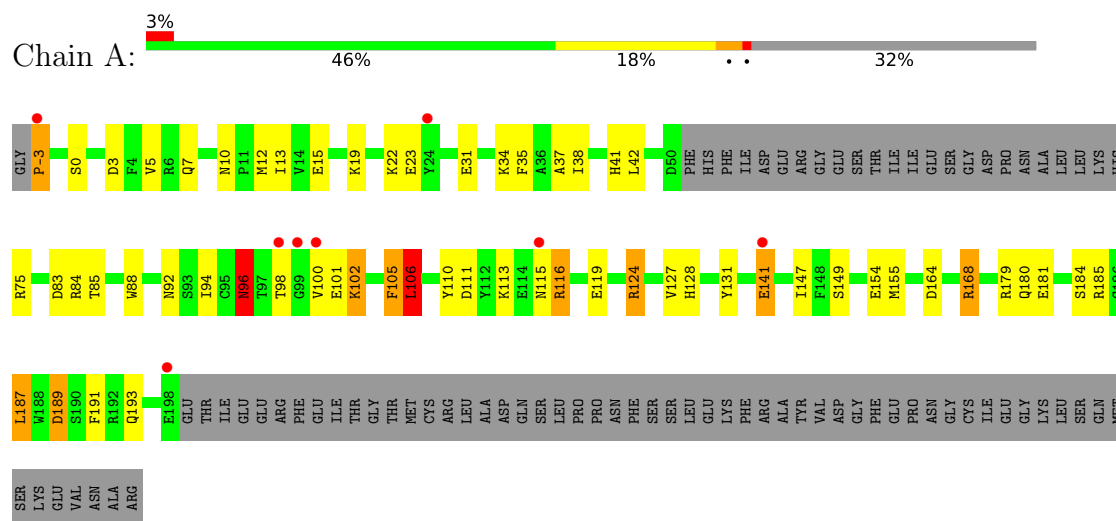
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total 127	O 127	0	0
4	B	104	Total 104	O 104	0	0
4	C	89	Total 89	O 89	0	0
4	D	90	Total 90	O 90	0	0

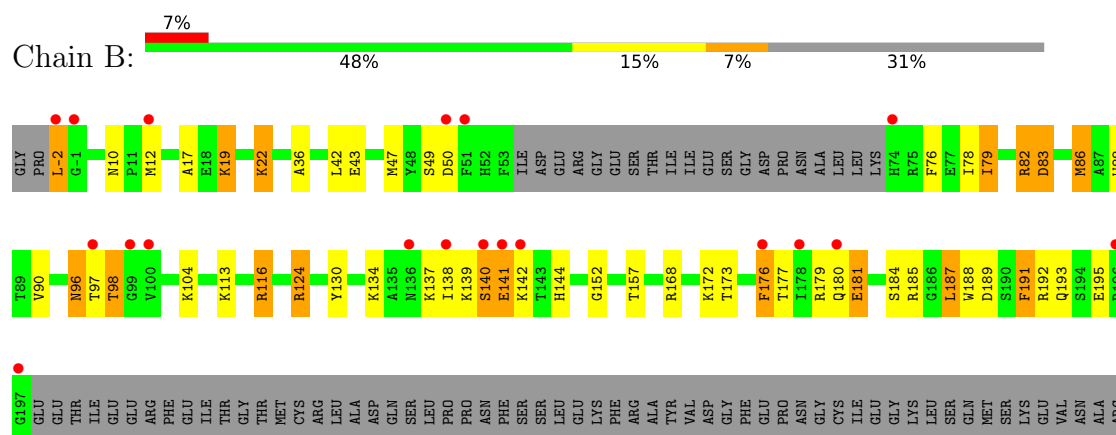
3 Residue-property plots

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

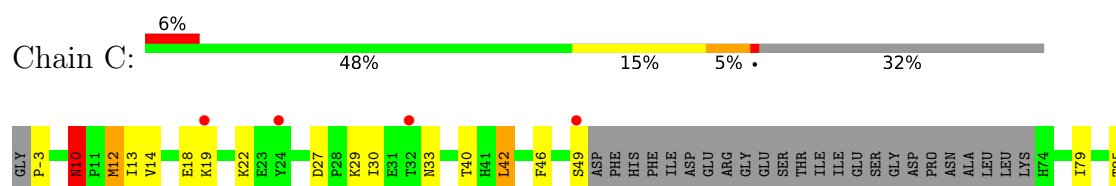
• Molecule 1: Polymerase acidic protein

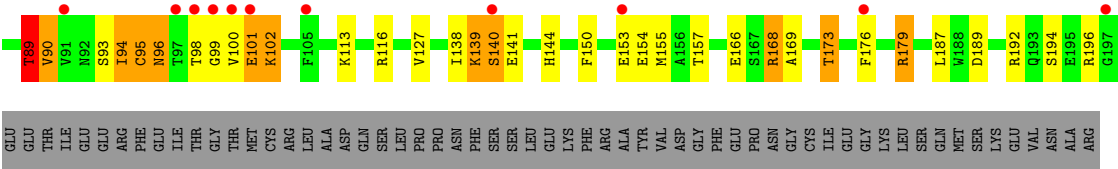


• Molecule 1: Polymerase acidic protein

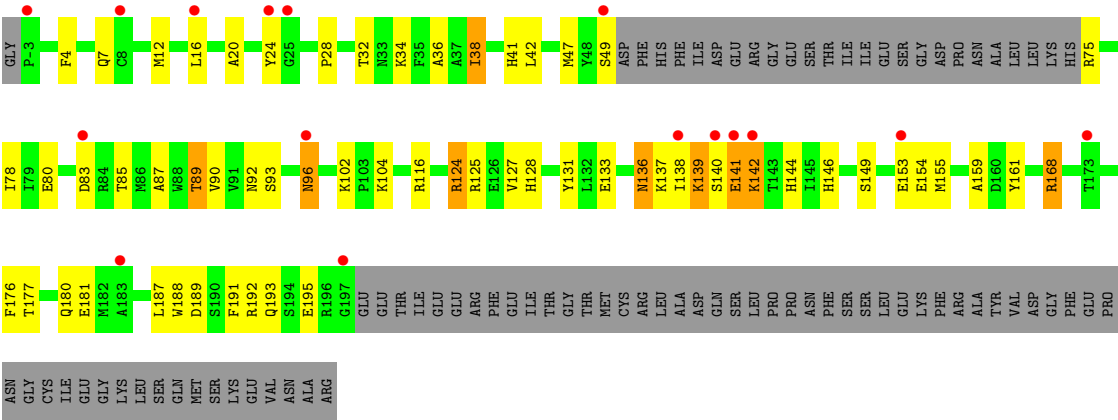


• Molecule 1: Polymerase acidic protein





● Molecule 1: Polymerase acidic protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.32Å 60.03Å 67.11Å 96.12° 96.36° 109.51°	Depositor
Resolution (Å)	47.78 – 1.90 47.78 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.5 (47.78-1.90) 93.8 (47.78-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.90 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.213 , 0.276 0.215 , 0.271	Depositor DCC
R_{free} test set	2794 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6359	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% 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: TMP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.33	6/1499 (0.4%)	1.43	15/2011 (0.7%)
1	B	1.33	4/1528 (0.3%)	1.31	12/2050 (0.6%)
1	C	1.18	2/1493 (0.1%)	1.22	9/2003 (0.4%)
1	D	1.25	4/1482 (0.3%)	1.23	5/1988 (0.3%)
All	All	1.27	16/6002 (0.3%)	1.30	41/8052 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	47	MET	SD-CE	-9.65	1.55	1.79
1	B	17	ALA	CA-CB	8.74	1.67	1.53
1	A	106	LEU	N-CA	7.74	1.57	1.46
1	D	36	ALA	CA-CB	7.13	1.64	1.53
1	A	116	ARG	CZ-NH1	6.89	1.42	1.32
1	A	94	ILE	CA-CB	6.16	1.61	1.54
1	B	191	PHE	C-O	-6.07	1.17	1.24
1	B	116	ARG	CZ-NH1	5.90	1.41	1.32
1	C	168	ARG	CD-NE	-5.60	1.38	1.46
1	A	37	ALA	CA-CB	5.39	1.61	1.53
1	A	168	ARG	CD-NE	-5.38	1.38	1.46
1	C	89	THR	CA-CB	5.30	1.61	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	159	ALA	CA-CB	5.15	1.61	1.53
1	B	36	ALA	CA-CB	5.07	1.61	1.53
1	A	147	ILE	CA-CB	5.07	1.61	1.54
1	D	38	ILE	CA-CB	5.04	1.60	1.54

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	THR	N-CA-C	-11.70	96.03	110.41
1	A	116	ARG	CD-NE-CZ	11.12	139.96	124.40
1	A	116	ARG	NE-CZ-NH2	-10.91	109.38	119.20
1	A	116	ARG	NE-CZ-NH1	10.63	132.13	121.50
1	B	50	ASP	CA-C-N	-10.35	105.75	123.25
1	B	50	ASP	C-N-CA	-10.35	105.75	123.25
1	A	105	PHE	O-C-N	-9.17	112.25	122.34
1	A	105	PHE	CA-C-N	-8.59	100.85	121.80
1	A	105	PHE	C-N-CA	-8.59	100.85	121.80
1	A	168	ARG	NE-CZ-NH2	-8.23	111.80	119.20
1	D	47	MET	CG-SD-CE	-7.90	83.51	100.90
1	B	116	ARG	NE-CZ-NH2	-7.60	112.36	119.20
1	B	168	ARG	NE-CZ-NH2	-6.94	112.95	119.20
1	A	168	ARG	CD-NE-CZ	6.94	134.11	124.40
1	C	10	ASN	CA-C-N	-6.89	112.53	119.56
1	C	10	ASN	C-N-CA	-6.89	112.53	119.56
1	D	161	TYR	N-CA-C	6.64	121.21	113.18
1	D	168	ARG	NE-CZ-NH2	-6.58	113.28	119.20
1	C	98	THR	N-CA-C	-6.54	99.81	109.81
1	A	116	ARG	CG-CD-NE	6.45	126.18	112.00
1	A	168	ARG	CG-CD-NE	-6.45	97.82	112.00
1	D	168	ARG	NE-CZ-NH1	6.42	127.92	121.50
1	C	168	ARG	CG-CD-NE	-6.41	97.90	112.00
1	C	140	SER	CB-CA-C	-6.27	102.86	111.51
1	D	142	LYS	N-CA-C	-6.23	104.16	112.94
1	A	168	ARG	NE-CZ-NH1	6.20	127.70	121.50
1	B	50	ASP	N-CA-C	6.06	117.75	111.03
1	B	116	ARG	CD-NE-CZ	6.03	132.85	124.40
1	A	96	ASN	N-CA-C	6.00	120.60	113.28
1	C	168	ARG	NE-CZ-NH2	-5.87	113.92	119.20
1	B	116	ARG	NE-CZ-NH1	5.75	127.25	121.50
1	B	96	ASN	N-CA-CB	5.65	119.26	110.44
1	C	100	VAL	N-CA-C	5.53	116.84	109.37
1	A	106	LEU	N-CA-CB	5.53	120.22	110.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	176	PHE	CB-CA-C	-5.44	101.81	110.84
1	A	164	ASP	N-CA-C	5.35	117.00	110.41
1	C	99	GLY	N-CA-C	5.30	120.77	113.99
1	C	166	GLU	N-CA-C	-5.26	105.62	111.36
1	A	96	ASN	N-CA-CB	5.19	118.61	110.46
1	B	83	ASP	N-CA-C	-5.17	103.32	110.35
1	B	184	SER	N-CA-C	5.14	117.55	111.33

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-3	PRO	Peptide
1	C	139	LYS	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	1470	0	1439	60	0
1	B	1496	0	1458	46	0
1	C	1463	0	1436	50	0
1	D	1453	0	1429	66	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	21	0	13	9	0
3	B	21	0	11	20	0
3	D	21	0	13	17	0
4	A	127	0	0	6	0
4	B	104	0	0	10	0
4	C	89	0	0	8	0
4	D	90	0	0	5	0
All	All	6359	0	5799	229	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 19.

All (229) 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:B:257:TMP:O5'	3:B:257:TMP:C5'	1.63	1.42
1:A:84:ARG:NH2	3:B:257:TMP:H51	1.35	1.39
1:A:105:PHE:O	1:A:106:LEU:CB	1.77	1.15
3:A:257:TMP:H5'1	3:A:257:TMP:C6	1.84	1.12
1:C:155:MET:HG3	4:C:1029:HOH:O	1.49	1.10
1:C:138:ILE:HG13	1:C:140:SER:HB3	1.22	1.10
1:D:128:HIS:HA	1:D:155:MET:HE1	1.31	1.09
1:D:125:ARG:NH1	1:D:195:GLU:HG2	1.68	1.08
1:D:42:LEU:HD21	3:D:257:TMP:C5M	1.83	1.08
1:C:94:ILE:HG22	1:C:95:CYS:H	1.16	1.07
1:A:84:ARG:HH22	3:B:257:TMP:C5M	1.64	1.07
3:B:257:TMP:C5'	3:B:257:TMP:P	2.51	0.99
1:A:41:HIS:ND1	3:A:257:TMP:H52	1.79	0.97
1:B:176:PHE:HD1	4:B:278:HOH:O	1.47	0.96
1:D:128:HIS:CA	1:D:155:MET:HE1	1.95	0.96
1:D:125:ARG:HH12	1:D:195:GLU:HG2	1.22	0.96
1:A:92:ASN:HD21	1:A:102:LYS:NZ	1.65	0.95
1:A:92:ASN:HD21	1:A:102:LYS:HZ2	1.17	0.93
1:A:75:ARG:N	4:A:341:HOH:O	2.01	0.92
1:B:86:MET:HG3	4:B:355:HOH:O	1.70	0.92
1:C:85:THR:O	1:C:89:THR:HG23	1.69	0.92
3:B:257:TMP:O3P	3:B:257:TMP:H5'2	1.70	0.90
1:B:192:ARG:HD2	4:B:1063:HOH:O	1.70	0.90
1:A:105:PHE:O	1:A:106:LEU:HB2	1.07	0.89
1:C:138:ILE:HG13	1:C:140:SER:CB	2.05	0.87
1:D:42:LEU:HD21	3:D:257:TMP:H53	1.57	0.87
1:A:84:ARG:NH2	3:B:257:TMP:C5M	2.31	0.86
1:C:94:ILE:HG22	1:C:95:CYS:N	1.92	0.85
1:C:154:GLU:OE2	1:C:168:ARG:HD2	1.77	0.84
1:B:177:THR:O	1:B:180:GLN:HG3	1.78	0.83
1:C:169:ALA:O	1:C:173:THR:HG22	1.79	0.83
3:B:257:TMP:O2	3:B:257:TMP:H2'1	1.80	0.82
1:D:75:ARG:N	4:D:326:HOH:O	2.13	0.81
1:C:154:GLU:OE2	1:C:168:ARG:CD	2.30	0.80
1:D:42:LEU:CD2	3:D:257:TMP:C5M	2.59	0.80
1:C:93:SER:C	1:C:94:ILE:O	2.24	0.80
1:C:94:ILE:CG2	1:C:95:CYS:H	1.95	0.79
1:D:138:ILE:O	4:D:358:HOH:O	2.02	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:LEU:HD11	3:D:257:TMP:H52	1.67	0.77
3:B:257:TMP:O2	3:B:257:TMP:C2'	2.32	0.77
1:D:92:ASN:HD21	1:D:102:LYS:HE2	1.50	0.76
1:C:94:ILE:O	1:C:96:ASN:N	2.19	0.76
1:B:88:TRP:CG	3:B:257:TMP:H53	2.21	0.76
1:B:176:PHE:CD1	4:B:278:HOH:O	2.28	0.75
1:D:141:GLU:HG3	1:D:142:LYS:H	1.52	0.75
1:C:79:ILE:CD1	1:C:90:VAL:CG1	2.65	0.75
1:C:140:SER:HA	4:C:356:HOH:O	1.88	0.74
1:B:124:ARG:HD2	1:B:191:PHE:O	1.88	0.74
1:A:127:VAL:HG23	1:A:155:MET:HE3	1.68	0.74
1:B:88:TRP:HB3	3:B:257:TMP:H53	1.68	0.74
1:C:189:ASP:HB2	4:C:1037:HOH:O	1.87	0.73
1:A:154:GLU:OE2	1:A:168:ARG:HD2	1.88	0.73
1:D:38:ILE:HG12	3:D:257:TMP:H1'	1.68	0.73
1:C:101:GLU:HG3	1:C:102:LYS:N	2.03	0.73
1:D:149:SER:OG	1:D:153:GLU:HG2	1.89	0.73
1:A:85:THR:HB	1:B:83:ASP:CG	2.14	0.73
3:A:257:TMP:C6	3:A:257:TMP:C5'	2.70	0.73
1:D:116:ARG:HD3	1:D:144:HIS:HB2	1.69	0.72
1:D:41:HIS:CE1	3:D:257:TMP:H5'1	2.25	0.72
1:D:42:LEU:HD21	3:D:257:TMP:H51	1.72	0.71
1:D:85:THR:O	1:D:89:THR:HG23	1.91	0.71
1:D:92:ASN:HD21	1:D:102:LYS:CE	2.04	0.71
1:D:42:LEU:CD2	3:D:257:TMP:H51	2.19	0.71
1:D:141:GLU:CG	1:D:142:LYS:H	2.04	0.71
3:A:257:TMP:H2'1	4:A:333:HOH:O	1.91	0.70
1:C:93:SER:O	1:C:94:ILE:O	2.09	0.70
1:A:119:GLU:OE2	4:A:1041:HOH:O	2.09	0.69
1:B:88:TRP:CB	3:B:257:TMP:H53	2.21	0.69
1:C:189:ASP:OD2	1:C:192:ARG:NH2	2.26	0.68
1:C:-3:PRO:CD	4:C:1034:HOH:O	2.41	0.68
1:C:116:ARG:HD3	1:C:144:HIS:HB2	1.74	0.68
1:A:10:ASN:ND2	1:A:12:MET:H	1.91	0.67
1:B:173:THR:O	1:B:176:PHE:HB2	1.93	0.67
3:B:257:TMP:C5'	3:B:257:TMP:O3P	2.37	0.66
1:A:41:HIS:ND1	3:A:257:TMP:C5M	2.57	0.66
1:D:92:ASN:ND2	1:D:102:LYS:HE2	2.09	0.66
1:D:128:HIS:HA	1:D:155:MET:CE	2.18	0.66
1:A:85:THR:HB	1:B:83:ASP:OD1	1.96	0.65
1:A:101:GLU:OE1	4:A:1031:HOH:O	2.14	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:GLU:OE2	4:B:1060:HOH:O	2.15	0.65
1:D:125:ARG:NH1	1:D:195:GLU:CG	2.54	0.65
1:C:79:ILE:CD1	1:C:90:VAL:HG11	2.27	0.64
1:A:128:HIS:CG	1:A:155:MET:HE1	2.33	0.64
1:D:177:THR:O	1:D:181:GLU:HG3	1.97	0.64
1:C:-3:PRO:HD2	4:C:1034:HOH:O	1.97	0.63
1:D:188:TRP:HE1	1:D:192:ARG:CZ	2.12	0.62
1:A:127:VAL:HG23	1:A:155:MET:CE	2.29	0.62
1:D:42:LEU:CG	3:D:257:TMP:H51	2.30	0.61
1:D:124:ARG:HD2	1:D:191:PHE:O	2.01	0.61
1:C:154:GLU:OE2	1:C:168:ARG:HD3	2.01	0.60
1:A:124:ARG:HD2	1:A:191:PHE:O	2.01	0.60
1:D:141:GLU:HG3	1:D:142:LYS:N	2.16	0.60
1:C:189:ASP:HA	1:C:192:ARG:HH21	1.65	0.60
1:D:189:ASP:O	1:D:193:GLN:HG3	2.02	0.60
3:B:257:TMP:O5'	3:B:257:TMP:C4'	2.43	0.59
1:D:137:LYS:C	1:D:139:LYS:H	2.10	0.59
1:D:176:PHE:HD1	4:D:1051:HOH:O	1.86	0.59
1:D:42:LEU:HG	3:D:257:TMP:H51	1.85	0.58
1:D:85:THR:O	1:D:89:THR:CG2	2.51	0.58
1:D:124:ARG:HG3	1:D:192:ARG:HA	1.85	0.58
1:A:128:HIS:ND1	1:A:155:MET:HE1	2.19	0.58
1:C:141:GLU:OE2	1:C:141:GLU:HA	2.04	0.58
1:C:116:ARG:CD	1:C:144:HIS:HB2	2.34	0.57
1:C:140:SER:CA	4:C:356:HOH:O	2.50	0.56
1:D:141:GLU:CG	1:D:142:LYS:N	2.68	0.56
1:B:144:HIS:CE1	1:B:157:THR:HB	2.41	0.56
1:D:20:ALA:O	1:D:24:TYR:HD1	1.88	0.56
1:C:79:ILE:HD11	1:C:90:VAL:CG1	2.34	0.56
1:A:110:TYR:OH	1:A:115:ASN:ND2	2.38	0.56
1:D:137:LYS:C	1:D:139:LYS:N	2.60	0.56
1:A:3:ASP:O	1:A:7:GLN:HG3	2.05	0.55
1:D:42:LEU:CG	3:D:257:TMP:C5M	2.84	0.55
1:C:19:LYS:HZ2	1:C:22:LYS:HE3	1.72	0.55
1:A:23:GLU:O	3:B:257:TMP:H52	2.07	0.55
1:C:79:ILE:HD12	1:C:90:VAL:HG12	1.89	0.54
1:A:23:GLU:O	3:B:257:TMP:C5M	2.55	0.54
1:B:116:ARG:HD2	1:B:144:HIS:HB2	1.90	0.54
1:D:137:LYS:O	1:D:139:LYS:N	2.40	0.54
1:B:88:TRP:CG	3:B:257:TMP:C5M	2.89	0.54
1:A:31:GLU:OE1	1:A:31:GLU:HA	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASN:HD21	1:A:102:LYS:HZ3	1.53	0.53
1:A:180:GLN:HG3	1:A:181:GLU:N	2.22	0.53
1:A:3:ASP:HB3	1:A:7:GLN:HE21	1.74	0.53
1:C:14:VAL:O	1:C:18:GLU:HG3	2.09	0.53
1:C:10:ASN:HD22	1:C:13:ILE:HG12	1.73	0.53
1:C:-3:PRO:N	4:C:1034:HOH:O	2.43	0.52
1:B:124:ARG:HG2	1:B:195:GLU:OE1	2.09	0.52
1:B:49:SER:OG	1:B:78:ILE:HD11	2.09	0.52
1:D:87:ALA:O	1:D:90:VAL:HG12	2.10	0.52
1:B:113:LYS:NZ	4:B:396:HOH:O	2.42	0.51
1:A:98:THR:OG1	1:A:100:VAL:HG23	2.09	0.51
1:D:116:ARG:HD2	4:D:1055:HOH:O	2.11	0.51
1:A:141:GLU:CD	1:A:141:GLU:H	2.19	0.51
1:B:43:GLU:HG2	1:B:47:MET:HE2	1.93	0.51
1:D:141:GLU:HA	4:D:1036:HOH:O	2.10	0.51
1:B:86:MET:CG	4:B:355:HOH:O	2.41	0.51
1:D:154:GLU:OE2	1:D:168:ARG:HD2	2.11	0.51
1:B:10:ASN:HD22	1:B:12:MET:H	1.58	0.50
1:C:127:VAL:CG2	1:C:153:GLU:HG2	2.41	0.50
1:A:88:TRP:CE2	1:A:106:LEU:HG	2.46	0.50
1:B:79:ILE:O	1:B:82:ARG:CG	2.60	0.50
1:D:49:SER:OG	1:D:78:ILE:HD11	2.12	0.50
1:A:38:ILE:HG12	3:A:257:TMP:C1'	2.42	0.49
1:B:-2:LEU:HB3	1:B:185:ARG:O	2.12	0.49
1:A:10:ASN:ND2	1:A:12:MET:HB3	2.26	0.49
1:A:19:LYS:NZ	1:A:22:LYS:HE2	2.27	0.49
1:B:124:ARG:HG3	1:B:192:ARG:HA	1.95	0.48
1:A:111:ASP:OD2	1:A:113:LYS:HB2	2.13	0.48
1:A:23:GLU:HG2	1:A:84:ARG:HH21	1.79	0.48
1:A:5:VAL:HG11	1:A:35:PHE:CE1	2.48	0.48
1:B:116:ARG:NH2	4:B:1053:HOH:O	2.36	0.48
1:A:127:VAL:CG1	1:A:149:SER:HB3	2.44	0.47
1:D:125:ARG:NH2	1:D:133:GLU:OE1	2.47	0.47
1:A:10:ASN:ND2	1:A:12:MET:N	2.62	0.47
1:B:130:TYR:OH	1:B:134:LYS:NZ	2.46	0.47
1:C:79:ILE:HD12	1:C:90:VAL:CG1	2.45	0.47
1:C:10:ASN:HD21	1:C:12:MET:HB3	1.79	0.47
1:B:10:ASN:ND2	1:B:12:MET:H	2.13	0.47
1:B:22:LYS:HB3	1:B:22:LYS:HE3	1.72	0.47
1:A:10:ASN:HD22	1:A:13:ILE:H	1.63	0.46
1:B:49:SER:HB2	1:B:76:PHE:HB2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASP:HB3	1:B:83:ASP:CG	2.41	0.46
1:A:41:HIS:HB3	3:A:257:TMP:H53	1.97	0.46
1:A:38:ILE:HG23	3:A:257:TMP:C5	2.50	0.46
1:B:180:GLN:CD	4:B:351:HOH:O	2.58	0.46
1:A:96:ASN:ND2	4:A:1053:HOH:O	2.47	0.46
1:C:27:ASP:OD1	1:C:30:ILE:CD1	2.64	0.46
1:D:80:GLU:OE1	3:D:257:TMP:C5	2.69	0.46
1:A:84:ARG:HH22	3:B:257:TMP:H51	0.71	0.46
1:C:27:ASP:HB3	1:C:30:ILE:HD13	1.97	0.46
1:D:137:LYS:O	1:D:138:ILE:C	2.59	0.46
1:B:139:LYS:O	1:B:141:GLU:N	2.49	0.45
1:C:40:THR:HG21	1:C:150:PHE:CZ	2.51	0.45
1:C:116:ARG:O	1:C:116:ARG:HG3	2.16	0.45
1:D:42:LEU:CD1	3:D:257:TMP:H52	2.43	0.45
3:A:257:TMP:H5'1	3:A:257:TMP:H6	1.68	0.45
1:C:79:ILE:CD1	1:C:90:VAL:HG12	2.43	0.45
1:A:19:LYS:HA	1:A:19:LYS:HD3	1.67	0.45
1:A:154:GLU:OE2	1:A:168:ARG:CD	2.61	0.45
1:B:19:LYS:HA	1:B:19:LYS:HD3	1.79	0.45
1:C:42:LEU:O	1:C:46:PHE:HD2	2.00	0.45
1:C:144:HIS:CE1	1:C:157:THR:HB	2.51	0.45
1:D:124:ARG:HG2	1:D:195:GLU:OE1	2.18	0.45
1:B:180:GLN:CG	4:B:351:HOH:O	2.65	0.44
1:D:92:ASN:ND2	1:D:102:LYS:CE	2.75	0.44
1:D:131:TYR:C	1:D:131:TYR:CD2	2.95	0.44
1:C:94:ILE:CG2	1:C:95:CYS:N	2.62	0.44
1:A:185:ARG:HB2	1:A:187:LEU:HD22	2.00	0.43
1:D:136:ASN:O	1:D:139:LYS:HD2	2.18	0.43
1:D:80:GLU:OE1	3:D:257:TMP:C4	2.72	0.43
1:A:92:ASN:ND2	1:A:102:LYS:HZ2	1.99	0.43
1:A:10:ASN:ND2	1:A:12:MET:CB	2.81	0.42
1:A:75:ARG:N	4:A:367:HOH:O	2.51	0.42
1:B:137:LYS:HG2	1:B:138:ILE:HD12	2.01	0.42
1:A:189:ASP:OD1	1:A:193:GLN:NE2	2.52	0.42
1:B:179:ARG:HG3	1:B:188:TRP:CE3	2.54	0.42
1:D:155:MET:HB3	1:D:155:MET:HE3	1.58	0.42
1:D:20:ALA:HB1	3:D:257:TMP:C4	2.54	0.42
1:A:84:ARG:HH12	3:B:257:TMP:H6	1.68	0.42
1:B:138:ILE:HG22	1:B:140:SER:HA	2.01	0.42
1:A:19:LYS:HZ2	1:A:22:LYS:HE2	1.85	0.42
1:B:152:GLY:O	1:B:172:LYS:HD2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ASN:HD22	1:C:13:ILE:H	1.68	0.42
1:B:79:ILE:O	1:B:82:ARG:HG2	2.20	0.41
1:B:97:THR:C	1:B:98:THR:O	2.54	0.41
1:C:10:ASN:ND2	1:C:13:ILE:H	2.18	0.41
1:D:28:PRO:O	1:D:32:THR:HG22	2.19	0.41
1:D:41:HIS:ND1	3:D:257:TMP:H5'1	2.34	0.41
1:B:88:TRP:CD2	3:B:257:TMP:C5	3.08	0.41
1:C:179:ARG:C	1:C:179:ARG:HD2	2.45	0.41
1:B:185:ARG:HB2	1:B:187:LEU:HD22	2.02	0.41
1:D:93:SER:HA	1:D:96:ASN:HD21	1.84	0.41
1:A:131:TYR:CD2	1:A:131:TYR:C	2.98	0.41
1:D:12:MET:HE2	1:D:16:LEU:HD11	2.02	0.41
1:D:92:ASN:HD22	1:D:92:ASN:HA	1.61	0.41
1:C:33:ASN:HD22	1:C:194:SER:CB	2.34	0.41
1:D:127:VAL:HG13	1:D:153:GLU:HG3	2.01	0.41
1:B:79:ILE:O	1:B:82:ARG:HG3	2.21	0.41
1:A:92:ASN:ND2	1:A:102:LYS:NZ	2.49	0.41
1:C:10:ASN:HD21	1:C:12:MET:CB	2.34	0.41
1:A:83:ASP:HB3	1:B:83:ASP:OD2	2.21	0.40
1:A:34:LYS:HB2	1:A:34:LYS:HE3	1.68	0.40
1:D:4:PHE:O	1:D:7:GLN:HG3	2.22	0.40
1:D:20:ALA:CB	3:D:257:TMP:C4	3.05	0.40
1:B:139:LYS:O	1:B:140:SER:C	2.64	0.40
1:C:96:ASN:O	4:C:1042:HOH:O	2.22	0.40
1:D:87:ALA:O	1:D:90:VAL:CG1	2.69	0.40
1:D:146:HIS:HE1	1:D:168:ARG:HD3	1.87	0.40
1:A:23:GLU:O	3:B:257:TMP:H53	2.22	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	174/261 (67%)	169 (97%)	4 (2%)	1 (1%)	21	13
1	B	176/261 (67%)	168 (96%)	5 (3%)	3 (2%)	7	2
1	C	173/261 (66%)	167 (96%)	3 (2%)	3 (2%)	7	2
1	D	172/261 (66%)	161 (94%)	9 (5%)	2 (1%)	10	4
All	All	695/1044 (67%)	665 (96%)	21 (3%)	9 (1%)	9	3

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	LEU
1	B	140	SER
1	B	141	GLU
1	C	94	ILE
1	D	140	SER
1	B	142	LYS
1	C	95	CYS
1	C	139	LYS
1	D	141	GLU

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	160/232 (69%)	146 (91%)	14 (9%)	9	4
1	B	162/232 (70%)	147 (91%)	15 (9%)	8	3
1	C	159/232 (68%)	143 (90%)	16 (10%)	7	3
1	D	158/232 (68%)	148 (94%)	10 (6%)	16	8
All	All	639/928 (69%)	584 (91%)	55 (9%)	10	4

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	PRO
1	A	0	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	15	GLU
1	A	42	LEU
1	A	96	ASN
1	A	102	LYS
1	A	106	LEU
1	A	116	ARG
1	A	124	ARG
1	A	141	GLU
1	A	179	ARG
1	A	184	SER
1	A	187	LEU
1	A	189	ASP
1	B	-2	LEU
1	B	19	LYS
1	B	22	LYS
1	B	42	LEU
1	B	79	ILE
1	B	82	ARG
1	B	86	MET
1	B	90	VAL
1	B	96	ASN
1	B	104	LYS
1	B	124	ARG
1	B	181	GLU
1	B	187	LEU
1	B	189	ASP
1	B	193	GLN
1	C	10	ASN
1	C	12	MET
1	C	29	LYS
1	C	42	LEU
1	C	49	SER
1	C	89	THR
1	C	90	VAL
1	C	96	ASN
1	C	101	GLU
1	C	102	LYS
1	C	113	LYS
1	C	173	THR
1	C	176	PHE
1	C	179	ARG
1	C	187	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	196	ARG
1	D	34	LYS
1	D	83	ASP
1	D	89	THR
1	D	96	ASN
1	D	104	LYS
1	D	124	ARG
1	D	136	ASN
1	D	139	LYS
1	D	180	GLN
1	D	187	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	10	ASN
1	A	92	ASN
1	A	115	ASN
1	A	136	ASN
1	B	10	ASN
1	B	33	ASN
1	B	52	HIS
1	B	92	ASN
1	B	128	HIS
1	B	136	ASN
1	C	10	ASN
1	C	33	ASN
1	C	92	ASN
1	C	128	HIS
1	D	41	HIS
1	D	92	ASN
1	D	96	ASN
1	D	115	ASN
1	D	180	GLN
1	D	193	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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$
3	TMP	D	257	2	22,22,22	1.72	4 (18%)	32,33,33	3.52	13 (40%)
3	TMP	A	257	2	22,22,22	1.64	7 (31%)	32,33,33	2.42	9 (28%)
3	TMP	B	257	-	22,22,22	2.85	9 (40%)	32,33,33	4.64	14 (43%)

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
3	TMP	D	257	2	-	3/10/22/22	0/2/2/2
3	TMP	A	257	2	-	6/10/22/22	0/2/2/2
3	TMP	B	257	-	-	7/10/22/22	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	257	TMP	C1'-N1	-5.77	1.33	1.48
3	B	257	TMP	C5'-C4'	-5.46	1.35	1.51
3	D	257	TMP	C2-N1	5.13	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	257	TMP	O5'-C5'	5.03	1.63	1.44
3	B	257	TMP	C2-N3	-4.22	1.30	1.38
3	B	257	TMP	C6-N1	-4.13	1.31	1.38
3	B	257	TMP	C4-N3	-4.03	1.31	1.38
3	A	257	TMP	C4-C5	3.77	1.51	1.44
3	B	257	TMP	C2'-C1'	3.29	1.61	1.52
3	B	257	TMP	O4'-C1'	3.22	1.49	1.42
3	A	257	TMP	C4-N3	-2.74	1.33	1.38
3	A	257	TMP	O4'-C4'	-2.70	1.39	1.45
3	A	257	TMP	C2-N3	-2.63	1.33	1.38
3	D	257	TMP	C6-N1	-2.49	1.33	1.38
3	D	257	TMP	O4'-C4'	-2.43	1.39	1.45
3	A	257	TMP	C6-C5	2.34	1.38	1.34
3	A	257	TMP	C6-N1	-2.24	1.34	1.38
3	D	257	TMP	P-O3P	-2.22	1.46	1.54
3	A	257	TMP	P-O3P	-2.13	1.46	1.54
3	B	257	TMP	P-O3P	-2.02	1.47	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	257	TMP	O4'-C1'-N1	18.45	140.61	107.86
3	D	257	TMP	C1'-N1-C2	10.09	137.40	117.66
3	B	257	TMP	O4'-C4'-C5'	9.57	139.99	109.33
3	D	257	TMP	C1'-N1-C6	-8.77	106.02	120.74
3	B	257	TMP	C5-C6-N1	-7.86	114.77	123.31
3	D	257	TMP	C2'-C1'-N1	7.57	132.74	113.81
3	A	257	TMP	C5M-C5-C4	6.92	126.17	118.78
3	B	257	TMP	C4-N3-C2	-6.30	119.08	127.34
3	B	257	TMP	C4'-O4'-C1'	-5.86	95.59	109.51
3	B	257	TMP	C5-C4-N3	5.28	119.91	115.32
3	D	257	TMP	O2-C2-N3	-5.22	111.87	121.49
3	A	257	TMP	C5M-C5-C6	-5.12	115.92	122.85
3	D	257	TMP	O4-C4-C5	-4.95	119.25	124.92
3	D	257	TMP	C6-N1-C2	-4.78	116.54	121.30
3	D	257	TMP	N3-C2-N1	4.49	120.74	114.89
3	B	257	TMP	N3-C2-N1	4.45	120.69	114.89
3	A	257	TMP	O2-C2-N1	-4.44	117.02	122.80
3	A	257	TMP	O4'-C1'-N1	-4.14	100.51	107.86
3	A	257	TMP	N3-C2-N1	4.05	120.16	114.89
3	D	257	TMP	C4-N3-C2	-3.76	122.40	127.34
3	A	257	TMP	C4-N3-C2	-3.53	122.71	127.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	257	TMP	O2-C2-N1	3.53	127.39	122.80
3	A	257	TMP	C5-C6-N1	-3.48	119.53	123.31
3	B	257	TMP	C1'-N1-C6	-3.47	114.91	120.74
3	B	257	TMP	C5'-C4'-C3'	-3.04	97.62	114.64
3	B	257	TMP	C6-N1-C2	2.74	124.03	121.30
3	B	257	TMP	O2-C2-N3	-2.60	116.69	121.49
3	A	257	TMP	C5-C4-N3	2.59	117.57	115.32
3	A	257	TMP	C1'-N1-C6	-2.50	116.54	120.74
3	B	257	TMP	O3'-C3'-C4'	2.49	119.49	110.07
3	D	257	TMP	O3'-C3'-C2'	2.39	119.17	110.88
3	D	257	TMP	C6-C5-C4	2.34	119.95	118.02
3	B	257	TMP	O4'-C1'-C2'	-2.23	102.08	106.25
3	D	257	TMP	O4-C4-N3	2.03	123.93	120.11
3	D	257	TMP	C2'-C3'-C4'	2.02	106.89	102.80
3	B	257	TMP	C6-C5-C4	2.01	119.68	118.02

There are no chirality outliers.

All (16) torsion outliers are listed below:

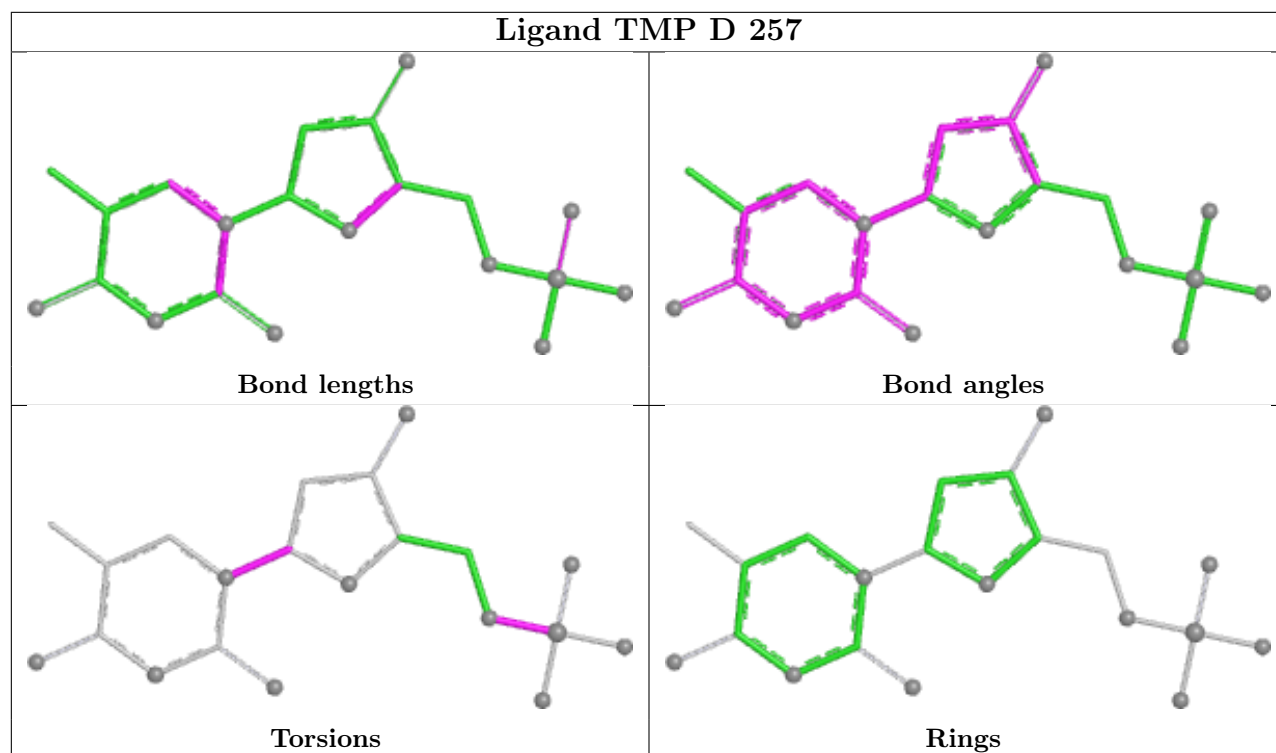
Mol	Chain	Res	Type	Atoms
3	A	257	TMP	C5'-O5'-P-O2P
3	A	257	TMP	C5'-O5'-P-O3P
3	A	257	TMP	O4'-C4'-C5'-O5'
3	B	257	TMP	C5'-O5'-P-O2P
3	B	257	TMP	C5'-O5'-P-O3P
3	B	257	TMP	O4'-C4'-C5'-O5'
3	B	257	TMP	C2'-C1'-N1-C2
3	B	257	TMP	C2'-C1'-N1-C6
3	D	257	TMP	C2'-C1'-N1-C2
3	D	257	TMP	C2'-C1'-N1-C6
3	A	257	TMP	C3'-C4'-C5'-O5'
3	B	257	TMP	C3'-C4'-C5'-O5'
3	A	257	TMP	C5'-O5'-P-O1P
3	B	257	TMP	C5'-O5'-P-O1P
3	D	257	TMP	C5'-O5'-P-O3P
3	A	257	TMP	C4'-C5'-O5'-P

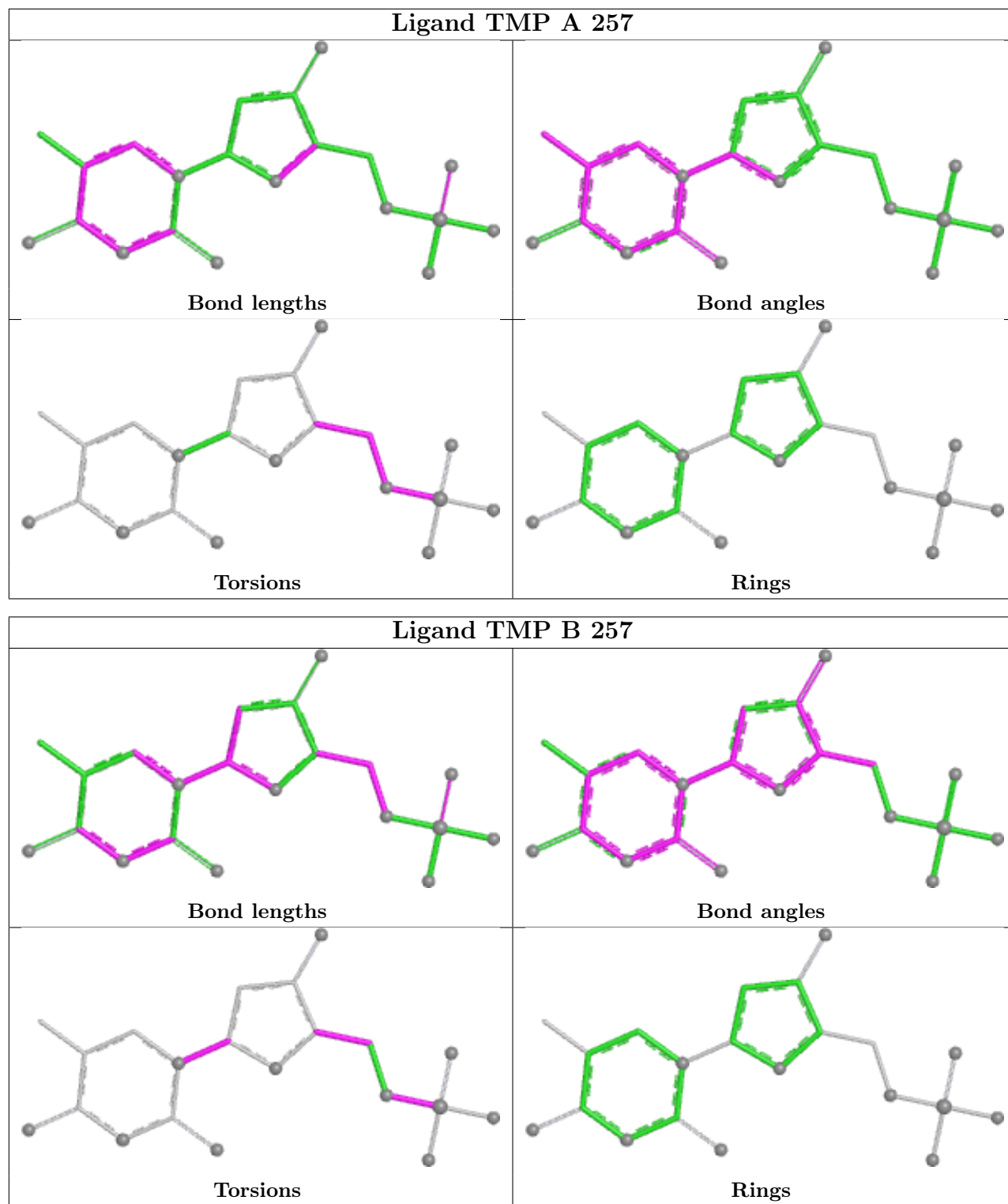
There are no ring outliers.

3 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	257	TMP	17	0
3	A	257	TMP	9	0
3	B	257	TMP	20	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	178/261 (68%)	0.52	8 (4%)	38 40	21, 31, 45, 49	0
1	B	180/261 (68%)	0.76	19 (10%)	11 12	21, 32, 49, 59	0
1	C	177/261 (67%)	0.77	15 (8%)	16 17	25, 36, 52, 66	0
1	D	176/261 (67%)	0.70	16 (9%)	15 15	23, 34, 53, 68	0
All	All	711/1044 (68%)	0.69	58 (8%)	17 18	21, 33, 50, 68	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	176	PHE	5.8
1	C	140	SER	5.4
1	B	51	PHE	4.9
1	B	197	GLY	4.7
1	B	196	ARG	4.4
1	C	99	GLY	4.4
1	D	138	ILE	4.2
1	C	176	PHE	4.1
1	C	100	VAL	4.1
1	A	100	VAL	4.0
1	A	-3	PRO	3.9
1	B	-1	GLY	3.9
1	A	24	TYR	3.7
1	D	96	ASN	3.5
1	C	197	GLY	3.4
1	D	153	GLU	3.3
1	D	197	GLY	3.3
1	B	138	ILE	3.2
1	A	99	GLY	3.2
1	B	136	ASN	3.1
1	D	24	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	49	SER	3.0
1	B	100	VAL	3.0
1	C	49	SER	2.9
1	B	97	THR	2.9
1	B	141	GLU	2.7
1	B	142	LYS	2.7
1	D	183	ALA	2.7
1	C	32	THR	2.7
1	B	-2	LEU	2.7
1	A	198	GLU	2.6
1	D	142	LYS	2.6
1	C	98	THR	2.6
1	C	24	TYR	2.5
1	D	83	ASP	2.5
1	B	50	ASP	2.4
1	B	178	ILE	2.4
1	B	74	HIS	2.4
1	C	19	LYS	2.3
1	D	-3	PRO	2.3
1	B	140	SER	2.3
1	A	141	GLU	2.3
1	D	8	CYS	2.3
1	C	105	PHE	2.2
1	B	12	MET	2.2
1	D	16	LEU	2.2
1	B	99	GLY	2.2
1	C	153	GLU	2.1
1	D	141	GLU	2.1
1	D	173	THR	2.1
1	C	101	GLU	2.1
1	A	115	ASN	2.1
1	D	140	SER	2.1
1	C	91	VAL	2.1
1	B	180	GLN	2.1
1	A	98	THR	2.0
1	C	97	THR	2.0
1	D	25	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

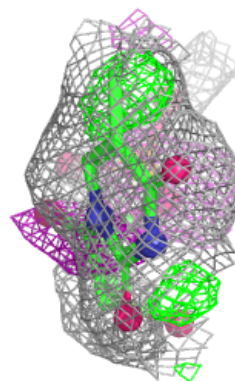
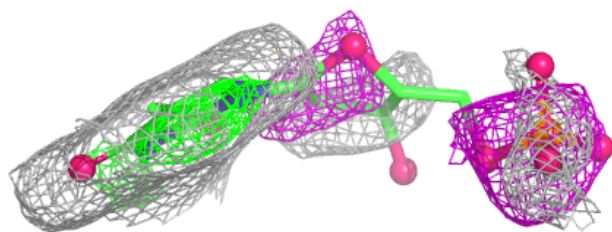
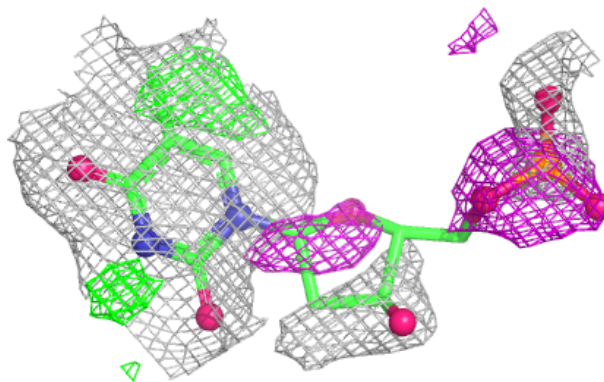
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TMP	B	257	21/21	0.41	0.19	49,70,88,89	0
3	TMP	D	257	21/21	0.64	0.21	33,61,65,67	0
3	TMP	A	257	21/21	0.66	0.16	20,20,20,20	0
2	MG	A	999	1/1	0.96	0.05	28,28,28,28	0
2	MG	B	999	1/1	0.96	0.05	33,33,33,33	0
2	MG	C	999	1/1	0.96	0.06	32,32,32,32	0
2	MG	D	999	1/1	0.98	0.04	36,36,36,36	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.

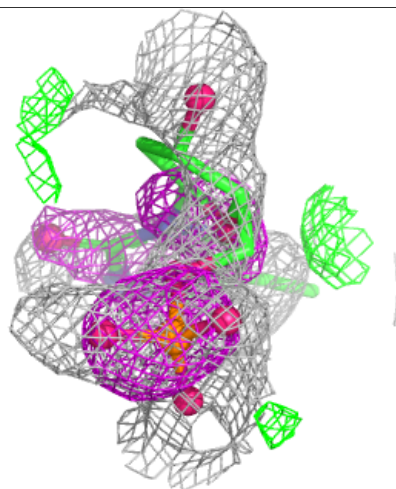
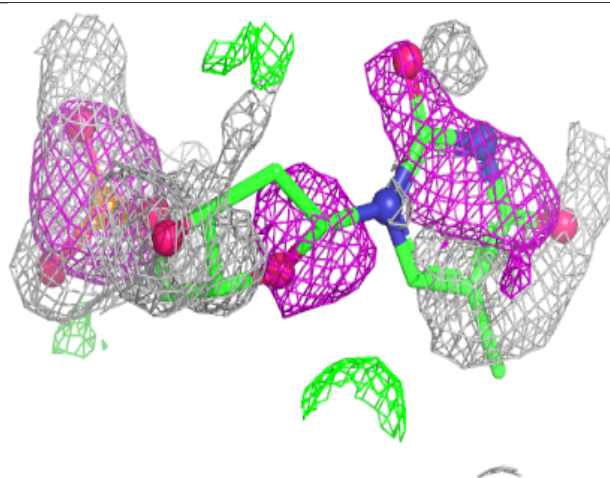
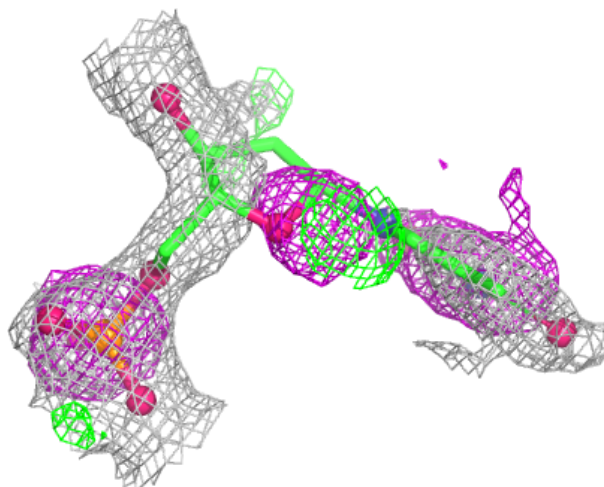
Electron density around TMP B 257:

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



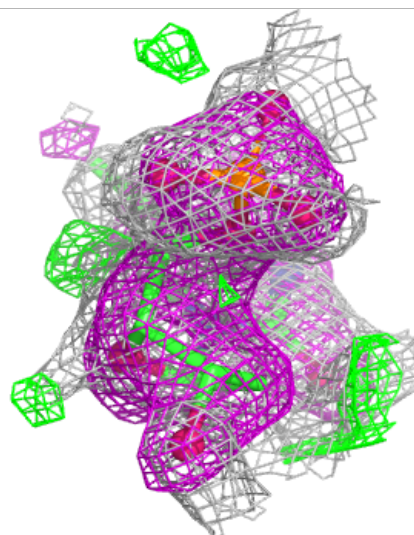
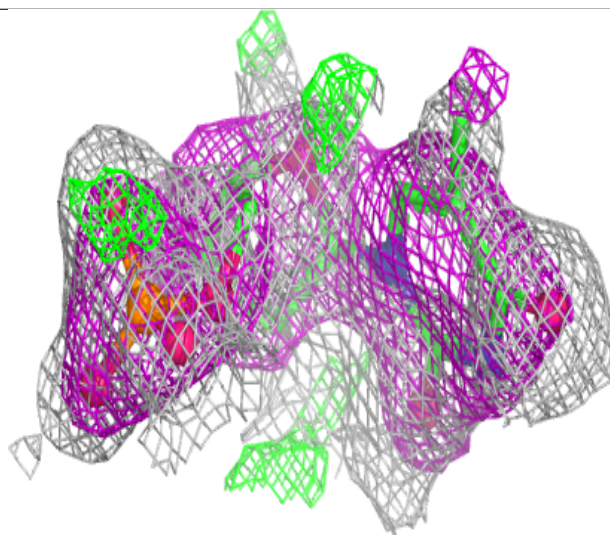
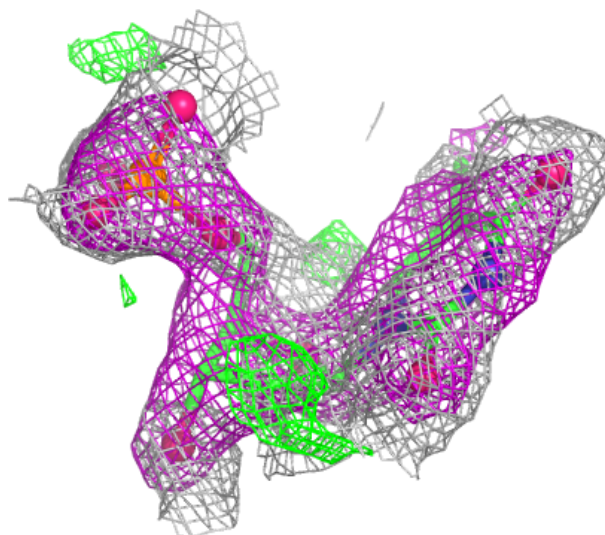
Electron density around TMP D 257:

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



Electron density around TMP A 257:

$2mF_o-DF_c$ (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.