Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2023 – 08:16 PM EDT

PDB ID	:	3HW4
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 (i) 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 (i)) were used in the production of this report:

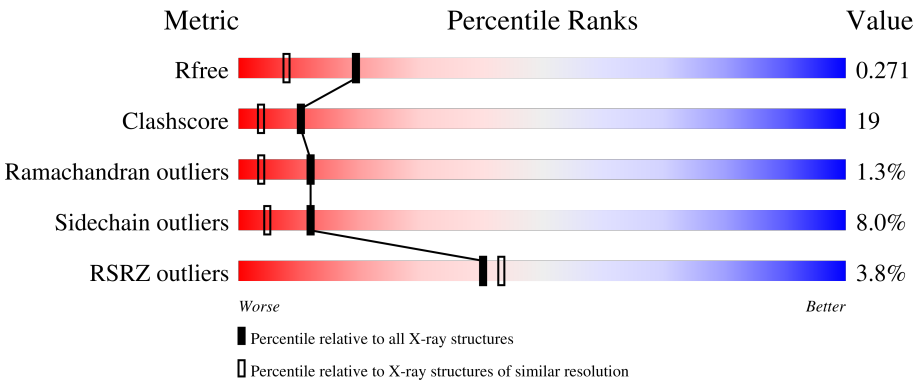
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 <=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	% 47% 16% • • 32%
1	B	261	4% 48% 15% 5% • 31%
1	C	261	3% 48% 15% 5% 32%
1	D	261	2% 45% 19% • 33%

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 (i)

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

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

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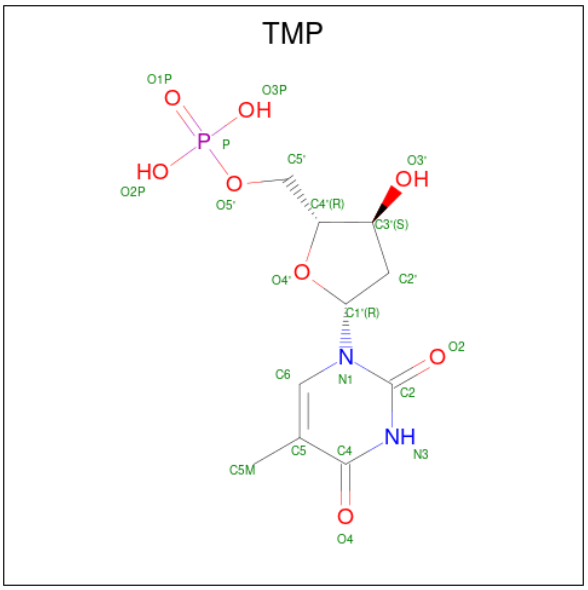
Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP Q9Q0U9
D	0	SER	-	expression tag	UNP Q9Q0U9
D	201	ILE	VAL	SEE REMARK 999	UNP Q9Q0U9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is THYMIDINE-5'-PHOSPHATE (three-letter code: TMP) (formula: $C_{10}H_{15}N_2O_8P$).



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

- Molecule 4 is water.

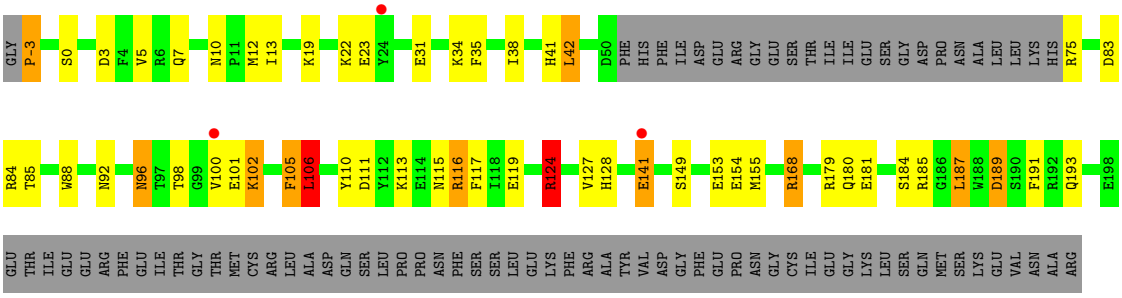
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	127	127	127	0	0
			Total	O		
4	B	104	104	104	0	0
			Total	O		
4	C	89	89	89	0	0
			Total	O		
4	D	90	90	90	0	0

3 Residue-property plots (i)

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

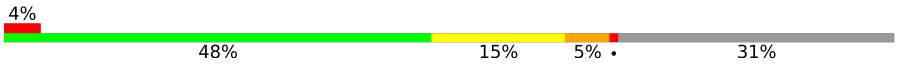
• Molecule 1: Polymerase acidic protein

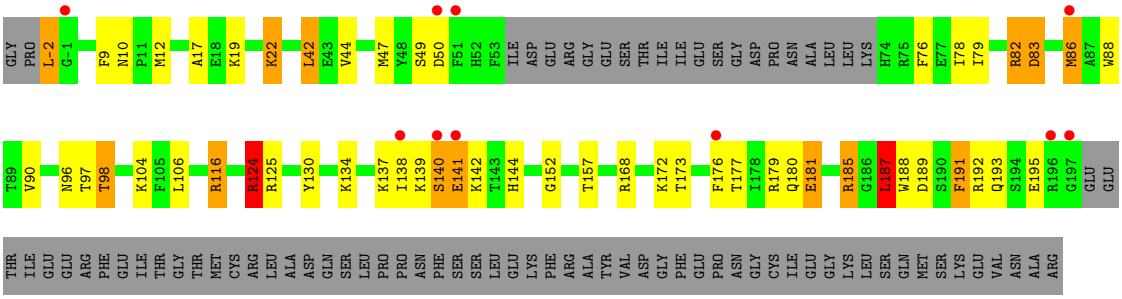
Chain A:



• Molecule 1: Polymerase acidic protein

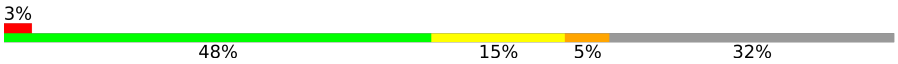
Chain B:

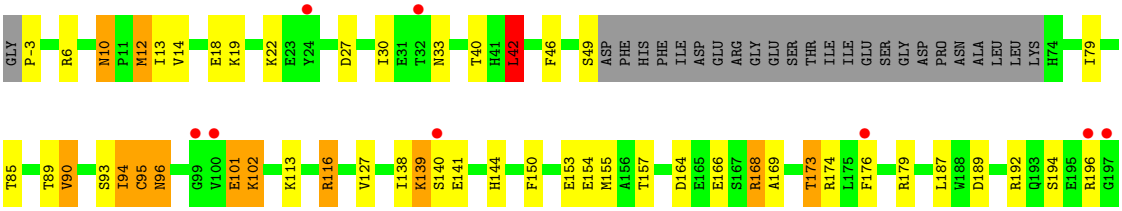




• Molecule 1: Polymerase acidic protein

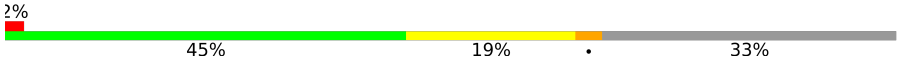
Chain C:

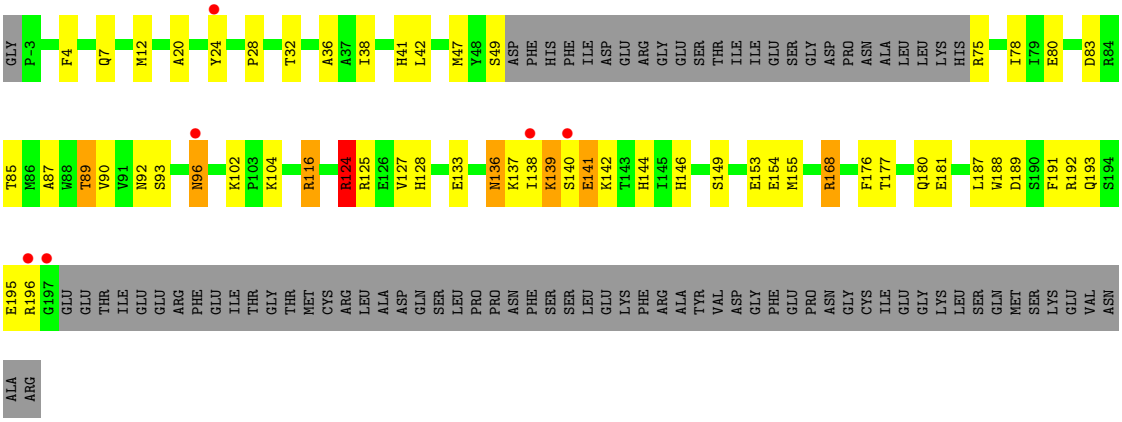




• Molecule 1: Polymerase acidic protein

Chain D:





4 Data and refinement statistics (i)

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) 93.5 (47.78-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.37 , 52.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	1.13	4/1499 (0.3%)	1.46	17/2011 (0.8%)
1	B	1.13	4/1528 (0.3%)	1.26	16/2050 (0.8%)
1	C	0.99	1/1493 (0.1%)	1.06	9/2003 (0.4%)
1	D	1.04	1/1482 (0.1%)	1.14	8/1988 (0.4%)
All	All	1.08	10/6002 (0.2%)	1.24	50/8052 (0.6%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	ARG	CZ-NH1	7.19	1.42	1.33
1	B	17	ALA	CA-CB	6.88	1.67	1.52
1	C	166	GLU	CG-CD	6.25	1.61	1.51
1	B	116	ARG	CZ-NH1	6.12	1.41	1.33
1	D	36	ALA	CA-CB	5.69	1.64	1.52
1	A	117	PHE	CD2-CE2	5.43	1.50	1.39
1	A	106	LEU	N-CA	5.35	1.57	1.46
1	B	191	PHE	CE2-CZ	5.21	1.47	1.37
1	B	9	PHE	CD2-CE2	5.20	1.49	1.39
1	A	153	GLU	CB-CG	-5.17	1.42	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	116	ARG	NE-CZ-NH1	23.66	132.13	120.30
1	A	116	ARG	NE-CZ-NH2	-21.84	109.38	120.30
1	A	168	ARG	NE-CZ-NH2	-17.01	111.80	120.30
1	B	116	ARG	NE-CZ-NH2	-15.88	112.36	120.30
1	D	168	ARG	NE-CZ-NH1	15.24	127.92	120.30
1	A	168	ARG	NE-CZ-NH1	14.81	127.70	120.30
1	B	168	ARG	NE-CZ-NH2	-14.69	112.95	120.30
1	D	168	ARG	NE-CZ-NH2	-14.04	113.28	120.30
1	B	116	ARG	NE-CZ-NH1	13.90	127.25	120.30
1	C	168	ARG	NE-CZ-NH2	-12.76	113.92	120.30
1	B	168	ARG	NE-CZ-NH1	12.25	126.43	120.30
1	D	116	ARG	NE-CZ-NH1	11.73	126.17	120.30
1	A	116	ARG	CD-NE-CZ	11.69	139.96	123.60
1	A	124	ARG	NE-CZ-NH2	-10.46	115.07	120.30
1	D	47	MET	CG-SD-CE	-10.43	83.51	100.20
1	A	124	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	C	168	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	D	116	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	A	105	PHE	C-N-CA	-8.34	100.85	121.70
1	B	185	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	B	124	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	168	ARG	CD-NE-CZ	7.51	134.11	123.60
1	C	164	ASP	CB-CG-OD2	7.10	124.69	118.30
1	B	124	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	116	ARG	CG-CD-NE	6.85	126.18	111.80
1	B	185	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	168	ARG	CG-CD-NE	-6.66	97.82	111.80
1	C	168	ARG	CG-CD-NE	-6.62	97.90	111.80
1	A	179	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	116	ARG	CD-NE-CZ	6.60	132.85	123.60
1	A	106	LEU	CA-CB-CG	6.60	130.48	115.30
1	A	105	PHE	O-C-N	-6.53	112.25	122.70
1	B	83	ASP	CB-CG-OD2	6.44	124.10	118.30
1	D	124	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	50	ASP	C-N-CA	-6.38	105.75	121.70
1	A	42	LEU	CA-CB-CG	6.30	129.79	115.30
1	C	174	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	B	187	LEU	CA-CB-CG	6.16	129.47	115.30
1	D	124	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	42	LEU	CB-CG-CD1	5.63	120.57	111.00
1	B	98	THR	N-CA-C	-5.55	96.03	111.00
1	C	6	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	C	164	ASP	CB-CG-OD1	-5.50	113.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	42	LEU	CB-CG-CD2	5.41	120.19	111.00
1	C	116	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	42	LEU	CA-CB-CG	5.26	127.41	115.30
1	D	168	ARG	CD-NE-CZ	5.13	130.78	123.60
1	A	179	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	106	LEU	CB-CG-CD1	-5.02	102.46	111.00
1	C	42	LEU	CA-CB-CG	5.01	126.83	115.30

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 (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	1470	0	1439	59	0
1	B	1496	0	1458	44	0
1	C	1463	0	1436	49	0
1	D	1453	0	1429	62	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	10	0
3	B	21	0	11	20	0
3	D	21	0	13	15	0
4	A	127	0	0	6	0
4	B	104	0	0	9	0
4	C	89	0	0	8	0
4	D	90	0	0	5	0
All	All	6359	0	5799	221	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 (221) 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: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:B:176:PHE:HD1	4:B:278:HOH:O	1.47	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:D:42:LEU:HD21	3:D:257:TMP:H53	1.51	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: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:D:42:LEU:HG	3:D:257:TMP:H51	1.64	0.79
1:D:42:LEU:CG	3:D:257:TMP:H51	2.12	0.79
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:127:VAL:HG23	1:A:155:MET:HE3	1.67	0.75
1:C:93:SER:C	1:C:94:ILE:O	2.24	0.75
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: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:128:HIS:HA	1:D:155:MET:CE	2.18	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
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: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: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:A:85:THR:HB	1:B:83:ASP:CG	2.14	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:A:41:HIS:ND1	3:A:257:TMP:C5M	2.57	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:D:92:ASN:ND2	1:D:102:LYS:HE2	2.09	0.66
1:A:128:HIS:CG	1:A:155:MET:HE1	2.31	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:HIS:CA	1:D:155:MET:HE1	2.27	0.64
1:D:177:THR:O	1:D:181:GLU:HG3	1.97	0.64
1:D:42:LEU:CD2	3:D:257:TMP:H51	2.27	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:128:HIS:HA	1:D:155:MET:HE1	1.82	0.61
1:D:124:ARG:HD2	1:D:191:PHE:O	2.01	0.61
1:D:128:HIS:HA	1:D:155:MET:HE3	1.83	0.61
1:A:128:HIS:ND1	1:A:155:MET:HE1	2.16	0.60
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:A:41:HIS:ND1	3:A:257:TMP:H51	2.17	0.59
1:D:176:PHE:HD1	4:D:1051:HOH:O	1.86	0.59
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: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:A:41:HIS:HB3	3:A:257:TMP:H51	1.86	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:41:HIS:ND1	3:A:257:TMP:H53	2.20	0.56
1:A:110:TYR:OH	1:A:115:ASN:ND2	2.38	0.56
1:A:3:ASP:O	1:A:7:GLN:HG3	2.05	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:D:137:LYS:C	1:D:139:LYS:N	2.60	0.54
1:D:137:LYS:C	1:D:139:LYS:H	2.10	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
1:B:44:VAL:HA	1:B:47:MET:HE2	1.91	0.53

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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:D:42:LEU:CG	3:D:257:TMP:C5M	2.84	0.52
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: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: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:D:42:LEU:HD11	3:D:257:TMP:H52	1.94	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
1:A:141:GLU:CD	1:A:141:GLU:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ILE:HG23	3:A:257:TMP:C5	2.50	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:C:19:LYS:HZ2	1:C:22:LYS:HE3	1.80	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
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: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: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:B:152:GLY:O	1:B:172:LYS:HD2	2.20	0.42
1:B:180:GLN:CD	4:B:351:HOH:O	2.58	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:92:ASN:HD22	1:D:92:ASN:HA	1.61	0.41
1:A:83:ASP:HB3	1:B:83:ASP:CG	2.41	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:D:137:LYS:O	1:D:138:ILE:C	2.59	0.41
1:B:79:ILE:O	1:B:82:ARG:HG3	2.21	0.41
1:B:97:THR:C	1:B:98:THR:O	2.54	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: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%)	25 15
1	B	176/261 (67%)	168 (96%)	5 (3%)	3 (2%)	9 2
1	C	173/261 (66%)	167 (96%)	3 (2%)	3 (2%)	9 2
1	D	172/261 (66%)	161 (94%)	9 (5%)	2 (1%)	13 4
All	All	695/1044 (67%)	665 (96%)	21 (3%)	9 (1%)	12 4

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 (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
1	A	160/232 (69%)	148 (92%)	12 (8%)	13 5
1	B	162/232 (70%)	148 (91%)	14 (9%)	10 4
1	C	159/232 (68%)	145 (91%)	14 (9%)	10 4
1	D	158/232 (68%)	147 (93%)	11 (7%)	15 7
All	All	639/928 (69%)	588 (92%)	51 (8%)	12 5

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	PRO
1	A	0	SER
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	184	SER
1	A	187	LEU

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Mol	Chain	Res	Type
1	A	189	ASP
1	B	-2	LEU
1	B	22	LYS
1	B	42	LEU
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	125	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	42	LEU
1	C	49	SER
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
1	C	196	ARG
1	D	12	MET
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
1	D	196	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) 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	193	GLN
1	B	10	ASN
1	B	52	HIS
1	B	92	ASN
1	B	136	ASN
1	C	10	ASN
1	C	33	ASN
1	C	92	ASN
1	D	92	ASN
1	D	96	ASN
1	D	115	ASN
1	D	193	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 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	1.70	4 (18%)	33,33,33	3.48	11 (33%)
3	TMP	A	257	2	22,22,22	1.62	7 (31%)	33,33,33	2.37	9 (27%)
3	TMP	B	257	-	22,22,22	2.80	8 (36%)	33,33,33	4.68	14 (42%)

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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	257	TMP	C1'-N1	-5.63	1.33	1.48
3	B	257	TMP	C5'-C4'	-5.28	1.35	1.51
3	D	257	TMP	C2-N1	5.02	1.46	1.38
3	B	257	TMP	O5'-C5'	4.90	1.63	1.44
3	B	257	TMP	C6-N1	-4.14	1.31	1.38
3	B	257	TMP	C2-N3	-4.13	1.30	1.38
3	B	257	TMP	C4-N3	-4.06	1.31	1.38
3	A	257	TMP	C4-C5	3.72	1.51	1.44
3	B	257	TMP	O4'-C1'	3.22	1.49	1.42
3	B	257	TMP	C2'-C1'	3.20	1.61	1.52
3	A	257	TMP	C4-N3	-2.75	1.33	1.38
3	A	257	TMP	O4'-C4'	-2.68	1.39	1.45
3	A	257	TMP	C2-N3	-2.58	1.33	1.38
3	D	257	TMP	C6-N1	-2.51	1.33	1.38
3	D	257	TMP	O4'-C4'	-2.42	1.39	1.45
3	A	257	TMP	C6-C5	2.34	1.38	1.34
3	A	257	TMP	C6-N1	-2.25	1.34	1.38
3	D	257	TMP	P-O3P	-2.15	1.46	1.54
3	A	257	TMP	P-O3P	-2.07	1.46	1.54

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	257	TMP	O4'-C1'-N1	18.32	140.61	107.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	257	TMP	C1'-N1-C2	10.03	137.40	117.64
3	B	257	TMP	O4'-C4'-C5'	9.31	139.99	109.37
3	D	257	TMP	C1'-N1-C6	-8.56	106.02	120.77
3	B	257	TMP	C5-C6-N1	-8.33	114.77	123.34
3	D	257	TMP	C2'-C1'-N1	8.24	132.74	113.77
3	A	257	TMP	C5M-C5-C4	6.73	126.17	118.77
3	B	257	TMP	C4-N3-C2	-6.38	119.08	127.35
3	B	257	TMP	P-O5'-C5'	-6.26	101.06	118.30
3	B	257	TMP	C4'-O4'-C1'	-5.74	95.59	109.45
3	B	257	TMP	C5-C4-N3	5.39	119.91	115.31
3	A	257	TMP	C5M-C5-C6	-5.19	115.92	122.85
3	D	257	TMP	O2-C2-N3	-5.17	111.87	121.50
3	D	257	TMP	O4-C4-C5	-4.87	119.25	124.90
3	D	257	TMP	C6-N1-C2	-4.69	116.54	121.30
3	D	257	TMP	N3-C2-N1	4.41	120.74	114.89
3	B	257	TMP	N3-C2-N1	4.37	120.69	114.89
3	A	257	TMP	O2-C2-N1	-4.34	117.02	122.79
3	A	257	TMP	O4'-C1'-N1	-4.11	100.51	107.86
3	A	257	TMP	N3-C2-N1	3.97	120.16	114.89
3	D	257	TMP	C4-N3-C2	-3.82	122.40	127.35
3	A	257	TMP	C5-C6-N1	-3.70	119.53	123.34
3	A	257	TMP	C4-N3-C2	-3.59	122.71	127.35
3	D	257	TMP	O2-C2-N1	3.46	127.39	122.79
3	B	257	TMP	C1'-N1-C6	-3.40	114.91	120.77
3	B	257	TMP	C5'-C4'-C3'	-2.91	97.62	114.74
3	B	257	TMP	C6-N1-C2	2.71	124.03	121.30
3	A	257	TMP	C5-C4-N3	2.65	117.57	115.31
3	B	257	TMP	O2-C2-N3	-2.59	116.69	121.50
3	A	257	TMP	C1'-N1-C6	-2.46	116.54	120.77
3	B	257	TMP	O3'-C3'-C4'	2.45	119.49	110.10
3	D	257	TMP	O3'-C3'-C2'	2.31	119.17	110.90
3	D	257	TMP	C6-C5-C4	2.29	119.95	118.03
3	B	257	TMP	O4'-C1'-C2'	-2.21	102.08	106.25

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

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Mol	Chain	Res	Type	Atoms
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

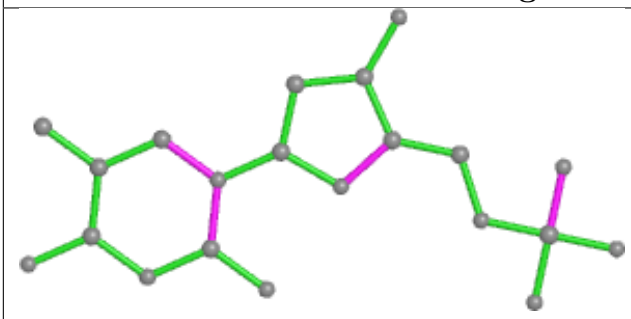
There are no ring outliers.

3 monomers are involved in 45 short contacts:

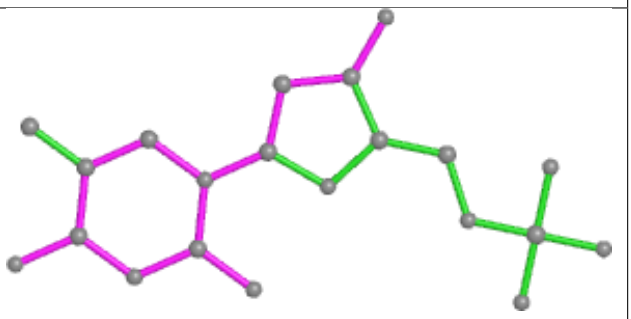
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	257	TMP	15	0
3	A	257	TMP	10	0
3	B	257	TMP	20	0

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 then 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.

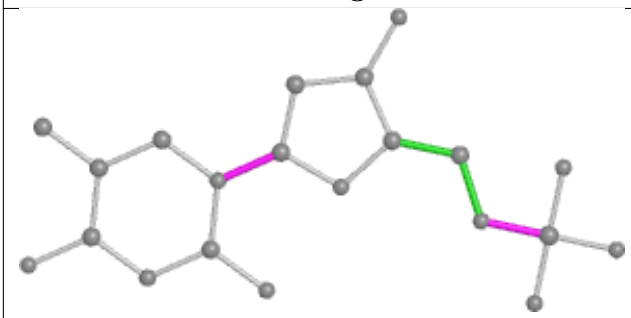
Ligand TMP D 257



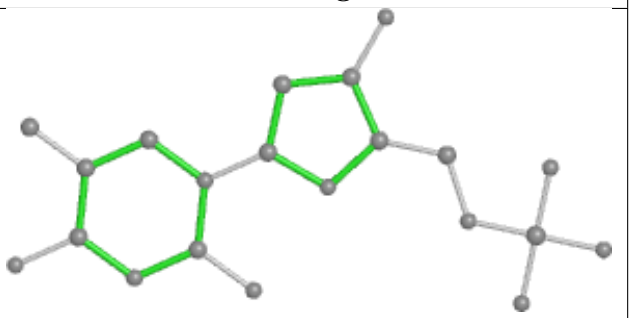
Bond lengths



Bond angles

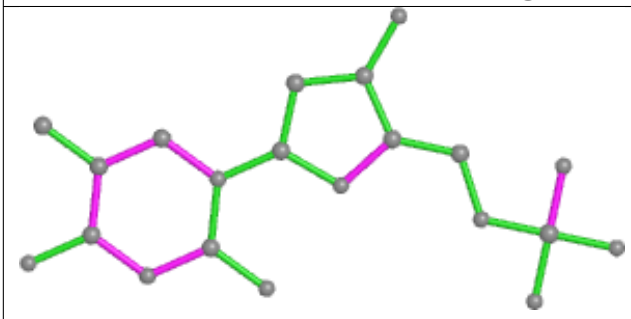


Torsions

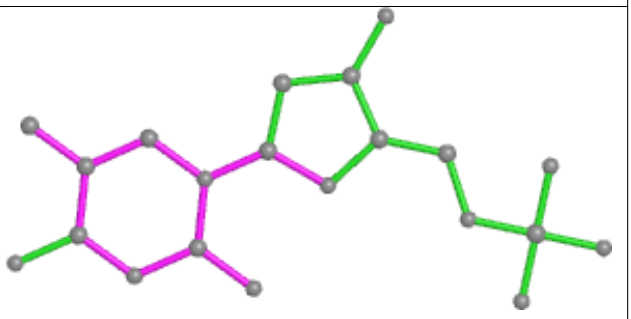


Rings

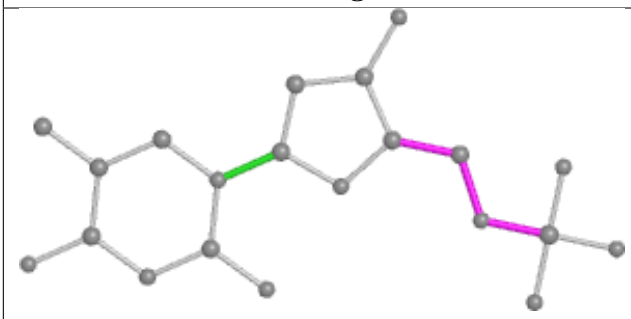
Ligand TMP A 257



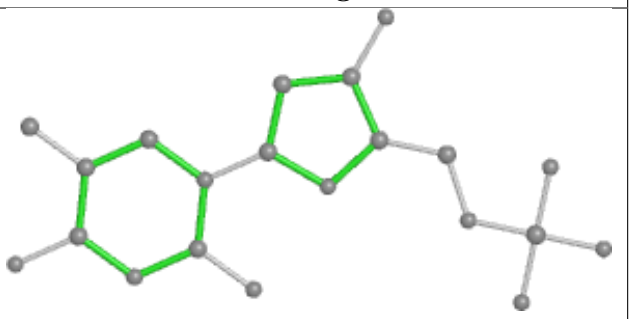
Bond lengths



Bond angles

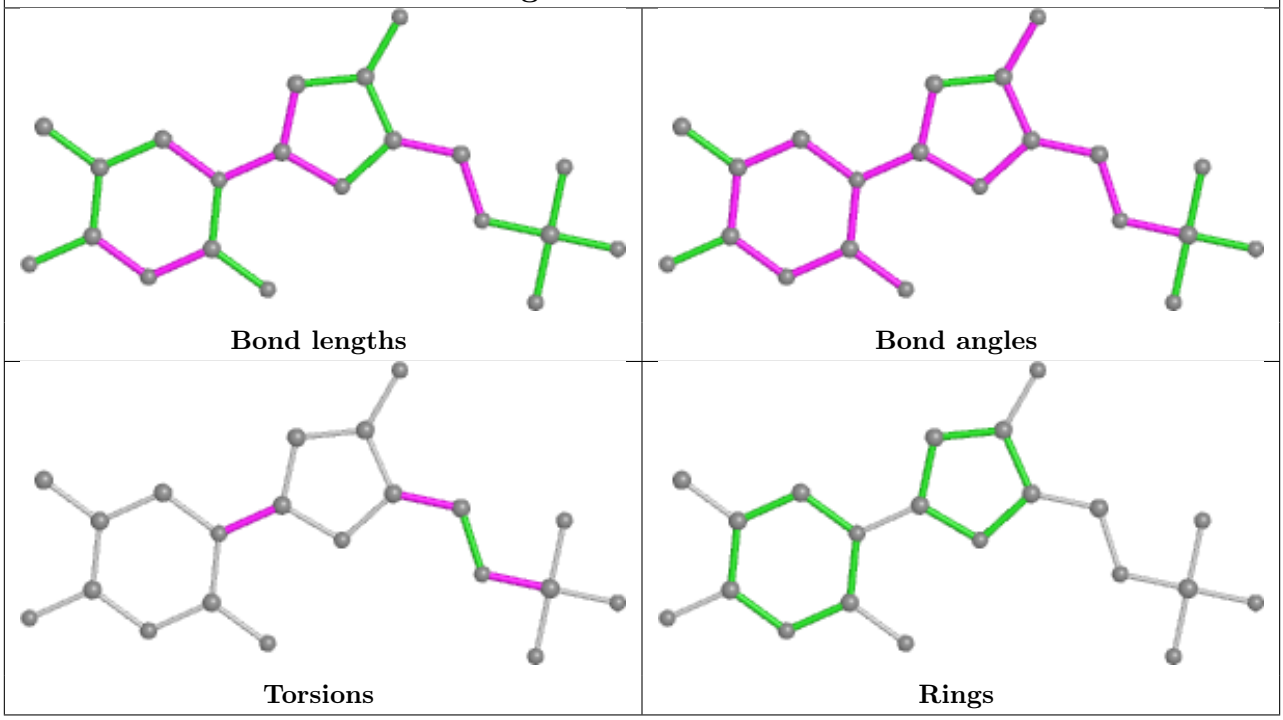


Torsions



Rings

Ligand TMP B 257



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.07	3 (1%)	70	72	21, 31, 45, 49	0
1	B	180/261 (68%)	0.31	10 (5%)	24	27	21, 32, 49, 59	0
1	C	177/261 (67%)	0.26	8 (4%)	33	36	25, 36, 52, 66	0
1	D	176/261 (67%)	0.23	6 (3%)	45	48	23, 34, 53, 68	0
All	All	711/1044 (68%)	0.22	27 (3%)	40	43	21, 33, 50, 68	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	197	GLY	8.6
1	C	197	GLY	7.6
1	B	196	ARG	6.8
1	B	197	GLY	6.1
1	B	176	PHE	5.9
1	C	100	VAL	4.9
1	B	51	PHE	4.3
1	B	141	GLU	4.2
1	D	196	ARG	3.7
1	C	196	ARG	3.7
1	B	138	ILE	3.3
1	C	99	GLY	3.3
1	C	176	PHE	3.2
1	C	140	SER	3.0
1	D	138	ILE	2.7
1	C	24	TYR	2.7
1	B	140	SER	2.7
1	B	-1	GLY	2.6
1	D	140	SER	2.3
1	A	141	GLU	2.3
1	A	24	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	24	TYR	2.2
1	C	32	THR	2.2
1	A	100	VAL	2.2
1	D	96	ASN	2.1
1	B	86	MET	2.1
1	B	50	ASP	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)

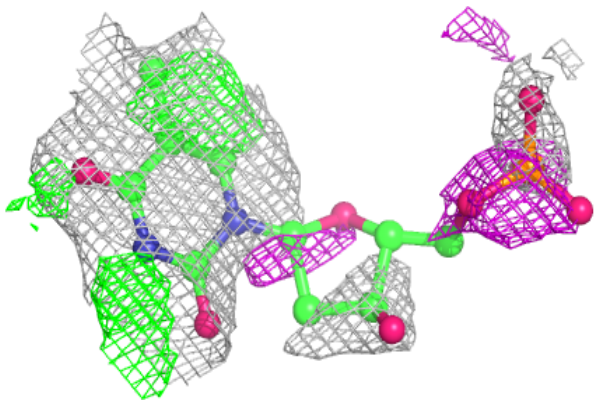
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

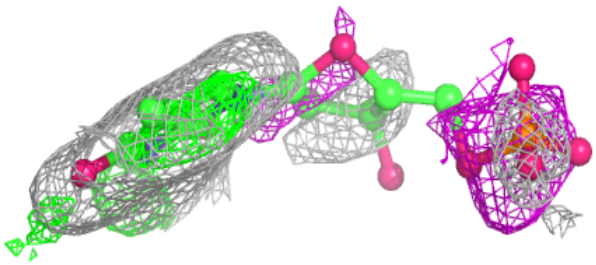
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TMP	B	257	21/21	0.57	0.40	49,70,88,89	0
3	TMP	D	257	21/21	0.72	0.38	33,61,65,67	0
3	TMP	A	257	21/21	0.77	0.40	20,20,20,20	0
2	MG	A	999	1/1	0.94	0.09	28,28,28,28	0
2	MG	B	999	1/1	0.95	0.08	33,33,33,33	0
2	MG	D	999	1/1	0.96	0.07	36,36,36,36	0
2	MG	C	999	1/1	0.96	0.04	32,32,32,32	0

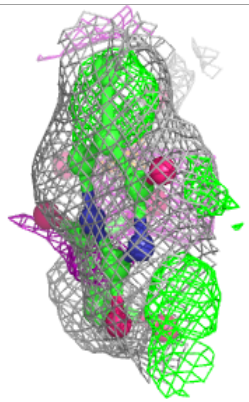
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

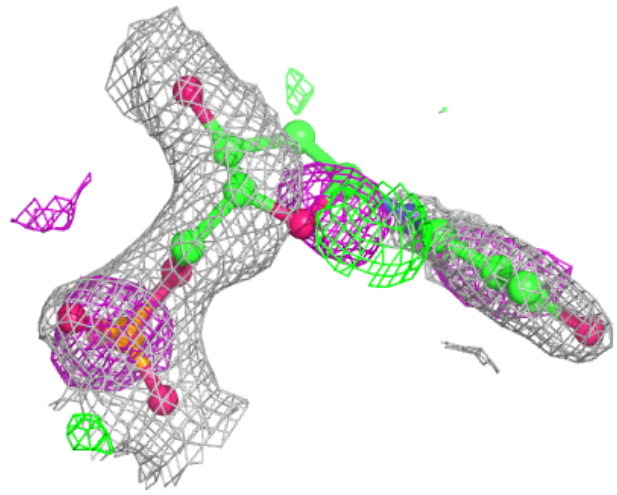


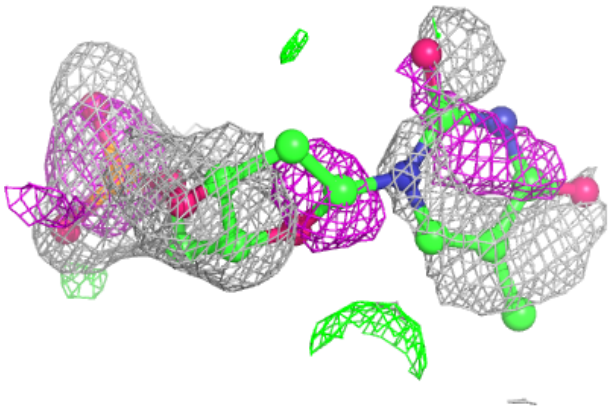


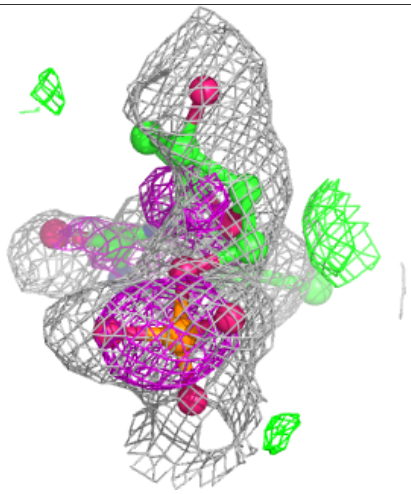


Electron density around TMP D 257:

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

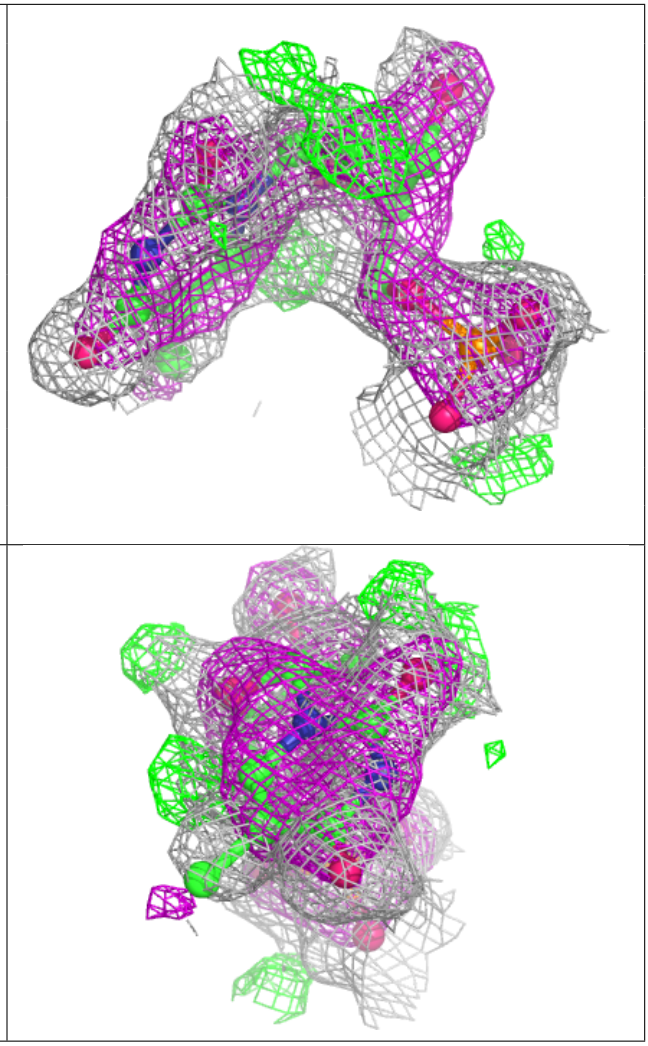






Electron density around TMP A 257:

$2mF_o$-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.