



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:08 AM UTC

PDB ID : 6TRQ / pdb_00006trq
Title : S.c. Scavenger Decapping Enzyme DcpS in complex with the capped RNA dinucleotide m7G-GU
Authors : Fuchs, A.-L.; Neu, A.; Sprangers, R.
Deposited on : 2019-12-19
Resolution : 2.94 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

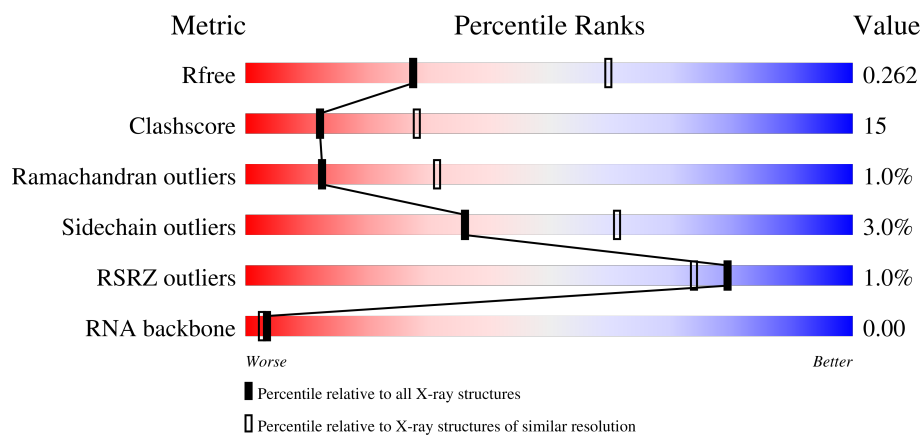
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)
RNA backbone	3983	1018 (3.14-2.74)

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	345	2% 70% 24% • •
1	B	345	67% 24% • 6%
1	C	345	68% 27% • •
1	D	345	2% 68% 23% • 8%

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Mol	Chain	Length	Quality of chain
2	E	2	 100%
2	F	2	 100%

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
2	0G	E	403	X	-	-	-
2	0G	F	403	X	-	-	-
4	2PO	F	501	-	-	X	-
5	M7G	E	502	X	-	-	-
5	M7G	F	502	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10991 atoms, of which 74 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 m7GpppX diphosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	0	0	0
			2722	1748	454	507	13			
1	B	323	Total	C	N	O	S	0	0	0
			2657	1708	443	494	12			
1	C	336	Total	C	N	O	S	0	0	0
			2758	1768	463	514	13			
1	D	318	Total	C	N	O	S	0	0	0
			2616	1684	433	487	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLY	-	expression tag	UNP Q06151
A	7	MET	-	expression tag	UNP Q06151
A	268	ASN	HIS	engineered mutation	UNP Q06151
B	6	GLY	-	expression tag	UNP Q06151
B	7	MET	-	expression tag	UNP Q06151
B	268	ASN	HIS	engineered mutation	UNP Q06151
C	6	GLY	-	expression tag	UNP Q06151
C	7	MET	-	expression tag	UNP Q06151
C	268	ASN	HIS	engineered mutation	UNP Q06151
D	6	GLY	-	expression tag	UNP Q06151
D	7	MET	-	expression tag	UNP Q06151
D	268	ASN	HIS	engineered mutation	UNP Q06151

- Molecule 2 is a RNA chain called Capped RNA dinucleotide.

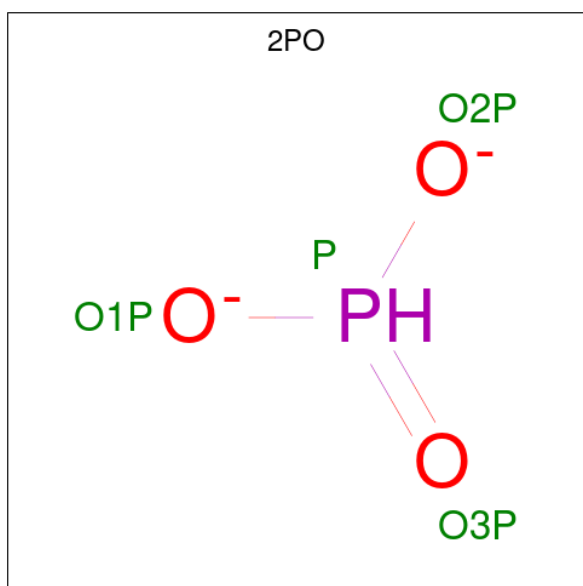
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	2	Total 64	C 19	H 21	N 7	O 15	P 2	0	0	0
2	F	2	Total 64	C 19	H 21	N 7	O 15	P 2	0	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is PHOSPHONATE (CCD ID: 2PO) (formula: HO₃P).



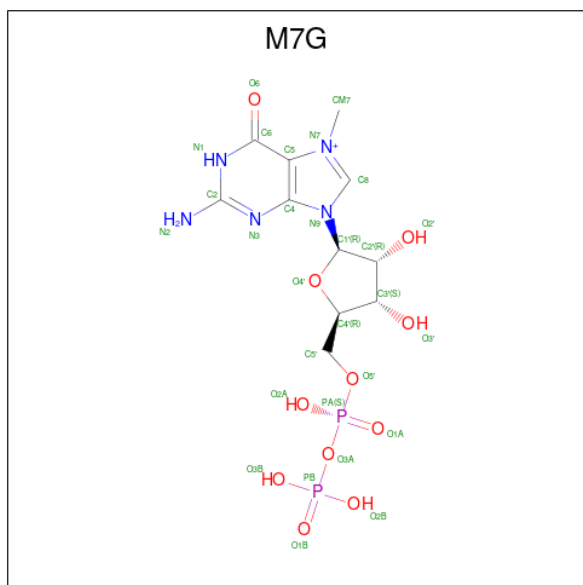
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	P	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	O	P	0	0
			4	3	1		

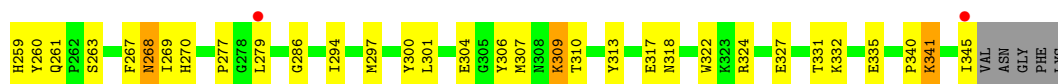
- Molecule 5 is 7N-METHYL-8-HYDROGUANOSINE-5'-DIPHOSPHATE (CCD ID: M7G) (formula: $C_{11}H_{18}N_5O_{11}P_2$).



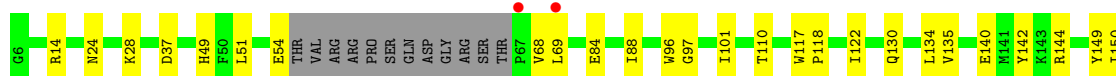
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	E	1	Total	C	H	N	O	P	0	0
			45	11	16	5	11	2		
5	F	1	Total	C	H	N	O	P	0	0
			45	11	16	5	11	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	2	Total	O	0	0
			2	2		



- Molecule 1: m7GpppX diphosphatase



- Molecule 2: Capped RNA dinucleotide



- Molecule 2: Capped RNA dinucleotide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.76Å 104.10Å 189.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.31 – 2.94 47.31 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.31-2.94) 99.7 (47.31-2.94)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.204 , 0.263 0.201 , 0.262	Depositor DCC
R_{free} test set	1872 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	67.1	Xtriage
Anisotropy	0.794	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10991	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: SO4, M7G, 0G, 2PO

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	0.37	0/2784	0.73	3/3773 (0.1%)
1	B	0.32	0/2717	0.63	0/3681
1	C	0.35	0/2821	0.63	0/3822
1	D	0.33	0/2675	0.67	0/3621
2	E	1.56	0/21	3.19	4/30 (13.3%)
2	F	1.47	0/21	2.25	1/30 (3.3%)
All	All	0.35	0/11039	0.69	8/14957 (0.1%)

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
2	E	1	0
2	F	1	0
All	All	2	0

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ARG	NE-CZ-NH1	-11.50	110.00	121.50
1	A	144	ARG	NE-CZ-NH2	9.74	127.97	119.20
2	E	404	U	O4'-C1'-C2'	-9.58	98.02	107.60
1	A	144	ARG	CD-NE-CZ	-9.35	111.32	124.40
2	E	404	U	C3'-C2'-C1'	8.29	109.59	101.30
2	E	404	U	N1-C1'-C2'	7.42	123.13	112.00
2	F	404	U	C4'-C3'-C2'	6.18	108.78	102.60
2	E	404	U	C4'-C3'-O3'	5.75	121.62	113.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	403	0G	C1'
2	F	403	0G	C1'

There are no planarity outliers.

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	2722	0	2693	111	0
1	B	2657	0	2639	101	0
1	C	2758	0	2735	99	0
1	D	2616	0	2597	87	0
2	E	43	21	21	5	0
2	F	43	21	21	8	0
3	D	10	0	0	1	0
4	E	4	0	0	0	0
4	F	4	0	0	3	0
5	E	29	16	16	5	0
5	F	29	16	16	4	0
6	C	2	0	0	0	0
All	All	10917	74	10738	335	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 15.

All (335) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:LYS:HE3	1:D:296:GLU:HG2	1.32	1.10
1:B:173:GLU:HG3	1:D:195:MET:HE3	1.39	1.05
1:D:170:ALA:O	1:D:172:SER:N	1.94	1.00
1:A:297:MET:HE2	1:B:297:MET:HE1	1.46	0.98
1:D:140:GLU:OE2	1:D:144:ARG:NH1	1.96	0.98
1:B:165:ILE:HD13	1:B:170:ALA:HB3	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:MET:HE1	1:A:158:ARG:HD2	1.46	0.94
1:D:282:SER:OG	3:D:401:SO4:O2	1.85	0.93
1:A:297:MET:CE	1:B:297:MET:HE1	1.99	0.92
1:C:335:GLU:HG2	1:C:341:LYS:HE3	1.51	0.90
2:F:404:U:O2'	4:F:501:2PO:O1P	1.89	0.89
1:C:138:THR:HA	1:C:310:THR:HG22	1.54	0.88
1:A:143:LYS:HE3	1:A:307:MET:HE3	1.54	0.87
1:A:296:GLU:OE1	1:B:310:THR:HB	1.76	0.84
1:D:153:MET:HE2	1:D:153:MET:HA	1.58	0.84
1:A:140:GLU:OE2	1:A:144:ARG:NH1	2.11	0.83
1:B:55:THR:HG22	1:B:56:VAL:H	1.45	0.81
1:B:125:LYS:HG2	1:B:126:LYS:H	1.46	0.79
1:D:174:ARG:NH2	1:D:193:PRO:HB2	1.97	0.79
1:A:30:MET:HE2	1:B:52:PHE:CZ	2.18	0.78
1:A:304:GLU:HG2	1:A:308:ASN:ND2	1.99	0.77
1:B:165:ILE:HD13	1:B:170:ALA:CB	2.14	0.77
1:D:154:CYS:O	1:D:160:LYS:HG3	1.85	0.76
1:A:9:ALA:O	1:A:13:LYS:HG3	1.85	0.76
1:D:272:VAL:HG11	1:D:279:LEU:HD11	1.65	0.76
1:C:309:LYS:CE	1:D:296:GLU:HG2	2.15	0.74
1:C:309:LYS:HD2	1:C:310:THR:H	1.53	0.73
1:D:195:MET:SD	1:D:195:MET:N	2.57	0.72
1:D:14:ARG:NH1	1:D:37:ASP:OD2	2.22	0.72
1:D:272:VAL:HG11	1:D:279:LEU:CD1	2.19	0.72
1:A:173:GLU:HG2	1:A:174:ARG:HG2	1.73	0.71
1:D:335:GLU:CG	1:D:341:LYS:HE2	2.22	0.70
1:A:280:GLY:HA2	2:E:404:U:H3'	1.74	0.70
1:A:55:THR:HG23	1:A:68:VAL:HG21	1.75	0.69
1:A:345:ILE:HD13	1:D:51:LEU:HD21	1.73	0.69
1:C:14:ARG:NH1	1:C:37:ASP:OD2	2.25	0.68
1:A:297:MET:CA	1:A:297:MET:HE3	2.22	0.68
1:C:309:LYS:HD2	1:C:310:THR:N	2.08	0.68
1:D:142:TYR:CE2	1:D:307:MET:HE1	2.30	0.66
1:C:143:LYS:HD3	1:C:147:GLN:OE1	1.96	0.66
1:D:142:TYR:HE2	1:D:307:MET:HE1	1.61	0.66
1:B:56:VAL:HG23	1:B:69:LEU:O	1.96	0.66
1:A:84:GLU:CB	1:A:100:VAL:HG12	2.26	0.65
1:A:84:GLU:HB3	1:A:100:VAL:HG12	1.78	0.65
1:D:176:VAL:HG23	1:D:193:PRO:HD3	1.79	0.65
1:A:55:THR:CG2	1:A:68:VAL:HG21	2.27	0.65
1:C:297:MET:SD	1:D:297:MET:HE1	2.37	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:HIS:NE2	1:A:317:GLU:HG3	2.12	0.65
1:D:178:LYS:HA	1:D:190:LEU:HB3	1.79	0.65
1:A:30:MET:HE1	1:B:50:PHE:CB	2.27	0.64
1:A:91:ASN:ND2	1:D:236:LYS:HG2	2.13	0.63
1:A:55:THR:HG23	1:A:68:VAL:CG2	2.28	0.63
1:A:55:THR:OG1	1:A:68:VAL:HG21	1.99	0.63
1:C:216:ILE:HD13	1:C:222:LEU:HD23	1.81	0.63
1:D:335:GLU:HG2	1:D:341:LYS:HE2	1.81	0.63
1:B:213:ARG:HD3	1:B:229:TRP:CH2	2.34	0.63
1:C:309:LYS:NZ	1:D:297:MET:HE2	2.14	0.62
1:D:182:GLU:OE2	1:D:185:LYS:NZ	2.25	0.62
1:A:315:ILE:HD11	1:A:319:HIS:CG	2.34	0.62
1:B:56:VAL:HG23	1:B:69:LEU:HB2	1.82	0.62
1:B:216:ILE:HG22	1:B:267:PHE:HB2	1.81	0.62
1:B:125:LYS:HG2	1:B:126:LYS:N	2.15	0.62
1:B:56:VAL:HG22	1:B:58:ARG:H	1.65	0.61
1:A:342:ILE:HD13	1:B:247:TYR:CD2	2.34	0.61
1:B:173:GLU:CG	1:D:195:MET:HE3	2.25	0.61
1:C:69:LEU:O	1:C:70:TYR:HB2	1.99	0.61
1:A:91:ASN:HD21	1:D:236:LYS:HG2	1.65	0.61
1:D:68:VAL:O	1:D:69:LEU:HG	2.01	0.61
1:C:286:GLY:HA2	1:D:290:LEU:HD11	1.83	0.61
1:A:142:TYR:CE1	1:A:220:ARG:HG3	2.35	0.61
1:D:154:CYS:C	1:D:160:LYS:HG3	2.25	0.61
1:A:149:TYR:CZ	1:A:153:MET:HG3	2.35	0.60
1:B:201:ASN:N	1:B:201:ASN:ND2	2.49	0.60
1:C:263:SER:OG	2:F:403:OG:OP1	2.15	0.60
1:B:327:GLU:O	1:B:331:THR:HG23	2.01	0.60
1:A:345:ILE:CD1	1:D:51:LEU:HD21	2.31	0.60
1:A:315:ILE:HD11	1:A:319:HIS:CD2	2.37	0.60
1:D:216:ILE:HD13	1:D:222:LEU:HD23	1.83	0.60
1:B:149:TYR:HD1	1:B:324:ARG:HH21	1.50	0.59
1:C:105:MET:HE2	1:D:84:GLU:HB3	1.84	0.59
1:A:239:SER:HA	1:B:340:PRO:HD2	1.85	0.59
1:C:7:MET:O	1:C:10:SER:N	2.35	0.59
1:A:270:HIS:CE1	5:E:502:M7G:H5'1	2.38	0.59
1:A:304:GLU:HG2	1:A:308:ASN:HD21	1.66	0.59
1:B:150:ILE:O	1:B:153:MET:HB2	2.03	0.59
1:A:279:LEU:HD13	2:E:403:OG:N2	2.17	0.59
1:C:258:VAL:HG12	1:C:259:HIS:N	2.18	0.59
1:C:114:ASN:ND2	2:F:403:OG:N7	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ILE:HG21	1:D:247:TYR:OH	2.03	0.58
1:A:297:MET:CE	1:A:297:MET:HA	2.31	0.58
1:A:342:ILE:CD1	1:B:247:TYR:HD2	2.16	0.58
1:A:70:TYR:OH	1:A:203:ASP:OD1	2.22	0.58
1:A:194:ASP:OD1	5:E:502:M7G:O2'	2.19	0.58
1:D:68:VAL:O	1:D:68:VAL:HG23	2.04	0.58
1:A:14:ARG:NH1	1:A:37:ASP:OD2	2.37	0.58
1:B:55:THR:HG22	1:B:56:VAL:N	2.19	0.57
1:B:125:LYS:O	1:B:127:TYR:N	2.33	0.57
1:A:342:ILE:HD13	1:B:247:TYR:HD2	1.69	0.57
1:B:189:PHE:C	1:B:212:TYR:HE1	2.12	0.57
1:A:89:THR:HB	1:C:340:PRO:HG3	1.86	0.57
1:B:84:GLU:CB	1:B:100:VAL:HG12	2.35	0.57
1:C:174:ARG:NH2	1:C:193:PRO:HB2	2.19	0.57
1:B:142:TYR:HE2	1:B:307:MET:HE1	1.70	0.56
1:C:177:TYR:CE2	1:C:179:ASP:HB2	2.40	0.56
1:A:30:MET:CE	1:B:50:PHE:HB2	2.35	0.56
1:A:344:LYS:O	1:A:344:LYS:HG3	2.04	0.56
1:A:297:MET:HE3	1:A:297:MET:HA	1.88	0.56
1:C:194:ASP:OD2	5:F:502:M7G:H2'	2.05	0.56
1:B:54:GLU:O	1:B:54:GLU:HG2	2.04	0.56
1:B:189:PHE:HE2	1:B:191:ILE:HD11	1.71	0.56
1:B:201:ASN:N	1:D:201:ASN:HD22	2.04	0.56
1:A:30:MET:HE1	1:B:50:PHE:HB3	1.87	0.56
1:C:190:LEU:HD12	1:C:190:LEU:C	2.32	0.55
1:D:161:TRP:H	1:D:161:TRP:CD1	2.23	0.55
1:B:57:ARG:HB3	1:B:71:ASN:ND2	2.21	0.55
1:B:142:TYR:CE2	1:B:307:MET:HE1	2.40	0.55
1:C:202:LEU:HD21	1:C:248:ALA:HB3	1.88	0.55
1:C:125:LYS:HB3	1:C:318:ASN:HB3	1.88	0.55
1:A:142:TYR:HE2	1:A:307:MET:HE1	1.72	0.55
1:A:297:MET:HE3	1:A:297:MET:O	2.07	0.55
1:C:322:TRP:CE2	1:C:327:GLU:HB2	2.42	0.55
1:A:194:ASP:OD1	1:A:195:MET:N	2.40	0.55
1:C:68:VAL:HG12	1:C:68:VAL:O	2.07	0.54
1:C:300:TYR:HB3	1:D:300:TYR:HB3	1.88	0.54
1:C:158:ARG:HG2	1:C:158:ARG:HH11	1.73	0.54
1:A:189:PHE:HE1	1:A:236:LYS:HD3	1.72	0.54
1:C:223:ARG:NH1	1:C:304:GLU:HA	2.22	0.54
1:B:84:GLU:HB3	1:B:100:VAL:HG12	1.88	0.54
1:A:158:ARG:HG3	1:A:158:ARG:HH11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ARG:CZ	1:A:311:ILE:HD12	2.38	0.53
1:C:110:THR:HG21	1:D:101:ILE:HB	1.90	0.53
1:C:62:ASP:OD1	1:C:62:ASP:N	2.41	0.53
1:D:122:ILE:HD12	1:D:122:ILE:H	1.73	0.53
1:A:216:ILE:HD13	1:A:222:LEU:CD2	2.39	0.53
1:A:304:GLU:HG2	1:A:308:ASN:CG	2.34	0.52
1:B:165:ILE:CD1	1:B:171:GLU:HG3	2.40	0.52
1:C:239:SER:HA	1:D:340:PRO:HD2	1.91	0.52
1:B:190:LEU:C	1:B:190:LEU:HD12	2.35	0.52
1:C:268:ASN:C	1:C:268:ASN:HD22	2.13	0.52
1:A:297:MET:HE2	1:B:297:MET:CE	2.30	0.52
1:C:133:HIS:NE2	1:C:317:GLU:HG3	2.25	0.52
1:C:79:ILE:HB	1:C:82:ILE:CD1	2.40	0.51
1:C:309:LYS:HZ3	1:D:297:MET:HE2	1.74	0.51
1:B:195:MET:SD	1:D:173:GLU:HG3	2.50	0.51
1:C:261:GLN:HG2	1:C:313:TYR:CE2	2.45	0.51
1:A:190:LEU:HD12	1:A:190:LEU:C	2.35	0.51
1:C:270:HIS:CE1	5:F:502:M7G:H5'1	2.45	0.51
1:C:304:GLU:OE2	1:C:304:GLU:N	2.40	0.51
1:A:103:GLN:HB3	1:B:100:VAL:HG23	1.92	0.51
1:A:177:TYR:CD1	1:A:240:ILE:HD13	2.46	0.51
1:B:56:VAL:CG2	1:B:69:LEU:HB2	2.40	0.51
1:A:229:TRP:CZ2	1:A:233:LEU:HD11	2.46	0.51
1:C:279:LEU:HD22	2:F:403:OG:N2	2.26	0.50
1:B:124:ILE:C	1:B:125:LYS:O	2.52	0.50
1:A:153:MET:HE1	1:A:158:ARG:CD	2.30	0.50
1:A:143:LYS:CE	1:A:307:MET:HE3	2.35	0.50
1:C:28:LYS:HD2	1:C:28:LYS:N	2.26	0.50
1:D:135:VAL:HG23	1:D:315:ILE:HG22	1.94	0.50
1:D:192:LEU:C	1:D:192:LEU:HD12	2.37	0.50
1:A:297:MET:CE	1:B:297:MET:CE	2.82	0.50
1:A:180:PHE:CE2	1:A:182:GLU:HG3	2.46	0.50
1:C:297:MET:SD	1:D:297:MET:SD	3.10	0.49
1:D:122:ILE:HD12	1:D:122:ILE:N	2.28	0.49
1:A:30:MET:CE	1:B:50:PHE:CB	2.90	0.49
1:B:125:LYS:C	1:B:127:TYR:H	2.19	0.49
1:B:129:GLN:OE1	1:B:129:GLN:HA	2.12	0.49
1:B:272:VAL:HG11	1:B:279:LEU:HD11	1.95	0.49
1:C:56:VAL:HA	1:C:67:PRO:HA	1.94	0.49
1:C:193:PRO:HA	1:C:207:LEU:HD23	1.95	0.49
1:A:48:THR:O	1:B:47:LYS:HE3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:ILE:HD11	1:D:171:GLU:CG	2.42	0.49
1:B:122:ILE:HD12	1:B:122:ILE:H	1.78	0.49
1:C:149:TYR:CZ	1:C:153:MET:HG3	2.47	0.49
1:D:166:LEU:HD21	1:D:210:ILE:HG22	1.95	0.49
1:A:220:ARG:NH1	1:A:309:LYS:O	2.41	0.48
1:B:125:LYS:CG	1:B:126:LYS:H	2.21	0.48
1:C:6:GLY:O	1:C:7:MET:HB3	2.13	0.48
1:A:133:HIS:CD2	1:A:317:GLU:HG3	2.49	0.48
1:A:179:ASP:O	1:A:188:GLY:HA3	2.13	0.48
1:B:144:ARG:NH2	1:B:329:GLU:OE2	2.41	0.48
1:B:189:PHE:HA	1:B:212:TYR:CD1	2.47	0.48
1:C:133:HIS:CD2	1:C:317:GLU:HG3	2.49	0.48
1:A:141:MET:SD	1:A:329:GLU:HG2	2.54	0.48
1:A:216:ILE:HD13	1:A:222:LEU:HD23	1.95	0.48
1:B:51:LEU:HD21	1:C:345:ILE:CD1	2.43	0.48
1:A:28:LYS:HE2	1:B:47:LYS:O	2.14	0.48
1:C:24:ASN:OD1	1:C:26:GLN:HB2	2.14	0.48
1:C:126:LYS:HZ3	1:C:263:SER:CB	2.26	0.48
1:A:252:ASP:CB	1:B:330:LEU:HD21	2.44	0.48
1:C:6:GLY:O	1:C:7:MET:CB	2.61	0.48
1:D:130:GLN:OE1	1:D:318:ASN:HB2	2.14	0.48
1:B:142:TYR:CE1	1:B:220:ARG:HG3	2.49	0.48
1:B:236:LYS:HE2	1:C:91:ASN:HD21	1.78	0.48
1:D:153:MET:HA	1:D:153:MET:CE	2.37	0.48
1:C:126:LYS:NZ	1:C:263:SER:HB3	2.29	0.48
1:A:300:TYR:HB3	1:B:300:TYR:HB3	1.94	0.47
1:C:101:ILE:HB	1:D:110:THR:HG21	1.96	0.47
1:A:149:TYR:CE1	1:A:153:MET:HG3	2.49	0.47
1:A:345:ILE:CG2	1:A:346:VAL:HG23	2.44	0.47
1:C:158:ARG:HG2	1:C:158:ARG:NH1	2.30	0.47
1:C:8:PHE:CE2	1:D:97:GLY:HA3	2.49	0.47
1:C:53:ASP:OD2	1:C:71:ASN:HB3	2.14	0.47
1:A:35:THR:HA	1:A:39:LYS:O	2.15	0.47
1:B:161:TRP:O	1:B:164:ASN:HB2	2.14	0.47
1:D:142:TYR:CE1	1:D:220:ARG:HG3	2.50	0.47
1:D:149:TYR:HD1	1:D:324:ARG:NH1	2.12	0.47
1:B:66:THR:O	1:B:69:LEU:HG	2.15	0.47
1:C:137:GLU:OE1	1:C:260:TYR:OH	2.24	0.47
1:A:189:PHE:CE1	1:A:236:LYS:HD3	2.50	0.46
1:D:170:ALA:C	1:D:172:SER:N	2.71	0.46
1:A:64:ARG:NH2	1:B:342:ILE:HD13	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:PHE:HE1	1:B:236:LYS:HD3	1.79	0.46
1:C:9:ALA:O	1:C:13:LYS:HG2	2.15	0.46
1:B:7:MET:HE3	1:B:11:LEU:HG	1.97	0.46
1:C:7:MET:O	1:C:8:PHE:C	2.58	0.46
1:A:193:PRO:HA	1:A:207:LEU:HD23	1.97	0.46
1:D:165:ILE:HD11	1:D:171:GLU:CD	2.39	0.46
1:D:272:VAL:CG1	1:D:279:LEU:HD11	2.39	0.46
1:B:15:PHE:CZ	1:B:34:GLY:HA3	2.51	0.46
1:B:122:ILE:HD12	1:B:122:ILE:N	2.31	0.46
1:D:192:LEU:HD12	1:D:193:PRO:O	2.15	0.46
1:A:126:LYS:NZ	1:A:263:SER:OG	2.49	0.46
1:A:346:VAL:HG11	1:B:246:ASN:O	2.16	0.45
1:C:250:HIS:HB3	1:C:251:PRO:HD2	1.97	0.45
1:C:258:VAL:HG12	1:C:259:HIS:H	1.81	0.45
1:D:28:LYS:HD2	1:D:28:LYS:N	2.32	0.45
1:D:194:ASP:O	1:D:195:MET:C	2.59	0.45
1:B:189:PHE:HA	1:B:212:TYR:HD1	1.80	0.45
1:C:297:MET:CE	1:D:297:MET:HE1	2.47	0.45
1:D:88:ILE:HG13	1:D:97:GLY:HA2	1.98	0.45
1:A:270:HIS:CE1	5:E:502:M7G:C5'	2.99	0.45
1:D:142:TYR:CD1	1:D:220:ARG:HG3	2.51	0.45
1:A:297:MET:SD	1:B:297:MET:SD	3.15	0.45
1:C:16:GLN:HA	1:C:16:GLN:OE1	2.17	0.45
1:C:286:GLY:CA	1:D:290:LEU:HD11	2.46	0.45
2:E:404:U:C6	2:E:404:U:H5''	2.51	0.45
1:C:195:MET:HG3	1:D:96:TRP:CD2	2.51	0.45
1:A:286:GLY:HA2	1:B:290:LEU:HD11	1.99	0.45
1:B:134:LEU:HD23	1:B:134:LEU:HA	1.62	0.45
1:C:153:MET:C	1:C:155:ASN:H	2.25	0.45
1:C:294:ILE:HD13	1:C:306:TYR:OH	2.16	0.45
1:A:48:THR:O	1:B:47:LYS:HG3	2.17	0.45
1:B:149:TYR:HA	1:B:324:ARG:NH2	2.32	0.45
1:B:192:LEU:HD12	1:B:193:PRO:O	2.16	0.45
1:D:134:LEU:HD23	1:D:134:LEU:HA	1.68	0.45
1:A:321:LEU:HA	1:A:324:ARG:HB2	2.00	0.44
1:A:84:GLU:CB	1:A:100:VAL:CG1	2.94	0.44
1:B:165:ILE:HD11	1:B:171:GLU:HG3	1.99	0.44
2:F:404:U:O2'	4:F:501:2PO:P	2.74	0.44
1:C:216:ILE:HD13	1:C:222:LEU:CD2	2.46	0.44
1:C:270:HIS:CE1	5:F:502:M7G:C5'	3.00	0.44
1:D:117:TRP:HA	1:D:118:PRO:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:GLU:O	1:D:296:GLU:HG3	2.15	0.44
1:D:150:ILE:HG21	1:D:217:LYS:HD3	2.00	0.44
1:A:55:THR:CB	1:A:68:VAL:HG21	2.47	0.44
1:C:28:LYS:HA	1:D:49:HIS:ND1	2.33	0.44
2:F:404:U:HO2'	4:F:501:2PO:P	2.29	0.44
1:C:209:ALA:HB3	1:C:269:ILE:HB	2.00	0.44
1:A:345:ILE:HG22	1:A:346:VAL:HG23	2.00	0.44
1:D:177:TYR:O	1:D:178:LYS:HB3	2.18	0.44
1:A:194:ASP:OD1	5:E:502:M7G:C2'	2.66	0.43
1:A:297:MET:HE3	1:A:297:MET:C	2.42	0.43
5:E:502:M7G:PB	5:E:502:M7G:H5'2	2.58	0.43
1:A:30:MET:HE2	1:B:52:PHE:HZ	1.75	0.43
1:D:178:LYS:HA	1:D:190:LEU:CB	2.46	0.43
1:C:301:LEU:HD13	1:C:306:TYR:HA	2.00	0.43
1:A:114:ASN:ND2	2:E:403:OG:N7	2.66	0.43
1:A:136:ARG:O	1:A:333:GLN:NE2	2.35	0.43
1:B:203:ASP:HA	1:B:273:ASN:ND2	2.33	0.43
1:A:342:ILE:CD1	1:B:247:TYR:CD2	2.98	0.43
1:A:84:GLU:HB3	1:B:105:MET:HE2	2.00	0.43
1:A:345:ILE:HD13	1:D:51:LEU:CD2	2.45	0.43
1:B:125:LYS:C	1:B:127:TYR:N	2.76	0.43
1:B:147:GLN:HB3	1:B:148:PRO:HD3	2.00	0.43
1:C:79:ILE:HB	1:C:82:ILE:HD12	2.01	0.43
1:B:257:LEU:CD1	1:B:259:HIS:HE1	2.32	0.43
1:C:53:ASP:OD1	1:C:77:SER:OG	2.29	0.43
2:F:403:OG:H2'	2:F:403:OG:N3	2.34	0.43
1:C:173:GLU:HG2	1:C:174:ARG:HG2	2.00	0.43
1:D:261:GLN:O	1:D:287:LYS:NZ	2.41	0.43
1:A:30:MET:HE3	1:A:30:MET:HB2	1.68	0.42
1:C:7:MET:O	1:C:9:ALA:N	2.51	0.42
1:B:180:PHE:H	1:C:92:ASP:CG	2.26	0.42
1:A:292:GLU:OE2	1:B:136:ARG:HD3	2.19	0.42
1:B:142:TYR:CD1	1:B:146:VAL:HB	2.54	0.42
1:C:252:ASP:CB	1:D:330:LEU:HD21	2.48	0.42
1:A:279:LEU:HD13	2:E:403:OG:C2	2.49	0.42
1:C:126:LYS:HZ1	1:C:263:SER:HB3	1.84	0.42
1:C:154:CYS:SG	1:C:217:LYS:HD2	2.60	0.42
1:C:247:TYR:CD2	1:D:342:ILE:HD11	2.53	0.42
1:C:277:PRO:HG2	1:D:24:ASN:OD1	2.18	0.42
1:C:297:MET:SD	1:D:297:MET:CE	3.07	0.42
1:D:165:ILE:HD13	1:D:170:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ASP:HB3	1:D:330:LEU:HD21	2.00	0.42
1:D:185:LYS:HG2	1:D:186:ASP:OD1	2.19	0.42
1:D:216:ILE:HD13	1:D:222:LEU:CD2	2.50	0.42
1:B:192:LEU:HD12	1:B:192:LEU:C	2.44	0.42
1:A:153:MET:HE3	1:A:153:MET:HB3	1.87	0.42
1:B:236:LYS:HE2	1:C:91:ASN:OD1	2.19	0.42
1:B:343:PRO:O	1:B:344:LYS:C	2.62	0.42
1:C:331:THR:O	1:C:335:GLU:HG3	2.18	0.42
1:A:261:GLN:HG2	1:A:313:TYR:CE2	2.55	0.42
1:C:213:ARG:HD3	1:C:229:TRP:CZ2	2.55	0.42
1:A:30:MET:HE1	1:B:50:PHE:HB2	1.94	0.41
1:A:158:ARG:HH11	1:A:158:ARG:CG	2.33	0.41
1:A:84:GLU:HB2	1:A:100:VAL:CG1	2.49	0.41
1:A:153:MET:CE	1:A:158:ARG:HD2	2.34	0.41
1:A:341:LYS:O	1:A:342:ILE:O	2.38	0.41
1:B:85:LEU:HD23	1:B:99:SER:HB3	2.01	0.41
1:C:332:LYS:HD2	1:C:332:LYS:HA	1.80	0.41
1:D:301:LEU:HB3	1:D:305:GLY:O	2.21	0.41
1:C:155:ASN:C	1:C:157:GLY:N	2.78	0.41
1:D:54:GLU:O	1:D:54:GLU:HG2	2.19	0.41
1:C:309:LYS:HE2	1:C:310:THR:O	2.20	0.41
1:A:93:ILE:HD11	1:B:123:HIS:CE1	2.55	0.41
1:B:51:LEU:HD21	1:C:345:ILE:HD12	2.01	0.41
1:A:20:VAL:O	1:B:68:VAL:HA	2.20	0.41
1:C:335:GLU:HG2	1:C:341:LYS:CE	2.35	0.41
1:B:57:ARG:HH22	1:B:58:ARG:NH1	2.19	0.41
1:B:173:GLU:HG2	1:B:174:ARG:HG2	2.02	0.41
1:B:201:ASN:N	1:B:201:ASN:HD22	2.19	0.41
1:C:64:ARG:H	1:C:64:ARG:HG2	1.63	0.41
1:C:196:LYS:HE2	2:F:403:OG:H5'	2.01	0.41
1:D:150:ILE:CG2	1:D:217:LYS:HD3	2.50	0.41
1:D:169:GLY:O	1:D:170:ALA:O	2.39	0.41
1:B:252:ASP:OD1	1:B:252:ASP:N	2.54	0.41
1:A:277:PRO:O	1:A:283:ILE:HD11	2.21	0.40
1:D:229:TRP:CZ2	1:D:233:LEU:HD11	2.56	0.40
1:B:260:TYR:HA	1:B:261:GLN:HA	1.85	0.40
1:C:297:MET:HE3	1:C:297:MET:HB3	1.78	0.40
1:B:130:GLN:OE1	1:B:318:ASN:HB2	2.21	0.40
1:C:194:ASP:CG	5:F:502:M7G:H2'	2.46	0.40
1:A:250:HIS:HB3	1:A:251:PRO:HD2	2.02	0.40
1:A:260:TYR:CZ	1:A:261:GLN:NE2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ILE:HG22	1:C:267:PHE:HB2	2.03	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	326/345 (94%)	312 (96%)	12 (4%)	2 (1%)	21	45
1	B	315/345 (91%)	302 (96%)	11 (4%)	2 (1%)	21	45
1	C	332/345 (96%)	315 (95%)	14 (4%)	3 (1%)	14	34
1	D	310/345 (90%)	292 (94%)	12 (4%)	6 (2%)	6	17
All	All	1283/1380 (93%)	1221 (95%)	49 (4%)	13 (1%)	12	31

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	125	LYS
1	C	7	MET
1	C	8	PHE
1	D	162	VAL
1	D	170	ALA
1	D	171	GLU
1	D	195	MET
1	D	343	PRO
1	A	342	ILE
1	D	178	LYS
1	B	343	PRO
1	C	70	TYR
1	A	155	ASN

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	302/314 (96%)	294 (97%)	8 (3%)	40	65
1	B	296/314 (94%)	286 (97%)	10 (3%)	32	58
1	C	306/314 (98%)	293 (96%)	13 (4%)	26	52
1	D	291/314 (93%)	286 (98%)	5 (2%)	53	73
All	All	1195/1256 (95%)	1159 (97%)	36 (3%)	36	61

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	THR
1	A	66	THR
1	A	68	VAL
1	A	158	ARG
1	A	182	GLU
1	A	296	GLU
1	A	304	GLU
1	A	345	ILE
1	B	56	VAL
1	B	57	ARG
1	B	69	LEU
1	B	160	LYS
1	B	183	GLU
1	B	195	MET
1	B	201	ASN
1	B	315	ILE
1	B	324	ARG
1	B	344	LYS
1	C	56	VAL
1	C	62	ASP
1	C	64	ARG
1	C	66	THR
1	C	68	VAL
1	C	140	GLU

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Mol	Chain	Res	Type
1	C	154	CYS
1	C	186	ASP
1	C	268	ASN
1	C	307	MET
1	C	309	LYS
1	C	324	ARG
1	C	341	LYS
1	D	152	GLU
1	D	153	MET
1	D	195	MET
1	D	196	LYS
1	D	328	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
1	A	268	ASN
1	A	318	ASN
1	B	38	ASN
1	B	114	ASN
1	B	147	GLN
1	B	201	ASN
1	B	268	ASN
1	D	103	GLN
1	D	234	ASN
1	D	250	HIS
1	D	268	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	0/2	-	-
2	F	0/2	-	-
All	All	0/4	-	-

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	0G	F	403	2,5	22,25,26	1.14	3 (13%)	32,37,40	2.28	14 (43%)
2	0G	E	403	2,5	22,25,26	1.36	3 (13%)	32,37,40	2.55	15 (46%)

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
2	0G	F	403	2,5	1/1/5/5	1/7/25/26	0/3/3/3
2	0G	E	403	2,5	1/1/5/5	3/7/25/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	403	0G	C5-C4	2.91	1.46	1.38
2	F	403	0G	C5-C4	2.79	1.46	1.38
2	E	403	0G	C6-N1	-2.42	1.34	1.38
2	F	403	0G	C4-N9	-2.20	1.32	1.38
2	E	403	0G	O4'-C1'	2.16	1.47	1.42
2	F	403	0G	C6-N1	-2.15	1.34	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	403	0G	C5'-C4'-C3'	5.34	134.45	115.21
2	E	403	0G	C5-C4-N3	-5.33	119.90	128.39
2	F	403	0G	C5-C4-N3	-4.58	121.09	128.39
2	F	403	0G	C2-N3-C4	4.43	119.93	112.30
2	E	403	0G	C2'-C1'-N9	4.40	125.51	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	403	0G	C2-N3-C4	4.37	119.83	112.30
2	F	403	0G	C6-C5-N7	4.15	137.84	130.29
2	E	403	0G	N9-C4-N3	3.95	133.85	125.95
2	F	403	0G	O4'-C1'-N9	3.92	117.24	108.36
2	E	403	0G	C6-C5-N7	3.77	137.15	130.29
2	F	403	0G	O4'-C1'-C2'	-3.25	99.66	106.62
2	F	403	0G	N9-C4-N3	3.21	132.38	125.95
2	E	403	0G	C3'-C2'-C1'	-3.16	95.48	101.46
2	E	403	0G	C4-C5-N7	-2.94	106.01	110.67
2	E	403	0G	O4'-C1'-C2'	-2.89	100.42	106.62
2	F	403	0G	C4-C5-N7	-2.82	106.21	110.67
2	F	403	0G	C4'-O4'-C1'	-2.62	103.69	109.47
2	E	403	0G	C8-N7-C5	2.61	108.91	104.26
2	E	403	0G	O4'-C4'-C3'	-2.55	100.10	105.15
2	E	403	0G	C2'-C3'-C4'	2.35	107.14	102.61
2	E	403	0G	N9-C8-N7	-2.31	109.12	113.40
2	F	403	0G	O6-C6-C5	-2.28	120.50	126.53
2	F	403	0G	N9-C8-N7	-2.24	109.24	113.40
2	F	403	0G	C8-N7-C5	2.22	108.21	104.26
2	E	403	0G	O6-C6-C5	-2.20	120.73	126.53
2	F	403	0G	C5'-C4'-C3'	2.20	123.12	115.21
2	E	403	0G	C1'-N9-C4	-2.15	120.12	126.49
2	F	403	0G	C1'-N9-C4	-2.14	120.16	126.49
2	F	403	0G	O4'-C4'-C5'	-2.02	102.86	109.33

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	403	0G	C1'
2	F	403	0G	C1'

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	403	0G	C4'-C5'-O5'-P
2	E	403	0G	O4'-C4'-C5'-O5'
2	E	403	0G	C3'-C4'-C5'-O5'
2	F	403	0G	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	403	0G	5	0
2	E	403	0G	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	401	-	4,4,4	0.14	0	6,6,6	0.40	0
4	2PO	E	501	2	0,3,3	-	-	0,3,3	-	-
5	M7G	E	502	2	30,31,31	2.33	8 (26%)	47,49,49	2.92	20 (42%)
3	SO4	D	402	-	4,4,4	0.21	0	6,6,6	0.26	0
4	2PO	F	501	2	0,3,3	-	-	0,3,3	-	-
5	M7G	F	502	2	30,31,31	2.29	5 (16%)	47,49,49	2.58	14 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	M7G	F	502	2	3/3/6/6	6/16/32/32	0/3/3/3
5	M7G	E	502	2	3/3/6/6	7/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	502	M7G	C8-N7	8.79	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	502	M7G	C8-N7	8.48	1.47	1.33
5	F	502	M7G	C8-N9	4.62	1.48	1.35
5	E	502	M7G	C8-N9	4.44	1.47	1.35
5	E	502	M7G	C5-N7	-4.13	1.34	1.39
5	E	502	M7G	PA-O3A	3.94	1.63	1.59
5	F	502	M7G	C5-C4	3.92	1.48	1.38
5	F	502	M7G	C5-N7	-3.89	1.34	1.39
5	E	502	M7G	C5-C4	3.69	1.47	1.38
5	F	502	M7G	C5-C6	2.28	1.49	1.43
5	E	502	M7G	C5-C6	2.18	1.49	1.43
5	E	502	M7G	C6-N1	-2.13	1.34	1.38
5	E	502	M7G	PB-O3B	2.05	1.62	1.54

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	502	M7G	CM7-N7-C8	-7.68	113.16	124.79
5	E	502	M7G	C8-N7-C5	7.23	116.83	107.78
5	F	502	M7G	CM7-N7-C8	-7.23	113.85	124.79
5	E	502	M7G	N9-C8-N7	-6.77	96.05	112.48
5	F	502	M7G	N9-C8-N7	-6.73	96.14	112.48
5	F	502	M7G	C8-N7-C5	6.69	116.15	107.78
5	E	502	M7G	C5-C4-N3	-6.06	116.69	128.15
5	E	502	M7G	N9-C4-N3	5.90	137.75	125.95
5	F	502	M7G	N9-C4-N3	5.87	137.70	125.95
5	F	502	M7G	C5-C4-N3	-5.80	117.19	128.15
5	E	502	M7G	C2-N3-C4	5.46	121.70	112.30
5	F	502	M7G	C2-N3-C4	5.28	121.39	112.30
5	E	502	M7G	O2A-PA-O3A	4.34	119.01	107.27
5	E	502	M7G	C2'-C1'-N9	4.13	124.76	113.25
5	F	502	M7G	C8-N9-C4	3.83	116.58	107.09
5	E	502	M7G	C8-N9-C4	3.66	116.14	107.09
5	E	502	M7G	O3A-PA-O1A	-2.90	101.97	110.70
5	F	502	M7G	C1'-N9-C8	-2.79	117.31	126.74
5	E	502	M7G	O4'-C4'-C3'	2.71	110.54	105.15
5	E	502	M7G	O6-C6-C5	-2.64	122.13	128.01
5	E	502	M7G	CM7-N7-C5	2.58	130.01	126.80
5	F	502	M7G	CM7-N7-C5	2.57	130.01	126.80
5	E	502	M7G	O3B-PB-O3A	2.46	112.89	104.64
5	F	502	M7G	O3'-C3'-C2'	-2.44	103.99	111.82
5	F	502	M7G	O4'-C4'-C3'	2.40	109.92	105.15
5	F	502	M7G	C5-C6-N1	2.40	116.79	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	502	M7G	C5-C6-N1	2.25	116.49	111.84
5	E	502	M7G	C6-C5-N7	2.25	134.99	132.17
5	E	502	M7G	O4'-C1'-N9	-2.22	103.33	108.36
5	F	502	M7G	C6-C5-N7	2.21	134.94	132.17
5	F	502	M7G	O6-C6-C5	-2.17	123.18	128.01
5	E	502	M7G	C1'-N9-C8	-2.16	119.43	126.74
5	E	502	M7G	O3'-C3'-C2'	-2.08	105.14	111.82
5	E	502	M7G	C3'-C2'-C1'	2.02	105.28	101.46

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	502	M7G	C3'
5	E	502	M7G	C4'
5	E	502	M7G	C2'
5	F	502	M7G	C3'
5	F	502	M7G	C4'
5	F	502	M7G	C2'

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	502	M7G	C5'-O5'-PA-O1A
5	E	502	M7G	C5'-O5'-PA-O3A
5	E	502	M7G	PA-O3A-PB-O3B
5	F	502	M7G	C5'-O5'-PA-O3A
5	E	502	M7G	C3'-C4'-C5'-O5'
5	E	502	M7G	C5'-O5'-PA-O2A
5	F	502	M7G	C5'-O5'-PA-O1A
5	F	502	M7G	C4'-C5'-O5'-PA
5	F	502	M7G	PA-O3A-PB-O1B
5	E	502	M7G	PA-O3A-PB-O2B
5	F	502	M7G	PA-O3A-PB-O2B
5	F	502	M7G	PA-O3A-PB-O3B
5	E	502	M7G	C4'-C5'-O5'-PA

There are no ring outliers.

4 monomers are involved in 13 short contacts:

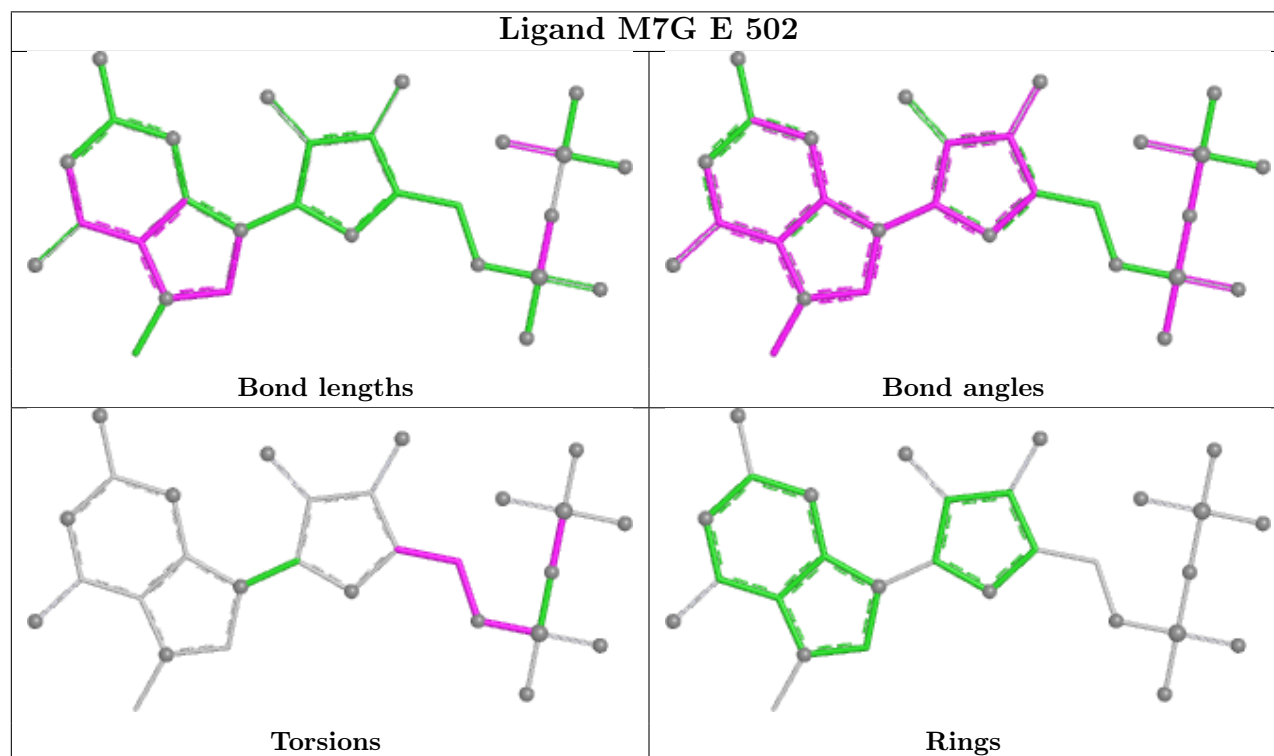
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	SO4	1	0

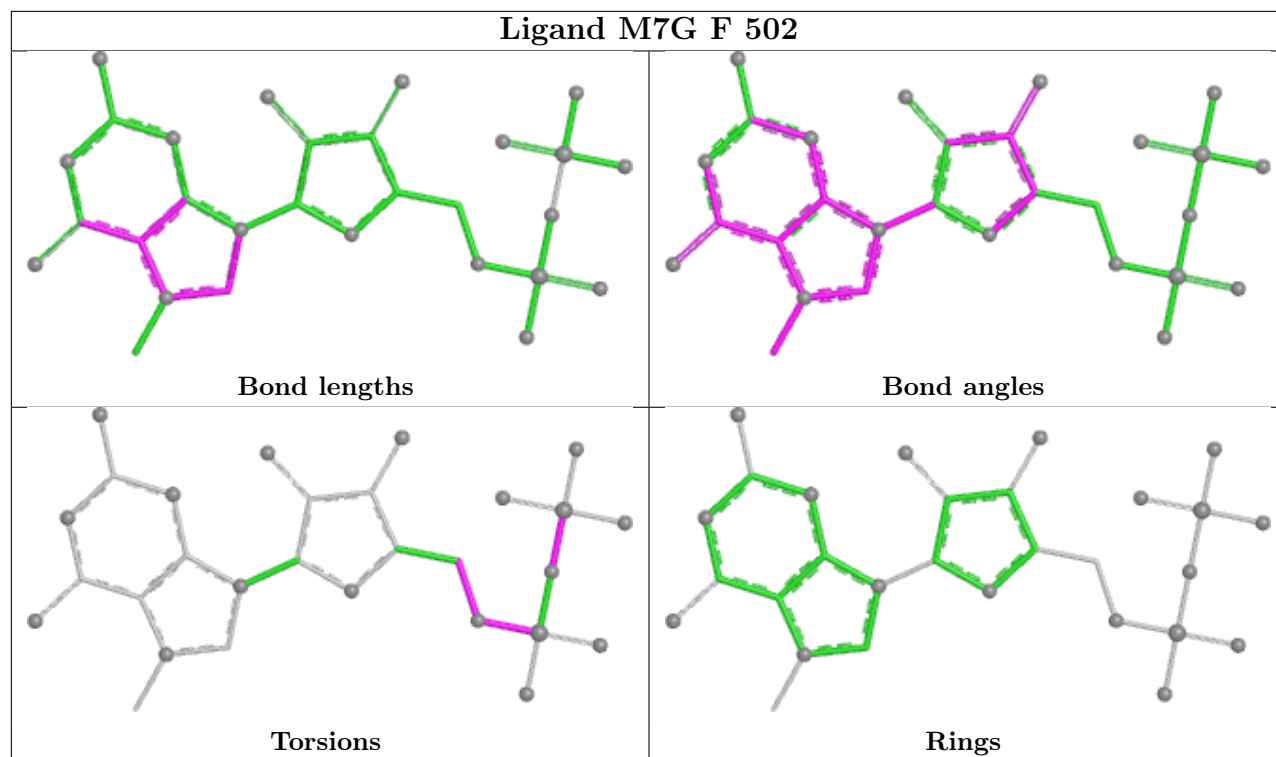
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	502	M7G	5	0
4	F	501	2PO	3	0
5	F	502	M7G	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	332/345 (96%)	-0.40	2 (0%) 85 81	44, 69, 115, 152	0
1	B	323/345 (93%)	-0.33	2 (0%) 85 81	44, 75, 121, 146	0
1	C	336/345 (97%)	-0.26	3 (0%) 81 75	45, 81, 126, 161	0
1	D	318/345 (92%)	-0.14	6 (1%) 66 58	49, 87, 138, 167	0
2	E	1/2 (50%)	-0.09	0 100 100	116, 116, 116, 116	0
2	F	1/2 (50%)	-0.93	0 100 100	104, 104, 104, 104	0
All	All	1311/1384 (94%)	-0.28	13 (0%) 79 74	44, 77, 127, 167	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	LEU	3.6
1	D	67	PRO	3.3
1	C	279	LEU	2.8
1	D	69	LEU	2.7
1	C	345	ILE	2.6
1	B	59	PRO	2.6
1	C	6	GLY	2.5
1	D	196	LYS	2.4
1	D	154	CYS	2.3
1	D	341	LYS	2.2
1	B	154	CYS	2.2
1	D	161	TRP	2.2
1	A	346	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	OG	F	403	23/24	0.91	0.10	65,107,130,138	0
2	OG	E	403	23/24	0.92	0.09	63,97,126,131	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

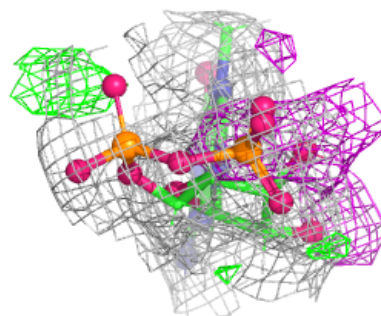
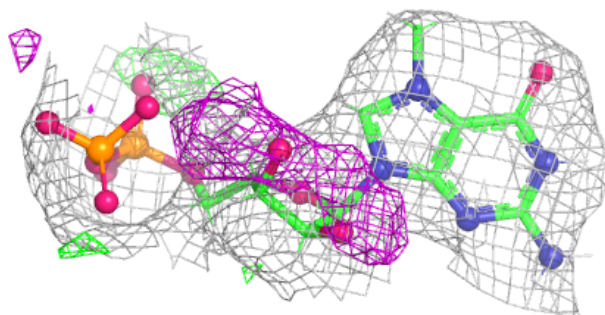
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	D	401	5/5	0.85	0.12	92,95,108,111	0
3	SO4	D	402	5/5	0.86	0.16	112,120,124,136	0
4	2PO	E	501	4/4	0.91	0.12	137,142,143,145	0
4	2PO	F	501	4/4	0.91	0.10	103,109,111,116	0
5	M7G	E	502	29/29	0.93	0.08	43,60,91,129	0
5	M7G	F	502	29/29	0.93	0.09	43,88,113,128	0

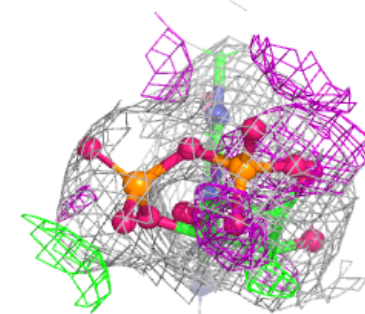
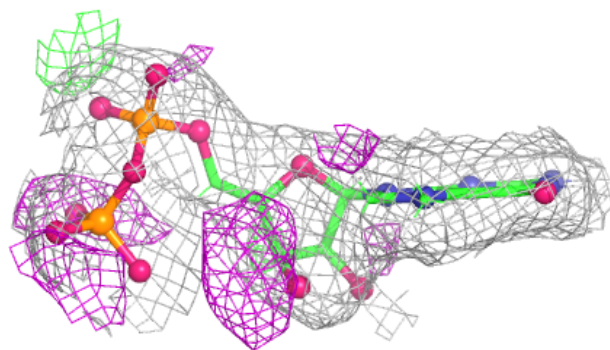
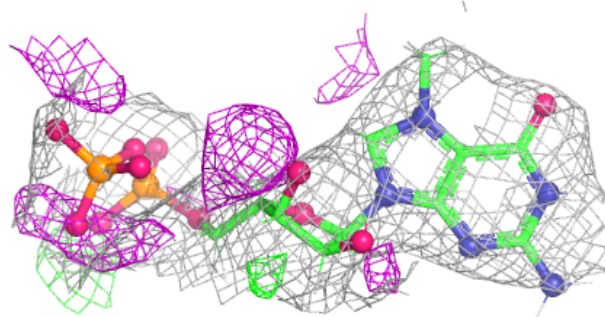
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around M7G E 502:

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

**Electron density around M7G F 502:**

$2mF_o-DF_c$ (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.