



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 07:05 am BST

PDB ID : 6SCX
Title : Crystal structure of the catalytic domain of human NUDT12 in complex with 7-methyl-guanosine-5'-triphosphate
Authors : McCarthy, A.A.; Chen, K.M.; Wu, H.; Li, L.; Homolka, D.; Gos, P.; Fleury-Olela, F.; Pillai, R.S.
Deposited on : 2019-07-25
Resolution : 2.92 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

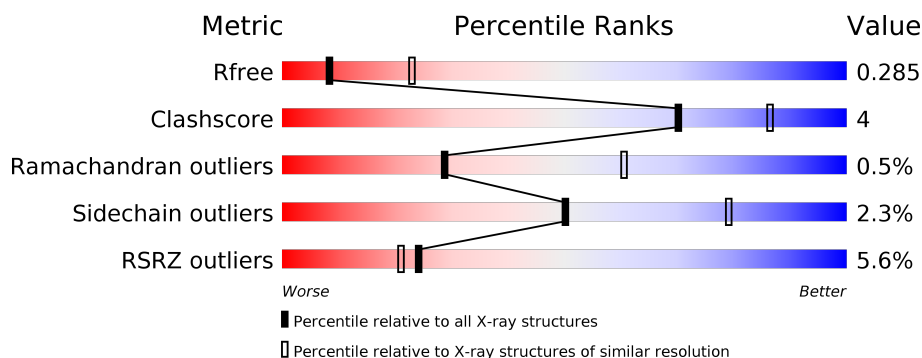
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	352	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>7%</div> </div> </div>
1	B	352	<div> <div>7%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>8%</div> </div> </div>
1	C	352	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>8%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7767 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.

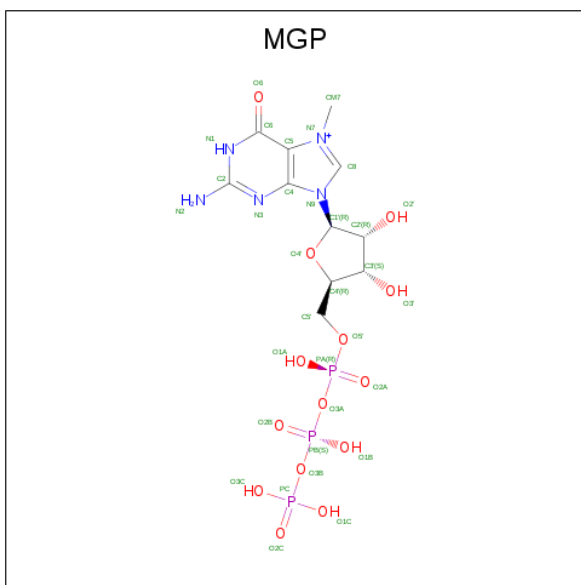
- Molecule 1 is a protein called Peroxisomal NADH pyrophosphatase NUDT12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2526	1616	429	465	16			
1	B	325	Total	C	N	O	S	0	0	0
			2522	1616	426	464	16			
1	C	323	Total	C	N	O	S	0	0	0
			2508	1604	426	462	16			

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Cd	0	0
			3	3		
2	A	4	Total	Cd	0	0
			4	4		
2	C	2	Total	Cd	0	0
			2	2		

- Molecule 3 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE (three-letter code: MGP) (formula: C₁₁H₁₉N₅O₁₄P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total 66	C 22	N 10	O 28	P 6	0	1
3	B	1	Total 66	C 22	N 10	O 28	P 6	0	1
3	C	1	Total 66	C 22	N 10	O 28	P 6	0	1

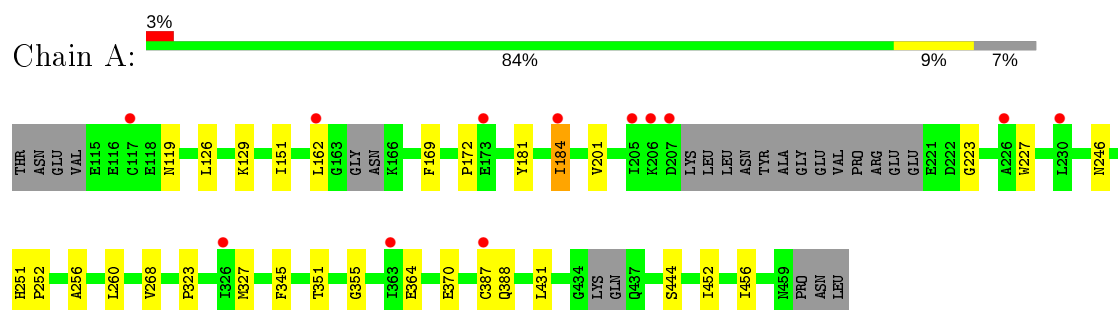
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	1	Total O 1 1	0	0
4	C	2	Total O 2 2	0	0

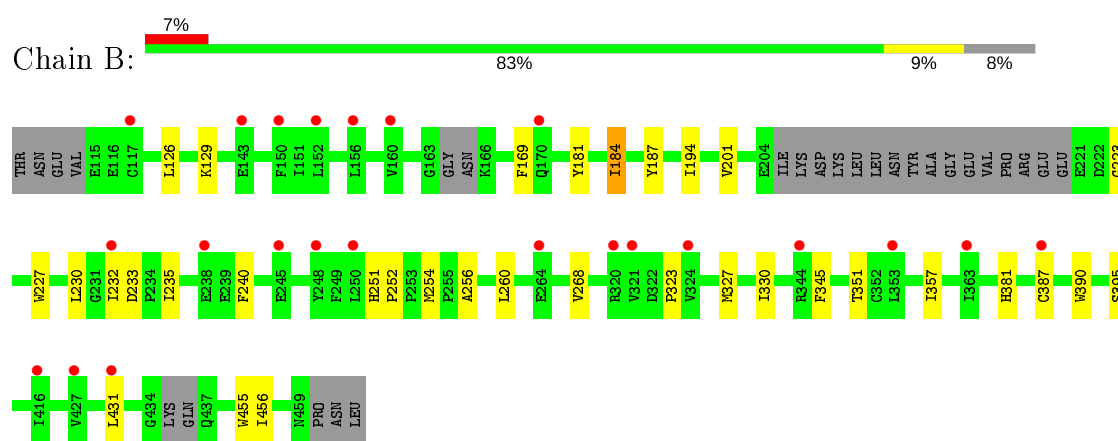
3 Residue-property plots [i](#)

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

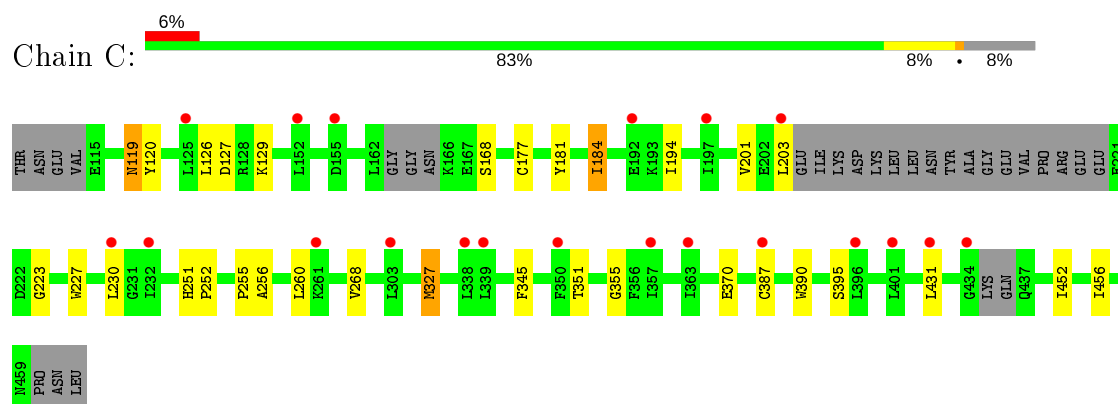
- Molecule 1: Peroxisomal NADH pyrophosphatase NUDT12



- Molecule 1: Peroxisomal NADH pyrophosphatase NUDT12



- Molecule 1: Peroxisomal NADH pyrophosphatase NUDT12



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	229.86Å 229.86Å 159.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	114.93 – 2.92 114.93 – 2.92	Depositor EDS
% Data completeness (in resolution range)	60.2 (114.93-2.92) 60.1 (114.93-2.92)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.232 , 0.260 0.248 , 0.285	Depositor DCC
R_{free} test set	1062 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	91.5	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7767	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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: MGP, CD

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	0.31	0/2584	0.54	0/3513
1	B	0.31	0/2582	0.53	0/3511
1	C	0.31	0/2566	0.54	0/3488
All	All	0.31	0/7732	0.54	0/10512

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	2526	0	2431	20	0
1	B	2522	0	2433	19	0
1	C	2508	0	2431	19	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
3	A	66	0	30	0	0
3	B	66	0	30	0	0
3	C	66	0	30	0	0
4	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	2	0	0	0	0
All	All	7767	0	7385	55	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (55) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LYS:HG3	1:B:201:VAL:HG22	1.87	0.57
1:C:252:PRO:O	1:C:256:ALA:HB3	2.07	0.55
1:B:252:PRO:O	1:B:256:ALA:HB3	2.06	0.55
1:B:345:PHE:HE2	1:B:351:THR:HG21	1.72	0.55
1:A:345:PHE:CE2	1:A:351:THR:HG21	2.43	0.52
1:A:162:LEU:HG	1:A:172:PRO:HB2	1.91	0.52
1:C:345:PHE:CE2	1:C:351:THR:HG21	2.45	0.52
1:A:345:PHE:HE2	1:A:351:THR:HG21	1.75	0.52
1:A:181:TYR:HA	1:A:184:ILE:HG22	1.91	0.52
1:B:345:PHE:CE2	1:B:351:THR:HG21	2.45	0.52
1:C:181:TYR:HA	1:C:184:ILE:HG22	1.92	0.52
1:B:187:TYR:HE2	1:B:240:PHE:CD2	2.27	0.51
1:C:129:LYS:HG3	1:C:201:VAL:HG22	1.92	0.51
1:B:181:TYR:HA	1:B:184:ILE:HG22	1.92	0.51
1:A:252:PRO:O	1:A:256:ALA:HB3	2.10	0.51
1:A:431:LEU:HD12	1:A:456:ILE:HD12	1.92	0.51
1:A:431:LEU:CD1	1:A:456:ILE:HD12	2.41	0.51
1:A:162:LEU:HD21	1:A:172:PRO:HG2	1.93	0.50
1:A:129:LYS:HG3	1:A:201:VAL:HG22	1.94	0.50
1:C:431:LEU:HD11	1:C:452:ILE:HG22	1.93	0.50
1:A:323:PRO:HG3	1:B:323:PRO:HG3	1.94	0.49
1:B:431:LEU:CD1	1:B:456:ILE:HD12	2.43	0.48
1:C:431:LEU:CD1	1:C:456:ILE:HD12	2.44	0.48
1:C:431:LEU:HD12	1:C:456:ILE:HD12	1.97	0.47
1:A:431:LEU:HD11	1:A:452:ILE:HG22	1.96	0.47
1:B:194:ILE:HG22	1:B:232:ILE:HG22	1.96	0.47
1:B:260:LEU:HD13	1:B:268:VAL:HG21	1.96	0.47
1:C:345:PHE:HE2	1:C:351:THR:HG21	1.80	0.46
1:A:431:LEU:HD12	1:A:456:ILE:CD1	2.45	0.46
1:A:119:ASN:HB3	1:A:388:GLN:HG3	1.98	0.45
1:B:431:LEU:HD12	1:B:456:ILE:HD12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:SER:OG	1:C:168:SER:HA	2.17	0.44
1:B:330:ILE:HD12	1:B:455:TRP:CD1	2.53	0.44
1:B:431:LEU:HD12	1:B:456:ILE:CD1	2.48	0.44
1:B:126:LEU:HD21	1:B:227:TRP:CG	2.53	0.43
1:C:431:LEU:HD12	1:C:456:ILE:CD1	2.48	0.43
1:B:233:ASP:HB3	1:B:235:ILE:HG12	2.00	0.43
1:A:126:LEU:HD21	1:A:227:TRP:CG	2.54	0.42
1:A:260:LEU:HD13	1:A:268:VAL:HG21	2.01	0.42
1:B:187:TYR:CE2	1:B:240:PHE:CD2	3.06	0.42
1:C:119:ASN:HD22	1:C:119:ASN:N	2.17	0.42
1:A:246:ASN:O	1:C:255:PRO:HG3	2.18	0.42
1:C:194:ILE:HB	1:C:230:LEU:HD11	2.02	0.42
1:C:260:LEU:HD13	1:C:268:VAL:HG21	2.00	0.42
1:A:355:GLY:HA3	1:A:370:GLU:HG3	2.02	0.42
1:B:323:PRO:HB2	1:B:357:ILE:HD12	2.01	0.42
1:C:355:GLY:HA3	1:C:370:GLU:HG3	2.02	0.41
1:B:194:ILE:HB	1:B:230:LEU:HD11	2.03	0.41
1:A:151:ILE:HD11	1:A:227:TRP:CZ3	2.56	0.41
1:B:390:TRP:HB3	1:B:395:SER:HB2	2.01	0.41
1:C:126:LEU:HD21	1:C:227:TRP:CG	2.56	0.41
1:C:327:MET:HE2	1:C:327:MET:HB3	1.82	0.41
1:C:390:TRP:HB3	1:C:395:SER:HB2	2.03	0.41
1:C:127:ASP:HB2	1:C:203:LEU:HD11	2.02	0.40
1:A:345:PHE:CE2	1:A:351:THR:CG2	3.05	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	320/352 (91%)	302 (94%)	17 (5%)	1 (0%)	41 70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	317/352 (90%)	301 (95%)	15 (5%)	1 (0%)	41 70
1	C	315/352 (90%)	298 (95%)	14 (4%)	3 (1%)	15 43
All	All	952/1056 (90%)	901 (95%)	46 (5%)	5 (0%)	29 60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	223	GLY
1	B	223	GLY
1	C	120	TYR
1	A	223	GLY
1	C	177	CYS

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	265/309 (86%)	259 (98%)	6 (2%)	50 79
1	B	267/309 (86%)	260 (97%)	7 (3%)	46 76
1	C	267/309 (86%)	262 (98%)	5 (2%)	57 83
All	All	799/927 (86%)	781 (98%)	18 (2%)	50 79

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	PHE
1	A	184	ILE
1	A	251	HIS
1	A	327	MET
1	A	364	GLU
1	A	387	CYS
1	B	169	PHE
1	B	184	ILE
1	B	251	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	254	MET
1	B	327	MET
1	B	381	HIS
1	B	387	CYS
1	C	119	ASN
1	C	184	ILE
1	C	251	HIS
1	C	327	MET
1	C	387	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	328	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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	MGP	B	504[A]	2	28,35,35	0.96	1 (3%)	33,56,56	2.11	3 (9%)
3	MGP	B	504[B]	-	28,35,35	0.91	1 (3%)	33,56,56	2.12	3 (9%)
3	MGP	C	503[B]	-	28,35,35	0.95	1 (3%)	33,56,56	2.12	3 (9%)
3	MGP	C	503[A]	-	28,35,35	0.96	1 (3%)	33,56,56	2.14	3 (9%)
3	MGP	A	505[B]	-	28,35,35	0.93	1 (3%)	33,56,56	2.14	4 (12%)
3	MGP	A	505[A]	-	28,35,35	0.99	1 (3%)	33,56,56	2.14	3 (9%)

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	MGP	B	504[A]	2	-	6/18/38/38	0/3/3/3
3	MGP	B	504[B]	-	-	9/18/38/38	0/3/3/3
3	MGP	C	503[B]	-	-	8/18/38/38	0/3/3/3
3	MGP	C	503[A]	-	-	6/18/38/38	0/3/3/3
3	MGP	A	505[B]	-	-	8/18/38/38	0/3/3/3
3	MGP	A	505[A]	-	-	6/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	505[A]	MGP	C6-N1	3.76	1.39	1.33
3	C	503[A]	MGP	C6-N1	3.75	1.39	1.33
3	A	505[B]	MGP	C6-N1	3.65	1.39	1.33
3	C	503[B]	MGP	C6-N1	3.60	1.39	1.33
3	B	504[A]	MGP	C6-N1	3.58	1.39	1.33
3	B	504[B]	MGP	C6-N1	3.43	1.39	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	505[A]	MGP	C5-C6-N1	-9.82	110.00	123.43
3	C	503[A]	MGP	C5-C6-N1	-9.65	110.23	123.43
3	A	505[B]	MGP	C5-C6-N1	-9.51	110.43	123.43
3	B	504[A]	MGP	C5-C6-N1	-9.42	110.55	123.43
3	C	503[B]	MGP	C5-C6-N1	-9.32	110.68	123.43
3	B	504[B]	MGP	C5-C6-N1	-9.00	111.11	123.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	504[B]	MGP	C6-N1-C2	6.26	125.88	115.93
3	C	503[A]	MGP	C6-N1-C2	6.10	125.62	115.93
3	A	505[B]	MGP	C6-N1-C2	6.08	125.59	115.93
3	C	503[B]	MGP	C6-N1-C2	6.03	125.52	115.93
3	B	504[A]	MGP	C6-N1-C2	5.99	125.44	115.93
3	A	505[A]	MGP	C6-N1-C2	5.98	125.44	115.93
3	B	504[B]	MGP	N3-C2-N1	-2.86	123.41	127.22
3	C	503[A]	MGP	N3-C2-N1	-2.84	123.43	127.22
3	B	504[A]	MGP	N3-C2-N1	-2.82	123.46	127.22
3	A	505[B]	MGP	N3-C2-N1	-2.80	123.48	127.22
3	C	503[B]	MGP	N3-C2-N1	-2.79	123.50	127.22
3	A	505[A]	MGP	N3-C2-N1	-2.76	123.54	127.22
3	A	505[B]	MGP	C1'-N9-C4	-2.06	123.03	126.64

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	504[A]	MGP	C5'-O5'-PA-O1A
3	B	504[A]	MGP	C5'-O5'-PA-O2A
3	B	504[B]	MGP	C5'-O5'-PA-O1A
3	B	504[B]	MGP	C5'-O5'-PA-O2A
3	B	504[B]	MGP	C5'-O5'-PA-O3A
3	C	503[A]	MGP	C5'-O5'-PA-O1A
3	C	503[A]	MGP	C5'-O5'-PA-O2A
3	C	503[A]	MGP	O4'-C4'-C5'-O5'
3	A	505[B]	MGP	C5'-O5'-PA-O1A
3	A	505[B]	MGP	C5'-O5'-PA-O2A
3	A	505[B]	MGP	C5'-O5'-PA-O3A
3	C	503[B]	MGP	C5'-O5'-PA-O1A
3	C	503[B]	MGP	C5'-O5'-PA-O2A
3	C	503[B]	MGP	C5'-O5'-PA-O3A
3	A	505[A]	MGP	C5'-O5'-PA-O1A
3	A	505[A]	MGP	C5'-O5'-PA-O2A
3	A	505[A]	MGP	PB-O3B-PC-O3C
3	A	505[A]	MGP	O4'-C4'-C5'-O5'
3	B	504[A]	MGP	O4'-C4'-C5'-O5'
3	A	505[B]	MGP	O4'-C4'-C5'-O5'
3	B	504[B]	MGP	O4'-C4'-C5'-O5'
3	C	503[B]	MGP	O4'-C4'-C5'-O5'
3	B	504[A]	MGP	PB-O3B-PC-O3C
3	B	504[A]	MGP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

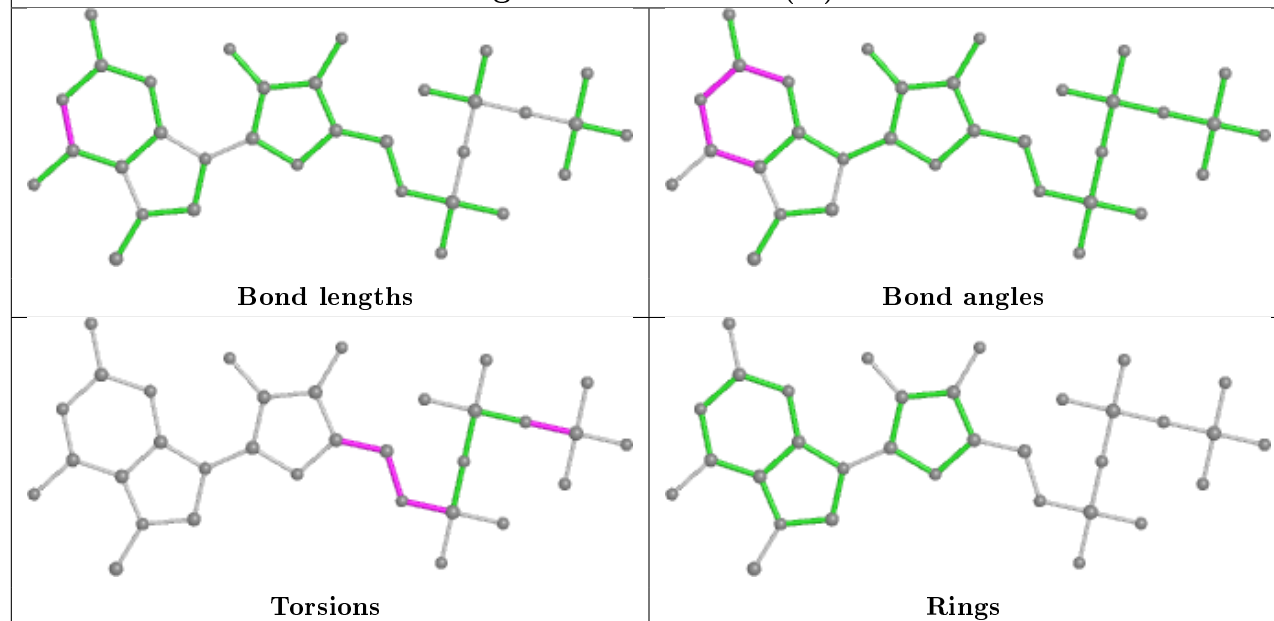
Mol	Chain	Res	Type	Atoms
3	C	503[A]	MGP	C5'-O5'-PA-O3A
3	A	505[A]	MGP	C5'-O5'-PA-O3A
3	B	504[B]	MGP	PA-O3A-PB-O1B
3	A	505[B]	MGP	PA-O3A-PB-O1B
3	C	503[B]	MGP	PA-O3A-PB-O1B
3	B	504[A]	MGP	C4'-C5'-O5'-PA
3	C	503[A]	MGP	C4'-C5'-O5'-PA
3	A	505[A]	MGP	C4'-C5'-O5'-PA
3	A	505[B]	MGP	C3'-C4'-C5'-O5'
3	B	504[B]	MGP	C3'-C4'-C5'-O5'
3	C	503[B]	MGP	C3'-C4'-C5'-O5'
3	C	503[A]	MGP	PB-O3B-PC-O3C
3	B	504[B]	MGP	PA-O3A-PB-O2B
3	B	504[B]	MGP	PC-O3B-PB-O1B
3	B	504[B]	MGP	PC-O3B-PB-O2B
3	A	505[B]	MGP	PA-O3A-PB-O2B
3	A	505[B]	MGP	PC-O3B-PB-O1B
3	C	503[B]	MGP	PA-O3A-PB-O2B
3	C	503[B]	MGP	PC-O3B-PB-O2B

There are no ring outliers.

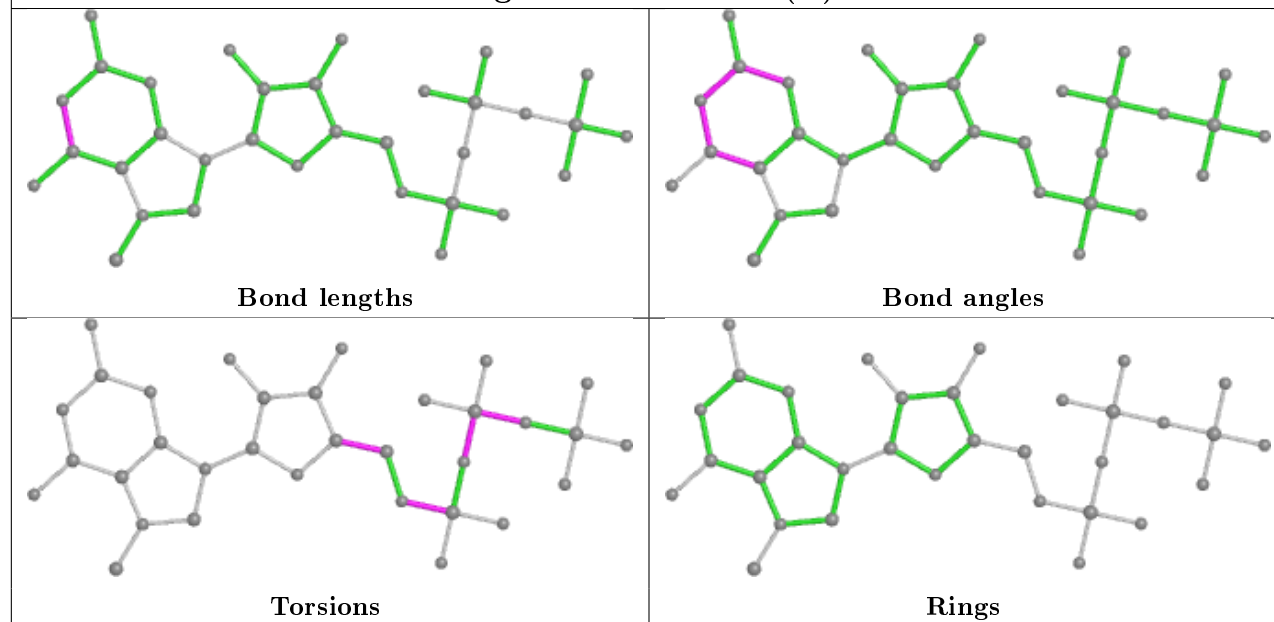
No monomer is involved in short contacts.

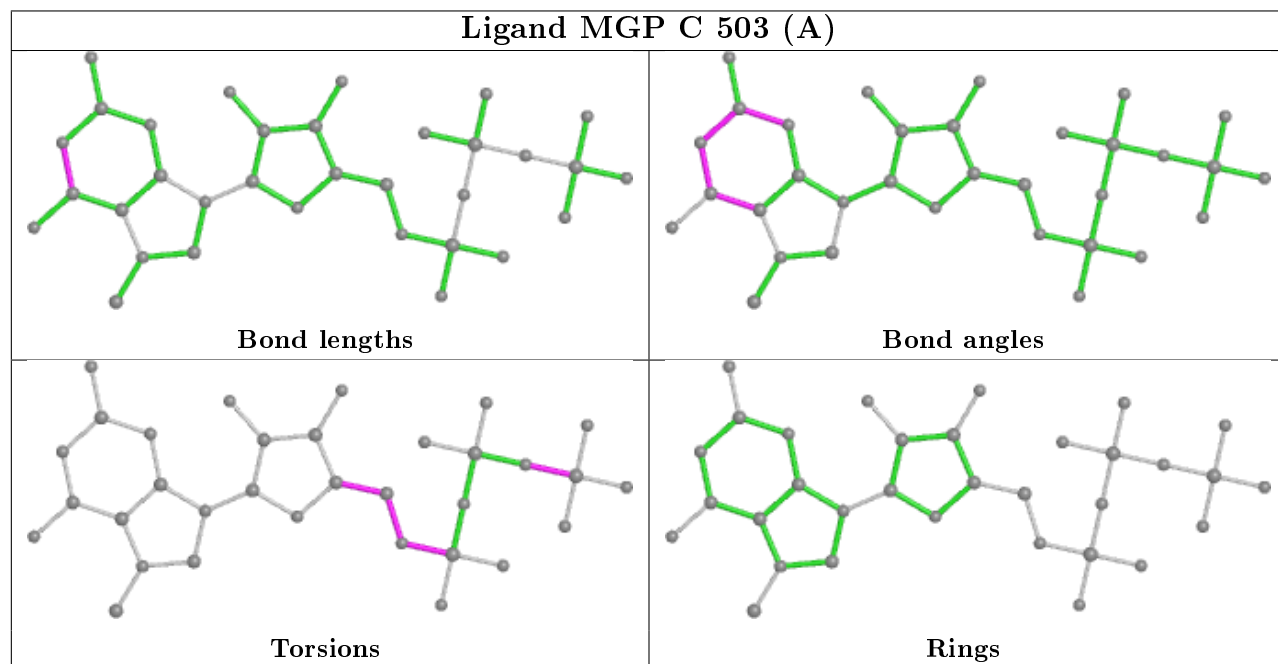
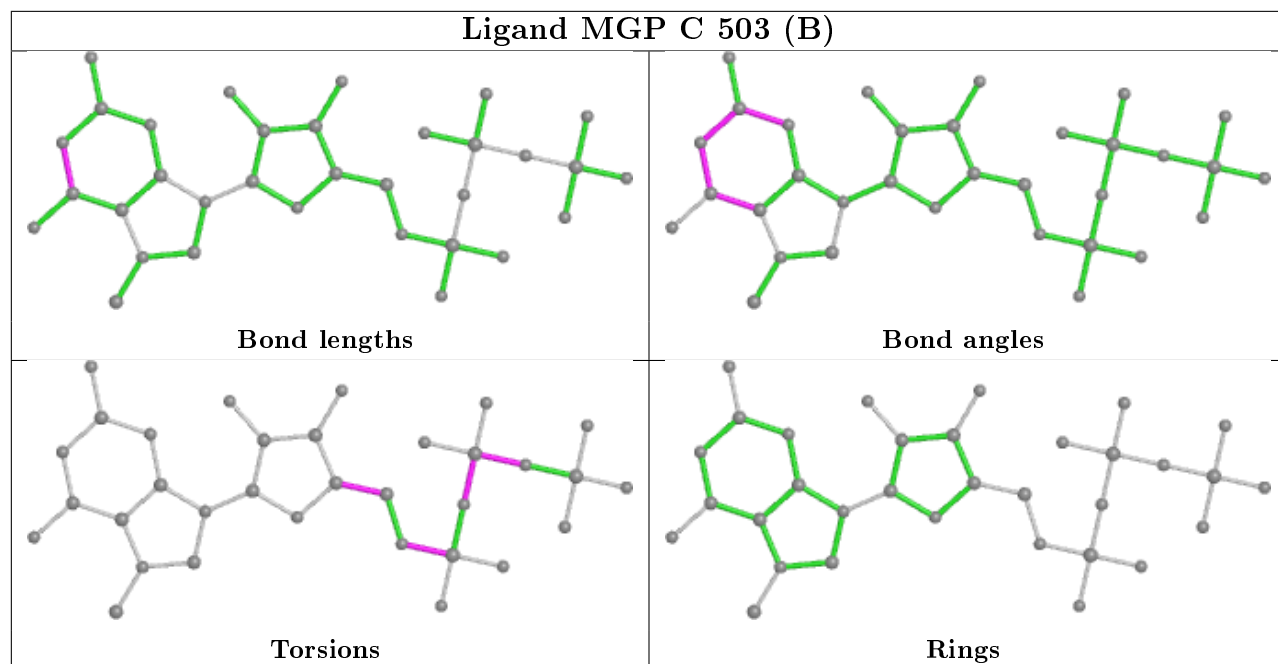
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

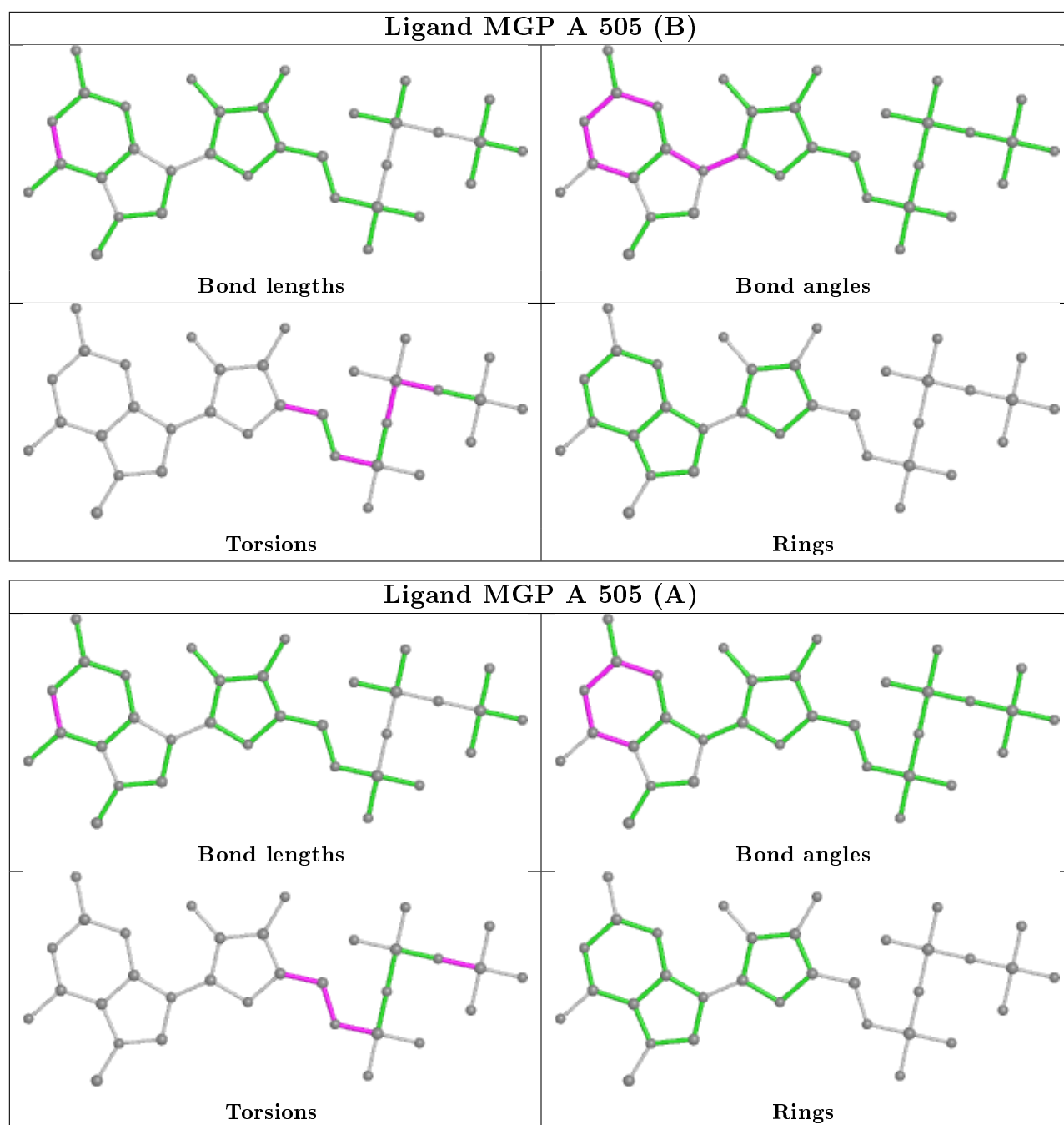
Ligand MGP B 504 (A)



Ligand MGP B 504 (B)







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 ⓘ

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	328/352 (93%)	0.34	12 (3%)	41 38	50, 90, 132, 161	0
1	B	325/352 (92%)	0.64	23 (7%)	16 13	48, 88, 126, 152	0
1	C	323/352 (91%)	0.55	20 (6%)	20 17	58, 99, 139, 155	0
All	All	976/1056 (92%)	0.51	55 (5%)	24 21	48, 93, 134, 161	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	ASP	4.5
1	B	250	LEU	4.2
1	A	206	LYS	4.0
1	C	396	LEU	3.7
1	B	387	CYS	3.6
1	B	431	LEU	3.4
1	C	232	ILE	3.4
1	C	363	ILE	3.4
1	C	357	ILE	3.2
1	C	338	LEU	3.0
1	A	387	CYS	2.7
1	B	156	LEU	2.7
1	A	205	ILE	2.7
1	C	152	LEU	2.7
1	C	387	CYS	2.6
1	B	152	LEU	2.6
1	C	230	LEU	2.6
1	C	431	LEU	2.5
1	C	434	GLY	2.5
1	A	117	CYS	2.5
1	B	232	ILE	2.4
1	B	248	TYR	2.4
1	B	416	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	203	LEU	2.4
1	B	143	GLU	2.4
1	B	238	GLU	2.3
1	B	264	GLU	2.3
1	A	173	GLU	2.3
1	C	125	LEU	2.3
1	B	245	GLU	2.3
1	A	363	ILE	2.3
1	C	197	ILE	2.3
1	C	401	LEU	2.2
1	B	117	CYS	2.2
1	B	320	ARG	2.2
1	A	326	ILE	2.2
1	B	427	VAL	2.2
1	B	363	ILE	2.2
1	A	162	LEU	2.2
1	B	344	ARG	2.2
1	C	303	LEU	2.1
1	C	339	LEU	2.1
1	C	192	GLU	2.1
1	A	230	LEU	2.1
1	A	226	ALA	2.1
1	B	321	VAL	2.1
1	B	353	LEU	2.1
1	B	170	GLN	2.1
1	B	324	VAL	2.1
1	C	155	ASP	2.0
1	B	160	VAL	2.0
1	B	150	PHE	2.0
1	C	350	PHE	2.0
1	A	184	ILE	2.0
1	C	261	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

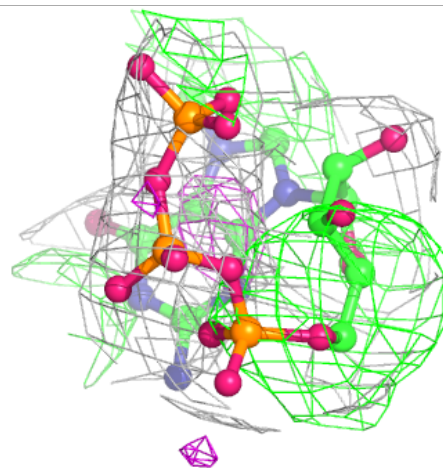
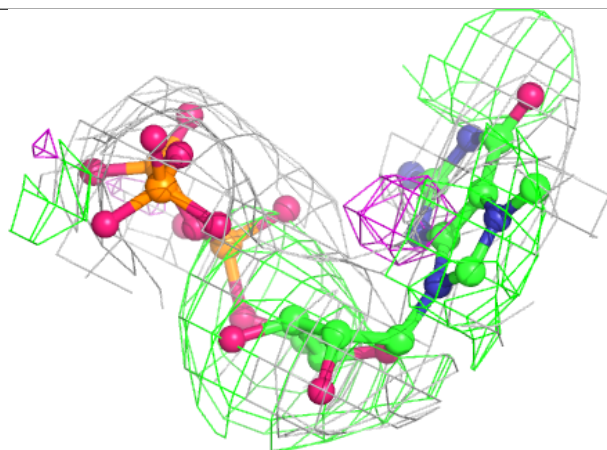
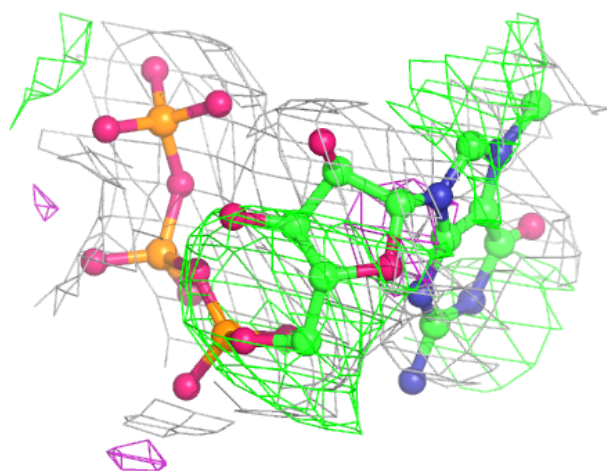
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CD	C	502	1/1	0.15	0.27	258,258,258,258	0
2	CD	B	502	1/1	0.41	0.14	199,199,199,199	1
2	CD	A	504	1/1	0.65	0.09	232,232,232,232	0
2	CD	A	503	1/1	0.72	0.13	237,237,237,237	0
3	MGP	C	503[A]	33/33	0.80	0.30	57,74,106,106	33
3	MGP	A	505[B]	33/33	0.80	0.30	44,68,78,80	33
3	MGP	C	503[B]	33/33	0.80	0.30	56,80,106,108	33
3	MGP	A	505[A]	33/33	0.80	0.30	50,62,70,70	33
3	MGP	B	504[B]	33/33	0.83	0.31	32,69,90,94	33
3	MGP	B	504[A]	33/33	0.83	0.31	50,59,91,92	33
2	CD	A	502	1/1	0.85	0.05	179,179,179,179	1
2	CD	B	503	1/1	0.94	0.08	200,200,200,200	1
2	CD	A	501	1/1	0.95	0.15	132,132,132,132	0
2	CD	B	501	1/1	0.98	0.16	136,136,136,136	0
2	CD	C	501	1/1	0.99	0.12	149,149,149,149	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.

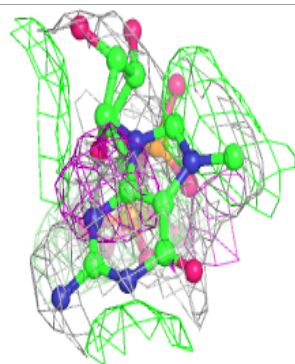
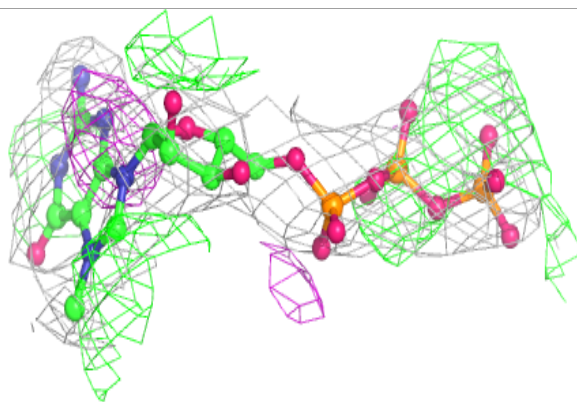
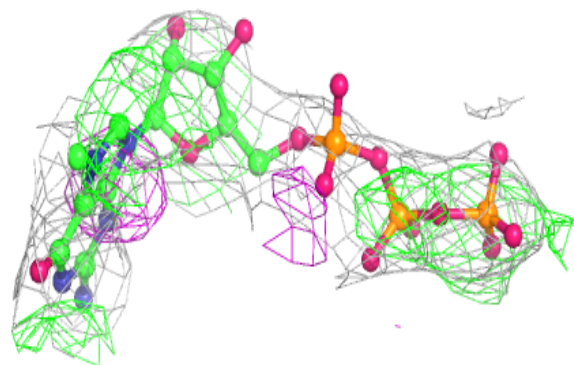
Electron density around MGP C 503 (A):

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

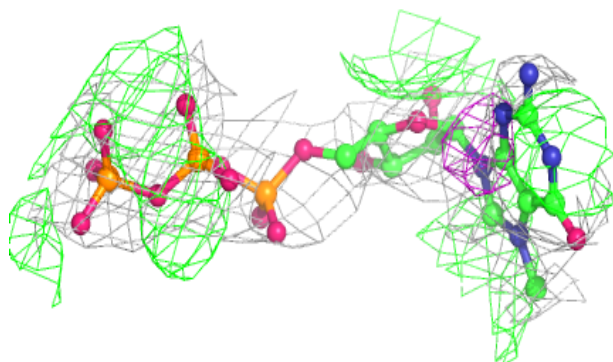
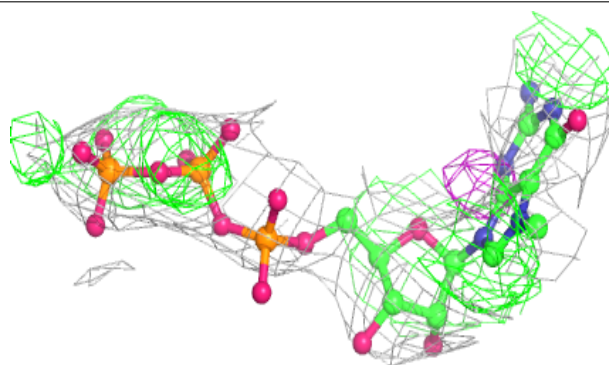


Electron density around MGP A 505 (B):

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

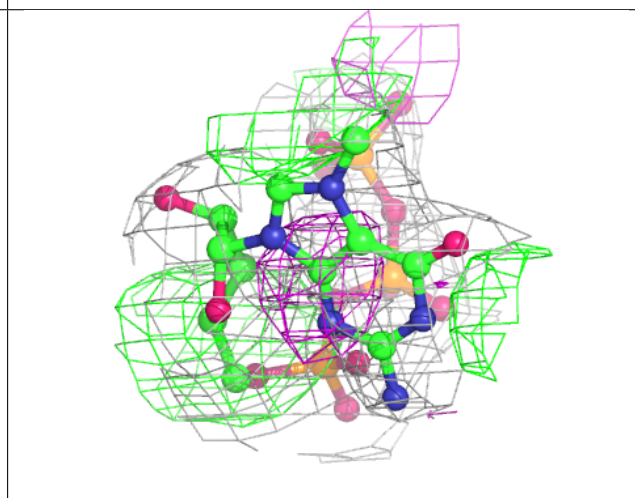
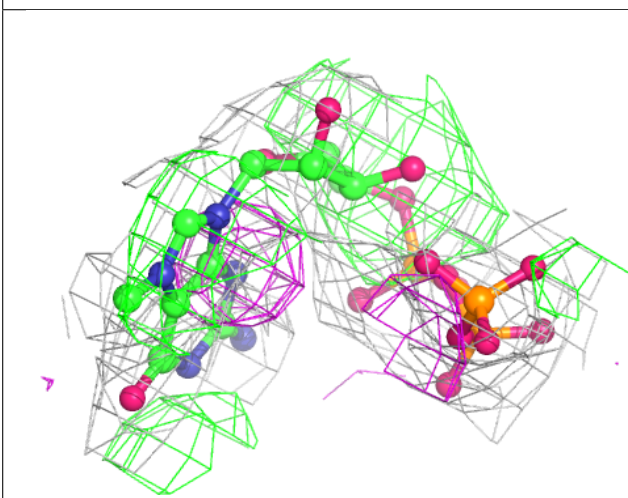
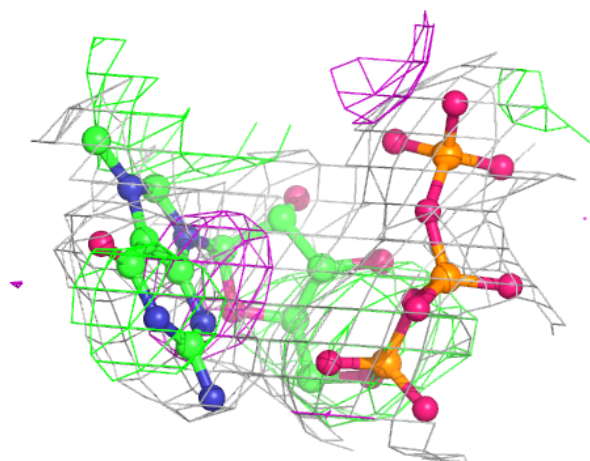
**Electron density around MGP C 503 (B):**

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



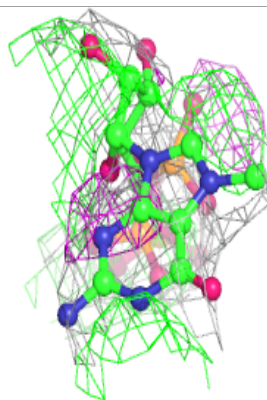
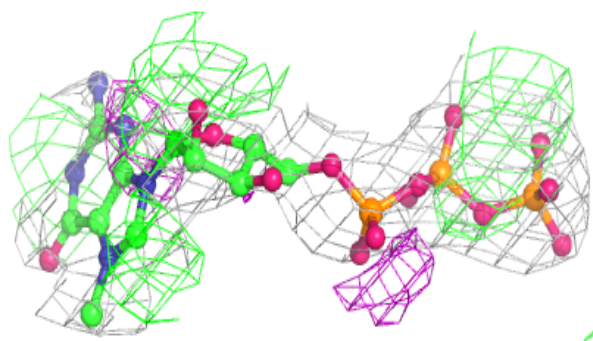
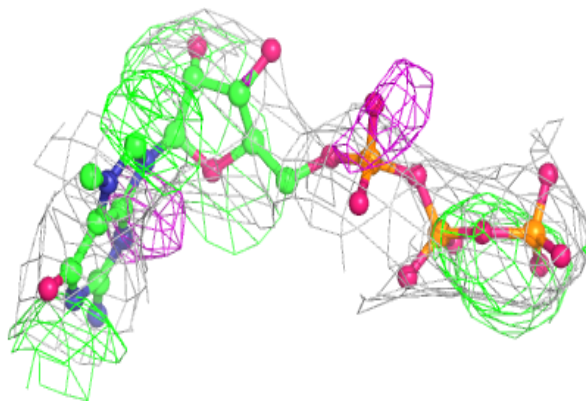
Electron density around MGP A 505 (A):

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



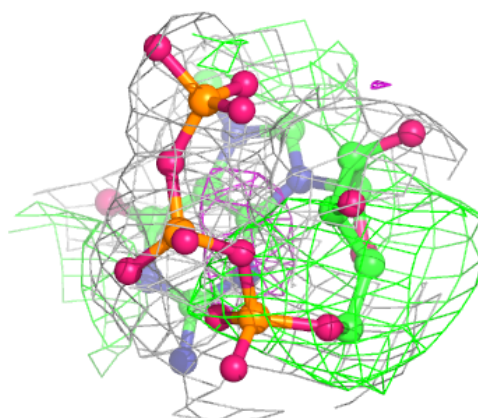
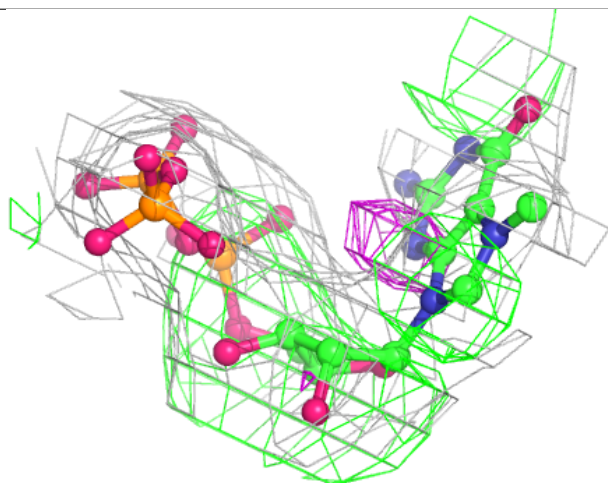
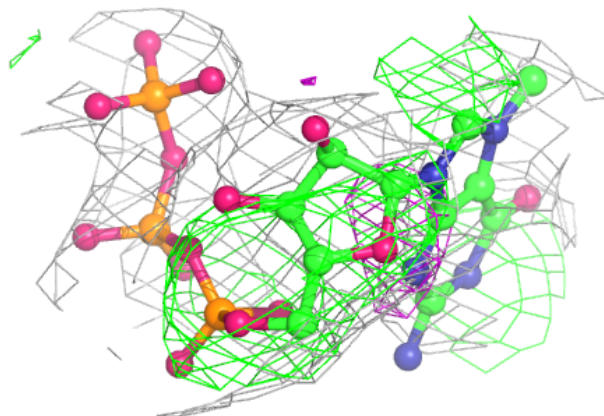
Electron density around MGP B 504 (B):

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



Electron density around MGP B 504 (A):

$2mF_o-DF_c$ (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.