



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 2, 2025 – 02:04 am BST

PDB ID : 5T5I / pdb\_00005t5i  
Title : TUNGSTEN-CONTAINING FORMYLMETHANOFURAN DEHYDROGENASE FROM METHANOTHERMOBACTER WOLFEII, ORTHORHOMBIC FORM AT 1.9 Å  
Authors : Wagner, T.; Ermler, U.; Shima, S.  
Deposited on : 2016-08-31  
Resolution : 1.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

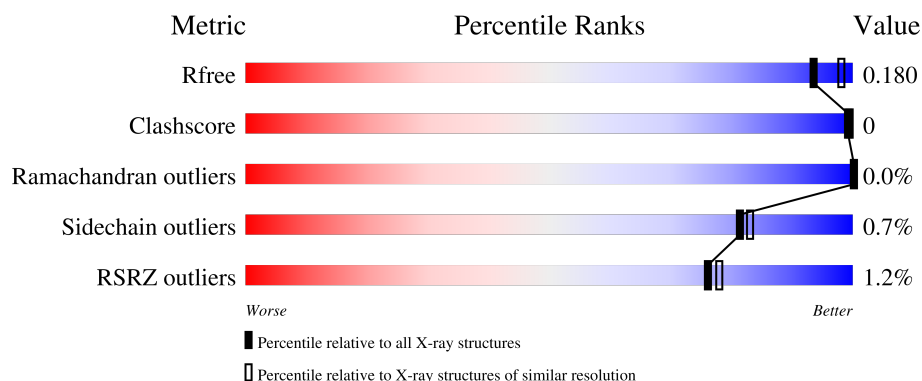
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (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  $\geq 3$ , 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	569	 99% .
1	I	569	 98% .
2	B	432	 98% .
2	J	432	 99% .

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Mol	Chain	Length	Quality of chain
3	C	270	<div><div></div><div>99%</div></div>
3	K	270	<div><div></div><div>100%</div></div>
4	D	130	<div><div><div>2%</div></div><div><div></div><div>98%</div></div><div>.</div></div>
4	L	130	<div><div><div>%</div></div><div><div></div><div>100%</div></div></div>
5	F	349	<div><div><div>5%</div></div><div><div></div><div>95%</div></div><div><div>.</div><div>.</div></div></div>
5	N	349	<div><div><div>2%</div></div><div><div></div><div>93%</div></div><div><div>.</div><div>6%</div></div></div>
6	G	82	<div><div><div>%</div></div><div><div></div><div>95%</div></div><div><div>.</div><div>.</div></div></div>
6	P	82	<div><div><div>%</div></div><div><div></div><div>93%</div></div><div><div>6%</div><div>.</div></div></div>

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 30815 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 Tungsten formylmethanofuran dehydrogenase subunit fwdA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	2	0
			4427	2818	735	851	23			
1	I	569	Total	C	N	O	S	0	2	0
			4437	2822	739	853	23			

- Molecule 2 is a protein called Tungsten formylmethanofuran dehydrogenase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	3	0
			3386	2130	594	632	30			
2	J	431	Total	C	N	O	S	0	3	0
			3393	2134	595	634	30			

- Molecule 3 is a protein called Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	269	Total	C	N	O	S	0	0	0
			1994	1254	336	391	13			
3	K	269	Total	C	N	O	S	0	0	0
			1994	1254	336	391	13			

- Molecule 4 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	130	Total	C	N	O	S	0	0	0
			1005	643	163	190	9			
4	L	130	Total	C	N	O	S	0	0	0
			1005	643	163	190	9			

- Molecule 5 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	335	Total	C	N	O	S	0	1	0
			2554	1577	428	508	41			
5	N	329	Total	C	N	O	S	0	1	0
			2503	1544	419	499	41			

- Molecule 6 is a protein called Tungsten formylmethanofuran dehydrogenase subunit fwdG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	80	Total	C	N	O	S	0	0	0
			572	354	96	113	9			
6	P	81	Total	C	N	O	S	0	1	0
			586	364	97	116	9			

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Zn	0	0
			2	2		
7	I	2	Total	Zn	0	0
			2	2		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mg	0	0
			1	1		
8	I	1	Total	Mg	0	0
			1	1		

- Molecule 9 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total	K	0	0
			2	2		
9	B	1	Total	K	0	0
			1	1		
9	F	5	Total	K	0	0
			5	5		
9	G	2	Total	K	0	0
			2	2		
9	I	2	Total	K	0	0
			2	2		

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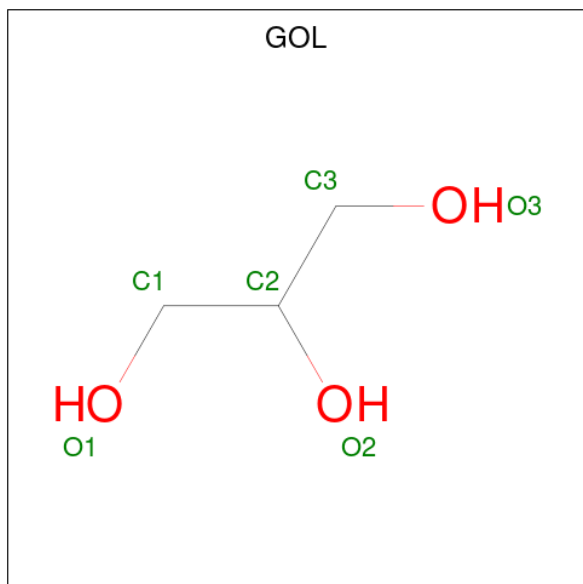
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	J	1	Total	K	0	0
			1	1		
9	N	4	Total	K	0	0
			4	4		
9	P	1	Total	K	0	0
			1	1		

- Molecule 10 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	2	Total	Na	0	0
			2	2		
10	I	2	Total	Na	0	0
			2	2		
10	L	1	Total	Na	0	0
			1	1		

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



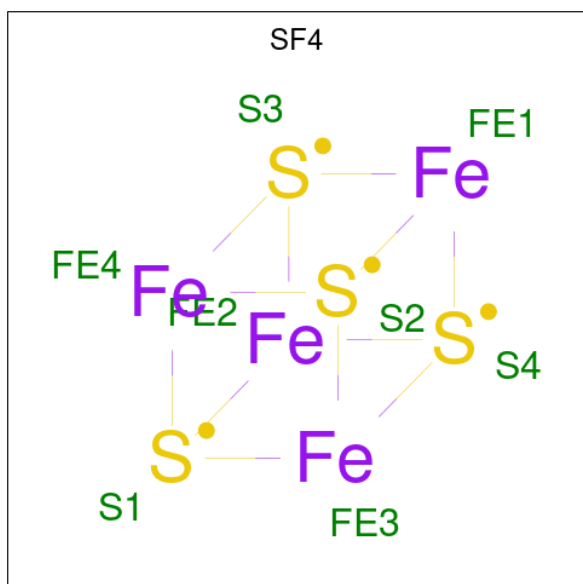
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			6	3	3		
11	A	1	Total	C	O	0	0
			6	3	3		
11	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			6	3	3		
11	I	1	Total	C	O	0	0
			6	3	3		
11	I	1	Total	C	O	0	0
			6	3	3		
11	I	1	Total	C	O	0	0
			6	3	3		
11	J	1	Total	C	O	0	0
			6	3	3		
11	N	1	Total	C	O	0	0
			6	3	3		

- Molecule 12 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	Fe	S	0	0
			8	4	4		
12	F	1	Total	Fe	S	0	0
			8	4	4		
12	F	1	Total	Fe	S	0	0
			8	4	4		
12	F	1	Total	Fe	S	0	0
			8	4	4		
12	F	1	Total	Fe	S	0	0
			8	4	4		

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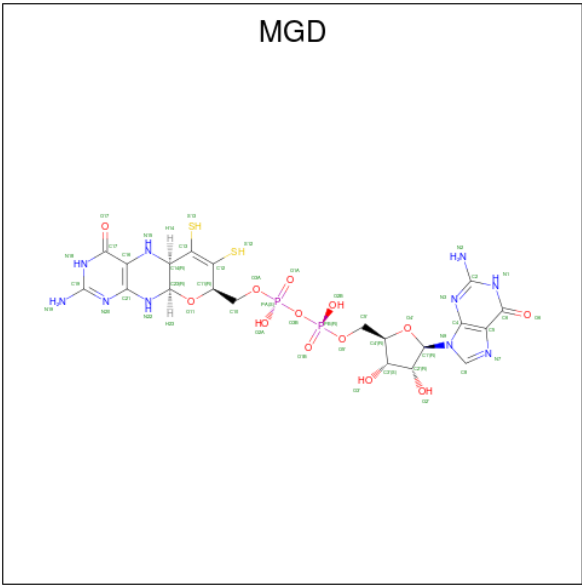
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	F	1	Total 8	Fe 4	S 4	0	0
12	F	1	Total 8	Fe 4	S 4	0	0
12	F	1	Total 8	Fe 4	S 4	0	0
12	F	1	Total 8	Fe 4	S 4	0	0
12	G	1	Total 8	Fe 4	S 4	0	0
12	G	1	Total 8	Fe 4	S 4	0	0
12	J	1	Total 8	Fe 4	S 4	0	0
12	N	1	Total 8	Fe 4	S 4	0	0
12	N	1	Total 8	Fe 4	S 4	0	0
12	N	1	Total 8	Fe 4	S 4	0	0
12	N	1	Total 8	Fe 4	S 4	0	0
12	N	1	Total 8	Fe 4	S 4	0	0
12	N	1	Total 8	Fe 4	S 4	0	0
12	N	1	Total 8	Fe 4	S 4	0	0
12	N	1	Total 8	Fe 4	S 4	0	0
12	P	1	Total 8	Fe 4	S 4	0	0
12	P	1	Total 8	Fe 4	S 4	0	0

- Molecule 13 is TUNGSTEN ION (CCD ID: W) (formula: W).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	B	1	Total 1	W 1	0	0
13	J	1	Total 1	W 1	0	0

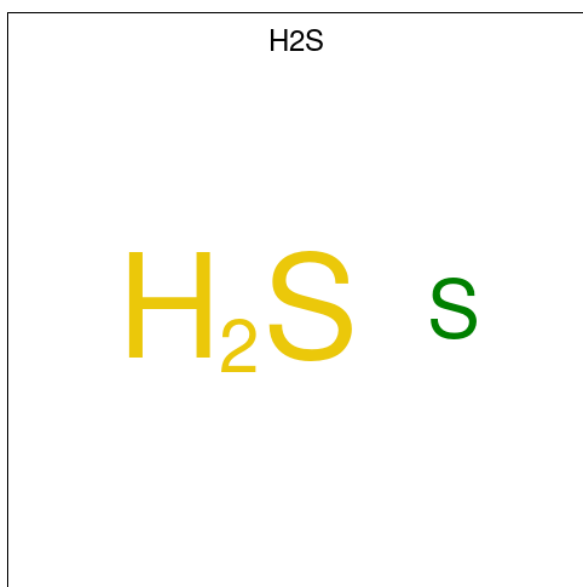


- Molecule 14 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	B	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
14	B	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
14	J	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
14	J	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 15 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H<sub>2</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	1	Total S 1 1	0	0
15	J	1	Total S 1 1	0	0

- Molecule 16 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total Ca 1 1	0	0
16	J	1	Total Ca 1 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	362	Total O 362 362	0	0
17	B	226	Total O 226 226	0	0
17	C	174	Total O 174 174	0	0
17	D	108	Total O 108 108	0	0
17	F	198	Total O 198 198	0	0

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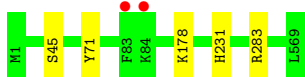
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	G	60	Total 60	O 60	0	0
17	I	445	Total 445	O 445	0	0
17	J	273	Total 273	O 273	0	0
17	K	187	Total 187	O 187	0	0
17	L	126	Total 126	O 126	0	0
17	N	283	Total 283	O 283	0	0
17	P	64	Total 64	O 64	0	0

### 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: Tungsten formylmethanofuran dehydrogenase subunit fwdA

Chain A:  99%



- Molecule 1: Tungsten formylmethanofuran dehydrogenase subunit fwdA

Chain I:  98%



- Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

Chain B:  98%



- Molecule 2: Tungsten formylmethanofuran dehydrogenase subunit B

Chain J:  99%



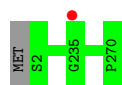
- Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C

Chain C:  99%



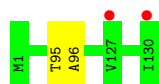
- Molecule 3: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C

Chain K:  100%



- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

Chain D:  98%



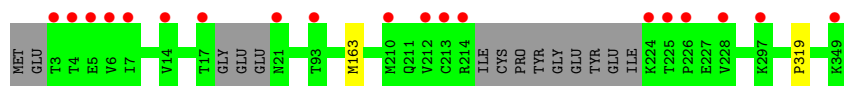
- Molecule 4: Tungsten formylmethanofuran dehydrogenase subunit fwdD

Chain L:  100%




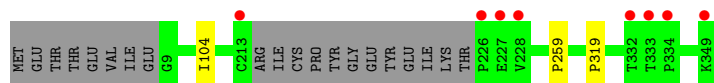
- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdF

Chain F:  95%



- Molecule 5: Tungsten formylmethanofuran dehydrogenase subunit fwdF

Chain N:  93% 6%



- Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdG

Chain G:  95%



- Molecule 6: Tungsten formylmethanofuran dehydrogenase subunit fwdG

Chain P:  93% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.64Å 174.58Å 205.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.49 – 1.90 48.49 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.49-1.90) 99.1 (48.49-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 1.90Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, $R_{free}$	0.152 , 0.172 0.162 , 0.180	Depositor DCC
$R_{free}$ test set	16949 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	30815	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0186e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, MG, SF4, CA, ZN, K, W, GOL, H2S, MGD, NA

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	0.46	0/4537	0.64	0/6179
1	I	0.46	0/4544	0.64	0/6187
2	B	0.45	0/3465	0.64	0/4689
2	J	0.46	0/3472	0.65	0/4699
3	C	0.41	0/2027	0.64	0/2729
3	K	0.43	0/2027	0.64	0/2729
4	D	0.45	0/1024	0.66	0/1390
4	L	0.46	0/1024	0.64	0/1390
5	F	0.44	0/2591	0.59	0/3511
5	N	0.45	0/2541	0.58	0/3443
6	G	0.44	0/579	0.66	0/787
6	P	0.46	0/596	0.67	0/810
All	All	0.45	0/28427	0.63	0/38543

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 [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	4427	0	4285	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	4437	0	4289	3	0
2	B	3386	0	3339	2	0
2	J	3393	0	3346	1	0
3	C	1994	0	1962	0	0
3	K	1994	0	1962	0	0
4	D	1005	0	1033	1	0
4	L	1005	0	1033	0	0
5	F	2554	0	2526	1	0
5	N	2503	0	2463	2	0
6	G	572	0	567	1	0
6	P	586	0	584	2	0
7	A	2	0	0	0	0
7	I	2	0	0	0	0
8	A	1	0	0	0	0
8	I	1	0	0	0	0
9	A	2	0	0	0	0
9	B	1	0	0	0	0
9	F	5	0	0	0	0
9	G	2	0	0	0	0
9	I	2	0	0	1	0
9	J	1	0	0	0	0
9	N	4	0	0	0	0
9	P	1	0	0	0	0
10	A	2	0	0	0	0
10	I	2	0	0	0	0
10	L	1	0	0	0	0
11	A	18	0	24	0	0
11	B	6	0	8	0	0
11	I	18	0	24	0	0
11	J	6	0	8	0	0
11	N	6	0	8	0	0
12	B	8	0	0	0	0
12	F	64	0	0	0	0
12	G	16	0	0	0	0
12	J	8	0	0	0	0
12	N	64	0	0	0	0
12	P	16	0	0	0	0
13	B	1	0	0	0	0
13	J	1	0	0	0	0
14	B	94	0	44	1	0
14	J	94	0	44	1	0
15	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	J	1	0	0	0	0
16	B	1	0	0	0	0
16	J	1	0	0	0	0
17	A	362	0	0	0	0
17	B	226	0	0	0	0
17	C	174	0	0	0	0
17	D	108	0	0	0	0
17	F	198	0	0	0	0
17	G	60	0	0	0	0
17	I	445	0	0	2	0
17	J	273	0	0	0	0
17	K	187	0	0	0	0
17	L	126	0	0	0	0
17	N	283	0	0	0	0
17	P	64	0	0	0	0
All	All	30815	0	27549	12	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 0.

The worst 5 of 12 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)
9:I:604:K:K	17:I:763:HOH:O	1.98	0.74
1:I:391:PRO:HB2	17:I:701:HOH:O	2.07	0.55
5:N:319:PRO:HG3	6:P:64:CYS:HB3	1.97	0.47
1:I:99:MET:O	1:I:103[B]:ARG:HG3	2.15	0.46
5:F:319:PRO:HG3	6:G:64:CYS:HB3	2.01	0.42

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	568/569 (100%)	550 (97%)	18 (3%)	0	100	100
1	I	568/569 (100%)	550 (97%)	18 (3%)	0	100	100
2	B	431/432 (100%)	415 (96%)	15 (4%)	1 (0%)	44	36
2	J	432/432 (100%)	416 (96%)	16 (4%)	0	100	100
3	C	267/270 (99%)	259 (97%)	8 (3%)	0	100	100
3	K	267/270 (99%)	259 (97%)	8 (3%)	0	100	100
4	D	128/130 (98%)	123 (96%)	5 (4%)	0	100	100
4	L	128/130 (98%)	124 (97%)	4 (3%)	0	100	100
5	F	330/349 (95%)	328 (99%)	2 (1%)	0	100	100
5	N	326/349 (93%)	325 (100%)	1 (0%)	0	100	100
6	G	78/82 (95%)	78 (100%)	0	0	100	100
6	P	80/82 (98%)	80 (100%)	0	0	100	100
All	All	3603/3664 (98%)	3507 (97%)	95 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	382	PRO

### 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	472/470 (100%)	468 (99%)	4 (1%)	79	80
1	I	472/470 (100%)	467 (99%)	5 (1%)	70	71
2	B	362/361 (100%)	358 (99%)	4 (1%)	70	71
2	J	363/361 (101%)	359 (99%)	4 (1%)	70	71
3	C	203/204 (100%)	202 (100%)	1 (0%)	86	88
3	K	203/204 (100%)	203 (100%)	0	100	100
4	D	111/111 (100%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	L	111/111 (100%)	111 (100%)	0	100	100
5	F	301/312 (96%)	300 (100%)	1 (0%)	91	92
5	N	294/312 (94%)	294 (100%)	0	100	100
6	G	65/67 (97%)	64 (98%)	1 (2%)	60	59
6	P	67/67 (100%)	65 (97%)	2 (3%)	36	30
All	All	3024/3050 (99%)	3002 (99%)	22 (1%)	81	83

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	424	SER
2	J	308	TYR
2	J	278	ASP
2	J	351	GLN
2	B	351	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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
1	KCX	I	178	1,7	9,11,12	0.77	0	5,12,14	0.35	0
1	KCX	A	178	1,7	9,11,12	1.90	1 (11%)	5,12,14	2.17	1 (20%)

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
1	KCX	I	178	1,7	-	0/9/10/12	-
1	KCX	A	178	1,7	-	0/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	KCX	OQ1-CX	5.51	1.31	1.21

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	KCX	OQ1-CX-NZ	-4.69	117.69	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 70 ligands modelled in this entry, 33 are monoatomic and 2 are modelled with single atom - leaving 35 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
12	SF4	F	407	5	0,12,12	-	-	-		
12	SF4	N	501	5	0,12,12	-	-	-		
12	SF4	F	408	5	0,12,12	-	-	-		
12	SF4	N	504	5	0,12,12	-	-	-		
11	GOL	A	608	-	5,5,5	0.19	0	5,5,5	0.26	0
11	GOL	I	609	-	5,5,5	0.19	0	5,5,5	0.27	0
12	SF4	F	402	5	0,12,12	-	-	-		
11	GOL	I	608	-	5,5,5	0.09	0	5,5,5	0.15	0
12	SF4	N	503	5	0,12,12	-	-	-		
11	GOL	A	609	-	5,5,5	0.14	0	5,5,5	0.33	0
12	SF4	F	401	5	0,12,12	-	-	-		
12	SF4	P	201	6	0,12,12	-	-	-		
12	SF4	B	501	2	0,12,12	-	-	-		
14	MGD	B	503	13	41,52,52	1.27	2 (4%)	40,81,81	1.54	8 (20%)
11	GOL	N	513	-	5,5,5	0.24	0	5,5,5	0.46	0
12	SF4	F	406	5	0,12,12	-	-	-		
14	MGD	J	503	13	41,52,52	1.21	3 (7%)	40,81,81	1.32	3 (7%)
12	SF4	P	200	6	0,12,12	-	-	-		
14	MGD	B	504	13	41,52,52	1.25	3 (7%)	40,81,81	1.44	6 (15%)
12	SF4	N	506	5	0,12,12	-	-	-		
12	SF4	F	403	5	0,12,12	-	-	-		
11	GOL	A	607	-	5,5,5	0.07	0	5,5,5	0.12	0
11	GOL	I	607	-	5,5,5	0.12	0	5,5,5	0.18	0
11	GOL	J	507	-	5,5,5	0.06	0	5,5,5	0.35	0
12	SF4	G	102	6	0,12,12	-	-	-		
12	SF4	N	508	5	0,12,12	-	-	-		
12	SF4	J	501	2	0,12,12	-	-	-		
12	SF4	N	505	5	0,12,12	-	-	-		
12	SF4	F	405	5	0,12,12	-	-	-		
11	GOL	B	507	-	5,5,5	0.07	0	5,5,5	0.21	0
12	SF4	N	507	5	0,12,12	-	-	-		
12	SF4	G	101	6	0,12,12	-	-	-		
12	SF4	N	502	5	0,12,12	-	-	-		
14	MGD	J	504	13	41,52,52	1.24	2 (4%)	40,81,81	1.52	9 (22%)
12	SF4	F	404	5	0,12,12	-	-	-		

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
12	SF4	F	407	5	-	-	0/6/5/5
12	SF4	N	501	5	-	-	0/6/5/5
12	SF4	F	408	5	-	-	0/6/5/5
12	SF4	N	504	5	-	-	0/6/5/5
11	GOL	A	608	-	-	2/4/4/4	-
11	GOL	I	609	-	-	0/4/4/4	-
12	SF4	F	402	5	-	-	0/6/5/5
11	GOL	I	608	-	-	0/4/4/4	-
12	SF4	N	503	5	-	-	0/6/5/5
11	GOL	A	609	-	-	0/4/4/4	-
12	SF4	F	401	5	-	-	0/6/5/5
12	SF4	P	201	6	-	-	0/6/5/5
12	SF4	B	501	2	-	-	0/6/5/5
14	MGD	B	503	13	-	7/18/66/66	0/6/6/6
11	GOL	N	513	-	-	2/4/4/4	-
12	SF4	F	406	5	-	-	0/6/5/5
14	MGD	J	503	13	-	2/18/66/66	0/6/6/6
14	MGD	B	504	13	-	0/18/66/66	0/6/6/6
12	SF4	P	200	6	-	-	0/6/5/5
12	SF4	N	506	5	-	-	0/6/5/5
12	SF4	F	403	5	-	-	0/6/5/5
11	GOL	A	607	-	-	0/4/4/4	-
11	GOL	I	607	-	-	0/4/4/4	-
11	GOL	J	507	-	-	0/4/4/4	-
12	SF4	G	102	6	-	-	0/6/5/5
12	SF4	N	508	5	-	-	0/6/5/5
12	SF4	J	501	2	-	-	0/6/5/5
12	SF4	N	505	5	-	-	0/6/5/5
12	SF4	F	405	5	-	-	0/6/5/5
11	GOL	B	507	-	-	1/4/4/4	-
12	SF4	N	507	5	-	-	0/6/5/5
12	SF4	G	101	6	-	-	0/6/5/5
12	SF4	N	502	5	-	-	0/6/5/5
14	MGD	J	504	13	-	7/18/66/66	0/6/6/6
12	SF4	F	404	5	-	-	0/6/5/5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	B	504	MGD	C16-C21	5.59	1.48	1.38
14	B	503	MGD	C16-C21	5.43	1.47	1.38
14	J	504	MGD	C16-C21	5.17	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	J	503	MGD	C16-C21	5.17	1.47	1.38
14	B	504	MGD	C16-C17	2.61	1.49	1.42

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	503	MGD	C19-N20-C21	4.11	120.84	113.43
14	J	504	MGD	C19-N20-C21	4.03	120.70	113.43
14	B	504	MGD	O11-C23-C14	3.63	111.39	108.96
14	B	503	MGD	O11-C23-C14	-3.54	106.60	108.96
14	B	504	MGD	C19-N20-C21	3.35	119.47	113.43

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

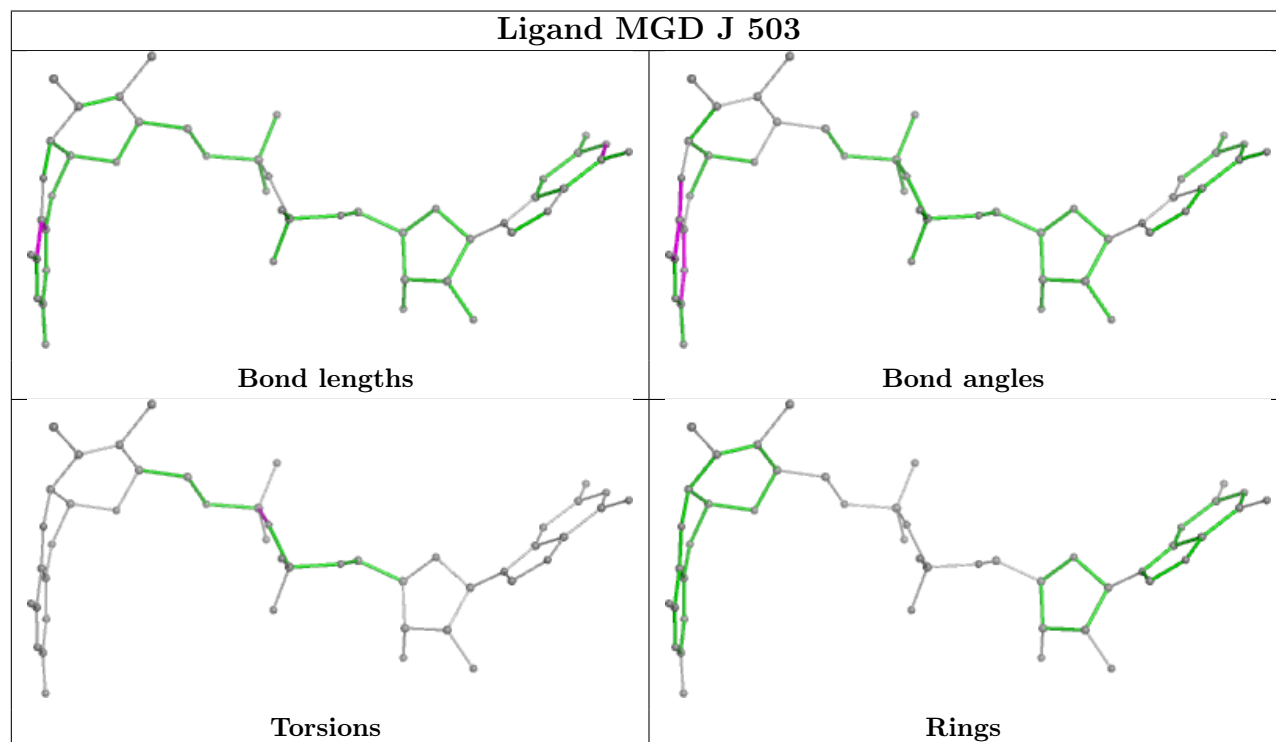
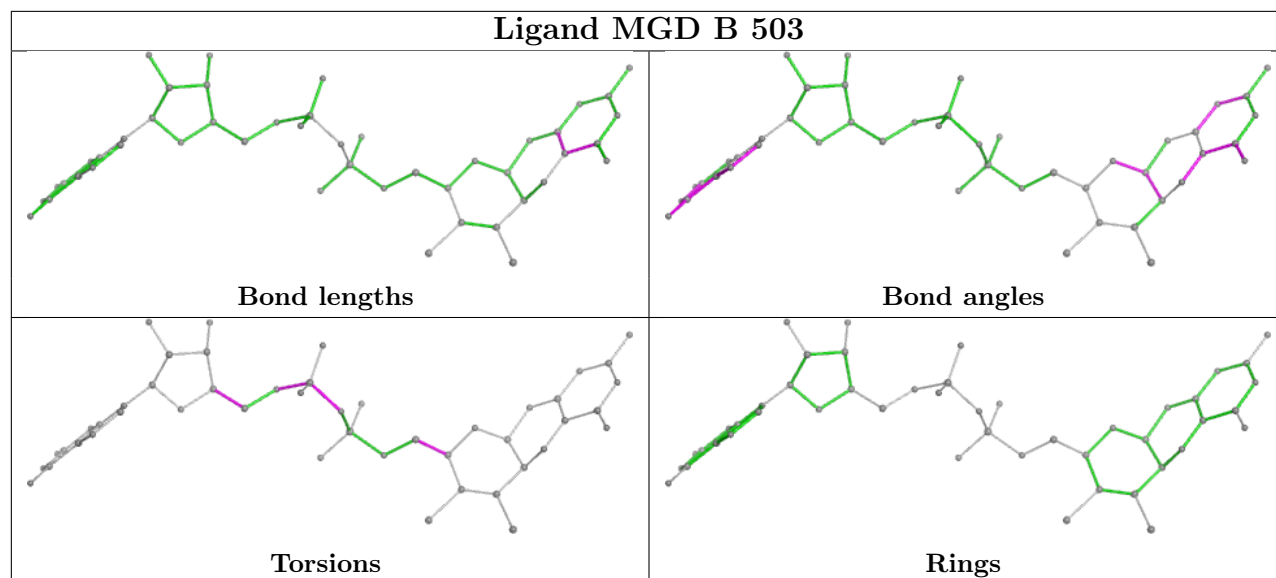
Mol	Chain	Res	Type	Atoms
11	A	608	GOL	C1-C2-C3-O3
11	A	608	GOL	O2-C2-C3-O3
11	N	513	GOL	O1-C1-C2-C3
14	B	503	MGD	C5'-O5'-PB-O2B
14	B	503	MGD	O3A-C10-C11-C12

There are no ring outliers.

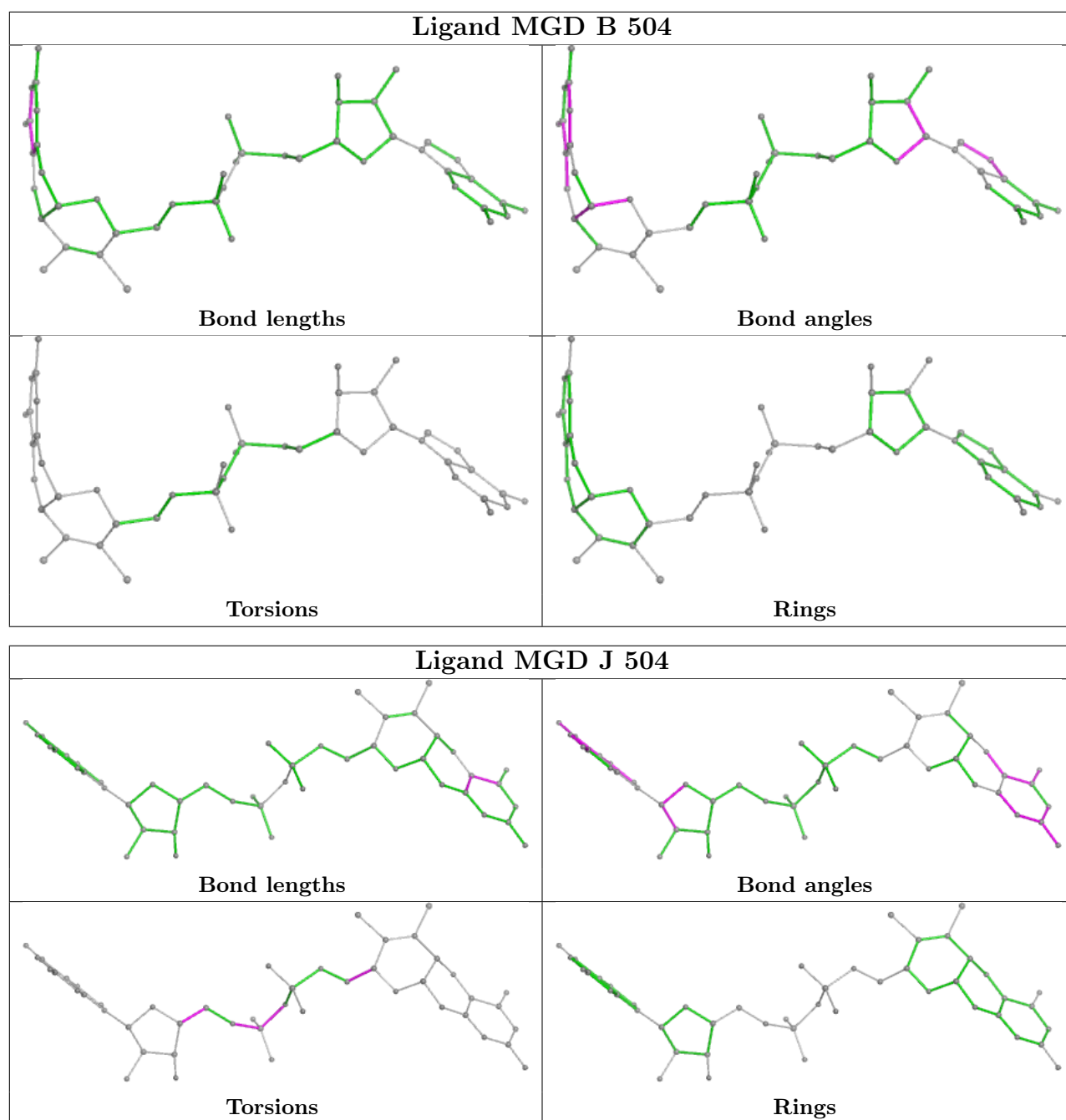
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	J	503	MGD	1	0
14	B	504	MGD	1	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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	568/569 (99%)	-0.26	2 (0%) 89 90	17, 28, 50, 73	2 (0%)
1	I	568/569 (99%)	-0.43	1 (0%) 92 92	15, 24, 44, 61	2 (0%)
2	B	430/432 (99%)	-0.29	2 (0%) 87 88	16, 25, 45, 85	3 (0%)
2	J	431/432 (99%)	-0.44	6 (1%) 73 75	15, 23, 43, 96	3 (0%)
3	C	269/270 (99%)	-0.11	1 (0%) 89 90	20, 30, 50, 66	0
3	K	269/270 (99%)	-0.32	1 (0%) 89 90	19, 27, 45, 59	0
4	D	130/130 (100%)	-0.16	2 (1%) 71 74	22, 29, 47, 78	0
4	L	130/130 (100%)	-0.35	1 (0%) 82 84	18, 25, 41, 72	0
5	F	335/349 (95%)	0.41	19 (5%) 30 32	20, 37, 71, 104	1 (0%)
5	N	329/349 (94%)	0.06	8 (2%) 59 61	15, 31, 56, 81	1 (0%)
6	G	80/82 (97%)	-0.24	1 (1%) 74 76	21, 27, 43, 49	0
6	P	81/82 (98%)	-0.43	1 (1%) 76 78	14, 23, 37, 90	1 (1%)
All	All	3620/3664 (98%)	-0.22	45 (1%) 76 78	14, 27, 51, 104	13 (0%)

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	N	213	CYS	6.3
2	B	430	ALA	6.2
1	A	83	PHE	4.8
5	F	225	THR	4.6
5	F	17	THR	4.5

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	KCX	A	178	12/13	0.98	0.04	17,19,23,23	0
1	KCX	I	178	12/13	0.98	0.04	15,17,19,21	0

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
11	GOL	A	609	6/6	0.75	0.20	74,76,77,77	0
11	GOL	I	609	6/6	0.80	0.20	44,52,55,55	0
11	GOL	A	608	6/6	0.84	0.18	40,49,52,54	0
11	GOL	I	608	6/6	0.85	0.19	68,68,70,72	0
11	GOL	N	513	6/6	0.85	0.18	36,40,49,55	0
11	GOL	A	607	6/6	0.86	0.14	43,45,45,46	0
11	GOL	I	607	6/6	0.90	0.11	37,39,39,40	0
11	GOL	B	507	6/6	0.90	0.12	51,53,58,61	0
11	GOL	J	507	6/6	0.91	0.11	46,47,50,51	0
9	K	F	410	1/1	0.94	0.10	42,42,42,42	0
9	K	N	511	1/1	0.95	0.09	39,39,39,39	0
9	K	I	604	1/1	0.96	0.14	45,45,45,45	0
9	K	F	413	1/1	0.97	0.09	42,42,42,42	0
9	K	F	409	1/1	0.97	0.09	38,38,38,38	0
9	K	A	605	1/1	0.97	0.10	49,49,49,49	0
15	H2S	J	505	1/1	0.97	0.06	19,19,19,19	0
9	K	N	509	1/1	0.98	0.07	32,32,32,32	0
9	K	G	104	1/1	0.98	0.05	46,46,46,46	0
9	K	N	512	1/1	0.98	0.04	35,35,35,35	0
10	NA	A	610	1/1	0.98	0.04	25,25,25,25	0
12	SF4	F	403	8/8	0.98	0.04	35,38,39,39	0
14	MGD	B	503	47/47	0.98	0.05	16,22,26,32	0
14	MGD	B	504	47/47	0.98	0.05	18,21,23,23	0
14	MGD	J	503	47/47	0.98	0.04	15,19,21,21	0

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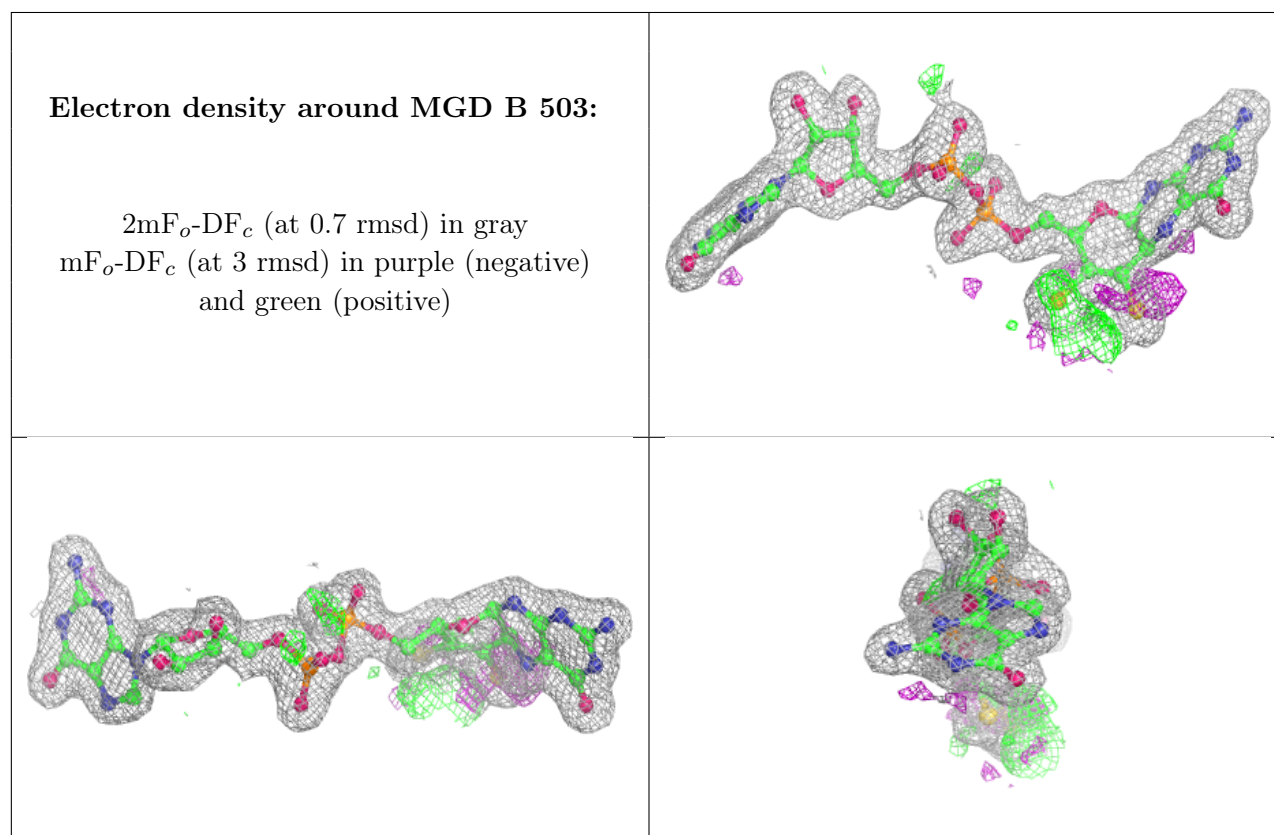
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	MGD	J	504	47/47	0.98	0.05	11,20,23,25	0
15	H2S	B	505	1/1	0.98	0.07	20,20,20,20	0
10	NA	I	606	1/1	0.98	0.08	20,20,20,20	0
9	K	F	411	1/1	0.99	0.06	37,37,37,37	0
9	K	J	506	1/1	0.99	0.03	26,26,26,26	0
10	NA	I	610	1/1	0.99	0.08	28,28,28,28	0
12	SF4	B	501	8/8	0.99	0.03	20,22,22,22	0
12	SF4	F	401	8/8	0.99	0.02	23,26,27,27	0
10	NA	L	201	1/1	0.99	0.08	22,22,22,22	0
12	SF4	F	404	8/8	0.99	0.03	28,28,30,32	0
12	SF4	F	405	8/8	0.99	0.03	26,28,30,30	0
12	SF4	F	406	8/8	0.99	0.02	28,29,30,31	0
12	SF4	F	407	8/8	0.99	0.03	28,29,32,32	0
12	SF4	F	408	8/8	0.99	0.03	30,31,32,33	0
12	SF4	G	101	8/8	0.99	0.02	22,23,25,25	0
12	SF4	N	504	8/8	0.99	0.03	22,23,24,26	0
12	SF4	N	505	8/8	0.99	0.03	29,31,31,33	0
12	SF4	N	506	8/8	0.99	0.03	30,31,33,33	0
12	SF4	N	507	8/8	0.99	0.02	22,23,25,26	0
12	SF4	P	200	8/8	0.99	0.02	20,21,22,22	0
9	K	F	412	1/1	0.99	0.06	34,34,34,34	0
9	K	N	510	1/1	0.99	0.06	28,28,28,28	0
9	K	A	604	1/1	0.99	0.03	21,21,21,21	0
9	K	B	506	1/1	0.99	0.05	32,32,32,32	0
9	K	P	202	1/1	0.99	0.03	25,25,25,25	0
10	NA	A	606	1/1	0.99	0.06	21,21,21,21	0
16	CA	B	508	1/1	0.99	0.04	25,25,25,25	0
12	SF4	N	502	8/8	1.00	0.02	19,19,20,21	0
12	SF4	N	503	8/8	1.00	0.02	19,21,21,22	0
7	ZN	I	601	1/1	1.00	0.03	22,22,22,22	0
12	SF4	F	402	8/8	1.00	0.02	23,24,25,26	0
7	ZN	I	602	1/1	1.00	0.02	24,24,24,24	0
9	K	I	605	1/1	1.00	0.02	20,20,20,20	0
12	SF4	N	508	8/8	1.00	0.02	20,21,22,22	0
8	MG	A	603	1/1	1.00	0.05	16,16,16,16	0
12	SF4	P	201	8/8	1.00	0.02	19,20,21,23	0
13	W	B	502	1/1	1.00	0.11	29,29,29,29	0
13	W	J	502	1/1	1.00	0.11	25,25,25,25	0
8	MG	I	603	1/1	1.00	0.07	13,13,13,13	0
7	ZN	A	601	1/1	1.00	0.02	25,25,25,25	0
7	ZN	A	602	1/1	1.00	0.02	24,24,24,24	0
9	K	G	103	1/1	1.00	0.04	27,27,27,27	0

*Continued on next page...*

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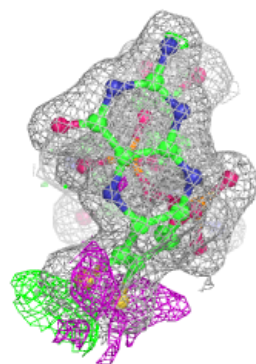
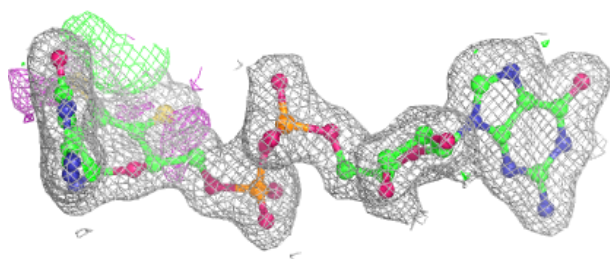
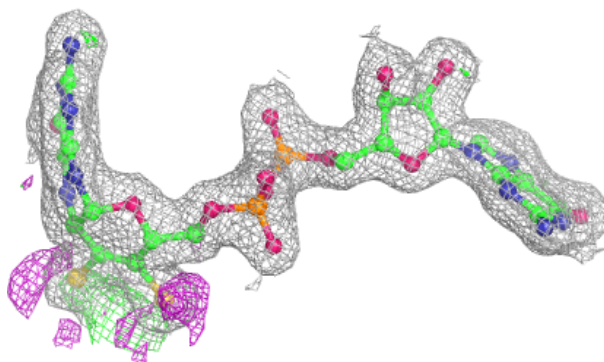
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	SF4	G	102	8/8	1.00	0.02	24,25,25,26	0
12	SF4	J	501	8/8	1.00	0.02	17,18,19,20	0
12	SF4	N	501	8/8	1.00	0.02	19,20,21,22	0
16	CA	J	508	1/1	1.00	0.02	24,24,24,24	0

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.

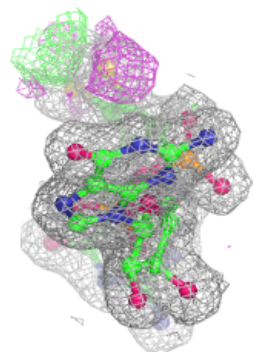
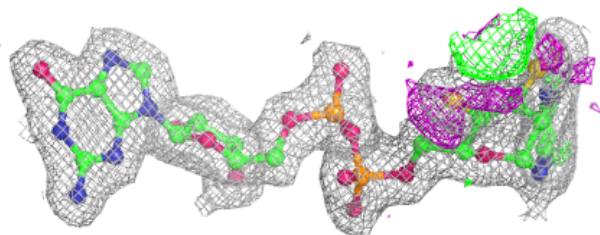
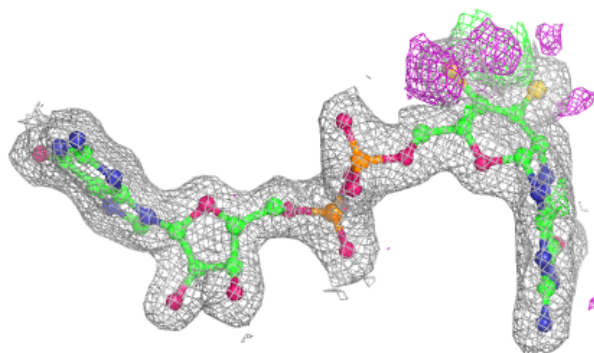


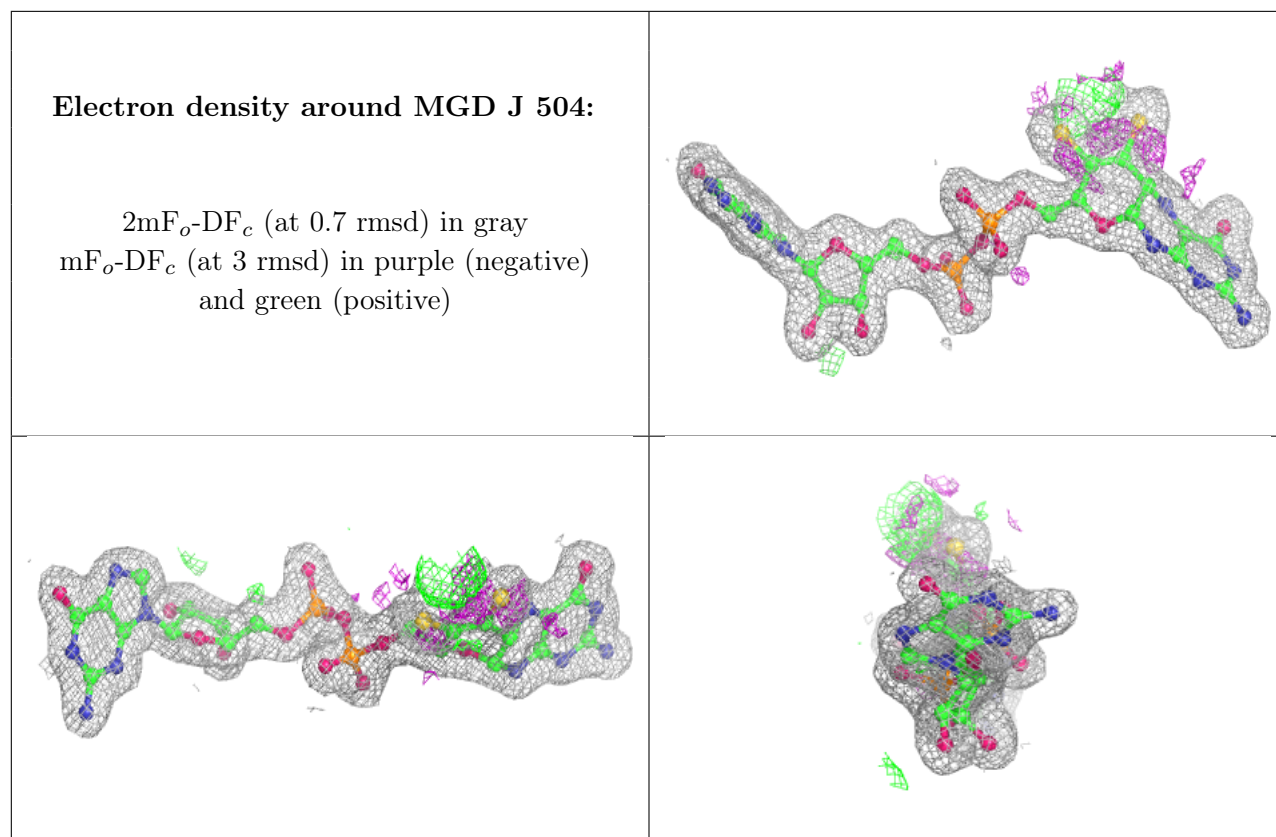
**Electron density around MGD B 504:**

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

**Electron density around MGD J 503:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.