



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2025 – 10:08 am BST

PDB ID : 8RAU / pdb\_00008rau  
Title : The crystal structure of DNA-bound human MutSbeta (MSH2/MSH3) in the canonical mismatch bound conformation with ADP bound in MSH2 and MSH3  
Authors : Thomsen, M.; Costanzi, E.  
Deposited on : 2023-12-01  
Resolution : 2.33 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](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>.

---

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
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) : 2.43.1

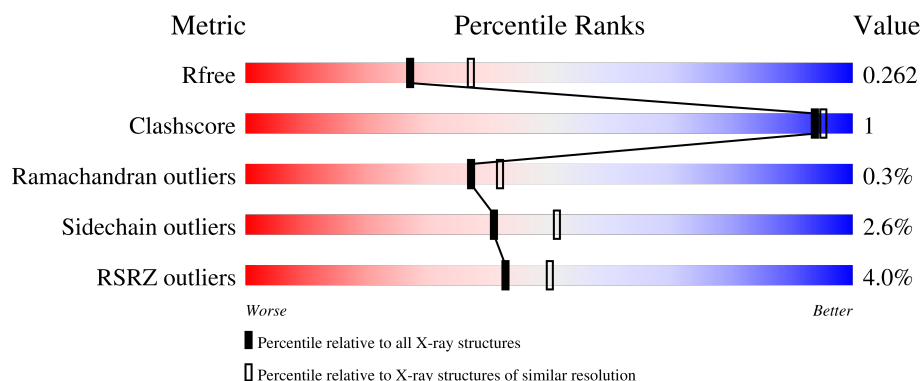
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

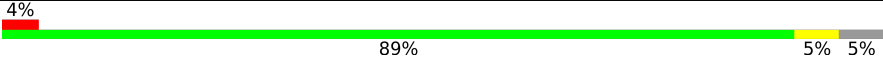
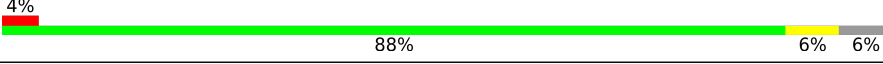
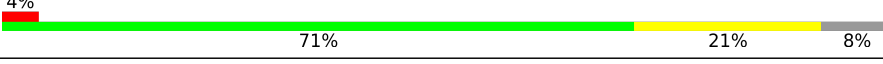

The reported resolution of this entry is 2.33 Å.

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	2747 (2.36-2.32)
Clashscore	180529	2936 (2.36-2.32)
Ramachandran outliers	177936	2912 (2.36-2.32)
Sidechain outliers	177891	2912 (2.36-2.32)
RSRZ outliers	164620	2747 (2.36-2.32)

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	934	
2	B	918	
3	C	24	
4	D	24	

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 15330 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 DNA mismatch repair protein Msh2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	883	Total	C	N	O	S	252	2	0
			6992	4433	1188	1333	38			

- Molecule 2 is a protein called DNA mismatch repair protein Msh3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	863	Total	C	N	O	S	201	3	0
			6934	4424	1187	1290	33			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	217	GLY	-	expression tag	UNP P20585
B	218	PRO	-	expression tag	UNP P20585
B	949	ARG	GLN	conflict	UNP P20585

- Molecule 3 is a DNA chain called DNA (5'-D(\*TP\*CP\*TP\*AP\*TP\*CP\*TP\*GP\*AP\*AP\*GP\*CP\*CP\*GP\*AP\*TP\*CP\*GP\*AP\*TP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	22	Total	C	N	O	P	0	0	0
			449	215	82	131	21			

- Molecule 4 is a DNA chain called DNA (5'-D(\*TP\*CP\*AP\*TP\*CP\*GP\*AP\*TP\*CP\*GP\*CP\*AP\*GP\*CP\*TP\*TP\*CP\*AP\*GP\*AP\*TP\*AP\*GP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	24	Total	C	N	O	P	0	0	0
			489	234	90	142	23			

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
5	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $\text{C}_2\text{H}_6\text{O}_2$ ).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	170	Total	O	0	0
			170	170		
8	B	182	Total	O	0	0
			182	182		
8	C	9	Total	O	0	0
			9	9		

*Continued on next page...*

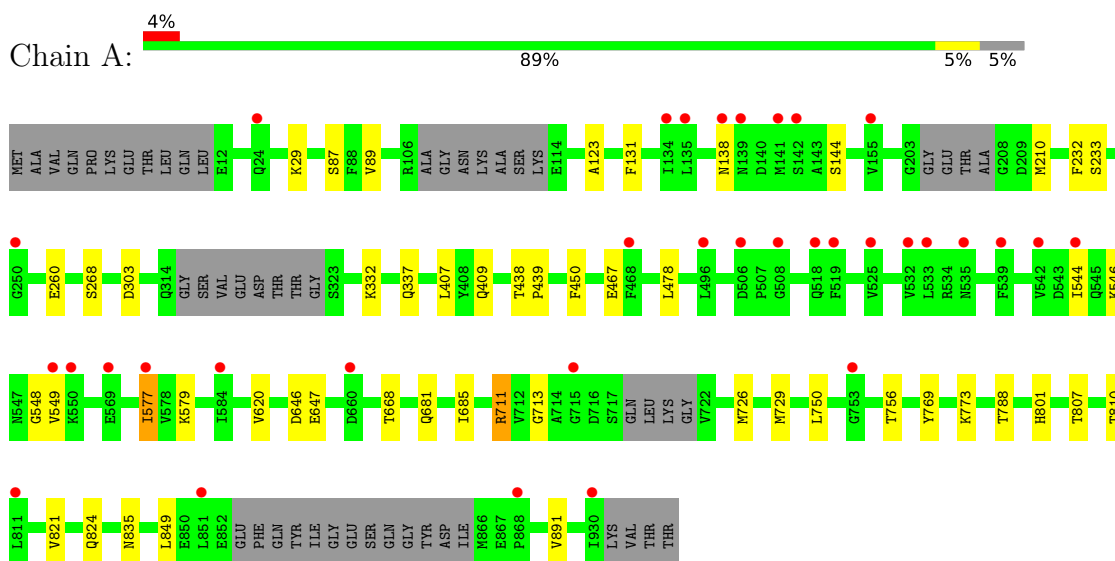
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	13	Total	O	0	0
			13	13		

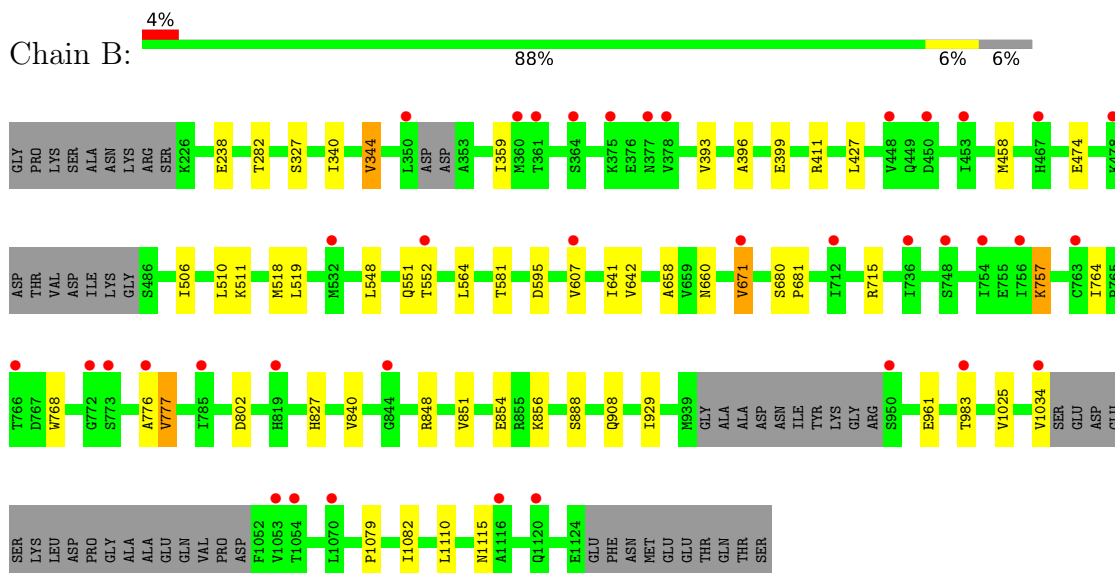
### 3 Residue-property plots [i](#)

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.

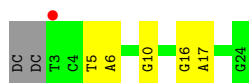
- Molecule 1: DNA mismatch repair protein Msh2



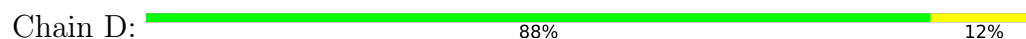
- Molecule 2: DNA mismatch repair protein Msh3



- Molecule 3: DNA (5'-D(\*TP\*CP\*TP\*AP\*TP\*CP\*TP\*GP\*AP\*AP\*GP\*CP\*CP\*GP\*AP\*TP\*CP\*GP\*AP\*TP\*GP\*G)-3')



● Molecule 4: DNA (5'-D(\*TP\*CP\*AP\*TP\*CP\*GP\*AP\*TP\*CP\*GP\*CP\*AP\*GP\*CP\*TP\*TP\*CP\*AP\*GP\*AP\*TP\*AP\*GP\*G)-3')





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.84Å 91.88Å 94.12Å 67.32° 86.93° 75.69°	Depositor
Resolution (Å)	46.45 – 2.33 46.45 – 2.33	Depositor EDS
% Data completeness (in resolution range)	94.2 (46.45-2.33) 94.2 (46.45-2.33)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.222 , 0.258 0.224 , 0.262	Depositor DCC
$R_{free}$ test set	1226 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.5	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 67.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15330	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.03	0/7100	1.54	8/9565 (0.1%)
2	B	1.03	0/7060	1.55	7/9529 (0.1%)
3	C	0.34	0/503	0.82	1/775 (0.1%)
4	D	0.34	0/548	0.83	1/844 (0.1%)
All	All	1.00	0/15211	1.50	17/20713 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	39	DC	C2'-C3'-O3'	6.92	121.88	111.50
2	B	1025	VAL	CA-C-N	5.97	126.21	121.61
2	B	1025	VAL	C-N-CA	5.97	126.21	121.61
2	B	344	VAL	CB-CA-C	5.92	116.19	110.63
1	A	579	LYS	CA-C-N	5.53	127.63	120.44
1	A	579	LYS	C-N-CA	5.53	127.63	120.44
3	C	10	DG	C4'-C3'-O3'	5.50	118.25	110.00
1	A	548	GLY	CA-C-O	-5.42	118.70	122.22
1	A	337	GLN	CA-C-N	5.26	125.68	119.94
1	A	337	GLN	C-N-CA	5.26	125.68	119.94
2	B	1079	PRO	CA-C-N	5.12	125.66	119.98
2	B	1079	PRO	C-N-CA	5.12	125.66	119.98
2	B	854	GLU	CA-C-N	5.08	128.32	121.05
2	B	854	GLU	C-N-CA	5.08	128.32	121.05
1	A	303	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	409	GLN	CA-C-N	5.02	125.52	119.94
1	A	409	GLN	C-N-CA	5.02	125.52	119.94

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	6992	0	7044	16	0
2	B	6934	0	7053	21	0
3	C	449	0	250	2	0
4	D	489	0	272	1	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	20	0	30	0	0
7	B	16	0	24	0	0
8	A	170	0	0	1	0
8	B	182	0	0	2	0
8	C	9	0	0	0	0
8	D	13	0	0	0	0
All	All	15330	0	14697	38	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 1.

All (38) 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)
2:B:581:THR:HG21	8:B:1320:HOH:O	1.97	0.64
2:B:393:VAL:HB	2:B:518:MET:CE	2.32	0.60
2:B:776:ALA:O	2:B:777:VAL:HG22	2.05	0.57
1:A:681:GLN:O	1:A:685:ILE:HG12	2.06	0.55
1:A:438:THR:HB	1:A:439:PRO:HD3	1.91	0.53
1:A:788:THR:HG21	1:A:821:VAL:HG13	1.89	0.53
2:B:595:ASP:OD1	2:B:848:ARG:NH2	2.38	0.53
1:A:407:LEU:HD23	1:A:450:PHE:CZ	2.44	0.52
2:B:427:LEU:HD11	2:B:458:MET:HE3	1.91	0.52
4:D:42:DC:H2"	4:D:43:DA:C8	2.46	0.50
2:B:548:LEU:HD21	2:B:581:THR:CG2	2.42	0.49
2:B:393:VAL:HB	2:B:518:MET:HE2	1.95	0.47
1:A:478:LEU:HD11	1:A:577:ILE:HD11	1.96	0.47

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PHE:O	1:A:268:SER:OG	2.27	0.47
3:C:5:DT:H2"	3:C:6:DA:C8	2.50	0.47
1:A:478:LEU:HD11	1:A:577:ILE:CD1	2.45	0.47
2:B:607:VAL:HG21	2:B:658:ALA:HB1	1.97	0.46
1:A:89:VAL:HG11	1:A:131:PHE:CD2	2.52	0.45
1:A:769:TYR:CZ	1:A:773:LYS:HG2	2.51	0.45
3:C:16:DG:H2'	3:C:17:DA:C8	2.52	0.44
2:B:393:VAL:HG21	2:B:510:LEU:HD11	1.99	0.44
2:B:511:LYS:NZ	8:B:1308:HOH:O	2.51	0.44
2:B:851:VAL:HA	2:B:929:ILE:O	2.18	0.44
2:B:671:VAL:HG22	2:B:827:HIS:ND1	2.33	0.43
2:B:715:ARG:NH1	2:B:802:ASP:OD2	2.51	0.43
1:A:824:GLN:NE2	8:A:1109:HOH:O	2.52	0.42
2:B:506:ILE:HG22	2:B:519:LEU:HD11	2.02	0.42
2:B:757:LYS:HA	2:B:777:VAL:HA	2.01	0.42
1:A:668:THR:O	1:A:801:HIS:HA	2.20	0.41
1:A:891:VAL:HG11	2:B:1110:LEU:HD11	2.02	0.41
2:B:340:ILE:HD12	2:B:396:ALA:HA	2.02	0.41
2:B:680:SER:N	2:B:681:PRO:CD	2.84	0.41
2:B:764:ILE:HG23	2:B:768:TRP:CE3	2.55	0.41
1:A:123:ALA:HB2	1:A:131:PHE:CD1	2.56	0.41
1:A:711:ARG:NH2	1:A:713:GLY:O	2.52	0.41
1:A:729:MET:HE1	1:A:750:LEU:HD11	2.02	0.41
2:B:564:LEU:HA	2:B:840:VAL:HG21	2.01	0.41
1:A:769:TYR:CG	2:B:1082:ILE:HD11	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	873/934 (94%)	845 (97%)	26 (3%)	2 (0%)	44 51

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	856/918 (93%)	818 (96%)	34 (4%)	4 (0%)	25	27
All	All	1729/1852 (93%)	1663 (96%)	60 (4%)	6 (0%)	37	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	757	LYS
1	A	138	ASN
2	B	359	ILE
2	B	777	VAL
2	B	888	SER
1	A	835	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	770/808 (95%)	749 (97%)	21 (3%)	40	50
2	B	776/818 (95%)	757 (98%)	19 (2%)	44	54
All	All	1546/1626 (95%)	1506 (97%)	40 (3%)	41	51

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	87	SER
1	A	144	SER
1	A	210	MET
1	A	233	SER
1	A	260	GLU
1	A	332	LYS
1	A	467	GLU
1	A	544	ILE
1	A	546	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	549	VAL
1	A	577	ILE
1	A	620	VAL
1	A	646	ASP
1	A	647	GLU
1	A	711	ARG
1	A	726	MET
1	A	756	THR
1	A	807	THR
1	A	810	THR
1	A	849	LEU
2	B	238	GLU
2	B	282	THR
2	B	327	SER
2	B	344	VAL
2	B	399	GLU
2	B	411	ARG
2	B	474	GLU
2	B	551	GLN
2	B	552	THR
2	B	641	ILE
2	B	642	VAL
2	B	660	ASN
2	B	671	VAL
2	B	856	LYS
2	B	908	GLN
2	B	961	GLU
2	B	983	THR
2	B	1034	VAL
2	B	1115	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	215	GLN
1	A	218	GLN
1	A	288	GLN
1	A	374	GLN
1	A	413	GLN
1	A	416	ASN
1	A	681	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	801	HIS
1	A	839	HIS
2	B	321	ASN
2	B	377	ASN
2	B	524	ASN
2	B	591	ASN
2	B	610	GLN
2	B	739	ASN
2	B	817	HIS
2	B	852	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\# Z  > 2$
7	EDO	A	1006	-	3,3,3	0.08	0	2,2,2	0.25	0
7	EDO	A	1007	-	3,3,3	0.06	0	2,2,2	0.26	0
7	EDO	B	1205	-	3,3,3	0.09	0	2,2,2	0.23	0
7	EDO	A	1004	-	3,3,3	0.13	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	EDO	B	1203	-	3,3,3	0.11	0	2,2,2	0.32	0
7	EDO	B	1204	-	3,3,3	0.08	0	2,2,2	0.25	0
5	ADP	B	1201	6	24,29,29	0.66	0	29,45,45	0.74	1 (3%)
5	ADP	A	1001	6	24,29,29	0.66	0	29,45,45	0.80	1 (3%)
7	EDO	B	1206	-	3,3,3	0.05	0	2,2,2	0.24	0
7	EDO	A	1005	-	3,3,3	0.09	0	2,2,2	0.31	0
7	EDO	A	1003	-	3,3,3	0.12	0	2,2,2	0.39	0

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
7	EDO	A	1006	-	-	0/1/1/1	-
7	EDO	A	1007	-	-	0/1/1/1	-
7	EDO	B	1205	-	-	0/1/1/1	-
7	EDO	A	1004	-	-	1/1/1/1	-
7	EDO	B	1203	-	-	1/1/1/1	-
7	EDO	B	1204	-	-	0/1/1/1	-
5	ADP	B	1201	6	-	2/12/32/32	0/3/3/3
5	ADP	A	1001	6	-	2/12/32/32	0/3/3/3
7	EDO	B	1206	-	-	0/1/1/1	-
7	EDO	A	1005	-	-	0/1/1/1	-
7	EDO	A	1003	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	ADP	C5-C6-N6	2.11	123.57	120.35
5	B	1201	ADP	C5-C6-N6	2.11	123.56	120.35

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	ADP	PA-O3A-PB-O2B
5	B	1201	ADP	PA-O3A-PB-O2B
7	A	1003	EDO	O1-C1-C2-O2

*Continued on next page...*



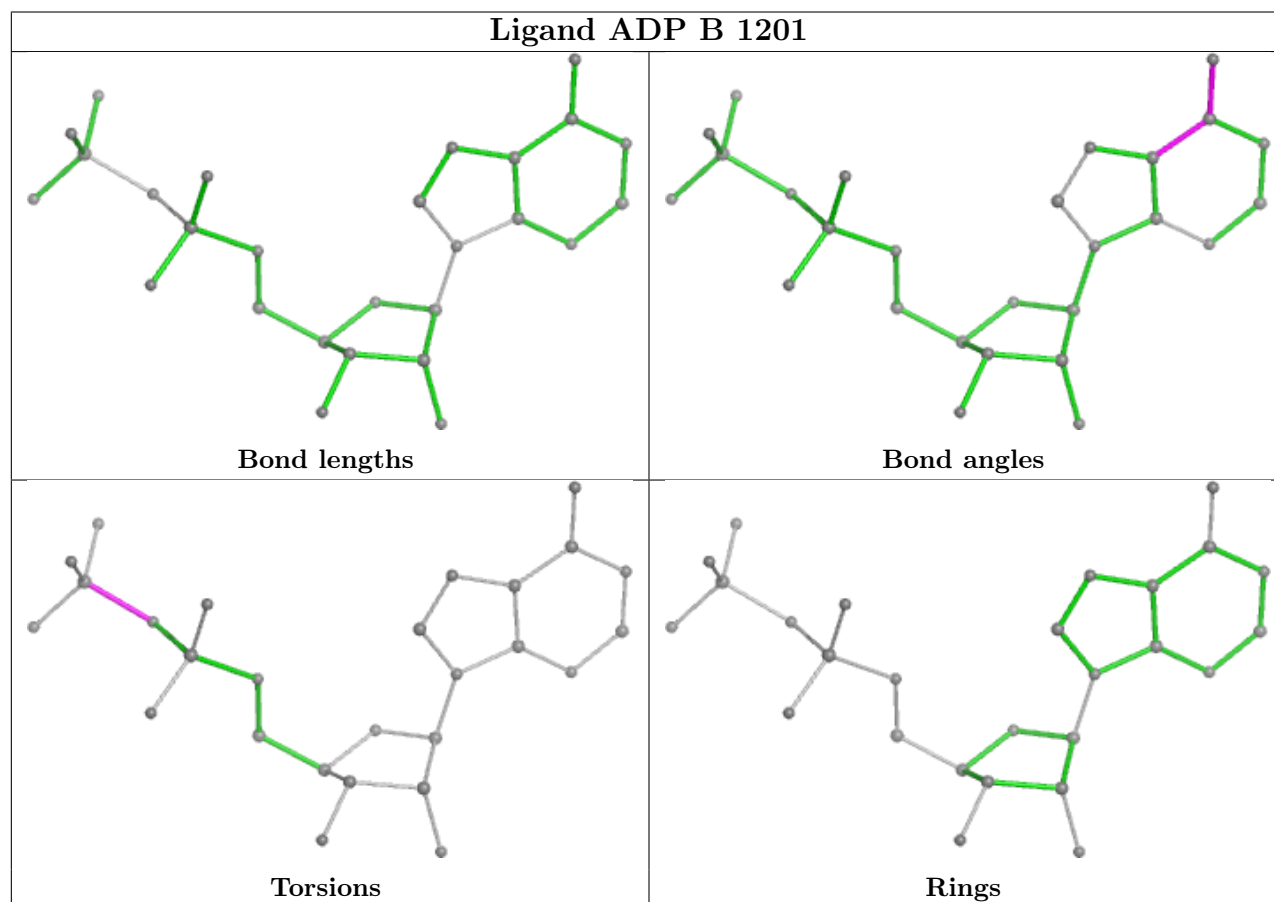
*Continued from previous page...*

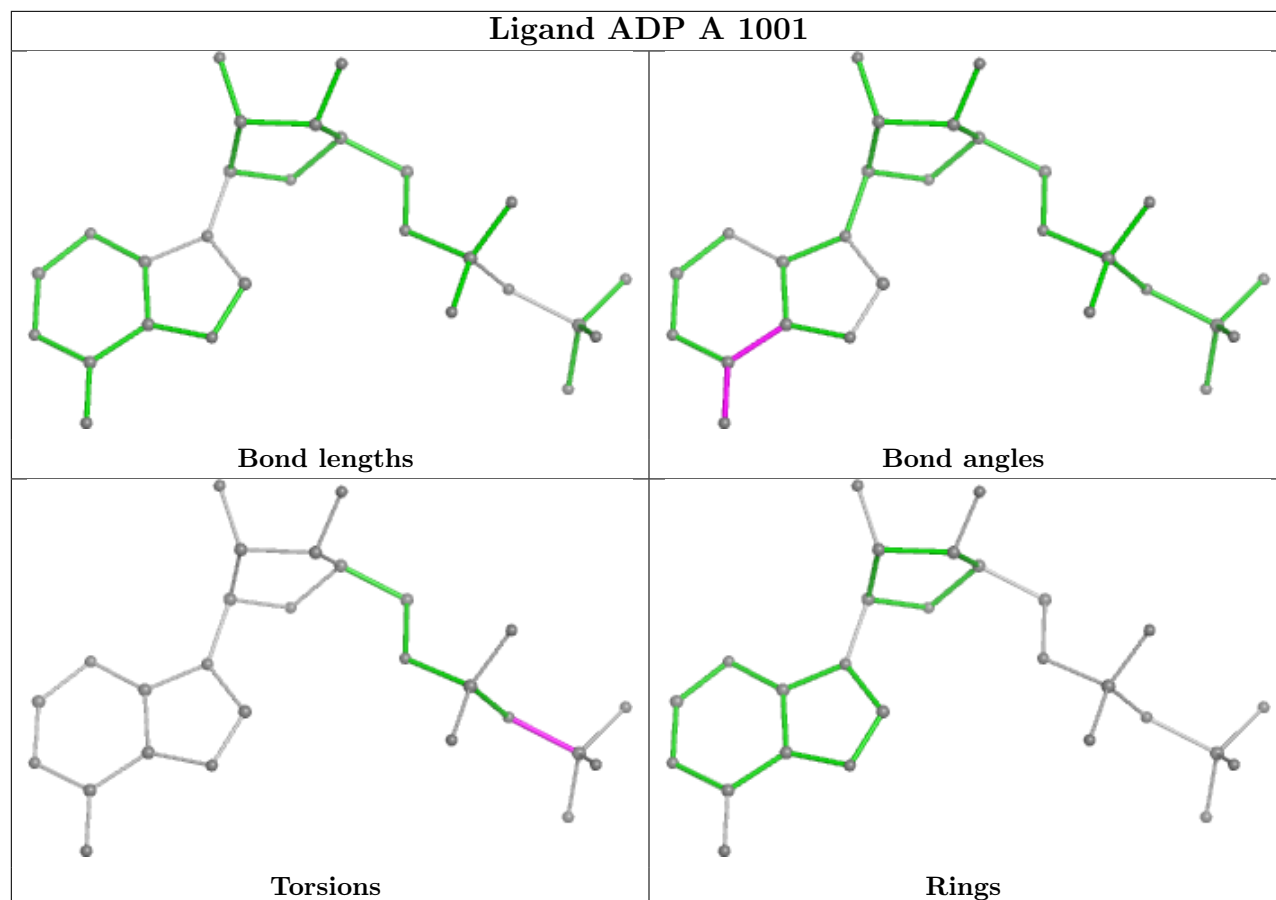
Mol	Chain	Res	Type	Atoms
7	A	1004	EDO	O1-C1-C2-O2
5	B	1201	ADP	PA-O3A-PB-O1B
7	B	1203	EDO	O1-C1-C2-O2
5	A	1001	ADP	PA-O3A-PB-O1B

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.





## 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, 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	883/934 (94%)	0.56	34 (3%) 44 51	27, 68, 114, 151	73 (8%)
2	B	863/918 (94%)	0.50	37 (4%) 40 48	26, 64, 106, 146	67 (7%)
3	C	22/24 (91%)	0.27	1 (4%) 39 46	58, 116, 181, 224	0
4	D	24/24 (100%)	0.22	0 100 100	56, 104, 187, 236	0
All	All	1792/1900 (94%)	0.52	72 (4%) 43 50	26, 67, 115, 236	140 (7%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1053	VAL	4.2
1	A	519	PHE	3.7
1	A	930	ILE	3.4
1	A	250	GLY	3.3
2	B	378	VAL	3.2
2	B	448	VAL	3.1
1	A	539	PHE	3.0
1	A	24	GLN	2.9
2	B	1120	GLN	2.9
1	A	544	ILE	2.9
2	B	1034	VAL	2.8
1	A	549	VAL	2.8
2	B	754	ILE	2.8
1	A	506	ASP	2.8
2	B	350	LEU	2.8
2	B	364	SER	2.7
1	A	468	PHE	2.7
1	A	135	LEU	2.6
2	B	712	ILE	2.6
1	A	142	SER	2.6
2	B	748	SER	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	785	ILE	2.6
2	B	1070	LEU	2.6
2	B	478	LYS	2.5
1	A	715	GLY	2.5
1	A	525	VAL	2.5
1	A	577	ILE	2.5
2	B	607	VAL	2.5
2	B	766	THR	2.5
1	A	141	MET	2.5
2	B	532	MET	2.5
1	A	753	GLY	2.5
1	A	496	LEU	2.5
1	A	660	ASP	2.4
2	B	844	GLY	2.4
2	B	377	ASN	2.4
2	B	756	ILE	2.4
2	B	1054	THR	2.4
2	B	467	HIS	2.4
1	A	535	ASN	2.4
2	B	950	SER	2.3
1	A	811	LEU	2.3
2	B	776	ALA	2.3
2	B	1116	ALA	2.3
2	B	360	MET	2.3
2	B	361	THR	2.3
1	A	518	GLN	2.3
1	A	139	ASN	2.3
2	B	375	LYS	2.3
2	B	453	ILE	2.3
3	C	3	DT	2.3
2	B	819[A]	HIS	2.2
1	A	138	ASN	2.2
2	B	763	CYS	2.2
1	A	542	VAL	2.2
2	B	736	ILE	2.2
1	A	569	GLU	2.2
1	A	868	PRO	2.2
1	A	532	VAL	2.2
1	A	550	LYS	2.2
1	A	533	LEU	2.1
2	B	671	VAL	2.1
2	B	450	ASP	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	508	GLY	2.1
2	B	772	GLY	2.1
2	B	773	SER	2.1
1	A	851	LEU	2.1
1	A	155	VAL	2.1
1	A	134	ILE	2.1
2	B	552	THR	2.1
1	A	584	ILE	2.0
2	B	983	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

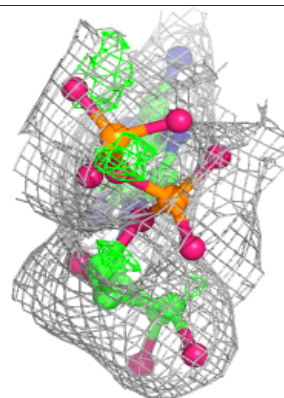
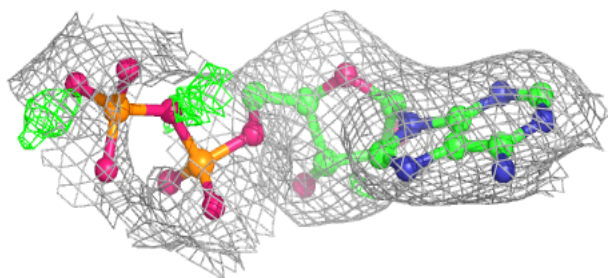
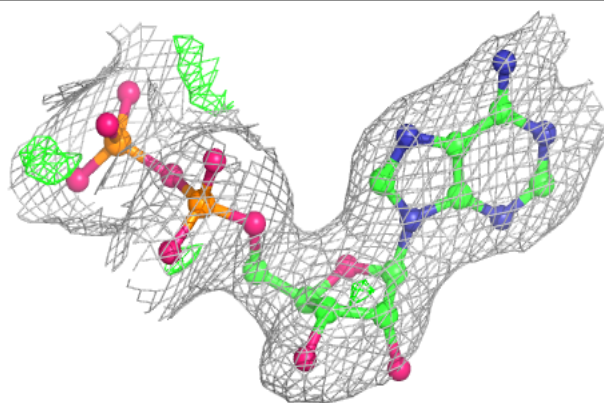
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	EDO	B	1204	4/4	0.73	0.13	91,94,94,95	0
7	EDO	A	1003	4/4	0.74	0.15	92,94,94,94	0
7	EDO	A	1007	4/4	0.83	0.16	95,96,97,98	0
7	EDO	B	1205	4/4	0.85	0.17	80,81,83,87	0
7	EDO	A	1005	4/4	0.86	0.12	88,89,89,90	0
7	EDO	A	1004	4/4	0.86	0.13	69,69,70,70	0
7	EDO	A	1006	4/4	0.87	0.14	62,63,66,68	0
7	EDO	B	1203	4/4	0.91	0.13	79,79,80,83	0
7	EDO	B	1206	4/4	0.93	0.12	69,69,71,72	0
5	ADP	B	1201	27/27	0.95	0.07	47,52,57,61	0
5	ADP	A	1001	27/27	0.95	0.07	48,53,59,63	0
6	MG	B	1202	1/1	0.96	0.04	49,49,49,49	0
6	MG	A	1002	1/1	0.99	0.02	52,52,52,52	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.

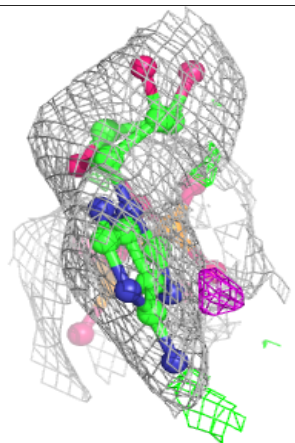
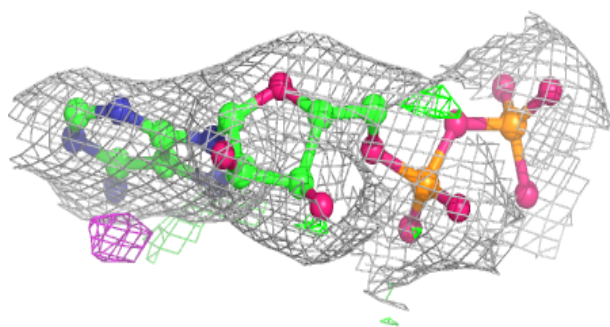
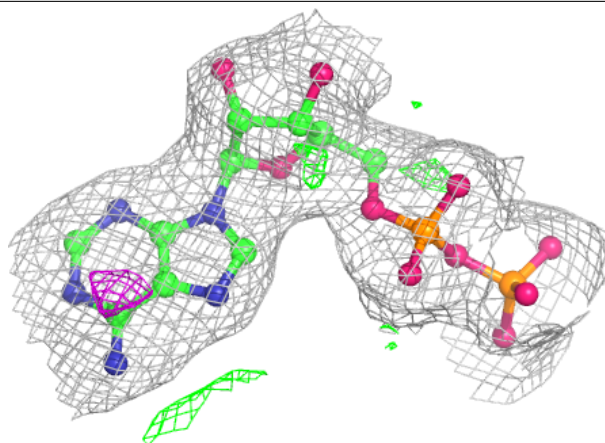
**Electron density around ADP B 1201:**

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



**Electron density around ADP A 1001:**

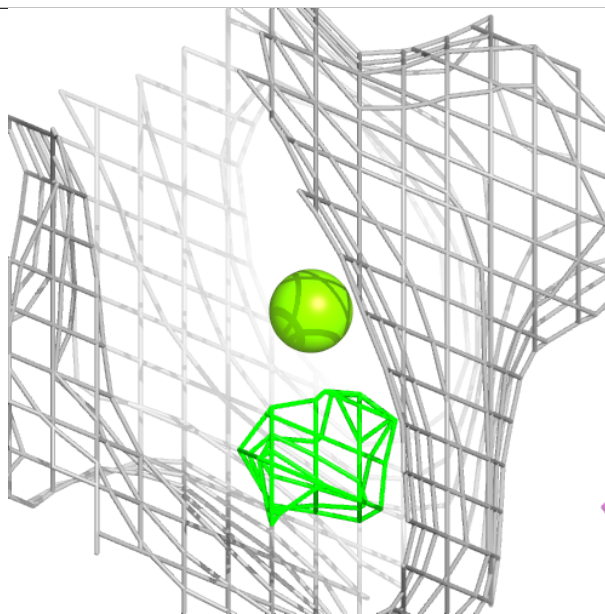
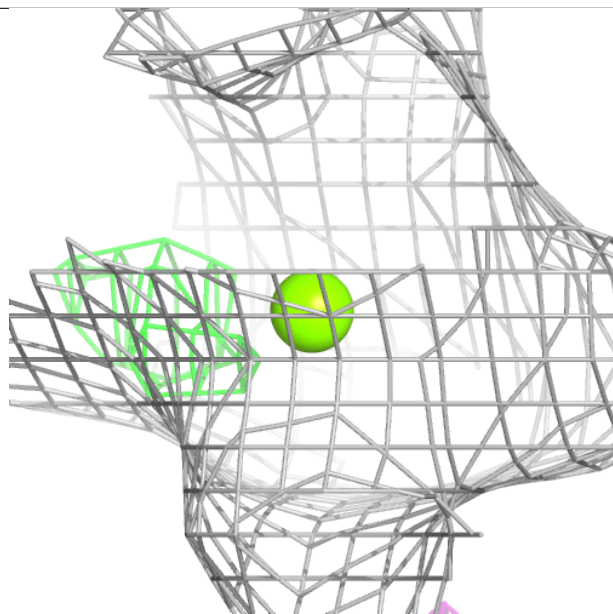
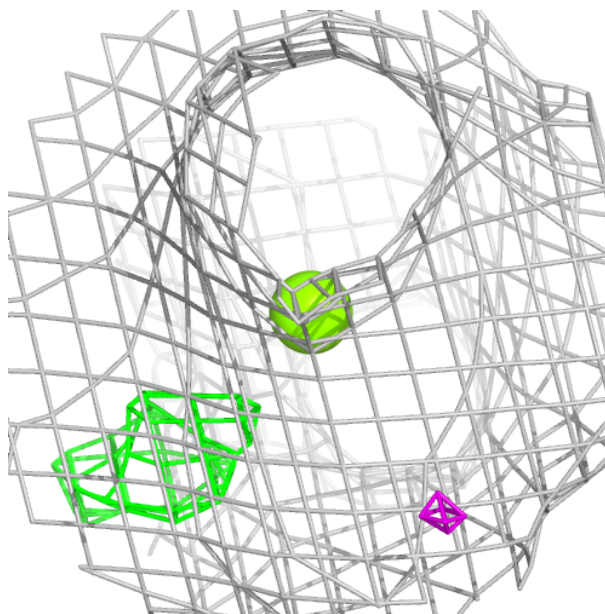
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MG B 1202:**

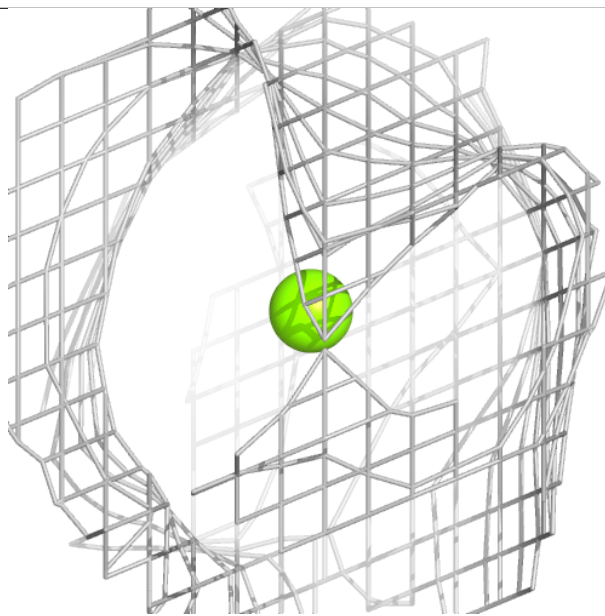
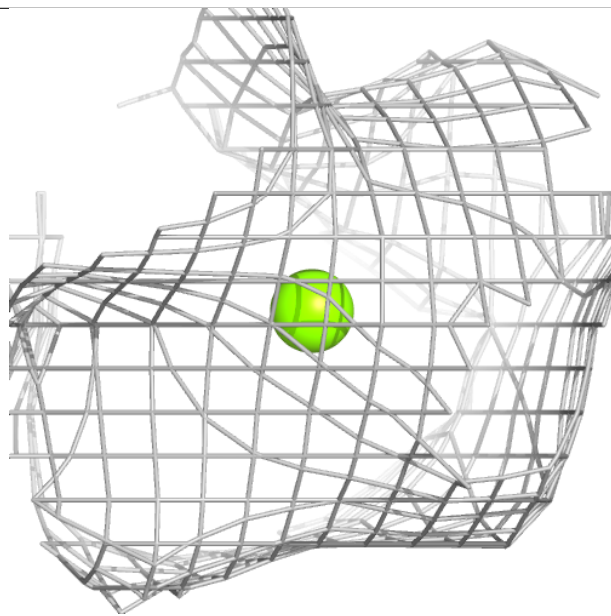
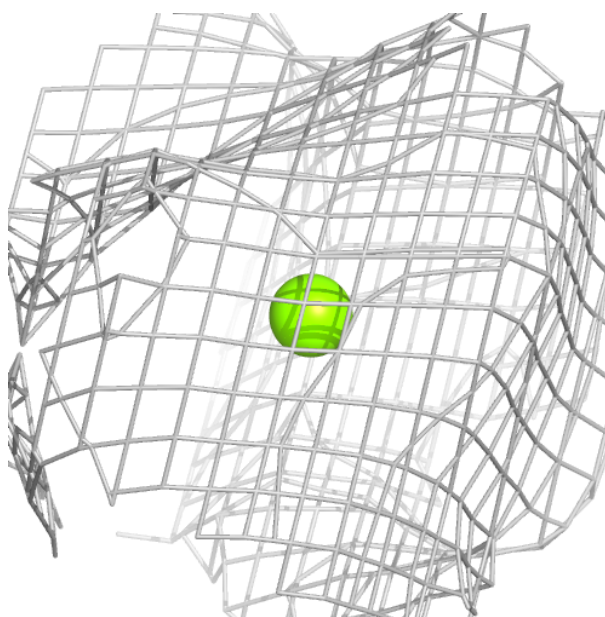
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around MG A 1002:**

$2mF_o-DF_c$  (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.