

wwPDB X-ray Structure Validation Summary Report (i)

Feb 8, 2023 - 09:28 am GMT

PDB ID : 8A3V

Title : Crystal structure of the Vibrio cholerae replicative helicase (VcDnaB) in com-

plex with its loader protein (VcDciA)

Authors: Walbott, H.; Quevillon-Cheruel, S.; Cargemel, C.

Deposited on : 2022-06-09

Resolution : 2.90 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
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.32.1 buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

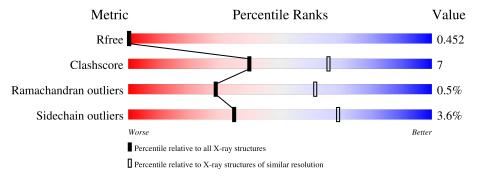
Validation Pipeline (wwPDB-VP) : 2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.90 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	Similar resolution
Wietric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain		
1	A	474	78%	16%	• 5%
1	В	474	77%	16%	6%
2	С	163	74%	15% •	9%
2	D	163	75%	14% •	9%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9367 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 Replicative DNA helicase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	450	Total 3509	C 2184	N 619	O 691	S 15	0	0	0
1	В	447	Total 3481	C 2168	N 611	O 687	S 15	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	HIS	-	expression tag	UNP A0A085R2T8
A	470	HIS	-	expression tag	UNP A0A085R2T8
A	471	HIS	-	expression tag	UNP A0A085R2T8
A	472	HIS	-	expression tag	UNP A0A085R2T8
A	473	HIS	-	expression tag	UNP A0A085R2T8
A	474	HIS	-	expression tag	UNP A0A085R2T8
В	469	HIS	-	expression tag	UNP A0A085R2T8
В	470	HIS	-	expression tag	UNP A0A085R2T8
В	471	HIS	-	expression tag	UNP A0A085R2T8
В	472	HIS	-	expression tag	UNP A0A085R2T8
В	473	HIS	_	expression tag	UNP A0A085R2T8
В	474	HIS	_	expression tag	UNP A0A085R2T8

• Molecule 2 is a protein called DUF721 domain-containing protein.

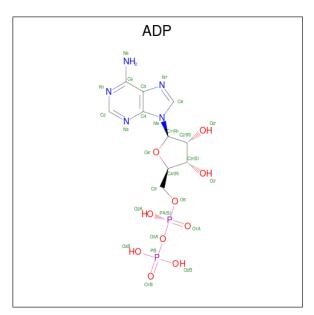
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
9	С	149	Total	С	N	О	S	0	0	0
		149	1162	726	224	211	1	0	U	U
9	D	148	Total	С	N	О	S	0	0	0
	D	140	1159	723	223	212	1	0	U	0

There are 14 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
С	-5	MET	-	initiating methionine	UNP A0A0H5ZA06
С	-4	HIS	-	expression tag	UNP A0A0H5ZA06
С	-3	HIS	-	expression tag	UNP A0A0H5ZA06
С	-2	HIS	-	expression tag	UNP A0A0H5ZA06
С	-1	HIS	-	expression tag	UNP A0A0H5ZA06
С	0	HIS	-	expression tag	UNP A0A0H5ZA06
С	1	HIS	-	expression tag	UNP A0A0H5ZA06
D	-5	MET	-	initiating methionine	UNP A0A0H5ZA06
D	-4	HIS	-	expression tag	UNP A0A0H5ZA06
D	-3	HIS	-	expression tag	UNP A0A0H5ZA06
D	-2	HIS	-	expression tag	UNP A0A0H5ZA06
D	-1	HIS	-	expression tag	UNP A0A0H5ZA06
D	0	HIS	-	expression tag	UNP A0A0H5ZA06
D	1	HIS	-	expression tag	UNP A0A0H5ZA06

• Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
9	Λ	1	Total	С	N	О	Р	0	0	
3	A	1	27	10	5	10	2	U		
9	D	1	Total	С	N	О	Р	0	0	
3	Б	1	27	10	5	10	2	U	0	

• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).



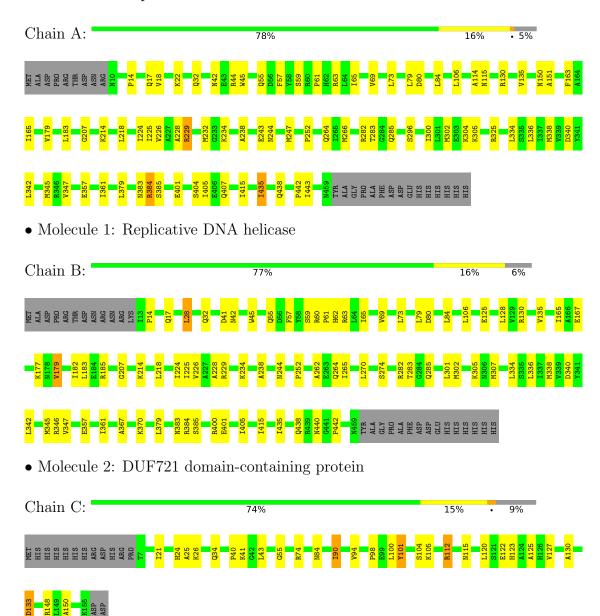
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	В	1	Total Mg 1 1	0	0



3 Residue-property plots (i)

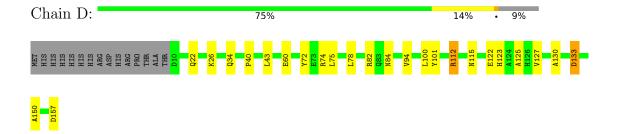
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: Replicative DNA helicase



• Molecule 2: DUF721 domain-containing protein







4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants	186.51Å 186.51Å 252.84Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.80 - 2.90	Depositor
Resolution (A)	40.80 - 2.90	EDS
% Data completeness	54.0 (40.80-2.90)	Depositor
(in resolution range)	54.0 (40.80-2.90)	EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.61 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
P. P.	0.279 , 0.290	Depositor
R, R_{free}	0.429 , 0.452	DCC
R_{free} test set	1229 reflections (6.05%)	wwPDB-VP
Wilson B-factor (Å ²)	84.7	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33, 68.5	EDS
L-test for twinning ²	$ < L > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	9367	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: ADP, MG

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

Mal	Mol Chain		lengths	Bond angles		
IVIOI	Chain	RMSZ # Z > 5		RMSZ	# Z > 5	
1	A	0.24	0/3558	0.41	0/4811	
1	В	0.24	0/3530	0.43	0/4775	
2	С	0.27	0/1174	0.48	0/1581	
2	D	0.25	0/1171	0.45	0/1576	
All	All	0.24	0/9433	0.43	0/12743	

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	3509	0	3522	56	0
1	В	3481	0	3490	53	0
2	С	1162	0	1235	21	0
2	D	1159	0	1224	24	0
3	A	27	0	12	0	0
3	В	27	0	12	0	0
4	A	1	0	0	0	0
4	В	1	0	0	0	0
All	All	9367	0	9495	138	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 7.

The worst 5 of 138 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:340:ASP:O	1:A:379:LEU:HB2	1.65	0.96
1:B:28:LEU:HD13	1:B:62:HIS:HE1	1.32	0.94
1:B:340:ASP:O	1:B:379:LEU:HB2	1.65	0.94
1:B:264:GLN:HG3	1:B:282:ARG:HH22	1.33	0.93
1:A:264:GLN:HG3	1:A:282:ARG:HH22	1.33	0.92

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	Perce	ntiles
1	A	448/474 (94%)	439 (98%)	9 (2%)	0	100	100
1	В	445/474 (94%)	432 (97%)	12 (3%)	1 (0%)	47	78
2	С	147/163 (90%)	137 (93%)	6 (4%)	4 (3%)	5	19
2	D	146/163 (90%)	138 (94%)	7 (5%)	1 (1%)	22	54
All	All	1186/1274 (93%)	1146 (97%)	34 (3%)	6 (0%)	29	61

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	177	LYS
2	С	41	LYS
2	С	98	PRO
2	С	24	HIS
2	С	112	ARG



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	A	383/403~(95%)	372 (97%)	11 (3%)	42	76
1	В	380/403~(94%)	368 (97%)	12 (3%)	39	73
2	C	123/137~(90%)	116 (94%)	7 (6%)	20	51
2	D	123/137~(90%)	117 (95%)	6 (5%)	25	57
All	All	1009/1080~(93%)	973 (96%)	36 (4%)	35	69

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	С	133	ASP
2	D	157	ASP
2	С	148	ARG
2	D	115	ASN
1	В	60	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	С	153	ASN
2	D	22	GLN
2	D	153	ASN
2	D	46	GLN
2	D	84	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	Trme	Chain	Dag	Res Link Bond lengths			В	ond ang	cles	
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	В	501	-	24,29,29	0.73	0	29,45,45	0.77	1 (3%)
3	ADP	A	501	-	24,29,29	0.74	0	29,45,45	0.76	1 (3%)

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	ADP	В	501	-	-	4/12/32/32	0/3/3/3
3	ADP	A	501	-	-	4/12/32/32	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
3	В	501	ADP	C5-C6-N6	2.28	123.82	120.35
3	A	501	ADP	C5-C6-N6	2.21	123.71	120.35

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ADP	C5'-O5'-PA-O2A

Continued on next page...



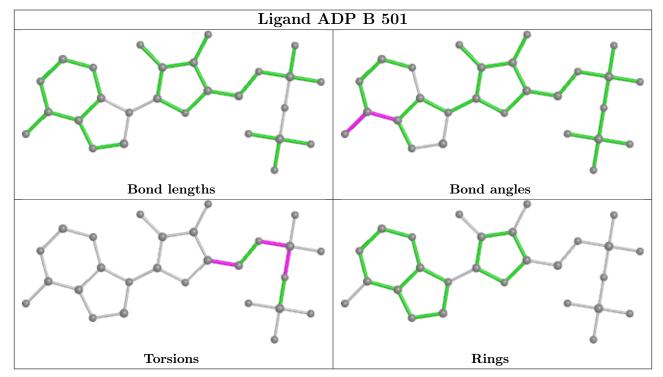
Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	501	ADP	C5'-O5'-PA-O3A
3	В	501	ADP	C5'-O5'-PA-O2A
3	В	501	ADP	C5'-O5'-PA-O3A
3	A	501	ADP	PB-O3A-PA-O2A

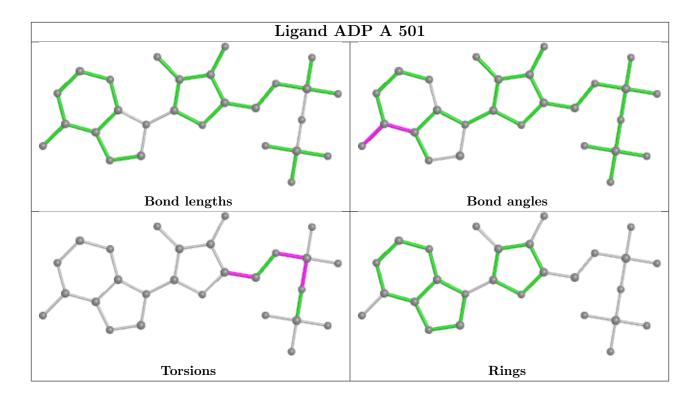
There are no ring outliers.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

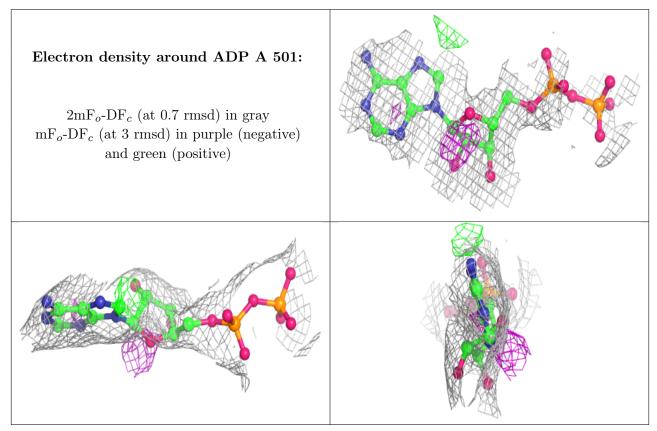
6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

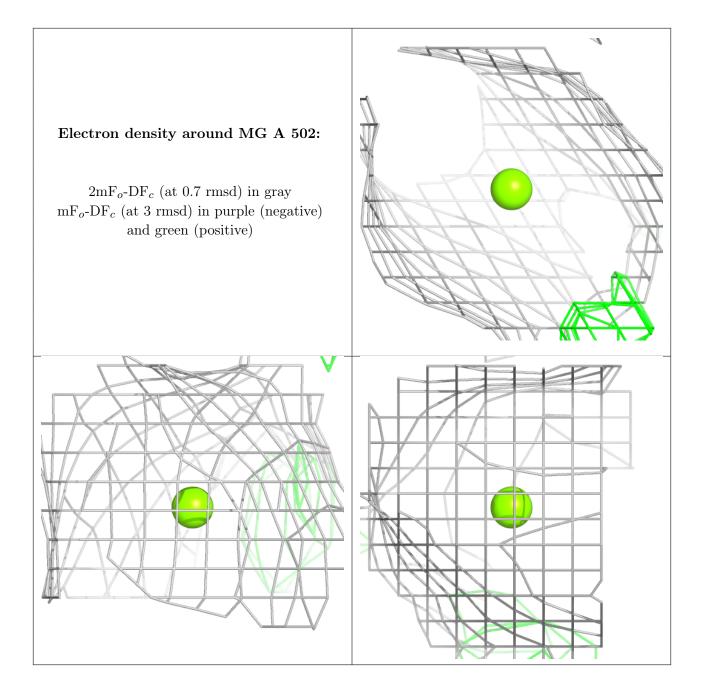
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

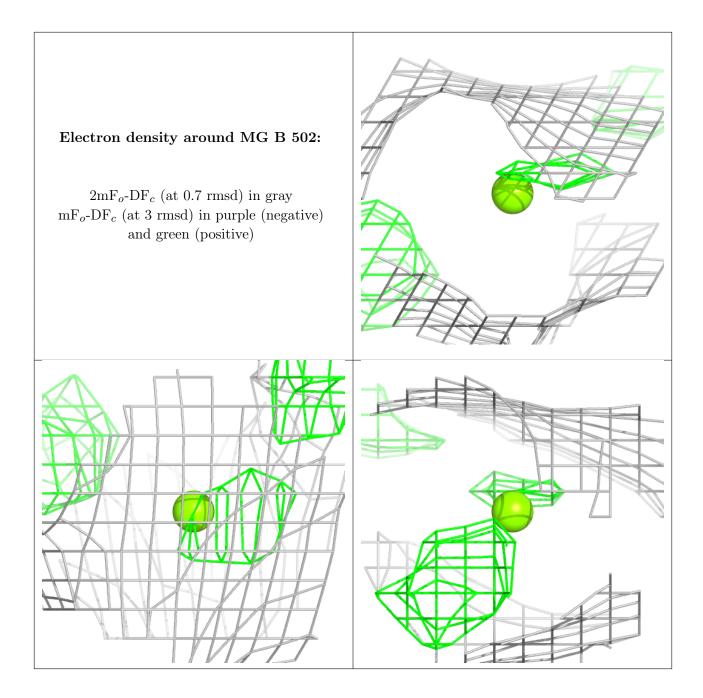












6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

