Full wwPDB X-ray Structure Validation Report ⓘ

Apr 6, 2023 – 04:24 pm BST

PDB ID	:	8ANP
Title	:	Legionella effector Lem3 mutant D190A in complex with Mg2+
Authors	:	Kaspers, M.S.; Pogenberg, V.; Ernst, S.; Ecker, F.; Pett, C.; Ochtrop, P.; Hedberg, C.; Groll, M.; Itzen, A.
Deposited on	:	2022-08-05
Resolution	:	2.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

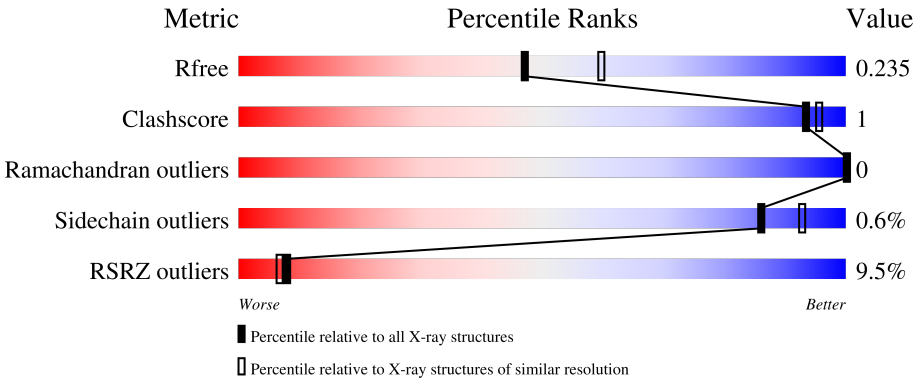
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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% 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	468	7% 85% · 11%
1	B	468	8% 93% · ·
1	C	468	10% 89% 5% 6%
1	D	468	10% 79% · 16%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13813 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 Phosphocholine hydrolase Lem3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	Se	0	0	0
			3306	2084	570	640	5	7			
1	B	454	Total	C	N	O	S	Se	0	0	0
			3603	2274	617	700	5	7			
1	C	442	Total	C	N	O	S	Se	0	0	0
			3509	2219	600	678	5	7			
1	D	391	Total	C	N	O	S	Se	0	0	0
			3083	1942	536	594	5	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP Q5ZXN5
A	20	HIS	-	expression tag	UNP Q5ZXN5
A	190	ALA	ASP	engineered mutation	UNP Q5ZXN5
B	19	GLY	-	expression tag	UNP Q5ZXN5
B	20	HIS	-	expression tag	UNP Q5ZXN5
B	190	ALA	ASP	engineered mutation	UNP Q5ZXN5
C	19	GLY	-	expression tag	UNP Q5ZXN5
C	20	HIS	-	expression tag	UNP Q5ZXN5
C	190	ALA	ASP	engineered mutation	UNP Q5ZXN5
D	19	GLY	-	expression tag	UNP Q5ZXN5
D	20	HIS	-	expression tag	UNP Q5ZXN5
D	190	ALA	ASP	engineered mutation	UNP Q5ZXN5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

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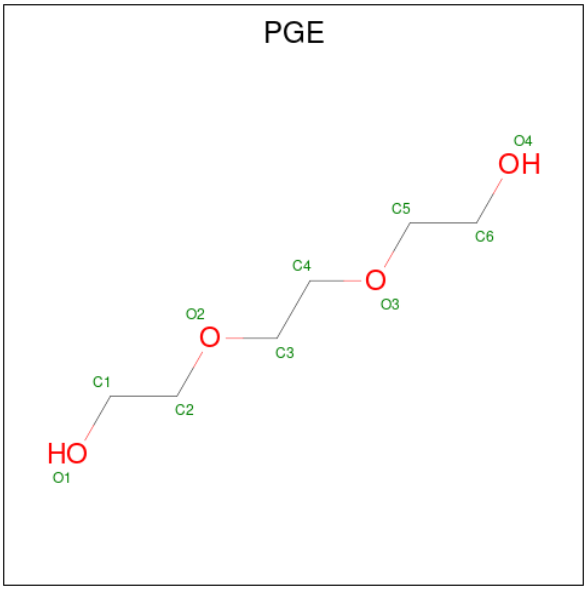
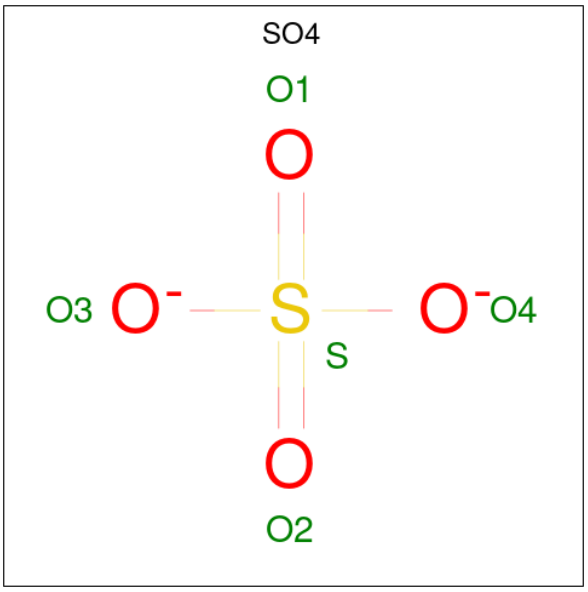
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 6 4	0	0
3	B	1	Total C O 10 6 4	0	0
3	C	1	Total C O 10 6 4	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

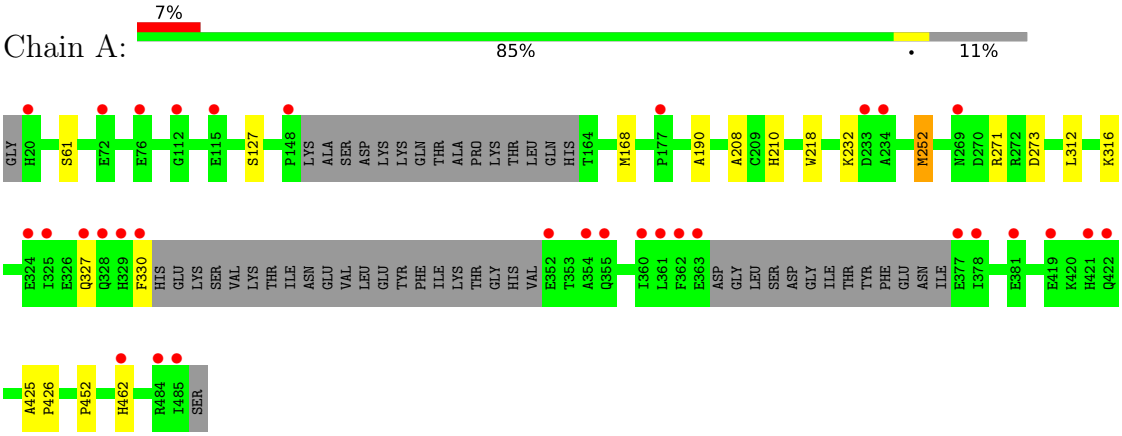
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	73	Total O 73 73	0	0
5	B	91	Total O 91 91	0	0
5	C	70	Total O 70 70	0	0
5	D	36	Total O 36 36	0	0

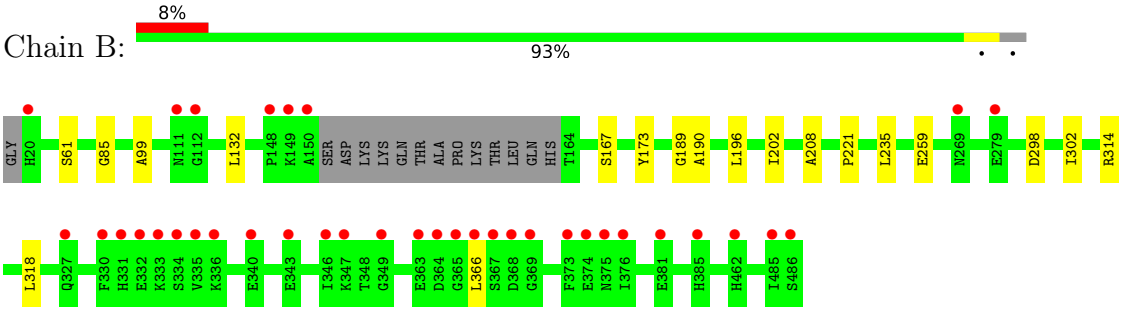
3 Residue-property plots (i)

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.

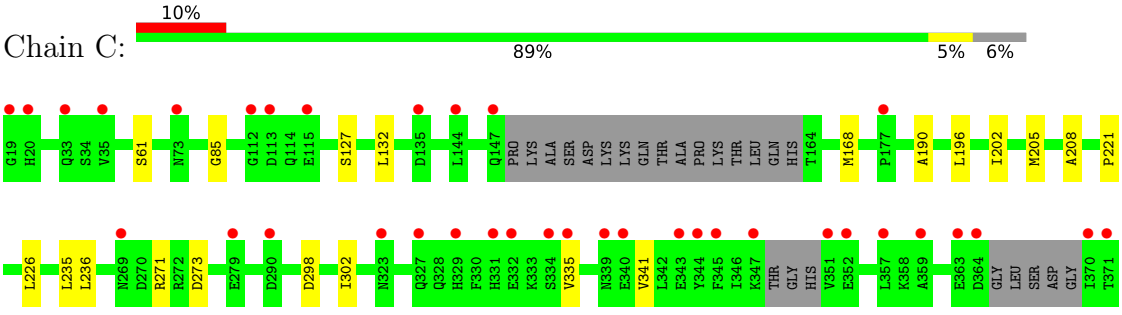
• Molecule 1: Phosphocholine hydrolase Lem3

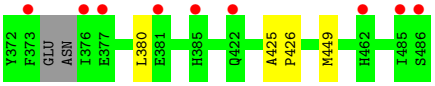


• Molecule 1: Phosphocholine hydrolase Lem3

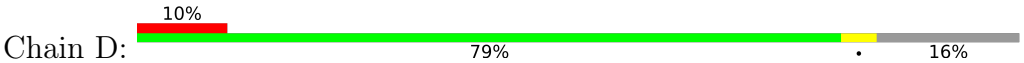


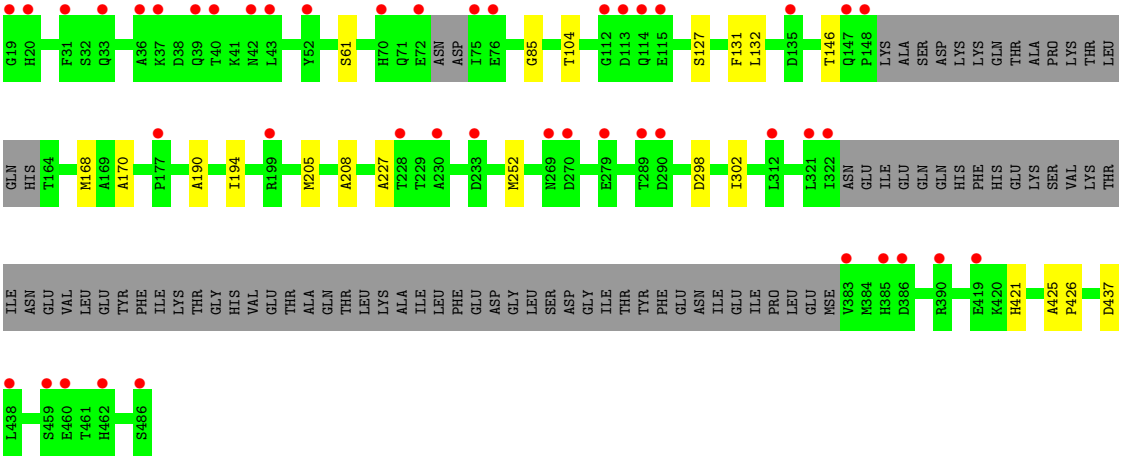
• Molecule 1: Phosphocholine hydrolase Lem3





• Molecule 1: Phosphocholine hydrolase Lem3





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	55.72Å 187.69Å 193.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.20 14.96 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (15.00-2.20) 99.8 (14.96-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.190 , 0.230 0.199 , 0.235	Depositor DCC
R_{free} test set	5165 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.005 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13813	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PGE, SO4

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	0.65	0/3356	0.73	1/4521 (0.0%)
1	B	0.65	0/3661	0.72	0/4936
1	C	0.66	0/3562	0.72	2/4798 (0.0%)
1	D	0.66	0/3130	0.73	1/4216 (0.0%)
All	All	0.65	0/13709	0.72	4/18471 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	449	MSE	CG-SE-CE	5.76	111.57	98.90
1	A	252	MSE	CG-SE-CE	5.65	111.33	98.90
1	C	205	MSE	CG-SE-CE	5.42	110.82	98.90
1	D	205	MSE	CG-SE-CE	5.31	110.58	98.90

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	3306	0	3281	9	0
1	B	3603	0	3577	9	0
1	C	3509	0	3479	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3083	0	3069	9	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	14	0	0
3	B	10	0	14	0	0
3	C	10	0	14	0	0
4	B	5	0	0	0	0
5	A	73	0	0	2	0
5	B	91	0	0	0	0
5	C	70	0	0	0	0
5	D	36	0	0	0	0
All	All	13813	0	13448	37	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 (37) 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:A:312:LEU:O	1:A:316:LYS:HG2	2.02	0.59
1:D:85:GLY:HA3	1:D:132:LEU:HD11	1.89	0.55
1:C:271:ARG:NH1	1:C:273:ASP:OD1	2.40	0.55
1:D:127:SER:O	1:D:168:MSE:HE1	2.09	0.52
1:A:127:SER:O	1:A:168:MSE:HE1	2.09	0.52
1:B:298:ASP:O	1:B:302:ILE:HG12	2.10	0.52
1:B:99:ALA:HB3	1:B:173:TYR:CE2	2.47	0.50
1:D:131:PHE:CZ	1:D:170:ALA:HB1	2.47	0.49
1:A:232:LYS:NZ	5:A:603:HOH:O	2.45	0.49
1:D:146:THR:HB	1:D:227:ALA:HB2	1.97	0.47
1:C:221:PRO:HB3	1:C:235:LEU:HD22	1.95	0.47
1:A:210:HIS:HB3	1:A:218:TRP:HB3	1.97	0.46
1:B:318:LEU:HD13	1:B:366:LEU:HD11	1.98	0.45
1:A:425:ALA:HB3	1:A:426:PRO:HD3	1.98	0.45
1:B:196:LEU:HD23	1:B:202:ILE:HA	1.97	0.44
1:C:341:VAL:HG21	1:C:380:LEU:HD12	2.00	0.44
1:C:425:ALA:HB3	1:C:426:PRO:HD3	1.98	0.44
1:D:194:ILE:HD12	1:D:252:MSE:HE1	1.99	0.44
1:A:452:PRO:HD2	1:A:462:HIS:O	2.17	0.44
1:B:259:GLU:OE1	1:B:314:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:HD23	1:C:202:ILE:HA	1.99	0.43
1:C:127:SER:O	1:C:168:MSE:HE1	2.18	0.43
1:B:190:ALA:HA	1:B:208:ALA:HB1	2.00	0.43
1:D:104:THR:CG2	1:D:168:MSE:HE3	2.48	0.43
1:A:252:MSE:HE2	5:A:611:HOH:O	2.19	0.42
1:D:425:ALA:HB3	1:D:426:PRO:HD3	2.01	0.42
1:C:85:GLY:HA3	1:C:132:LEU:HD11	2.01	0.42
1:D:298:ASP:O	1:D:302:ILE:HG12	2.20	0.42
1:B:167:SER:HB2	1:B:189:GLY:HA3	2.01	0.42
1:A:271:ARG:NH1	1:A:273:ASP:OD1	2.53	0.41
1:C:226:LEU:HD11	1:C:236:LEU:HB2	2.01	0.41
1:B:85:GLY:HA3	1:B:132:LEU:HD11	2.03	0.41
1:C:298:ASP:O	1:C:302:ILE:HG12	2.21	0.40
1:C:190:ALA:HA	1:C:208:ALA:HB1	2.03	0.40
1:B:221:PRO:HB3	1:B:235:LEU:HD22	2.02	0.40
1:A:190:ALA:HA	1:A:208:ALA:HB1	2.02	0.40
1:D:190:ALA:HA	1:D:208:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	409/468 (87%)	402 (98%)	7 (2%)	0	100	100
1	B	450/468 (96%)	441 (98%)	9 (2%)	0	100	100
1	C	432/468 (92%)	421 (98%)	11 (2%)	0	100	100
1	D	383/468 (82%)	379 (99%)	4 (1%)	0	100	100
All	All	1674/1872 (89%)	1643 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	Percentiles
1	A	367/406 (90%)	364 (99%)	3 (1%)	81 90
1	B	401/406 (99%)	400 (100%)	1 (0%)	93 97
1	C	389/406 (96%)	387 (100%)	2 (0%)	88 94
1	D	342/406 (84%)	339 (99%)	3 (1%)	78 88
All	All	1499/1624 (92%)	1490 (99%)	9 (1%)	86 93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	SER
1	A	327	GLN
1	A	330	PHE
1	B	61	SER
1	C	61	SER
1	C	335	VAL
1	D	61	SER
1	D	421	HIS
1	D	437	ASP

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

Mol	Chain	Res	Type
1	B	339	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 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 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	PGE	A	503	-	9,9,9	0.15	0	8,8,8	0.10	0
4	SO4	B	504	-	4,4,4	0.41	0	6,6,6	0.05	0
3	PGE	B	503	-	9,9,9	0.16	0	8,8,8	0.07	0
3	PGE	C	503	-	9,9,9	0.16	0	8,8,8	0.10	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
3	PGE	A	503	-	-	0/7/7/7	-
3	PGE	B	503	-	-	4/7/7/7	-
3	PGE	C	503	-	-	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	503	PGE	C6-C5-O3-C4
3	B	503	PGE	O1-C1-C2-O2
3	B	503	PGE	O3-C5-C6-O4
3	B	503	PGE	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
3	B	503	PGE	O2-C3-C4-O3

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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	410/468 (87%)	0.28	32 (7%)	13	11	31, 48, 90, 118	0
1	B	447/468 (95%)	0.22	37 (8%)	11	10	28, 44, 96, 119	0
1	C	435/468 (92%)	0.38	45 (10%)	6	5	30, 52, 102, 136	0
1	D	385/468 (82%)	0.45	45 (11%)	4	4	33, 59, 96, 120	0
All	All	1677/1872 (89%)	0.33	159 (9%)	8	7	28, 50, 96, 136	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	385	HIS	8.6
1	B	20	HIS	6.0
1	A	363	GLU	5.9
1	D	148	PRO	5.6
1	A	362	PHE	5.5
1	C	364	ASP	5.5
1	B	367	SER	5.5
1	B	150	ALA	5.5
1	C	370	ILE	5.4
1	C	334	SER	5.3
1	C	352	GLU	5.3
1	B	365	GLY	5.3
1	C	332	GLU	5.2
1	A	269	ASN	5.2
1	D	72	GLU	5.2
1	C	331	HIS	5.0
1	B	373	PHE	4.8
1	D	462	HIS	4.8
1	B	334	SER	4.7
1	D	486	SER	4.7
1	B	332	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	419	GLU	4.6
1	C	147	GLN	4.5
1	A	328	GLN	4.4
1	C	112	GLY	4.4
1	B	149	LYS	4.4
1	A	112	GLY	4.4
1	A	422	GLN	4.3
1	B	269	ASN	4.2
1	A	378	ILE	4.2
1	C	20	HIS	4.2
1	A	354	ALA	4.1
1	A	330	PHE	4.1
1	B	331	HIS	4.1
1	D	322	ILE	4.1
1	B	364	ASP	4.0
1	D	269	ASN	4.0
1	C	485	ILE	4.0
1	C	329	HIS	4.0
1	B	369	GLY	3.9
1	D	19	GLY	3.9
1	A	329	HIS	3.9
1	C	363	GLU	3.9
1	C	486	SER	3.8
1	B	347	LYS	3.8
1	B	381	GLU	3.7
1	B	343	GLU	3.7
1	B	363	GLU	3.7
1	C	351	VAL	3.7
1	B	374	GLU	3.7
1	D	147	GLN	3.6
1	D	112	GLY	3.6
1	D	321	LEU	3.6
1	D	228	THR	3.6
1	D	289	THR	3.6
1	B	368	ASP	3.6
1	B	336	LYS	3.6
1	C	177	PRO	3.6
1	D	20	HIS	3.5
1	B	486	SER	3.5
1	A	355	GLN	3.4
1	B	366	LEU	3.4
1	A	462	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	148	PRO	3.3
1	C	269	ASN	3.2
1	D	31	PHE	3.2
1	C	290	ASP	3.2
1	D	383	VAL	3.1
1	C	33	GLN	3.1
1	C	339	ASN	3.1
1	D	290	ASP	3.1
1	B	462	HIS	3.0
1	A	361	LEU	3.0
1	B	148	PRO	3.0
1	A	20	HIS	3.0
1	D	36	ALA	3.0
1	A	360	ILE	3.0
1	D	233	ASP	3.0
1	B	333	LYS	3.0
1	A	327	GLN	2.9
1	B	327	GLN	2.9
1	C	377	GLU	2.9
1	C	19	GLY	2.9
1	D	459	SER	2.9
1	D	43	LEU	2.9
1	A	72	GLU	2.9
1	D	113	ASP	2.9
1	C	462	HIS	2.8
1	D	70	HIS	2.8
1	C	340	GLU	2.8
1	A	115	GLU	2.8
1	A	377	GLU	2.7
1	C	113	ASP	2.7
1	D	230	ALA	2.7
1	A	234	ALA	2.7
1	D	39	GLN	2.7
1	B	385	HIS	2.6
1	C	144	LEU	2.6
1	C	343	GLU	2.6
1	B	375	ASN	2.6
1	B	340	GLU	2.6
1	B	376	ILE	2.6
1	C	422	GLN	2.6
1	A	76	GLU	2.6
1	C	371	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	279	GLU	2.5
1	D	52	TYR	2.5
1	D	42	ASN	2.5
1	D	312	LEU	2.5
1	D	438	LEU	2.5
1	D	75	ILE	2.5
1	D	279	GLU	2.5
1	D	114	GLN	2.5
1	D	390	ARG	2.4
1	D	76	GLU	2.4
1	C	135	ASP	2.4
1	C	376	ILE	2.4
1	A	324	GLU	2.4
1	B	335	VAL	2.4
1	D	270	ASP	2.4
1	A	484	ARG	2.3
1	A	352	GLU	2.3
1	B	112	GLY	2.3
1	B	346	ILE	2.3
1	B	279	GLU	2.3
1	B	111	ASN	2.3
1	D	386	ASP	2.3
1	A	421	HIS	2.3
1	C	115	GLU	2.3
1	A	177	PRO	2.3
1	C	347	LYS	2.3
1	C	35	VAL	2.2
1	D	33	GLN	2.2
1	C	373	PHE	2.2
1	B	485	ILE	2.2
1	B	330	PHE	2.2
1	A	233	ASP	2.2
1	A	381	GLU	2.2
1	C	73	ASN	2.2
1	D	177	PRO	2.2
1	B	349	GLY	2.2
1	C	357	LEU	2.2
1	C	323	ASN	2.1
1	C	327	GLN	2.1
1	A	419	GLU	2.1
1	D	135	ASP	2.1
1	A	325	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	485	ILE	2.1
1	C	335	VAL	2.1
1	C	381	GLU	2.1
1	C	385	HIS	2.1
1	D	40	THR	2.1
1	C	359	ALA	2.1
1	C	345	PHE	2.1
1	D	460	GLU	2.0
1	C	344	TYR	2.0
1	D	37	LYS	2.0
1	D	115	GLU	2.0
1	D	199	ARG	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)

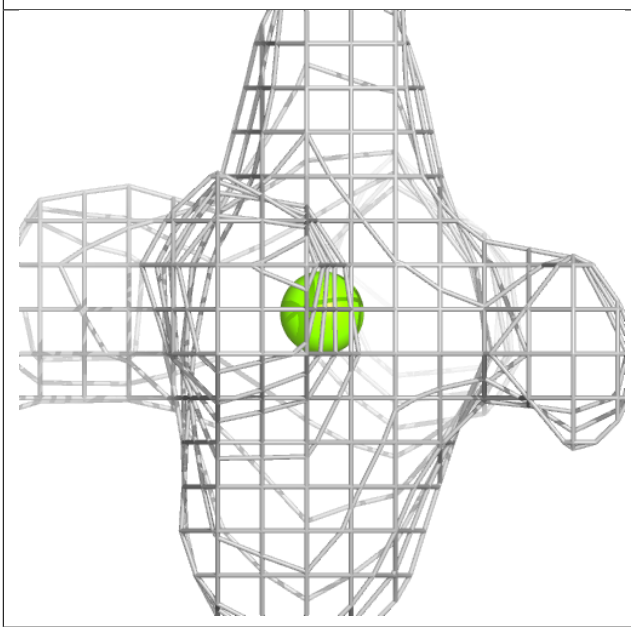
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

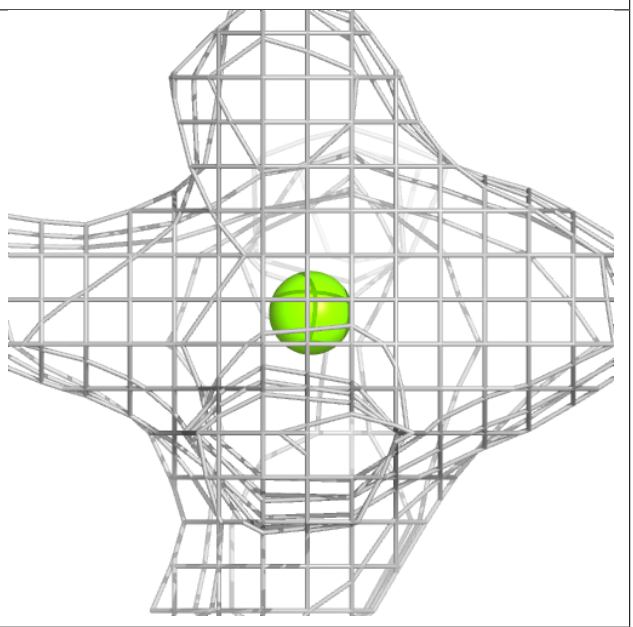
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PGE	B	503	10/10	0.81	0.23	59,61,65,65	0
3	PGE	C	503	10/10	0.87	0.13	68,70,74,75	0
2	MG	B	502	1/1	0.89	0.06	58,58,58,58	0
3	PGE	A	503	10/10	0.92	0.09	58,61,65,67	0
2	MG	A	502	1/1	0.95	0.07	51,51,51,51	0
2	MG	A	501	1/1	0.95	0.03	37,37,37,37	0
2	MG	C	501	1/1	0.95	0.06	36,36,36,36	0
2	MG	C	502	1/1	0.96	0.16	76,76,76,76	0
2	MG	D	501	1/1	0.98	0.05	33,33,33,33	0
2	MG	B	501	1/1	0.98	0.03	35,35,35,35	0
4	SO4	B	504	5/5	0.99	0.12	53,54,59,63	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 MG B 502:

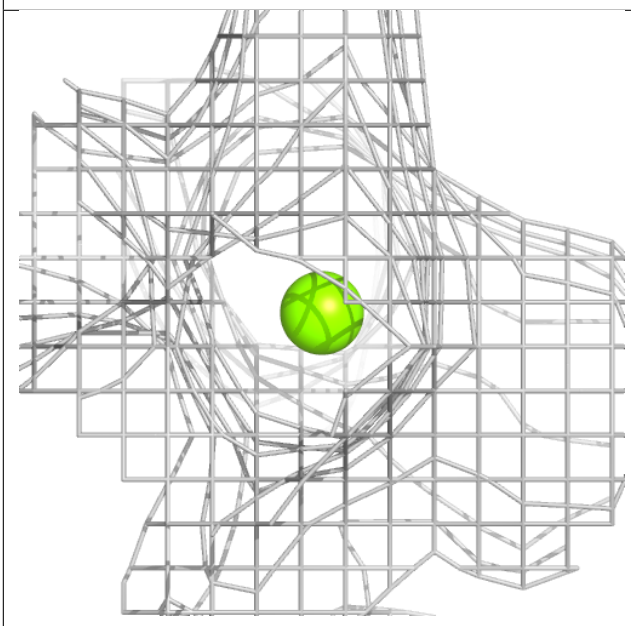
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

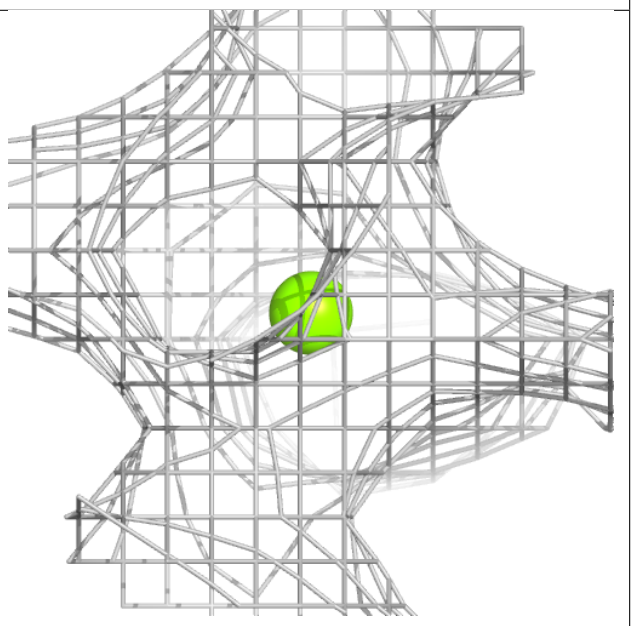




Electron density around MG A 502:

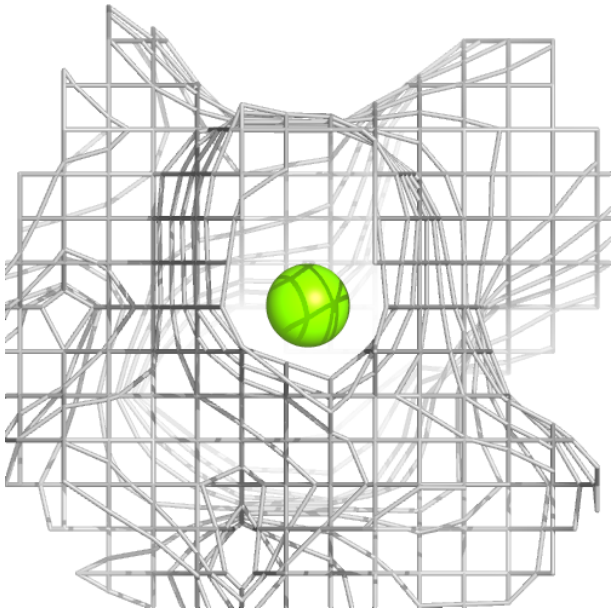
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

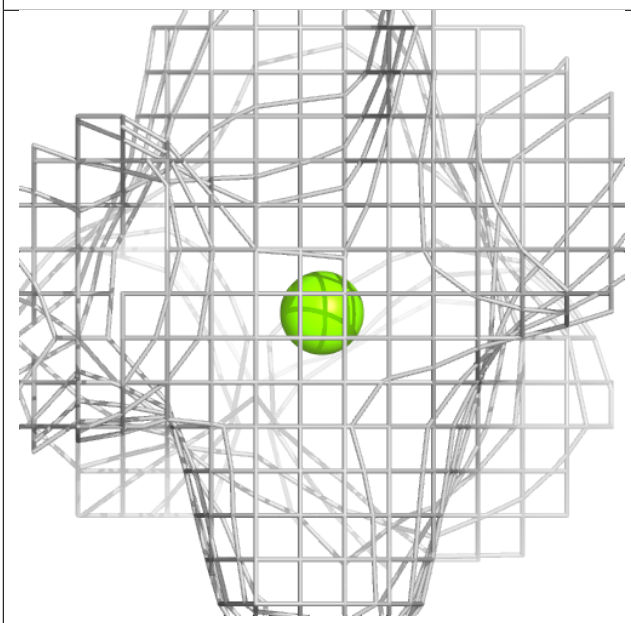


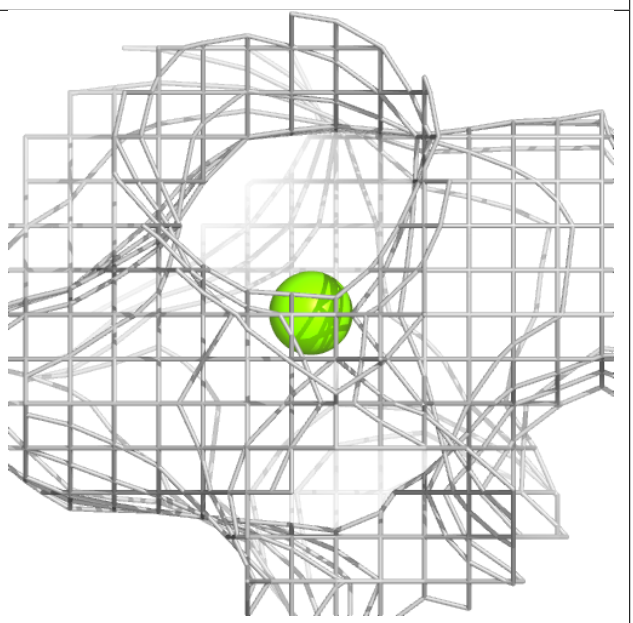


Electron density around MG A 501:

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

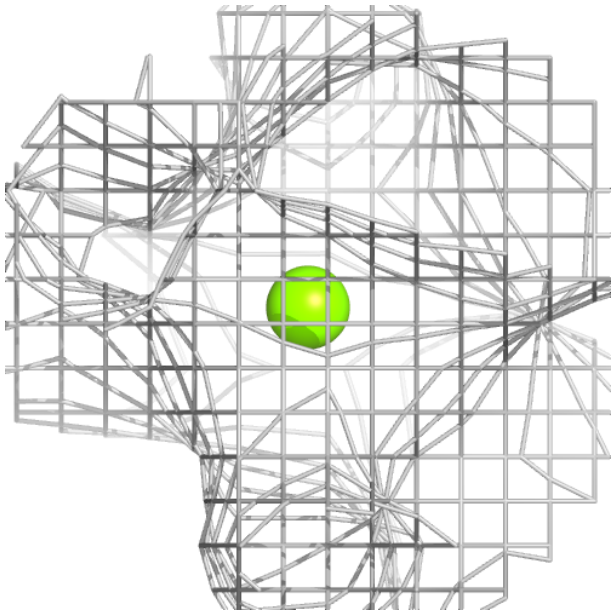


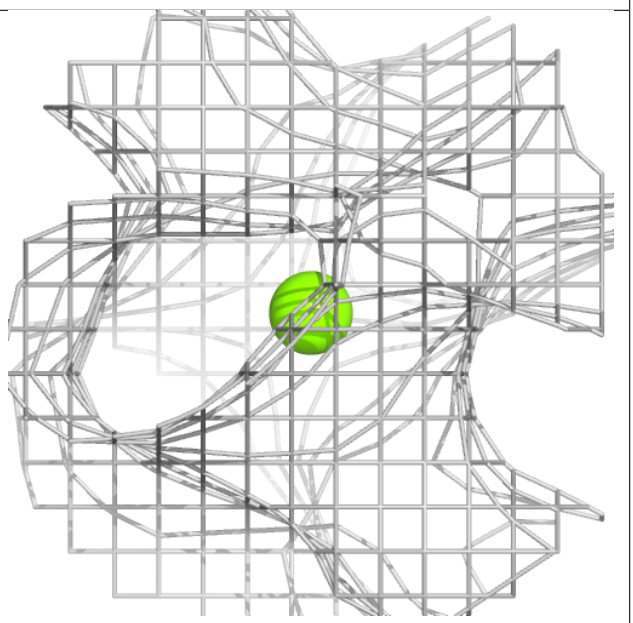




Electron density around MG C 501:

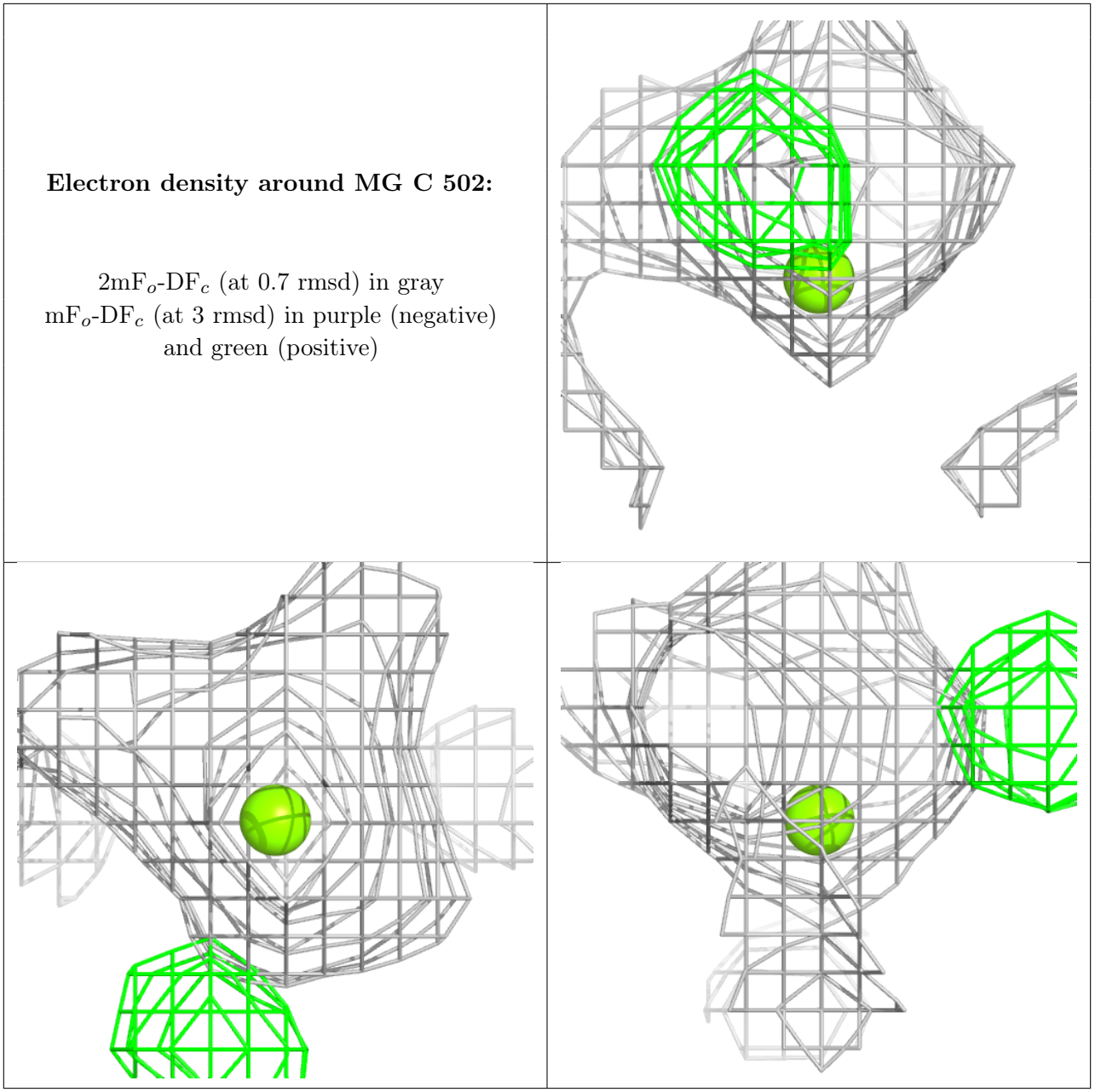
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





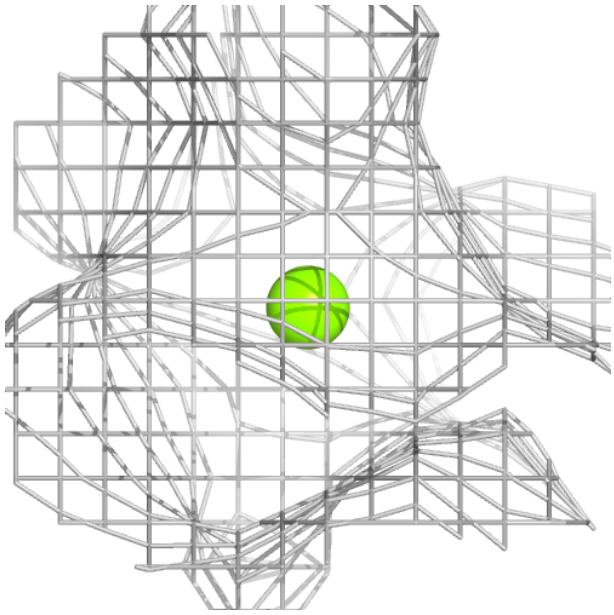
Electron density around MG C 502:

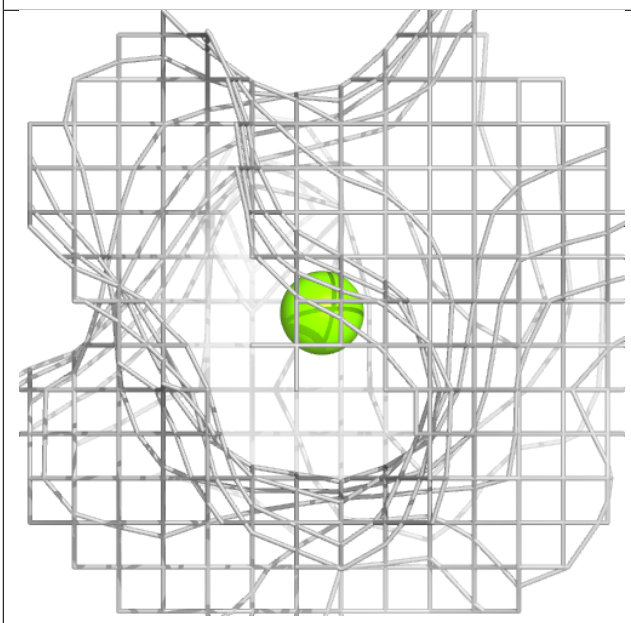
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

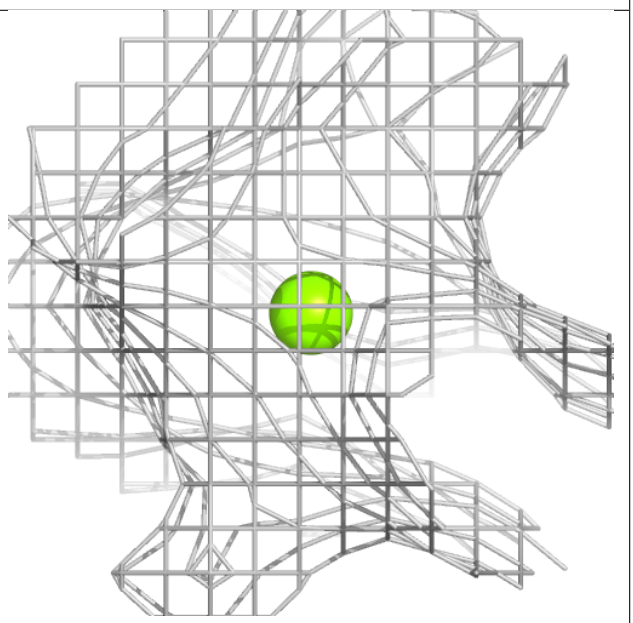


Electron density around MG D 501:

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

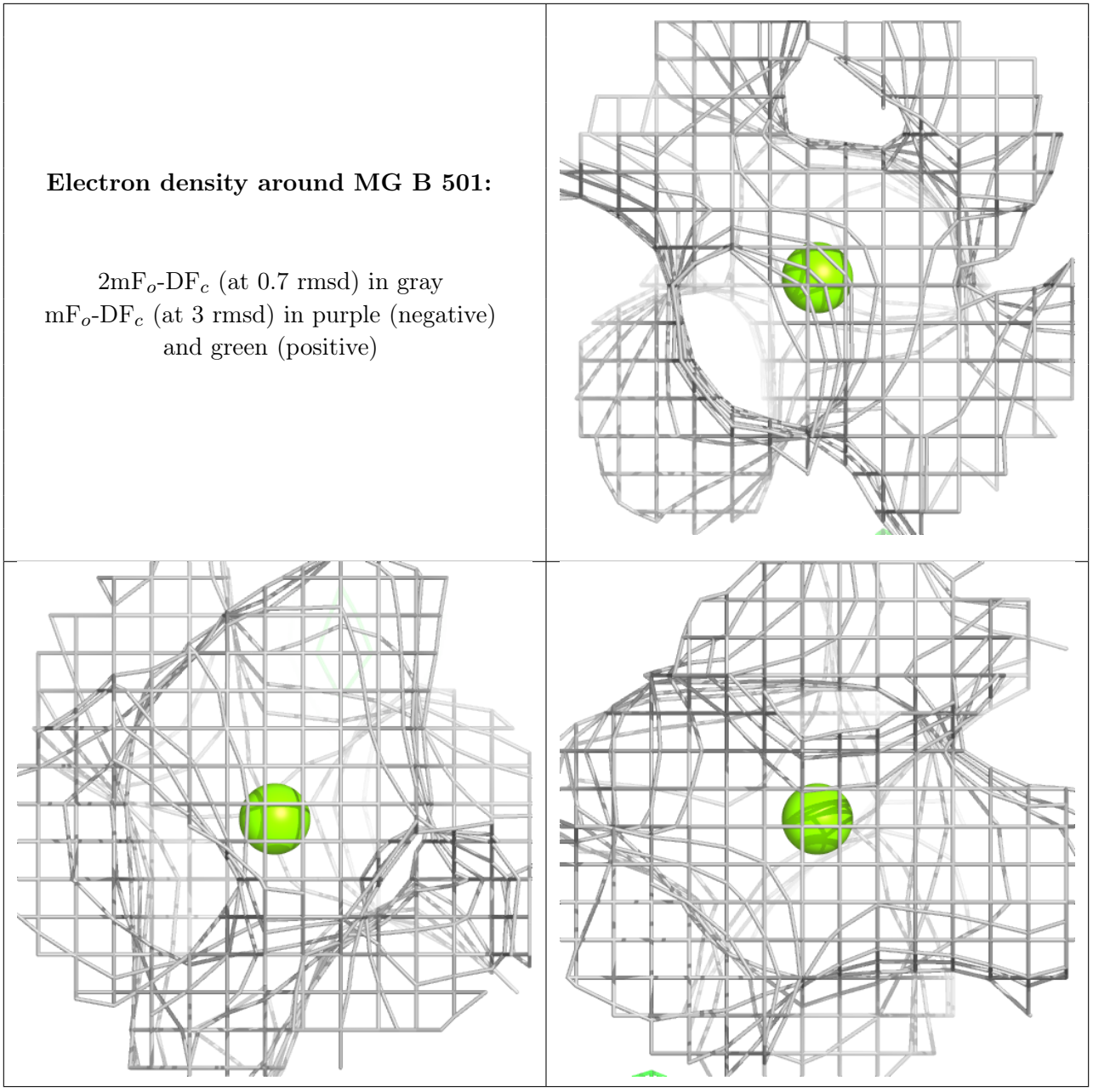






Electron density around MG B 501:

$2mF_o$-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.