



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2026 – 09:41 PM UTC

PDB ID : 22ZA / pdb_000022za
Title : crystal structures of RipN from Ralstonia solanacearum
Authors : Ge, H.
Deposited on : 2026-01-28
Resolution : 2.28 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

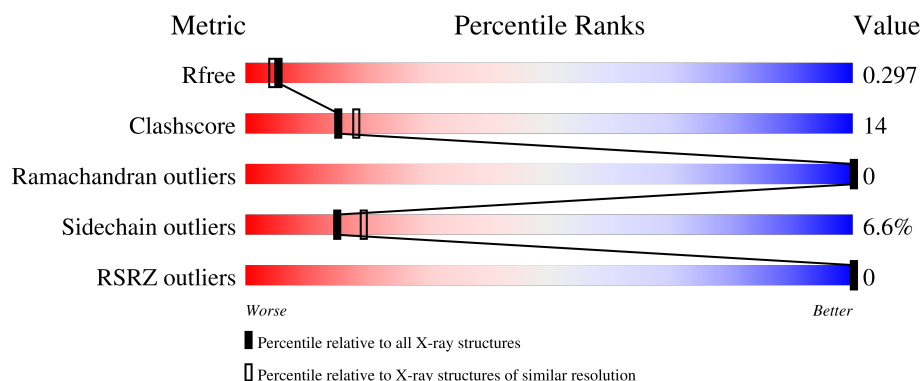
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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 $\leq 5\%$. 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	482	
1	B	482	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5750 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 Type III effector protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2751	1711	489	538	13			
1	B	361	Total	C	N	O	S	0	0	0
			2754	1714	489	538	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q8XQT8
A	-6	GLY	-	expression tag	UNP Q8XQT8
A	-5	HIS	-	expression tag	UNP Q8XQT8
A	-4	HIS	-	expression tag	UNP Q8XQT8
A	-3	HIS	-	expression tag	UNP Q8XQT8
A	-2	HIS	-	expression tag	UNP Q8XQT8
A	-1	HIS	-	expression tag	UNP Q8XQT8
A	0	HIS	-	expression tag	UNP Q8XQT8
B	-7	MET	-	initiating methionine	UNP Q8XQT8
B	-6	GLY	-	expression tag	UNP Q8XQT8
B	-5	HIS	-	expression tag	UNP Q8XQT8
B	-4	HIS	-	expression tag	UNP Q8XQT8
B	-3	HIS	-	expression tag	UNP Q8XQT8
B	-2	HIS	-	expression tag	UNP Q8XQT8
B	-1	HIS	-	expression tag	UNP Q8XQT8
B	0	HIS	-	expression tag	UNP Q8XQT8

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total 3	Mg 3	0	0

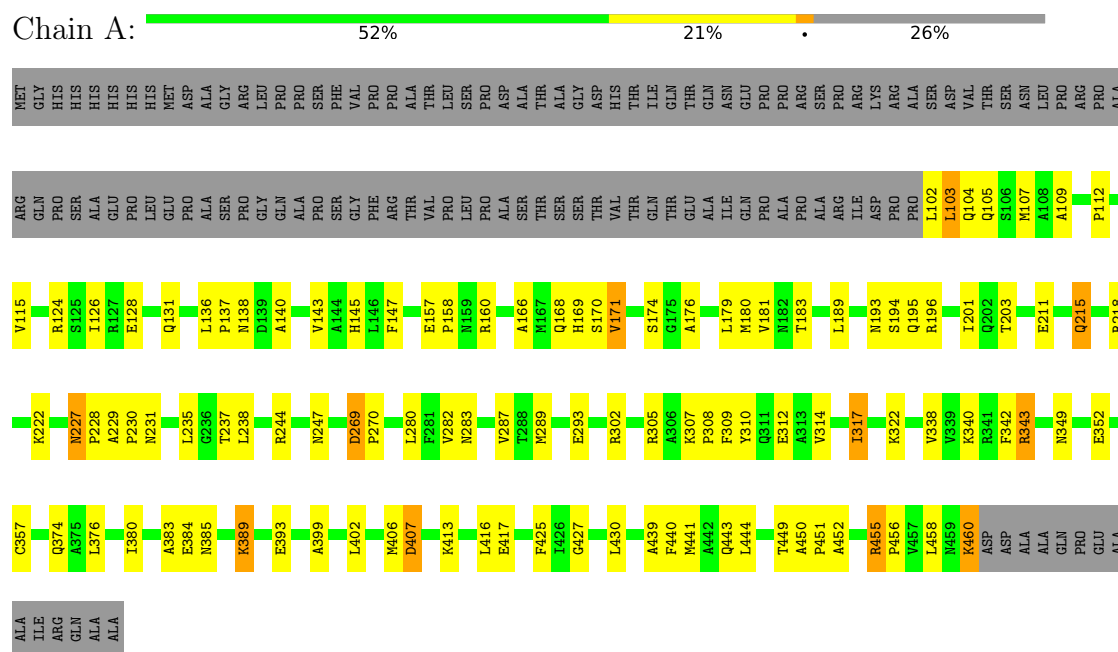
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0
3	B	118	Total 118	O 118	0	0

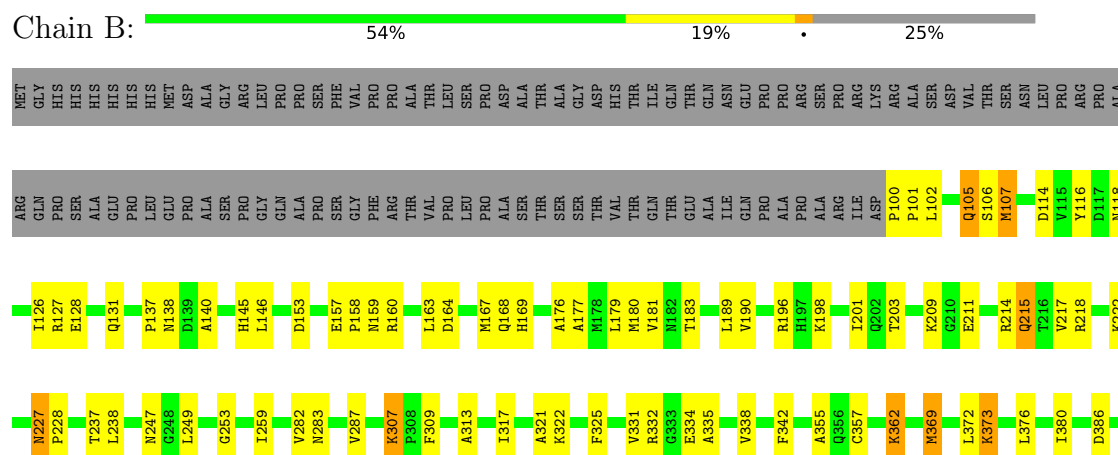
3 Residue-property plots

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: Type III effector protein



• Molecule 1: Type III effector protein



E393	P394	M400	M406	K413	E417	N418	F421	D422	M423	I426	L430	H431	L432	F440	Q443	L444	K445	P451	A452	I453	G454	R455	P456	K460	ASP	ASP	ALA	ALA	GLN	PRO	GLU	ALA	ALA	ILE	ARG	GLN	ALA	ALA
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	127.36Å 127.36Å 104.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.28 20.00 – 2.28	Depositor EDS
% Data completeness (in resolution range)	89.7 (20.00-2.28) 89.8 (20.00-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.93 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.264 , 0.290 0.267 , 0.297	Depositor DCC
R_{free} test set	2031 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 14.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.468 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5750	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.63	0/2794	1.14	8/3789 (0.2%)
1	B	0.63	0/2799	1.11	3/3798 (0.1%)
All	All	0.63	0/5593	1.13	11/7587 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASN	CA-C-N	6.52	126.50	119.78
1	A	227	ASN	C-N-CA	6.52	126.50	119.78
1	A	269	ASP	CA-C-N	6.05	125.93	119.28
1	A	269	ASP	C-N-CA	6.05	125.93	119.28
1	A	136	LEU	CA-C-N	5.80	125.77	120.03
1	A	136	LEU	C-N-CA	5.80	125.77	120.03
1	A	229	ALA	CA-C-N	5.35	124.53	118.97
1	A	229	ALA	C-N-CA	5.35	124.53	118.97
1	B	153	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	227	ASN	CA-C-N	5.18	125.11	119.78
1	B	227	ASN	C-N-CA	5.18	125.11	119.78

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	2751	0	2702	71	0
1	B	2754	0	2696	80	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	121	0	0	5	0
3	B	118	0	0	4	0
All	All	5750	0	5398	148	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 14.

All (148) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:PRO:HB2	1:B:101:PRO:CD	1.40	1.49
1:B:100:PRO:CB	1:B:101:PRO:CD	2.28	1.11
1:A:102:LEU:HB2	3:A:625:HOH:O	1.48	1.09
1:B:100:PRO:HB2	1:B:101:PRO:HD2	1.10	1.06
1:B:100:PRO:HB2	1:B:101:PRO:HD3	1.33	1.05
1:B:332:ARG:HD3	1:B:369:MET:HG3	1.45	0.98
1:A:105:GLN:O	1:A:452:ALA:HB1	1.69	0.93
1:A:451:PRO:HD2	1:A:455:ARG:HB2	1.52	0.91
1:B:105:GLN:O	1:B:452:ALA:HB1	1.73	0.89
1:B:100:PRO:CB	1:B:101:PRO:HD2	2.01	0.81
1:B:332:ARG:CD	1:B:369:MET:HG3	2.11	0.80
1:B:443:GLN:OE1	1:B:460:LYS:HA	1.81	0.79
1:A:309:PHE:CD1	1:A:342:PHE:HB2	2.18	0.78
1:B:247:ASN:HB3	1:B:430:LEU:HD23	1.68	0.76
1:B:114:ASP:OD2	1:B:118:ASN:HB2	1.86	0.76
1:B:102:LEU:H	1:B:102:LEU:HD23	1.48	0.75
1:A:282:VAL:HG21	1:A:444:LEU:HD22	1.67	0.75
1:B:100:PRO:CB	1:B:101:PRO:HD3	2.04	0.74
1:B:309:PHE:CD1	1:B:342:PHE:HB2	2.23	0.73
1:B:164:ASP:O	1:B:168:GLN:NE2	2.21	0.73
1:B:400:MET:HG2	1:B:432:LEU:HD22	1.75	0.69
1:A:451:PRO:HD3	1:A:456:PRO:O	1.92	0.69
1:B:126:ILE:HD12	1:B:169:HIS:HB2	1.75	0.67
1:B:102:LEU:H	1:B:102:LEU:CD2	2.07	0.67
1:B:309:PHE:CZ	1:B:342:PHE:HA	2.34	0.63
1:B:179:LEU:HD11	1:B:237:THR:HB	1.79	0.63
1:A:413:LYS:O	1:A:417:GLU:HG3	1.99	0.63
1:B:102:LEU:HD23	1:B:102:LEU:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASN:N	1:A:228:PRO:HD3	2.14	0.63
1:A:440:PHE:CZ	1:A:444:LEU:HD11	2.34	0.62
1:B:440:PHE:CZ	1:B:444:LEU:HD11	2.34	0.62
1:B:105:GLN:NE2	1:B:107:MET:SD	2.74	0.61
1:B:440:PHE:CE1	1:B:444:LEU:HD11	2.36	0.61
1:A:126:ILE:HD12	1:A:169:HIS:HB2	1.83	0.61
1:A:450:ALA:HB1	1:A:451:PRO:CD	2.31	0.60
1:A:109:ALA:HB2	3:A:694:HOH:O	2.02	0.60
1:A:309:PHE:CZ	1:A:342:PHE:HA	2.36	0.59
1:A:340:LYS:HG3	1:A:343:ARG:NH2	2.17	0.59
1:A:440:PHE:CE1	1:A:444:LEU:HD11	2.38	0.58
1:A:402:LEU:HB2	1:A:416:LEU:HD13	1.84	0.58
1:A:128:GLU:HA	1:A:131:GLN:OE1	2.03	0.58
1:A:317:ILE:HD11	1:A:376:LEU:HB2	1.86	0.58
1:A:145:HIS:HD2	1:B:145:HIS:O	1.88	0.57
1:B:102:LEU:O	1:B:453:ILE:HG13	2.05	0.57
1:A:450:ALA:HB1	1:A:451:PRO:HD2	1.86	0.56
1:B:331:VAL:O	1:B:334:GLU:HG2	2.05	0.56
1:B:413:LYS:O	1:B:417:GLU:HG3	2.06	0.56
1:A:189:LEU:HD21	1:A:201:ILE:HB	1.87	0.56
1:A:307:LYS:N	1:A:308:PRO:HD2	2.19	0.56
1:A:179:LEU:HD11	1:A:237:THR:HB	1.87	0.55
1:A:195:GLN:HG3	1:A:384:GLU:O	2.07	0.55
1:A:406:MET:HG2	1:A:413:LYS:HA	1.89	0.55
1:A:112:PRO:HG2	1:A:115:VAL:HB	1.88	0.54
1:B:137:PRO:HG2	1:B:140:ALA:HB2	1.89	0.54
1:B:146:LEU:HD12	1:B:167:MET:HE3	1.89	0.54
1:A:280:LEU:HD21	1:A:444:LEU:HD21	1.90	0.54
1:B:198:LYS:HE2	3:B:656:HOH:O	2.06	0.54
1:A:137:PRO:HG2	1:A:140:ALA:HB2	1.89	0.54
1:B:106:SER:HA	1:B:453:ILE:HB	1.90	0.53
1:A:312:GLU:OE1	1:A:338:VAL:HG13	2.08	0.53
1:B:183:THR:HA	1:B:287:VAL:O	2.09	0.53
1:A:427:GLY:O	1:A:430:LEU:HB2	2.08	0.53
1:A:302:ARG:HB3	1:A:349:ASN:OD1	2.10	0.52
1:A:230:PRO:HD2	3:A:601:HOH:O	2.08	0.52
1:A:145:HIS:O	1:B:145:HIS:HD2	1.92	0.52
1:A:393:GLU:HG2	1:A:441:MET:SD	2.49	0.52
1:A:231:ASN:OD1	1:A:231:ASN:N	2.34	0.51
1:B:309:PHE:CE1	1:B:342:PHE:HA	2.45	0.51
1:B:107:MET:HG2	1:B:455:ARG:CG	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ALA:O	1:B:325:PHE:HB2	2.11	0.51
1:A:282:VAL:CG2	1:A:444:LEU:HD22	2.38	0.50
1:A:389:LYS:NZ	3:A:604:HOH:O	2.33	0.50
1:B:253:GLY:HA3	1:B:259:ILE:HG13	1.93	0.50
1:B:218:ARG:HE	1:B:222:LYS:HZ2	1.60	0.50
1:B:334:GLU:O	1:B:338:VAL:HG23	2.12	0.49
1:B:309:PHE:CE1	1:B:342:PHE:CA	2.95	0.49
1:A:449:THR:O	1:A:458:LEU:HD12	2.13	0.49
1:B:432:LEU:HD11	1:B:440:PHE:CE2	2.47	0.49
1:A:310:TYR:HB2	1:A:383:ALA:HB3	1.95	0.49
1:A:289:MET:HE3	1:A:293:GLU:CG	2.44	0.48
1:B:249:LEU:HD21	1:B:426:ILE:HG22	1.96	0.48
1:A:102:LEU:C	1:A:102:LEU:HD23	2.39	0.47
1:B:400:MET:HG2	1:B:432:LEU:CD2	2.43	0.47
1:B:127:ARG:HB2	1:B:167:MET:HB3	1.97	0.47
1:B:189:LEU:HD21	1:B:201:ILE:HB	1.97	0.47
1:B:393:GLU:HB2	1:B:394:PRO:CD	2.45	0.46
1:B:421:PHE:CE2	1:B:423:MET:HB2	2.50	0.46
1:A:247:ASN:HB3	1:A:430:LEU:HD23	1.97	0.46
1:B:179:LEU:HD23	1:B:190:VAL:HG21	1.96	0.46
1:A:124:ARG:O	1:A:171:VAL:HG22	2.16	0.46
1:A:126:ILE:HD12	1:A:166:ALA:O	2.15	0.46
1:A:218:ARG:NH1	1:A:235:LEU:HD22	2.32	0.45
1:A:460:LYS:HD2	1:A:460:LYS:HA	1.79	0.45
1:B:180:MET:HB2	1:B:282:VAL:HG22	1.97	0.45
1:B:451:PRO:HD2	1:B:456:PRO:O	2.16	0.45
1:A:181:VAL:HA	1:A:283:ASN:OD1	2.16	0.45
1:B:307:LYS:HG3	1:B:386:ASP:HB3	1.99	0.45
1:A:310:TYR:O	1:A:314:VAL:HG23	2.17	0.45
1:B:332:ARG:O	1:B:372:LEU:HD21	2.16	0.45
1:A:439:ALA:O	1:A:443:GLN:HG2	2.17	0.45
1:B:126:ILE:CD1	1:B:169:HIS:HB2	2.43	0.45
1:B:227:ASN:N	1:B:228:PRO:HD3	2.31	0.45
1:B:406:MET:HG2	1:B:413:LYS:HA	1.99	0.45
1:B:211:GLU:HA	1:B:215:GLN:OE1	2.18	0.44
1:A:174:SER:HB3	3:A:683:HOH:O	2.16	0.44
1:B:307:LYS:HG3	1:B:386:ASP:CB	2.46	0.44
1:B:335:ALA:HB1	1:B:376:LEU:HD11	1.99	0.44
1:B:355:ALA:N	3:B:617:HOH:O	2.49	0.44
1:A:157:GLU:N	1:A:158:PRO:CD	2.81	0.44
1:B:406:MET:HE2	1:B:406:MET:HB2	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ASN:O	1:B:163:LEU:HG	2.18	0.43
1:A:194:SER:C	1:A:196:ARG:H	2.26	0.43
1:A:211:GLU:HA	1:A:215:GLN:OE1	2.18	0.43
1:A:309:PHE:CE1	1:A:342:PHE:CA	3.00	0.43
1:A:183:THR:HA	1:A:287:VAL:O	2.18	0.43
1:A:102:LEU:HD23	1:A:103:LEU:N	2.33	0.43
1:A:131:GLN:HE21	1:A:138:ASN:HA	1.84	0.43
1:A:179:LEU:HD11	1:A:237:THR:CG2	2.49	0.43
1:A:455:ARG:HA	1:A:455:ARG:HE	1.84	0.43
1:B:317:ILE:CD1	1:B:373:LYS:HD2	2.49	0.43
1:A:180:MET:HB2	1:A:282:VAL:HG22	2.00	0.43
1:B:116:TYR:CE2	1:B:214:ARG:HG3	2.53	0.43
1:B:146:LEU:CD1	1:B:167:MET:HE3	2.49	0.43
1:B:181:VAL:HA	1:B:283:ASN:OD1	2.18	0.42
1:B:107:MET:HE3	1:B:107:MET:HA	2.01	0.42
1:B:218:ARG:HH11	1:B:218:ARG:HG3	1.84	0.42
1:A:193:ASN:O	1:A:385:ASN:HA	2.20	0.42
1:A:176:ALA:HA	1:A:203:THR:O	2.19	0.42
1:B:157:GLU:HG2	1:B:160:ARG:HH22	1.83	0.42
1:B:393:GLU:N	1:B:394:PRO:HD2	2.35	0.42
1:A:269:ASP:HA	1:A:270:PRO:HD2	1.82	0.41
1:A:399:ALA:HB1	1:A:425:PHE:CZ	2.55	0.41
1:A:147:PHE:CD1	1:A:160:ARG:HB2	2.55	0.41
1:A:244:ARG:HG3	1:A:444:LEU:HD23	2.02	0.41
1:B:313:ALA:HA	1:B:376:LEU:HD22	2.02	0.41
1:A:451:PRO:CD	1:A:455:ARG:HB2	2.37	0.41
1:B:128:GLU:HA	1:B:131:GLN:OE1	2.20	0.41
1:B:102:LEU:HD22	3:B:643:HOH:O	2.21	0.41
1:A:222:LYS:NZ	1:A:352:GLU:OE2	2.47	0.41
1:A:407:ASP:OD1	1:A:407:ASP:N	2.53	0.41
1:B:131:GLN:HE21	1:B:138:ASN:HA	1.85	0.41
1:B:177:ALA:HB2	1:B:217:VAL:HG13	2.02	0.41
1:B:362:LYS:HE3	3:B:638:HOH:O	2.21	0.41
1:A:145:HIS:NE2	1:B:145:HIS:NE2	2.69	0.41
1:B:393:GLU:HB2	1:B:394:PRO:HD3	2.02	0.41
1:A:289:MET:HE3	1:A:293:GLU:HG3	2.04	0.40
1:B:176:ALA:HA	1:B:203:THR:O	2.22	0.40
1:B:157:GLU:N	1:B:158:PRO:CD	2.85	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	357/482 (74%)	347 (97%)	10 (3%)	0	100	100
1	B	359/482 (74%)	355 (99%)	4 (1%)	0	100	100
All	All	716/964 (74%)	702 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	282/381 (74%)	262 (93%)	20 (7%)	13	17
1	B	281/381 (74%)	264 (94%)	17 (6%)	17	23
All	All	563/762 (74%)	526 (93%)	37 (7%)	15	19

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LEU
1	A	104	GLN
1	A	107	MET
1	A	143	VAL
1	A	168	GLN
1	A	170	SER
1	A	171	VAL
1	A	215	GLN

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Mol	Chain	Res	Type
1	A	238	LEU
1	A	305	ARG
1	A	317	ILE
1	A	322	LYS
1	A	343	ARG
1	A	357	CYS
1	A	374	GLN
1	A	380	ILE
1	A	389	LYS
1	A	407	ASP
1	A	455	ARG
1	A	460	LYS
1	B	105	GLN
1	B	107	MET
1	B	196	ARG
1	B	209	LYS
1	B	215	GLN
1	B	238	LEU
1	B	307	LYS
1	B	322	LYS
1	B	357	CYS
1	B	362	LYS
1	B	369	MET
1	B	373	LYS
1	B	380	ILE
1	B	406	MET
1	B	418	ASN
1	B	445	LYS
1	B	460	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	HIS
1	A	197	HIS
1	A	247	ASN
1	A	276	ASN
1	A	443	GLN
1	B	154	GLN
1	B	197	HIS
1	B	202	GLN
1	B	247	ASN

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Mol	Chain	Res	Type
1	B	398	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	359/482 (74%)	-1.57	0 100 100	14, 36, 59, 87	3 (0%)
1	B	361/482 (74%)	-1.54	0 100 100	14, 38, 62, 79	4 (1%)
All	All	720/964 (74%)	-1.56	0 100 100	14, 37, 60, 87	7 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

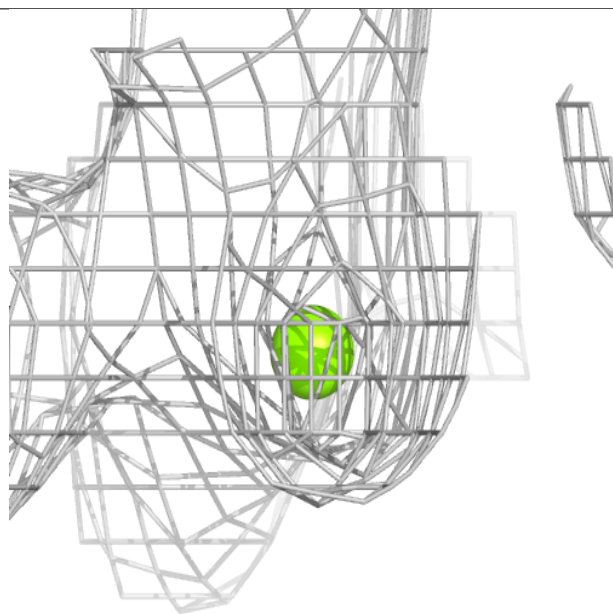
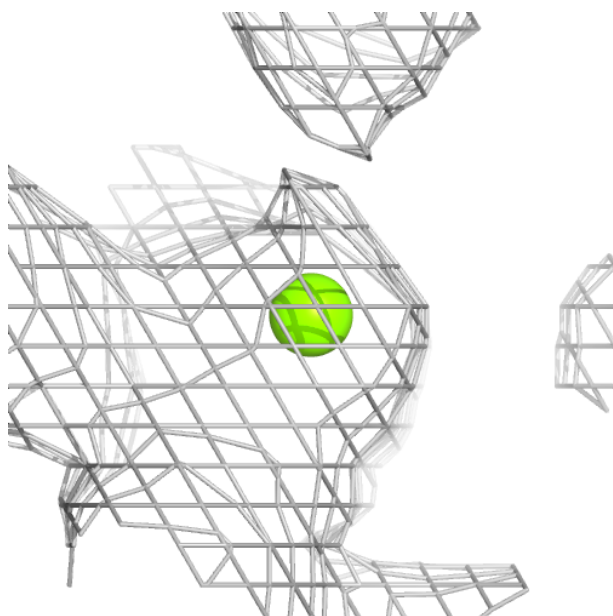
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	A	501	1/1	0.99	0.05	30,30,30,30	1
2	MG	B	501	1/1	0.99	0.05	30,30,30,30	0
2	MG	A	503	1/1	1.00	0.02	30,30,30,30	1
2	MG	A	502	1/1	1.00	0.02	30,30,30,30	0
2	MG	B	502	1/1	1.00	0.02	30,30,30,30	0
2	MG	B	503	1/1	1.00	0.02	30,30,30,30	1

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.

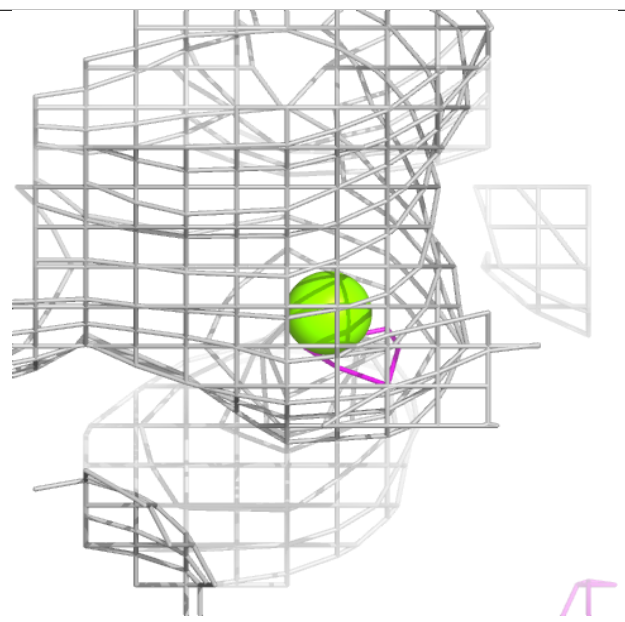
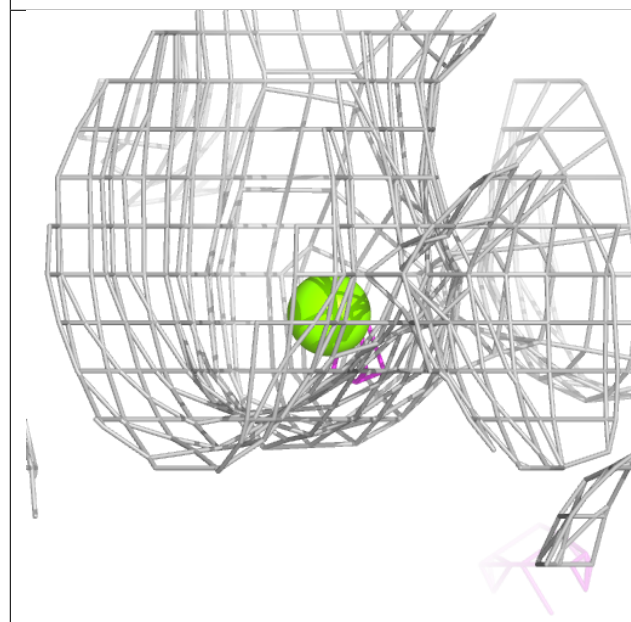
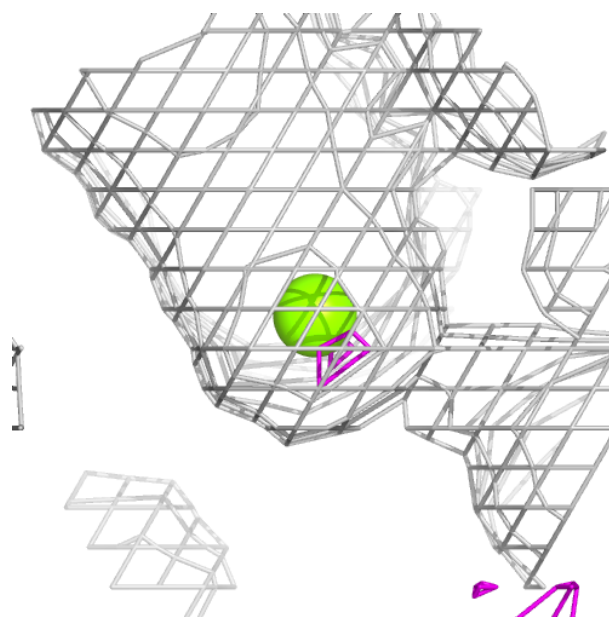
Electron density around MG A 501:

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



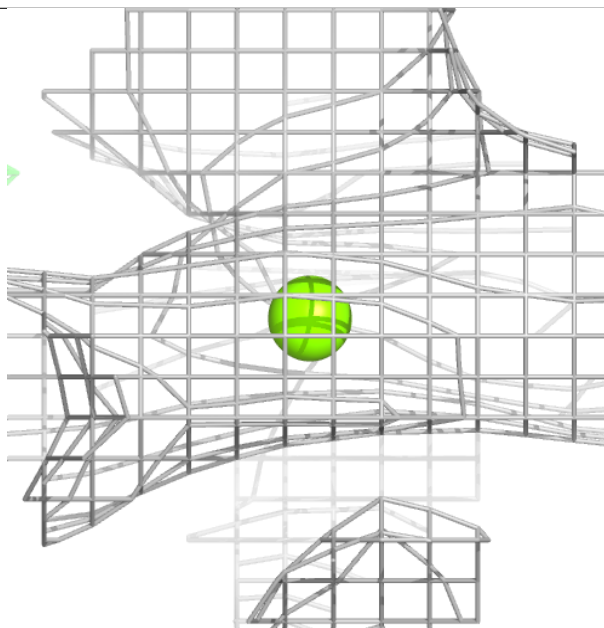
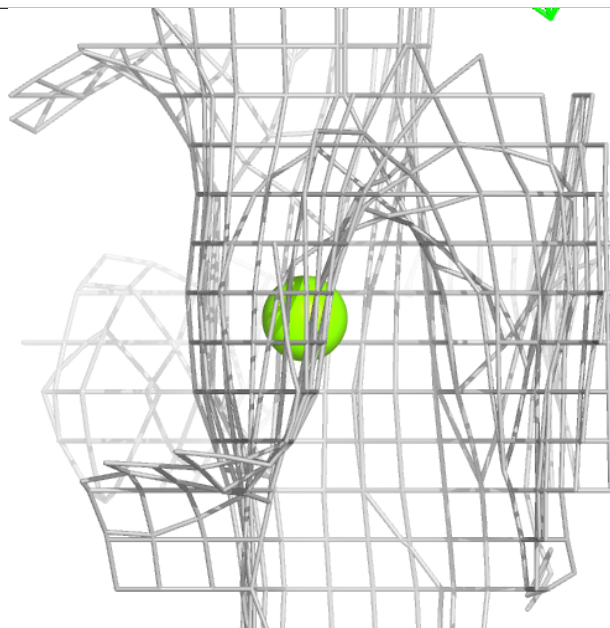
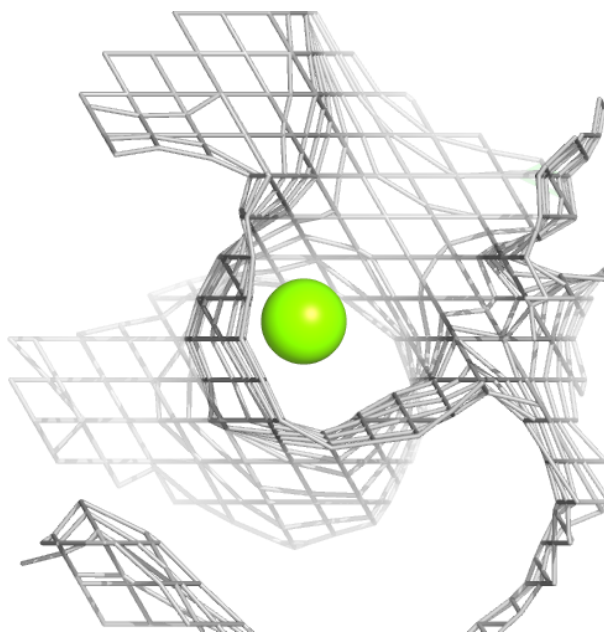
Electron density around MG B 501:

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



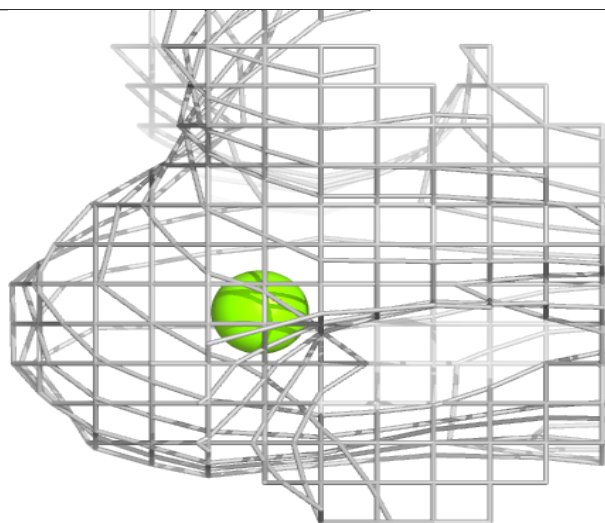
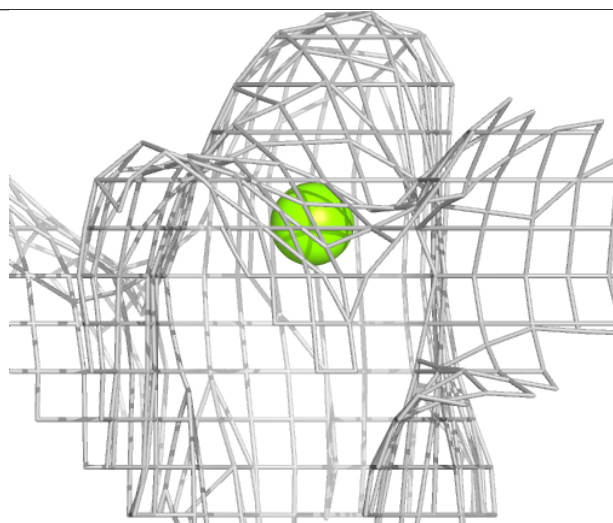
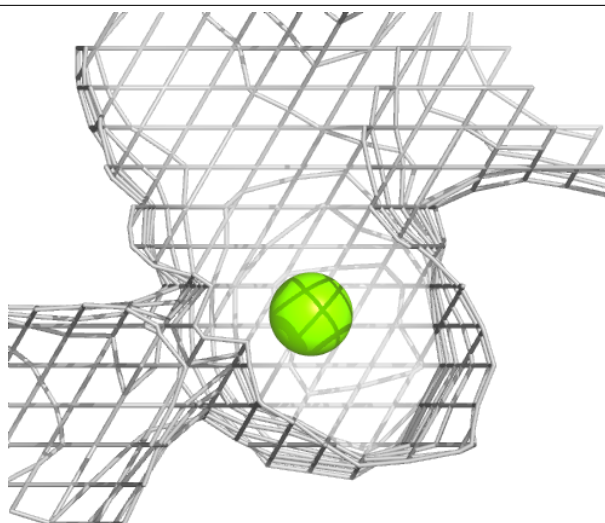
Electron density around MG A 503:

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



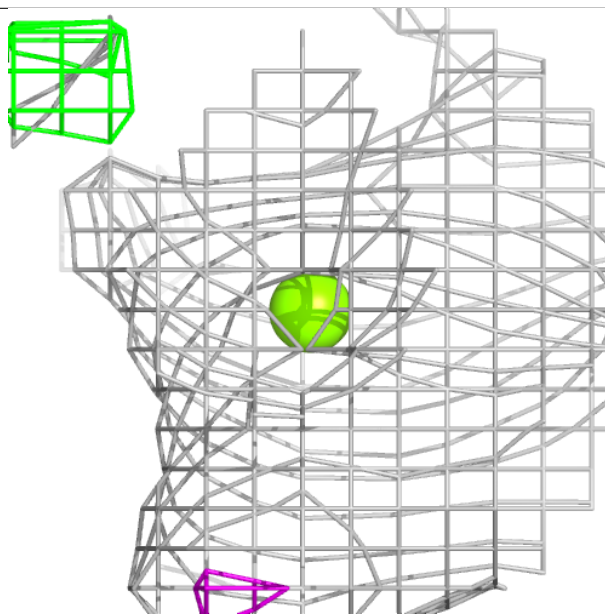
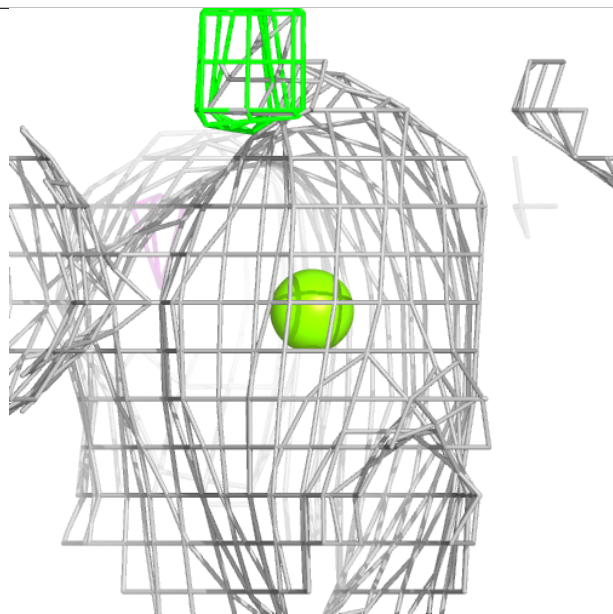
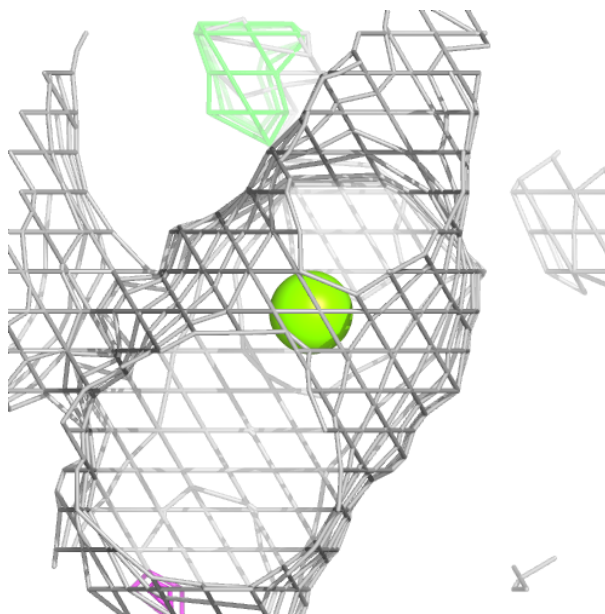
Electron density around MG A 502:

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and green (positive)



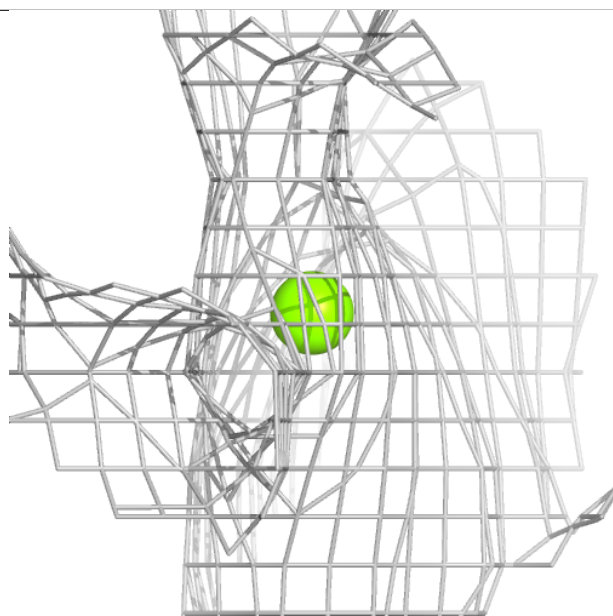
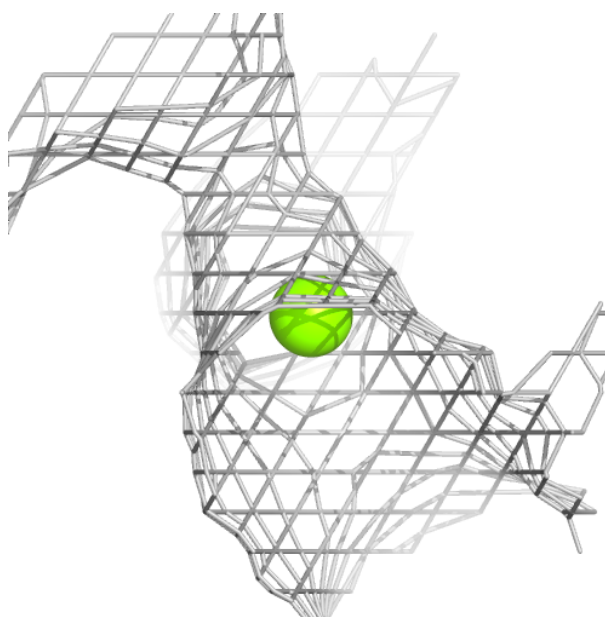
Electron density around MG B 502:

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



Electron density around MG B 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.