



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 04:17 PM EDT

PDB ID : 8QL1 / pdb_00008ql1
Title : Crystal structure of the human MDN1-MIDAS/NLE1-UBL complex
Authors : Wild, K.; Fiorentino, F.; Hurt, E.; Sinning, I.
Deposited on : 2023-09-19
Resolution : 2.30 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

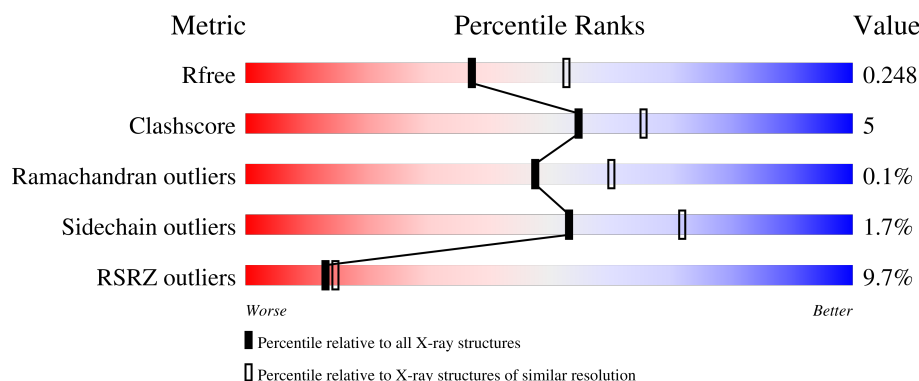
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	279	8% 76% 10% 14%
1	C	279	7% 76% 11% 12%
1	E	279	7% 72% 15% 12%
1	G	279	8% 77% 8% 15%
2	B	103	8% 78% 10% 13%

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Mol	Chain	Length	Quality of chain
2	D	103	20% 73% 9% 18%
2	F	103	4% 73% 8% 18%
2	H	103	11% 80% 7% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10770 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 NDE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1909	1228	316	356	9			
1	C	245	Total	C	N	O	S	0	0	0
			1935	1242	321	363	9			
1	E	245	Total	C	N	O	S	0	0	0
			1935	1242	321	363	9			
1	G	236	Total	C	N	O	S	0	0	0
			1862	1200	305	348	9			

- Molecule 2 is a protein called Notchless protein homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	90	Total	C	N	O	S	0	0	0
			704	451	116	136	1			
2	D	84	Total	C	N	O	S	0	0	0
			651	416	104	130	1			
2	F	84	Total	C	N	O	S	0	0	0
			651	416	104	130	1			
2	H	90	Total	C	N	O	S	0	0	0
			704	451	116	136	1			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	HIS	-	expression tag	UNP Q9NVX2
B	3	HIS	-	expression tag	UNP Q9NVX2
B	4	HIS	-	expression tag	UNP Q9NVX2
B	5	HIS	-	expression tag	UNP Q9NVX2
B	6	HIS	-	expression tag	UNP Q9NVX2
B	7	HIS	-	expression tag	UNP Q9NVX2
B	8	GLY	-	expression tag	UNP Q9NVX2
B	9	SER	-	expression tag	UNP Q9NVX2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2	HIS	-	expression tag	UNP Q9NVX2
D	3	HIS	-	expression tag	UNP Q9NVX2
D	4	HIS	-	expression tag	UNP Q9NVX2
D	5	HIS	-	expression tag	UNP Q9NVX2
D	6	HIS	-	expression tag	UNP Q9NVX2
D	7	HIS	-	expression tag	UNP Q9NVX2
D	8	GLY	-	expression tag	UNP Q9NVX2
D	9	SER	-	expression tag	UNP Q9NVX2
F	2	HIS	-	expression tag	UNP Q9NVX2
F	3	HIS	-	expression tag	UNP Q9NVX2
F	4	HIS	-	expression tag	UNP Q9NVX2
F	5	HIS	-	expression tag	UNP Q9NVX2
F	6	HIS	-	expression tag	UNP Q9NVX2
F	7	HIS	-	expression tag	UNP Q9NVX2
F	8	GLY	-	expression tag	UNP Q9NVX2
F	9	SER	-	expression tag	UNP Q9NVX2
H	2	HIS	-	expression tag	UNP Q9NVX2
H	3	HIS	-	expression tag	UNP Q9NVX2
H	4	HIS	-	expression tag	UNP Q9NVX2
H	5	HIS	-	expression tag	UNP Q9NVX2
H	6	HIS	-	expression tag	UNP Q9NVX2
H	7	HIS	-	expression tag	UNP Q9NVX2
H	8	GLY	-	expression tag	UNP Q9NVX2
H	9	SER	-	expression tag	UNP Q9NVX2

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0

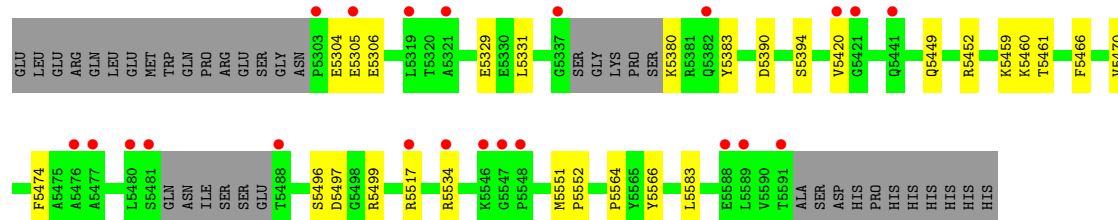
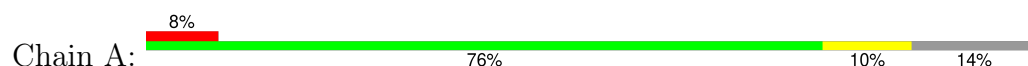
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	80	Total 80	O 80	0	0
4	B	27	Total 27	O 27	0	0
4	C	64	Total 64	O 64	0	0
4	D	13	Total 13	O 13	0	0
4	E	97	Total 97	O 97	0	0
4	F	28	Total 28	O 28	0	0
4	G	61	Total 61	O 61	0	0
4	H	45	Total 45	O 45	0	0

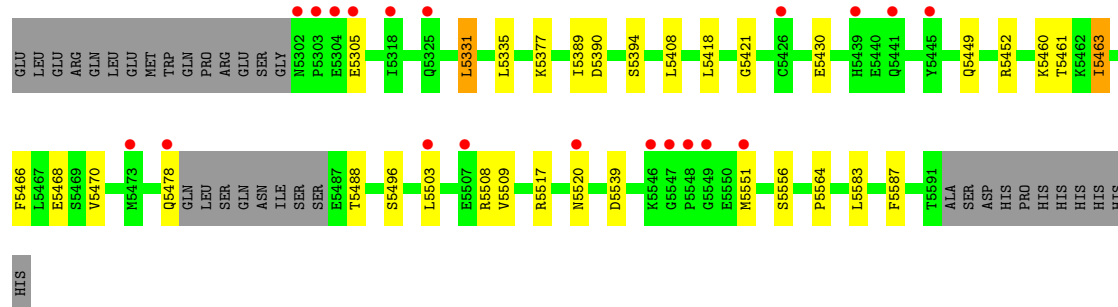
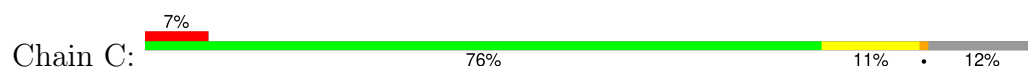
3 Residue-property plots [i](#)

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.

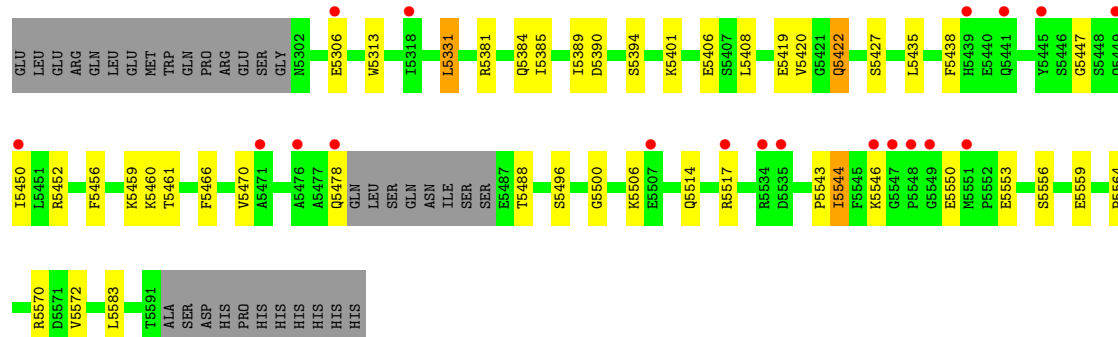
• Molecule 1: NDE1



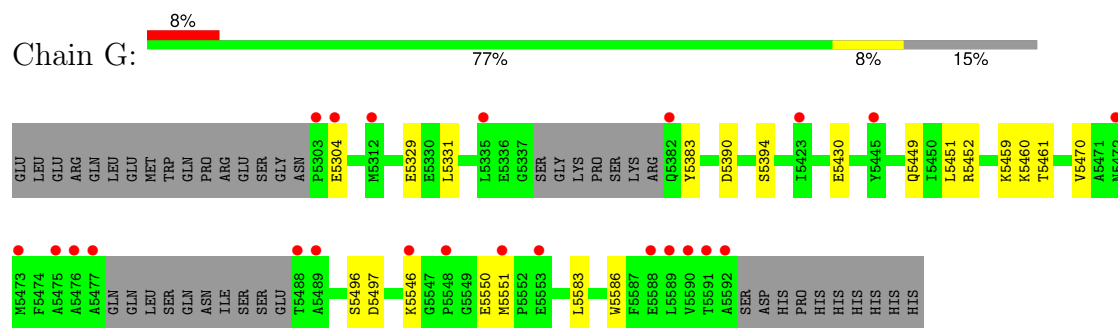
• Molecule 1: NDE1



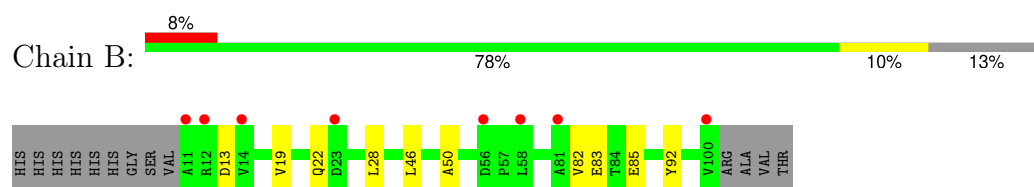
• Molecule 1: NDE1



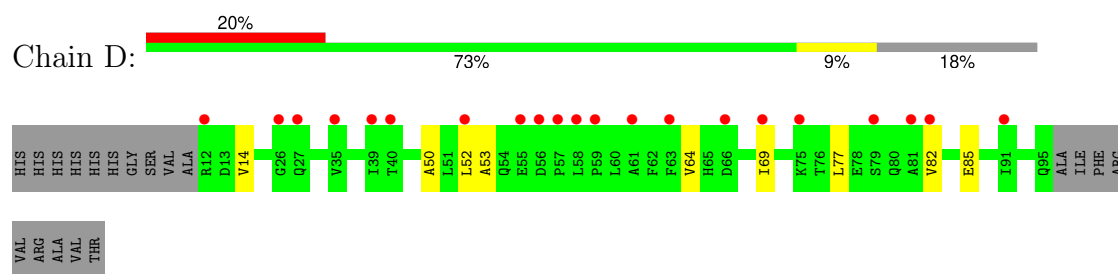
- Molecule 1: NDE1



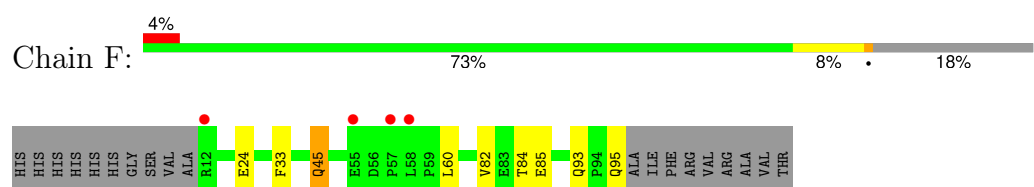
- Molecule 2: Notchless protein homolog 1



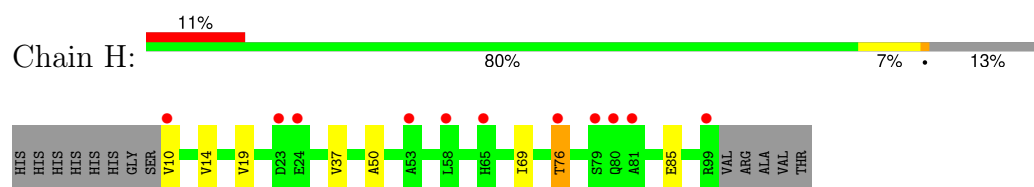
- Molecule 2: Notchless protein homolog 1



- Molecule 2: Notchless protein homolog 1



- Molecule 2: Notchless protein homolog 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	237.16Å 69.82Å 103.18Å 90.00° 91.79° 90.00°	Depositor
Resolution (Å)	118.52 – 2.30 118.52 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (118.52-2.30) 99.7 (118.52-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.19_4092: ???)	Depositor
R, R_{free}	0.214 , 0.248 0.216 , 0.248	Depositor DCC
R_{free} test set	3813 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10770	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5003e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.11	0/1943	0.31	0/2626
1	C	0.11	0/1971	0.29	0/2666
1	E	0.12	0/1971	0.31	0/2666
1	G	0.11	0/1896	0.30	0/2565
2	B	0.16	0/716	0.36	0/976
2	D	0.23	0/662	0.37	0/904
2	F	0.10	0/662	0.30	0/904
2	H	0.16	0/716	0.37	0/976
All	All	0.13	0/10537	0.31	0/14283

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	1909	0	1927	20	0
1	C	1935	0	1949	20	0
1	E	1935	0	1949	31	0
1	G	1862	0	1874	14	0
2	B	704	0	707	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	651	0	644	7	0
2	F	651	0	644	7	0
2	H	704	0	707	5	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	80	0	0	5	0
4	B	27	0	0	5	0
4	C	64	0	0	4	0
4	D	13	0	0	1	0
4	E	97	0	0	9	0
4	F	28	0	0	2	0
4	G	61	0	0	3	0
4	H	45	0	0	2	0
All	All	10770	0	10401	100	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 5.

All (100) 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:E:5381:ARG:NH1	4:E:5801:HOH:O	2.04	0.85
1:A:5534:ARG:NH1	4:A:5801:HOH:O	2.07	0.85
1:A:5449:GLN:OE1	1:A:5452:ARG:NH2	2.15	0.79
1:C:5556:SER:OG	4:C:5801:HOH:O	2.00	0.79
1:G:5551:MET:SD	4:H:242:HOH:O	2.43	0.76
2:F:84:THR:O	4:F:201:HOH:O	2.05	0.75
2:B:13:ASP:OD2	4:B:201:HOH:O	2.04	0.73
1:E:5506:LYS:NZ	4:E:5805:HOH:O	2.20	0.73
1:A:5566:TYR:OH	4:A:5802:HOH:O	2.07	0.72
2:D:77:LEU:HD22	2:D:82:VAL:HG21	1.71	0.71
1:G:5449:GLN:OE1	1:G:5452:ARG:NH2	2.24	0.71
1:E:5559:GLU:OE2	4:E:5802:HOH:O	2.09	0.70
1:A:5551:MET:SD	4:B:224:HOH:O	2.49	0.70
1:C:5463:ILE:HD11	1:C:5509:VAL:HG13	1.73	0.70
1:G:5451:LEU:O	4:G:5801:HOH:O	2.10	0.69
2:B:83:GLU:OE2	4:B:202:HOH:O	2.10	0.69
1:A:5497:ASP:OD1	4:A:5803:HOH:O	2.11	0.69
1:C:5449:GLN:OE1	1:C:5452:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5514:GLN:OE1	4:E:5803:HOH:O	2.12	0.67
1:E:5419:GLU:OE1	4:E:5804:HOH:O	2.13	0.67
1:E:5517:ARG:HH22	1:E:5564:PRO:HG3	1.61	0.66
1:G:5551:MET:HE1	2:H:50:ALA:HB2	1.78	0.66
2:F:24:GLU:OE2	2:F:93:GLN:NE2	2.30	0.65
2:H:10:VAL:N	4:H:203:HOH:O	2.30	0.64
1:G:5459:LYS:C	1:G:5460:LYS:HD2	2.24	0.62
1:C:5389:ILE:HD11	1:C:5408:LEU:HD13	1.82	0.62
1:E:5500:GLY:N	4:E:5811:HOH:O	2.31	0.61
1:C:5478:GLN:NE2	1:C:5488:THR:OG1	2.32	0.59
1:A:5466:PHE:O	1:A:5470:VAL:HG23	2.03	0.58
1:A:5329:GLU:OE2	4:A:5804:HOH:O	2.17	0.57
1:C:5517:ARG:HH22	1:C:5564:PRO:HG3	1.68	0.56
1:G:5497:ASP:OD1	4:G:5802:HOH:O	2.18	0.54
2:B:92:TYR:OH	4:B:203:HOH:O	2.19	0.54
1:E:5517:ARG:NH1	4:E:5803:HOH:O	2.40	0.53
2:H:69:ILE:HG12	2:H:76:THR:HG21	1.90	0.53
1:A:5551:MET:HE1	2:B:50:ALA:HB2	1.91	0.53
2:D:64:VAL:HG12	2:D:69:ILE:HD11	1.91	0.52
1:C:5331:LEU:HD11	1:C:5583:LEU:HD12	1.90	0.52
1:A:5394:SER:HB3	2:B:85:GLU:HG3	1.91	0.52
1:E:5466:PHE:O	1:E:5470:VAL:HG23	2.10	0.52
1:G:5394:SER:HB3	2:H:85:GLU:HG3	1.92	0.51
1:G:5390:ASP:HB2	1:G:5496:SER:HB2	1.93	0.51
1:E:5394:SER:HB3	2:F:85:GLU:HG3	1.92	0.51
1:E:5422:GLN:HG3	1:E:5438:PHE:HB3	1.93	0.51
1:E:5517:ARG:NH2	1:E:5564:PRO:HG3	2.25	0.50
1:C:5430:GLU:HG2	1:C:5460:LYS:HB2	1.92	0.50
1:C:5539:ASP:OD2	4:C:5802:HOH:O	2.20	0.50
1:C:5551:MET:HE1	2:D:50:ALA:HB2	1.93	0.50
1:C:5466:PHE:O	1:C:5470:VAL:HG23	2.12	0.49
1:E:5331:LEU:HD11	1:E:5583:LEU:HD12	1.94	0.49
1:E:5546:LYS:O	1:E:5550:GLU:HB2	2.11	0.49
1:E:5390:ASP:HB2	1:E:5496:SER:HB2	1.95	0.48
1:A:5552:PRO:HD3	2:B:46:LEU:HB3	1.96	0.48
1:E:5459:LYS:O	1:E:5460:LYS:HD2	2.13	0.48
1:A:5459:LYS:O	1:A:5460:LYS:HD2	2.13	0.48
1:E:5461:THR:OG1	2:F:85:GLU:OE2	2.32	0.48
1:A:5390:ASP:HB2	1:A:5496:SER:HB2	1.95	0.48
1:C:5503:LEU:HB2	4:C:5814:HOH:O	2.14	0.47
1:E:5384:GLN:NE2	4:E:5812:HOH:O	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5331:LEU:HD21	1:A:5583:LEU:HD12	1.96	0.47
1:E:5306:GLU:OE2	1:E:5452:ARG:NH2	2.48	0.47
1:G:5331:LEU:HD21	1:G:5583:LEU:HD12	1.97	0.47
1:A:5470:VAL:HG12	1:A:5474:PHE:CD2	2.50	0.46
1:C:5335:LEU:HD12	1:C:5418:LEU:HD21	1.96	0.46
1:C:5377:LYS:HG3	1:C:5587:PHE:HZ	1.80	0.46
1:A:5304:GLU:C	1:A:5306:GLU:H	2.24	0.46
2:B:83:GLU:HG2	4:B:218:HOH:O	2.14	0.46
1:C:5390:ASP:HB2	1:C:5496:SER:HB2	1.98	0.45
1:A:5517:ARG:NH2	1:A:5564:PRO:HG3	2.32	0.45
1:C:5461:THR:OG1	2:D:85:GLU:OE2	2.34	0.45
1:E:5570:ARG:NH2	4:E:5824:HOH:O	2.50	0.45
1:G:5304:GLU:O	1:G:5304:GLU:HG3	2.17	0.45
1:E:5544:ILE:HG23	1:E:5553:GLU:HB3	1.99	0.44
1:G:5430:GLU:O	4:G:5803:HOH:O	2.21	0.44
1:E:5389:ILE:HD11	1:E:5408:LEU:HD13	1.99	0.44
2:D:14:VAL:O	4:D:201:HOH:O	2.21	0.44
1:A:5383:TYR:HB2	1:A:5420:VAL:HG12	1.99	0.44
1:C:5394:SER:HB3	2:D:85:GLU:HG3	2.00	0.43
1:A:5517:ARG:HH22	1:A:5564:PRO:HG3	1.83	0.43
1:E:5478:GLN:OE1	1:E:5488:THR:OG1	2.30	0.43
2:B:22:GLN:HB3	2:B:28:LEU:HD23	2.00	0.43
1:A:5499:ARG:NH1	4:A:5805:HOH:O	2.21	0.43
1:C:5421:GLY:N	4:C:5803:HOH:O	2.21	0.42
1:E:5313:TRP:CH2	1:E:5408:LEU:HD23	2.55	0.42
1:A:5461:THR:OG1	2:B:85:GLU:OE2	2.37	0.42
1:G:5461:THR:OG1	2:H:85:GLU:OE2	2.38	0.42
2:F:45:GLN:HE22	2:F:60:LEU:H	1.68	0.41
1:G:5546:LYS:O	1:G:5550:GLU:HB2	2.19	0.41
1:E:5313:TRP:CE2	1:E:5447:GLY:HA3	2.55	0.41
1:G:5383:TYR:HD2	1:G:5586:TRP:CH2	2.38	0.41
1:C:5468:GLU:OE2	1:C:5508:ARG:NH2	2.47	0.41
2:F:95:GLN:HB2	4:F:217:HOH:O	2.21	0.41
1:E:5543:PRO:HD3	2:F:33:PHE:HD2	1.85	0.41
1:C:5331:LEU:HB3	1:C:5418:LEU:HD22	2.03	0.41
1:E:5401:LYS:HG3	1:E:5456:PHE:CD2	2.56	0.41
1:E:5385:ILE:HD12	1:E:5420:VAL:HG11	2.03	0.40
2:D:52:LEU:O	2:D:53:ALA:C	2.64	0.40
1:E:5406:GLU:HB3	1:E:5572:VAL:HG21	2.02	0.40
1:E:5556:SER:OG	1:E:5559:GLU:HG3	2.21	0.40
1:E:5427:SER:HB3	1:E:5435:LEU:HD11	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	235/279 (84%)	232 (99%)	2 (1%)	1 (0%)	30	38
1	C	241/279 (86%)	239 (99%)	2 (1%)	0	100	100
1	E	241/279 (86%)	239 (99%)	2 (1%)	0	100	100
1	G	230/279 (82%)	228 (99%)	2 (1%)	0	100	100
2	B	88/103 (85%)	87 (99%)	1 (1%)	0	100	100
2	D	82/103 (80%)	81 (99%)	1 (1%)	0	100	100
2	F	82/103 (80%)	82 (100%)	0	0	100	100
2	H	88/103 (85%)	87 (99%)	1 (1%)	0	100	100
All	All	1287/1528 (84%)	1275 (99%)	11 (1%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5305	GLU

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	210/245 (86%)	209 (100%)	1 (0%)	81	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	213/245 (87%)	209 (98%)	4 (2%)	50	69
1	E	213/245 (87%)	209 (98%)	4 (2%)	50	69
1	G	204/245 (83%)	202 (99%)	2 (1%)	68	82
2	B	79/90 (88%)	77 (98%)	2 (2%)	42	60
2	D	74/90 (82%)	74 (100%)	0	100	100
2	F	74/90 (82%)	72 (97%)	2 (3%)	39	58
2	H	79/90 (88%)	75 (95%)	4 (5%)	21	32
All	All	1146/1340 (86%)	1127 (98%)	19 (2%)	53	72

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5380	LYS
2	B	19	VAL
2	B	82	VAL
1	C	5305	GLU
1	C	5331	LEU
1	C	5463	ILE
1	C	5520	ASN
1	E	5331	LEU
1	E	5422	GLN
1	E	5450	ILE
1	E	5544	ILE
2	F	45	GLN
2	F	82	VAL
1	G	5329	GLU
1	G	5470	VAL
2	H	14	VAL
2	H	19	VAL
2	H	37	VAL
2	H	76	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5399	HIS
1	A	5479	GLN
2	B	15	GLN

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Mol	Chain	Res	Type
1	C	5399	HIS
1	C	5413	ASN
1	C	5465	GLN
1	E	5314	GLN
1	E	5384	GLN
1	E	5399	HIS
1	E	5413	ASN
1	E	5490	GLN
2	F	93	GLN
1	G	5399	HIS
2	H	15	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 4 ligands modelled in this entry, 4 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 [i](#)

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 ⓘ

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, 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	241/279 (86%)	0.54	22 (9%) 15 16	29, 45, 81, 101	0
1	C	245/279 (87%)	0.63	20 (8%) 17 19	29, 49, 86, 101	0
1	E	245/279 (87%)	0.48	19 (7%) 19 21	28, 44, 72, 100	0
1	G	236/279 (84%)	0.64	23 (9%) 13 15	29, 46, 79, 89	0
2	B	90/103 (87%)	0.65	8 (8%) 15 17	32, 44, 70, 87	0
2	D	84/103 (81%)	1.49	21 (25%) 2 2	49, 79, 103, 126	0
2	F	84/103 (81%)	0.71	4 (4%) 35 37	38, 54, 81, 95	0
2	H	90/103 (87%)	0.68	11 (12%) 8 9	32, 42, 74, 93	0
All	All	1315/1528 (86%)	0.65	128 (9%) 13 15	28, 48, 87, 126	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	81	ALA	5.3
2	B	100	VAL	5.2
1	A	5591	THR	5.2
1	G	5303	PRO	4.8
1	G	5477	ALA	4.7
1	G	5589	LEU	4.6
2	F	58	LEU	4.4
1	G	5592	ALA	4.3
1	A	5589	LEU	4.3
2	D	12	ARG	4.1
1	A	5488	THR	4.1
1	A	5303	PRO	4.0
1	C	5439	HIS	3.9
2	D	75	LYS	3.8
2	D	58	LEU	3.8
1	C	5478	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	5503	LEU	3.7
1	A	5548	PRO	3.7
2	H	10	VAL	3.7
1	C	5441	GLN	3.6
2	D	81	ALA	3.5
1	C	5303	PRO	3.5
1	G	5548	PRO	3.5
2	F	55	GLU	3.5
1	A	5546	LYS	3.4
1	A	5305	GLU	3.4
2	D	82	VAL	3.4
1	G	5488	THR	3.3
1	G	5591	THR	3.3
1	A	5337	GLY	3.3
1	E	5547	GLY	3.2
1	A	5547	GLY	3.2
1	G	5588	GLU	3.1
2	D	56	ASP	3.1
1	G	5476	ALA	3.1
2	B	11	ALA	3.1
1	A	5534	ARG	3.0
1	E	5548	PRO	3.0
1	E	5478	GLN	3.0
1	A	5517	ARG	2.9
2	H	76	THR	2.9
2	B	81	ALA	2.9
1	E	5551	MET	2.9
1	E	5439	HIS	2.9
1	E	5476	ALA	2.9
1	G	5335	LEU	2.9
2	D	63	PHE	2.9
2	H	80	GLN	2.8
1	C	5305	GLU	2.8
1	C	5547	GLY	2.8
1	G	5551	MET	2.8
1	E	5507	GLU	2.7
1	G	5546	LYS	2.7
1	C	5318	ILE	2.7
1	E	5471	ALA	2.7
1	C	5549	GLY	2.7
1	C	5302	ASN	2.7
1	C	5304	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	5520	ASN	2.6
2	D	69	ILE	2.6
2	F	12	ARG	2.6
2	D	61	ALA	2.6
2	H	99	ARG	2.6
1	G	5489	ALA	2.6
1	C	5473	MET	2.6
1	A	5481	SER	2.6
1	E	5441	GLN	2.5
1	E	5534	ARG	2.5
1	A	5476	ALA	2.5
1	C	5551	MET	2.5
1	G	5473	MET	2.5
1	A	5319	LEU	2.5
1	E	5549	GLY	2.5
1	E	5449	GLN	2.5
1	C	5445	TYR	2.5
2	H	58	LEU	2.5
2	D	26	GLY	2.5
1	A	5441	GLN	2.5
1	E	5306	GLU	2.4
1	C	5546	LYS	2.4
1	E	5517	ARG	2.4
2	D	55	GLU	2.4
2	B	23	ASP	2.3
1	C	5548	PRO	2.3
1	E	5546	LYS	2.3
2	D	35	VAL	2.3
1	A	5321	ALA	2.3
2	D	79	SER	2.3
2	H	65	HIS	2.3
2	F	57	PRO	2.3
2	B	14	VAL	2.3
1	A	5421	GLY	2.2
1	E	5445	TYR	2.2
1	G	5304	GLU	2.2
2	H	79	SER	2.2
1	E	5535	ASP	2.2
2	D	59	PRO	2.2
1	A	5382	GLN	2.2
1	G	5445	TYR	2.2
2	B	58	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	5590	VAL	2.2
1	C	5426	CYS	2.2
2	D	52	LEU	2.2
2	D	66	ASP	2.2
1	G	5382	GLN	2.2
2	H	24	GLU	2.1
2	D	27	GLN	2.1
1	G	5475	ALA	2.1
2	D	40	THR	2.1
1	G	5312	MET	2.1
1	C	5507	GLU	2.1
1	G	5553	GLU	2.1
1	A	5420	VAL	2.1
1	A	5588	GLU	2.1
2	D	39	ILE	2.1
2	D	91	ILE	2.1
1	A	5477	ALA	2.0
2	H	53	ALA	2.0
1	C	5325	GLN	2.0
1	A	5480	LEU	2.0
1	G	5472	ASN	2.0
2	B	56	ASP	2.0
2	H	23	ASP	2.0
1	G	5423	ILE	2.0
2	D	57	PRO	2.0
1	E	5318	ILE	2.0
1	E	5450	ILE	2.0
2	B	12	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 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,

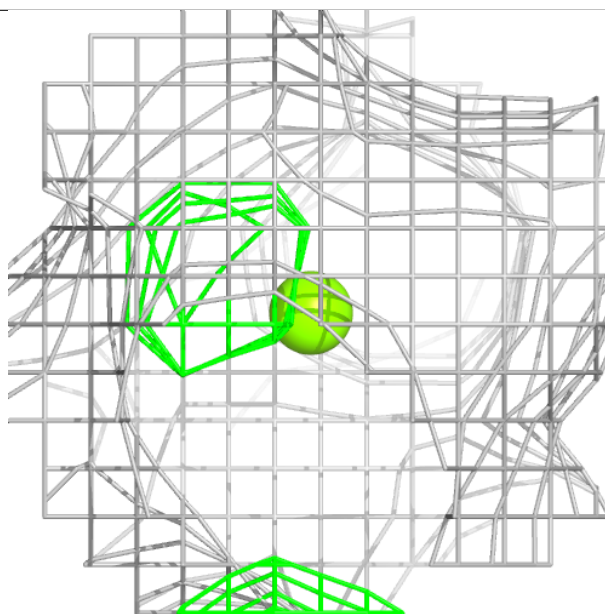
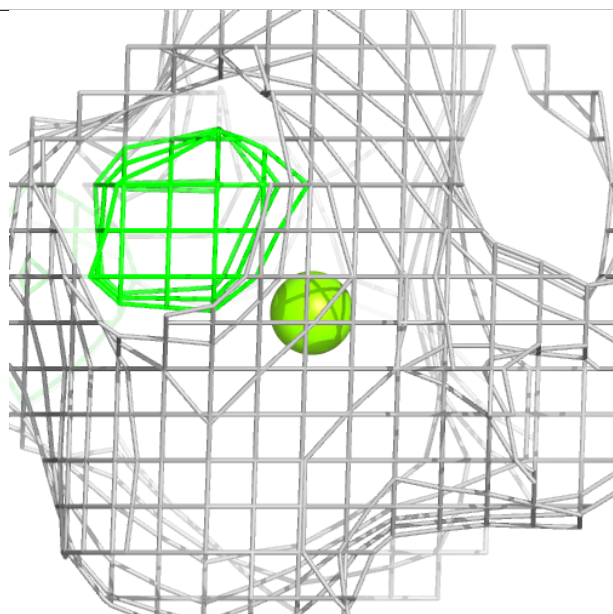
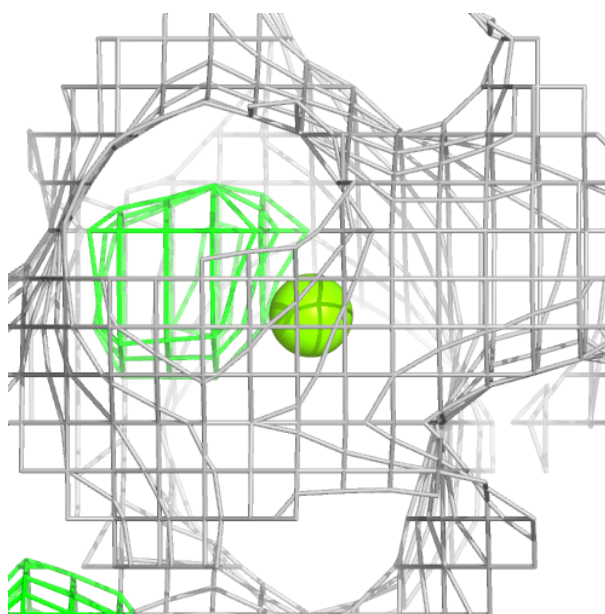
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	C	5701	1/1	0.97	0.07	45,45,45,45	0
3	MG	A	5701	1/1	0.98	0.05	29,29,29,29	0
3	MG	E	5701	1/1	0.99	0.07	35,35,35,35	0
3	MG	G	5701	1/1	0.99	0.03	26,26,26,26	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.

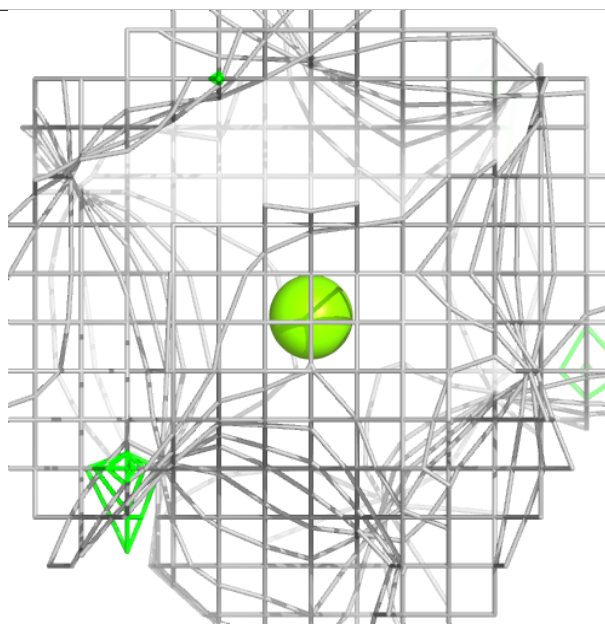
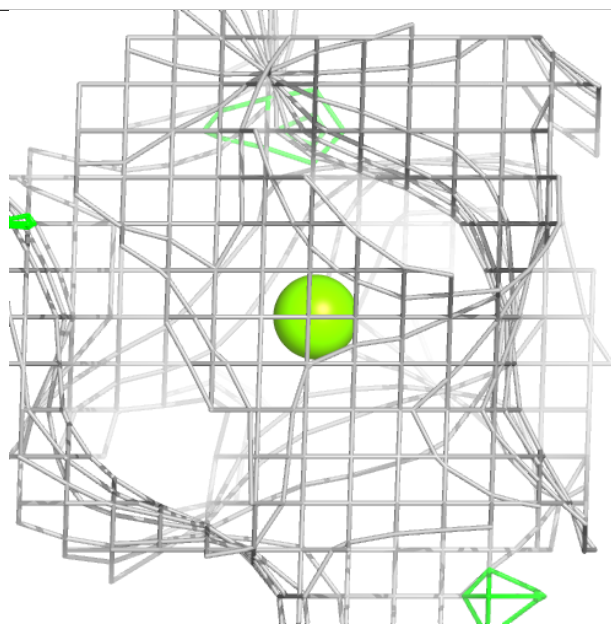
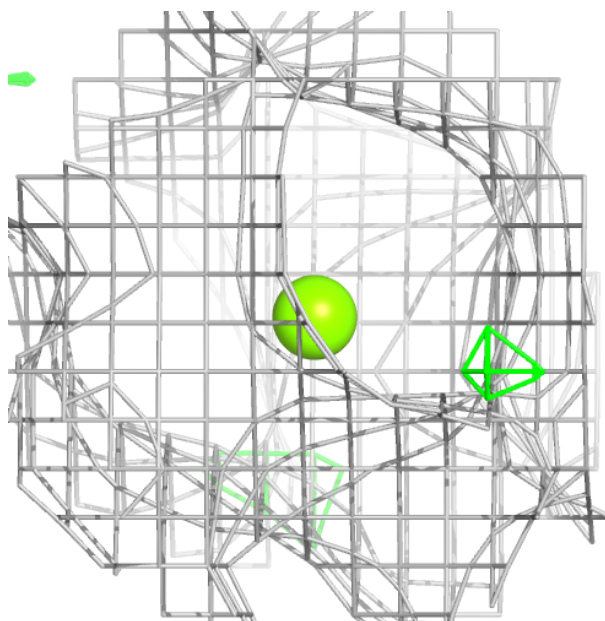
Electron density around MG C 5701:

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



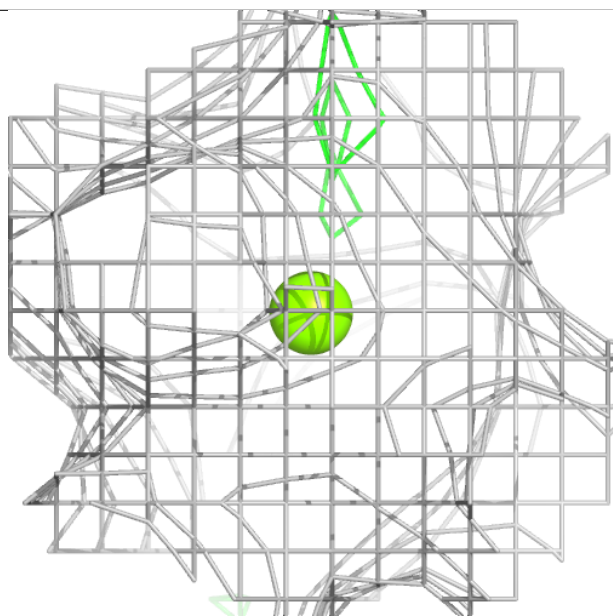
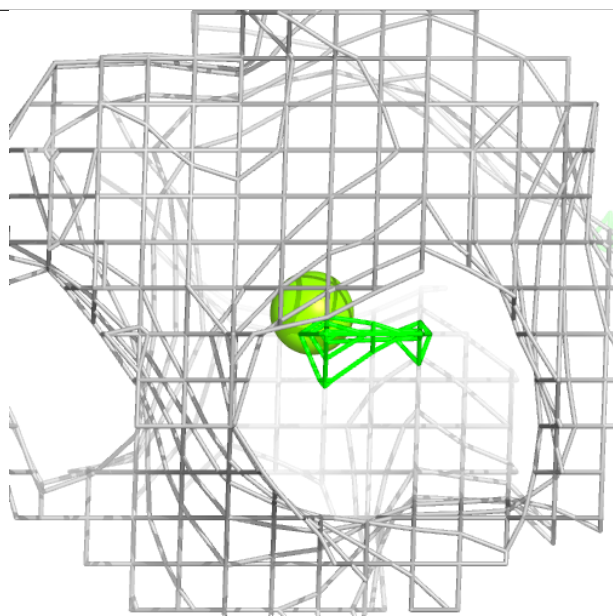
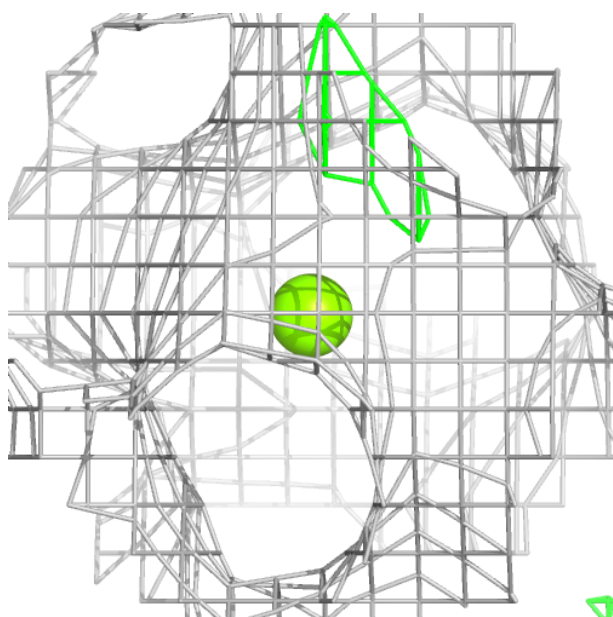
Electron density around MG A 5701:

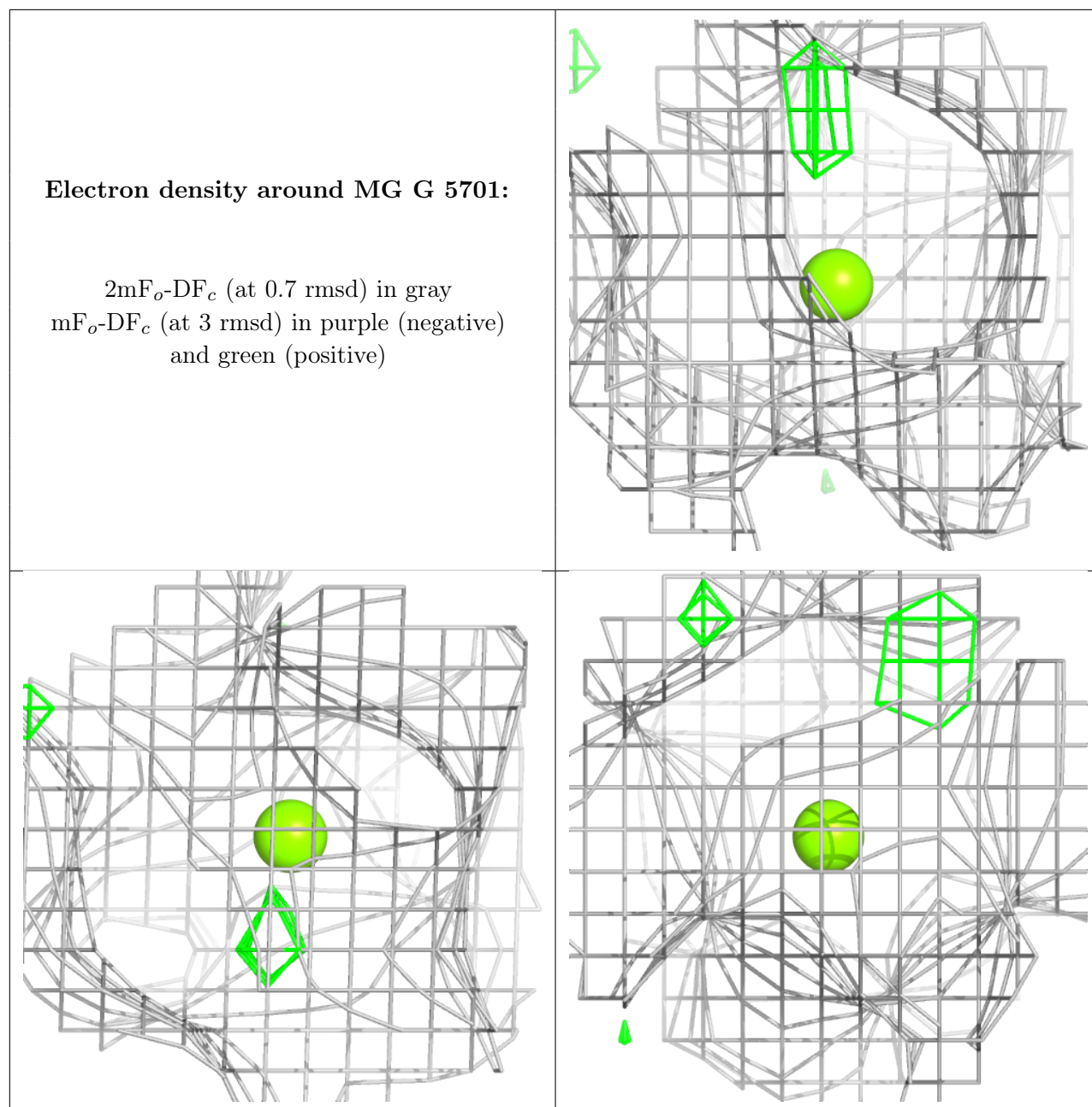
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG E 5701:

$2mF_o-DF_c$ (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.