



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:22 AM UTC

PDB ID : 7YOS / pdb_00007yos
Title : Recj2 and Mn complex from Methanocaldococcus jannaschii
Authors : Wang, W.W.; Liu, X.P.
Deposited on : 2022-08-02
Resolution : 2.17 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

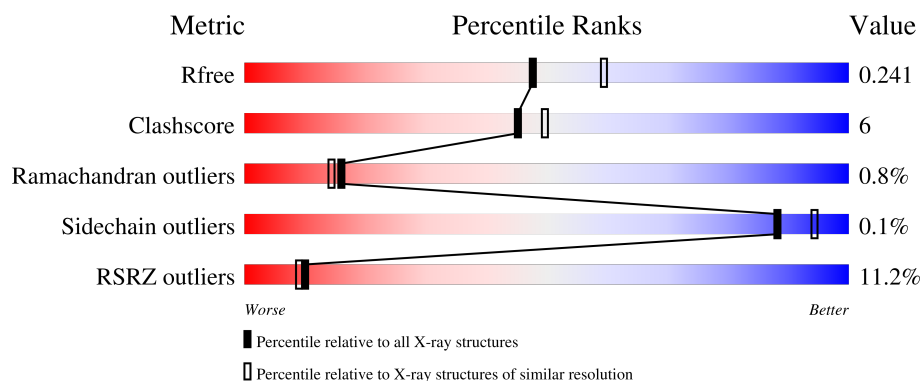
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	432	19% 83% 16%
1	B	432	4% 89% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6919 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 nuclease RecJ2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3406	2200	571	621	14			
1	B	431	Total	C	N	O	S	0	0	0
			3421	2209	575	623	14			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

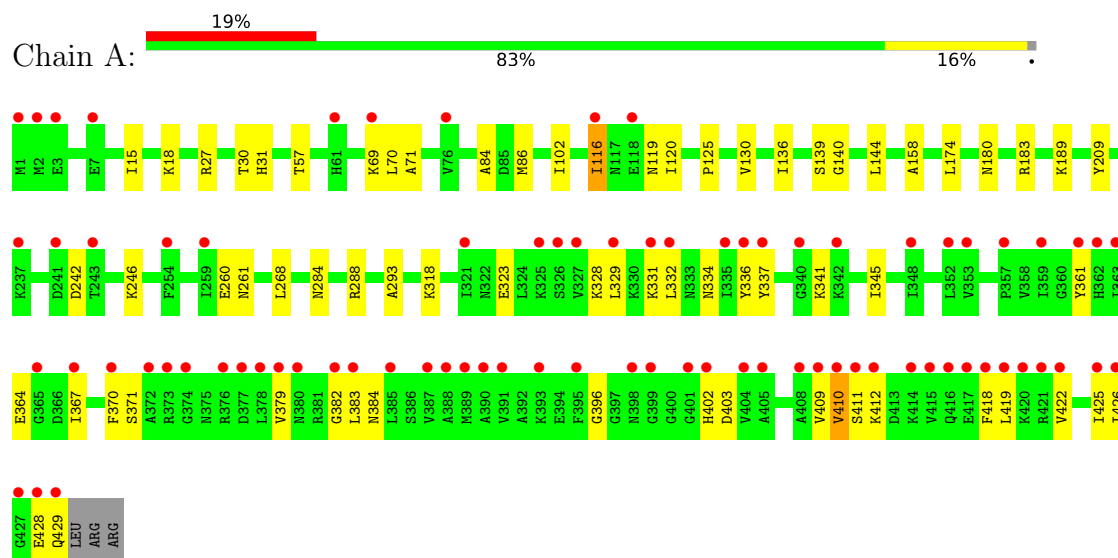
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		
3	B	62	Total	O	0	0
			62	62		

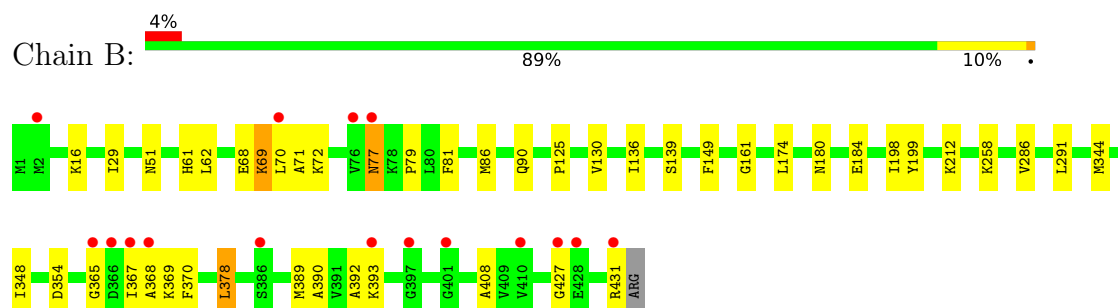
3 Residue-property plots

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: nuclease RecJ2



• Molecule 1: nuclease RecJ2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	83.91Å 175.82Å 66.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.05 – 2.17 48.05 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.05-2.17) 92.4 (48.05-2.17)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.205 , 0.240 0.206 , 0.241	Depositor DCC
R_{free} test set	1982 reflections (3.76%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6919	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.33	0/3465	0.51	2/4662 (0.0%)
1	B	0.39	0/3480	0.55	0/4683
All	All	0.36	0/6945	0.53	2/9345 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	VAL	CA-C-N	5.21	131.34	121.97
1	A	409	VAL	C-N-CA	5.21	131.34	121.97

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	3406	0	3512	53	0
1	B	3421	0	3525	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	28	0	0	2	0
3	B	62	0	0	6	0
All	All	6919	0	7037	82	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 6.

All (82) 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:90:GLN:CG	3:B:652:HOH:O	1.96	1.09
1:B:90:GLN:HG3	3:B:652:HOH:O	1.52	1.01
1:A:30:THR:HG22	1:A:84:ALA:HB3	1.55	0.88
1:A:402:HIS:HE1	3:A:621:HOH:O	1.56	0.86
1:A:27:ARG:HH12	1:A:57:THR:HG23	1.43	0.83
1:B:69:LYS:O	1:B:71:ALA:N	2.12	0.82
1:A:419:LEU:HA	1:A:422:VAL:HG12	1.64	0.78
1:B:61:HIS:CD2	3:B:621:HOH:O	2.44	0.70
1:A:345:ILE:HG22	1:A:371:SER:HB2	1.74	0.69
1:A:125:PRO:HB2	1:A:130:VAL:HB	1.77	0.67
1:A:209:TYR:CE1	1:A:318:LYS:HG2	2.31	0.67
1:B:90:GLN:HG2	3:B:652:HOH:O	1.75	0.66
1:A:139:SER:HB3	1:A:158:ALA:HA	1.78	0.66
1:A:331:LYS:HG2	1:A:336:TYR:HE1	1.62	0.64
1:A:331:LYS:HG2	1:A:336:TYR:CE1	2.34	0.63
1:A:402:HIS:CE1	3:A:621:HOH:O	2.40	0.63
1:A:334:ASN:H	1:A:422:VAL:CG2	2.13	0.61
1:A:410:VAL:HB	1:A:411:SER:HB3	1.81	0.61
1:B:427:GLY:O	1:B:431:ARG:HD2	2.04	0.57
1:A:425:ILE:O	1:A:429:GLN:HG2	2.04	0.57
1:A:411:SER:OG	1:A:412:LYS:N	2.32	0.56
1:B:258:LYS:HE3	1:B:354:ASP:OD1	2.05	0.55
1:A:332:LEU:HD11	1:A:337:TYR:HE2	1.76	0.51
1:B:61:HIS:HD2	3:B:621:HOH:O	1.86	0.51
1:A:334:ASN:H	1:A:422:VAL:HG21	1.75	0.51
1:B:390:ALA:O	1:B:393:LYS:HG3	2.11	0.51
1:A:180:ASN:OD1	1:A:183:ARG:NH2	2.44	0.51
1:B:77:ASN:O	1:B:79:PRO:HD3	2.11	0.50
1:A:293:ALA:HB3	1:B:51:ASN:HA	1.94	0.49
1:A:426:ILE:HA	1:A:429:GLN:HB2	1.94	0.49
1:B:286:VAL:HG13	1:B:291:LEU:HB2	1.95	0.48
1:A:361:TYR:HB3	1:A:370:PHE:CD2	2.48	0.48
1:B:212:LYS:HE3	3:B:640:HOH:O	2.12	0.48
1:A:27:ARG:NH1	1:A:57:THR:HG23	2.21	0.48
1:B:79:PRO:HG2	1:B:81:PHE:CE1	2.49	0.47
1:A:69:LYS:O	1:A:70:LEU:HB2	2.15	0.47
1:B:68:GLU:C	1:B:69:LYS:O	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:ASN:CG	1:A:426:ILE:HG12	2.40	0.47
1:A:364:GLU:O	1:A:367:ILE:HG22	2.16	0.46
1:A:328:LYS:HA	1:A:328:LYS:HD3	1.75	0.45
1:A:31:HIS:CE1	1:A:86:MET:HE2	2.51	0.45
1:A:189:LYS:HE2	1:A:268:LEU:HD12	1.98	0.45
1:A:260:GLU:CD	1:A:261:ASN:H	2.23	0.45
1:A:15:ILE:HG23	1:A:102:ILE:HD13	1.97	0.45
1:B:136:ILE:HD12	1:B:174:LEU:HB3	1.99	0.45
1:A:367:ILE:HG13	1:A:410:VAL:HA	2.00	0.44
1:B:16:LYS:HG3	1:B:149:PHE:CZ	2.52	0.44
1:A:382:GLY:O	1:A:428:GLU:HB3	2.18	0.44
1:B:198:ILE:HD11	1:B:199:TYR:CZ	2.53	0.44
1:A:367:ILE:HG13	1:A:410:VAL:HG12	2.00	0.44
1:A:116:ILE:HB	1:A:120:ILE:HB	1.99	0.43
1:A:125:PRO:HG3	1:A:136:ILE:HG21	1.99	0.43
1:B:369:LYS:HD2	1:B:370:PHE:N	2.32	0.43
1:B:29:ILE:HG22	1:B:86:MET:SD	2.57	0.43
1:A:242:ASP:O	1:A:246:LYS:HG3	2.18	0.43
1:A:379:VAL:HA	1:A:383:LEU:H	1.84	0.43
1:B:389:MET:HE3	1:B:408:ALA:HB3	2.01	0.42
1:A:140:GLY:O	1:A:144:LEU:HG	2.19	0.42
1:A:396:GLY:O	1:A:410:VAL:HG21	2.20	0.42
1:B:72:LYS:HA	1:B:72:LYS:HD3	1.85	0.42
1:B:344:MET:O	1:B:348:ILE:HG12	2.19	0.42
1:B:367:ILE:HD13	1:B:367:ILE:HA	1.79	0.41
1:A:69:LYS:O	1:A:71:ALA:N	2.49	0.41
1:B:62:LEU:HD12	1:B:62:LEU:HA	1.90	0.41
1:B:139:SER:OG	1:B:161:GLY:HA3	2.19	0.41
1:A:125:PRO:HG3	1:A:136:ILE:CG2	2.50	0.41
1:A:334:ASN:H	1:A:422:VAL:HG23	1.86	0.41
1:A:370:PHE:HE2	1:A:418:PHE:CZ	2.37	0.41
1:A:331:LYS:NZ	1:A:336:TYR:OH	2.54	0.41
1:B:125:PRO:HB2	1:B:130:VAL:HB	2.02	0.41
1:A:384:ASN:HA	1:A:403:ASP:HA	2.02	0.41
1:A:18:LYS:NZ	1:A:119:ASN:O	2.50	0.40
1:A:284:ASN:O	1:A:288:ARG:HG2	2.21	0.40
1:A:332:LEU:HD13	1:A:419:LEU:HG	2.03	0.40
1:B:378:LEU:HD12	1:B:378:LEU:HA	1.95	0.40
1:A:174:LEU:HD23	1:A:174:LEU:HA	1.81	0.40
1:A:323:GLU:OE2	1:A:341:LYS:HD2	2.20	0.40
1:B:180:ASN:O	1:B:184:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ALA:C	1:B:392:ALA:H	2.28	0.40
1:A:332:LEU:HD22	1:A:419:LEU:HD21	2.03	0.40
1:A:379:VAL:HG21	1:A:403:ASP:CG	2.46	0.40
1:A:329:LEU:HD23	1:A:329:LEU:HA	1.94	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	427/432 (99%)	406 (95%)	19 (4%)	2 (0%)	24	25
1	B	429/432 (99%)	411 (96%)	13 (3%)	5 (1%)	10	7
All	All	856/864 (99%)	817 (95%)	32 (4%)	7 (1%)	16	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	VAL
1	A	116	ILE
1	B	69	LYS
1	B	77	ASN
1	B	368	ALA
1	B	70	LEU
1	B	365	GLY

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	369/373 (99%)	369 (100%)	0	100	100
1	B	370/373 (99%)	369 (100%)	1 (0%)	86	92
All	All	739/746 (99%)	738 (100%)	1 (0%)	88	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	378	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	74	ASN
1	A	97	HIS
1	A	192	ASN
1	A	239	GLN
1	A	310	ASN
1	A	402	HIS
1	B	61	HIS
1	B	77	ASN
1	B	119	ASN
1	B	122	GLN
1	B	126	HIS
1	B	261	ASN

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 2 ligands modelled in this entry, 2 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

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	429/432 (99%)	0.94	80 (18%) 3 3	22, 45, 89, 97	0
1	B	431/432 (99%)	0.18	16 (3%) 45 44	18, 33, 62, 81	0
All	All	860/864 (99%)	0.56	96 (11%) 10 9	18, 38, 83, 97	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	PHE	6.3
1	A	382	GLY	6.0
1	B	367	ILE	5.8
1	A	426	ILE	5.5
1	A	379	VAL	5.3
1	A	410	VAL	4.9
1	A	1	MET	4.7
1	B	410	VAL	4.2
1	A	415	VAL	4.2
1	A	422	VAL	4.2
1	A	254	PHE	4.0
1	A	337	TYR	3.9
1	A	335	ILE	3.9
1	A	419	LEU	3.9
1	A	361	TYR	3.8
1	A	427	GLY	3.7
1	A	373	ARG	3.7
1	A	383	LEU	3.6
1	A	417	GLU	3.6
1	A	390	ALA	3.6
1	B	365	GLY	3.5
1	A	387	VAL	3.4
1	A	393	LYS	3.4
1	A	365	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	412	LYS	3.4
1	A	352	LEU	3.3
1	A	402	HIS	3.3
1	A	409	VAL	3.3
1	A	76	VAL	3.2
1	A	326	SER	3.2
1	A	416	GLN	3.1
1	A	336	TYR	3.1
1	A	2	MET	3.1
1	A	388	ALA	3.1
1	A	421	ARG	3.0
1	B	368	ALA	2.9
1	A	391	VAL	2.9
1	A	61	HIS	2.9
1	A	405	ALA	2.9
1	A	374	GLY	2.9
1	A	370	PHE	2.9
1	A	408	ALA	2.9
1	A	380	ASN	2.8
1	A	376	ARG	2.8
1	A	353	VAL	2.8
1	A	3	GLU	2.8
1	A	332	LEU	2.8
1	A	362	HIS	2.7
1	A	7	GLU	2.7
1	A	429	GLN	2.7
1	A	329	LEU	2.7
1	B	70	LEU	2.7
1	A	428	GLU	2.6
1	A	331	LYS	2.6
1	A	357	PRO	2.6
1	B	76	VAL	2.6
1	B	366	ASP	2.6
1	A	116	ILE	2.5
1	A	420	LYS	2.5
1	A	425	ILE	2.5
1	B	77	ASN	2.5
1	A	118	GLU	2.5
1	A	372	ALA	2.5
1	A	348	ILE	2.5
1	A	367	ILE	2.4
1	A	69	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	397	GLY	2.4
1	B	401	GLY	2.4
1	A	395	PHE	2.4
1	A	378	LEU	2.4
1	A	385	LEU	2.4
1	A	327	VAL	2.4
1	A	363	ILE	2.4
1	A	237	LYS	2.4
1	A	377	ASP	2.3
1	A	404	VAL	2.3
1	A	243	THR	2.3
1	A	241	ASP	2.3
1	B	386	SER	2.3
1	A	340	GLY	2.3
1	A	325	LYS	2.2
1	A	389	MET	2.2
1	A	342	LYS	2.2
1	A	399	GLY	2.2
1	A	359	ILE	2.1
1	B	393	LYS	2.1
1	B	2	MET	2.1
1	B	431	ARG	2.1
1	A	411	SER	2.1
1	A	259	ILE	2.1
1	B	427	GLY	2.1
1	B	428	GLU	2.1
1	A	401	GLY	2.1
1	A	414	LYS	2.1
1	A	398	ASN	2.0
1	A	321	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

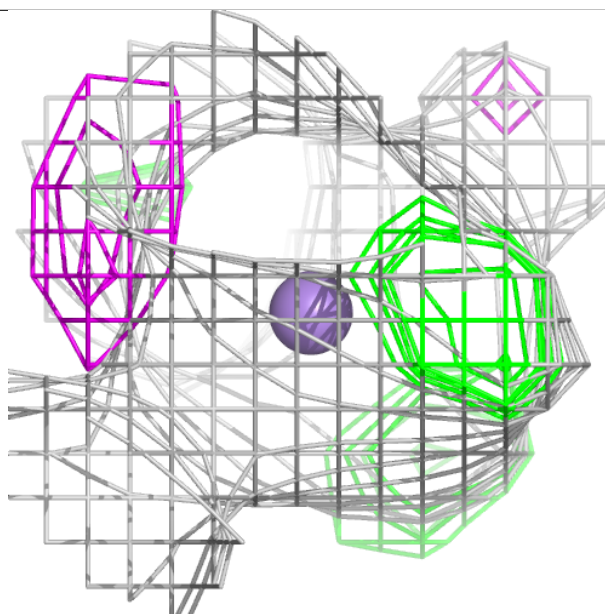
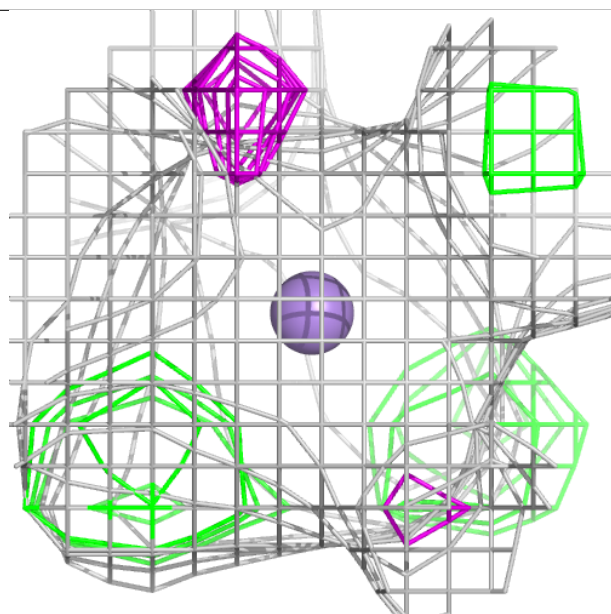
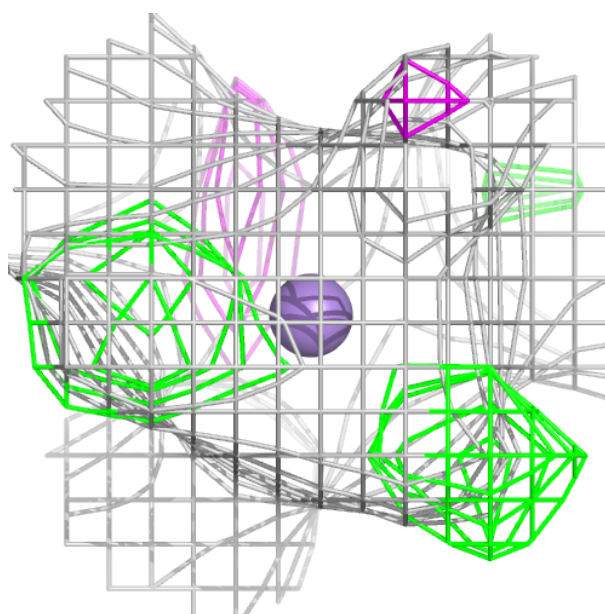
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MN	A	501	1/1	0.93	0.07	52,52,52,52	0
2	MN	B	501	1/1	0.99	0.03	35,35,35,35	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.

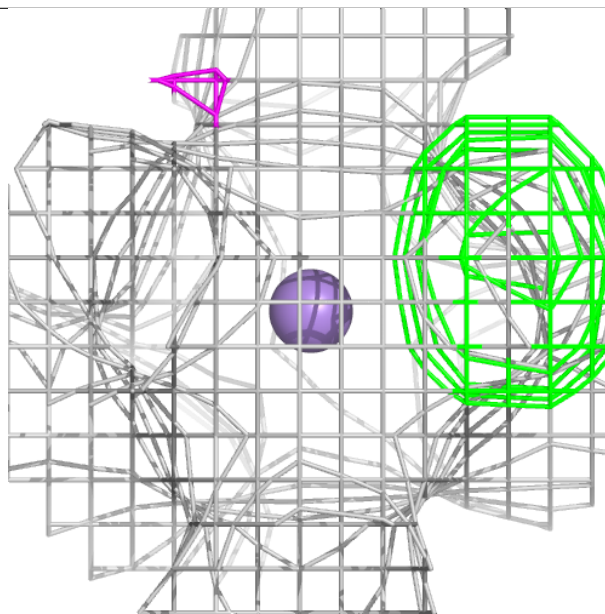
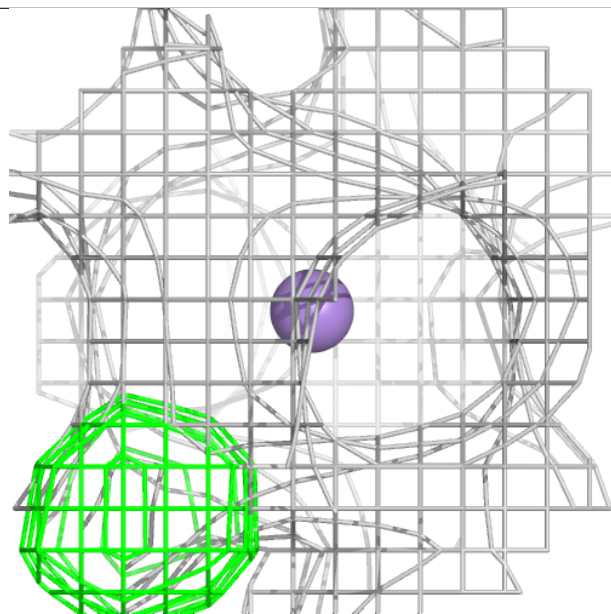
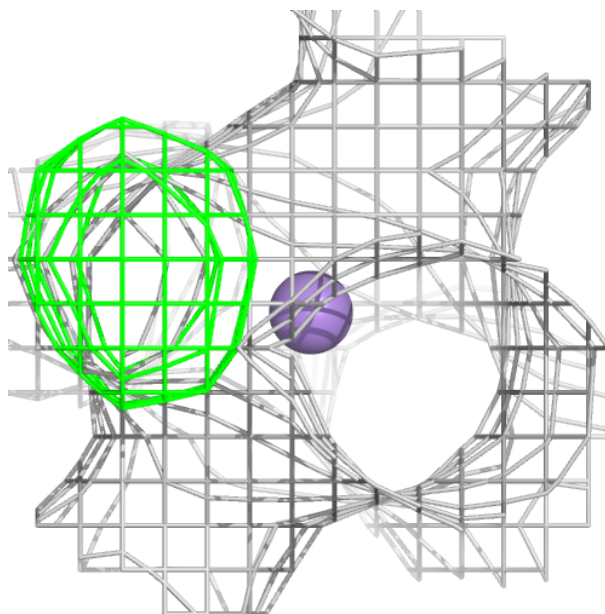
Electron density around MN A 501:

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



Electron density around MN 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 ⓘ

There are no such residues in this entry.