



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:35 PM UTC

PDB ID : 7VW5 / pdb_00007vw5
Title : Crystal structures of alphavirus nonstructural protein 4 (nsP4) reveal an intrinsically dynamic RNA-dependent RNA polymerase fold
Authors : Tan, Y.B.; Luo, D.
Deposited on : 2021-11-09
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

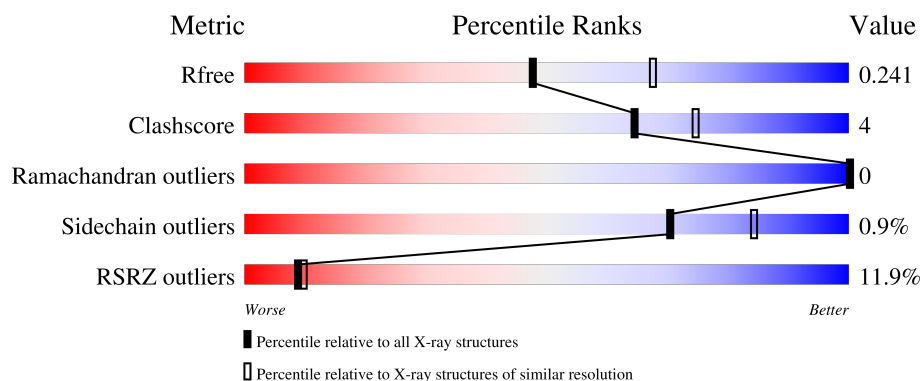
1 Overall quality at a glance

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	520	11% 79% 10% 11%
1	B	520	11% 80% 9% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7615 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 RNA-directed RNA polymerase nsP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3626	2302	611	689	24			
1	B	466	Total	C	N	O	S	0	0	0
			3641	2313	613	691	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	SER	CYS	engineered mutation	UNP P03317
B	164	SER	CYS	engineered mutation	UNP P03317

- 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	1	Total	Mg	1	0
			1	1		
2	B	1	Total	Mg	1	0
			1	1		

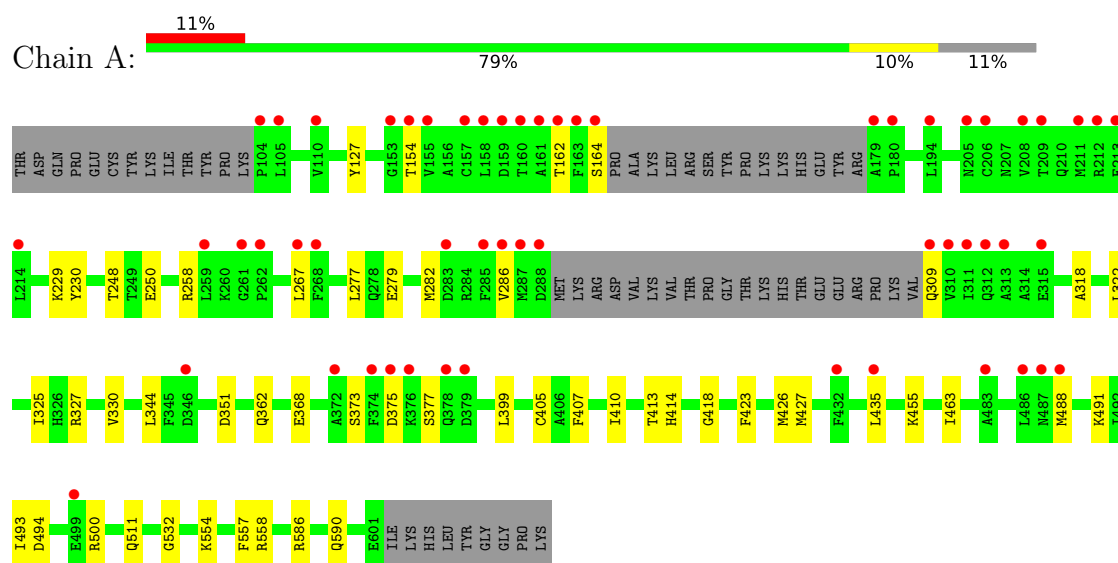
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	168	Total	O	0	0
			168	168		
3	B	178	Total	O	0	0
			178	178		

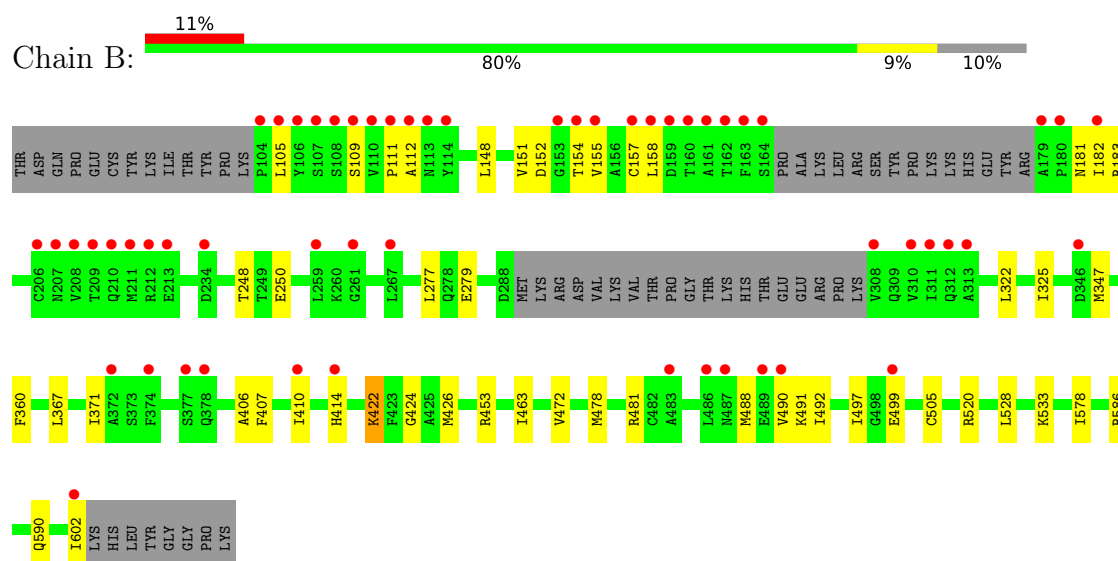
3 Residue-property plots [i](#)

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: RNA-directed RNA polymerase nsP4



• Molecule 1: RNA-directed RNA polymerase nsP4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.45Å 68.94Å 71.42Å 116.31° 107.05° 95.10°	Depositor
Resolution (Å)	36.27 – 2.30 36.27 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.4 (36.27-2.30) 94.5 (36.27-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, R_{free}	0.197 , 0.240 0.197 , 0.241	Depositor DCC
R_{free} test set	2000 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7615	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 6.03% 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 [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	0.08	0/3695	0.25	0/5020
1	B	0.08	0/3710	0.23	0/5041
All	All	0.08	0/7405	0.24	0/10061

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	3626	0	3607	31	0
1	B	3641	0	3627	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	168	0	0	1	0
3	B	178	0	0	1	0
All	All	7615	0	7234	56	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 4.

All (56) 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:286:VAL:HB	1:A:309:GLN:HG3	1.76	0.67
1:A:554:LYS:HG2	1:A:586:ARG:HH12	1.60	0.66
1:A:164:SER:HB3	1:A:330:VAL:HG11	1.78	0.66
1:A:322:LEU:HA	1:A:325:ILE:HD12	1.76	0.66
1:A:322:LEU:HD13	1:A:426:MET:HE1	1.78	0.65
1:B:488:MET:O	1:B:491:LYS:NZ	2.32	0.62
1:B:155:VAL:HG22	1:B:463:ILE:HG12	1.83	0.61
1:A:407:PHE:HD1	1:A:410:ILE:HD11	1.67	0.58
1:B:151:VAL:HG21	1:B:157:CYS:HB2	1.85	0.57
1:B:152:ASP:HB3	1:B:183:ARG:HB3	1.87	0.56
1:A:154:THR:HG23	1:A:435:LEU:HD13	1.88	0.55
1:B:586:ARG:HH21	1:B:590:GLN:HE22	1.53	0.55
1:B:155:VAL:HB	1:B:182:ILE:HD11	1.90	0.54
1:A:455:LYS:NZ	3:A:803:HOH:O	2.41	0.53
1:A:418:GLY:HA2	1:B:602:ILE:HD11	1.93	0.51
1:B:371:ILE:HA	1:B:490:VAL:HG22	1.93	0.50
1:A:423:PHE:HA	1:A:427:MET:HE2	1.94	0.50
1:A:248:THR:HA	1:A:279:GLU:HA	1.93	0.49
1:B:586:ARG:NE	1:B:590:GLN:OE1	2.45	0.49
1:A:407:PHE:CD1	1:A:410:ILE:HD11	2.46	0.49
1:A:282:MET:HE1	1:A:399:LEU:HD22	1.94	0.48
1:A:414:HIS:HE1	1:B:528:LEU:O	1.97	0.48
1:B:478:MET:HG2	1:B:492:ILE:HD13	1.96	0.48
1:B:347:MET:HE3	1:B:347:MET:HB2	1.73	0.48
1:A:375:ASP:OD1	1:A:377:SER:OG	2.30	0.47
1:B:499:GLU:N	1:B:499:GLU:OE1	2.48	0.47
1:A:344:LEU:HB2	1:A:463:ILE:HB	1.96	0.47
1:B:406:ALA:HB1	1:B:426:MET:HE1	1.96	0.47
1:A:410:ILE:O	1:A:413:THR:OG1	2.32	0.46
1:B:360:PHE:HD2	1:B:497:ILE:HD11	1.79	0.46
1:A:586:ARG:NE	1:A:590:GLN:OE1	2.49	0.45
1:B:248:THR:HA	1:B:279:GLU:HA	1.98	0.45
1:B:367:LEU:HD13	1:B:472:VAL:HG12	1.98	0.45
1:B:505:CYS:O	1:B:520:ARG:NH2	2.42	0.45
1:B:322:LEU:HD23	1:B:325:ILE:HD12	1.98	0.45
1:A:127:TYR:CZ	1:B:578:ILE:HD12	2.52	0.44
1:B:148:LEU:HD22	1:B:154:THR:HA	1.99	0.44
1:A:250:GLU:CD	1:A:277:LEU:H	2.26	0.43
1:A:558:ARG:HA	1:B:109:SER:HA	1.99	0.43
1:A:532:GLY:HA3	1:B:414:HIS:CE1	2.53	0.43
1:B:533:LYS:NZ	3:B:814:HOH:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ARG:HH22	1:B:481:ARG:HH22	1.65	0.43
1:B:105:LEU:HD12	1:B:105:LEU:HA	1.89	0.42
1:A:494:ASP:O	1:A:500:ARG:NH1	2.52	0.42
1:A:258:ARG:HA	1:A:258:ARG:HD3	1.76	0.42
1:A:362:GLN:HB2	1:A:511:GLN:OE1	2.20	0.42
1:A:488:MET:SD	1:A:491:LYS:NZ	2.88	0.42
1:A:229:LYS:HD2	1:A:230:TYR:CZ	2.55	0.42
1:B:109:SER:O	1:B:111:PRO:HD3	2.19	0.42
1:B:422:LYS:HD2	1:B:424:GLY:H	1.85	0.42
1:B:250:GLU:CD	1:B:277:LEU:H	2.27	0.41
1:A:318:ALA:O	1:A:322:LEU:HD12	2.21	0.41
1:A:557:PHE:CE1	1:B:112:ALA:HB3	2.56	0.41
1:A:162:THR:HB	1:A:327:ARG:NH1	2.36	0.41
1:B:407:PHE:HA	1:B:410:ILE:HG12	2.03	0.40
1:A:368:GLU:HB3	1:A:493:ILE:HB	2.02	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	458/520 (88%)	442 (96%)	16 (4%)	0	100	100
1	B	460/520 (88%)	449 (98%)	11 (2%)	0	100	100
All	All	918/1040 (88%)	891 (97%)	27 (3%)	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	394/446 (88%)	390 (99%)	4 (1%)	68	82
1	B	396/446 (89%)	393 (99%)	3 (1%)	73	86
All	All	790/892 (89%)	783 (99%)	7 (1%)	70	84

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	267	LEU
1	A	351	ASP
1	A	373	SER
1	A	405	CYS
1	B	158	LEU
1	B	181	ASN
1	B	422	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	126	ASN
1	A	207	ASN
1	A	340	ASN
1	A	414	HIS
1	A	596	GLN
1	B	113	ASN
1	B	191	GLN
1	B	511	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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, 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	464/520 (89%)	0.63	55 (11%) 9 10	17, 38, 94, 133	0
1	B	466/520 (89%)	0.59	56 (12%) 9 9	17, 34, 87, 119	0
All	All	930/1040 (89%)	0.61	111 (11%) 9 10	17, 36, 91, 133	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	164	SER	8.7
1	B	112	ALA	7.8
1	B	111	PRO	7.1
1	A	157	CYS	6.6
1	B	158	LEU	5.9
1	B	157	CYS	5.7
1	B	155	VAL	5.1
1	B	110	VAL	5.0
1	B	105	LEU	4.9
1	A	163	PHE	4.7
1	B	104	PRO	4.7
1	B	154	THR	4.7
1	B	182	ILE	4.6
1	A	158	LEU	4.5
1	A	208	VAL	4.4
1	B	108	SER	4.3
1	A	209	THR	4.3
1	A	310	VAL	4.2
1	B	106	TYR	4.2
1	B	163	PHE	4.2
1	A	110	VAL	4.2
1	A	179	ALA	4.1
1	B	602	ILE	4.1
1	A	313	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	209	THR	3.9
1	A	164	SER	3.9
1	B	208	VAL	3.9
1	A	262	PRO	3.8
1	B	308	VAL	3.8
1	B	179	ALA	3.7
1	B	207	ASN	3.6
1	A	162	THR	3.4
1	A	374	PHE	3.4
1	B	213	GLU	3.4
1	B	180	PRO	3.4
1	B	161	ALA	3.4
1	B	113	ASN	3.4
1	A	155	VAL	3.3
1	A	488	MET	3.3
1	B	312	GLN	3.3
1	B	211	MET	3.3
1	B	114	TYR	3.3
1	A	212	ARG	3.2
1	B	210	GLN	3.2
1	A	211	MET	3.2
1	B	159	ASP	3.2
1	A	486	LEU	3.2
1	B	162	THR	3.2
1	A	283	ASP	3.0
1	A	285	PHE	3.0
1	A	180	PRO	3.0
1	A	346	ASP	3.0
1	A	287	MET	2.9
1	A	161	ALA	2.8
1	A	315	GLU	2.8
1	A	311	ILE	2.8
1	A	205	ASN	2.8
1	A	483	ALA	2.8
1	B	377	SER	2.8
1	A	154	THR	2.8
1	B	153	GLY	2.7
1	A	213	GLU	2.7
1	A	288	ASP	2.7
1	B	234	ASP	2.6
1	B	109	SER	2.6
1	A	105	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	267	LEU	2.6
1	B	346	ASP	2.6
1	B	489	GLU	2.5
1	B	160	THR	2.5
1	A	499	GLU	2.5
1	B	483	ALA	2.5
1	B	374	PHE	2.5
1	A	432	PHE	2.4
1	B	310	VAL	2.4
1	B	267	LEU	2.4
1	A	309	GLN	2.4
1	A	153	GLY	2.4
1	A	268	PHE	2.4
1	A	379	ASP	2.4
1	A	104	PRO	2.4
1	A	261	GLY	2.4
1	A	160	THR	2.4
1	B	410	ILE	2.4
1	A	214	LEU	2.3
1	B	378	GLN	2.3
1	A	286	VAL	2.3
1	B	414	HIS	2.3
1	B	490	VAL	2.3
1	A	206	CYS	2.3
1	A	372	ALA	2.3
1	B	212	ARG	2.3
1	A	435	LEU	2.2
1	B	261	GLY	2.2
1	B	259	LEU	2.2
1	A	159	ASP	2.2
1	A	487	ASN	2.2
1	B	311	ILE	2.2
1	A	376	LYS	2.2
1	A	259	LEU	2.1
1	B	313	ALA	2.1
1	B	372	ALA	2.1
1	A	378	GLN	2.1
1	B	206	CYS	2.1
1	B	499	GLU	2.1
1	A	312	GLN	2.1
1	A	194	LEU	2.0
1	B	486	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	107	SER	2.0
1	A	375	ASP	2.0
1	B	487	ASN	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](#)

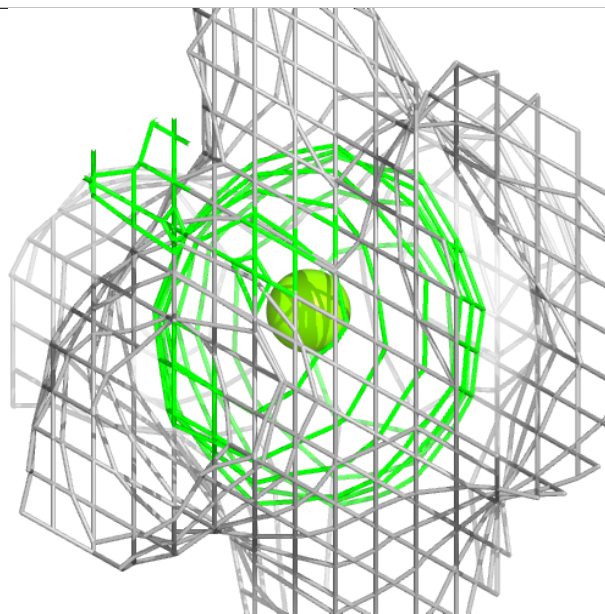
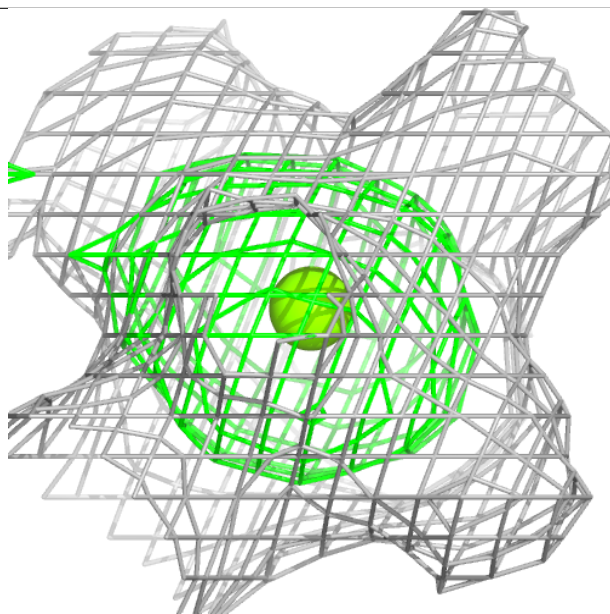
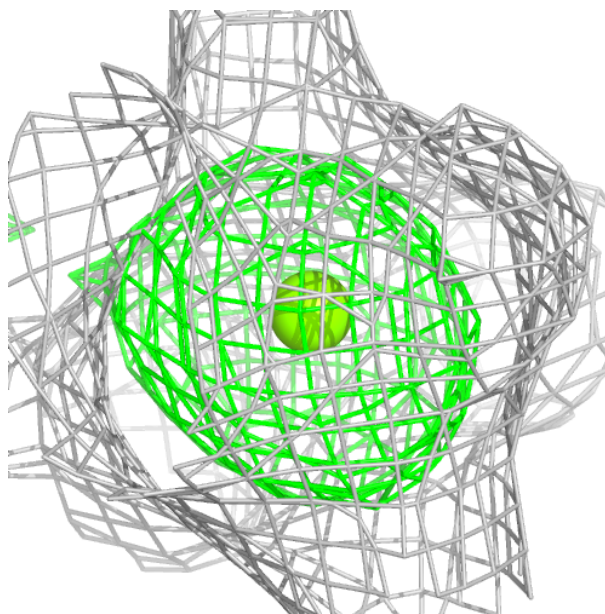
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	MG	A	701	1/1	-	-	30,30,30,30	1
2	MG	B	701	1/1	-	-	26,26,26,26	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.

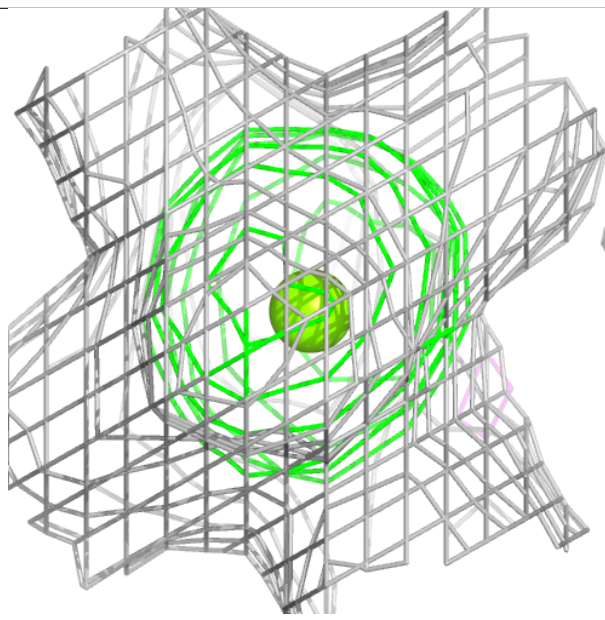
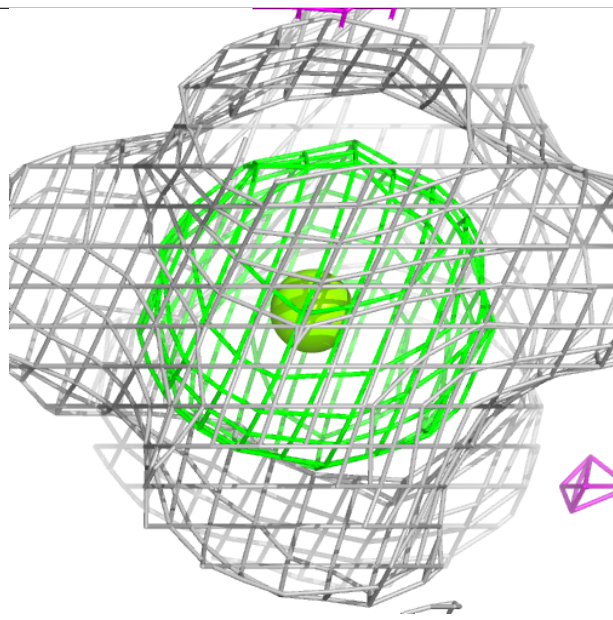
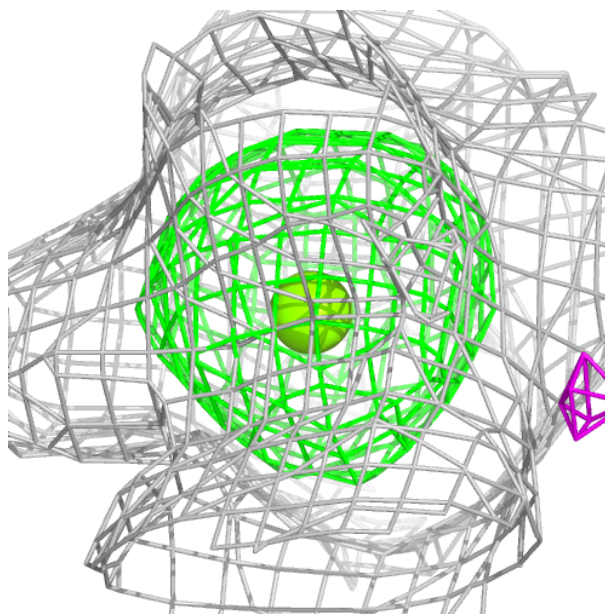
Electron density around MG A 701:

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



Electron density around MG B 701:

$2mF_o-DF_c$ (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.