



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:20 AM UTC

PDB ID : 7CK1 / pdb_00007ck1
Title : Crystal structure of arabidopsis CESA3 catalytic domain
Authors : Qiao, Z.; Gao, Y.G.
Deposited on : 2020-07-15
Resolution : 2.35 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

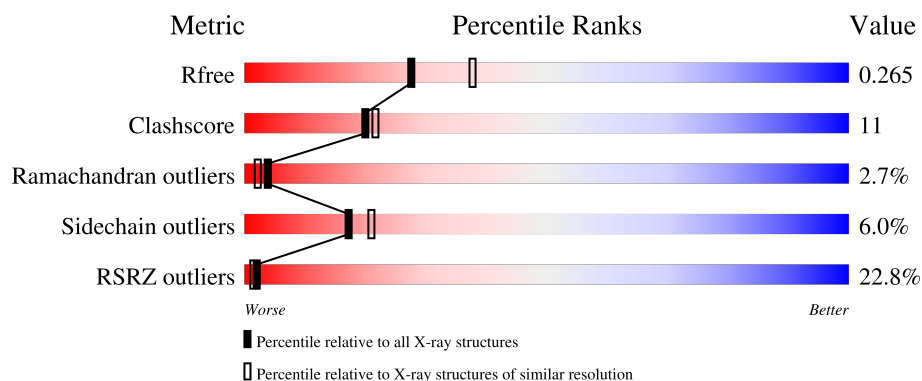
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	410	19% 61% 21% • • 14%
1	B	410	20% 62% 20% • • 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5573 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 Cellulose synthase A catalytic subunit 3 [UDP-forming], Cellulose synthase A catalytic subunit 3 [UDP-forming].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2788	1781	473	515	19			
1	B	351	Total	C	N	O	S	0	0	0
			2764	1767	469	509	19			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	697	GLY	-	linker	UNP Q941L0
A	698	SER	-	linker	UNP Q941L0
A	699	GLY	-	linker	UNP Q941L0
A	700	SER	-	linker	UNP Q941L0
A	701	GLY	-	linker	UNP Q941L0
B	697	GLY	-	linker	UNP Q941L0
B	698	SER	-	linker	UNP Q941L0
B	699	GLY	-	linker	UNP Q941L0
B	700	SER	-	linker	UNP Q941L0
B	701	GLY	-	linker	UNP Q941L0

- 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		

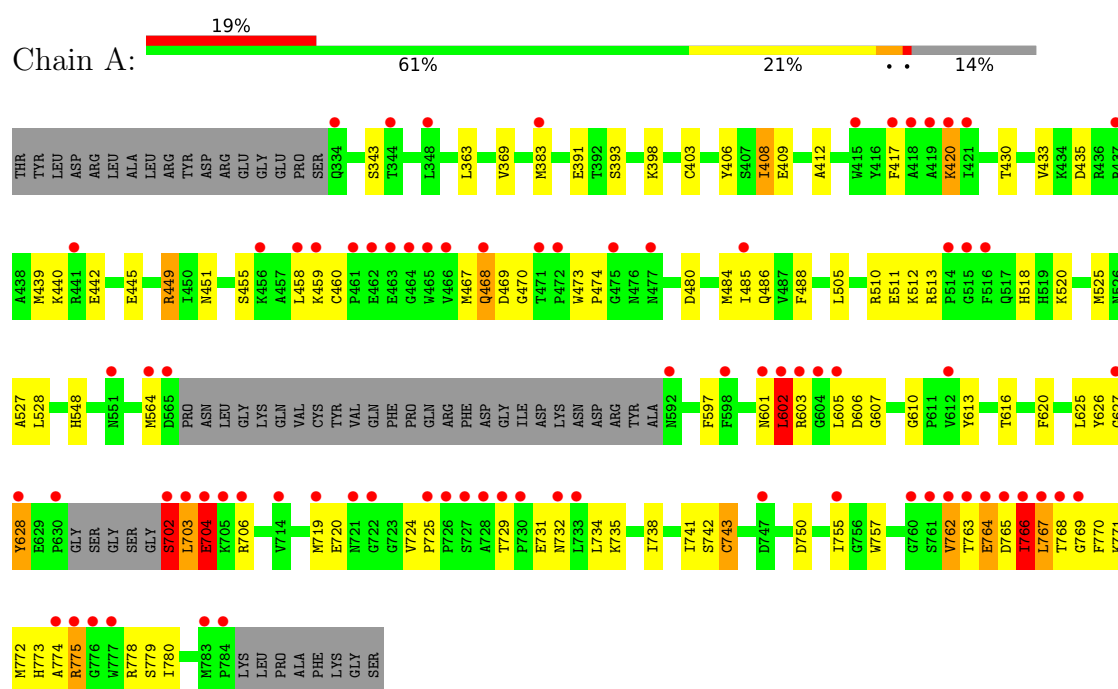
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total 8	O 8	0	0
3	B	11	Total 11	O 11	0	0

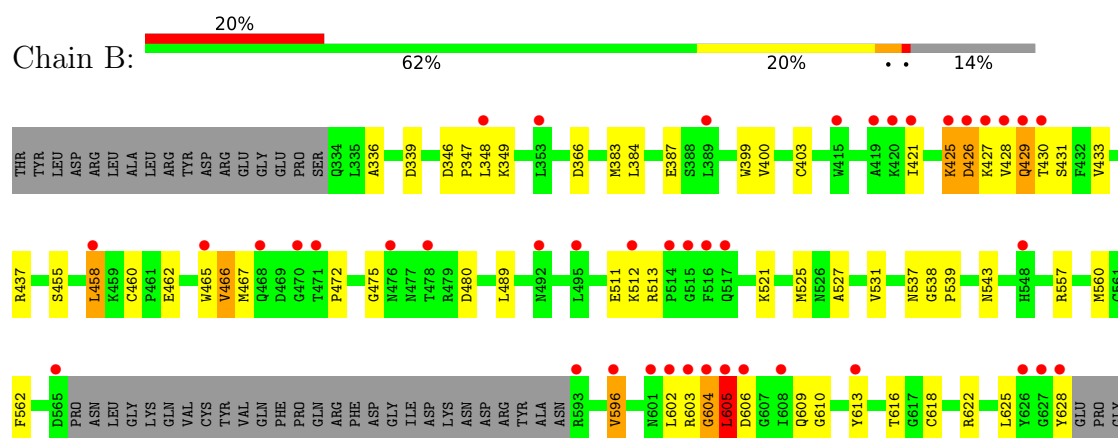
3 Residue-property plots

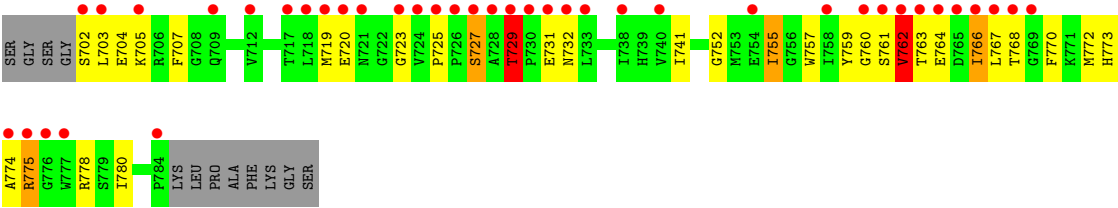
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cellulose synthase A catalytic subunit 3 [UDP-forming], Cellulose synthase A catalytic subunit 3 [UDP-forming]



- Molecule 1: Cellulose synthase A catalytic subunit 3 [UDP-forming], Cellulose synthase A catalytic subunit 3 [UDP-forming]





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.62Å 147.03Å 92.51Å 90.00° 102.05° 90.00°	Depositor
Resolution (Å)	48.08 – 2.35 48.08 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.08-2.35) 99.8 (48.08-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.237 , 0.264 0.239 , 0.265	Depositor DCC
R_{free} test set	2961 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.6	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5573	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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: 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	0.59	0/2856	1.00	9/3869 (0.2%)
1	B	0.60	0/2831	0.94	4/3834 (0.1%)
All	All	0.60	0/5687	0.97	13/7703 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
All	All	0	6

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	769	GLY	N-CA-C	6.68	120.87	110.91
1	A	602	LEU	CA-CB-CG	6.20	137.98	116.30
1	A	764	GLU	N-CA-C	5.47	119.05	112.38
1	B	460	CYS	CA-C-N	5.44	125.42	120.03
1	B	460	CYS	C-N-CA	5.44	125.42	120.03
1	A	548	HIS	CB-CA-C	-5.43	102.55	111.68
1	B	604	GLY	N-CA-C	5.39	125.95	113.18
1	A	412	ALA	CA-C-N	5.29	124.74	119.24
1	A	412	ALA	C-N-CA	5.29	124.74	119.24
1	A	468	GLN	N-CA-C	-5.23	106.16	112.54
1	A	626	TYR	N-CA-C	5.13	119.18	113.02
1	A	767	LEU	CA-CB-CG	5.05	133.99	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	762	VAL	N-CA-C	5.00	119.75	109.34

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	602	LEU	Peptide
1	A	702	SER	Peptide
1	A	742	SER	Peptide
1	A	766	ILE	Peptide
1	B	603	ARG	Peptide
1	B	729	THR	Peptide

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	2788	0	2738	71	0
1	B	2764	0	2719	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	0	2	0
3	B	11	0	0	5	0
All	All	5573	0	5457	125	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 11.

All (125) 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:732:ASN:HA	1:A:735:LYS:HG2	1.47	0.94
1:A:766:ILE:HA	1:A:768:THR:HG22	1.54	0.88
1:B:387:GLU:N	3:B:901:HOH:O	2.09	0.85
1:A:764:GLU:HB3	1:A:766:ILE:HD12	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ALA:H	1:B:560:MET:HE2	1.44	0.81
1:B:429:GLN:O	1:B:431:SER:N	2.17	0.78
1:B:761:SER:O	1:B:763:THR:N	2.19	0.74
1:A:603:ARG:HB3	1:A:606:ASP:OD1	1.89	0.72
1:B:475:GLY:O	3:B:902:HOH:O	2.09	0.70
1:A:628:TYR:C	1:A:775:ARG:HD2	2.17	0.69
1:B:527:ALA:HB1	1:B:741:ILE:HG22	1.75	0.68
1:A:430:THR:HG22	1:A:433:VAL:HG13	1.77	0.65
1:B:772:MET:HE1	1:B:780:ILE:HD11	1.81	0.61
1:A:766:ILE:HG22	1:A:767:LEU:N	2.15	0.61
1:A:627:GLY:O	1:A:628:TYR:HB2	2.00	0.60
1:B:384:LEU:O	3:B:901:HOH:O	2.17	0.60
1:A:702:SER:O	1:A:704:GLU:N	2.34	0.60
1:B:384:LEU:C	3:B:901:HOH:O	2.44	0.59
1:A:459:LYS:HD2	1:A:460:CYS:N	2.18	0.59
1:A:602:LEU:HB3	1:A:603:ARG:HG2	1.85	0.59
1:B:625:LEU:HD21	1:B:770:PHE:HB3	1.84	0.59
1:A:628:TYR:O	1:A:775:ARG:NH1	2.35	0.58
1:A:719:MET:HE1	1:A:725:PRO:HD3	1.84	0.58
1:A:518:HIS:HE1	1:A:520:LYS:HD3	1.67	0.58
1:B:339:ASP:OD2	1:B:622:ARG:NH2	2.37	0.57
1:A:720:GLU:OE1	1:A:720:GLU:N	2.37	0.57
1:B:537:ASN:HB3	1:B:723:GLY:H	1.69	0.57
1:B:628:TYR:C	1:B:775:ARG:HE	2.13	0.56
1:A:729:THR:HG23	1:A:731:GLU:HG2	1.88	0.56
1:A:750:ASP:HB2	1:A:755:ILE:HD12	1.86	0.56
1:B:336:ALA:H	1:B:560:MET:CE	2.14	0.56
1:B:763:THR:HG23	1:B:764:GLU:H	1.71	0.55
1:A:510:ARG:HD2	3:A:902:HOH:O	2.06	0.55
1:A:403:CYS:HA	1:A:408:ILE:HD13	1.89	0.55
1:B:604:GLY:O	1:B:606:ASP:N	2.37	0.54
1:A:398:LYS:HE2	1:A:442:GLU:OE2	2.07	0.54
1:A:625:LEU:HD21	1:A:770:PHE:HB3	1.90	0.54
1:A:602:LEU:HB3	1:A:603:ARG:CG	2.37	0.53
1:A:774:ALA:HA	1:A:778:ARG:CZ	2.38	0.53
1:A:757:TRP:HE1	1:A:767:LEU:C	2.15	0.53
1:A:602:LEU:CD2	1:A:603:ARG:H	2.22	0.53
1:A:606:ASP:OD1	1:A:606:ASP:N	2.37	0.52
1:B:760:GLY:O	1:B:767:LEU:HD12	2.10	0.52
1:A:527:ALA:HB1	1:A:741:ILE:HG22	1.93	0.51
1:B:347:PRO:HB2	1:B:384:LEU:HD23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:GLU:HB3	1:A:766:ILE:CD1	2.36	0.51
1:B:707:PHE:CE1	1:B:755:ILE:HD13	2.47	0.50
1:A:779:SER:C	1:A:780:ILE:HD13	2.36	0.50
1:A:597:PHE:HB3	1:A:780:ILE:HG12	1.94	0.50
1:A:607:GLY:HA2	1:B:618:CYS:SG	2.52	0.49
1:B:383:MET:HE1	1:B:467:MET:HA	1.93	0.49
1:B:366:ASP:OD1	1:B:557:ARG:NH1	2.44	0.49
1:B:562:PHE:CZ	1:B:596:VAL:HG13	2.48	0.49
1:B:426:ASP:O	1:B:428:VAL:N	2.46	0.48
1:B:729:THR:O	1:B:731:GLU:N	2.46	0.48
1:A:439:MET:HE3	1:A:439:MET:HA	1.94	0.48
1:A:772:MET:SD	1:A:780:ILE:HD11	2.52	0.48
1:A:343:SER:HB3	1:A:525:MET:HE3	1.94	0.48
1:B:480:ASP:HA	1:B:512:LYS:O	2.14	0.48
1:A:420:LYS:HA	1:A:420:LYS:HD2	1.58	0.47
1:B:521:LYS:O	1:B:525:MET:HG2	2.14	0.47
1:A:391:GLU:CD	1:A:449:ARG:HH21	2.22	0.47
1:A:485:ILE:HD12	1:A:738:ILE:HG13	1.96	0.47
1:A:613:TYR:HB2	1:B:609:GLN:O	2.14	0.47
1:B:702:SER:O	1:B:704:GLU:N	2.47	0.47
1:B:527:ALA:O	1:B:531:VAL:HG23	2.15	0.47
1:B:610:GLY:O	1:B:774:ALA:HB2	2.15	0.47
1:A:473:TRP:CH2	1:A:484:MET:HE1	2.49	0.47
1:B:466:VAL:HA	1:B:472:PRO:HA	1.96	0.46
1:B:752:GLY:HA3	1:B:759:TYR:CD2	2.51	0.46
1:A:406:TYR:OH	1:A:435:ASP:OD2	2.23	0.46
1:A:735:LYS:N	1:A:735:LYS:HD3	2.30	0.46
1:A:601:ASN:OD1	1:A:603:ARG:HD2	2.16	0.46
1:A:445:GLU:O	1:A:449:ARG:HG2	2.16	0.46
1:B:383:MET:O	3:B:901:HOH:O	2.20	0.46
1:B:613:TYR:CD1	1:B:766:ILE:HD11	2.51	0.45
1:A:766:ILE:CG2	1:A:768:THR:H	2.30	0.45
1:B:772:MET:HE1	1:B:780:ILE:CD1	2.44	0.45
1:A:518:HIS:CE1	1:A:520:LYS:HD3	2.50	0.45
1:A:451:ASN:H	1:A:451:ASN:HD22	1.65	0.45
1:A:393:SER:HB3	1:A:505:LEU:HD23	1.98	0.45
1:A:731:GLU:C	1:A:735:LYS:HE2	2.42	0.45
1:A:486:GLN:HG2	1:A:488:PHE:CZ	2.51	0.44
1:B:346:ASP:CG	1:B:349:LYS:HE3	2.42	0.44
1:A:480:ASP:OD1	1:A:513:ARG:NH1	2.48	0.44
1:A:773:HIS:O	1:A:778:ARG:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:MET:CE	1:B:467:MET:HA	2.48	0.44
1:A:528:LEU:HD23	1:A:528:LEU:HA	1.87	0.44
1:A:610:GLY:O	1:A:774:ALA:HB2	2.18	0.44
1:A:731:GLU:O	1:A:734:LEU:N	2.51	0.44
1:B:704:GLU:HB2	1:B:705:LYS:HZ2	1.82	0.44
1:B:752:GLY:HA3	1:B:759:TYR:CE2	2.53	0.44
1:B:543:ASN:OD1	1:B:616:THR:HG22	2.18	0.43
1:A:510:ARG:HG2	3:A:907:HOH:O	2.19	0.43
1:B:725:PRO:C	1:B:727:SER:H	2.27	0.43
1:A:391:GLU:OE1	1:A:449:ARG:NH2	2.49	0.42
1:A:762:VAL:HG13	1:A:764:GLU:OE1	2.19	0.42
1:B:433:VAL:O	1:B:437:ARG:HG3	2.19	0.42
1:A:468:GLN:N	1:A:468:GLN:CD	2.76	0.42
1:B:707:PHE:HE1	1:B:755:ILE:HD13	1.82	0.42
1:A:613:TYR:OH	1:A:771:LYS:HD2	2.19	0.42
1:B:763:THR:HG23	1:B:764:GLU:N	2.34	0.42
1:A:383:MET:CE	1:A:467:MET:HG2	2.50	0.42
1:A:764:GLU:O	1:A:766:ILE:HD12	2.19	0.42
1:A:602:LEU:HD22	1:A:603:ARG:H	1.85	0.42
1:A:473:TRP:HA	1:A:474:PRO:HD3	1.91	0.42
1:B:336:ALA:HB3	1:B:560:MET:HE1	2.02	0.42
1:A:430:THR:CG2	1:A:433:VAL:HG13	2.45	0.41
1:A:512:LYS:O	1:A:513:ARG:HD3	2.20	0.41
1:A:511:GLU:CG	1:A:743:CYS:HB2	2.50	0.41
1:B:605:LEU:HD13	1:B:605:LEU:HA	1.81	0.41
1:B:772:MET:HE3	1:B:772:MET:HB2	1.75	0.41
1:A:417:PHE:CE1	1:A:440:LYS:HB2	2.56	0.41
1:B:383:MET:SD	1:B:465:TRP:HB3	2.61	0.41
1:B:752:GLY:HA2	1:B:757:TRP:O	2.21	0.41
1:B:538:GLY:HA2	1:B:539:PRO:HD3	1.95	0.41
1:B:773:HIS:O	1:B:778:ARG:HD3	2.21	0.41
1:B:399:TRP:CE2	1:B:403:CYS:SG	3.14	0.41
1:B:511:GLU:OE2	1:B:513:ARG:NE	2.50	0.40
1:A:620:PHE:HA	1:A:779:SER:O	2.22	0.40
1:B:425:LYS:O	1:B:426:ASP:O	2.40	0.40
1:A:473:TRP:CZ3	1:A:484:MET:HE1	2.56	0.40
1:A:764:GLU:O	1:A:765:ASP:HB2	2.21	0.40
1:A:511:GLU:HG2	1:A:743:CYS:HB2	2.02	0.40
1:B:455:SER:HA	1:B:458:LEU:HD23	2.04	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	348/410 (85%)	319 (92%)	19 (6%)	10 (3%)	3	2
1	B	345/410 (84%)	312 (90%)	24 (7%)	9 (3%)	4	2
All	All	693/820 (84%)	631 (91%)	43 (6%)	19 (3%)	4	2

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	ASP
1	A	602	LEU
1	A	628	TYR
1	A	703	LEU
1	A	704	GLU
1	A	743	CYS
1	A	775	ARG
1	B	426	ASP
1	B	430	THR
1	B	703	LEU
1	B	720	GLU
1	B	762	VAL
1	B	427	LYS
1	B	605	LEU
1	A	763	THR
1	A	766	ILE
1	B	429	GLN
1	B	775	ARG
1	A	470	GLY

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	300/346 (87%)	283 (94%)	17 (6%)	18	23
1	B	297/346 (86%)	278 (94%)	19 (6%)	16	18
All	All	597/692 (86%)	561 (94%)	36 (6%)	17	21

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	363	LEU
1	A	369	VAL
1	A	408	ILE
1	A	409	GLU
1	A	420	LYS
1	A	449	ARG
1	A	455	SER
1	A	458	LEU
1	A	564	MET
1	A	605	LEU
1	A	616	THR
1	A	702	SER
1	A	703	LEU
1	A	704	GLU
1	A	706	ARG
1	A	724	VAL
1	A	762	VAL
1	B	348	LEU
1	B	400	VAL
1	B	421	ILE
1	B	425	LYS
1	B	458	LEU
1	B	462	GLU
1	B	466	VAL
1	B	489	LEU
1	B	596	VAL
1	B	602	LEU
1	B	605	LEU
1	B	719	MET
1	B	727	SER
1	B	729	THR
1	B	732	ASN
1	B	755	ILE

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Mol	Chain	Res	Type
1	B	762	VAL
1	B	766	ILE
1	B	768	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	451	ASN
1	A	721	ASN
1	B	551	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 [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	354/410 (86%)	1.41	79 (22%) 2 2	56, 73, 113, 135	0
1	B	351/410 (85%)	1.41	82 (23%) 2 1	54, 72, 110, 144	0
All	All	705/820 (85%)	1.41	161 (22%) 2 1	54, 72, 111, 144	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	602	LEU	10.7
1	A	767	LEU	9.4
1	B	767	LEU	7.8
1	A	703	LEU	7.6
1	B	727	SER	6.6
1	B	728	ALA	6.6
1	A	766	ILE	6.6
1	B	762	VAL	6.4
1	A	630	PRO	6.2
1	A	768	THR	6.2
1	A	762	VAL	6.2
1	B	766	ILE	5.9
1	B	726	PRO	5.9
1	B	760	GLY	5.3
1	B	763	THR	5.3
1	B	515	GLY	5.2
1	A	602	LEU	5.0
1	B	730	PRO	4.9
1	B	761	SER	4.5
1	A	705	LYS	4.4
1	B	628	TYR	4.4
1	A	775	ARG	4.3
1	A	784	PRO	4.3
1	A	702	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	763	THR	4.1
1	B	601	ASN	4.1
1	A	704	GLU	4.1
1	A	726	PRO	4.1
1	A	760	GLY	4.0
1	B	776	GLY	3.9
1	B	429	GLN	3.9
1	B	729	THR	3.9
1	B	468	GLN	3.8
1	B	627	GLY	3.8
1	B	702	SER	3.8
1	A	592	ASN	3.7
1	A	764	GLU	3.7
1	B	718	LEU	3.7
1	A	514	PRO	3.7
1	B	427	LYS	3.7
1	A	765	ASP	3.7
1	A	464	GLY	3.7
1	A	551	ASN	3.7
1	B	514	PRO	3.7
1	A	334	GLN	3.6
1	A	468	GLN	3.6
1	A	729	THR	3.6
1	B	784	PRO	3.6
1	A	761	SER	3.6
1	B	775	ARG	3.5
1	A	465	TRP	3.4
1	A	598	PHE	3.4
1	A	461	PRO	3.4
1	B	725	PRO	3.4
1	B	606	ASP	3.4
1	A	418	ALA	3.3
1	B	723	GLY	3.3
1	B	605	LEU	3.2
1	A	421	ILE	3.2
1	A	769	GLY	3.1
1	B	516	PHE	3.1
1	B	430	THR	3.1
1	B	719	MET	3.1
1	B	428	VAL	3.1
1	B	712	VAL	3.1
1	B	764	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	709	GLN	3.0
1	A	714	VAL	3.0
1	B	470	GLY	3.0
1	A	437	ARG	3.0
1	A	603	ARG	3.0
1	A	604	GLY	3.0
1	B	458	LEU	2.9
1	A	458	LEU	2.9
1	A	605	LEU	2.9
1	B	732	ASN	2.9
1	A	456	LYS	2.8
1	A	348	LEU	2.8
1	B	420	LYS	2.8
1	B	565	ASP	2.8
1	A	628	TYR	2.8
1	A	728	ALA	2.8
1	A	564	MET	2.8
1	A	565	ASP	2.8
1	B	768	THR	2.7
1	B	492	ASN	2.7
1	B	608	ILE	2.7
1	B	415	TRP	2.7
1	A	727	SER	2.6
1	B	548	HIS	2.6
1	A	466	VAL	2.6
1	B	769	GLY	2.6
1	B	758	ILE	2.6
1	A	706	ARG	2.5
1	A	415	TRP	2.5
1	A	471	THR	2.5
1	A	783	MET	2.5
1	B	765	ASP	2.5
1	A	472	PRO	2.5
1	A	732	ASN	2.5
1	A	627	GLY	2.5
1	A	721	ASN	2.5
1	B	495	LEU	2.4
1	B	476	ASN	2.4
1	A	777	TRP	2.4
1	B	348	LEU	2.4
1	B	593	ARG	2.4
1	A	601	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	730	PRO	2.4
1	A	383	MET	2.4
1	B	731	GLU	2.4
1	A	344	THR	2.3
1	A	719	MET	2.3
1	A	485	ILE	2.3
1	B	426	ASP	2.3
1	B	465	TRP	2.3
1	B	478	THR	2.3
1	A	463	GLU	2.3
1	B	517	GLN	2.3
1	A	774	ALA	2.3
1	B	705	LYS	2.3
1	A	419	ALA	2.2
1	B	717	THR	2.2
1	A	516	PHE	2.2
1	A	747	ASP	2.2
1	A	441	ARG	2.2
1	A	475	GLY	2.2
1	B	471	THR	2.2
1	A	733	LEU	2.2
1	B	353	LEU	2.2
1	B	733	LEU	2.2
1	B	425	LYS	2.2
1	B	738	ILE	2.2
1	A	417	PHE	2.2
1	B	754	GLU	2.2
1	B	604	GLY	2.2
1	A	462	GLU	2.1
1	B	419	ALA	2.1
1	B	703	LEU	2.1
1	B	721	ASN	2.1
1	B	596	VAL	2.1
1	B	724	VAL	2.1
1	B	777	TRP	2.1
1	A	722	GLY	2.1
1	A	459	LYS	2.1
1	B	512	LYS	2.1
1	A	477	ASN	2.1
1	B	613	TYR	2.1
1	A	515	GLY	2.1
1	A	776	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	603	ARG	2.1
1	B	774	ALA	2.0
1	B	626	TYR	2.0
1	A	612	VAL	2.0
1	B	740	VAL	2.0
1	B	720	GLU	2.0
1	B	389	LEU	2.0
1	A	725	PRO	2.0
1	A	755	ILE	2.0
1	B	421	ILE	2.0
1	A	420	LYS	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](#)

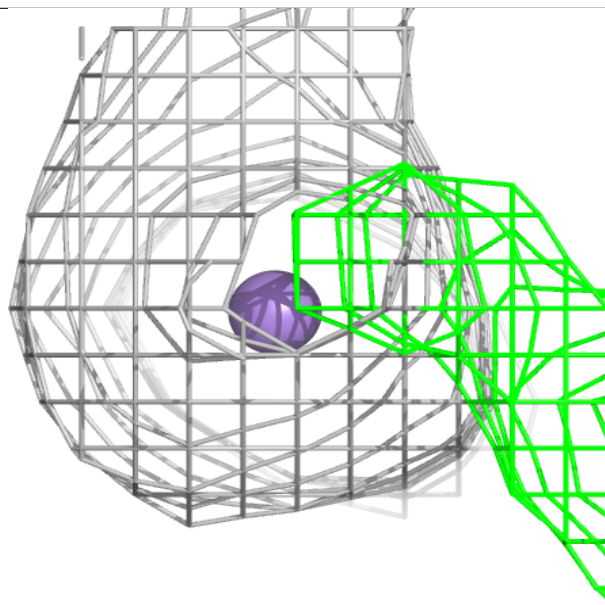
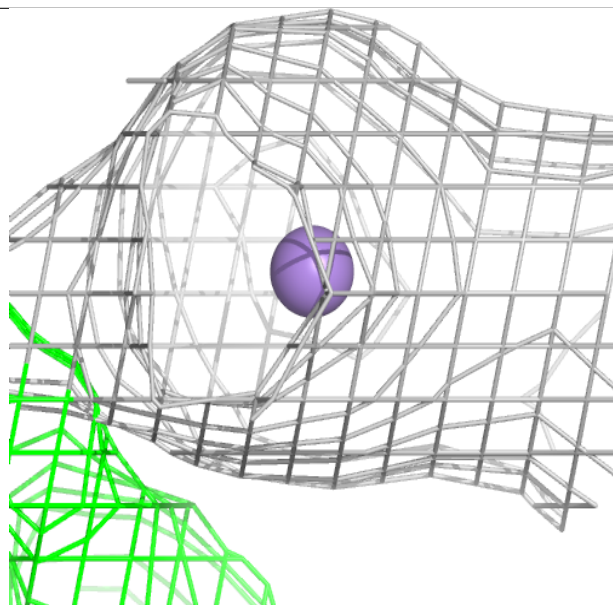
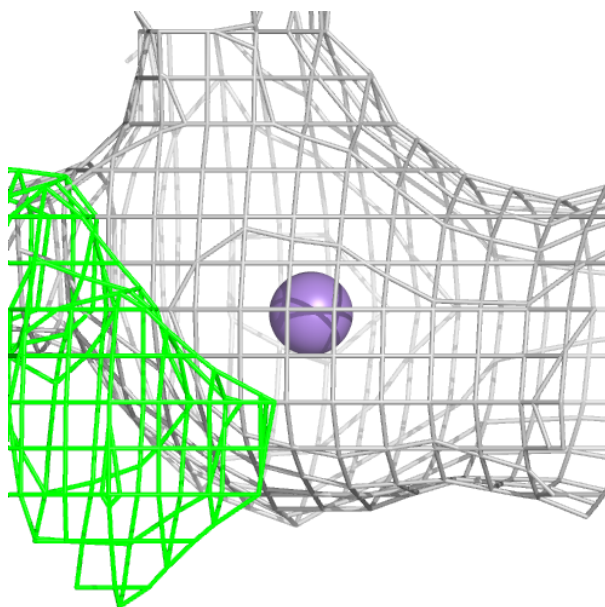
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MN	B	801	1/1	0.94	0.19	93,93,93,93	1
2	MN	A	801	1/1	0.96	0.17	85,85,85,85	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.

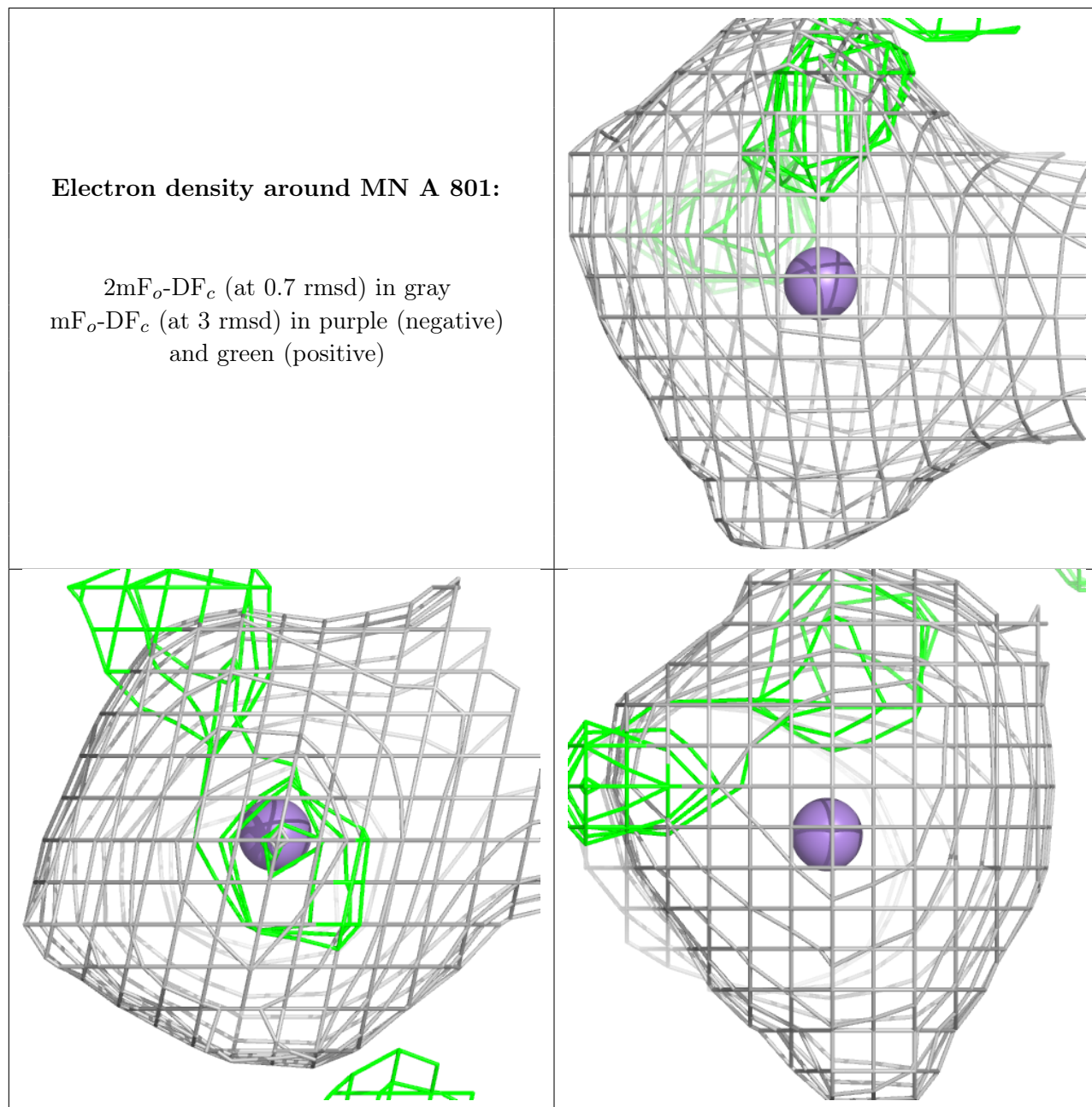
Electron density around MN B 801:

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



Electron density around MN A 801:

$2mF_o-DF_c$ (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.