



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:52 PM UTC

PDB ID : 8R9O / pdb_00008r9o
Title : A soakable crystal form of human CDK7 in complex with AMP-PNP
Authors : Mukherjee, M.; Cleasby, A.
Deposited on : 2023-11-30
Resolution : 2.22 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

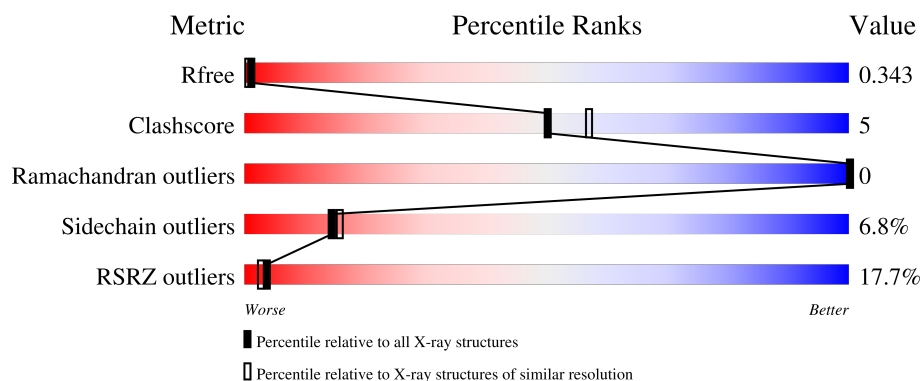
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	371	14% 59% 13% 26%
1	B	371	13% 60% 16% 23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4799 atoms, of which 70 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 Cyclin-dependent kinase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	5	0
			2225	1441	373	396	15			
1	B	284	Total	C	N	O	S	0	4	0
			2289	1481	387	408	13			

There are 56 discrepancies between the modelled and reference sequences:

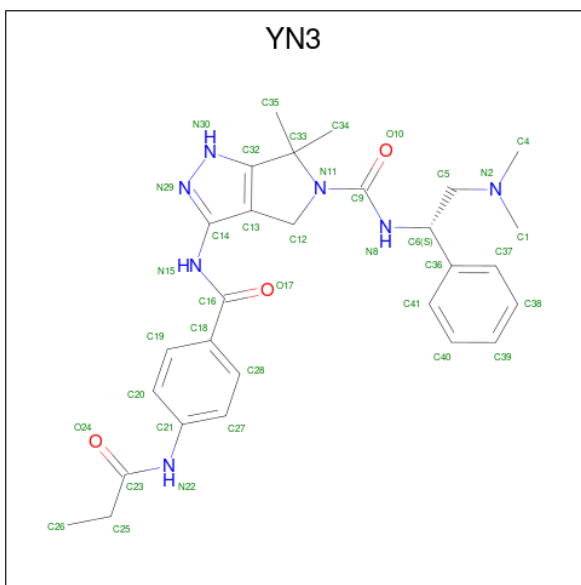
Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP P50613
A	-23	SER	-	expression tag	UNP P50613
A	-22	TYR	-	expression tag	UNP P50613
A	-21	TYR	-	expression tag	UNP P50613
A	-20	HIS	-	expression tag	UNP P50613
A	-19	HIS	-	expression tag	UNP P50613
A	-18	HIS	-	expression tag	UNP P50613
A	-17	HIS	-	expression tag	UNP P50613
A	-16	HIS	-	expression tag	UNP P50613
A	-15	HIS	-	expression tag	UNP P50613
A	-14	ASP	-	expression tag	UNP P50613
A	-13	TYR	-	expression tag	UNP P50613
A	-12	ASP	-	expression tag	UNP P50613
A	-11	ILE	-	expression tag	UNP P50613
A	-10	PRO	-	expression tag	UNP P50613
A	-9	THR	-	expression tag	UNP P50613
A	-8	THR	-	expression tag	UNP P50613
A	-7	GLU	-	expression tag	UNP P50613
A	-6	ASN	-	expression tag	UNP P50613
A	-5	LEU	-	expression tag	UNP P50613
A	-4	TYR	-	expression tag	UNP P50613
A	-3	PHE	-	expression tag	UNP P50613
A	-2	GLN	-	expression tag	UNP P50613
A	-1	GLY	-	expression tag	UNP P50613
A	0	SER	-	expression tag	UNP P50613

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Chain	Residue	Modelled	Actual	Comment	Reference
A	132	ARG	TRP	engineered mutation	UNP P50613
A	164	ASP	SER	engineered mutation	UNP P50613
A	170	GLU	THR	engineered mutation	UNP P50613
B	-24	MET	-	initiating methionine	UNP P50613
B	-23	SER	-	expression tag	UNP P50613
B	-22	TYR	-	expression tag	UNP P50613
B	-21	TYR	-	expression tag	UNP P50613
B	-20	HIS	-	expression tag	UNP P50613
B	-19	HIS	-	expression tag	UNP P50613
B	-18	HIS	-	expression tag	UNP P50613
B	-17	HIS	-	expression tag	UNP P50613
B	-16	HIS	-	expression tag	UNP P50613
B	-15	HIS	-	expression tag	UNP P50613
B	-14	ASP	-	expression tag	UNP P50613
B	-13	TYR	-	expression tag	UNP P50613
B	-12	ASP	-	expression tag	UNP P50613
B	-11	ILE	-	expression tag	UNP P50613
B	-10	PRO	-	expression tag	UNP P50613
B	-9	THR	-	expression tag	UNP P50613
B	-8	THR	-	expression tag	UNP P50613
B	-7	GLU	-	expression tag	UNP P50613
B	-6	ASN	-	expression tag	UNP P50613
B	-5	LEU	-	expression tag	UNP P50613
B	-4	TYR	-	expression tag	UNP P50613
B	-3	PHE	-	expression tag	UNP P50613
B	-2	GLN	-	expression tag	UNP P50613
B	-1	GLY	-	expression tag	UNP P50613
B	0	SER	-	expression tag	UNP P50613
B	132	ARG	TRP	engineered mutation	UNP P50613
B	164	ASP	SER	engineered mutation	UNP P50613
B	170	GLU	THR	engineered mutation	UNP P50613

- Molecule 2 is {N}-[(1 {S})-2-(dimethylamino)-1-phenyl-ethyl]-6,6-dimethyl-3-[[4-(propanoyl amino)phenyl]carbonylamino]-1,4-dihydropyrrolo[3,4-c]pyrazole-5-carboxamide (CCD ID: YN3) (formula: C₂₈H₃₅N₇O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 73	C 28	H 35	N 7	O 3	0	0
2	B	1	Total 73	C 28	H 35	N 7	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	74	Total O 74 74	0	0
3	B	65	Total O 65 65	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	40.14Å 123.74Å 142.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.73 – 2.22 56.73 – 2.22	Depositor EDS
% Data completeness (in resolution range)	43.1 (56.73-2.22) 43.1 (56.73-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.22Å)	Xtriage
Refinement program	BUSTER 2.11.8 (16-JUL-2021)	Depositor
R, R_{free}	0.253 , 0.344 0.251 , 0.343	Depositor DCC
R_{free} test set	795 reflections (1.75%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4799	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 34.59 % 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 6.6589e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: YN3

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	0.99	5/2283 (0.2%)	1.13	7/3091 (0.2%)
1	B	1.01	2/2346 (0.1%)	1.15	4/3177 (0.1%)
All	All	1.00	7/4629 (0.2%)	1.14	11/6268 (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	B	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	ILE	CA-C	6.05	1.59	1.52
1	A	196	MET	SD-CE	-5.56	1.65	1.79
1	A	24	ALA	CA-C	5.50	1.60	1.52
1	A	162	PHE	CA-C	5.44	1.60	1.52
1	A	292	MET	SD-CE	-5.42	1.66	1.79
1	B	196	MET	SD-CE	-5.32	1.66	1.79
1	B	23	PHE	CA-C	5.29	1.57	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ASP	CA-CB-CG	9.11	121.71	112.60
1	B	162	PHE	CA-CB-CG	6.86	120.66	113.80
1	A	162	PHE	CA-CB-CG	6.52	120.32	113.80
1	B	164	ASP	CA-CB-CG	6.42	119.02	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	HIS	CA-CB-CG	5.78	119.58	113.80
1	B	131	HIS	CA-CB-CG	-5.31	108.49	113.80
1	A	33	ASN	CA-CB-CG	5.20	117.80	112.60
1	A	131	HIS	CA-CB-CG	-5.10	108.70	113.80
1	A	67	GLN	CA-C-N	5.07	129.25	121.19
1	A	67	GLN	C-N-CA	5.07	129.25	121.19
1	B	17	PHE	CA-CB-CG	5.04	118.84	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	23	PHE	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	2225	0	2259	21	0
1	B	2289	0	2322	28	0
2	A	38	35	0	2	0
2	B	38	35	0	2	0
3	A	74	0	0	0	0
3	B	65	0	0	0	0
All	All	4729	70	4581	49	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 (49) 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:40:ILE:HD13	1:A:90:VAL:HG22	1.57	0.86
1:B:98:LEU:HD12	1:B:143:LEU:HD12	1.72	0.72
1:A:155:ASP:OD2	2:A:401:YN3:N2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:MET:N	2:B:401:YN3:N29	2.44	0.61
1:B:143:LEU:HD11	1:B:202:ILE:HD13	1.82	0.61
1:B:81:PHE:O	1:B:87:ILE:HG23	1.99	0.61
1:A:185:PHE:O	1:A:245:ASP:HB2	2.00	0.61
1:A:65:LEU:O	1:A:68:GLU:HB2	2.01	0.59
1:A:56:ASN:O	1:A:60:LEU:HB2	2.02	0.58
1:B:176:ARG:HD2	1:B:217:SER:O	2.07	0.55
1:A:118[A]:MET:HE2	1:A:118[A]:MET:HA	1.89	0.54
1:B:118[A]:MET:HA	1:B:118[A]:MET:HE2	1.89	0.54
1:B:143:LEU:HD22	1:B:153:LEU:HD22	1.88	0.54
1:B:182:GLU:OE1	1:B:280:PRO:HG3	2.09	0.53
1:A:129:HIS:CE1	1:A:192:VAL:HB	2.45	0.52
1:A:104:ASP:O	1:A:209:ARG:NH2	2.43	0.51
1:B:155:ASP:OD2	2:B:401:YN3:N2	2.44	0.51
1:B:102:ILE:HG21	1:B:205:GLU:HG2	1.92	0.50
1:B:139:LYS:HG3	1:B:141:ASN:OD1	2.13	0.49
1:B:95:GLU:HG3	1:B:96:THR:N	2.29	0.47
1:A:190:TYR:CD1	1:A:194:VAL:HG21	2.50	0.46
1:A:289:ALA:O	1:A:292:MET:HB2	2.16	0.46
1:B:118[A]:MET:HE1	1:B:199:VAL:HG13	1.98	0.46
1:A:213:LEU:HD13	1:A:225:ILE:HG12	1.99	0.45
1:A:118[A]:MET:HE1	1:A:199:VAL:HG13	1.99	0.45
1:B:98:LEU:O	1:B:102:ILE:HG13	2.16	0.45
1:B:122:LEU:HD21	1:B:199:VAL:HG11	1.98	0.45
1:A:227:GLU:O	1:A:254:GLY:HA2	2.17	0.45
1:B:174:VAL:HG22	1:B:175:THR:N	2.31	0.45
1:B:213:LEU:HD13	1:B:225:ILE:HG12	1.99	0.45
1:A:221:GLN:O	1:A:225:ILE:HG13	2.18	0.44
1:A:237:TRP:CE3	1:A:240:MET:SD	3.11	0.44
1:B:227:GLU:O	1:B:254:GLY:HA2	2.18	0.44
1:A:174:VAL:HG22	1:A:175:THR:N	2.33	0.44
1:B:204:ALA:O	1:B:208:LEU:HG	2.16	0.44
1:A:234:GLU:HG3	1:A:240:MET:HE2	2.00	0.43
1:B:221:GLN:O	1:B:225:ILE:HG13	2.19	0.43
1:B:113:HIS:CD2	1:B:308:PRO:HD3	2.53	0.43
1:B:128:LEU:HD21	1:B:156:PHE:HE2	1.84	0.43
1:B:190:TYR:CD1	1:B:194:VAL:HG21	2.54	0.43
1:A:92:ASP:O	2:A:401:YN3:N30	2.53	0.42
1:B:173:VAL:HG12	1:B:183:LEU:HD13	2.01	0.42
1:A:220:ASP:O	1:A:224:ARG:HG3	2.21	0.41
1:A:66:LEU:HD21	1:A:156:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ILE:O	1:B:118[B]:MET:HG2	2.21	0.41
1:B:183:LEU:HD11	1:B:194:VAL:HG13	2.03	0.41
1:B:220:ASP:O	1:B:224:ARG:HG3	2.21	0.40
1:A:125:LEU:HD23	1:A:196:MET:HE1	2.03	0.40
1:B:181:PRO:HA	1:B:184:LEU:HD12	2.04	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	273/371 (74%)	253 (93%)	20 (7%)	0	100	100
1	B	280/371 (76%)	262 (94%)	18 (6%)	0	100	100
All	All	553/742 (74%)	515 (93%)	38 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	245/323 (76%)	227 (93%)	18 (7%)	13	13
1	B	252/323 (78%)	237 (94%)	15 (6%)	17	20
All	All	497/646 (77%)	464 (93%)	33 (7%)	14	17

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	PHE
1	A	22	GLN
1	A	33	ASN
1	A	40	ILE
1	A	57	ARG
1	A	60	LEU
1	A	65	LEU
1	A	81	PHE
1	A	87	ILE
1	A	88	SER
1	A	95	GLU
1	A	139	LYS
1	A	145	LEU
1	A	148	ASN
1	A	153	LEU
1	A	210	VAL
1	A	249	PHE
1	A	307	LEU
1	B	60	LEU
1	B	61	ARG
1	B	88	SER
1	B	145	LEU
1	B	148	ASN
1	B	160	LYS
1	B	173	VAL
1	B	179	ARG
1	B	210	VAL
1	B	219	LEU
1	B	249	PHE
1	B	292	MET
1	B	293	LYS
1	B	307	LEU
1	B	309	ARG

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	113	HIS
1	A	259	HIS
1	A	273	GLN
1	B	129	HIS

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Mol	Chain	Res	Type
1	B	130	GLN
1	B	142	ASN
1	B	172	GLN
1	B	259	HIS
1	B	288	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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	YN3	A	401	1	38,41,41	0.71	0	46,59,59	1.68	3 (6%)
2	YN3	B	401	1	38,41,41	0.88	1 (2%)	46,59,59	2.22	6 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	YN3	A	401	1	-	6/30/46/46	0/4/4/4
2	YN3	B	401	1	-	6/30/46/46	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	YN3	C14-N29	4.03	1.38	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	YN3	C32-C13-C14	11.12	109.02	104.22
2	B	401	YN3	C13-C14-N29	-8.29	108.39	113.57
2	A	401	YN3	C32-C13-C14	7.76	107.57	104.22
2	A	401	YN3	C13-C14-N29	-6.67	109.40	113.57
2	B	401	YN3	C14-N29-N30	3.26	105.82	103.32
2	A	401	YN3	C14-N29-N30	2.88	105.52	103.32
2	B	401	YN3	C12-C13-C14	-2.70	138.81	142.85
2	B	401	YN3	C21-N22-C23	-2.36	123.35	127.52
2	B	401	YN3	C33-C32-C13	-2.01	109.69	112.45

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	YN3	N2-C5-C6-C36
2	A	401	YN3	N2-C5-C6-N8
2	A	401	YN3	C13-C14-N15-C16
2	B	401	YN3	C20-C21-N22-C23
2	B	401	YN3	C27-C21-N22-C23
2	B	401	YN3	N2-C5-C6-C36
2	B	401	YN3	N2-C5-C6-N8
2	B	401	YN3	N22-C23-C25-C26
2	A	401	YN3	N29-C14-N15-C16
2	B	401	YN3	O24-C23-C25-C26
2	A	401	YN3	C27-C21-N22-C23
2	A	401	YN3	C20-C21-N22-C23

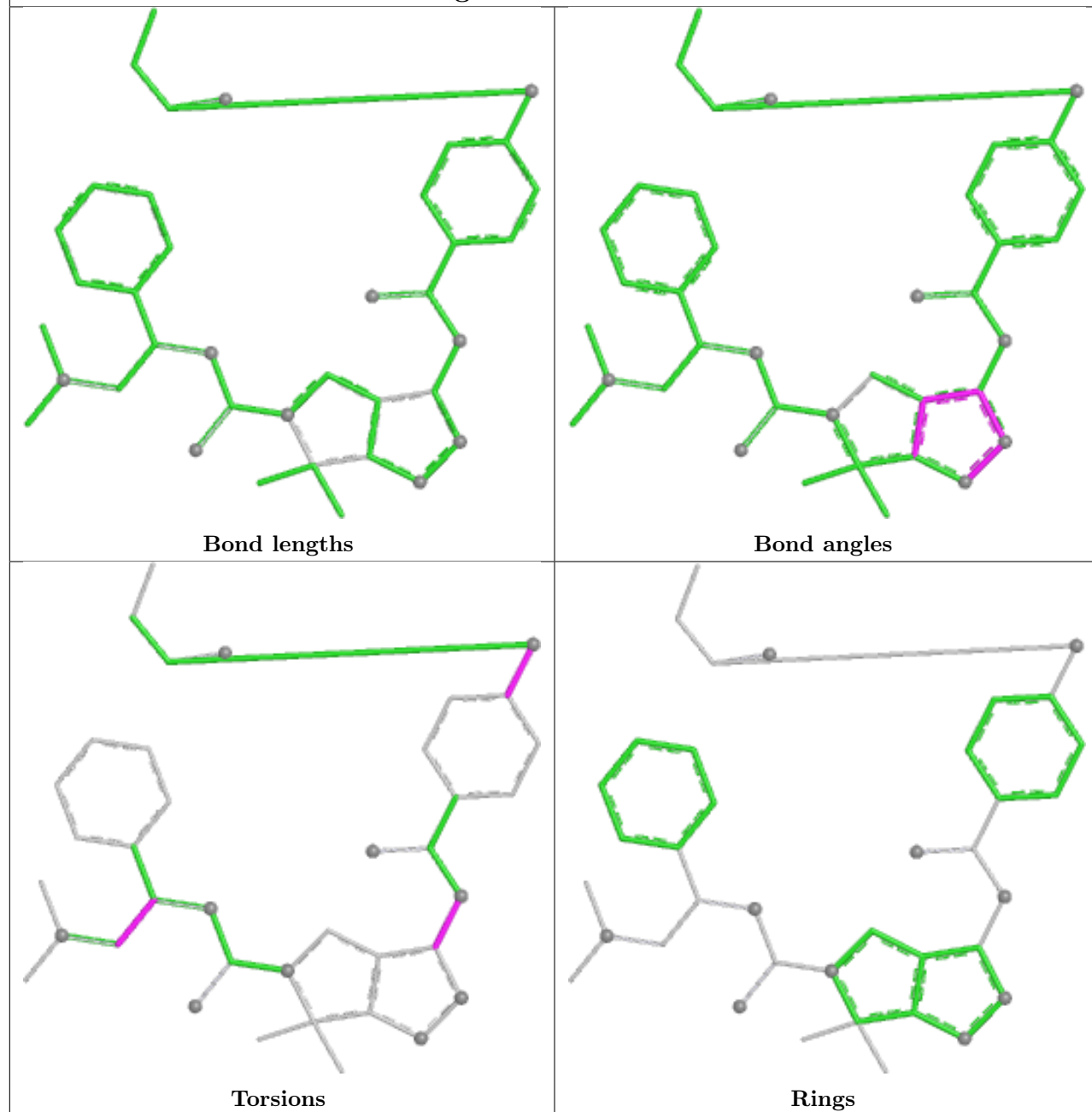
There are no ring outliers.

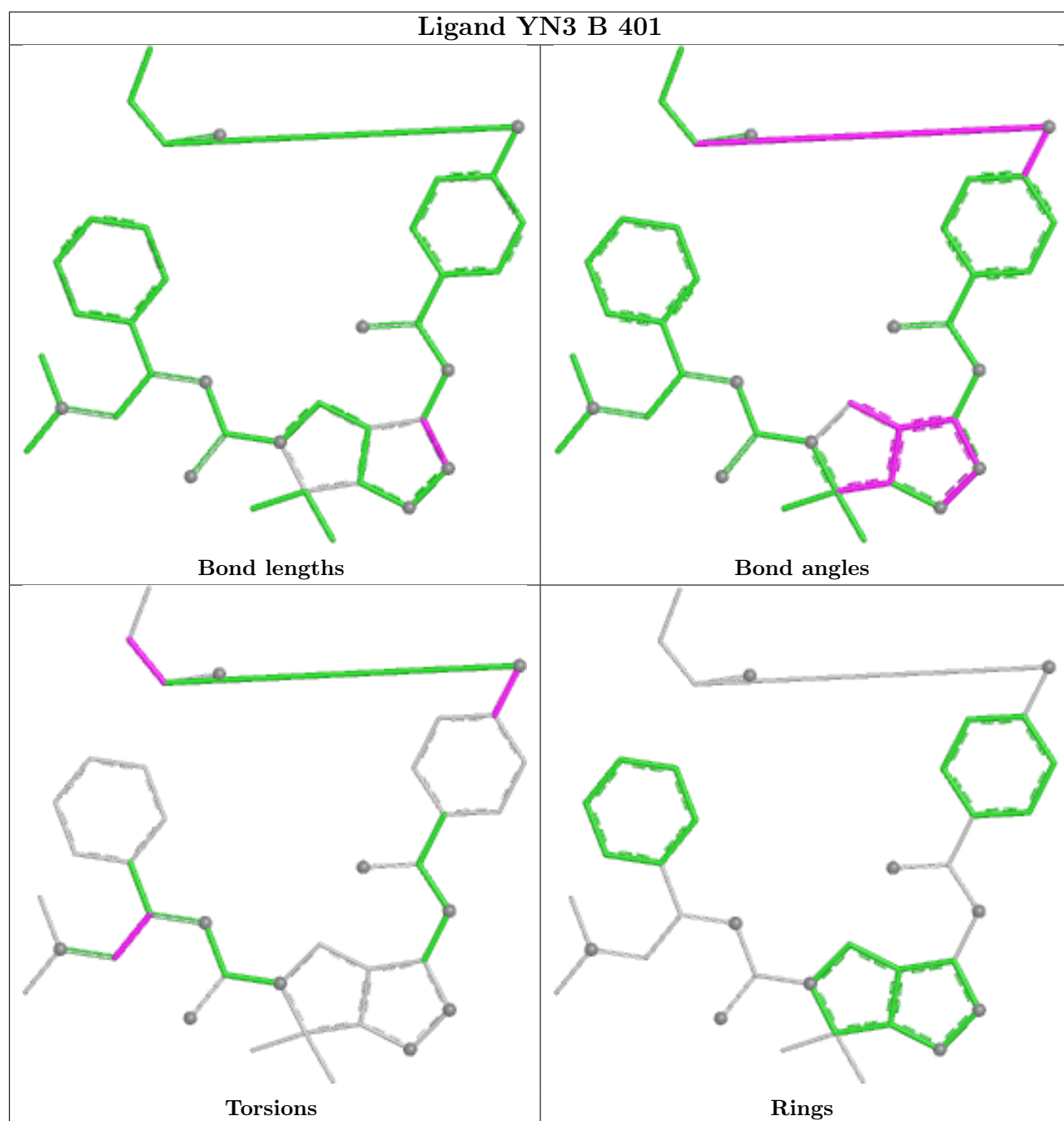
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	YN3	2	0
2	B	401	YN3	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand YN3 A 401





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	276/371 (74%)	1.34	52 (18%)	3 2	12, 42, 89, 97	5 (1%)
1	B	284/371 (76%)	1.06	47 (16%)	4 3	12, 39, 78, 84	4 (1%)
All	All	560/742 (75%)	1.20	99 (17%)	4 3	12, 40, 83, 97	9 (1%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	PRO	6.5
1	A	15	LEU	6.2
1	A	247	VAL	5.4
1	A	244	PRO	4.8
1	A	246	TYR	4.8
1	B	243	LEU	4.7
1	A	66	LEU	4.6
1	A	238	PRO	4.6
1	B	14	LYS	4.1
1	B	274	GLY	3.9
1	B	26	VAL	3.9
1	B	63	ILE	3.8
1	A	61	ARG	3.7
1	A	27	TYR	3.7
1	A	312	CYS	3.6
1	A	237	TRP	3.5
1	B	27	TYR	3.5
1	A	30	ARG	3.5
1	A	29	ALA	3.4
1	A	12	TYR	3.3
1	B	237	TRP	3.3
1	A	38	VAL	3.3
1	B	24	ALA	3.2
1	B	59	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	58	THR	3.2
1	B	29	ALA	3.2
1	A	265	GLY	3.1
1	A	255	ILE	3.1
1	A	80	ALA	3.1
1	B	60	LEU	3.1
1	B	271	LEU	3.1
1	B	163	GLY	3.0
1	A	174	VAL	3.0
1	B	15	LEU	3.0
1	B	242	SER	3.0
1	A	26	VAL	3.0
1	B	175	THR	2.9
1	A	24	ALA	2.9
1	A	36	GLN	2.9
1	A	59	ALA	2.9
1	A	245	ASP	2.9
1	A	163	GLY	2.8
1	B	284[A]	ILE	2.8
1	B	247	VAL	2.8
1	A	86	ASN	2.8
1	A	18	LEU	2.8
1	B	268	LEU	2.8
1	B	43	ILE	2.7
1	B	173	VAL	2.7
1	A	16	ASP	2.7
1	A	242	SER	2.7
1	A	226	PHE	2.6
1	A	37	ILE	2.6
1	A	249	PHE	2.6
1	B	21	GLY	2.6
1	B	189	MET	2.6
1	A	25	THR	2.5
1	B	38	VAL	2.5
1	A	62	GLU	2.5
1	B	99	GLU	2.5
1	A	10	LYS	2.5
1	A	74	ILE	2.5
1	B	12	TYR	2.5
1	B	16	ASP	2.5
1	A	248	THR	2.4
1	B	23	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	234	GLU	2.4
1	B	241	CYS	2.4
1	A	87	ILE	2.4
1	A	102	ILE	2.4
1	A	240	MET	2.4
1	A	28	LYS	2.4
1	A	241	CYS	2.4
1	A	22	GLN	2.4
1	B	236	GLN	2.4
1	A	23	PHE	2.3
1	B	65	LEU	2.3
1	B	18	LEU	2.3
1	A	33	ASN	2.3
1	B	190	TYR	2.3
1	B	240	MET	2.3
1	B	13	GLU	2.3
1	A	216	ASP	2.3
1	A	40	ILE	2.3
1	B	258	HIS	2.2
1	A	65	LEU	2.2
1	A	234	GLU	2.2
1	A	21	GLY	2.1
1	B	58	THR	2.1
1	B	245	ASP	2.1
1	B	174	VAL	2.1
1	B	249	PHE	2.1
1	B	30	ARG	2.1
1	B	96	THR	2.1
1	B	66	LEU	2.1
1	A	77	LEU	2.0
1	A	194	VAL	2.0
1	B	188	ARG	2.0
1	B	253	PRO	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 ⓘ

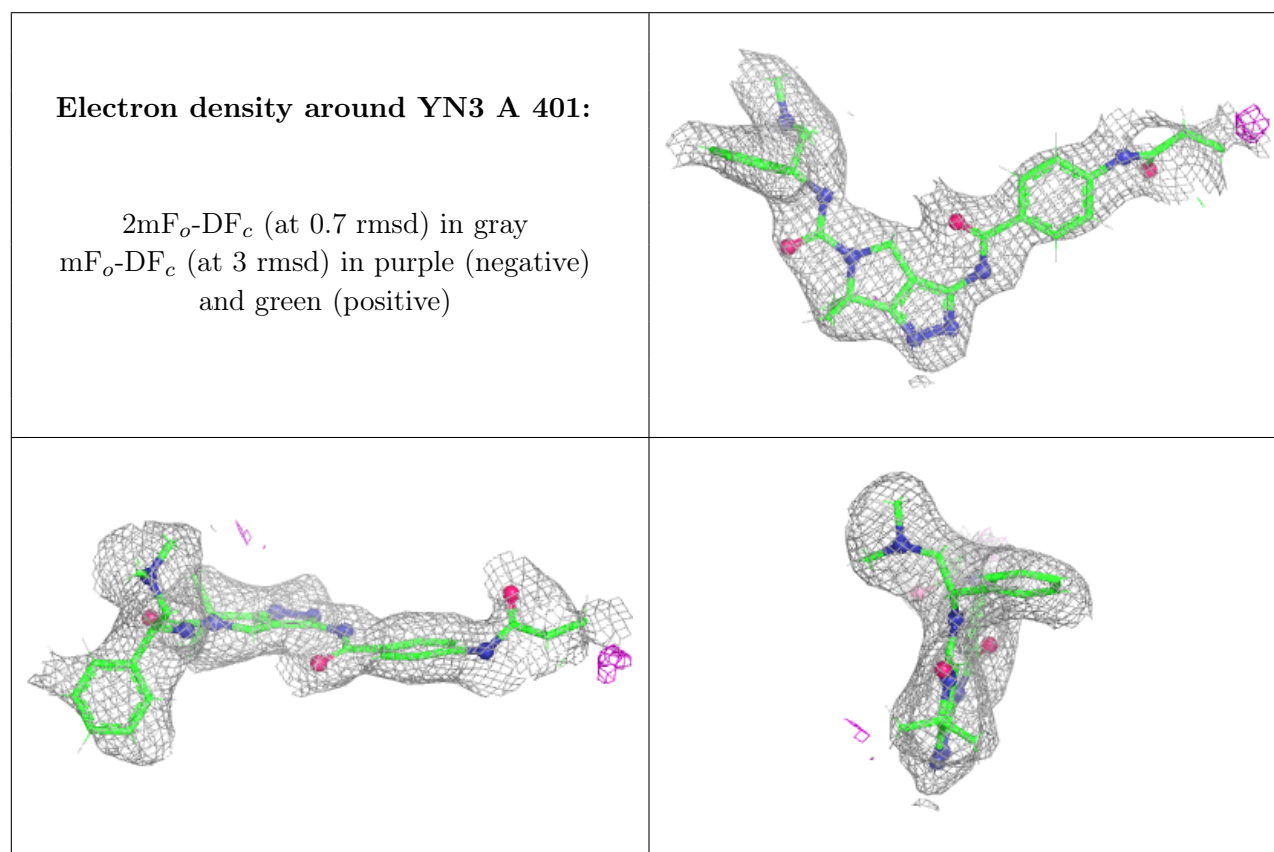
There are no oligosaccharides in this entry.

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.

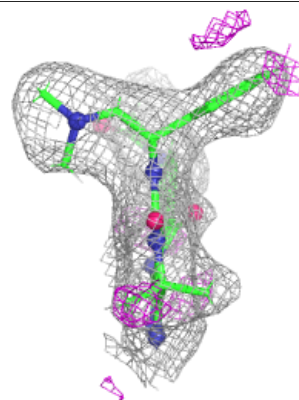
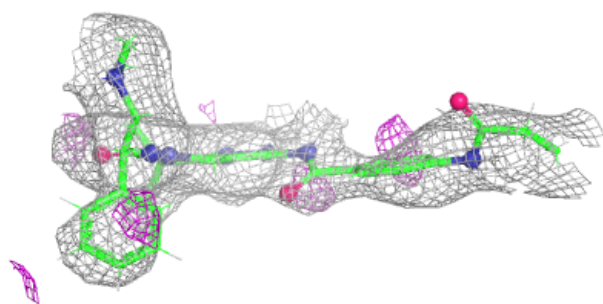
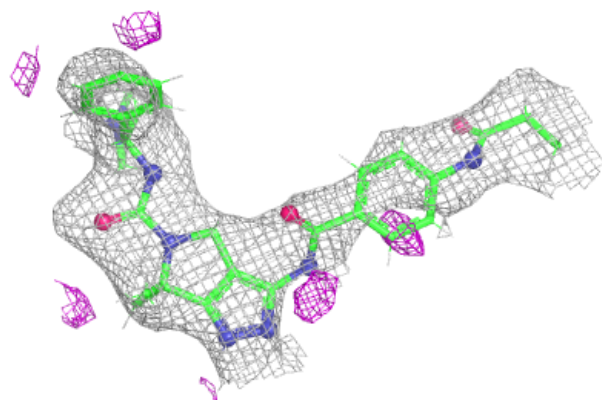
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	YN3	A	401	38/38	0.89	0.11	14,44,80,83	0
2	YN3	B	401	38/38	0.90	0.14	10,35,77,86	0

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 YN3 B 401:

$2mF_o-DF_c$ (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.