Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 07:00 PM EDT

PDB ID	:	6WXX
Title	:	crystal structure of cA4-activated Card1
Authors	:	Rostol, J.; Xie, W.; Patel, D.J.; Marraffini, L.
Deposited on	:	2020-05-12
Resolution	:	3.00 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:

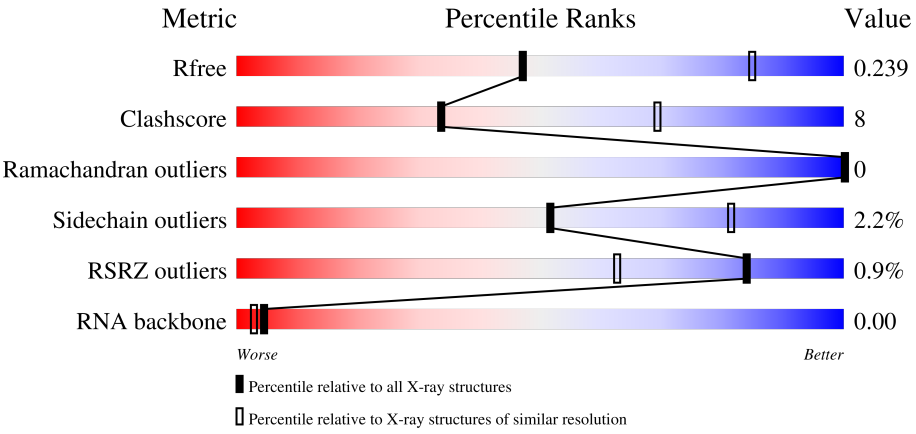
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 <=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	382	% 79% 17%
1	B	382	% 79% 18%
1	C	382	% 77% 20%
1	D	382	% 75% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	X	4	25% 50% 25%
2	Y	4	75% 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MN	A	901	-	-	-	X
3	MN	C	901	-	-	-	X
3	MN	D	901	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12548 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 Card1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	372	Total	C	N	O	S	0	0	0
			3092	1991	506	585	10			
1	A	372	Total	C	N	O	S	0	0	0
			3092	1991	506	585	10			
1	D	372	Total	C	N	O	S	0	0	0
			3092	1991	506	585	10			
1	C	372	Total	C	N	O	S	0	0	0
			3092	1991	506	585	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	374	GLY	-	expression tag	UNP F2NWD3
B	375	SER	-	expression tag	UNP F2NWD3
B	376	GLY	-	expression tag	UNP F2NWD3
B	377	HIS	-	expression tag	UNP F2NWD3
B	378	HIS	-	expression tag	UNP F2NWD3
B	379	HIS	-	expression tag	UNP F2NWD3
B	380	HIS	-	expression tag	UNP F2NWD3
B	381	HIS	-	expression tag	UNP F2NWD3
B	382	HIS	-	expression tag	UNP F2NWD3
A	374	GLY	-	expression tag	UNP F2NWD3
A	375	SER	-	expression tag	UNP F2NWD3
A	376	GLY	-	expression tag	UNP F2NWD3
A	377	HIS	-	expression tag	UNP F2NWD3
A	378	HIS	-	expression tag	UNP F2NWD3
A	379	HIS	-	expression tag	UNP F2NWD3
A	380	HIS	-	expression tag	UNP F2NWD3
A	381	HIS	-	expression tag	UNP F2NWD3
A	382	HIS	-	expression tag	UNP F2NWD3
D	374	GLY	-	expression tag	UNP F2NWD3
D	375	SER	-	expression tag	UNP F2NWD3
D	376	GLY	-	expression tag	UNP F2NWD3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	377	HIS	-	expression tag	UNP F2NWD3
D	378	HIS	-	expression tag	UNP F2NWD3
D	379	HIS	-	expression tag	UNP F2NWD3
D	380	HIS	-	expression tag	UNP F2NWD3
D	381	HIS	-	expression tag	UNP F2NWD3
D	382	HIS	-	expression tag	UNP F2NWD3
C	374	GLY	-	expression tag	UNP F2NWD3
C	375	SER	-	expression tag	UNP F2NWD3
C	376	GLY	-	expression tag	UNP F2NWD3
C	377	HIS	-	expression tag	UNP F2NWD3
C	378	HIS	-	expression tag	UNP F2NWD3
C	379	HIS	-	expression tag	UNP F2NWD3
C	380	HIS	-	expression tag	UNP F2NWD3
C	381	HIS	-	expression tag	UNP F2NWD3
C	382	HIS	-	expression tag	UNP F2NWD3

- Molecule 2 is a RNA chain called cA4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	4	Total	C	N	O	P	0	0	0
			88	40	20	24	4			
2	X	4	Total	C	N	O	P	0	0	0
			88	40	20	24	4			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

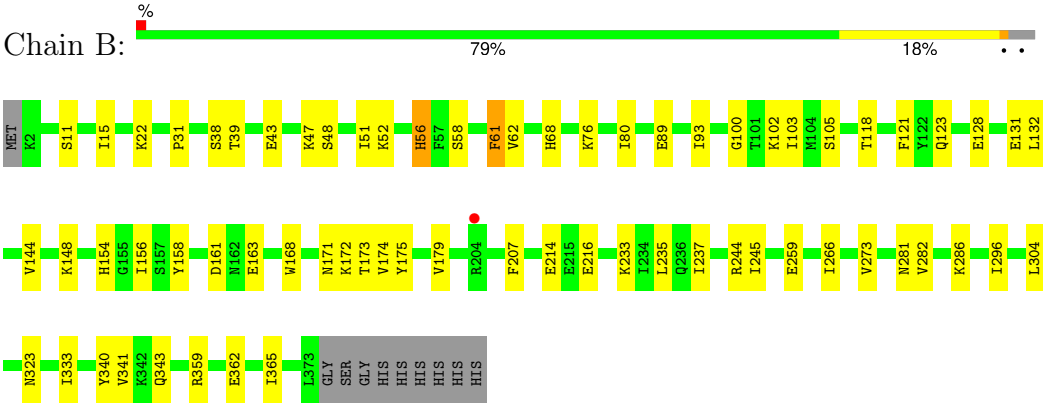
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

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.

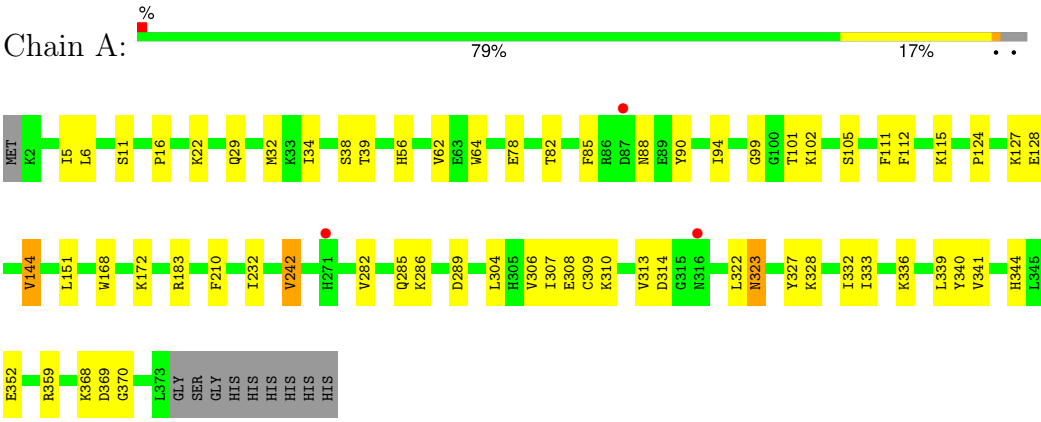
• Molecule 1: Card1

Chain B:



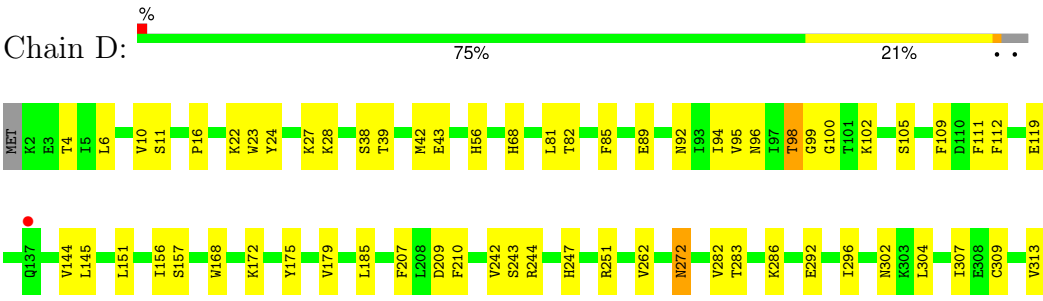
• Molecule 1: Card1

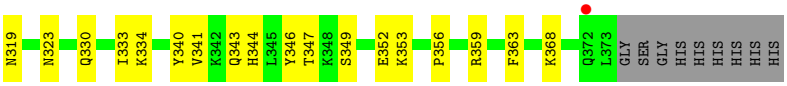
Chain A:



• Molecule 1: Card1

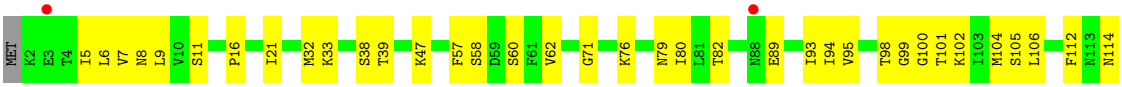
Chain D:

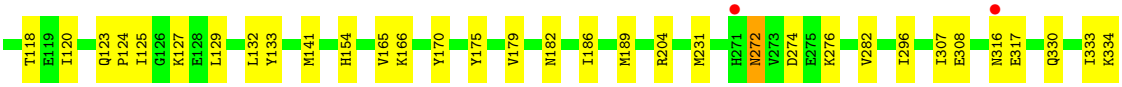


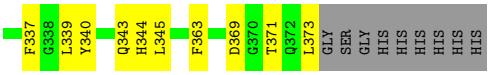


• Molecule 1: Card1

Chain C:





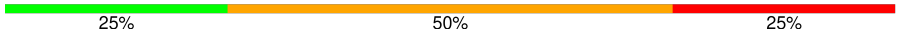


• Molecule 2: cA4

Chain Y:

• Molecule 2: cA4

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.06Å 121.22Å 103.71Å 90.00° 113.06° 90.00°	Depositor
Resolution (Å)	28.88 – 3.00 28.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.88-3.00) 98.8 (28.88-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.18_3855, PHENIX 1.18_3855	Depositor
R, R_{free}	0.204 , 0.237 0.207 , 0.239	Depositor DCC
R_{free} test set	1886 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	80.0	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12548	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.32	0/3157	0.50	0/4257
1	B	0.39	0/3157	0.53	0/4257
1	C	0.35	0/3157	0.51	0/4257
1	D	0.33	0/3157	0.49	0/4257
2	X	1.62	2/99 (2.0%)	0.96	0/152
2	Y	1.56	2/99 (2.0%)	1.08	0/152
All	All	0.40	4/12826 (0.0%)	0.52	0/17332

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	2	A	O3'-P	-7.17	1.52	1.61
2	Y	3	A	O3'-P	-6.88	1.52	1.61
2	Y	1	A	O3'-P	-6.49	1.53	1.61
2	X	3	A	O3'-P	-5.96	1.53	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3092	0	3063	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3092	0	3063	69	0
1	C	3092	0	3063	58	0
1	D	3092	0	3063	58	0
2	X	88	0	44	3	0
2	Y	88	0	44	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	12548	0	12340	211	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 8.

All (211) 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:31:PRO:HB3	1:B:61:PHE:CD2	2.01	0.95
1:B:31:PRO:CD	1:B:61:PHE:HE2	1.80	0.93
1:B:31:PRO:HB3	1:B:61:PHE:CE2	2.08	0.89
1:B:31:PRO:CB	1:B:61:PHE:CE2	2.56	0.88
1:B:31:PRO:CA	1:B:61:PHE:CE2	2.57	0.87
1:B:31:PRO:CA	1:B:61:PHE:HE2	1.90	0.85
1:B:31:PRO:N	1:B:61:PHE:HE2	1.76	0.83
1:B:31:PRO:CB	1:B:61:PHE:HE2	1.93	0.82
1:D:347:THR:HG22	1:D:349:SER:H	1.43	0.82
1:B:31:PRO:CD	1:B:61:PHE:CE2	2.64	0.80
1:D:22:LYS:NZ	1:D:144:VAL:O	2.15	0.80
1:C:274:ASP:OD2	1:C:276:LYS:HG2	1.84	0.77
1:B:31:PRO:HD3	1:B:61:PHE:CE2	2.21	0.75
1:B:89:GLU:HB2	1:C:204:ARG:HD2	1.68	0.75
1:C:101:THR:HG22	1:C:104:MET:HE2	1.71	0.73
1:B:31:PRO:N	1:B:61:PHE:CE2	2.57	0.71
1:A:306:VAL:HB	1:A:333:ILE:HD11	1.74	0.70
1:C:307:ILE:HG12	1:C:344:HIS:HB2	1.74	0.70
1:D:283:THR:HG22	1:D:292:GLU:HG2	1.73	0.69
1:C:95:VAL:HB	1:C:120:ILE:HG22	1.75	0.69
1:D:247:HIS:HD2	1:D:251:ARG:HE	1.42	0.68
1:A:22:LYS:NZ	1:A:144:VAL:O	2.24	0.68
1:B:259:GLU:OE1	1:B:281:ASN:OD1	2.15	0.64
1:C:98:THR:HG21	1:C:123:GLN:HB3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:THR:HG22	1:D:92:ASN:HB2	1.81	0.63
1:C:93:ILE:HG13	1:C:118:THR:HG23	1.80	0.62
1:A:168:TRP:O	1:A:172:LYS:HG3	2.00	0.62
1:A:369:ASP:OD2	1:A:370:GLY:N	2.33	0.62
1:B:31:PRO:CB	1:B:61:PHE:CD2	2.77	0.61
1:B:11:SER:HB3	1:B:100:GLY:H	1.66	0.61
1:B:31:PRO:HA	1:B:61:PHE:CE2	2.36	0.60
1:B:76:LYS:O	1:B:80:ILE:HG13	2.01	0.60
1:A:56:HIS:O	1:A:56:HIS:ND1	2.34	0.60
1:D:10:VAL:HB	1:D:38:SER:HB2	1.83	0.60
1:B:304:LEU:HB3	1:B:341:VAL:HG12	1.84	0.60
1:B:343:GLN:HG2	1:B:365:ILE:HA	1.84	0.60
1:C:98:THR:CG2	1:C:123:GLN:H	2.15	0.60
1:D:156:ILE:HD13	1:D:286:LYS:HB2	1.83	0.59
1:B:102:LYS:HE2	1:A:99:GLY:O	2.03	0.59
1:C:101:THR:HG23	1:C:104:MET:H	1.68	0.59
1:D:307:ILE:HG12	1:D:344:HIS:HB2	1.84	0.58
1:B:123:GLN:O	2:X:4:A:H8	1.85	0.58
1:B:58:SER:OG	1:B:61:PHE:HB2	2.03	0.58
1:C:79:ASN:O	1:C:82:THR:OG1	2.21	0.58
1:B:31:PRO:HB3	1:B:61:PHE:HD2	1.63	0.57
1:A:6:LEU:HD13	1:A:94:ILE:HB	1.86	0.57
1:A:304:LEU:HB3	1:A:341:VAL:HG12	1.86	0.57
1:A:327:TYR:OH	1:A:359:ARG:NH1	2.37	0.57
1:A:350:ILE:HA	1:A:369:ASP:OD2	2.04	0.57
1:D:347:THR:HG22	1:D:349:SER:N	2.16	0.56
1:B:31:PRO:HA	1:B:61:PHE:CD2	2.39	0.56
1:A:307:ILE:HG12	1:A:344:HIS:HB2	1.86	0.56
1:B:333:ILE:HD13	1:B:343:GLN:HB3	1.87	0.56
1:B:207:PHE:CD1	1:B:244:ARG:HB2	2.40	0.56
1:D:6:LEU:HD23	1:D:94:ILE:HB	1.88	0.56
1:D:42:MET:HG2	2:Y:1:A:C2	2.40	0.56
1:C:330:GLN:HG3	1:C:363:PHE:CG	2.41	0.56
1:A:232:ILE:HG23	1:A:242:VAL:HG11	1.88	0.55
1:A:82:THR:HG22	1:A:111:PHE:CE1	2.41	0.55
1:C:98:THR:HG22	1:C:123:GLN:H	1.72	0.55
1:D:81:LEU:HB3	1:D:111:PHE:CD1	2.41	0.55
1:D:330:GLN:HG3	1:D:363:PHE:CD2	2.42	0.55
1:C:330:GLN:HG3	1:C:363:PHE:CD1	2.42	0.55
1:B:43:GLU:HG3	1:B:68:HIS:NE2	2.22	0.54
1:C:129:LEU:HD22	1:C:141:MET:HE2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:ILE:HD13	1:B:286:LYS:HB2	1.89	0.53
1:D:102:LYS:HD3	1:C:105:SER:CB	2.38	0.53
1:D:210:PHE:HB2	1:D:242:VAL:HG13	1.91	0.53
1:C:16:PRO:HG3	2:Y:4:A:C4	2.43	0.53
1:B:31:PRO:CA	1:B:61:PHE:CD2	2.91	0.53
1:D:207:PHE:CD2	1:D:244:ARG:HB3	2.43	0.53
1:B:343:GLN:N	1:B:343:GLN:OE1	2.42	0.53
1:D:16:PRO:HG3	2:Y:2:A:C4	2.44	0.53
1:C:7:VAL:HG13	1:C:95:VAL:HA	1.91	0.53
1:A:124:PRO:HG2	1:A:127:LYS:HB2	1.91	0.53
1:B:362:GLU:HG2	1:A:336:LYS:NZ	2.23	0.52
1:B:31:PRO:CG	1:B:61:PHE:HE2	2.22	0.52
1:A:313:VAL:HG21	1:A:322:LEU:HB2	1.92	0.52
1:D:105:SER:CB	1:C:102:LYS:HD3	2.39	0.52
1:D:262:VAL:HG21	1:D:309:CYS:SG	2.49	0.52
1:D:272:ASN:O	1:D:272:ASN:ND2	2.42	0.52
1:D:353:LYS:HB2	1:D:356:PRO:HD2	1.91	0.52
1:C:11:SER:HB3	1:C:100:GLY:H	1.75	0.52
1:D:43:GLU:HG3	1:D:68:HIS:NE2	2.25	0.52
1:D:304:LEU:HB3	1:D:341:VAL:HG12	1.92	0.52
1:D:11:SER:HB3	1:D:100:GLY:H	1.76	0.51
1:B:343:GLN:HG3	1:B:365:ILE:HG12	1.93	0.51
1:D:96:ASN:OD1	1:D:98:THR:OG1	2.27	0.51
1:A:6:LEU:HB2	1:A:34:ILE:HD13	1.92	0.50
1:B:31:PRO:HD3	1:B:61:PHE:CZ	2.45	0.50
1:B:61:PHE:HD2	1:B:61:PHE:O	1.94	0.50
1:A:323:ASN:OD1	1:A:359:ARG:NH1	2.45	0.50
1:D:323:ASN:OD1	1:D:359:ARG:NH1	2.40	0.50
1:B:172:LYS:O	1:B:173:THR:OG1	2.24	0.49
1:B:15:ILE:HD11	1:B:154:HIS:CE1	2.47	0.49
1:D:95:VAL:HB	1:D:120:ILE:HG23	1.94	0.49
1:D:207:PHE:HD2	1:D:244:ARG:HB3	1.77	0.49
1:D:120:ILE:HG13	1:D:133:TYR:HB3	1.94	0.49
1:D:334:LYS:HG2	1:C:334:LYS:HB3	1.95	0.49
1:C:9:LEU:O	1:C:99:GLY:HA3	2.12	0.49
1:C:282:VAL:HG21	1:C:296:ILE:HG12	1.94	0.49
1:B:15:ILE:H	1:B:15:ILE:HD12	1.78	0.48
1:C:369:ASP:OD1	1:C:371:THR:OG1	2.20	0.48
1:B:22:LYS:HE3	1:B:144:VAL:O	2.14	0.48
1:A:38:SER:OG	1:A:39:THR:N	2.46	0.48
1:D:330:GLN:HG3	1:D:363:PHE:CG	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ILE:HA	1:C:337:PHE:HD2	1.79	0.48
1:D:56:HIS:O	1:D:56:HIS:ND1	2.45	0.48
1:C:189:MET:HE2	1:C:231:MET:SD	2.53	0.48
1:D:145:LEU:H	1:D:302:ASN:HD21	1.62	0.48
1:C:5:ILE:HD12	1:C:33:LYS:HB3	1.96	0.48
1:B:121:PHE:CE1	1:B:131:GLU:HB3	2.48	0.48
1:C:57:PHE:HD2	1:C:62:VAL:HG21	1.79	0.47
1:C:166:LYS:HB3	1:C:170:TYR:HD1	1.78	0.47
1:C:175:TYR:HA	1:C:179:VAL:HB	1.95	0.47
1:B:105:SER:CB	1:A:102:LYS:HD3	2.45	0.47
1:A:32:MET:O	1:A:62:VAL:HA	2.14	0.47
1:D:168:TRP:O	1:D:172:LYS:HG3	2.15	0.47
1:C:38:SER:OG	1:C:39:THR:N	2.46	0.47
1:B:38:SER:OG	1:B:39:THR:N	2.48	0.47
1:B:61:PHE:CD2	1:B:61:PHE:O	2.68	0.47
1:B:168:TRP:O	1:B:172:LYS:HG2	2.14	0.47
1:B:282:VAL:HG11	1:B:296:ILE:HG12	1.96	0.47
1:C:6:LEU:CD2	1:C:94:ILE:HB	2.44	0.47
1:B:58:SER:HG	1:B:61:PHE:H	1.63	0.47
1:A:141:MET:HE3	1:A:144:VAL:HG21	1.97	0.47
1:A:183:ARG:NH1	1:A:314:ASP:OD2	2.33	0.47
1:A:308:GLU:HG3	1:A:310:LYS:HE2	1.97	0.46
1:C:114:ASN:HA	1:C:133:TYR:CZ	2.50	0.46
1:A:128:GLU:HB2	1:A:139:TYR:O	2.14	0.46
1:C:154:HIS:NE2	1:C:337:PHE:O	2.48	0.46
1:B:323:ASN:OD1	1:B:359:ARG:NH2	2.48	0.46
1:D:99:GLY:O	1:C:102:LYS:HE2	2.14	0.46
1:D:313:VAL:HG22	1:D:347:THR:HG21	1.97	0.46
1:D:109:PHE:CD2	1:C:106:LEU:HD11	2.50	0.46
1:D:346:TYR:CZ	1:D:368:LYS:HD2	2.50	0.46
1:A:346:TYR:CZ	1:A:368:LYS:HD2	2.50	0.46
1:D:144:VAL:HG23	1:D:145:LEU:HG	1.96	0.46
1:B:133:TYR:CD1	1:B:134:PRO:HA	2.51	0.46
1:B:362:GLU:OE2	1:A:286:LYS:HD2	2.15	0.46
1:A:328:LYS:O	1:A:332:ILE:HG12	2.15	0.46
1:C:95:VAL:HG21	1:C:112:PHE:CG	2.51	0.46
1:B:102:LYS:HD3	1:A:105:SER:CB	2.47	0.45
1:C:8:ASN:OD1	1:C:21:ILE:HD11	2.16	0.45
1:C:71:GLY:O	1:C:101:THR:HG21	2.16	0.45
1:C:272:ASN:O	1:C:272:ASN:ND2	2.49	0.45
1:B:62:VAL:O	1:B:62:VAL:HG13	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:PRO:HG3	2:X:2:A:C4	2.51	0.45
1:D:175:TYR:HA	1:D:179:VAL:HB	1.98	0.45
1:B:56:HIS:O	1:B:56:HIS:ND1	2.49	0.45
1:C:89:GLU:OE2	1:C:89:GLU:N	2.47	0.45
1:B:128:GLU:HB3	1:B:139:TYR:O	2.16	0.45
1:B:214:GLU:HB3	1:B:216:GLU:OE1	2.17	0.45
1:A:112:PHE:HA	1:A:115:LYS:HG3	1.99	0.45
1:D:102:LYS:HD3	1:C:105:SER:OG	2.17	0.45
1:B:11:SER:HB3	1:B:100:GLY:N	2.32	0.45
1:A:34:ILE:HG21	1:A:64:TRP:CZ3	2.52	0.45
1:D:282:VAL:HG21	1:D:296:ILE:HG12	1.99	0.45
1:C:125:ILE:HA	2:Y:4:A:N7	2.32	0.45
1:D:247:HIS:HD2	1:D:251:ARG:NE	2.11	0.44
1:C:120:ILE:HG12	1:C:133:TYR:HB3	2.00	0.44
1:C:124:PRO:HG2	1:C:127:LYS:HB2	1.98	0.44
1:C:165:VAL:HG12	1:C:166:LYS:HG2	1.99	0.44
1:B:235:LEU:HD13	1:B:245:ILE:HG13	1.99	0.44
1:B:161:ASP:C	1:B:163:GLU:H	2.20	0.43
1:B:48:SER:O	1:B:52:LYS:HG3	2.18	0.43
1:A:85:PHE:HD1	1:A:88:ASN:HD22	1.65	0.43
1:D:247:HIS:CD2	1:D:251:ARG:HE	2.29	0.43
1:C:5:ILE:HG22	1:C:93:ILE:HG22	2.00	0.43
1:B:233:LYS:O	1:B:237:ILE:HG13	2.18	0.43
1:B:175:TYR:HA	1:B:179:VAL:HB	2.00	0.43
1:D:247:HIS:CD2	1:D:251:ARG:NE	2.86	0.43
1:D:333:ILE:HG12	1:D:343:GLN:HG2	1.99	0.43
1:C:6:LEU:HD23	1:C:94:ILE:HB	2.00	0.43
1:C:16:PRO:HG3	2:Y:4:A:C5	2.53	0.43
1:B:266:ILE:HG23	1:B:273:VAL:HG11	2.00	0.43
1:D:102:LYS:HE2	1:C:99:GLY:O	2.19	0.43
1:C:333:ILE:HG12	1:C:343:GLN:HG2	2.01	0.43
1:D:352:GLU:O	1:D:353:LYS:HD3	2.19	0.42
1:C:316:ASN:OD1	1:C:317:GLU:N	2.52	0.42
1:D:6:LEU:CD2	1:D:94:ILE:HB	2.48	0.42
1:D:23:TRP:O	1:D:27:LYS:HG2	2.19	0.42
1:B:133:TYR:CG	1:B:134:PRO:HA	2.54	0.42
1:B:296:ILE:HG22	1:B:306:VAL:HA	2.01	0.42
1:A:309:CYS:O	1:A:310:LYS:HD2	2.19	0.42
1:A:210:PHE:HB2	1:A:242:VAL:HG12	2.02	0.42
1:B:93:ILE:HB	1:B:118:THR:HG22	2.01	0.42
1:B:148:LYS:HG3	1:B:158:TYR:OH	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:LYS:O	1:C:80:ILE:HG23	2.19	0.42
1:D:119:GLU:HG2	1:D:121:PHE:CE2	2.55	0.42
1:B:105:SER:HB2	1:A:102:LYS:HD3	2.02	0.42
1:D:145:LEU:HB2	1:D:302:ASN:ND2	2.35	0.42
1:B:47:LYS:O	1:B:51:ILE:HG13	2.20	0.41
1:D:85:PHE:HE2	1:D:112:PHE:CZ	2.38	0.41
1:A:5:ILE:HB	1:A:90:TYR:CD2	2.55	0.41
1:D:89:GLU:OE1	1:D:89:GLU:N	2.40	0.41
1:C:32:MET:O	1:C:62:VAL:HA	2.20	0.41
1:B:171:ASN:O	1:B:174:VAL:HG12	2.20	0.41
1:A:285:GLN:HA	1:A:289:ASP:O	2.20	0.41
1:C:47:LYS:HA	1:C:47:LYS:HD3	1.83	0.41
1:D:85:PHE:HE2	1:D:112:PHE:HZ	1.68	0.41
1:D:209:ASP:OD1	1:D:243:SER:HA	2.20	0.41
1:C:11:SER:HB2	2:Y:3:A:H1'	2.02	0.41
1:C:308:GLU:O	1:C:345:LEU:HD12	2.21	0.41
1:A:11:SER:OG	2:X:2:A:OP2	2.26	0.41
1:C:182:ASN:O	1:C:186:ILE:HG13	2.21	0.41
1:B:103:ILE:HD13	1:B:103:ILE:HA	1.90	0.41
1:D:24:TYR:CE2	1:D:28:LYS:HG3	2.57	0.40
1:C:93:ILE:HD11	1:C:118:THR:OG1	2.21	0.40
1:A:78:GLU:O	1:A:82:THR:HG23	2.22	0.40
1:D:38:SER:OG	1:D:39:THR:N	2.54	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	370/382 (97%)	359 (97%)	11 (3%)	0	100	100
1	B	370/382 (97%)	362 (98%)	8 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	370/382 (97%)	364 (98%)	6 (2%)	0	100	100
1	D	370/382 (97%)	361 (98%)	9 (2%)	0	100	100
All	All	1480/1528 (97%)	1446 (98%)	34 (2%)	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	344/352 (98%)	334 (97%)	10 (3%)	42	76
1	B	344/352 (98%)	340 (99%)	4 (1%)	71	90
1	C	344/352 (98%)	337 (98%)	7 (2%)	55	83
1	D	344/352 (98%)	335 (97%)	9 (3%)	46	78
All	All	1376/1408 (98%)	1346 (98%)	30 (2%)	52	81

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	56	HIS
1	B	61	PHE
1	B	132	LEU
1	B	340	TYR
1	A	29	GLN
1	A	101	THR
1	A	144	VAL
1	A	151	LEU
1	A	242	VAL
1	A	282	VAL
1	A	323	ASN
1	A	339	LEU
1	A	340	TYR
1	A	352	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	82	THR
1	D	98	THR
1	D	120	ILE
1	D	151	LEU
1	D	157	SER
1	D	185	LEU
1	D	272	ASN
1	D	319	ASN
1	D	340	TYR
1	C	58	SER
1	C	60	SER
1	C	132	LEU
1	C	272	ASN
1	C	339	LEU
1	C	340	TYR
1	C	373	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	GLN
1	B	281	ASN
1	B	330	GLN
1	A	26	ASN
1	D	247	HIS
1	D	272	ASN
1	D	330	GLN
1	C	272	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	X	3/4 (75%)	3 (100%)	0
2	Y	3/4 (75%)	3 (100%)	1 (33%)
All	All	6/8 (75%)	6 (100%)	1 (16%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	Y	2	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Y	3	A
2	Y	4	A
2	X	2	A
2	X	3	A
2	X	4	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	Y	3	A

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 monosaccharides 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 (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, 95^{th} 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	372/382 (97%)	-0.24	3 (0%) 86 65	49, 74, 102, 137	0
1	B	372/382 (97%)	-0.21	2 (0%) 91 75	50, 72, 106, 128	0
1	C	372/382 (97%)	-0.18	4 (1%) 80 56	45, 80, 106, 142	0
1	D	372/382 (97%)	-0.15	4 (1%) 80 56	52, 76, 102, 123	0
2	X	4/4 (100%)	0.32	0 100 100	52, 52, 52, 52	0
2	Y	4/4 (100%)	0.34	0 100 100	52, 52, 52, 52	0
All	All	1496/1536 (97%)	-0.19	13 (0%) 84 63	45, 75, 104, 142	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	ASP	3.8
1	C	271	HIS	3.6
1	C	3	GLU	3.0
1	B	204	ARG	2.9
1	D	317	GLU	2.8
1	D	316	ASN	2.6
1	C	316	ASN	2.5
1	A	316	ASN	2.5
1	B	316	ASN	2.5
1	D	372	GLN	2.4
1	C	88	ASN	2.2
1	D	137	GLN	2.2
1	A	271	HIS	2.1

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

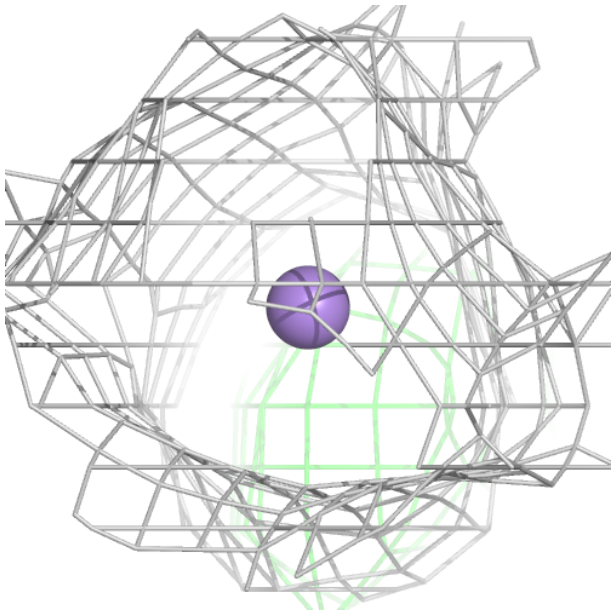
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

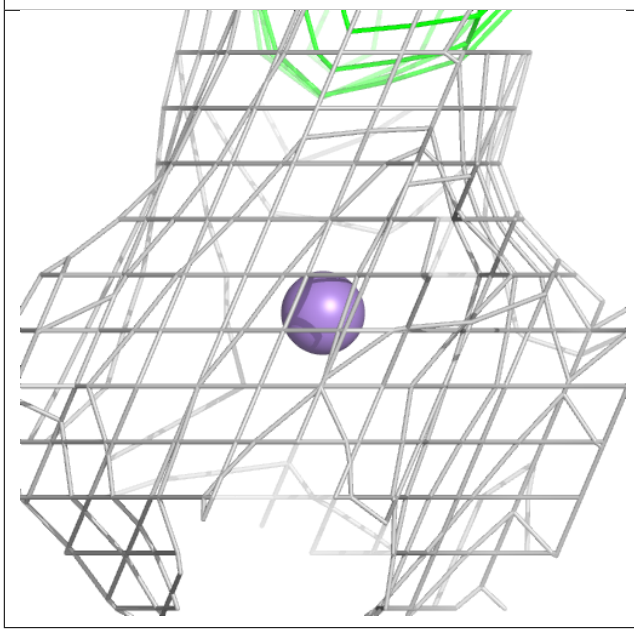
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MN	B	901	1/1	0.63	0.30	123,123,123,123	0
3	MN	C	901	1/1	0.65	0.65	135,135,135,135	0
3	MN	A	901	1/1	0.74	0.44	124,124,124,124	0
3	MN	D	901	1/1	0.75	0.40	110,110,110,110	0

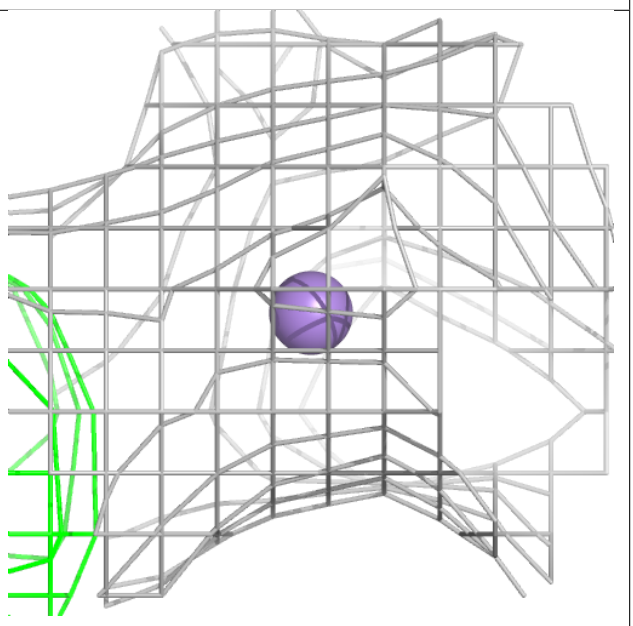
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MN B 901:

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

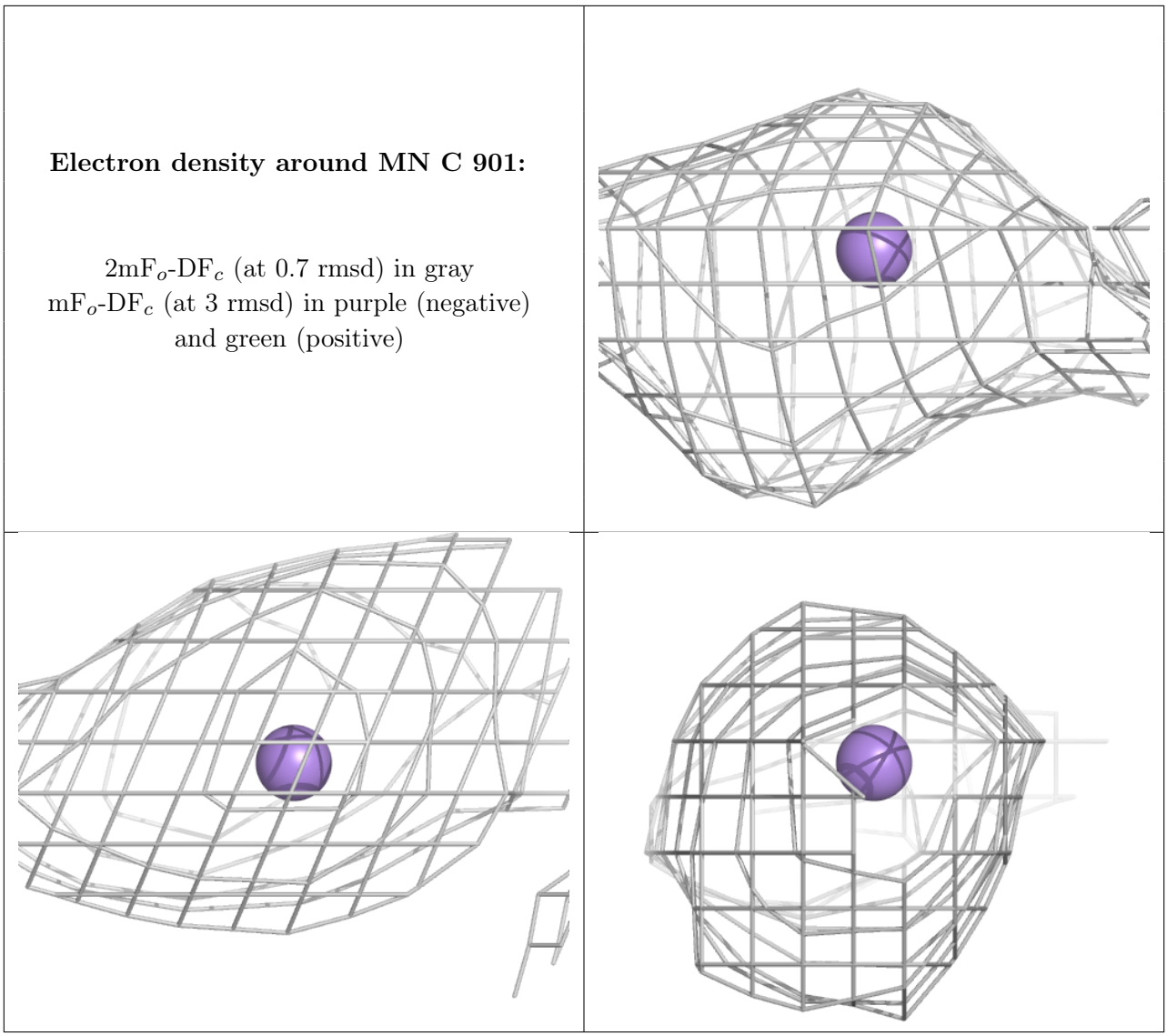






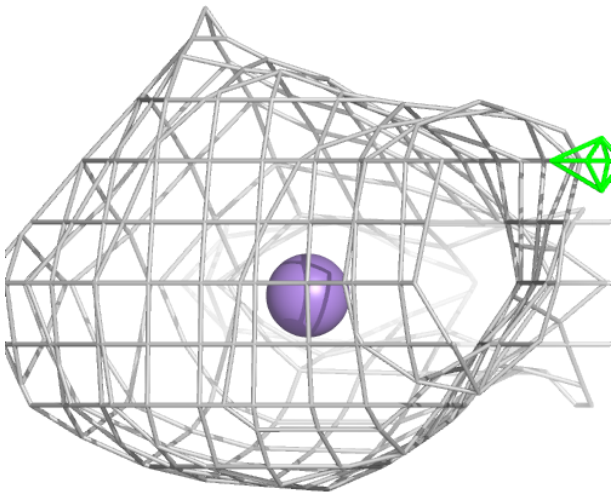
Electron density around MN C 901:

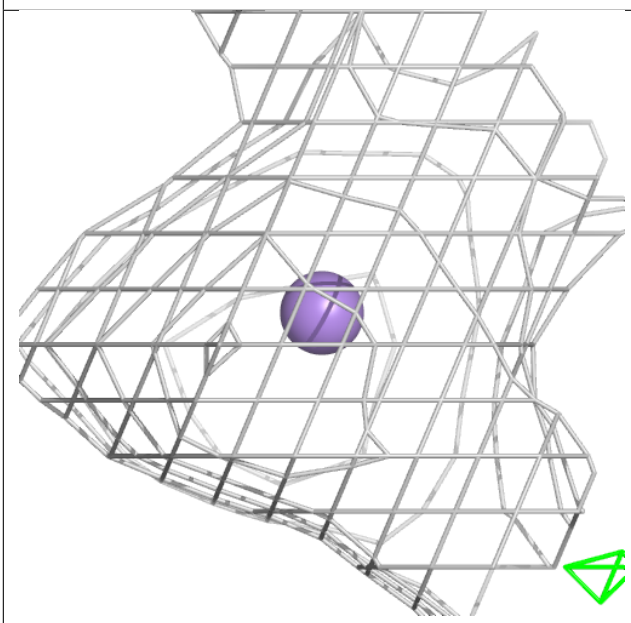
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

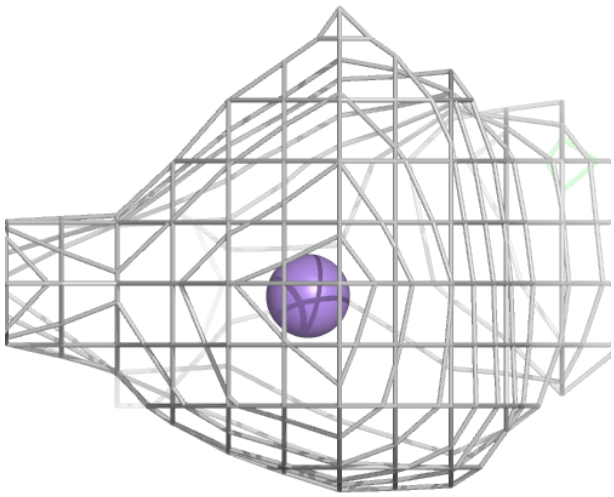


Electron density around MN A 901:

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

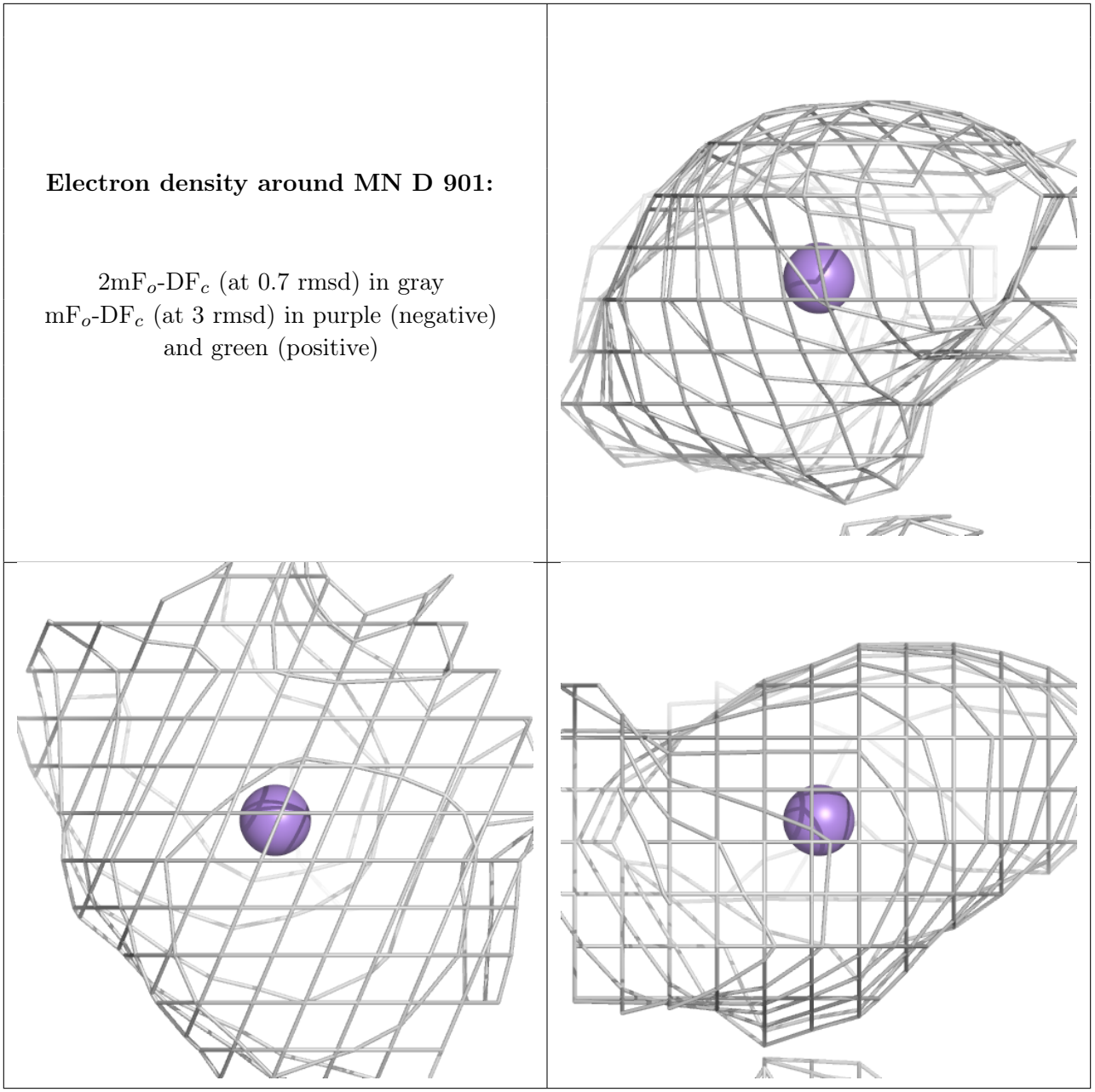






Electron density around MN D 901:

$2mF_o$-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 (i)

There are no such residues in this entry.