WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jan 14, 2024 – 09:29 am GMT

PDB ID	:	6SNA
Title	:	Crystal structure of Antirestriction ArdC protein from R388 plasmid. Mn(II)-bound structure.
Authors	:	Gonzalez-Montes, L.; Moncalian, G.
Deposited on	:	2019-08-23
Resolution	:	2.70 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

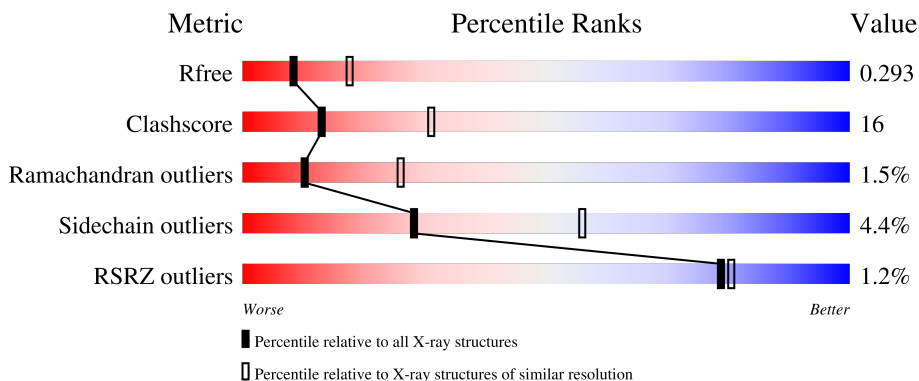|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	Percentile Ranks	Value
Rfree		0.293
Clashscore		16
Ramachandran outliers		1.5%
Sidechain outliers		4.4%
RSRZ outliers		1.2%

Worse ▬ *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	305	63% / 21% / • / 13%
1	B	305	62% / 23% / • / 13%
1	F	305	3% / 46% / 30% / • / 22%
1	G	305	67% / 17% / • / 13%
1	J	305	% / 46% / 30% / • / 22%

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Mol	Chain	Length	Quality of chain
1	K	305	62% 24% 13%
1	N	305	2% 45% 30% 22%
1	X	305	% 51% 26% 22%

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 16349 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 ArdC protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2118	1351	369	392	6			
1	B	265	Total	C	N	O	S	0	0	0
			2118	1351	369	392	6			
1	F	237	Total	C	N	O	S	0	0	0
			1885	1204	327	348	6			
1	G	265	Total	C	N	O	S	0	0	0
			2118	1351	369	392	6			
1	J	237	Total	C	N	O	S	0	0	0
			1885	1204	327	348	6			
1	K	265	Total	C	N	O	S	0	0	0
			2118	1351	369	392	6			
1	N	237	Total	C	N	O	S	0	0	0
			1885	1204	327	348	6			
1	X	237	Total	C	N	O	S	0	0	0
			1885	1204	327	348	6			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	LEU	-	expression tag	UNP Q6I6B2
A	299	GLU	-	expression tag	UNP Q6I6B2
A	300	HIS	-	expression tag	UNP Q6I6B2
A	301	HIS	-	expression tag	UNP Q6I6B2
A	302	HIS	-	expression tag	UNP Q6I6B2
A	303	HIS	-	expression tag	UNP Q6I6B2
A	304	HIS	-	expression tag	UNP Q6I6B2
A	305	HIS	-	expression tag	UNP Q6I6B2
B	298	LEU	-	expression tag	UNP Q6I6B2
B	299	GLU	-	expression tag	UNP Q6I6B2
B	300	HIS	-	expression tag	UNP Q6I6B2
B	301	HIS	-	expression tag	UNP Q6I6B2
B	302	HIS	-	expression tag	UNP Q6I6B2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	303	HIS	-	expression tag	UNP Q6I6B2
B	304	HIS	-	expression tag	UNP Q6I6B2
B	305	HIS	-	expression tag	UNP Q6I6B2
F	298	LEU	-	expression tag	UNP Q6I6B2
F	299	GLU	-	expression tag	UNP Q6I6B2
F	300	HIS	-	expression tag	UNP Q6I6B2
F	301	HIS	-	expression tag	UNP Q6I6B2
F	302	HIS	-	expression tag	UNP Q6I6B2
F	303	HIS	-	expression tag	UNP Q6I6B2
F	304	HIS	-	expression tag	UNP Q6I6B2
F	305	HIS	-	expression tag	UNP Q6I6B2
G	298	LEU	-	expression tag	UNP Q6I6B2
G	299	GLU	-	expression tag	UNP Q6I6B2
G	300	HIS	-	expression tag	UNP Q6I6B2
G	301	HIS	-	expression tag	UNP Q6I6B2
G	302	HIS	-	expression tag	UNP Q6I6B2
G	303	HIS	-	expression tag	UNP Q6I6B2
G	304	HIS	-	expression tag	UNP Q6I6B2
G	305	HIS	-	expression tag	UNP Q6I6B2
J	298	LEU	-	expression tag	UNP Q6I6B2
J	299	GLU	-	expression tag	UNP Q6I6B2
J	300	HIS	-	expression tag	UNP Q6I6B2
J	301	HIS	-	expression tag	UNP Q6I6B2
J	302	HIS	-	expression tag	UNP Q6I6B2
J	303	HIS	-	expression tag	UNP Q6I6B2
J	304	HIS	-	expression tag	UNP Q6I6B2
J	305	HIS	-	expression tag	UNP Q6I6B2
K	298	LEU	-	expression tag	UNP Q6I6B2
K	299	GLU	-	expression tag	UNP Q6I6B2
K	300	HIS	-	expression tag	UNP Q6I6B2
K	301	HIS	-	expression tag	UNP Q6I6B2
K	302	HIS	-	expression tag	UNP Q6I6B2
K	303	HIS	-	expression tag	UNP Q6I6B2
K	304	HIS	-	expression tag	UNP Q6I6B2
K	305	HIS	-	expression tag	UNP Q6I6B2
N	298	LEU	-	expression tag	UNP Q6I6B2
N	299	GLU	-	expression tag	UNP Q6I6B2
N	300	HIS	-	expression tag	UNP Q6I6B2
N	301	HIS	-	expression tag	UNP Q6I6B2
N	302	HIS	-	expression tag	UNP Q6I6B2
N	303	HIS	-	expression tag	UNP Q6I6B2
N	304	HIS	-	expression tag	UNP Q6I6B2

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Chain	Residue	Modelled	Actual	Comment	Reference
N	305	HIS	-	expression tag	UNP Q6I6B2
X	298	LEU	-	expression tag	UNP Q6I6B2
X	299	GLU	-	expression tag	UNP Q6I6B2
X	300	HIS	-	expression tag	UNP Q6I6B2
X	301	HIS	-	expression tag	UNP Q6I6B2
X	302	HIS	-	expression tag	UNP Q6I6B2
X	303	HIS	-	expression tag	UNP Q6I6B2
X	304	HIS	-	expression tag	UNP Q6I6B2
X	305	HIS	-	expression tag	UNP Q6I6B2

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	F	1	Total 1	Mn 1	0	0
2	G	1	Total 1	Mn 1	0	0
2	J	1	Total 1	Mn 1	0	0
2	K	1	Total 1	Mn 1	0	0
2	N	1	Total 1	Mn 1	0	0
2	X	1	Total 1	Mn 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total 61	O 61	0	0
3	B	47	Total 47	O 47	0	0
3	F	21	Total 21	O 21	0	0
3	G	54	Total 54	O 54	0	0

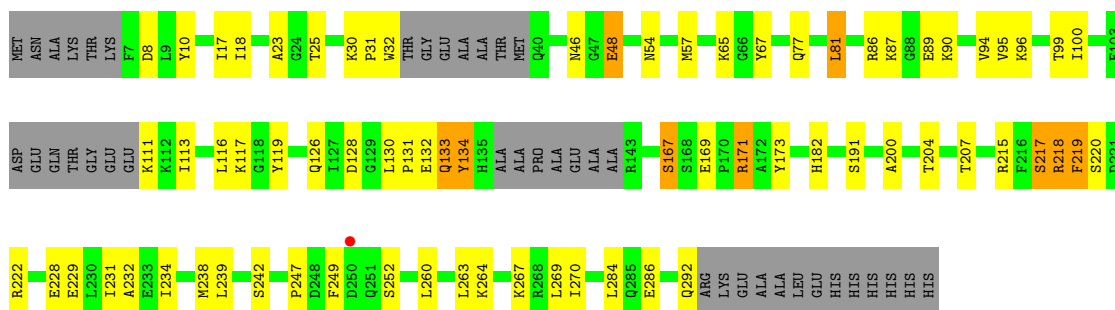*Continued on next page...*

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	28	Total 28	O 28	0	0
3	K	46	Total 46	O 46	0	0
3	N	26	Total 26	O 26	0	0
3	X	46	Total 46	O 46	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.
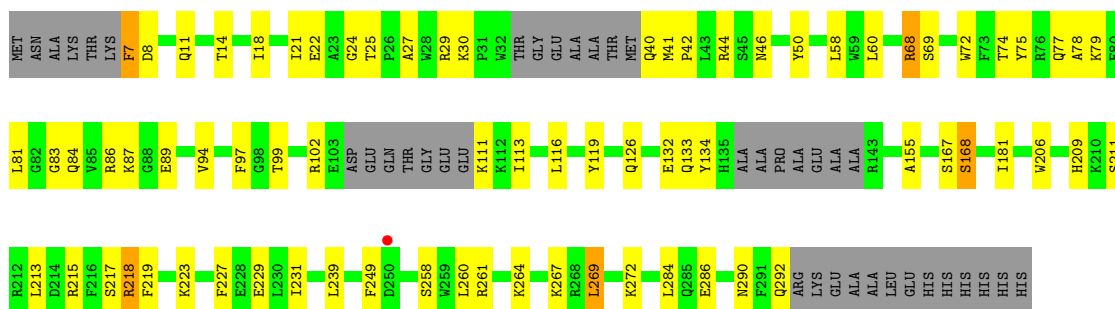
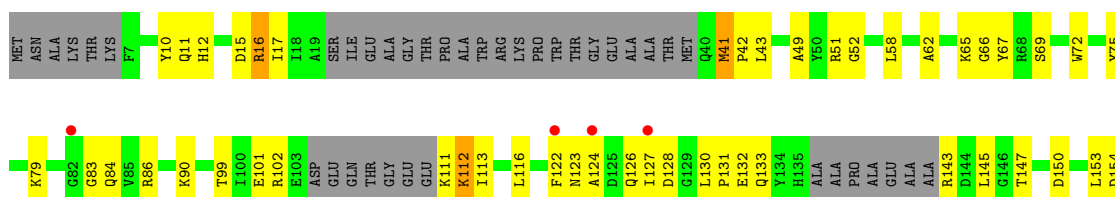- Molecule 1: ArdC protein
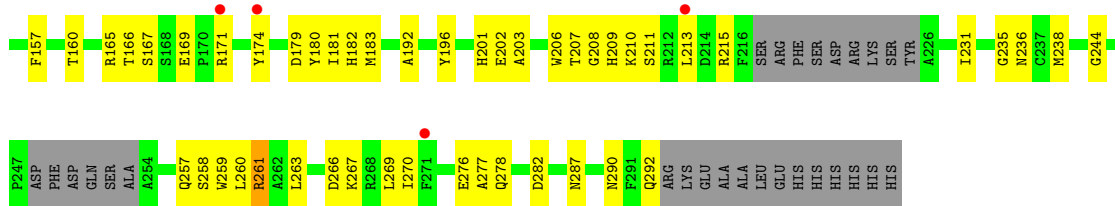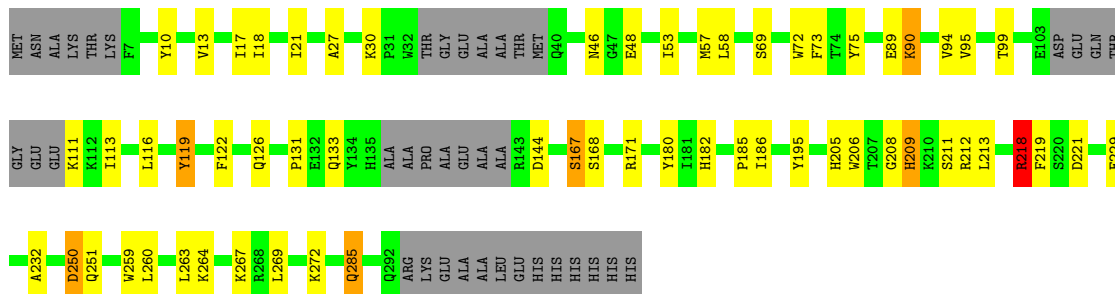
Chain A:

- Molecule 1: ArdC protein
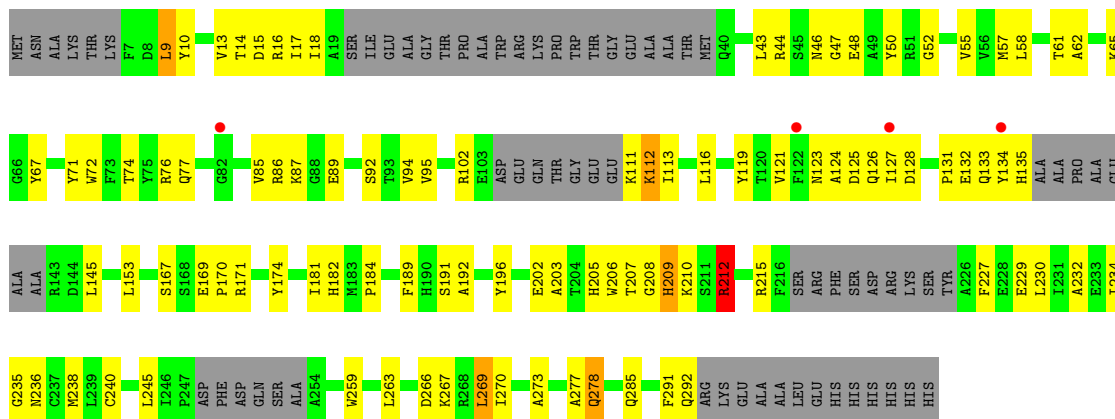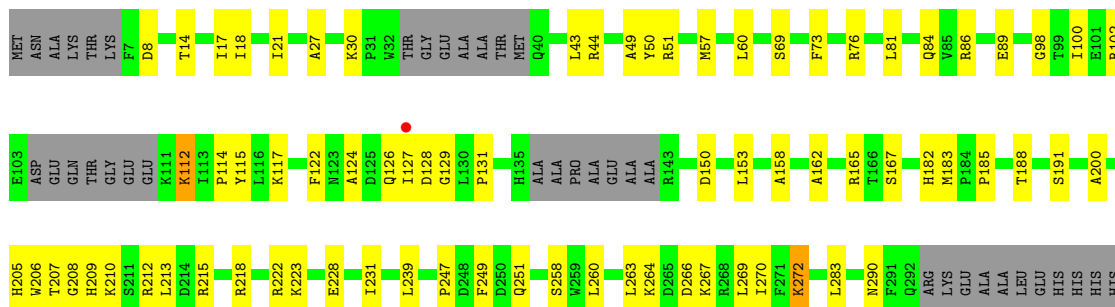
Chain B:

- Molecule 1: ArdC protein

Chain F:

F157 T160 R165 T166 S167 S168 E169 P170 R171 Y174 D179 Y180 I181 H182 M183 A192 Y196 H201 E202 A203 W206 T207 G208 H209 K210 S211 R212 L213 D214 R215 F216 SER ARG PHE SER ASP LYS SER TYR A226 I231 G235 N236 C237 M238 G244

P247 ASP PHE GLN SER ALA A254 Q257 S258 W259 L260 R261 A262 L263 D266 K267 R268 L269 I270 F271 E276 A277 Q278 D282 N287 N290 F291 Q292 ARG LYS GLU ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: ArdC protein

Chain G: 67% 17% • 13%

MET ASN ALA LYS THR LYS F7 Y10 V13 I17 I18 I21 A27 K30 P31 W32 THR GLY GLU ALA ALA THR MET Q40 N46 G47 E48 I53 M57 L58 S69 W72 T73 T74 Y75 E89 K90 V94 V95 T99 E103 ASP GLU GLN THR

GLY GLU GLU K111 K112 I113 L116 Y119 F122 Q126 P131 E132 Q133 Y134 H135 ALA ALA PRO ALA GLU ALA ALA R143 D144 S167 S168 R171 Y180 I181 H182 P185 I186 Y195 H205 W206 T207 G208 H209 K210 S211 R212 L213 H218 F219 S220 D221 E229

A232 D250 Q251 W259 L260 L263 K264 K267 R268 L269 K272 Q285 Q292 ARG LYS GLU ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: ArdC protein

Chain J: .% 46% 30% • 22%

MET ASN ALA THR LYS F7 D8 L9 Y10 V13 T14 D15 R16 I17 I18 A19 SER ILE GLU ALA GLY THR PRO ALA TRP ARG LYS PRO TRP THR THR GLY GLU ALA ALA THR MET Q40 L43 R44 S45 N46 G47 E48 A49 Y50 R51 G52 V55 V56 M57 L58 T61 A62 K65

G66 Y67 V71 W72 F73 T74 Y75 R76 Q77 G82 V85 R86 K87 G88 E89 S92 T93 V94 V95 R102 E103 ASP GLU GLN THR GLY GLU K111 K112 I113 L116 Y119 T120 V121 F122 N123 A124 D125 Q126 I127 D128 P131 E132 Q133 Y134 H135 ALA PRO ALA GLU

ALA ALA R143 D144 L145 L153 S167 S168 E169 P170 R171 Y174 I181 H182 M183 P184 F189 H190 S191 A192 Y196 E202 A203 T204 H205 W206 T207 G208 H209 K210 S211 R212 R215 F216 SER ARG PHE SER ASP ARG LYS SER TYR A226 F227 E228 E229 L230 I231 A232 E233 I234

G235 N236 C237 M238 L239 C240 L245 T246 P247 ASP PHE GLN SER ALA A254 W259 L263 D266 K267 R268 I269 I270 A273 A277 Q278 Q285 F291 Q292 ARG LYS GLU ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

• Molecule 1: ArdC protein

Chain K: 62% 24% • 13%

MET ASN ALA LYS THR LYS F7 D8 T14 I17 I18 I21 A27 K30 P31 W32 THR GLY GLU ALA ALA THR MET Q40 L43 R44 A49 Y50 R51 M57 L60 S69 F73 R76 L81 Q84 V85 R86 E89 G98 T99 I100 E101 R102

E103 ASP GLU GLN THR GLY GLU GLU K111 K112 I113 P114 Y115 L116 K117 F122 N123 A124 D125 Q126 I127 D128 G129 L130 P131 H135 ALA ALA PRO ALA GLU ALA ALA R143 D150 L153 A158 A162 R165 T166 S167 H182 M183 P184 P185 T188 S191 A200

H205 W206 T207 G208 H209 K210 S211 R212 L213 D214 R215 R218 R222 K223 E228 I231 L239 P247 D248 F249 D250 Q251 S258 W259 L260 L263 K264 D265 D266 K267 R268 L269 I270 F271 K272 L283 N290 F291 Q292 ARG LYS GLU ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS
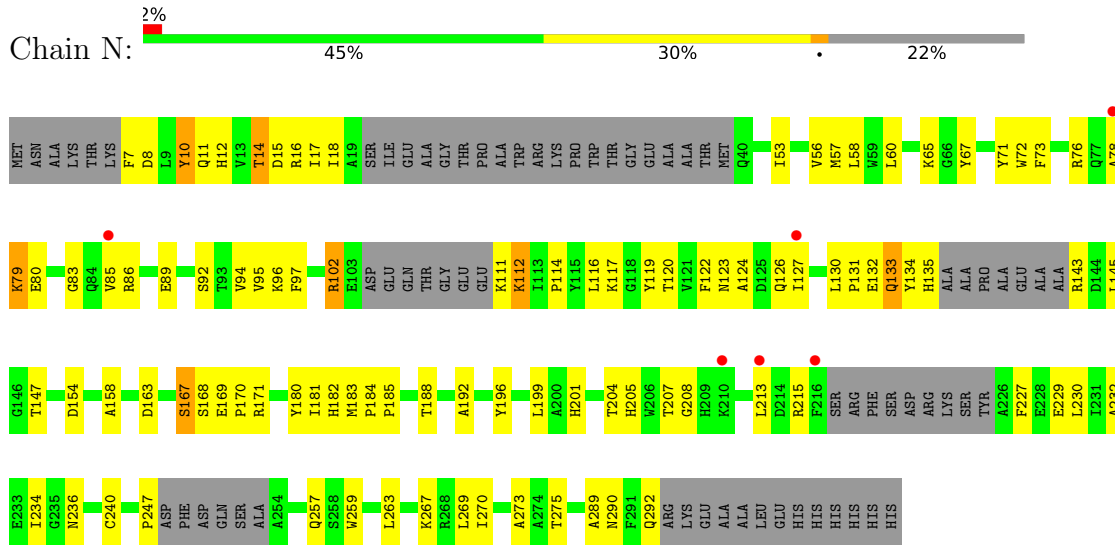
HIS
HIS

● Molecule 1: ArdC protein

Chain N:

● Molecule 1: ArdC protein

Chain X:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	116.50Å　　116.50Å　　162.12Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	54.82　–　2.70 54.82　–　2.70	Depositor EDS
% Data completeness (in resolution range)	95.5 (54.82-2.70) 96.6 (54.82-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.222　,　0.294 0.220　,　0.293	Depositor DCC
R_{free} test set	3008 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.9	EDS
L-test for twinning[2]	$< |L| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.047 for -h,-k,l 0.467 for h,-h-k,-l 0.047 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16349	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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 27.79 % 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 2.0662e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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	0.61	0/2172	0.70	0/2938
1	B	0.54	0/2172	0.69	0/2938
1	F	0.50	0/1928	0.62	0/2604
1	G	0.54	0/2172	0.66	0/2938
1	J	0.49	0/1928	0.63	0/2604
1	K	0.54	0/2172	0.67	0/2938
1	N	0.50	0/1928	0.65	0/2604
1	X	0.49	0/1928	0.64	0/2604
All	All	0.53	0/16400	0.66	0/22168

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 ⓘ

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	2118	0	2043	55	0
1	B	2118	0	2043	55	0
1	F	1885	0	1828	78	0
1	G	2118	0	2043	47	0
1	J	1885	0	1828	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	2118	0	2043	53	0
1	N	1885	0	1828	96	0
1	X	1885	0	1828	72	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	N	1	0	0	0	0
2	X	1	0	0	0	0
3	A	61	0	0	0	0
3	B	47	0	0	2	0
3	F	21	0	0	0	0
3	G	54	0	0	0	0
3	J	28	0	0	0	0
3	K	46	0	0	0	0
3	N	26	0	0	0	0
3	X	46	0	0	3	0
All	All	16349	0	15484	518	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 16.

All (518) 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:N:111:LYS:O	1:N:112:LYS:HG3	1.17	1.27
1:N:85:VAL:CA	1:N:127:ILE:HG22	1.68	1.24
1:N:67:TYR:HB3	1:N:123:ASN:ND2	1.54	1.22
1:N:85:VAL:HA	1:N:127:ILE:HG22	1.12	1.08
1:N:85:VAL:CB	1:N:127:ILE:HG22	1.82	1.07
1:N:111:LYS:O	1:N:112:LYS:CG	2.09	1.01
1:N:85:VAL:HB	1:N:127:ILE:CG2	1.95	0.96
1:N:78:ALA:HB1	1:N:127:ILE:CD1	1.96	0.96
1:N:85:VAL:CB	1:N:127:ILE:CG2	2.43	0.95
1:N:85:VAL:HA	1:N:127:ILE:CG2	1.97	0.94
1:J:95:VAL:HG13	1:J:116:LEU:HD11	1.54	0.88
1:A:25:THR:HB	1:A:30:LYS:HE2	1.57	0.86
1:G:27:ALA:O	1:G:30:LYS:HG2	1.77	0.85
1:N:67:TYR:HB3	1:N:123:ASN:HD22	1.36	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:181:ILE:HD11	1:F:206:TRP:HB2	1.59	0.84
1:N:67:TYR:CB	1:N:123:ASN:ND2	2.40	0.84
1:G:99:THR:HG1	1:G:111:LYS:N	1.76	0.83
1:J:112:LYS:HB3	1:J:113:ILE:HD12	1.60	0.83
1:N:85:VAL:CA	1:N:127:ILE:CG2	2.55	0.81
1:K:215:ARG:HD2	1:K:231:ILE:HD13	1.64	0.80
1:X:258:SER:HA	1:X:261:ARG:HE	1.48	0.77
1:A:17:ILE:HD12	1:A:270:ILE:HG12	1.67	0.77
1:X:127:ILE:HB	1:X:130:LEU:HD11	1.66	0.76
1:B:8:ASP:HB3	1:B:11:GLN:HB2	1.68	0.76
1:N:85:VAL:HB	1:N:127:ILE:HG21	1.66	0.76
1:N:78:ALA:CB	1:N:127:ILE:CD1	2.64	0.75
1:X:79:LYS:HE3	1:X:84:GLN:HA	1.69	0.75
1:G:17:ILE:N	1:G:17:ILE:HD12	2.03	0.74
1:G:89:GLU:HB3	1:G:126:GLN:HE21	1.52	0.73
1:X:112:LYS:HB3	1:X:113:ILE:HD12	1.68	0.73
1:N:86:ARG:HB2	1:N:89:GLU:HG3	1.70	0.73
1:J:10:TYR:HB2	1:J:267:LYS:HD2	1.69	0.72
1:J:86:ARG:HB3	1:J:89:GLU:HG3	1.71	0.72
1:N:259:TRP:O	1:N:263:LEU:N	2.21	0.72
1:N:67:TYR:CB	1:N:123:ASN:HD22	2.02	0.72
1:N:67:TYR:HB3	1:N:123:ASN:HD21	1.50	0.71
1:A:169:GLU:OE1	1:A:171:ARG:NH1	2.23	0.71
1:F:123:ASN:OD1	1:F:124:ALA:N	2.22	0.71
1:A:200:ALA:HB1	1:A:239:LEU:HD23	1.73	0.71
1:B:239:LEU:HD22	1:B:284:LEU:HD23	1.73	0.71
1:N:201:HIS:NE2	1:N:229:GLU:OE2	2.23	0.71
1:J:145:LEU:HB3	1:J:192:ALA:HB3	1.72	0.70
1:J:67:TYR:OH	1:J:126:GLN:NE2	2.24	0.70
1:N:85:VAL:HG23	1:N:127:ILE:CG2	2.21	0.69
1:N:78:ALA:CB	1:N:127:ILE:HD13	2.21	0.69
1:F:65:LYS:NZ	1:F:126:GLN:OE1	2.25	0.69
1:N:85:VAL:CG2	1:N:127:ILE:HG22	2.23	0.69
1:K:266:ASP:HB3	1:K:269:LEU:HB2	1.75	0.69
1:F:65:LYS:NZ	1:F:90:LYS:O	2.25	0.68
1:J:95:VAL:CG1	1:J:116:LEU:HD11	2.23	0.68
1:G:218:ARG:HH11	1:G:218:ARG:HG2	1.58	0.68
1:F:209:HIS:ND1	1:F:211:SER:OG	2.24	0.68
1:F:10:TYR:HB2	1:F:267:LYS:HE3	1.75	0.68
1:N:78:ALA:HB1	1:N:127:ILE:HD12	1.75	0.67
1:K:115:TYR:OH	1:K:117:LYS:HE2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:75:TYR:CE1	1:X:79:LYS:HD3	2.29	0.67
1:F:17:ILE:HD12	1:F:270:ILE:HG12	1.77	0.67
1:J:62:ALA:O	1:J:67:TYR:N	2.28	0.67
1:J:17:ILE:HD13	1:J:270:ILE:HG12	1.76	0.66
1:G:13:VAL:O	1:G:17:ILE:CD1	2.43	0.66
1:G:131:PRO:HB2	1:G:133:GLN:HG3	1.77	0.66
1:N:85:VAL:CG2	1:N:127:ILE:CG2	2.73	0.65
1:J:266:ASP:OD2	1:J:269:LEU:HB2	1.97	0.65
1:N:132:GLU:O	1:N:134:TYR:N	2.29	0.65
1:A:133:GLN:O	1:A:133:GLN:HG3	1.97	0.65
1:F:266:ASP:HB3	1:F:269:LEU:HB2	1.78	0.65
1:X:281:ALA:O	1:X:285:GLN:HG3	1.97	0.65
1:B:8:ASP:OD2	1:B:267:LYS:NZ	2.27	0.65
1:B:86:ARG:HG2	1:B:126:GLN:O	1.96	0.64
1:G:209:HIS:ND1	1:G:211:SER:OG	2.29	0.64
1:K:86:ARG:NH2	1:K:89:GLU:OE2	2.31	0.64
1:N:183:MET:SD	1:N:199:LEU:HD13	2.37	0.64
1:B:89:GLU:OE2	1:B:126:GLN:NE2	2.27	0.64
1:X:235:GLY:HA2	1:X:238:MET:HE2	1.79	0.64
1:X:238:MET:HE1	1:X:277:ALA:C	2.18	0.64
1:F:143:ARG:HD2	1:F:244:GLY:O	1.98	0.63
1:G:17:ILE:HD12	1:G:17:ILE:H	1.63	0.63
1:J:62:ALA:HA	1:J:67:TYR:CD2	2.34	0.63
1:J:259:TRP:O	1:J:263:LEU:N	2.31	0.63
1:K:98:GLY:HA3	1:K:117:LYS:HE3	1.80	0.63
1:A:292:GLN:HG2	1:X:116:LEU:HD22	1.80	0.62
1:F:65:LYS:HB2	1:F:67:TYR:CE2	2.34	0.62
1:N:85:VAL:HG23	1:N:127:ILE:HG23	1.79	0.62
1:X:207:THR:HG22	1:X:283:LEU:HD23	1.82	0.62
1:B:27:ALA:HA	1:B:30:LYS:HD3	1.81	0.62
1:B:25:THR:O	1:B:30:LYS:HE2	1.99	0.62
1:B:25:THR:HG23	1:B:30:LYS:NZ	2.14	0.62
1:G:208:GLY:HA2	1:G:213:LEU:HB2	1.82	0.62
1:J:85:VAL:HA	1:J:127:ILE:HG12	1.82	0.62
1:X:13:VAL:HG11	1:X:271:PHE:HZ	1.65	0.62
1:A:234:ILE:O	1:A:238:MET:HG3	2.01	0.61
1:J:62:ALA:HA	1:J:67:TYR:HD2	1.65	0.61
1:J:202:GLU:O	1:J:206:TRP:N	2.34	0.61
1:J:86:ARG:HG2	1:J:89:GLU:HG2	1.83	0.61
1:N:132:GLU:C	1:N:134:TYR:H	2.03	0.61
1:J:58:LEU:HD23	1:J:72:TRP:CD2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:258:SER:HA	1:F:261:ARG:HB3	1.82	0.61
1:N:8:ASP:HB3	1:N:11:GLN:HB3	1.82	0.61
1:F:160:THR:HA	1:F:287:ASN:HB3	1.83	0.61
1:F:62:ALA:HA	1:F:67:TYR:HD2	1.65	0.60
1:G:89:GLU:HB3	1:G:126:GLN:NE2	2.16	0.60
1:J:94:VAL:HG23	1:J:119:TYR:CE1	2.37	0.60
1:B:290:ASN:HB3	1:B:292:GLN:OE1	2.02	0.60
1:A:8:ASP:OD2	1:A:267:LYS:NZ	2.31	0.60
1:J:86:ARG:NH2	1:J:128:ASP:OD1	2.34	0.60
1:J:291:PHE:O	1:J:292:GLN:HG3	2.01	0.59
1:A:17:ILE:HD11	1:A:57:MET:CE	2.32	0.59
1:A:18:ILE:HD13	1:A:264:LYS:HG3	1.84	0.59
1:A:95:VAL:HG13	1:A:116:LEU:HD11	1.85	0.59
1:A:218:ARG:NH1	1:A:219:PHE:H	2.00	0.59
1:K:200:ALA:HB1	1:K:239:LEU:HD23	1.83	0.59
1:X:14:THR:HG21	1:X:267:LYS:HA	1.84	0.59
1:A:46:ASN:HD21	1:A:48:GLU:HB2	1.68	0.59
1:B:209:HIS:ND1	1:B:211:SER:OG	2.29	0.59
1:N:56:VAL:O	1:N:60:LEU:HG	2.03	0.59
1:F:86:ARG:NH2	1:F:128:ASP:OD2	2.36	0.59
1:X:175:ASN:O	1:X:179:ASP:N	2.34	0.59
1:N:17:ILE:HD12	1:N:270:ILE:HG12	1.85	0.58
1:X:167:SER:O	1:X:185:PRO:HD3	2.02	0.58
1:B:79:LYS:HG2	1:B:84:GLN:HA	1.84	0.58
1:K:21:ILE:HG21	1:K:260:LEU:HG	1.85	0.58
1:K:124:ALA:HA	1:K:127:ILE:HD12	1.86	0.58
1:F:201:HIS:HB2	1:F:236:ASN:HD21	1.69	0.58
1:G:90:LYS:HD3	1:G:90:LYS:H	1.67	0.58
1:J:230:LEU:O	1:J:234:ILE:HG13	2.03	0.58
1:J:263:LEU:HD11	1:J:270:ILE:HD13	1.86	0.58
1:K:206:TRP:O	1:K:212:ARG:NH2	2.22	0.58
1:J:240:CYS:HB3	1:J:245:LEU:HB2	1.86	0.58
1:X:13:VAL:HG11	1:X:271:PHE:CZ	2.38	0.58
1:X:258:SER:HA	1:X:261:ARG:NE	2.19	0.58
1:K:115:TYR:CZ	1:K:117:LYS:HE2	2.38	0.58
1:J:266:ASP:CG	1:J:269:LEU:HB2	2.25	0.57
1:X:10:TYR:HB2	1:X:267:LYS:HD2	1.85	0.57
1:B:99:THR:HG23	3:B:513:HOH:O	2.03	0.57
1:F:102:ARG:HB2	1:F:113:ILE:HD13	1.85	0.57
1:N:208:GLY:H	1:N:213:LEU:HB2	1.69	0.57
1:B:58:LEU:HD22	1:B:72:TRP:CD2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:17:ILE:CD1	1:K:270:ILE:HG12	2.34	0.57
1:G:46:ASN:OD1	1:G:48:GLU:HB2	2.04	0.57
1:J:74:THR:H	1:J:77:GLN:HE21	1.52	0.57
1:A:286:GLU:HG3	1:X:282:ASP:OD2	2.04	0.57
1:A:239:LEU:HD22	1:A:284:LEU:HD23	1.85	0.57
1:B:18:ILE:O	1:B:22:GLU:HG3	2.05	0.56
1:B:77:GLN:O	1:B:81:LEU:HD23	2.05	0.56
1:A:77:GLN:O	1:A:81:LEU:HB2	2.06	0.56
1:F:112:LYS:HB3	1:F:113:ILE:HD12	1.86	0.56
1:J:181:ILE:HD11	1:J:206:TRP:HB2	1.87	0.56
1:K:263:LEU:CD2	1:K:269:LEU:HD12	2.34	0.56
1:A:130:LEU:HD12	1:A:130:LEU:H	1.70	0.56
1:N:131:PRO:O	1:N:134:TYR:HD1	1.89	0.56
1:X:130:LEU:HD12	1:X:130:LEU:H	1.69	0.56
1:G:133:GLN:OE1	1:J:135:HIS:ND1	2.38	0.56
1:J:208:GLY:O	1:J:215:ARG:N	2.39	0.56
1:J:52:GLY:HA2	1:J:278:GLN:HG3	1.87	0.56
1:K:17:ILE:HD12	1:K:270:ILE:HG12	1.88	0.56
1:K:272:LYS:HG3	1:N:292:GLN:HE21	1.70	0.56
1:N:58:LEU:HD22	1:N:72:TRP:CD2	2.40	0.56
1:X:127:ILE:CB	1:X:130:LEU:HD11	2.35	0.56
1:X:285:GLN:NE2	3:X:501:HOH:O	2.37	0.56
1:X:260:LEU:O	1:X:264:LYS:HE2	2.06	0.55
1:A:247:PRO:HB2	1:A:249:PHE:CZ	2.42	0.55
1:K:263:LEU:HD23	1:K:269:LEU:HD12	1.88	0.55
1:X:10:TYR:CD1	1:X:268:ARG:HG2	2.42	0.55
1:X:174:TYR:OH	1:X:209:HIS:HB2	2.06	0.55
1:A:228:GLU:OE1	1:A:228:GLU:HA	2.05	0.55
1:G:18:ILE:HD13	1:G:264:LYS:HG3	1.88	0.55
1:X:13:VAL:HG23	1:X:57:MET:SD	2.47	0.55
1:B:132:GLU:C	1:B:134:TYR:H	2.09	0.55
1:J:266:ASP:N	1:J:266:ASP:OD1	2.39	0.55
1:B:79:LYS:HA	1:B:83:GLY:O	2.07	0.55
1:F:174:TYR:OH	1:F:179:ASP:OD1	2.20	0.55
1:X:79:LYS:CE	1:X:84:GLN:HA	2.37	0.55
1:X:207:THR:HB	1:X:213:LEU:HD12	1.88	0.55
1:A:10:TYR:HB3	1:A:267:LYS:O	2.07	0.54
1:F:15:ASP:HB2	1:F:16:ARG:HH21	1.73	0.54
1:F:238:MET:SD	1:F:278:GLN:HG2	2.47	0.54
1:F:207:THR:HB	1:F:215:ARG:HH12	1.71	0.54
1:F:259:TRP:O	1:F:263:LEU:N	2.30	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:185:PRO:HB2	1:N:188:THR:HG23	1.88	0.54
1:J:238:MET:HE1	1:J:277:ALA:C	2.27	0.54
1:K:27:ALA:HB1	1:K:60:LEU:HB2	1.89	0.54
1:A:46:ASN:ND2	1:A:48:GLU:HB2	2.23	0.54
1:J:207:THR:O	1:J:215:ARG:NH2	2.41	0.54
1:X:11:GLN:HG3	1:X:15:ASP:OD2	2.08	0.54
1:J:207:THR:HG23	1:J:215:ARG:HH22	1.73	0.54
1:F:52:GLY:H	1:F:278:GLN:HG3	1.72	0.53
1:B:86:ARG:HG3	1:B:89:GLU:HG3	1.90	0.53
1:B:18:ILE:HD13	1:B:264:LYS:HG2	1.89	0.53
1:F:169:GLU:HG3	1:F:182:HIS:CE1	2.43	0.53
1:A:95:VAL:CG1	1:A:116:LEU:HD11	2.39	0.53
1:F:101:GLU:O	1:F:102:ARG:HG3	2.09	0.53
1:X:200:ALA:HB1	1:X:239:LEU:HD23	1.90	0.53
1:F:207:THR:HG21	1:F:213:LEU:HD12	1.90	0.53
1:G:13:VAL:O	1:G:17:ILE:HD13	2.09	0.53
1:N:92:SER:O	1:N:120:THR:HA	2.09	0.53
1:A:263:LEU:HD23	1:A:269:LEU:HD23	1.90	0.52
1:B:58:LEU:HD22	1:B:72:TRP:CE2	2.44	0.52
1:F:207:THR:HG22	1:F:208:GLY:H	1.73	0.52
1:N:263:LEU:HD23	1:N:269:LEU:HD12	1.91	0.52
1:J:44:ARG:HG2	1:J:50:TYR:CE1	2.43	0.52
1:X:73:PHE:HE1	1:X:124:ALA:HB2	1.74	0.52
1:J:67:TYR:CD1	1:J:125:ASP:HB2	2.44	0.52
1:X:79:LYS:NZ	1:X:85:VAL:HG23	2.25	0.52
1:N:169:GLU:O	1:N:182:HIS:HE1	1.92	0.52
1:X:132:GLU:C	1:X:134:TYR:H	2.13	0.52
1:F:201:HIS:HB2	1:F:236:ASN:ND2	2.25	0.52
1:N:85:VAL:HG23	1:N:127:ILE:HG22	1.88	0.52
1:X:208:GLY:HA2	1:X:213:LEU:HB2	1.92	0.52
1:G:218:ARG:HG2	1:G:218:ARG:NH1	2.25	0.51
1:F:257:GLN:HA	1:F:260:LEU:HB2	1.91	0.51
1:N:95:VAL:HG13	1:N:116:LEU:HD11	1.92	0.51
1:J:153:LEU:HD23	1:J:196:TYR:CD2	2.45	0.51
1:B:29:ARG:HG2	1:B:249:PHE:CZ	2.46	0.51
1:F:52:GLY:HA2	1:F:278:GLN:HG3	1.91	0.51
1:N:204:THR:HG21	1:N:232:ALA:HA	1.92	0.51
1:G:272:LYS:HA	1:J:292:GLN:HE21	1.76	0.51
1:N:169:GLU:OE1	1:N:171:ARG:HD2	2.11	0.51
1:N:8:ASP:OD2	1:N:267:LYS:NZ	2.31	0.51
1:B:181:ILE:HD11	1:B:206:TRP:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:213:LEU:HD13	1:K:283:LEU:HD22	1.92	0.50
1:B:272:LYS:HG2	1:F:292:GLN:OE1	2.11	0.50
1:K:205:HIS:O	1:K:207:THR:O	2.30	0.50
1:A:65:LYS:NZ	1:A:90:LYS:O	2.41	0.50
1:F:235:GLY:HA2	1:F:238:MET:HE2	1.94	0.50
1:J:52:GLY:O	1:J:55:VAL:HB	2.11	0.50
1:X:92:SER:O	1:X:120:THR:HA	2.12	0.50
1:F:169:GLU:HG3	1:F:169:GLU:O	2.11	0.50
1:X:18:ILE:HG12	1:X:263:LEU:HD23	1.93	0.50
1:B:44:ARG:HG2	1:B:50:TYR:CZ	2.47	0.50
1:J:207:THR:OG1	1:J:208:GLY:N	2.45	0.50
1:N:240:CYS:SG	1:N:247:PRO:HG3	2.51	0.50
1:J:95:VAL:HG13	1:J:116:LEU:CD1	2.35	0.49
1:J:133:GLN:N	1:J:133:GLN:OE1	2.45	0.49
1:K:114:PRO:HD3	1:N:158:ALA:HB1	1.94	0.49
1:N:290:ASN:ND2	1:N:292:GLN:OE1	2.45	0.49
1:N:58:LEU:HD22	1:N:72:TRP:CE2	2.47	0.49
1:N:94:VAL:HG23	1:N:119:TYR:CE1	2.47	0.49
1:N:133:GLN:HG3	1:N:134:TYR:CE1	2.47	0.49
1:B:286:GLU:OE1	1:F:51:ARG:NH2	2.41	0.49
1:K:8:ASP:OD2	1:K:267:LYS:NZ	2.36	0.49
1:N:78:ALA:HB1	1:N:127:ILE:HD13	1.79	0.49
1:N:15:ASP:HA	1:N:18:ILE:CG1	2.43	0.49
1:F:131:PRO:C	1:F:133:GLN:H	2.15	0.49
1:G:250:ASP:OD1	1:G:251:GLN:N	2.46	0.49
1:K:272:LYS:HG3	1:N:292:GLN:NE2	2.27	0.49
1:N:10:TYR:O	1:N:14:THR:OG1	2.30	0.49
1:F:154:ASP:OD1	1:F:196:TYR:OH	2.28	0.49
1:X:127:ILE:CG2	1:X:130:LEU:HD11	2.43	0.49
1:N:227:PHE:CE1	1:N:273:ALA:HB2	2.47	0.48
1:A:17:ILE:HD11	1:A:57:MET:HE3	1.95	0.48
1:J:206:TRP:O	1:J:212:ARG:NH2	2.32	0.48
1:K:89:GLU:HB3	1:K:126:GLN:HE21	1.78	0.48
1:G:17:ILE:HD11	1:G:57:MET:HE1	1.94	0.48
1:K:158:ALA:HB1	1:N:114:PRO:HD3	1.95	0.48
1:A:111:LYS:HB3	1:X:154:ASP:OD2	2.14	0.48
1:F:127:ILE:HG23	1:F:130:LEU:HD11	1.94	0.48
1:A:167:SER:OG	1:A:169:GLU:HG3	2.13	0.48
1:B:27:ALA:HB1	1:B:60:LEU:HB2	1.94	0.48
1:X:111:LYS:O	1:X:112:LYS:HG3	2.12	0.48
1:N:96:LYS:HG2	1:N:97:PHE:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:207:THR:HG22	1:F:213:LEU:HB2	1.94	0.48
1:A:17:ILE:CD1	1:A:270:ILE:HG12	2.42	0.48
1:G:95:VAL:CG1	1:G:116:LEU:HD11	2.44	0.48
1:X:173:TYR:HA	1:X:202:GLU:OE1	2.14	0.48
1:N:232:ALA:O	1:N:236:ASN:HB2	2.14	0.47
1:G:17:ILE:N	1:G:17:ILE:CD1	2.74	0.47
1:G:58:LEU:HD22	1:G:72:TRP:CD2	2.49	0.47
1:B:7:PHE:N	3:B:504:HOH:O	2.47	0.47
1:F:181:ILE:HD11	1:F:206:TRP:CB	2.39	0.47
1:J:15:ASP:O	1:J:18:ILE:N	2.48	0.47
1:X:232:ALA:O	1:X:236:ASN:HB2	2.15	0.47
1:F:147:THR:HG22	1:F:147:THR:O	2.15	0.47
1:N:201:HIS:NE2	1:N:205:HIS:CE1	2.83	0.47
1:A:17:ILE:HD11	1:A:57:MET:HE1	1.97	0.47
1:A:100:ILE:HG22	1:K:100:ILE:HG22	1.97	0.47
1:F:145:LEU:HB3	1:F:192:ALA:HB3	1.96	0.47
1:N:167:SER:HB3	1:N:182:HIS:NE2	2.29	0.47
1:B:227:PHE:HE1	1:B:269:LEU:HG	1.80	0.47
1:K:213:LEU:CD1	1:K:283:LEU:HD22	2.45	0.47
1:N:53:ILE:O	1:N:57:MET:HG2	2.15	0.47
1:N:73:PHE:HE1	1:N:124:ALA:HB2	1.79	0.47
1:A:94:VAL:HG23	1:A:119:TYR:CE1	2.49	0.47
1:G:167:SER:HB3	1:G:182:HIS:NE2	2.30	0.47
1:K:98:GLY:CA	1:K:117:LYS:HE3	2.45	0.47
1:X:88:GLY:O	1:X:90:LYS:HE3	2.14	0.47
1:X:96:LYS:HG2	1:X:97:PHE:N	2.30	0.47
1:B:227:PHE:CE1	1:B:269:LEU:HG	2.50	0.47
1:B:258:SER:HA	1:B:261:ARG:NH1	2.29	0.47
1:J:52:GLY:CA	1:J:278:GLN:HG3	2.45	0.47
1:J:189:PHE:C	1:J:191:SER:H	2.18	0.47
1:N:8:ASP:HB3	1:N:11:GLN:CB	2.44	0.47
1:B:25:THR:HG23	1:B:30:LYS:HZ1	1.80	0.46
1:G:209:HIS:CE1	1:G:211:SER:HG	2.30	0.46
1:J:71:TYR:CD1	1:J:134:TYR:HD1	2.33	0.46
1:J:235:GLY:HA2	1:J:238:MET:HE2	1.97	0.46
1:N:116:LEU:HD12	1:N:116:LEU:HA	1.73	0.46
1:A:65:LYS:HD2	1:A:67:TYR:OH	2.15	0.46
1:A:167:SER:HB3	1:A:182:HIS:NE2	2.30	0.46
1:J:17:ILE:HG22	1:J:263:LEU:HD21	1.97	0.46
1:J:46:ASN:OD1	1:J:48:GLU:HG3	2.15	0.46
1:F:65:LYS:HE2	1:F:90:LYS:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:ILE:CD1	1:G:17:ILE:H	2.27	0.46
1:J:13:VAL:HG13	1:J:57:MET:SD	2.55	0.46
1:A:96:LYS:CE	1:A:117:LYS:HE2	2.45	0.46
1:A:218:ARG:HA	1:A:218:ARG:HH11	1.81	0.46
1:F:12:HIS:CE1	1:F:16:ARG:NH1	2.83	0.46
1:F:62:ALA:HB1	1:F:67:TYR:HB2	1.96	0.46
1:N:201:HIS:CE1	1:N:232:ALA:HB1	2.51	0.46
1:X:165:ARG:O	1:X:182:HIS:HA	2.15	0.46
1:J:86:ARG:HE	1:J:86:ARG:HB2	1.41	0.46
1:X:44:ARG:HG2	1:X:50:TYR:CE2	2.51	0.46
1:A:30:LYS:N	1:A:31:PRO:HD2	2.30	0.46
1:G:13:VAL:HG13	1:G:57:MET:HE3	1.98	0.46
1:G:269:LEU:HD12	1:G:269:LEU:HA	1.84	0.46
1:J:227:PHE:CE1	1:J:273:ALA:HB2	2.51	0.46
1:K:162:ALA:HB2	1:K:206:TRP:CE2	2.51	0.46
1:N:208:GLY:HA3	1:N:215:ARG:HG2	1.97	0.46
1:X:14:THR:O	1:X:18:ILE:HG13	2.16	0.46
1:A:215:ARG:HD2	1:A:231:ILE:HD13	1.98	0.46
1:F:211:SER:H	1:F:211:SER:HG	1.49	0.46
1:B:14:THR:O	1:B:18:ILE:HG13	2.16	0.46
1:G:211:SER:HG	1:G:211:SER:H	1.57	0.46
1:J:111:LYS:O	1:J:112:LYS:HG2	2.15	0.46
1:N:154:ASP:OD1	1:N:196:TYR:OH	2.20	0.46
1:X:9:LEU:HD21	1:X:95:VAL:HG22	1.97	0.46
1:J:72:TRP:HB3	1:J:121:VAL:HB	1.98	0.46
1:J:238:MET:HE2	1:J:238:MET:HB2	1.63	0.46
1:K:290:ASN:HA	1:N:275:THR:HG23	1.98	0.46
1:F:58:LEU:HD22	1:F:72:TRP:CD2	2.51	0.45
1:F:202:GLU:O	1:F:206:TRP:N	2.49	0.45
1:N:167:SER:OG	1:N:168:SER:N	2.48	0.45
1:A:133:GLN:O	1:A:134:TYR:CD1	2.69	0.45
1:X:132:GLU:C	1:X:134:TYR:N	2.70	0.45
1:G:13:VAL:O	1:G:17:ILE:HD12	2.15	0.45
1:J:9:LEU:O	1:J:13:VAL:HG23	2.16	0.45
1:X:44:ARG:HG2	1:X:50:TYR:CZ	2.51	0.45
1:A:133:GLN:O	1:A:134:TYR:CG	2.70	0.45
1:K:150:ASP:HB3	1:K:153:LEU:HB2	1.98	0.45
1:K:167:SER:O	1:K:185:PRO:HD3	2.16	0.45
1:F:150:ASP:HB3	1:F:153:LEU:HD23	1.99	0.45
1:J:116:LEU:HA	1:J:116:LEU:HD12	1.53	0.45
1:A:171:ARG:NH1	1:A:173:TYR:HE2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:GLY:C	1:F:127:ILE:HD11	2.36	0.45
1:J:203:ALA:O	1:J:206:TRP:HB3	2.17	0.45
1:A:54:ASN:OD1	1:A:95:VAL:N	2.49	0.45
1:F:52:GLY:N	1:F:278:GLN:HG3	2.31	0.45
1:G:229:GLU:HA	1:G:232:ALA:HB3	1.97	0.45
1:K:208:GLY:HA2	1:K:213:LEU:HB2	1.99	0.45
1:X:208:GLY:N	1:X:213:LEU:HB2	2.32	0.45
1:A:86:ARG:HH21	1:A:128:ASP:CG	2.18	0.45
1:F:171:ARG:O	1:F:182:HIS:ND1	2.48	0.45
1:F:238:MET:HE1	1:F:277:ALA:C	2.38	0.45
1:X:228:GLU:O	1:X:231:ILE:N	2.50	0.45
1:X:17:ILE:HD13	1:X:270:ILE:HG12	1.99	0.45
1:B:21:ILE:HG21	1:B:260:LEU:HD13	1.99	0.45
1:J:174:TYR:OH	1:J:209:HIS:HB2	2.17	0.45
1:X:14:THR:HG23	1:X:263:LEU:HD11	1.98	0.45
1:F:12:HIS:CD2	1:F:16:ARG:HH12	2.35	0.44
1:N:79:LYS:HA	1:N:83:GLY:O	2.17	0.44
1:N:95:VAL:CG1	1:N:116:LEU:HD11	2.48	0.44
1:X:130:LEU:HD12	1:X:130:LEU:N	2.33	0.44
1:X:175:ASN:ND2	1:X:180:TYR:OH	2.50	0.44
1:B:97:PHE:HZ	1:F:290:ASN:O	2.00	0.44
1:F:62:ALA:HA	1:F:67:TYR:CD2	2.50	0.44
1:F:213:LEU:HD23	1:F:213:LEU:HA	1.79	0.44
1:N:76:ARG:O	1:N:80:GLU:HG3	2.18	0.44
1:X:235:GLY:HA2	1:X:238:MET:CE	2.47	0.44
1:N:15:ASP:HA	1:N:18:ILE:HG12	2.00	0.44
1:N:132:GLU:C	1:N:134:TYR:N	2.70	0.44
1:N:145:LEU:HB3	1:N:192:ALA:HB3	1.98	0.44
1:N:170:PRO:HA	1:N:184:PRO:HG3	1.98	0.44
1:B:167:SER:OG	1:B:168:SER:N	2.50	0.44
1:B:102:ARG:HB3	1:B:113:ILE:HD12	1.99	0.44
1:F:43:LEU:HD23	1:F:49:ALA:HA	2.00	0.44
1:F:79:LYS:HG3	1:F:84:GLN:HE22	1.82	0.44
1:F:102:ARG:HB2	1:F:113:ILE:CD1	2.48	0.44
1:K:27:ALA:O	1:K:30:LYS:HB2	2.17	0.44
1:G:218:ARG:CZ	1:G:219:PHE:CZ	3.00	0.44
1:J:43:LEU:HD22	1:J:47:GLY:O	2.17	0.44
1:J:46:ASN:CG	1:J:48:GLU:HG3	2.38	0.44
1:J:205:HIS:CE1	1:J:229:GLU:HG2	2.52	0.44
1:K:81:LEU:HD22	1:K:131:PRO:HG2	1.99	0.44
1:B:74:THR:O	1:B:78:ALA:N	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:LYS:HA	1:B:87:LYS:HD2	1.87	0.43
1:B:94:VAL:HG23	1:B:119:TYR:CE1	2.52	0.43
1:B:116:LEU:HD12	1:B:116:LEU:HA	1.68	0.43
1:B:215:ARG:HD2	1:B:231:ILE:HG21	2.00	0.43
1:J:153:LEU:HD23	1:J:196:TYR:CG	2.53	0.43
1:J:171:ARG:O	1:J:184:PRO:HD3	2.18	0.43
1:X:79:LYS:HZ1	1:X:85:VAL:HG23	1.81	0.43
1:A:25:THR:HB	1:A:30:LYS:CE	2.39	0.43
1:N:181:ILE:HG21	1:N:199:LEU:CD1	2.48	0.43
1:X:95:VAL:HG13	1:X:116:LEU:HD11	1.99	0.43
1:K:73:PHE:O	1:K:122:PHE:N	2.37	0.43
1:K:205:HIS:HE1	1:K:228:GLU:HG3	1.83	0.43
1:F:167:SER:HB3	1:F:182:HIS:NE2	2.33	0.43
1:J:131:PRO:O	1:J:133:GLN:N	2.50	0.43
1:X:208:GLY:H	1:X:213:LEU:HB2	1.83	0.43
1:F:203:ALA:O	1:F:206:TRP:HB3	2.18	0.43
1:G:21:ILE:HG21	1:G:260:LEU:HD13	2.01	0.43
1:G:73:PHE:O	1:G:122:PHE:N	2.44	0.43
1:J:95:VAL:O	1:J:119:TYR:HE1	2.01	0.43
1:K:51:ARG:HD3	1:N:289:ALA:CB	2.48	0.43
1:K:207:THR:HB	1:K:213:LEU:HD22	2.01	0.43
1:N:132:GLU:O	1:N:132:GLU:HG3	2.18	0.43
1:N:230:LEU:O	1:N:234:ILE:HG13	2.18	0.43
1:X:230:LEU:HB2	1:X:259:TRP:CE2	2.54	0.43
1:K:102:ARG:O	1:K:112:LYS:HE2	2.18	0.43
1:B:68:ARG:HG3	1:B:68:ARG:HH11	1.84	0.43
1:G:94:VAL:HG23	1:G:119:TYR:CE1	2.53	0.43
1:G:285:GLN:HE21	1:G:285:GLN:HA	1.84	0.43
1:N:147:THR:HG22	1:N:147:THR:O	2.19	0.43
1:K:222:ARG:NH2	1:K:258:SER:HB2	2.33	0.43
1:X:96:LYS:HG2	1:X:97:PHE:H	1.84	0.43
1:K:247:PRO:HB2	1:K:249:PHE:CE1	2.54	0.43
1:N:163:ASP:HB3	1:N:180:TYR:HA	2.01	0.43
1:N:205:HIS:CD2	1:N:232:ALA:HB2	2.54	0.43
1:X:85:VAL:HG12	1:X:89:GLU:HB2	1.99	0.43
1:X:157:PHE:CD2	1:X:199:LEU:HD13	2.54	0.43
1:B:155:ALA:HB2	1:F:99:THR:HB	2.01	0.42
1:J:71:TYR:CD1	1:J:134:TYR:CD1	3.07	0.42
1:K:247:PRO:HB2	1:K:249:PHE:CZ	2.54	0.42
1:N:85:VAL:HG23	1:N:126:GLN:O	2.19	0.42
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:133:GLN:NE2	3:X:505:HOH:O	2.52	0.42
1:A:252:SER:O	1:A:252:SER:OG	2.27	0.42
1:G:259:TRP:O	1:G:263:LEU:HG	2.19	0.42
1:J:123:ASN:OD1	1:J:124:ALA:N	2.52	0.42
1:N:183:MET:CG	1:N:199:LEU:HD13	2.49	0.42
1:A:239:LEU:HD22	1:A:284:LEU:CD2	2.49	0.42
1:F:165:ARG:HG3	1:F:180:TYR:CD1	2.54	0.42
1:J:227:PHE:HE1	1:J:273:ALA:HB2	1.84	0.42
1:K:8:ASP:CG	1:K:267:LYS:HZ3	2.20	0.42
1:K:153:LEU:HA	1:K:153:LEU:HD23	1.79	0.42
1:K:183:MET:HB3	1:K:183:MET:HE3	1.80	0.42
1:N:85:VAL:HG21	1:N:122:PHE:CD2	2.55	0.42
1:A:217:SER:O	1:A:218:ARG:HB3	2.20	0.42
1:B:58:LEU:HD23	1:B:58:LEU:HA	1.83	0.42
1:B:78:ALA:O	1:B:81:LEU:HB2	2.19	0.42
1:B:111:LYS:HB3	1:F:154:ASP:OD2	2.19	0.42
1:F:10:TYR:HB2	1:F:267:LYS:CE	2.44	0.42
1:F:111:LYS:HE2	1:F:111:LYS:HB2	1.81	0.42
1:K:185:PRO:O	1:K:188:THR:OG1	2.28	0.42
1:F:52:GLY:CA	1:F:278:GLN:HG3	2.48	0.42
1:J:62:ALA:CB	1:J:67:TYR:HB2	2.50	0.42
1:J:102:ARG:HB2	1:J:113:ILE:HD13	2.02	0.42
1:X:75:TYR:O	1:X:79:LYS:HD2	2.20	0.42
1:F:51:ARG:NH2	1:F:282:ASP:OD2	2.53	0.42
1:F:231:ILE:CD1	1:F:276:GLU:HB2	2.50	0.42
1:J:14:THR:HG22	1:J:18:ILE:CD1	2.49	0.42
1:N:71:TYR:CD1	1:N:134:TYR:HD2	2.38	0.42
1:X:44:ARG:H	1:X:44:ARG:HG3	1.69	0.42
1:X:94:VAL:HG23	1:X:119:TYR:CE1	2.55	0.42
1:A:260:LEU:HD23	1:A:260:LEU:HA	1.76	0.42
1:F:157:PHE:HA	1:F:160:THR:HG23	2.01	0.42
1:F:166:THR:HG23	1:F:183:MET:O	2.19	0.42
1:G:167:SER:O	1:G:185:PRO:HD3	2.20	0.42
1:N:111:LYS:C	1:N:112:LYS:HG3	2.17	0.42
1:X:178:GLY:O	1:X:180:TYR:HD2	2.03	0.42
1:J:205:HIS:HE1	1:J:229:GLU:HG2	1.85	0.41
1:X:208:GLY:CA	1:X:213:LEU:HB2	2.50	0.41
1:A:169:GLU:HB2	1:A:182:HIS:CE1	2.55	0.41
1:B:111:LYS:HE3	1:B:111:LYS:HB2	1.84	0.41
1:F:10:TYR:CD1	1:F:10:TYR:N	2.88	0.41
1:F:167:SER:HB3	1:F:169:GLU:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:HIS:CE1	1:G:232:ALA:HB2	2.55	0.41
1:J:169:GLU:HA	1:J:170:PRO:HD3	1.89	0.41
1:K:89:GLU:OE1	1:K:126:GLN:HG2	2.20	0.41
1:X:238:MET:HE2	1:X:238:MET:HB2	1.61	0.41
1:A:204:THR:O	1:A:207:THR:OG1	2.34	0.41
1:B:99:THR:HA	1:B:113:ILE:O	2.19	0.41
1:G:218:ARG:NE	1:G:219:PHE:CE2	2.88	0.41
1:N:127:ILE:HD11	1:N:130:LEU:HD21	2.01	0.41
1:X:290:ASN:ND2	3:X:506:HOH:O	2.52	0.41
1:B:132:GLU:C	1:B:134:TYR:N	2.73	0.41
1:K:14:THR:O	1:K:18:ILE:HG13	2.20	0.41
1:N:65:LYS:HD3	1:N:67:TYR:OH	2.19	0.41
1:F:99:THR:HG1	1:F:111:LYS:N	2.18	0.41
1:N:126:GLN:HE21	1:N:126:GLN:HB3	1.56	0.41
1:A:31:PRO:HG2	1:A:32:TRP:CZ3	2.55	0.41
1:F:116:LEU:HD12	1:F:116:LEU:HA	1.69	0.41
1:G:53:ILE:HA	1:G:53:ILE:HD12	1.73	0.41
1:G:99:THR:HA	1:G:113:ILE:O	2.21	0.41
1:N:116:LEU:HG	1:N:117:LYS:H	1.86	0.41
1:A:239:LEU:CD2	1:A:284:LEU:HD23	2.49	0.41
1:B:218:ARG:O	1:B:218:ARG:CG	2.69	0.41
1:N:12:HIS:CE1	1:N:16:ARG:HG3	2.56	0.41
1:A:99:THR:HA	1:A:113:ILE:O	2.20	0.41
1:B:24:GLY:HA3	1:G:180:TYR:CZ	2.56	0.41
1:B:79:LYS:HB3	1:B:79:LYS:HE2	1.94	0.41
1:G:10:TYR:HB3	1:G:267:LYS:O	2.21	0.41
1:J:232:ALA:O	1:J:236:ASN:HB2	2.21	0.41
1:K:17:ILE:HD11	1:K:57:MET:CE	2.49	0.41
1:K:260:LEU:HA	1:K:260:LEU:HD23	1.74	0.41
1:F:41:MET:HA	1:F:42:PRO:HD3	1.94	0.41
1:G:186:ILE:HA	1:G:195:TYR:CD2	2.56	0.41
1:K:44:ARG:HG2	1:K:50:TYR:CE2	2.56	0.41
1:K:165:ARG:O	1:K:182:HIS:HA	2.21	0.41
1:N:169:GLU:CD	1:N:171:ARG:HD2	2.41	0.41
1:X:263:LEU:HA	1:X:263:LEU:HD12	1.89	0.41
1:F:15:ASP:HB2	1:F:16:ARG:NH2	2.36	0.40
1:G:218:ARG:NE	1:G:219:PHE:CZ	2.89	0.40
1:J:65:LYS:HB2	1:J:67:TYR:CE2	2.56	0.40
1:B:58:LEU:HD11	1:B:94:VAL:HG11	2.03	0.40
1:J:52:GLY:N	1:J:278:GLN:HG3	2.36	0.40
1:J:167:SER:HB3	1:J:182:HIS:NE2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:264:LYS:HD3	1:K:264:LYS:HA	1.74	0.40
1:B:213:LEU:HA	1:B:213:LEU:HD23	1.86	0.40
1:G:206:TRP:CZ2	1:G:212:ARG:NH1	2.90	0.40
1:X:201:HIS:CE1	1:X:229:GLU:OE2	2.73	0.40
1:B:41:MET:HG3	1:B:42:PRO:HD2	2.03	0.40
1:F:83:GLY:O	1:F:127:ILE:HD11	2.21	0.40
1:K:43:LEU:HD23	1:K:49:ALA:HA	2.03	0.40
1:A:89:GLU:HG3	1:A:126:GLN:HB3	2.03	0.40
1:A:229:GLU:HA	1:A:232:ALA:HB3	2.04	0.40
1:J:61:THR:HG23	1:J:65:LYS:HD2	2.03	0.40
1:J:263:LEU:HD12	1:J:269:LEU:HD23	2.02	0.40
1:N:201:HIS:CE1	1:N:229:GLU:OE2	2.73	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	257/305 (84%)	237 (92%)	12 (5%)	8 (3%)	4	9
1	B	257/305 (84%)	241 (94%)	14 (5%)	2 (1%)	19	43
1	F	225/305 (74%)	207 (92%)	14 (6%)	4 (2%)	8	21
1	G	257/305 (84%)	239 (93%)	16 (6%)	2 (1%)	19	43
1	J	225/305 (74%)	205 (91%)	15 (7%)	5 (2%)	6	17
1	K	257/305 (84%)	238 (93%)	15 (6%)	4 (2%)	9	24
1	N	225/305 (74%)	211 (94%)	10 (4%)	4 (2%)	8	21
1	X	225/305 (74%)	211 (94%)	14 (6%)	0	100	100
All	All	1928/2440 (79%)	1789 (93%)	110 (6%)	29 (2%)	10	26

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	133	GLN
1	A	134	TYR
1	B	133	GLN
1	B	219	PHE
1	F	66	GLY
1	J	112	LYS
1	J	132	GLU
1	K	218	ARG
1	N	112	LYS
1	A	132	GLU
1	A	218	ARG
1	A	219	PHE
1	F	41	MET
1	F	132	GLU
1	G	209	HIS
1	J	87	LYS
1	N	207	THR
1	A	23	ALA
1	A	133	GLN
1	F	112	LYS
1	G	218	ARG
1	J	209	HIS
1	J	212	ARG
1	K	191	SER
1	A	131	PRO
1	K	209	HIS
1	A	191	SER
1	N	102	ARG
1	K	129	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	212/240 (88%)	203 (96%)	9 (4%)	30	58
1	B	212/240 (88%)	200 (94%)	12 (6%)	20	44
1	F	188/240 (78%)	181 (96%)	7 (4%)	34	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	212/240 (88%)	200 (94%)	12 (6%)	20	44
1	J	188/240 (78%)	179 (95%)	9 (5%)	25	53
1	K	212/240 (88%)	203 (96%)	9 (4%)	30	58
1	N	188/240 (78%)	179 (95%)	9 (5%)	25	53
1	X	188/240 (78%)	184 (98%)	4 (2%)	53	80
All	All	1600/1920 (83%)	1529 (96%)	71 (4%)	28	56

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	81	LEU
1	A	87	LYS
1	A	167	SER
1	A	171	ARG
1	A	217	SER
1	A	220	SER
1	A	222	ARG
1	A	242	SER
1	B	7	PHE
1	B	40	GLN
1	B	46	ASN
1	B	68	ARG
1	B	69	SER
1	B	75	TYR
1	B	168	SER
1	B	217	SER
1	B	218	ARG
1	B	223	LYS
1	B	229	GLU
1	B	269	LEU
1	F	11	GLN
1	F	16	ARG
1	F	69	SER
1	F	75	TYR
1	F	122	PHE
1	F	210	LYS
1	F	261	ARG
1	G	69	SER
1	G	75	TYR

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Mol	Chain	Res	Type
1	G	90	LYS
1	G	119	TYR
1	G	144	ASP
1	G	167	SER
1	G	168	SER
1	G	171	ARG
1	G	218	ARG
1	G	221	ASP
1	G	250	ASP
1	G	285	GLN
1	J	9	LEU
1	J	16	ARG
1	J	76	ARG
1	J	92	SER
1	J	210	LYS
1	J	212	ARG
1	J	269	LEU
1	J	278	GLN
1	J	285	GLN
1	K	69	SER
1	K	76	ARG
1	K	84	GLN
1	K	112	LYS
1	K	128	ASP
1	K	210	LYS
1	K	223	LYS
1	K	251	GLN
1	K	272	LYS
1	N	7	PHE
1	N	10	TYR
1	N	14	THR
1	N	79	LYS
1	N	102	ARG
1	N	135	HIS
1	N	143	ARG
1	N	167	SER
1	N	257	GLN
1	X	11	GLN
1	X	41	MET
1	X	79	LYS
1	X	84	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	G	126	GLN
1	J	126	GLN
1	N	123	ASN
1	N	290	ASN
1	N	292	GLN
1	X	126	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues (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	265/305 (86%)	-0.34	1 (0%)	92	93	19, 31, 65, 85	0
1	B	265/305 (86%)	-0.32	1 (0%)	92	93	24, 37, 73, 87	0
1	F	237/305 (77%)	0.10	8 (3%)	45	45	34, 59, 88, 96	0
1	G	265/305 (86%)	-0.32	0	100	100	19, 36, 68, 90	0
1	J	237/305 (77%)	-0.13	4 (1%)	70	72	28, 55, 86, 96	0
1	K	265/305 (86%)	-0.29	1 (0%)	92	93	22, 35, 62, 80	0
1	N	237/305 (77%)	-0.11	6 (2%)	57	59	29, 54, 78, 92	0
1	X	237/305 (77%)	-0.15	3 (1%)	77	78	23, 48, 71, 88	0
All	All	2008/2440 (82%)	-0.20	24 (1%)	79	80	19, 44, 77, 96	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	82	GLY	5.4
1	N	127	ILE	4.0
1	F	171	ARG	2.8
1	N	213	LEU	2.7
1	A	250	ASP	2.7
1	N	210	LYS	2.6
1	K	127	ILE	2.6
1	F	127	ILE	2.5
1	X	135	HIS	2.5
1	N	216	PHE	2.5
1	N	78	ALA	2.5
1	F	213	LEU	2.4
1	J	82	GLY	2.3
1	F	271	PHE	2.3
1	J	127	ILE	2.3
1	B	250	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	N	85	VAL	2.3
1	F	122	PHE	2.3
1	J	134	TYR	2.2
1	F	174	TYR	2.2
1	X	213	LEU	2.2
1	F	124	ALA	2.2
1	J	122	PHE	2.2
1	X	216	PHE	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 monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	MN	F	401	1/1	0.80	0.11	73,73,73,73	0
2	MN	G	401	1/1	0.81	0.18	46,46,46,46	0
2	MN	A	401	1/1	0.85	0.17	40,40,40,40	0
2	MN	K	401	1/1	0.85	0.21	45,45,45,45	0
2	MN	X	401	1/1	0.92	0.12	49,49,49,49	0
2	MN	N	401	1/1	0.95	0.10	60,60,60,60	0
2	MN	B	401	1/1	0.95	0.18	32,32,32,32	0
2	MN	J	401	1/1	0.98	0.13	52,52,52,52	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.
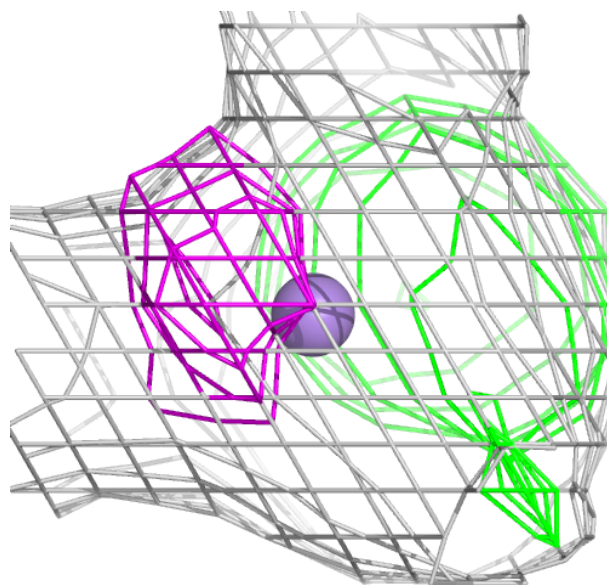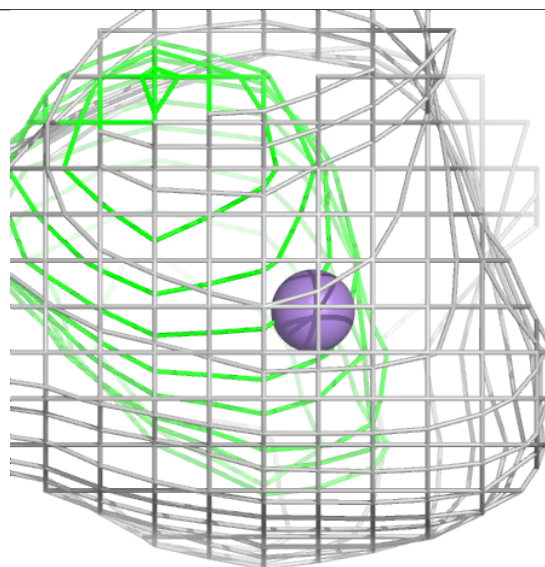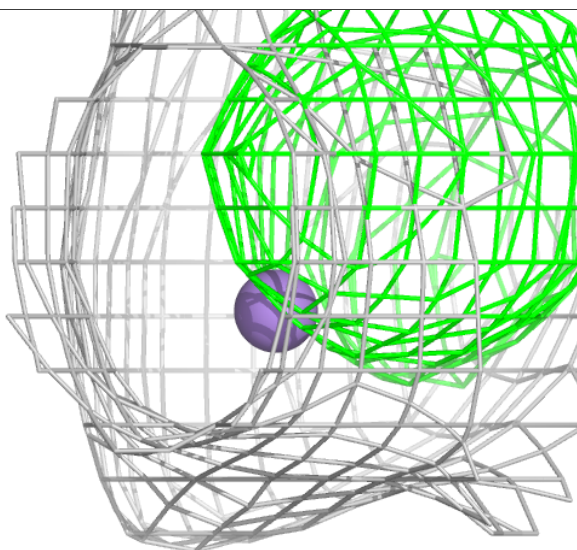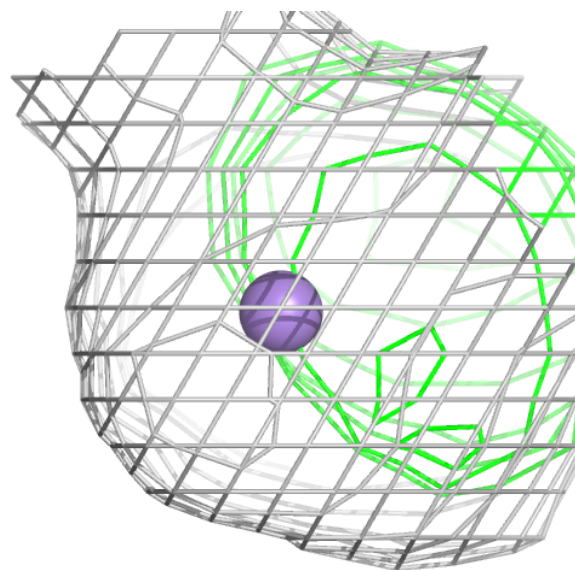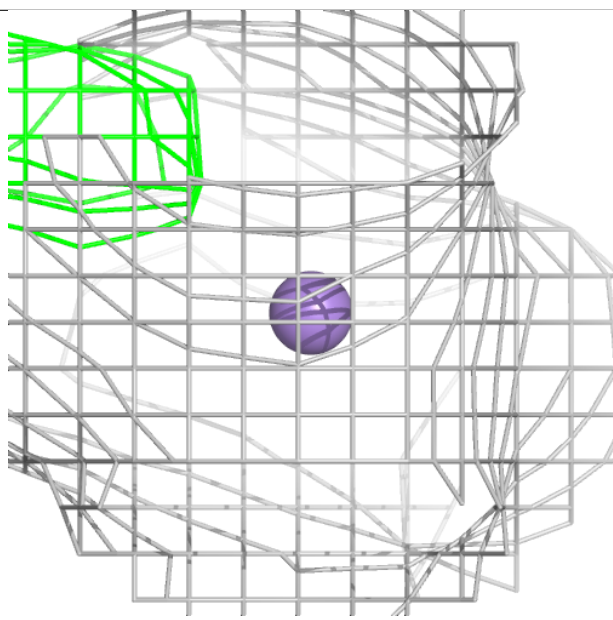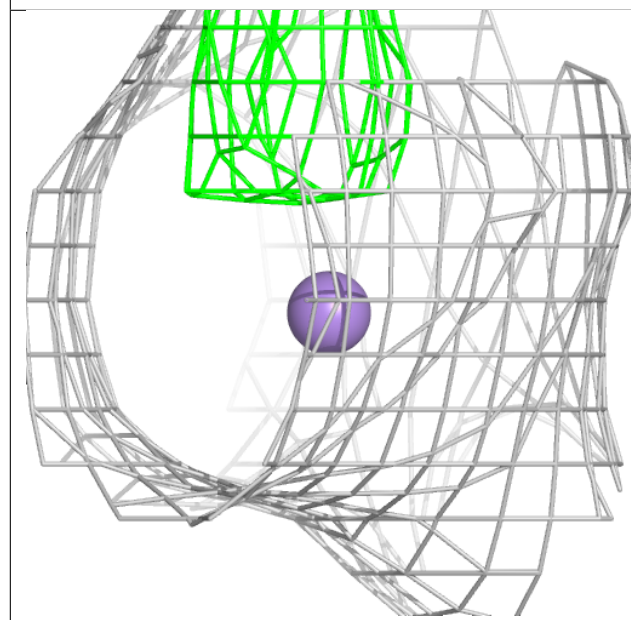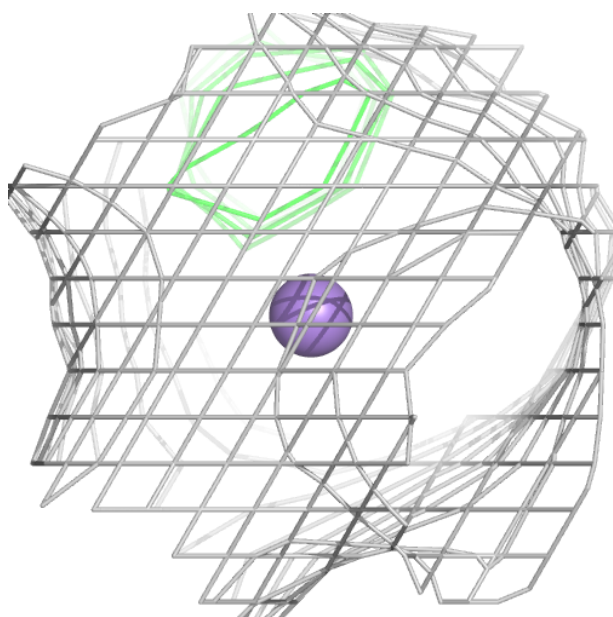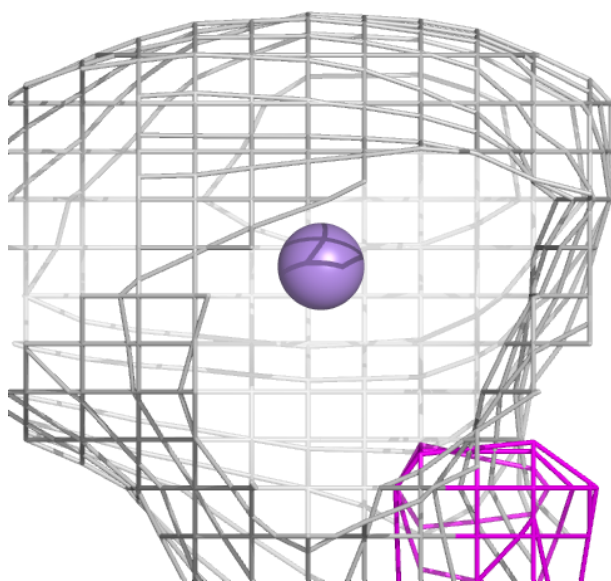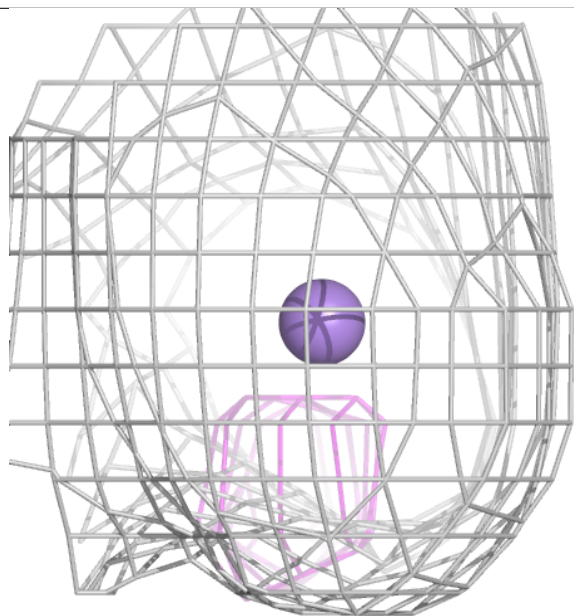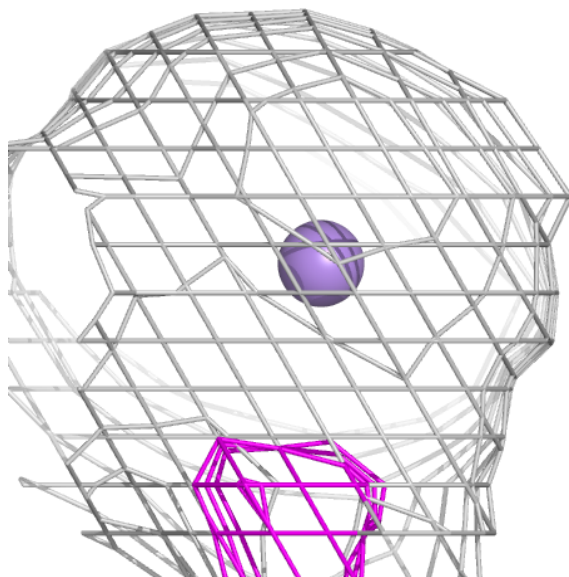
Electron density around MN F 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
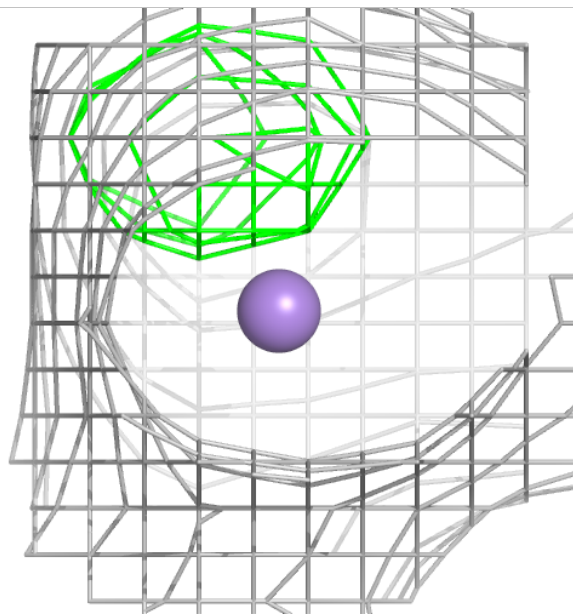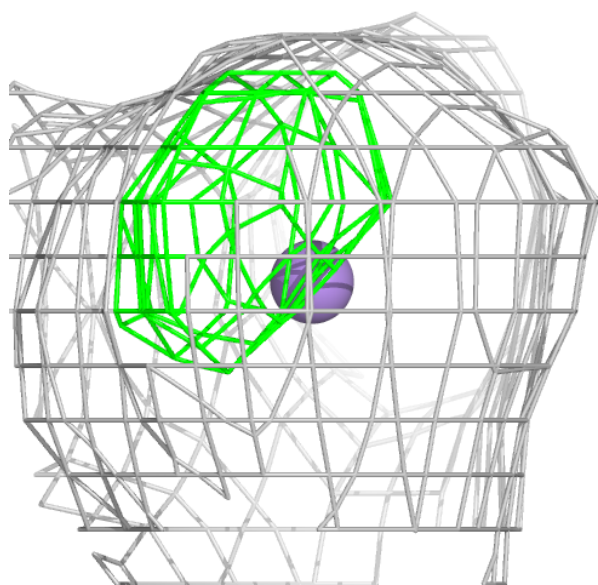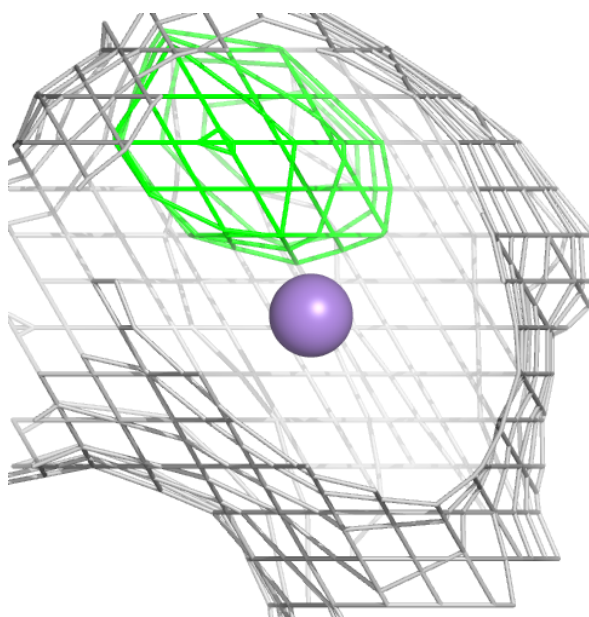
Electron density around MN G 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
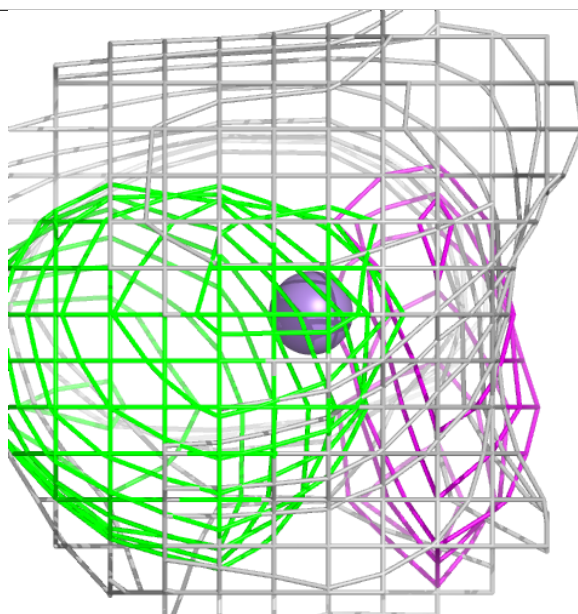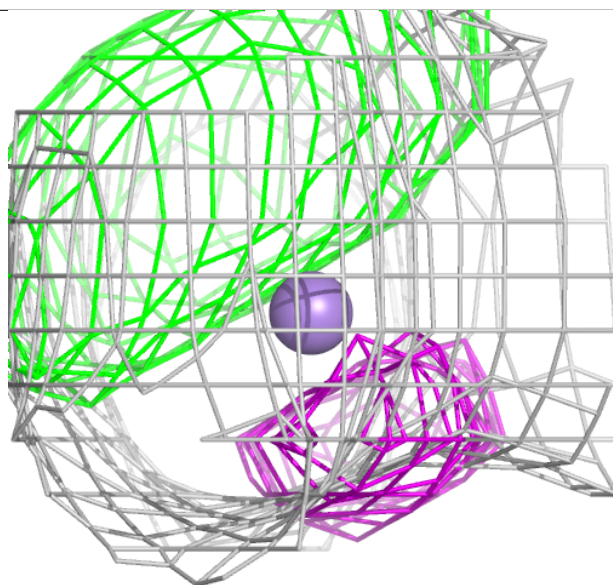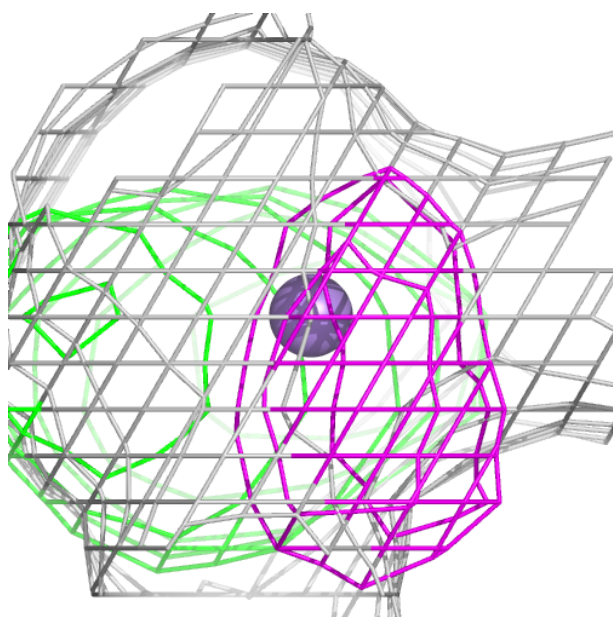
Electron density around MN A 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
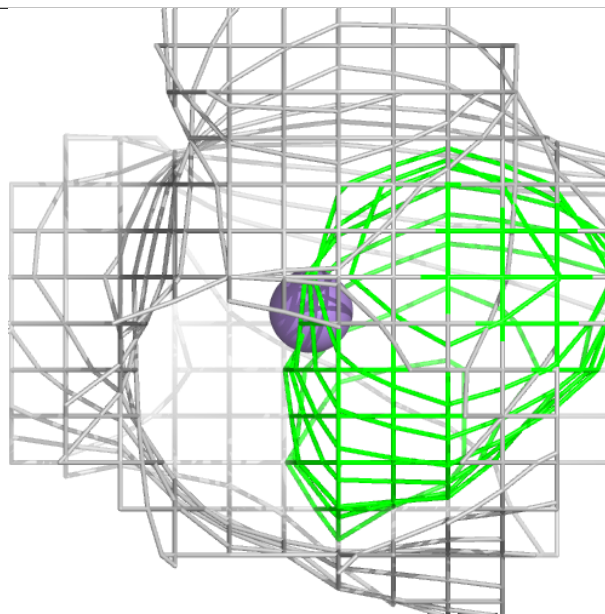$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
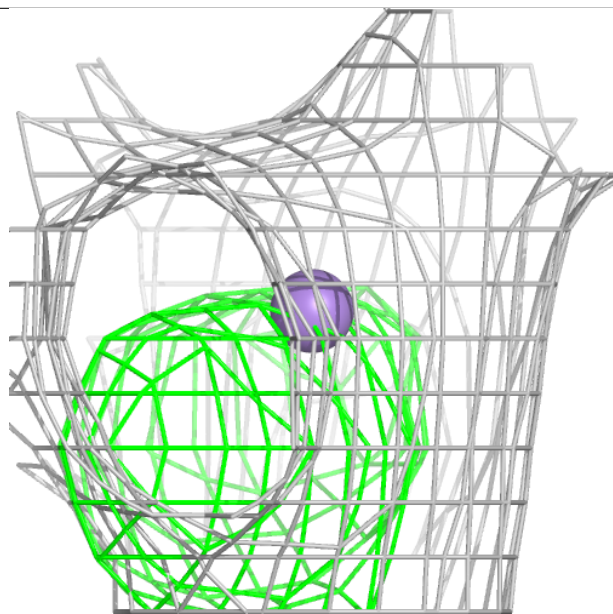and green (positive)
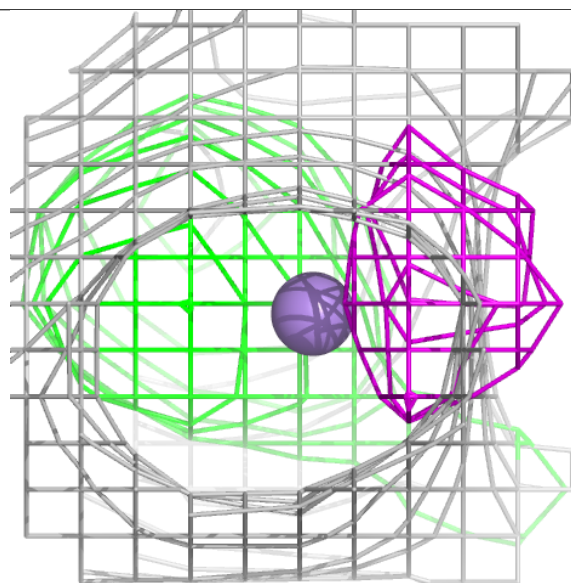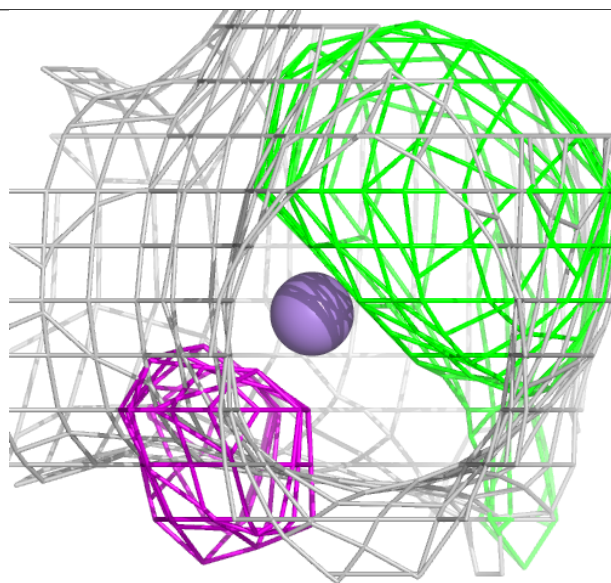
Electron density around MN K 401:

$2mF_o$-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 X 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
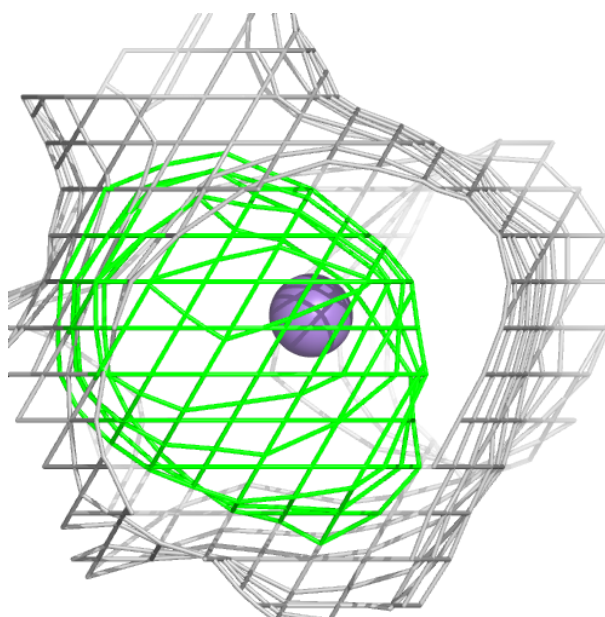and green (positive)

Electron density around MN N 401:

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

Electron density around MN B 401:
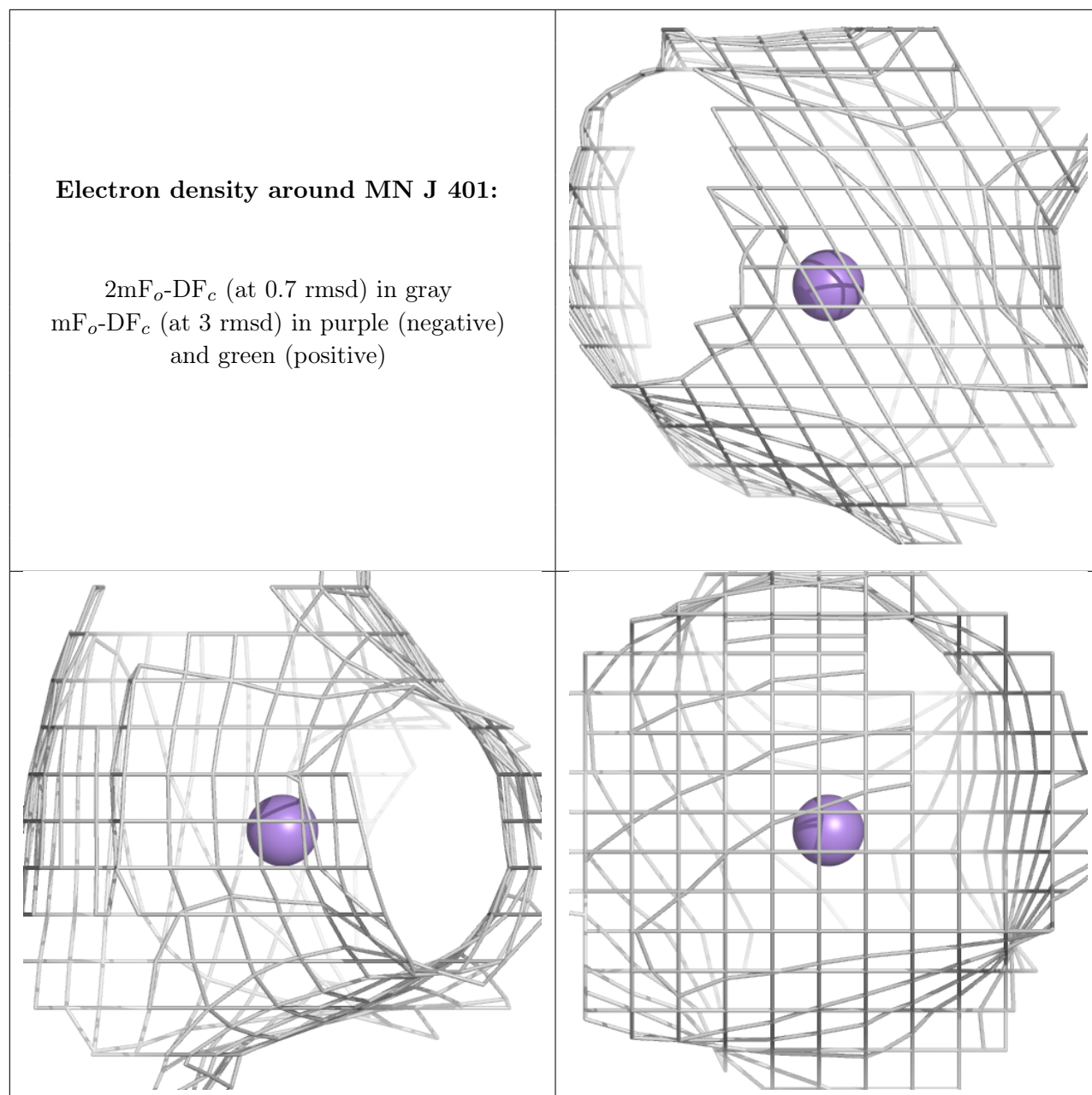
$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around MN J 401:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.