Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2024 – 02:40 PM EST

PDB ID	:	8SP2
Title	:	Crystal structure of metformin hydrolase (MfmAB) from Pseudomonas mendocina sp. MET-2 apo form
Authors	:	Tassoulas, L.J.; Rankin, J.A.; Elias, M.H.; Wackett, L.P.
Deposited on	:	2023-05-01
Resolution	:	2.20 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:

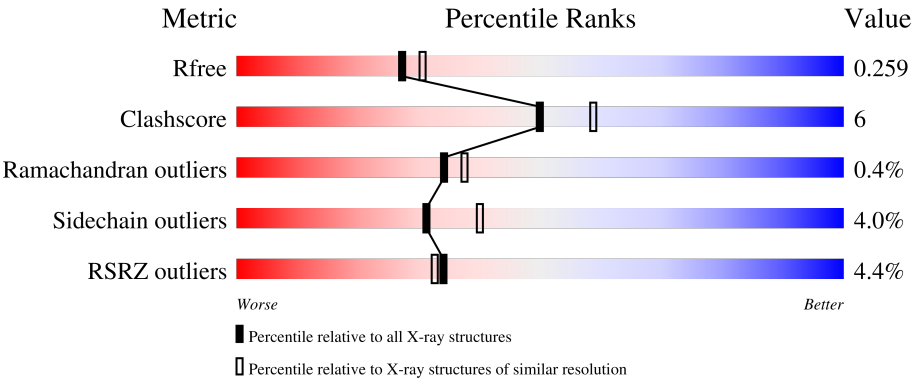
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	348	3% 85% 9% • 5%
1	B	348	4% 83% 10% •• 5%
1	C	348	4% 83% 11% • 5%
1	D	348	4% 79% 14% • 5%
1	E	348	5% 83% 11% • 5%

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Mol	Chain	Length	Quality of chain
1	F	348	8% 79% 15% • 5%
1	K	348	14% 78% 16% • 5%
1	L	348	5% 82% 11% • 5%
2	G	364	% 82% 12% • 5%
2	H	364	% 84% 10% • 5%
2	I	364	2% 79% 15% • 5%
2	J	364	% 79% 13% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 32022 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 metformin hydrolase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2535	1595	444	477	19			
1	B	331	Total	C	N	O	S	0	0	0
			2535	1595	444	477	19			
1	C	331	Total	C	N	O	S	0	0	0
			2535	1595	444	477	19			
1	D	331	Total	C	N	O	S	0	0	0
			2535	1595	444	477	19			
1	E	331	Total	C	N	O	S	0	0	0
			2535	1595	444	477	19			
1	F	331	Total	C	N	O	S	0	0	0
			2535	1595	444	477	19			
1	K	331	Total	C	N	O	S	0	0	0
			2535	1595	444	477	19			
1	L	331	Total	C	N	O	S	0	0	0
			2535	1595	444	477	19			

- Molecule 2 is a protein called metformin hydrolase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	346	Total	C	N	O	S	0	0	0
			2706	1706	474	503	23			
2	H	346	Total	C	N	O	S	0	0	0
			2706	1706	474	503	23			
2	I	346	Total	C	N	O	S	0	0	0
			2706	1706	474	503	23			
2	J	346	Total	C	N	O	S	0	0	0
			2706	1706	474	503	23			

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	2	Total Ni 2 2	0	0
3	H	2	Total Ni 2 2	0	0
3	I	2	Total Ni 2 2	0	0
3	J	2	Total Ni 2 2	0	0

- Molecule 4 is water.

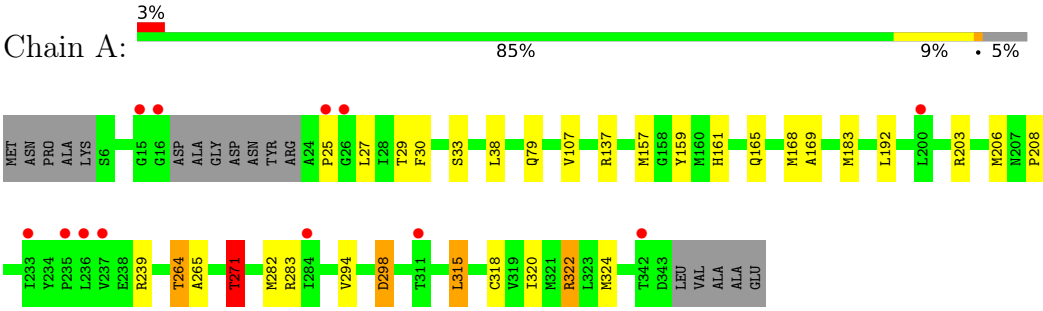
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	89	Total O 89 89	0	0
4	B	100	Total O 100 100	0	0
4	C	79	Total O 79 79	0	0
4	D	76	Total O 76 76	0	0
4	E	42	Total O 42 42	0	0
4	F	40	Total O 40 40	0	0
4	G	114	Total O 114 114	0	0
4	H	112	Total O 112 112	0	0
4	I	88	Total O 88 88	0	0
4	J	87	Total O 87 87	0	0
4	K	35	Total O 35 35	0	0
4	L	48	Total O 48 48	0	0

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.

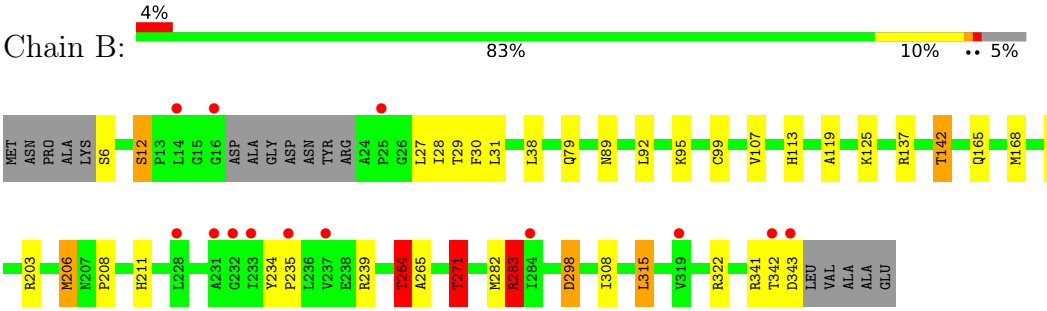
• Molecule 1: metformin hydrolase subunit B

Chain A:



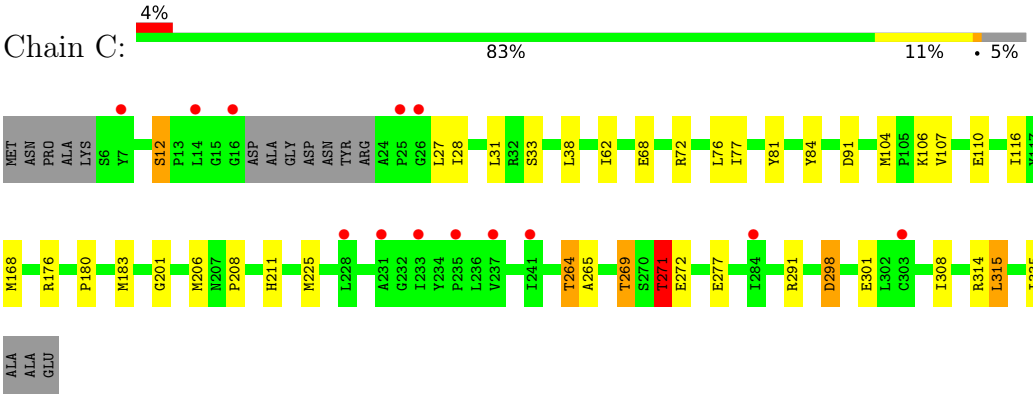
• Molecule 1: metformin hydrolase subunit B

Chain B:



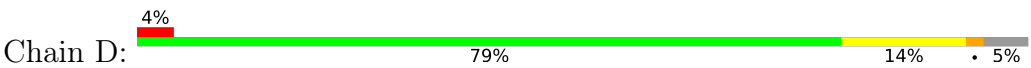
• Molecule 1: metformin hydrolase subunit B

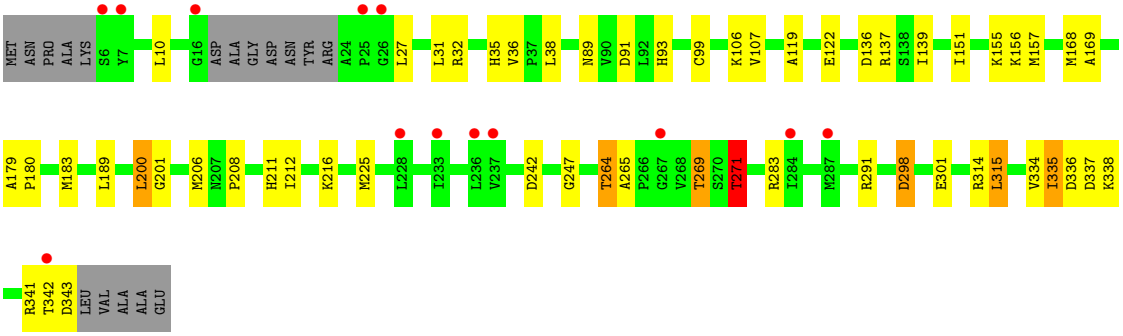
Chain C:



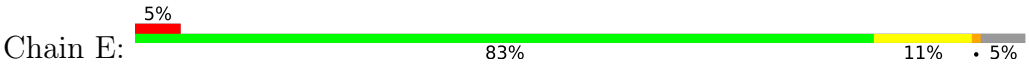
• Molecule 1: metformin hydrolase subunit B

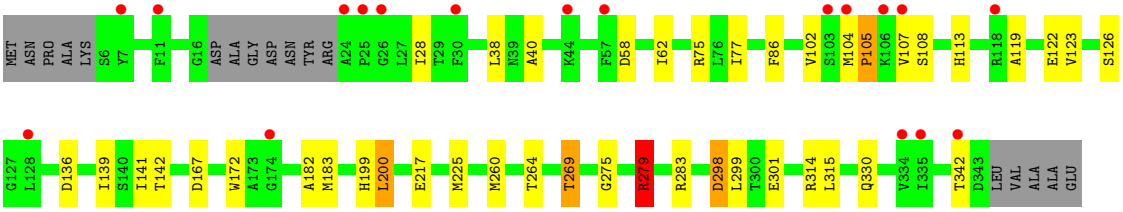
Chain D:



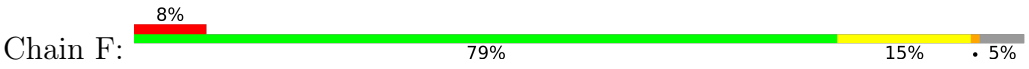


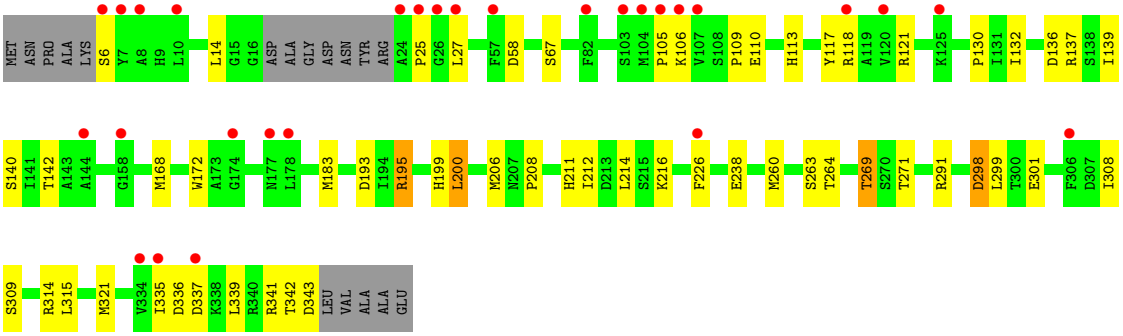
• Molecule 1: metformin hydrolase subunit B



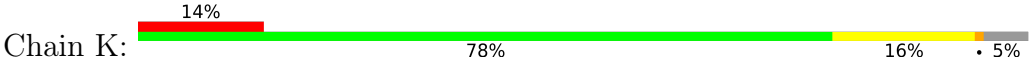


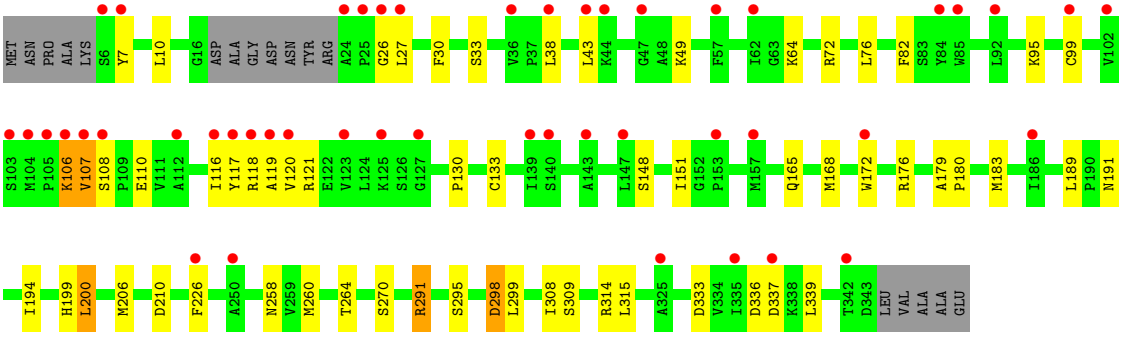
• Molecule 1: metformin hydrolase subunit B





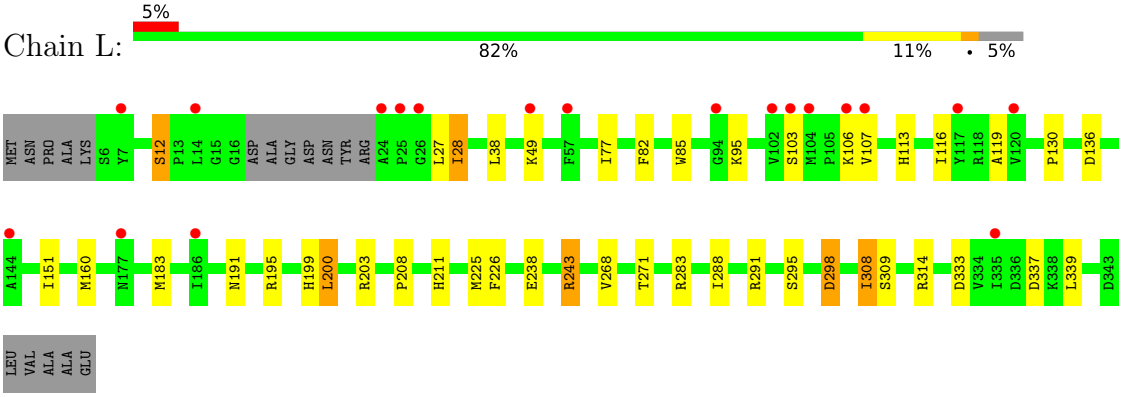
• Molecule 1: metformin hydrolase subunit B





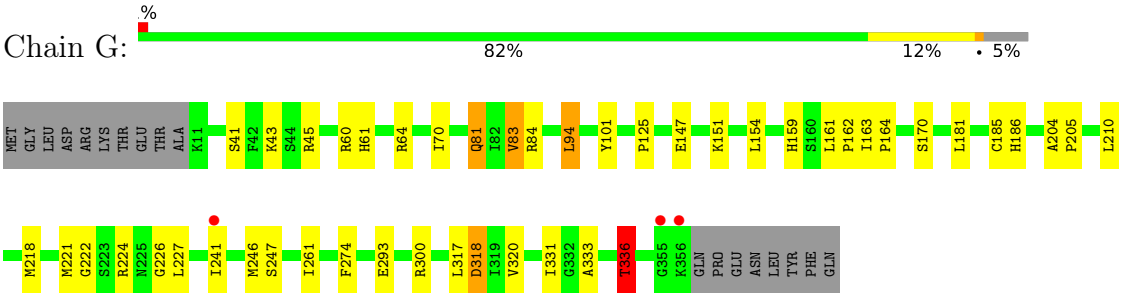
• Molecule 1: metformin hydrolase subunit B

Chain L:



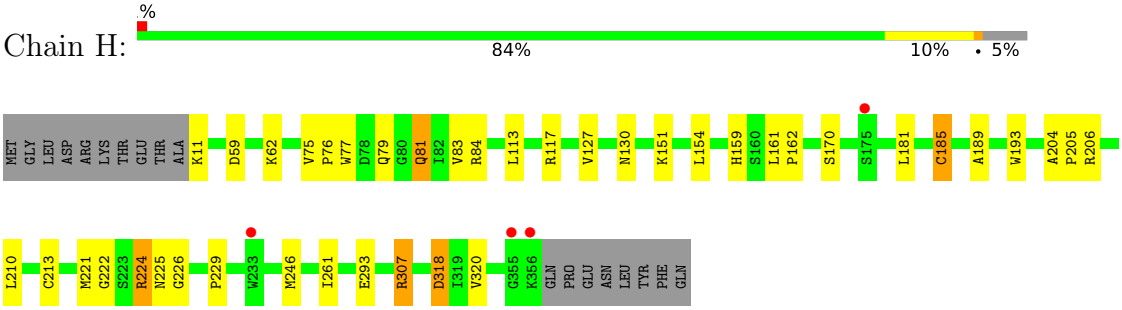
• Molecule 2: metformin hydrolase subunit A

Chain G:



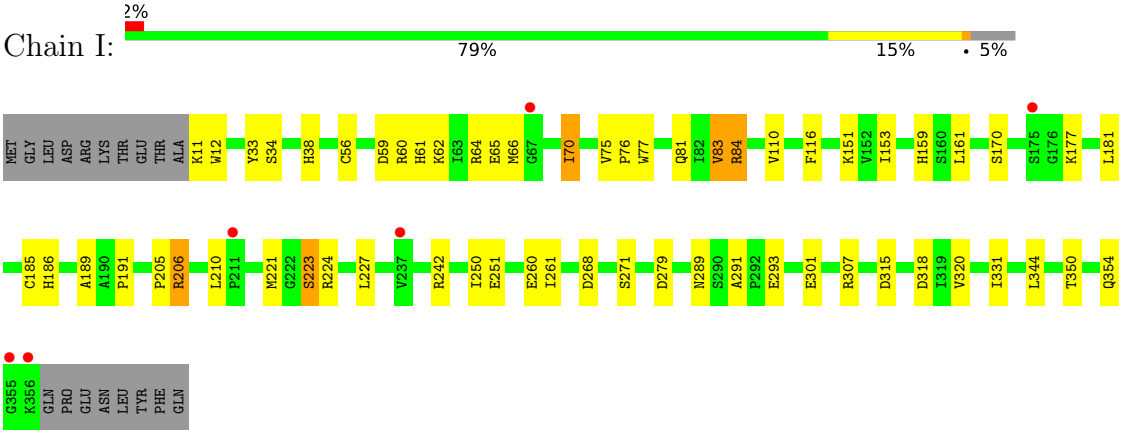
• Molecule 2: metformin hydrolase subunit A

Chain H:



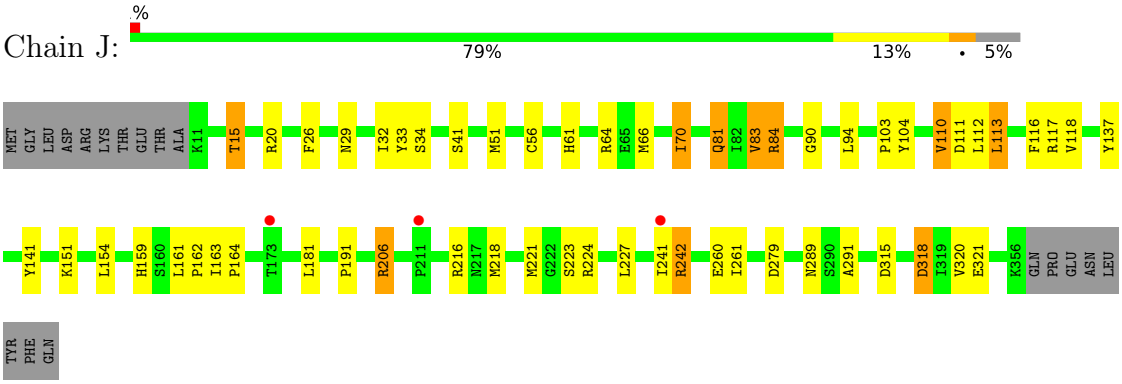
• Molecule 2: metformin hydrolase subunit A

Chain I:



• Molecule 2: metformin hydrolase subunit A

Chain J:


%
79%
13%
5%
MET GLY LEU ASP ARG LYS THR GLU THR ALA K11 T15 R20 F26 N29 I32 Y33 S34 S41 M51 C56 H61 R64 E65 M66 I70 Q81 I82 V83 R84 G90 L94 P103 Y104 V110 D111 L112 L113 F116 R117 V118 Y137
Y141 K151 L154 H159 S160 L161 P162 I163 P164 T173 L181 P191 R206 P211 R216 N217 M218 M221 G222 S223 R224 L227 I241 R242 E260 I261 D279 N289 S290 A291 D315 D318 I319 V320 E321 K356 GLN PRO GLU ASN LEU
TYR PHE GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	103.53Å 107.88Å 114.51Å 93.43° 97.62° 98.11°	Depositor
Resolution (Å)	74.61 – 2.20 74.61 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.2 (74.61-2.20) 91.2 (74.61-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.212 , 0.257 0.218 , 0.259	Depositor DCC
R_{free} test set	11220 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	32022	wwPDB-VP
Average B, all atoms (Å^2)	52.0	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 76.81 % 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 9.6659e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: NI

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	0.37	0/2587	0.68	1/3499 (0.0%)
1	B	0.37	0/2587	0.69	2/3499 (0.1%)
1	C	0.38	0/2587	0.70	1/3499 (0.0%)
1	D	0.35	0/2587	0.67	1/3499 (0.0%)
1	E	0.33	0/2587	0.65	1/3499 (0.0%)
1	F	0.33	0/2587	0.62	0/3499
1	K	0.32	0/2587	0.61	0/3499
1	L	0.32	0/2587	0.63	1/3499 (0.0%)
2	G	0.37	0/2778	0.71	2/3765 (0.1%)
2	H	0.36	0/2778	0.70	0/3765
2	I	0.35	0/2778	0.68	0/3765
2	J	0.34	0/2778	0.68	0/3765
All	All	0.35	0/31808	0.67	9/43052 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	3
1	E	0	1
1	F	0	2
1	K	0	1
2	G	0	1
2	H	0	3
2	I	0	1
2	J	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	18

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	279	ARG	CB-CG-CD	-6.85	93.79	111.60
1	B	271	THR	CB-CA-C	-6.54	93.93	111.60
1	C	271	THR	CB-CA-C	-6.35	94.45	111.60
1	D	271	THR	CB-CA-C	-6.10	95.14	111.60
1	A	271	THR	CB-CA-C	-5.74	96.09	111.60
2	G	43	LYS	CB-CA-C	-5.67	99.05	110.40
2	G	336	THR	N-CA-CB	-5.16	100.50	110.30
1	B	264	THR	CB-CA-C	-5.04	97.98	111.60
1	L	226	PHE	CB-CA-C	5.04	120.48	110.40

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ARG	Sidechain
1	B	283	ARG	Sidechain
1	C	137	ARG	Sidechain
1	C	291	ARG	Sidechain
1	D	137	ARG	Sidechain
1	D	283	ARG	Sidechain
1	D	314	ARG	Sidechain
1	E	279	ARG	Sidechain
1	F	137	ARG	Sidechain
1	F	58	ASP	Peptide
2	G	45	ARG	Sidechain
2	H	117	ARG	Sidechain
2	H	206	ARG	Sidechain
2	H	307	ARG	Sidechain
2	I	206	ARG	Sidechain
2	J	117	ARG	Sidechain
2	J	206	ARG	Sidechain
1	K	291	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2535	0	2497	22	0
1	B	2535	0	2497	27	0
1	C	2535	0	2497	30	0
1	D	2535	0	2497	29	0
1	E	2535	0	2497	26	0
1	F	2535	0	2497	33	0
1	K	2535	0	2497	42	0
1	L	2535	0	2497	29	0
2	G	2706	0	2592	28	0
2	H	2706	0	2592	30	0
2	I	2706	0	2592	38	0
2	J	2706	0	2592	46	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
4	A	89	0	0	1	0
4	B	100	0	0	4	0
4	C	79	0	0	2	0
4	D	76	0	0	0	0
4	E	42	0	0	0	0
4	F	40	0	0	1	0
4	G	114	0	0	1	0
4	H	112	0	0	5	0
4	I	88	0	0	0	0
4	J	87	0	0	3	0
4	K	35	0	0	2	0
4	L	48	0	0	1	0
All	All	32022	0	30344	357	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 6.

All (357) 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)
2:J:56:CYS:SG	2:J:66:MET:HE3	2.09	0.92
2:J:56:CYS:SG	2:J:66:MET:CE	2.63	0.87
2:G:333:ALA:O	2:G:336:THR:HG22	1.79	0.83
1:C:104:MET:HE3	1:C:116:ILE:HG13	1.62	0.80
2:H:185:CYS:SG	2:H:293:GLU:HG3	2.22	0.80
2:I:12:TRP:HA	2:I:66:MET:HE2	1.68	0.74
1:A:318:CYS:O	1:A:322:ARG:HG3	1.87	0.74
1:D:269:THR:HG21	1:D:301:GLU:OE1	1.88	0.74
2:J:70:ILE:CD1	2:J:116:PHE:CD1	2.71	0.74
1:E:199:HIS:C	1:E:200:LEU:HD23	2.09	0.73
1:K:199:HIS:C	1:K:200:LEU:HD23	2.09	0.72
2:I:185:CYS:SG	2:I:293:GLU:HG3	2.30	0.72
1:C:264:THR:HG21	1:C:315:LEU:HD13	1.70	0.71
2:I:81:GLN:NE2	2:I:84:ARG:O	2.24	0.71
1:C:269:THR:HG21	1:C:301:GLU:OE1	1.91	0.71
1:K:199:HIS:HD2	4:K:430:HOH:O	1.73	0.71
1:L:199:HIS:C	1:L:200:LEU:HD23	2.11	0.70
1:F:269:THR:HG21	1:F:301:GLU:OE1	1.92	0.69
2:J:32:ILE:HD12	2:J:104:TYR:HB2	1.73	0.69
1:A:165:GLN:HE21	1:A:206:MET:CE	2.06	0.69
1:K:30:PHE:O	1:K:33:SER:OG	2.10	0.68
1:E:269:THR:HG21	1:E:301:GLU:OE1	1.93	0.68
2:J:32:ILE:CD1	2:J:104:TYR:HB2	2.23	0.68
1:F:263:SER:OG	4:F:401:HOH:O	2.11	0.68
1:D:151:ILE:O	1:D:155:LYS:HG3	1.94	0.67
2:I:221:MET:SD	2:I:261:ILE:HG12	2.35	0.67
2:I:350:THR:O	2:I:354:GLN:HG3	1.94	0.67
2:J:242:ARG:NH2	2:J:260:GLU:OE2	2.23	0.67
2:J:32:ILE:HD11	2:J:111:ASP:CG	2.14	0.67
1:A:239:ARG:HD2	4:A:459:HOH:O	1.94	0.66
2:G:181:LEU:HD13	2:G:261:ILE:CD1	2.26	0.65
2:G:181:LEU:HD13	2:G:261:ILE:HD13	1.77	0.65
2:H:213:CYS:O	4:H:501:HOH:O	2.14	0.65
1:A:271:THR:HG21	2:I:331:ILE:HG22	1.76	0.65
2:J:181:LEU:HD13	2:J:261:ILE:CD1	2.26	0.65
2:J:191:PRO:O	2:J:206:ARG:NH2	2.29	0.65
1:K:133:CYS:SG	1:K:299:LEU:HD11	2.36	0.65
2:H:307:ARG:NH1	4:H:502:HOH:O	2.30	0.65
1:E:279:ARG:HD2	2:I:250:ILE:HD13	1.77	0.64
2:H:81:GLN:HE22	2:H:84:ARG:N	1.95	0.64
1:L:38:LEU:HD21	1:L:119:ALA:HB1	1.79	0.64
1:B:208:PRO:HG2	1:B:211:HIS:CD2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ILE:HG22	1:A:324:MET:CE	2.27	0.64
2:H:181:LEU:HD13	2:H:261:ILE:HD13	1.80	0.64
1:F:199:HIS:C	1:F:200:LEU:HD23	2.17	0.64
1:E:113:HIS:CD2	1:E:142:THR:HG21	2.33	0.63
1:L:195:ARG:O	1:L:243:ARG:HG2	1.99	0.62
1:C:81:TYR:HA	1:K:206:MET:HE1	1.81	0.62
1:F:113:HIS:ND1	1:F:142:THR:HG21	2.14	0.62
1:F:200:LEU:HD23	1:F:200:LEU:N	2.14	0.62
1:A:165:GLN:HE21	1:A:206:MET:HE3	1.65	0.61
2:J:151:LYS:HD2	2:J:315:ASP:HA	1.82	0.61
2:I:12:TRP:HA	2:I:66:MET:CE	2.29	0.61
1:C:271:THR:HG21	2:G:331:ILE:HG22	1.81	0.61
2:J:81:GLN:HE22	2:J:84:ARG:N	1.99	0.61
1:F:130:PRO:HB2	1:F:132:ILE:HD11	1.81	0.61
1:F:336:ASP:HB3	1:F:339:LEU:CD1	2.31	0.60
2:I:242:ARG:NH2	2:I:260:GLU:OE2	2.29	0.60
2:J:56:CYS:CB	2:J:66:MET:HE1	2.32	0.60
1:K:95:LYS:HE2	1:K:333:ASP:OD2	2.01	0.60
1:B:38:LEU:HD21	1:B:119:ALA:HB1	1.84	0.60
1:D:208:PRO:HG2	1:D:211:HIS:CD2	2.37	0.60
2:J:110:VAL:HG22	2:J:112:LEU:HD23	1.83	0.60
1:A:157:MET:HG2	1:A:192:LEU:HD13	1.84	0.60
1:K:165:GLN:HE21	1:K:258:ASN:HD21	1.50	0.60
1:L:49:LYS:HE2	1:L:49:LYS:HA	1.84	0.59
1:B:38:LEU:HD21	1:B:119:ALA:CB	2.32	0.59
1:C:208:PRO:HG2	1:C:211:HIS:CD2	2.37	0.59
1:L:200:LEU:HD23	1:L:200:LEU:N	2.17	0.59
2:I:181:LEU:HD13	2:I:261:ILE:HD13	1.84	0.59
1:A:208:PRO:HG2	1:A:211:HIS:CD2	2.37	0.59
2:I:191:PRO:O	2:I:206:ARG:NH2	2.35	0.59
2:G:60:ARG:NH1	2:G:147:GLU:HG2	2.17	0.59
1:D:264:THR:HG21	1:D:315:LEU:HD13	1.83	0.58
1:B:264:THR:HG21	1:B:315:LEU:HD13	1.84	0.58
1:E:200:LEU:HD23	1:E:200:LEU:N	2.18	0.58
2:J:56:CYS:SG	2:J:66:MET:HE1	2.43	0.58
2:H:222:GLY:HA2	2:H:246:MET:HE2	1.85	0.58
1:A:29:THR:O	1:A:79:GLN:NE2	2.37	0.58
2:G:221:MET:SD	2:G:261:ILE:HG12	2.42	0.58
2:G:81:GLN:HE22	2:G:84:ARG:N	2.01	0.58
1:K:264:THR:HG22	1:K:315:LEU:HD22	1.85	0.58
1:D:212:ILE:HG22	1:D:216:LYS:HE2	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:226:GLY:O	1:K:82:PHE:HB2	2.04	0.57
1:C:91:ASP:N	1:C:335:ILE:HD11	2.19	0.57
1:E:264:THR:HG22	1:E:315:LEU:HD22	1.85	0.57
2:G:218:MET:CE	2:G:241:ILE:HD13	2.34	0.57
2:I:11:LYS:HE3	2:I:65:GLU:OE1	2.03	0.57
2:H:59:ASP:OD2	2:H:62:LYS:HG2	2.04	0.57
1:K:38:LEU:HD21	1:K:119:ALA:HB1	1.86	0.56
1:K:336:ASP:HB3	1:K:339:LEU:HD13	1.86	0.56
1:A:318:CYS:O	1:A:322:ARG:CG	2.53	0.56
2:H:181:LEU:HD13	2:H:261:ILE:CD1	2.36	0.56
1:E:40:ALA:N	1:E:122:GLU:OE1	2.39	0.56
2:I:59:ASP:OD2	2:I:62:LYS:HG2	2.05	0.56
1:F:208:PRO:HG2	1:F:211:HIS:CD2	2.41	0.56
2:I:181:LEU:HD13	2:I:261:ILE:CD1	2.36	0.56
2:J:218:MET:HE2	2:J:241:ILE:HD13	1.88	0.56
1:L:49:LYS:O	1:L:49:LYS:HD3	2.06	0.56
1:K:148:SER:CB	1:K:189:LEU:HD12	2.36	0.55
2:G:61:HIS:ND1	2:G:64:ARG:NH2	2.54	0.55
2:G:222:GLY:HA2	2:G:246:MET:HE2	1.89	0.55
2:H:226:GLY:O	1:L:82:PHE:HB2	2.07	0.55
2:I:12:TRP:CA	2:I:66:MET:HE2	2.37	0.55
1:L:95:LYS:HE2	1:L:333:ASP:OD2	2.07	0.55
1:K:200:LEU:HD23	1:K:200:LEU:N	2.20	0.55
1:D:200:LEU:HD23	1:D:200:LEU:N	2.22	0.54
1:F:168:MET:HG3	1:F:214:LEU:HD23	1.89	0.54
1:C:264:THR:CG2	1:C:315:LEU:HD13	2.37	0.54
2:J:15:THR:HG21	2:J:20:ARG:HG2	1.88	0.54
1:E:62:ILE:HD13	1:E:172:TRP:CZ2	2.43	0.54
2:J:242:ARG:HG3	2:J:242:ARG:HH11	1.72	0.54
2:I:61:HIS:ND1	2:I:64:ARG:NH2	2.55	0.54
2:I:307:ARG:HG2	2:I:307:ARG:HH11	1.73	0.53
2:J:61:HIS:ND1	2:J:64:ARG:NH2	2.56	0.53
1:K:151:ILE:HD11	1:K:191:ASN:ND2	2.23	0.53
1:F:269:THR:HG23	1:F:301:GLU:HB3	1.91	0.53
2:H:221:MET:SD	2:H:261:ILE:HG12	2.48	0.53
1:L:308:ILE:HD12	1:L:308:ILE:N	2.23	0.53
1:B:30:PHE:CE2	1:B:31:LEU:HD12	2.43	0.53
1:E:123:VAL:O	1:E:126:SER:OG	2.20	0.53
1:K:308:ILE:N	1:K:308:ILE:HD12	2.24	0.53
1:B:239:ARG:HD2	4:B:441:HOH:O	2.09	0.53
2:J:56:CYS:HB2	2:J:66:MET:HE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:320:VAL:HG23	2:J:321:GLU:HG2	1.91	0.53
2:J:70:ILE:HD12	2:J:116:PHE:CD1	2.43	0.53
1:F:264:THR:HG22	1:F:315:LEU:HD22	1.90	0.52
1:F:109:PRO:HD2	1:F:110:GLU:OE2	2.09	0.52
1:F:238:GLU:OE2	1:F:291:ARG:NH2	2.43	0.52
2:G:185:CYS:SG	2:G:293:GLU:HG3	2.50	0.52
1:D:38:LEU:HD13	1:D:99:CYS:HB3	1.91	0.52
2:I:75:VAL:HG11	2:I:161:LEU:HD13	1.90	0.52
2:I:159:HIS:CD2	2:I:320:VAL:HG21	2.45	0.52
1:K:26:GLY:O	1:K:27:LEU:HB2	2.10	0.52
2:J:56:CYS:HB2	2:J:66:MET:CE	2.40	0.51
1:B:29:THR:O	1:B:79:GLN:NE2	2.43	0.51
1:F:110:GLU:OE2	1:F:110:GLU:N	2.42	0.51
2:H:159:HIS:CD2	2:H:320:VAL:HG21	2.45	0.51
1:L:283:ARG:NH1	4:L:403:HOH:O	2.42	0.51
2:J:159:HIS:CG	2:J:320:VAL:HG21	2.45	0.51
1:F:130:PRO:HB2	1:F:132:ILE:CD1	2.40	0.51
1:B:12:SER:HB3	1:F:172:TRP:CE3	2.45	0.51
1:B:298:ASP:C	1:B:298:ASP:OD1	2.50	0.51
1:C:269:THR:HG23	1:C:301:GLU:HB3	1.93	0.51
1:K:298:ASP:OD1	1:K:298:ASP:C	2.49	0.51
1:A:298:ASP:OD1	1:A:298:ASP:C	2.50	0.50
1:D:269:THR:HG23	1:D:301:GLU:HB3	1.93	0.50
1:E:102:VAL:HG12	1:E:104:MET:CE	2.42	0.50
2:I:170:SER:HB2	2:I:210:LEU:HD13	1.93	0.50
1:B:113:HIS:ND1	1:B:142:THR:HG21	2.26	0.49
1:F:14:LEU:HD23	1:F:341:ARG:NH2	2.27	0.49
2:G:170:SER:HB2	2:G:210:LEU:HD13	1.93	0.49
1:C:265:ALA:O	1:C:271:THR:HG23	2.13	0.49
1:E:279:ARG:NH2	2:I:301:GLU:OE2	2.40	0.49
1:F:168:MET:SD	1:F:183:MET:HB3	2.52	0.49
2:I:81:GLN:NE2	2:I:84:ARG:C	2.65	0.49
2:J:70:ILE:HD13	2:J:116:PHE:CG	2.47	0.49
2:J:159:HIS:CD2	2:J:320:VAL:HG21	2.47	0.49
2:H:185:CYS:HB2	2:H:224:ARG:HD3	1.95	0.49
2:J:56:CYS:CB	2:J:66:MET:CE	2.90	0.49
1:C:106:LYS:NZ	4:C:408:HOH:O	2.45	0.49
1:E:298:ASP:C	1:E:298:ASP:OD1	2.51	0.48
2:I:159:HIS:CG	2:I:320:VAL:HG21	2.48	0.48
1:K:49:LYS:NZ	4:K:404:HOH:O	2.45	0.48
1:L:160:MET:HE3	1:L:288:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:193:TRP:CE3	1:L:12:SER:HB2	2.48	0.48
1:F:117:TYR:CE2	1:F:121:ARG:HG3	2.48	0.48
2:H:307:ARG:NH2	4:H:509:HOH:O	2.45	0.48
1:B:168:MET:SD	1:B:183:MET:HB3	2.53	0.48
1:C:298:ASP:OD1	1:C:298:ASP:C	2.52	0.48
1:F:200:LEU:N	1:F:200:LEU:CD2	2.77	0.48
2:J:279:ASP:HB3	2:J:289:ASN:ND2	2.28	0.48
1:L:77:ILE:HG21	1:L:314:ARG:HA	1.95	0.48
2:J:181:LEU:HD13	2:J:261:ILE:HD13	1.96	0.47
2:H:189:ALA:HA	2:H:205:PRO:CD	2.44	0.47
2:I:186:HIS:NE2	2:I:227:LEU:HD23	2.28	0.47
1:B:27:LEU:HD12	1:B:28:ILE:H	1.79	0.47
1:D:168:MET:SD	1:D:183:MET:HB3	2.55	0.47
1:D:298:ASP:OD1	1:D:298:ASP:C	2.53	0.47
2:G:70:ILE:HD13	2:G:151:LYS:HB2	1.97	0.47
2:H:189:ALA:HA	2:H:205:PRO:HD3	1.96	0.47
2:I:279:ASP:HB3	2:I:289:ASN:ND2	2.29	0.47
1:L:268:VAL:HG22	1:L:271:THR:HG22	1.96	0.47
1:C:308:ILE:HG23	1:K:308:ILE:HG12	1.97	0.47
2:J:29:ASN:ND2	4:J:508:HOH:O	2.47	0.47
1:D:201:GLY:HA2	1:D:225:MET:HE1	1.96	0.47
2:G:218:MET:HE2	2:G:241:ILE:HD13	1.95	0.47
2:I:177:LYS:NZ	2:I:268:ASP:O	2.46	0.47
1:L:106:LYS:O	1:L:107:VAL:C	2.53	0.47
1:A:264:THR:HG21	1:A:315:LEU:HD13	1.97	0.47
1:C:272:GLU:OE1	2:G:101:TYR:OH	2.28	0.47
1:D:200:LEU:N	1:D:200:LEU:CD2	2.78	0.47
1:F:309:SER:O	1:F:314:ARG:NH1	2.48	0.47
2:H:170:SER:HB2	2:H:210:LEU:HD13	1.95	0.47
2:I:70:ILE:CD1	2:I:116:PHE:CD1	2.98	0.47
1:B:137:ARG:NH1	4:B:406:HOH:O	2.48	0.47
1:L:298:ASP:C	1:L:298:ASP:OD1	2.53	0.47
1:K:309:SER:O	1:K:314:ARG:NH1	2.44	0.46
1:F:298:ASP:OD1	1:F:298:ASP:C	2.54	0.46
2:J:161:LEU:N	2:J:162:PRO:HD2	2.31	0.46
1:F:260:MET:HG3	1:F:315:LEU:HD21	1.96	0.46
2:G:159:HIS:CG	2:G:320:VAL:HG21	2.50	0.46
1:C:110:GLU:CD	1:C:110:GLU:H	2.18	0.46
2:G:274:PHE:CD2	2:G:317:LEU:HD13	2.51	0.46
1:D:91:ASP:OD2	1:D:93:HIS:HB3	2.16	0.46
2:G:161:LEU:N	2:G:162:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PRO:O	1:K:27:LEU:HD12	2.15	0.46
1:B:283:ARG:NH1	4:B:401:HOH:O	2.25	0.46
1:C:176:ARG:NH1	4:C:409:HOH:O	2.46	0.46
1:E:77:ILE:HG21	1:E:314:ARG:HA	1.97	0.46
1:A:168:MET:SD	1:A:183:MET:HB3	2.55	0.46
1:A:320:ILE:HG22	1:A:324:MET:HE2	1.97	0.46
2:J:70:ILE:CD1	2:J:116:PHE:CG	2.99	0.46
1:K:116:ILE:O	1:K:120:VAL:HG23	2.16	0.46
1:E:86:PHE:HZ	2:I:223:SER:HB2	1.80	0.46
2:G:204:ALA:HB3	2:G:205:PRO:HD3	1.97	0.46
2:H:225:ASN:HA	1:L:85:TRP:CZ3	2.51	0.46
2:I:153:ILE:HD11	2:I:344:LEU:HD21	1.98	0.46
2:H:76:PRO:HD2	4:H:582:HOH:O	2.15	0.45
2:I:56:CYS:HB2	2:I:66:MET:SD	2.55	0.45
1:E:113:HIS:CG	1:E:142:THR:HG21	2.51	0.45
2:J:32:ILE:HD11	2:J:111:ASP:CB	2.47	0.45
2:J:103:PRO:O	2:J:112:LEU:HG	2.16	0.45
1:L:200:LEU:N	1:L:200:LEU:CD2	2.80	0.45
2:H:204:ALA:HB3	2:H:205:PRO:HD3	1.97	0.45
2:J:32:ILE:HD13	2:J:104:TYR:HB2	1.98	0.45
1:D:336:ASP:OD2	1:D:338:LYS:HB2	2.17	0.45
1:D:264:THR:CG2	1:D:315:LEU:HD13	2.47	0.45
1:D:35:HIS:CD2	1:D:35:HIS:C	2.90	0.45
1:B:264:THR:CG2	1:B:315:LEU:HD13	2.46	0.45
1:F:193:ASP:OD1	1:F:195:ARG:HB2	2.17	0.45
2:H:159:HIS:CG	2:H:320:VAL:HG21	2.51	0.45
1:B:234:TYR:N	1:B:235:PRO:CD	2.80	0.45
1:F:140:SER:OG	1:F:298:ASP:OD2	2.23	0.45
1:K:38:LEU:HD13	1:K:99:CYS:HB3	1.97	0.45
1:B:308:ILE:HG23	1:F:308:ILE:HG12	1.97	0.45
1:F:212:ILE:HG22	1:F:216:LYS:HE2	1.97	0.45
1:K:38:LEU:HD21	1:K:119:ALA:CB	2.47	0.45
1:K:7:TYR:HB3	1:K:10:LEU:HD23	1.98	0.44
4:G:547:HOH:O	1:K:264:THR:HG23	2.17	0.44
2:J:51:MET:O	2:J:51:MET:HG2	2.17	0.44
1:C:201:GLY:HA2	1:C:225:MET:HE1	1.98	0.44
2:H:154:LEU:O	2:H:318:ASP:HA	2.18	0.44
2:J:33:TYR:O	2:J:34:SER:C	2.56	0.44
1:K:260:MET:HG3	1:K:315:LEU:HD21	1.98	0.44
1:B:179:ALA:N	1:B:180:PRO:HD2	2.33	0.44
1:D:136:ASP:O	1:D:139:ILE:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:ASP:O	1:E:139:ILE:HG23	2.18	0.44
2:G:159:HIS:CD2	2:G:320:VAL:HG21	2.53	0.44
1:C:104:MET:HE3	1:C:116:ILE:CG1	2.40	0.44
1:C:308:ILE:CG2	1:K:308:ILE:HD13	2.48	0.44
1:E:28:ILE:HG22	1:E:75:ARG:HD3	1.99	0.44
1:E:107:VAL:HG12	1:E:107:VAL:O	2.17	0.44
2:G:163:ILE:HB	2:G:164:PRO:CD	2.48	0.44
2:H:307:ARG:CZ	4:H:502:HOH:O	2.64	0.44
1:C:84:TYR:CE1	1:C:335:ILE:HD13	2.53	0.44
1:F:113:HIS:ND1	1:F:142:THR:CG2	2.78	0.44
1:D:38:LEU:HD21	1:D:119:ALA:HB1	1.99	0.44
1:A:159:TYR:CE1	1:A:161:HIS:HB2	2.53	0.43
2:H:193:TRP:CZ3	1:L:12:SER:HB2	2.52	0.43
2:J:90:GLY:HA3	4:J:540:HOH:O	2.17	0.43
2:J:94:LEU:HD13	2:J:94:LEU:C	2.38	0.43
1:A:165:GLN:HE21	1:A:206:MET:HE2	1.81	0.43
1:B:265:ALA:O	1:B:271:THR:HG23	2.17	0.43
1:F:321:MET:HB2	1:F:321:MET:HE2	1.85	0.43
2:J:83:VAL:HG12	2:J:84:ARG:HG3	2.01	0.43
1:C:12:SER:HB3	1:K:172:TRP:CE3	2.54	0.43
2:H:76:PRO:O	2:H:77:TRP:C	2.55	0.43
1:A:265:ALA:O	1:A:271:THR:HG23	2.17	0.43
1:B:203:ARG:HB2	4:B:430:HOH:O	2.18	0.43
1:D:179:ALA:N	1:D:180:PRO:HD2	2.33	0.43
2:I:189:ALA:HA	2:I:205:PRO:CD	2.49	0.43
1:D:341:ARG:C	1:D:343:ASP:H	2.21	0.43
1:E:225:MET:HE3	1:E:275:GLY:HA2	2.01	0.43
2:G:94:LEU:HG	2:G:336:THR:HG23	1.99	0.43
2:G:154:LEU:O	2:G:318:ASP:HA	2.19	0.43
1:K:117:TYR:CE1	1:K:121:ARG:HG3	2.53	0.43
2:H:75:VAL:HG11	2:H:161:LEU:HD13	2.00	0.43
1:L:309:SER:O	1:L:314:ARG:NH1	2.40	0.43
1:D:269:THR:CG2	1:D:301:GLU:OE1	2.63	0.43
1:A:203:ARG:HH11	1:A:225:MET:HE2	1.83	0.42
1:C:168:MET:SD	1:C:183:MET:HB3	2.59	0.42
1:B:38:LEU:HD13	1:B:99:CYS:HB3	2.02	0.42
1:C:84:TYR:HE1	1:C:335:ILE:HD13	1.83	0.42
2:J:41:SER:HB2	4:J:570:HOH:O	2.18	0.42
1:L:203:ARG:HH11	1:L:225:MET:HE2	1.84	0.42
1:C:27:LEU:HD13	1:C:28:ILE:N	2.34	0.42
2:I:289:ASN:HD22	2:I:291:ALA:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:ALA:O	1:D:271:THR:HG23	2.18	0.42
2:H:77:TRP:CH2	2:H:79:GLN:HB2	2.55	0.42
1:B:92:LEU:HA	1:B:95:LYS:HG3	2.00	0.42
1:B:165:GLN:HE21	1:B:206:MET:HE2	1.84	0.42
1:K:64:LYS:N	1:K:64:LYS:HD2	2.34	0.42
1:C:269:THR:CG2	1:C:301:GLU:OE1	2.65	0.42
2:H:127:VAL:HG12	2:H:130:ASN:HB3	2.01	0.42
2:H:161:LEU:N	2:H:162:PRO:HD2	2.34	0.42
2:J:113:LEU:HA	2:J:118:VAL:HG13	2.01	0.42
2:J:137:TYR:O	2:J:141:TYR:HD1	2.03	0.42
1:D:242:ASP:OD2	1:D:291:ARG:NH2	2.52	0.42
2:J:163:ILE:HB	2:J:164:PRO:CD	2.49	0.42
1:B:27:LEU:HD12	1:B:28:ILE:N	2.35	0.42
1:E:141:ILE:HD11	1:E:182:ALA:HA	2.01	0.41
2:I:33:TYR:O	2:I:34:SER:C	2.58	0.41
1:K:106:LYS:O	1:K:107:VAL:C	2.58	0.41
1:L:203:ARG:NH1	1:L:225:MET:HE2	2.35	0.41
1:D:89:ASN:O	1:D:334:VAL:HG13	2.20	0.41
2:J:289:ASN:HD22	2:J:291:ALA:H	1.68	0.41
1:L:199:HIS:C	1:L:200:LEU:CD2	2.85	0.41
1:C:62:ILE:HG12	1:C:180:PRO:HG3	2.01	0.41
1:E:200:LEU:N	1:E:200:LEU:CD2	2.83	0.41
1:F:136:ASP:O	1:F:139:ILE:HG23	2.21	0.41
2:I:151:LYS:CD	2:I:315:ASP:HA	2.50	0.41
2:J:221:MET:CE	2:J:261:ILE:HG12	2.50	0.41
1:K:43:LEU:HD21	1:K:99:CYS:SG	2.60	0.41
1:L:151:ILE:HD11	1:L:191:ASN:ND2	2.36	0.41
1:A:169:ALA:HB2	1:A:211:HIS:HE2	1.85	0.41
1:B:341:ARG:C	1:B:343:ASP:H	2.23	0.41
1:D:35:HIS:CD2	1:D:36:VAL:N	2.89	0.41
1:E:167:ASP:O	1:E:183:MET:HB2	2.20	0.41
1:K:179:ALA:N	1:K:180:PRO:CD	2.83	0.41
1:C:72:ARG:O	1:C:76:LEU:HG	2.20	0.41
2:I:271:SER:HA	2:I:315:ASP:OD2	2.19	0.41
1:L:130:PRO:HD2	1:L:295:SER:O	2.20	0.41
1:L:208:PRO:HD2	1:L:211:HIS:CD2	2.55	0.41
1:E:105:PRO:HG2	1:E:108:SER:HB3	2.02	0.41
1:F:199:HIS:C	1:F:200:LEU:CD2	2.87	0.41
1:F:269:THR:CG2	1:F:301:GLU:OE1	2.67	0.41
1:L:113:HIS:HA	1:L:116:ILE:HD12	2.02	0.41
1:C:277:GLU:HG2	2:G:300:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:186:HIS:CD2	2:G:227:LEU:HD23	2.55	0.41
2:I:76:PRO:O	2:I:77:TRP:C	2.58	0.41
1:L:238:GLU:OE2	1:L:291:ARG:NH2	2.53	0.41
1:K:200:LEU:N	1:K:200:LEU:CD2	2.84	0.41
1:A:30:PHE:HZ	1:A:324:MET:CE	2.34	0.41
1:B:12:SER:HB3	1:F:172:TRP:CZ3	2.56	0.41
1:E:260:MET:HG3	1:E:315:LEU:HD21	2.02	0.41
1:A:315:LEU:O	1:A:315:LEU:HG	2.21	0.40
2:J:154:LEU:O	2:J:318:ASP:HA	2.21	0.40
1:B:282:MET:SD	1:B:322:ARG:HD3	2.61	0.40
1:C:12:SER:OG	1:K:210:ASP:OD2	2.40	0.40
1:C:77:ILE:HG21	1:C:314:ARG:HA	2.03	0.40
1:D:10:LEU:CD1	1:D:335:ILE:HD13	2.51	0.40
1:D:157:MET:HE1	1:D:189:LEU:HD13	2.03	0.40
1:E:38:LEU:HD21	1:E:119:ALA:HB1	2.03	0.40
2:H:229:PRO:HG3	1:L:82:PHE:CZ	2.56	0.40
2:I:60:ARG:O	2:I:64:ARG:HB2	2.22	0.40
1:D:156:LYS:HE2	1:D:247:GLY:O	2.21	0.40
1:D:169:ALA:HB2	1:D:211:HIS:NE2	2.36	0.40
2:G:125:PRO:HB3	2:I:38:HIS:CG	2.56	0.40
1:K:130:PRO:HD2	1:K:295:SER:O	2.21	0.40
1:K:168:MET:SD	1:K:183:MET:HB3	2.61	0.40
1:K:194:ILE:HD12	1:K:194:ILE:HA	1.92	0.40
1:K:76:LEU:HD13	1:K:76:LEU:HA	1.91	0.40
1:E:269:THR:HG23	1:E:301:GLU:HB3	2.03	0.40
2:G:218:MET:HE2	2:G:241:ILE:CD1	2.51	0.40
1:K:110:GLU:CD	1:K:110:GLU:H	2.25	0.40
1:K:199:HIS:C	1:K:200:LEU:CD2	2.87	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	327/348 (94%)	319 (98%)	7 (2%)	1 (0%)	41	46
1	B	327/348 (94%)	316 (97%)	9 (3%)	2 (1%)	25	26
1	C	327/348 (94%)	317 (97%)	9 (3%)	1 (0%)	41	46
1	D	327/348 (94%)	318 (97%)	7 (2%)	2 (1%)	25	26
1	E	327/348 (94%)	315 (96%)	10 (3%)	2 (1%)	25	26
1	F	327/348 (94%)	316 (97%)	8 (2%)	3 (1%)	17	16
1	K	327/348 (94%)	314 (96%)	12 (4%)	1 (0%)	41	46
1	L	327/348 (94%)	316 (97%)	10 (3%)	1 (0%)	41	46
2	G	344/364 (94%)	327 (95%)	16 (5%)	1 (0%)	41	46
2	H	344/364 (94%)	330 (96%)	13 (4%)	1 (0%)	41	46
2	I	344/364 (94%)	322 (94%)	21 (6%)	1 (0%)	41	46
2	J	344/364 (94%)	328 (95%)	15 (4%)	1 (0%)	41	46
All	All	3992/4240 (94%)	3838 (96%)	137 (3%)	17 (0%)	34	37

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	342	THR
1	B	342	THR
1	F	105	PRO
1	F	342	THR
1	E	105	PRO
1	E	342	THR
1	D	107	VAL
2	J	83	VAL
1	K	106	LYS
1	A	107	VAL
1	B	107	VAL
2	H	83	VAL
1	L	28	ILE
1	C	107	VAL
2	G	83	VAL
2	I	83	VAL
1	F	25	PRO

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	267/279 (96%)	256 (96%)	11 (4%)	30	39
1	B	267/279 (96%)	256 (96%)	11 (4%)	30	39
1	C	267/279 (96%)	255 (96%)	12 (4%)	27	34
1	D	267/279 (96%)	253 (95%)	14 (5%)	23	28
1	E	267/279 (96%)	259 (97%)	8 (3%)	41	53
1	F	267/279 (96%)	251 (94%)	16 (6%)	19	22
1	K	267/279 (96%)	256 (96%)	11 (4%)	30	39
1	L	267/279 (96%)	255 (96%)	12 (4%)	27	34
2	G	286/302 (95%)	278 (97%)	8 (3%)	43	56
2	H	286/302 (95%)	279 (98%)	7 (2%)	49	62
2	I	286/302 (95%)	278 (97%)	8 (3%)	43	56
2	J	286/302 (95%)	273 (96%)	13 (4%)	27	34
All	All	3280/3440 (95%)	3149 (96%)	131 (4%)	31	40

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	33	SER
1	A	38	LEU
1	A	264	THR
1	A	271	THR
1	A	282	MET
1	A	283	ARG
1	A	294	VAL
1	A	298	ASP
1	A	315	LEU
1	A	322	ARG
1	B	6	SER
1	B	12	SER
1	B	89	ASN

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Mol	Chain	Res	Type
1	B	125	LYS
1	B	142	THR
1	B	206	MET
1	B	264	THR
1	B	271	THR
1	B	283	ARG
1	B	298	ASP
1	B	315	LEU
1	C	12	SER
1	C	31	LEU
1	C	33	SER
1	C	38	LEU
1	C	68	GLU
1	C	118	ARG
1	C	206	MET
1	C	264	THR
1	C	269	THR
1	C	271	THR
1	C	298	ASP
1	C	315	LEU
1	D	27	LEU
1	D	31	LEU
1	D	32	ARG
1	D	106	LYS
1	D	122	GLU
1	D	200	LEU
1	D	206	MET
1	D	264	THR
1	D	269	THR
1	D	271	THR
1	D	298	ASP
1	D	315	LEU
1	D	335	ILE
1	D	337	ASP
1	E	58	ASP
1	E	200	LEU
1	E	217	GLU
1	E	269	THR
1	E	283	ARG
1	E	298	ASP
1	E	299	LEU
1	E	330	GLN

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Mol	Chain	Res	Type
1	F	6	SER
1	F	27	LEU
1	F	67	SER
1	F	106	LYS
1	F	118	ARG
1	F	195	ARG
1	F	200	LEU
1	F	206	MET
1	F	226	PHE
1	F	269	THR
1	F	271	THR
1	F	298	ASP
1	F	299	LEU
1	F	335	ILE
1	F	337	ASP
1	F	343	ASP
2	G	41	SER
2	G	81	GLN
2	G	83	VAL
2	G	94	LEU
2	G	224	ARG
2	G	247	SER
2	G	318	ASP
2	G	336	THR
2	H	11	LYS
2	H	81	GLN
2	H	113	LEU
2	H	151	LYS
2	H	185	CYS
2	H	224	ARG
2	H	318	ASP
2	I	70	ILE
2	I	83	VAL
2	I	84	ARG
2	I	110	VAL
2	I	223	SER
2	I	224	ARG
2	I	251	GLU
2	I	318	ASP
2	J	15	THR
2	J	26	PHE
2	J	70	ILE

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Mol	Chain	Res	Type
2	J	81	GLN
2	J	84	ARG
2	J	110	VAL
2	J	113	LEU
2	J	216	ARG
2	J	223	SER
2	J	224	ARG
2	J	227	LEU
2	J	242	ARG
2	J	318	ASP
1	K	72	ARG
1	K	107	VAL
1	K	108	SER
1	K	118	ARG
1	K	176	ARG
1	K	200	LEU
1	K	226	PHE
1	K	270	SER
1	K	291	ARG
1	K	298	ASP
1	K	337	ASP
1	L	12	SER
1	L	27	LEU
1	L	28	ILE
1	L	103	SER
1	L	136	ASP
1	L	183	MET
1	L	200	LEU
1	L	243	ARG
1	L	298	ASP
1	L	308	ILE
1	L	337	ASP
1	L	339	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	B	165	GLN
1	B	258	ASN
1	C	196	ASN
1	D	35	HIS

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Mol	Chain	Res	Type
1	E	113	HIS
1	E	330	GLN
2	G	81	GLN
2	G	353	GLN
2	H	81	GLN
2	H	353	GLN
2	I	81	GLN
2	J	17	HIS
2	J	81	GLN
2	J	100	GLN
2	J	354	GLN
1	K	165	GLN
1	L	196	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (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	331/348 (95%)	0.18	12 (3%)	42	41	24, 44, 77, 106	0
1	B	331/348 (95%)	0.19	13 (3%)	39	37	23, 43, 76, 106	0
1	C	331/348 (95%)	0.23	13 (3%)	39	37	22, 47, 84, 118	0
1	D	331/348 (95%)	0.28	13 (3%)	39	37	25, 53, 83, 110	0
1	E	331/348 (95%)	0.41	18 (5%)	25	24	34, 58, 85, 130	0
1	F	331/348 (95%)	0.61	28 (8%)	10	9	31, 61, 91, 148	0
1	K	331/348 (95%)	0.89	47 (14%)	2	2	34, 64, 92, 137	0
1	L	331/348 (95%)	0.53	19 (5%)	23	22	35, 57, 86, 138	0
2	G	346/364 (95%)	-0.11	3 (0%)	84	83	24, 43, 62, 117	0
2	H	346/364 (95%)	-0.12	4 (1%)	79	77	26, 44, 62, 96	0
2	I	346/364 (95%)	-0.08	6 (1%)	70	68	27, 46, 64, 116	0
2	J	346/364 (95%)	-0.03	3 (0%)	84	83	28, 48, 69, 93	0
All	All	4032/4240 (95%)	0.25	179 (4%)	34	32	22, 50, 81, 148	0

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	105	PRO	8.0
1	F	24	ALA	7.7
1	F	26	GLY	6.8
1	K	107	VAL	5.5
1	K	7	TYR	5.4
1	L	25	PRO	5.4
2	G	356	LYS	5.2
1	K	25	PRO	5.2
1	K	120	VAL	5.1
1	K	106	LYS	4.9
1	A	16	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	L	7	TYR	4.9
1	L	104	MET	4.9
1	L	107	VAL	4.8
1	K	92	LEU	4.8
1	E	7	TYR	4.8
1	F	7	TYR	4.8
2	H	356	LYS	4.7
1	L	24	ALA	4.5
1	D	26	GLY	4.4
1	K	24	ALA	4.4
1	K	118	ARG	4.3
1	F	25	PRO	4.3
2	I	355	GLY	4.3
1	K	26	GLY	4.2
1	K	117	TYR	4.1
1	F	335	ILE	4.0
1	A	342	THR	4.0
1	F	10	LEU	3.9
1	L	106	LYS	3.9
1	K	337	ASP	3.9
1	B	16	GLY	3.8
1	E	25	PRO	3.8
1	K	116	ILE	3.7
1	L	14	LEU	3.6
1	F	103	SER	3.6
1	K	104	MET	3.6
1	E	107	VAL	3.5
1	F	105	PRO	3.5
1	C	26	GLY	3.3
1	K	102	VAL	3.3
1	K	112	ALA	3.3
1	F	104	MET	3.3
1	A	237	VAL	3.2
1	E	174	GLY	3.2
1	K	123	VAL	3.2
1	D	342	THR	3.2
1	E	128	LEU	3.1
1	K	6	SER	3.1
1	L	335	ILE	3.1
1	D	237	VAL	3.0
1	L	117	TYR	3.0
1	K	36	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	153	PRO	3.0
1	K	147	LEU	3.0
1	D	7	TYR	3.0
1	K	335	ILE	3.0
2	H	355	GLY	3.0
2	J	211	PRO	3.0
1	E	103	SER	2.9
1	B	237	VAL	2.9
1	A	25	PRO	2.9
1	A	15	GLY	2.9
1	C	7	TYR	2.8
1	F	118	ARG	2.8
1	K	139	ILE	2.7
1	D	25	PRO	2.7
1	F	107	VAL	2.7
1	F	82	PHE	2.7
1	L	103	SER	2.7
1	F	57	PHE	2.7
1	E	30	PHE	2.7
1	K	108	SER	2.7
1	K	157	MET	2.7
1	E	335	ILE	2.6
1	K	44	LYS	2.6
1	F	8	ALA	2.6
2	H	233	TRP	2.6
1	K	119	ALA	2.6
1	F	6	SER	2.6
2	I	356	LYS	2.6
1	A	26	GLY	2.5
1	E	106	LYS	2.5
1	F	106	LYS	2.5
1	B	342	THR	2.5
1	C	233	ILE	2.5
1	L	102	VAL	2.5
1	D	6	SER	2.5
1	K	62	ILE	2.5
1	K	127	GLY	2.5
1	L	120	VAL	2.5
1	F	120	VAL	2.5
1	K	325	ALA	2.5
1	D	16	GLY	2.5
1	E	104	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	14	LEU	2.5
1	C	237	VAL	2.4
1	K	125	LYS	2.4
1	A	233	ILE	2.4
1	D	284	ILE	2.4
1	A	284	ILE	2.4
1	A	235	PRO	2.4
1	E	334	VAL	2.4
1	F	226	PHE	2.4
1	B	343	ASP	2.4
1	F	178	LEU	2.4
1	L	177	ASN	2.4
2	I	67	GLY	2.4
1	E	24	ALA	2.4
1	K	226	PHE	2.4
2	J	241	ILE	2.4
1	F	27	LEU	2.4
1	F	174	GLY	2.3
1	C	14	LEU	2.3
1	K	43	LEU	2.3
1	K	57	PHE	2.3
2	I	237	VAL	2.3
1	B	232	GLY	2.3
1	D	228	LEU	2.3
1	F	125	LYS	2.3
1	E	118	ARG	2.3
1	F	306	PHE	2.3
1	C	16	GLY	2.3
1	L	94	GLY	2.3
1	C	235	PRO	2.3
1	K	85	TRP	2.3
1	E	26	GLY	2.3
1	B	235	PRO	2.3
1	C	241	ILE	2.3
1	D	236	LEU	2.3
1	E	342	THR	2.3
1	K	140	SER	2.3
1	C	303	CYS	2.3
1	C	231	ALA	2.2
2	G	241	ILE	2.2
1	A	200	LEU	2.2
1	F	158	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	284	ILE	2.2
1	B	228	LEU	2.2
1	F	334	VAL	2.2
1	E	57	PHE	2.2
1	D	267	GLY	2.2
1	K	143	ALA	2.2
1	K	186	ILE	2.2
1	K	342	THR	2.2
2	J	173	THR	2.2
1	D	233	ILE	2.2
1	L	49	LYS	2.2
1	K	47	GLY	2.2
1	K	172	TRP	2.2
1	C	228	LEU	2.1
1	B	319	VAL	2.1
1	L	186	ILE	2.1
1	D	287	MET	2.1
1	K	99	CYS	2.1
1	B	231	ALA	2.1
1	B	25	PRO	2.1
1	B	233	ILE	2.1
1	K	27	LEU	2.1
1	L	26	GLY	2.1
2	H	175	SER	2.1
1	F	144	ALA	2.1
1	E	11	PHE	2.1
1	C	284	ILE	2.1
1	A	311	THR	2.1
1	K	250	ALA	2.1
1	K	84	TYR	2.1
1	L	57	PHE	2.1
1	E	44	LYS	2.1
1	K	103	SER	2.1
1	K	38	LEU	2.0
1	L	144	ALA	2.0
2	I	211	PRO	2.0
1	A	236	LEU	2.0
1	F	177	ASN	2.0
2	G	355	GLY	2.0
1	C	25	PRO	2.0
1	F	337	ASP	2.0
2	I	175	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

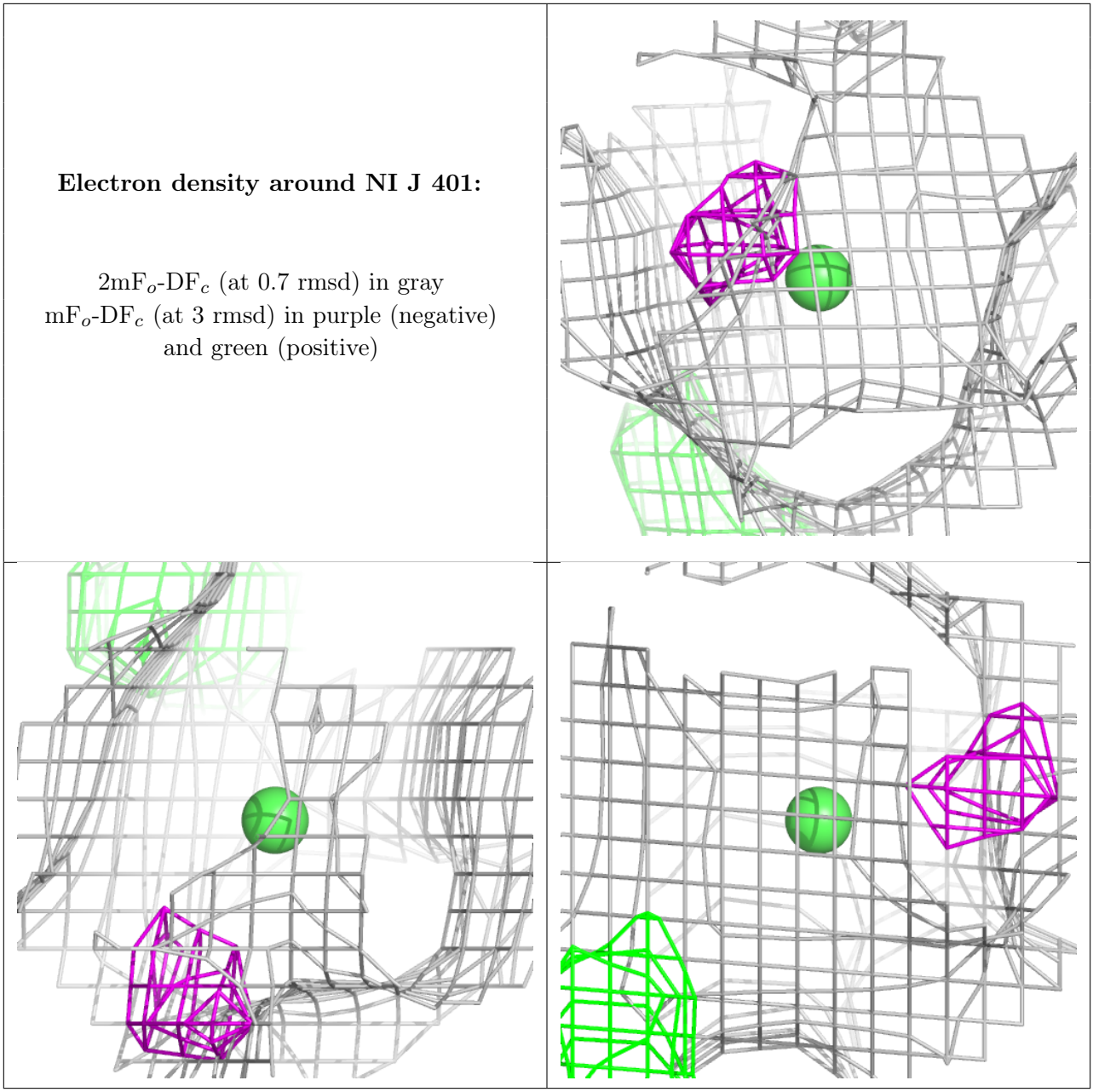
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	NI	J	401	1/1	0.97	0.09	59,59,59,59	0
3	NI	I	401	1/1	0.98	0.09	55,55,55,55	0
3	NI	G	401	1/1	0.98	0.09	49,49,49,49	0
3	NI	H	402	1/1	0.99	0.09	47,47,47,47	0
3	NI	G	402	1/1	0.99	0.10	49,49,49,49	0
3	NI	I	402	1/1	0.99	0.09	56,56,56,56	0
3	NI	H	401	1/1	0.99	0.10	50,50,50,50	0
3	NI	J	402	1/1	0.99	0.07	63,63,63,63	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.

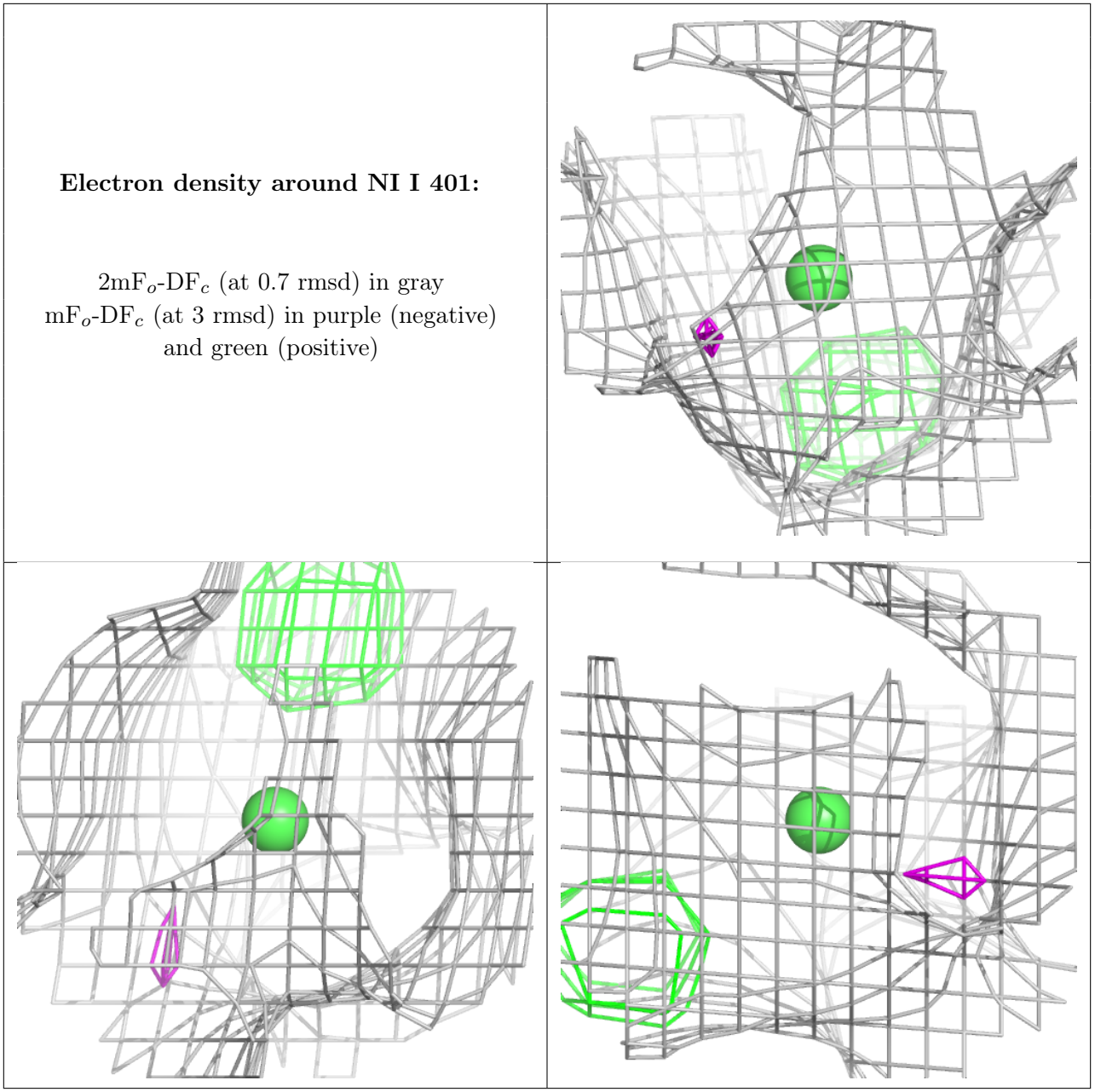
Electron density around NI J 401:

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



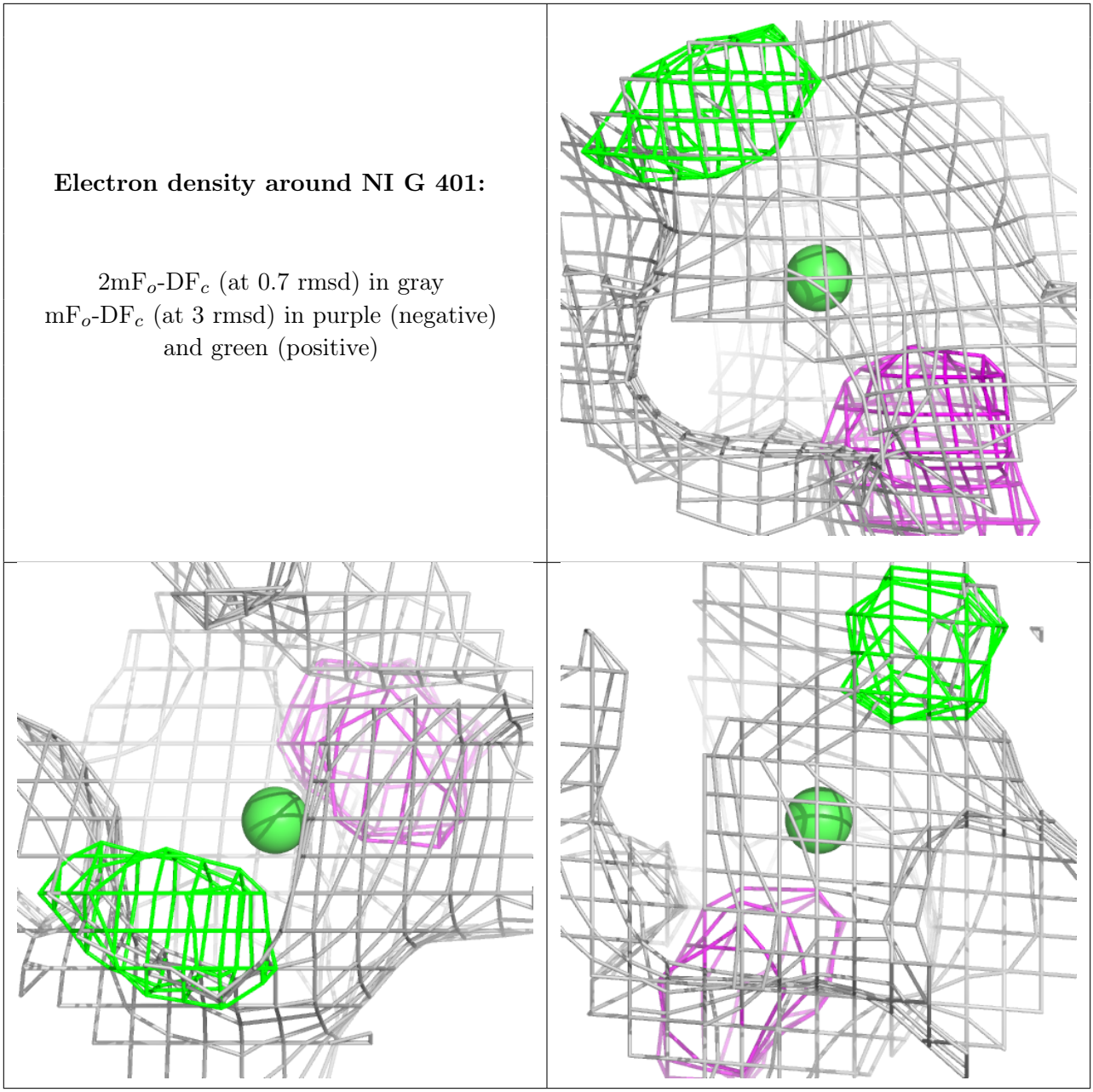
Electron density around NI I 401:

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



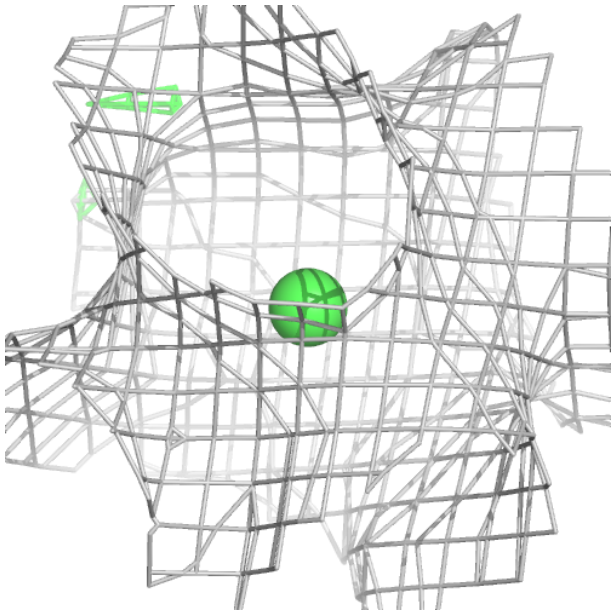
Electron density around NI G 401:

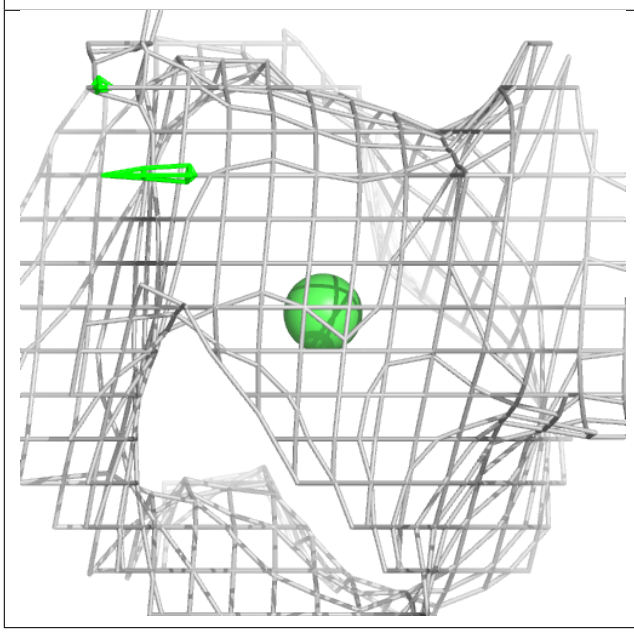
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

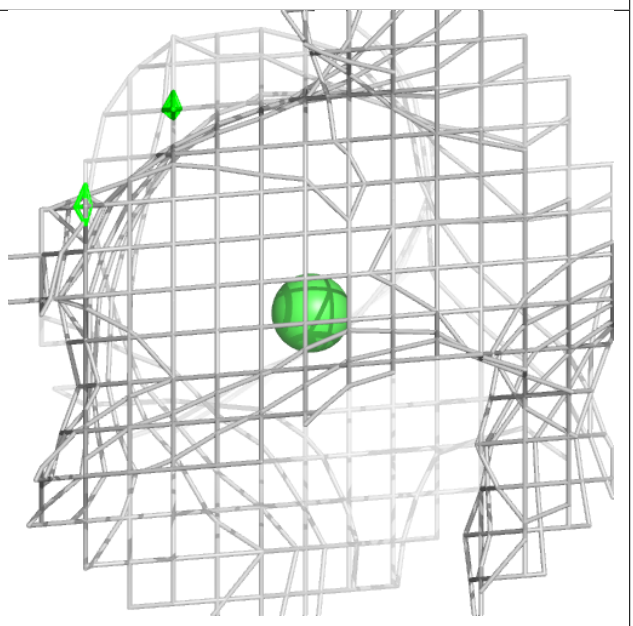


Electron density around NI H 402:

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

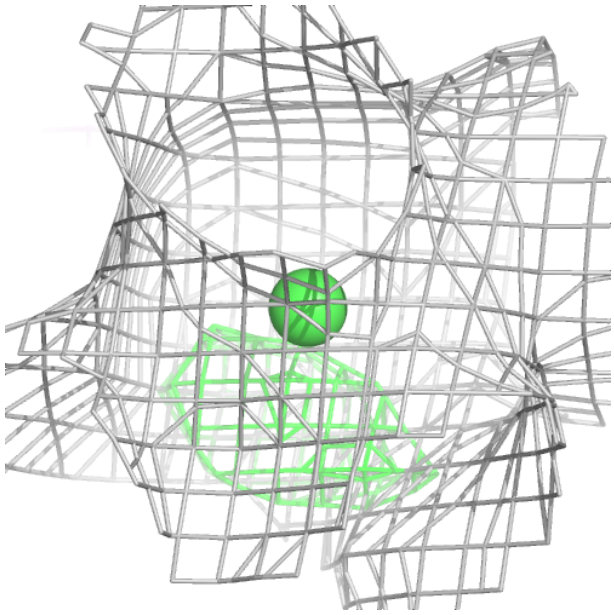


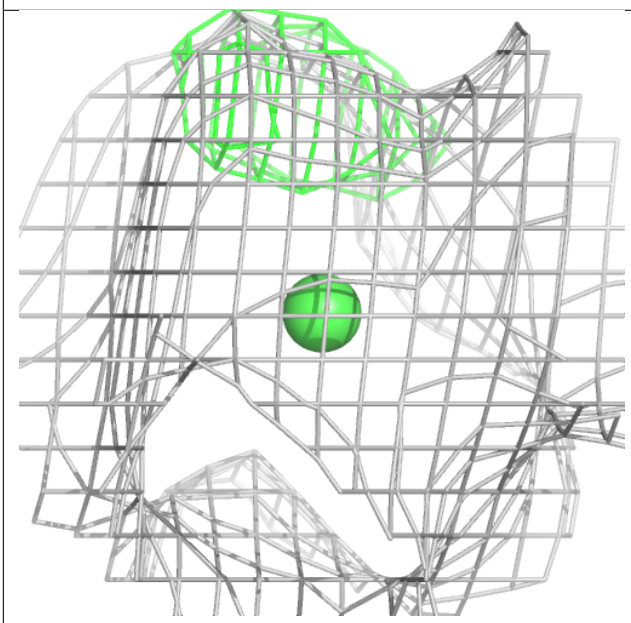


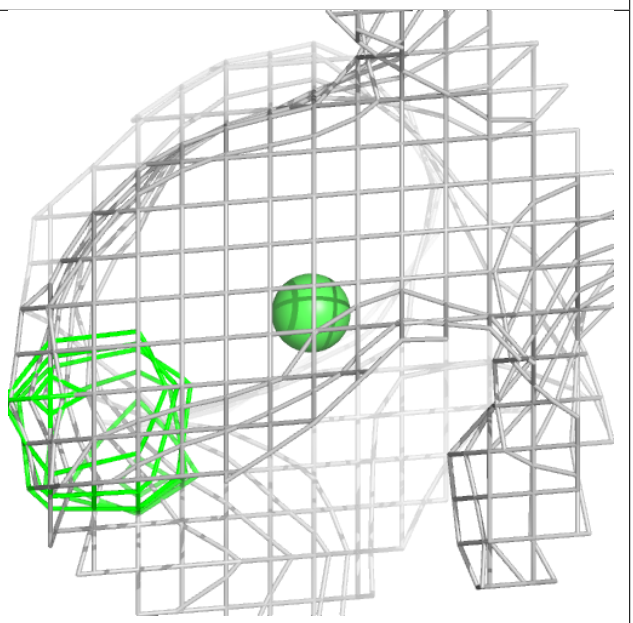


Electron density around NI G 402:

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

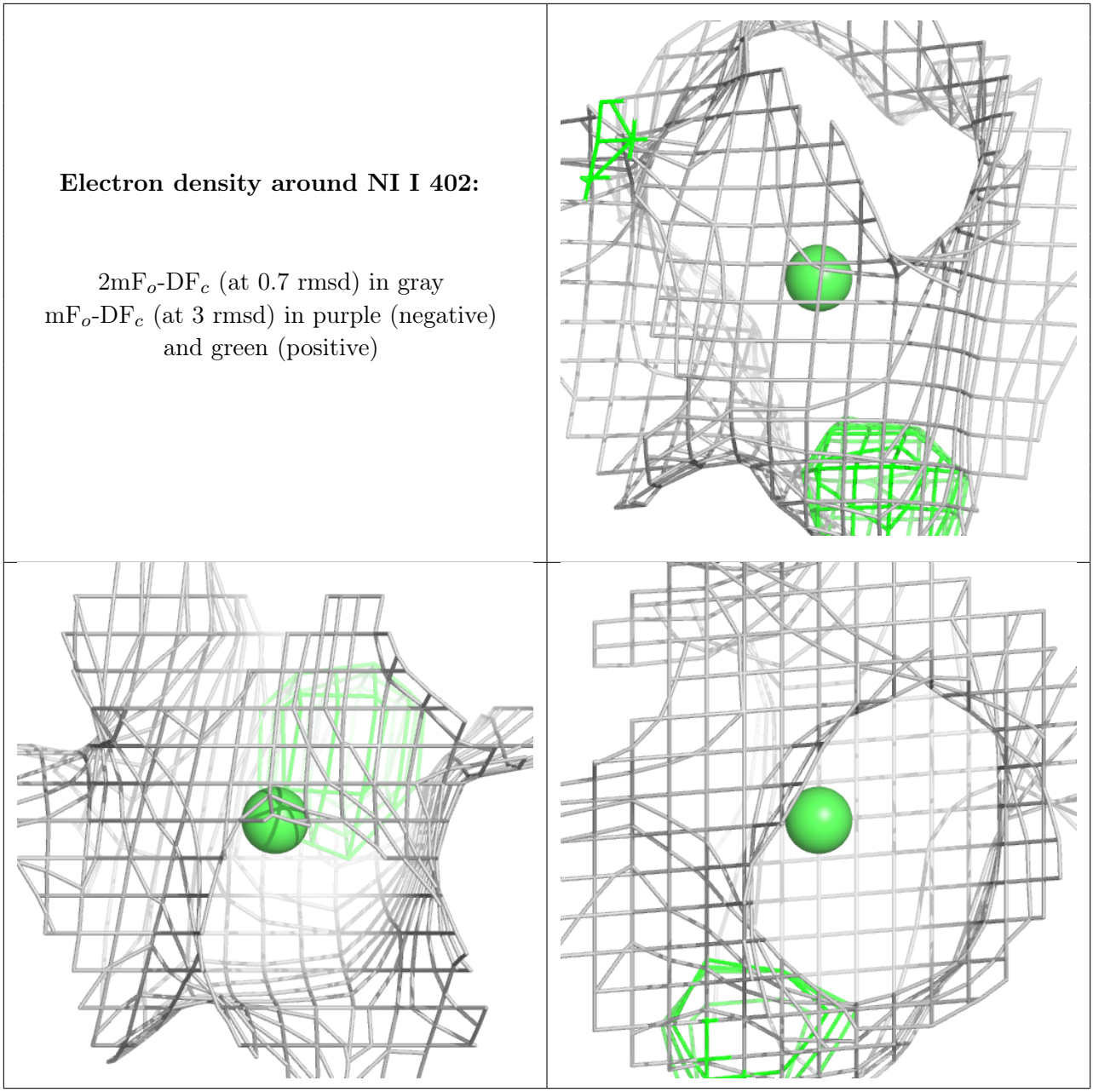






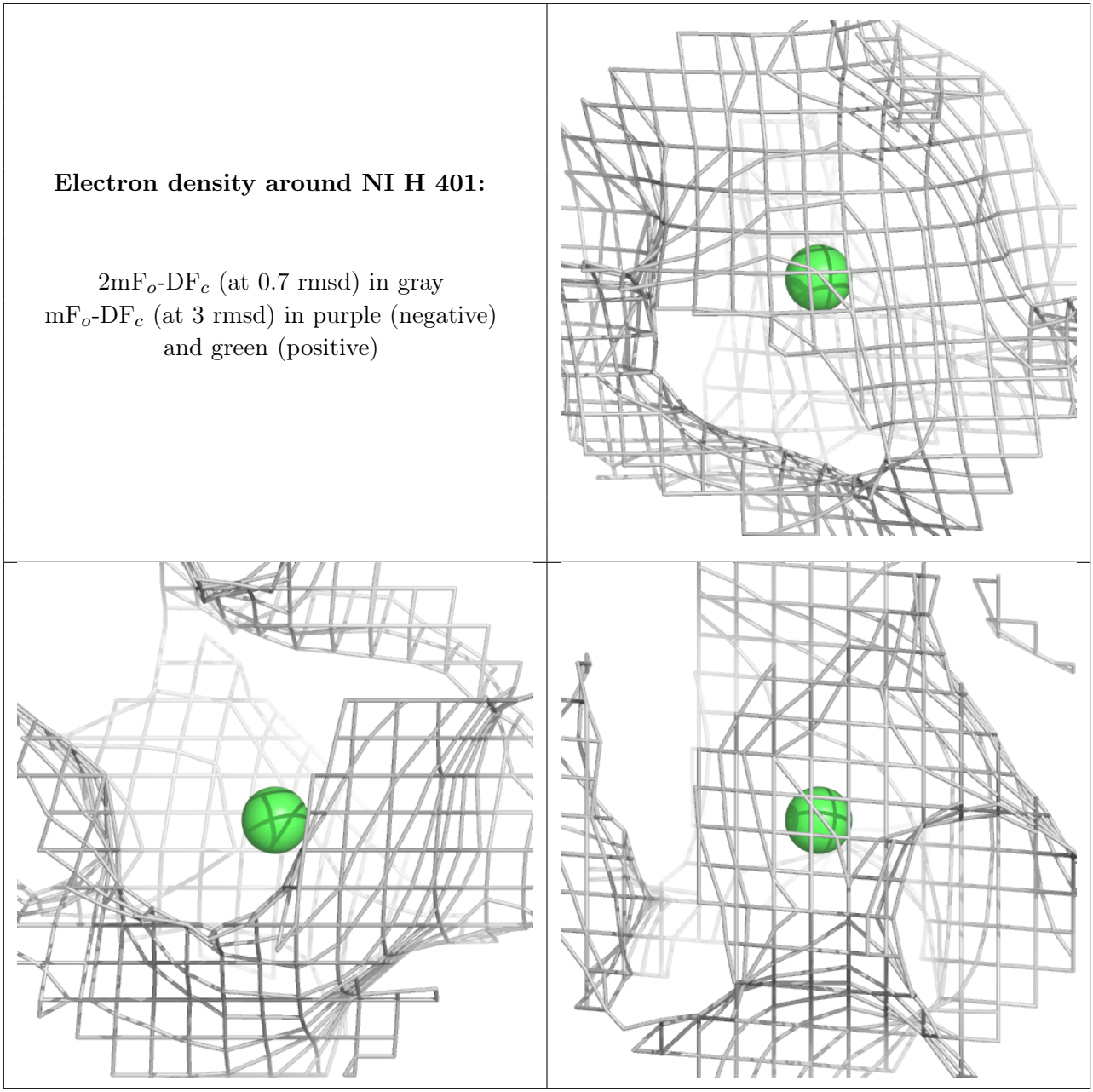
Electron density around NI I 402:

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



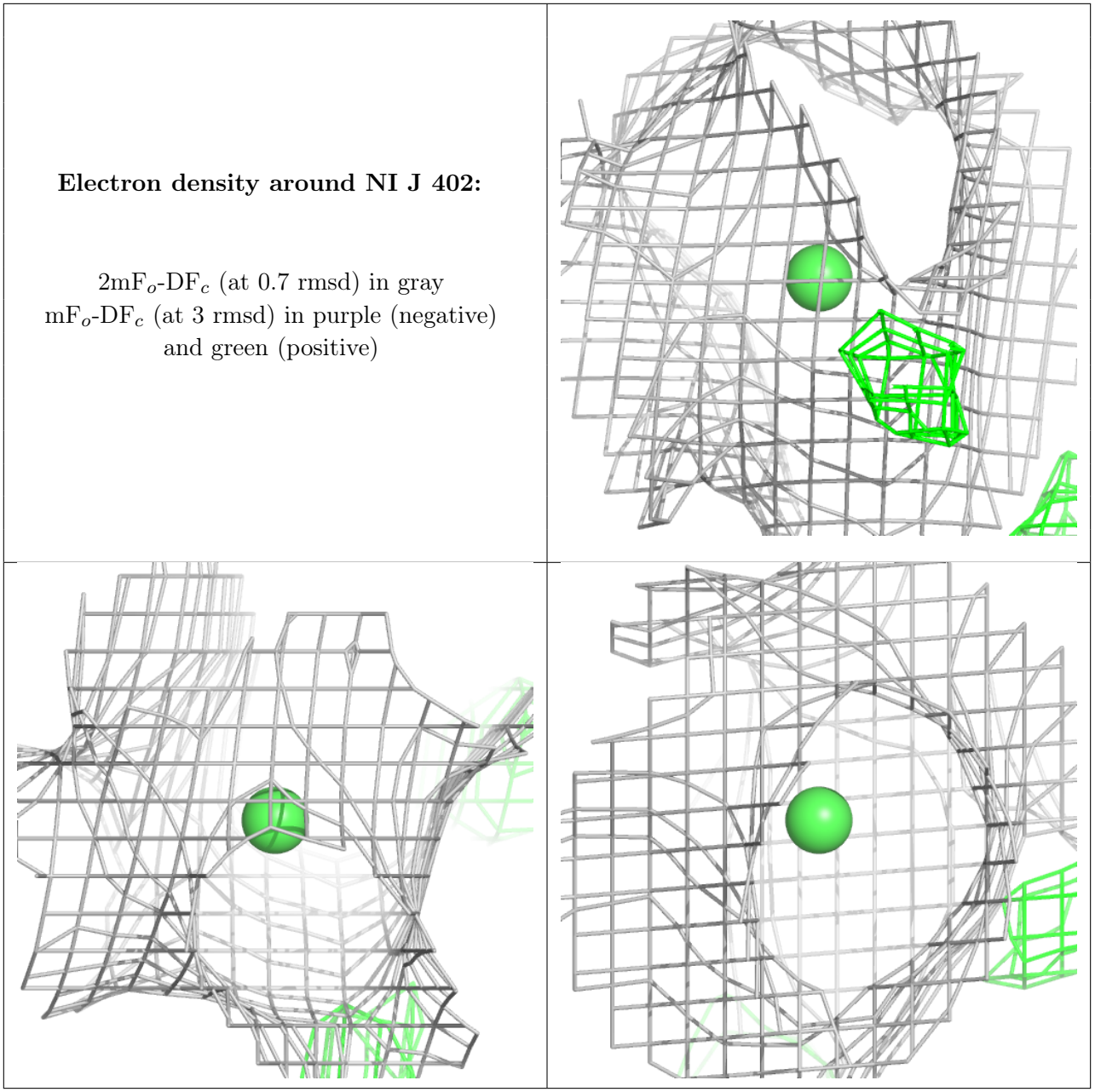
Electron density around NI H 401:

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



Electron density around NI J 402:

$2mF_o$-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.