



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:35 AM UTC

PDB ID : 8SP2 / pdb_00008sp2
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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

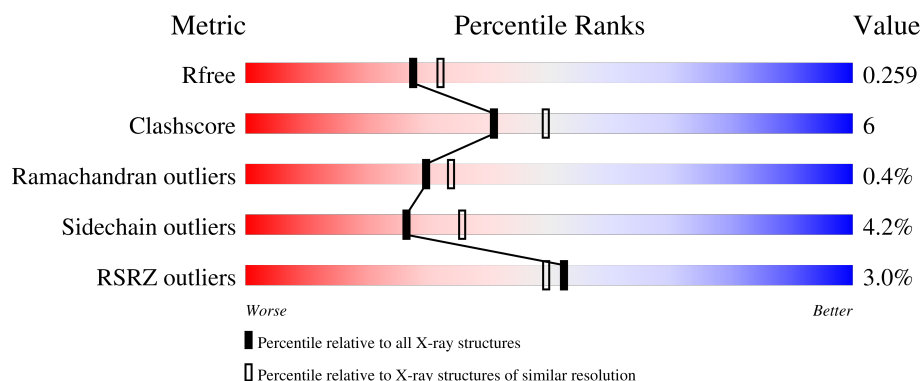
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

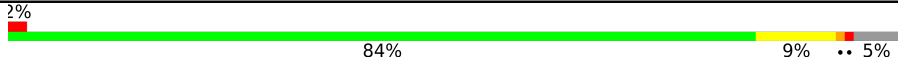
The reported resolution of this entry is 2.20 Å.

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	348	
1	B	348	
1	C	348	
1	D	348	
1	E	348	

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Mol	Chain	Length	Quality of chain
1	F	348	8% 77% 16% • 5%
1	K	348	7% 75% 18% • 5%
1	L	348	4% 82% 11% • 5%
2	G	364	81% 12% • 5%
2	H	364	% 84% 10% • 5%
2	I	364	% 78% 15% • 5%
2	J	364	% 78% 14% • 5%

2 Entry composition

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 (CCD ID: 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

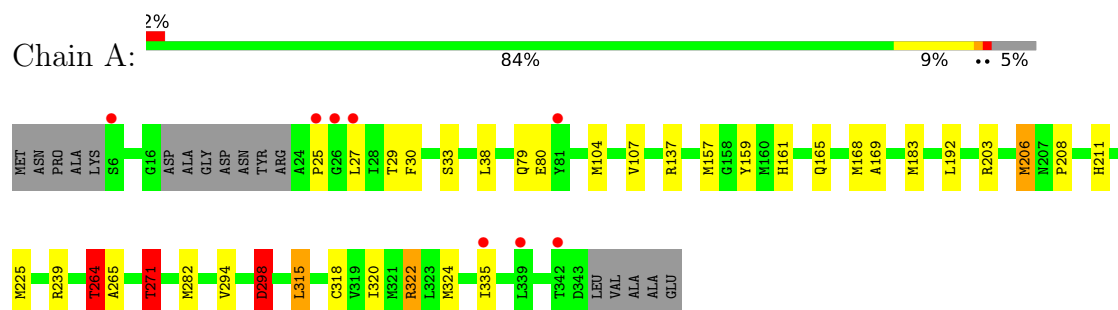
- Molecule 4 is water.

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

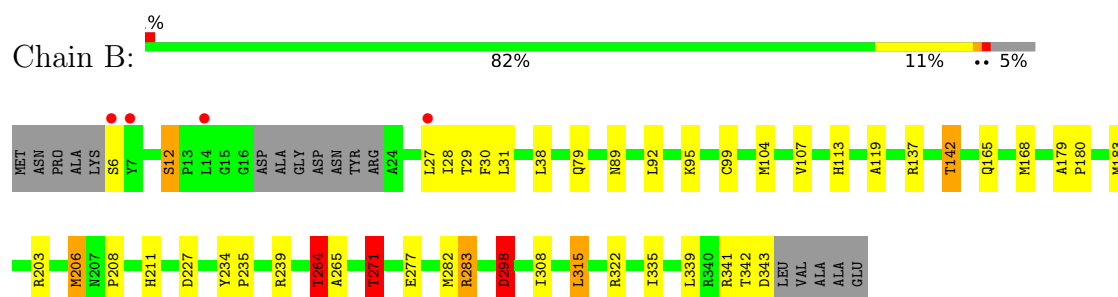
3 Residue-property plots [i](#)

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.

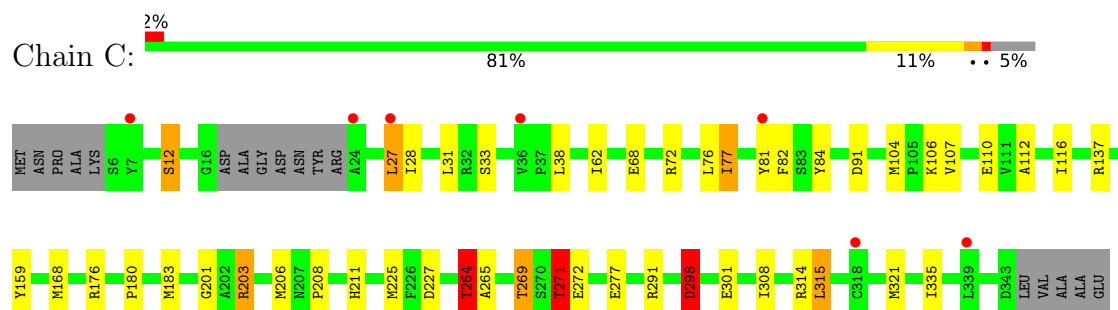
- Molecule 1: metformin hydrolase subunit B



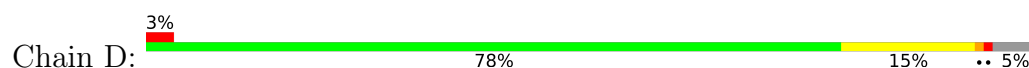
- Molecule 1: metformin hydrolase subunit B

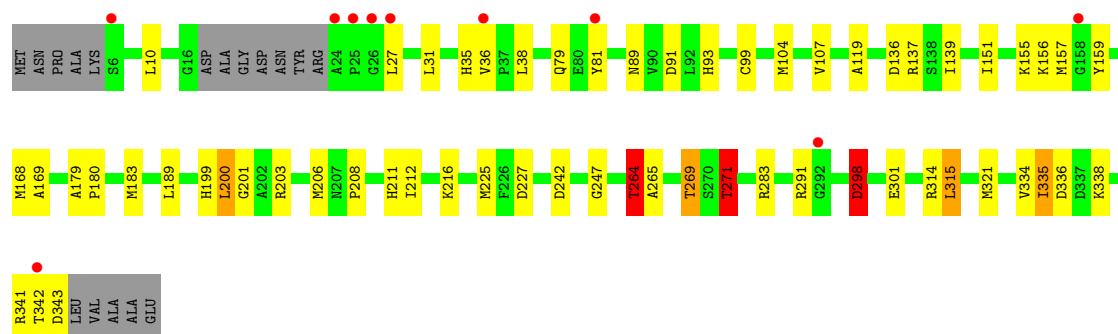


- Molecule 1: metformin hydrolase subunit B

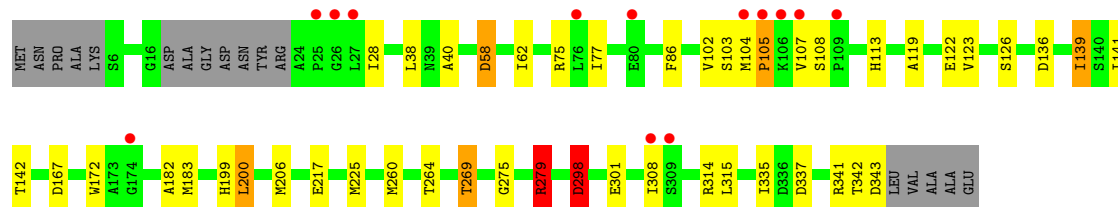
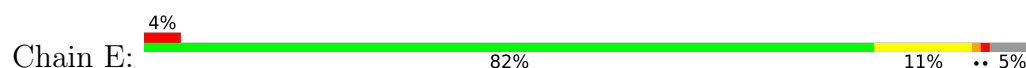


- Molecule 1: metformin hydrolase subunit B

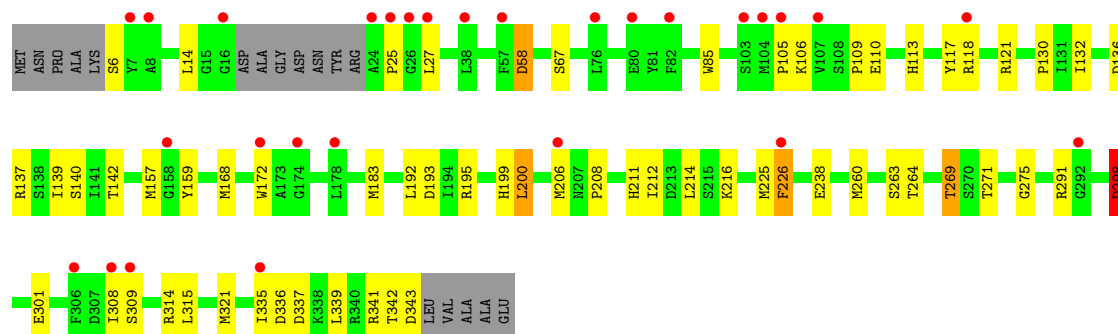
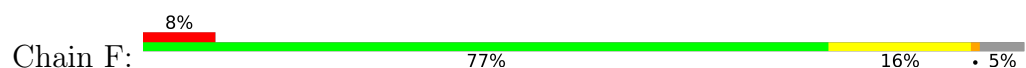




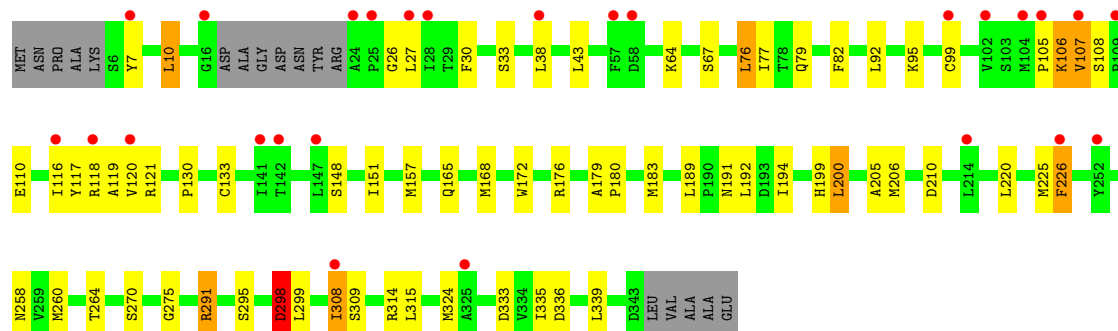
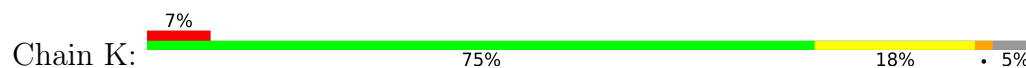
• Molecule 1: metformin hydrolase subunit B



• Molecule 1: metformin hydrolase subunit B

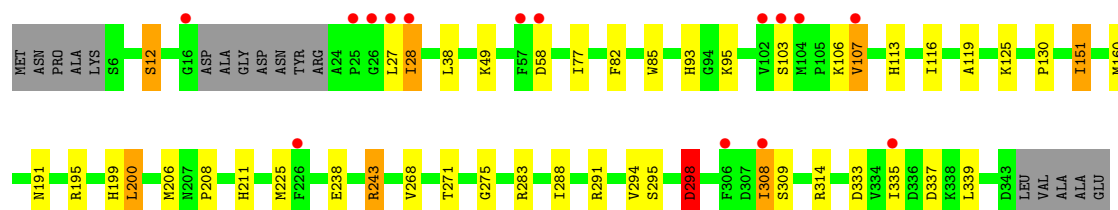


• Molecule 1: metformin hydrolase subunit B



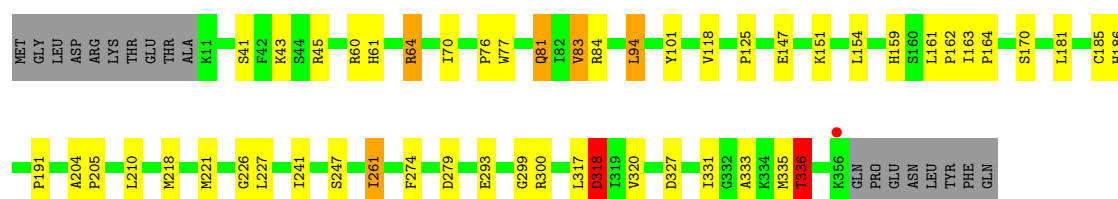
- Molecule 1: metformin hydrolase subunit B

Chain L: 



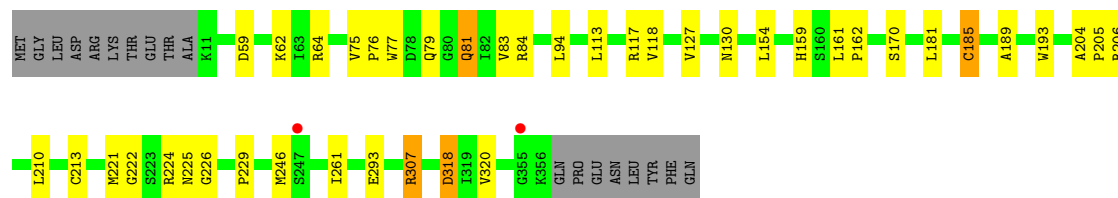
- Molecule 2: metformin hydrolase subunit A

Chain G: 



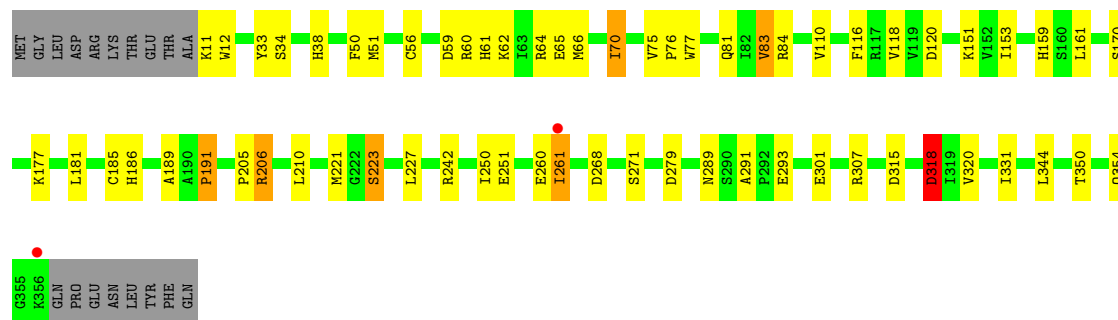
- Molecule 2: metformin hydrolase subunit A

Chain H: 



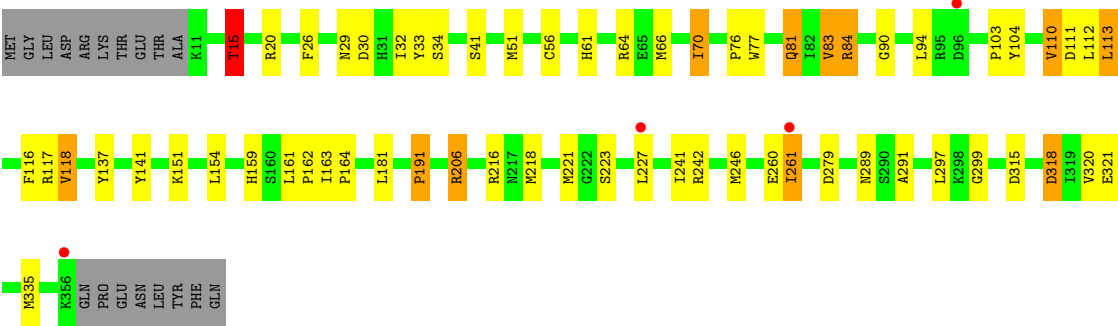
- Molecule 2: metformin hydrolase subunit A

Chain I: 



- Molecule 2: metformin hydrolase subunit A

Chain J: 



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.20Å)	Xtrriage
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	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.56	0/2587	0.96	4/3499 (0.1%)
1	B	0.55	0/2587	0.97	6/3499 (0.2%)
1	C	0.57	0/2587	0.96	5/3499 (0.1%)
1	D	0.54	0/2587	0.95	4/3499 (0.1%)
1	E	0.51	0/2587	0.93	4/3499 (0.1%)
1	F	0.52	0/2587	0.92	3/3499 (0.1%)
1	K	0.51	0/2587	0.92	2/3499 (0.1%)
1	L	0.51	0/2587	0.91	3/3499 (0.1%)
2	G	0.56	0/2778	1.01	6/3765 (0.2%)
2	H	0.55	0/2778	0.98	1/3765 (0.0%)
2	I	0.54	0/2778	0.97	3/3765 (0.1%)
2	J	0.52	0/2778	0.97	3/3765 (0.1%)
All	All	0.54	0/31808	0.96	44/43052 (0.1%)

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 (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	THR	CB-CA-C	-8.76	93.93	109.62
1	D	271	THR	CB-CA-C	-8.09	95.14	109.62
1	F	226	PHE	CA-CB-CG	7.94	121.74	113.80
1	E	279	ARG	CB-CG-CD	-7.61	93.79	111.30
1	E	58	ASP	CA-CB-CG	7.54	120.14	112.60
1	C	271	THR	CB-CA-C	-7.34	94.45	109.65
1	B	264	THR	CB-CA-C	-7.25	97.98	110.09
1	K	226	PHE	CA-CB-CG	7.15	120.95	113.80
1	L	298	ASP	CA-CB-CG	6.85	119.45	112.60
1	C	264	THR	CB-CA-C	-6.69	98.92	110.09
2	G	336	THR	CB-CA-C	6.61	123.36	110.67
1	A	271	THR	CB-CA-C	-6.55	96.09	109.65
1	F	298	ASP	CA-CB-CG	6.48	119.08	112.60
1	E	298	ASP	CA-CB-CG	6.34	118.94	112.60
1	C	227	ASP	CA-CB-CG	6.32	118.92	112.60
1	D	298	ASP	CA-CB-CG	6.32	118.92	112.60
2	G	336	THR	N-CA-CB	-6.31	100.50	110.28
2	G	43	LYS	CB-CA-C	-6.29	99.05	110.56
1	A	264	THR	CB-CA-C	-6.22	99.70	110.09
1	L	93	HIS	CA-CB-CG	-6.21	107.59	113.80
1	D	227	ASP	CA-CB-CG	6.16	118.76	112.60
2	H	64	ARG	CB-CA-C	-6.12	101.02	110.81
2	J	15	THR	CB-CA-C	6.07	116.78	109.31
1	C	298	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	298	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	277	GLU	CB-CA-C	5.84	119.44	109.80
1	K	298	ASP	CA-CB-CG	5.75	118.35	112.60
1	B	298	ASP	CA-CB-CG	5.68	118.28	112.60
2	G	327	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	271	THR	N-CA-CB	5.53	118.17	110.26
2	G	191	PRO	N-CA-C	-5.43	105.98	113.53
1	B	227	ASP	CA-CB-CG	5.35	117.95	112.60
2	I	191	PRO	N-CA-C	-5.31	106.15	113.53
2	J	30	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	203	ARG	O-C-N	5.27	128.56	123.29
2	J	191	PRO	N-CA-C	-5.25	106.22	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	58	ASP	CA-CB-CG	5.25	117.85	112.60
2	G	318	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	271	THR	N-CA-CB	5.16	117.63	110.04
1	L	58	ASP	CA-CB-CG	5.13	117.73	112.60
1	D	264	THR	CB-CA-C	-5.10	101.57	110.09
1	E	337	ASP	CB-CA-C	-5.10	102.01	110.68
2	I	318	ASP	CA-CB-CG	5.05	117.65	112.60
2	I	120	ASP	CA-CB-CG	5.00	117.60	112.60

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

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	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2535	0	2497	29	0
1	C	2535	0	2497	37	0
1	D	2535	0	2497	35	0
1	E	2535	0	2497	29	0
1	F	2535	0	2497	38	0
1	K	2535	0	2497	48	0
1	L	2535	0	2497	29	0
2	G	2706	0	2592	30	0
2	H	2706	0	2592	32	0
2	I	2706	0	2592	42	0
2	J	2706	0	2592	50	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	1	0
4	L	48	0	0	1	0
All	All	32022	0	30344	397	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 (397) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLN:HE21	1:A:206:MET:HE2	1.22	1.04
2:J:56:CYS:SG	2:J:66:MET:CE	2.63	0.87
1:A:30:PHE:HZ	1:A:324:MET:HE1	1.38	0.87
2:G:333:ALA:O	2:G:336:THR:HG22	1.79	0.83
2:J:56:CYS:CB	2:J:66:MET:HE1	2.09	0.82
1:A:165:GLN:NE2	1:A:206:MET:HE2	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:185:CYS:SG	2:H:293:GLU:HG3	2.22	0.80
1:B:165:GLN:HE21	1:B:206:MET:HE2	1.48	0.78
2:J:56:CYS:HB2	2:J:66:MET:HE1	1.66	0.78
1:E:199:HIS:C	1:E:200:LEU:HD23	2.09	0.78
1:K:199:HIS:C	1:K:200:LEU:HD23	2.09	0.77
2:J:56:CYS:SG	2:J:66:MET:HE1	2.24	0.77
2:J:221:MET:HE2	2:J:261:ILE:HG12	1.67	0.77
2:J:56:CYS:SG	2:J:66:MET:HE3	2.26	0.76
1:L:199:HIS:C	1:L:200:LEU:HD23	2.11	0.74
1:D:81:TYR:CD2	1:D:321:MET:HE1	2.23	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:K:168:MET:HE2	1:K:220:LEU:HD22	1.69	0.72
2:I:185:CYS:SG	2:I:293:GLU:HG3	2.30	0.72
1:C:201:GLY:HA2	1:C:225:MET:HE2	1.70	0.71
2:J:32:ILE:HD11	2:J:111:ASP:CG	2.14	0.71
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:A:30:PHE:CZ	1:A:324:MET:HE1	2.24	0.70
2:I:12:TRP:HA	2:I:66:MET:HE3	1.74	0.69
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: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
1:F:199:HIS:C	1:F:200:LEU:HD23	2.17	0.68
1:D:201:GLY:HA2	1:D:225:MET:HE2	1.74	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:81:TYR:CD2	1:C:321:MET:HE1	2.34	0.63
1:E:113:HIS:CD2	1:E:142:THR:HG21	2.33	0.63
1:A:165:GLN:HE21	1:A:206:MET:CE	2.06	0.63
1:C:104:MET:HE2	1:C:112:ALA:HB1	1.81	0.63
1:L:195:ARG:O	1:L:243:ARG:HG2	1.99	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
2:I:12:TRP:HA	2:I:66:MET:CE	2.29	0.61
2:J:151:LYS:HD2	2:J:315:ASP:HA	1.82	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:159:TYR:CE2	1:F:183:MET:HE1	2.35	0.61
2:J:218:MET:HE2	2:J:241:ILE:HD13	1.82	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
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
1:L:225:MET:HE3	1:L:275:GLY:HA2	1.84	0.59
2:J:221:MET:HE2	2:J:261:ILE:CG1	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:MET:HE3	1:C:116:ILE:HG13	1.85	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
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
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
2:I:12:TRP:HD1	2:I:66:MET:HE2	1.69	0.57
2:I:12:TRP:CD1	2:I:66:MET:HE2	2.39	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
1:E:225:MET:HE3	1:E:275:GLY:HA2	1.88	0.56
1:F:225:MET:HE3	1:F:275:GLY:HA2	1.88	0.56
2:H:181:LEU:HD13	2:H:261:ILE:CD1	2.36	0.56
1:C:203:ARG:NH1	1:C:225:MET:HE3	2.21	0.56
1:K:157:MET:HE2	1:K:192:LEU:HB2	1.88	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
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
1:K:298:ASP:OD1	1:K:298:ASP:C	2.49	0.55
1:C:201:GLY:CA	1:C:225:MET:HE2	2.36	0.55
2:G:61:HIS:ND1	2:G:64:ARG:NH2	2.54	0.55
1:A:298:ASP:OD1	1:A:298:ASP:C	2.50	0.55
2:H:226:GLY:O	1:L:82:PHE:HB2	2.07	0.55
1:L:95:LYS:HE2	1:L:333:ASP:OD2	2.07	0.55
1:B:298:ASP:C	1:B:298:ASP:OD1	2.50	0.55
2:I:81:GLN:NE2	2:I:84:ARG:C	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:203:ARG:NH1	1:D:225:MET:HE3	2.23	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:246:MET:HE1	2:J:297:LEU:HD23	1.90	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:F:85:TRP:HZ2	1:F:321:MET:HE3	1.73	0.53
1:K:308:ILE:N	1:K:308:ILE:HD12	2.24	0.53
1:C:298:ASP:OD1	1:C:298:ASP:C	2.52	0.53
1:K:205:ALA:C	1:K:206:MET:HE2	2.33	0.53
1:B:239:ARG:HD2	4:B:441:HOH:O	2.09	0.53
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:E:298:ASP:C	1:E:298:ASP:OD1	2.51	0.52
1:F:264:THR:HG22	1:F:315:LEU:HD22	1.90	0.52
1:C:104:MET:HE1	1:C:116:ILE:HD11	1.90	0.52
1:F:109:PRO:HD2	1:F:110:GLU:OE2	2.09	0.52
1:K:225:MET:HE3	1:K:275:GLY:HA2	1.92	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
1:D:201:GLY:CA	1:D:225:MET:HE2	2.37	0.52
1:D:298:ASP:OD1	1:D:298:ASP:C	2.53	0.52
2:I:75:VAL:HG11	2:I:161:LEU:HD13	1.90	0.52
1:L:106:LYS:O	1:L:107:VAL:C	2.53	0.52
2:I:159:HIS:CD2	2:I:320:VAL:HG21	2.45	0.52
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:206:MET:HE2	1:L:206:MET:HA	1.92	0.51
1:L:283:ARG:NH1	4:L:403:HOH:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:110:GLU:CD	1:C:110:GLU:H	2.18	0.51
1:F:298:ASP:OD1	1:F:298:ASP:C	2.54	0.51
1:C:269:THR:HG23	1:C:301:GLU:HB3	1.93	0.51
1:K:26:GLY:O	1:K:27:LEU:HB2	2.10	0.50
1:L:298:ASP:C	1:L:298:ASP:OD1	2.53	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:D:35:HIS:CD2	1:D:35:HIS:C	2.90	0.49
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
1:B:206:MET:HE3	1:B:206:MET:O	2.12	0.49
1:C:81:TYR:HA	1:K:206:MET:HE1	1.94	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:J:56:CYS:HB2	2:J:66:MET:CE	2.40	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:33:TYR:O	2:J:34:SER:C	2.56	0.49
1:C:106:LYS:NZ	4:C:408:HOH:O	2.45	0.49
2:I:159:HIS:CG	2:I:320:VAL:HG21	2.48	0.48
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
2:J:94:LEU:HD13	2:J:94:LEU:C	2.38	0.48
1:D:341:ARG:C	1:D:343:ASP:H	2.21	0.48
1:C:82:PHE:H	1:K:206:MET:HE1	1.77	0.48
1:F:200:LEU:N	1:F:200:LEU:CD2	2.77	0.48
2:H:76:PRO:O	2:H:77:TRP:C	2.55	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:11:LYS:O	2:I:66:MET:HE3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:I:177:LYS:NZ	2:I:268:ASP:O	2.46	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:K:309:SER:O	1:K:314:ARG:NH1	2.44	0.46
2:I:33:TYR:O	2:I:34:SER:C	2.58	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:L:199:HIS:C	1:L:200:LEU:CD2	2.85	0.46
2:G:274:PHE:CD2	2:G:317:LEU:HD13	2.51	0.46
1:B:341:ARG:C	1:B:343:ASP:H	2.23	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
1:K:106:LYS:O	1:K:107:VAL:C	2.58	0.46
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:F:199:HIS:C	1:F:200:LEU:CD2	2.87	0.46
2:I:76:PRO:O	2:I:77:TRP:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:218:MET:HE2	2:G:241:ILE:HD13	1.97	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: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
2:I:50:PHE:CE2	2:I:51:MET:HE3	2.51	0.45
1:K:38:LEU:HD13	1:K:99:CYS:HB3	1.97	0.45
1:K:110:GLU:CD	1:K:110:GLU:H	2.25	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
2:H:154:LEU:O	2:H:318:ASP:HA	2.18	0.44
2:G:76:PRO:O	2:G:77:TRP:C	2.60	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
1:E:136:ASP:O	1:E:139:ILE:HG23	2.18	0.44
1:E:341:ARG:C	1:E:343:ASP:H	2.26	0.44
2:G:159:HIS:CD2	2:G:320:VAL:HG21	2.53	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:K:199:HIS:C	1:K:200:LEU:CD2	2.87	0.44
1:A:80:GLU:O	1:E:206:MET:HE1	2.18	0.44
1:C:104:MET:CE	1:C:116:ILE:HG13	2.47	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
2:J:76:PRO:O	2:J:77:TRP:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:199:HIS:C	1:D:200:LEU:HD23	2.42	0.43
2:H:193:TRP:CZ3	1:L:12:SER:HB2	2.52	0.43
2:G:218:MET:HE2	2:G:241:ILE:CD1	2.48	0.43
2:J:90:GLY:HA3	4:J:540:HOH:O	2.17	0.43
1:B:265:ALA:O	1:B:271:THR:HG23	2.17	0.43
2:J:32:ILE:HD11	2:J:111:ASP:CB	2.47	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
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
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
2:G:299:GLY:HA2	2:G:335:MET:HE1	2.00	0.43
1:K:117:TYR:CE1	1:K:121:ARG:HG3	2.53	0.43
1:F:85:TRP:CZ2	1:F:321:MET:HE3	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
2:H:222:GLY:HA2	2:H:246:MET:HE2	2.00	0.43
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:B:104:MET:HE3	1:B:104:MET:HB2	1.94	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: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
1:A:203:ARG:NH1	1:A:225:MET:HE3	2.33	0.42
1:D:104:MET:HE3	1:D:104:MET:HB2	1.95	0.42
1:D:265:ALA:O	1:D:271:THR:HG23	2.18	0.42
1:F:157:MET:HE2	1:F:192:LEU:HD13	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:299:GLY:HA2	2:J:335:MET:HE1	2.01	0.42
1:L:160:MET:HE1	1:L:288:ILE:HG12	2.02	0.42
1:B:27:LEU:HD12	1:B:28:ILE:N	2.35	0.42
2:H:94:LEU:HD13	2:H:94:LEU:C	2.45	0.42
1:E:141:ILE:HD11	1:E:182:ALA:HA	2.01	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:C:62:ILE:HG12	1:C:180:PRO:HG3	2.01	0.41
1:E:199:HIS:C	1:E:200:LEU:CD2	2.86	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
1:F:159:TYR:CD2	1:F:183:MET:HE1	2.56	0.41
2:I:151:LYS:CD	2:I:315:ASP:HA	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: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:269:THR:CG2	1:F:301:GLU:OE1	2.67	0.41
1:K:105:PRO:O	1:K:106:LYS:C	2.63	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
1:D:159:TYR:CE1	1:D:183:MET:HE1	2.56	0.41
2:G:186:HIS:CD2	2:G:227:LEU:HD23	2.55	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:104:MET:HE3	1:A:104:MET:HB2	1.99	0.41
1:B:12:SER:HB3	1:F:172:TRP:CZ3	2.56	0.41
1:C:159:TYR:CE1	1:C:183:MET:HE1	2.56	0.41
1:E:260:MET:HG3	1:E:315:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:318:ASP:C	2:I:318:ASP:OD1	2.64	0.41
1:K:92:LEU:HD13	1:K:324:MET:HE2	2.03	0.41
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: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
2:H:318:ASP:OD1	2:H:318:ASP:C	2.64	0.40
2:J:318:ASP:OD1	2:J:318:ASP:C	2.64	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:D:157:MET:HE1	1:D:189:LEU:HD13	2.02	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:279:ASP:OD1	2:G:279:ASP:C	2.64	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%)	36	42
1	B	327/348 (94%)	316 (97%)	9 (3%)	2 (1%)	21	23
1	C	327/348 (94%)	317 (97%)	9 (3%)	1 (0%)	36	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	327/348 (94%)	318 (97%)	7 (2%)	2 (1%)	21	23
1	E	327/348 (94%)	315 (96%)	10 (3%)	2 (1%)	21	23
1	F	327/348 (94%)	316 (97%)	8 (2%)	3 (1%)	14	14
1	K	327/348 (94%)	314 (96%)	12 (4%)	1 (0%)	36	42
1	L	327/348 (94%)	316 (97%)	10 (3%)	1 (0%)	36	42
2	G	344/364 (94%)	327 (95%)	16 (5%)	1 (0%)	36	42
2	H	344/364 (94%)	330 (96%)	13 (4%)	1 (0%)	36	42
2	I	344/364 (94%)	322 (94%)	21 (6%)	1 (0%)	36	42
2	J	344/364 (94%)	328 (95%)	15 (4%)	1 (0%)	36	42
All	All	3992/4240 (94%)	3838 (96%)	137 (3%)	17 (0%)	30	34

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 ⓘ

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%)	255 (96%)	12 (4%)	24	33
1	B	267/279 (96%)	256 (96%)	11 (4%)	27	37
1	C	267/279 (96%)	254 (95%)	13 (5%)	22	29
1	D	267/279 (96%)	256 (96%)	11 (4%)	27	37
1	E	267/279 (96%)	258 (97%)	9 (3%)	32	44
1	F	267/279 (96%)	253 (95%)	14 (5%)	21	26
1	K	267/279 (96%)	251 (94%)	16 (6%)	17	21
1	L	267/279 (96%)	252 (94%)	15 (6%)	19	24
2	G	286/302 (95%)	276 (96%)	10 (4%)	32	43
2	H	286/302 (95%)	281 (98%)	5 (2%)	53	69
2	I	286/302 (95%)	278 (97%)	8 (3%)	38	52
2	J	286/302 (95%)	273 (96%)	13 (4%)	24	33
All	All	3280/3440 (95%)	3143 (96%)	137 (4%)	26	36

All (137) 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	206	MET
1	A	264	THR
1	A	271	THR
1	A	282	MET
1	A	294	VAL
1	A	298	ASP
1	A	315	LEU
1	A	322	ARG
1	A	335	ILE
1	B	6	SER
1	B	12	SER
1	B	89	ASN
1	B	142	THR
1	B	206	MET
1	B	264	THR
1	B	271	THR
1	B	298	ASP

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Mol	Chain	Res	Type
1	B	315	LEU
1	B	335	ILE
1	B	339	LEU
1	C	12	SER
1	C	27	LEU
1	C	31	LEU
1	C	33	SER
1	C	38	LEU
1	C	68	GLU
1	C	77	ILE
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	79	GLN
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	E	58	ASP
1	E	103	SER
1	E	139	ILE
1	E	200	LEU
1	E	217	GLU
1	E	269	THR
1	E	298	ASP
1	E	308	ILE
1	E	335	ILE
1	F	6	SER
1	F	27	LEU
1	F	67	SER
1	F	106	LYS
1	F	118	ARG
1	F	200	LEU

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Mol	Chain	Res	Type
1	F	206	MET
1	F	226	PHE
1	F	269	THR
1	F	271	THR
1	F	298	ASP
1	F	335	ILE
1	F	337	ASP
1	F	343	ASP
2	G	41	SER
2	G	64	ARG
2	G	81	GLN
2	G	83	VAL
2	G	94	LEU
2	G	118	VAL
2	G	247	SER
2	G	261	ILE
2	G	318	ASP
2	G	336	THR
2	H	81	GLN
2	H	113	LEU
2	H	118	VAL
2	H	185	CYS
2	H	318	ASP
2	I	70	ILE
2	I	83	VAL
2	I	110	VAL
2	I	118	VAL
2	I	223	SER
2	I	251	GLU
2	I	261	ILE
2	I	318	ASP
2	J	15	THR
2	J	26	PHE
2	J	70	ILE
2	J	81	GLN
2	J	84	ARG
2	J	110	VAL
2	J	113	LEU
2	J	118	VAL
2	J	216	ARG
2	J	223	SER
2	J	227	LEU

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Mol	Chain	Res	Type
2	J	261	ILE
2	J	318	ASP
1	K	10	LEU
1	K	67	SER
1	K	76	LEU
1	K	77	ILE
1	K	79	GLN
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	308	ILE
1	K	335	ILE
1	L	12	SER
1	L	27	LEU
1	L	28	ILE
1	L	103	SER
1	L	107	VAL
1	L	125	LYS
1	L	151	ILE
1	L	200	LEU
1	L	243	ARG
1	L	294	VAL
1	L	298	ASP
1	L	308	ILE
1	L	335	ILE
1	L	337	ASP
1	L	339	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	89	ASN
1	A	161	HIS
1	A	165	GLN
1	A	177	ASN

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Mol	Chain	Res	Type
1	A	258	ASN
1	B	161	HIS
1	B	165	GLN
1	B	177	ASN
1	B	258	ASN
1	C	89	ASN
1	C	154	GLN
1	C	177	ASN
1	D	161	HIS
1	D	177	ASN
1	E	113	HIS
1	E	330	GLN
1	F	61	ASN
1	F	177	ASN
2	G	81	GLN
2	G	353	GLN
2	H	39	ASN
2	H	81	GLN
2	H	89	GLN
2	H	353	GLN
2	I	81	GLN
2	I	239	ASN
2	I	354	GLN
2	J	13	GLN
2	J	29	ASN
2	J	81	GLN
2	J	100	GLN
2	J	330	GLN
2	J	349	GLN
2	J	354	GLN
1	K	161	HIS
1	K	165	GLN
1	K	177	ASN
1	L	177	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	331/348 (95%)	0.15	8 (2%) 59 56	24, 44, 77, 106	0
1	B	331/348 (95%)	0.15	4 (1%) 76 74	23, 43, 76, 106	0
1	C	331/348 (95%)	0.26	7 (2%) 63 60	22, 47, 84, 118	0
1	D	331/348 (95%)	0.34	10 (3%) 52 49	25, 53, 83, 110	0
1	E	331/348 (95%)	0.46	13 (3%) 43 40	34, 58, 85, 130	0
1	F	331/348 (95%)	0.68	28 (8%) 16 14	31, 61, 91, 148	0
1	K	331/348 (95%)	0.80	26 (7%) 18 16	34, 64, 92, 137	0
1	L	331/348 (95%)	0.49	15 (4%) 38 35	35, 57, 86, 138	0
2	G	346/364 (95%)	-0.00	1 (0%) 90 88	24, 43, 62, 117	0
2	H	346/364 (95%)	-0.03	2 (0%) 85 83	26, 44, 62, 96	0
2	I	346/364 (95%)	0.12	2 (0%) 85 83	27, 46, 64, 116	0
2	J	346/364 (95%)	0.23	4 (1%) 76 74	28, 48, 69, 93	0
All	All	4032/4240 (95%)	0.30	120 (2%) 52 49	22, 50, 81, 148	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	24	ALA	4.5
1	F	25	PRO	4.4
1	K	24	ALA	4.2
1	B	27	LEU	3.9
1	K	25	PRO	3.8
1	L	28	ILE	3.8
1	E	25	PRO	3.7
1	K	325	ALA	3.7
1	E	107	VAL	3.5
1	L	27	LEU	3.3
1	K	107	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	292	GLY	3.3
1	F	226	PHE	3.2
2	I	356	LYS	3.2
1	E	308	ILE	3.2
1	L	308	ILE	3.2
1	K	226	PHE	3.2
1	F	57	PHE	3.1
1	A	26	GLY	3.1
1	L	102	VAL	3.1
1	K	308	ILE	3.1
1	C	24	ALA	3.0
1	F	105	PRO	3.0
1	D	81	TYR	3.0
1	C	27	LEU	2.9
1	L	104	MET	2.9
1	A	27	LEU	2.9
1	L	16	GLY	2.8
2	G	356	LYS	2.8
1	F	82	PHE	2.8
1	K	102	VAL	2.8
1	E	109	PRO	2.7
1	D	26	GLY	2.7
1	F	178	LEU	2.7
1	K	104	MET	2.7
1	D	24	ALA	2.7
1	F	26	GLY	2.7
1	L	226	PHE	2.6
1	E	80	GLU	2.6
1	K	120	VAL	2.6
1	D	342	THR	2.6
1	F	103	SER	2.6
1	K	38	LEU	2.6
1	A	81	TYR	2.6
1	F	306	PHE	2.6
2	I	261	ILE	2.6
1	K	109	PRO	2.6
1	A	6	SER	2.5
1	F	308	ILE	2.5
1	F	38	LEU	2.5
1	F	174	GLY	2.5
1	L	25	PRO	2.5
1	K	57	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	107	VAL	2.4
1	F	27	LEU	2.4
1	K	147	LEU	2.4
1	A	25	PRO	2.4
1	C	318	CYS	2.4
1	E	76	LEU	2.4
1	F	7	TYR	2.3
1	D	25	PRO	2.3
1	D	158	GLY	2.3
1	E	309	SER	2.3
1	F	107	VAL	2.3
1	D	27	LEU	2.3
1	F	80	GLU	2.3
1	E	105	PRO	2.3
2	J	356	LYS	2.3
1	L	306	PHE	2.3
1	C	7	TYR	2.3
1	K	7	TYR	2.3
1	B	14	LEU	2.3
2	J	96	ASP	2.3
2	H	355	GLY	2.3
1	A	342	THR	2.3
1	L	103	SER	2.3
1	K	252	TYR	2.2
1	K	28	ILE	2.2
1	C	339	LEU	2.2
1	E	27	LEU	2.2
1	K	99	CYS	2.2
1	E	26	GLY	2.2
1	A	335	ILE	2.2
1	K	141	ILE	2.2
1	K	27	LEU	2.2
1	F	158	GLY	2.2
1	F	309	SER	2.2
1	F	76	LEU	2.2
1	K	118	ARG	2.2
1	E	104	MET	2.2
1	E	106	LYS	2.2
1	F	104	MET	2.1
1	K	142	THR	2.1
1	C	81	TYR	2.1
1	F	206	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	105	PRO	2.1
1	F	16	GLY	2.1
1	F	118	ARG	2.1
1	D	6	SER	2.1
1	B	7	TYR	2.1
1	F	335	ILE	2.1
1	L	58	ASP	2.1
2	J	261	ILE	2.1
2	H	247	SER	2.1
1	K	58	ASP	2.1
1	C	36	VAL	2.1
1	E	174	GLY	2.1
1	L	26	GLY	2.1
1	F	8	ALA	2.0
1	A	339	LEU	2.0
1	K	116	ILE	2.0
1	D	36	VAL	2.0
1	F	292	GLY	2.0
1	K	16	GLY	2.0
1	L	57	PHE	2.0
1	F	172	TRP	2.0
1	B	6	SER	2.0
1	K	214	LEU	2.0
2	J	227	LEU	2.0
1	L	335	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

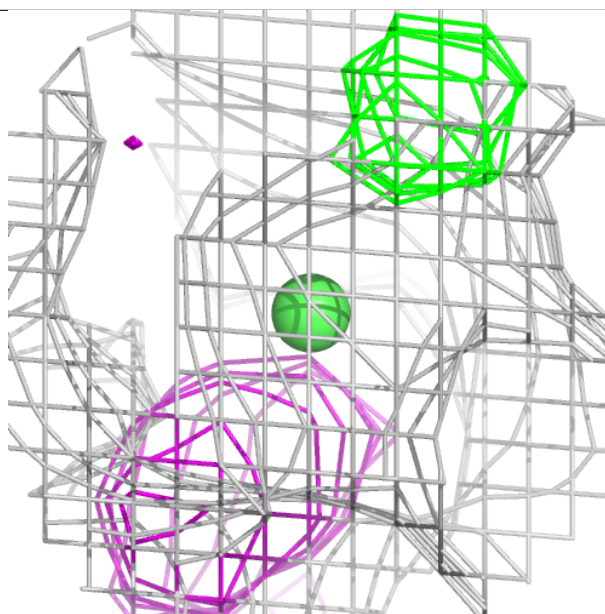
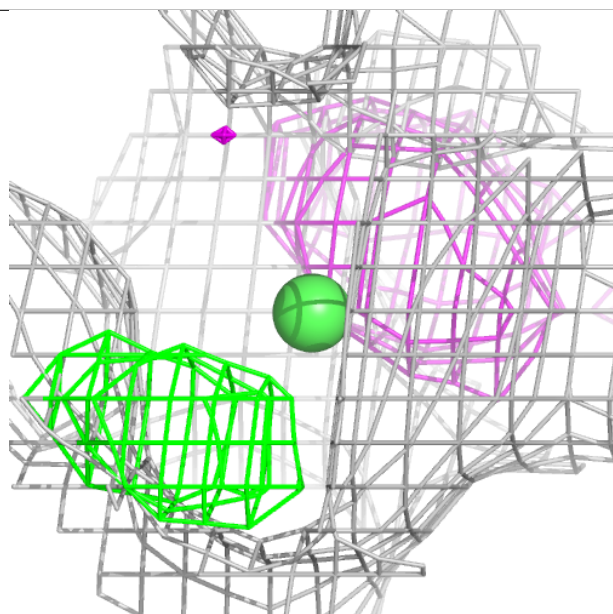
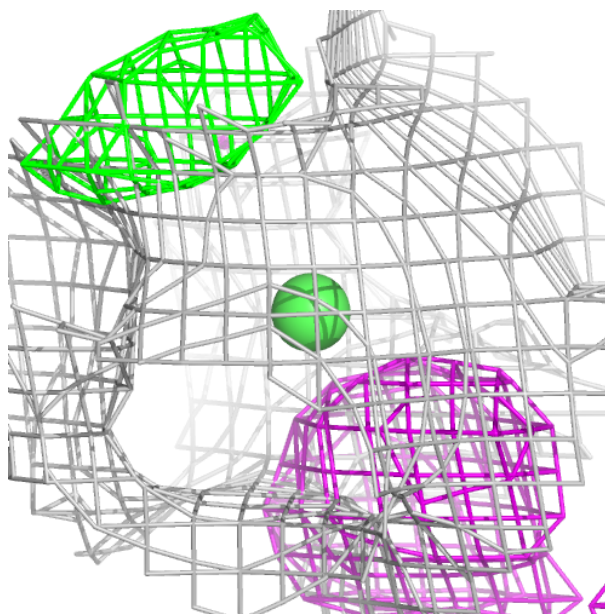
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NI	G	401	1/1	0.98	0.05	49,49,49,49	0
3	NI	G	402	1/1	0.98	0.03	49,49,49,49	0
3	NI	I	401	1/1	0.98	0.04	55,55,55,55	0
3	NI	H	402	1/1	0.99	0.03	47,47,47,47	0
3	NI	H	401	1/1	0.99	0.03	50,50,50,50	0
3	NI	I	402	1/1	0.99	0.03	56,56,56,56	0
3	NI	J	401	1/1	0.99	0.04	59,59,59,59	0
3	NI	J	402	1/1	0.99	0.04	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.

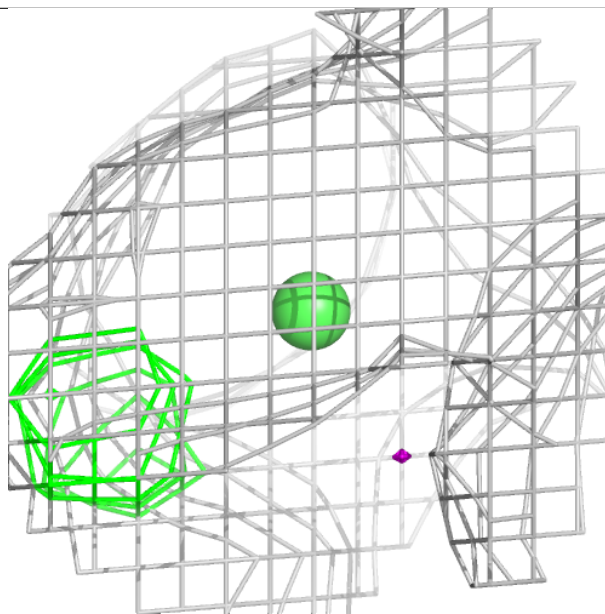
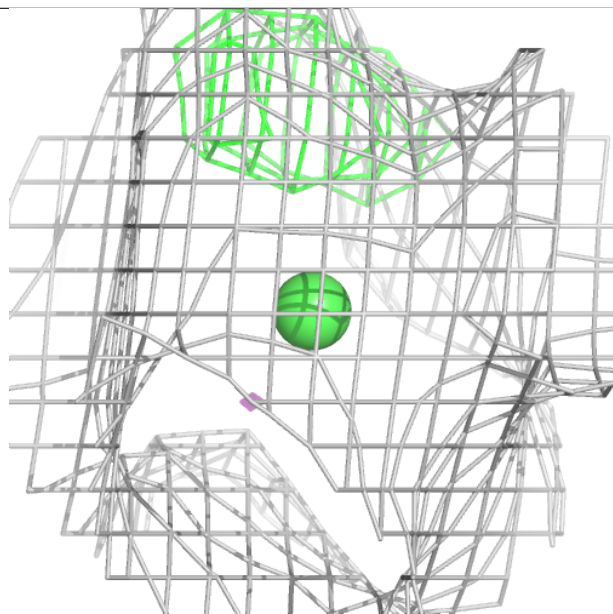
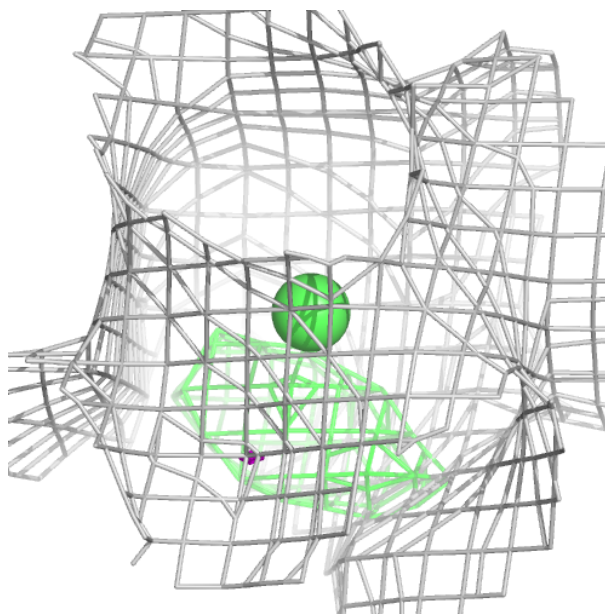
Electron density around NI G 401:

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



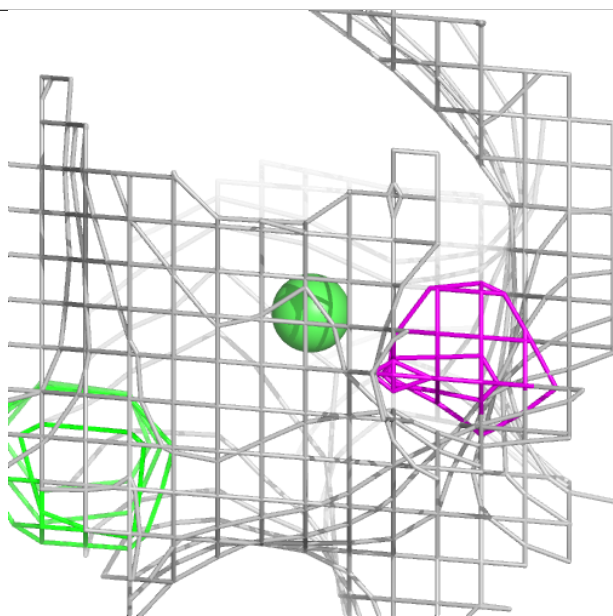
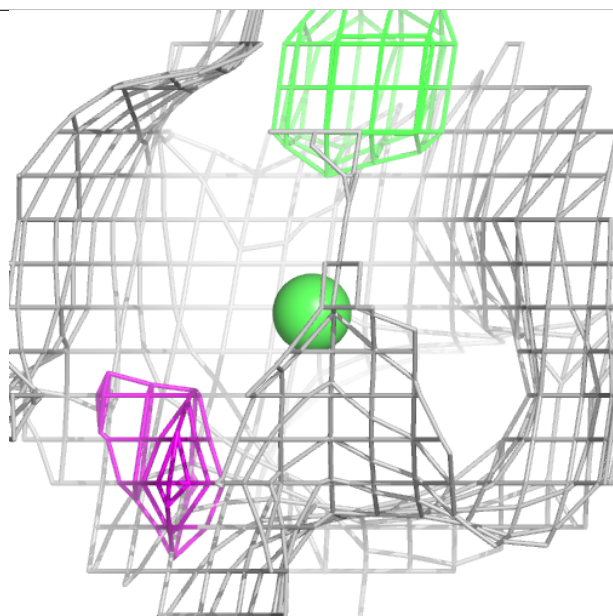
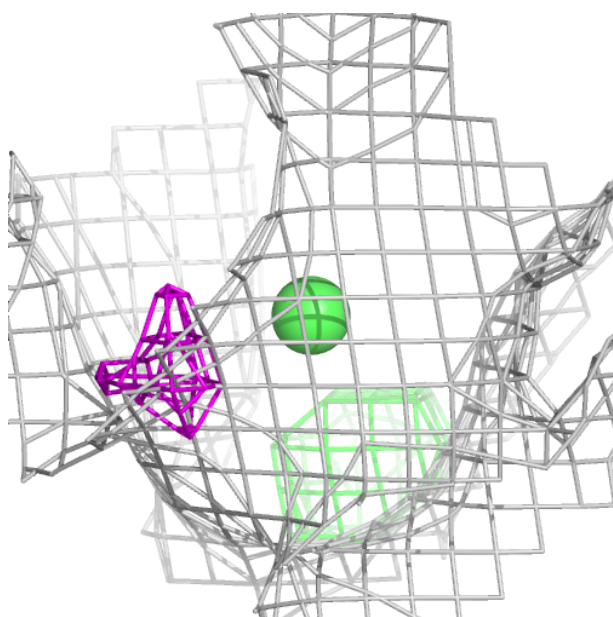
Electron density around NI G 402:

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



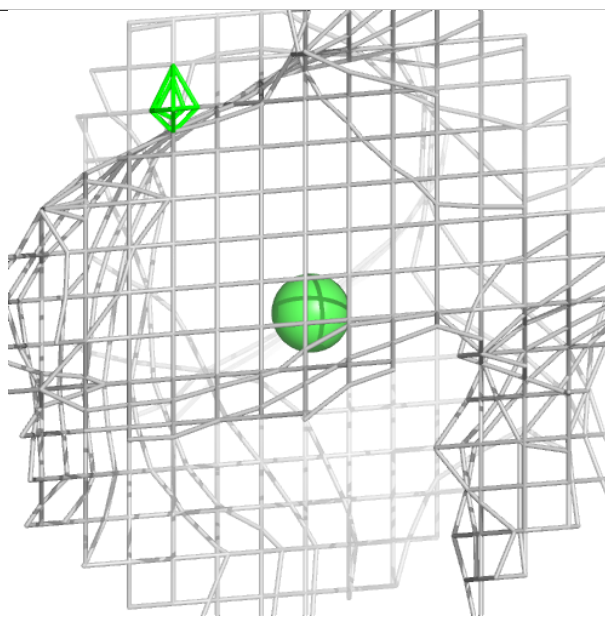
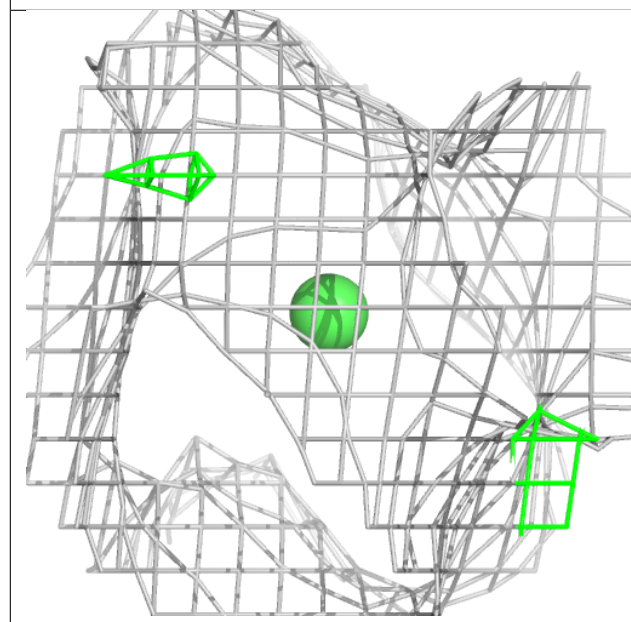
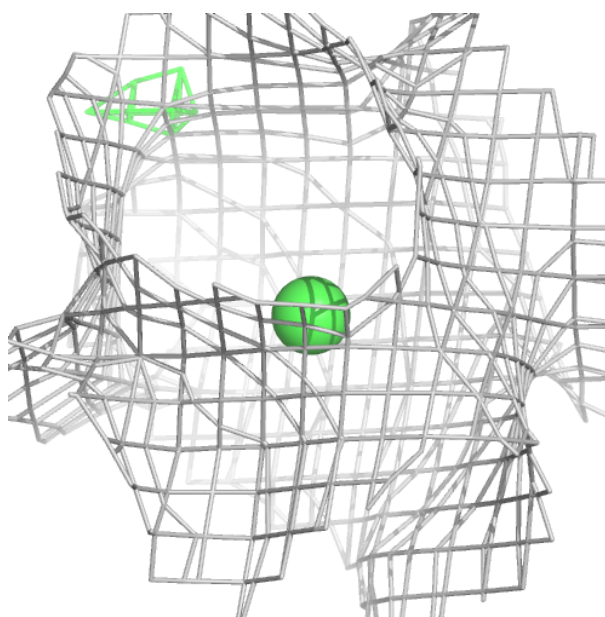
Electron density around NI I 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



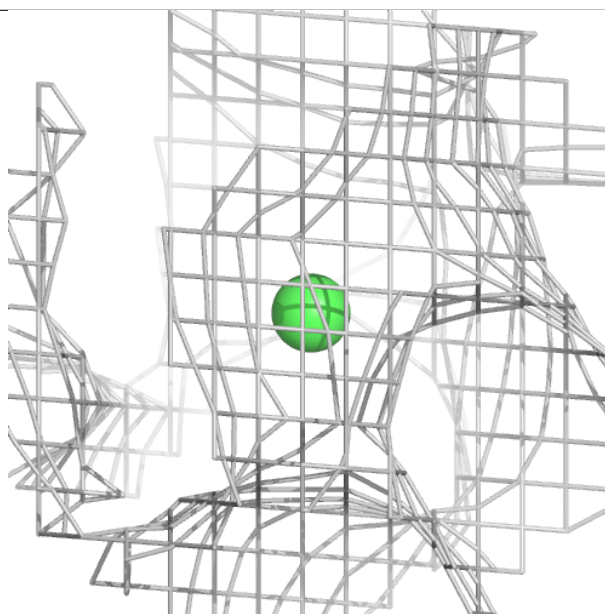
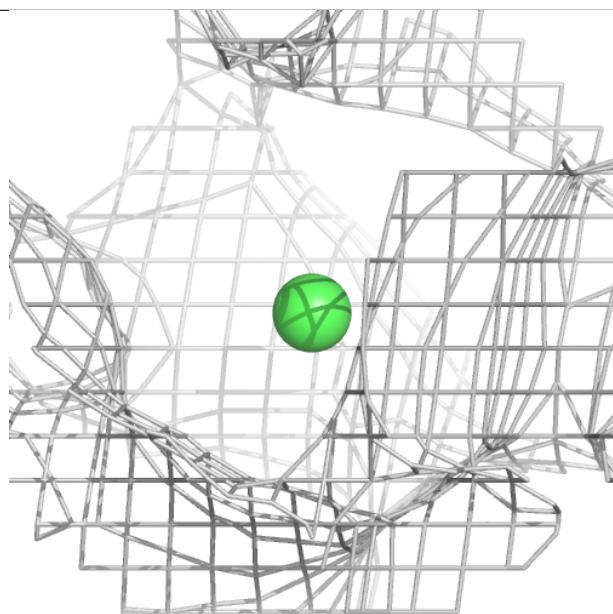
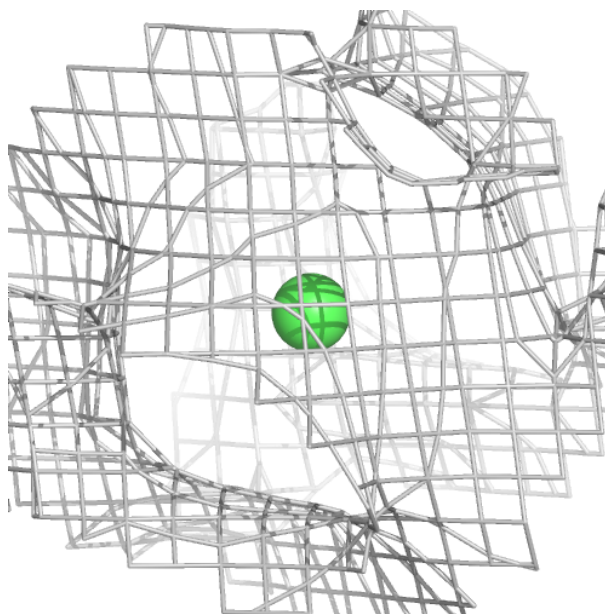
Electron density around NI H 402:

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and green (positive)



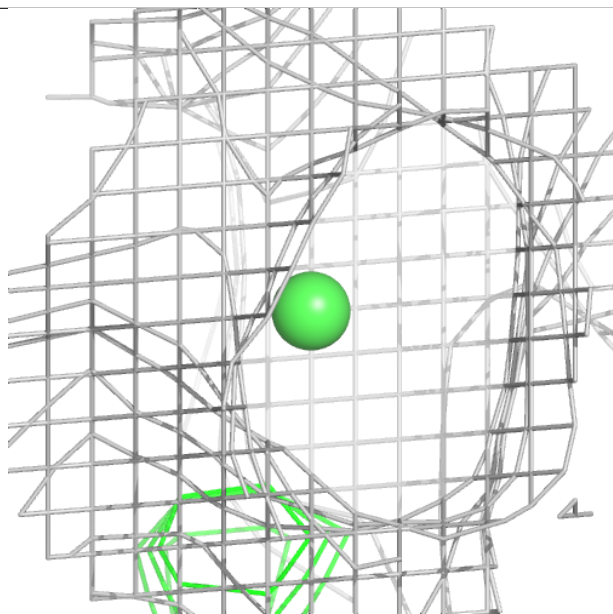
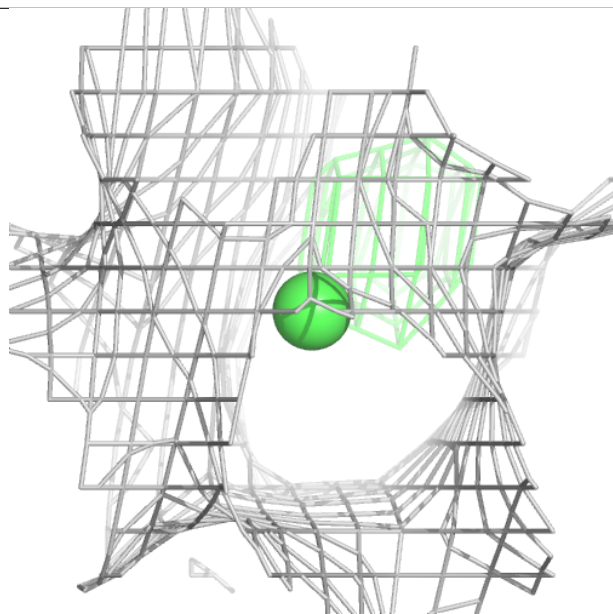
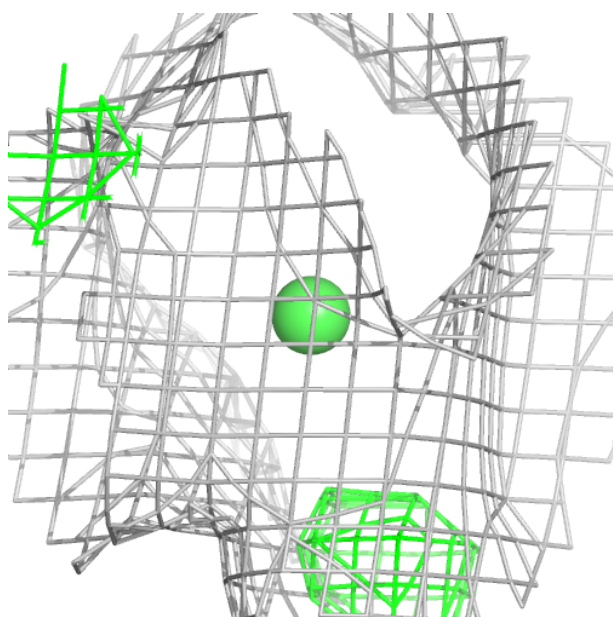
Electron density around NI H 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



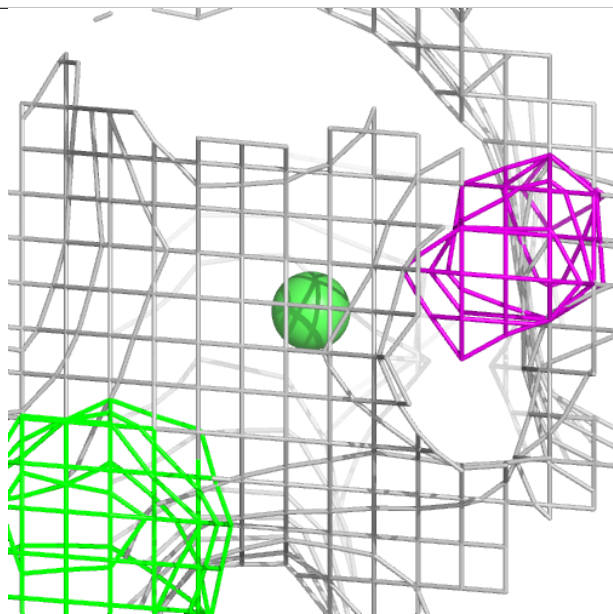
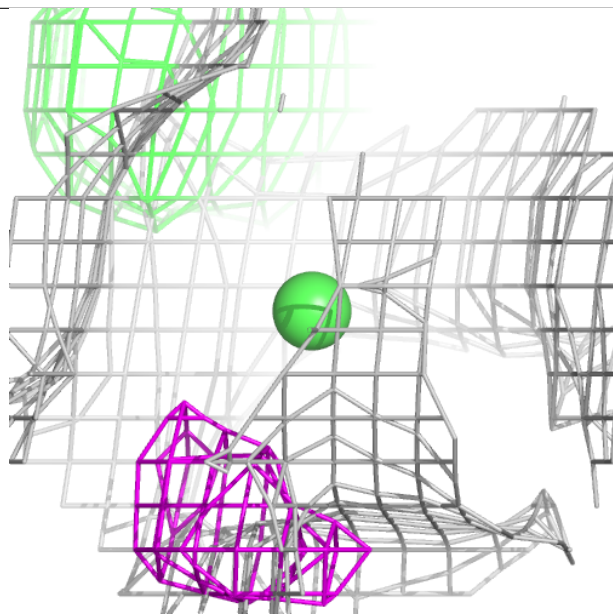
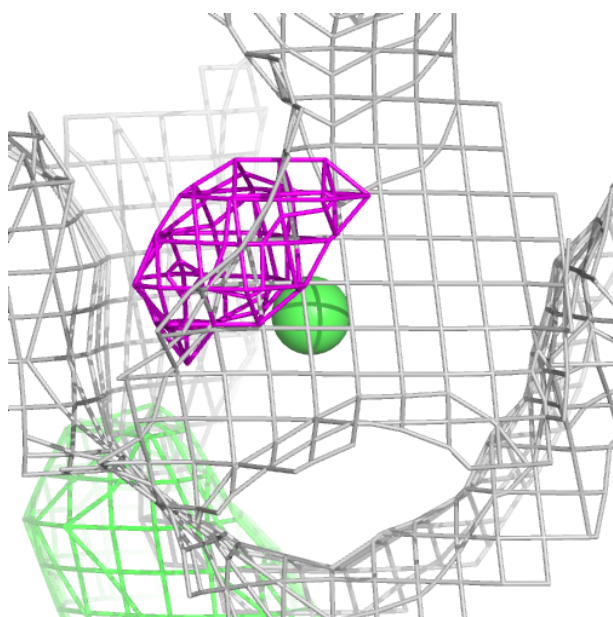
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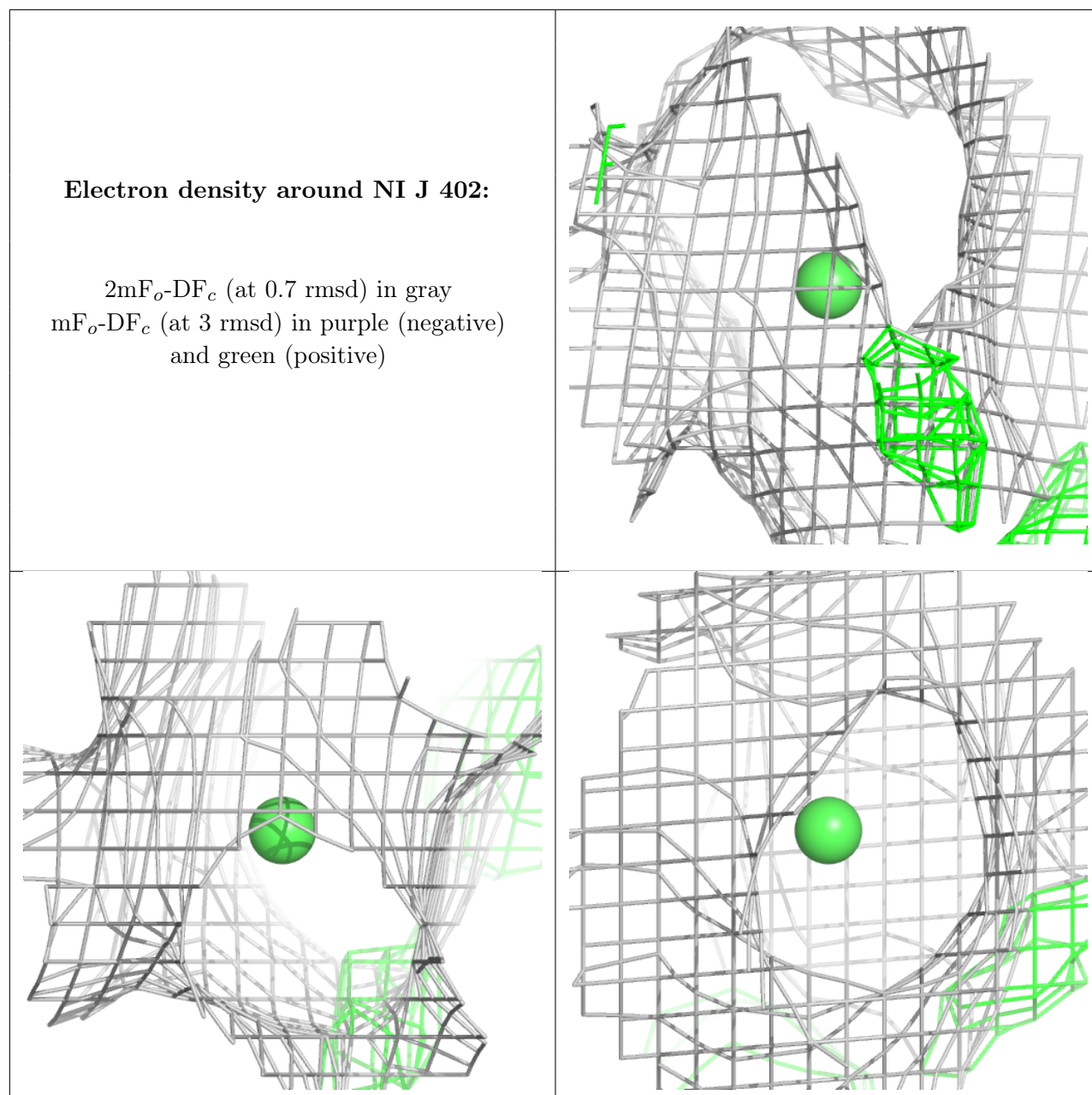
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NI J 401:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.