



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:58 PM UTC

PDB ID : 9CCK / pdb_00009cck
Title : Multi-copper oxidase with a C-terminal cupredoxin domain from *Nitrosopumilus maritimus*
Authors : Volland, R.W.; Lancaster, K.M.
Deposited on : 2024-06-21
Resolution : 1.84 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

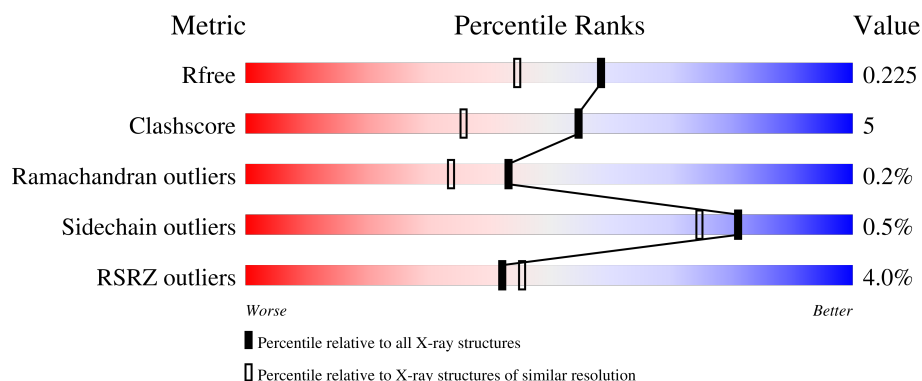
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	409	4% 92% 8%
1	B	409	4% 90% 9%
1	D	409	3% 92% 7%
1	E	409	2% 90% 9%
1	G	409	4% 88% 12%

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Mol	Chain	Length	Quality of chain
1	H	409	 3% 92% 7%
1	J	409	 4% 89% 11%
1	K	409	 3% 89% 11%
2	C	309	 5% 91% 9%
2	F	309	 4% 90% 10%
2	I	309	 6% 91% 9%
2	L	309	 6% 88% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 39687 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 Copper-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3239	2061	523	639	16			
1	B	409	Total	C	N	O	S	0	0	0
			3239	2061	523	639	16			
1	D	409	Total	C	N	O	S	0	0	0
			3239	2061	523	639	16			
1	E	409	Total	C	N	O	S	0	0	0
			3239	2061	523	639	16			
1	G	409	Total	C	N	O	S	0	0	0
			3239	2061	523	639	16			
1	H	409	Total	C	N	O	S	0	0	0
			3239	2061	523	639	16			
1	J	409	Total	C	N	O	S	0	0	0
			3239	2061	523	639	16			
1	K	409	Total	C	N	O	S	0	0	0
			3239	2061	523	639	16			

- Molecule 2 is a protein called Copper-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	309	Total	C	N	O	S	0	0	0
			2463	1576	402	471	14			
2	F	309	Total	C	N	O	S	0	0	0
			2463	1576	402	471	14			
2	I	309	Total	C	N	O	S	0	0	0
			2463	1576	402	471	14			
2	L	309	Total	C	N	O	S	0	0	0
			2463	1576	402	471	14			

- Molecule 3 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total Cu 6 6	0	0
3	B	5	Total Cu 5 5	0	0
3	C	3	Total Cu 3 3	0	0
3	D	5	Total Cu 5 5	0	0
3	E	5	Total Cu 5 5	0	0
3	F	4	Total Cu 4 4	0	0
3	G	5	Total Cu 5 5	0	0
3	H	5	Total Cu 5 5	0	0
3	I	4	Total Cu 4 4	0	0
3	J	5	Total Cu 5 5	0	0
3	K	5	Total Cu 5 5	0	0
3	L	4	Total Cu 4 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	314	Total O 314 314	0	0
4	B	399	Total O 399 399	0	0
4	C	282	Total O 282 282	0	0
4	D	323	Total O 323 323	0	0
4	E	427	Total O 427 427	0	0
4	F	304	Total O 304 304	0	0
4	G	319	Total O 319 319	0	0
4	H	363	Total O 363 363	0	0

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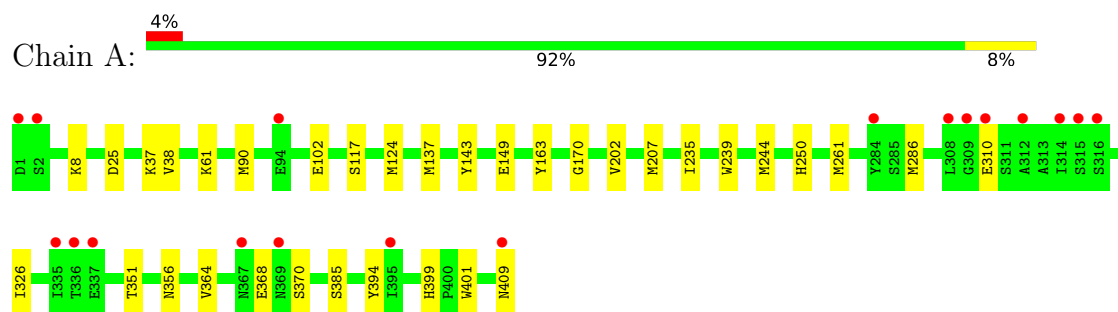
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	268	Total 268	O 268	0	0
4	J	296	Total 296	O 296	0	0
4	K	353	Total 353	O 353	0	0
4	L	219	Total 219	O 219	0	0

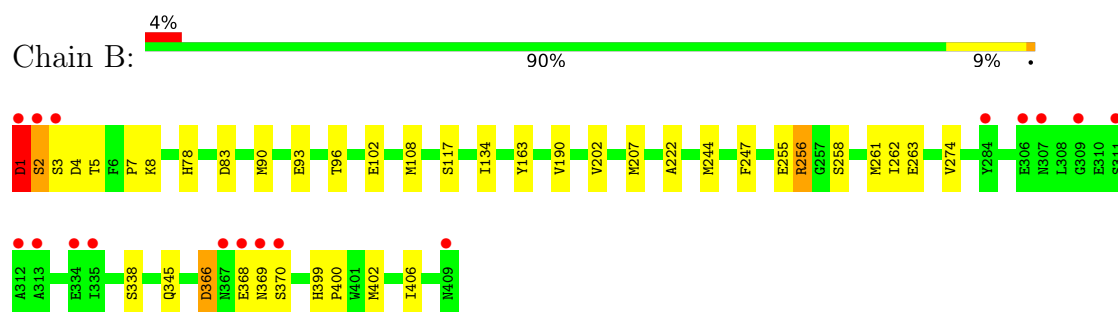
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

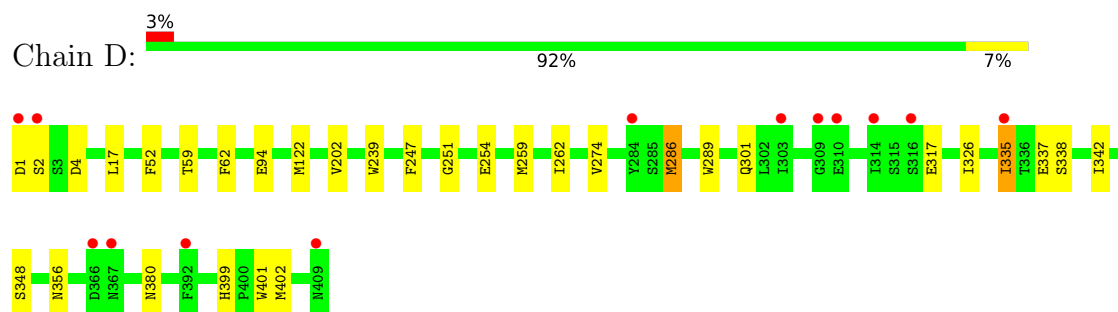
- Molecule 1: Copper-containing nitrite reductase



- Molecule 1: Copper-containing nitrite reductase

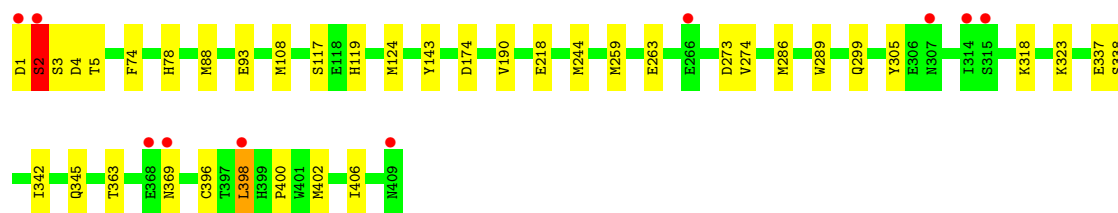


- Molecule 1: Copper-containing nitrite reductase

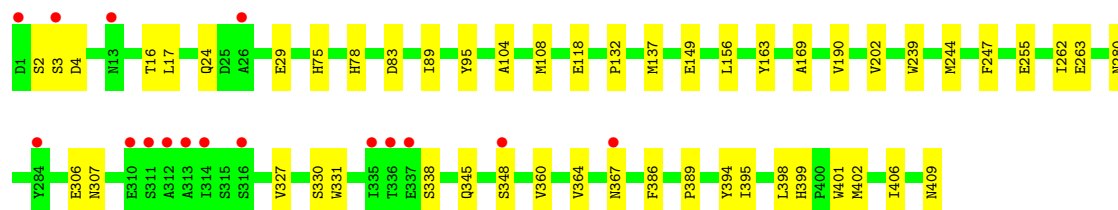
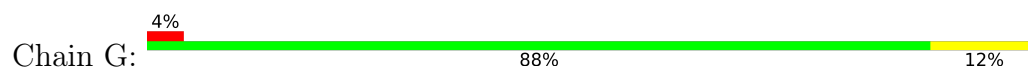


- Molecule 1: Copper-containing nitrite reductase

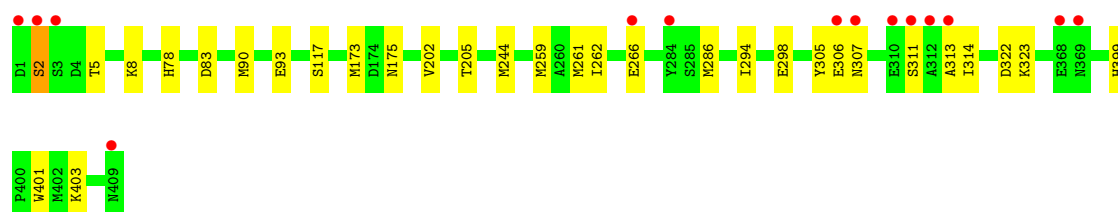




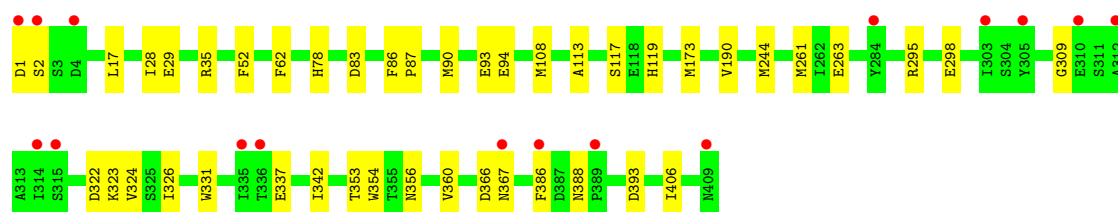
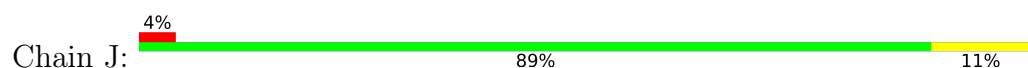
- Molecule 1: Copper-containing nitrite reductase



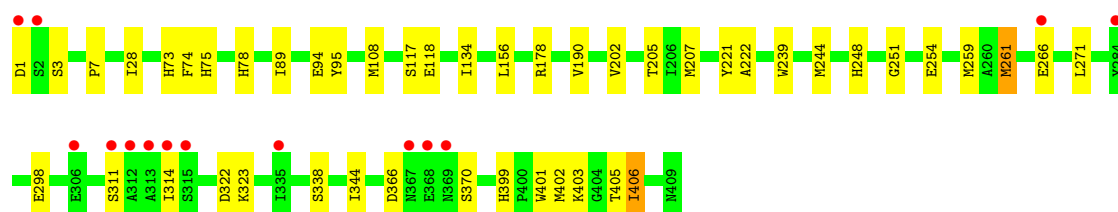
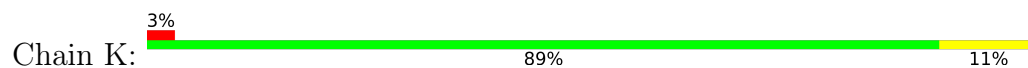
- Molecule 1: Copper-containing nitrite reductase



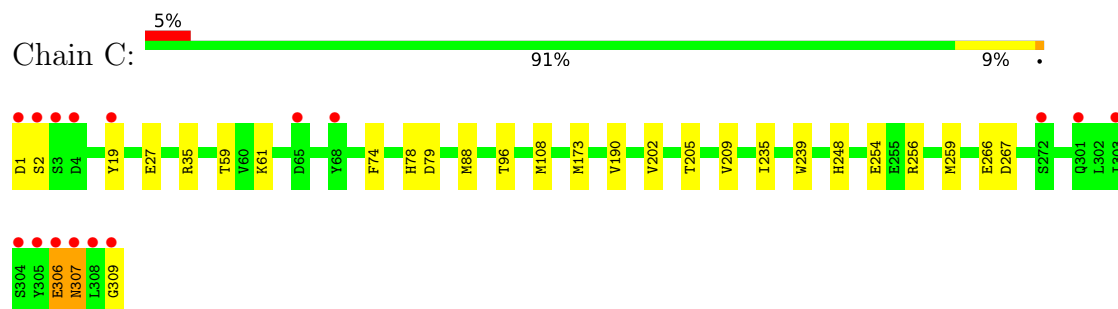
- Molecule 1: Copper-containing nitrite reductase



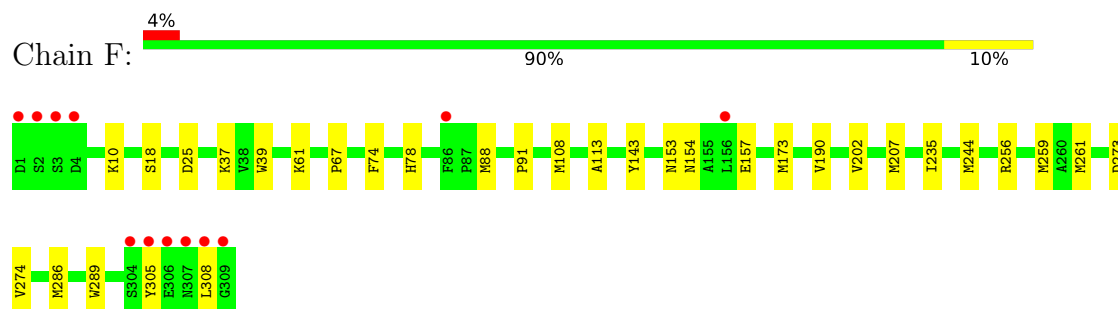
- Molecule 1: Copper-containing nitrite reductase



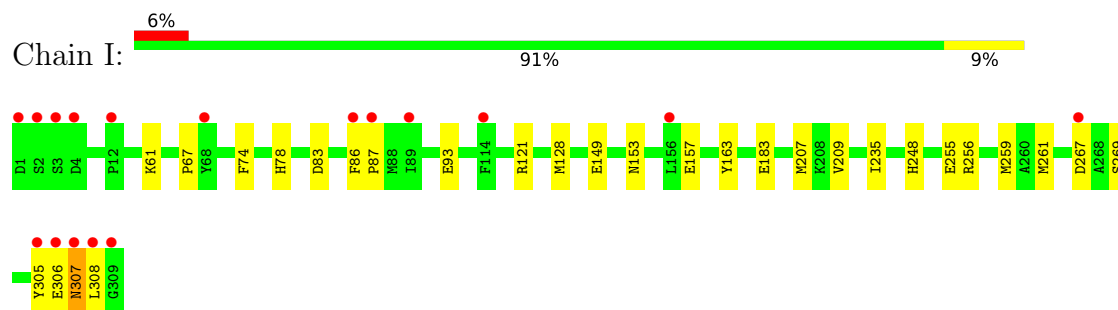
● Molecule 2: Copper-containing nitrite reductase



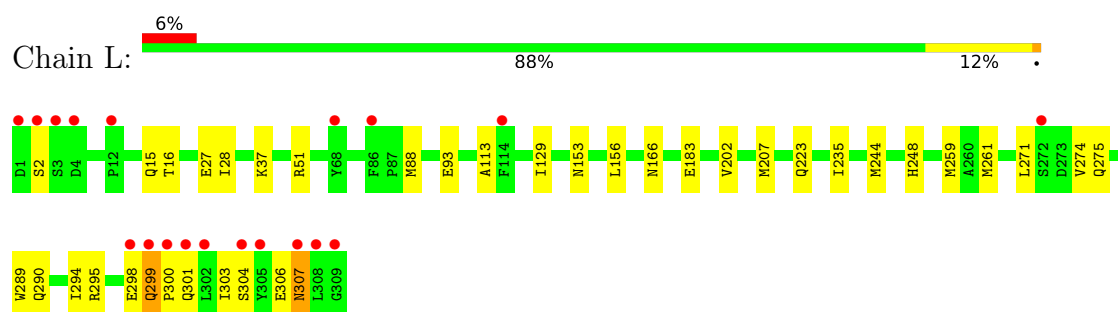
● Molecule 2: Copper-containing nitrite reductase



● Molecule 2: Copper-containing nitrite reductase



● Molecule 2: Copper-containing nitrite reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	173.29Å 92.98Å 204.48Å 90.00° 95.79° 90.00°	Depositor
Resolution (Å)	84.56 – 1.84 84.56 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.1 (84.56-1.84) 99.1 (84.56-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.199 , 0.226 0.199 , 0.225	Depositor DCC
R_{free} test set	27687 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	39687	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 42.65 % 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 1.9767e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.35	0/3338	0.57	2/4560 (0.0%)
1	B	0.38	0/3338	0.62	2/4560 (0.0%)
1	D	0.37	0/3338	0.58	1/4560 (0.0%)
1	E	0.39	0/3338	0.61	1/4560 (0.0%)
1	G	0.36	0/3338	0.54	0/4560
1	H	0.37	0/3338	0.59	0/4560
1	J	0.32	0/3338	0.55	0/4560
1	K	0.37	0/3338	0.58	1/4560 (0.0%)
2	C	0.39	0/2541	0.60	0/3466
2	F	0.40	0/2541	0.60	0/3466
2	I	0.35	0/2541	0.57	0/3466
2	L	0.34	0/2541	0.56	0/3466
All	All	0.37	0/36868	0.58	7/50344 (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	B	0	3
2	L	0	1
All	All	0	4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	261	MET	CG-SD-CE	5.48	112.95	100.90
1	D	286	MET	CB-CG-SD	-5.21	97.08	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	ASP	CA-C-N	-5.11	112.67	121.66
1	B	366	ASP	C-N-CA	-5.11	112.67	121.66
1	E	398	LEU	N-CA-C	-5.11	102.20	110.32
1	A	368	GLU	CA-C-N	-5.04	113.60	123.13
1	A	368	GLU	C-N-CA	-5.04	113.60	123.13

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1	ASP	Peptide
1	B	256	ARG	Sidechain
1	B	368	GLU	Peptide
2	L	299	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3239	0	3014	25	0
1	B	3239	0	3014	30	1
1	D	3239	0	3014	23	0
1	E	3239	0	3014	35	0
1	G	3239	0	3014	38	0
1	H	3239	0	3014	23	0
1	J	3239	0	3014	27	0
1	K	3239	0	3014	36	1
2	C	2463	0	2310	22	1
2	F	2463	0	2310	25	0
2	I	2463	0	2310	23	0
2	L	2463	0	2310	30	1
3	A	6	0	0	0	0
3	B	5	0	0	0	0
3	C	3	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	5	0	0	0	0
3	H	5	0	0	0	0
3	I	4	0	0	0	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	4	0	0	0	0
4	A	314	0	0	7	3
4	B	399	0	0	6	0
4	C	282	0	0	10	0
4	D	323	0	0	3	0
4	E	427	0	0	13	0
4	F	304	0	0	9	0
4	G	319	0	0	9	1
4	H	363	0	0	7	0
4	I	268	0	0	8	1
4	J	296	0	0	6	3
4	K	353	0	0	2	0
4	L	219	0	0	7	0
All	All	39687	0	33352	333	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (333) 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:D:301:GLN:OE1	4:D:601:HOH:O	1.90	0.89
1:J:337:GLU:HB2	1:J:342:ILE:HD11	1.54	0.89
1:E:345:GLN:NE2	4:E:603:HOH:O	2.09	0.86
1:E:244:MET:HE1	1:E:263:GLU:HG3	1.58	0.85
1:K:75:HIS:HD1	2:L:223:GLN:HE21	1.24	0.82
2:F:153:ASN:ND2	4:F:501:HOH:O	2.06	0.82
1:E:363:THR:O	4:E:601:HOH:O	1.99	0.81
1:G:338:SER:HB3	1:G:402:MET:HG2	1.61	0.80
1:B:117:SER:HB3	4:C:528:HOH:O	1.83	0.78
1:A:370:SER:OG	4:A:601:HOH:O	2.01	0.78
1:E:273:ASP:OD1	4:E:602:HOH:O	2.01	0.77
1:G:2:SER:O	1:G:4:ASP:N	2.16	0.77
1:A:117:SER:HB3	4:B:602:HOH:O	1.84	0.77
2:C:19:TYR:OH	4:C:501:HOH:O	2.02	0.76
2:I:61:LYS:NZ	4:I:502:HOH:O	2.17	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:GLY:O	1:D:254:GLU:HG2	1.85	0.76
2:F:244:MET:HE2	2:F:261:MET:SD	2.26	0.74
2:L:93:GLU:OE2	4:L:501:HOH:O	2.05	0.74
1:H:266:GLU:CD	1:H:266:GLU:H	1.96	0.74
2:F:256:ARG:NE	4:F:504:HOH:O	2.19	0.73
1:G:24:GLN:OE1	4:G:601:HOH:O	2.05	0.73
2:C:267:ASP:OD2	4:C:502:HOH:O	2.06	0.73
1:A:61:LYS:HG3	4:A:604:HOH:O	1.88	0.73
2:I:267:ASP:OD2	2:I:269:SER:OG	2.05	0.72
2:F:273:ASP:OD1	4:F:502:HOH:O	2.06	0.71
1:B:202:VAL:HG22	4:B:646:HOH:O	1.91	0.71
1:E:93:GLU:HG3	4:E:920:HOH:O	1.90	0.71
2:C:205:THR:O	4:C:503:HOH:O	2.08	0.71
1:B:90:MET:HE3	1:B:400:PRO:HB3	1.71	0.71
2:L:244:MET:HE2	2:L:261:MET:HG2	1.71	0.71
1:K:244:MET:HE2	1:K:261:MET:CE	2.21	0.70
1:H:175:ASN:ND2	4:H:601:HOH:O	2.23	0.70
1:K:311:SER:OG	1:K:403:LYS:HE2	1.91	0.70
1:E:2:SER:HB2	1:E:218:GLU:OE2	1.92	0.69
2:L:28:ILE:HG22	2:L:300:PRO:HA	1.73	0.69
1:H:90:MET:HB2	1:H:93:GLU:HG3	1.74	0.69
2:F:25:ASP:OD2	4:F:503:HOH:O	2.10	0.69
4:H:708:HOH:O	2:I:259:MET:HE1	1.92	0.69
1:E:299:GLN:NE2	4:E:606:HOH:O	2.16	0.69
1:K:266:GLU:H	1:K:266:GLU:CD	2.01	0.69
2:L:244:MET:HE2	2:L:261:MET:CG	2.23	0.68
1:G:29:GLU:OE2	4:G:602:HOH:O	2.12	0.67
1:G:78:HIS:HE1	1:G:83:ASP:OD1	1.77	0.67
1:B:90:MET:HB2	1:B:93:GLU:CD	2.20	0.66
1:B:1:ASP:OD2	4:B:601:HOH:O	2.13	0.66
1:D:399:HIS:O	1:D:402:MET:HB2	1.94	0.66
2:I:93:GLU:OE1	4:I:501:HOH:O	2.12	0.66
1:E:174:ASP:OD2	4:E:604:HOH:O	2.13	0.65
1:G:327:VAL:O	1:G:330:SER:OG	2.11	0.65
2:L:271:LEU:O	2:L:275:GLN:HG2	1.96	0.65
1:B:244:MET:SD	1:B:261:MET:HE3	2.37	0.64
1:G:399:HIS:N	4:G:604:HOH:O	2.31	0.63
1:H:8:LYS:HE2	4:H:660:HOH:O	1.99	0.63
1:D:59:THR:HG23	4:D:644:HOH:O	1.98	0.63
1:J:117:SER:OG	4:J:601:HOH:O	1.89	0.63
2:L:183:GLU:OE1	4:L:502:HOH:O	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:TYR:O	4:E:605:HOH:O	2.16	0.62
1:B:244:MET:HE1	1:B:263:GLU:HG3	1.80	0.62
2:C:267:ASP:CG	4:C:502:HOH:O	2.43	0.62
2:C:88:MET:HE2	2:C:88:MET:HA	1.82	0.61
1:D:338:SER:HB3	1:D:402:MET:HG2	1.83	0.61
1:E:259:MET:HE1	4:E:625:HOH:O	2.02	0.60
2:F:202:VAL:HG22	4:F:511:HOH:O	2.01	0.60
2:C:307:ASN:ND2	4:C:512:HOH:O	2.34	0.60
2:I:256:ARG:NE	4:I:509:HOH:O	2.33	0.60
1:J:244:MET:HE3	1:J:261:MET:SD	2.42	0.59
1:J:244:MET:SD	1:J:263:GLU:HG3	2.42	0.59
1:E:117:SER:HB3	4:F:508:HOH:O	2.02	0.59
2:L:153:ASN:ND2	4:L:505:HOH:O	2.29	0.59
1:B:338:SER:CB	1:B:402:MET:HG2	2.32	0.59
2:L:244:MET:HE3	2:L:244:MET:HA	1.85	0.59
4:J:871:HOH:O	2:L:156:LEU:HD12	2.01	0.59
1:G:399:HIS:HB3	1:G:401:TRP:CZ2	2.37	0.59
1:K:117:SER:HB3	4:L:510:HOH:O	2.01	0.59
1:K:366:ASP:OD2	1:K:370:SER:HB3	2.03	0.59
2:C:306:GLU:OE1	4:C:504:HOH:O	2.17	0.58
2:C:27:GLU:HG3	2:C:35:ARG:HG2	1.86	0.58
1:E:274:VAL:HG22	1:E:289:TRP:HB2	1.85	0.58
1:H:202:VAL:HG22	4:H:641:HOH:O	2.04	0.58
1:A:37:LYS:HE2	1:A:38:VAL:O	2.04	0.58
1:J:295:ARG:NH2	4:J:602:HOH:O	2.17	0.58
1:G:169:ALA:O	4:G:603:HOH:O	2.17	0.57
1:H:78:HIS:HE1	1:H:83:ASP:OD1	1.87	0.57
1:B:255:GLU:OE2	4:B:602:HOH:O	2.18	0.57
2:L:290:GLN:O	2:L:294:ILE:HG12	2.05	0.57
1:B:366:ASP:OD2	1:B:370:SER:HB3	2.05	0.57
2:C:256:ARG:NE	4:C:514:HOH:O	2.37	0.57
1:K:254:GLU:HB2	1:K:259:MET:HE3	1.86	0.57
1:H:314:ILE:HD11	1:H:403:LYS:HG3	1.86	0.56
1:G:78:HIS:HD2	4:G:860:HOH:O	1.87	0.56
2:L:28:ILE:HB	2:L:298:GLU:HG3	1.86	0.56
1:K:75:HIS:HD1	2:L:223:GLN:NE2	2.01	0.56
2:I:256:ARG:CZ	4:I:509:HOH:O	2.54	0.55
2:F:91:PRO:HB3	2:F:308:LEU:HD22	1.88	0.55
1:H:244:MET:HE2	1:H:261:MET:SD	2.46	0.55
1:G:75:HIS:HA	4:H:773:HOH:O	2.06	0.55
1:G:338:SER:CB	1:G:402:MET:HG2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLY:HA2	4:A:730:HOH:O	2.06	0.55
1:K:248:HIS:CG	1:K:259:MET:HE2	2.42	0.55
1:H:294:ILE:O	1:H:298:GLU:HG3	2.07	0.55
1:B:2:SER:HB2	1:B:5:THR:H	1.71	0.55
1:K:254:GLU:HB2	1:K:259:MET:CE	2.36	0.54
2:L:15:GLN:HE21	2:L:16:THR:H	1.55	0.54
1:E:323:LYS:HD2	4:E:972:HOH:O	2.06	0.54
1:K:207:MET:HB2	1:K:222:ALA:O	2.08	0.54
1:A:202:VAL:CG1	1:A:239:TRP:HZ2	2.21	0.54
2:C:266:GLU:OE2	4:C:505:HOH:O	2.18	0.54
2:F:37:LYS:NZ	2:F:39:TRP:HE1	2.04	0.54
2:I:207:MET:HB3	2:I:235:ILE:HG23	1.89	0.54
1:K:108:MET:HE2	1:K:190:VAL:HG13	1.90	0.54
1:J:323:LYS:NZ	4:J:611:HOH:O	2.39	0.54
2:L:244:MET:CE	2:L:261:MET:HG2	2.38	0.54
1:J:323:LYS:HE3	1:J:353:THR:HB	1.89	0.54
1:K:244:MET:HE2	1:K:261:MET:HE3	1.89	0.54
2:F:88:MET:HE1	2:F:113:ALA:HA	1.89	0.54
1:K:74:PHE:O	1:K:78:HIS:HE1	1.91	0.54
2:F:143:TYR:CZ	2:F:286:MET:HG3	2.43	0.53
2:L:202:VAL:HG22	4:L:508:HOH:O	2.08	0.53
1:B:244:MET:HE1	1:B:263:GLU:CG	2.38	0.53
1:E:338:SER:CB	1:E:402:MET:HG2	2.38	0.53
2:I:61:LYS:HG3	4:I:505:HOH:O	2.09	0.53
2:I:74:PHE:HB3	2:I:128:MET:HE1	1.91	0.53
1:B:78:HIS:HE1	1:B:83:ASP:OD1	1.89	0.53
1:D:335:ILE:O	1:D:335:ILE:HG13	2.06	0.53
1:E:2:SER:C	1:E:4:ASP:H	2.17	0.52
1:E:88:MET:HG3	1:E:398:LEU:HD23	1.91	0.52
1:K:338:SER:CB	1:K:402:MET:HG2	2.39	0.52
1:E:74:PHE:O	1:E:78:HIS:HE1	1.93	0.52
2:I:121:ARG:NH1	2:I:157:GLU:O	2.33	0.52
1:J:322:ASP:O	1:J:323:LYS:HD2	2.10	0.52
2:C:173:MET:SD	2:C:259:MET:HG2	2.49	0.52
1:D:380:ASN:ND2	4:E:604:HOH:O	2.43	0.51
2:I:78:HIS:HE1	2:I:83:ASP:OD1	1.92	0.51
1:G:399:HIS:CG	4:G:604:HOH:O	2.61	0.51
1:E:1:ASP:O	1:E:3:SER:N	2.44	0.51
2:L:27:GLU:OE2	2:L:37:LYS:HG2	2.10	0.51
2:F:173:MET:SD	2:F:259:MET:HG3	2.50	0.51
1:H:259:MET:HE1	4:H:614:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:HG11	1:A:239:TRP:HZ2	1.76	0.50
1:D:1:ASP:HA	1:D:4:ASP:OD2	2.11	0.50
1:E:400:PRO:HA	4:E:687:HOH:O	2.12	0.50
1:B:207:MET:HB2	1:B:222:ALA:O	2.10	0.50
2:C:108:MET:HE2	2:C:190:VAL:HG13	1.93	0.50
1:H:244:MET:CE	1:H:261:MET:HG2	2.42	0.50
1:K:344:ILE:HD11	1:K:406:ILE:HD12	1.94	0.50
1:B:8:LYS:NZ	1:B:102:GLU:O	2.45	0.50
1:D:274:VAL:HG22	1:D:289:TRP:HB2	1.94	0.50
2:F:37:LYS:HZ1	2:F:39:TRP:HE1	1.59	0.50
2:I:267:ASP:CG	4:I:503:HOH:O	2.55	0.50
1:B:7:PRO:HG2	1:B:134:ILE:HD13	1.94	0.49
2:F:61:LYS:HG3	4:F:657:HOH:O	2.11	0.49
1:G:202:VAL:HG11	1:G:239:TRP:HZ2	1.77	0.49
1:A:37:LYS:NZ	4:A:602:HOH:O	2.23	0.49
2:F:256:ARG:CZ	4:F:504:HOH:O	2.57	0.49
1:G:367:ASN:HD21	1:G:395:ILE:HG23	1.75	0.49
1:A:310:GLU:HG3	4:A:661:HOH:O	2.13	0.49
1:D:17:LEU:HD12	1:D:52:PHE:HB3	1.94	0.49
1:H:2:SER:HB2	1:H:5:THR:HG23	1.94	0.49
1:B:2:SER:OG	1:B:3:SER:N	2.46	0.49
1:K:338:SER:HB3	1:K:402:MET:HG2	1.94	0.49
2:C:74:PHE:O	2:C:78:HIS:HE1	1.95	0.49
1:A:250:HIS:ND1	4:A:606:HOH:O	2.33	0.49
1:K:244:MET:HE2	1:K:261:MET:HE2	1.94	0.49
2:C:1:ASP:O	2:C:2:SER:C	2.56	0.49
1:E:1:ASP:C	1:E:3:SER:N	2.70	0.48
1:G:348:SER:HB3	1:G:389:PRO:HD3	1.94	0.48
2:F:108:MET:HE2	2:F:190:VAL:HG13	1.95	0.48
1:A:207:MET:HB3	1:A:235:ILE:HG23	1.95	0.48
1:B:338:SER:HB3	1:B:402:MET:HG2	1.95	0.48
1:G:149:GLU:HG2	1:G:163:TYR:CE2	2.49	0.48
1:B:2:SER:C	1:B:4:ASP:H	2.22	0.48
2:L:298:GLU:O	2:L:298:GLU:HG2	2.14	0.48
2:L:207:MET:HB3	2:L:235:ILE:HG23	1.95	0.48
1:B:1:ASP:CG	4:B:601:HOH:O	2.56	0.47
2:L:303:ILE:HA	4:L:504:HOH:O	2.13	0.47
1:B:366:ASP:CG	1:B:369:ASN:H	2.22	0.47
1:E:108:MET:HE2	1:E:190:VAL:HG13	1.95	0.47
1:A:399:HIS:HB3	1:A:401:TRP:CZ2	2.50	0.47
1:B:399:HIS:O	1:B:402:MET:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2:SER:C	1:G:4:ASP:N	2.72	0.47
1:J:62:PHE:O	1:J:94:GLU:HG2	2.15	0.47
1:K:322:ASP:O	1:K:323:LYS:HE2	2.15	0.47
1:G:16:THR:C	1:G:17:LEU:HD23	2.39	0.47
2:I:153:ASN:ND2	4:I:508:HOH:O	2.33	0.46
1:B:2:SER:HB3	1:B:5:THR:HG23	1.96	0.46
1:E:2:SER:CB	1:E:218:GLU:HG2	2.45	0.46
1:J:309:GLY:O	4:J:603:HOH:O	2.20	0.46
1:A:25:ASP:HB3	1:A:37:LYS:HE3	1.97	0.46
1:G:78:HIS:CE1	1:G:83:ASP:HA	2.51	0.46
1:J:331:TRP:HB3	1:J:360:VAL:HG21	1.98	0.46
1:K:7:PRO:HG2	1:K:134:ILE:HD13	1.96	0.46
2:L:295:ARG:NH1	2:L:300:PRO:HG2	2.29	0.46
1:E:274:VAL:HG21	1:E:289:TRP:CD1	2.51	0.46
1:G:137:MET:HG3	1:G:280:ASN:HD21	1.80	0.46
1:E:143:TYR:CZ	1:E:286:MET:HG3	2.51	0.46
1:G:306:GLU:HG2	1:G:307:ASN:N	2.29	0.46
2:C:254:GLU:HB2	2:C:259:MET:HE3	1.97	0.46
1:D:317:GLU:HG2	1:H:305:TYR:CE2	2.51	0.46
2:F:274:VAL:CG2	2:F:289:TRP:HB2	2.45	0.45
1:D:202:VAL:CG1	1:D:239:TRP:HZ2	2.29	0.45
2:I:149:GLU:HG2	2:I:163:TYR:CE2	2.51	0.45
1:J:28:ILE:HB	1:J:298:GLU:HB3	1.98	0.45
2:I:261:MET:HE3	2:I:261:MET:HB2	1.79	0.45
2:F:154:ASN:ND2	2:F:157:GLU:OE1	2.50	0.45
1:G:202:VAL:CG1	1:G:239:TRP:HZ2	2.29	0.45
1:H:399:HIS:HB3	1:H:401:TRP:CZ2	2.51	0.45
1:K:399:HIS:HB3	1:K:401:TRP:CZ2	2.51	0.45
1:E:396:CYS:SG	1:E:398:LEU:O	2.75	0.45
1:K:322:ASP:C	1:K:323:LYS:HE2	2.42	0.45
2:F:244:MET:CE	2:F:261:MET:HG2	2.47	0.45
1:J:17:LEU:HD12	1:J:52:PHE:HB3	1.98	0.45
1:K:73:HIS:HA	4:K:690:HOH:O	2.15	0.45
1:A:202:VAL:HG11	1:A:239:TRP:CZ2	2.51	0.45
1:A:244:MET:HE3	1:A:261:MET:HE3	1.99	0.45
1:H:117:SER:OG	2:I:255:GLU:OE1	2.34	0.45
1:D:326:ILE:HB	1:D:356:ASN:HA	1.98	0.45
1:B:247:PHE:HD2	1:B:262:ILE:HD11	1.81	0.44
1:H:173:MET:HE3	1:H:173:MET:HB3	1.85	0.44
1:J:29:GLU:OE1	1:J:35:ARG:HG2	2.17	0.44
1:D:337:GLU:HG3	1:D:342:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:248:HIS:CD2	2:L:259:MET:HE2	2.52	0.44
1:B:2:SER:CB	1:B:5:THR:HG23	2.48	0.44
1:E:1:ASP:C	1:E:3:SER:H	2.24	0.44
1:J:90:MET:HB2	1:J:93:GLU:HG3	1.98	0.44
1:B:90:MET:CE	1:B:400:PRO:HB3	2.45	0.44
1:E:1:ASP:HA	1:E:5:THR:OG1	2.17	0.44
1:E:93:GLU:HA	1:E:93:GLU:OE1	2.18	0.44
2:I:86:PHE:HB3	2:I:87:PRO:HD3	1.99	0.44
2:I:306:GLU:HG2	2:I:307:ASN:N	2.33	0.44
1:K:314:ILE:HD12	1:K:405:THR:HG23	2.00	0.44
2:L:51:ARG:HG3	2:L:129:ILE:HB	2.00	0.44
1:G:398:LEU:HB2	4:G:604:HOH:O	2.16	0.44
1:B:256:ARG:NH1	1:B:256:ARG:HG2	2.33	0.44
1:K:75:HIS:HA	4:K:608:HOH:O	2.17	0.44
1:A:364:VAL:HG13	1:A:394:TYR:CD2	2.53	0.44
2:C:309:GLY:N	4:C:517:HOH:O	2.45	0.44
2:I:248:HIS:HB3	2:I:259:MET:HG3	2.00	0.43
1:K:178:ARG:HD2	1:K:271:LEU:HD21	1.99	0.43
1:D:399:HIS:HB3	1:D:401:TRP:CZ2	2.52	0.43
1:A:351:THR:HA	1:A:385:SER:HA	2.00	0.43
1:A:244:MET:CE	1:A:261:MET:HE3	2.48	0.43
2:C:209:VAL:HG22	2:C:235:ILE:HG12	2.00	0.43
2:F:207:MET:HB3	2:F:235:ILE:HG23	2.00	0.43
1:G:202:VAL:HG11	1:G:239:TRP:CZ2	2.53	0.43
2:I:209:VAL:HG22	2:I:235:ILE:HG12	2.01	0.43
1:J:366:ASP:OD1	1:J:367:ASN:N	2.51	0.43
1:K:202:VAL:CG1	1:K:239:TRP:HZ2	2.31	0.43
1:D:254:GLU:HB2	1:D:259:MET:HE3	1.99	0.43
1:J:393:ASP:HB3	4:J:801:HOH:O	2.18	0.43
1:B:108:MET:HE2	1:B:190:VAL:HG13	2.01	0.43
1:E:337:GLU:HG2	1:E:342:ILE:CD1	2.49	0.43
2:F:259:MET:HB2	2:F:259:MET:HE2	1.60	0.43
1:G:89:ILE:HD12	1:G:95:TYR:HB2	1.99	0.43
1:G:118:GLU:HA	1:G:156:LEU:HD21	2.01	0.43
1:K:314:ILE:HG13	1:K:403:LYS:HD2	2.01	0.43
1:G:202:VAL:HB	4:G:610:HOH:O	2.18	0.43
1:K:89:ILE:HD12	1:K:95:TYR:HB2	2.00	0.43
1:A:149:GLU:HG2	1:A:163:TYR:CE2	2.53	0.43
1:G:331:TRP:HB3	1:G:360:VAL:HG21	2.01	0.43
1:H:286:MET:HE3	1:H:286:MET:HB3	1.87	0.43
2:L:304:SER:N	4:L:504:HOH:O	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:GLU:OE2	4:D:603:HOH:O	2.21	0.42
2:F:74:PHE:O	2:F:78:HIS:HE1	2.02	0.42
1:G:244:MET:SD	1:G:263:GLU:HB2	2.58	0.42
1:J:1:ASP:O	1:J:2:SER:HB2	2.19	0.42
1:J:108:MET:HE2	1:J:190:VAL:HG13	2.01	0.42
1:A:326:ILE:HB	1:A:356:ASN:HA	2.01	0.42
1:K:1:ASP:C	1:K:3:SER:H	2.27	0.42
1:A:8:LYS:NZ	1:A:102:GLU:O	2.52	0.42
2:I:67:PRO:HD3	2:I:305:TYR:CE2	2.54	0.42
1:J:326:ILE:HB	1:J:356:ASN:HA	2.01	0.42
2:L:88:MET:HE1	2:L:113:ALA:HA	2.01	0.42
2:L:299:GLN:HA	2:L:300:PRO:HD3	1.88	0.42
2:C:202:VAL:CG1	2:C:239:TRP:HZ2	2.31	0.42
1:J:173:MET:HE3	1:J:173:MET:HB3	1.90	0.42
1:J:322:ASP:C	1:J:323:LYS:HD2	2.44	0.42
1:K:118:GLU:HA	1:K:156:LEU:HD21	2.01	0.42
1:D:286:MET:HE3	1:D:286:MET:HB3	1.81	0.42
2:F:274:VAL:HG21	2:F:289:TRP:CD1	2.55	0.42
1:A:124:MET:HE2	1:A:124:MET:HB3	1.98	0.42
1:A:143:TYR:CZ	1:A:286:MET:HG3	2.55	0.42
2:C:248:HIS:CD2	2:C:259:MET:HE2	2.54	0.42
1:D:122:MET:HE3	1:D:122:MET:HB3	1.68	0.42
1:G:255:GLU:HG3	4:G:854:HOH:O	2.18	0.42
1:J:78:HIS:HE1	1:J:83:ASP:OD1	2.03	0.42
2:C:59:THR:HG21	2:C:61:LYS:NZ	2.35	0.42
1:K:314:ILE:HD11	1:K:403:LYS:HG3	2.01	0.42
2:L:166:ASN:HB3	2:L:294:ILE:HD11	2.02	0.42
1:D:62:PHE:O	1:D:94:GLU:HG2	2.19	0.41
1:H:323:LYS:NZ	4:H:607:HOH:O	2.42	0.41
2:I:78:HIS:CE1	2:I:83:ASP:HA	2.55	0.41
1:G:364:VAL:HG13	1:G:394:TYR:CD2	2.55	0.41
1:K:207:MET:O	1:K:221:TYR:HA	2.20	0.41
1:H:307:ASN:OD1	1:H:307:ASN:N	2.53	0.41
1:K:202:VAL:HG11	1:K:239:TRP:HZ2	1.85	0.41
2:L:274:VAL:CG2	2:L:289:TRP:HB2	2.50	0.41
2:L:299:GLN:H	2:L:299:GLN:HG3	1.56	0.41
1:E:174:ASP:CG	4:E:604:HOH:O	2.60	0.41
1:G:247:PHE:HD2	1:G:262:ILE:HD11	1.85	0.41
1:G:345:GLN:NE2	1:G:409:ASN:HB2	2.36	0.41
1:H:244:MET:HE3	1:H:262:ILE:O	2.20	0.41
1:E:318:LYS:NZ	4:E:627:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:274:VAL:HG22	2:F:289:TRP:HB2	2.02	0.41
1:H:78:HIS:CE1	1:H:83:ASP:HA	2.55	0.41
2:L:306:GLU:HG2	2:L:307:ASN:OD1	2.20	0.41
1:J:86:PHE:HA	1:J:87:PRO:HA	1.96	0.41
1:J:386:PHE:CZ	1:J:406:ILE:HD13	2.55	0.41
1:A:90:MET:HE3	1:A:90:MET:HB3	1.78	0.41
1:E:2:SER:HB3	1:E:218:GLU:HG2	2.03	0.41
1:E:124:MET:HE2	1:E:124:MET:HB3	1.88	0.41
1:G:104:ALA:HB2	1:G:132:PRO:HA	2.03	0.41
1:G:386:PHE:CZ	1:G:406:ILE:HD13	2.56	0.41
1:J:113:ALA:HB3	1:J:119:HIS:CE1	2.56	0.41
1:K:251:GLY:O	1:K:254:GLU:HG2	2.21	0.41
1:D:247:PHE:HD2	1:D:262:ILE:HD11	1.85	0.41
1:D:274:VAL:HG21	1:D:289:TRP:CD1	2.55	0.41
1:D:274:VAL:CG2	1:D:289:TRP:HB2	2.51	0.41
1:E:119:HIS:O	1:E:124:MET:HG3	2.21	0.41
1:E:338:SER:HB3	1:E:402:MET:HG2	2.02	0.41
1:A:137:MET:HE2	1:A:137:MET:HB3	1.91	0.40
2:I:183:GLU:OE1	4:I:504:HOH:O	2.22	0.40
1:B:345:GLN:HB3	4:B:612:HOH:O	2.21	0.40
1:H:266:GLU:CD	1:H:266:GLU:N	2.74	0.40
1:H:322:ASP:O	1:H:323:LYS:HD3	2.21	0.40
1:J:324:VAL:HB	1:J:354:TRP:CD1	2.56	0.40
2:C:59:THR:HG23	2:C:96:THR:CG2	2.51	0.40
2:F:10:LYS:NZ	4:F:516:HOH:O	2.54	0.40
2:F:67:PRO:HD3	2:F:305:TYR:CE2	2.56	0.40
1:G:108:MET:HE2	1:G:190:VAL:HG13	2.03	0.40
4:A:762:HOH:O	2:C:79:ASP:HB2	2.22	0.40
1:G:399:HIS:HB3	1:G:401:TRP:CE2	2.56	0.40
1:B:163:TYR:O	1:B:258:SER:HB2	2.21	0.40
1:K:28:ILE:HB	1:K:298:GLU:HB3	2.03	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:THR:N	2:C:1:ASP:OD2[2_545]	1.77	0.43
4:G:721:HOH:O	4:I:689:HOH:O[2_646]	1.82	0.38
4:A:738:HOH:O	4:J:824:HOH:O[2_555]	2.11	0.09
4:A:901:HOH:O	4:J:868:HOH:O[2_555]	2.16	0.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:703:HOH:O	4:J:657:HOH:O[2_555]	2.19	0.01
1:K:94:GLU:O	2:L:2:SER:OG[2_556]	2.19	0.01

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	407/409 (100%)	396 (97%)	11 (3%)	0	100	100
1	B	407/409 (100%)	398 (98%)	8 (2%)	1 (0%)	43	34
1	D	407/409 (100%)	399 (98%)	8 (2%)	0	100	100
1	E	407/409 (100%)	399 (98%)	7 (2%)	1 (0%)	43	34
1	G	407/409 (100%)	396 (97%)	10 (2%)	1 (0%)	43	34
1	H	407/409 (100%)	398 (98%)	8 (2%)	1 (0%)	43	34
1	J	407/409 (100%)	395 (97%)	11 (3%)	1 (0%)	43	34
1	K	407/409 (100%)	401 (98%)	6 (2%)	0	100	100
2	C	307/309 (99%)	301 (98%)	6 (2%)	0	100	100
2	F	307/309 (99%)	301 (98%)	6 (2%)	0	100	100
2	I	307/309 (99%)	296 (96%)	9 (3%)	2 (1%)	18	7
2	L	307/309 (99%)	290 (94%)	15 (5%)	2 (1%)	18	7
All	All	4484/4508 (100%)	4370 (98%)	105 (2%)	9 (0%)	43	34

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	SER
1	G	3	SER
2	L	301	GLN
1	H	313	ALA
2	I	307	ASN

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Mol	Chain	Res	Type
2	I	308	LEU
1	E	2	SER
1	J	388	ASN
2	L	307	ASN

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	358/358 (100%)	357 (100%)	1 (0%)	86	81
1	B	358/358 (100%)	355 (99%)	3 (1%)	73	65
1	D	358/358 (100%)	355 (99%)	3 (1%)	73	65
1	E	358/358 (100%)	355 (99%)	3 (1%)	73	65
1	G	358/358 (100%)	358 (100%)	0	100	100
1	H	358/358 (100%)	354 (99%)	4 (1%)	65	54
1	J	358/358 (100%)	358 (100%)	0	100	100
1	K	358/358 (100%)	356 (99%)	2 (1%)	78	72
2	C	268/268 (100%)	266 (99%)	2 (1%)	76	68
2	F	268/268 (100%)	267 (100%)	1 (0%)	84	78
2	I	268/268 (100%)	268 (100%)	0	100	100
2	L	268/268 (100%)	268 (100%)	0	100	100
All	All	3936/3936 (100%)	3917 (100%)	19 (0%)	81	75

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	409	ASN
1	B	1	ASP
1	B	274	VAL
1	B	406	ILE
2	C	306	GLU
2	C	307	ASN

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Mol	Chain	Res	Type
1	D	2	SER
1	D	335	ILE
1	D	348	SER
1	E	2	SER
1	E	369	ASN
1	E	406	ILE
2	F	18	SER
1	H	2	SER
1	H	205	THR
1	H	306	GLU
1	H	311	SER
1	K	205	THR
1	K	406	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	345	GLN
1	B	377	GLN
1	B	409	ASN
1	D	13	ASN
1	E	301	GLN
1	E	345	GLN
1	E	388	ASN
1	G	78	HIS
1	G	345	GLN
1	G	367	ASN
1	H	24	GLN
1	H	153	ASN
1	H	299	GLN
2	I	78	HIS
2	I	307	ASN
1	J	78	HIS
1	J	158	HIS
1	J	345	GLN
1	J	367	ASN
1	J	388	ASN
1	J	409	ASN
1	K	153	ASN
2	L	15	GLN
2	L	223	GLN
2	L	299	GLN

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Mol	Chain	Res	Type
2	L	301	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 56 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	409/409 (100%)	0.20	18 (4%)	39	42	18, 27, 47, 55	0
1	B	409/409 (100%)	0.01	17 (4%)	40	43	17, 25, 42, 63	0
1	D	409/409 (100%)	0.16	13 (3%)	50	54	18, 26, 48, 58	0
1	E	409/409 (100%)	0.02	10 (2%)	59	66	18, 24, 42, 53	0
1	G	409/409 (100%)	0.26	16 (3%)	43	46	21, 29, 48, 62	0
1	H	409/409 (100%)	0.11	14 (3%)	48	52	20, 27, 42, 68	0
1	J	409/409 (100%)	0.34	16 (3%)	43	46	21, 30, 47, 63	0
1	K	409/409 (100%)	0.19	14 (3%)	48	52	20, 29, 44, 76	0
2	C	309/309 (100%)	0.16	16 (5%)	33	34	17, 25, 39, 71	0
2	F	309/309 (100%)	0.05	12 (3%)	43	46	17, 23, 38, 78	0
2	I	309/309 (100%)	0.22	17 (5%)	30	33	21, 29, 46, 83	0
2	L	309/309 (100%)	0.34	19 (6%)	27	28	22, 31, 50, 101	0
All	All	4508/4508 (100%)	0.17	182 (4%)	42	45	17, 27, 45, 101	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1	ASP	8.8
2	L	300	PRO	8.6
2	L	2	SER	7.7
2	I	86	PHE	5.8
1	A	1	ASP	5.6
1	E	1	ASP	5.5
2	F	308	LEU	5.4
2	F	305	TYR	5.1
1	E	369	ASN	5.1
1	A	310	GLU	5.1
2	I	2	SER	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	314	ILE	5.0
1	G	1	ASP	4.8
1	G	310	GLU	4.7
2	L	3	SER	4.6
1	G	314	ILE	4.5
2	I	1	ASP	4.4
2	F	2	SER	4.4
2	C	308	LEU	4.3
2	I	308	LEU	4.3
1	H	313	ALA	4.3
2	C	309	GLY	4.2
2	L	309	GLY	4.2
1	E	2	SER	4.2
2	C	307	ASN	4.1
1	D	314	ILE	4.0
1	J	314	ILE	4.0
1	B	1	ASP	4.0
1	J	336	THR	3.9
1	B	368	GLU	3.9
2	F	1	ASP	3.9
1	K	1	ASP	3.9
1	A	2	SER	3.8
1	G	336	THR	3.8
1	D	310	GLU	3.7
2	C	305	TYR	3.7
1	B	2	SER	3.7
1	H	1	ASP	3.7
1	B	369	ASN	3.6
2	F	306	GLU	3.5
1	B	312	ALA	3.5
2	F	309	GLY	3.5
2	C	2	SER	3.4
2	F	307	ASN	3.4
1	D	367	ASN	3.4
2	I	87	PRO	3.4
1	E	368	GLU	3.4
1	A	309	GLY	3.4
2	I	3	SER	3.4
1	H	307	ASN	3.4
1	K	367	ASN	3.3
1	H	368	GLU	3.3
2	F	3	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	L	304	SER	3.3
1	E	398	LEU	3.3
2	L	308	LEU	3.3
2	I	307	ASN	3.2
1	G	311	SER	3.2
1	J	312	ALA	3.2
2	I	12	PRO	3.1
1	J	284	TYR	3.1
1	J	310	GLU	3.1
1	K	312	ALA	3.1
2	L	301	GLN	3.0
1	J	386	PHE	3.0
1	J	2	SER	3.0
2	L	68	TYR	3.0
2	L	305	TYR	3.0
2	I	306	GLU	3.0
1	J	1	ASP	3.0
2	L	307	ASN	2.9
1	E	314	ILE	2.9
2	L	299	GLN	2.9
1	B	284	TYR	2.9
1	A	337	GLU	2.9
1	A	367	ASN	2.9
2	L	114	PHE	2.9
1	D	1	ASP	2.9
1	D	409	ASN	2.8
1	H	409	ASN	2.8
1	D	284	TYR	2.8
1	B	3	SER	2.8
1	H	311	SER	2.8
2	C	3	SER	2.8
1	A	315	SER	2.8
2	C	272	SER	2.8
2	L	1	ASP	2.8
1	K	368	GLU	2.8
1	B	409	ASN	2.7
1	G	312	ALA	2.7
2	L	12	PRO	2.7
1	A	409	ASN	2.7
1	K	369	ASN	2.7
1	K	284	TYR	2.7
2	I	309	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	369	ASN	2.7
1	D	335	ILE	2.7
1	K	266	GLU	2.7
1	A	284	TYR	2.6
1	D	366	ASP	2.6
2	C	301	GLN	2.6
2	L	4	ASP	2.6
1	K	311	SER	2.6
1	B	307	ASN	2.6
1	E	307	ASN	2.6
1	K	314	ILE	2.6
1	H	306	GLU	2.6
1	H	2	SER	2.6
1	J	367	ASN	2.6
1	H	284	TYR	2.6
1	H	266	GLU	2.6
1	A	369	ASN	2.6
2	C	304	SER	2.6
2	L	298	GLU	2.5
1	B	367	ASN	2.5
2	F	304	SER	2.5
2	C	306	GLU	2.5
1	B	311	SER	2.5
1	H	3	SER	2.5
1	G	313	ALA	2.5
1	E	266	GLU	2.5
1	H	312	ALA	2.5
1	J	4	ASP	2.5
2	I	4	ASP	2.5
2	C	68	TYR	2.4
2	L	302	LEU	2.4
1	K	315	SER	2.4
1	A	316	SER	2.4
1	G	367	ASN	2.4
2	F	4	ASP	2.4
1	J	335	ILE	2.4
1	G	13	ASN	2.4
1	J	315	SER	2.4
1	G	284	TYR	2.3
1	B	334	GLU	2.3
1	A	312	ALA	2.3
1	A	94	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	I	156	LEU	2.3
1	A	336	THR	2.3
2	C	19	TYR	2.3
2	F	86	PHE	2.3
2	I	305	TYR	2.3
1	J	389	PRO	2.3
1	H	310	GLU	2.3
1	K	306	GLU	2.3
2	C	4	ASP	2.3
1	E	409	ASN	2.3
1	G	335	ILE	2.2
1	K	335	ILE	2.2
1	G	26	ALA	2.2
2	I	267	ASP	2.2
1	J	305	TYR	2.2
2	L	86	PHE	2.2
1	D	316	SER	2.2
1	G	3	SER	2.2
2	I	68	TYR	2.2
2	I	114	PHE	2.1
1	D	2	SER	2.1
2	L	272	SER	2.1
1	B	309	GLY	2.1
1	A	308	LEU	2.1
2	F	156	LEU	2.1
1	B	313	ALA	2.1
1	J	409	ASN	2.1
1	K	313	ALA	2.1
1	B	335	ILE	2.1
1	J	303	ILE	2.1
1	D	309	GLY	2.1
1	D	303	ILE	2.1
2	I	89	ILE	2.1
1	E	315	SER	2.0
2	C	65	ASP	2.0
1	B	306	GLU	2.0
1	G	337	GLU	2.0
1	B	370	SER	2.0
1	G	316	SER	2.0
1	G	348	SER	2.0
1	K	2	SER	2.0
1	A	335	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	395	ILE	2.0
1	D	392	PHE	2.0
2	C	303	ILE	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CU	F	404	1/1	0.97	0.04	25,25,25,25	0
3	CU	L	403	1/1	0.97	0.07	35,35,35,35	0
3	CU	D	505	1/1	0.98	0.04	25,25,25,25	0
3	CU	F	402	1/1	0.98	0.04	29,29,29,29	0
3	CU	F	403	1/1	0.98	0.04	27,27,27,27	0
3	CU	A	506	1/1	0.98	0.04	29,29,29,29	0
3	CU	G	501	1/1	0.98	0.05	31,31,31,31	0
3	CU	C	403	1/1	0.98	0.04	28,28,28,28	0
3	CU	C	401	1/1	0.99	0.03	23,23,23,23	0
3	CU	C	402	1/1	0.99	0.04	30,30,30,30	0
3	CU	A	503	1/1	0.99	0.02	25,25,25,25	0
3	CU	D	501	1/1	0.99	0.04	29,29,29,29	0
3	CU	D	502	1/1	0.99	0.04	29,29,29,29	0
3	CU	D	503	1/1	0.99	0.03	24,24,24,24	0
3	CU	D	504	1/1	0.99	0.03	27,27,27,27	0
3	CU	A	505	1/1	0.99	0.04	25,25,25,25	0
3	CU	E	501	1/1	0.99	0.03	24,24,24,24	0
3	CU	E	502	1/1	0.99	0.03	27,27,27,27	0
3	CU	E	503	1/1	0.99	0.04	27,27,27,27	0
3	CU	E	504	1/1	0.99	0.03	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CU	F	401	1/1	0.99	0.06	27,27,27,27	0
3	CU	A	501	1/1	0.99	0.03	31,31,31,31	0
3	CU	B	501	1/1	0.99	0.02	25,25,25,25	0
3	CU	B	503	1/1	0.99	0.02	27,27,27,27	0
3	CU	B	504	1/1	0.99	0.06	22,22,22,22	0
3	CU	G	502	1/1	0.99	0.08	30,30,30,30	0
3	CU	H	501	1/1	0.99	0.02	27,27,27,27	0
3	CU	H	502	1/1	0.99	0.04	29,29,29,29	0
3	CU	I	402	1/1	0.99	0.06	34,34,34,34	0
3	CU	I	403	1/1	0.99	0.06	32,32,32,32	0
3	CU	I	404	1/1	0.99	0.04	34,34,34,34	0
3	CU	J	501	1/1	0.99	0.05	32,32,32,32	0
3	CU	J	502	1/1	0.99	0.05	31,31,31,31	0
3	CU	J	503	1/1	0.99	0.02	26,26,26,26	0
3	CU	J	504	1/1	0.99	0.03	28,28,28,28	0
3	CU	J	505	1/1	0.99	0.02	31,31,31,31	0
3	CU	K	501	1/1	0.99	0.03	29,29,29,29	0
3	CU	K	502	1/1	0.99	0.04	31,31,31,31	0
3	CU	K	504	1/1	0.99	0.03	22,22,22,22	0
3	CU	K	505	1/1	0.99	0.02	28,28,28,28	0
3	CU	B	505	1/1	0.99	0.02	24,24,24,24	0
3	CU	G	503	1/1	1.00	0.02	25,25,25,25	0
3	CU	G	504	1/1	1.00	0.03	27,27,27,27	0
3	CU	G	505	1/1	1.00	0.02	30,30,30,30	0
3	CU	B	502	1/1	1.00	0.02	27,27,27,27	0
3	CU	E	505	1/1	1.00	0.01	23,23,23,23	0
3	CU	H	503	1/1	1.00	0.06	30,30,30,30	0
3	CU	H	504	1/1	1.00	0.01	23,23,23,23	0
3	CU	H	505	1/1	1.00	0.01	26,26,26,26	0
3	CU	K	503	1/1	1.00	0.07	31,31,31,31	0
3	CU	I	401	1/1	1.00	0.01	26,26,26,26	0
3	CU	A	504	1/1	1.00	0.03	28,28,28,28	0
3	CU	L	401	1/1	1.00	0.02	26,26,26,26	0
3	CU	L	402	1/1	1.00	0.06	35,35,35,35	0
3	CU	A	502	1/1	1.00	0.04	29,29,29,29	0
3	CU	L	404	1/1	1.00	0.02	35,35,35,35	0

6.5 Other polymers

There are no such residues in this entry.