Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 09:07 PM EST

PDB ID	:	3RFR
Title	:	Crystal Structure of particulate methane monooxygenase (pMMO) from Methylocystis sp. strain M
Authors	:	Smith, S.M.; Rosenzweig, A.C.
Deposited on	:	2011-04-06
Resolution	:	2.68 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 (i) 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 (i)) were used in the production of this report:

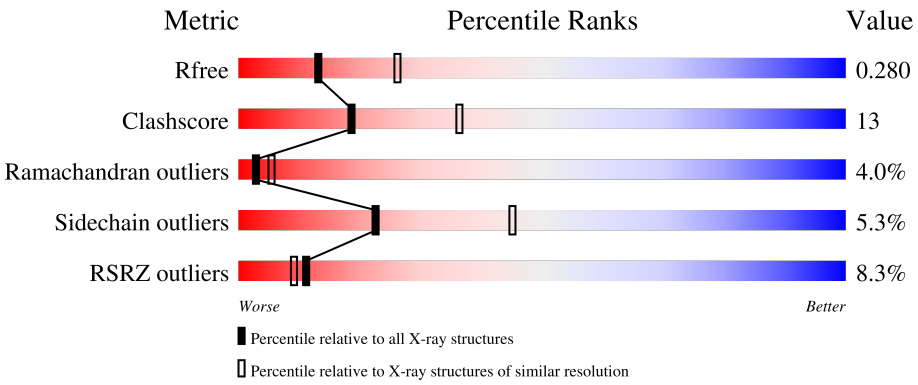
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.68 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	419	9% 68% 19% • • 8%
1	E	419	9% 68% 19% • • 8%
1	I	419	11% 56% 31% • • 8%
2	D	19	11% 74% 26%
2	H	19	26% 68% 16% 16%

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Mol	Chain	Length	Quality of chain
3	B	252	6% 70% 22%
3	F	252	7% 69% 22%
3	J	252	3% 69% 21% 5%
4	C	256	7% 60% 19% 18%
4	G	256	5% 60% 20% 18%
4	K	256	7% 63% 17% 18%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 20224 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 PmoB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	386	3012	1937	521	551	3	0	0	0
1	E	386	3012	1937	521	551	3	0	0	0
1	I	386	3012	1937	521	551	3	0	0	0

- Molecule 2 is a protein called peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	19	94	57	19	18	0	0	0
2	H	16	79	48	16	15	0	0	0

- Molecule 3 is a protein called PmoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	J	242	1964	1326	312	313	13	0	0	0
3	B	242	1964	1326	312	313	13	0	0	0
3	F	242	1964	1326	312	313	13	0	0	0

- Molecule 4 is a protein called PmoC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	210	1695	1137	271	280	7	0	0	0
4	G	211	1706	1146	272	281	7	0	0	0

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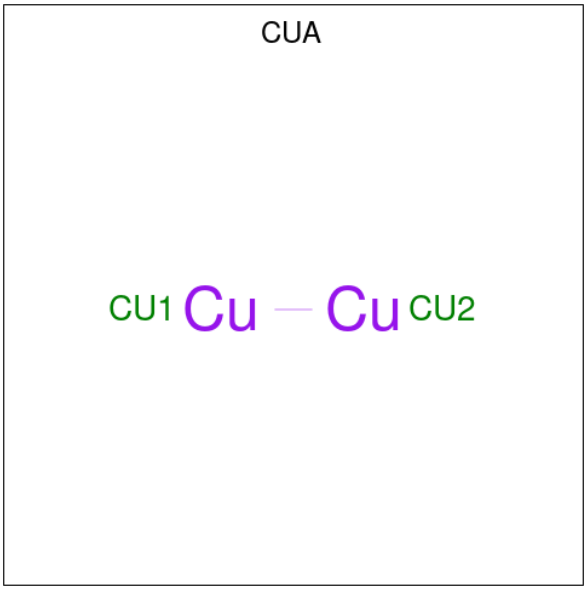
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	K	211	1706	1146	272	281	7	0	0	0

- Molecule 5 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
5	A	1	2	2	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	A	1	1	1	0	0
6	C	2	2	2	0	0
6	G	2	2	2	0	0
6	K	2	2	2	0	0
6	E	1	1	1	0	0
6	I	1	1	1	0	0

- Molecule 7 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
7	E	1	1	1	0	0
7	I	1	1	1	0	0

- Molecule 8 is water.

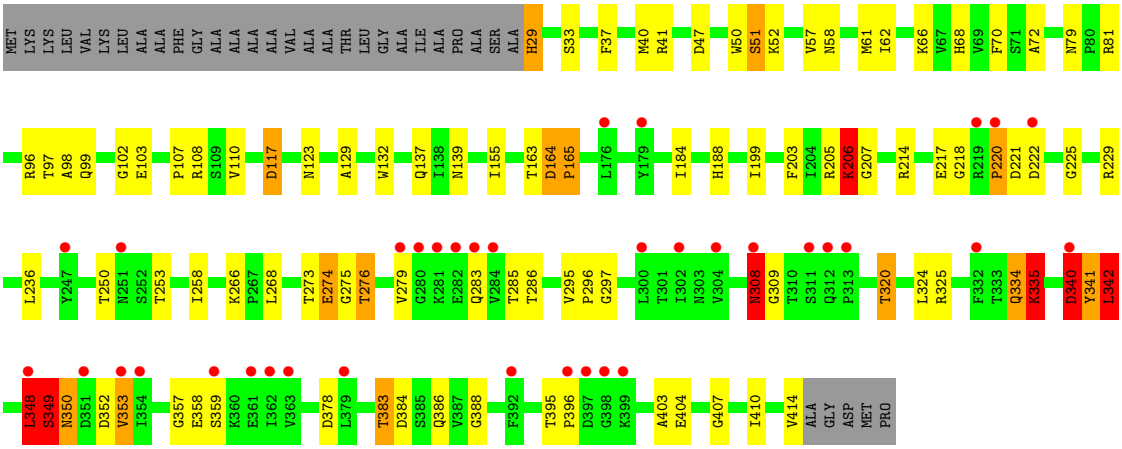
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	C	1	1	1	0	0
8	G	1	1	1	0	0
8	K	1	1	1	0	0

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.

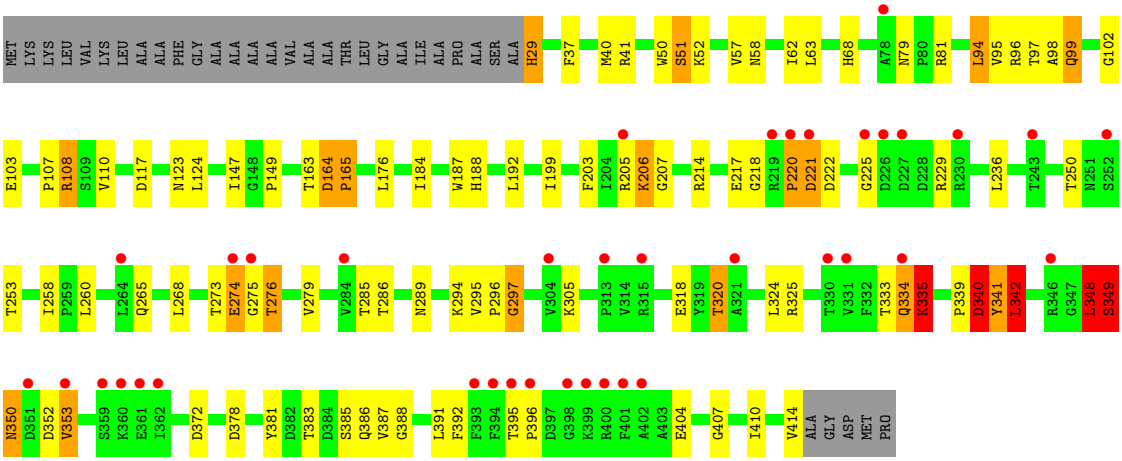
• Molecule 1: PmoB

Chain A: 9% 68% 19% • • 8%



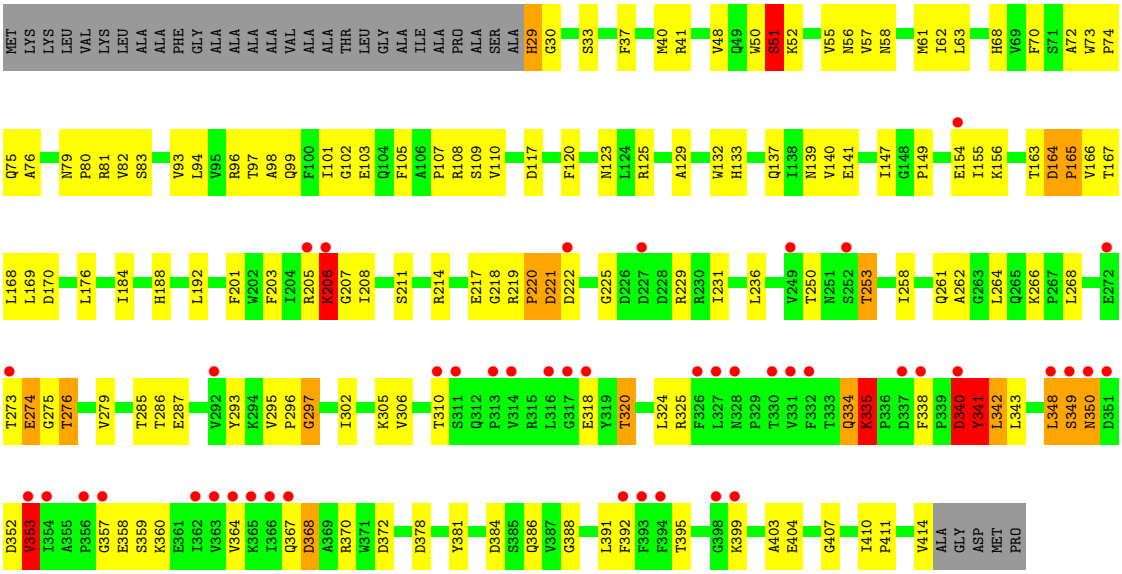
• Molecule 1: PmoB

Chain E: 9% 68% 19% • • 8%



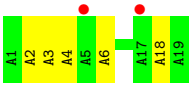
• Molecule 1: PmoB

Chain I: 11% 56% 31% • • 8%



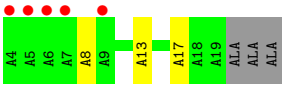
- Molecule 2: peptide

Chain D:



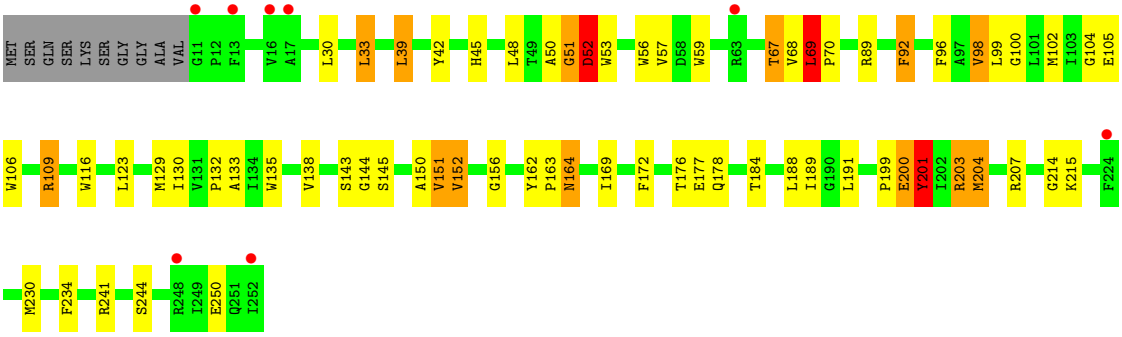
- Molecule 2: peptide

Chain H:



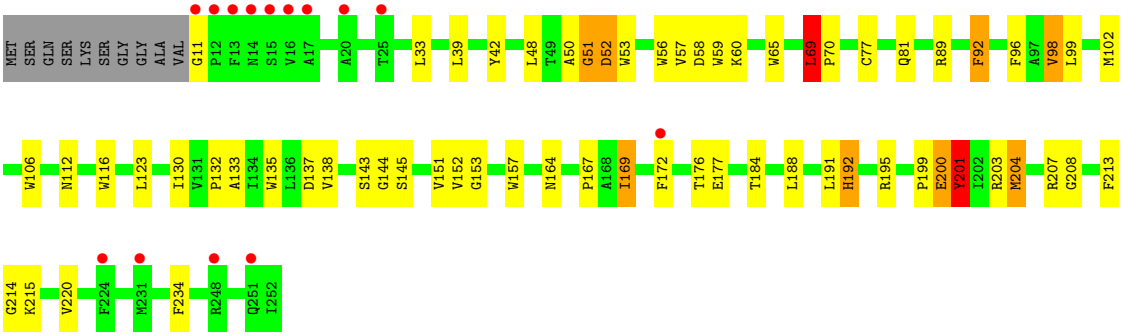
- Molecule 3: PmoA

Chain J:



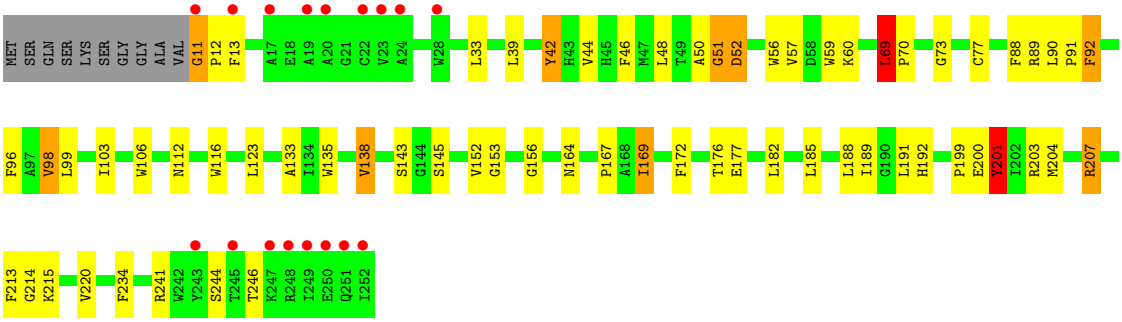
- Molecule 3: PmoA

Chain B:



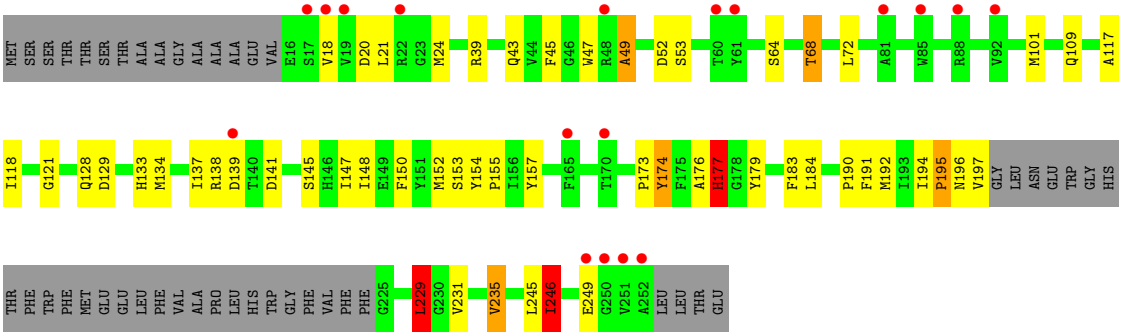
- Molecule 3: PmoA

Chain F:



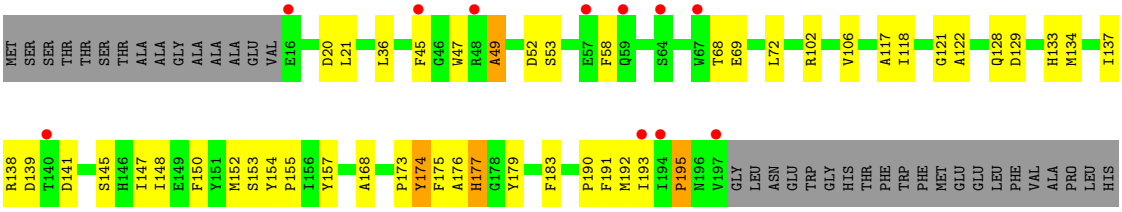
- Molecule 4: PmoC

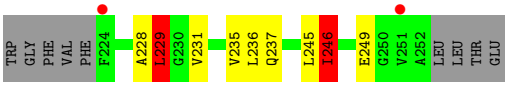
Chain C:



- Molecule 4: PmoC

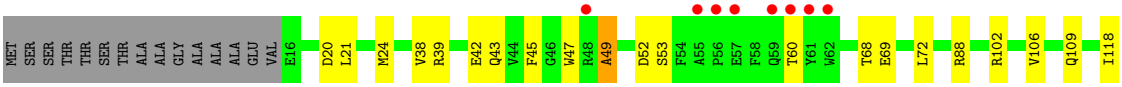
Chain G:





• Molecule 4: PmoC

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.72Å 178.31Å 183.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.79 – 2.68 45.79 – 2.68	Depositor EDS
% Data completeness (in resolution range)	88.9 (45.79-2.68) 88.9 (45.79-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.249 , 0.281 0.250 , 0.280	Depositor DCC
R_{free} test set	4440 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	61.2	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	20224	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.66	0/3087	0.81	4/4205 (0.1%)
1	E	0.69	0/3087	0.81	5/4205 (0.1%)
1	I	1.04	1/3087 (0.0%)	0.94	4/4205 (0.1%)
2	D	1.00	0/93	1.02	0/129
2	H	0.84	0/78	0.67	0/108
3	B	0.79	0/2041	0.81	2/2795 (0.1%)
3	F	0.86	0/2041	0.86	2/2795 (0.1%)
3	J	0.92	0/2041	0.89	3/2795 (0.1%)
4	C	0.70	0/1749	0.70	1/2386 (0.0%)
4	G	0.66	0/1761	0.69	1/2402 (0.0%)
4	K	0.72	0/1761	0.72	2/2402 (0.1%)
All	All	0.80	1/20826 (0.0%)	0.82	24/28427 (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	4
1	E	0	3
1	I	0	4
3	B	0	3
3	F	0	3
3	J	0	2
4	G	0	1
4	K	0	1
All	All	0	21

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	154	GLU	CG-CD	5.42	1.60	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	69	LEU	CA-CB-CG	-7.86	97.23	115.30
3	F	69	LEU	CA-CB-CG	-7.58	97.87	115.30
3	J	69	LEU	CA-CB-CG	-7.37	98.34	115.30
4	G	229	LEU	CA-CB-CG	6.79	130.93	115.30
4	C	229	LEU	CA-CB-CG	6.76	130.85	115.30
3	J	200	GLU	OE1-CD-OE2	-6.22	115.83	123.30
1	E	348	LEU	CA-CB-CG	6.15	129.45	115.30
3	J	109	ARG	NE-CZ-NH1	6.09	123.34	120.30
3	F	207	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	E	342	LEU	N-CA-C	6.01	127.23	111.00
4	K	225	GLY	N-CA-C	5.97	128.03	113.10
1	I	192	LEU	CA-CB-CG	5.93	128.95	115.30
1	A	342	LEU	N-CA-C	5.92	126.98	111.00
1	A	348	LEU	CA-CB-CG	5.73	128.49	115.30
1	E	341	TYR	C-N-CA	5.54	135.56	121.70
3	B	195	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	341	TYR	C-N-CA	5.50	135.45	121.70
1	I	169	LEU	CA-CB-CG	5.30	127.50	115.30
1	I	63	LEU	CA-CB-CG	5.29	127.45	115.30
4	K	229	LEU	CA-CB-CG	5.24	127.35	115.30
1	E	192	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	308	ASN	C-N-CA	5.16	133.14	122.30
1	I	341	TYR	C-N-CA	5.04	134.31	121.70
1	E	108	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	LYS	Peptide
1	A	308	ASN	Peptide
1	A	335	LYS	Peptide
1	A	340	ASP	Peptide
3	B	11	GLY	Peptide
3	B	50	ALA	Peptide
3	B	51	GLY	Peptide
1	E	206	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	E	335	LYS	Peptide
1	E	340	ASP	Peptide
3	F	11	GLY	Peptide
3	F	50	ALA	Peptide
3	F	51	GLY	Peptide
4	G	228	ALA	Peptide
1	I	206	LYS	Peptide
1	I	335	LYS	Peptide
1	I	340	ASP	Peptide
1	I	341	TYR	Peptide
3	J	50	ALA	Peptide
3	J	51	GLY	Peptide
4	K	224	PHE	Peptide

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	3012	0	3009	94	0
1	E	3012	0	3009	95	0
1	I	3012	0	3009	136	0
2	D	94	0	97	2	0
2	H	79	0	79	2	0
3	B	1964	0	1924	55	0
3	F	1964	0	1924	62	0
3	J	1964	0	1924	55	0
4	C	1695	0	1692	36	0
4	G	1706	0	1701	36	0
4	K	1706	0	1701	36	0
5	A	2	0	0	0	0
6	A	1	0	0	0	0
6	C	2	0	0	0	0
6	E	1	0	0	0	0
6	G	2	0	0	0	0
6	I	1	0	0	0	0
6	K	2	0	0	0	0
7	E	1	0	0	0	0
7	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	1	0	0	0	0
8	G	1	0	0	0	0
8	K	1	0	0	0	0
All	All	20224	0	20069	533	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 13.

All (533) 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)
3:J:116:TRP:O	4:K:47:TRP:HH2	1.31	1.13
1:I:275:GLY:HA3	1:I:276:THR:HG22	1.29	1.11
3:F:11:GLY:HA3	3:F:13:PHE:H	1.02	1.10
1:A:340:ASP:HB3	1:A:341:TYR:HB3	1.33	1.09
3:B:51:GLY:HA3	3:B:52:ASP:HB2	1.28	1.08
1:A:274:GLU:H	1:A:275:GLY:CA	1.66	1.08
1:A:275:GLY:HA3	1:A:276:THR:HG22	1.28	1.08
1:E:340:ASP:HB3	1:E:341:TYR:HB3	1.28	1.07
3:J:116:TRP:O	4:K:47:TRP:CH2	2.08	1.07
3:J:51:GLY:HA3	3:J:52:ASP:HB2	1.36	1.06
1:E:274:GLU:H	1:E:275:GLY:CA	1.67	1.06
3:B:116:TRP:O	4:C:47:TRP:HH2	1.38	1.06
4:K:245:LEU:O	4:K:246:ILE:HG13	1.54	1.05
3:F:51:GLY:HA3	3:F:52:ASP:HB2	1.36	1.05
3:B:116:TRP:O	4:C:47:TRP:CH2	2.12	1.02
1:A:348:LEU:HB2	1:A:349:SER:HB3	1.44	1.00
1:I:274:GLU:H	1:I:275:GLY:CA	1.74	0.99
1:A:274:GLU:H	1:A:275:GLY:HA3	1.30	0.97
4:C:245:LEU:O	4:C:246:ILE:HG13	1.64	0.97
4:K:121:GLY:HA2	4:K:153:SER:OG	1.63	0.97
1:I:340:ASP:HB3	1:I:341:TYR:HB3	1.46	0.96
4:G:245:LEU:O	4:G:246:ILE:HG13	1.65	0.95
1:A:275:GLY:HA3	1:A:276:THR:CG2	1.95	0.94
1:I:96:ARG:HH21	1:I:99:GLN:HE22	1.02	0.93
1:I:58:ASN:HD21	1:I:163:THR:H	1.16	0.92
4:G:245:LEU:C	4:G:246:ILE:HG13	1.90	0.92
1:I:275:GLY:HA3	1:I:276:THR:CG2	2.00	0.91
1:I:274:GLU:H	1:I:275:GLY:HA3	1.34	0.91
3:F:116:TRP:O	4:G:47:TRP:HH2	1.54	0.89
2:D:3:ALA:HA	2:D:6:ALA:HB3	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:11:GLY:HA3	3:F:13:PHE:N	1.87	0.88
3:F:116:TRP:O	4:G:47:TRP:CH2	2.27	0.88
4:C:121:GLY:HA2	4:C:153:SER:OG	1.73	0.88
4:K:245:LEU:C	4:K:246:ILE:HG13	1.89	0.88
1:E:340:ASP:HB3	1:E:341:TYR:CB	2.02	0.88
1:I:164:ASP:CB	1:I:165:PRO:HA	2.02	0.87
3:F:11:GLY:CA	3:F:13:PHE:H	1.88	0.87
1:I:137:GLN:HE21	1:I:139:ASN:HD21	1.23	0.86
1:A:340:ASP:HB3	1:A:341:TYR:CB	2.07	0.85
1:I:205:ARG:O	1:I:206:LYS:HB2	1.77	0.84
4:C:245:LEU:C	4:C:246:ILE:HG13	1.95	0.83
1:E:274:GLU:H	1:E:275:GLY:HA3	1.42	0.83
1:I:348:LEU:HB2	1:I:349:SER:HB3	1.61	0.81
4:K:245:LEU:O	4:K:246:ILE:CG1	2.30	0.80
1:A:164:ASP:CB	1:A:165:PRO:HA	2.12	0.80
3:J:143:SER:O	3:J:145:SER:N	2.14	0.80
3:B:51:GLY:CA	3:B:52:ASP:HB2	2.12	0.80
3:J:214:GLY:HA2	3:J:215:LYS:HB2	1.62	0.79
1:E:68:HIS:HE1	1:E:404:GLU:OE1	1.66	0.79
1:A:58:ASN:HD21	1:A:163:THR:H	1.30	0.79
1:I:96:ARG:HH21	1:I:99:GLN:NE2	1.80	0.79
4:G:148:ILE:HG23	4:G:152:MET:HE1	1.66	0.78
4:C:148:ILE:HG23	4:C:152:MET:HE1	1.64	0.78
3:F:214:GLY:HA2	3:F:215:LYS:HB2	1.65	0.78
1:E:58:ASN:HD21	1:E:163:THR:H	1.30	0.78
3:B:200:GLU:O	3:B:201:TYR:HB3	1.83	0.77
4:K:148:ILE:HG23	4:K:152:MET:HE1	1.64	0.77
4:G:245:LEU:O	4:G:246:ILE:CG1	2.32	0.77
4:G:53:SER:OG	4:G:139:ASP:HB2	1.84	0.77
1:I:68:HIS:HE1	1:I:404:GLU:OE1	1.67	0.76
1:I:164:ASP:HB2	1:I:165:PRO:HA	1.67	0.76
1:A:164:ASP:HB2	1:A:165:PRO:HA	1.68	0.76
1:E:274:GLU:N	1:E:275:GLY:CA	2.47	0.76
1:I:225:GLY:HA2	1:I:229:ARG:NH2	2.00	0.76
1:E:164:ASP:CB	1:E:165:PRO:HA	2.16	0.75
3:B:98:VAL:HG21	3:B:133:ALA:HB2	1.66	0.75
1:E:274:GLU:H	1:E:275:GLY:HA2	1.48	0.75
1:A:98:ALA:HB3	1:A:123:ASN:HD22	1.52	0.75
1:I:220:PRO:O	1:I:222:ASP:N	2.16	0.75
3:J:106:TRP:HE1	1:I:188:HIS:CD2	2.04	0.75
1:E:340:ASP:CB	1:E:341:TYR:HB3	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:8:ALA:HB1	4:G:68:THR:HG21	1.68	0.74
3:J:98:VAL:HG21	3:J:133:ALA:HB2	1.67	0.74
4:C:53:SER:OG	4:C:139:ASP:HB2	1.85	0.74
1:E:275:GLY:HA3	1:E:276:THR:HG22	1.68	0.74
1:A:348:LEU:CB	1:A:349:SER:HB3	2.18	0.73
1:E:334:GLN:HA	1:E:335:LYS:HB2	1.71	0.73
3:J:177:GLU:HG3	1:E:410:ILE:HG12	1.69	0.73
3:B:214:GLY:HA2	3:B:215:LYS:HB2	1.70	0.73
1:A:220:PRO:O	1:A:222:ASP:N	2.15	0.73
1:I:70:PHE:HE1	1:I:72:ALA:HB3	1.53	0.72
3:B:143:SER:O	3:B:145:SER:N	2.21	0.72
1:E:348:LEU:HB2	1:E:349:SER:HB3	1.72	0.72
3:B:60:LYS:HD2	3:B:169:ILE:HD11	1.70	0.72
4:K:52:ASP:HB2	1:I:29:HIS:HD2	1.55	0.72
4:C:245:LEU:O	4:C:246:ILE:CG1	2.39	0.71
1:I:334:GLN:HA	1:I:335:LYS:HB2	1.71	0.71
1:E:220:PRO:O	1:E:222:ASP:N	2.20	0.71
3:J:203:ARG:O	3:J:204:MET:HB2	1.89	0.71
1:A:188:HIS:CD2	3:B:106:TRP:HE1	2.08	0.70
3:J:184:THR:HG22	1:I:258:ILE:HG13	1.74	0.70
1:I:68:HIS:HD2	1:I:117:ASP:OD1	1.75	0.69
3:F:200:GLU:O	3:F:201:TYR:HB3	1.92	0.69
1:E:164:ASP:HB2	1:E:165:PRO:HA	1.73	0.69
3:J:51:GLY:CA	3:J:52:ASP:HB2	2.19	0.69
1:E:40:MET:HE2	1:E:388:GLY:H	1.58	0.68
1:I:164:ASP:CB	1:I:165:PRO:CA	2.71	0.68
1:E:50:TRP:O	1:E:52:LYS:N	2.26	0.68
1:E:98:ALA:HB3	1:E:123:ASN:HD22	1.59	0.68
1:E:275:GLY:HA3	1:E:276:THR:CG2	2.23	0.68
1:A:334:GLN:HA	1:A:335:LYS:HB2	1.76	0.67
3:F:60:LYS:HD2	3:F:169:ILE:HD11	1.76	0.67
3:B:203:ARG:O	3:B:204:MET:HB2	1.94	0.67
1:I:68:HIS:CD2	1:I:117:ASP:OD1	2.48	0.67
4:G:121:GLY:HA2	4:G:153:SER:OG	1.95	0.67
4:K:45:PHE:O	4:K:49:ALA:HB3	1.94	0.67
1:I:96:ARG:NH2	1:I:99:GLN:HE22	1.86	0.66
1:I:276:THR:HG23	1:I:279:VAL:HB	1.77	0.66
1:I:70:PHE:CE1	1:I:72:ALA:HB3	2.30	0.66
1:I:225:GLY:HA2	1:I:229:ARG:HH21	1.58	0.66
1:A:68:HIS:HD2	1:A:117:ASP:OD1	1.79	0.66
1:A:340:ASP:CB	1:A:341:TYR:HB3	2.18	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:53:SER:OG	4:K:139:ASP:HB2	1.96	0.65
1:A:274:GLU:N	1:A:275:GLY:CA	2.48	0.65
1:A:274:GLU:H	1:A:275:GLY:HA2	1.60	0.65
3:J:214:GLY:CA	3:J:215:LYS:HB2	2.27	0.65
1:A:29:HIS:HD2	4:C:52:ASP:HB2	1.62	0.64
1:A:96:ARG:HH21	1:A:99:GLN:HE22	1.45	0.64
4:K:52:ASP:HB2	1:I:29:HIS:CD2	2.31	0.64
1:A:68:HIS:HE1	1:A:404:GLU:OE1	1.81	0.64
3:B:213:PHE:HA	1:I:33:SER:O	1.98	0.64
4:C:246:ILE:HB	4:C:249:GLU:HG2	1.78	0.64
3:J:59:TRP:CZ3	3:J:203:ARG:O	2.51	0.63
4:G:45:PHE:O	4:G:49:ALA:HB3	1.98	0.63
1:A:275:GLY:HA3	1:A:276:THR:CB	2.28	0.63
3:B:143:SER:C	3:B:145:SER:H	2.01	0.63
3:F:214:GLY:CA	3:F:215:LYS:HB2	2.29	0.63
1:I:164:ASP:OD2	1:I:176:LEU:HB2	1.99	0.63
1:I:250:THR:O	1:I:253:THR:O	2.17	0.63
1:A:410:ILE:HG12	3:F:177:GLU:HG3	1.79	0.62
4:G:246:ILE:HB	4:G:249:GLU:HG2	1.79	0.62
1:A:274:GLU:N	1:A:275:GLY:HA3	2.11	0.62
1:A:276:THR:HG23	1:A:279:VAL:HB	1.80	0.62
3:F:98:VAL:HG21	3:F:133:ALA:HB2	1.81	0.62
1:I:110:VAL:HB	1:I:268:LEU:HD11	1.81	0.62
3:J:138:VAL:HG21	1:I:236:LEU:HB2	1.80	0.62
4:K:246:ILE:HB	4:K:249:GLU:HG2	1.81	0.62
1:E:274:GLU:N	1:E:275:GLY:HA3	2.13	0.62
1:E:275:GLY:HA3	1:E:276:THR:CB	2.30	0.62
1:E:225:GLY:HA2	1:E:229:ARG:NH2	2.15	0.61
3:F:106:TRP:HE1	1:E:188:HIS:CD2	2.18	0.61
1:A:236:LEU:HB2	3:B:138:VAL:HG21	1.83	0.61
3:B:214:GLY:CA	3:B:215:LYS:HB2	2.31	0.61
3:F:46:PHE:HZ	3:F:69:LEU:HD11	1.65	0.61
3:F:51:GLY:CA	3:F:52:ASP:HB2	2.22	0.61
3:F:138:VAL:HG21	1:E:236:LEU:HB2	1.82	0.61
1:A:220:PRO:C	1:A:222:ASP:H	2.02	0.61
1:A:225:GLY:HA2	1:A:229:ARG:NH2	2.15	0.61
1:A:283:GLN:O	1:A:309:GLY:HA3	2.00	0.61
4:C:150:PHE:CZ	4:C:195:PRO:HG3	2.36	0.61
3:F:69:LEU:HB3	3:F:70:PRO:HD3	1.81	0.61
1:I:386:GLN:HG3	1:I:407:GLY:C	2.21	0.61
4:G:150:PHE:CZ	4:G:195:PRO:HG3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:348:LEU:CA	1:I:349:SER:HB3	2.31	0.60
1:A:348:LEU:CA	1:A:349:SER:HB3	2.30	0.60
3:B:69:LEU:HB3	3:B:70:PRO:HD3	1.82	0.60
1:E:205:ARG:O	1:E:206:LYS:HB2	2.01	0.60
1:I:164:ASP:HB3	1:I:165:PRO:HA	1.81	0.60
1:I:48:VAL:HG21	1:I:149:PRO:HG2	1.83	0.60
1:I:50:TRP:O	1:I:52:LYS:N	2.35	0.60
4:K:20:ASP:O	4:K:21:LEU:HB2	2.02	0.60
1:E:214:ARG:NH1	1:E:222:ASP:O	2.34	0.60
1:I:164:ASP:HB3	1:I:165:PRO:CA	2.31	0.60
3:B:207:ARG:HD3	1:I:75:GLN:NE2	2.15	0.60
1:E:348:LEU:HB2	1:E:349:SER:CB	2.30	0.60
4:G:138:ARG:NH1	4:G:141:ASP:HA	2.17	0.60
1:I:320:THR:HG22	1:I:324:LEU:O	2.01	0.60
3:J:203:ARG:O	3:J:204:MET:CB	2.50	0.60
1:I:348:LEU:CB	1:I:349:SER:HB3	2.31	0.60
3:J:143:SER:C	3:J:145:SER:H	2.05	0.59
1:A:205:ARG:O	1:A:206:LYS:HB2	2.01	0.59
1:A:275:GLY:CA	1:A:276:THR:HG22	2.20	0.59
4:K:69:GLU:OE1	4:K:152:MET:HB2	2.02	0.59
4:C:45:PHE:O	4:C:49:ALA:HB3	2.02	0.59
1:I:340:ASP:HB3	1:I:341:TYR:CB	2.27	0.59
1:I:207:GLY:O	1:I:211:SER:HB2	2.03	0.59
1:A:164:ASP:CB	1:A:165:PRO:CA	2.80	0.59
3:J:172:PHE:CE2	1:I:184:ILE:HD11	2.37	0.59
3:B:59:TRP:CZ3	3:B:203:ARG:O	2.55	0.59
4:K:150:PHE:CZ	4:K:195:PRO:HG3	2.38	0.59
3:J:176:THR:HG21	3:J:188:LEU:HD22	1.84	0.59
3:F:191:LEU:HD13	1:E:107:PRO:HA	1.85	0.59
1:I:214:ARG:NH1	1:I:222:ASP:O	2.36	0.59
1:E:275:GLY:CA	1:E:276:THR:HB	2.31	0.59
1:E:275:GLY:HA3	1:E:276:THR:HB	1.84	0.59
1:I:349:SER:OG	1:I:350:ASN:N	2.36	0.59
4:G:52:ASP:HB2	1:E:29:HIS:HD2	1.67	0.58
1:A:352:ASP:O	1:A:353:VAL:C	2.41	0.58
3:B:215:LYS:HA	1:I:381:TYR:CZ	2.39	0.58
3:J:200:GLU:O	3:J:201:TYR:HB3	2.03	0.58
1:I:102:GLY:HA3	1:I:268:LEU:HD22	1.85	0.58
4:K:137:ILE:HD13	1:I:147:ILE:CD1	2.34	0.58
1:E:320:THR:HG22	1:E:324:LEU:O	2.04	0.57
1:I:219:ARG:HB3	1:I:221:ASP:OD1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:138:ARG:NH1	4:C:141:ASP:HA	2.19	0.57
1:I:96:ARG:CD	1:I:99:GLN:NE2	2.68	0.57
3:F:203:ARG:O	3:F:204:MET:HB2	2.04	0.57
4:G:176:ALA:O	4:G:177:HIS:CD2	2.58	0.57
1:E:352:ASP:O	1:E:353:VAL:C	2.43	0.56
3:F:167:PRO:HA	1:E:250:THR:HG21	1.85	0.56
1:E:68:HIS:HD2	1:E:117:ASP:OD1	1.88	0.56
1:I:220:PRO:C	1:I:222:ASP:H	2.03	0.56
1:I:68:HIS:CE1	1:I:404:GLU:OE1	2.54	0.56
1:A:214:ARG:NH1	1:A:222:ASP:O	2.39	0.56
1:E:395:THR:OG1	1:E:396:PRO:HD2	2.05	0.56
1:A:68:HIS:CD2	1:A:117:ASP:OD1	2.57	0.56
4:K:176:ALA:O	4:K:177:HIS:CD2	2.59	0.56
1:I:170:ASP:OD1	1:I:170:ASP:C	2.44	0.56
3:B:208:GLY:O	1:I:76:ALA:HB1	2.06	0.56
1:I:51:SER:HB3	1:I:62:ILE:O	2.05	0.55
3:J:98:VAL:HG12	3:J:99:LEU:N	2.20	0.55
3:B:203:ARG:O	3:B:204:MET:CB	2.53	0.55
1:I:203:PHE:O	1:I:207:GLY:HA2	2.07	0.55
1:A:349:SER:OG	1:A:350:ASN:N	2.39	0.54
3:F:143:SER:C	3:F:145:SER:H	2.09	0.54
1:A:220:PRO:HB3	3:B:89:ARG:HG3	1.89	0.54
3:F:46:PHE:CZ	3:F:69:LEU:HD11	2.41	0.54
3:F:96:PHE:HA	1:E:199:ILE:HD11	1.88	0.54
1:E:164:ASP:CB	1:E:165:PRO:CA	2.84	0.54
1:I:274:GLU:N	1:I:275:GLY:CA	2.55	0.54
3:F:89:ARG:HG3	1:E:220:PRO:HB3	1.89	0.54
1:I:275:GLY:HA3	1:I:276:THR:CB	2.38	0.54
4:K:24:MET:HB2	4:K:109:GLN:HG2	1.90	0.54
1:I:58:ASN:HD22	1:I:125:ARG:HH21	1.56	0.54
1:I:367:GLN:O	1:I:368:ASP:HB2	2.07	0.54
3:J:57:VAL:HG12	3:J:123:LEU:HD12	1.90	0.54
1:I:358:GLU:HG2	1:I:359:SER:N	2.23	0.54
1:A:70:PHE:HE1	1:A:72:ALA:HB3	1.73	0.53
3:F:57:VAL:HG12	3:F:123:LEU:HD12	1.90	0.53
3:B:200:GLU:O	3:B:201:TYR:CB	2.55	0.53
1:I:334:GLN:HA	1:I:335:LYS:CB	2.37	0.53
1:A:102:GLY:HA3	1:A:268:LEU:HD22	1.89	0.53
3:F:200:GLU:HG2	3:F:203:ARG:HH11	1.73	0.53
1:A:395:THR:OG1	1:A:396:PRO:HD2	2.09	0.53
1:E:110:VAL:HB	1:E:268:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:57:VAL:HG12	3:B:123:LEU:HD12	1.91	0.53
1:E:320:THR:CG2	1:E:325:ARG:HG2	2.39	0.53
3:F:135:TRP:NE1	3:F:156:GLY:HA3	2.24	0.53
3:J:92:PHE:O	3:J:96:PHE:HB2	2.09	0.52
1:I:352:ASP:O	1:I:353:VAL:C	2.46	0.52
1:A:40:MET:HE2	1:A:388:GLY:H	1.73	0.52
4:K:180:SER:HB3	4:K:183:PHE:HB2	1.92	0.52
1:I:82:VAL:HG11	1:I:141:GLU:OE1	2.08	0.52
1:I:286:THR:HG21	1:I:391:LEU:HD12	1.91	0.52
1:I:358:GLU:HG2	1:I:359:SER:H	1.73	0.52
1:A:275:GLY:CA	1:A:276:THR:CB	2.87	0.52
3:B:132:PRO:HB2	3:B:157:TRP:CE3	2.45	0.52
1:I:273:THR:HB	1:I:274:GLU:HB2	1.91	0.52
1:E:340:ASP:HB3	1:E:341:TYR:CA	2.38	0.52
1:E:386:GLN:HG3	1:E:407:GLY:C	2.29	0.52
1:I:348:LEU:HA	1:I:349:SER:HB3	1.92	0.52
1:I:395:THR:HG22	1:I:399:LYS:O	2.10	0.52
1:E:318:GLU:HB3	1:E:392:PHE:HB2	1.91	0.52
1:A:50:TRP:O	1:A:52:LYS:N	2.43	0.51
2:D:2:ALA:O	2:D:6:ALA:HB2	2.11	0.51
1:A:250:THR:HG21	3:B:167:PRO:HA	1.93	0.51
3:J:69:LEU:HB3	3:J:70:PRO:HD3	1.92	0.51
3:F:204:MET:H	3:F:207:ARG:HH12	1.59	0.51
1:E:276:THR:HG23	1:E:279:VAL:HB	1.92	0.51
3:F:77:CYS:SG	3:F:98:VAL:HG23	2.50	0.51
4:G:246:ILE:HG21	4:G:249:GLU:OE2	2.11	0.51
3:J:89:ARG:HG3	1:I:220:PRO:HB3	1.91	0.51
1:A:203:PHE:O	1:A:207:GLY:HA2	2.10	0.51
4:C:246:ILE:HG21	4:C:249:GLU:OE2	2.11	0.51
3:F:59:TRP:CZ3	3:F:203:ARG:O	2.64	0.51
3:F:176:THR:HG21	3:F:188:LEU:HD22	1.93	0.51
4:C:173:PRO:O	4:C:174:TYR:CB	2.59	0.51
4:G:102:ARG:O	4:G:106:VAL:HG23	2.10	0.51
1:E:102:GLY:HA3	1:E:268:LEU:HD22	1.92	0.51
4:K:121:GLY:HA2	4:K:153:SER:HG	1.71	0.51
1:E:37:PHE:O	1:E:41:ARG:HG3	2.12	0.50
1:A:341:TYR:H	1:A:342:LEU:CA	2.24	0.50
3:J:56:TRP:CH2	4:K:134:MET:HG3	2.46	0.50
4:G:53:SER:OG	4:G:139:ASP:CB	2.59	0.50
1:I:96:ARG:HD3	1:I:99:GLN:NE2	2.26	0.50
2:H:13:ALA:O	2:H:17:ALA:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:176:THR:HG21	3:B:188:LEU:HD22	1.93	0.50
3:B:204:MET:H	3:B:207:ARG:HH12	1.58	0.50
1:E:57:VAL:O	1:E:58:ASN:HB2	2.12	0.50
1:I:273:THR:CA	1:I:274:GLU:HB2	2.40	0.50
1:A:184:ILE:HD11	3:B:172:PHE:CE2	2.47	0.50
1:E:149:PRO:HB3	1:E:342:LEU:HD21	1.93	0.50
1:A:47:ASP:OD2	1:A:66:LYS:NZ	2.36	0.50
4:C:231:VAL:O	4:C:235:VAL:HG13	2.11	0.50
1:I:274:GLU:H	1:I:275:GLY:HA2	1.70	0.50
1:A:275:GLY:CA	1:A:276:THR:HB	2.41	0.50
3:J:201:TYR:CD1	3:J:201:TYR:C	2.85	0.50
1:E:341:TYR:H	1:E:342:LEU:CA	2.25	0.50
1:A:386:GLN:HG3	1:A:407:GLY:C	2.32	0.49
4:G:168:ALA:O	4:G:175:PHE:HB2	2.12	0.49
4:K:137:ILE:HD13	1:I:147:ILE:HD11	1.93	0.49
1:E:349:SER:OG	1:E:350:ASN:N	2.45	0.49
1:A:33:SER:O	3:F:213:PHE:HA	2.12	0.49
1:A:96:ARG:HH21	1:A:99:GLN:NE2	2.09	0.49
1:I:58:ASN:ND2	1:I:163:THR:H	1.97	0.49
1:I:205:ARG:O	1:I:206:LYS:CB	2.52	0.49
1:I:96:ARG:HD2	1:I:99:GLN:NE2	2.27	0.49
3:J:184:THR:CG2	1:I:258:ILE:HG13	2.42	0.49
3:F:246:THR:HG22	4:G:237:GLN:HG3	1.93	0.49
1:E:348:LEU:HA	1:E:349:SER:HB2	1.94	0.49
1:I:56:ASN:HA	1:I:156:LYS:O	2.12	0.49
1:I:101:ILE:HG13	1:I:120:PHE:HB3	1.95	0.49
1:I:79:ASN:C	1:I:81:ARG:H	2.14	0.49
1:A:70:PHE:CE1	1:A:72:ALA:HB3	2.48	0.49
3:J:191:LEU:HD13	1:I:107:PRO:HA	1.95	0.49
3:F:135:TRP:CD1	3:F:153:GLY:O	2.66	0.49
3:F:138:VAL:CG2	1:E:236:LEU:HD22	2.43	0.49
4:G:20:ASP:O	4:G:21:LEU:HB2	2.13	0.49
1:E:334:GLN:HG2	1:E:335:LYS:HB2	1.95	0.49
1:I:338:PHE:HB3	1:I:343:LEU:HD22	1.95	0.49
1:A:334:GLN:HA	1:A:335:LYS:CB	2.42	0.48
1:A:340:ASP:HB3	1:A:341:TYR:CA	2.42	0.48
1:E:203:PHE:O	1:E:207:GLY:HA2	2.13	0.48
3:J:102:MET:HG3	3:J:130:ILE:CD1	2.43	0.48
1:E:107:PRO:HD2	1:E:265:GLN:HE22	1.79	0.48
1:I:320:THR:CG2	1:I:325:ARG:HG2	2.43	0.48
4:K:39:ARG:NH2	4:K:43:GLN:HB2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:176:ALA:O	4:C:177:HIS:CD2	2.67	0.48
1:I:334:GLN:HG2	1:I:335:LYS:HB2	1.96	0.48
1:A:108:ARG:NH2	1:I:384:ASP:OD1	2.46	0.48
1:A:320:THR:CG2	1:A:325:ARG:HG2	2.44	0.48
3:F:172:PHE:CZ	1:E:184:ILE:HD11	2.48	0.48
1:E:220:PRO:C	1:E:222:ASP:H	2.13	0.48
1:I:410:ILE:HG23	1:I:411:PRO:HD2	1.95	0.48
3:B:201:TYR:CD1	3:B:201:TYR:C	2.86	0.48
3:F:99:LEU:HG	3:F:103:ILE:HD12	1.95	0.48
4:C:129:ASP:O	4:C:133:HIS:HD2	1.96	0.48
1:A:188:HIS:HD2	3:B:106:TRP:HE1	1.60	0.48
3:J:53:TRP:CE3	3:J:68:VAL:HG21	2.49	0.48
1:I:58:ASN:HD21	1:I:163:THR:N	1.98	0.48
3:F:203:ARG:O	3:F:204:MET:CB	2.62	0.48
1:I:80:PRO:HA	1:I:140:VAL:HG13	1.96	0.48
3:F:185:LEU:O	3:F:189:ILE:HG13	2.13	0.47
1:A:384:ASP:OD1	1:E:108:ARG:NH2	2.46	0.47
3:J:215:LYS:HA	1:E:381:TYR:CZ	2.49	0.47
3:J:39:LEU:HD11	3:J:104:GLY:HA3	1.97	0.47
1:I:105:PHE:CE2	1:I:107:PRO:HG3	2.50	0.47
1:A:110:VAL:HB	1:A:268:LEU:HD11	1.97	0.47
1:E:275:GLY:CA	1:E:276:THR:CB	2.92	0.47
1:A:258:ILE:HG13	3:B:184:THR:HG22	1.97	0.47
3:B:199:PRO:HB2	3:B:201:TYR:CE2	2.49	0.47
3:F:192:HIS:HD2	1:E:164:ASP:OD2	1.98	0.47
4:K:20:ASP:O	4:K:21:LEU:CB	2.62	0.47
3:F:42:TYR:OH	3:F:73:GLY:O	2.25	0.47
3:F:200:GLU:HG2	3:F:203:ARG:NH1	2.30	0.47
3:F:192:HIS:CD2	1:E:164:ASP:OD2	2.68	0.46
3:F:199:PRO:HB2	3:F:201:TYR:CE2	2.50	0.46
3:F:59:TRP:CZ2	3:F:203:ARG:HA	2.51	0.46
3:F:167:PRO:HG2	1:E:187:TRP:CZ2	2.50	0.46
1:I:55:VAL:O	1:I:155:ILE:HA	2.15	0.46
1:A:132:TRP:CD1	1:A:155:ILE:HD12	2.50	0.46
3:J:151:VAL:HG12	3:J:152:VAL:N	2.29	0.46
4:G:173:PRO:O	4:G:174:TYR:CB	2.63	0.46
3:B:177:GLU:HG3	1:I:410:ILE:HG12	1.97	0.46
1:I:58:ASN:ND2	1:I:125:ARG:HH21	2.13	0.46
1:A:273:THR:HB	1:A:274:GLU:HB2	1.97	0.46
3:B:98:VAL:HG12	3:B:99:LEU:N	2.29	0.46
1:E:79:ASN:OD1	1:E:81:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:HA	1:A:349:SER:CB	2.45	0.46
4:C:173:PRO:O	4:C:174:TYR:HB2	2.15	0.46
4:K:138:ARG:NH1	4:K:141:ASP:HA	2.31	0.46
3:F:98:VAL:HG12	3:F:99:LEU:N	2.30	0.46
1:E:339:PRO:O	1:E:340:ASP:C	2.54	0.46
1:I:40:MET:HE2	1:I:388:GLY:H	1.81	0.46
1:A:137:GLN:HE21	1:A:139:ASN:HD21	1.64	0.46
3:B:135:TRP:CD1	3:B:153:GLY:O	2.69	0.46
4:G:69:GLU:OE1	4:G:152:MET:HB2	2.15	0.46
1:E:334:GLN:HA	1:E:335:LYS:CB	2.38	0.46
4:C:24:MET:HB2	4:C:109:GLN:HG2	1.98	0.45
1:I:275:GLY:CA	1:I:276:THR:CB	2.94	0.45
4:C:20:ASP:O	4:C:21:LEU:HB2	2.15	0.45
4:C:53:SER:OG	4:C:139:ASP:CB	2.60	0.45
1:E:385:SER:H	1:I:261:GLN:HE22	1.63	0.45
3:J:39:LEU:HD22	3:J:100:GLY:HA2	1.97	0.45
3:B:59:TRP:CZ2	3:B:203:ARG:HA	2.51	0.45
1:E:96:ARG:HH21	1:E:99:GLN:HE22	1.63	0.45
3:J:98:VAL:HG22	3:J:129:MET:CE	2.47	0.45
4:G:53:SER:HA	4:G:58:PHE:CG	2.52	0.45
1:E:94:LEU:HB3	1:E:124:LEU:HB3	1.98	0.45
1:I:302:ILE:HG13	1:I:364:VAL:HB	1.98	0.45
1:E:68:HIS:CE1	1:E:404:GLU:OE1	2.57	0.45
3:J:39:LEU:HD22	3:J:100:GLY:CA	2.47	0.45
1:E:220:PRO:HB2	1:E:221:ASP:H	1.51	0.45
3:J:123:LEU:HD13	3:J:189:ILE:HG22	1.99	0.45
1:A:308:ASN:O	1:A:357:GLY:N	2.50	0.45
1:A:341:TYR:CG	1:A:342:LEU:HB2	2.51	0.45
3:J:67:THR:HG22	3:J:68:VAL:N	2.31	0.45
3:F:172:PHE:CE2	1:E:184:ILE:HD11	2.51	0.45
4:C:18:VAL:HG11	4:C:101:MET:HG3	1.98	0.45
4:K:184:LEU:HD23	4:K:184:LEU:HA	1.88	0.45
1:E:341:TYR:CG	1:E:342:LEU:HB2	2.52	0.45
1:I:274:GLU:N	1:I:275:GLY:HA3	2.17	0.45
1:A:348:LEU:CA	1:A:349:SER:CB	2.95	0.45
1:E:348:LEU:CA	1:E:349:SER:CB	2.95	0.45
1:A:358:GLU:HG2	1:A:359:SER:N	2.33	0.44
1:A:61:MET:O	1:A:61:MET:HG3	2.17	0.44
1:A:79:ASN:OD1	1:A:81:ARG:HB2	2.17	0.44
1:A:199:ILE:HD11	3:B:96:PHE:HA	2.00	0.44
3:J:105:GLU:O	3:J:109:ARG:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:154:TYR:HB2	4:G:155:PRO:HD3	2.00	0.44
4:K:137:ILE:HG22	4:K:137:ILE:O	2.17	0.44
1:I:94:LEU:HG	1:I:155:ILE:HD11	1.99	0.44
1:E:297:GLY:O	1:E:372:ASP:HB2	2.18	0.44
1:E:289:ASN:ND2	1:E:305:LYS:HE2	2.33	0.44
1:I:293:TYR:CZ	1:I:411:PRO:HB3	2.53	0.44
1:A:225:GLY:HA2	1:A:229:ARG:HH21	1.80	0.44
1:A:79:ASN:C	1:A:81:ARG:H	2.20	0.44
1:A:184:ILE:HD11	3:B:172:PHE:CZ	2.52	0.44
3:J:132:PRO:HD3	3:J:164:ASN:ND2	2.33	0.44
4:K:38:VAL:O	4:K:42:GLU:HG2	2.17	0.44
1:I:93:VAL:HG11	1:I:132:TRP:CE2	2.52	0.44
1:A:164:ASP:HB3	1:A:165:PRO:CA	2.48	0.44
4:G:231:VAL:O	4:G:235:VAL:HG13	2.18	0.44
1:I:318:GLU:HB3	1:I:392:PHE:HB2	1.99	0.44
1:A:37:PHE:O	1:A:41:ARG:HG3	2.17	0.44
3:J:135:TRP:NE1	3:J:156:GLY:HA3	2.33	0.44
3:J:172:PHE:HE2	1:I:184:ILE:HD11	1.79	0.44
3:B:77:CYS:SG	3:B:98:VAL:HG23	2.58	0.43
3:B:81:GLN:HE21	3:B:137:ASP:HA	1.84	0.43
1:A:96:ARG:HD2	1:A:99:GLN:NE2	2.33	0.43
1:A:320:THR:HG22	1:A:324:LEU:O	2.18	0.43
3:J:178:GLN:HG3	3:J:188:LEU:HD11	2.00	0.43
3:B:188:LEU:HD12	3:B:188:LEU:HA	1.86	0.43
4:G:137:ILE:HD13	1:E:147:ILE:CD1	2.49	0.43
1:I:61:MET:O	1:I:61:MET:HG3	2.17	0.43
3:F:192:HIS:HA	1:E:96:ARG:O	2.18	0.43
1:E:273:THR:O	1:E:273:THR:OG1	2.36	0.43
3:F:185:LEU:HD22	1:E:176:LEU:HD21	2.01	0.43
1:I:167:THR:HG22	1:I:168:LEU:O	2.18	0.43
1:A:295:VAL:HA	1:A:296:PRO:HA	1.92	0.43
3:J:204:MET:H	3:J:207:ARG:HH12	1.65	0.43
1:E:295:VAL:HA	1:E:296:PRO:HA	1.90	0.43
4:C:184:LEU:HD23	4:C:184:LEU:HA	1.76	0.43
1:I:306:VAL:HG12	1:I:360:LYS:O	2.19	0.43
3:J:59:TRP:CH2	3:J:203:ARG:O	2.71	0.43
3:B:143:SER:C	3:B:145:SER:N	2.67	0.43
1:I:98:ALA:HB3	1:I:123:ASN:HD22	1.82	0.43
1:I:341:TYR:CG	1:I:342:LEU:HB2	2.53	0.43
3:F:90:LEU:HA	3:F:91:PRO:HD3	1.87	0.43
4:K:139:ASP:OD1	1:I:30:GLY:HA2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:190:PRO:C	4:G:192:MET:H	2.20	0.42
1:I:129:ALA:HA	1:I:155:ILE:O	2.19	0.42
1:I:276:THR:CG2	1:I:279:VAL:HB	2.48	0.42
1:A:107:PRO:HA	3:B:191:LEU:HD13	2.01	0.42
1:A:334:GLN:HG2	1:A:335:LYS:HB2	2.00	0.42
3:J:116:TRP:CD1	4:K:47:TRP:CZ3	3.07	0.42
3:B:98:VAL:O	3:B:102:MET:HG2	2.19	0.42
3:B:112:ASN:CG	4:C:128:GLN:HE21	2.22	0.42
4:C:196:ASN:HA	4:C:197:VAL:HA	1.81	0.42
1:A:57:VAL:O	1:A:58:ASN:HB2	2.19	0.42
3:F:92:PHE:O	3:F:96:PHE:HB2	2.19	0.42
1:I:58:ASN:HD22	1:I:125:ARG:NH2	2.17	0.42
3:J:178:GLN:HG3	3:J:188:LEU:CD1	2.49	0.42
4:C:39:ARG:NH2	4:C:43:GLN:HB2	2.34	0.42
4:C:64:SER:O	4:C:68:THR:HB	2.20	0.42
4:K:196:ASN:HA	4:K:197:VAL:HA	1.87	0.42
1:E:225:GLY:HA2	1:E:229:ARG:HH21	1.81	0.42
1:I:149:PRO:HB3	1:I:342:LEU:HD21	2.02	0.42
3:F:44:VAL:HG23	4:G:122:ALA:HB1	2.00	0.42
4:K:88:ARG:HB2	4:K:170:THR:HB	2.01	0.42
1:E:333:THR:O	1:E:334:GLN:CB	2.68	0.42
3:J:241:ARG:O	3:J:244:SER:HB2	2.19	0.42
3:F:182:LEU:HD21	1:E:258:ILE:HD13	2.02	0.42
1:I:201:PHE:HZ	1:I:231:ILE:HD13	1.84	0.42
3:F:56:TRP:CZ2	4:G:134:MET:HG3	2.55	0.42
3:F:112:ASN:CG	4:G:128:GLN:HE21	2.23	0.42
1:I:220:PRO:C	1:I:222:ASP:N	2.68	0.42
1:I:273:THR:CB	1:I:274:GLU:HB2	2.49	0.42
1:A:286:THR:OG1	1:A:403:ALA:HB1	2.19	0.42
3:B:116:TRP:CD1	4:C:47:TRP:CZ3	3.07	0.42
4:C:137:ILE:HG22	4:C:137:ILE:O	2.20	0.42
1:I:37:PHE:O	1:I:41:ARG:HG3	2.20	0.42
1:I:342:LEU:H	1:I:370:ARG:HD3	1.84	0.42
1:I:56:ASN:O	1:I:57:VAL:C	2.56	0.42
1:I:108:ARG:HD2	1:I:262:ALA:HA	2.02	0.42
4:C:190:PRO:C	4:C:192:MET:H	2.23	0.42
1:E:62:ILE:HG22	1:E:123:ASN:OD1	2.20	0.42
1:I:297:GLY:O	1:I:372:ASP:HB2	2.20	0.42
3:B:53:TRP:O	3:B:60:LYS:NZ	2.53	0.41
3:F:201:TYR:CD1	3:F:201:TYR:C	2.93	0.41
1:I:201:PHE:CZ	1:I:231:ILE:HD13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:TYR:CZ	1:A:342:LEU:HD22	2.56	0.41
4:K:246:ILE:HG21	4:K:249:GLU:OE2	2.19	0.41
1:E:276:THR:CG2	1:E:279:VAL:HB	2.50	0.41
1:I:102:GLY:HA3	1:I:268:LEU:HB3	2.02	0.41
1:A:51:SER:HB3	1:A:62:ILE:O	2.21	0.41
4:G:129:ASP:O	4:G:133:HIS:HD2	2.02	0.41
1:E:40:MET:HE2	1:E:387:VAL:HB	2.01	0.41
1:I:275:GLY:CA	1:I:276:THR:HB	2.50	0.41
1:I:286:THR:OG1	1:I:403:ALA:HB1	2.20	0.41
1:A:164:ASP:OD2	3:B:192:HIS:CD2	2.73	0.41
3:J:45:HIS:HE1	4:K:224:PHE:HA	1.85	0.41
4:K:137:ILE:HD13	1:I:147:ILE:HD12	2.02	0.41
1:I:73:TRP:HA	1:I:74:PRO:HD3	1.91	0.41
3:B:92:PHE:O	3:B:96:PHE:HB2	2.20	0.41
1:E:348:LEU:HA	1:E:349:SER:CB	2.50	0.41
1:A:129:ALA:HA	1:A:155:ILE:O	2.21	0.41
4:C:154:TYR:HB2	4:C:155:PRO:HD3	2.03	0.41
1:E:286:THR:HG21	1:E:391:LEU:HD12	2.02	0.41
1:I:295:VAL:HA	1:I:296:PRO:HA	1.92	0.41
3:B:56:TRP:CH2	4:C:134:MET:HG3	2.56	0.41
3:B:59:TRP:CH2	3:B:203:ARG:O	2.74	0.41
4:G:117:ALA:HB1	4:G:157:TYR:HB3	2.03	0.41
1:E:294:LYS:O	1:E:297:GLY:HA2	2.21	0.41
1:I:83:SER:O	1:I:109:SER:HB2	2.21	0.41
1:A:96:ARG:NH2	1:A:99:GLN:HE22	2.16	0.41
3:J:30:LEU:HD23	3:J:33:LEU:HD21	2.03	0.41
3:B:98:VAL:HG11	3:B:130:ILE:HA	2.03	0.41
3:F:51:GLY:HA3	3:F:52:ASP:CB	2.26	0.41
3:F:244:SER:O	4:G:236:LEU:HD12	2.20	0.41
3:J:162:TYR:O	3:J:163:PRO:C	2.56	0.40
3:B:58:ASP:HB2	3:B:203:ARG:HH21	1.86	0.40
3:B:60:LYS:HD3	3:B:65:TRP:CZ2	2.56	0.40
3:F:188:LEU:HD12	3:F:188:LEU:HA	1.97	0.40
4:C:117:ALA:HB1	4:C:157:TYR:HB3	2.02	0.40
4:G:190:PRO:O	4:G:193:ILE:HG13	2.21	0.40
1:A:102:GLY:HA3	1:A:268:LEU:HB3	2.03	0.40
3:F:44:VAL:CG2	4:G:122:ALA:HB1	2.51	0.40
1:E:163:THR:HG22	1:E:164:ASP:N	2.36	0.40
3:J:150:ALA:O	3:J:230:MET:HG2	2.22	0.40
3:J:199:PRO:HB2	3:J:201:TYR:CE2	2.57	0.40
1:A:334:GLN:HG2	1:A:335:LYS:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:129:MET:O	3:J:132:PRO:HD2	2.21	0.40
3:J:172:PHE:CZ	1:I:184:ILE:HD11	2.57	0.40
3:F:241:ARG:O	3:F:244:SER:HB2	2.21	0.40
1:E:51:SER:HB3	1:E:62:ILE:O	2.21	0.40
1:I:48:VAL:HG21	1:I:149:PRO:CG	2.51	0.40
1:A:383:THR:HG22	1:E:260:LEU:O	2.22	0.40
4:C:39:ARG:HH22	4:C:43:GLN:HB2	1.86	0.40
4:C:194:ILE:HA	4:C:195:PRO:HD3	2.00	0.40
4:K:102:ARG:O	4:K:106:VAL:HG23	2.22	0.40
1:I:275:GLY:CA	1:I:276:THR:HG22	2.22	0.40
1:I:287:GLU:HB2	1:I:305:LYS:HB2	2.03	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	384/419 (92%)	338 (88%)	27 (7%)	19 (5%)	2 3
1	E	384/419 (92%)	340 (88%)	26 (7%)	18 (5%)	2 4
1	I	384/419 (92%)	330 (86%)	31 (8%)	23 (6%)	1 2
2	D	17/19 (90%)	13 (76%)	2 (12%)	2 (12%)	0 0
2	H	14/19 (74%)	12 (86%)	2 (14%)	0	100 100
3	B	240/252 (95%)	218 (91%)	16 (7%)	6 (2%)	5 12
3	F	240/252 (95%)	215 (90%)	22 (9%)	3 (1%)	12 27
3	J	240/252 (95%)	214 (89%)	19 (8%)	7 (3%)	4 9
4	C	206/256 (80%)	188 (91%)	10 (5%)	8 (4%)	3 6
4	G	207/256 (81%)	181 (87%)	18 (9%)	8 (4%)	3 6
4	K	207/256 (81%)	184 (89%)	16 (8%)	7 (3%)	3 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2523/2819 (90%)	2233 (88%)	189 (8%)	101 (4%)	3 5

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	GLU
1	A	164	ASP
1	A	220	PRO
1	A	221	ASP
1	A	274	GLU
1	A	276	THR
1	A	340	ASP
1	A	342	LEU
1	A	349	SER
2	D	4	ALA
3	J	52	ASP
3	J	201	TYR
3	B	201	TYR
3	F	12	PRO
3	F	52	ASP
4	C	229	LEU
4	G	49	ALA
4	G	229	LEU
4	K	229	LEU
1	E	51	SER
1	E	103	GLU
1	E	164	ASP
1	E	217	GLU
1	E	220	PRO
1	E	221	ASP
1	E	276	THR
1	E	334	GLN
1	E	340	ASP
1	E	342	LEU
1	E	349	SER
1	I	51	SER
1	I	103	GLU
1	I	164	ASP
1	I	220	PRO
1	I	221	ASP
1	I	274	GLU
1	I	276	THR

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Mol	Chain	Res	Type
1	I	335	LYS
1	I	340	ASP
1	I	342	LEU
1	I	349	SER
1	I	353	VAL
1	A	51	SER
1	A	217	GLU
1	A	353	VAL
3	J	204	MET
3	B	52	ASP
3	F	201	TYR
4	C	49	ALA
4	C	174	TYR
4	C	177	HIS
4	C	246	ILE
4	G	174	TYR
4	G	177	HIS
4	G	246	ILE
4	K	49	ALA
4	K	174	TYR
4	K	177	HIS
1	E	274	GLU
1	E	353	VAL
1	A	218	GLY
1	A	297	GLY
1	A	335	LYS
3	B	204	MET
4	G	195	PRO
4	K	179	TYR
1	E	297	GLY
1	E	335	LYS
1	I	217	GLU
1	I	218	GLY
1	I	264	LEU
1	I	334	GLN
1	I	350	ASN
1	A	334	GLN
1	A	350	ASN
4	C	179	TYR
4	C	191	PHE
4	C	195	PRO
4	G	191	PHE

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Mol	Chain	Res	Type
4	K	246	ILE
1	E	218	GLY
1	E	350	ASN
1	I	165	PRO
1	I	206	LYS
1	I	297	GLY
3	J	144	GLY
3	J	250	GLU
4	G	179	TYR
4	K	195	PRO
1	A	206	LYS
2	D	18	ALA
3	J	203	ARG
3	B	144	GLY
3	B	200	GLU
1	I	368	ASP
3	J	151	VAL
1	I	357	GLY
3	B	151	VAL
1	I	208	ILE
1	A	165	PRO
1	E	165	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	318/335 (95%)	305 (96%)	13 (4%)	30	56
1	E	318/335 (95%)	304 (96%)	14 (4%)	28	53
1	I	318/335 (95%)	304 (96%)	14 (4%)	28	53
3	B	201/208 (97%)	187 (93%)	14 (7%)	15	32
3	F	201/208 (97%)	186 (92%)	15 (8%)	13	29
3	J	201/208 (97%)	187 (93%)	14 (7%)	15	32
4	C	173/209 (83%)	163 (94%)	10 (6%)	20	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	174/209 (83%)	166 (95%)	8 (5%)	27	51
4	K	174/209 (83%)	165 (95%)	9 (5%)	23	46
All	All	2078/2256 (92%)	1967 (95%)	111 (5%)	22	45

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	97	THR
1	A	117	ASP
1	A	253	THR
1	A	266	LYS
1	A	285	THR
1	A	320	THR
1	A	340	ASP
1	A	348	LEU
1	A	349	SER
1	A	378	ASP
1	A	383	THR
1	A	414	VAL
3	J	33	LEU
3	J	39	LEU
3	J	42	TYR
3	J	48	LEU
3	J	52	ASP
3	J	67	THR
3	J	69	LEU
3	J	92	PHE
3	J	98	VAL
3	J	152	VAL
3	J	164	ASN
3	J	169	ILE
3	J	201	TYR
3	J	234	PHE
3	B	33	LEU
3	B	39	LEU
3	B	42	TYR
3	B	48	LEU
3	B	69	LEU
3	B	92	PHE
3	B	98	VAL

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Mol	Chain	Res	Type
3	B	152	VAL
3	B	164	ASN
3	B	169	ILE
3	B	192	HIS
3	B	201	TYR
3	B	220	VAL
3	B	234	PHE
3	F	33	LEU
3	F	39	LEU
3	F	42	TYR
3	F	48	LEU
3	F	69	LEU
3	F	88	PHE
3	F	92	PHE
3	F	98	VAL
3	F	138	VAL
3	F	152	VAL
3	F	164	ASN
3	F	169	ILE
3	F	201	TYR
3	F	220	VAL
3	F	234	PHE
4	C	68	THR
4	C	72	LEU
4	C	118	ILE
4	C	145	SER
4	C	147	ILE
4	C	177	HIS
4	C	183	PHE
4	C	229	LEU
4	C	235	VAL
4	C	246	ILE
4	G	36	LEU
4	G	72	LEU
4	G	118	ILE
4	G	145	SER
4	G	147	ILE
4	G	183	PHE
4	G	229	LEU
4	G	246	ILE
4	K	60	THR
4	K	68	THR

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Mol	Chain	Res	Type
4	K	72	LEU
4	K	118	ILE
4	K	145	SER
4	K	183	PHE
4	K	229	LEU
4	K	235	VAL
4	K	246	ILE
1	E	29	HIS
1	E	63	LEU
1	E	94	LEU
1	E	95	VAL
1	E	97	THR
1	E	99	GLN
1	E	253	THR
1	E	285	THR
1	E	320	THR
1	E	348	LEU
1	E	349	SER
1	E	378	ASP
1	E	383	THR
1	E	414	VAL
1	I	29	HIS
1	I	51	SER
1	I	97	THR
1	I	133	HIS
1	I	166	VAL
1	I	253	THR
1	I	266	LYS
1	I	285	THR
1	I	310	THR
1	I	320	THR
1	I	348	LEU
1	I	353	VAL
1	I	378	ASP
1	I	414	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	44	ASN
1	A	58	ASN

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Mol	Chain	Res	Type
1	A	68	HIS
1	A	99	GLN
1	A	137	GLN
1	A	188	HIS
1	A	261	GLN
3	J	45	HIS
3	B	192	HIS
3	F	45	HIS
3	F	174	GLN
3	F	192	HIS
4	C	109	GLN
4	C	128	GLN
4	C	177	HIS
4	G	109	GLN
4	G	128	GLN
4	G	177	HIS
4	K	109	GLN
4	K	128	GLN
4	K	177	HIS
1	E	44	ASN
1	E	58	ASN
1	E	68	HIS
1	E	99	GLN
1	E	104	GLN
1	E	188	HIS
1	E	261	GLN
1	E	265	GLN
1	I	58	ASN
1	I	68	HIS
1	I	99	GLN
1	I	139	ASN
1	I	188	HIS
1	I	261	GLN
1	I	386	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 11 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	CUA	A	420	1	0,1,1	-	-	-		

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	386/419 (92%)	0.48	36 (9%)	8	6	50, 69, 98, 114	0
1	E	386/419 (92%)	0.48	38 (9%)	7	5	48, 68, 101, 123	0
1	I	386/419 (92%)	0.42	45 (11%)	4	3	34, 50, 74, 90	0
2	D	19/19 (100%)	0.37	2 (10%)	6	4	78, 80, 83, 83	0
2	H	16/19 (84%)	1.45	5 (31%)	0	0	97, 99, 104, 104	0
3	B	242/252 (96%)	0.25	14 (5%)	23	21	43, 58, 90, 109	0
3	F	242/252 (96%)	0.41	17 (7%)	16	14	42, 57, 93, 117	0
3	J	242/252 (96%)	0.08	8 (3%)	46	45	40, 55, 89, 109	0
4	C	210/256 (82%)	0.52	18 (8%)	10	8	53, 69, 101, 114	0
4	G	211/256 (82%)	0.42	13 (6%)	20	18	53, 78, 112, 125	0
4	K	211/256 (82%)	0.46	17 (8%)	12	10	54, 72, 106, 119	0
All	All	2551/2819 (90%)	0.41	213 (8%)	11	9	34, 63, 100, 125	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	394	PHE	8.4
1	I	349	SER	7.3
4	K	56	PRO	7.3
1	I	365	LYS	6.9
3	B	11	GLY	6.8
3	F	248	ARG	6.7
3	J	13	PHE	6.3
4	K	60	THR	6.2
4	K	48	ARG	6.2
1	I	311	SER	6.0
3	F	251	GLN	5.5
1	E	226	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	222	ASP	5.4
1	I	348	LEU	5.3
2	H	5	ALA	5.3
4	C	251	VAL	5.0
1	I	354	ILE	5.0
1	E	393	PHE	4.9
1	E	359	SER	4.9
1	E	396	PRO	4.8
1	I	351	ASP	4.8
1	A	399	LYS	4.7
1	I	316	LEU	4.7
1	E	275	GLY	4.7
1	I	364	VAL	4.6
1	A	398	GLY	4.6
2	H	6	ALA	4.6
1	I	350	ASN	4.4
3	F	11	GLY	4.3
4	K	197	VAL	4.3
3	F	250	GLU	4.3
4	C	19	VAL	4.1
4	K	59	GLN	4.0
1	I	332	PHE	4.0
3	F	249	ILE	4.0
1	E	402	ALA	3.8
4	C	85	TRP	3.8
4	G	48	ARG	3.8
1	A	397	ASP	3.7
1	E	353	VAL	3.7
4	C	250	GLY	3.7
3	F	252	ILE	3.6
1	E	205	ARG	3.6
1	I	357	GLY	3.6
3	B	251	GLN	3.6
4	G	67	TRP	3.5
1	A	280	GLY	3.5
3	B	16	VAL	3.5
3	B	231	MET	3.4
4	C	139	ASP	3.4
4	G	45	PHE	3.4
1	E	274	GLU	3.3
3	F	13	PHE	3.3
1	A	353	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	I	331	VAL	3.3
1	E	362	ILE	3.3
1	E	264	LEU	3.3
4	K	178	GLY	3.3
1	E	399	LYS	3.3
1	E	330	THR	3.3
4	C	60	THR	3.2
3	B	13	PHE	3.2
4	K	61	TYR	3.2
1	I	273	THR	3.2
4	K	57	GLU	3.2
1	E	219	ARG	3.2
1	E	360	LYS	3.2
1	I	366	ILE	3.1
3	J	17	ALA	3.1
3	F	20	ALA	3.1
3	B	17	ALA	3.1
4	C	61	TYR	3.1
1	I	393	PHE	3.1
1	I	363	VAL	3.1
1	A	176	LEU	3.1
1	I	362	ILE	3.1
4	C	249	GLU	3.1
3	F	17	ALA	3.1
1	I	338	PHE	3.1
4	C	17	SER	3.1
1	I	353	VAL	3.0
4	C	92	VAL	3.0
2	H	7	ALA	3.0
1	E	304	VAL	3.0
4	G	251	VAL	3.0
1	A	312	GLN	3.0
1	I	399	LYS	3.0
3	F	245	THR	3.0
4	G	16	GLU	3.0
3	F	22	CYS	3.0
3	B	25	THR	3.0
2	H	4	ALA	3.0
1	A	363	VAL	3.0
1	E	252	SER	2.9
1	E	400	ARG	2.9
1	I	394	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
4	K	55	ALA	2.9
1	I	313	PRO	2.9
1	I	252	SER	2.9
4	C	48	ARG	2.9
3	B	248	ARG	2.9
1	I	272	GLU	2.9
1	E	225	GLY	2.8
1	A	247	TYR	2.8
4	G	59	GLN	2.8
1	A	281	LYS	2.8
1	I	310	THR	2.8
4	C	170	THR	2.8
1	I	328	ASN	2.8
1	E	315	ARG	2.8
1	I	314	VAL	2.7
4	K	62	TRP	2.7
4	C	252	ALA	2.7
4	K	226	TRP	2.7
1	A	354	ILE	2.7
1	A	359	SER	2.7
3	B	15	SER	2.7
1	E	351	ASP	2.7
1	A	348	LEU	2.7
1	A	396	PRO	2.7
1	I	356	PRO	2.7
4	K	196	ASN	2.7
1	A	220	PRO	2.6
3	B	224	PHE	2.6
3	F	247	LYS	2.6
4	G	64	SER	2.6
4	G	194	ILE	2.6
1	I	318	GLU	2.6
1	E	321	ALA	2.6
1	A	340	ASP	2.6
1	A	311	SER	2.6
1	A	279	VAL	2.6
1	E	398	GLY	2.6
1	A	361	GLU	2.6
3	B	172	PHE	2.6
1	A	283	GLN	2.6
2	D	5	ALA	2.6
2	D	17	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	230	ARG	2.5
1	A	179	TYR	2.5
1	E	395	THR	2.5
1	I	340	ASP	2.5
3	F	23	VAL	2.5
1	I	327	LEU	2.5
3	B	14	ASN	2.5
4	K	139	ASP	2.5
4	K	252	ALA	2.5
1	I	227	ASP	2.5
1	A	304	VAL	2.4
3	J	16	VAL	2.4
1	I	206	LYS	2.4
3	J	224	PHE	2.4
1	E	220	PRO	2.4
4	G	197	VAL	2.4
1	E	346	ARG	2.4
3	B	20	ALA	2.4
1	I	154	GLU	2.4
1	A	379	LEU	2.4
1	E	78	ALA	2.4
1	E	401	PHE	2.4
1	I	330	THR	2.3
4	C	165	PHE	2.3
3	F	19	ALA	2.3
3	F	28	TRP	2.3
1	A	313	PRO	2.3
1	E	313	PRO	2.3
1	A	219	ARG	2.3
4	C	81	ALA	2.3
1	E	221	ASP	2.3
1	I	337	ASP	2.3
4	K	140	THR	2.3
1	I	249	VAL	2.3
3	J	63	ARG	2.3
4	G	57	GLU	2.3
4	C	22	ARG	2.3
3	J	11	GLY	2.3
1	E	334	GLN	2.3
1	A	282	GLU	2.3
1	I	292	VAL	2.3
3	F	24	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	317	GLY	2.2
1	I	222	ASP	2.2
1	A	284	VAL	2.2
1	E	361	GLU	2.2
4	C	18	VAL	2.2
1	A	392	PHE	2.2
3	F	243	TYR	2.2
1	A	351	ASP	2.2
1	E	331	VAL	2.2
4	G	193	ILE	2.2
3	B	12	PRO	2.1
1	A	251	ASN	2.1
1	I	392	PHE	2.1
4	G	224	PHE	2.1
1	I	398	GLY	2.1
1	E	243	THR	2.1
1	I	367	GLN	2.1
3	J	248	ARG	2.1
1	E	227	ASP	2.1
1	E	284	VAL	2.1
4	K	194	ILE	2.1
1	I	326	PHE	2.1
1	A	332	PHE	2.1
1	A	300	LEU	2.1
4	C	88	ARG	2.1
1	A	302	ILE	2.1
2	H	9	ALA	2.1
4	G	140	THR	2.0
1	A	362	ILE	2.0
3	J	252	ILE	2.0
4	K	192	MET	2.0
1	A	308	ASN	2.0
1	I	205	ARG	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, 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
6	ZN	K	258	1/1	0.80	0.21	141,141,141,141	0
6	ZN	G	258	1/1	0.82	0.11	129,129,129,129	0
6	ZN	A	421	1/1	0.93	0.09	88,88,88,88	0
7	CU	I	420	1/1	0.95	0.08	76,76,76,76	0
7	CU	E	420	1/1	0.96	0.04	63,63,63,63	0
5	CUA	A	420	2/2	0.96	0.11	72,72,72,93	0
6	ZN	C	258	1/1	0.97	0.03	87,87,87,87	0
6	ZN	I	421	1/1	0.97	0.28	70,70,70,70	0
6	ZN	E	421	1/1	0.98	0.08	90,90,90,90	0
6	ZN	K	257	1/1	0.99	0.10	70,70,70,70	0
6	ZN	G	257	1/1	0.99	0.14	64,64,64,64	0
6	ZN	C	257	1/1	0.99	0.11	57,57,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.