



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2016 – 05:07 PM EDT

PDB ID : 4PI0
Title : Crystal structure of particulate methane monooxygenase from *Methylocystis* sp. ATCC 49242 (Rockwell) soaked in copper
Authors : Sirajuddin, S.; Rosenzweig, A.C.
Deposited on : 2014-05-07
Resolution : 3.15 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

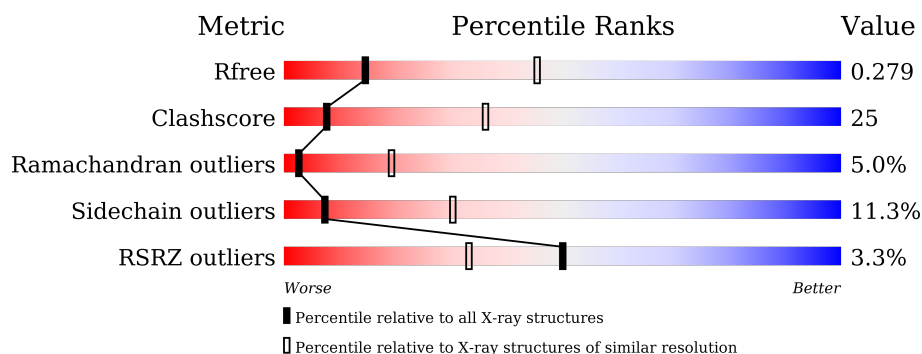
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	D	25	<div> <div>60%</div> <div>16%</div> <div>24%</div> </div>
1	H	25	<div> <div>64%</div> <div>16%</div> <div>20%</div> </div>
1	N	25	<div> <div>60%</div> <div>40%</div> </div>
2	B	252	<div> <div>%</div> <div>56%</div> <div>36%</div> <div>• • •</div> </div>
2	F	252	<div> <div>%</div> <div>57%</div> <div>34%</div> <div>5% • •</div> </div>
2	J	252	<div> <div>55%</div> <div>37%</div> <div>• • •</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	256	<div><div></div><div>3%</div><div>46%</div><div>29%</div><div>10%</div><div>15%</div></div>
3	G	256	<div><div></div><div>4%</div><div>43%</div><div>32%</div><div>8%</div><div>17%</div></div>
3	K	256	<div><div></div><div>5%</div><div>43%</div><div>32%</div><div>11%</div><div>15%</div></div>
4	A	420	<div><div></div><div>7%</div><div>51%</div><div>33%</div><div>7%</div><div>7%</div></div>
4	E	420	<div><div></div><div></div><div>51%</div><div>33%</div><div>8%</div><div>7%</div></div>
4	I	420	<div><div></div><div>4%</div><div>52%</div><div>34%</div><div>6%</div><div>7%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20630 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 unknown peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	D	19	Total	C	N	O	0	0	0
			95	57	19	19			
1	H	20	Total	C	N	O	0	0	0
			100	60	20	20			
1	N	25	Total	C	N	O	0	0	0
			125	75	25	25			

- Molecule 2 is a protein called Particulate methane monooxygenase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	244	Total	C	N	O	S	0	0	0
			1974	1336	311	316	11			
2	J	244	Total	C	N	O	S	0	0	0
			1974	1336	311	316	11			
2	B	244	Total	C	N	O	S	0	0	0
			1974	1336	311	316	11			

- Molecule 3 is a protein called Particulate methane monooxygenase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	217	Total	C	N	O	S	0	0	0
			1765	1185	279	293	8			
3	C	217	Total	C	N	O	S	0	0	0
			1765	1185	279	293	8			
3	G	213	Total	C	N	O	S	0	0	0
			1738	1168	274	288	8			

- Molecule 4 is a protein called Particulate methane monooxygenase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	390	Total	C	N	O	S	0	0	0
			3038	1952	523	559	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	390	Total	C	N	O	S	0	0	0
			3038	1952	523	559	4			
4	I	390	Total	C	N	O	S	0	0	0
			3038	1952	523	559	4			

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

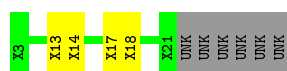
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Cu	0	0
			1	1		
5	K	1	Total	Cu	0	0
			1	1		
5	E	1	Total	Cu	0	0
			1	1		
5	I	1	Total	Cu	0	0
			1	1		
5	C	1	Total	Cu	0	0
			1	1		
5	A	1	Total	Cu	0	0
			1	1		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: unknown peptide

Chain D: 



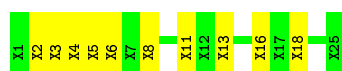
- Molecule 1: unknown peptide

Chain H: 



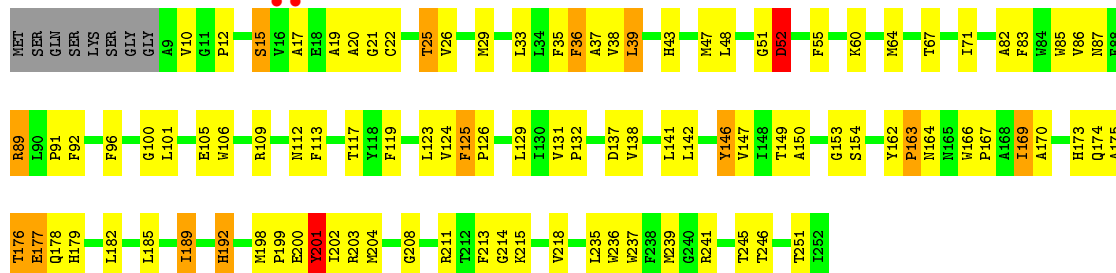
- Molecule 1: unknown peptide

Chain N: 



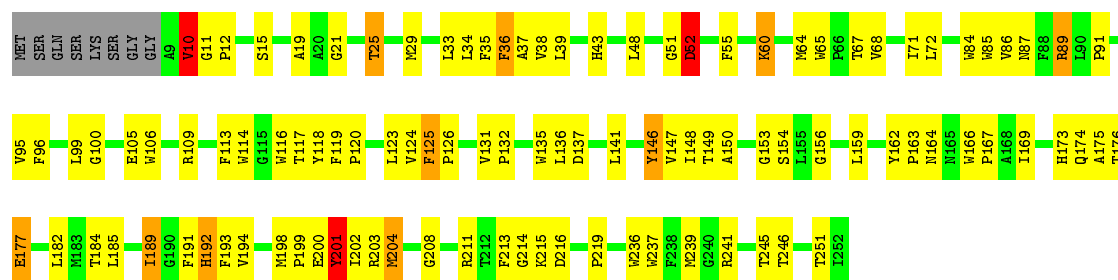
- Molecule 2: Particulate methane monooxygenase subunit A

Chain F: 

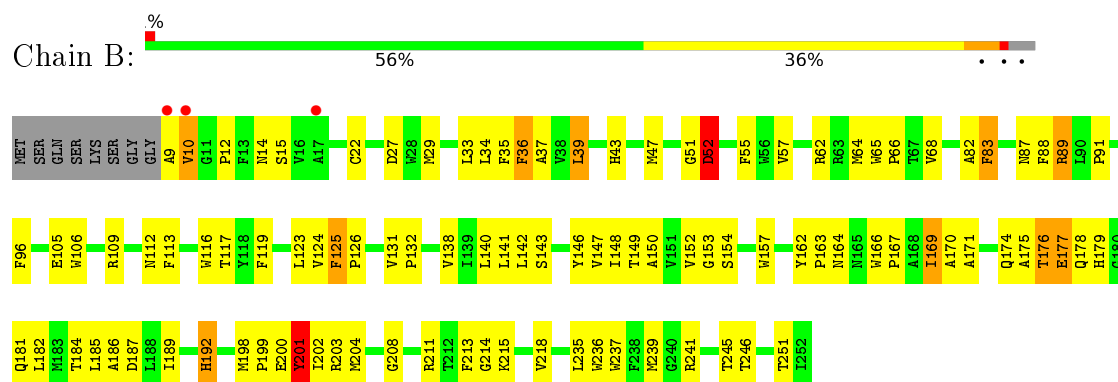


- Molecule 2: Particulate methane monooxygenase subunit A

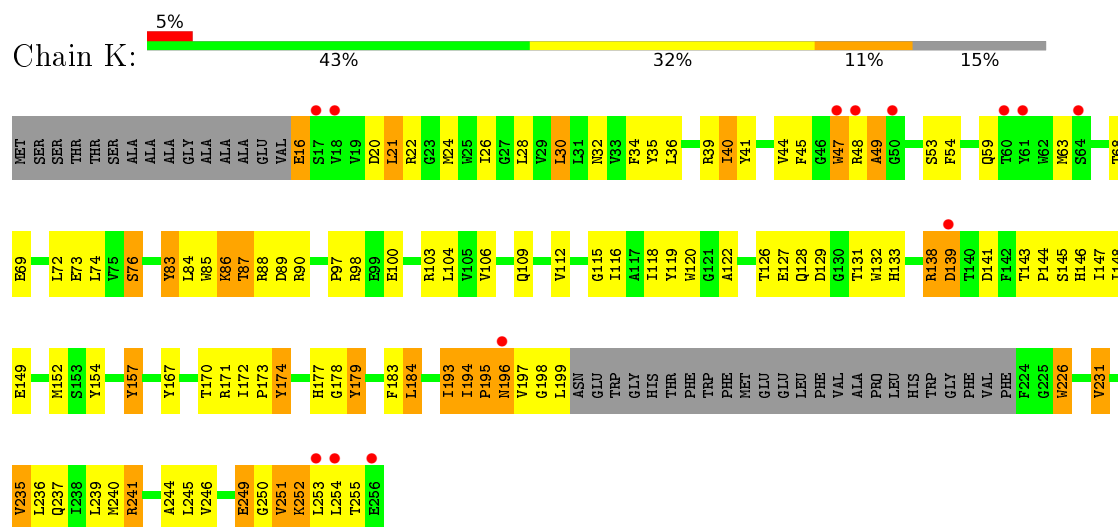
Chain J: 



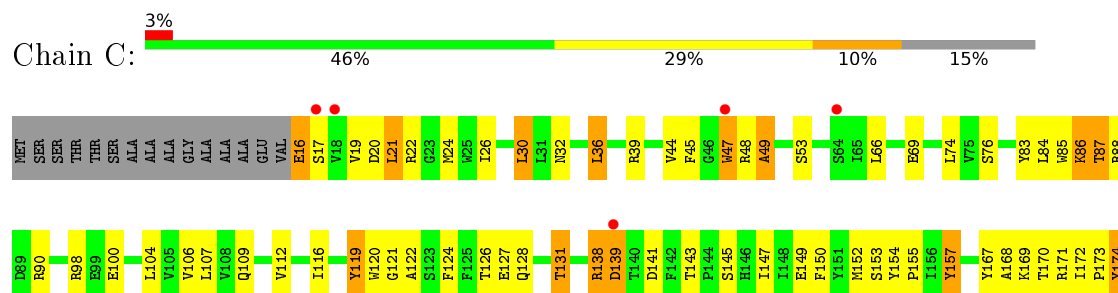
• Molecule 2: Particulate methane monooxygenase subunit A

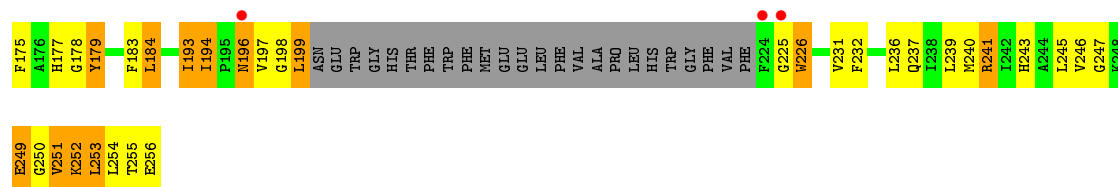


• Molecule 3: Particulate methane monooxygenase subunit C

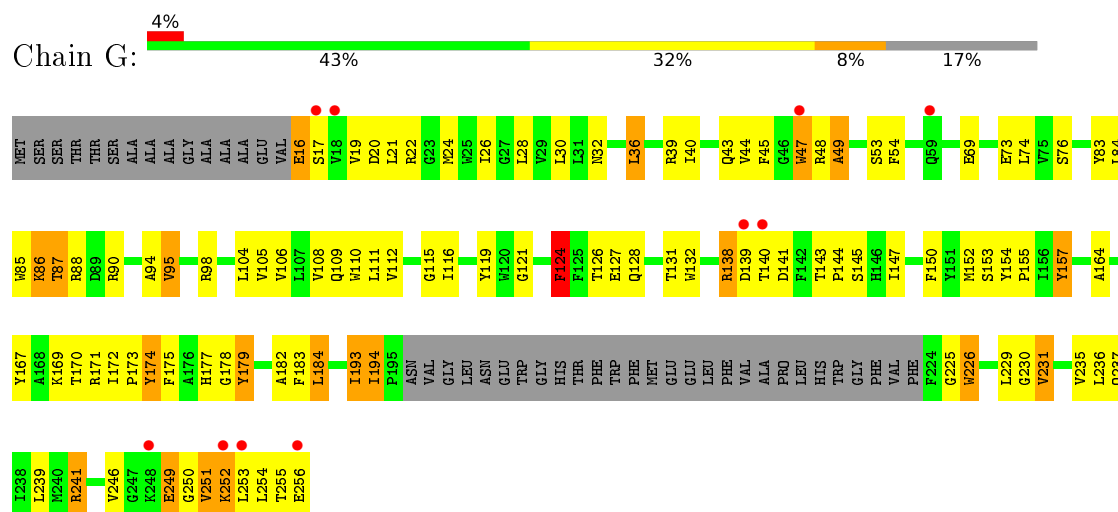


• Molecule 3: Particulate methane monooxygenase subunit C

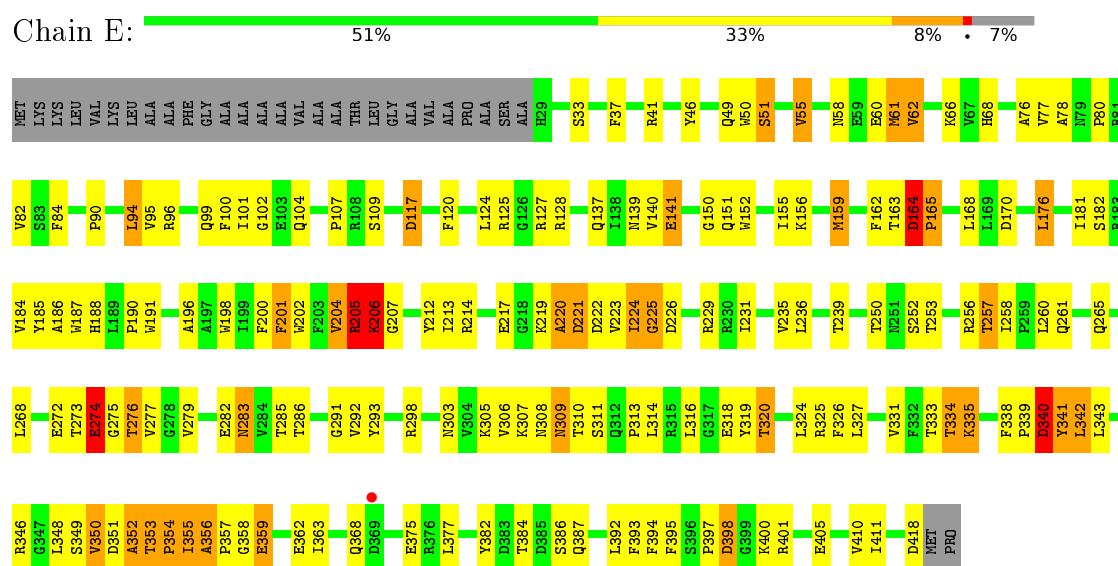




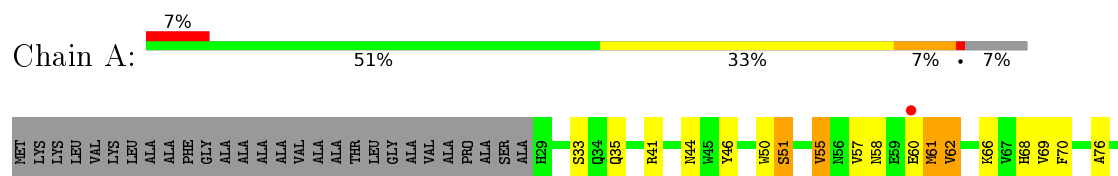
• Molecule 3: Particulate methane monooxygenase subunit C

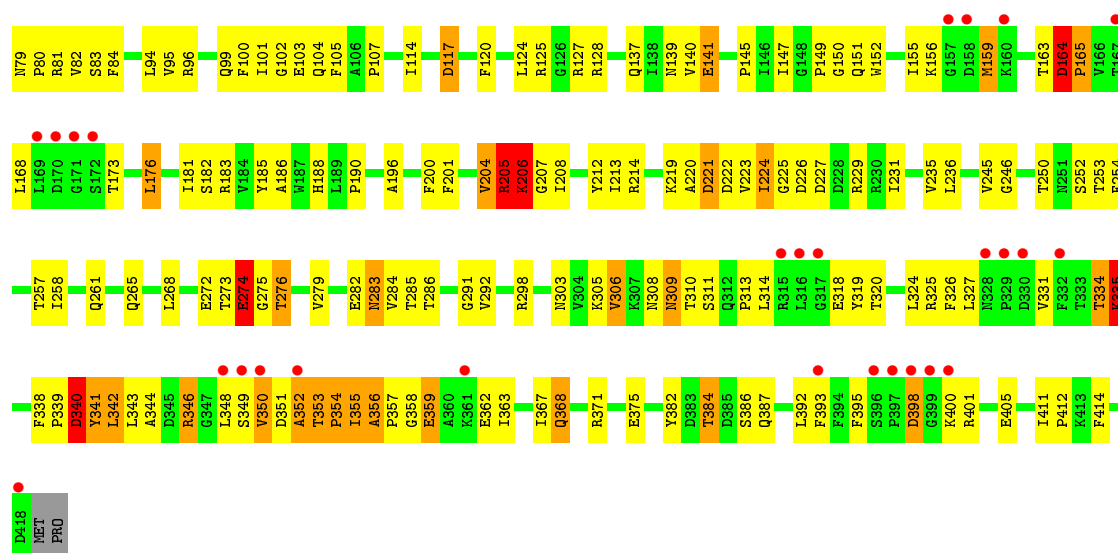


• Molecule 4: Particulate methane monooxygenase subunit B

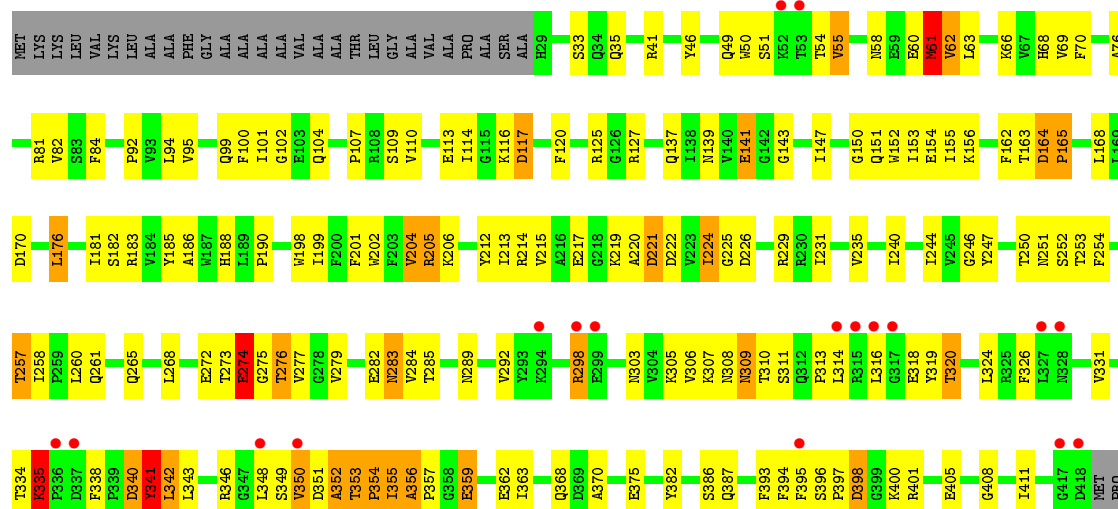


• Molecule 4: Particulate methane monooxygenase subunit B





• Molecule 4: Particulate methane monooxygenase subunit B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.36Å 184.74Å 188.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.15 49.52 – 3.15	Depositor EDS
% Data completeness (in resolution range)	78.2 (50.00-3.15) 78.5 (49.52-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.221 , 0.280 0.221 , 0.279	Depositor DCC
R_{free} test set	2796 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.2	EDS
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 55807 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	20630	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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
2	B	0.64	0/2052	0.79	0/2814
2	F	0.75	1/2052 (0.0%)	0.84	0/2814
2	J	0.74	0/2052	0.86	0/2814
3	C	0.61	2/1820 (0.1%)	0.75	1/2481 (0.0%)
3	G	0.65	2/1793 (0.1%)	0.78	1/2444 (0.0%)
3	K	0.67	0/1820	0.82	1/2481 (0.0%)
4	A	0.60	0/3115	0.80	0/4243
4	E	0.67	0/3115	0.83	0/4243
4	I	0.60	0/3115	0.81	0/4243
All	All	0.66	5/20934 (0.0%)	0.81	3/28577 (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
4	A	0	2
4	E	0	3
4	I	0	2
All	All	0	7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	119	TYR	CE1-CZ	-6.83	1.29	1.38
3	C	119	TYR	CG-CD2	-6.31	1.30	1.39
3	G	119	TYR	CG-CD1	-5.63	1.31	1.39
3	C	119	TYR	CE1-CZ	-5.62	1.31	1.38
2	F	83	PHE	CG-CD1	-5.54	1.30	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	229	LEU	CA-CB-CG	5.37	127.65	115.30
3	K	199	LEU	CA-CB-CG	5.14	127.13	115.30
3	C	199	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	340	ASP	Peptide
4	A	341	TYR	Peptide
4	E	333	THR	Peptide
4	E	340	ASP	Peptide
4	E	341	TYR	Peptide
4	I	340	ASP	Peptide
4	I	341	TYR	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	D	95	0	22	4	0
1	H	100	0	23	3	0
1	N	125	0	27	7	0
2	B	1974	0	1932	116	0
2	F	1974	0	1932	110	0
2	J	1974	0	1932	115	0
3	C	1765	0	1772	94	0
3	G	1738	0	1743	91	0
3	K	1765	0	1772	103	0
4	A	3038	0	3022	182	0
4	E	3038	0	3022	178	0
4	I	3038	0	3022	160	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	1	0	0	0	0
5	K	1	0	0	0	0
All	All	20630	0	20221	1032	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 25.

All (1032) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:51:GLY:CA	2:F:52:ASP:HB2	1.63	1.26
2:J:51:GLY:CA	2:J:52:ASP:HB2	1.72	1.16
2:B:51:GLY:CA	2:B:52:ASP:HB2	1.76	1.15
2:J:146:TYR:HD2	2:J:237:TRP:CE2	1.63	1.15
4:E:352:ALA:O	4:E:354:PRO:HD3	1.46	1.13
2:F:51:GLY:HA3	2:F:52:ASP:CB	1.71	1.11
2:B:51:GLY:HA3	2:B:52:ASP:HB2	1.13	1.10
2:J:51:GLY:HA3	2:J:52:ASP:CB	1.79	1.10
4:E:334:THR:HA	4:E:335:LYS:HB2	1.15	1.10
4:A:334:THR:HA	4:A:335:LYS:HB2	1.13	1.10
4:I:334:THR:HA	4:I:335:LYS:HB2	1.08	1.07
2:B:51:GLY:HA3	2:B:52:ASP:CB	1.80	1.06
2:J:200:GLU:HG2	2:J:203:ARG:HD2	1.37	1.06
4:A:352:ALA:O	4:A:354:PRO:HD3	1.54	1.04
4:I:352:ALA:O	4:I:354:PRO:HD3	1.55	1.03
2:F:51:GLY:HA3	2:F:52:ASP:HB2	1.08	1.03
2:F:200:GLU:HG2	2:F:203:ARG:HD2	1.41	1.03
3:K:104:LEU:HD23	3:K:172:ILE:HD13	1.37	1.02
4:E:356:ALA:HB1	4:E:357:PRO:CA	1.90	1.02
4:A:356:ALA:HB1	4:A:357:PRO:C	1.77	1.02
3:C:104:LEU:HD23	3:C:172:ILE:HD13	1.41	1.02
4:E:275:GLY:HA2	4:E:276:THR:HB	1.41	1.01
4:I:334:THR:CA	4:I:335:LYS:HB2	1.90	1.00
4:I:220:ALA:O	4:I:222:ASP:N	1.93	1.00
2:B:200:GLU:HG2	2:B:203:ARG:HD2	1.43	0.99
4:A:356:ALA:HB1	4:A:357:PRO:CA	1.92	0.98
2:J:51:GLY:HA3	2:J:52:ASP:HB2	1.01	0.98
4:E:356:ALA:HB1	4:E:357:PRO:C	1.84	0.97
4:I:356:ALA:HB1	4:I:357:PRO:CA	1.95	0.96
3:G:246:VAL:HG11	3:G:250:GLY:HA3	1.48	0.96
4:E:308:ASN:HA	4:E:309:ASN:HB2	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:334:THR:CA	4:E:335:LYS:HB2	1.95	0.95
4:I:356:ALA:HB1	4:I:357:PRO:C	1.87	0.95
4:A:308:ASN:HA	4:A:309:ASN:HB2	1.49	0.94
4:E:350:VAL:HG12	4:E:351:ASP:H	1.32	0.94
4:A:334:THR:CA	4:A:335:LYS:HB2	1.97	0.94
4:I:331:VAL:HG11	4:I:395:PHE:HD2	1.30	0.93
2:F:213:PHE:HD1	4:A:33:SER:HG	0.95	0.93
2:J:146:TYR:CD2	2:J:237:TRP:CE2	2.56	0.92
4:I:58:ASN:HD21	4:I:163:THR:H	1.15	0.92
4:A:219:LYS:HA	4:A:220:ALA:HB3	1.51	0.92
3:G:246:VAL:CG1	3:G:250:GLY:HA3	1.99	0.92
4:I:308:ASN:HA	4:I:309:ASN:HB2	1.49	0.92
4:E:58:ASN:HD21	4:E:163:THR:H	1.08	0.92
3:K:83:TYR:O	3:K:83:TYR:HD1	1.51	0.91
4:A:188:HIS:HD2	2:B:106:TRP:HE1	1.19	0.90
4:I:58:ASN:HD22	4:I:125:ARG:NH2	1.69	0.90
4:I:58:ASN:HD22	4:I:125:ARG:HH21	1.18	0.90
4:E:382:TYR:CD1	2:J:215:LYS:HE3	2.07	0.90
4:A:350:VAL:HG12	4:A:351:ASP:H	1.34	0.89
2:J:146:TYR:CE1	2:J:147:VAL:HG23	2.07	0.89
2:J:146:TYR:HD1	2:J:147:VAL:N	1.70	0.89
4:A:58:ASN:HD21	4:A:163:THR:H	1.14	0.88
4:I:60:GLU:HG3	4:I:60:GLU:O	1.71	0.88
4:A:58:ASN:HD22	4:A:125:ARG:HH21	1.18	0.88
4:I:219:LYS:HA	4:I:220:ALA:HB3	1.56	0.88
4:A:100:PHE:HD1	4:A:105:PHE:HA	1.38	0.87
3:C:246:VAL:HG11	3:C:250:GLY:HA3	1.53	0.86
4:I:350:VAL:HG12	4:I:351:ASP:H	1.39	0.86
4:I:276:THR:HG22	4:I:279:VAL:HB	1.57	0.86
4:E:219:LYS:HA	4:E:220:ALA:HB3	1.58	0.86
4:I:275:GLY:HA2	4:I:276:THR:HB	1.58	0.86
4:A:220:ALA:O	4:A:222:ASP:N	2.09	0.85
3:G:104:LEU:HD23	3:G:172:ILE:HD13	1.58	0.85
2:F:106:TRP:HE1	4:E:188:HIS:HD2	1.22	0.85
4:E:356:ALA:HB1	4:E:357:PRO:HA	1.56	0.85
4:I:334:THR:HA	4:I:335:LYS:CB	2.03	0.85
3:K:44:VAL:HG12	3:K:45:PHE:CD1	2.11	0.85
4:E:331:VAL:HG11	4:E:395:PHE:HD2	1.42	0.84
4:E:137:GLN:HE21	4:E:139:ASN:HD21	1.25	0.84
4:A:137:GLN:HE21	4:A:139:ASN:HD21	1.25	0.84
3:C:83:TYR:HE1	3:C:87:THR:HG21	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:356:ALA:HB1	4:I:357:PRO:HA	1.60	0.83
4:A:324:LEU:HD11	4:A:375:GLU:HG3	1.60	0.83
3:C:246:VAL:CG1	3:C:250:GLY:HA3	2.07	0.83
4:I:324:LEU:HD11	4:I:375:GLU:HG3	1.60	0.83
2:J:146:TYR:CD2	2:J:237:TRP:NE1	2.46	0.83
4:A:275:GLY:HA2	4:A:276:THR:HB	1.59	0.83
2:J:146:TYR:HD2	2:J:237:TRP:NE1	1.76	0.83
4:E:220:ALA:O	4:E:222:ASP:N	2.10	0.83
3:G:138:ARG:HH12	3:G:141:ASP:HA	1.43	0.83
4:E:33:SER:HG	2:J:213:PHE:HD1	1.25	0.83
4:A:188:HIS:CD2	2:B:106:TRP:HE1	1.97	0.82
4:E:276:THR:HG22	4:E:279:VAL:HB	1.59	0.82
4:E:356:ALA:CB	4:E:357:PRO:CA	2.57	0.82
3:K:246:VAL:HG11	3:K:250:GLY:HA3	1.61	0.82
4:I:231:ILE:O	4:I:235:VAL:HG23	1.80	0.82
4:E:324:LEU:HD11	4:E:375:GLU:HG3	1.62	0.81
4:E:60:GLU:O	4:E:60:GLU:HG3	1.77	0.81
3:K:83:TYR:C	3:K:83:TYR:HD1	1.81	0.81
4:A:219:LYS:HD3	4:A:220:ALA:HB3	1.61	0.81
2:J:146:TYR:HD1	2:J:147:VAL:H	1.25	0.81
4:E:308:ASN:CA	4:E:309:ASN:HB2	2.12	0.80
3:C:26:ILE:O	3:C:30:LEU:HB2	1.81	0.80
2:F:177:GLU:HG3	4:A:411:ILE:HG12	1.62	0.80
3:K:83:TYR:C	3:K:83:TYR:CD1	2.52	0.80
3:K:246:VAL:CG1	3:K:250:GLY:HA3	2.11	0.80
4:E:308:ASN:ND2	4:E:356:ALA:HB3	1.97	0.80
4:A:231:ILE:O	4:A:235:VAL:HG23	1.82	0.80
4:I:219:LYS:HD3	4:I:220:ALA:HB3	1.63	0.80
4:E:356:ALA:CB	4:E:357:PRO:HA	2.13	0.79
4:I:188:HIS:HD2	2:J:106:TRP:HE1	1.28	0.79
2:J:146:TYR:HE1	2:J:147:VAL:HG23	1.47	0.79
4:A:58:ASN:HD22	4:A:125:ARG:NH2	1.80	0.78
3:K:26:ILE:O	3:K:30:LEU:HB2	1.83	0.78
4:A:356:ALA:HB1	4:A:357:PRO:HA	1.63	0.78
2:F:51:GLY:HA2	2:F:52:ASP:HB2	1.64	0.78
3:G:85:TRP:O	3:G:88:ARG:HB3	1.84	0.78
4:A:356:ALA:CB	4:A:357:PRO:CA	2.61	0.77
2:B:185:LEU:O	2:B:189:ILE:HD12	1.84	0.77
2:J:200:GLU:O	2:J:201:TYR:HB3	1.83	0.77
2:F:106:TRP:HE1	4:E:188:HIS:CD2	2.03	0.77
3:G:86:LYS:HE3	3:G:86:LYS:HA	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:137:GLN:HE21	4:I:139:ASN:HD21	1.31	0.77
4:A:308:ASN:CA	4:A:309:ASN:HB2	2.15	0.76
3:K:138:ARG:HH12	3:K:141:ASP:HA	1.50	0.76
4:A:60:GLU:O	4:A:60:GLU:HG3	1.85	0.76
4:E:231:ILE:O	4:E:235:VAL:HG23	1.86	0.76
3:G:53:SER:OG	3:G:139:ASP:HB3	1.85	0.76
3:K:83:TYR:HE1	3:K:87:THR:HG21	1.50	0.76
3:C:86:LYS:HE3	3:C:86:LYS:HA	1.68	0.75
4:I:58:ASN:ND2	4:I:125:ARG:HH21	1.84	0.75
3:C:83:TYR:CE1	3:C:87:THR:HG21	2.22	0.75
3:C:138:ARG:HH12	3:C:141:ASP:HA	1.52	0.74
4:E:58:ASN:HD22	4:E:125:ARG:HH21	1.32	0.74
4:A:308:ASN:ND2	4:A:356:ALA:HB3	2.03	0.74
4:A:276:THR:HG22	4:A:279:VAL:HB	1.69	0.74
2:J:200:GLU:HG2	2:J:203:ARG:CD	2.17	0.74
3:K:69:GLU:OE1	3:K:152:MET:HG3	1.87	0.74
4:A:334:THR:HA	4:A:335:LYS:CB	2.06	0.73
2:B:198:MET:HG3	2:B:198:MET:O	1.86	0.73
3:K:197:VAL:HG22	3:K:198:GLY:H	1.52	0.73
4:E:164:ASP:CB	4:E:165:PRO:HA	2.17	0.73
3:K:122:ALA:O	3:K:126:THR:HB	1.89	0.73
4:E:320:THR:HG22	4:E:324:LEU:O	1.89	0.73
4:I:341:TYR:CZ	4:I:342:LEU:HD22	2.23	0.72
2:B:201:TYR:HE1	2:B:202:ILE:HD13	1.54	0.72
3:C:44:VAL:HG12	3:C:45:PHE:CD1	2.24	0.72
2:F:213:PHE:HD1	4:A:33:SER:OG	1.70	0.72
2:J:146:TYR:CD1	2:J:147:VAL:N	2.54	0.72
3:G:44:VAL:HG12	3:G:45:PHE:CD1	2.25	0.72
3:G:83:TYR:CE1	3:G:87:THR:HG21	2.24	0.72
4:I:308:ASN:CA	4:I:309:ASN:HB2	2.20	0.72
4:E:331:VAL:HG11	4:E:395:PHE:CD2	2.25	0.72
4:I:356:ALA:CB	4:I:357:PRO:CA	2.66	0.72
2:B:200:GLU:HG2	2:B:203:ARG:CD	2.20	0.72
2:F:198:MET:HG3	2:F:198:MET:O	1.90	0.72
4:A:356:ALA:CB	4:A:357:PRO:HA	2.20	0.72
2:F:185:LEU:O	2:F:189:ILE:HD12	1.89	0.71
3:C:85:TRP:O	3:C:88:ARG:HB3	1.91	0.71
4:I:188:HIS:CD2	2:J:106:TRP:HE1	2.09	0.71
3:C:194:ILE:H	3:C:194:ILE:HD13	1.54	0.71
3:K:86:LYS:HE3	3:K:86:LYS:HA	1.72	0.70
3:C:109:GLN:HG3	2:B:29:MET:CE	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:224:ILE:HG22	4:E:225:GLY:N	2.07	0.70
4:E:58:ASN:HD22	4:E:125:ARG:NH2	1.90	0.70
2:B:125:PHE:HD1	2:B:125:PHE:H	1.37	0.69
2:F:215:LYS:HE3	4:A:382:TYR:CD1	2.27	0.69
2:J:198:MET:O	2:J:198:MET:HG3	1.91	0.69
3:K:83:TYR:CE1	3:K:87:THR:HG21	2.27	0.69
2:B:174:GLN:HB2	2:B:185:LEU:HD12	1.74	0.69
4:A:224:ILE:HG22	4:A:225:GLY:N	2.06	0.69
4:A:341:TYR:H	4:A:342:LEU:CB	2.06	0.69
3:C:225:GLY:O	3:C:226:TRP:HE3	1.76	0.69
4:A:283:ASN:O	4:A:309:ASN:HB3	1.93	0.68
4:E:96:ARG:HH21	4:E:99:GLN:NE2	1.89	0.68
2:F:200:GLU:O	2:F:201:TYR:HB3	1.93	0.68
4:I:311:SER:HA	4:I:357:PRO:HB3	1.74	0.68
4:E:353:THR:O	4:E:355:ILE:N	2.26	0.68
4:I:331:VAL:HG11	4:I:395:PHE:CD2	2.21	0.68
3:G:138:ARG:NH1	3:G:141:ASP:HA	2.09	0.68
4:I:204:VAL:HG12	4:I:204:VAL:O	1.92	0.68
4:I:341:TYR:CE2	4:I:342:LEU:HD22	2.29	0.68
2:F:201:TYR:C	2:F:201:TYR:HD1	1.96	0.68
2:J:166:TRP:HB3	2:J:167:PRO:HD3	1.76	0.68
2:B:235:LEU:HG	2:B:239:MET:HE2	1.76	0.68
2:F:146:TYR:CD1	2:F:147:VAL:N	2.61	0.68
3:K:143:THR:O	3:K:147:ILE:HG12	1.92	0.68
1:N:3:UNK:C	1:N:5:UNK:N	2.55	0.68
3:C:119:TYR:CD1	3:C:119:TYR:C	2.66	0.67
4:I:168:LEU:HD12	4:I:168:LEU:N	2.09	0.67
4:I:341:TYR:H	4:I:342:LEU:CA	2.07	0.67
3:K:104:LEU:HD23	3:K:172:ILE:CD1	2.22	0.67
4:A:219:LYS:HB3	4:A:220:ALA:O	1.94	0.67
2:J:201:TYR:C	2:J:201:TYR:HD1	1.97	0.67
3:G:143:THR:O	3:G:147:ILE:HG12	1.94	0.67
4:I:356:ALA:CB	4:I:357:PRO:HA	2.24	0.67
4:E:283:ASN:O	4:E:309:ASN:HB3	1.94	0.67
2:F:146:TYR:HD1	2:F:147:VAL:N	1.92	0.67
2:B:35:PHE:HA	2:B:96:PHE:CZ	2.29	0.67
2:F:175:ALA:HB1	2:F:182:LEU:HD11	1.77	0.67
3:G:45:PHE:O	3:G:49:ALA:HB3	1.95	0.67
4:I:274:GLU:N	4:I:275:GLY:HA2	2.09	0.67
4:E:311:SER:HA	4:E:357:PRO:HB3	1.77	0.67
4:E:341:TYR:H	4:E:342:LEU:CA	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:382:TYR:CD1	2:B:215:LYS:HE3	2.29	0.66
3:K:194:ILE:HD13	3:K:194:ILE:N	2.10	0.66
4:E:260:LEU:O	4:A:384:THR:HG22	1.95	0.66
2:F:10:VAL:HG21	3:G:254:LEU:HD11	1.77	0.66
4:I:338:PHE:HB3	4:I:343:LEU:HD22	1.77	0.66
3:K:194:ILE:HD13	3:K:194:ILE:H	1.60	0.66
3:C:193:ILE:HG13	3:C:194:ILE:HD13	1.77	0.66
3:C:194:ILE:N	3:C:194:ILE:HD13	2.10	0.66
4:E:164:ASP:HB3	4:E:165:PRO:CA	2.26	0.66
4:E:219:LYS:HB3	4:E:220:ALA:O	1.95	0.66
3:G:225:GLY:O	3:G:226:TRP:HE3	1.78	0.66
2:J:120:PRO:HG3	2:J:193:PHE:CE2	2.31	0.66
2:F:146:TYR:CD2	2:F:237:TRP:CE2	2.83	0.66
4:A:164:ASP:CB	4:A:165:PRO:HA	2.26	0.66
4:A:186:ALA:O	4:A:190:PRO:HG2	1.94	0.66
3:C:53:SER:OG	3:C:139:ASP:HB3	1.95	0.66
4:E:164:ASP:HB3	4:E:165:PRO:HA	1.76	0.65
3:G:26:ILE:O	3:G:30:LEU:HB2	1.96	0.65
3:K:83:TYR:HE1	3:K:87:THR:CG2	2.08	0.65
4:E:101:ILE:HG13	4:E:120:PHE:HB3	1.79	0.65
2:F:201:TYR:CD1	2:F:201:TYR:C	2.70	0.65
2:F:246:THR:HG22	3:G:237:GLN:HG3	1.78	0.65
4:A:356:ALA:HA	4:A:359:GLU:HB2	1.78	0.65
4:E:204:VAL:HG12	4:E:204:VAL:O	1.97	0.65
4:E:261:GLN:HE22	4:A:386:SER:H	1.42	0.65
2:J:201:TYR:C	2:J:201:TYR:CD1	2.70	0.65
3:K:241:ARG:HA	3:K:241:ARG:HE	1.62	0.65
3:C:109:GLN:HG3	2:B:29:MET:HE3	1.79	0.65
4:A:100:PHE:CD1	4:A:105:PHE:HA	2.29	0.65
2:F:235:LEU:HG	2:F:239:MET:HE2	1.77	0.65
4:I:164:ASP:CB	4:I:165:PRO:HA	2.27	0.65
4:E:219:LYS:HD3	4:E:220:ALA:HB3	1.78	0.65
4:I:219:LYS:HD2	4:I:221:ASP:HB2	1.77	0.65
4:A:363:ILE:O	4:A:363:ILE:HG13	1.96	0.64
3:C:83:TYR:HE1	3:C:87:THR:CG2	2.10	0.64
2:J:146:TYR:CD1	2:J:147:VAL:HG23	2.32	0.64
4:A:311:SER:HA	4:A:357:PRO:HB3	1.78	0.64
2:B:150:ALA:O	2:B:154:SER:OG	2.14	0.64
4:I:33:SER:HG	2:B:213:PHE:HD1	1.46	0.64
4:I:341:TYR:CG	4:I:342:LEU:HB2	2.32	0.64
2:J:175:ALA:HB1	2:J:182:LEU:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:200:GLU:O	2:J:201:TYR:CB	2.45	0.63
2:B:36:PHE:HB3	2:B:39:LEU:HB3	1.80	0.63
3:G:24:MET:HB2	3:G:109:GLN:HG2	1.78	0.63
2:J:203:ARG:O	2:J:204:MET:HB2	1.98	0.63
3:C:128:GLN:HG3	2:B:112:ASN:CG	2.18	0.63
2:B:83:PHE:CD1	2:B:83:PHE:C	2.72	0.63
4:A:212:TYR:CD2	3:C:239:LEU:HD22	2.33	0.63
2:F:10:VAL:O	2:F:10:VAL:HG12	1.98	0.63
2:F:125:PHE:H	2:F:125:PHE:HD1	1.44	0.63
2:F:146:TYR:HD2	2:F:237:TRP:CZ2	2.16	0.63
1:N:2:UNK:O	1:N:4:UNK:N	2.31	0.63
4:A:94:LEU:HD22	4:A:124:LEU:HB3	1.80	0.63
2:B:203:ARG:O	2:B:204:MET:HB2	1.98	0.63
4:A:219:LYS:HA	4:A:220:ALA:CB	2.27	0.63
3:C:24:MET:HB2	3:C:109:GLN:HG2	1.80	0.63
4:A:58:ASN:ND2	4:A:125:ARG:HH21	1.93	0.63
2:B:64:MET:HG3	2:B:204:MET:O	1.99	0.63
2:F:91:PRO:HB3	2:F:141:LEU:HD13	1.80	0.63
3:G:226:TRP:CE3	3:G:226:TRP:HA	2.34	0.63
2:B:119:PHE:HB3	2:B:123:LEU:HD23	1.79	0.63
4:A:261:GLN:HE22	4:I:386:SER:H	1.45	0.63
4:A:101:ILE:HG13	4:A:120:PHE:HB3	1.79	0.62
4:A:82:VAL:HB	4:A:141:GLU:HB2	1.80	0.62
4:I:51:SER:CB	4:I:62:VAL:H	2.12	0.62
3:C:154:TYR:HD1	3:C:157:TYR:HE2	1.47	0.62
4:I:308:ASN:ND2	4:I:356:ALA:HB3	2.13	0.62
4:A:204:VAL:O	4:A:204:VAL:HG12	2.00	0.62
2:B:91:PRO:HB3	2:B:141:LEU:HD13	1.80	0.62
4:E:51:SER:HB3	4:E:62:VAL:H	1.64	0.62
3:C:251:VAL:HG12	3:C:252:LYS:N	2.14	0.62
3:G:39:ARG:HH22	3:G:43:GLN:HB2	1.64	0.62
4:I:341:TYR:CD1	4:I:342:LEU:HB2	2.35	0.62
3:K:24:MET:HB2	3:K:109:GLN:HG2	1.82	0.62
3:K:44:VAL:HG12	3:K:45:PHE:CE1	2.33	0.62
4:A:273:THR:HA	4:A:274:GLU:CB	2.30	0.62
4:A:212:TYR:CE2	3:C:239:LEU:HB3	2.34	0.62
4:A:224:ILE:HG22	4:A:225:GLY:H	1.64	0.62
4:A:341:TYR:CD1	4:A:342:LEU:HB2	2.35	0.62
4:A:341:TYR:CZ	4:A:342:LEU:HD22	2.35	0.62
2:B:201:TYR:C	2:B:201:TYR:HD1	2.03	0.62
4:I:224:ILE:HG22	4:I:225:GLY:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:16:GLU:N	3:K:16:GLU:OE2	2.33	0.62
4:E:334:THR:HA	4:E:335:LYS:CB	2.09	0.61
4:E:411:ILE:HG12	2:J:177:GLU:HG3	1.81	0.61
3:K:226:TRP:HA	3:K:226:TRP:CE3	2.34	0.61
4:E:341:TYR:CG	4:E:342:LEU:HB2	2.35	0.61
2:J:201:TYR:HE1	2:J:202:ILE:HD13	1.64	0.61
4:I:151:GLN:HE21	4:I:152:TRP:H	1.48	0.61
4:I:51:SER:HB3	4:I:62:VAL:H	1.63	0.61
4:I:164:ASP:OD2	2:J:192:HIS:HD2	1.83	0.61
3:G:249:GLU:O	3:G:253:LEU:HB2	2.00	0.61
3:G:83:TYR:CE1	3:G:87:THR:CG2	2.83	0.61
4:A:273:THR:HA	4:A:274:GLU:CG	2.31	0.61
4:E:55:VAL:HG23	4:E:155:ILE:HG12	1.83	0.61
4:I:168:LEU:CD1	4:I:168:LEU:N	2.64	0.61
4:I:95:VAL:HG23	4:I:127:ARG:HD2	1.82	0.61
2:J:236:TRP:CE2	2:J:239:MET:HE3	2.35	0.61
3:K:47:TRP:CH2	2:J:117:THR:HA	2.35	0.61
4:I:33:SER:OG	2:B:213:PHE:HD1	1.84	0.60
4:A:51:SER:HB3	4:A:62:VAL:H	1.66	0.60
4:A:341:TYR:CG	4:A:342:LEU:HB2	2.36	0.60
4:I:411:ILE:HG12	2:B:177:GLU:HG3	1.82	0.60
4:E:58:ASN:ND2	4:E:125:ARG:HH21	2.00	0.60
4:E:82:VAL:HB	4:E:141:GLU:HB2	1.83	0.60
2:F:150:ALA:O	2:F:154:SER:OG	2.20	0.60
4:E:58:ASN:ND2	4:E:163:THR:H	1.88	0.60
4:E:273:THR:HA	4:E:274:GLU:CB	2.31	0.60
4:I:353:THR:O	4:I:355:ILE:N	2.33	0.60
4:A:151:GLN:HE21	4:A:152:TRP:H	1.50	0.60
4:A:341:TYR:H	4:A:342:LEU:HB3	1.64	0.60
4:A:55:VAL:HG23	4:A:155:ILE:HG12	1.84	0.60
4:E:275:GLY:CA	4:E:276:THR:HB	2.25	0.60
4:A:164:ASP:OD2	2:B:192:HIS:CD2	2.54	0.60
3:G:193:ILE:HG13	3:G:194:ILE:HD13	1.84	0.60
4:I:50:TRP:HD1	4:I:61:MET:HE1	1.66	0.60
4:I:250:THR:HG21	2:J:167:PRO:HA	1.83	0.60
4:E:224:ILE:HG22	4:E:225:GLY:H	1.67	0.59
4:E:363:ILE:HG13	4:E:363:ILE:O	2.01	0.59
2:F:146:TYR:CD1	2:F:146:TYR:C	2.76	0.59
3:G:121:GLY:HA2	3:G:153:SER:OG	2.02	0.59
2:B:201:TYR:C	2:B:201:TYR:CD1	2.75	0.59
3:C:98:ARG:HA	2:B:12:PRO:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:143:THR:O	3:C:147:ILE:HG12	2.02	0.59
3:C:226:TRP:CE3	3:C:226:TRP:HA	2.35	0.59
3:C:83:TYR:CE1	3:C:87:THR:CG2	2.85	0.59
2:F:189:ILE:HG13	4:E:176:LEU:HD13	1.84	0.59
4:A:107:PRO:HD2	4:A:265:GLN:HE22	1.68	0.59
4:A:341:TYR:H	4:A:342:LEU:CA	2.16	0.59
3:K:85:TRP:O	3:K:88:ARG:HB3	2.03	0.59
4:A:250:THR:HG21	2:B:167:PRO:HA	1.84	0.59
2:F:51:GLY:CA	2:F:52:ASP:CB	2.44	0.59
4:I:101:ILE:HG13	4:I:120:PHE:HB3	1.84	0.59
3:C:138:ARG:NH1	3:C:141:ASP:HA	2.17	0.59
2:F:51:GLY:HA3	2:F:52:ASP:HB3	1.80	0.59
2:F:35:PHE:HA	2:F:96:PHE:CZ	2.38	0.59
4:E:219:LYS:HD2	4:E:221:ASP:HB2	1.85	0.59
4:I:219:LYS:HA	4:I:220:ALA:CB	2.30	0.59
4:I:164:ASP:HB3	4:I:165:PRO:HA	1.84	0.59
3:K:195:PRO:O	3:K:196:ASN:C	2.41	0.58
3:C:104:LEU:HD23	3:C:172:ILE:CD1	2.26	0.58
4:I:164:ASP:OD2	2:J:192:HIS:CD2	2.55	0.58
2:F:192:HIS:CD2	4:E:164:ASP:OD2	2.56	0.58
2:F:201:TYR:HE1	2:F:202:ILE:HD13	1.68	0.58
2:F:64:MET:HG3	2:F:204:MET:O	2.02	0.58
3:G:88:ARG:HB2	3:G:170:THR:HB	1.86	0.58
4:E:33:SER:HB3	3:G:54:PHE:HE2	1.68	0.58
4:E:341:TYR:CD1	4:E:342:LEU:HB2	2.37	0.58
3:K:231:VAL:O	3:K:235:VAL:HG13	2.02	0.58
2:B:82:ALA:HB1	2:B:241:ARG:HD2	1.84	0.58
4:E:356:ALA:HA	4:E:359:GLU:HB2	1.85	0.58
2:F:146:TYR:HD1	2:F:146:TYR:C	2.07	0.58
3:G:154:TYR:HD1	3:G:157:TYR:HE2	1.50	0.58
3:K:157:TYR:CD1	3:K:157:TYR:C	2.77	0.58
3:C:237:GLN:HG3	2:B:246:THR:HG22	1.86	0.58
2:F:166:TRP:HB3	2:F:167:PRO:HD3	1.85	0.58
2:J:125:PHE:HD1	2:J:125:PHE:H	1.52	0.58
3:C:48:ARG:O	3:C:49:ALA:HB2	2.04	0.57
4:E:350:VAL:HG12	4:E:351:ASP:N	2.12	0.57
4:A:314:LEU:N	4:A:354:PRO:O	2.36	0.57
3:C:112:VAL:HG22	2:B:33:LEU:HB3	1.85	0.57
4:E:96:ARG:HH21	4:E:99:GLN:HE22	1.50	0.57
4:E:386:SER:H	4:I:261:GLN:HE22	1.50	0.57
2:J:64:MET:HG3	2:J:204:MET:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:241:ARG:HH21	3:K:244:ALA:HB3	1.69	0.57
4:E:341:TYR:H	4:E:342:LEU:CB	2.17	0.57
2:F:29:MET:CE	3:G:109:GLN:HG3	2.34	0.57
3:K:178:GLY:O	3:K:179:TYR:CD2	2.57	0.57
3:K:39:ARG:NH1	2:J:116:TRP:HB2	2.19	0.57
2:F:200:GLU:O	2:F:201:TYR:CB	2.52	0.57
4:A:326:PHE:HD1	4:A:344:ALA:HB3	1.69	0.57
4:E:341:TYR:CZ	4:E:342:LEU:HD22	2.40	0.57
4:E:51:SER:CB	4:E:62:VAL:H	2.18	0.57
4:I:137:GLN:HG3	4:I:147:ILE:HD13	1.86	0.57
4:E:334:THR:CA	4:E:335:LYS:CB	2.76	0.57
2:F:33:LEU:HB3	3:G:112:VAL:HG22	1.86	0.57
3:K:236:LEU:HD11	2:J:87:ASN:ND2	2.20	0.57
4:A:150:GLY:O	4:A:341:TYR:HE2	1.87	0.57
3:C:249:GLU:O	3:C:253:LEU:HB2	2.05	0.57
4:I:313:PRO:HB2	4:I:354:PRO:HB3	1.87	0.57
4:E:313:PRO:HB2	4:E:354:PRO:HB3	1.87	0.57
4:A:236:LEU:HB2	2:B:138:VAL:HG11	1.87	0.56
2:J:33:LEU:O	2:J:37:ALA:HB2	2.05	0.56
4:A:331:VAL:HG11	4:A:395:PHE:CD2	2.39	0.56
4:I:283:ASN:O	4:I:309:ASN:HB3	2.05	0.56
2:J:150:ALA:O	2:J:154:SER:OG	2.22	0.56
4:I:35:GLN:OE1	2:B:208:GLY:HA2	2.06	0.56
4:I:151:GLN:HE21	4:I:152:TRP:N	2.04	0.56
2:J:85:TRP:CE2	2:J:89:ARG:HD3	2.41	0.56
2:F:199:PRO:HB3	4:E:84:PHE:HB3	1.87	0.56
4:A:340:ASP:HB3	4:A:341:TYR:HA	1.86	0.56
4:E:340:ASP:HB3	4:E:341:TYR:HA	1.86	0.56
3:G:170:THR:O	3:G:171:ARG:HD2	2.06	0.56
4:I:274:GLU:H	4:I:275:GLY:HA2	1.70	0.56
3:K:138:ARG:NH1	3:K:141:ASP:HA	2.18	0.56
4:I:273:THR:HA	4:I:274:GLU:CB	2.34	0.56
4:E:76:ALA:HB1	2:J:208:GLY:O	2.05	0.56
3:K:83:TYR:CE1	3:K:87:THR:CG2	2.86	0.56
3:C:178:GLY:O	3:C:179:TYR:CD2	2.59	0.56
3:C:44:VAL:HG12	3:C:45:PHE:CE1	2.41	0.56
4:E:164:ASP:CB	4:E:165:PRO:CA	2.82	0.56
2:F:125:PHE:CZ	2:F:169:ILE:CD1	2.88	0.56
3:K:173:PRO:O	3:K:174:TYR:HB2	2.06	0.56
2:B:33:LEU:O	2:B:37:ALA:HB2	2.05	0.56
2:F:167:PRO:HA	4:E:250:THR:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:47:MET:SD	3:G:126:THR:HG22	2.47	0.56
4:A:338:PHE:HB3	4:A:343:LEU:HD22	1.88	0.55
2:B:214:GLY:HA2	2:B:215:LYS:HB2	1.88	0.55
4:E:226:ASP:H	4:E:229:ARG:NH2	2.04	0.55
4:A:68:HIS:HD2	4:A:117:ASP:OD1	1.89	0.55
2:F:117:THR:HA	3:G:47:TRP:CH2	2.41	0.55
2:J:146:TYR:CE2	2:J:237:TRP:NE1	2.75	0.55
4:A:282:GLU:HB3	4:A:310:THR:HG22	1.88	0.55
4:E:219:LYS:HA	4:E:220:ALA:CB	2.35	0.55
2:F:125:PHE:HZ	2:F:169:ILE:CD1	2.19	0.55
3:K:237:GLN:HG3	2:J:246:THR:HG22	1.88	0.55
4:A:353:THR:O	4:A:355:ILE:N	2.36	0.55
4:E:94:LEU:HD22	4:E:124:LEU:HB3	1.89	0.55
3:K:241:ARG:HH21	3:K:244:ALA:CB	2.20	0.55
3:G:173:PRO:O	3:G:174:TYR:HB2	2.07	0.55
3:C:47:TRP:CH2	2:B:117:THR:HA	2.41	0.55
3:G:44:VAL:HG12	3:G:45:PHE:CE1	2.42	0.55
4:E:282:GLU:HB3	4:E:310:THR:HA	1.89	0.55
4:E:58:ASN:HD21	4:E:163:THR:N	1.90	0.55
4:I:314:LEU:N	4:I:354:PRO:O	2.40	0.55
2:J:174:GLN:HB2	2:J:185:LEU:HD12	1.87	0.55
2:J:36:PHE:HB3	2:J:39:LEU:HB3	1.89	0.55
3:K:251:VAL:HG12	3:K:252:LYS:N	2.21	0.55
2:F:200:GLU:HG2	2:F:203:ARG:CD	2.28	0.54
3:K:254:LEU:HD11	2:J:10:VAL:HG11	1.89	0.54
4:E:273:THR:HA	4:E:274:GLU:CG	2.37	0.54
2:F:87:ASN:ND2	3:G:236:LEU:HD11	2.22	0.54
3:G:246:VAL:HG12	3:G:250:GLY:HA3	1.84	0.54
4:E:33:SER:OG	2:J:213:PHE:HD1	1.89	0.54
3:K:129:ASP:O	3:K:133:HIS:CD2	2.60	0.54
3:K:154:TYR:HD1	3:K:157:TYR:HE2	1.54	0.54
4:A:96:ARG:HH21	4:A:99:GLN:NE2	2.04	0.54
4:E:68:HIS:HD2	4:E:117:ASP:OD1	1.89	0.54
2:F:138:VAL:HG11	4:E:236:LEU:HB2	1.88	0.54
4:E:95:VAL:HG21	4:E:162:PHE:CZ	2.43	0.54
4:I:350:VAL:HG12	4:I:351:ASP:N	2.17	0.54
4:A:164:ASP:CB	4:A:165:PRO:CA	2.85	0.54
4:A:214:ARG:HD3	4:A:222:ASP:HB2	1.88	0.54
4:I:204:VAL:O	4:I:204:VAL:CG1	2.56	0.54
4:I:348:LEU:HB2	4:I:349:SER:HB2	1.89	0.54
4:I:84:PHE:HB3	2:J:199:PRO:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:164:ASP:HB3	4:A:165:PRO:CA	2.37	0.54
4:A:313:PRO:HB2	4:A:354:PRO:CB	2.37	0.54
2:B:43:HIS:HE2	2:B:105:GLU:HG2	1.72	0.54
4:I:164:ASP:HB3	4:I:165:PRO:CA	2.38	0.54
4:I:68:HIS:HD2	4:I:117:ASP:OD1	1.90	0.54
2:J:185:LEU:O	2:J:189:ILE:HD12	2.08	0.54
3:K:178:GLY:O	3:K:179:TYR:CG	2.61	0.54
2:B:162:TYR:HB3	2:B:163:PRO:HD3	1.90	0.54
2:B:200:GLU:O	2:B:201:TYR:HB3	2.08	0.54
3:G:84:LEU:HD22	3:G:167:TYR:HA	1.90	0.54
1:N:5:UNK:O	1:N:6:UNK:O	2.25	0.54
4:E:350:VAL:CG1	4:E:351:ASP:H	2.12	0.54
4:E:212:TYR:CE2	3:G:239:LEU:HB3	2.43	0.54
4:I:313:PRO:HB2	4:I:354:PRO:CB	2.38	0.54
4:I:46:TYR:CE2	4:I:66:LYS:HD2	2.43	0.54
4:A:181:ILE:HG22	4:A:185:TYR:CE2	2.43	0.53
2:F:12:PRO:HB2	3:G:98:ARG:HA	1.90	0.53
4:A:168:LEU:HD12	4:A:168:LEU:N	2.22	0.53
2:B:201:TYR:CE1	2:B:202:ILE:HD13	2.38	0.53
2:B:36:PHE:O	2:B:36:PHE:HD1	1.90	0.53
4:A:102:GLY:HA3	4:A:268:LEU:HB3	1.90	0.53
3:C:150:PHE:O	3:C:155:PRO:HD3	2.07	0.53
3:C:173:PRO:O	3:C:174:TYR:HB2	2.08	0.53
4:I:331:VAL:CG1	4:I:395:PHE:HD2	2.12	0.53
2:B:201:TYR:HD1	2:B:202:ILE:N	2.06	0.53
3:C:16:GLU:OE2	3:C:16:GLU:N	2.41	0.53
3:C:254:LEU:HD11	2:B:10:VAL:HG21	1.91	0.53
4:E:316:LEU:HB2	4:E:394:PHE:CE1	2.43	0.53
2:F:149:THR:O	2:F:153:GLY:HA3	2.09	0.53
4:I:41:ARG:NE	4:I:387:GLN:HG2	2.24	0.53
3:K:20:ASP:O	3:K:21:LEU:HB2	2.09	0.53
4:E:318:GLU:OE2	4:E:325:ARG:HG2	2.07	0.53
2:B:175:ALA:HB1	2:B:182:LEU:HD11	1.90	0.53
4:I:341:TYR:H	4:I:342:LEU:CB	2.21	0.53
4:A:350:VAL:HG12	4:A:351:ASP:N	2.14	0.53
2:F:192:HIS:HD2	4:E:164:ASP:OD2	1.92	0.53
1:H:12:UNK:O	1:H:16:UNK:CB	2.56	0.53
4:I:110:VAL:HG12	4:I:265:GLN:HB2	1.90	0.53
4:E:33:SER:HB3	3:G:54:PHE:CE2	2.44	0.53
3:K:54:PHE:HE2	4:I:33:SER:HB3	1.74	0.53
4:E:382:TYR:HD1	2:J:215:LYS:HE3	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:ARG:HG3	2:B:12:PRO:O	2.09	0.52
2:F:36:PHE:HB3	2:F:39:LEU:HB3	1.90	0.52
3:G:48:ARG:O	3:G:49:ALA:HB2	2.08	0.52
4:I:58:ASN:ND2	4:I:125:ARG:NH2	2.45	0.52
4:I:224:ILE:HG22	4:I:225:GLY:H	1.74	0.52
2:J:146:TYR:CE1	2:J:147:VAL:CG2	2.88	0.52
4:I:226:ASP:H	4:I:229:ARG:NH2	2.06	0.52
4:A:164:ASP:OD2	2:B:192:HIS:HD2	1.93	0.52
2:B:237:TRP:O	2:B:241:ARG:HG2	2.10	0.52
2:F:236:TRP:CD2	2:F:239:MET:HE3	2.43	0.52
4:A:168:LEU:CD1	4:A:168:LEU:N	2.72	0.52
4:I:151:GLN:O	4:I:153:ILE:HG12	2.09	0.52
4:I:356:ALA:HA	4:I:359:GLU:HB2	1.91	0.52
4:E:274:GLU:N	4:E:275:GLY:HA2	2.25	0.52
4:I:82:VAL:HB	4:I:141:GLU:HB2	1.91	0.52
3:K:193:ILE:HG13	3:K:194:ILE:HD13	1.90	0.52
3:C:236:LEU:HD11	2:B:87:ASN:ND2	2.24	0.52
4:A:219:LYS:HD2	4:A:221:ASP:HB2	1.92	0.52
4:E:95:VAL:HG21	4:E:162:PHE:HZ	1.74	0.52
2:F:214:GLY:HA2	2:F:215:LYS:HB2	1.92	0.52
3:K:249:GLU:O	3:K:253:LEU:HB2	2.10	0.52
3:C:109:GLN:HG3	2:B:29:MET:HE1	1.90	0.52
4:E:314:LEU:N	4:E:354:PRO:O	2.42	0.52
4:A:292:VAL:HA	4:A:411:ILE:O	2.10	0.52
2:F:213:PHE:CD1	4:A:33:SER:OG	2.54	0.52
2:J:146:TYR:HE1	2:J:147:VAL:CG2	2.18	0.52
4:A:188:HIS:CD2	2:B:106:TRP:NE1	2.73	0.52
4:A:274:GLU:N	4:A:275:GLY:HA2	2.24	0.52
2:B:200:GLU:CG	2:B:203:ARG:HH11	2.23	0.52
4:E:151:GLN:HE21	4:E:152:TRP:H	1.56	0.52
2:F:162:TYR:HB3	2:F:163:PRO:HD3	1.91	0.52
4:I:92:PRO:O	4:I:127:ARG:HD3	2.10	0.52
4:E:223:VAL:O	4:E:224:ILE:HD13	2.10	0.51
4:E:96:ARG:NH2	4:E:99:GLN:HE22	2.08	0.51
2:F:101:LEU:O	2:F:105:GLU:HG3	2.09	0.51
2:F:119:PHE:HB3	2:F:123:LEU:HD23	1.91	0.51
3:G:150:PHE:O	3:G:155:PRO:HD3	2.10	0.51
3:K:98:ARG:HA	2:J:12:PRO:HB2	1.91	0.51
2:B:36:PHE:O	2:B:36:PHE:CD1	2.62	0.51
3:C:246:VAL:HG12	3:C:250:GLY:HA3	1.91	0.51
4:I:183:ARG:O	4:I:186:ALA:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:285:THR:HB	4:I:307:LYS:HB3	1.93	0.51
4:E:41:ARG:NE	4:E:387:GLN:HG2	2.25	0.51
2:F:174:GLN:HB2	2:F:185:LEU:HD12	1.92	0.51
2:F:112:ASN:CG	3:G:128:GLN:HG3	2.31	0.51
3:G:69:GLU:O	3:G:73:GLU:N	2.32	0.51
4:I:363:ILE:HG13	4:I:363:ILE:O	2.09	0.51
4:A:308:ASN:CG	4:A:356:ALA:HB3	2.31	0.51
2:F:201:TYR:HD1	2:F:202:ILE:N	2.08	0.51
2:F:67:THR:O	2:F:71:ILE:HD12	2.11	0.51
2:B:132:PRO:HB3	2:B:157:TRP:HA	1.93	0.51
2:J:67:THR:O	2:J:71:ILE:HD12	2.10	0.51
4:A:291:GLY:O	4:A:292:VAL:CG2	2.58	0.51
3:C:232:PHE:CD1	2:B:83:PHE:CD2	2.99	0.51
4:E:327:LEU:HD11	4:E:343:LEU:HD11	1.93	0.51
3:G:48:ARG:O	3:G:49:ALA:CB	2.58	0.51
2:F:125:PHE:CZ	2:F:169:ILE:HD11	2.45	0.51
2:F:131:VAL:HB	2:F:132:PRO:HD3	1.93	0.51
2:F:149:THR:O	2:F:153:GLY:CA	2.59	0.51
2:F:36:PHE:O	3:G:115:GLY:O	2.28	0.51
2:F:82:ALA:HB1	2:F:241:ARG:HD2	1.93	0.51
3:K:48:ARG:O	3:K:49:ALA:HB2	2.11	0.51
4:A:348:LEU:HB2	4:A:349:SER:HB2	1.92	0.51
4:A:331:VAL:HG11	4:A:395:PHE:HD2	1.75	0.51
3:C:197:VAL:HG22	3:C:198:GLY:N	2.26	0.51
3:C:48:ARG:O	3:C:49:ALA:CB	2.59	0.51
4:E:168:LEU:N	4:E:168:LEU:HD12	2.27	0.51
3:K:34:PHE:HE2	3:K:152:MET:HE3	1.76	0.51
4:I:313:PRO:HG2	4:I:397:PRO:HD3	1.92	0.50
4:I:260:LEU:HD13	2:J:203:ARG:HH21	1.76	0.50
3:K:86:LYS:CE	3:K:86:LYS:HA	2.36	0.50
4:I:76:ALA:HB1	2:B:208:GLY:O	2.12	0.50
3:C:250:GLY:HA2	3:C:254:LEU:HG	1.93	0.50
4:E:292:VAL:HA	4:E:411:ILE:O	2.11	0.50
2:F:166:TRP:CE2	2:F:170:ALA:HB2	2.46	0.50
4:I:308:ASN:ND2	4:I:314:LEU:HD12	2.25	0.50
4:E:313:PRO:HB2	4:E:354:PRO:CB	2.42	0.50
2:J:135:TRP:NE1	2:J:156:GLY:HA3	2.27	0.50
4:E:382:TYR:CZ	2:J:215:LYS:HA	2.45	0.50
3:K:236:LEU:O	3:K:240:MET:HG3	2.11	0.50
3:C:69:GLU:OE1	3:C:152:MET:HG3	2.12	0.50
4:E:214:ARG:HD3	4:E:222:ASP:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:275:GLY:CA	4:I:276:THR:HB	2.37	0.50
1:N:5:UNK:O	1:N:6:UNK:C	2.59	0.50
4:A:313:PRO:HB2	4:A:354:PRO:HB3	1.93	0.50
4:A:84:PHE:HB3	2:B:199:PRO:HB3	1.93	0.50
2:F:201:TYR:HB3	4:E:109:SER:HB3	1.94	0.50
2:F:43:HIS:HE1	3:G:127:GLU:HB2	1.76	0.50
3:G:86:LYS:C	3:G:88:ARG:H	2.14	0.50
4:I:109:SER:HB3	2:J:201:TYR:HB3	1.93	0.50
2:J:68:VAL:HG23	2:J:72:LEU:HD12	1.92	0.50
2:J:34:LEU:HD13	2:J:84:TRP:CZ2	2.46	0.50
1:N:16:UNK:C	1:N:18:UNK:N	2.75	0.50
4:E:181:ILE:HG22	4:E:185:TYR:CE2	2.47	0.50
4:I:107:PRO:HD2	4:I:265:GLN:HE22	1.76	0.50
3:K:53:SER:OG	3:K:139:ASP:HB3	2.10	0.50
2:B:201:TYR:CD1	2:B:202:ILE:N	2.80	0.50
4:I:141:GLU:OE2	4:I:141:GLU:HA	2.10	0.50
3:K:119:TYR:C	3:K:119:TYR:CD1	2.83	0.50
3:C:241:ARG:HE	3:C:241:ARG:HA	1.76	0.50
3:C:39:ARG:NH1	2:B:116:TRP:HB2	2.27	0.50
4:I:199:ILE:HD11	2:J:95:VAL:HG12	1.93	0.50
4:A:117:ASP:N	4:A:117:ASP:OD1	2.45	0.50
4:A:285:THR:O	4:A:306:VAL:HA	2.11	0.50
2:B:166:TRP:HB3	2:B:167:PRO:HD3	1.94	0.50
3:G:178:GLY:O	3:G:179:TYR:CD2	2.65	0.50
4:I:246:GLY:O	4:I:250:THR:OG1	2.23	0.50
2:J:162:TYR:HB3	2:J:163:PRO:HD3	1.93	0.50
4:E:37:PHE:O	4:E:41:ARG:HG3	2.12	0.49
4:E:68:HIS:HE1	4:E:405:GLU:OE1	1.95	0.49
2:F:146:TYR:HD2	2:F:237:TRP:CE2	2.25	0.49
3:K:154:TYR:HD1	3:K:157:TYR:CE2	2.30	0.49
4:E:275:GLY:HA2	4:E:276:THR:CB	2.28	0.49
4:E:96:ARG:NH2	4:E:99:GLN:NE2	2.59	0.49
4:A:149:PRO:HB3	4:A:342:LEU:HD21	1.94	0.49
4:A:318:GLU:HB3	4:A:393:PHE:HB2	1.94	0.49
4:E:95:VAL:HG23	4:E:127:ARG:HD2	1.94	0.49
4:I:273:THR:HA	4:I:274:GLU:CG	2.42	0.49
4:I:55:VAL:HG23	4:I:155:ILE:HG12	1.94	0.49
4:A:46:TYR:CE2	4:A:66:LYS:HD2	2.48	0.49
3:K:104:LEU:CD2	3:K:172:ILE:HD13	2.25	0.49
4:A:291:GLY:O	4:A:292:VAL:HG23	2.13	0.49
2:B:125:PHE:CD1	2:B:125:PHE:N	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:250:GLY:HA2	3:K:254:LEU:HG	1.94	0.49
3:K:83:TYR:O	3:K:83:TYR:CD1	2.44	0.49
4:A:50:TRP:HB3	4:A:61:MET:HE1	1.94	0.49
3:C:100:GLU:OE1	3:C:245:LEU:HD11	2.12	0.49
4:E:170:ASP:C	4:E:170:ASP:OD1	2.50	0.49
2:F:146:TYR:CE1	2:F:147:VAL:HG23	2.48	0.49
4:I:170:ASP:C	4:I:170:ASP:OD1	2.49	0.49
3:C:154:TYR:HD1	3:C:157:TYR:CE2	2.27	0.49
3:C:86:LYS:C	3:C:88:ARG:H	2.16	0.49
4:E:305:LYS:HD3	4:E:362:GLU:OE1	2.13	0.49
2:J:201:TYR:HD1	2:J:202:ILE:N	2.09	0.49
3:K:167:TYR:CE1	3:K:171:ARG:HG2	2.48	0.49
4:I:257:THR:HA	2:J:173:HIS:O	2.13	0.49
4:I:334:THR:CA	4:I:335:LYS:CB	2.71	0.49
2:B:55:PHE:O	2:B:124:VAL:HA	2.13	0.49
3:C:66:LEU:HD13	3:C:147:ILE:HD13	1.95	0.49
2:J:131:VAL:HB	2:J:132:PRO:HD3	1.94	0.49
2:J:200:GLU:CG	2:J:203:ARG:HH11	2.25	0.49
3:K:106:VAL:O	3:K:109:GLN:HB2	2.13	0.49
2:B:178:GLN:O	2:B:179:HIS:C	2.51	0.49
2:B:162:TYR:CD2	2:B:218:VAL:HG11	2.48	0.49
2:J:91:PRO:HB3	2:J:141:LEU:HD13	1.94	0.49
4:I:176:LEU:HD13	2:J:189:ILE:HG13	1.94	0.49
3:K:126:THR:HA	3:K:149:GLU:OE1	2.13	0.49
3:K:246:VAL:HG12	3:K:250:GLY:HA3	1.93	0.49
3:C:126:THR:HA	3:C:149:GLU:OE1	2.13	0.48
2:F:149:THR:O	2:F:153:GLY:N	2.46	0.48
3:G:32:ASN:O	3:G:36:LEU:HB2	2.13	0.48
4:I:150:GLY:O	4:I:341:TYR:HE2	1.96	0.48
4:I:186:ALA:O	4:I:190:PRO:HG2	2.12	0.48
4:A:214:ARG:HH21	3:C:256:GLU:CD	2.16	0.48
4:E:117:ASP:N	4:E:117:ASP:OD1	2.45	0.48
2:F:21:GLY:O	2:F:25:THR:HG23	2.13	0.48
2:J:43:HIS:HE2	2:J:105:GLU:HG2	1.78	0.48
2:J:35:PHE:HA	2:J:96:PHE:CZ	2.48	0.48
3:K:127:GLU:HB2	2:J:43:HIS:HE1	1.78	0.48
3:K:84:LEU:HD22	3:K:167:TYR:HA	1.95	0.48
4:A:80:PRO:HA	4:A:140:VAL:HG13	1.94	0.48
3:C:106:VAL:O	3:C:109:GLN:HB2	2.13	0.48
3:C:121:GLY:HA2	3:C:153:SER:OG	2.13	0.48
4:A:319:TYR:HD2	4:A:326:PHE:HD2	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:TYR:HB3	3:C:184:LEU:HD23	1.96	0.48
4:E:308:ASN:HA	4:E:309:ASN:CB	2.31	0.48
2:F:146:TYR:CD2	2:F:237:TRP:NE1	2.81	0.48
4:I:69:VAL:HG12	4:I:114:ILE:HA	1.96	0.48
4:A:314:LEU:O	4:A:355:ILE:HD12	2.14	0.48
4:A:57:VAL:HG12	4:A:58:ASN:OD1	2.14	0.48
1:H:5:UNK:O	1:H:9:UNK:N	2.46	0.48
2:J:174:GLN:HB2	2:J:185:LEU:CD1	2.44	0.48
2:J:245:THR:O	2:J:245:THR:HG23	2.14	0.48
2:F:33:LEU:O	2:F:37:ALA:HB2	2.14	0.48
4:I:292:VAL:HA	4:I:411:ILE:O	2.13	0.48
4:E:341:TYR:CE2	4:E:342:LEU:HD22	2.49	0.48
3:K:131:THR:OG1	2:J:113:PHE:HA	2.14	0.48
2:B:125:PHE:CZ	2:B:169:ILE:CD1	2.96	0.48
4:I:247:TYR:O	4:I:251:ASN:HB2	2.14	0.48
4:A:398:ASP:N	4:A:398:ASP:OD1	2.39	0.47
3:C:122:ALA:O	3:C:126:THR:HB	2.15	0.47
3:K:98:ARG:HG3	2:J:12:PRO:O	2.14	0.47
4:E:186:ALA:O	4:E:190:PRO:HG2	2.14	0.47
4:E:273:THR:CA	4:E:274:GLU:HB2	2.44	0.47
3:G:182:ALA:HB1	3:G:230:GLY:O	2.14	0.47
3:G:250:GLY:HA2	3:G:254:LEU:HG	1.97	0.47
2:J:236:TRP:CD2	2:J:239:MET:HE3	2.48	0.47
3:C:20:ASP:O	3:C:21:LEU:HB2	2.14	0.47
1:D:13:UNK:O	1:D:17:UNK:CB	2.62	0.47
4:E:204:VAL:CG1	4:E:204:VAL:O	2.61	0.47
4:A:58:ASN:ND2	4:A:163:THR:H	1.95	0.47
4:A:205:ARG:O	4:A:206:LYS:HE2	2.13	0.47
3:G:174:TYR:CD1	3:G:174:TYR:C	2.88	0.47
3:G:194:ILE:HD13	3:G:194:ILE:N	2.29	0.47
4:I:305:LYS:HD3	4:I:362:GLU:OE1	2.15	0.47
2:B:235:LEU:HG	2:B:239:MET:CE	2.42	0.47
2:B:43:HIS:NE2	2:B:105:GLU:HG2	2.29	0.47
4:E:151:GLN:HE21	4:E:152:TRP:N	2.12	0.47
2:F:29:MET:HE1	3:G:109:GLN:HG3	1.96	0.47
4:I:298:ARG:HH11	4:I:370:ALA:HA	1.78	0.47
4:I:340:ASP:HB3	4:I:341:TYR:HA	1.96	0.47
2:B:149:THR:O	2:B:153:GLY:HA3	2.14	0.47
3:C:45:PHE:O	3:C:49:ALA:HB3	2.14	0.47
3:K:68:THR:HG21	1:N:8:UNK:O	2.15	0.47
4:A:181:ILE:O	4:A:185:TYR:CD2	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:283:ASN:O	4:A:309:ASN:CB	2.63	0.47
4:A:79:ASN:OD1	4:A:81:ARG:HB2	2.15	0.47
1:D:13:UNK:HA	3:C:30:LEU:CD2	2.44	0.47
3:G:124:PHE:HD1	3:G:124:PHE:C	2.17	0.47
3:G:251:VAL:HG12	3:G:252:LYS:N	2.30	0.47
3:K:28:LEU:O	3:K:32:ASN:ND2	2.42	0.47
4:I:58:ASN:ND2	4:I:163:THR:H	1.98	0.47
4:A:207:GLY:HA3	2:B:27:ASP:OD2	2.15	0.47
2:B:65:TRP:CE3	2:B:66:PRO:HD3	2.50	0.47
3:G:124:PHE:C	3:G:124:PHE:CD1	2.88	0.47
3:K:128:GLN:O	3:K:131:THR:HG22	2.15	0.47
4:A:342:LEU:H	4:A:371:ARG:HD3	1.79	0.47
4:I:289:ASN:ND2	4:I:305:LYS:HE3	2.29	0.47
4:A:226:ASP:H	4:A:229:ARG:NH2	2.13	0.46
4:E:273:THR:CA	4:E:274:GLU:CB	2.93	0.46
2:B:131:VAL:HB	2:B:132:PRO:HD3	1.97	0.46
2:B:169:ILE:HA	2:B:169:ILE:HD12	1.65	0.46
2:B:200:GLU:O	2:B:201:TYR:CB	2.63	0.46
3:C:157:TYR:C	3:C:157:TYR:CD1	2.89	0.46
2:F:208:GLY:HA2	4:A:35:GLN:OE1	2.14	0.46
3:G:194:ILE:H	3:G:194:ILE:HD13	1.79	0.46
4:I:127:ARG:HG3	4:I:162:PHE:CG	2.51	0.46
1:N:11:UNK:C	1:N:13:UNK:N	2.76	0.46
3:C:126:THR:HG22	2:B:47:MET:SD	2.55	0.46
2:F:29:MET:HE3	3:G:109:GLN:HG3	1.97	0.46
4:I:164:ASP:CB	4:I:165:PRO:CA	2.94	0.46
3:K:47:TRP:CZ3	2:J:116:TRP:O	2.69	0.46
2:J:214:GLY:HA2	2:J:215:LYS:HB2	1.95	0.46
2:B:109:ARG:HG3	2:B:126:PRO:HD3	1.98	0.46
3:C:154:TYR:CD1	3:C:157:TYR:HE2	2.30	0.46
2:J:149:THR:O	2:J:153:GLY:N	2.48	0.46
4:A:41:ARG:NE	4:A:387:GLN:HG2	2.30	0.46
2:B:162:TYR:HB3	2:B:163:PRO:CD	2.44	0.46
3:K:179:TYR:HB3	3:K:184:LEU:HD23	1.97	0.46
2:B:149:THR:O	2:B:153:GLY:CA	2.64	0.46
4:I:396:SER:HB2	4:I:397:PRO:HD2	1.98	0.46
3:K:194:ILE:H	3:K:194:ILE:CD1	2.16	0.46
3:C:232:PHE:CG	2:B:83:PHE:CD2	3.03	0.46
3:C:32:ASN:O	3:C:36:LEU:HB2	2.16	0.46
2:F:200:GLU:CG	2:F:203:ARG:HH11	2.29	0.46
2:F:203:ARG:O	2:F:204:MET:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:148:ILE:N	2:J:148:ILE:HD12	2.30	0.46
2:J:237:TRP:O	2:J:241:ARG:HG2	2.16	0.46
3:K:194:ILE:O	3:K:197:VAL:O	2.34	0.46
4:I:164:ASP:HB2	4:I:176:LEU:H	1.79	0.46
2:J:109:ARG:HG3	2:J:126:PRO:HD3	1.98	0.46
3:K:241:ARG:HA	3:K:241:ARG:NE	2.28	0.46
2:F:175:ALA:HB2	4:E:258:ILE:HG12	1.98	0.46
3:G:53:SER:HG	3:G:139:ASP:HB3	1.80	0.46
3:G:194:ILE:H	3:G:194:ILE:CD1	2.28	0.46
4:A:164:ASP:HB2	4:A:165:PRO:HA	1.98	0.46
4:A:226:ASP:HA	4:A:229:ARG:H	1.81	0.46
2:B:51:GLY:HA2	2:B:52:ASP:HB2	1.82	0.46
2:B:87:ASN:HB2	2:B:88:PHE:CE1	2.50	0.46
4:E:285:THR:HB	4:E:307:LYS:HB3	1.97	0.46
4:I:198:TRP:HZ3	4:I:235:VAL:HG21	1.79	0.46
2:B:34:LEU:O	2:B:37:ALA:HB3	2.15	0.45
4:E:282:GLU:HB3	4:E:310:THR:HG22	1.98	0.45
4:E:393:PHE:CD1	4:E:401:ARG:HD2	2.52	0.45
3:G:128:GLN:O	3:G:131:THR:HG22	2.17	0.45
4:I:214:ARG:HD3	4:I:222:ASP:HB2	1.99	0.45
3:K:54:PHE:CE2	4:I:33:SER:HB3	2.51	0.45
4:I:355:ILE:HG22	4:I:356:ALA:N	2.30	0.45
4:E:318:GLU:HB3	4:E:393:PHE:HB2	1.98	0.45
3:K:85:TRP:HA	3:K:170:THR:HG21	1.97	0.45
4:A:151:GLN:HE21	4:A:152:TRP:N	2.14	0.45
2:B:105:GLU:O	2:B:109:ARG:HG2	2.16	0.45
2:B:146:TYR:CD1	2:B:147:VAL:N	2.84	0.45
2:F:55:PHE:O	2:F:124:VAL:HA	2.16	0.45
4:A:68:HIS:HE1	4:A:405:GLU:OE1	1.99	0.45
4:A:102:GLY:O	4:A:103:GLU:HB2	2.17	0.45
3:C:119:TYR:CD1	3:C:120:TRP:N	2.85	0.45
3:G:241:ARG:HA	3:G:241:ARG:HE	1.82	0.45
4:I:398:ASP:N	4:I:398:ASP:OD1	2.42	0.45
3:K:109:GLN:HG3	2:J:29:MET:CE	2.46	0.45
3:K:239:LEU:HB3	4:I:212:TYR:CE2	2.51	0.45
4:A:411:ILE:HG23	4:A:412:PRO:HD2	1.97	0.45
2:F:176:THR:O	2:F:182:LEU:HD12	2.17	0.45
3:K:239:LEU:HD22	4:I:212:TYR:CD2	2.52	0.45
4:A:212:TYR:CD2	3:C:239:LEU:HB3	2.52	0.45
4:E:100:PHE:HA	4:E:104:GLN:O	2.17	0.45
3:K:167:TYR:CD1	3:K:171:ARG:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:245:VAL:HG12	4:A:246:GLY:N	2.30	0.45
4:A:273:THR:CA	4:A:274:GLU:CB	2.95	0.45
4:E:168:LEU:N	4:E:168:LEU:CD1	2.80	0.45
2:F:237:TRP:O	2:F:241:ARG:HG2	2.16	0.45
3:G:83:TYR:HE1	3:G:87:THR:HG21	1.73	0.45
4:I:181:ILE:HG22	4:I:185:TYR:CE2	2.52	0.45
4:A:128:ARG:HG2	4:A:159:MET:HG3	1.98	0.45
2:B:125:PHE:HZ	2:B:169:ILE:CD1	2.29	0.45
2:B:236:TRP:CD2	2:B:239:MET:HE3	2.52	0.45
4:E:354:PRO:O	4:E:355:ILE:HB	2.16	0.45
4:I:318:GLU:HB3	4:I:393:PHE:HB2	1.99	0.45
4:E:348:LEU:HA	4:E:349:SER:HA	1.77	0.45
2:F:201:TYR:CD1	2:F:202:ILE:N	2.85	0.45
3:G:85:TRP:HA	3:G:170:THR:HG21	1.99	0.45
4:I:320:THR:HG22	4:I:324:LEU:O	2.16	0.45
3:K:173:PRO:O	3:K:174:TYR:CB	2.64	0.45
4:E:341:TYR:H	4:E:342:LEU:HB3	1.81	0.44
4:I:395:PHE:HD1	4:I:401:ARG:HA	1.82	0.44
2:J:203:ARG:O	2:J:204:MET:CB	2.64	0.44
3:K:35:TYR:CD2	3:K:120:TRP:CG	3.05	0.44
4:A:204:VAL:O	4:A:204:VAL:CG1	2.64	0.44
4:A:363:ILE:O	4:A:363:ILE:CG1	2.63	0.44
2:B:148:ILE:N	2:B:148:ILE:HD12	2.31	0.44
3:C:247:GLY:O	3:C:251:VAL:HG23	2.17	0.44
4:E:137:GLN:HE21	4:E:139:ASN:ND2	2.04	0.44
4:E:212:TYR:CD2	3:G:239:LEU:HD22	2.53	0.44
4:I:54:THR:HA	4:I:154:GLU:O	2.18	0.44
4:I:69:VAL:CG1	4:I:114:ILE:HA	2.47	0.44
2:J:33:LEU:O	2:J:37:ALA:CB	2.64	0.44
4:A:164:ASP:HB3	4:A:165:PRO:HA	1.97	0.44
4:A:339:PRO:O	4:A:340:ASP:C	2.55	0.44
4:E:164:ASP:HB2	4:E:176:LEU:H	1.82	0.44
4:E:198:TRP:O	4:E:202:TRP:HD1	2.00	0.44
3:G:20:ASP:O	3:G:21:LEU:HB2	2.17	0.44
2:J:146:TYR:CD2	2:J:237:TRP:CD1	3.05	0.44
3:K:115:GLY:O	2:J:36:PHE:O	2.34	0.44
4:A:176:LEU:HD13	2:B:189:ILE:HG13	1.98	0.44
2:B:65:TRP:HE3	2:B:66:PRO:HD3	1.83	0.44
3:C:169:LYS:HD2	3:C:175:PHE:O	2.17	0.44
3:C:85:TRP:HA	3:C:170:THR:HG21	1.99	0.44
3:G:106:VAL:O	3:G:109:GLN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:114:TRP:CE3	2:J:118:TYR:HA	2.53	0.44
3:K:174:TYR:C	3:K:174:TYR:CD1	2.91	0.44
2:B:176:THR:O	2:B:182:LEU:HD12	2.17	0.44
2:B:62:ARG:HB3	2:B:218:VAL:HG22	2.00	0.44
4:E:201:PHE:CZ	4:E:231:ILE:HD13	2.53	0.44
3:G:154:TYR:HD1	3:G:157:TYR:CE2	2.33	0.44
4:I:100:PHE:HA	4:I:104:GLN:O	2.17	0.44
3:K:48:ARG:O	3:K:49:ALA:CB	2.65	0.44
4:A:223:VAL:O	4:A:224:ILE:HD13	2.17	0.44
4:A:305:LYS:HD3	4:A:362:GLU:OE1	2.18	0.44
2:B:214:GLY:CA	2:B:215:LYS:HB2	2.48	0.44
2:F:85:TRP:CE2	2:F:89:ARG:HD3	2.53	0.44
3:G:28:LEU:O	3:G:32:ASN:ND2	2.43	0.44
2:B:64:MET:O	2:B:68:VAL:HG13	2.17	0.44
2:F:35:PHE:CZ	2:F:100:GLY:HA2	2.53	0.44
2:J:21:GLY:O	2:J:25:THR:HG23	2.17	0.44
3:K:154:TYR:CD1	3:K:157:TYR:HE2	2.33	0.44
3:K:89:ASP:OD2	3:K:103:ARG:NH1	2.41	0.44
3:G:21:LEU:HD23	3:G:109:GLN:NE2	2.33	0.44
1:H:9:UNK:HA	1:H:12:UNK:CB	2.48	0.44
3:C:104:LEU:CD2	3:C:172:ILE:HD13	2.29	0.43
4:E:350:VAL:CG1	4:E:351:ASP:N	2.77	0.43
3:G:121:GLY:HA2	3:G:153:SER:CB	2.48	0.43
2:J:192:HIS:O	2:J:194:VAL:HG23	2.18	0.43
2:J:52:ASP:H	2:J:55:PHE:H	1.65	0.43
3:K:45:PHE:O	3:K:49:ALA:HB3	2.17	0.43
4:A:273:THR:CA	4:A:274:GLU:HB2	2.48	0.43
4:E:213:ILE:O	4:E:217:GLU:HG2	2.17	0.43
3:G:231:VAL:O	3:G:235:VAL:HG13	2.18	0.43
4:I:316:LEU:HB2	4:I:394:PHE:CE2	2.53	0.43
4:I:68:HIS:HE1	4:I:405:GLU:OE1	2.00	0.43
3:C:167:TYR:CD1	3:C:171:ARG:HD3	2.53	0.43
1:D:14:UNK:O	1:D:18:UNK:N	2.52	0.43
2:F:106:TRP:NE1	4:E:188:HIS:CD2	2.80	0.43
4:E:226:ASP:HA	4:E:229:ARG:H	1.83	0.43
4:E:340:ASP:HB3	4:E:341:TYR:CA	2.46	0.43
2:F:113:PHE:HA	3:G:131:THR:OG1	2.19	0.43
4:I:188:HIS:HD2	2:J:106:TRP:NE1	2.04	0.43
4:A:96:ARG:HH21	4:A:99:GLN:HE22	1.65	0.43
2:J:99:LEU:O	2:J:100:GLY:C	2.56	0.43
4:E:313:PRO:HG2	4:E:397:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:46:TYR:CE2	4:E:66:LYS:HD2	2.54	0.43
3:G:16:GLU:N	3:G:16:GLU:OE2	2.51	0.43
2:J:120:PRO:HG3	2:J:193:PHE:CD2	2.52	0.43
4:A:348:LEU:HA	4:A:349:SER:HA	1.76	0.43
3:C:84:LEU:HD22	3:C:167:TYR:HA	2.00	0.43
3:G:252:LYS:O	3:G:256:GLU:C	2.56	0.43
4:I:258:ILE:HG13	2:J:184:THR:HG22	2.00	0.43
2:J:119:PHE:HB3	2:J:123:LEU:HD23	1.99	0.43
3:K:72:LEU:O	3:K:76:SER:HB2	2.19	0.43
4:E:127:ARG:HG3	4:E:162:PHE:CG	2.53	0.43
4:E:363:ILE:CG1	4:E:363:ILE:O	2.65	0.43
3:G:179:TYR:HB3	3:G:184:LEU:HD23	2.00	0.43
4:A:318:GLU:OE2	4:A:325:ARG:HG2	2.18	0.43
2:F:125:PHE:CD1	2:F:125:PHE:N	2.82	0.43
4:I:219:LYS:HD2	4:I:221:ASP:OD2	2.18	0.43
4:E:398:ASP:OD1	4:E:398:ASP:N	2.41	0.43
4:A:95:VAL:HG23	4:A:127:ARG:HD2	2.01	0.43
4:A:196:ALA:O	4:A:200:PHE:HD1	2.02	0.43
4:A:308:ASN:HA	4:A:309:ASN:CB	2.33	0.43
4:A:319:TYR:CD2	4:A:326:PHE:HD2	2.36	0.43
4:A:341:TYR:CE2	4:A:342:LEU:HD22	2.54	0.43
2:B:166:TRP:CE2	2:B:170:ALA:HB2	2.54	0.43
2:F:129:LEU:O	2:F:132:PRO:HD2	2.19	0.43
3:K:122:ALA:O	3:K:126:THR:CB	2.62	0.43
3:K:132:TRP:CZ2	3:K:144:PRO:HG2	2.54	0.43
4:A:212:TYR:OH	3:C:240:MET:HG2	2.19	0.42
4:A:105:PHE:HD2	2:B:181:GLN:OE1	2.01	0.42
4:E:128:ARG:HG2	4:E:159:MET:HG3	2.01	0.42
4:A:183:ARG:O	4:A:186:ALA:HB3	2.19	0.42
2:B:57:VAL:HG12	2:B:123:LEU:HD12	2.02	0.42
4:E:50:TRP:CE2	4:E:151:GLN:HB3	2.55	0.42
4:E:80:PRO:HA	4:E:140:VAL:HG13	2.02	0.42
2:F:117:THR:HG22	3:G:47:TRP:CH2	2.54	0.42
4:A:313:PRO:HB2	4:A:354:PRO:HB2	2.00	0.42
4:A:327:LEU:HD11	4:A:343:LEU:HD11	2.02	0.42
4:A:44:ASN:HD21	4:A:70:PHE:HD1	1.68	0.42
2:B:198:MET:O	2:B:198:MET:CG	2.57	0.42
3:K:148:ILE:HD13	3:K:148:ILE:N	2.34	0.42
3:C:47:TRP:CZ3	2:B:116:TRP:O	2.72	0.42
4:I:198:TRP:O	4:I:202:TRP:HD1	2.02	0.42
2:J:146:TYR:C	2:J:146:TYR:CD1	2.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:100:PHE:HA	4:A:104:GLN:O	2.18	0.42
4:A:213:ILE:HG12	3:C:243:HIS:CD2	2.55	0.42
4:A:334:THR:CA	4:A:335:LYS:CB	2.78	0.42
3:C:174:TYR:C	3:C:174:TYR:CD1	2.93	0.42
4:E:95:VAL:CG2	4:E:162:PHE:CZ	3.02	0.42
2:F:245:THR:O	2:F:245:THR:HG23	2.20	0.42
4:I:273:THR:CA	4:I:274:GLU:HB2	2.49	0.42
3:K:138:ARG:HH11	3:K:146:HIS:CE1	2.37	0.42
4:A:99:GLN:O	4:A:100:PHE:CD1	2.73	0.42
4:E:196:ALA:O	4:E:200:PHE:HD1	2.03	0.42
4:E:319:TYR:CD2	4:E:326:PHE:HD2	2.37	0.42
3:G:138:ARG:NH2	3:G:140:THR:O	2.52	0.42
4:I:274:GLU:H	4:I:275:GLY:CA	2.33	0.42
4:A:100:PHE:O	4:A:120:PHE:HA	2.20	0.42
4:A:137:GLN:HG3	4:A:147:ILE:HD13	2.01	0.42
4:E:256:ARG:HG2	4:A:414:PHE:CD2	2.54	0.42
2:F:146:TYR:CE1	2:F:147:VAL:CG2	3.02	0.42
3:K:86:LYS:C	3:K:88:ARG:H	2.22	0.42
4:I:314:LEU:O	4:I:355:ILE:HD12	2.19	0.42
3:C:88:ARG:HB2	3:C:170:THR:HB	2.01	0.42
4:E:286:THR:HG21	4:E:392:LEU:HD12	2.02	0.42
4:E:318:GLU:HG3	4:E:327:LEU:HD23	2.02	0.42
2:F:26:VAL:HG21	3:G:105:VAL:HG22	2.00	0.42
3:K:35:TYR:HE1	3:K:152:MET:CE	2.32	0.42
4:A:318:GLU:HG3	4:A:327:LEU:HD23	2.02	0.41
4:E:308:ASN:CG	4:E:356:ALA:HB3	2.39	0.41
4:E:375:GLU:O	4:E:377:LEU:N	2.52	0.41
2:F:82:ALA:O	2:F:86:VAL:HB	2.19	0.41
2:J:201:TYR:CD1	2:J:202:ILE:N	2.86	0.41
4:A:188:HIS:HD2	2:B:106:TRP:NE1	2.02	0.41
4:A:274:GLU:H	4:A:275:GLY:HA2	1.85	0.41
4:A:291:GLY:C	4:A:292:VAL:HG23	2.41	0.41
1:D:13:UNK:HA	3:C:30:LEU:HD22	2.03	0.41
2:F:178:GLN:O	2:F:179:HIS:C	2.58	0.41
3:G:132:TRP:CZ2	3:G:144:PRO:HG2	2.55	0.41
3:G:184:LEU:HD13	3:G:184:LEU:HA	1.81	0.41
4:I:113:GLU:HB2	4:I:116:LYS:HG3	2.01	0.41
3:K:112:VAL:HG22	2:J:33:LEU:HB3	2.02	0.41
4:A:69:VAL:CG1	4:A:114:ILE:HA	2.50	0.41
4:A:227:ASP:OD1	4:A:227:ASP:N	2.49	0.41
4:A:346:ARG:HB3	4:A:368:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:382:TYR:CZ	2:B:215:LYS:HA	2.55	0.41
3:C:131:THR:OG1	2:B:113:PHE:HA	2.21	0.41
4:E:291:GLY:O	4:E:292:VAL:CG2	2.68	0.41
2:F:125:PHE:N	2:F:125:PHE:HD1	2.13	0.41
2:J:125:PHE:HD1	2:J:125:PHE:N	2.17	0.41
4:A:219:LYS:HA	4:A:219:LYS:HD3	1.89	0.41
2:B:245:THR:HG23	2:B:245:THR:O	2.21	0.41
2:B:39:LEU:C	2:B:39:LEU:HD12	2.40	0.41
4:E:68:HIS:HB2	4:E:117:ASP:OD2	2.21	0.41
2:J:43:HIS:NE2	2:J:105:GLU:HG2	2.35	0.41
2:J:149:THR:O	2:J:153:GLY:CA	2.68	0.41
4:E:225:GLY:HA2	4:E:229:ARG:HH22	1.84	0.41
2:F:162:TYR:HB3	2:F:163:PRO:CD	2.50	0.41
2:F:167:PRO:HG2	4:E:187:TRP:CZ2	2.56	0.41
3:K:59:GLN:HA	3:K:63:MET:HB2	2.02	0.41
4:A:83:SER:HA	4:A:139:ASN:O	2.20	0.41
4:A:342:LEU:N	4:A:371:ARG:HD3	2.35	0.41
2:B:9:ALA:N	2:B:14:ASN:O	2.53	0.41
3:C:178:GLY:O	3:C:179:TYR:CG	2.74	0.41
3:C:241:ARG:NE	3:C:241:ARG:HA	2.36	0.41
3:C:86:LYS:CE	3:C:86:LYS:HA	2.38	0.41
4:E:339:PRO:O	4:E:340:ASP:C	2.59	0.41
2:F:202:ILE:HD12	2:F:202:ILE:HA	1.82	0.41
3:G:110:TRP:HB3	3:G:164:ALA:HB2	2.01	0.41
3:G:86:LYS:O	3:G:88:ARG:N	2.53	0.41
2:J:113:PHE:HB3	2:J:124:VAL:HG21	2.02	0.41
2:J:159:LEU:HD23	2:J:159:LEU:HA	1.88	0.41
4:A:340:ASP:HB3	4:A:341:TYR:CA	2.48	0.41
3:C:107:LEU:CD1	3:C:168:ALA:HB2	2.51	0.41
4:I:213:ILE:O	4:I:217:GLU:HG2	2.21	0.41
4:I:273:THR:CA	4:I:274:GLU:CB	2.96	0.41
3:K:83:TYR:HE1	3:K:87:THR:HG1	1.68	0.41
4:A:58:ASN:HD21	4:A:163:THR:N	1.97	0.41
3:C:173:PRO:O	3:C:174:TYR:CB	2.69	0.41
3:C:252:LYS:O	3:C:256:GLU:C	2.59	0.41
4:E:102:GLY:HA3	4:E:268:LEU:HB3	2.01	0.41
4:E:348:LEU:HB2	4:E:349:SER:HB2	2.02	0.41
2:F:166:TRP:HB3	2:F:167:PRO:CD	2.48	0.41
3:G:69:GLU:OE1	3:G:152:MET:HG3	2.20	0.41
4:I:215:VAL:O	4:I:217:GLU:O	2.39	0.41
4:I:319:TYR:CD2	4:I:326:PHE:HD2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:34:LEU:O	2:J:37:ALA:HB3	2.21	0.41
2:J:60:LYS:HB3	2:J:65:TRP:CE3	2.56	0.41
3:K:100:GLU:OE1	3:K:245:LEU:HD11	2.20	0.41
4:A:310:THR:O	4:A:357:PRO:HB3	2.21	0.41
4:E:150:GLY:O	4:E:341:TYR:HE2	2.03	0.41
4:E:351:ASP:O	4:E:353:THR:N	2.54	0.41
2:F:173:HIS:O	4:E:257:THR:HA	2.21	0.41
3:G:39:ARG:NH2	3:G:43:GLN:HB2	2.32	0.41
2:J:64:MET:HG2	2:J:64:MET:H	1.64	0.41
3:K:34:PHE:HE2	3:K:152:MET:CE	2.32	0.41
4:A:286:THR:HG21	4:A:392:LEU:HD12	2.02	0.41
2:J:136:LEU:HA	2:J:136:LEU:HD12	1.84	0.41
4:I:99:GLN:HG2	2:J:191:PHE:CZ	2.56	0.41
4:A:51:SER:CB	4:A:62:VAL:H	2.32	0.41
2:B:149:THR:O	2:B:153:GLY:N	2.54	0.41
4:E:191:TRP:CZ3	4:E:239:THR:HG23	2.56	0.41
4:E:338:PHE:HB3	4:E:343:LEU:HD22	2.03	0.41
2:F:109:ARG:HG3	2:F:126:PRO:HD3	2.02	0.41
2:F:162:TYR:CD2	2:F:218:VAL:HG11	2.56	0.41
4:I:102:GLY:HA3	4:I:268:LEU:HB3	2.03	0.41
4:I:348:LEU:HA	4:I:349:SER:HA	1.86	0.41
4:I:95:VAL:HG21	4:I:162:PHE:CZ	2.56	0.41
4:A:393:PHE:CD1	4:A:401:ARG:HD2	2.56	0.40
4:E:219:LYS:HA	4:E:219:LYS:HD3	1.92	0.40
4:E:338:PHE:CG	4:E:339:PRO:HD2	2.56	0.40
2:F:15:SER:HB2	2:F:17:ALA:H	1.86	0.40
2:F:33:LEU:HD13	3:G:111:LEU:HB3	2.01	0.40
3:G:226:TRP:HE3	3:G:226:TRP:HA	1.86	0.40
4:I:308:ASN:CG	4:I:356:ALA:HB3	2.40	0.40
4:I:387:GLN:HG3	4:I:408:GLY:C	2.41	0.40
2:B:162:TYR:N	2:B:163:PRO:HD2	2.36	0.40
2:B:186:ALA:O	2:B:187:ASP:C	2.59	0.40
4:A:208:ILE:HG23	2:B:88:PHE:CE2	2.56	0.40
4:E:198:TRP:HZ3	4:E:235:VAL:HG21	1.86	0.40
4:E:205:ARG:O	4:E:206:LYS:HE2	2.21	0.40
4:E:293:TYR:CE1	4:E:410:VAL:HG23	2.56	0.40
3:G:94:ALA:O	3:G:95:VAL:C	2.60	0.40
4:A:139:ASN:OD1	4:A:145:PRO:HA	2.22	0.40
4:A:326:PHE:CD2	4:A:367:ILE:HG21	2.57	0.40
4:E:107:PRO:HD2	4:E:265:GLN:HE22	1.87	0.40
4:I:240:ILE:O	4:I:244:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:40:ILE:HG22	3:K:41:TYR:N	2.36	0.40
4:A:392:LEU:HD23	4:A:392:LEU:HA	1.86	0.40
2:B:140:LEU:O	2:B:143:SER:O	2.40	0.40
2:B:199:PRO:O	2:B:200:GLU:C	2.57	0.40
3:C:109:GLN:CG	2:B:29:MET:HE3	2.49	0.40
3:C:225:GLY:O	3:C:226:TRP:CE3	2.66	0.40
4:I:282:GLU:HB3	4:I:310:THR:HG22	2.04	0.40
2:J:123:LEU:HD13	2:J:189:ILE:HG22	2.04	0.40
2:J:216:ASP:O	2:J:219:PRO:HD2	2.21	0.40
2:J:35:PHE:CZ	2:J:100:GLY:HA2	2.57	0.40
3:K:69:GLU:O	3:K:73:GLU:N	2.48	0.40
2:B:125:PHE:CZ	2:B:169:ILE:HD11	2.56	0.40
4:A:258:ILE:HG13	2:B:184:THR:HG22	2.03	0.40
4:E:77:VAL:O	4:E:78:ALA:C	2.59	0.40
3:G:104:LEU:O	3:G:108:VAL:HG23	2.22	0.40
3:G:169:LYS:HD2	3:G:175:PHE:O	2.22	0.40
2:J:60:LYS:HB3	2:J:65:TRP:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	242/252 (96%)	197 (81%)	40 (16%)	5 (2%)	9	44
2	F	242/252 (96%)	204 (84%)	32 (13%)	6 (2%)	7	39
2	J	242/252 (96%)	200 (83%)	35 (14%)	7 (3%)	6	35
3	C	213/256 (83%)	171 (80%)	31 (15%)	11 (5%)	2	18
3	G	209/256 (82%)	172 (82%)	28 (13%)	9 (4%)	3	23
3	K	213/256 (83%)	167 (78%)	36 (17%)	10 (5%)	3	21
4	A	388/420 (92%)	310 (80%)	53 (14%)	25 (6%)	2	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	388/420 (92%)	315 (81%)	43 (11%)	30 (8%)	1	7
4	I	388/420 (92%)	315 (81%)	50 (13%)	23 (6%)	2	15
All	All	2525/2784 (91%)	2051 (81%)	348 (14%)	126 (5%)	3	19

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	52	ASP
3	K	174	TYR
3	K	179	TYR
3	K	251	VAL
4	E	141	GLU
4	E	164	ASP
4	E	205	ARG
4	E	221	ASP
4	E	257	THR
4	E	274	GLU
4	E	335	LYS
4	E	342	LEU
4	E	352	ALA
4	E	353	THR
4	E	354	PRO
4	E	356	ALA
4	A	205	ARG
4	A	221	ASP
4	A	257	THR
4	A	274	GLU
4	A	335	LYS
4	A	342	LEU
4	A	352	ALA
4	A	354	PRO
4	A	356	ALA
4	I	141	GLU
4	I	164	ASP
4	I	205	ARG
4	I	221	ASP
4	I	257	THR
4	I	274	GLU
4	I	335	LYS
4	I	342	LEU
4	I	352	ALA

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Mol	Chain	Res	Type
4	I	353	THR
4	I	354	PRO
3	C	174	TYR
3	C	179	TYR
3	C	251	VAL
3	G	174	TYR
3	G	251	VAL
2	J	52	ASP
2	B	52	ASP
2	F	201	TYR
3	K	49	ALA
3	K	87	THR
3	K	138	ARG
3	K	177	HIS
3	K	196	ASN
4	E	206	LYS
4	E	298	ARG
4	E	309	ASN
4	E	355	ILE
4	A	141	GLU
4	A	164	ASP
4	A	298	ARG
4	A	355	ILE
4	I	298	ARG
4	I	309	ASN
4	I	355	ILE
4	I	356	ALA
3	C	49	ALA
3	C	87	THR
3	C	138	ARG
3	C	196	ASN
3	G	49	ALA
3	G	87	THR
3	G	138	ARG
3	G	179	TYR
2	J	19	ALA
2	J	201	TYR
2	B	142	LEU
2	B	201	TYR
2	F	19	ALA
2	F	20	ALA
2	F	142	LEU

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Mol	Chain	Res	Type
3	K	21	LEU
4	E	51	SER
4	A	309	ASN
4	A	340	ASP
4	A	353	THR
4	A	400	LYS
4	I	400	LYS
3	C	177	HIS
3	G	177	HIS
2	J	60	LYS
2	B	89	ARG
2	B	171	ALA
4	E	61	MET
4	E	224	ILE
4	E	225	GLY
4	E	400	LYS
4	A	51	SER
4	A	224	ILE
4	I	61	MET
4	I	224	ILE
3	C	21	LEU
3	C	124	PHE
3	G	95	VAL
2	J	11	GLY
2	F	60	LYS
4	E	201	PHE
4	E	220	ALA
4	A	76	ALA
4	A	201	PHE
4	A	206	LYS
4	I	70	PHE
4	I	201	PHE
3	G	124	PHE
2	J	10	VAL
4	E	340	ASP
4	A	165	PRO
4	A	350	VAL
3	C	253	LEU
2	J	204	MET
4	E	350	VAL
4	A	358	GLY
4	I	143	GLY

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Mol	Chain	Res	Type
4	E	184	VAL
4	I	350	VAL
4	E	358	GLY
3	K	195	PRO
4	E	207	GLY
4	E	90	PRO
4	E	165	PRO
4	I	165	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/208 (97%)	184 (91%)	18 (9%)	12	42
2	F	202/208 (97%)	179 (89%)	23 (11%)	7	30
2	J	202/208 (97%)	181 (90%)	21 (10%)	9	33
3	C	184/213 (86%)	155 (84%)	29 (16%)	3	14
3	G	181/213 (85%)	156 (86%)	25 (14%)	4	20
3	K	184/213 (86%)	156 (85%)	28 (15%)	3	16
4	A	320/336 (95%)	289 (90%)	31 (10%)	10	37
4	E	320/336 (95%)	289 (90%)	31 (10%)	10	37
4	I	320/336 (95%)	288 (90%)	32 (10%)	9	36
All	All	2115/2271 (93%)	1877 (89%)	238 (11%)	7	30

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	15	SER
2	F	22	CYS
2	F	25	THR
2	F	36	PHE
2	F	38	VAL
2	F	39	LEU

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Mol	Chain	Res	Type
2	F	48	LEU
2	F	52	ASP
2	F	89	ARG
2	F	92	PHE
2	F	125	PHE
2	F	137	ASP
2	F	146	TYR
2	F	163	PRO
2	F	164	ASN
2	F	169	ILE
2	F	176	THR
2	F	177	GLU
2	F	189	ILE
2	F	192	HIS
2	F	201	TYR
2	F	211	ARG
2	F	251	THR
3	K	16	GLU
3	K	22	ARG
3	K	30	LEU
3	K	36	LEU
3	K	40	ILE
3	K	47	TRP
3	K	74	LEU
3	K	76	SER
3	K	83	TYR
3	K	86	LYS
3	K	90	ARG
3	K	97	PRO
3	K	116	ILE
3	K	118	ILE
3	K	139	ASP
3	K	145	SER
3	K	157	TYR
3	K	183	PHE
3	K	184	LEU
3	K	193	ILE
3	K	194	ILE
3	K	226	TRP
3	K	231	VAL
3	K	235	VAL
3	K	241	ARG

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Mol	Chain	Res	Type
3	K	249	GLU
3	K	252	LYS
3	K	255	THR
4	E	49	GLN
4	E	55	VAL
4	E	61	MET
4	E	62	VAL
4	E	94	LEU
4	E	117	ASP
4	E	156	LYS
4	E	159	MET
4	E	164	ASP
4	E	176	LEU
4	E	182	SER
4	E	204	VAL
4	E	205	ARG
4	E	206	LYS
4	E	252	SER
4	E	253	THR
4	E	272	GLU
4	E	274	GLU
4	E	276	THR
4	E	277	VAL
4	E	283	ASN
4	E	303	ASN
4	E	306	VAL
4	E	320	THR
4	E	334	THR
4	E	346	ARG
4	E	359	GLU
4	E	368	GLN
4	E	384	THR
4	E	398	ASP
4	E	418	ASP
4	A	55	VAL
4	A	61	MET
4	A	62	VAL
4	A	117	ASP
4	A	156	LYS
4	A	159	MET
4	A	164	ASP
4	A	173	THR

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Mol	Chain	Res	Type
4	A	176	LEU
4	A	182	SER
4	A	204	VAL
4	A	205	ARG
4	A	206	LYS
4	A	252	SER
4	A	253	THR
4	A	254	PHE
4	A	272	GLU
4	A	274	GLU
4	A	276	THR
4	A	283	ASN
4	A	284	VAL
4	A	303	ASN
4	A	306	VAL
4	A	320	THR
4	A	334	THR
4	A	335	LYS
4	A	346	ARG
4	A	359	GLU
4	A	368	GLN
4	A	384	THR
4	A	398	ASP
4	I	49	GLN
4	I	55	VAL
4	I	61	MET
4	I	62	VAL
4	I	63	LEU
4	I	81	ARG
4	I	94	LEU
4	I	117	ASP
4	I	156	LYS
4	I	176	LEU
4	I	182	SER
4	I	204	VAL
4	I	205	ARG
4	I	206	LYS
4	I	252	SER
4	I	253	THR
4	I	254	PHE
4	I	272	GLU
4	I	274	GLU

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Mol	Chain	Res	Type
4	I	276	THR
4	I	277	VAL
4	I	283	ASN
4	I	284	VAL
4	I	303	ASN
4	I	306	VAL
4	I	320	THR
4	I	335	LYS
4	I	341	TYR
4	I	346	ARG
4	I	359	GLU
4	I	368	GLN
4	I	398	ASP
3	C	16	GLU
3	C	17	SER
3	C	19	VAL
3	C	22	ARG
3	C	30	LEU
3	C	36	LEU
3	C	47	TRP
3	C	74	LEU
3	C	76	SER
3	C	86	LYS
3	C	90	ARG
3	C	116	ILE
3	C	127	GLU
3	C	131	THR
3	C	139	ASP
3	C	145	SER
3	C	157	TYR
3	C	183	PHE
3	C	184	LEU
3	C	193	ILE
3	C	194	ILE
3	C	196	ASN
3	C	199	LEU
3	C	226	TRP
3	C	231	VAL
3	C	241	ARG
3	C	249	GLU
3	C	252	LYS
3	C	255	THR

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Mol	Chain	Res	Type
3	G	16	GLU
3	G	17	SER
3	G	19	VAL
3	G	22	ARG
3	G	36	LEU
3	G	40	ILE
3	G	47	TRP
3	G	74	LEU
3	G	76	SER
3	G	86	LYS
3	G	90	ARG
3	G	116	ILE
3	G	124	PHE
3	G	145	SER
3	G	157	TYR
3	G	183	PHE
3	G	184	LEU
3	G	193	ILE
3	G	194	ILE
3	G	226	TRP
3	G	231	VAL
3	G	241	ARG
3	G	249	GLU
3	G	252	LYS
3	G	255	THR
2	J	10	VAL
2	J	15	SER
2	J	25	THR
2	J	36	PHE
2	J	38	VAL
2	J	48	LEU
2	J	52	ASP
2	J	86	VAL
2	J	89	ARG
2	J	125	PHE
2	J	137	ASP
2	J	146	TYR
2	J	164	ASN
2	J	169	ILE
2	J	176	THR
2	J	177	GLU
2	J	189	ILE

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Mol	Chain	Res	Type
2	J	192	HIS
2	J	201	TYR
2	J	211	ARG
2	J	251	THR
2	B	10	VAL
2	B	15	SER
2	B	22	CYS
2	B	36	PHE
2	B	39	LEU
2	B	52	ASP
2	B	83	PHE
2	B	89	ARG
2	B	125	PHE
2	B	152	VAL
2	B	164	ASN
2	B	169	ILE
2	B	176	THR
2	B	177	GLU
2	B	192	HIS
2	B	201	TYR
2	B	211	ARG
2	B	251	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	45	HIS
2	F	173	HIS
2	F	178	GLN
2	F	192	HIS
3	K	133	HIS
3	K	177	HIS
4	E	44	ASN
4	E	58	ASN
4	E	68	HIS
4	E	99	GLN
4	E	137	GLN
4	E	151	GLN
4	E	188	HIS
4	E	261	GLN
4	E	265	GLN
4	E	283	ASN

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Mol	Chain	Res	Type
4	A	44	ASN
4	A	58	ASN
4	A	68	HIS
4	A	99	GLN
4	A	137	GLN
4	A	151	GLN
4	A	188	HIS
4	A	261	GLN
4	A	265	GLN
4	A	283	ASN
4	I	44	ASN
4	I	58	ASN
4	I	68	HIS
4	I	75	GLN
4	I	99	GLN
4	I	137	GLN
4	I	151	GLN
4	I	188	HIS
4	I	261	GLN
4	I	265	GLN
4	I	283	ASN
3	C	133	HIS
3	C	177	HIS
3	C	196	ASN
3	G	109	GLN
3	G	133	HIS
2	J	87	ASN
2	J	174	GLN
2	J	178	GLN
2	J	192	HIS
2	B	192	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	D	0/25	-	-	-	-
1	H	0/25	-	-	-	-
1	N	0/25	-	-	-	-
2	B	244/252 (96%)	-0.40	3 (1%) 81 69	29, 55, 88, 135	0
2	F	244/252 (96%)	-0.53	2 (0%) 87 79	19, 37, 78, 118	0
2	J	244/252 (96%)	-0.55	0 100 100	21, 38, 69, 115	0
3	C	217/256 (84%)	-0.18	8 (3%) 45 28	35, 67, 127, 170	0
3	G	213/256 (83%)	-0.19	10 (4%) 35 20	26, 56, 108, 176	0
3	K	217/256 (84%)	-0.26	13 (5%) 25 13	23, 50, 123, 166	0
4	A	390/420 (92%)	0.03	28 (7%) 18 9	30, 66, 102, 159	0
4	E	390/420 (92%)	-0.43	1 (0%) 94 92	22, 41, 71, 120	0
4	I	390/420 (92%)	-0.12	18 (4%) 36 21	27, 60, 106, 160	0
All	All	2549/2859 (89%)	-0.28	83 (3%) 50 33	19, 52, 102, 176	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	418	ASP	5.7
3	G	253	LEU	5.3
3	C	18	VAL	5.3
3	G	252	LYS	5.2
4	A	328	ASN	5.1
3	G	139	ASP	4.8
4	I	418	ASP	4.4
4	I	316	LEU	4.4
3	C	17	SER	4.4
3	G	256	GLU	4.3
3	C	196	ASN	4.3
3	K	139	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
4	A	399	GLY	4.1
3	G	47	TRP	3.9
4	I	337	ASP	3.9
3	G	140	THR	3.8
4	I	350	VAL	3.6
3	K	196	ASN	3.6
3	C	139	ASP	3.6
4	A	317	GLY	3.5
4	A	348	LEU	3.4
4	I	348	LEU	3.4
4	A	170	ASP	3.4
3	K	48	ARG	3.4
4	A	315	ARG	3.3
4	A	157	GLY	3.2
4	A	316	LEU	3.2
3	K	17	SER	3.1
4	I	417	GLY	3.0
3	K	64	SER	3.0
4	I	317	GLY	3.0
4	A	400	LYS	2.9
4	A	396	SER	2.9
4	A	352	ALA	2.9
4	A	397	PRO	2.8
4	I	327	LEU	2.8
4	A	169	LEU	2.8
3	G	18	VAL	2.8
3	K	61	TYR	2.7
4	I	395	PHE	2.7
3	G	17	SER	2.7
3	K	47	TRP	2.7
4	I	328	ASN	2.7
2	B	9	ALA	2.7
4	A	60	GLU	2.6
3	K	50	GLY	2.6
4	A	349	SER	2.5
4	A	350	VAL	2.5
4	I	294	LYS	2.5
3	K	254	LEU	2.5
3	C	47	TRP	2.5
2	F	16	VAL	2.4
4	A	171	GLY	2.4
4	A	398	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
4	A	330	ASP	2.3
2	B	17	ALA	2.3
4	A	361	LYS	2.3
4	A	332	PHE	2.3
3	C	64	SER	2.3
4	E	369	ASP	2.3
4	A	160	LYS	2.3
4	I	53	THR	2.3
4	I	336	PRO	2.3
4	A	329	PRO	2.2
3	G	248	LYS	2.2
3	K	18	VAL	2.2
4	A	172	SER	2.2
4	A	393	PHE	2.2
4	I	299	GLU	2.2
3	K	253	LEU	2.2
4	A	158	ASP	2.2
3	K	60	THR	2.2
4	I	314	LEU	2.2
3	C	225	GLY	2.2
3	K	256	GLU	2.2
2	B	10	VAL	2.1
4	I	298	ARG	2.1
2	F	17	ALA	2.1
3	G	59	GLN	2.1
4	A	167	THR	2.1
4	I	52	LYS	2.1
4	I	315	ARG	2.0
3	C	224	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
5	CU	C	301	1/1	0.99	0.06	-	71,71,71,71	0
5	CU	E	501	1/1	0.99	0.07	-	53,53,53,53	0
5	CU	A	501	1/1	0.95	0.06	-	108,108,108,108	0
5	CU	K	301	1/1	0.98	0.11	-	85,85,85,85	0
5	CU	I	501	1/1	0.97	0.06	-	85,85,85,85	0
5	CU	G	301	1/1	0.97	0.08	-	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.