



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:59 am BST

PDB ID : 4PI2
Title : Crystal structure of particulate methane monooxygenase from *Methylocystis* sp. ATCC 49242 (Rockwell) soaked in zinc
Authors : Sirajuddin, S.; Rosenzweig, A.C.
Deposited on : 2014-05-07
Resolution : 3.33 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

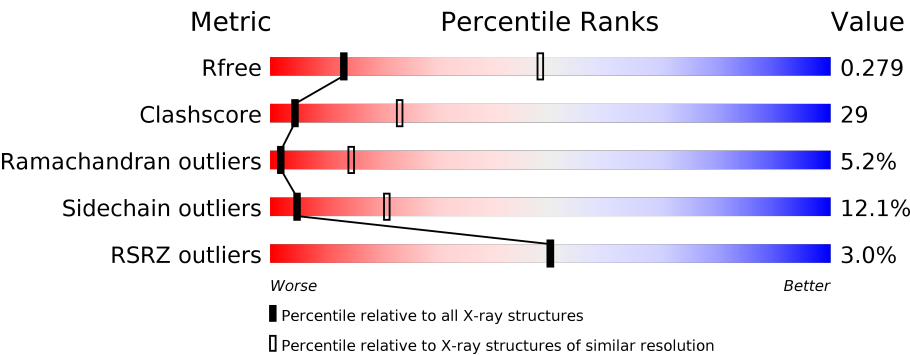
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.33 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	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	25	<div><div></div><div>64%12%24%</div></div>
1	H	25	<div><div></div><div>76%.20%</div></div>
1	N	25	<div><div></div><div>64%32%.5%</div></div>
2	B	252	<div><div></div><div>55%37%5%.2%</div></div>
2	F	252	<div><div></div><div>51%39%6%.2%</div></div>
2	J	252	<div><div>2%</div><div>46%42%8%.2%</div></div>

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Mol	Chain	Length	Quality of chain
3	A	420	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>7%</div><div>46%</div><div>38%</div><div>9%</div><div>7%</div></div>
3	E	420	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%</div><div>47%</div><div>35%</div><div>9%</div><div>7%</div></div>
3	I	420	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>3%</div><div>46%</div><div>37%</div><div>9%</div><div>7%</div></div>
4	C	256	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>5%</div><div>39%</div><div>37%</div><div>12%</div><div>11%</div></div>
4	G	256	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%</div><div>38%</div><div>39%</div><div>11%</div><div>11%</div></div>
4	K	256	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>4%</div><div>34%</div><div>44%</div><div>11%</div><div>11%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20979 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 B.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	228	Total	C	N	O	S	0	0	0
			1870	1256	295	310	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	228	Total	C	N	O	S	0	0	0
			1870	1256	295	310	9			
4	C	228	Total	C	N	O	S	0	0	0
			1870	1256	295	310	9			

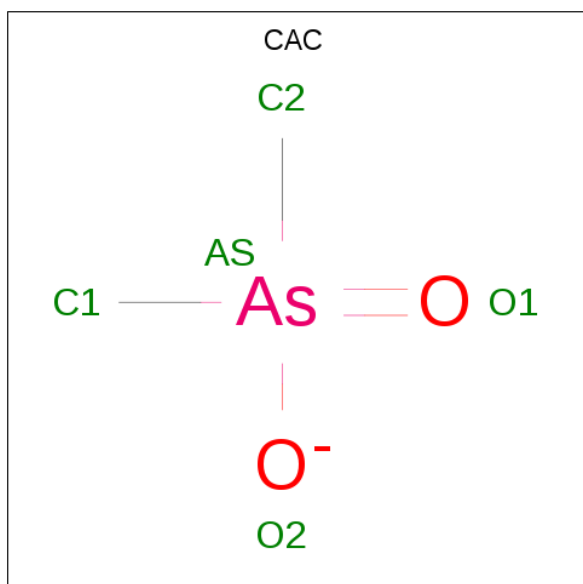
- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

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

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

- Molecule 7 is CACODYLATE ION (three-letter code: CAC) (formula: C₂H₆AsO₂).



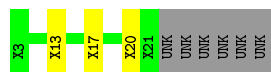
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	As	C	O	0	0
			5	1	2	2		

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 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: unknown peptide

Chain D: 



- Molecule 1: unknown peptide

Chain H: 



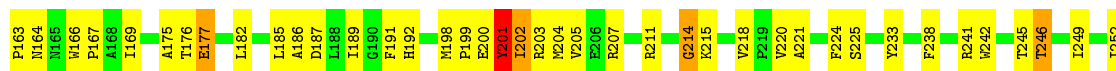
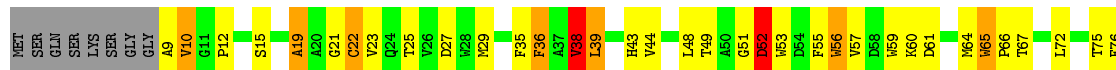
- Molecule 1: unknown peptide

Chain N: 



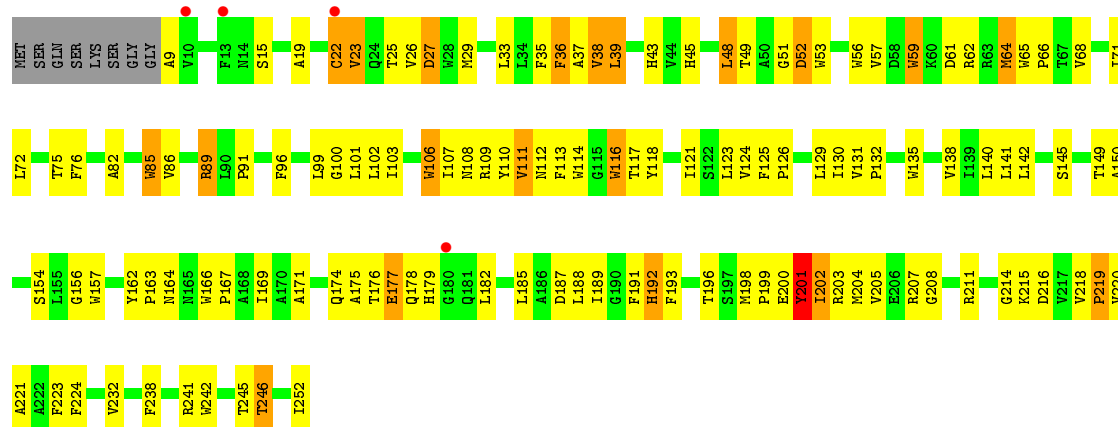
- Molecule 2: Particulate methane monooxygenase subunit A

Chain F: 



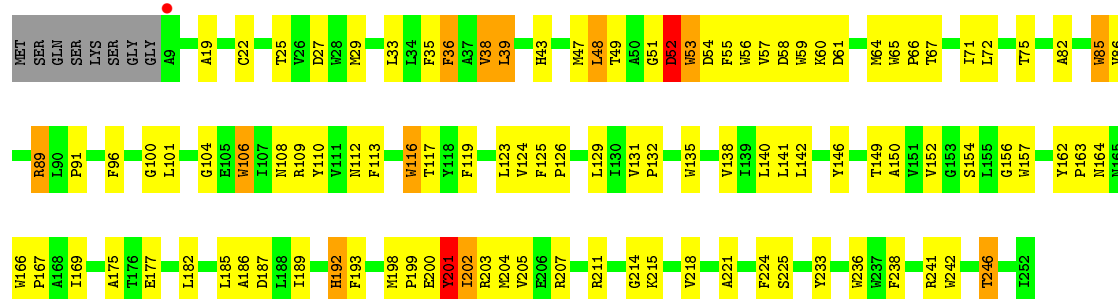
- Molecule 2: Particulate methane monooxygenase subunit A

Chain J: 



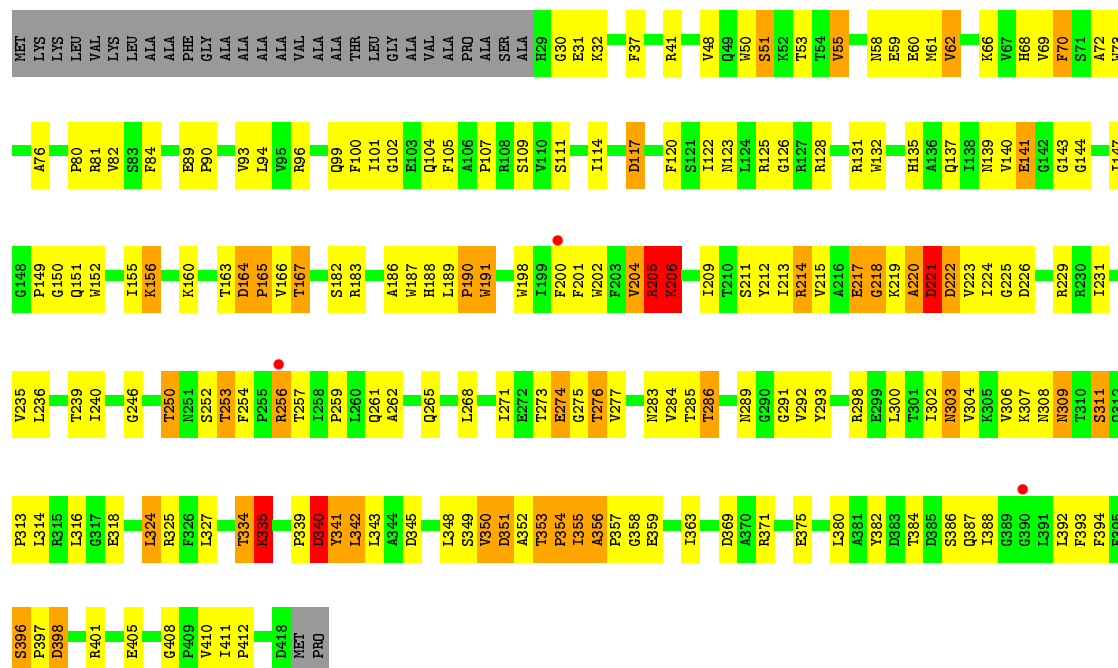
• Molecule 2: Particulate methane monooxygenase subunit A

Chain B: 55% 37% 5% ..

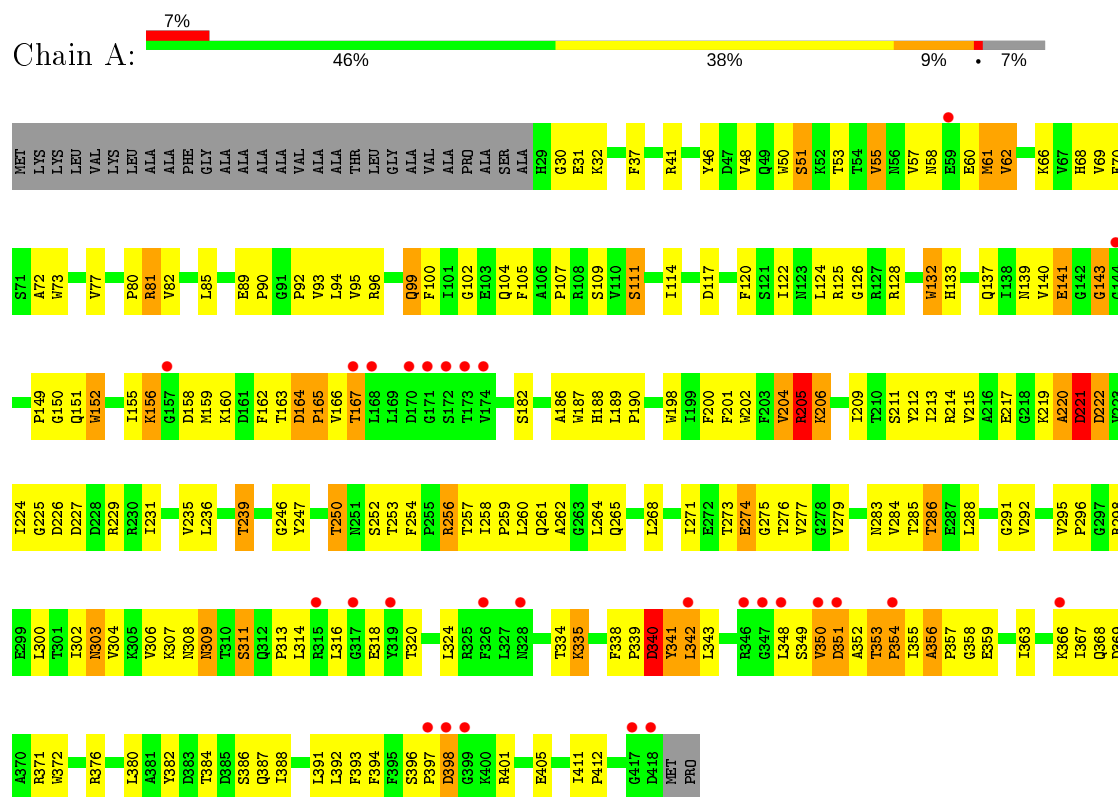


• Molecule 3: Particulate methane monooxygenase subunit B

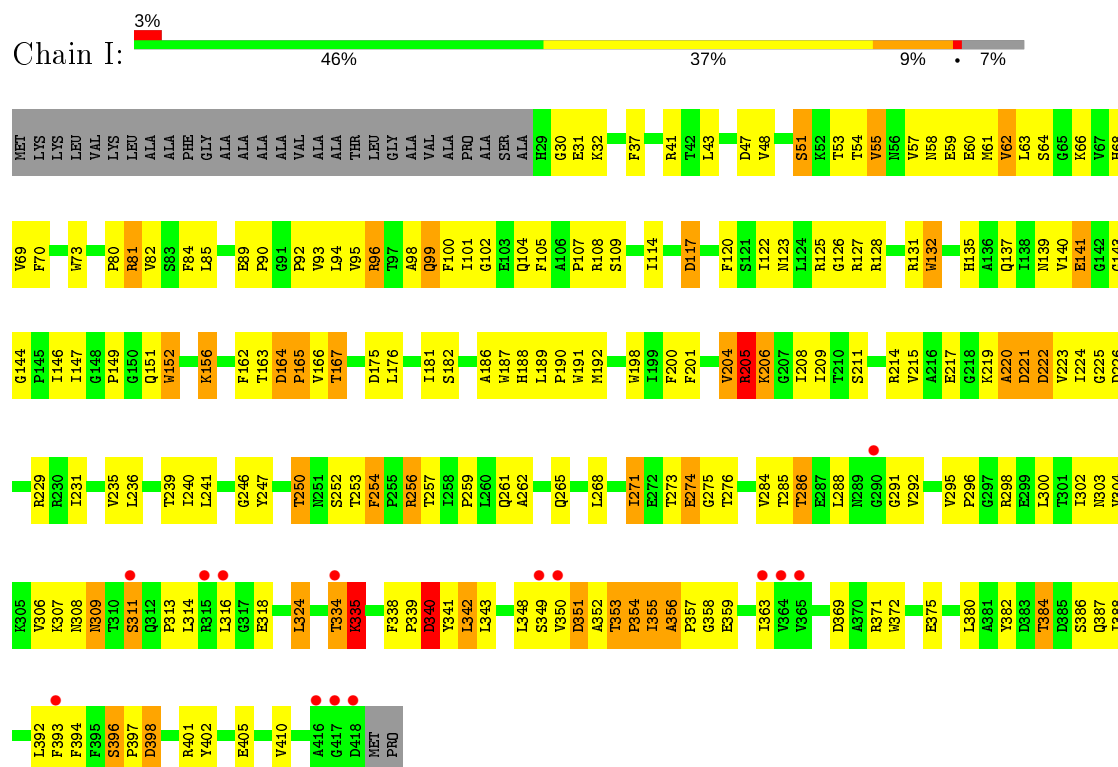
Chain E: 47% 35% 9% 7%



- Molecule 3: Particulate methane monooxygenase subunit B



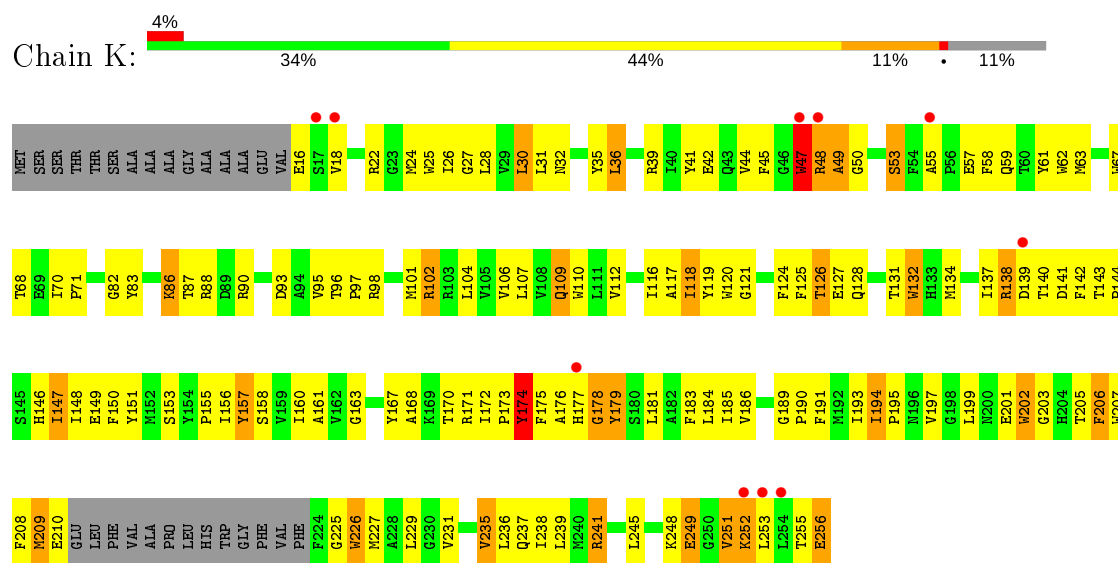
- Molecule 3: Particulate methane monooxygenase subunit B



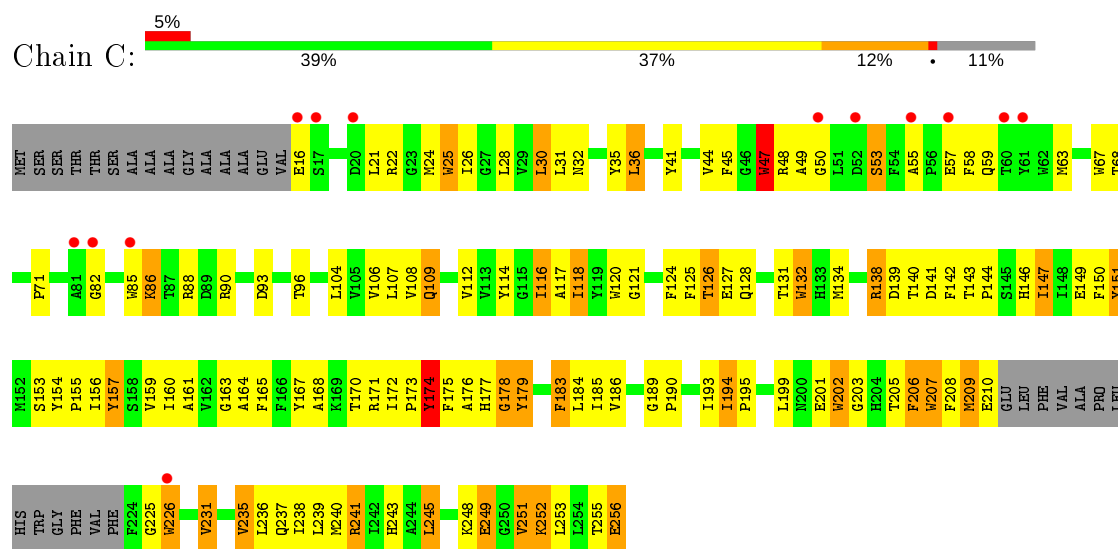
- Molecule 4: Particulate methane monooxygenase subunit C



• Molecule 4: Particulate methane monooxygenase subunit C



• Molecule 4: Particulate methane monooxygenase subunit C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.86Å 185.45Å 192.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.33 48.97 – 3.33	Depositor EDS
% Data completeness (in resolution range)	80.7 (50.00-3.33) 80.9 (48.97-3.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.67 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.225 , 0.282 0.223 , 0.279	Depositor DCC
R_{free} test set	2599 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.029 for -h,l,k	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	20979	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 4.27% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, ZN, 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	0.84	6/2052 (0.3%)	0.82	0/2814
2	F	0.91	5/2052 (0.2%)	0.87	1/2814 (0.0%)
2	J	0.91	6/2052 (0.3%)	0.88	0/2814
3	A	0.67	4/3115 (0.1%)	0.82	1/4243 (0.0%)
3	E	0.72	1/3115 (0.0%)	0.84	1/4243 (0.0%)
3	I	0.70	3/3115 (0.1%)	0.85	3/4243 (0.1%)
4	C	0.80	7/1932 (0.4%)	0.80	1/2634 (0.0%)
4	G	0.80	5/1932 (0.3%)	0.85	1/2634 (0.0%)
4	K	0.81	6/1932 (0.3%)	0.89	2/2634 (0.1%)
All	All	0.79	43/21297 (0.2%)	0.84	10/29073 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	N	0	1
3	A	0	1
3	E	0	2
3	I	0	1
4	C	0	1
4	G	0	1
4	K	0	1
All	All	0	8

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	106	TRP	CD2-CE2	6.74	1.49	1.41
4	K	132	TRP	CD2-CE2	6.64	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	132	TRP	CD2-CE2	6.39	1.49	1.41
3	A	372	TRP	CD2-CE2	5.97	1.48	1.41
2	B	106	TRP	CD2-CE2	5.95	1.48	1.41
2	F	106	TRP	CD2-CE2	5.89	1.48	1.41
3	I	152	TRP	CD2-CE2	5.89	1.48	1.41
4	C	25	TRP	CD2-CE2	5.87	1.48	1.41
2	F	65	TRP	CD2-CE2	5.84	1.48	1.41
4	C	85	TRP	CD2-CE2	5.79	1.48	1.41
2	F	242	TRP	CD2-CE2	5.73	1.48	1.41
3	I	372	TRP	CD2-CE2	5.72	1.48	1.41
2	J	85	TRP	CD2-CE2	5.65	1.48	1.41
4	K	25	TRP	CD2-CE2	5.64	1.48	1.41
4	C	132	TRP	CD2-CE2	5.60	1.48	1.41
2	B	53	TRP	CD2-CE2	5.58	1.48	1.41
4	G	207	TRP	CD2-CE2	5.55	1.48	1.41
2	J	242	TRP	CD2-CE2	5.47	1.48	1.41
4	C	207	TRP	CD2-CE2	5.46	1.48	1.41
4	G	62	TRP	CD2-CE2	5.45	1.47	1.41
2	B	85	TRP	CD2-CE2	5.43	1.47	1.41
4	K	67	TRP	CD2-CE2	5.43	1.47	1.41
4	K	47	TRP	CD2-CE2	5.40	1.47	1.41
4	K	207	TRP	CD2-CE2	5.40	1.47	1.41
2	B	242	TRP	CD2-CE2	5.39	1.47	1.41
3	A	132	TRP	CD2-CE2	5.29	1.47	1.41
2	F	56	TRP	CD2-CE2	5.27	1.47	1.41
4	C	47	TRP	CD2-CE2	5.27	1.47	1.41
3	A	152	TRP	CD2-CE2	5.26	1.47	1.41
2	B	236	TRP	CD2-CE2	5.25	1.47	1.41
2	B	116	TRP	CD2-CE2	5.24	1.47	1.41
2	J	116	TRP	CD2-CE2	5.23	1.47	1.41
4	G	132	TRP	CD2-CE2	5.23	1.47	1.41
4	G	226	TRP	CD2-CE2	5.20	1.47	1.41
4	G	85	TRP	CD2-CE2	5.20	1.47	1.41
4	K	202	TRP	CD2-CE2	5.20	1.47	1.41
2	J	157	TRP	CD2-CE2	5.17	1.47	1.41
3	E	191	TRP	CD2-CE2	5.16	1.47	1.41
3	A	50	TRP	CD2-CE2	5.14	1.47	1.41
2	J	59	TRP	CD2-CE2	5.13	1.47	1.41
2	F	85	TRP	CD2-CE2	5.08	1.47	1.41
4	C	202	TRP	CD2-CE2	5.08	1.47	1.41
4	C	67	TRP	CD2-CE2	5.05	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	96	ARG	NE-CZ-NH1	-7.62	116.49	120.30
4	G	138	ARG	NE-CZ-NH2	7.53	124.07	120.30
4	K	98	ARG	NE-CZ-NH1	6.15	123.38	120.30
3	I	96	ARG	NE-CZ-NH2	6.01	123.30	120.30
4	K	102	ARG	NE-CZ-NH2	5.60	123.10	120.30
3	A	342	LEU	N-CA-C	5.51	125.88	111.00
3	E	342	LEU	N-CA-C	5.39	125.57	111.00
4	C	138	ARG	NE-CZ-NH2	5.25	122.92	120.30
3	I	342	LEU	N-CA-C	5.17	124.95	111.00
2	F	214	GLY	N-CA-C	-5.10	100.35	113.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	340	ASP	Peptide
4	C	178	GLY	Peptide
3	E	340	ASP	Peptide
3	E	341	TYR	Peptide
4	G	178	GLY	Peptide
3	I	340	ASP	Peptide
4	K	178	GLY	Peptide
1	N	3	UNK	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	21	4	0
1	H	100	0	23	1	0
1	N	125	0	28	10	0
2	B	1974	0	1932	126	0
2	F	1974	0	1932	126	0
2	J	1974	0	1932	141	0
3	A	3038	0	3022	186	0
3	E	3038	0	3022	191	0
3	I	3038	0	3022	192	0
4	C	1870	0	1854	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	1870	0	1854	127	0
4	K	1870	0	1854	133	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
5	I	1	0	0	0	0
6	C	2	0	0	0	0
6	G	2	0	0	0	0
6	K	1	0	0	0	0
7	C	5	0	0	0	0
All	All	20979	0	20496	1196	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 29.

All (1196) 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:B:51:GLY:HA3	2:B:52:ASP:CB	1.70	1.21
3:A:334:THR:HA	3:A:335:LYS:HB2	1.24	1.18
2:J:51:GLY:HA3	2:J:52:ASP:CB	1.73	1.18
2:F:51:GLY:HA3	2:F:52:ASP:CB	1.75	1.16
2:B:51:GLY:CA	2:B:52:ASP:HB2	1.75	1.16
3:E:334:THR:HA	3:E:335:LYS:HB2	1.27	1.14
3:E:164:ASP:HB2	3:E:165:PRO:HA	1.25	1.14
4:G:104:LEU:HD23	4:G:172:ILE:HD13	1.29	1.13
3:E:224:ILE:HG22	3:E:225:GLY:H	1.05	1.13
2:J:51:GLY:CA	2:J:52:ASP:HB2	1.79	1.12
2:F:51:GLY:CA	2:F:52:ASP:HB2	1.80	1.11
3:A:164:ASP:HB2	3:A:165:PRO:HA	1.23	1.09
3:I:99:GLN:C	3:I:100:PHE:HD2	1.56	1.09
3:I:334:THR:HA	3:I:335:LYS:HB2	1.32	1.08
4:K:194:ILE:HG12	4:K:195:PRO:CD	1.84	1.08
3:I:164:ASP:HB2	3:I:165:PRO:HA	1.35	1.07
4:C:194:ILE:HG12	4:C:195:PRO:CD	1.87	1.05
4:G:194:ILE:HG12	4:G:195:PRO:HD3	1.37	1.05
3:E:396:SER:HB2	3:E:397:PRO:HD2	1.34	1.05
4:C:104:LEU:HD23	4:C:172:ILE:HD13	1.34	1.04
3:A:224:ILE:HG22	3:A:225:GLY:H	1.21	1.04
4:G:194:ILE:HG12	4:G:195:PRO:CD	1.87	1.03
2:F:51:GLY:HA3	2:F:52:ASP:HB2	1.02	1.02
2:F:10:VAL:HG21	4:G:254:LEU:HD11	1.37	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:104:LEU:HD23	4:K:172:ILE:HD13	1.36	1.01
3:E:107:PRO:HD2	3:E:265:GLN:HE22	1.25	1.01
3:I:308:ASN:HA	3:I:309:ASN:HB2	1.40	1.01
4:G:104:LEU:HD23	4:G:172:ILE:CD1	1.92	0.99
3:A:107:PRO:HD2	3:A:265:GLN:HE22	1.28	0.98
3:I:58:ASN:HD22	3:I:125:ARG:HH21	1.03	0.98
4:K:194:ILE:HG12	4:K:195:PRO:HD2	1.46	0.97
3:E:308:ASN:HA	3:E:309:ASN:HB2	1.47	0.96
3:E:224:ILE:HG22	3:E:225:GLY:N	1.81	0.96
3:I:224:ILE:HG22	3:I:225:GLY:H	1.27	0.95
3:E:318:GLU:HB3	3:E:393:PHE:HB2	1.48	0.95
3:A:334:THR:CA	3:A:335:LYS:HB2	1.97	0.94
4:G:104:LEU:CD2	4:G:172:ILE:HD13	1.96	0.94
3:I:318:GLU:HB3	3:I:393:PHE:HB2	1.47	0.94
2:F:246:THR:HG22	4:G:237:GLN:HG3	1.48	0.94
3:E:60:GLU:O	3:E:60:GLU:HG3	1.67	0.93
3:I:396:SER:HB2	3:I:397:PRO:HD2	1.46	0.93
3:A:58:ASN:HD22	3:A:125:ARG:HH21	0.97	0.93
3:E:334:THR:CA	3:E:335:LYS:HB2	1.98	0.93
3:A:396:SER:HB2	3:A:397:PRO:HD2	1.50	0.93
2:B:51:GLY:HA3	2:B:52:ASP:HB2	0.94	0.93
3:E:224:ILE:CG2	3:E:225:GLY:H	1.81	0.93
3:I:219:LYS:HA	3:I:220:ALA:HB3	1.50	0.92
2:B:246:THR:HG22	4:C:237:GLN:HG3	1.47	0.92
3:E:219:LYS:HB3	3:E:220:ALA:O	1.69	0.92
3:I:219:LYS:HB3	3:I:220:ALA:O	1.69	0.92
3:E:286:THR:HG22	3:E:304:VAL:CG1	2.00	0.92
3:E:352:ALA:O	3:E:354:PRO:HD3	1.69	0.92
3:A:318:GLU:HB3	3:A:393:PHE:HB2	1.52	0.91
4:K:44:VAL:HG12	4:K:45:PHE:CD1	2.04	0.91
3:I:286:THR:HG22	3:I:304:VAL:CG1	2.01	0.90
3:E:164:ASP:HB2	3:E:165:PRO:CA	2.02	0.90
3:A:308:ASN:HA	3:A:309:ASN:HB2	1.54	0.90
2:B:199:PRO:HB2	2:B:201:TYR:CE1	2.06	0.89
3:I:334:THR:CA	3:I:335:LYS:HB2	2.03	0.89
3:E:219:LYS:HA	3:E:220:ALA:HB3	1.52	0.89
3:A:352:ALA:O	3:A:354:PRO:HD3	1.72	0.89
4:G:24:MET:HB2	4:G:109:GLN:HG2	1.53	0.89
4:C:194:ILE:HG12	4:C:195:PRO:HD3	1.52	0.89
3:E:58:ASN:HD22	3:E:125:ARG:HH21	1.15	0.88
3:E:137:GLN:HE21	3:E:139:ASN:HD21	1.19	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:24:MET:HB2	4:K:109:GLN:HG2	1.53	0.88
4:C:104:LEU:HD23	4:C:172:ILE:CD1	2.02	0.88
3:A:219:LYS:HA	3:A:220:ALA:HB3	1.52	0.88
3:A:219:LYS:HB3	3:A:220:ALA:O	1.74	0.88
2:J:199:PRO:HB2	2:J:201:TYR:CE1	2.09	0.88
3:A:286:THR:HG22	3:A:304:VAL:CG1	2.04	0.87
3:A:164:ASP:HB2	3:A:165:PRO:CA	2.04	0.87
2:J:246:THR:HG22	4:K:237:GLN:HG3	1.53	0.87
2:J:200:GLU:O	2:J:201:TYR:HB3	1.74	0.87
3:A:60:GLU:HG3	3:A:60:GLU:O	1.74	0.86
4:K:104:LEU:HD23	4:K:172:ILE:CD1	2.04	0.86
4:G:194:ILE:H	4:G:194:ILE:HD13	1.41	0.86
3:E:225:GLY:HA2	3:E:229:ARG:NH2	1.90	0.86
3:I:352:ALA:O	3:I:354:PRO:HD3	1.74	0.85
3:E:356:ALA:HB1	3:E:357:PRO:CA	2.06	0.85
2:F:10:VAL:HG21	4:G:254:LEU:CD1	2.06	0.85
3:I:99:GLN:C	3:I:100:PHE:CD2	2.47	0.85
1:N:8:UNK:O	4:K:68:THR:HG21	1.77	0.85
3:A:224:ILE:HG22	3:A:225:GLY:N	1.92	0.84
4:C:194:ILE:HG12	4:C:195:PRO:HD2	1.58	0.84
3:I:340:ASP:O	3:I:343:LEU:HB3	1.77	0.84
3:I:164:ASP:HB2	3:I:165:PRO:CA	2.06	0.84
3:I:205:ARG:O	3:I:206:LYS:HE2	1.77	0.84
2:B:64:MET:HG3	2:B:204:MET:O	1.77	0.84
4:C:24:MET:HB2	4:C:109:GLN:HG2	1.60	0.84
2:F:29:MET:HE3	4:G:109:GLN:HG3	1.60	0.84
3:I:298:ARG:HG2	3:I:369:ASP:O	1.78	0.84
3:A:224:ILE:CG2	3:A:225:GLY:H	1.90	0.84
4:C:104:LEU:CD2	4:C:172:ILE:HD13	2.07	0.83
3:E:225:GLY:HA2	3:E:229:ARG:HH22	1.41	0.83
2:F:199:PRO:HB2	2:F:201:TYR:CE1	2.13	0.83
4:K:194:ILE:HG12	4:K:195:PRO:HD3	1.59	0.83
3:E:396:SER:HB2	3:E:397:PRO:CD	2.09	0.82
3:E:356:ALA:HB1	3:E:357:PRO:HA	1.61	0.82
3:A:58:ASN:HD22	3:A:125:ARG:NH2	1.76	0.82
2:J:51:GLY:HA3	2:J:52:ASP:HB2	0.88	0.81
3:A:225:GLY:HA2	3:A:229:ARG:NH2	1.96	0.81
3:E:286:THR:HG22	3:E:304:VAL:HG12	1.62	0.81
3:I:356:ALA:HB1	3:I:357:PRO:CA	2.11	0.81
3:I:137:GLN:HE21	3:I:139:ASN:HD21	1.29	0.80
3:I:308:ASN:CA	3:I:309:ASN:HB2	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:286:THR:HG22	3:I:304:VAL:HG12	1.64	0.80
3:A:236:LEU:HB2	2:B:138:VAL:HG11	1.63	0.80
3:A:356:ALA:HB1	3:A:357:PRO:CA	2.12	0.80
3:A:225:GLY:HA2	3:A:229:ARG:HH22	1.46	0.79
3:I:313:PRO:HG2	3:I:397:PRO:HD3	1.64	0.79
2:F:203:ARG:NH1	3:E:262:ALA:HB2	1.97	0.79
3:I:58:ASN:HD22	3:I:125:ARG:NH2	1.79	0.79
3:A:356:ALA:HB1	3:A:357:PRO:HA	1.64	0.78
4:K:93:ASP:OD1	4:K:177:HIS:HE1	1.67	0.78
3:A:188:HIS:HD2	2:B:106:TRP:HE1	1.31	0.78
3:I:356:ALA:HB1	3:I:357:PRO:HA	1.64	0.78
3:A:340:ASP:O	3:A:343:LEU:HB3	1.83	0.78
3:A:137:GLN:HE21	3:A:139:ASN:HD21	1.30	0.78
2:F:200:GLU:O	2:F:201:TYR:HB3	1.84	0.78
2:B:36:PHE:HE1	4:C:116:ILE:CD1	1.96	0.77
3:E:353:THR:O	3:E:355:ILE:N	2.16	0.77
2:F:106:TRP:HE1	3:E:188:HIS:HD2	1.31	0.77
3:E:58:ASN:HD21	3:E:163:THR:H	1.30	0.77
3:I:224:ILE:HG22	3:I:225:GLY:N	1.99	0.77
4:K:104:LEU:CD2	4:K:172:ILE:HD13	2.13	0.77
3:I:60:GLU:HG3	3:I:60:GLU:O	1.83	0.77
2:J:199:PRO:HB2	2:J:201:TYR:CD1	2.18	0.76
3:A:231:ILE:O	3:A:235:VAL:HG23	1.85	0.76
3:A:308:ASN:ND2	3:A:356:ALA:HB3	2.01	0.76
3:E:205:ARG:O	3:E:206:LYS:HE2	1.86	0.76
3:I:224:ILE:CG2	3:I:225:GLY:H	1.97	0.76
3:A:164:ASP:CB	3:A:165:PRO:HA	2.09	0.76
2:B:175:ALA:HB1	2:B:182:LEU:HD11	1.68	0.75
2:B:185:LEU:O	2:B:189:ILE:HG13	1.85	0.75
3:E:308:ASN:CA	3:E:309:ASN:HB2	2.16	0.75
3:E:273:THR:CA	3:E:274:GLU:HB2	2.16	0.75
3:E:340:ASP:O	3:E:343:LEU:HB3	1.87	0.75
3:I:94:LEU:HD23	3:I:126:GLY:HA2	1.68	0.75
3:I:273:THR:CA	3:I:274:GLU:HB2	2.16	0.75
4:C:194:ILE:H	4:C:194:ILE:HD13	1.51	0.75
3:E:73:TRP:CZ2	3:E:80:PRO:HG3	2.23	0.74
3:I:101:ILE:HG13	3:I:120:PHE:HB3	1.70	0.74
3:A:286:THR:HG22	3:A:304:VAL:HG12	1.67	0.74
3:I:273:THR:HA	3:I:274:GLU:HB2	1.68	0.74
3:A:94:LEU:HD23	3:A:126:GLY:HA2	1.70	0.74
2:F:175:ALA:HB1	2:F:182:LEU:HD11	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:PHE:CE1	4:C:116:ILE:HD12	2.24	0.73
4:K:209:MET:O	4:K:209:MET:HG2	1.88	0.73
3:E:107:PRO:HD2	3:E:265:GLN:NE2	2.00	0.73
3:I:99:GLN:O	3:I:100:PHE:HD2	1.72	0.73
3:I:48:VAL:HG21	3:I:149:PRO:HG2	1.70	0.73
2:B:150:ALA:O	2:B:154:SER:OG	2.06	0.72
3:I:68:HIS:HE1	3:I:405:GLU:OE1	1.71	0.72
3:E:356:ALA:HB1	3:E:357:PRO:C	2.09	0.72
3:E:273:THR:HA	3:E:274:GLU:HB2	1.71	0.72
3:I:353:THR:O	3:I:355:ILE:N	2.21	0.72
2:J:246:THR:HG22	4:K:237:GLN:CG	2.20	0.72
3:I:100:PHE:HA	3:I:104:GLN:O	1.90	0.72
3:E:48:VAL:HG21	3:E:149:PRO:HG2	1.71	0.72
2:J:203:ARG:O	2:J:204:MET:HB2	1.89	0.72
2:B:64:MET:HG3	2:B:205:VAL:HA	1.71	0.72
2:F:64:MET:HG3	2:F:204:MET:O	1.90	0.72
2:B:36:PHE:CE1	4:C:116:ILE:CD1	2.72	0.72
2:F:138:VAL:HG11	3:E:236:LEU:HB2	1.71	0.72
2:J:162:TYR:HB3	2:J:163:PRO:CD	2.19	0.71
4:K:117:ALA:HB1	4:K:157:TYR:HA	1.72	0.71
4:C:117:ALA:HB1	4:C:157:TYR:HA	1.73	0.71
3:E:324:LEU:H	3:E:324:LEU:HD12	1.55	0.71
4:G:44:VAL:HG12	4:G:45:PHE:CD1	2.25	0.71
2:J:29:MET:HE3	4:K:109:GLN:HG3	1.72	0.71
3:A:220:ALA:C	3:A:222:ASP:H	1.93	0.71
3:I:356:ALA:HB1	3:I:357:PRO:C	2.10	0.71
4:G:193:ILE:HD12	4:G:194:ILE:N	2.06	0.70
3:A:308:ASN:CA	3:A:309:ASN:HB2	2.20	0.70
3:E:100:PHE:HD2	3:E:105:PHE:HA	1.57	0.70
2:B:29:MET:HE3	4:C:109:GLN:HG3	1.71	0.70
2:F:162:TYR:HB3	2:F:163:PRO:HD3	1.73	0.70
2:F:199:PRO:HB2	2:F:201:TYR:CD1	2.26	0.70
3:I:380:LEU:HG	3:I:380:LEU:O	1.91	0.70
4:G:143:THR:O	4:G:147:ILE:HG12	1.91	0.70
2:B:214:GLY:HA2	2:B:215:LYS:HB2	1.72	0.70
3:A:73:TRP:CZ2	3:A:80:PRO:HG3	2.26	0.69
4:G:26:ILE:O	4:G:30:LEU:HB2	1.92	0.69
3:E:273:THR:HA	3:E:274:GLU:CB	2.22	0.69
4:C:251:VAL:HG12	4:C:252:LYS:N	2.08	0.69
3:I:188:HIS:HD2	2:J:106:TRP:HE1	1.40	0.69
3:A:58:ASN:HD21	3:A:163:THR:H	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:231:VAL:O	4:G:235:VAL:HG13	1.93	0.69
3:E:94:LEU:HD23	3:E:126:GLY:HA2	1.75	0.69
3:I:340:ASP:HB3	3:I:341:TYR:CB	2.22	0.69
3:I:73:TRP:CZ2	3:I:80:PRO:HG3	2.27	0.69
2:J:200:GLU:O	2:J:201:TYR:CB	2.41	0.69
4:C:32:ASN:O	4:C:36:LEU:HB2	1.93	0.69
2:F:36:PHE:HE1	4:G:116:ILE:CD1	2.06	0.69
3:E:308:ASN:ND2	3:E:356:ALA:HB3	2.08	0.68
4:K:193:ILE:HD12	4:K:194:ILE:N	2.08	0.68
3:I:273:THR:HA	3:I:274:GLU:CB	2.22	0.68
2:B:129:LEU:O	2:B:132:PRO:HD2	1.93	0.68
3:A:324:LEU:HD12	3:A:324:LEU:H	1.56	0.68
2:B:125:PHE:HZ	2:B:169:ILE:HD12	1.57	0.68
2:J:214:GLY:HA2	2:J:215:LYS:HB2	1.76	0.68
3:I:206:LYS:HB2	3:I:211:SER:OG	1.94	0.68
3:A:273:THR:CA	3:A:274:GLU:HB2	2.24	0.68
4:C:143:THR:O	4:C:147:ILE:HG12	1.93	0.68
2:J:9:ALA:HB3	2:J:15:SER:HA	1.76	0.67
3:A:273:THR:HA	3:A:274:GLU:HB2	1.75	0.67
4:C:138:ARG:NH1	4:C:141:ASP:HA	2.09	0.67
3:A:58:ASN:ND2	3:A:125:ARG:HH21	1.81	0.67
3:E:285:THR:HB	3:E:307:LYS:HB3	1.77	0.67
3:E:58:ASN:HD22	3:E:125:ARG:NH2	1.91	0.67
4:K:241:ARG:HA	4:K:241:ARG:HE	1.59	0.67
4:C:26:ILE:O	4:C:30:LEU:HB2	1.94	0.67
3:I:151:GLN:HE21	3:I:152:TRP:H	1.43	0.67
4:C:93:ASP:OD1	4:C:177:HIS:HE1	1.78	0.67
3:I:58:ASN:ND2	3:I:125:ARG:HH21	1.86	0.67
2:J:112:ASN:ND2	4:K:128:GLN:HG3	2.10	0.67
4:G:150:PHE:O	4:G:155:PRO:HD3	1.93	0.67
3:A:380:LEU:HD11	3:A:387:GLN:H	1.59	0.66
4:C:59:GLN:HA	4:C:63:MET:HB2	1.77	0.66
2:F:39:LEU:HD13	2:F:100:GLY:O	1.94	0.66
3:A:151:GLN:HE21	3:A:152:TRP:H	1.42	0.66
3:A:48:VAL:HG21	3:A:149:PRO:HG2	1.77	0.66
4:K:28:LEU:O	4:K:32:ASN:ND2	2.20	0.66
3:E:340:ASP:HB3	3:E:341:TYR:CB	2.25	0.66
3:A:261:GLN:HE22	3:I:386:SER:H	1.44	0.66
2:J:162:TYR:HB3	2:J:163:PRO:HD3	1.78	0.66
4:K:59:GLN:HA	4:K:63:MET:HB2	1.78	0.66
2:B:109:ARG:HG3	2:B:126:PRO:HD3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:29:MET:CE	4:G:109:GLN:HG3	2.25	0.66
3:A:353:THR:O	3:A:355:ILE:N	2.28	0.66
3:I:298:ARG:HG2	3:I:369:ASP:C	2.17	0.66
4:C:226:TRP:CE3	4:C:226:TRP:HA	2.31	0.65
4:G:194:ILE:HG12	4:G:195:PRO:HD2	1.75	0.65
3:A:69:VAL:CG1	3:A:114:ILE:HA	2.25	0.65
4:C:31:LEU:HD23	4:C:116:ILE:HG22	1.78	0.65
4:G:251:VAL:HG12	4:G:252:LYS:N	2.10	0.65
2:B:211:ARG:HG3	2:B:211:ARG:HH11	1.60	0.65
3:E:151:GLN:HE21	3:E:152:TRP:H	1.42	0.65
2:F:211:ARG:HH11	2:F:211:ARG:HG3	1.62	0.65
2:F:64:MET:HG3	2:F:205:VAL:HA	1.78	0.65
3:I:380:LEU:HD11	3:I:387:GLN:H	1.61	0.65
2:J:109:ARG:HG3	2:J:126:PRO:HD3	1.77	0.65
4:K:26:ILE:O	4:K:30:LEU:HB2	1.95	0.65
2:F:214:GLY:HA2	2:F:215:LYS:HB2	1.77	0.65
3:A:285:THR:HB	3:A:307:LYS:HB3	1.79	0.65
3:A:356:ALA:HB1	3:A:357:PRO:C	2.17	0.65
4:G:209:MET:HG2	4:G:209:MET:O	1.97	0.65
3:I:396:SER:HB2	3:I:397:PRO:CD	2.20	0.65
3:E:382:TYR:CD1	2:J:215:LYS:HE3	2.32	0.65
3:E:220:ALA:C	3:E:222:ASP:H	2.00	0.64
4:C:193:ILE:HD12	4:C:194:ILE:N	2.12	0.64
3:A:273:THR:HA	3:A:274:GLU:CB	2.28	0.64
3:A:396:SER:HB2	3:A:397:PRO:CD	2.26	0.64
2:F:246:THR:HG22	4:G:237:GLN:CG	2.23	0.64
3:A:206:LYS:HB2	3:A:211:SER:OG	1.98	0.64
2:F:162:TYR:HB3	2:F:163:PRO:CD	2.27	0.64
3:I:262:ALA:HB2	2:J:203:ARG:NH1	2.13	0.64
4:K:226:TRP:HA	4:K:226:TRP:CE3	2.32	0.64
3:E:151:GLN:HE21	3:E:152:TRP:N	1.96	0.64
3:I:85:LEU:HD23	3:I:99:GLN:HG3	1.79	0.64
4:C:241:ARG:HE	4:C:241:ARG:HA	1.62	0.64
2:F:36:PHE:CE1	4:G:116:ILE:CD1	2.81	0.64
2:J:36:PHE:O	2:J:36:PHE:HD1	1.80	0.64
3:E:380:LEU:O	3:E:380:LEU:HG	1.97	0.63
2:F:36:PHE:CE1	4:G:116:ILE:HD12	2.33	0.63
3:A:201:PHE:HZ	3:A:231:ILE:HD13	1.64	0.63
2:F:185:LEU:O	2:F:189:ILE:HG13	1.99	0.63
4:K:143:THR:O	4:K:147:ILE:HG12	1.98	0.63
4:K:251:VAL:HG12	4:K:252:LYS:N	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:44:VAL:HG12	4:C:45:PHE:CD1	2.33	0.63
4:G:138:ARG:NH1	4:G:141:ASP:HA	2.14	0.63
3:I:37:PHE:O	3:I:41:ARG:HG3	1.99	0.63
3:I:144:GLY:CA	2:B:211:ARG:HH12	2.10	0.63
2:J:113:PHE:HB3	2:J:124:VAL:HG21	1.81	0.63
3:A:69:VAL:HG11	3:A:114:ILE:HA	1.79	0.63
3:E:100:PHE:HA	3:E:104:GLN:O	1.97	0.63
3:I:225:GLY:HA2	3:I:229:ARG:NH2	2.14	0.63
2:F:44:VAL:HG23	4:G:122:ALA:O	1.99	0.62
2:J:61:ASP:OD2	2:J:64:MET:HG2	1.99	0.62
2:B:49:THR:OG1	2:B:72:LEU:HD22	1.99	0.62
2:F:36:PHE:HB3	2:F:39:LEU:HB3	1.81	0.62
3:I:275:GLY:HA2	3:I:276:THR:HB	1.81	0.62
4:K:121:GLY:HA2	4:K:153:SER:HB2	1.81	0.62
3:E:231:ILE:O	3:E:235:VAL:HG23	1.99	0.62
2:F:221:ALA:HA	4:C:206:PHE:HZ	1.64	0.62
3:E:68:HIS:HE1	3:E:405:GLU:OE1	1.82	0.62
2:B:29:MET:CE	4:C:109:GLN:HG3	2.28	0.62
3:A:224:ILE:CG2	3:A:225:GLY:N	2.58	0.62
4:C:209:MET:HG2	4:C:209:MET:O	2.00	0.62
4:C:189:GLY:N	4:C:190:PRO:HD2	2.15	0.62
3:I:189:LEU:N	3:I:190:PRO:HD2	2.15	0.62
2:F:203:ARG:O	2:F:204:MET:HB2	1.98	0.61
4:G:226:TRP:CE3	4:G:226:TRP:HA	2.34	0.61
2:F:10:VAL:CG2	4:G:254:LEU:HD11	2.22	0.61
3:E:164:ASP:CB	3:E:165:PRO:CA	2.74	0.61
3:I:220:ALA:C	3:I:222:ASP:H	2.02	0.61
3:E:275:GLY:HA2	3:E:276:THR:HB	1.82	0.61
3:E:356:ALA:CB	3:E:357:PRO:HA	2.31	0.61
3:A:107:PRO:HD2	3:A:265:GLN:NE2	2.08	0.61
3:A:259:PRO:HG3	3:I:382:TYR:O	2.01	0.61
2:F:221:ALA:HA	4:C:206:PHE:CZ	2.35	0.61
3:I:107:PRO:HD2	3:I:265:GLN:HE22	1.65	0.61
2:J:200:GLU:CG	2:J:203:ARG:HH11	2.14	0.61
3:I:30:GLY:O	3:I:32:LYS:N	2.33	0.61
4:G:117:ALA:HB1	4:G:157:TYR:HA	1.81	0.61
2:J:64:MET:HG3	2:J:205:VAL:HA	1.82	0.61
3:A:68:HIS:HE1	3:A:405:GLU:OE1	1.84	0.60
4:K:138:ARG:NH1	4:K:141:ASP:HA	2.16	0.60
2:B:224:PHE:CD2	4:K:199:LEU:HD22	2.36	0.60
2:J:200:GLU:HG2	2:J:203:ARG:HH11	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:117:ALA:HB2	4:C:160:ILE:HD13	1.83	0.60
4:G:152:MET:O	4:G:155:PRO:HD2	2.01	0.60
4:C:150:PHE:O	4:C:155:PRO:HD3	2.01	0.60
1:N:3:UNK:CB	4:K:41:TYR:OH	2.50	0.60
3:A:151:GLN:HE21	3:A:152:TRP:N	2.00	0.60
4:G:241:ARG:HA	4:G:241:ARG:HE	1.66	0.60
3:I:284:VAL:HG11	3:I:394:PHE:CE2	2.37	0.60
2:B:140:LEU:HD13	2:B:149:THR:OG1	2.02	0.60
3:E:380:LEU:HD11	3:E:387:GLN:H	1.66	0.60
3:E:261:GLN:HE22	3:A:386:SER:H	1.48	0.60
3:A:262:ALA:HB2	2:B:203:ARG:NH1	2.16	0.60
4:G:170:THR:O	4:G:171:ARG:HD2	2.01	0.60
3:I:225:GLY:HA2	3:I:229:ARG:HH22	1.67	0.60
1:D:13:UNK:HA	4:C:30:LEU:CD2	2.32	0.60
3:E:37:PHE:O	3:E:41:ARG:HG3	2.02	0.60
3:I:236:LEU:HB2	2:J:138:VAL:HG11	1.84	0.60
3:E:286:THR:CG2	3:E:304:VAL:CG1	2.78	0.59
4:G:206:PHE:HZ	2:J:221:ALA:HA	1.67	0.59
3:I:164:ASP:CB	3:I:165:PRO:CA	2.80	0.59
3:A:205:ARG:O	3:A:206:LYS:HE2	2.01	0.59
4:C:209:MET:O	4:C:210:GLU:O	2.20	0.59
2:F:109:ARG:HG3	2:F:126:PRO:HD3	1.84	0.59
4:K:189:GLY:N	4:K:190:PRO:HD2	2.16	0.59
3:A:201:PHE:CZ	3:A:231:ILE:HD13	2.37	0.59
2:B:200:GLU:O	2:B:201:TYR:HB3	2.02	0.59
3:A:313:PRO:HG2	3:A:397:PRO:HD3	1.85	0.59
2:B:200:GLU:HG2	2:B:203:ARG:CD	2.32	0.59
2:B:200:GLU:HG2	2:B:203:ARG:HH11	1.67	0.59
3:I:340:ASP:HB3	3:I:341:TYR:HA	1.84	0.59
2:B:39:LEU:HD13	2:B:100:GLY:O	2.02	0.59
2:B:199:PRO:HB2	2:B:201:TYR:CD1	2.36	0.59
2:F:135:TRP:NE1	2:F:156:GLY:HA3	2.16	0.59
3:I:151:GLN:HE21	3:I:152:TRP:N	2.01	0.59
2:F:106:TRP:HE1	3:E:188:HIS:CD2	2.19	0.59
3:E:284:VAL:HG11	3:E:394:PHE:CE2	2.38	0.59
3:I:137:GLN:HG3	3:I:147:ILE:HD13	1.84	0.59
4:G:206:PHE:CZ	2:J:221:ALA:HA	2.38	0.59
4:G:59:GLN:HA	4:G:63:MET:HB2	1.85	0.59
3:I:200:PHE:O	3:I:204:VAL:HG23	2.01	0.59
4:C:53:SER:HB3	4:C:139:ASP:HB2	1.85	0.59
4:G:32:ASN:O	4:G:36:LEU:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:55:VAL:HG12	3:I:59:GLU:HB3	1.84	0.59
3:I:58:ASN:HD21	3:I:163:THR:H	1.50	0.59
2:J:36:PHE:CE1	4:K:116:ILE:HD12	2.37	0.59
3:E:340:ASP:HB3	3:E:341:TYR:HB3	1.84	0.58
3:E:51:SER:HB3	3:E:62:VAL:H	1.68	0.58
3:A:213:ILE:HG12	4:C:243:HIS:CD2	2.37	0.58
3:E:198:TRP:O	3:E:202:TRP:HD1	1.86	0.58
2:J:166:TRP:HA	2:J:169:ILE:HG22	1.85	0.58
3:E:356:ALA:CB	3:E:357:PRO:CA	2.80	0.58
3:A:286:THR:CG2	3:A:304:VAL:CG1	2.80	0.58
3:E:339:PRO:O	3:E:340:ASP:C	2.41	0.58
3:I:219:LYS:HA	3:I:220:ALA:CB	2.28	0.58
3:I:51:SER:HB3	3:I:62:VAL:H	1.66	0.58
3:A:348:LEU:HB2	3:A:349:SER:HB2	1.86	0.58
4:K:32:ASN:O	4:K:36:LEU:HB2	2.02	0.58
2:B:203:ARG:O	2:B:204:MET:HB2	2.03	0.58
3:E:316:LEU:HD11	3:E:392:LEU:HD22	1.86	0.58
2:B:162:TYR:HB3	2:B:163:PRO:HD3	1.86	0.58
3:E:189:LEU:N	3:E:190:PRO:HD2	2.18	0.58
3:I:340:ASP:HB3	3:I:341:TYR:HB3	1.83	0.58
2:J:252:ILE:HA	2:B:146:TYR:HE1	1.68	0.58
4:K:146:HIS:CE1	4:K:201:GLU:OE1	2.56	0.58
3:I:340:ASP:HB3	3:I:341:TYR:CA	2.34	0.58
3:A:51:SER:HB3	3:A:62:VAL:H	1.69	0.57
2:F:200:GLU:O	2:F:201:TYR:CB	2.52	0.57
2:J:36:PHE:O	2:J:36:PHE:CD1	2.56	0.57
3:A:164:ASP:CB	3:A:165:PRO:CA	2.74	0.57
2:B:113:PHE:HB3	2:B:124:VAL:HG21	1.86	0.57
2:J:204:MET:CE	2:J:204:MET:HA	2.34	0.57
1:N:3:UNK:C	1:N:5:UNK:N	2.66	0.57
4:K:170:THR:O	4:K:171:ARG:HD2	2.04	0.57
3:E:137:GLN:NE2	3:E:139:ASN:HD21	1.97	0.57
4:C:108:VAL:O	4:C:112:VAL:HG23	2.05	0.57
3:I:339:PRO:O	3:I:340:ASP:C	2.42	0.57
3:I:286:THR:CG2	3:I:304:VAL:CG1	2.81	0.57
2:J:150:ALA:O	2:J:154:SER:OG	2.23	0.57
4:K:176:ALA:O	4:K:177:HIS:CD2	2.58	0.57
2:B:125:PHE:HZ	2:B:169:ILE:CD1	2.17	0.57
3:A:292:VAL:O	3:A:300:LEU:HD12	2.04	0.57
2:B:200:GLU:CG	2:B:203:ARG:HH11	2.17	0.57
3:E:201:PHE:CZ	3:E:231:ILE:HD13	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:200:GLU:HG2	2:F:203:ARG:HH11	1.69	0.57
2:F:200:GLU:HG2	2:F:203:ARG:HD2	1.87	0.57
2:J:220:VAL:HG23	2:J:221:ALA:N	2.20	0.57
3:A:219:LYS:HA	3:A:220:ALA:CB	2.29	0.57
3:A:46:TYR:HE2	3:A:66:LYS:HD2	1.70	0.57
4:G:241:ARG:O	4:G:245:LEU:HG	2.04	0.57
3:I:188:HIS:CD2	2:J:106:TRP:HE1	2.23	0.57
3:A:334:THR:CA	3:A:335:LYS:CB	2.80	0.56
3:I:99:GLN:O	3:I:100:PHE:CD2	2.55	0.56
3:I:229:ARG:HG3	3:I:229:ARG:HH11	1.70	0.56
3:E:206:LYS:HB2	3:E:211:SER:OG	2.05	0.56
3:I:382:TYR:CD1	2:B:215:LYS:HE3	2.40	0.56
2:B:214:GLY:CA	2:B:215:LYS:HB2	2.35	0.56
4:K:194:ILE:CG1	4:K:195:PRO:HD3	2.33	0.56
3:A:209:ILE:HG13	2:B:27:ASP:OD1	2.06	0.56
4:C:121:GLY:HA2	4:C:153:SER:HB2	1.88	0.56
4:G:53:SER:HB3	4:G:139:ASP:HB2	1.86	0.56
3:I:341:TYR:CE2	3:I:342:LEU:HD22	2.40	0.56
2:F:113:PHE:HB3	2:F:124:VAL:HG21	1.87	0.56
2:J:175:ALA:HB1	2:J:182:LEU:HD11	1.87	0.56
3:E:313:PRO:HG2	3:E:397:PRO:HD3	1.87	0.56
3:A:156:LYS:HB3	3:A:156:LYS:NZ	2.21	0.56
3:A:198:TRP:O	3:A:202:TRP:HD1	1.88	0.56
3:A:339:PRO:O	3:A:340:ASP:C	2.44	0.56
3:A:341:TYR:H	3:A:342:LEU:CA	2.18	0.56
3:A:341:TYR:CE2	3:A:342:LEU:HD22	2.41	0.56
4:G:128:GLN:O	4:G:131:THR:HG22	2.06	0.56
4:K:168:ALA:HB1	4:K:175:PHE:CD2	2.41	0.56
3:I:164:ASP:OD2	3:I:176:LEU:HB2	2.05	0.56
3:I:41:ARG:NE	3:I:387:GLN:HG2	2.19	0.56
2:J:214:GLY:CA	2:J:215:LYS:HB2	2.36	0.56
3:A:316:LEU:HD11	3:A:392:LEU:HD22	1.87	0.56
4:G:169:LYS:HD2	4:G:175:PHE:O	2.06	0.56
4:G:93:ASP:OD1	4:G:177:HIS:HE1	1.88	0.56
3:I:93:VAL:HA	3:I:128:ARG:HB2	1.88	0.56
3:A:356:ALA:CB	3:A:357:PRO:HA	2.36	0.56
2:F:167:PRO:HG2	3:E:187:TRP:CZ2	2.41	0.56
3:E:259:PRO:HG3	3:A:382:TYR:O	2.05	0.55
4:G:35:TYR:HE1	4:G:152:MET:HE2	1.71	0.55
4:G:86:LYS:HE3	4:G:86:LYS:HA	1.88	0.55
3:I:186:ALA:O	3:I:190:PRO:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:86:LYS:HE3	4:C:86:LYS:HA	1.88	0.55
3:E:69:VAL:CG1	3:E:114:ILE:HA	2.36	0.55
2:B:91:PRO:HB3	2:B:141:LEU:HD13	1.88	0.55
4:C:126:THR:HA	4:C:149:GLU:OE1	2.05	0.55
3:I:393:PHE:CD1	3:I:401:ARG:HD2	2.40	0.55
3:A:30:GLY:O	3:A:32:LYS:N	2.40	0.55
3:E:55:VAL:HG23	3:E:155:ILE:HG12	1.88	0.55
2:J:36:PHE:HB3	2:J:39:LEU:HB3	1.89	0.55
4:C:151:TYR:CD1	4:C:151:TYR:N	2.74	0.55
4:C:170:THR:O	4:C:171:ARG:HD2	2.06	0.55
2:F:36:PHE:HD1	2:F:36:PHE:O	1.90	0.55
2:F:200:GLU:HG2	2:F:203:ARG:CD	2.36	0.55
4:G:140:THR:HG23	4:G:142:PHE:H	1.70	0.55
2:J:203:ARG:HB3	2:J:205:VAL:HG22	1.89	0.55
2:B:221:ALA:HA	4:K:206:PHE:HZ	1.72	0.55
2:F:177:GLU:HG2	3:A:411:ILE:HG12	1.89	0.55
4:K:137:ILE:HG22	4:K:137:ILE:O	2.07	0.55
3:A:284:VAL:HG11	3:A:394:PHE:CE2	2.42	0.55
4:K:86:LYS:HE3	4:K:86:LYS:HA	1.89	0.55
1:D:13:UNK:HA	4:C:30:LEU:HD21	1.87	0.55
3:A:220:ALA:O	3:A:222:ASP:N	2.39	0.54
2:B:36:PHE:HB3	2:B:39:LEU:HB3	1.88	0.54
3:A:246:GLY:O	3:A:250:THR:OG1	2.25	0.54
1:N:7:UNK:O	1:N:9:UNK:N	2.41	0.54
3:A:93:VAL:HB	3:A:132:TRP:CD1	2.42	0.54
3:I:316:LEU:HD11	3:I:392:LEU:HD22	1.89	0.54
4:C:140:THR:HG23	4:C:142:PHE:H	1.71	0.54
2:J:64:MET:HG3	2:J:204:MET:O	2.06	0.54
1:N:7:UNK:C	1:N:9:UNK:N	2.67	0.54
3:A:212:TYR:CE2	4:C:239:LEU:HB3	2.42	0.54
3:A:291:GLY:HA3	3:A:302:ILE:HG22	1.88	0.54
2:B:162:TYR:HB3	2:B:163:PRO:CD	2.38	0.54
4:C:118:ILE:HG12	4:C:157:TYR:CE1	2.43	0.54
3:E:102:GLY:HA3	3:E:268:LEU:HD13	1.89	0.54
4:G:132:TRP:CZ2	4:G:144:PRO:HG2	2.43	0.54
4:K:88:ARG:HB2	4:K:170:THR:HB	1.90	0.54
2:B:198:MET:N	2:B:199:PRO:HD3	2.22	0.54
2:F:214:GLY:CA	2:F:215:LYS:HB2	2.38	0.54
4:G:143:THR:O	4:G:147:ILE:CG1	2.56	0.54
4:K:150:PHE:O	4:K:155:PRO:HD3	2.08	0.54
3:A:220:ALA:C	3:A:222:ASP:N	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:ALA:HA	4:K:206:PHE:CZ	2.42	0.54
3:E:298:ARG:HG2	3:E:369:ASP:O	2.08	0.54
4:K:126:THR:HA	4:K:149:GLU:OE1	2.07	0.54
2:F:191:PHE:CE1	3:E:107:PRO:HA	2.43	0.54
3:E:58:ASN:ND2	3:E:125:ARG:HH21	1.96	0.54
2:F:203:ARG:HH12	3:E:262:ALA:HB2	1.68	0.54
4:G:249:GLU:O	4:G:253:LEU:HB2	2.07	0.54
2:J:22:CYS:O	2:J:23:VAL:C	2.47	0.54
3:A:200:PHE:O	3:A:204:VAL:HG23	2.08	0.53
4:K:137:ILE:CG2	4:K:137:ILE:O	2.56	0.53
4:K:194:ILE:HD13	4:K:194:ILE:H	1.71	0.53
3:A:89:GLU:OE1	3:A:93:VAL:CG2	2.56	0.53
2:B:35:PHE:CZ	2:B:100:GLY:HA2	2.43	0.53
3:E:200:PHE:O	3:E:204:VAL:HG23	2.08	0.53
2:F:117:THR:HA	4:G:47:TRP:CH2	2.43	0.53
3:I:166:VAL:HG12	3:I:167:THR:N	2.23	0.53
3:A:186:ALA:O	3:A:190:PRO:HG3	2.09	0.53
3:I:125:ARG:HD3	3:I:162:PHE:CE2	2.42	0.53
3:I:188:HIS:HD2	2:J:106:TRP:NE1	2.04	0.53
3:A:340:ASP:HB3	3:A:341:TYR:CB	2.38	0.53
3:A:109:SER:HB3	2:B:201:TYR:HB3	1.91	0.53
4:C:252:LYS:O	4:C:256:GLU:HA	2.09	0.53
3:I:100:PHE:N	3:I:100:PHE:CD2	2.71	0.53
3:I:341:TYR:H	3:I:342:LEU:CA	2.21	0.53
4:K:209:MET:CG	4:K:209:MET:O	2.56	0.53
3:I:311:SER:HA	3:I:357:PRO:HB3	1.90	0.53
4:G:108:VAL:O	4:G:112:VAL:HG23	2.08	0.53
3:I:246:GLY:O	3:I:250:THR:OG1	2.25	0.53
2:J:125:PHE:HZ	2:J:169:ILE:CD1	2.22	0.53
3:A:66:LYS:HD3	3:A:271:ILE:HD13	1.89	0.53
3:A:55:VAL:HG23	3:A:155:ILE:HG12	1.91	0.53
4:G:174:TYR:CD1	4:G:174:TYR:C	2.82	0.53
3:I:308:ASN:ND2	3:I:356:ALA:HB3	2.23	0.53
3:E:137:GLN:HE21	3:E:139:ASN:ND2	1.99	0.53
3:E:340:ASP:HB3	3:E:341:TYR:CA	2.39	0.53
3:I:231:ILE:O	3:I:235:VAL:HG23	2.09	0.53
2:J:33:LEU:HB3	4:K:112:VAL:HG22	1.91	0.53
3:A:141:GLU:OE2	3:A:141:GLU:HA	2.09	0.52
3:E:166:VAL:HG12	3:E:167:THR:N	2.24	0.52
3:E:93:VAL:HB	3:E:132:TRP:CD1	2.44	0.52
2:J:82:ALA:HB1	2:J:241:ARG:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:21:LEU:O	4:G:25:TRP:CD1	2.63	0.52
4:K:35:TYR:OH	4:K:153:SER:HA	2.09	0.52
4:K:231:VAL:O	4:K:235:VAL:HG13	2.10	0.52
3:A:219:LYS:HD3	3:A:220:ALA:HB3	1.90	0.52
3:A:247:TYR:CE1	2:B:166:TRP:CD1	2.98	0.52
3:A:298:ARG:HG2	3:A:369:ASP:O	2.09	0.52
4:C:146:HIS:CE1	4:C:201:GLU:OE1	2.62	0.52
3:E:341:TYR:CE2	3:E:342:LEU:HD22	2.44	0.52
3:E:66:LYS:HD3	3:E:271:ILE:HD13	1.90	0.52
4:G:152:MET:C	4:G:155:PRO:HD2	2.30	0.52
4:G:156:ILE:O	4:G:159:VAL:N	2.41	0.52
3:I:201:PHE:CZ	3:I:231:ILE:HD13	2.44	0.52
2:J:102:LEU:HD12	2:J:130:ILE:HD12	1.91	0.52
2:F:125:PHE:HZ	2:F:169:ILE:HD12	1.74	0.52
3:E:101:ILE:HG13	3:E:120:PHE:HB3	1.92	0.52
3:I:356:ALA:CB	3:I:357:PRO:HA	2.36	0.52
3:A:356:ALA:CB	3:A:357:PRO:CA	2.86	0.52
2:B:82:ALA:HB1	2:B:241:ARG:HD2	1.91	0.52
3:E:340:ASP:HB3	3:E:341:TYR:HA	1.92	0.52
3:I:131:ARG:HB3	4:K:48:ARG:HH12	1.75	0.52
3:A:81:ARG:O	3:A:111:SER:HA	2.10	0.52
1:H:3:UNK:HA	4:G:61:TYR:HE1	1.74	0.52
3:I:108:ARG:HB3	2:J:200:GLU:OE1	2.09	0.52
4:K:50:GLY:HA2	4:K:58:PHE:HD1	1.75	0.52
4:C:16:GLU:N	4:C:16:GLU:CD	2.63	0.52
2:F:200:GLU:CG	2:F:203:ARG:HH11	2.21	0.52
2:F:215:LYS:HE3	3:A:382:TYR:CD1	2.45	0.52
3:I:285:THR:HB	3:I:307:LYS:HB3	1.92	0.52
3:A:340:ASP:HB3	3:A:341:TYR:HA	1.92	0.51
3:E:236:LEU:HG	3:E:240:ILE:HD12	1.92	0.51
3:I:209:ILE:HG13	2:J:27:ASP:OD1	2.10	0.51
4:K:174:TYR:C	4:K:174:TYR:CD1	2.83	0.51
4:C:121:GLY:HA2	4:C:153:SER:CB	2.40	0.51
4:C:55:ALA:HB1	4:C:57:GLU:OE1	2.11	0.51
4:K:174:TYR:C	4:K:174:TYR:HD1	2.13	0.51
3:A:298:ARG:HG2	3:A:369:ASP:C	2.30	0.51
3:A:366:LYS:HB2	3:A:366:LYS:HZ2	1.74	0.51
4:C:132:TRP:CZ2	4:C:144:PRO:HG2	2.46	0.51
4:C:167:TYR:CE1	4:C:171:ARG:HG2	2.45	0.51
3:E:58:ASN:ND2	3:E:163:THR:H	2.04	0.51
3:E:30:GLY:O	3:E:32:LYS:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:224:ILE:CG2	3:I:225:GLY:N	2.65	0.51
3:I:292:VAL:O	3:I:300:LEU:HD12	2.11	0.51
3:I:107:PRO:HA	2:J:191:PHE:CE1	2.45	0.51
3:I:176:LEU:HD12	2:J:192:HIS:CD2	2.45	0.51
4:K:120:TRP:HE3	4:K:125:PHE:CE2	2.29	0.51
3:E:69:VAL:HG11	3:E:114:ILE:HA	1.93	0.51
2:F:186:ALA:O	2:F:187:ASP:C	2.48	0.51
2:F:201:TYR:HD1	2:F:202:ILE:N	2.08	0.51
4:G:16:GLU:CD	4:G:16:GLU:N	2.64	0.51
4:G:178:GLY:O	4:G:179:TYR:CD2	2.64	0.51
3:I:298:ARG:CG	3:I:369:ASP:O	2.55	0.51
2:J:53:TRP:HB3	2:J:65:TRP:CD1	2.46	0.51
4:K:31:LEU:HD23	4:K:116:ILE:HG22	1.92	0.51
4:K:173:PRO:O	4:K:174:TYR:HB2	2.11	0.51
4:K:68:THR:O	4:K:71:PRO:HG2	2.10	0.51
3:A:77:VAL:HG13	3:A:143:GLY:HA3	1.92	0.51
2:B:60:LYS:HD3	2:B:65:TRP:CE2	2.46	0.51
4:C:168:ALA:HB1	4:C:175:PHE:CD2	2.46	0.51
3:E:292:VAL:O	3:E:300:LEU:HD12	2.09	0.51
3:I:98:ALA:HB1	3:I:100:PHE:HE2	1.76	0.51
3:A:46:TYR:CE2	3:A:66:LYS:HB2	2.46	0.51
2:B:198:MET:HG3	2:B:198:MET:O	2.11	0.51
2:B:200:GLU:HG2	2:B:203:ARG:HD3	1.93	0.51
2:F:38:VAL:CG2	2:F:39:LEU:N	2.73	0.51
3:I:144:GLY:HA3	2:B:211:ARG:HH12	1.74	0.51
3:A:275:GLY:HA2	3:A:276:THR:HB	1.93	0.51
2:B:61:ASP:OD2	2:B:64:MET:HG2	2.11	0.51
4:G:174:TYR:HD1	4:G:174:TYR:C	2.14	0.51
2:J:43:HIS:HD2	2:J:101:LEU:CD1	2.23	0.51
2:J:35:PHE:HD2	2:J:36:PHE:CD2	2.28	0.51
2:F:150:ALA:O	2:F:154:SER:OG	2.26	0.50
2:F:61:ASP:OD2	2:F:64:MET:HG2	2.11	0.50
3:I:57:VAL:HG12	3:I:58:ASN:OD1	2.11	0.50
4:K:44:VAL:HG12	4:K:45:PHE:CE1	2.43	0.50
3:A:366:LYS:HB2	3:A:366:LYS:NZ	2.26	0.50
3:A:393:PHE:CD1	3:A:401:ARG:HD2	2.46	0.50
2:B:238:PHE:HA	2:B:241:ARG:HG2	1.92	0.50
2:F:35:PHE:CZ	2:F:100:GLY:HA2	2.46	0.50
3:E:386:SER:H	3:I:261:GLN:HE22	1.60	0.50
2:J:131:VAL:HB	2:J:132:PRO:HD3	1.92	0.50
4:K:199:LEU:HD23	4:K:202:TRP:CZ3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:252:LYS:O	4:K:256:GLU:HA	2.11	0.50
4:K:35:TYR:CD2	4:K:120:TRP:CG	2.98	0.50
2:B:116:TRP:O	4:C:47:TRP:CZ3	2.64	0.50
2:B:162:TYR:CD2	2:B:218:VAL:HG11	2.46	0.50
2:B:36:PHE:HE1	4:C:116:ILE:HD12	1.64	0.50
2:F:201:TYR:HB3	3:E:109:SER:HB3	1.93	0.50
2:F:57:VAL:HG12	2:F:123:LEU:HA	1.94	0.50
2:B:150:ALA:HB2	2:B:233:TYR:CD1	2.47	0.50
4:C:225:GLY:C	4:C:226:TRP:HE3	2.15	0.50
3:E:298:ARG:HG2	3:E:369:ASP:C	2.32	0.50
3:E:284:VAL:HG11	3:E:394:PHE:CD2	2.46	0.50
2:F:82:ALA:HB1	2:F:241:ARG:HD2	1.94	0.50
4:G:169:LYS:O	4:G:176:ALA:HB2	2.11	0.50
3:I:308:ASN:ND2	3:I:314:LEU:HD12	2.26	0.50
2:J:116:TRP:HB2	4:K:39:ARG:NH1	2.26	0.50
3:A:41:ARG:NE	3:A:387:GLN:HG2	2.27	0.50
2:B:117:THR:HA	4:C:47:TRP:CH2	2.46	0.50
3:E:41:ARG:NE	3:E:387:GLN:HG2	2.26	0.50
3:I:356:ALA:CB	3:I:357:PRO:CA	2.84	0.50
4:K:178:GLY:O	4:K:179:TYR:CG	2.64	0.50
4:K:185:ILE:HG22	4:K:186:VAL:N	2.27	0.50
4:K:140:THR:HG23	4:K:142:PHE:H	1.76	0.50
2:B:65:TRP:CE3	2:B:66:PRO:HD3	2.47	0.50
2:J:39:LEU:HD13	2:J:100:GLY:O	2.12	0.50
2:J:99:LEU:HD11	2:J:103:ILE:HD11	1.93	0.50
4:K:117:ALA:HB2	4:K:160:ILE:HD13	1.94	0.50
3:A:94:LEU:HD22	3:A:124:LEU:HB3	1.94	0.50
3:E:341:TYR:H	3:E:342:LEU:CA	2.25	0.50
4:G:16:GLU:OE2	4:G:16:GLU:N	2.45	0.50
4:K:41:TYR:C	4:K:41:TYR:CD1	2.84	0.50
2:B:36:PHE:CE1	4:C:116:ILE:HD11	2.47	0.50
3:E:140:VAL:O	3:E:141:GLU:C	2.50	0.50
4:C:173:PRO:O	4:C:174:TYR:HB2	2.11	0.49
3:E:82:VAL:HB	3:E:141:GLU:HB2	1.94	0.49
2:F:204:MET:CE	2:F:204:MET:HA	2.42	0.49
4:G:120:TRP:HE3	4:G:125:PHE:CE2	2.30	0.49
4:G:118:ILE:HG12	4:G:157:TYR:CE1	2.47	0.49
2:J:252:ILE:HA	2:B:146:TYR:CE1	2.46	0.49
2:F:201:TYR:CD1	2:F:202:ILE:N	2.79	0.49
3:A:100:PHE:HD2	3:A:105:PHE:HA	1.78	0.49
3:A:93:VAL:HA	3:A:128:ARG:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:166:VAL:HG12	3:A:167:THR:N	2.28	0.49
3:A:188:HIS:HD2	2:B:106:TRP:NE1	2.03	0.49
4:C:194:ILE:CG1	4:C:195:PRO:HD3	2.35	0.49
3:E:198:TRP:O	3:E:202:TRP:CD1	2.65	0.49
4:K:93:ASP:OD1	4:K:177:HIS:CE1	2.57	0.49
3:A:188:HIS:CD2	2:B:106:TRP:HE1	2.20	0.49
2:B:57:VAL:HG12	2:B:123:LEU:HA	1.95	0.49
2:F:211:ARG:CG	2:F:211:ARG:HH11	2.25	0.49
2:J:140:LEU:HD13	2:J:149:THR:OG1	2.12	0.49
2:J:62:ARG:HB3	2:J:218:VAL:HG22	1.95	0.49
4:K:194:ILE:CG1	4:K:195:PRO:CD	2.74	0.49
3:E:246:GLY:O	3:E:250:THR:OG1	2.31	0.49
3:E:96:ARG:NH2	3:E:99:GLN:HE22	2.09	0.49
2:F:140:LEU:HD13	2:F:149:THR:OG1	2.12	0.49
2:F:224:PHE:CD2	4:C:199:LEU:HD22	2.48	0.49
3:A:94:LEU:HD23	3:A:126:GLY:CA	2.41	0.49
4:C:21:LEU:O	4:C:25:TRP:CD1	2.66	0.49
3:E:60:GLU:OE2	3:E:123:ASN:HB3	2.12	0.49
3:E:191:TRP:CZ3	3:E:239:THR:HG23	2.48	0.49
3:E:219:LYS:HA	3:E:220:ALA:CB	2.31	0.49
3:E:224:ILE:CG2	3:E:225:GLY:N	2.50	0.49
3:E:393:PHE:CD1	3:E:401:ARG:HD2	2.48	0.49
4:G:225:GLY:C	4:G:226:TRP:HE3	2.16	0.49
4:G:225:GLY:O	4:G:226:TRP:HE3	1.96	0.49
3:A:341:TYR:CG	3:A:342:LEU:HB2	2.48	0.49
3:I:141:GLU:OE2	3:I:141:GLU:HA	2.12	0.49
3:I:226:ASP:HA	3:I:229:ARG:H	1.78	0.49
2:J:252:ILE:O	2:B:146:TYR:HD1	1.96	0.49
4:C:231:VAL:O	4:C:235:VAL:HG13	2.12	0.49
2:F:39:LEU:HD11	2:F:104:GLY:HA3	1.94	0.49
3:I:250:THR:HG21	2:J:167:PRO:HA	1.94	0.49
2:J:36:PHE:HE1	4:K:116:ILE:HD12	1.76	0.49
3:A:100:PHE:HA	3:A:104:GLN:O	2.12	0.49
3:A:261:GLN:NE2	3:I:386:SER:H	2.08	0.49
2:B:65:TRP:HE3	2:B:66:PRO:HD3	1.77	0.49
3:E:58:ASN:HD21	3:E:163:THR:N	2.05	0.49
2:F:56:TRP:HB2	2:F:59:TRP:CD1	2.48	0.49
2:J:245:THR:HG23	2:J:245:THR:O	2.12	0.49
2:B:55:PHE:O	2:B:124:VAL:HA	2.13	0.48
2:B:200:GLU:HG2	2:B:203:ARG:HD2	1.94	0.48
3:I:109:SER:HB3	2:J:201:TYR:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:46:TYR:CE2	3:A:66:LYS:HD2	2.46	0.48
4:C:28:LEU:O	4:C:32:ASN:ND2	2.31	0.48
3:E:131:ARG:HB3	4:G:48:ARG:HH12	1.77	0.48
3:E:351:ASP:HB2	3:E:353:THR:OG1	2.13	0.48
1:N:3:UNK:CB	4:K:61:TYR:HD1	2.26	0.48
3:E:311:SER:HA	3:E:357:PRO:HB3	1.96	0.48
2:J:45:HIS:HB2	4:K:227:MET:CE	2.43	0.48
3:A:89:GLU:OE1	3:A:93:VAL:HG23	2.14	0.48
2:F:166:TRP:HA	2:F:169:ILE:HG22	1.94	0.48
4:G:104:LEU:HD23	4:G:172:ILE:HD11	1.87	0.48
2:J:135:TRP:NE1	2:J:156:GLY:HA3	2.28	0.48
4:C:178:GLY:O	4:C:179:TYR:CD2	2.66	0.48
4:C:50:GLY:HA2	4:C:58:PHE:HD1	1.78	0.48
4:C:88:ARG:HB2	4:C:170:THR:HB	1.96	0.48
3:E:339:PRO:HB2	3:E:341:TYR:HD2	1.78	0.48
3:I:32:LYS:HG2	3:I:375:GLU:HA	1.96	0.48
3:A:283:ASN:O	3:A:309:ASN:HB3	2.13	0.48
3:A:340:ASP:HB3	3:A:341:TYR:CA	2.44	0.48
4:C:68:THR:O	4:C:71:PRO:HG2	2.14	0.48
3:A:284:VAL:HG11	3:A:394:PHE:CD2	2.48	0.48
4:G:167:TYR:CE1	4:G:171:ARG:HG2	2.49	0.48
4:G:31:LEU:HD23	4:G:116:ILE:HG22	1.96	0.48
3:I:192:MET:CE	2:J:103:ILE:HG13	2.44	0.48
4:K:110:TRP:CZ3	4:K:163:GLY:HA3	2.49	0.48
3:A:140:VAL:O	3:A:141:GLU:C	2.52	0.48
4:C:165:PHE:HA	4:C:183:PHE:CE1	2.49	0.48
3:E:334:THR:CA	3:E:335:LYS:CB	2.81	0.48
4:G:240:MET:HB2	4:G:240:MET:HE2	1.61	0.48
3:I:198:TRP:HZ3	3:I:235:VAL:HG21	1.79	0.48
3:I:99:GLN:OE1	2:J:191:PHE:HE1	1.97	0.48
1:N:9:UNK:C	1:N:11:UNK:N	2.77	0.48
2:J:116:TRP:O	4:K:47:TRP:CZ3	2.66	0.48
2:F:252:ILE:O	2:J:145:SER:HA	2.14	0.48
3:A:311:SER:HA	3:A:357:PRO:HB3	1.95	0.47
2:B:132:PRO:HB2	2:B:157:TRP:CE3	2.49	0.47
3:A:92:PRO:HB3	2:B:193:PHE:HA	1.95	0.47
2:B:201:TYR:HA	2:B:207:ARG:NH2	2.29	0.47
2:B:85:TRP:CE2	2:B:89:ARG:HD3	2.48	0.47
4:C:226:TRP:CE3	4:C:226:TRP:CA	2.96	0.47
4:C:35:TYR:CD2	4:C:120:TRP:CG	3.01	0.47
3:E:201:PHE:HZ	3:E:231:ILE:HD13	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:49:THR:OG1	2:F:72:LEU:HD22	2.14	0.47
4:G:148:ILE:N	4:G:148:ILE:HD13	2.27	0.47
4:G:126:THR:HA	4:G:149:GLU:OE1	2.14	0.47
3:A:69:VAL:HG12	3:A:114:ILE:HA	1.95	0.47
2:B:57:VAL:CG1	2:B:123:LEU:HA	2.44	0.47
4:C:174:TYR:C	4:C:174:TYR:CD1	2.87	0.47
2:F:55:PHE:O	2:F:124:VAL:HA	2.14	0.47
3:I:388:ILE:HD13	3:I:410:VAL:HG21	1.94	0.47
2:B:125:PHE:CZ	2:B:169:ILE:CD1	2.96	0.47
2:F:65:TRP:N	2:F:66:PRO:HD2	2.29	0.47
3:I:101:ILE:O	3:I:104:GLN:N	2.43	0.47
4:K:124:PHE:HD2	4:K:125:PHE:CE2	2.32	0.47
4:K:121:GLY:HA2	4:K:153:SER:CB	2.43	0.47
4:K:201:GLU:C	4:K:203:GLY:H	2.17	0.47
4:K:225:GLY:C	4:K:226:TRP:HE3	2.17	0.47
1:N:7:UNK:O	1:N:8:UNK:C	2.62	0.47
3:E:201:PHE:CE1	3:E:205:ARG:HG3	2.48	0.47
4:G:88:ARG:HB2	4:G:170:THR:HB	1.96	0.47
4:G:178:GLY:O	4:G:179:TYR:CG	2.66	0.47
4:K:236:LEU:HD23	4:K:236:LEU:HA	1.68	0.47
4:K:256:GLU:N	4:K:256:GLU:CD	2.67	0.47
3:A:380:LEU:O	3:A:380:LEU:HG	2.15	0.47
3:E:226:ASP:HA	3:E:229:ARG:H	1.80	0.47
3:E:286:THR:CG2	3:E:304:VAL:HG11	2.44	0.47
4:G:252:LYS:O	4:G:256:GLU:HA	2.15	0.47
2:J:200:GLU:HG2	2:J:203:ARG:CD	2.44	0.47
3:A:235:VAL:O	3:A:239:THR:OG1	2.33	0.47
4:C:120:TRP:HE3	4:C:125:PHE:CE2	2.32	0.47
4:G:100:GLU:HG2	4:G:245:LEU:HD11	1.95	0.47
4:G:70:ILE:HB	4:G:71:PRO:CD	2.44	0.47
2:J:43:HIS:HD2	2:J:101:LEU:HD11	1.79	0.47
2:F:22:CYS:O	2:F:23:VAL:C	2.52	0.47
2:F:36:PHE:CD1	2:F:36:PHE:O	2.67	0.47
4:G:19:VAL:HA	4:G:105:VAL:HG11	1.97	0.47
4:G:165:PHE:HA	4:G:183:PHE:CE1	2.50	0.47
4:G:68:THR:O	4:G:71:PRO:HG2	2.14	0.47
3:A:261:GLN:HE22	3:I:386:SER:N	2.10	0.47
3:E:411:ILE:HG12	2:J:177:GLU:HG2	1.96	0.47
2:F:67:THR:HG1	4:C:206:PHE:HE1	1.62	0.47
4:G:209:MET:O	4:G:210:GLU:O	2.32	0.47
3:I:80:PRO:HA	3:I:140:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:291:GLY:HA3	3:I:302:ILE:HG22	1.96	0.47
2:J:245:THR:HG21	4:K:181:LEU:HD23	1.96	0.47
3:E:220:ALA:C	3:E:222:ASP:N	2.67	0.47
3:E:308:ASN:ND2	3:E:314:LEU:HD12	2.30	0.47
3:I:187:TRP:CZ2	2:J:167:PRO:HG2	2.49	0.47
4:C:128:GLN:O	4:C:131:THR:HG22	2.14	0.47
4:C:163:GLY:O	4:C:164:ALA:C	2.51	0.47
4:C:82:GLY:O	4:C:86:LYS:HB2	2.14	0.47
2:J:53:TRP:HB3	2:J:65:TRP:HD1	1.79	0.47
4:K:226:TRP:CA	4:K:226:TRP:CE3	2.96	0.47
3:A:313:PRO:HB2	3:A:354:PRO:HB3	1.97	0.47
4:K:149:GLU:OE2	4:K:150:PHE:CE1	2.68	0.47
4:C:178:GLY:O	4:C:179:TYR:CG	2.69	0.46
2:J:199:PRO:CB	2:J:201:TYR:CE1	2.91	0.46
4:K:117:ALA:HB1	4:K:157:TYR:CA	2.45	0.46
4:K:53:SER:HB3	4:K:139:ASP:HB2	1.97	0.46
2:B:117:THR:HG22	4:C:47:TRP:HH2	1.80	0.46
3:E:101:ILE:HG23	3:E:268:LEU:HD11	1.95	0.46
2:F:57:VAL:CG1	2:F:123:LEU:HA	2.45	0.46
3:I:137:GLN:HG3	3:I:147:ILE:CD1	2.44	0.46
3:I:82:VAL:HB	3:I:141:GLU:HB2	1.97	0.46
3:I:236:LEU:HG	3:I:240:ILE:HD12	1.98	0.46
2:J:102:LEU:HA	2:J:102:LEU:HD23	1.47	0.46
2:B:132:PRO:HB3	2:B:157:TRP:HA	1.97	0.46
4:C:240:MET:HE2	4:C:240:MET:HB2	1.77	0.46
2:F:238:PHE:HA	2:F:241:ARG:HG2	1.97	0.46
4:G:209:MET:CG	4:G:209:MET:O	2.62	0.46
3:I:141:GLU:H	2:J:201:TYR:HE2	1.62	0.46
2:J:53:TRP:CD1	2:J:65:TRP:HB2	2.50	0.46
4:K:18:VAL:HG11	4:K:101:MET:CE	2.46	0.46
2:F:27:ASP:OD1	3:E:209:ILE:HG13	2.15	0.46
3:E:214:ARG:HB3	3:E:220:ALA:H	1.79	0.46
3:E:273:THR:CA	3:E:274:GLU:CB	2.84	0.46
3:I:324:LEU:HD12	3:I:324:LEU:H	1.80	0.46
2:J:29:MET:CE	4:K:109:GLN:HG3	2.41	0.46
4:K:44:VAL:CG1	4:K:45:PHE:CE1	2.98	0.46
3:E:135:HIS:HA	3:E:149:PRO:O	2.16	0.46
3:A:189:LEU:N	3:A:190:PRO:HD2	2.31	0.46
3:A:262:ALA:HB2	2:B:203:ARG:HH12	1.81	0.46
4:C:41:TYR:C	4:C:41:TYR:CD1	2.89	0.46
2:F:44:VAL:CG2	4:G:122:ALA:O	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:201:TYR:HA	2:J:207:ARG:NH2	2.31	0.46
4:K:27:GLY:O	4:K:31:LEU:HB2	2.16	0.46
3:A:411:ILE:HG23	3:A:412:PRO:HD2	1.98	0.46
2:B:117:THR:HG22	4:C:47:TRP:CH2	2.51	0.46
3:E:186:ALA:O	3:E:190:PRO:HG3	2.16	0.46
3:E:187:TRP:O	3:E:191:TRP:HD1	1.99	0.46
3:E:213:ILE:HG12	4:G:243:HIS:CD2	2.51	0.46
4:G:39:ARG:O	4:G:39:ARG:NH2	2.46	0.46
2:J:125:PHE:HZ	2:J:169:ILE:HD12	1.80	0.46
2:B:129:LEU:C	2:B:132:PRO:HD2	2.36	0.46
2:B:204:MET:HA	2:B:204:MET:CE	2.46	0.46
2:B:108:ASN:ND2	4:C:127:GLU:OE2	2.39	0.46
3:E:93:VAL:HA	3:E:128:ARG:HB2	1.98	0.46
4:K:119:TYR:C	4:K:119:TYR:CD2	2.87	0.46
2:J:108:ASN:ND2	4:K:127:GLU:HB3	2.31	0.46
2:B:109:ARG:O	2:B:113:PHE:HB2	2.16	0.46
2:B:200:GLU:O	2:B:201:TYR:CB	2.64	0.46
2:B:43:HIS:HD2	2:B:101:LEU:CD1	2.29	0.46
3:E:96:ARG:HH21	3:E:99:GLN:HE22	1.63	0.46
4:G:194:ILE:H	4:G:194:ILE:CD1	2.18	0.46
4:G:39:ARG:HH22	4:G:43:GLN:HB2	1.81	0.46
2:J:65:TRP:N	2:J:66:PRO:HD2	2.31	0.46
3:A:286:THR:CG2	3:A:304:VAL:HG11	2.45	0.45
3:I:96:ARG:NH2	3:I:99:GLN:HE22	2.14	0.45
2:J:117:THR:HA	4:K:47:TRP:CH2	2.50	0.45
3:A:308:ASN:ND2	3:A:314:LEU:HD12	2.32	0.45
2:B:135:TRP:NE1	2:B:156:GLY:HA3	2.31	0.45
2:B:56:TRP:HB2	2:B:59:TRP:CD1	2.51	0.45
3:I:220:ALA:C	3:I:222:ASP:N	2.69	0.45
2:J:76:PHE:CE2	4:K:229:LEU:HD21	2.51	0.45
3:A:60:GLU:O	3:A:60:GLU:CG	2.52	0.45
2:F:38:VAL:HG23	2:F:39:LEU:N	2.31	0.45
2:F:60:LYS:HD3	2:F:65:TRP:CE2	2.52	0.45
3:I:219:LYS:CB	3:I:220:ALA:O	2.53	0.45
4:K:18:VAL:HG13	4:K:102:ARG:HA	1.98	0.45
3:E:229:ARG:HH11	3:E:229:ARG:HG3	1.82	0.45
3:E:273:THR:OG1	3:E:273:THR:O	2.33	0.45
4:G:168:ALA:HB1	4:G:175:PHE:CD2	2.52	0.45
3:I:156:LYS:HB3	3:I:156:LYS:NZ	2.31	0.45
3:I:221:ASP:OD1	3:I:221:ASP:N	2.50	0.45
2:J:108:ASN:OD1	2:J:112:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:51:GLY:CA	2:J:52:ASP:CB	2.59	0.45
2:F:43:HIS:HD2	2:F:101:LEU:CD1	2.29	0.45
2:F:91:PRO:HB3	2:F:141:LEU:HD13	1.98	0.45
2:F:44:VAL:HG22	4:G:126:THR:HG21	1.99	0.45
3:I:219:LYS:HD3	3:I:220:ALA:HB3	1.98	0.45
3:I:247:TYR:CE1	2:J:166:TRP:CD1	3.04	0.45
2:J:71:ILE:HG23	2:J:232:VAL:HG21	1.99	0.45
2:J:45:HIS:HB2	4:K:227:MET:HE3	1.99	0.45
3:A:70:PHE:HE2	3:A:72:ALA:HB3	1.81	0.45
2:B:119:PHE:HB3	2:B:123:LEU:HD23	1.97	0.45
4:G:117:ALA:HB2	4:G:160:ILE:HD13	1.97	0.45
3:I:163:THR:HG22	3:I:175:ASP:OD2	2.16	0.45
3:A:300:LEU:HD23	3:A:367:ILE:HD13	1.99	0.45
2:B:166:TRP:HA	2:B:169:ILE:HG22	1.99	0.45
3:E:308:ASN:HA	3:E:309:ASN:CB	2.32	0.45
2:F:131:VAL:HB	2:F:132:PRO:HD3	1.98	0.45
2:F:249:ILE:O	4:G:178:GLY:O	2.35	0.45
3:I:191:TRP:CZ3	3:I:239:THR:HG23	2.52	0.45
3:I:60:GLU:CG	3:I:60:GLU:O	2.61	0.45
2:J:114:TRP:O	2:J:118:TYR:N	2.46	0.45
4:K:107:LEU:HD23	4:K:238:ILE:HD11	1.99	0.45
2:B:38:VAL:CG2	2:B:39:LEU:N	2.79	0.45
2:B:71:ILE:HD11	2:B:225:SER:HA	1.97	0.45
1:D:20:UNK:CB	4:C:26:ILE:HD13	2.47	0.45
3:E:291:GLY:HA3	3:E:302:ILE:HG22	1.97	0.45
3:E:342:LEU:N	3:E:371:ARG:HD3	2.31	0.45
4:K:120:TRP:HE3	4:K:125:PHE:HE2	1.64	0.45
3:A:102:GLY:HA3	3:A:268:LEU:HD13	1.99	0.45
4:C:249:GLU:O	4:C:253:LEU:HB2	2.16	0.45
4:K:148:ILE:HD13	4:K:148:ILE:N	2.32	0.45
4:K:158:SER:O	4:K:161:ALA:HB3	2.17	0.45
3:A:303:ASN:OD1	3:A:303:ASN:N	2.50	0.45
3:A:32:LYS:O	3:A:376:ARG:HD3	2.17	0.45
3:A:96:ARG:NH2	3:A:99:GLN:HE22	2.15	0.45
3:E:286:THR:HG22	3:E:304:VAL:HG11	1.94	0.45
2:F:199:PRO:HB3	3:E:84:PHE:CB	2.47	0.45
3:I:43:LEU:HG	3:I:146:ILE:HD12	1.99	0.45
2:J:36:PHE:CE1	4:K:116:ILE:CD1	3.00	0.45
3:A:227:ASP:O	3:A:231:ILE:HG13	2.16	0.44
3:A:89:GLU:OE1	3:A:93:VAL:HG22	2.18	0.44
3:A:236:LEU:CB	2:B:138:VAL:HG11	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:144:GLY:CA	2:J:211:ARG:HH12	2.30	0.44
2:F:119:PHE:HB3	2:F:123:LEU:HD23	1.98	0.44
2:F:198:MET:N	2:F:199:PRO:HD3	2.32	0.44
4:G:147:ILE:H	4:G:147:ILE:HG12	1.53	0.44
3:I:140:VAL:O	3:I:141:GLU:C	2.54	0.44
2:J:36:PHE:HE1	4:K:116:ILE:CD1	2.30	0.44
4:C:176:ALA:O	4:C:177:HIS:CD2	2.70	0.44
2:F:116:TRP:O	4:G:47:TRP:CZ3	2.71	0.44
4:G:44:VAL:HG12	4:G:45:PHE:CE1	2.52	0.44
3:I:98:ALA:HA	2:J:191:PHE:HE2	1.82	0.44
2:J:198:MET:N	2:J:199:PRO:HD3	2.31	0.44
4:K:249:GLU:O	4:K:253:LEU:HB2	2.17	0.44
3:A:82:VAL:HG13	3:A:264:LEU:HD13	2.00	0.44
3:A:339:PRO:HB2	3:A:341:TYR:HD2	1.83	0.44
3:E:392:LEU:HA	3:E:392:LEU:HD23	1.64	0.44
3:I:93:VAL:HB	3:I:132:TRP:CD1	2.53	0.44
4:K:146:HIS:HE1	4:K:201:GLU:OE1	1.99	0.44
2:B:186:ALA:O	2:B:187:ASP:C	2.56	0.44
3:E:411:ILE:HG23	3:E:412:PRO:HD2	2.00	0.44
2:F:102:LEU:HD23	2:F:102:LEU:HA	1.54	0.44
2:F:201:TYR:CD1	2:F:201:TYR:C	2.90	0.44
3:I:100:PHE:HZ	2:J:179:HIS:NE2	2.15	0.44
3:I:284:VAL:HG11	3:I:394:PHE:CD2	2.51	0.44
2:J:198:MET:O	2:J:198:MET:HG3	2.17	0.44
4:K:209:MET:O	4:K:210:GLU:O	2.35	0.44
3:E:223:VAL:HG12	3:E:224:ILE:HG12	1.99	0.44
3:E:382:TYR:O	3:I:259:PRO:HG3	2.18	0.44
2:F:201:TYR:HD2	3:E:82:VAL:HG12	1.82	0.44
2:F:176:THR:O	2:F:182:LEU:HD12	2.18	0.44
2:F:199:PRO:CB	2:F:201:TYR:CE1	2.94	0.44
2:F:201:TYR:HA	2:F:207:ARG:NH2	2.33	0.44
3:I:135:HIS:HA	3:I:149:PRO:O	2.17	0.44
4:K:151:TYR:CD1	4:K:151:TYR:N	2.85	0.44
2:F:35:PHE:HD2	2:F:36:PHE:CD2	2.35	0.44
4:G:173:PRO:O	4:G:174:TYR:HB2	2.18	0.44
4:G:226:TRP:CA	4:G:226:TRP:CE3	3.00	0.44
2:F:117:THR:HG22	4:G:47:TRP:HH2	1.81	0.44
1:N:5:UNK:O	1:N:6:UNK:C	2.66	0.44
3:A:340:ASP:HB3	3:A:341:TYR:HB3	1.99	0.44
3:E:221:ASP:OD1	3:E:221:ASP:N	2.51	0.44
3:E:349:SER:OG	3:E:350:VAL:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:9:ALA:HB3	2:F:15:SER:HA	2.00	0.44
3:I:84:PHE:CB	2:J:199:PRO:HB3	2.48	0.44
2:J:48:LEU:HD12	2:J:48:LEU:HA	1.67	0.44
4:K:106:VAL:HB	4:K:167:TYR:OH	2.17	0.44
3:A:37:PHE:O	3:A:41:ARG:HG3	2.18	0.44
4:C:118:ILE:HG12	4:C:157:TYR:CD1	2.52	0.44
4:C:226:TRP:HE3	4:C:226:TRP:HA	1.81	0.44
2:F:88:PHE:N	2:F:88:PHE:CD1	2.85	0.44
4:G:194:ILE:CG1	4:G:195:PRO:HD3	2.27	0.44
3:I:69:VAL:CG1	3:I:114:ILE:HA	2.48	0.44
3:I:313:PRO:HB2	3:I:354:PRO:HB3	2.00	0.44
2:J:111:VAL:HG12	2:J:112:ASN:OD1	2.17	0.44
2:J:38:VAL:CG2	2:J:39:LEU:N	2.81	0.44
2:B:67:THR:HG1	4:K:206:PHE:HE1	1.65	0.43
3:E:354:PRO:O	3:E:355:ILE:HB	2.17	0.43
3:I:47:ASP:OD2	3:I:401:ARG:NH1	2.45	0.43
3:I:85:LEU:O	3:I:99:GLN:NE2	2.51	0.43
3:A:250:THR:HG21	2:B:167:PRO:HA	1.99	0.43
3:A:348:LEU:HA	3:A:349:SER:HA	1.77	0.43
2:B:201:TYR:HD1	2:B:202:ILE:N	2.17	0.43
2:B:211:ARG:CG	2:B:211:ARG:HH11	2.27	0.43
2:B:36:PHE:O	2:B:36:PHE:HD1	2.01	0.43
3:E:89:GLU:OE1	3:E:93:VAL:CG2	2.67	0.43
2:F:19:ALA:O	2:F:21:GLY:N	2.50	0.43
4:G:226:TRP:HE3	4:G:226:TRP:HA	1.82	0.43
3:A:341:TYR:CD1	3:A:342:LEU:HB2	2.53	0.43
2:B:38:VAL:O	2:B:39:LEU:C	2.57	0.43
4:C:174:TYR:C	4:C:174:TYR:HD1	2.20	0.43
4:C:236:LEU:HA	4:C:236:LEU:HD23	1.80	0.43
2:F:78:ALA:HB2	2:F:233:TYR:CD2	2.52	0.43
3:I:286:THR:CG2	3:I:304:VAL:HG11	2.48	0.43
2:J:36:PHE:HA	2:J:37:ALA:C	2.38	0.43
2:J:49:THR:OG1	2:J:72:LEU:HD22	2.19	0.43
3:A:198:TRP:O	3:A:202:TRP:CD1	2.71	0.43
4:C:190:PRO:O	4:C:193:ILE:HG13	2.17	0.43
3:E:212:TYR:OH	4:G:240:MET:HG2	2.17	0.43
3:E:96:ARG:HH21	3:E:99:GLN:NE2	2.15	0.43
3:I:60:GLU:OE2	3:I:123:ASN:HB3	2.18	0.43
3:I:348:LEU:HB2	3:I:349:SER:HB2	2.01	0.43
3:I:94:LEU:HD23	3:I:126:GLY:CA	2.42	0.43
3:A:133:HIS:NE2	3:A:150:GLY:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:TRP:CD1	2:B:65:TRP:HB2	2.54	0.43
3:E:141:GLU:OE2	3:E:141:GLU:HA	2.18	0.43
3:E:60:GLU:O	3:E:60:GLU:CG	2.45	0.43
4:G:199:LEU:HD23	4:G:202:TRP:CZ3	2.54	0.43
3:I:308:ASN:HA	3:I:309:ASN:CB	2.27	0.43
2:J:176:THR:HG21	2:J:188:LEU:HD22	2.00	0.43
2:J:39:LEU:C	2:J:39:LEU:HD12	2.39	0.43
2:B:201:TYR:CD1	2:B:202:ILE:N	2.87	0.43
2:F:125:PHE:HZ	2:F:169:ILE:CD1	2.32	0.43
2:F:220:VAL:HG23	2:F:221:ALA:N	2.34	0.43
4:G:119:TYR:CD2	4:G:119:TYR:C	2.90	0.43
2:F:117:THR:HG22	4:G:47:TRP:CH2	2.54	0.43
3:I:254:PHE:HD1	2:J:174:GLN:NE2	2.16	0.43
3:I:342:LEU:N	3:I:371:ARG:HD3	2.33	0.43
3:I:96:ARG:HH21	3:I:99:GLN:HE22	1.67	0.43
2:J:26:VAL:O	2:J:29:MET:N	2.52	0.43
2:B:43:HIS:HE1	4:C:127:GLU:HB2	1.83	0.43
3:E:99:GLN:HB2	3:E:122:ILE:HG12	2.00	0.43
2:F:35:PHE:HA	2:F:96:PHE:CZ	2.54	0.43
3:I:229:ARG:NH1	3:I:229:ARG:HG3	2.32	0.43
2:J:91:PRO:HB3	2:J:141:LEU:HD13	1.99	0.43
4:K:88:ARG:CB	4:K:170:THR:HB	2.49	0.43
3:A:99:GLN:HE21	3:A:122:ILE:HG12	1.83	0.43
3:A:343:LEU:H	3:A:371:ARG:HD3	1.84	0.43
2:B:138:VAL:O	2:B:142:LEU:HG	2.18	0.43
2:F:64:MET:H	2:F:64:MET:HG2	1.63	0.43
4:G:146:HIS:CE1	4:G:201:GLU:OE1	2.71	0.43
3:A:214:ARG:HB3	3:A:220:ALA:H	1.84	0.43
2:B:56:TRP:HB3	2:B:58:ASP:OD1	2.19	0.43
3:E:131:ARG:HB3	4:G:48:ARG:HH22	1.83	0.43
2:F:76:PHE:CE2	4:G:229:LEU:HD21	2.54	0.43
2:F:90:LEU:HA	2:F:90:LEU:HD23	1.87	0.43
4:G:189:GLY:N	4:G:190:PRO:HD2	2.34	0.43
4:G:251:VAL:O	4:G:252:LYS:C	2.56	0.43
4:K:193:ILE:O	4:K:197:VAL:N	2.52	0.43
3:A:57:VAL:O	3:A:58:ASN:HB2	2.18	0.43
2:F:202:ILE:HD12	2:F:202:ILE:HA	1.66	0.43
2:J:114:TRP:CE3	2:J:118:TYR:HA	2.53	0.43
4:K:82:GLY:O	4:K:86:LYS:HB2	2.18	0.43
4:C:143:THR:O	4:C:147:ILE:CG1	2.65	0.42
2:F:245:THR:O	2:F:245:THR:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:151:TYR:N	4:G:151:TYR:CD1	2.87	0.42
3:I:96:ARG:HH21	3:I:99:GLN:NE2	2.16	0.42
2:J:57:VAL:HG12	2:J:123:LEU:HD12	1.99	0.42
4:K:132:TRP:CZ2	4:K:144:PRO:HG2	2.53	0.42
2:B:33:LEU:HB3	4:C:112:VAL:HG22	2.01	0.42
2:F:35:PHE:HA	2:F:96:PHE:CE1	2.55	0.42
3:I:392:LEU:HD23	3:I:392:LEU:HA	1.64	0.42
2:J:203:ARG:O	2:J:204:MET:CB	2.59	0.42
4:K:178:GLY:O	4:K:179:TYR:CD2	2.72	0.42
4:K:41:TYR:CD1	4:K:41:TYR:O	2.73	0.42
4:K:83:TYR:CZ	4:K:87:THR:HG21	2.54	0.42
3:A:158:ASP:OD1	3:A:159:MET:N	2.52	0.42
3:A:324:LEU:HG	3:A:342:LEU:HD12	2.01	0.42
2:B:35:PHE:HA	2:B:96:PHE:CZ	2.55	0.42
3:E:220:ALA:O	3:E:222:ASP:N	2.50	0.42
3:E:293:TYR:CE1	3:E:410:VAL:HG23	2.54	0.42
2:F:135:TRP:CE2	2:F:156:GLY:HA3	2.54	0.42
4:G:41:TYR:CD1	4:G:41:TYR:C	2.92	0.42
4:K:235:VAL:HG23	4:K:239:LEU:HD12	2.01	0.42
4:K:42:GLU:HA	4:K:62:TRP:HH2	1.82	0.42
3:A:187:TRP:CZ2	2:B:167:PRO:HG2	2.54	0.42
2:B:48:LEU:HD12	2:B:48:LEU:HA	1.84	0.42
4:C:154:TYR:O	4:C:155:PRO:C	2.56	0.42
3:E:273:THR:HB	3:E:274:GLU:HB2	2.01	0.42
3:E:55:VAL:HG12	3:E:59:GLU:HB3	2.01	0.42
3:I:223:VAL:HG12	3:I:224:ILE:HG12	2.00	0.42
2:J:238:PHE:HA	2:J:241:ARG:HG2	2.01	0.42
3:I:131:ARG:HB3	4:K:48:ARG:HH22	1.85	0.42
3:A:295:VAL:HA	3:A:296:PRO:HA	1.91	0.42
2:B:189:ILE:O	2:B:193:PHE:HD1	2.02	0.42
2:B:54:ASP:O	2:B:109:ARG:NH1	2.52	0.42
3:E:219:LYS:CB	3:E:220:ALA:O	2.55	0.42
3:E:334:THR:CB	3:E:335:LYS:HB2	2.50	0.42
2:F:204:MET:HE2	2:F:204:MET:HA	2.00	0.42
2:F:85:TRP:CE2	2:F:89:ARG:HD3	2.54	0.42
3:I:66:LYS:HD3	3:I:271:ILE:HD13	2.00	0.42
3:I:307:LYS:HG3	3:I:309:ASN:ND2	2.35	0.42
3:A:214:ARG:NE	3:A:222:ASP:HB3	2.35	0.42
3:A:276:THR:O	3:A:279:VAL:HB	2.19	0.42
2:B:39:LEU:HD11	2:B:104:GLY:HA3	2.00	0.42
3:E:70:PHE:HE2	3:E:72:ALA:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:85:TRP:CE2	2:J:89:ARG:HD3	2.54	0.42
4:K:167:TYR:CD1	4:K:171:ARG:HD3	2.55	0.42
3:A:392:LEU:HD23	3:A:392:LEU:HA	1.67	0.42
4:C:107:LEU:CD1	4:C:168:ALA:HB2	2.50	0.42
4:C:209:MET:O	4:C:209:MET:CG	2.66	0.42
4:G:104:LEU:O	4:G:108:VAL:HG23	2.20	0.42
2:F:108:ASN:ND2	4:G:127:GLU:OE2	2.39	0.42
1:N:24:UNK:O	1:N:25:UNK:CB	2.67	0.42
2:B:200:GLU:HA	2:B:203:ARG:HD2	2.02	0.42
2:B:113:PHE:CE1	4:C:131:THR:HB	2.55	0.42
4:C:185:ILE:HG22	4:C:186:VAL:N	2.35	0.42
4:C:199:LEU:HD23	4:C:202:TRP:CZ3	2.55	0.42
3:E:183:ARG:HH22	3:E:253:THR:HG21	1.84	0.42
3:I:137:GLN:HE21	3:I:139:ASN:ND2	2.07	0.42
2:J:220:VAL:CG2	2:J:221:ALA:N	2.83	0.42
2:J:35:PHE:HA	2:J:96:PHE:CZ	2.55	0.42
3:A:288:LEU:HA	3:A:288:LEU:HD12	1.94	0.42
3:A:350:VAL:HG12	3:A:351:ASP:H	1.84	0.42
4:G:116:ILE:HA	4:G:116:ILE:HD12	1.80	0.42
4:G:35:TYR:HE1	4:G:152:MET:CE	2.31	0.42
3:I:99:GLN:HB2	3:I:122:ILE:HG12	2.01	0.42
2:F:177:GLU:CG	3:A:411:ILE:HG12	2.50	0.42
4:C:107:LEU:HD23	4:C:238:ILE:HD11	2.01	0.42
4:C:155:PRO:O	4:C:159:VAL:HG23	2.20	0.42
3:E:100:PHE:CD2	3:E:105:PHE:HA	2.46	0.42
4:K:24:MET:HB2	4:K:109:GLN:CG	2.37	0.42
3:A:391:LEU:HA	3:A:391:LEU:HD23	1.83	0.41
3:E:100:PHE:CA	3:E:104:GLN:O	2.66	0.41
3:E:117:ASP:N	3:E:117:ASP:OD1	2.52	0.41
3:E:316:LEU:HB2	3:E:394:PHE:CE1	2.54	0.41
2:F:182:LEU:HD22	3:A:412:PRO:HD3	2.02	0.41
3:I:117:ASP:N	3:I:117:ASP:OD1	2.52	0.41
2:J:185:LEU:O	2:J:189:ILE:HG13	2.20	0.41
2:F:162:TYR:CD2	2:F:218:VAL:HG11	2.55	0.41
4:G:203:GLY:O	4:G:207:TRP:HB2	2.20	0.41
4:K:16:GLU:CD	4:K:16:GLU:N	2.73	0.41
4:K:44:VAL:CG1	4:K:45:PHE:CD1	2.89	0.41
3:A:125:ARG:HD3	3:A:162:PHE:CE2	2.55	0.41
3:E:318:GLU:OE2	3:E:325:ARG:HG2	2.20	0.41
3:E:32:LYS:HG2	3:E:375:GLU:HA	2.02	0.41
4:G:118:ILE:HG12	4:G:157:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:35:TYR:CD2	4:G:120:TRP:CG	3.08	0.41
3:E:131:ARG:O	4:G:48:ARG:NH2	2.54	0.41
3:I:84:PHE:HB3	2:J:199:PRO:HB3	2.02	0.41
3:I:95:VAL:HG23	3:I:127:ARG:HD2	2.02	0.41
2:J:129:LEU:O	2:J:132:PRO:HD2	2.21	0.41
3:A:85:LEU:HD21	3:A:120:PHE:HB2	2.03	0.41
2:B:117:THR:HB	2:B:119:PHE:HE1	1.85	0.41
2:B:56:TRP:CH2	4:C:134:MET:HG3	2.55	0.41
4:C:146:HIS:HE1	4:C:201:GLU:OE1	2.00	0.41
4:C:114:TYR:HE1	4:C:161:ALA:HB2	1.85	0.41
3:E:69:VAL:HG12	3:E:114:ILE:HA	2.01	0.41
3:E:156:LYS:NZ	3:E:156:LYS:HB3	2.35	0.41
4:G:42:GLU:HA	4:G:62:TRP:HH2	1.86	0.41
3:I:311:SER:HA	3:I:357:PRO:CB	2.50	0.41
2:J:200:GLU:HG2	2:J:203:ARG:HD3	2.03	0.41
4:K:45:PHE:O	4:K:49:ALA:HB3	2.19	0.41
4:K:70:ILE:HB	4:K:71:PRO:CD	2.51	0.41
3:E:135:HIS:HA	3:E:150:GLY:HA2	2.03	0.41
3:A:61:MET:SD	3:A:62:VAL:N	2.94	0.41
4:C:114:TYR:CE1	4:C:161:ALA:HB2	2.55	0.41
2:F:12:PRO:O	4:G:98:ARG:NH1	2.52	0.41
3:I:102:GLY:HA3	3:I:268:LEU:HD13	2.02	0.41
3:I:92:PRO:HB3	2:J:193:PHE:HA	2.03	0.41
2:J:211:ARG:HG3	2:J:211:ARG:HH11	1.86	0.41
2:J:76:PHE:HE2	4:K:229:LEU:HD21	1.85	0.41
2:J:56:TRP:CH2	4:K:134:MET:HG3	2.55	0.41
3:A:198:TRP:HZ3	3:A:235:VAL:HG21	1.85	0.41
3:A:221:ASP:N	3:A:221:ASP:OD1	2.54	0.41
3:E:307:LYS:HG3	3:E:309:ASN:ND2	2.36	0.41
2:F:150:ALA:HB2	2:F:233:TYR:CD1	2.55	0.41
4:G:55:ALA:HB1	4:G:57:GLU:OE1	2.20	0.41
2:J:103:ILE:CG2	2:J:107:ILE:HD11	2.51	0.41
2:J:204:MET:HE2	2:J:204:MET:HA	2.03	0.41
2:J:223:PHE:O	2:J:224:PHE:C	2.59	0.41
4:K:118:ILE:HG22	4:K:119:TYR:N	2.35	0.41
2:B:112:ASN:CG	4:C:128:GLN:HG3	2.41	0.41
1:D:13:UNK:O	1:D:17:UNK:CB	2.69	0.41
3:E:212:TYR:CE2	4:G:239:LEU:HB3	2.55	0.41
3:E:327:LEU:HB2	3:E:345:ASP:HA	2.02	0.41
3:I:295:VAL:HA	3:I:296:PRO:HA	1.89	0.41
3:A:95:VAL:HG11	2:B:192:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:24:MET:HB2	4:C:109:GLN:CG	2.42	0.41
4:C:256:GLU:N	4:C:256:GLU:CD	2.74	0.41
3:E:50:TRP:CE2	3:E:151:GLN:HB3	2.55	0.41
3:E:348:LEU:HA	3:E:349:SER:HA	1.75	0.41
2:F:112:ASN:ND2	4:G:128:GLN:HG3	2.36	0.41
4:G:137:ILE:O	4:G:137:ILE:CG2	2.69	0.41
4:G:146:HIS:HE1	4:G:201:GLU:OE1	2.03	0.41
3:I:288:LEU:HD12	3:I:288:LEU:HA	1.88	0.41
3:A:260:LEU:O	3:I:384:THR:HG22	2.20	0.41
2:J:26:VAL:O	2:J:27:ASP:C	2.58	0.41
4:K:117:ALA:HB1	4:K:157:TYR:HB2	2.02	0.41
3:A:96:ARG:HH21	3:A:99:GLN:HE22	1.68	0.41
4:C:124:PHE:HD2	4:C:125:PHE:CE2	2.39	0.41
4:C:241:ARG:O	4:C:245:LEU:HG	2.21	0.41
4:C:53:SER:HB3	4:C:139:ASP:CB	2.51	0.41
3:E:217:GLU:O	3:E:218:GLY:C	2.59	0.41
3:E:289:ASN:O	3:E:303:ASN:HB2	2.21	0.41
3:I:351:ASP:HB2	3:I:353:THR:OG1	2.20	0.41
3:I:284:VAL:HG23	3:I:402:TYR:HB3	2.03	0.41
2:J:182:LEU:HD12	2:J:182:LEU:HA	1.95	0.41
2:B:53:TRP:HB3	2:B:65:TRP:HD1	1.86	0.41
4:C:172:ILE:HA	4:C:173:PRO:HD3	1.98	0.41
3:E:387:GLN:HG3	3:E:408:GLY:C	2.41	0.41
2:F:53:TRP:HB3	2:F:65:TRP:CD1	2.56	0.41
4:G:251:VAL:HG12	4:G:252:LYS:H	1.84	0.41
3:I:89:GLU:OE1	3:I:93:VAL:CG2	2.69	0.41
4:K:167:TYR:CE1	4:K:171:ARG:HG2	2.56	0.41
3:A:70:PHE:CE2	3:A:72:ALA:HB3	2.56	0.40
2:B:131:VAL:HB	2:B:132:PRO:HD3	2.03	0.40
2:B:52:ASP:H	2:B:55:PHE:H	1.70	0.40
2:B:82:ALA:O	2:B:86:VAL:HB	2.21	0.40
4:C:106:VAL:HB	4:C:167:TYR:OH	2.20	0.40
3:I:105:PHE:CE2	2:J:178:GLN:O	2.73	0.40
3:I:204:VAL:O	3:I:205:ARG:HG2	2.19	0.40
2:J:187:ASP:OD1	2:J:203:ARG:NH2	2.53	0.40
3:A:229:ARG:HH11	3:A:229:ARG:HG3	1.86	0.40
4:C:138:ARG:HH12	4:C:141:ASP:HA	1.83	0.40
3:E:273:THR:CB	3:E:274:GLU:HB2	2.51	0.40
3:E:283:ASN:O	3:E:309:ASN:HB3	2.21	0.40
3:I:144:GLY:HA3	2:B:211:ARG:NH1	2.35	0.40
2:J:202:ILE:HD12	2:J:202:ILE:HA	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:147:ILE:HG12	4:K:147:ILE:H	1.77	0.40
4:K:174:TYR:O	4:K:174:TYR:HD1	2.03	0.40
3:A:351:ASP:HB2	3:A:353:THR:OG1	2.21	0.40
4:C:156:ILE:O	4:C:159:VAL:N	2.52	0.40
3:E:101:ILE:HG23	3:E:268:LEU:CD1	2.51	0.40
4:C:201:GLU:C	4:C:203:GLY:H	2.24	0.40
4:C:203:GLY:O	4:C:207:TRP:HB2	2.22	0.40
2:F:101:LEU:O	2:F:105:GLU:HG3	2.22	0.40
2:F:132:PRO:HB3	2:F:157:TRP:HA	2.02	0.40
2:F:198:MET:HG3	2:F:198:MET:O	2.21	0.40
4:G:31:LEU:HD12	4:G:31:LEU:HA	1.86	0.40
3:I:69:VAL:HG11	3:I:114:ILE:HA	2.03	0.40
2:B:224:PHE:HD2	4:K:199:LEU:HD22	1.86	0.40
3:E:137:GLN:HG3	3:E:147:ILE:HD13	2.03	0.40
3:E:303:ASN:OD1	3:E:303:ASN:N	2.55	0.40
4:G:121:GLY:HA2	4:G:153:SER:CB	2.51	0.40
3:I:54:THR:CG2	3:I:156:LYS:HE2	2.51	0.40
3:I:89:GLU:OE1	3:I:93:VAL:HG22	2.22	0.40
2:J:135:TRP:CE2	2:J:156:GLY:HA3	2.57	0.40
3:E:76:ALA:HB1	2:J:208:GLY:O	2.21	0.40
2:J:216:ASP:O	2:J:219:PRO:HD2	2.22	0.40
2:J:56:TRP:HB2	2:J:59:TRP:CD1	2.56	0.40
4:K:191:PHE:HA	4:K:194:ILE:HD11	2.04	0.40
4:K:55:ALA:HB1	4:K:57:GLU:OE1	2.21	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
2	B	242/252 (96%)	189 (78%)	48 (20%)	5 (2%)	7 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	242/252 (96%)	197 (81%)	36 (15%)	9 (4%)	3	22
2	J	242/252 (96%)	200 (83%)	29 (12%)	13 (5%)	2	13
3	A	388/420 (92%)	307 (79%)	56 (14%)	25 (6%)	1	10
3	E	388/420 (92%)	314 (81%)	44 (11%)	30 (8%)	1	7
3	I	388/420 (92%)	308 (79%)	53 (14%)	27 (7%)	1	9
4	C	224/256 (88%)	169 (75%)	49 (22%)	6 (3%)	5	28
4	G	224/256 (88%)	172 (77%)	44 (20%)	8 (4%)	3	23
4	K	224/256 (88%)	163 (73%)	52 (23%)	9 (4%)	3	20
All	All	2562/2784 (92%)	2019 (79%)	411 (16%)	132 (5%)	2	14

All (132) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	52	ASP
3	E	31	GLU
3	E	51	SER
3	E	141	GLU
3	E	164	ASP
3	E	257	THR
3	E	274	GLU
3	E	335	LYS
3	E	353	THR
3	E	354	PRO
3	A	31	GLU
3	A	51	SER
3	A	141	GLU
3	A	164	ASP
3	A	257	THR
3	A	274	GLU
3	A	335	LYS
3	A	354	PRO
3	I	31	GLU
3	I	51	SER
3	I	141	GLU
3	I	164	ASP
3	I	257	THR
3	I	274	GLU
3	I	335	LYS
3	I	354	PRO

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Mol	Chain	Res	Type
4	G	49	ALA
4	G	174	TYR
4	G	251	VAL
2	J	52	ASP
2	B	52	ASP
4	K	174	TYR
4	K	251	VAL
4	C	49	ALA
4	C	174	TYR
4	C	251	VAL
2	F	201	TYR
3	E	143	GLY
3	E	205	ARG
3	E	256	ARG
3	E	309	ASN
3	E	340	ASP
3	E	350	VAL
3	A	143	GLY
3	A	205	ARG
3	A	309	ASN
3	A	340	ASP
3	A	350	VAL
3	I	70	PHE
3	I	81	ARG
3	I	143	GLY
3	I	205	ARG
3	I	309	ASN
3	I	340	ASP
3	I	353	THR
4	G	48	ARG
2	J	110	TYR
2	J	111	VAL
2	J	201	TYR
2	B	201	TYR
4	K	49	ALA
4	K	245	LEU
2	F	19	ALA
2	F	75	THR
3	E	81	ARG
3	E	90	PRO
3	E	398	ASP
3	A	398	ASP

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Mol	Chain	Res	Type
3	I	90	PRO
3	I	220	ALA
3	I	256	ARG
3	I	350	VAL
3	I	398	ASP
2	J	75	THR
2	J	121	ILE
2	J	196	THR
2	B	75	THR
4	K	138	ARG
4	C	48	ARG
3	E	160	LYS
3	E	206	LYS
3	E	220	ALA
3	E	356	ALA
3	A	81	ARG
3	A	90	PRO
3	A	160	LYS
3	A	165	PRO
3	A	226	ASP
3	A	256	ARG
3	A	353	THR
3	I	396	SER
2	J	19	ALA
2	J	142	LEU
4	C	179	TYR
4	C	245	LEU
2	F	110	TYR
2	F	142	LEU
3	E	221	ASP
3	E	276	THR
3	A	221	ASP
3	I	356	ALA
4	G	179	TYR
2	J	27	ASP
2	J	171	ALA
2	B	19	ALA
2	B	110	TYR
4	K	179	TYR
2	F	10	VAL
3	E	70	PHE
3	E	165	PRO

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Mol	Chain	Res	Type
3	E	396	SER
3	A	220	ALA
3	A	356	ALA
4	K	48	ARG
3	A	358	GLY
3	I	208	ILE
3	I	358	GLY
4	G	95	VAL
2	J	23	VAL
2	J	38	VAL
4	K	95	VAL
2	F	111	VAL
3	I	165	PRO
4	G	156	ILE
4	G	178	GLY
2	F	38	VAL
3	E	218	GLY
3	E	355	ILE
3	E	358	GLY
3	I	355	ILE
4	K	156	ILE
3	I	181	ILE

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%)	186 (92%)	16 (8%)	12	40
2	F	202/208 (97%)	186 (92%)	16 (8%)	12	40
2	J	202/208 (97%)	186 (92%)	16 (8%)	12	40
3	A	320/336 (95%)	281 (88%)	39 (12%)	5	20
3	E	320/336 (95%)	283 (88%)	37 (12%)	5	22
3	I	320/336 (95%)	280 (88%)	40 (12%)	4	19
4	C	194/213 (91%)	162 (84%)	32 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	194/213 (91%)	161 (83%)	33 (17%)	2	9
4	K	194/213 (91%)	163 (84%)	31 (16%)	2	11
All	All	2148/2271 (95%)	1888 (88%)	260 (12%)	5	21

All (260) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	22	CYS
2	F	25	THR
2	F	36	PHE
2	F	38	VAL
2	F	39	LEU
2	F	48	LEU
2	F	52	ASP
2	F	86	VAL
2	F	89	ARG
2	F	164	ASN
2	F	177	GLU
2	F	192	HIS
2	F	201	TYR
2	F	202	ILE
2	F	225	SER
2	F	246	THR
3	E	53	THR
3	E	55	VAL
3	E	61	MET
3	E	62	VAL
3	E	111	SER
3	E	117	ASP
3	E	156	LYS
3	E	167	THR
3	E	182	SER
3	E	190	PRO
3	E	204	VAL
3	E	205	ARG
3	E	206	LYS
3	E	214	ARG
3	E	215	VAL
3	E	217	GLU
3	E	221	ASP
3	E	222	ASP

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Mol	Chain	Res	Type
3	E	250	THR
3	E	252	SER
3	E	253	THR
3	E	254	PHE
3	E	256	ARG
3	E	277	VAL
3	E	286	THR
3	E	303	ASN
3	E	306	VAL
3	E	311	SER
3	E	324	LEU
3	E	334	THR
3	E	335	LYS
3	E	351	ASP
3	E	359	GLU
3	E	363	ILE
3	E	384	THR
3	E	388	ILE
3	E	398	ASP
3	A	53	THR
3	A	55	VAL
3	A	61	MET
3	A	62	VAL
3	A	99	GLN
3	A	111	SER
3	A	117	ASP
3	A	156	LYS
3	A	167	THR
3	A	182	SER
3	A	204	VAL
3	A	205	ARG
3	A	206	LYS
3	A	215	VAL
3	A	217	GLU
3	A	221	ASP
3	A	222	ASP
3	A	239	THR
3	A	250	THR
3	A	252	SER
3	A	253	THR
3	A	254	PHE
3	A	256	ARG

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Mol	Chain	Res	Type
3	A	258	ILE
3	A	277	VAL
3	A	286	THR
3	A	303	ASN
3	A	306	VAL
3	A	311	SER
3	A	320	THR
3	A	338	PHE
3	A	341	TYR
3	A	351	ASP
3	A	359	GLU
3	A	363	ILE
3	A	368	GLN
3	A	384	THR
3	A	388	ILE
3	A	398	ASP
3	I	53	THR
3	I	55	VAL
3	I	61	MET
3	I	62	VAL
3	I	63	LEU
3	I	64	SER
3	I	81	ARG
3	I	99	GLN
3	I	117	ASP
3	I	156	LYS
3	I	167	THR
3	I	182	SER
3	I	204	VAL
3	I	205	ARG
3	I	206	LYS
3	I	214	ARG
3	I	215	VAL
3	I	217	GLU
3	I	221	ASP
3	I	222	ASP
3	I	241	LEU
3	I	250	THR
3	I	252	SER
3	I	253	THR
3	I	254	PHE
3	I	256	ARG

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Mol	Chain	Res	Type
3	I	271	ILE
3	I	286	THR
3	I	303	ASN
3	I	306	VAL
3	I	311	SER
3	I	324	LEU
3	I	334	THR
3	I	335	LYS
3	I	338	PHE
3	I	351	ASP
3	I	359	GLU
3	I	363	ILE
3	I	384	THR
3	I	398	ASP
4	G	22	ARG
4	G	30	LEU
4	G	36	LEU
4	G	40	ILE
4	G	47	TRP
4	G	53	SER
4	G	74	LEU
4	G	86	LYS
4	G	90	ARG
4	G	96	THR
4	G	109	GLN
4	G	116	ILE
4	G	118	ILE
4	G	126	THR
4	G	137	ILE
4	G	147	ILE
4	G	157	TYR
4	G	174	TYR
4	G	183	PHE
4	G	184	LEU
4	G	194	ILE
4	G	205	THR
4	G	206	PHE
4	G	208	PHE
4	G	209	MET
4	G	226	TRP
4	G	231	VAL
4	G	241	ARG

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Mol	Chain	Res	Type
4	G	248	LYS
4	G	249	GLU
4	G	252	LYS
4	G	255	THR
4	G	256	GLU
2	J	22	CYS
2	J	25	THR
2	J	36	PHE
2	J	39	LEU
2	J	48	LEU
2	J	64	MET
2	J	68	VAL
2	J	86	VAL
2	J	89	ARG
2	J	164	ASN
2	J	177	GLU
2	J	192	HIS
2	J	201	TYR
2	J	202	ILE
2	J	219	PRO
2	J	246	THR
2	B	22	CYS
2	B	25	THR
2	B	36	PHE
2	B	38	VAL
2	B	39	LEU
2	B	47	MET
2	B	48	LEU
2	B	52	ASP
2	B	89	ARG
2	B	152	VAL
2	B	164	ASN
2	B	177	GLU
2	B	192	HIS
2	B	201	TYR
2	B	202	ILE
2	B	246	THR
4	K	22	ARG
4	K	30	LEU
4	K	36	LEU
4	K	47	TRP
4	K	53	SER

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Mol	Chain	Res	Type
4	K	86	LYS
4	K	90	ARG
4	K	96	THR
4	K	97	PRO
4	K	109	GLN
4	K	118	ILE
4	K	126	THR
4	K	131	THR
4	K	147	ILE
4	K	157	TYR
4	K	174	TYR
4	K	183	PHE
4	K	184	LEU
4	K	194	ILE
4	K	205	THR
4	K	206	PHE
4	K	208	PHE
4	K	209	MET
4	K	226	TRP
4	K	235	VAL
4	K	241	ARG
4	K	248	LYS
4	K	249	GLU
4	K	252	LYS
4	K	255	THR
4	K	256	GLU
4	C	22	ARG
4	C	30	LEU
4	C	36	LEU
4	C	47	TRP
4	C	53	SER
4	C	86	LYS
4	C	90	ARG
4	C	96	THR
4	C	109	GLN
4	C	116	ILE
4	C	118	ILE
4	C	126	THR
4	C	147	ILE
4	C	151	TYR
4	C	157	TYR
4	C	174	TYR

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Mol	Chain	Res	Type
4	C	183	PHE
4	C	184	LEU
4	C	194	ILE
4	C	205	THR
4	C	206	PHE
4	C	208	PHE
4	C	209	MET
4	C	226	TRP
4	C	231	VAL
4	C	235	VAL
4	C	241	ARG
4	C	248	LYS
4	C	249	GLU
4	C	252	LYS
4	C	255	THR
4	C	256	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	178	GLN
3	E	44	ASN
3	E	58	ASN
3	E	68	HIS
3	E	99	GLN
3	E	137	GLN
3	E	151	GLN
3	E	188	HIS
3	E	261	GLN
3	E	265	GLN
3	E	283	ASN
3	A	44	ASN
3	A	58	ASN
3	A	68	HIS
3	A	99	GLN
3	A	137	GLN
3	A	151	GLN
3	A	188	HIS
3	A	261	GLN
3	A	265	GLN
3	A	283	ASN
3	I	44	ASN

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Mol	Chain	Res	Type
3	I	58	ASN
3	I	68	HIS
3	I	99	GLN
3	I	137	GLN
3	I	151	GLN
3	I	188	HIS
3	I	261	GLN
3	I	265	GLN
4	G	109	GLN
4	G	177	HIS
2	J	178	GLN
2	J	192	HIS
2	B	178	GLN
2	B	192	HIS
4	K	91	ASN
4	K	109	GLN
4	K	177	HIS
4	C	109	GLN
4	C	177	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 9 ligands modelled in this entry, 8 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	$\# Z > 2$
7	CAC	C	303	6	0,4,4	0.00	-	0,6,6	0.00	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	D	0/25	-	-	-	-
1	H	0/25	-	-	-	-
1	N	0/25	-	-	-	-
2	B	244/252 (96%)	-0.54	1 (0%) 92 94	27, 51, 92, 117	0
2	F	244/252 (96%)	-0.63	0 100 100	14, 31, 66, 95	0
2	J	244/252 (96%)	-0.58	4 (1%) 72 71	16, 33, 67, 104	0
3	A	390/420 (92%)	0.14	28 (7%) 15 16	35, 72, 112, 153	0
3	E	390/420 (92%)	-0.29	3 (0%) 86 87	24, 47, 85, 129	0
3	I	390/420 (92%)	-0.13	14 (3%) 42 41	25, 64, 117, 179	0
4	C	228/256 (89%)	-0.20	13 (5%) 23 25	31, 59, 111, 148	0
4	G	228/256 (89%)	-0.30	5 (2%) 62 61	20, 48, 101, 153	0
4	K	228/256 (89%)	-0.17	10 (4%) 34 35	24, 47, 115, 160	0
All	All	2586/2859 (90%)	-0.27	78 (3%) 50 50	14, 52, 107, 179	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	418	ASP	6.1
4	K	253	LEU	5.3
3	A	417	GLY	5.0
4	C	17	SER	4.6
4	K	254	LEU	4.2
2	J	180	GLY	3.8
3	I	363	ILE	3.8
3	A	418	ASP	3.8
4	K	17	SER	3.7
4	C	82	GLY	3.6
3	I	417	GLY	3.6
3	E	256	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
4	G	195	PRO	3.3
4	C	55	ALA	3.3
4	G	224	PHE	3.3
3	A	173	THR	3.2
4	K	55	ALA	3.2
3	A	397	PRO	3.2
3	I	350	VAL	3.1
3	I	290	GLY	3.1
4	K	139	ASP	3.1
4	C	16	GLU	3.1
3	A	172	SER	3.0
3	I	334	THR	2.9
3	A	170	ASP	2.9
3	A	342	LEU	2.9
3	A	319	TYR	2.8
4	K	252	LYS	2.8
3	A	399	GLY	2.8
3	I	315	ARG	2.7
3	A	351	ASP	2.7
3	A	350	VAL	2.6
3	I	393	PHE	2.6
2	B	9	ALA	2.6
3	I	364	VAL	2.6
4	K	18	VAL	2.6
3	I	349	SER	2.5
2	J	10	VAL	2.5
3	A	347	GLY	2.5
3	A	348	LEU	2.5
3	I	316	LEU	2.5
4	C	52	ASP	2.4
4	C	85	TRP	2.4
3	A	315	ARG	2.4
2	J	13	PHE	2.3
4	C	50	GLY	2.3
3	A	157	GLY	2.3
4	K	47	TRP	2.3
3	A	174	VAL	2.3
4	G	207	TRP	2.3
4	C	20	ASP	2.3
3	A	171	GLY	2.3
4	K	48	ARG	2.3
4	C	57	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
3	E	390	GLY	2.2
4	G	196	ASN	2.2
4	C	81	ALA	2.2
4	C	61	TYR	2.2
3	A	366	LYS	2.2
3	A	326	PHE	2.2
3	I	365	VAL	2.2
3	A	168	LEU	2.1
4	C	226	TRP	2.1
3	A	398	ASP	2.1
3	I	311	SER	2.1
3	E	200	PHE	2.1
3	A	167	THR	2.1
3	A	144	GLY	2.1
3	A	317	GLY	2.1
3	A	59	GLU	2.1
3	A	346	ARG	2.1
3	A	354	PRO	2.1
4	C	60	THR	2.1
3	I	416	ALA	2.0
4	G	228	ALA	2.0
3	A	328	ASN	2.0
4	K	177	HIS	2.0
2	J	22	CYS	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 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. 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(\AA^2)	Q<0.9
6	ZN	G	302	1/1	0.93	0.04	153,153,153,153	0
7	CAC	C	303	5/5	0.97	0.12	92,95,102,107	0
5	CU	A	501	1/1	0.97	0.04	85,85,85,85	0
6	ZN	C	302	1/1	0.98	0.04	106,106,106,106	0
6	ZN	G	301	1/1	0.99	0.09	64,64,64,64	0
6	ZN	C	301	1/1	0.99	0.07	66,66,66,66	0
6	ZN	K	301	1/1	0.99	0.03	67,67,67,67	0
5	CU	I	501	1/1	0.99	0.05	63,63,63,63	0
5	CU	E	501	1/1	0.99	0.05	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.