



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:43 PM UTC

PDB ID : 4PI2 / pdb_00004pi2
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

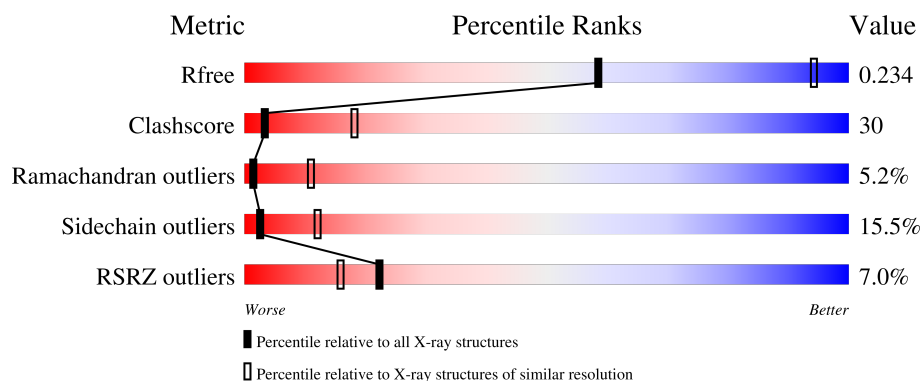
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	D	25	
1	H	25	
1	N	25	
2	B	252	
2	F	252	

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Mol	Chain	Length	Quality of chain
2	J	252	
3	A	420	
3	E	420	
3	I	420	
4	C	256	
4	G	256	
4	K	256	

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			

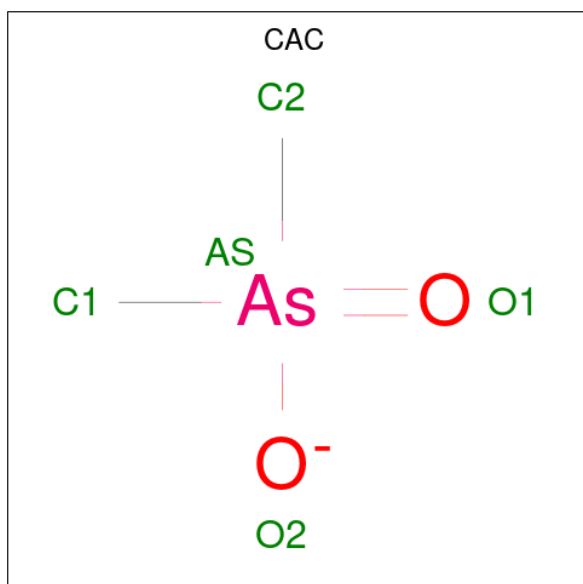
- Molecule 5 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

- Molecule 6 is ZINC ION (CCD ID: 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 (CCD ID: CAC) (formula: C₂H₆AsO₂).



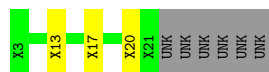
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	As	C	O	0	0
			5	1	2	2		

3 Residue-property plots [i](#)

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

- Molecule 1: unknown peptide

Chain D: 



- Molecule 1: unknown peptide

Chain H: 



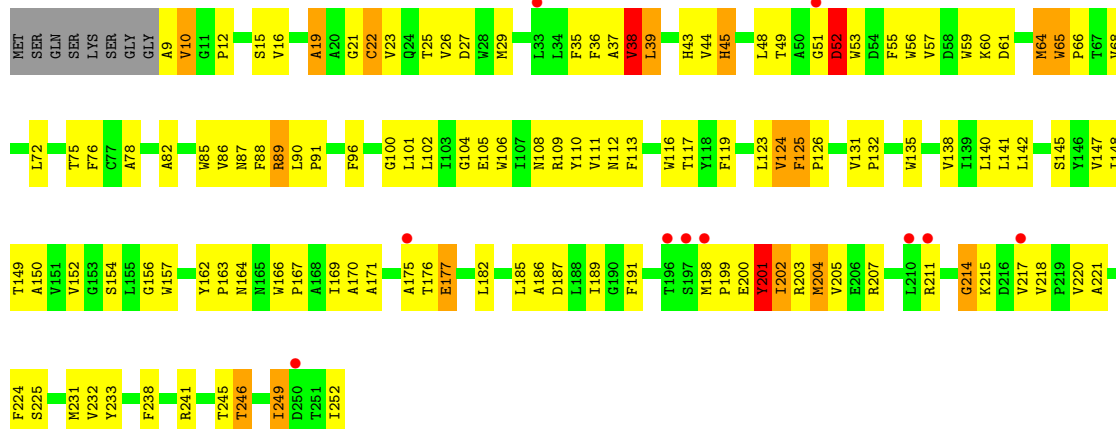
- Molecule 1: unknown peptide

Chain N: 

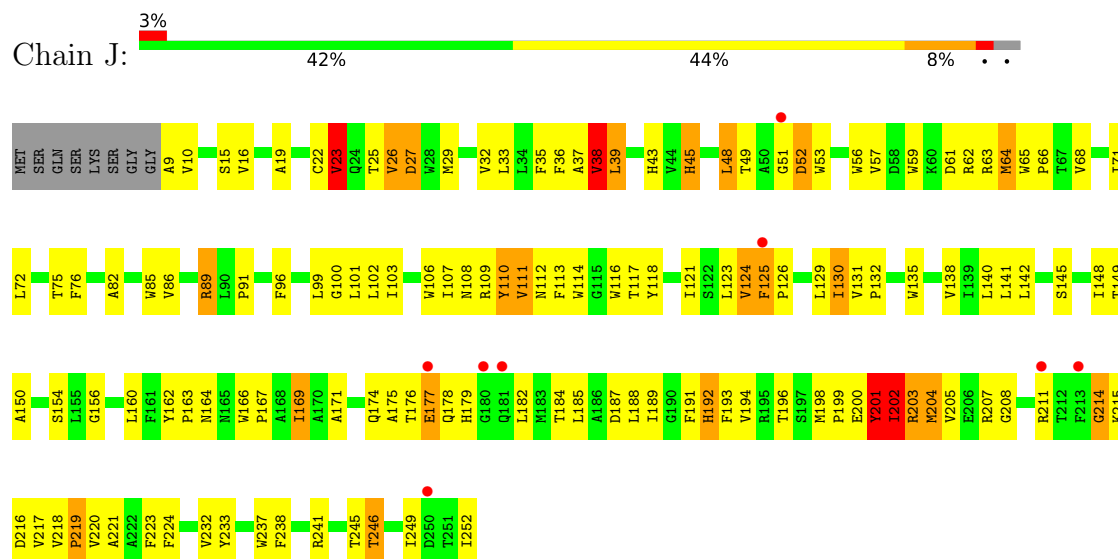


- Molecule 2: Particulate methane monooxygenase subunit A

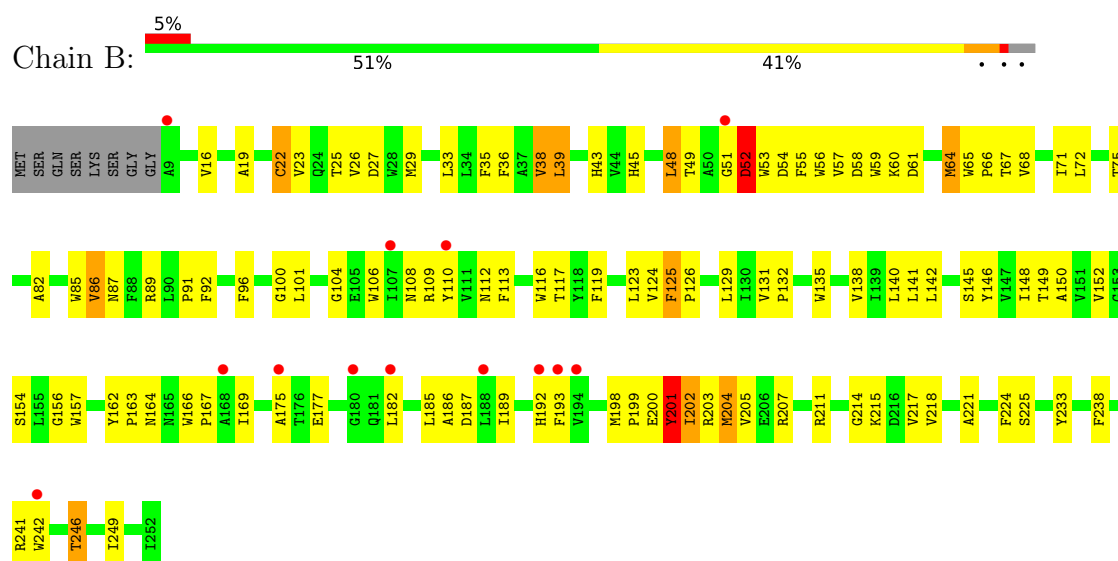
Chain F: 



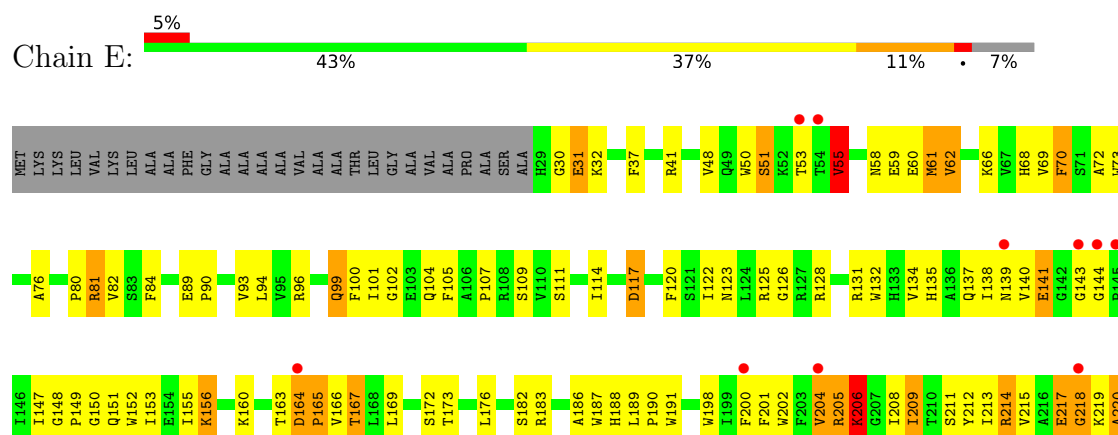
• Molecule 2: Particulate methane monooxygenase subunit A

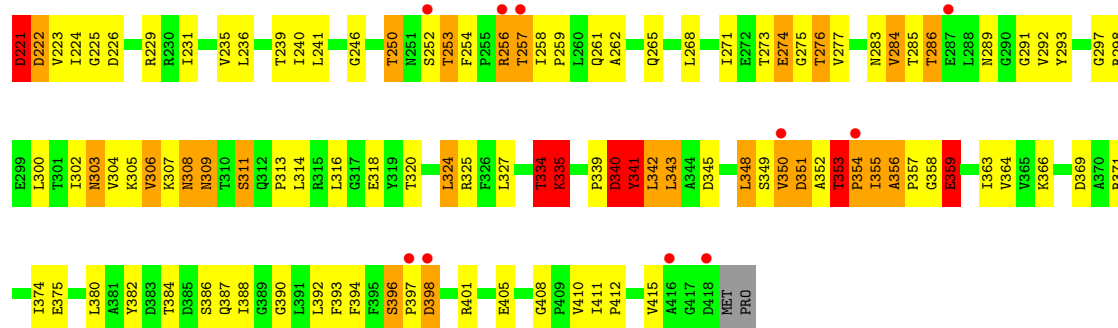


• Molecule 2: Particulate methane monooxygenase subunit A

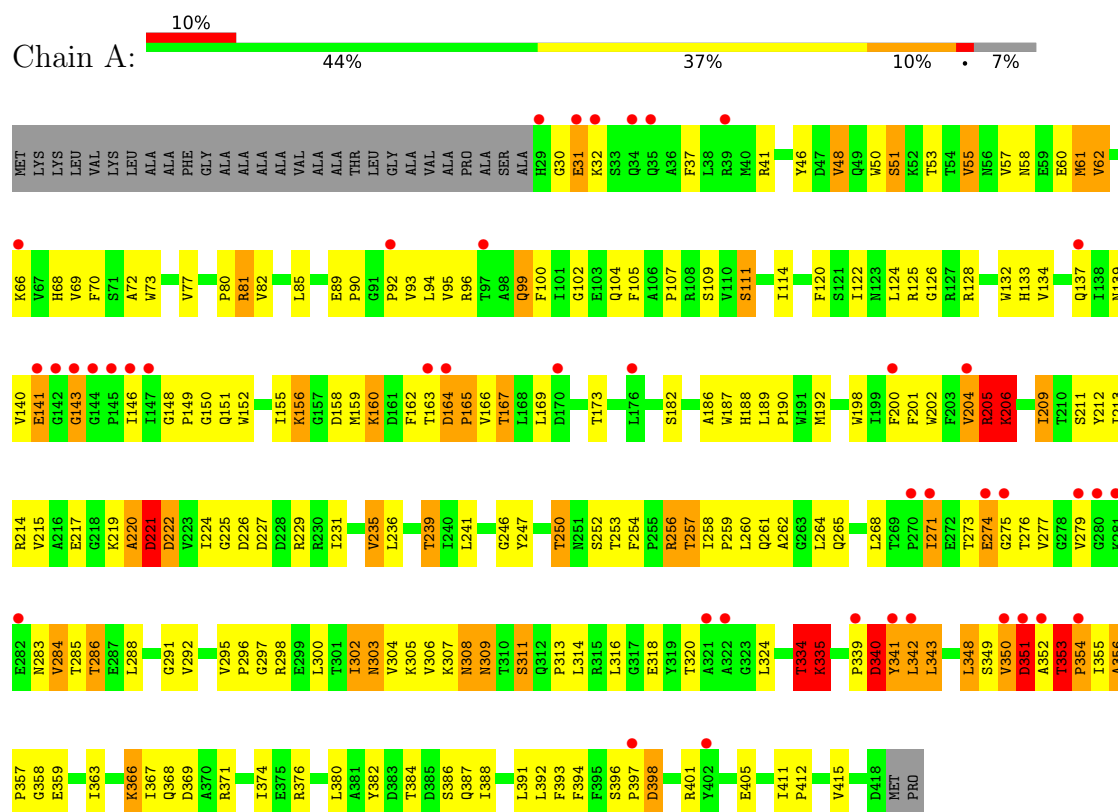


• Molecule 3: Particulate methane monooxygenase subunit B

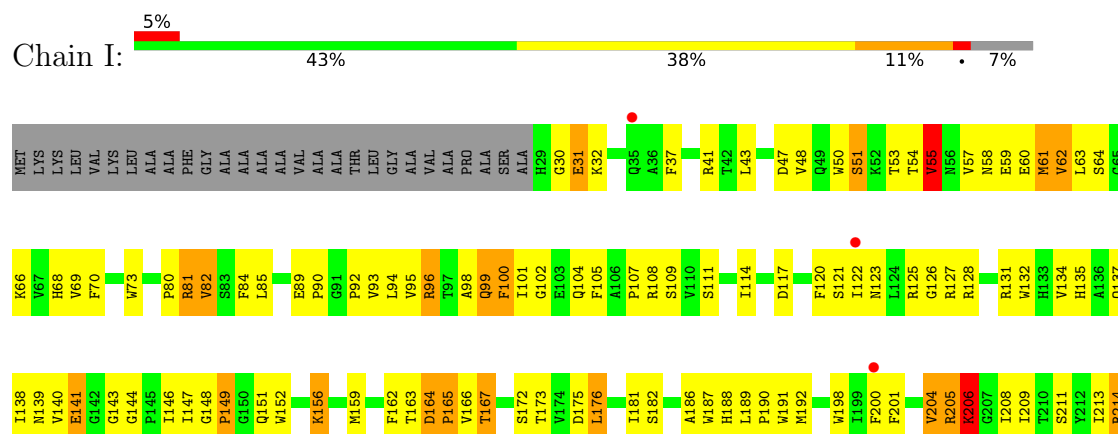


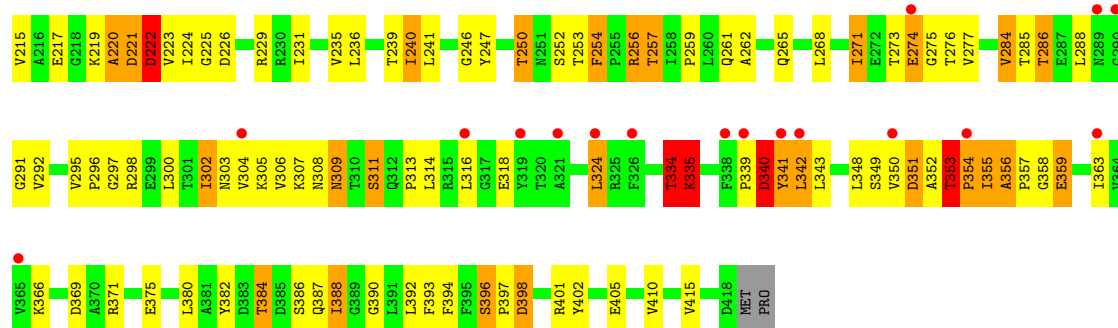


• Molecule 3: Particulate methane monooxygenase subunit B

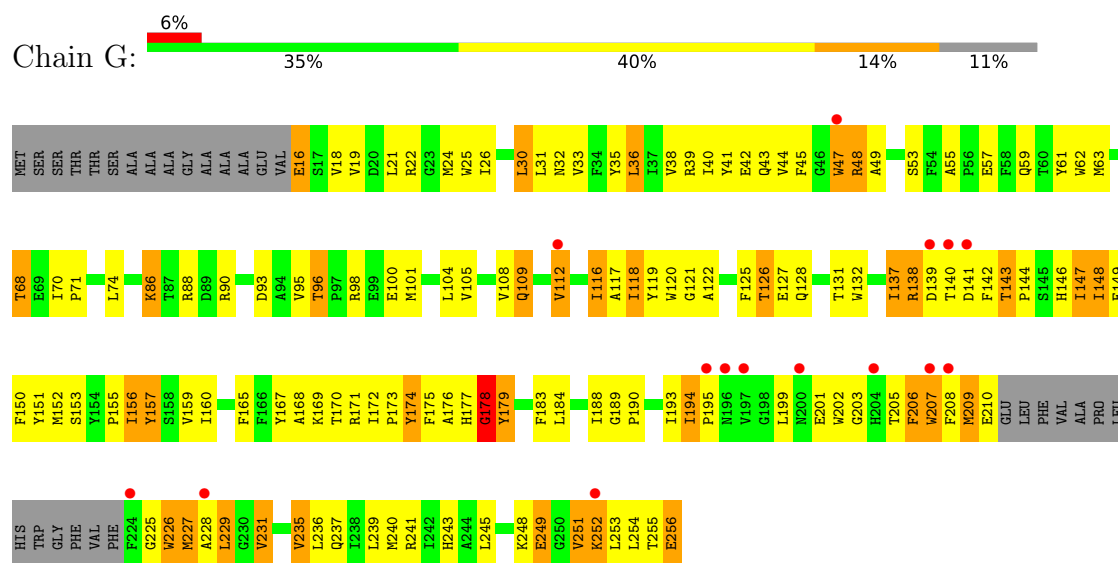


• Molecule 3: Particulate methane monooxygenase subunit B

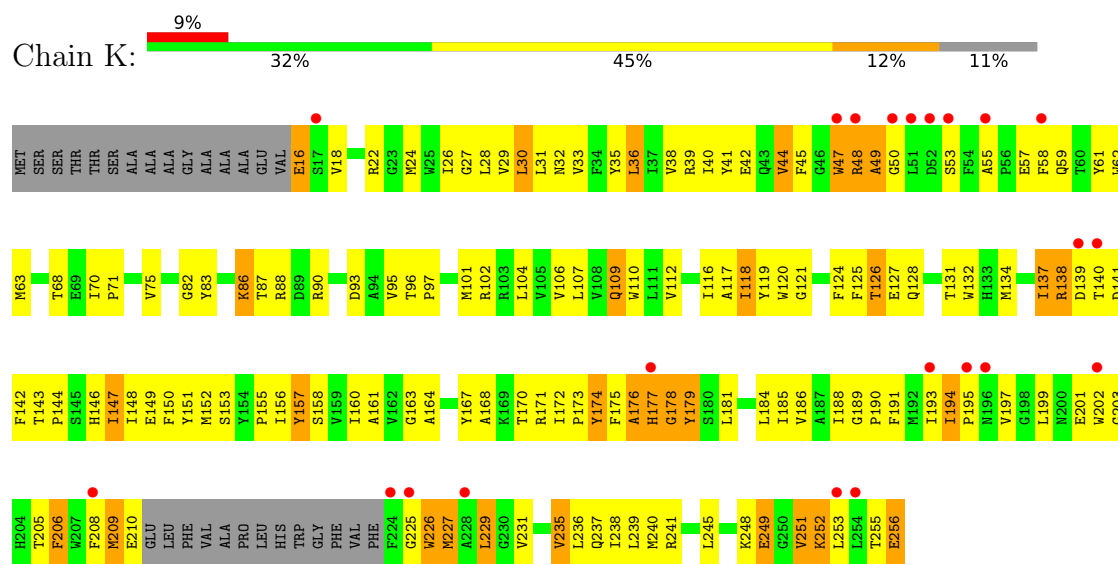




• Molecule 4: Particulate methane monooxygenase subunit C

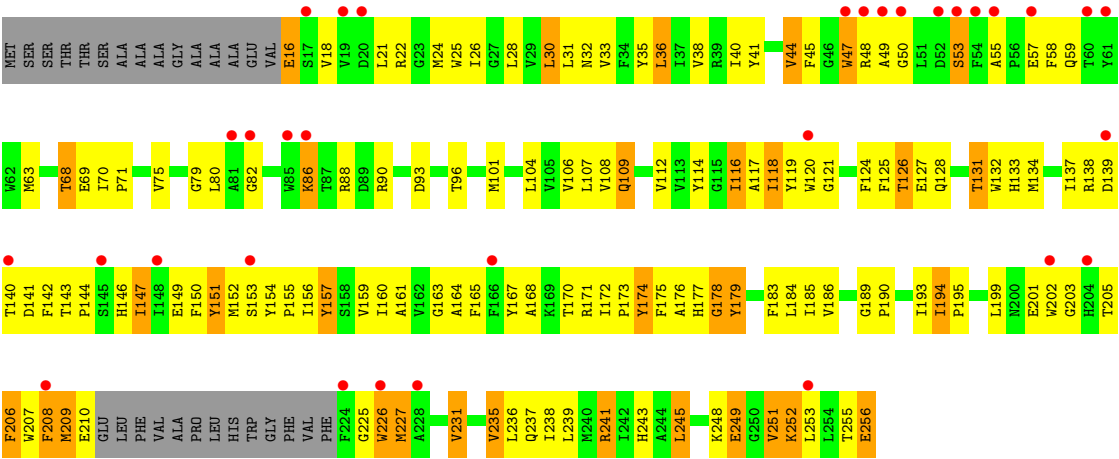


• Molecule 4: Particulate methane monooxygenase subunit C



• 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 50.00 – 3.33	Depositor EDS
% Data completeness (in resolution range)	80.7 (50.00-3.33) 80.9 (50.00-3.33)	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 (Not available) , 0.234	Depositor DCC
R_{free} test set	2599 reflections (4.07%)	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)	0.25 , 36.2	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	0.86	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: CU, CAC, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
2	B	0.96	0/2052	1.10	3/2814 (0.1%)
2	F	1.08	2/2052 (0.1%)	1.18	6/2814 (0.2%)
2	J	1.07	1/2052 (0.0%)	1.21	10/2814 (0.4%)
3	A	0.85	0/3115	1.15	19/4243 (0.4%)
3	E	0.93	0/3115	1.18	23/4243 (0.5%)
3	I	0.88	0/3115	1.19	21/4243 (0.5%)
4	C	0.95	1/1932 (0.1%)	1.09	2/2634 (0.1%)
4	G	0.97	2/1932 (0.1%)	1.14	6/2634 (0.2%)
4	K	0.98	1/1932 (0.1%)	1.18	4/2634 (0.2%)
All	All	0.95	7/21297 (0.0%)	1.16	94/29073 (0.3%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	228	ALA	CA-C	6.34	1.60	1.53
4	G	207	TRP	CA-C	-5.80	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	177	HIS	CG-CD2	5.47	1.41	1.35
2	F	65	TRP	CA-CB	-5.43	1.47	1.53
4	C	133	HIS	CG-CD2	5.11	1.41	1.35
2	F	45	HIS	CG-CD2	5.02	1.41	1.35
2	J	45	HIS	CG-CD2	5.02	1.41	1.35

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	125	PHE	CA-C-N	8.68	128.62	120.03
2	F	125	PHE	C-N-CA	8.68	128.62	120.03
3	E	134	VAL	N-CA-C	7.96	119.38	107.51
2	J	10	VAL	N-CA-C	7.90	119.24	107.15
2	J	125	PHE	CA-C-N	7.49	127.44	120.03
2	J	125	PHE	C-N-CA	7.49	127.44	120.03
3	E	148	GLY	CA-C-N	7.38	127.42	119.90
3	E	148	GLY	C-N-CA	7.38	127.42	119.90
2	F	214	GLY	N-CA-C	-7.34	100.35	112.83
3	I	172	SER	N-CA-C	7.33	119.28	110.19
2	J	124	VAL	N-CA-C	7.33	119.18	112.29
4	G	143	THR	N-CA-C	-6.88	102.06	110.31
3	E	172	SER	N-CA-C	6.83	118.66	110.19
3	A	353	THR	CA-C-N	6.80	128.34	119.84
3	A	353	THR	C-N-CA	6.80	128.34	119.84
3	A	297	GLY	N-CA-C	6.75	120.32	110.80
2	B	125	PHE	CA-C-N	6.74	127.13	119.92
2	B	125	PHE	C-N-CA	6.74	127.13	119.92
2	J	214	GLY	N-CA-C	-6.62	100.78	112.77
4	K	229	LEU	N-CA-C	-6.54	104.61	112.59
3	E	341	TYR	CA-C-N	6.37	133.17	121.70
3	E	341	TYR	C-N-CA	6.37	133.17	121.70
3	I	359	GLU	N-CA-C	6.25	118.78	109.59
3	I	341	TYR	CA-C-N	6.24	132.93	121.70
3	I	341	TYR	C-N-CA	6.24	132.93	121.70
3	I	353	THR	CA-C-N	6.19	127.58	119.84
3	I	353	THR	C-N-CA	6.19	127.58	119.84
3	I	206	LYS	N-CA-C	-6.18	97.64	110.80
3	A	351	ASP	N-CA-C	-6.17	103.91	112.30
3	I	297	GLY	N-CA-C	6.01	118.98	110.74
4	G	227	MET	N-CA-C	5.96	118.47	109.41
3	I	334	THR	CA-C-N	5.93	132.38	121.70
3	I	334	THR	C-N-CA	5.93	132.38	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	334	THR	N-CA-C	-5.92	99.70	108.99
3	A	341	TYR	CA-C-N	5.87	132.27	121.70
3	A	341	TYR	C-N-CA	5.87	132.27	121.70
3	E	206	LYS	N-CA-C	-5.87	98.31	110.80
3	A	206	LYS	N-CA-C	-5.85	98.33	110.80
3	I	222	ASP	N-CA-C	-5.83	105.26	112.90
3	I	55	VAL	N-CA-C	5.83	115.93	107.88
3	A	222	ASP	N-CA-C	-5.82	104.90	112.23
4	K	227	MET	N-CA-C	5.80	118.22	109.41
4	C	44	VAL	N-CA-C	5.80	115.98	110.53
3	E	359	GLU	N-CA-C	5.72	118.00	109.59
3	I	257	THR	N-CA-C	5.68	122.90	110.80
3	A	148	GLY	CA-C-N	5.66	125.67	119.90
3	A	148	GLY	C-N-CA	5.66	125.67	119.90
3	A	134	VAL	N-CA-C	5.59	116.44	107.73
4	G	229	LEU	N-CA-C	-5.54	105.83	112.59
2	J	32	VAL	N-CA-C	5.53	115.73	110.53
3	I	148	GLY	CA-C-N	5.48	126.69	119.84
3	I	148	GLY	C-N-CA	5.48	126.69	119.84
3	A	257	THR	N-CA-C	5.47	122.45	110.80
3	E	297	GLY	N-CA-C	5.45	119.92	111.08
3	E	222	ASP	N-CA-C	-5.44	105.78	112.90
3	E	257	THR	N-CA-C	5.43	122.38	110.80
3	E	353	THR	CA-C-N	5.42	126.61	119.84
3	E	353	THR	C-N-CA	5.42	126.61	119.84
4	G	138	ARG	NE-CZ-NH2	5.41	124.07	119.20
2	F	147	VAL	N-CA-C	-5.40	105.45	110.53
3	A	334	THR	N-CA-C	-5.38	100.90	109.23
3	A	308	ASN	CA-C-N	5.37	131.37	121.70
3	A	308	ASN	C-N-CA	5.37	131.37	121.70
4	K	176	ALA	N-CA-C	-5.36	102.55	110.48
3	I	351	ASP	N-CA-C	-5.35	104.46	112.54
2	J	194	VAL	N-CA-C	5.35	120.47	109.34
3	A	334	THR	CA-C-N	5.34	131.32	121.70
3	A	334	THR	C-N-CA	5.34	131.32	121.70
3	E	306	VAL	N-CA-C	5.34	116.47	109.21
2	F	145	SER	N-CA-C	5.32	118.29	109.46
3	A	342	LEU	N-CA-C	5.31	125.88	111.00
2	J	237	TRP	N-CA-C	-5.30	105.19	110.97
3	E	390	GLY	N-CA-C	5.30	118.50	110.97
3	E	308	ASN	CA-C-N	5.28	131.21	121.70
3	E	308	ASN	C-N-CA	5.28	131.21	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	227	MET	N-CA-C	5.26	117.40	109.41
3	E	55	VAL	N-CA-C	5.25	115.93	108.42
3	I	302	ILE	N-CA-C	5.24	116.27	108.46
3	E	334	THR	N-CA-C	-5.20	100.82	108.99
3	E	342	LEU	N-CA-C	5.20	125.57	111.00
3	E	334	THR	CA-C-N	5.17	131.01	121.70
3	E	334	THR	C-N-CA	5.17	131.01	121.70
3	I	134	VAL	N-CA-C	5.17	115.80	107.73
4	K	44	VAL	N-CA-C	5.17	115.38	110.42
2	B	145	SER	N-CA-C	5.16	118.03	109.46
4	G	96	THR	CA-C-N	5.15	125.45	119.47
4	G	96	THR	C-N-CA	5.15	125.45	119.47
3	A	302	ILE	N-CA-C	5.13	116.10	108.46
2	J	160	LEU	N-CA-C	5.12	118.31	111.75
2	F	124	VAL	N-CA-C	5.12	116.47	111.91
2	J	202	ILE	N-CA-C	-5.06	106.99	113.22
3	I	390	GLY	N-CA-C	5.02	118.10	110.97
3	I	96	ARG	NE-CZ-NH1	-5.01	116.49	121.50
3	E	153	ILE	N-CA-C	-5.00	101.29	108.89

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	134	0
2	F	1974	0	1932	135	0
2	J	1974	0	1932	145	0
3	A	3038	0	3022	192	0
3	E	3038	0	3022	196	0
3	I	3038	0	3022	200	0
4	C	1870	0	1854	130	0
4	G	1870	0	1854	136	0
4	K	1870	0	1854	141	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	1255	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 30.

All (1255) 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:I:99:GLN:C	3:I:100:PHE:HD2	1.56	1.14
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: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: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
2:J:51:GLY:CA	2:J:52:ASP:HB2	1.79	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:164:ASP:HB2	3:I:165:PRO:HA	1.35	1.07
4:G:194:ILE:HG12	4:G:195:PRO:HD3	1.37	1.05
4:C:194:ILE:HG12	4:C:195:PRO:CD	1.87	1.05
3:E:396:SER:HB2	3:E:397:PRO:HD2	1.34	1.05
3:A:224:ILE:HG22	3:A:225:GLY:H	1.21	1.04
4:C:104:LEU:HD23	4:C:172:ILE:HD13	1.34	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
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: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
3:I:318:GLU:HB3	3:I:393:PHE:HB2	1.47	0.94
4:G:104:LEU:CD2	4:G:172:ILE:HD13	1.96	0.94
2:F:246:THR:HG22	4:G:237:GLN:HG3	1.48	0.94
3:E:60:GLU:HG3	3:E:60:GLU:O	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
3:E:219:LYS:HB3	3:E:220:ALA:O	1.69	0.92
2:B:246:THR:HG22	4:C:237:GLN:HG3	1.47	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
2:J:45:HIS:HB2	4:K:227:MET:HE3	1.48	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:99:GLN:C	3:I:100:PHE:CD2	2.47	0.91
3:E:224:ILE:HG22	3:E:225:GLY:N	1.81	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:334:THR:CA	3:I:335:LYS:HB2	2.03	0.89
2:B:199:PRO:HB2	2:B:201:TYR:CE1	2.06	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
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:O	3:A:60:GLU:HG3	1.74	0.86
4:K:104:LEU:HD23	4:K:172:ILE:CD1	2.04	0.86
4:G:194:ILE:HD13	4:G:194:ILE:H	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
2:F:10:VAL:HG21	4:G:254:LEU:CD1	2.06	0.85
3:E:356:ALA:HB1	3:E:357:PRO:CA	2.06	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
3:I:340:ASP:O	3:I:343:LEU:HB3	1.77	0.84
4:C:194:ILE:HG12	4:C:195:PRO:HD2	1.58	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
3:I:298:ARG:HG2	3:I:369:ASP:O	1.78	0.84
4:C:24:MET:HB2	4:C:109:GLN:HG2	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:204:MET:HA	2:J:204:MET:HE2	1.61	0.81
3:E:286:THR:HG22	3:E:304:VAL:HG12	1.62	0.81
3:A:225:GLY:HA2	3:A:229:ARG:NH2	1.96	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
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:F:106:TRP:HE1	3:E:188:HIS:HD2	1.31	0.77
3:E:353:THR:O	3:E:355:ILE:N	2.16	0.77
2:B:36:PHE:HE1	4:C:116:ILE:CD1	1.96	0.77
3:E:58:ASN:HD21	3:E:163:THR:H	1.30	0.77
3:E:356:ALA:HB1	3:E:357:PRO:C	2.09	0.77
4:K:104:LEU:CD2	4:K:172:ILE:HD13	2.13	0.77
3:I:60:GLU:O	3:I:60:GLU:HG3	1.83	0.77
2:J:199:PRO:HB2	2:J:201:TYR:CD1	2.18	0.76
3:E:205:ARG:O	3:E:206:LYS:HE2	1.86	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: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
3:A:220:ALA:C	3:A:222:ASP:H	1.93	0.76
3:I:356:ALA:HB1	3:I:357:PRO:C	2.10	0.76
3:E:308:ASN:CA	3:E:309:ASN:HB2	2.16	0.75
2:B:175:ALA:HB1	2:B:182:LEU:HD11	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:LEU:O	2:B:189:ILE:HG13	1.85	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:HD13	4:C:194:ILE:H	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
2:B:36:PHE:CE1	4:C:116:ILE:HD12	2.24	0.73
4:K:209:MET:HG2	4:K:209:MET:O	1.88	0.73
3:E:107:PRO:HD2	3:E:265:GLN:NE2	2.00	0.73
3:I:48:VAL:HG21	3:I:149:PRO:HG2	1.70	0.73
3:I:99:GLN:O	3:I:100:PHE:HD2	1.72	0.73
3:I:68:HIS:HE1	3:I:405:GLU:OE1	1.71	0.72
2:B:150:ALA:O	2:B:154:SER:OG	2.06	0.72
3:E:273:THR:HA	3:E:274:GLU:HB2	1.71	0.72
3:I:224:ILE:HG22	3:I:225:GLY:N	1.99	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
2:B:204:MET:HE2	2:B:204:MET:HA	1.71	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:F:64:MET:HG3	2:F:204:MET:O	1.90	0.72
2:B:64:MET:HG3	2:B:205:VAL:HA	1.71	0.72
2:F:138:VAL:HG11	3:E:236:LEU:HB2	1.71	0.72
2:B:36:PHE:CE1	4:C:116:ILE:CD1	2.72	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
3:E:324:LEU:H	3:E:324:LEU:HD12	1.55	0.71
4:C:117:ALA:HB1	4:C:157:TYR:HA	1.73	0.71
4:G:44:VAL:HG12	4:G:45:PHE:CD1	2.25	0.71
4:G:193:ILE:HD12	4:G:194:ILE:N	2.06	0.70
3:E:100:PHE:HD2	3:E:105:PHE:HA	1.57	0.70
3:A:308:ASN:CA	3:A:309:ASN:HB2	2.20	0.70
3:I:298:ARG:HG2	3:I:369:ASP:C	2.17	0.70
2:F:162:TYR:HB3	2:F:163:PRO:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:204:MET:HE2	2:F:204:MET:HA	1.73	0.70
2:F:199:PRO:HB2	2:F:201:TYR:CD1	2.26	0.70
3:I:380:LEU:O	3:I:380:LEU:HG	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
3:A:356:ALA:HB1	3:A:357:PRO:C	2.17	0.69
3:E:220:ALA:C	3:E:222:ASP:H	2.00	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
3:E:94:LEU:HD23	3:E:126:GLY:HA2	1.75	0.69
4:G:231:VAL:O	4:G:235:VAL:HG13	1.93	0.69
3:I:73:TRP:CZ2	3:I:80:PRO:HG3	2.27	0.69
3:I:340:ASP:HB3	3:I:341:TYR:CB	2.22	0.69
2:J:200:GLU:O	2:J:201:TYR:CB	2.41	0.69
2:F:36:PHE:HE1	4:G:116:ILE:CD1	2.06	0.69
4:C:32:ASN:O	4:C:36:LEU:HB2	1.93	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
3:A:366:LYS:HZ2	3:A:366:LYS:HB2	1.59	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
4:C:251:VAL:HG12	4:C:252:LYS:N	2.08	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
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:273:THR:CA	3:A:274:GLU:HB2	2.24	0.67
3:E:58:ASN:HD22	3:E:125:ARG:NH2	1.91	0.67
3:E:285:THR:HB	3:E:307:LYS:HB3	1.77	0.67
3:A:58:ASN:ND2	3:A:125:ARG:HH21	1.81	0.67
4:K:241:ARG:HE	4:K:241:ARG:HA	1.59	0.67
3:I:50:TRP:HB3	3:I:61:MET:HE1	1.75	0.67
3:I:151:GLN:HE21	3:I:152:TRP:H	1.43	0.67
4:C:26:ILE:O	4:C:30:LEU:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:93:ASP:OD1	4:C:177:HIS:HE1	1.78	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:I:220:ALA:C	3:I:222:ASP:H	2.02	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:F:29:MET:CE	4:G:109:GLN:HG3	2.25	0.66
2:B:109:ARG:HG3	2:B:126:PRO:HD3	1.77	0.66
3:A:353:THR:O	3:A:355:ILE:N	2.28	0.66
4:G:194:ILE:HG12	4:G:195:PRO:HD2	1.75	0.65
4:C:226:TRP:HA	4:C:226:TRP:CE3	2.31	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
3:E:151:GLN:HE21	3:E:152:TRP:H	1.42	0.65
2:B:211:ARG:HG3	2:B:211:ARG:HH11	1.60	0.65
2:F:211:ARG:HG3	2:F:211:ARG:HH11	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
4:G:38:VAL:HG21	4:G:152:MET:HE1	1.79	0.65
2:F:214:GLY:HA2	2:F:215:LYS:HB2	1.77	0.65
3:E:382:TYR:CD1	2:J:215:LYS:HE3	2.32	0.65
3:A:285:THR:HB	3:A:307:LYS:HB3	1.79	0.65
3:I:396:SER:HB2	3:I:397:PRO:CD	2.20	0.65
4:G:209:MET:O	4:G:209:MET:HG2	1.97	0.65
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
2:F:246:THR:HG22	4:G:237:GLN:CG	2.23	0.64
3:A:396:SER:HB2	3:A:397:PRO:CD	2.26	0.64
2:F:162:TYR:HB3	2:F:163:PRO:CD	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:206:LYS:HB2	3:A:211:SER:OG	1.98	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:HD1	2:J:36:PHE:O	1.80	0.64
2:F:36:PHE:CE1	4:G:116:ILE:HD12	2.33	0.63
2:F:185:LEU:O	2:F:189:ILE:HG13	1.99	0.63
3:A:201:PHE:HZ	3:A:231:ILE:HD13	1.64	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
3:E:380:LEU:O	3:E:380:LEU:HG	1.97	0.63
3:I:37:PHE:O	3:I:41:ARG:HG3	1.99	0.63
4:G:138:ARG:NH1	4:G:141:ASP:HA	2.14	0.63
4:C:44:VAL:HG12	4:C:45:PHE:CD1	2.33	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:E:100:PHE:HA	3:E:104:GLN:O	1.97	0.63
3:E:339:PRO:O	3:E:340:ASP:C	2.41	0.63
3:A:69:VAL:HG11	3:A:114:ILE:HA	1.79	0.63
3:I:225:GLY:HA2	3:I:229:ARG:NH2	2.14	0.63
2:B:29:MET:CE	4:C:109:GLN:HG3	2.28	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: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
2:B:49:THR:OG1	2:B:72:LEU:HD22	1.99	0.62
4:K:121:GLY:HA2	4:K:153:SER:HB2	1.81	0.62
2:F:221:ALA:HA	4:C:206:PHE:HZ	1.64	0.62
3:E:231:ILE:O	3:E:235:VAL:HG23	1.99	0.62
3:E:68:HIS:HE1	3:E:405:GLU:OE1	1.82	0.62
3:I:339:PRO:O	3:I:340:ASP:C	2.42	0.62
4:C:209:MET:O	4:C:209:MET:HG2	2.00	0.62
3:I:189:LEU:N	3:I:190:PRO:HD2	2.15	0.62
4:C:189:GLY:N	4:C:190:PRO:HD2	2.15	0.62
2:F:203:ARG:O	2:F:204:MET:HB2	1.98	0.61
2:F:45:HIS:HB2	4:G:227:MET:HE3	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:164:ASP:CB	3:E:165:PRO:CA	2.74	0.61
4:G:18:VAL:HG11	4:G:101:MET:HE3	1.83	0.61
2:J:29:MET:HE3	4:K:109:GLN:HG3	1.82	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
2:F:221:ALA:HA	4:C:206:PHE:CZ	2.35	0.61
3:A:259:PRO:HG3	3:I:382:TYR:O	2.01	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
3:A:339:PRO:O	3:A:340:ASP:C	2.44	0.60
4:K:138:ARG:NH1	4:K:141:ASP:HA	2.16	0.60
2:J:200:GLU:HG2	2:J:203:ARG:HH11	1.66	0.60
2:B:224:PHE:CD2	4:K:199:LEU:HD22	2.36	0.60
4:G:152:MET:O	4:G:155:PRO:HD2	2.01	0.60
4:C:117:ALA:HB2	4:C:160:ILE:HD13	1.83	0.60
1:N:3:UNK:CB	4:K:41:TYR:OH	2.50	0.60
4:C:150:PHE:O	4:C:155:PRO:HD3	2.01	0.60
3:A:151:GLN:HE21	3:A:152:TRP:N	2.00	0.60
3:I:284:VAL:HG11	3:I:394:PHE:CE2	2.37	0.60
4:G:241:ARG:HE	4:G:241:ARG:HA	1.66	0.60
3:E:380:LEU:HD11	3:E:387:GLN:H	1.66	0.60
2:B:140:LEU:HD13	2:B:149:THR:OG1	2.02	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
3:I:225:GLY:HA2	3:I:229:ARG:HH22	1.67	0.60
4:G:170:THR:O	4:G:171:ARG:HD2	2.01	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
3:I:164:ASP:CB	3:I:165:PRO:CA	2.80	0.59
4:G:206:PHE:HZ	2:J:221:ALA:HA	1.67	0.59
2:F:109:ARG:HG3	2:F:126:PRO:HD3	1.84	0.59
3:A:205:ARG:O	3:A:206:LYS:HE2	2.01	0.59
4:K:189:GLY:N	4:K:190:PRO:HD2	2.16	0.59
4:C:209:MET:O	4:C:210:GLU:O	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:I:340:ASP:HB3	3:I:341:TYR:HA	1.84	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
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: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: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
3:I:200:PHE:O	3:I:204:VAL:HG23	2.01	0.59
4:G:59:GLN:HA	4:G:63:MET:HB2	1.85	0.59
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
4:G:32:ASN:O	4:G:36:LEU:HB2	2.02	0.59
2:J:36:PHE:CE1	4:K:116:ILE:HD12	2.37	0.59
4:C:53:SER:HB3	4:C:139:ASP:HB2	1.85	0.59
3:E:51:SER:HB3	3:E:62:VAL:H	1.68	0.58
3:E:340:ASP:HB3	3:E:341:TYR:HB3	1.84	0.58
3:A:213:ILE:HG12	4:C:243:HIS:CD2	2.37	0.58
2:F:29:MET:HE3	4:G:109:GLN:HG3	1.85	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
2:J:22:CYS:O	2:J:23:VAL:C	2.47	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:I:51:SER:HB3	3:I:62:VAL:H	1.66	0.58
3:I:219:LYS:HA	3:I:220:ALA:CB	2.28	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
3:E:316:LEU:HD11	3:E:392:LEU:HD22	1.86	0.58
2:B:203:ARG:O	2:B:204:MET:HB2	2.03	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
2:B:162:TYR:HB3	2:B:163:PRO:HD3	1.86	0.58
4:K:146:HIS:CE1	4:K:201:GLU:OE1	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:340:ASP:HB3	3:I:341:TYR:CA	2.34	0.58
2:F:200:GLU:O	2:F:201:TYR:CB	2.52	0.57
3:A:51:SER:HB3	3:A:62:VAL:H	1.69	0.57
2:J:36:PHE:O	2:J:36:PHE:CD1	2.56	0.57
1:N:3:UNK:C	1:N:5:UNK:N	2.66	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
4:G:174:TYR:CD1	4:G:174:TYR:C	2.82	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: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
4:G:152:MET:C	4:G:155:PRO:HD2	2.30	0.57
2:B:125:PHE:HZ	2:B:169:ILE:CD1	2.17	0.57
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
3:E:201:PHE:CZ	3:E:231:ILE:HD13	2.40	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:A:46:TYR:HE2	3:A:66:LYS:HD2	1.70	0.57
3:A:219:LYS:HA	3:A:220:ALA:CB	2.29	0.57
3:I:188:HIS:CD2	2:J:106:TRP:HE1	2.23	0.57
4:G:241:ARG:O	4:G:245:LEU:HG	2.04	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:J:220:VAL:HG23	2:J:221:ALA:N	2.20	0.56
3:A:209:ILE:HG13	2:B:27:ASP:OD1	2.06	0.56
3:I:341:TYR:CE2	3:I:342:LEU:HD22	2.40	0.56
4:G:53:SER:HB3	4:G:139:ASP:HB2	1.86	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
4:C:16:GLU:N	4:C:16:GLU:CD	2.63	0.56
4:C:121:GLY:HA2	4:C:153:SER:HB2	1.88	0.56
2:F:113:PHE:HB3	2:F:124:VAL:HG21	1.87	0.56
4:G:174:TYR:C	4:G:174:TYR:HD1	2.14	0.56
2:J:175:ALA:HB1	2:J:182:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:174:TYR:CD1	4:K:174:TYR:C	2.83	0.56
3:E:313:PRO:HG2	3:E:397:PRO:HD3	1.87	0.56
3:A:298:ARG:HG2	3:A:369:ASP:C	2.30	0.56
4:K:174:TYR:C	4:K:174:TYR:HD1	2.13	0.56
3:A:156:LYS:NZ	3:A:156:LYS:HB3	2.21	0.56
3:A:198:TRP:O	3:A:202:TRP:HD1	1.88	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
2:F:186:ALA:O	2:F:187:ASP:C	2.48	0.56
3:I:41:ARG:NE	3:I:387:GLN:HG2	2.19	0.56
3:I:164:ASP:OD2	3:I:176:LEU:HB2	2.05	0.56
2:J:214:GLY:CA	2:J:215:LYS:HB2	2.36	0.56
2:B:45:HIS:HB2	4:C:227:MET:HE3	1.87	0.56
3:A:316:LEU:HD11	3:A:392:LEU:HD22	1.87	0.56
3:I:93:VAL:HA	3:I:128:ARG:HB2	1.88	0.56
4:G:16:GLU:N	4:G:16:GLU:CD	2.64	0.56
4:G:93:ASP:OD1	4:G:177:HIS:HE1	1.88	0.56
4:G:169:LYS:HD2	4:G:175:PHE:O	2.06	0.56
2:F:167:PRO:HG2	3:E:187:TRP:CZ2	2.41	0.56
3:A:356:ALA:CB	3:A:357:PRO:HA	2.36	0.56
4:G:209:MET:HE2	4:G:209:MET:H	1.70	0.56
2:J:204:MET:HA	2:J:204:MET:CE	2.34	0.56
3:E:259:PRO:HG3	3:A:382:TYR:O	2.05	0.55
3:I:186:ALA:O	3:I:190:PRO:HG3	2.06	0.55
4:G:86:LYS:HE3	4:G:86:LYS:HA	1.88	0.55
3:E:69:VAL:CG1	3:E:114:ILE:HA	2.36	0.55
4:C:86:LYS:HE3	4:C:86:LYS:HA	1.88	0.55
3:I:393:PHE:CD1	3:I:401:ARG:HD2	2.40	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:A:30:GLY:O	3:A:32:LYS:N	2.40	0.55
3:E:50:TRP:HB3	3:E:61:MET:HE1	1.89	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
2:F:36:PHE:HD1	2:F:36:PHE:O	1.90	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:200:GLU:HG2	2:F:203:ARG:CD	2.36	0.55
3:E:298:ARG:HG2	3:E:369:ASP:C	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:C:225:GLY:C	4:C:226:TRP:HE3	2.15	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
4:K:41:TYR:CD1	4:K:41:TYR:C	2.84	0.54
3:E:140:VAL:O	3:E:141:GLU:C	2.50	0.54
1:N:7:UNK:O	1:N:9:UNK:N	2.41	0.54
3:A:246:GLY:O	3:A:250:THR:OG1	2.25	0.54
4:G:225:GLY:C	4:G:226:TRP:HE3	2.16	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
1:N:7:UNK:C	1:N:9:UNK:N	2.67	0.54
2:J:64:MET:HG3	2:J:204:MET:O	2.06	0.54
4:C:140:THR:HG23	4:C:142:PHE:H	1.71	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
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
2:B:162:TYR:HB3	2:B:163:PRO:CD	2.38	0.54
4:K:88:ARG:HB2	4:K:170:THR:HB	1.90	0.54
4:C:118:ILE:HG12	4:C:157:TYR:CE1	2.43	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
2:B:198:MET:N	2:B:199:PRO:HD3	2.22	0.54
4:K:150:PHE:O	4:K:155:PRO:HD3	2.08	0.54
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
2:B:29:MET:HE1	4:C:109:GLN:HG3	1.90	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
2:F:203:ARG:HH12	3:E:262:ALA:HB2	1.68	0.54
3:E:58:ASN:ND2	3:E:125:ARG:HH21	1.96	0.54
4:G:249:GLU:O	4:G:253:LEU:HB2	2.07	0.54
3:A:200:PHE:O	3:A:204:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:137:ILE:O	4:K:137:ILE:CG2	2.56	0.53
4:K:194:ILE:HD13	4:K:194:ILE:H	1.71	0.53
2:F:117:THR:HA	4:G:47:TRP:CH2	2.43	0.53
3:E:200:PHE:O	3:E:204:VAL:HG23	2.08	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: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
3:I:100:PHE:CD2	3:I:100:PHE:N	2.71	0.53
3:I:341:TYR:H	3:I:342:LEU:CA	2.21	0.53
4:K:209:MET:O	4:K:209:MET:CG	2.56	0.53
4:C:252:LYS:O	4:C:256:GLU:HA	2.09	0.53
3:I:311:SER:HA	3:I:357:PRO:HB3	1.90	0.53
3:I:246:GLY:O	3:I:250:THR:OG1	2.25	0.53
4:G:108:VAL:O	4:G:112:VAL:HG23	2.08	0.53
2:J:125:PHE:HZ	2:J:169:ILE:CD1	2.22	0.53
3:A:55:VAL:HG23	3:A:155:ILE:HG12	1.91	0.53
3:A:66:LYS:HD3	3:A:271:ILE:HD13	1.89	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:E:93:VAL:HB	3:E:132:TRP:CD1	2.44	0.52
3:E:166:VAL:HG12	3:E:167:THR:N	2.24	0.52
3:A:140:VAL:O	3:A:141:GLU:C	2.52	0.52
3:A:141:GLU:OE2	3:A:141:GLU:HA	2.09	0.52
2:J:82:ALA:HB1	2:J:241:ARG:HD2	1.90	0.52
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
2:F:29:MET:HE1	4:G:109:GLN:HE21	1.74	0.52
3:E:66:LYS:HD3	3:E:271:ILE:HD13	1.90	0.52
3:E:341:TYR:CE2	3:E:342:LEU:HD22	2.44	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
3:I:201:PHE:CZ	3:I:231:ILE:HD13	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:156:ILE:O	4:G:159:VAL:N	2.41	0.52
2:J:102:LEU:HD12	2:J:130:ILE:HD12	1.91	0.52
4:C:146:HIS:CE1	4:C:201:GLU:OE1	2.62	0.52
2:F:29:MET:HE1	4:G:109:GLN:HG3	1.92	0.52
2:F:125:PHE:HZ	2:F:169:ILE:HD12	1.74	0.52
4:K:201:GLU:C	4:K:203:GLY:H	2.17	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
4:K:225:GLY:C	4:K:226:TRP:HE3	2.17	0.52
4:K:256:GLU:N	4:K:256:GLU:CD	2.67	0.52
3:E:340:ASP:HB3	3:E:341:TYR:HA	1.92	0.52
3:A:356:ALA:CB	3:A:357:PRO:CA	2.86	0.52
3:I:131:ARG:HB3	4:K:48:ARG:HH12	1.75	0.52
3:I:166:VAL:HG12	3:I:167:THR:N	2.23	0.52
2:B:82:ALA:HB1	2:B:241:ARG:HD2	1.91	0.52
1:H:3:UNK:HA	4:G:61:TYR:HE1	1.74	0.52
3:A:81:ARG:O	3:A:111:SER:HA	2.10	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
2:F:22:CYS:O	2:F:23:VAL:C	2.52	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
4:C:18:VAL:HG11	4:C:101:MET:HE3	1.91	0.52
3:I:285:THR:HB	3:I:307:LYS:HB3	1.92	0.52
3:E:236:LEU:HG	3:E:240:ILE:HD12	1.92	0.51
3:A:340:ASP:HB3	3:A:341:TYR:HA	1.92	0.51
3:I:209:ILE:HG13	2:J:27:ASP:OD1	2.10	0.51
4:C:55:ALA:HB1	4:C:57:GLU:OE1	2.11	0.51
4:C:121:GLY:HA2	4:C:153:SER:CB	2.40	0.51
4:C:163:GLY:O	4:C:164:ALA:C	2.51	0.51
3:E:30:GLY:O	3:E:32:LYS:N	2.43	0.51
3:E:58:ASN:ND2	3:E:163:THR:H	2.04	0.51
3:I:224:ILE:CG2	3:I:225:GLY:N	2.65	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
2:F:150:ALA:O	2:F:154:SER:OG	2.26	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
3:I:292:VAL:O	3:I:300:LEU:HD12	2.11	0.51
4:K:120:TRP:HE3	4:K:125:PHE:CE2	2.29	0.51
4:C:174:TYR:C	4:C:174:TYR:CD1	2.87	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:201:TYR:HD1	2:F:202:ILE:N	2.08	0.51
3:E:69:VAL:HG11	3:E:114:ILE:HA	1.93	0.51
3:I:298:ARG:CG	3:I:369:ASP:O	2.55	0.51
4:G:178:GLY:O	4:G:179:TYR:CD2	2.64	0.51
2:J:29:MET:CE	4:K:109:GLN:HG3	2.41	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:68:THR:O	4:K:71:PRO:HG2	2.10	0.51
4:K:173:PRO:O	4:K:174:TYR:HB2	2.11	0.51
3:E:292:VAL:O	3:E:300:LEU:HD12	2.09	0.51
3:A:77:VAL:HG13	3:A:143:GLY:HA3	1.92	0.51
3:I:98:ALA:HB1	3:I:100:PHE:HE2	1.76	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:A:46:TYR:CE2	3:A:66:LYS:HB2	2.46	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
2:B:198:MET:O	2:B:198:MET:HG3	2.11	0.51
2:B:200:GLU:HG2	2:B:203:ARG:HD3	1.93	0.51
4:C:41:TYR:CD1	4:C:41:TYR:C	2.89	0.51
3:A:275:GLY:HA2	3:A:276:THR:HB	1.93	0.51
2:J:35:PHE:HD2	2:J:36:PHE:CD2	2.28	0.51
2:J:43:HIS:HD2	2:J:101:LEU:CD1	2.23	0.51
2:B:61:ASP:OD2	2:B:64:MET:HG2	2.11	0.51
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
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
3:A:393:PHE:CD1	3:A:401:ARG:HD2	2.46	0.50
2:J:131:VAL:HB	2:J:132:PRO:HD3	1.92	0.50
2:B:129:LEU:C	2:B:132:PRO:HD2	2.36	0.50
2:B:238:PHE:HA	2:B:241:ARG:HG2	1.92	0.50
4:K:35:TYR:CD2	4:K:120:TRP:CG	2.98	0.50
4:K:119:TYR:C	4:K:119:TYR:CD2	2.87	0.50
4:K:199:LEU:HD23	4:K:202:TRP:CZ3	2.46	0.50
4:K:252:LYS:O	4:K:256:GLU:HA	2.11	0.50
2:F:57:VAL:HG12	2:F:123:LEU:HA	1.94	0.50
2:F:201:TYR:HB3	3:E:109:SER:HB3	1.93	0.50
2:B:36:PHE:HE1	4:C:116:ILE:HD12	1.64	0.50
2:B:116:TRP:O	4:C:47:TRP:CZ3	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:TYR:CD2	2:B:218:VAL:HG11	2.46	0.50
2:F:82:ALA:HB1	2:F:241:ARG:HD2	1.94	0.50
3:E:284:VAL:HG11	3:E:394:PHE:CD2	2.46	0.50
3:I:308:ASN:ND2	3:I:314:LEU:HD12	2.26	0.50
4:G:169:LYS:O	4:G:176:ALA:HB2	2.11	0.50
2:J:116:TRP:HB2	4:K:39:ARG:NH1	2.26	0.50
2:B:150:ALA:HB2	2:B:233:TYR:CD1	2.47	0.50
3:E:41:ARG:NE	3:E:387:GLN:HG2	2.26	0.50
3:A:41:ARG:NE	3:A:387:GLN:HG2	2.27	0.50
3:I:220:ALA:C	3:I:222:ASP:N	2.69	0.50
3:I:356:ALA:CB	3:I:357:PRO:CA	2.84	0.50
2:B:117:THR:HA	4:C:47:TRP:CH2	2.46	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: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
2:B:65:TRP:CE3	2:B:66:PRO:HD3	2.47	0.50
4:K:18:VAL:HG11	4:K:101:MET:HE3	1.92	0.50
4:K:117:ALA:HB2	4:K:160:ILE:HD13	1.94	0.50
3:E:341:TYR:H	3:E:342:LEU:CA	2.25	0.50
3:A:94:LEU:HD22	3:A:124:LEU:HB3	1.94	0.50
3:A:220:ALA:C	3:A:222:ASP:N	2.61	0.50
4:G:16:GLU:N	4:G:16:GLU:OE2	2.45	0.50
2:B:36:PHE:CE1	4:C:116:ILE:HD11	2.47	0.50
3:E:82:VAL:HB	3:E:141:GLU:HB2	1.94	0.49
4:G:118:ILE:HG12	4:G:157:TYR:CE1	2.47	0.49
4:G:120:TRP:HE3	4:G:125:PHE:CE2	2.30	0.49
2:J:252:ILE:HA	2:B:146:TYR:CE1	2.46	0.49
4:C:173:PRO:O	4:C:174:TYR:HB2	2.11	0.49
2:F:201:TYR:CD1	2:F:202:ILE:N	2.79	0.49
3:E:198:TRP:O	3:E:202:TRP:CD1	2.65	0.49
3:A:93:VAL:HA	3:A:128:ARG:HB2	1.95	0.49
3:A:100:PHE:HD2	3:A:105:PHE:HA	1.78	0.49
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:K:93:ASP:OD1	4:K:177:HIS:CE1	2.57	0.49
4:C:174:TYR:C	4:C:174:TYR:HD1	2.20	0.49
4:C:194:ILE:CG1	4:C:195:PRO:HD3	2.35	0.49
2:F:211:ARG:HH11	2:F:211:ARG:CG	2.25	0.49
3:A:188:HIS:CD2	2:B:106:TRP:HE1	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:62:ARG:HB3	2:J:218:VAL:HG22	1.95	0.49
2:J:140:LEU:HD13	2:J:149:THR:OG1	2.12	0.49
2:B:57:VAL:HG12	2:B:123:LEU:HA	1.95	0.49
4:K:194:ILE:CG1	4:K:195:PRO:CD	2.74	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:E:96:ARG:NH2	3:E:99:GLN:HE22	2.09	0.49
3:E:246:GLY:O	3:E:250:THR:OG1	2.31	0.49
3:I:140:VAL:O	3:I:141:GLU:C	2.54	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: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: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:O	4:G:226:TRP:HE3	1.96	0.49
2:F:201:TYR:CD1	2:F:201:TYR:C	2.90	0.49
3:E:220:ALA:C	3:E:222:ASP:N	2.67	0.49
3:A:341:TYR:CG	3:A:342:LEU:HB2	2.48	0.49
3:I:141:GLU:HA	3:I:141:GLU:OE2	2.12	0.49
3:I:226:ASP:HA	3:I:229:ARG:H	1.78	0.49
2:B:186:ALA:O	2:B:187:ASP:C	2.56	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
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:56:TRP:HB2	2:F:59:TRP:CD1	2.48	0.49
3:E:58:ASN:HD21	3:E:163:THR:N	2.05	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:J:245:THR:HG23	2:J:245:THR:O	2.12	0.49
2:B:65:TRP:HE3	2:B:66:PRO:HD3	1.77	0.49
3:I:109:SER:HB3	2:J:201:TYR:HB3	1.94	0.48
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:E:131:ARG:HB3	4:G:48:ARG:HH12	1.77	0.48
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:351:ASP:HB2	3:E:353:THR:OG1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:3:UNK:CB	4:K:61:TYR:HD1	2.26	0.48
2:B:29:MET:HE3	4:C:109:GLN:HG3	1.95	0.48
3:E:311:SER:HA	3:E:357:PRO:HB3	1.96	0.48
2:F:166:TRP:HA	2:F:169:ILE:HG22	1.94	0.48
3:A:89:GLU:OE1	3:A:93:VAL:HG23	2.14	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
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
2:J:36:PHE:HA	2:J:37:ALA:C	2.38	0.48
2:B:38:VAL:O	2:B:39:LEU:C	2.57	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
4:C:178:GLY:O	4:C:179:TYR:CD2	2.66	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
3:I:192:MET:CE	2:J:103:ILE:HG13	2.44	0.48
4:G:31:LEU:HD23	4:G:116:ILE:HG22	1.96	0.48
4:G:167:TYR:CE1	4:G:171:ARG:HG2	2.49	0.48
2:J:39:LEU:C	2:J:39:LEU:HD12	2.39	0.48
4:K:110:TRP:CZ3	4:K:163:GLY:HA3	2.49	0.48
3:E:334:THR:CA	3:E:335:LYS:CB	2.81	0.48
1:N:9:UNK:C	1:N:11:UNK:N	2.77	0.48
3:A:50:TRP:HB3	3:A:61:MET:HE1	1.94	0.48
3:I:99:GLN:OE1	2:J:191:PHE:HE1	1.97	0.48
3:I:198:TRP:HZ3	3:I:235:VAL:HG21	1.79	0.48
4:G:119:TYR:C	4:G:119:TYR:CD2	2.90	0.48
4:C:165:PHE:HA	4:C:183:PHE:CE1	2.49	0.48
2:F:252:ILE:O	2:J:145:SER:HA	2.14	0.48
3:A:366:LYS:HB2	3:A:366:LYS:NZ	2.26	0.48
2:J:116:TRP:O	4:K:47:TRP:CZ3	2.66	0.48
2:F:49:THR:OG1	2:F:72:LEU:HD22	2.14	0.47
3:E:201:PHE:HZ	3:E:231:ILE:HD13	1.78	0.47
3:A:92:PRO:HB3	2:B:193:PHE:HA	1.95	0.47
3:A:311:SER:HA	3:A:357:PRO:HB3	1.95	0.47
4:G:126:THR:HA	4:G:149:GLU:OE1	2.14	0.47
4:G:148:ILE:HD13	4:G:148:ILE:N	2.27	0.47
2:B:85:TRP:CE2	2:B:89:ARG:HD3	2.48	0.47
2:B:132:PRO:HB2	2:B:157:TRP:CE3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:TYR:HA	2:B:207:ARG:NH2	2.29	0.47
4:C:35:TYR:CD2	4:C:120:TRP:CG	3.01	0.47
4:C:226:TRP:CE3	4:C:226:TRP:CA	2.96	0.47
2:F:55:PHE:O	2:F:124:VAL:HA	2.14	0.47
3:A:69:VAL:HG12	3:A:114:ILE:HA	1.95	0.47
3:I:388:ILE:HD13	3:I:410:VAL:HG21	1.94	0.47
4:G:251:VAL:O	4:G:252:LYS:C	2.56	0.47
2:B:57:VAL:CG1	2:B:123:LEU:HA	2.44	0.47
2:F:65:TRP:N	2:F:66:PRO:HD2	2.29	0.47
1:N:7:UNK:O	1:N:8:UNK:C	2.62	0.47
3:I:101:ILE:O	3:I:104:GLN:N	2.43	0.47
2:B:125:PHE:CZ	2:B:169:ILE:CD1	2.96	0.47
4:K:121:GLY:HA2	4:K:153:SER:CB	2.43	0.47
4:K:124:PHE:HD2	4:K:125:PHE:CE2	2.32	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
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
3:A:380:LEU:HG	3:A:380:LEU:O	2.15	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:G:35:TYR:HE1	4:G:152:MET:HE3	1.79	0.47
4:G:41:TYR:C	4:G:41:TYR:CD1	2.92	0.47
4:G:70:ILE:HB	4:G:71:PRO:CD	2.44	0.47
4:G:100:GLU:HG2	4:G:245:LEU:HD11	1.95	0.47
2:J:43:HIS:HD2	2:J:101:LEU:HD11	1.79	0.47
4:C:120:TRP:HE3	4:C:125:PHE:CE2	2.32	0.47
2:F:36:PHE:O	2:F:36:PHE:CD1	2.67	0.47
3:E:411:ILE:HG12	2:J:177:GLU:HG2	1.96	0.47
3:A:261:GLN:HE22	3:I:386:SER:N	2.10	0.47
3:I:80:PRO:HA	3:I:140:VAL:HG13	1.96	0.47
3:I:291:GLY:HA3	3:I:302:ILE:HG22	1.96	0.47
4:G:19:VAL:HA	4:G:105:VAL:HG11	1.97	0.47
4:G:68:THR:O	4:G:71:PRO:HG2	2.14	0.47
4:G:165:PHE:HA	4:G:183:PHE:CE1	2.50	0.47
4:G:209:MET:O	4:G:210:GLU:O	2.32	0.47
2:J:245:THR:HG21	4:K:181:LEU:HD23	1.96	0.47
4:C:154:TYR:O	4:C:155:PRO:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:53:TRP:HB3	2:J:65:TRP:HD1	1.79	0.47
4:K:226:TRP:CE3	4:K:226:TRP:CA	2.96	0.47
4:C:82:GLY:O	4:C:86:LYS:HB2	2.14	0.47
4:C:128:GLN:O	4:C:131:THR:HG22	2.14	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
2:F:204:MET:HA	2:F:204:MET:CE	2.42	0.46
2:J:199:PRO:CB	2:J:201:TYR:CE1	2.91	0.46
4:K:53:SER:HB3	4:K:139:ASP:HB2	1.97	0.46
4:K:117:ALA:HB1	4:K:157:TYR:CA	2.45	0.46
4:C:178:GLY:O	4:C:179:TYR:CG	2.69	0.46
2:F:57:VAL:CG1	2:F:123:LEU:HA	2.45	0.46
3:E:101:ILE:HG23	3:E:268:LEU:HD11	1.95	0.46
3:I:82:VAL:HB	3:I:141:GLU:HB2	1.97	0.46
3:I:137:GLN:HG3	3:I:147:ILE:CD1	2.44	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:117:THR:HG22	4:C:47:TRP:HH2	1.80	0.46
2:B:132:PRO:HB3	2:B:157:TRP:HA	1.97	0.46
2:F:238:PHE:HA	2:F:241:ARG:HG2	1.97	0.46
3:I:141:GLU:H	2:J:201:TYR:HE2	1.62	0.46
4:G:209:MET:O	4:G:209:MET:CG	2.62	0.46
2:J:53:TRP:CD1	2:J:65:TRP:HB2	2.50	0.46
4:K:16:GLU:CD	4:K:16:GLU:N	2.73	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:235:VAL:O	3:I:239:THR:OG1	2.34	0.46
3:I:324:LEU:HD12	3:I:324:LEU:H	1.80	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
2:F:44:VAL:CG2	4:G:122:ALA:O	2.64	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:213:ILE:HG12	4:G:243:HIS:CD2	2.51	0.46
3:A:411:ILE:HG23	3:A:412:PRO:HD2	1.98	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:117:THR:HG22	4:C:47:TRP:CH2	2.51	0.46
3:E:93:VAL:HA	3:E:128:ARG:HB2	1.98	0.46
2:J:63:ARG:HB3	2:J:64:MET:HE2	1.98	0.46
2:J:108:ASN:ND2	4:K:127:GLU:HB3	2.31	0.46
2:J:223:PHE:O	2:J:224:PHE:C	2.59	0.46
2:B:108:ASN:ND2	4:C:127:GLU:OE2	2.39	0.46
3:E:96:ARG:HH21	3:E:99:GLN:HE22	1.63	0.46
4:G:39:ARG:HH22	4:G:43:GLN:HB2	1.81	0.46
4:G:194:ILE:H	4:G:194:ILE:CD1	2.18	0.46
2:J:65:TRP:N	2:J:66:PRO:HD2	2.31	0.46
2:B:43:HIS:HD2	2:B:101:LEU:CD1	2.29	0.46
2:B:109:ARG:O	2:B:113:PHE:HB2	2.16	0.46
2:B:112:ASN:CG	4:C:128:GLN:HG3	2.41	0.46
2:B:200:GLU:O	2:B:201:TYR:CB	2.64	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:26:VAL:O	2:J:27:ASP:C	2.58	0.45
2:J:117:THR:HA	4:K:47:TRP:CH2	2.50	0.45
4:C:256:GLU:N	4:C:256:GLU:CD	2.74	0.45
3:E:387:GLN:HG3	3:E:408:GLY:C	2.41	0.45
3:A:308:ASN:ND2	3:A:314:LEU:HD12	2.32	0.45
2:J:76:PHE:CE2	4:K:229:LEU:HD21	2.51	0.45
2:B:56:TRP:HB2	2:B:59:TRP:CD1	2.51	0.45
2:B:135:TRP:NE1	2:B:156:GLY:HA3	2.31	0.45
2:F:60:LYS:HD3	2:F:65:TRP:CE2	2.52	0.45
3:A:60:GLU:O	3:A:60:GLU:CG	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:HG3	3:E:229:ARG:HH11	1.82	0.45
3:E:273:THR:O	3:E:273:THR:OG1	2.33	0.45
3:I:156:LYS:NZ	3:I:156:LYS:HB3	2.31	0.45
4:G:168:ALA:HB1	4:G:175:PHE:CD2	2.52	0.45
2:J:51:GLY:CA	2:J:52:ASP:CB	2.59	0.45
2:J:108:ASN:OD1	2:J:112:ASN:ND2	2.50	0.45
2:F:43:HIS:HD2	2:F:101:LEU:CD1	2.29	0.45
2:F:44:VAL:HG22	4:G:126:THR:HG21	1.99	0.45
2:F:91:PRO:HB3	2:F:141:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:70:PHE:HE2	3:A:72:ALA:HB3	1.81	0.45
3:I:128:ARG:HH22	4:K:47:TRP:NE1	2.15	0.45
3:I:163:THR:HG22	3:I:175:ASP:OD2	2.16	0.45
4:G:117:ALA:HB2	4:G:160:ILE:HD13	1.97	0.45
2:B:119:PHE:HB3	2:B:123:LEU:HD23	1.97	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:E:308:ASN:HA	3:E:309:ASN:CB	2.32	0.45
3:A:300:LEU:HD23	3:A:367:ILE:HD13	1.99	0.45
3:I:60:GLU:O	3:I:60:GLU:CG	2.61	0.45
3:I:191:TRP:CZ3	3:I:239:THR:HG23	2.52	0.45
2:J:114:TRP:O	2:J:118:TYR:N	2.46	0.45
2:B:166:TRP:HA	2:B:169:ILE:HG22	1.99	0.45
4:K:107:LEU:HD23	4:K:238:ILE:HD11	1.99	0.45
4:C:201:GLU:C	4:C:203:GLY:H	2.24	0.45
1:D:20:UNK:CB	4:C:26:ILE:HD13	2.47	0.45
3:E:217:GLU:O	3:E:218:GLY:C	2.59	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
3:A:156:LYS:HB3	3:A:156:LYS:HZ2	1.82	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
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
3:A:341:TYR:H	3:A:342:LEU:C	2.25	0.45
4:K:148:ILE:N	4:K:148:ILE:HD13	2.32	0.45
4:K:158:SER:O	4:K:161:ALA:HB3	2.17	0.45
4:C:249:GLU:O	4:C:253:LEU:HB2	2.16	0.45
2:F:199:PRO:HB3	3:E:84:PHE:CB	2.47	0.45
2:F:231:MET:O	2:F:232:VAL:C	2.60	0.45
3:E:286:THR:HG22	3:E:304:VAL:HG11	1.94	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:A:303:ASN:OD1	3:A:303:ASN:N	2.50	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:30:GLY:O	3:E:31:GLU:C	2.60	0.44
3:E:144:GLY:CA	2:J:211:ARG:HH12	2.30	0.44
3:A:89:GLU:OE1	3:A:93:VAL:HG22	2.18	0.44
3:A:227:ASP:O	3:A:231:ILE:HG13	2.16	0.44
3:A:236:LEU:CB	2:B:138:VAL:HG11	2.43	0.44
4:G:147:ILE:HG12	4:G:147:ILE:H	1.53	0.44
2:J:36:PHE:HE1	4:K:116:ILE:CD1	2.30	0.44
2:B:29:MET:HE1	4:C:109:GLN:HE21	1.81	0.44
4:C:152:MET:C	4:C:155:PRO:HD2	2.42	0.44
2:F:116:TRP:O	4:G:47:TRP:CZ3	2.71	0.44
3:A:50:TRP:O	3:A:51:SER:C	2.60	0.44
3:I:98:ALA:HA	2:J:191:PHE:HE2	1.82	0.44
4:G:44:VAL:HG12	4:G:45:PHE:CE1	2.52	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
4:C:176:ALA:O	4:C:177:HIS:CD2	2.70	0.44
3:E:392:LEU:HD23	3:E:392:LEU:HA	1.64	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:I:93:VAL:HB	3:I:132:TRP:CD1	2.53	0.44
3:I:213:ILE:O	3:I:214:ARG:C	2.60	0.44
4:K:146:HIS:HE1	4:K:201:GLU:OE1	1.99	0.44
2:F:102:LEU:HD23	2:F:102:LEU:HA	1.54	0.44
3:E:411:ILE:HG23	3:E:412:PRO:HD2	2.00	0.44
3:I:100:PHE:HZ	2:J:179:HIS:NE2	2.15	0.44
3:I:221:ASP:N	3:I:221:ASP:OD1	2.50	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
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:HD2	3:E:82:VAL:HG12	1.82	0.44
2:F:201:TYR:HA	2:F:207:ARG:NH2	2.33	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
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
4:C:79:GLY:O	4:C:80:LEU:C	2.61	0.44
2:F:35:PHE:HD2	2:F:36:PHE:CD2	2.35	0.44
2:F:87:ASN:CG	4:G:236:LEU:HD11	2.42	0.44
2:F:117:THR:HG22	4:G:47:TRP:HH2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:5:UNK:O	1:N:6:UNK:C	2.66	0.44
4:G:173:PRO:O	4:G:174:TYR:HB2	2.18	0.44
4:G:226:TRP:CE3	4:G:226:TRP:CA	3.00	0.44
4:C:119:TYR:CD2	4:C:119:TYR:C	2.95	0.44
2:F:9:ALA:HB3	2:F:15:SER:HA	2.00	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
3:A:340:ASP:HB3	3:A:341:TYR:HB3	1.99	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
2:F:88:PHE:CD1	2:F:88:PHE:N	2.85	0.44
3:A:37:PHE:O	3:A:41:ARG:HG3	2.18	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
4:G:194:ILE:CG1	4:G:195:PRO:HD3	2.27	0.44
2:J:111:VAL:HG12	2:J:112:ASN:OD1	2.17	0.44
2:B:39:LEU:C	2:B:39:LEU:HD12	2.43	0.44
4:C:118:ILE:HG12	4:C:157:TYR:CD1	2.52	0.44
4:C:226:TRP:HA	4:C:226:TRP:HE3	1.81	0.44
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
2:F:19:ALA:O	2:F:21:GLY:N	2.50	0.43
3:E:89:GLU:OE1	3:E:93:VAL:CG2	2.67	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
4:G:226:TRP:HA	4:G:226:TRP:HE3	1.82	0.43
2:B:22:CYS:O	2:B:23:VAL:C	2.60	0.43
2:B:36:PHE:HD1	2:B:36:PHE:O	2.01	0.43
2:B:201:TYR:HD1	2:B:202:ILE:N	2.17	0.43
2:B:211:ARG:HH11	2:B:211:ARG:CG	2.27	0.43
2:F:78:ALA:HB2	2:F:233:TYR:CD2	2.52	0.43
3:A:341:TYR:CD1	3:A:342:LEU:HB2	2.53	0.43
3:I:286:THR:CG2	3:I:304:VAL:HG11	2.48	0.43
2:J:49:THR:OG1	2:J:72:LEU:HD22	2.19	0.43
4:C:236:LEU:HD23	4:C:236:LEU:HA	1.80	0.43
3:E:96:ARG:HH21	3:E:99:GLN:NE2	2.15	0.43
3:E:212:TYR:OH	4:G:240:MET:HG2	2.17	0.43
3:A:198:TRP:O	3:A:202:TRP:CD1	2.71	0.43
3:I:60:GLU:OE2	3:I:123:ASN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:94:LEU:HD23	3:I:126:GLY:CA	2.42	0.43
3:I:348:LEU:HB2	3:I:349:SER:HB2	2.01	0.43
4:C:190:PRO:O	4:C:193:ILE:HG13	2.17	0.43
3:E:60:GLU:O	3:E:60:GLU:CG	2.45	0.43
3:E:141:GLU:OE2	3:E:141:GLU:HA	2.18	0.43
3:A:133:HIS:NE2	3:A:150:GLY:O	2.52	0.43
3:I:308:ASN:HA	3:I:309:ASN:CB	2.27	0.43
4:G:199:LEU:HD23	4:G:202:TRP:CZ3	2.54	0.43
2:J:38:VAL:CG2	2:J:39:LEU:N	2.81	0.43
2:J:176:THR:HG21	2:J:188:LEU:HD22	2.00	0.43
2:B:53:TRP:CD1	2:B:65:TRP:HB2	2.54	0.43
2:F:38:VAL:HG23	2:F:39:LEU:N	2.31	0.43
2:F:117:THR:HG22	4:G:47:TRP:CH2	2.54	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
3:I:96:ARG:HH21	3:I:99:GLN:HE22	1.67	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
2:J:26:VAL:O	2:J:29:MET:N	2.52	0.43
2:B:201:TYR:CD1	2:B:202:ILE:N	2.87	0.43
4:K:163:GLY:O	4:K:164:ALA:C	2.61	0.43
2:F:35:PHE:HA	2:F:96:PHE:CZ	2.54	0.43
3:E:99:GLN:HB2	3:E:122:ILE:HG12	2.00	0.43
3:I:229:ARG:HG3	3:I:229:ARG:NH1	2.32	0.43
2:J:91:PRO:HB3	2:J:141:LEU:HD13	1.99	0.43
2:B:43:HIS:HE1	4:C:127:GLU:HB2	1.83	0.43
4:K:88:ARG:CB	4:K:170:THR:HB	2.49	0.43
4:C:38:VAL:HG21	4:C:152:MET:HE1	2.01	0.43
2:F:64:MET:HG2	2:F:64:MET:H	1.63	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
4:G:146:HIS:CE1	4:G:201:GLU:OE1	2.71	0.43
4:G:201:GLU:C	4:G:203:GLY:H	2.27	0.43
2:B:138:VAL:O	2:B:142:LEU:HG	2.18	0.43
4:K:201:GLU:C	4:K:203:GLY:N	2.77	0.43
2:F:76:PHE:CE2	4:G:229:LEU:HD21	2.54	0.43
2:F:90:LEU:HD23	2:F:90:LEU:HA	1.87	0.43
2:F:170:ALA:O	2:F:171:ALA:C	2.62	0.43
3:E:131:ARG:HB3	4:G:48:ARG:HH22	1.83	0.43
3:A:214:ARG:HB3	3:A:220:ALA:H	1.84	0.43
4:G:189:GLY:N	4:G:190:PRO:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:TRP:HB3	2:B:58:ASP:OD1	2.19	0.43
2:B:87:ASN:CG	4:C:236:LEU:HD11	2.44	0.43
4:K:193:ILE:O	4:K:197:VAL:N	2.52	0.43
2:F:202:ILE:HD12	2:F:202:ILE:HA	1.66	0.43
3:A:57:VAL:O	3:A:58:ASN:HB2	2.18	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
2:F:245:THR:HG23	2:F:245:THR:O	2.18	0.42
3:I:30:GLY:O	3:I:31:GLU:C	2.62	0.42
3:I:96:ARG:HH21	3:I:99:GLN:NE2	2.16	0.42
4:G:151:TYR:N	4:G:151:TYR:CD1	2.87	0.42
4:G:256:GLU:CD	4:G:256:GLU:N	2.77	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
4:C:143:THR:O	4:C:147:ILE:CG1	2.65	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
2:B:33:LEU:HB3	4:C:112:VAL:HG22	2.01	0.42
2:B:241:ARG:O	2:B:242:TRP:C	2.59	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
4:K:178:GLY:O	4:K:179:TYR:CD2	2.72	0.42
2:F:135:TRP:CE2	2:F:156:GLY:HA3	2.54	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
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
4:K:42:GLU:HA	4:K:62:TRP:HH2	1.82	0.42
4:K:235:VAL:HG23	4:K:239:LEU:HD12	2.01	0.42
3:E:55:VAL:HG12	3:E:59:GLU:HB3	2.01	0.42
3:E:273:THR:HB	3:E:274:GLU:HB2	2.01	0.42
3:A:187:TRP:CZ2	2:B:167:PRO:HG2	2.54	0.42
3:I:121:SER:C	3:I:122:ILE:HG13	2.44	0.42
3:I:131:ARG:HB3	4:K:48:ARG:HH22	1.85	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
2:B:48:LEU:HD12	2:B:48:LEU:HA	1.84	0.42
2:F:38:VAL:O	2:F:39:LEU:C	2.62	0.42
2:F:85:TRP:CE2	2:F:89:ARG:HD3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:192:MET:HE2	3:A:192:MET:HB3	1.94	0.42
3:A:295:VAL:HA	3:A:296:PRO:HA	1.91	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
2:B:54:ASP:O	2:B:109:ARG:NH1	2.52	0.42
2:B:189:ILE:O	2:B:193:PHE:HD1	2.02	0.42
2:F:112:ASN:CG	4:G:128:GLN:HG3	2.45	0.42
3:E:70:PHE:HE2	3:E:72:ALA:HB3	1.85	0.42
3:E:357:PRO:C	3:E:359:GLU:H	2.28	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:J:85:TRP:CE2	2:J:89:ARG:HD3	2.54	0.42
2:B:39:LEU:HD11	2:B:104:GLY:HA3	2.00	0.42
4:K:167:TYR:CD1	4:K:171:ARG:HD3	2.55	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
3:A:392:LEU:HD23	3:A:392:LEU:HA	1.67	0.42
4:G:104:LEU:O	4:G:108:VAL:HG23	2.20	0.42
4:C:69:GLU:O	4:C:70:ILE:C	2.61	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:C:209:MET:HE2	4:C:209:MET:H	1.85	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:35:PHE:HA	2:J:96:PHE:CZ	2.55	0.42
2:J:220:VAL:CG2	2:J:221:ALA:N	2.83	0.42
2:B:113:PHE:CE1	4:C:131:THR:HB	2.55	0.42
2:B:200:GLU:HA	2:B:203:ARG:HD2	2.02	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:A:288:LEU:HD12	3:A:288:LEU:HA	1.94	0.42
3:A:350:VAL:HG12	3:A:351:ASP:H	1.84	0.42
3:I:99:GLN:HB2	3:I:122:ILE:HG12	2.01	0.42
4:G:35:TYR:HE1	4:G:152:MET:CE	2.31	0.42
4:G:116:ILE:HD12	4:G:116:ILE:HA	1.80	0.42
2:F:36:PHE:HA	2:F:37:ALA:C	2.44	0.42
2:F:177:GLU:CG	3:A:411:ILE:HG12	2.50	0.42
3:E:100:PHE:CD2	3:E:105:PHE:HA	2.46	0.42
3:A:158:ASP:CG	3:A:160:LYS:HB2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:24:MET:HB2	4:K:109:GLN:CG	2.37	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
2:F:182:LEU:HD22	3:A:412:PRO:HD3	2.02	0.41
3:E:100:PHE:CA	3:E:104:GLN:O	2.66	0.41
3:E:117:ASP:OD1	3:E:117:ASP:N	2.52	0.41
3:E:316:LEU:HB2	3:E:394:PHE:CE1	2.54	0.41
3:A:391:LEU:HD23	3:A:391:LEU:HA	1.83	0.41
3:I:117:ASP:OD1	3:I:117:ASP:N	2.52	0.41
2:J:37:ALA:O	2:J:38:VAL:C	2.62	0.41
2:J:112:ASN:CG	4:K:128:GLN:HG3	2.44	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
3:E:205:ARG:C	3:E:206:LYS:HG2	2.44	0.41
4:G:203:GLY:O	4:G:207:TRP:HB2	2.20	0.41
4:K:44:VAL:CG1	4:K:45:PHE:CD1	2.89	0.41
4:K:101:MET:HE3	4:K:101:MET:HB3	1.79	0.41
3:E:32:LYS:HG2	3:E:375:GLU:HA	2.02	0.41
3:E:131:ARG:O	4:G:48:ARG:NH2	2.54	0.41
3:E:318:GLU:OE2	3:E:325:ARG:HG2	2.20	0.41
3:A:125:ARG:HD3	3:A:162:PHE:CE2	2.55	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
3:I:219:LYS:HD2	3:I:221:ASP:CG	2.45	0.41
4:G:35:TYR:CD2	4:G:120:TRP:CG	3.08	0.41
4:G:118:ILE:HG12	4:G:157:TYR:CD1	2.55	0.41
2:J:129:LEU:O	2:J:132:PRO:HD2	2.21	0.41
3:E:69:VAL:HG12	3:E:114:ILE:HA	2.01	0.41
3:E:156:LYS:HB3	3:E:156:LYS:NZ	2.35	0.41
3:E:208:ILE:O	3:E:209:ILE:C	2.63	0.41
3:A:85:LEU:HD21	3:A:120:PHE:HB2	2.03	0.41
3:I:311:SER:HA	3:I:357:PRO:CB	2.50	0.41
4:G:42:GLU:HA	4:G:62:TRP:HH2	1.86	0.41
2:J:200:GLU:HG2	2:J:203:ARG:HD3	2.03	0.41
2:B:56:TRP:CH2	4:C:134:MET:HG3	2.55	0.41
2:B:117:THR:HB	2:B:119:PHE:HE1	1.85	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
4:C:114:TYR:HE1	4:C:161:ALA:HB2	1.85	0.41
4:C:146:HIS:HE1	4:C:201:GLU:OE1	2.00	0.41
3:E:135:HIS:HA	3:E:150:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:MET:HA	2:B:204:MET:CE	2.46	0.41
2:F:12:PRO:O	4:G:98:ARG:NH1	2.52	0.41
3:A:61:MET:SD	3:A:62:VAL:N	2.94	0.41
3:I:92:PRO:HB3	2:J:193:PHE:HA	2.03	0.41
3:I:102:GLY:HA3	3:I:268:LEU:HD13	2.02	0.41
2:J:56:TRP:CH2	4:K:134:MET:HG3	2.55	0.41
2:J:76:PHE:HE2	4:K:229:LEU:HD21	1.85	0.41
2:J:211:ARG:HG3	2:J:211:ARG:HH11	1.86	0.41
2:J:233:TYR:CD1	2:J:233:TYR:C	2.98	0.41
4:C:114:TYR:CE1	4:C:161:ALA:HB2	2.55	0.41
4:C:207:TRP:O	4:C:208:PHE:C	2.63	0.41
2:F:150:ALA:HB2	2:F:233:TYR:CD1	2.55	0.41
3:E:307:LYS:HG3	3:E:309:ASN:ND2	2.36	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
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
4:K:118:ILE:HG22	4:K:119:TYR:N	2.35	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
2:F:37:ALA:O	2:F:38:VAL:C	2.62	0.41
2:F:112:ASN:ND2	4:G:128:GLN:HG3	2.36	0.41
3:E:50:TRP:CE2	3:E:151:GLN:HB3	2.55	0.41
3:E:289:ASN:O	3:E:303:ASN:HB2	2.21	0.41
3:E:348:LEU:HA	3:E:349:SER:HA	1.75	0.41
3:A:95:VAL:HG11	2:B:192:HIS:CD2	2.55	0.41
3:A:96:ARG:HH21	3:A:99:GLN:HE22	1.68	0.41
3:A:260:LEU:O	3:I:384:THR:HG22	2.20	0.41
3:I:284:VAL:HG23	3:I:402:TYR:HB3	2.03	0.41
3:I:288:LEU:HD12	3:I:288:LEU:HA	1.88	0.41
3:I:351:ASP:HB2	3:I:353:THR:OG1	2.20	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
2:J:182:LEU:HD12	2:J:182:LEU:HA	1.95	0.41
4:K:117:ALA:HB1	4:K:157:TYR:HB2	2.02	0.41
4:K:193:ILE:HD12	4:K:193:ILE:C	2.46	0.41
4:K:251:VAL:O	4:K:252:LYS:C	2.63	0.41
4:C:24:MET:HB2	4:C:109:GLN:CG	2.42	0.41
4:C:53:SER:HB3	4:C:139:ASP:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:53:TRP:HB3	2:F:65:TRP:CD1	2.56	0.41
3:I:89:GLU:OE1	3:I:93:VAL:CG2	2.69	0.41
4:G:251:VAL:HG12	4:G:252:LYS:H	1.84	0.41
2:B:53:TRP:HB3	2:B:65:TRP:HD1	1.86	0.41
4:K:29:VAL:O	4:K:30:LEU:C	2.62	0.41
4:K:167:TYR:CE1	4:K:171:ARG:HG2	2.56	0.41
4:C:172:ILE:HA	4:C:173:PRO:HD3	1.98	0.41
3:A:70:PHE:CE2	3:A:72:ALA:HB3	2.56	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
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
2:B:131:VAL:HB	2:B:132:PRO:HD3	2.03	0.40
4:C:106:VAL:HB	4:C:167:TYR:OH	2.20	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:A:229:ARG:HH11	3:A:229:ARG:HG3	1.86	0.40
3:I:144:GLY:HA3	2:B:211:ARG:NH1	2.35	0.40
2:J:110:TYR:O	2:J:111:VAL:C	2.65	0.40
2:J:202:ILE:HA	2:J:202:ILE:HD12	1.65	0.40
4:K:147:ILE:HG12	4:K:147:ILE:H	1.77	0.40
4:K:174:TYR:HD1	4:K:174:TYR:O	2.03	0.40
4:C:138:ARG:HH12	4:C:141:ASP:HA	1.83	0.40
3:E:101:ILE:HG23	3:E:268:LEU:CD1	2.51	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
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:O	2:F:198:MET:HG3	2.21	0.40
3:A:30:GLY:O	3:A:31:GLU:C	2.64	0.40
3:I:69:VAL:HG11	3:I:114:ILE:HA	2.03	0.40
4:G:31:LEU:HD12	4:G:31:LEU:HA	1.86	0.40
2:B:224:PHE:HD2	4:K:199:LEU:HD22	1.86	0.40
4:K:38:VAL:HG21	4:K:152:MET:HE1	2.03	0.40
4:C:203:GLY:O	4:C:207:TRP:HB2	2.22	0.40
3:E:76:ALA:HB1	2:J:208:GLY:O	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:50:TRP:O	3:I:51:SER:C	2.64	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
4:G:121:GLY:HA2	4:G:153:SER:CB	2.51	0.40
2:J:56:TRP:HB2	2:J:59:TRP:CD1	2.56	0.40
2:J:135:TRP:CE2	2:J:156:GLY:HA3	2.57	0.40
2:J:216:ASP:O	2:J:219:PRO:HD2	2.22	0.40
2:B:92:PHE:CD1	2:B:92:PHE:C	2.99	0.40
4:K:55:ALA:HB1	4:K:57:GLU:OE1	2.21	0.40
4:K:191:PHE:HA	4:K:194:ILE:HD11	2.04	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%)	5	27
2	F	242/252 (96%)	197 (81%)	36 (15%)	9 (4%)	2	17
2	J	242/252 (96%)	200 (83%)	29 (12%)	13 (5%)	1	10
3	A	388/420 (92%)	307 (79%)	56 (14%)	25 (6%)	1	8
3	E	388/420 (92%)	314 (81%)	44 (11%)	30 (8%)	1	5
3	I	388/420 (92%)	308 (79%)	53 (14%)	27 (7%)	1	7
4	C	224/256 (88%)	169 (75%)	49 (22%)	6 (3%)	4	22
4	G	224/256 (88%)	172 (77%)	44 (20%)	8 (4%)	2	18
4	K	224/256 (88%)	163 (73%)	52 (23%)	9 (4%)	2	16
All	All	2562/2784 (92%)	2019 (79%)	411 (16%)	132 (5%)	1	11

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	180 (89%)	22 (11%)	6	24
2	F	202/208 (97%)	179 (89%)	23 (11%)	5	22
2	J	202/208 (97%)	176 (87%)	26 (13%)	4	18
3	A	320/336 (95%)	268 (84%)	52 (16%)	2	11
3	E	320/336 (95%)	268 (84%)	52 (16%)	2	11
3	I	320/336 (95%)	268 (84%)	52 (16%)	2	11
4	C	194/213 (91%)	157 (81%)	37 (19%)	1	6
4	G	194/213 (91%)	158 (81%)	36 (19%)	1	7
4	K	194/213 (91%)	160 (82%)	34 (18%)	2	9
All	All	2148/2271 (95%)	1814 (84%)	334 (16%)	2	12

All (334) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	16	VAL
2	F	22	CYS
2	F	25	THR
2	F	26	VAL
2	F	38	VAL
2	F	39	LEU
2	F	48	LEU
2	F	52	ASP
2	F	64	MET

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Mol	Chain	Res	Type
2	F	68	VAL
2	F	86	VAL
2	F	89	ARG
2	F	148	ILE
2	F	152	VAL
2	F	164	ASN
2	F	177	GLU
2	F	201	TYR
2	F	202	ILE
2	F	204	MET
2	F	217	VAL
2	F	225	SER
2	F	246	THR
2	F	249	ILE
3	E	53	THR
3	E	55	VAL
3	E	61	MET
3	E	62	VAL
3	E	81	ARG
3	E	99	GLN
3	E	111	SER
3	E	117	ASP
3	E	138	ILE
3	E	156	LYS
3	E	167	THR
3	E	169	LEU
3	E	173	THR
3	E	176	LEU
3	E	182	SER
3	E	204	VAL
3	E	206	LYS
3	E	209	ILE
3	E	214	ARG
3	E	215	VAL
3	E	217	GLU
3	E	221	ASP
3	E	241	LEU
3	E	250	THR
3	E	252	SER
3	E	253	THR
3	E	254	PHE
3	E	256	ARG

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Mol	Chain	Res	Type
3	E	258	ILE
3	E	277	VAL
3	E	284	VAL
3	E	286	THR
3	E	303	ASN
3	E	305	LYS
3	E	306	VAL
3	E	311	SER
3	E	320	THR
3	E	324	LEU
3	E	334	THR
3	E	335	LYS
3	E	343	LEU
3	E	348	LEU
3	E	351	ASP
3	E	359	GLU
3	E	363	ILE
3	E	364	VAL
3	E	366	LYS
3	E	374	ILE
3	E	384	THR
3	E	388	ILE
3	E	398	ASP
3	E	415	VAL
3	A	48	VAL
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	146	ILE
3	A	156	LYS
3	A	167	THR
3	A	169	LEU
3	A	173	THR
3	A	182	SER
3	A	204	VAL
3	A	205	ARG
3	A	206	LYS
3	A	209	ILE
3	A	215	VAL

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Mol	Chain	Res	Type
3	A	217	GLU
3	A	221	ASP
3	A	235	VAL
3	A	239	THR
3	A	241	LEU
3	A	250	THR
3	A	252	SER
3	A	253	THR
3	A	254	PHE
3	A	256	ARG
3	A	258	ILE
3	A	271	ILE
3	A	277	VAL
3	A	284	VAL
3	A	286	THR
3	A	303	ASN
3	A	305	LYS
3	A	306	VAL
3	A	311	SER
3	A	320	THR
3	A	334	THR
3	A	335	LYS
3	A	343	LEU
3	A	348	LEU
3	A	351	ASP
3	A	359	GLU
3	A	363	ILE
3	A	366	LYS
3	A	368	GLN
3	A	374	ILE
3	A	384	THR
3	A	388	ILE
3	A	398	ASP
3	A	415	VAL
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	82	VAL

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Mol	Chain	Res	Type
3	I	99	GLN
3	I	100	PHE
3	I	111	SER
3	I	138	ILE
3	I	149	PRO
3	I	156	LYS
3	I	159	MET
3	I	167	THR
3	I	173	THR
3	I	176	LEU
3	I	182	SER
3	I	204	VAL
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	240	ILE
3	I	241	LEU
3	I	250	THR
3	I	252	SER
3	I	253	THR
3	I	254	PHE
3	I	256	ARG
3	I	271	ILE
3	I	277	VAL
3	I	284	VAL
3	I	286	THR
3	I	303	ASN
3	I	305	LYS
3	I	306	VAL
3	I	311	SER
3	I	324	LEU
3	I	334	THR
3	I	335	LYS
3	I	342	LEU
3	I	359	GLU
3	I	363	ILE
3	I	366	LYS
3	I	384	THR
3	I	388	ILE

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Mol	Chain	Res	Type
3	I	398	ASP
3	I	415	VAL
4	G	16	GLU
4	G	22	ARG
4	G	30	LEU
4	G	33	VAL
4	G	36	LEU
4	G	40	ILE
4	G	47	TRP
4	G	68	THR
4	G	74	LEU
4	G	86	LYS
4	G	90	ARG
4	G	96	THR
4	G	109	GLN
4	G	112	VAL
4	G	116	ILE
4	G	118	ILE
4	G	126	THR
4	G	137	ILE
4	G	147	ILE
4	G	148	ILE
4	G	157	TYR
4	G	184	LEU
4	G	188	ILE
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	235	VAL
4	G	248	LYS
4	G	249	GLU
4	G	252	LYS
4	G	255	THR
4	G	256	GLU
2	J	16	VAL
2	J	23	VAL
2	J	25	THR
2	J	26	VAL

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Mol	Chain	Res	Type
2	J	38	VAL
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	130	ILE
2	J	148	ILE
2	J	164	ASN
2	J	169	ILE
2	J	177	GLU
2	J	184	THR
2	J	192	HIS
2	J	201	TYR
2	J	202	ILE
2	J	203	ARG
2	J	204	MET
2	J	217	VAL
2	J	219	PRO
2	J	246	THR
2	J	249	ILE
2	B	16	VAL
2	B	22	CYS
2	B	25	THR
2	B	26	VAL
2	B	38	VAL
2	B	39	LEU
2	B	48	LEU
2	B	52	ASP
2	B	64	MET
2	B	67	THR
2	B	68	VAL
2	B	86	VAL
2	B	148	ILE
2	B	152	VAL
2	B	164	ASN
2	B	177	GLU
2	B	201	TYR
2	B	202	ILE
2	B	204	MET
2	B	217	VAL

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Mol	Chain	Res	Type
2	B	246	THR
2	B	249	ILE
4	K	16	GLU
4	K	22	ARG
4	K	30	LEU
4	K	33	VAL
4	K	36	LEU
4	K	40	ILE
4	K	47	TRP
4	K	75	VAL
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	137	ILE
4	K	147	ILE
4	K	157	TYR
4	K	184	LEU
4	K	188	ILE
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	240	MET
4	K	248	LYS
4	K	249	GLU
4	K	252	LYS
4	K	255	THR
4	K	256	GLU
4	C	16	GLU
4	C	22	ARG
4	C	30	LEU
4	C	33	VAL
4	C	36	LEU
4	C	40	ILE

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Mol	Chain	Res	Type
4	C	47	TRP
4	C	53	SER
4	C	68	THR
4	C	75	VAL
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	131	THR
4	C	137	ILE
4	C	147	ILE
4	C	151	TYR
4	C	157	TYR
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	174	GLN
2	F	178	GLN
3	E	44	ASN
3	E	58	ASN
3	E	68	HIS
3	E	99	GLN
3	E	137	GLN

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Mol	Chain	Res	Type
3	E	151	GLN
3	E	188	HIS
3	E	261	GLN
3	E	289	ASN
3	E	368	GLN
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	312	GLN
3	A	328	ASN
3	A	368	GLN
3	I	44	ASN
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
3	I	368	GLN
4	G	59	GLN
4	G	109	GLN
4	G	177	HIS
2	J	174	GLN
2	J	178	GLN
2	J	192	HIS
2	B	174	GLN
2	B	178	GLN
2	B	192	HIS
4	K	43	GLN
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 oligosaccharides 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	2,4,4	3.14	2 (100%)	4,6,6	1.45	1 (25%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	303	CAC	AS-C2	3.23	1.98	1.90
7	C	303	CAC	AS-C1	3.04	1.97	1.90

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	303	CAC	O1-AS-C2	-2.03	108.98	111.50

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%)	0.24	13 (5%) 32 22	27, 51, 92, 117	0
2	F	244/252 (96%)	-0.02	10 (4%) 41 27	14, 31, 66, 95	0
2	J	244/252 (96%)	-0.03	8 (3%) 49 33	16, 33, 67, 104	0
3	A	390/420 (92%)	0.67	42 (10%) 11 10	35, 72, 112, 153	0
3	E	390/420 (92%)	0.17	20 (5%) 33 23	24, 47, 85, 129	0
3	I	390/420 (92%)	0.31	20 (5%) 33 23	25, 64, 117, 179	0
4	C	228/256 (89%)	0.70	32 (14%) 6 6	31, 59, 111, 148	0
4	G	228/256 (89%)	0.17	15 (6%) 24 16	20, 48, 101, 153	0
4	K	228/256 (89%)	0.31	22 (9%) 13 12	24, 47, 115, 160	0
All	All	2586/2859 (90%)	0.30	182 (7%) 22 16	14, 52, 107, 179	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	180	GLY	8.0
4	K	139	ASP	6.1
4	G	195	PRO	6.0
3	E	200	PHE	5.9
4	C	82	GLY	5.7
3	A	144	GLY	5.6
4	K	208	PHE	5.3
4	C	52	ASP	5.2
4	C	54	PHE	5.0
4	G	224	PHE	5.0
3	I	274	GLU	5.0
4	K	225	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
4	K	55	ALA	4.8
2	B	180	GLY	4.8
2	J	211	ARG	4.7
4	C	55	ALA	4.6
3	E	256	ARG	4.6
4	C	17	SER	4.5
3	I	290	GLY	4.5
4	K	224	PHE	4.3
4	C	81	ALA	4.3
4	C	226	TRP	4.3
2	F	197	SER	4.3
4	C	204	HIS	4.2
2	F	51	GLY	4.1
2	F	175	ALA	4.1
2	F	250	ASP	4.0
2	B	194	VAL	4.0
3	A	146	ILE	4.0
4	G	228	ALA	4.0
3	I	363	ILE	3.9
4	G	140	THR	3.9
4	C	20	ASP	3.9
3	A	141	GLU	3.8
3	A	39	ARG	3.8
2	F	211	ARG	3.8
3	A	34	GLN	3.8
4	C	50	GLY	3.7
3	A	397	PRO	3.7
4	K	253	LEU	3.6
4	K	53	SER	3.5
4	K	51	LEU	3.5
4	C	53	SER	3.5
3	A	145	PRO	3.5
2	B	193	PHE	3.4
4	G	196	ASN	3.4
3	E	145	PRO	3.4
3	I	200	PHE	3.4
3	A	97	THR	3.3
4	C	85	TRP	3.3
3	I	350	VAL	3.3
3	A	280	GLY	3.3
4	C	139	ASP	3.3
4	K	17	SER	3.3

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Mol	Chain	Res	Type	RSRZ
4	C	57	GLU	3.3
3	A	147	ILE	3.2
2	J	51	GLY	3.2
3	A	31	GLU	3.2
4	K	140	THR	3.2
3	A	92	PRO	3.1
3	A	354	PRO	3.1
3	A	342	LEU	3.1
4	C	140	THR	3.1
3	A	281	LYS	3.1
3	E	218	GLY	3.1
4	K	47	TRP	3.1
2	B	175	ALA	3.1
2	B	242	TRP	3.1
4	G	139	ASP	3.1
3	E	139	ASN	3.0
4	K	254	LEU	3.0
4	K	193	ILE	3.0
3	A	204	VAL	3.0
2	F	33	LEU	3.0
3	I	338	PHE	3.0
3	E	350	VAL	2.9
4	G	207	TRP	2.9
3	A	352	ALA	2.9
3	E	418	ASP	2.9
3	A	351	ASP	2.9
4	K	202	TRP	2.9
4	C	47	TRP	2.9
2	B	110	TYR	2.9
2	F	210	LEU	2.9
3	E	54	THR	2.8
3	A	270	PRO	2.8
4	C	86	LYS	2.8
4	C	60	THR	2.8
2	B	192	HIS	2.8
3	E	287	GLU	2.8
2	F	198	MET	2.8
4	C	253	LEU	2.8
4	C	19	VAL	2.8
3	A	142	GLY	2.7
4	K	228	ALA	2.7
4	C	228	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
3	I	342	LEU	2.7
3	I	316	LEU	2.7
3	A	275	GLY	2.7
3	A	350	VAL	2.7
3	I	304	VAL	2.7
4	K	48	ARG	2.6
3	A	402	TYR	2.6
3	A	164	ASP	2.6
3	A	322	ALA	2.6
4	G	141	ASP	2.6
2	J	181	GLN	2.6
3	I	341	TYR	2.6
4	C	61	TYR	2.6
4	C	224	PHE	2.5
4	K	58	PHE	2.5
4	C	208	PHE	2.5
3	A	341	TYR	2.5
3	A	271	ILE	2.5
4	C	202	TRP	2.5
3	A	279	VAL	2.5
3	A	321	ALA	2.5
3	E	354	PRO	2.5
3	I	319	TYR	2.5
4	C	148	ILE	2.4
2	B	182	LEU	2.4
3	A	32	LYS	2.4
4	C	48	ARG	2.4
3	A	282	GLU	2.4
3	A	170	ASP	2.4
4	K	177	HIS	2.4
2	J	213	PHE	2.4
3	I	354	PRO	2.4
2	F	217	VAL	2.4
4	C	120	TRP	2.3
3	E	143	GLY	2.3
3	A	143	GLY	2.3
4	G	200	ASN	2.3
3	E	164	ASP	2.3
3	I	35	GLN	2.3
3	A	274	GLU	2.3
3	E	397	PRO	2.3
3	I	122	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
4	G	47	TRP	2.3
3	E	53	THR	2.3
4	C	145	SER	2.3
4	K	196	ASN	2.3
3	A	339	PRO	2.3
3	E	416	ALA	2.3
2	J	125	PHE	2.3
2	B	107	ILE	2.3
2	B	9	ALA	2.3
2	B	168	ALA	2.3
4	K	52	ASP	2.3
2	F	196	THR	2.2
4	C	153	SER	2.2
3	E	398	ASP	2.2
4	G	204	HIS	2.2
3	I	289	ASN	2.2
4	G	252	LYS	2.2
4	G	208	PHE	2.2
4	C	166	PHE	2.2
4	G	112	VAL	2.1
3	A	137	GLN	2.1
3	I	321	ALA	2.1
3	E	257	THR	2.1
3	I	324	LEU	2.1
4	C	49	ALA	2.1
4	K	195	PRO	2.1
3	A	200	PHE	2.1
3	E	204	VAL	2.1
3	E	144	GLY	2.1
4	K	50	GLY	2.1
3	E	252	SER	2.1
3	I	326	PHE	2.1
4	G	197	VAL	2.1
2	J	250	ASP	2.1
2	B	51	GLY	2.1
3	I	339	PRO	2.1
3	A	66	LYS	2.1
3	A	29	HIS	2.0
2	J	177	GLU	2.0
3	I	365	VAL	2.0
3	A	163	THR	2.0
3	A	35	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	188	LEU	2.0
3	A	176	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ZN	G	302	1/1	0.83	0.11	153,153,153,153	0
7	CAC	C	303	5/5	0.96	0.11	92,95,102,107	0
5	CU	A	501	1/1	0.98	0.03	85,85,85,85	0
5	CU	I	501	1/1	0.98	0.03	63,63,63,63	0
6	ZN	C	301	1/1	0.99	0.08	66,66,66,66	0
6	ZN	C	302	1/1	0.99	0.05	106,106,106,106	0
6	ZN	G	301	1/1	0.99	0.05	64,64,64,64	0
6	ZN	K	301	1/1	1.00	0.03	67,67,67,67	0
5	CU	E	501	1/1	1.00	0.03	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.