



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:50 AM UTC

PDB ID : 1YEW / pdb_00001yew
Title : Crystal structure of particulate methane monooxygenase
Authors : Lieberman, R.L.; Rosenzweig, A.C.
Deposited on : 2004-12-28
Resolution : 2.80 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:

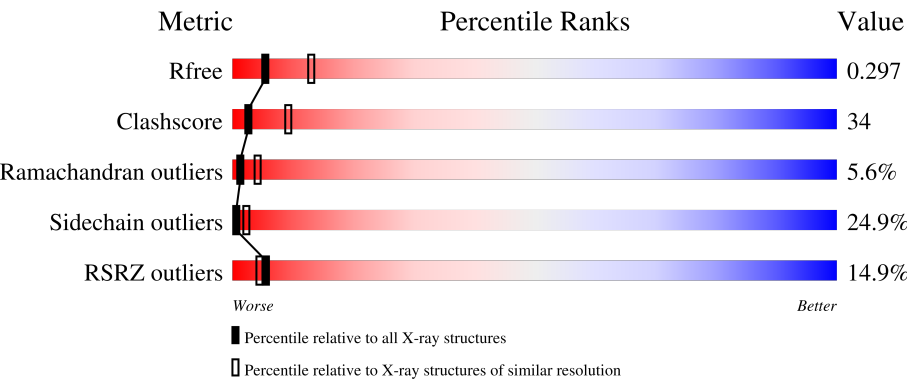
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	382	5% 53%31%14%.
1	E	382	7% 51%33%15%.
1	I	382	8% 50%35%14%.
2	B	247	19% 33%38%17%8%.
2	F	247	13% 29%40%19%7%.

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Mol	Chain	Length	Quality of chain
2	J	247	14%31%40%17%7%•
3	C	289	20%26%24%13%•35%
3	G	289	21%27%24%12%•35%
3	K	289	18%28%22%13%•35%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19772 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 particulate methane monooxygenase, B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			3018	1938	513	552	15			
1	E	382	Total	C	N	O	S	0	0	0
			3018	1938	513	552	15			
1	I	382	Total	C	N	O	S	0	0	0
			3018	1938	513	552	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1955	1317	311	316	11			
2	F	238	Total	C	N	O	S	0	0	0
			1955	1317	311	316	11			
2	J	238	Total	C	N	O	S	0	0	0
			1955	1317	311	316	11			

- Molecule 3 is a protein called particulate methane monooxygenase subunit C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	188	Total	C	N	O	S	0	0	0
			1612	1101	244	264	3			
3	G	188	Total	C	N	O	S	0	0	0
			1612	1101	244	264	3			
3	K	188	Total	C	N	O	S	0	0	0
			1612	1101	244	264	3			

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

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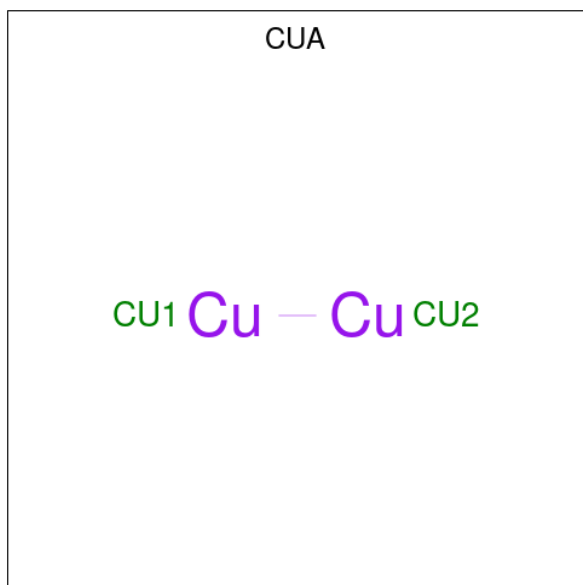
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	Cu 1	0	0
4	I	1	Total 1	Cu 1	0	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Zn 1	0	0
5	C	2	Total 2	Zn 2	0	0
5	E	3	Total 3	Zn 3	0	0
5	G	1	Total 1	Zn 1	0	0
5	K	1	Total 1	Zn 1	0	0

- Molecule 6 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

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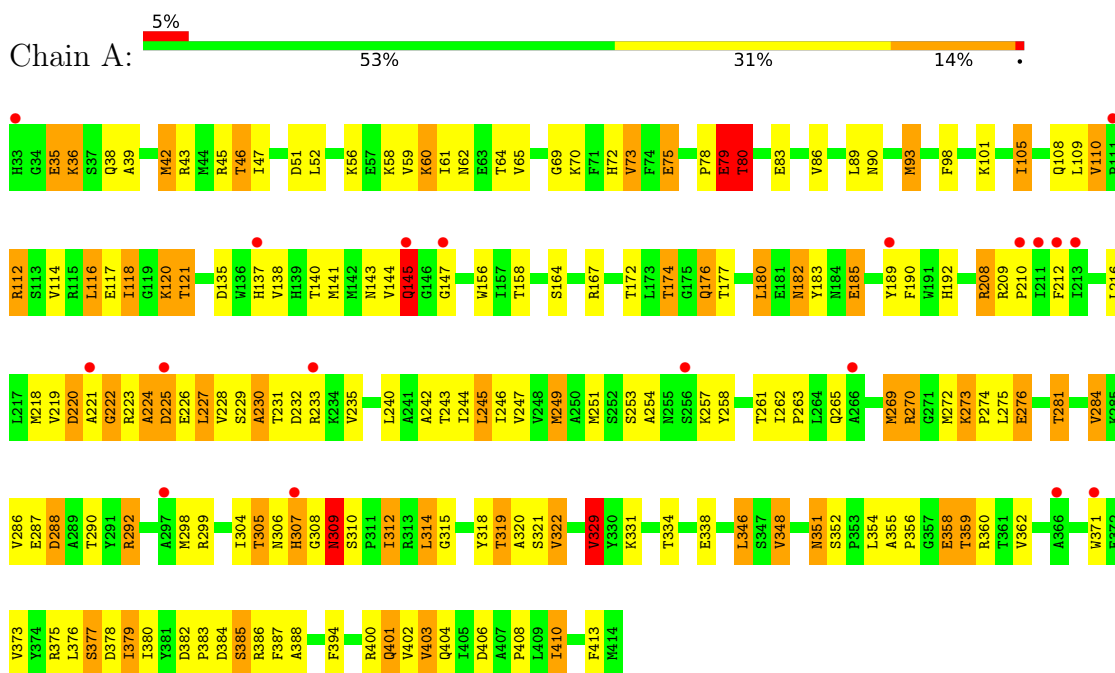
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	1	Total	Cu	0	0
			2	2		

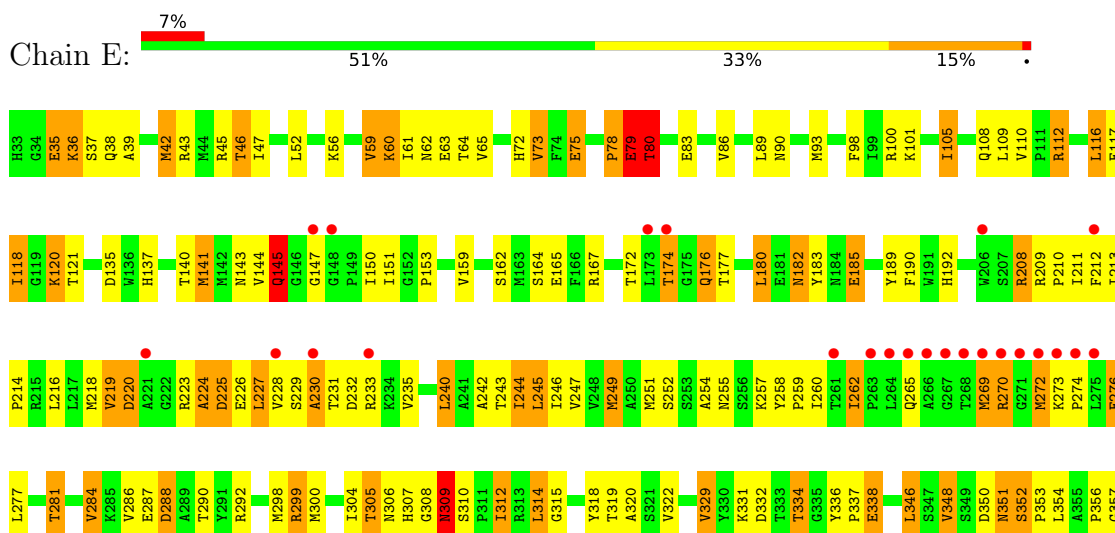
3 Residue-property plots

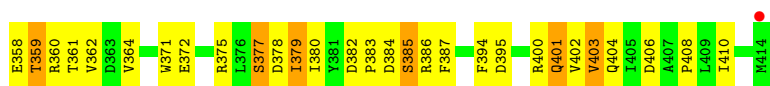
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: particulate methane monooxygenase, B subunit

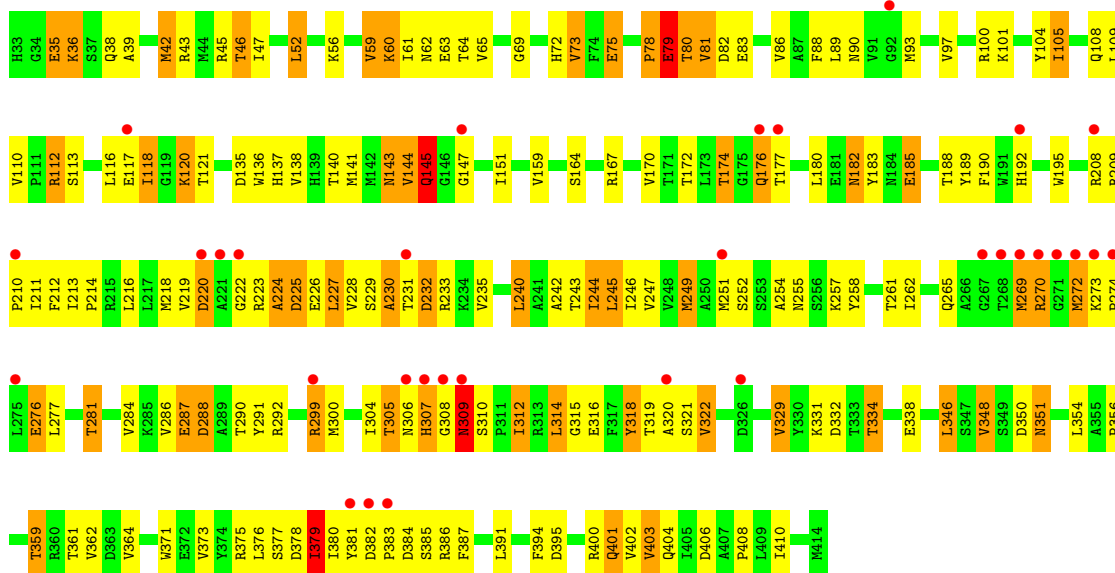


- Molecule 1: particulate methane monooxygenase, B subunit

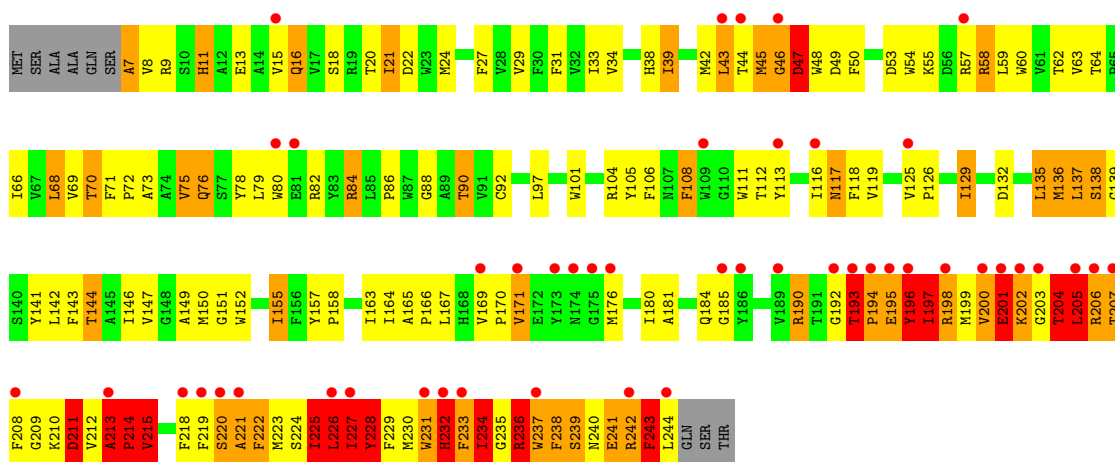




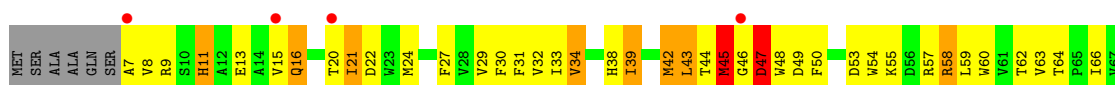
- Molecule 1: particulate methane monooxygenase, B subunit

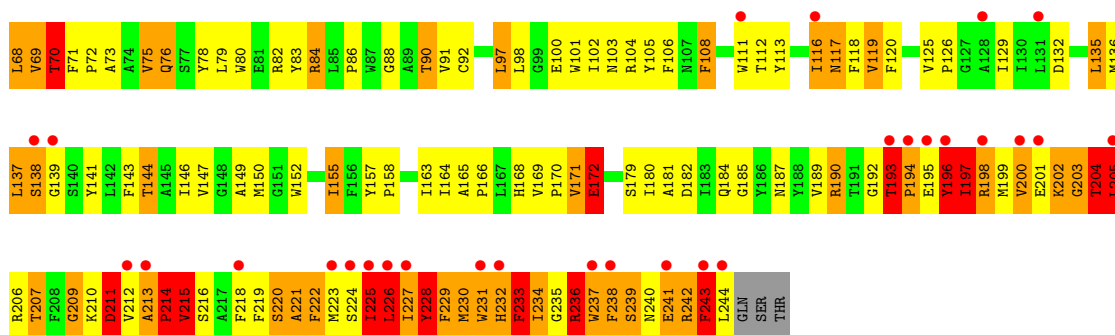


- Molecule 2: particulate methane monooxygenase, A subunit

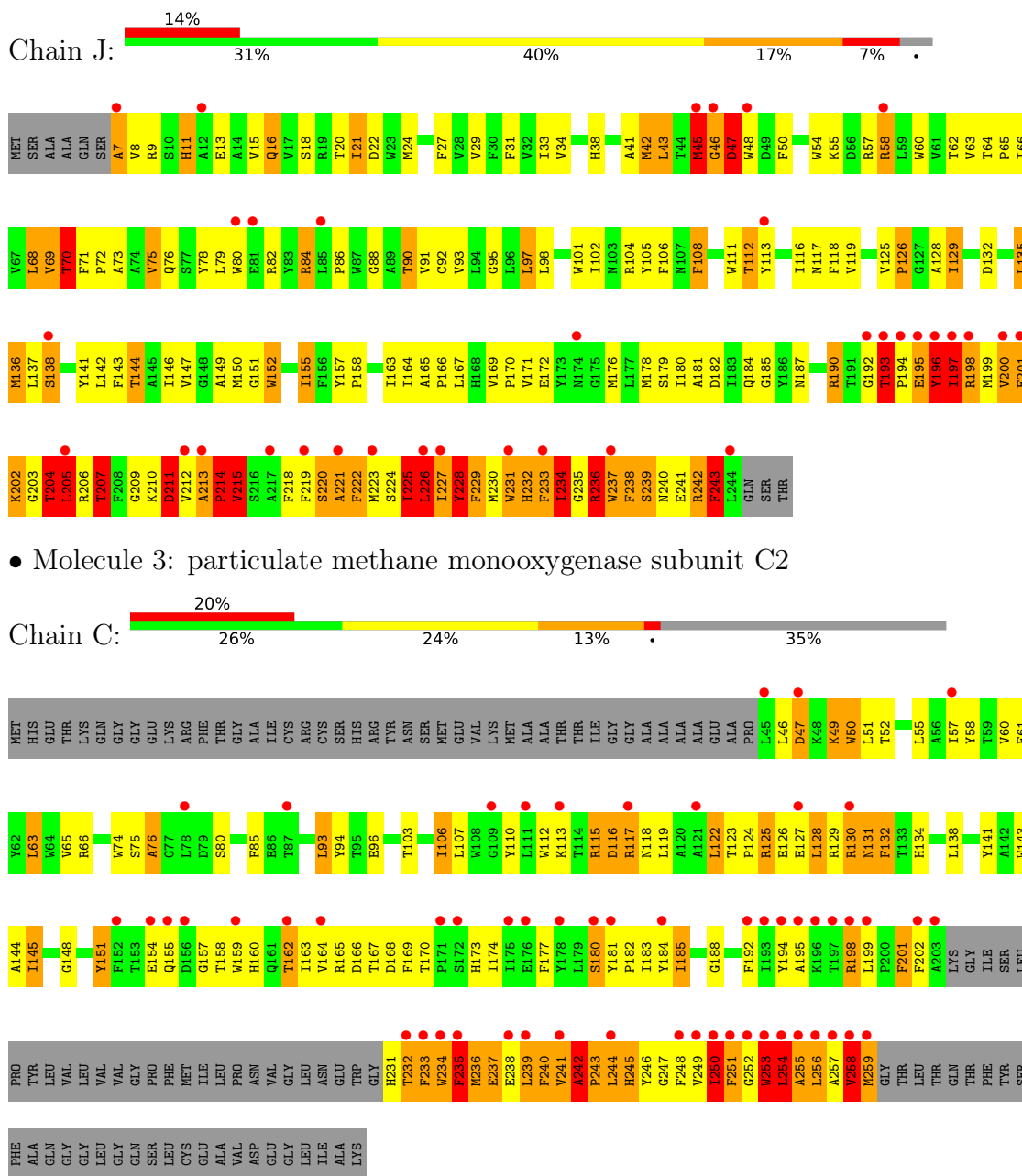


- Molecule 2: particulate methane monooxygenase, A subunit

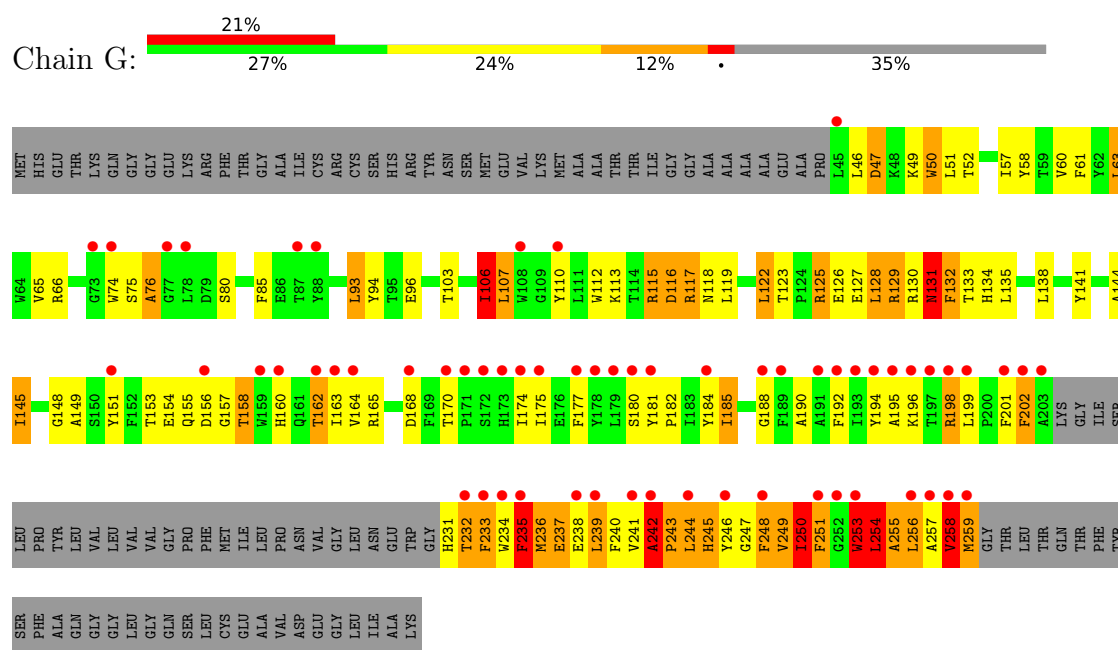




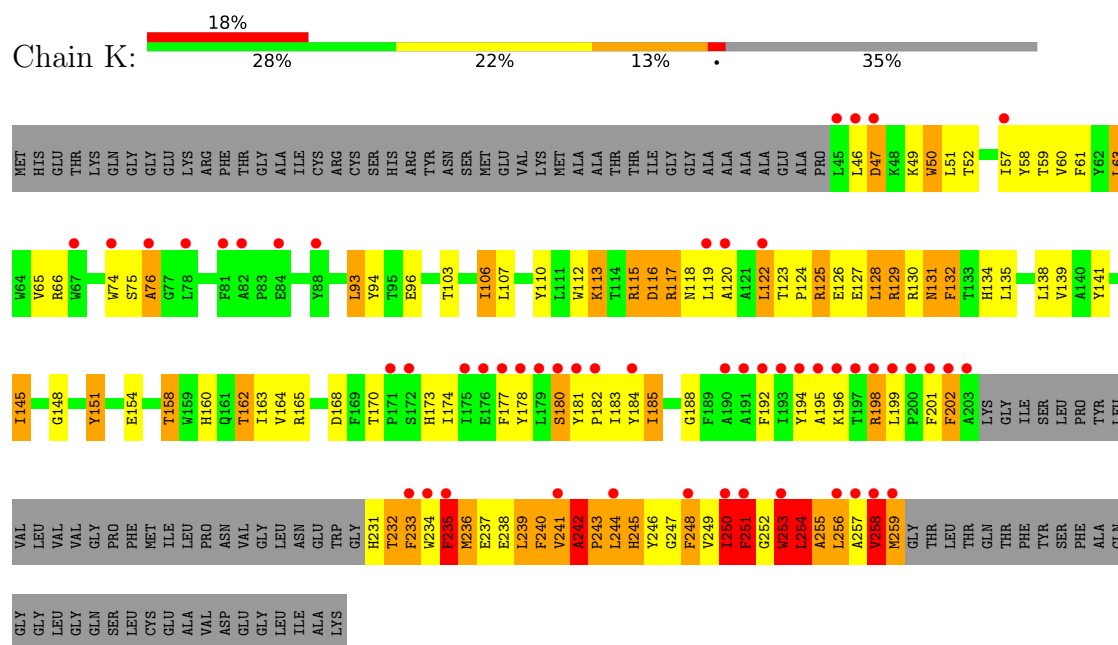
- Molecule 2: particulate methane monooxygenase, A subunit



- Molecule 3: particulate methane monooxygenase subunit C2



- Molecule 3: particulate methane monooxygenase subunit C2



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	264.14Å 264.14Å 150.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.55 – 2.80 29.55 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (29.55-2.80) 91.1 (29.55-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.272 , 0.302 (Not available) , 0.297	Depositor DCC
R_{free} test set	5932 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	19772	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.17	3/3100 (0.1%)	1.28	15/4215 (0.4%)
1	E	1.18	3/3100 (0.1%)	1.32	20/4215 (0.5%)
1	I	1.09	2/3100 (0.1%)	1.25	21/4215 (0.5%)
2	B	1.31	16/2031 (0.8%)	1.51	29/2780 (1.0%)
2	F	1.27	16/2031 (0.8%)	1.45	29/2780 (1.0%)
2	J	1.28	14/2031 (0.7%)	1.45	28/2780 (1.0%)
3	C	1.00	3/1680 (0.2%)	1.30	12/2302 (0.5%)
3	G	0.89	1/1680 (0.1%)	1.25	16/2302 (0.7%)
3	K	0.96	2/1680 (0.1%)	1.27	13/2302 (0.6%)
All	All	1.15	60/20433 (0.3%)	1.34	183/27891 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	E	0	4
1	I	0	4
2	B	0	11
2	F	0	9
2	J	0	10
3	C	0	3
3	G	0	3
3	K	0	3
All	All	0	50

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	200	VAL	CA-CB	10.14	1.68	1.54
2	J	200	VAL	CA-CB	10.10	1.68	1.54
2	B	200	VAL	CA-CB	9.97	1.68	1.54
2	B	243	PHE	CA-C	8.76	1.64	1.52
2	J	243	PHE	CA-C	8.00	1.63	1.52
2	F	243	PHE	CA-C	7.97	1.63	1.52
2	F	193	THR	CA-CB	7.17	1.64	1.53
1	E	150	ILE	CA-CB	-7.09	1.45	1.53
2	B	193	THR	CA-CB	7.01	1.64	1.53
2	F	242	ARG	N-CA	6.95	1.54	1.46
2	J	195	GLU	N-CA	6.90	1.54	1.46
2	B	193	THR	CA-C	6.83	1.61	1.52
2	B	242	ARG	CB-CG	6.67	1.72	1.52
2	J	193	THR	CA-C	6.57	1.61	1.52
2	F	242	ARG	CB-CG	6.37	1.71	1.52
2	B	242	ARG	N-CA	6.34	1.53	1.46
2	J	242	ARG	CB-CG	6.34	1.71	1.52
2	B	195	GLU	N-CA	6.22	1.54	1.46
3	C	241	VAL	CA-CB	6.21	1.62	1.54
2	J	165	ALA	CA-CB	-6.17	1.46	1.53
2	B	227	ILE	CA-CB	6.15	1.62	1.54
1	E	320	ALA	CA-C	-6.12	1.46	1.53
2	J	227	ILE	CA-CB	6.04	1.62	1.54
2	B	196	TYR	CA-C	6.00	1.60	1.52
2	B	201	GLU	CA-C	6.00	1.61	1.52
2	J	193	THR	CA-CB	5.97	1.62	1.53
2	J	241	GLU	CG-CD	5.79	1.66	1.52
1	A	110	VAL	CA-C	5.78	1.58	1.52
3	K	202	PHE	CA-C	5.73	1.58	1.53
2	B	225	ILE	CA-CB	5.69	1.62	1.54
2	B	241	GLU	CG-CD	5.68	1.66	1.52
2	J	201	GLU	CA-C	5.67	1.60	1.52
2	B	234	ILE	CA-CB	5.65	1.61	1.54
2	J	234	ILE	CA-CB	5.64	1.62	1.54
1	A	288	ASP	CB-CG	5.64	1.66	1.52
3	K	241	VAL	CA-CB	5.58	1.62	1.54
2	F	233	PHE	N-CA	-5.56	1.39	1.46
3	C	251	PHE	CB-CG	5.52	1.63	1.50
2	F	200	VAL	N-CA	5.47	1.53	1.46
2	F	168	HIS	N-CA	-5.44	1.39	1.46
2	F	45	MET	CA-C	5.41	1.60	1.52
2	B	200	VAL	N-CA	5.38	1.53	1.46
2	F	119	VAL	CA-CB	-5.37	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	288	ASP	CA-C	5.28	1.59	1.52
2	J	242	ARG	N-CA	5.21	1.52	1.46
2	F	225	ILE	CA-CB	5.19	1.61	1.54
3	C	49	LYS	CA-C	5.16	1.59	1.52
1	A	410	ILE	CA-CB	-5.15	1.48	1.54
2	F	227	ILE	CA-C	5.14	1.59	1.52
1	I	318	TYR	CA-C	-5.14	1.46	1.52
2	B	204	THR	CA-CB	5.14	1.62	1.53
2	B	46	GLY	N-CA	5.12	1.52	1.45
2	F	241	GLU	CG-CD	5.10	1.64	1.52
2	F	193	THR	CA-C	5.10	1.59	1.52
1	E	288	ASP	CB-CG	5.09	1.64	1.52
3	G	106	ILE	CA-CB	5.09	1.60	1.54
2	F	227	ILE	CA-CB	5.07	1.61	1.54
2	J	45	MET	CA-C	5.04	1.59	1.52
2	F	172	GLU	CA-C	-5.00	1.46	1.52
2	J	46	GLY	N-CA	5.00	1.52	1.45

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	47	ASP	N-CA-C	16.39	133.62	110.50
2	J	47	ASP	N-CA-C	16.30	133.48	110.50
2	B	213	ALA	CA-C-N	16.18	140.06	119.84
2	B	213	ALA	C-N-CA	16.18	140.06	119.84
2	B	47	ASP	N-CA-C	15.62	132.53	110.50
3	K	251	PHE	N-CA-C	-14.10	95.50	111.71
3	G	251	PHE	N-CA-C	-13.94	95.64	111.82
3	C	251	PHE	N-CA-C	-13.87	95.73	111.82
2	F	216	SER	N-CA-C	10.48	125.88	113.20
3	G	50	TRP	N-CA-C	-10.37	99.32	112.90
3	C	50	TRP	N-CA-C	-10.14	99.61	112.90
3	K	50	TRP	N-CA-C	-10.04	99.75	112.90
3	C	254	LEU	N-CA-C	-10.02	98.52	112.45
3	K	254	LEU	N-CA-C	-9.74	98.91	112.45
2	J	228	TYR	N-CA-C	-9.31	98.63	112.04
3	G	254	LEU	N-CA-C	-9.26	99.57	112.45
2	F	228	TYR	N-CA-C	-9.18	98.82	112.04
1	A	79	GLU	N-CA-C	9.02	125.02	111.04
2	F	212	VAL	N-CA-C	-8.73	94.50	107.51
2	B	212	VAL	N-CA-C	-8.64	94.64	107.51
1	I	309	ASN	N-CA-C	8.61	122.40	108.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	ASN	N-CA-C	8.57	122.34	108.63
1	E	42	MET	N-CA-C	-8.49	102.10	111.36
1	E	79	GLU	N-CA-C	8.44	124.13	111.04
2	J	212	VAL	N-CA-C	-8.44	94.94	107.51
1	I	79	GLU	N-CA-C	8.37	124.02	111.04
3	K	258	VAL	N-CA-C	8.25	119.60	106.32
3	K	233	PHE	N-CA-C	-8.18	102.30	111.71
2	F	215	VAL	N-CA-C	7.99	125.96	109.34
2	B	228	TYR	N-CA-C	-7.91	100.66	112.04
3	C	245	HIS	N-CA-C	-7.78	102.88	111.36
3	G	250	ILE	N-CA-C	7.66	118.55	112.12
1	A	79	GLU	CA-C-N	7.56	135.31	121.70
1	A	79	GLU	C-N-CA	7.56	135.31	121.70
3	G	245	HIS	N-CA-C	-7.55	103.13	111.36
3	C	258	VAL	N-CA-C	7.53	118.44	106.32
2	B	215	VAL	N-CA-C	7.50	124.93	109.34
3	C	168	ASP	N-CA-C	-7.48	103.89	113.16
3	K	250	ILE	N-CA-C	7.46	118.39	112.12
1	I	42	MET	N-CA-C	-7.45	102.52	111.69
3	G	233	PHE	N-CA-C	-7.38	103.22	111.71
3	K	245	HIS	N-CA-C	-7.36	103.33	111.36
3	C	233	PHE	N-CA-C	-7.20	103.43	111.28
1	E	230	ALA	N-CA-C	-7.09	100.15	110.64
2	J	232	HIS	CB-CA-C	7.02	120.55	111.50
1	E	372	GLU	N-CA-C	-7.00	104.38	113.12
2	J	215	VAL	N-CA-C	7.00	123.89	109.34
2	J	196	TYR	N-CA-C	6.97	125.64	110.80
2	F	232	HIS	CB-CA-C	6.86	121.56	111.88
2	B	215	VAL	CA-C-N	6.85	134.02	121.70
2	B	215	VAL	C-N-CA	6.85	134.02	121.70
1	I	230	ALA	N-CA-C	-6.84	100.51	110.64
2	J	215	VAL	CA-C-N	6.78	133.90	121.70
2	J	215	VAL	C-N-CA	6.78	133.90	121.70
3	C	242	ALA	CA-C-N	6.75	126.71	119.76
3	C	242	ALA	C-N-CA	6.75	126.71	119.76
2	F	232	HIS	N-CA-C	6.71	120.01	110.68
2	F	193	THR	CA-C-N	6.71	143.09	127.00
2	F	193	THR	C-N-CA	6.71	143.09	127.00
3	G	258	VAL	N-CA-C	6.66	117.05	106.32
2	F	196	TYR	N-CA-C	6.63	124.92	110.80
3	G	168	ASP	N-CA-C	-6.51	105.09	113.16
1	A	230	ALA	N-CA-C	-6.49	101.03	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	113	TYR	N-CA-C	6.48	119.69	110.68
2	J	212	VAL	CB-CA-C	6.45	120.34	111.31
1	E	309	ASN	N-CA-C	6.45	118.95	108.63
2	B	193	THR	N-CA-C	6.42	124.01	109.81
1	A	35	GLU	N-CA-C	-6.39	102.26	110.19
2	J	193	THR	CA-C-N	6.38	142.31	127.00
2	J	193	THR	C-N-CA	6.38	142.31	127.00
2	J	232	HIS	N-CA-C	6.35	120.96	111.81
2	F	225	ILE	N-CA-C	-6.35	104.75	113.00
2	B	226	LEU	CB-CA-C	6.32	119.65	111.50
2	B	232	HIS	N-CA-C	6.31	120.89	111.81
2	B	211	ASP	CA-C-N	-6.28	114.71	122.93
2	B	211	ASP	C-N-CA	-6.28	114.71	122.93
3	C	250	ILE	N-CA-C	6.27	117.39	112.12
2	B	232	HIS	CB-CA-C	6.26	119.58	111.50
2	B	242	ARG	N-CA-C	6.25	118.65	111.02
2	F	120	PHE	CA-C-N	6.25	126.71	120.52
2	F	120	PHE	C-N-CA	6.25	126.71	120.52
1	I	319	THR	N-CA-C	6.25	120.49	112.12
2	J	225	ILE	N-CA-C	-6.25	104.88	113.00
2	J	235	GLY	N-CA-C	-6.22	104.97	112.49
1	I	79	GLU	CA-C-N	6.20	134.20	123.91
1	I	79	GLU	C-N-CA	6.20	134.20	123.91
1	I	144	VAL	N-CA-C	6.20	116.54	107.37
2	B	113	TYR	N-CA-C	6.19	120.72	111.81
1	A	79	GLU	CA-C-O	-6.17	114.42	120.89
2	B	196	TYR	N-CA-C	6.14	123.88	110.80
2	F	211	ASP	CA-C-N	-6.14	114.89	122.93
2	F	211	ASP	C-N-CA	-6.14	114.89	122.93
2	B	193	THR	CA-C-N	6.12	141.70	127.00
2	B	193	THR	C-N-CA	6.12	141.70	127.00
2	J	193	THR	N-CA-C	6.12	123.33	109.81
2	J	112	THR	CA-C-N	-6.10	113.33	122.24
2	J	112	THR	C-N-CA	-6.10	113.33	122.24
2	F	212	VAL	CB-CA-C	6.08	119.83	111.31
1	E	35	GLU	N-CA-C	-6.08	102.66	110.19
3	G	242	ALA	CA-C-N	6.04	125.98	119.76
3	G	242	ALA	C-N-CA	6.04	125.98	119.76
1	I	212	PHE	N-CA-C	6.02	118.42	108.48
3	K	168	ASP	N-CA-C	-6.02	105.80	113.02
2	B	235	GLY	N-CA-C	-6.00	105.09	112.77
1	E	319	THR	N-CA-C	5.97	120.12	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	151	ILE	N-CA-C	5.96	116.38	107.51
3	K	253	TRP	N-CA-C	5.94	119.04	109.83
1	A	319	THR	CA-C-N	-5.94	113.60	123.04
1	A	319	THR	C-N-CA	-5.94	113.60	123.04
2	F	213	ALA	CA-C-N	5.92	141.21	127.00
2	F	213	ALA	C-N-CA	5.92	141.21	127.00
1	E	212	PHE	N-CA-C	5.89	118.19	108.48
2	B	212	VAL	CB-CA-C	5.83	119.48	111.31
3	K	248	PHE	CA-C-N	-5.83	113.12	121.52
3	K	248	PHE	C-N-CA	-5.83	113.12	121.52
2	J	242	ARG	N-CA-C	5.83	118.13	111.02
2	J	213	ALA	CA-C-N	5.76	140.82	127.00
2	J	213	ALA	C-N-CA	5.76	140.82	127.00
2	J	211	ASP	CA-C-N	-5.74	115.41	122.93
2	J	211	ASP	C-N-CA	-5.74	115.41	122.93
2	F	242	ARG	N-CA-C	5.72	118.00	111.02
1	I	319	THR	CA-C-N	-5.72	113.94	123.04
1	I	319	THR	C-N-CA	-5.72	113.94	123.04
1	I	232	ASP	N-CA-C	-5.68	104.99	111.07
1	E	98	PHE	N-CA-C	-5.67	100.73	109.52
2	B	234	ILE	N-CA-C	-5.66	105.00	110.72
2	F	226	LEU	CB-CA-C	5.62	118.75	111.50
3	G	248	PHE	CA-C-N	-5.59	113.46	121.52
3	G	248	PHE	C-N-CA	-5.59	113.46	121.52
2	B	137	LEU	N-CA-C	-5.58	103.12	110.43
2	F	193	THR	N-CA-C	5.53	122.04	109.81
1	E	79	GLU	CA-C-N	5.53	133.09	123.91
1	E	79	GLU	C-N-CA	5.53	133.09	123.91
1	A	212	PHE	N-CA-C	5.50	117.56	108.48
1	E	358	GLU	N-CA-C	5.50	117.63	110.53
2	B	204	THR	CB-CA-C	5.49	121.35	110.42
3	C	201	PHE	N-CA-C	-5.48	106.57	113.20
2	F	193	THR	C-N-CD	-5.47	108.56	120.60
1	E	37	SER	N-CA-C	-5.45	106.63	113.28
2	B	225	ILE	N-CA-C	-5.44	104.42	112.04
2	J	113	TYR	N-CA-C	5.43	117.50	110.65
3	G	175	ILE	N-CA-C	5.43	116.50	111.45
2	B	227	ILE	N-CA-C	-5.41	98.08	109.34
1	I	151	ILE	N-CA-C	5.41	115.56	107.51
1	A	358	GLU	N-CA-C	5.40	117.84	110.55
3	K	242	ALA	CA-C-N	5.38	125.32	119.78
3	K	242	ALA	C-N-CA	5.38	125.32	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	207	THR	N-CA-C	-5.37	99.36	110.80
2	J	226	LEU	CB-CA-C	5.34	118.39	111.50
3	G	253	TRP	N-CA-C	5.34	118.11	109.83
1	I	35	GLU	N-CA-C	-5.34	103.57	110.19
1	E	352	SER	N-CA-C	-5.34	102.28	110.07
1	A	42	MET	N-CA-C	-5.33	105.55	111.36
1	E	153	PRO	CA-C-N	-5.33	117.14	122.20
1	E	153	PRO	C-N-CA	-5.33	117.14	122.20
2	B	208	PHE	CB-CA-C	5.33	118.37	111.50
3	C	253	TRP	N-CA-C	5.32	118.08	109.83
1	I	113	SER	N-CA-C	-5.30	102.68	110.52
2	F	227	ILE	CB-CA-C	5.28	119.95	111.29
3	G	202	PHE	N-CA-C	5.26	115.95	108.54
2	B	242	ARG	CB-CG-CD	5.25	123.37	111.30
1	E	79	GLU	CA-C-O	-5.24	115.39	120.89
2	J	204	THR	CB-CA-C	5.21	120.80	110.42
1	I	81	VAL	N-CA-C	-5.21	98.50	109.34
2	F	241	GLU	CA-C-N	5.18	127.99	120.79
2	F	241	GLU	C-N-CA	5.18	127.99	120.79
1	A	121	THR	CB-CA-C	5.17	119.06	109.70
1	E	288	ASP	N-CA-C	5.17	121.81	110.80
1	I	379	ILE	N-CA-C	-5.17	104.45	111.89
1	A	329	VAL	N-CA-C	5.16	116.08	111.90
2	B	214	PRO	N-CA-C	5.14	123.07	112.47
1	A	352	SER	N-CA-C	-5.14	102.57	110.07
2	F	235	GLY	N-CA-C	-5.14	106.20	112.77
2	J	195	GLU	N-CA-C	5.13	119.29	112.72
2	J	242	ARG	CB-CG-CD	5.10	123.04	111.30
1	I	316	GLU	N-CA-C	5.10	116.81	108.55
2	F	215	VAL	CA-C-N	5.09	132.13	121.94
2	F	215	VAL	C-N-CA	5.09	132.13	121.94
1	I	143	ASN	CA-C-N	-5.09	116.18	123.11
1	I	143	ASN	C-N-CA	-5.09	116.18	123.11
1	E	357	GLY	N-CA-C	-5.08	108.14	113.58
1	I	79	GLU	CA-C-O	-5.01	115.62	120.89
3	G	249	VAL	N-CA-C	-5.01	107.04	112.80

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	79	GLU	Peptide
1	A	80	THR	Peptide
2	B	193	THR	Peptide
2	B	204	THR	Peptide
2	B	211	ASP	Peptide
2	B	213	ALA	Peptide
2	B	215	VAL	Peptide
2	B	221	ALA	Peptide
2	B	226	LEU	Peptide
2	B	227	ILE	Peptide
2	B	232	HIS	Peptide
2	B	46	GLY	Peptide
2	B	7	ALA	Peptide
3	C	243	PRO	Peptide
3	C	244	LEU	Peptide
3	C	253	TRP	Peptide
1	E	144	VAL	Peptide
1	E	78	PRO	Peptide
1	E	79	GLU	Peptide
1	E	80	THR	Peptide
2	F	193	THR	Peptide
2	F	204	THR	Peptide
2	F	211	ASP	Peptide
2	F	213	ALA	Peptide
2	F	215	VAL	Peptide
2	F	221	ALA	Peptide
2	F	226	LEU	Peptide
2	F	46	GLY	Peptide
2	F	7	ALA	Peptide
3	G	243	PRO	Peptide
3	G	244	LEU	Peptide
3	G	253	TRP	Peptide
1	I	144	VAL	Peptide
1	I	287	GLU	Peptide
1	I	78	PRO	Peptide
1	I	79	GLU	Peptide
2	J	193	THR	Peptide
2	J	204	THR	Peptide
2	J	211	ASP	Peptide
2	J	213	ALA	Peptide
2	J	215	VAL	Peptide
2	J	221	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	J	226	LEU	Peptide
2	J	46	GLY	Peptide
2	J	47	ASP	Peptide
2	J	7	ALA	Peptide
3	K	243	PRO	Peptide
3	K	244	LEU	Peptide
3	K	253	TRP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3018	0	2980	146	1
1	E	3018	0	2980	141	1
1	I	3018	0	2980	155	0
2	B	1955	0	1916	220	2
2	F	1955	0	1916	219	0
2	J	1955	0	1916	226	0
3	C	1612	0	1541	137	0
3	G	1612	0	1541	140	0
3	K	1612	0	1541	129	0
4	A	1	0	0	0	0
4	E	1	0	0	0	0
4	I	1	0	0	0	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
5	E	3	0	0	0	0
5	G	1	0	0	0	0
5	K	1	0	0	0	0
6	A	2	0	0	0	0
6	E	2	0	0	0	0
6	I	2	0	0	0	0
All	All	19772	0	19311	1327	3

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 34.

All (1327) 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:70:THR:CG2	2:B:227:ILE:HD11	1.47	1.42
2:J:70:THR:CG2	2:J:227:ILE:HD11	1.54	1.34
2:B:70:THR:HG22	2:B:227:ILE:CD1	1.57	1.33
2:F:195:GLU:HG2	3:G:160:HIS:CE1	1.65	1.30
2:F:70:THR:CG2	2:F:227:ILE:HD11	1.61	1.29
2:F:62:THR:HA	2:F:236:ARG:NH1	1.49	1.26
2:J:62:THR:HA	2:J:236:ARG:NH1	1.48	1.26
2:J:70:THR:HG22	2:J:227:ILE:CD1	1.65	1.26
2:B:62:THR:HA	2:B:236:ARG:NH1	1.49	1.24
2:F:70:THR:HG22	2:F:227:ILE:CD1	1.66	1.24
1:A:112:ARG:HB2	1:A:269:MET:CE	1.70	1.21
2:J:236:ARG:NH2	2:J:237:TRP:HA	1.56	1.19
2:F:236:ARG:NH2	2:F:237:TRP:HA	1.59	1.17
1:I:112:ARG:HB2	1:I:269:MET:CE	1.76	1.16
2:B:236:ARG:NH2	2:B:237:TRP:HA	1.62	1.13
2:F:112:THR:HG21	3:G:162:THR:HG21	1.25	1.10
1:E:272:MET:HE2	1:E:272:MET:HA	1.32	1.09
2:F:236:ARG:HE	2:F:236:ARG:C	1.61	1.06
2:B:195:GLU:HG2	3:C:160:HIS:CE1	1.90	1.06
1:E:79:GLU:HB3	1:E:80:THR:HG23	1.38	1.06
2:J:112:THR:HG21	3:K:162:THR:HG21	1.31	1.06
1:E:112:ARG:HB2	1:E:269:MET:CE	1.85	1.05
2:F:222:PHE:HA	3:G:256:LEU:HB2	1.34	1.05
2:B:236:ARG:HE	2:B:236:ARG:C	1.64	1.05
2:F:70:THR:HG22	2:F:227:ILE:HD11	1.15	1.04
1:I:272:MET:HE2	1:I:272:MET:HA	1.36	1.04
2:J:70:THR:HG22	2:J:227:ILE:HD11	1.10	1.04
3:C:231:HIS:HA	3:C:233:PHE:H	1.24	1.03
2:B:222:PHE:HA	3:C:256:LEU:HB2	1.39	1.02
2:B:70:THR:HG22	2:B:227:ILE:HD11	1.06	1.02
2:J:236:ARG:C	2:J:236:ARG:HE	1.66	1.02
2:F:8:VAL:HG23	3:G:125:ARG:HH22	1.20	1.02
1:I:79:GLU:HB3	1:I:80:THR:HG23	1.38	1.01
2:B:112:THR:HG21	3:C:162:THR:HG21	1.38	1.01
2:J:8:VAL:HG23	3:K:125:ARG:HH22	1.24	1.01
2:J:195:GLU:HG2	3:K:160:HIS:CE1	1.94	1.00
2:B:230:MET:O	2:B:232:HIS:N	1.94	1.00
2:J:62:THR:HA	2:J:236:ARG:HH12	0.85	1.00
2:B:62:THR:CA	2:B:236:ARG:HH12	1.75	1.00
2:F:230:MET:O	2:F:232:HIS:N	1.94	1.00
1:A:105:ILE:HG23	1:A:110:VAL:HG21	1.42	1.00
1:A:272:MET:HA	1:A:272:MET:HE2	1.40	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:222:PHE:HA	3:K:256:LEU:HB2	1.42	0.99
2:F:62:THR:CA	2:F:236:ARG:HH12	1.76	0.98
1:I:35:GLU:O	1:I:36:LYS:HB2	1.63	0.98
2:F:195:GLU:CG	3:G:160:HIS:CE1	2.47	0.97
3:K:231:HIS:HA	3:K:233:PHE:H	1.28	0.97
1:I:105:ILE:HG23	1:I:110:VAL:HG21	1.44	0.97
2:J:62:THR:CA	2:J:236:ARG:HH12	1.76	0.97
2:F:236:ARG:C	2:F:236:ARG:NE	2.23	0.97
1:A:35:GLU:O	1:A:36:LYS:HB2	1.63	0.96
1:I:112:ARG:HB2	1:I:269:MET:HE1	1.46	0.96
3:C:254:LEU:O	3:C:257:ALA:HB3	1.65	0.96
1:A:112:ARG:HB2	1:A:269:MET:HE1	1.45	0.95
2:B:62:THR:HA	2:B:236:ARG:HH12	0.80	0.95
3:G:231:HIS:HA	3:G:233:PHE:H	1.29	0.94
1:A:145:GLN:HE21	1:A:145:GLN:HA	1.30	0.94
2:B:90:THR:HG23	2:B:132:ASP:OD1	1.67	0.94
1:E:272:MET:HA	1:E:272:MET:CE	1.98	0.94
1:A:79:GLU:HB3	1:A:80:THR:HG23	1.49	0.93
2:B:70:THR:HG23	2:B:227:ILE:HD11	1.48	0.93
2:J:236:ARG:CZ	2:J:237:TRP:HA	1.99	0.93
2:J:225:ILE:HD13	2:J:225:ILE:O	1.67	0.93
2:J:70:THR:HG23	2:J:227:ILE:HD11	1.51	0.92
2:J:230:MET:O	2:J:232:HIS:N	2.01	0.92
2:B:214:PRO:O	2:B:215:VAL:HG23	1.69	0.92
2:F:236:ARG:CZ	2:F:237:TRP:HA	2.00	0.92
2:B:219:PHE:HD1	2:B:219:PHE:O	1.53	0.91
2:B:236:ARG:C	2:B:236:ARG:NE	2.26	0.91
2:J:236:ARG:C	2:J:236:ARG:NE	2.28	0.91
3:G:254:LEU:O	3:G:257:ALA:HB3	1.69	0.91
2:B:236:ARG:CZ	2:B:237:TRP:HA	2.00	0.90
2:B:239:SER:O	2:B:242:ARG:HB3	1.71	0.90
1:E:145:GLN:HE21	1:E:145:GLN:HA	1.33	0.90
2:J:236:ARG:HH21	2:J:237:TRP:HA	1.33	0.90
2:B:236:ARG:NH2	2:B:240:ASN:H	1.71	0.89
2:F:214:PRO:O	2:F:215:VAL:HG23	1.72	0.89
2:J:228:TYR:HD1	2:J:228:TYR:C	1.79	0.89
2:J:90:THR:HG23	2:J:132:ASP:OD1	1.73	0.89
1:E:35:GLU:O	1:E:36:LYS:HB2	1.73	0.89
3:C:131:ASN:HB3	3:C:199:LEU:HD21	1.54	0.89
2:J:202:LYS:NZ	2:J:202:LYS:HA	1.87	0.89
1:E:112:ARG:HB2	1:E:269:MET:HE1	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:66:ARG:HD3	3:C:151:TYR:OH	1.74	0.88
2:B:8:VAL:HG23	3:C:125:ARG:HH22	1.36	0.88
2:F:90:THR:HG23	2:F:132:ASP:OD1	1.73	0.88
3:K:66:ARG:HD3	3:K:151:TYR:OH	1.73	0.88
2:B:236:ARG:HH21	2:B:237:TRP:HA	1.35	0.87
2:J:214:PRO:O	2:J:215:VAL:HG23	1.75	0.87
1:I:145:GLN:HE21	1:I:145:GLN:HA	1.38	0.87
3:G:131:ASN:HB3	3:G:199:LEU:HD21	1.55	0.87
1:E:73:VAL:CG2	1:E:118:ILE:HA	2.04	0.87
1:E:105:ILE:HG23	1:E:110:VAL:HG21	1.54	0.87
2:F:219:PHE:HD1	2:F:219:PHE:O	1.57	0.87
2:B:70:THR:HG22	2:B:227:ILE:HD12	1.52	0.87
3:C:234:TRP:HA	3:C:237:GLU:CG	2.05	0.86
3:C:181:TYR:O	3:C:185:ILE:HG23	1.75	0.86
1:E:309:ASN:H	1:E:309:ASN:ND2	1.73	0.86
2:B:8:VAL:O	2:B:8:VAL:HG22	1.76	0.86
1:I:110:VAL:HG12	1:I:110:VAL:O	1.75	0.86
1:A:90:ASN:HD22	1:A:143:ASN:HD21	1.24	0.86
2:B:228:TYR:C	2:B:228:TYR:HD1	1.83	0.86
2:J:228:TYR:C	2:J:228:TYR:CD1	2.51	0.86
2:F:195:GLU:HG2	3:G:160:HIS:HE1	1.38	0.86
2:F:236:ARG:NH2	2:F:240:ASN:H	1.73	0.86
1:I:73:VAL:CG2	1:I:118:ILE:HA	2.05	0.85
2:J:219:PHE:HD1	2:J:219:PHE:O	1.59	0.85
2:F:236:ARG:HH21	2:F:237:TRP:HA	1.36	0.85
1:E:110:VAL:HG12	1:E:110:VAL:O	1.77	0.85
2:B:219:PHE:O	2:B:219:PHE:CD1	2.30	0.85
2:F:70:THR:HG22	2:F:227:ILE:HD12	1.59	0.84
2:J:236:ARG:NH2	2:J:240:ASN:H	1.75	0.84
1:A:110:VAL:HG12	1:A:110:VAL:O	1.77	0.84
2:F:62:THR:HA	2:F:236:ARG:HH12	0.79	0.84
2:F:70:THR:HG23	2:F:227:ILE:HD11	1.59	0.84
2:J:135:LEU:HB2	2:J:144:THR:HG21	1.59	0.84
3:C:234:TRP:HA	3:C:237:GLU:HG3	1.58	0.83
2:J:70:THR:HG22	2:J:227:ILE:HD12	1.60	0.83
3:G:232:THR:HG22	3:G:235:PHE:H	1.42	0.83
3:K:254:LEU:O	3:K:257:ALA:HB3	1.79	0.83
3:K:232:THR:HG22	3:K:235:PHE:H	1.44	0.83
2:B:70:THR:CG2	2:B:227:ILE:CD1	2.31	0.82
2:F:219:PHE:O	2:F:219:PHE:CD1	2.31	0.82
1:A:112:ARG:HB2	1:A:269:MET:HE3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:HIS:CE1	1:A:75:GLU:OE1	2.33	0.82
2:B:236:ARG:NE	2:B:239:SER:HB3	1.94	0.82
2:F:58:ARG:HH21	2:F:58:ARG:HG2	1.43	0.82
1:A:249:MET:HE2	1:A:249:MET:HA	1.60	0.81
2:F:225:ILE:HD13	2:F:225:ILE:O	1.80	0.81
2:F:228:TYR:HD1	2:F:228:TYR:C	1.87	0.81
3:G:66:ARG:HD3	3:G:151:TYR:OH	1.80	0.81
2:B:206:ARG:HG2	3:C:184:TYR:CE2	2.16	0.81
3:C:231:HIS:HA	3:C:233:PHE:N	1.96	0.80
1:I:112:ARG:HB2	1:I:269:MET:HE3	1.62	0.80
1:A:73:VAL:CG2	1:A:118:ILE:HA	2.10	0.80
2:J:219:PHE:O	2:J:219:PHE:CD1	2.34	0.80
2:J:239:SER:O	2:J:242:ARG:HB3	1.82	0.80
2:B:58:ARG:HG2	2:B:58:ARG:HH21	1.47	0.79
2:B:228:TYR:C	2:B:228:TYR:CD1	2.55	0.79
2:B:199:MET:O	2:B:202:LYS:N	2.15	0.79
3:C:254:LEU:O	3:C:255:ALA:O	1.99	0.79
1:I:72:HIS:CE1	1:I:75:GLU:OE1	2.35	0.79
2:F:58:ARG:HH12	2:F:237:TRP:HH2	1.28	0.79
3:G:231:HIS:HA	3:G:233:PHE:N	1.98	0.79
1:E:35:GLU:HA	1:E:38:GLN:HG2	1.66	0.78
1:I:254:ALA:O	1:I:257:LYS:O	2.01	0.78
2:B:135:LEU:HB2	2:B:144:THR:HG21	1.66	0.78
2:J:38:HIS:HE2	3:K:154:GLU:CD	1.92	0.78
1:E:315:GLY:HA2	1:E:329:VAL:HG22	1.65	0.78
1:A:315:GLY:HA2	1:A:329:VAL:HG22	1.66	0.78
2:F:206:ARG:HG2	3:G:184:TYR:CE2	2.18	0.77
2:B:225:ILE:HD13	2:B:225:ILE:O	1.83	0.77
2:F:228:TYR:C	2:F:228:TYR:CD1	2.58	0.77
1:A:265:GLN:HE22	1:I:385:SER:H	1.33	0.77
2:J:199:MET:O	2:J:202:LYS:N	2.17	0.77
2:B:11:HIS:H	2:B:11:HIS:CD2	2.03	0.77
2:F:190:ARG:HG2	2:F:190:ARG:HH11	1.49	0.77
2:J:206:ARG:HG2	3:K:184:TYR:CE2	2.18	0.77
1:I:272:MET:HA	1:I:272:MET:CE	2.12	0.76
2:F:199:MET:O	2:F:202:LYS:N	2.16	0.76
1:E:254:ALA:O	1:E:257:LYS:O	2.03	0.76
2:B:202:LYS:NZ	2:B:202:LYS:HA	2.01	0.76
1:E:262:ILE:HG12	2:F:170:PRO:HB3	1.67	0.76
3:C:232:THR:HG22	3:C:235:PHE:H	1.51	0.76
2:J:62:THR:CA	2:J:236:ARG:NH1	2.41	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:231:HIS:HA	3:K:233:PHE:N	2.00	0.75
2:B:38:HIS:HE2	3:C:154:GLU:CD	1.93	0.75
3:G:234:TRP:HA	3:G:237:GLU:CG	2.16	0.75
3:G:234:TRP:HA	3:G:237:GLU:HG3	1.66	0.75
1:I:315:GLY:HA2	1:I:329:VAL:HG22	1.68	0.75
2:J:58:ARG:HH12	2:J:237:TRP:HH2	1.33	0.75
1:I:72:HIS:HE1	1:I:75:GLU:OE1	1.70	0.75
3:K:234:TRP:HA	3:K:237:GLU:HG3	1.67	0.75
1:E:90:ASN:HD22	1:E:143:ASN:HD21	1.31	0.74
2:F:202:LYS:HA	2:F:202:LYS:NZ	2.02	0.74
1:E:112:ARG:HB2	1:E:269:MET:HE3	1.68	0.74
1:A:46:THR:HG22	1:A:47:ILE:H	1.52	0.74
1:E:182:ASN:C	1:E:182:ASN:HD22	1.95	0.74
3:G:115:ARG:HD2	3:G:117:ARG:HH22	1.52	0.74
3:K:131:ASN:HB3	3:K:199:LEU:HD21	1.69	0.74
3:G:47:ASP:C	3:G:47:ASP:OD1	2.30	0.74
1:E:145:GLN:HA	1:E:145:GLN:NE2	2.03	0.74
1:I:249:MET:HA	1:I:249:MET:HE2	1.70	0.74
1:E:309:ASN:HD22	1:E:309:ASN:N	1.85	0.73
2:F:104:ARG:HA	2:F:108:PHE:HB2	1.71	0.73
1:E:249:MET:HE2	1:E:249:MET:HA	1.71	0.73
1:A:62:ASN:HD21	1:A:167:ARG:H	1.36	0.73
2:B:58:ARG:HH12	2:B:237:TRP:HH2	1.34	0.73
2:B:234:ILE:HD11	2:J:199:MET:CG	2.19	0.73
1:A:145:GLN:HA	1:A:145:GLN:NE2	2.03	0.73
1:I:35:GLU:HA	1:I:38:GLN:HG2	1.70	0.73
2:J:210:LYS:HD3	3:K:141:TYR:HE2	1.53	0.73
3:K:181:TYR:O	3:K:185:ILE:HG23	1.88	0.73
1:I:230:ALA:HB2	1:I:233:ARG:HG2	1.70	0.73
3:G:254:LEU:O	3:G:255:ALA:O	2.06	0.73
2:F:8:VAL:HG23	3:G:125:ARG:NH2	2.00	0.72
2:B:90:THR:HG21	2:B:129:ILE:HD12	1.72	0.72
2:J:8:VAL:O	2:J:8:VAL:HG22	1.89	0.72
3:K:234:TRP:HA	3:K:237:GLU:CG	2.18	0.72
1:A:315:GLY:HA2	1:A:329:VAL:CG2	2.19	0.72
3:C:131:ASN:HD22	3:C:131:ASN:H	1.36	0.72
2:F:222:PHE:HA	3:G:256:LEU:CB	2.16	0.72
3:C:254:LEU:O	3:C:255:ALA:C	2.33	0.72
1:I:46:THR:CG2	1:I:47:ILE:N	2.52	0.72
2:J:58:ARG:HG2	2:J:58:ARG:HH21	1.53	0.72
1:E:315:GLY:HA2	1:E:329:VAL:CG2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:315:GLY:HA2	1:I:329:VAL:CG2	2.19	0.72
2:J:104:ARG:NH1	3:K:154:GLU:OE1	2.23	0.71
2:F:62:THR:CA	2:F:236:ARG:NH1	2.44	0.71
2:B:224:SER:HB3	3:C:256:LEU:HD12	1.73	0.71
1:A:224:ALA:O	1:A:226:GLU:N	2.23	0.71
1:A:245:LEU:HD13	1:A:249:MET:HG3	1.73	0.71
3:K:130:ARG:HE	3:K:198:ARG:HG3	1.56	0.71
1:A:90:ASN:ND2	1:A:143:ASN:HD21	1.88	0.71
1:A:272:MET:HA	1:A:272:MET:CE	2.19	0.71
1:E:79:GLU:CB	1:E:80:THR:HG23	2.19	0.70
2:J:20:THR:O	2:J:24:MET:HG3	1.91	0.70
2:F:227:ILE:HG12	2:F:230:MET:HB2	1.73	0.70
1:A:384:ASP:OD1	1:E:112:ARG:NH2	2.24	0.70
2:B:222:PHE:HA	3:C:256:LEU:CB	2.18	0.70
2:F:195:GLU:HG2	3:G:160:HIS:NE2	2.06	0.70
1:I:46:THR:HG22	1:I:47:ILE:H	1.56	0.70
2:B:199:MET:HG3	2:F:234:ILE:HD11	1.72	0.70
1:A:230:ALA:HB2	1:A:233:ARG:HG2	1.73	0.70
2:B:211:ASP:CG	2:B:211:ASP:O	2.34	0.70
3:K:47:ASP:OD1	3:K:47:ASP:C	2.35	0.69
1:A:42:MET:O	1:A:46:THR:HB	1.92	0.69
1:E:332:ASP:OD2	1:E:334:THR:HG23	1.91	0.69
2:F:224:SER:HB3	3:G:256:LEU:HD12	1.73	0.69
2:J:202:LYS:HA	2:J:202:LYS:HZ2	1.54	0.69
1:E:73:VAL:HG23	1:E:118:ILE:HA	1.73	0.69
2:F:38:HIS:HE2	3:G:154:GLU:CD	1.99	0.69
2:F:199:MET:HG3	2:J:234:ILE:HD11	1.74	0.69
1:E:192:HIS:CD2	2:F:101:TRP:HE1	2.10	0.69
3:G:130:ARG:HE	3:G:198:ARG:HG3	1.57	0.69
3:G:239:LEU:C	3:G:243:PRO:HG2	2.18	0.69
2:J:227:ILE:HG12	2:J:230:MET:HB2	1.73	0.69
3:K:254:LEU:O	3:K:255:ALA:O	2.09	0.69
2:F:135:LEU:HB2	2:F:144:THR:HG21	1.74	0.69
2:J:236:ARG:NE	2:J:239:SER:HB3	2.07	0.69
2:B:79:LEU:HD12	2:B:88:GLY:HA2	1.75	0.69
2:B:227:ILE:HG12	2:B:230:MET:HB2	1.75	0.69
3:G:201:PHE:HE2	3:G:248:PHE:HB3	1.57	0.69
1:I:182:ASN:C	1:I:182:ASN:HD22	2.00	0.69
3:K:131:ASN:H	3:K:131:ASN:HD22	1.41	0.69
2:B:210:LYS:HD3	3:C:141:TYR:HE2	1.56	0.68
1:E:309:ASN:ND2	1:E:309:ASN:N	2.35	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:62:ASN:HD21	1:I:167:ARG:H	1.41	0.68
1:I:230:ALA:CB	1:I:233:ARG:HG2	2.22	0.68
2:F:239:SER:O	2:F:242:ARG:HB3	1.93	0.68
3:C:131:ASN:H	3:C:131:ASN:ND2	1.91	0.68
1:E:75:GLU:OE1	1:E:404:GLN:NE2	2.26	0.68
2:B:234:ILE:HD11	2:J:199:MET:HG3	1.72	0.68
3:C:201:PHE:HE2	3:C:248:PHE:HB3	1.57	0.68
1:A:35:GLU:HA	1:A:38:GLN:HG2	1.76	0.68
2:F:112:THR:CG2	3:G:162:THR:HG21	2.15	0.68
1:I:247:VAL:HG21	2:J:155:ILE:HD11	1.76	0.68
2:J:222:PHE:HA	3:K:256:LEU:CB	2.19	0.68
1:A:72:HIS:HE1	1:A:75:GLU:OE1	1.75	0.68
1:A:220:ASP:OD1	2:B:82:ARG:NH1	2.27	0.68
2:F:228:TYR:HD1	2:F:228:TYR:O	1.76	0.68
1:I:220:ASP:OD1	2:J:82:ARG:NH1	2.26	0.68
2:J:104:ARG:HA	2:J:108:PHE:HB2	1.76	0.68
2:J:228:TYR:HD1	2:J:228:TYR:O	1.76	0.68
2:B:206:ARG:HG2	3:C:184:TYR:CZ	2.28	0.67
1:E:72:HIS:CE1	1:E:75:GLU:OE1	2.47	0.67
2:F:236:ARG:NE	2:F:239:SER:HB3	2.07	0.67
1:A:120:LYS:HG3	1:A:274:PRO:HB3	1.76	0.67
2:J:8:VAL:HG23	3:K:125:ARG:NH2	2.04	0.67
1:E:276:GLU:OE2	1:E:276:GLU:HA	1.94	0.67
1:I:145:GLN:HA	1:I:145:GLN:NE2	2.09	0.67
1:E:247:VAL:HG21	2:F:155:ILE:HD11	1.76	0.67
1:I:243:THR:O	1:I:247:VAL:HG23	1.94	0.67
2:J:210:LYS:HD3	3:K:141:TYR:CE2	2.29	0.67
2:J:224:SER:HB3	3:K:256:LEU:HD12	1.76	0.67
3:K:131:ASN:H	3:K:131:ASN:ND2	1.93	0.67
2:B:228:TYR:HD1	2:B:228:TYR:O	1.76	0.67
1:E:230:ALA:HB2	1:E:233:ARG:HG2	1.76	0.67
1:I:120:LYS:HG3	1:I:274:PRO:HB3	1.75	0.67
3:G:231:HIS:CA	3:G:233:PHE:H	2.06	0.67
1:I:192:HIS:CD2	2:J:101:TRP:HE1	2.13	0.67
2:F:210:LYS:HD3	3:G:141:TYR:HE2	1.59	0.67
1:A:112:ARG:CB	1:A:269:MET:CE	2.63	0.67
3:G:181:TYR:O	3:G:185:ILE:HG23	1.95	0.66
1:E:385:SER:H	1:I:265:GLN:HE22	1.41	0.66
2:F:79:LEU:HD12	2:F:88:GLY:HA2	1.76	0.66
1:E:172:THR:C	1:E:174:THR:H	2.02	0.66
1:A:46:THR:CG2	1:A:47:ILE:N	2.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ILE:HA	1:A:382:ASP:OD2	1.96	0.66
2:F:105:TYR:HD2	2:F:106:PHE:CE2	2.13	0.66
3:G:234:TRP:C	3:G:236:MET:H	2.03	0.66
2:F:220:SER:HB2	2:F:222:PHE:HB3	1.77	0.66
1:A:230:ALA:CB	1:A:233:ARG:HG2	2.26	0.66
2:J:211:ASP:O	2:J:211:ASP:CG	2.39	0.66
2:B:104:ARG:HA	2:B:108:PHE:HB2	1.76	0.66
3:K:239:LEU:C	3:K:243:PRO:HG2	2.21	0.66
2:B:195:GLU:HG2	3:C:160:HIS:NE2	2.11	0.66
2:F:181:ALA:O	2:F:184:GLN:HB2	1.95	0.66
1:E:46:THR:HG22	1:E:47:ILE:H	1.60	0.66
2:F:47:ASP:HB3	2:F:50:PHE:H	1.60	0.66
2:J:206:ARG:HG2	3:K:184:TYR:CZ	2.30	0.66
2:B:86:PRO:HB3	2:B:136:MET:HG3	1.78	0.65
2:B:20:THR:O	2:B:24:MET:HG3	1.95	0.65
3:C:130:ARG:HE	3:C:198:ARG:HG3	1.60	0.65
1:E:120:LYS:HG3	1:E:274:PRO:HB3	1.79	0.65
1:E:220:ASP:OD1	2:F:82:ARG:NH1	2.29	0.65
1:E:379:ILE:HA	1:E:382:ASP:OD2	1.96	0.65
1:I:73:VAL:HG23	1:I:118:ILE:HA	1.78	0.65
3:C:234:TRP:C	3:C:236:MET:H	2.04	0.65
2:F:206:ARG:HD3	3:G:185:ILE:HG22	1.78	0.65
1:I:245:LEU:HD13	1:I:249:MET:HG3	1.77	0.65
2:B:210:LYS:HD3	3:C:141:TYR:CE2	2.31	0.65
3:C:231:HIS:CA	3:C:233:PHE:H	2.07	0.65
1:E:110:VAL:O	1:E:110:VAL:CG1	2.45	0.65
1:A:243:THR:O	1:A:247:VAL:HG23	1.96	0.65
1:A:182:ASN:C	1:A:182:ASN:HD22	2.05	0.65
1:E:83:GLU:OE1	1:I:270:ARG:NH2	2.30	0.65
2:F:222:PHE:CA	3:G:256:LEU:HB2	2.22	0.65
2:F:44:THR:O	2:F:45:MET:HG2	1.95	0.65
2:F:221:ALA:C	2:F:223:MET:H	2.04	0.65
2:J:79:LEU:HD12	2:J:88:GLY:HA2	1.79	0.65
1:E:61:ILE:O	1:E:62:ASN:HB2	1.96	0.65
3:G:254:LEU:O	3:G:255:ALA:C	2.39	0.65
1:I:42:MET:O	1:I:46:THR:HB	1.97	0.65
2:F:205:LEU:O	2:F:207:THR:N	2.29	0.65
2:J:221:ALA:C	2:J:223:MET:H	2.05	0.65
3:K:61:PHE:O	3:K:65:VAL:HG23	1.97	0.65
3:K:201:PHE:HE2	3:K:248:PHE:HB3	1.60	0.65
1:A:385:SER:H	1:E:265:GLN:HE22	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:ASN:HD21	1:E:167:ARG:H	1.44	0.64
2:F:146:ILE:O	2:F:150:MET:HB2	1.97	0.64
2:B:62:THR:CA	2:B:236:ARG:NH1	2.43	0.64
1:E:46:THR:CG2	1:E:47:ILE:N	2.60	0.64
2:J:90:THR:HG21	2:J:129:ILE:HD12	1.79	0.64
3:C:239:LEU:C	3:C:243:PRO:HG2	2.22	0.64
2:F:210:LYS:HD3	3:G:141:TYR:CE2	2.32	0.64
3:C:231:HIS:N	3:C:233:PHE:CD2	2.66	0.64
2:F:206:ARG:HG2	3:G:184:TYR:CZ	2.32	0.64
1:A:83:GLU:OE1	1:E:270:ARG:NH2	2.31	0.64
2:B:220:SER:HB2	2:B:222:PHE:HB3	1.79	0.63
1:E:46:THR:CG2	1:E:47:ILE:H	2.12	0.63
1:A:247:VAL:HG21	2:B:155:ILE:HD11	1.80	0.63
1:E:384:ASP:CG	1:I:112:ARG:HH22	2.06	0.63
1:I:79:GLU:CB	1:I:80:THR:HG23	2.21	0.63
2:J:64:THR:O	2:J:68:LEU:HB2	1.98	0.63
1:I:213:ILE:HD11	2:J:21:ILE:HD13	1.80	0.63
2:J:195:GLU:HG2	3:K:160:HIS:NE2	2.12	0.63
1:E:224:ALA:O	1:E:226:GLU:N	2.32	0.63
2:B:236:ARG:HH21	2:B:237:TRP:C	2.06	0.63
2:J:105:TYR:HD2	2:J:106:PHE:CE2	2.15	0.63
2:F:8:VAL:HG22	2:F:8:VAL:O	1.98	0.63
3:G:242:ALA:N	3:G:243:PRO:CD	2.62	0.63
3:K:254:LEU:O	3:K:255:ALA:C	2.41	0.63
2:F:73:ALA:HB1	2:F:229:PHE:HB3	1.79	0.62
3:G:131:ASN:H	3:G:131:ASN:ND2	1.97	0.62
2:J:220:SER:HB2	2:J:222:PHE:HB3	1.81	0.62
3:C:131:ASN:HD22	3:C:131:ASN:N	1.95	0.62
2:F:13:GLU:O	2:F:16:GLN:HB2	2.00	0.62
2:F:117:ASN:HD22	2:F:184:GLN:NE2	1.97	0.62
3:G:115:ARG:CZ	3:G:117:ARG:HH12	2.13	0.62
1:I:110:VAL:O	1:I:110:VAL:CG1	2.47	0.62
2:J:42:MET:HG2	2:J:198:ARG:HH21	1.63	0.62
2:B:202:LYS:HA	2:B:202:LYS:HZ1	1.63	0.62
2:B:222:PHE:CA	3:C:256:LEU:HB2	2.23	0.62
1:E:384:ASP:CG	1:I:112:ARG:NH2	2.58	0.62
2:J:135:LEU:HB2	2:J:144:THR:CG2	2.30	0.62
1:I:190:PHE:CD1	1:I:190:PHE:C	2.77	0.62
3:C:234:TRP:HA	3:C:237:GLU:HG2	1.81	0.61
1:E:230:ALA:CB	1:E:233:ARG:HG2	2.29	0.61
1:E:233:ARG:HH12	2:F:137:LEU:HA	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:371:TRP:CH2	1:E:377:SER:HA	2.35	0.61
3:G:258:VAL:O	3:G:259:MET:HB3	1.99	0.61
2:B:146:ILE:O	2:B:150:MET:HB2	2.01	0.61
1:A:46:THR:CG2	1:A:47:ILE:H	2.13	0.61
1:A:309:ASN:H	1:A:309:ASN:ND2	1.96	0.61
3:C:248:PHE:O	3:C:248:PHE:CG	2.53	0.61
1:I:172:THR:C	1:I:174:THR:H	2.08	0.61
1:I:309:ASN:ND2	1:I:309:ASN:H	1.98	0.61
1:A:90:ASN:HB2	1:A:143:ASN:ND2	2.15	0.61
3:C:234:TRP:O	3:C:237:GLU:HG3	2.01	0.61
3:G:131:ASN:OD1	3:G:244:LEU:HB3	2.00	0.61
2:J:228:TYR:O	2:J:231:TRP:N	2.34	0.61
2:J:205:LEU:O	2:J:207:THR:N	2.34	0.61
2:J:206:ARG:HD3	3:K:185:ILE:HG22	1.82	0.61
3:K:234:TRP:C	3:K:236:MET:H	2.08	0.61
2:B:7:ALA:HB3	3:C:124:PRO:HG2	1.81	0.61
3:C:131:ASN:HB3	3:C:199:LEU:CD2	2.29	0.61
3:G:170:THR:O	3:G:174:ILE:HG12	2.01	0.61
2:J:163:ILE:O	2:J:166:PRO:HD2	2.01	0.61
2:F:211:ASP:CG	2:F:211:ASP:O	2.44	0.61
3:G:131:ASN:H	3:G:131:ASN:HD22	1.47	0.61
1:E:290:THR:HA	1:E:410:ILE:O	2.01	0.60
2:F:149:ALA:CB	2:F:232:HIS:HB2	2.31	0.60
2:J:196:TYR:C	2:J:196:TYR:CD2	2.79	0.60
2:B:105:TYR:HD2	2:B:106:PHE:CE2	2.19	0.60
1:A:192:HIS:CD2	2:B:101:TRP:HE1	2.19	0.60
2:B:228:TYR:CD1	2:B:228:TYR:O	2.54	0.60
2:F:238:PHE:C	2:F:238:PHE:HD1	2.09	0.60
3:G:49:LYS:HB2	3:G:52:THR:OG1	2.01	0.60
3:G:131:ASN:HB3	3:G:199:LEU:CD2	2.30	0.60
3:C:242:ALA:N	3:C:243:PRO:CD	2.64	0.60
2:F:86:PRO:HB3	2:F:136:MET:HG3	1.82	0.60
2:J:202:LYS:HA	2:J:202:LYS:HZ3	1.67	0.60
2:J:214:PRO:HD3	2:J:220:SER:HB3	1.83	0.60
3:C:117:ARG:HA	3:C:117:ARG:HH21	1.67	0.60
2:F:238:PHE:C	2:F:238:PHE:CD1	2.80	0.60
2:F:199:MET:CG	2:J:234:ILE:HD11	2.32	0.60
3:K:242:ALA:N	3:K:243:PRO:CD	2.65	0.60
2:B:53:ASP:OD2	2:B:190:ARG:NH2	2.35	0.60
2:F:190:ARG:HG2	2:F:190:ARG:NH1	2.12	0.60
2:F:236:ARG:HH21	2:F:237:TRP:C	2.10	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:143:PHE:CZ	2:J:147:VAL:HG21	2.37	0.60
1:E:42:MET:O	1:E:46:THR:HB	2.00	0.60
1:E:281:THR:HG23	1:E:307:HIS:O	2.01	0.60
2:J:13:GLU:O	2:J:16:GLN:HB2	2.02	0.60
3:K:195:ALA:HB1	3:K:202:PHE:CE1	2.37	0.60
2:B:202:LYS:HD3	3:C:181:TYR:CE2	2.37	0.60
2:B:236:ARG:NH2	2:B:240:ASN:N	2.47	0.59
2:B:238:PHE:HD1	2:B:238:PHE:C	2.10	0.59
2:F:20:THR:O	2:F:24:MET:HG3	2.01	0.59
3:K:131:ASN:HD22	3:K:131:ASN:N	1.99	0.59
2:J:228:TYR:CD1	2:J:228:TYR:O	2.53	0.59
2:B:117:ASN:HD22	2:B:184:GLN:NE2	2.00	0.59
1:E:90:ASN:ND2	1:E:143:ASN:HD21	1.99	0.59
2:F:112:THR:HG21	3:G:162:THR:CG2	2.18	0.59
2:F:236:ARG:NE	2:F:236:ARG:O	2.23	0.59
1:I:281:THR:HG23	1:I:307:HIS:O	2.02	0.59
2:B:214:PRO:HD3	2:B:220:SER:HB3	1.83	0.59
3:G:119:LEU:HA	3:G:122:LEU:HD12	1.83	0.59
2:B:238:PHE:C	2:B:238:PHE:CD1	2.81	0.59
1:E:72:HIS:HE1	1:E:75:GLU:OE1	1.84	0.59
2:F:228:TYR:CD1	2:F:228:TYR:O	2.54	0.59
1:A:249:MET:HA	1:A:249:MET:CE	2.32	0.59
2:B:13:GLU:O	2:B:16:GLN:HB2	2.03	0.59
1:E:174:THR:CG2	1:E:174:THR:O	2.50	0.59
2:F:196:TYR:C	2:F:196:TYR:CD2	2.80	0.59
2:B:64:THR:O	2:B:68:LEU:HB2	2.03	0.59
2:F:64:THR:O	2:F:68:LEU:HB2	2.03	0.59
2:F:71:PHE:O	2:F:72:PRO:C	2.45	0.59
3:G:158:THR:O	3:G:162:THR:HG22	2.03	0.59
1:I:224:ALA:O	1:I:226:GLU:N	2.36	0.59
2:J:236:ARG:HH21	2:J:237:TRP:CA	2.13	0.59
1:A:145:GLN:HE21	1:A:145:GLN:CA	2.06	0.59
3:C:131:ASN:OD1	3:C:244:LEU:HB3	2.02	0.59
1:I:145:GLN:HE21	1:I:145:GLN:CA	2.14	0.59
2:J:222:PHE:CA	3:K:256:LEU:HB2	2.26	0.59
3:C:47:ASP:C	3:C:47:ASP:OD1	2.45	0.58
3:C:201:PHE:CE2	3:C:248:PHE:HB3	2.37	0.58
3:K:116:ASP:OD1	3:K:122:LEU:HD13	2.02	0.58
3:K:117:ARG:HA	3:K:117:ARG:HH21	1.68	0.58
3:K:231:HIS:CA	3:K:233:PHE:H	2.11	0.58
2:F:230:MET:C	2:F:232:HIS:H	2.09	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:146:ILE:O	2:J:150:MET:HB2	2.03	0.58
3:K:131:ASN:OD1	3:K:244:LEU:HB3	2.03	0.58
3:C:126:GLU:C	3:C:128:LEU:H	2.09	0.58
3:G:117:ARG:HA	3:G:117:ARG:HH21	1.66	0.58
2:J:149:ALA:CB	2:J:232:HIS:HB2	2.33	0.58
1:A:309:ASN:ND2	1:A:309:ASN:N	2.50	0.58
2:B:230:MET:C	2:B:232:HIS:H	2.11	0.58
2:J:236:ARG:HH21	2:J:237:TRP:C	2.11	0.58
1:A:315:GLY:CA	1:A:329:VAL:CG2	2.81	0.58
2:B:62:THR:O	2:B:66:ILE:HG13	2.04	0.58
3:C:195:ALA:HB1	3:C:202:PHE:CE1	2.38	0.58
1:I:309:ASN:ND2	1:I:309:ASN:N	2.50	0.58
2:J:47:ASP:HB3	2:J:50:PHE:H	1.69	0.58
2:J:190:ARG:HG2	2:J:190:ARG:HH11	1.69	0.58
2:B:199:MET:CG	2:F:234:ILE:HD11	2.32	0.58
2:B:229:PHE:HD2	2:B:229:PHE:O	1.87	0.58
1:E:281:THR:H	1:E:401:GLN:HG2	1.68	0.58
3:G:126:GLU:C	3:G:128:LEU:H	2.12	0.58
3:G:195:ALA:HB1	3:G:202:PHE:CE1	2.39	0.58
2:J:70:THR:CG2	2:J:227:ILE:CD1	2.39	0.58
1:A:75:GLU:OE1	1:A:404:GLN:NE2	2.34	0.57
2:B:167:LEU:O	2:B:180:ILE:HB	2.04	0.57
3:G:201:PHE:CE2	3:G:248:PHE:HB3	2.38	0.57
1:I:90:ASN:HD22	1:I:143:ASN:HD21	1.52	0.57
1:I:270:ARG:HH11	1:I:270:ARG:HG2	1.68	0.57
2:J:224:SER:O	2:J:227:ILE:HG22	2.04	0.57
3:C:119:LEU:HA	3:C:122:LEU:HD12	1.86	0.57
2:F:236:ARG:NH2	2:F:240:ASN:N	2.48	0.57
2:B:206:ARG:HD3	3:C:185:ILE:HG22	1.86	0.57
3:G:234:TRP:O	3:G:236:MET:N	2.37	0.57
2:J:236:ARG:NH2	2:J:237:TRP:CA	2.50	0.57
2:F:104:ARG:NH1	3:G:154:GLU:OE1	2.37	0.57
2:J:7:ALA:HB3	3:K:124:PRO:HG2	1.86	0.57
3:C:61:PHE:O	3:C:65:VAL:HG23	2.03	0.57
1:I:211:ILE:HD12	2:J:22:ASP:HB3	1.85	0.57
3:K:126:GLU:C	3:K:128:LEU:H	2.12	0.57
1:A:110:VAL:O	1:A:110:VAL:CG1	2.51	0.57
3:K:201:PHE:CE2	3:K:248:PHE:HB3	2.40	0.57
2:J:238:PHE:HD1	2:J:238:PHE:C	2.13	0.57
1:A:229:SER:O	1:A:232:ASP:N	2.28	0.57
2:J:202:LYS:HD3	3:K:181:TYR:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:LYS:HB2	3:C:52:THR:OG1	2.04	0.56
1:A:172:THR:C	1:A:174:THR:H	2.11	0.56
2:B:206:ARG:O	2:B:206:ARG:HG3	2.05	0.56
2:F:70:THR:CG2	2:F:227:ILE:CD1	2.42	0.56
2:F:197:ILE:O	2:F:199:MET:N	2.39	0.56
2:F:214:PRO:HD3	2:F:220:SER:HB3	1.88	0.56
2:F:224:SER:O	2:F:227:ILE:HG22	2.06	0.56
1:I:90:ASN:HB3	1:I:141:MET:HG3	1.87	0.56
1:A:290:THR:HA	1:A:410:ILE:O	2.06	0.56
1:I:350:ASP:C	1:I:350:ASP:OD2	2.46	0.56
1:A:276:GLU:HA	1:A:276:GLU:OE2	2.05	0.56
2:F:88:GLY:O	2:F:91:VAL:HG12	2.05	0.56
3:C:250:ILE:C	3:C:253:TRP:H	2.13	0.56
2:J:238:PHE:C	2:J:238:PHE:CD1	2.83	0.56
1:A:262:ILE:HG12	2:B:170:PRO:HB3	1.86	0.56
2:B:230:MET:C	2:B:232:HIS:N	2.63	0.56
3:G:231:HIS:N	3:G:233:PHE:CD2	2.74	0.56
1:I:306:ASN:ND2	1:I:312:ILE:HD13	2.21	0.56
3:K:192:PHE:HD1	3:K:251:PHE:CZ	2.24	0.56
2:B:38:HIS:NE2	3:C:154:GLU:CD	2.62	0.56
2:B:149:ALA:CB	2:B:232:HIS:HB2	2.36	0.56
2:B:197:ILE:HG12	2:B:197:ILE:O	2.05	0.56
1:E:245:LEU:HD13	1:E:249:MET:HG3	1.87	0.56
2:B:18:SER:HB2	3:C:236:MET:HE1	1.88	0.56
2:B:236:ARG:NH2	2:B:237:TRP:CA	2.53	0.56
2:F:204:THR:HG22	2:F:205:LEU:N	2.21	0.56
2:J:71:PHE:O	2:J:72:PRO:C	2.49	0.56
2:J:86:PRO:HB3	2:J:136:MET:HG3	1.87	0.56
3:K:250:ILE:C	3:K:253:TRP:H	2.14	0.56
2:F:204:THR:O	2:F:206:ARG:N	2.39	0.56
1:I:108:GLN:HG3	1:I:109:LEU:N	2.21	0.56
3:K:231:HIS:N	3:K:233:PHE:CD2	2.74	0.56
1:I:108:GLN:HG3	1:I:109:LEU:O	2.07	0.55
1:I:249:MET:HA	1:I:249:MET:CE	2.35	0.55
2:J:230:MET:C	2:J:232:HIS:H	2.14	0.55
2:J:231:TRP:O	2:J:231:TRP:CD1	2.59	0.55
3:C:234:TRP:O	3:C:236:MET:N	2.39	0.55
3:K:119:LEU:HA	3:K:122:LEU:HD12	1.87	0.55
2:B:90:THR:CG2	2:B:129:ILE:HD12	2.37	0.55
2:F:98:LEU:O	2:F:102:ILE:HG13	2.06	0.55
2:F:105:TYR:HD2	2:F:106:PHE:CD2	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:38:HIS:NE2	3:K:154:GLU:CD	2.61	0.55
2:F:137:LEU:O	2:F:138:SER:C	2.48	0.55
2:F:143:PHE:CZ	2:F:147:VAL:HG21	2.41	0.55
2:F:204:THR:CG2	2:F:205:LEU:N	2.69	0.55
1:I:61:ILE:O	1:I:62:ASN:HB2	2.07	0.55
1:I:75:GLU:OE1	1:I:404:GLN:NE2	2.39	0.55
2:B:236:ARG:NE	2:B:237:TRP:HA	2.21	0.55
2:F:80:TRP:CZ3	2:F:84:ARG:HG3	2.42	0.55
3:G:234:TRP:C	3:G:236:MET:N	2.64	0.55
1:A:112:ARG:CB	1:A:269:MET:HE3	2.33	0.55
1:A:386:ARG:HG2	1:A:408:PRO:HA	1.87	0.55
2:B:105:TYR:HD2	2:B:106:PHE:CD2	2.24	0.55
2:J:55:LYS:HD2	2:J:60:TRP:CE2	2.41	0.55
2:J:86:PRO:CB	2:J:136:MET:HG3	2.37	0.55
2:B:205:LEU:O	2:B:207:THR:N	2.37	0.55
3:C:236:MET:HG3	3:C:237:GLU:N	2.21	0.55
3:G:248:PHE:CG	3:G:248:PHE:O	2.59	0.55
2:F:69:VAL:HG13	2:F:152:TRP:NE1	2.22	0.55
1:E:249:MET:HA	1:E:249:MET:CE	2.37	0.55
1:I:90:ASN:ND2	1:I:143:ASN:HD21	2.05	0.55
2:B:78:TYR:CD1	3:C:253:TRP:CE3	2.94	0.55
2:B:143:PHE:CZ	2:B:147:VAL:HG21	2.42	0.55
1:I:174:THR:O	1:I:174:THR:CG2	2.54	0.55
2:F:206:ARG:NH2	3:G:188:GLY:HA3	2.23	0.54
1:I:315:GLY:CA	1:I:329:VAL:CG2	2.84	0.54
2:B:8:VAL:O	2:B:8:VAL:CG2	2.51	0.54
2:B:27:PHE:CE2	2:B:31:PHE:CE2	2.95	0.54
1:A:305:THR:HB	1:A:359:THR:CB	2.37	0.54
2:F:236:ARG:HH21	2:F:237:TRP:CA	2.15	0.54
2:B:199:MET:HA	2:B:202:LYS:HB2	1.88	0.54
1:I:46:THR:HG23	1:I:47:ILE:N	2.23	0.54
2:J:204:THR:CG2	2:J:205:LEU:N	2.71	0.54
3:K:112:TRP:O	3:K:115:ARG:HB3	2.07	0.54
3:K:234:TRP:O	3:K:236:MET:N	2.40	0.54
1:A:182:ASN:O	1:A:185:GLU:HB2	2.06	0.54
2:B:196:TYR:C	2:B:196:TYR:CD2	2.86	0.54
2:F:243:PHE:O	2:F:243:PHE:CD1	2.61	0.54
1:I:394:PHE:CD1	1:I:400:ARG:HB3	2.42	0.54
2:B:43:LEU:HG	2:B:196:TYR:OH	2.06	0.54
2:F:86:PRO:CB	2:F:136:MET:HG3	2.38	0.54
2:F:165:ALA:HB3	2:F:166:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:115:ARG:CD	3:G:117:ARG:HH22	2.19	0.54
1:I:182:ASN:O	1:I:185:GLU:HB2	2.08	0.54
3:K:248:PHE:CG	3:K:248:PHE:O	2.60	0.54
1:A:371:TRP:CH2	1:A:377:SER:HA	2.43	0.54
2:F:45:MET:HB2	2:F:47:ASP:OD1	2.08	0.54
2:F:202:LYS:HA	2:F:202:LYS:HZ2	1.71	0.54
3:G:131:ASN:HA	3:G:134:HIS:HB3	1.90	0.54
2:J:11:HIS:CD2	2:J:11:HIS:H	2.24	0.54
2:J:157:TYR:HB3	2:J:158:PRO:CD	2.38	0.54
2:B:181:ALA:O	2:B:184:GLN:HB2	2.08	0.54
3:C:254:LEU:O	3:C:257:ALA:CB	2.49	0.54
2:J:204:THR:HG22	2:J:205:LEU:N	2.23	0.54
3:K:131:ASN:HB3	3:K:199:LEU:CD2	2.38	0.54
2:B:72:PRO:O	2:B:76:GLN:HB2	2.08	0.54
2:F:206:ARG:HD3	3:G:185:ILE:CG2	2.37	0.54
3:G:47:ASP:OD1	3:G:47:ASP:O	2.26	0.54
1:A:145:GLN:NE2	1:A:145:GLN:CA	2.69	0.53
2:B:135:LEU:HB2	2:B:144:THR:CG2	2.37	0.53
3:C:234:TRP:C	3:C:236:MET:N	2.65	0.53
3:G:117:ARG:HA	3:G:117:ARG:NH2	2.23	0.53
3:G:131:ASN:HD22	3:G:131:ASN:N	2.03	0.53
2:B:118:PHE:CZ	2:B:185:GLY:HA2	2.43	0.53
1:E:243:THR:O	1:E:247:VAL:HG23	2.07	0.53
3:G:250:ILE:C	3:G:253:TRP:H	2.16	0.53
2:J:45:MET:HB2	2:J:47:ASP:OD1	2.07	0.53
1:A:281:THR:HG23	1:A:307:HIS:O	2.09	0.53
2:B:73:ALA:HB1	2:B:229:PHE:HB3	1.89	0.53
3:C:116:ASP:OD1	3:C:122:LEU:HD13	2.07	0.53
3:C:258:VAL:O	3:C:259:MET:HB3	2.07	0.53
1:E:299:ARG:CB	1:E:299:ARG:HH11	2.21	0.53
3:G:158:THR:O	3:G:162:THR:CG2	2.57	0.53
2:B:234:ILE:HD11	2:J:199:MET:HG2	1.89	0.53
3:C:192:PHE:HD1	3:C:251:PHE:CZ	2.25	0.53
3:C:249:VAL:HG12	3:C:249:VAL:O	2.08	0.53
2:F:157:TYR:N	2:F:158:PRO:HD2	2.22	0.53
1:I:262:ILE:HG12	2:J:170:PRO:HB3	1.91	0.53
1:I:291:TYR:HD2	1:I:371:TRP:HH2	1.56	0.53
2:F:42:MET:HG2	2:F:198:ARG:HH21	1.73	0.53
2:F:48:TRP:HA	2:F:54:TRP:HB3	1.90	0.53
2:F:240:ASN:C	2:F:242:ARG:N	2.63	0.53
2:J:105:TYR:HD2	2:J:106:PHE:CD2	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:116:ASP:OD1	3:G:122:LEU:HD13	2.08	0.53
2:B:228:TYR:O	2:B:231:TRP:N	2.42	0.53
3:K:148:GLY:HA2	3:K:180:SER:OG	2.08	0.53
1:A:183:TYR:HE1	2:B:166:PRO:O	1.92	0.53
2:B:71:PHE:O	2:B:72:PRO:C	2.51	0.53
2:B:236:ARG:O	2:B:238:PHE:N	2.42	0.53
2:F:221:ALA:HB3	3:G:253:TRP:CD1	2.44	0.53
1:I:309:ASN:HA	1:I:356:PRO:HB3	1.91	0.53
2:B:11:HIS:CE1	3:C:237:GLU:OE2	2.62	0.53
2:B:69:VAL:HG13	2:B:152:TRP:NE1	2.23	0.53
1:E:145:GLN:HE21	1:E:145:GLN:CA	2.11	0.53
1:I:90:ASN:HB2	1:I:143:ASN:ND2	2.24	0.53
2:J:21:ILE:HG22	2:J:22:ASP:N	2.22	0.53
2:J:43:LEU:HG	2:J:196:TYR:OH	2.08	0.53
3:C:233:PHE:O	3:C:236:MET:HB3	2.08	0.53
2:F:75:VAL:HA	3:G:253:TRP:CH2	2.44	0.53
2:J:206:ARG:HD3	3:K:185:ILE:CG2	2.39	0.53
3:K:132:PHE:O	3:K:135:LEU:N	2.42	0.53
1:A:380:ILE:HG13	1:A:380:ILE:O	2.07	0.52
2:B:233:PHE:O	2:B:237:TRP:N	2.29	0.52
2:B:236:ARG:HH21	2:B:237:TRP:CA	2.13	0.52
2:J:243:PHE:O	2:J:243:PHE:CD1	2.62	0.52
1:A:73:VAL:HG21	1:A:118:ILE:HA	1.91	0.52
2:F:202:LYS:HD3	3:G:181:TYR:CE2	2.44	0.52
2:F:203:GLY:HA3	2:J:234:ILE:CD1	2.39	0.52
3:G:75:SER:O	3:G:76:ALA:CB	2.57	0.52
3:K:75:SER:O	3:K:76:ALA:CB	2.58	0.52
3:K:117:ARG:HA	3:K:117:ARG:NH2	2.24	0.52
2:B:86:PRO:CB	2:B:136:MET:HG3	2.39	0.52
1:E:211:ILE:HD12	2:F:22:ASP:HB3	1.91	0.52
1:I:379:ILE:HA	1:I:382:ASP:OD2	2.09	0.52
3:K:47:ASP:OD1	3:K:47:ASP:O	2.28	0.52
1:A:265:GLN:HA	1:I:383:PRO:O	2.10	0.52
1:A:314:LEU:HD13	1:A:346:LEU:HD11	1.92	0.52
1:E:174:THR:O	1:E:174:THR:HG23	2.08	0.52
1:E:383:PRO:O	1:I:265:GLN:HA	2.09	0.52
2:F:8:VAL:CG2	3:G:125:ARG:HH22	2.09	0.52
2:F:72:PRO:O	2:F:76:GLN:HB2	2.08	0.52
1:I:90:ASN:HB3	1:I:141:MET:CG	2.40	0.52
2:J:222:PHE:CG	2:J:222:PHE:O	2.63	0.52
1:A:270:ARG:NH2	1:I:83:GLU:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:ILE:HD13	3:C:184:TYR:CE2	2.45	0.52
1:I:35:GLU:HB2	1:I:43:ARG:HD3	1.91	0.52
1:A:245:LEU:HD13	1:A:249:MET:CG	2.39	0.52
2:B:8:VAL:HG23	3:C:125:ARG:NH2	2.16	0.52
2:B:141:TYR:O	2:B:142:LEU:C	2.52	0.52
2:F:205:LEU:C	2:F:207:THR:H	2.16	0.52
2:F:229:PHE:HD2	2:F:229:PHE:O	1.92	0.52
1:A:35:GLU:HB2	1:A:43:ARG:HD3	1.92	0.52
1:E:174:THR:HG22	1:E:176:GLN:HG3	1.92	0.52
2:F:11:HIS:H	2:F:11:HIS:CD2	2.26	0.52
1:A:309:ASN:HA	1:A:356:PRO:HB3	1.91	0.52
2:J:230:MET:C	2:J:232:HIS:N	2.67	0.52
1:A:70:LYS:HE3	1:A:275:LEU:HD21	1.92	0.52
2:F:8:VAL:HB	3:G:125:ARG:HH12	1.74	0.52
2:J:149:ALA:CB	2:J:232:HIS:CB	2.88	0.52
2:B:224:SER:O	2:B:227:ILE:HG22	2.08	0.52
1:E:242:ALA:O	1:E:246:ILE:HG13	2.09	0.52
3:G:93:LEU:O	3:G:96:GLU:HG2	2.09	0.52
1:I:174:THR:O	1:I:174:THR:HG23	2.09	0.52
3:K:192:PHE:HD1	3:K:251:PHE:HZ	1.57	0.52
2:B:11:HIS:ND1	3:C:237:GLU:OE2	2.43	0.51
2:B:104:ARG:NH1	3:C:154:GLU:OE1	2.43	0.51
2:B:231:TRP:O	2:B:231:TRP:CD1	2.63	0.51
2:F:38:HIS:NE2	3:G:154:GLU:CD	2.68	0.51
2:F:236:ARG:C	2:F:236:ARG:CD	2.80	0.51
1:I:281:THR:H	1:I:401:GLN:HG2	1.75	0.51
1:I:291:TYR:CD2	1:I:371:TRP:HH2	2.28	0.51
2:J:66:ILE:HG23	2:J:233:PHE:HB2	1.91	0.51
1:A:93:MET:HE1	1:A:98:PHE:HB2	1.92	0.51
3:C:115:ARG:HD2	3:C:117:ARG:HH22	1.74	0.51
2:J:243:PHE:CD1	2:J:243:PHE:C	2.87	0.51
1:E:299:ARG:HH11	1:E:299:ARG:HB3	1.74	0.51
2:B:137:LEU:O	2:B:138:SER:C	2.52	0.51
3:G:232:THR:HG22	3:G:235:PHE:N	2.20	0.51
2:J:73:ALA:HB1	2:J:229:PHE:HB3	1.91	0.51
2:B:47:ASP:HB3	2:B:50:PHE:H	1.76	0.51
3:C:126:GLU:C	3:C:128:LEU:N	2.65	0.51
3:C:131:ASN:HA	3:C:134:HIS:HB3	1.92	0.51
3:C:231:HIS:CE1	3:C:234:TRP:CD1	2.98	0.51
1:E:182:ASN:O	1:E:185:GLU:HB2	2.10	0.51
2:F:149:ALA:CB	2:F:232:HIS:CB	2.89	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:57:ARG:O	2:J:240:ASN:ND2	2.44	0.51
1:A:371:TRP:CD1	1:A:376:LEU:HD12	2.45	0.51
1:E:73:VAL:HG21	1:E:118:ILE:HA	1.90	0.51
1:E:284:VAL:HG13	1:E:403:VAL:HG21	1.92	0.51
2:F:38:HIS:CE1	3:G:154:GLU:HB2	2.45	0.51
2:F:195:GLU:CG	3:G:160:HIS:NE2	2.70	0.51
3:G:145:ILE:HD13	3:G:184:TYR:CE2	2.46	0.51
3:G:181:TYR:CD1	3:G:184:TYR:HE1	2.28	0.51
2:J:229:PHE:HD2	2:J:229:PHE:O	1.94	0.51
1:E:209:ARG:HB2	1:E:210:PRO:HD2	1.93	0.51
2:F:118:PHE:CZ	2:F:185:GLY:HA2	2.46	0.51
2:F:236:ARG:NH2	2:F:237:TRP:CA	2.52	0.51
1:I:276:GLU:OE2	1:I:276:GLU:HA	2.10	0.51
2:B:233:PHE:HA	2:B:236:ARG:HB3	1.93	0.51
1:I:213:ILE:CD1	2:J:21:ILE:HD13	2.40	0.51
3:K:115:ARG:HD2	3:K:117:ARG:HH22	1.75	0.51
1:E:348:VAL:HG22	1:E:351:ASN:HB2	1.93	0.51
1:I:332:ASP:OD2	1:I:334:THR:HG23	2.11	0.51
2:J:205:LEU:C	2:J:207:THR:H	2.16	0.51
3:K:158:THR:O	3:K:162:THR:HG22	2.11	0.51
2:B:78:TYR:OH	3:C:249:VAL:HG12	2.11	0.50
1:E:218:MET:HE2	1:E:226:GLU:OE2	2.11	0.50
3:G:144:ALA:HB1	3:G:184:TYR:CB	2.39	0.50
1:I:380:ILE:O	1:I:380:ILE:HG13	2.10	0.50
3:K:115:ARG:CZ	3:K:117:ARG:HH12	2.24	0.50
1:A:242:ALA:O	1:A:246:ILE:HG13	2.11	0.50
2:B:236:ARG:NE	2:B:236:ARG:O	2.26	0.50
3:K:170:THR:O	3:K:174:ILE:HG12	2.12	0.50
1:A:375:ARG:O	1:A:378:ASP:HB2	2.11	0.50
2:B:236:ARG:C	2:B:236:ARG:CD	2.83	0.50
2:F:111:TRP:CD1	3:G:74:TRP:HZ3	2.28	0.50
2:F:231:TRP:O	2:F:231:TRP:CD1	2.64	0.50
3:G:192:PHE:HD1	3:G:251:PHE:CZ	2.30	0.50
3:G:194:TYR:O	3:G:198:ARG:HB2	2.11	0.50
1:A:112:ARG:NH2	1:I:384:ASP:CG	2.70	0.50
2:B:205:LEU:C	2:B:207:THR:H	2.19	0.50
1:E:105:ILE:HD11	1:E:116:LEU:HD11	1.93	0.50
2:J:199:MET:HA	2:J:202:LYS:HB2	1.94	0.50
2:J:221:ALA:HB3	3:K:253:TRP:CD1	2.47	0.50
3:G:234:TRP:HA	3:G:237:GLU:HG2	1.94	0.50
2:J:190:ARG:HG2	2:J:190:ARG:NH1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:234:TRP:O	3:K:237:GLU:HG3	2.11	0.50
3:K:258:VAL:O	3:K:259:MET:HB3	2.12	0.50
3:C:115:ARG:CZ	3:C:117:ARG:HH12	2.25	0.50
1:I:299:ARG:HH11	1:I:299:ARG:CB	2.24	0.50
1:A:190:PHE:CD1	1:A:190:PHE:C	2.89	0.50
1:A:284:VAL:HG13	1:A:403:VAL:HG21	1.94	0.50
1:A:318:TYR:CD1	1:A:318:TYR:C	2.90	0.50
3:C:117:ARG:HA	3:C:117:ARG:NH2	2.27	0.50
2:F:149:ALA:HB3	2:F:232:HIS:CB	2.41	0.50
1:I:214:PRO:HD3	2:J:18:SER:OG	2.12	0.50
1:I:371:TRP:CH2	1:I:377:SER:HA	2.47	0.50
2:J:33:ILE:HG21	2:J:92:CYS:HA	1.94	0.50
2:B:149:ALA:HB3	2:B:232:HIS:CB	2.42	0.50
2:B:240:ASN:C	2:B:242:ARG:N	2.67	0.50
2:F:135:LEU:HB2	2:F:144:THR:CG2	2.39	0.50
2:F:233:PHE:O	2:F:237:TRP:N	2.32	0.50
3:G:141:TYR:CD1	3:G:188:GLY:HA2	2.47	0.50
1:I:183:TYR:HE1	2:J:166:PRO:O	1.95	0.50
2:J:206:ARG:HD3	3:K:185:ILE:HB	1.94	0.50
1:A:394:PHE:CD1	1:A:400:ARG:HB3	2.46	0.49
3:C:170:THR:O	3:C:174:ILE:HG12	2.12	0.49
2:J:58:ARG:HH22	2:J:237:TRP:HZ3	1.56	0.49
2:J:69:VAL:O	2:J:70:THR:C	2.55	0.49
3:K:131:ASN:HA	3:K:134:HIS:HB3	1.94	0.49
2:B:135:LEU:O	2:B:135:LEU:HD22	2.11	0.49
1:E:108:GLN:HG3	1:E:109:LEU:O	2.12	0.49
1:E:252:SER:HA	1:E:255:ASN:HB2	1.95	0.49
1:I:305:THR:HB	1:I:359:THR:HB	1.93	0.49
2:J:38:HIS:CD2	2:J:42:MET:HE1	2.47	0.49
2:B:149:ALA:HB3	2:B:232:HIS:HB2	1.93	0.49
2:B:165:ALA:HB3	2:B:166:PRO:HD3	1.93	0.49
2:F:21:ILE:HG22	2:F:22:ASP:N	2.27	0.49
1:I:233:ARG:HH12	2:J:137:LEU:HA	1.76	0.49
3:K:234:TRP:C	3:K:236:MET:N	2.69	0.49
1:A:108:GLN:HG3	1:A:109:LEU:N	2.28	0.49
1:A:305:THR:HB	1:A:359:THR:HB	1.93	0.49
2:B:195:GLU:CG	3:C:160:HIS:CE1	2.81	0.49
2:F:125:VAL:O	2:F:126:PRO:C	2.56	0.49
2:F:163:ILE:O	2:F:166:PRO:HD2	2.12	0.49
3:K:49:LYS:HB2	3:K:52:THR:OG1	2.12	0.49
2:B:57:ARG:O	2:B:240:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:ALA:HB3	3:C:253:TRP:CD1	2.46	0.49
1:E:315:GLY:CA	1:E:329:VAL:CG2	2.89	0.49
1:E:318:TYR:CD1	1:E:318:TYR:C	2.90	0.49
1:I:309:ASN:N	1:I:309:ASN:HD22	2.09	0.49
3:K:173:HIS:CD2	3:K:177:PHE:CE1	3.00	0.49
1:A:383:PRO:O	1:E:265:GLN:HA	2.12	0.49
2:B:149:ALA:O	2:B:150:MET:C	2.55	0.49
1:E:385:SER:H	1:I:265:GLN:NE2	2.10	0.49
3:C:141:TYR:CD1	3:C:188:GLY:HA2	2.48	0.49
2:F:236:ARG:NE	2:F:237:TRP:HA	2.25	0.49
3:G:132:PHE:O	3:G:135:LEU:N	2.46	0.49
2:B:221:ALA:C	2:B:223:MET:H	2.20	0.49
2:F:233:PHE:HA	2:F:236:ARG:HB3	1.95	0.49
3:G:234:TRP:O	3:G:237:GLU:HG3	2.12	0.49
1:I:320:ALA:O	1:I:321:SER:HB2	2.12	0.49
2:B:80:TRP:CZ3	2:B:84:ARG:HG3	2.48	0.49
2:F:206:ARG:HG3	2:F:206:ARG:O	2.12	0.49
3:G:75:SER:O	3:G:76:ALA:HB3	2.13	0.49
3:G:148:GLY:HA2	3:G:180:SER:OG	2.13	0.49
2:J:149:ALA:O	2:J:150:MET:C	2.56	0.49
1:A:108:GLN:HG3	1:A:109:LEU:O	2.13	0.49
2:B:243:PHE:CD1	2:B:243:PHE:O	2.66	0.49
1:E:375:ARG:O	1:E:378:ASP:HB2	2.12	0.49
2:F:222:PHE:CG	2:F:222:PHE:O	2.65	0.49
3:G:231:HIS:CE1	3:G:234:TRP:CD1	3.01	0.49
2:J:137:LEU:O	2:J:138:SER:C	2.55	0.49
3:K:231:HIS:CE1	3:K:234:TRP:CD1	3.01	0.49
1:A:254:ALA:O	1:A:257:LYS:O	2.30	0.48
2:B:204:THR:O	2:B:206:ARG:N	2.46	0.48
1:E:395:ASP:OD2	1:E:395:ASP:C	2.55	0.48
3:G:250:ILE:O	3:G:254:LEU:N	2.46	0.48
1:I:386:ARG:HG2	1:I:408:PRO:HA	1.93	0.48
2:J:48:TRP:HA	2:J:54:TRP:HB3	1.95	0.48
1:E:90:ASN:HB2	1:E:143:ASN:ND2	2.28	0.48
3:G:181:TYR:HA	3:G:184:TYR:CE1	2.47	0.48
3:K:250:ILE:O	3:K:254:LEU:N	2.46	0.48
2:B:222:PHE:CG	2:B:222:PHE:O	2.65	0.48
2:F:171:VAL:HG23	2:F:172:GLU:N	2.28	0.48
2:F:202:LYS:HA	2:F:202:LYS:HZ3	1.79	0.48
2:J:90:THR:CG2	2:J:129:ILE:HD12	2.42	0.48
2:J:207:THR:C	2:J:209:GLY:H	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:MET:HB2	2:B:47:ASP:OD1	2.13	0.48
2:B:71:PHE:O	2:B:75:VAL:HG13	2.13	0.48
1:E:305:THR:HB	1:E:359:THR:CB	2.44	0.48
3:G:246:TYR:O	3:G:247:GLY:C	2.55	0.48
1:I:60:LYS:O	1:I:63:GLU:HB2	2.12	0.48
2:J:38:HIS:CD2	2:J:42:MET:CE	2.96	0.48
2:J:72:PRO:O	2:J:76:GLN:HB2	2.12	0.48
2:J:75:VAL:HA	3:K:253:TRP:CH2	2.47	0.48
2:J:236:ARG:NE	2:J:237:TRP:HA	2.27	0.48
3:K:126:GLU:C	3:K:128:LEU:N	2.70	0.48
2:B:204:THR:CG2	2:B:205:LEU:N	2.76	0.48
1:E:120:LYS:HA	1:E:120:LYS:HD3	1.53	0.48
3:G:181:TYR:HD1	3:G:184:TYR:HE1	1.61	0.48
1:I:36:LYS:HE2	1:I:373:VAL:O	2.13	0.48
1:I:59:VAL:O	1:I:159:VAL:HA	2.14	0.48
3:K:75:SER:O	3:K:76:ALA:HB3	2.13	0.48
3:K:249:VAL:HG12	3:K:249:VAL:O	2.14	0.48
3:K:253:TRP:O	3:K:253:TRP:CE3	2.67	0.48
1:A:306:ASN:ND2	1:A:312:ILE:HD13	2.28	0.48
2:B:21:ILE:HG22	2:B:22:ASP:N	2.28	0.48
1:E:190:PHE:CD1	1:E:190:PHE:C	2.91	0.48
2:J:149:ALA:HB3	2:J:232:HIS:CB	2.43	0.48
2:J:230:MET:HE3	2:J:231:TRP:HA	1.96	0.48
3:K:236:MET:HG3	3:K:237:GLU:N	2.28	0.48
2:F:55:LYS:HD2	2:F:60:TRP:CE2	2.48	0.48
2:F:106:PHE:CD2	2:F:106:PHE:N	2.82	0.48
2:F:204:THR:O	2:F:205:LEU:C	2.57	0.48
1:E:90:ASN:HB3	1:E:141:MET:CG	2.44	0.48
2:F:53:ASP:OD2	2:F:190:ARG:NH2	2.46	0.48
1:I:209:ARG:HB2	1:I:210:PRO:HD2	1.94	0.48
1:I:290:THR:HA	1:I:410:ILE:O	2.14	0.48
2:J:111:TRP:O	3:K:74:TRP:CH2	2.66	0.48
2:J:233:PHE:HA	2:J:236:ARG:HB3	1.95	0.48
2:J:236:ARG:C	2:J:236:ARG:CD	2.87	0.48
2:J:236:ARG:O	2:J:238:PHE:N	2.47	0.48
1:A:90:ASN:HB3	1:A:141:MET:HG3	1.96	0.48
3:C:232:THR:HG22	3:C:235:PHE:N	2.26	0.48
2:F:30:PHE:O	2:F:34:VAL:HG23	2.13	0.48
2:F:106:PHE:N	2:F:106:PHE:HD2	2.12	0.48
2:F:149:ALA:HB3	2:F:232:HIS:HB2	1.94	0.48
2:F:199:MET:HA	2:F:202:LYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:135:LEU:O	2:J:135:LEU:HD22	2.13	0.48
2:F:58:ARG:HH21	2:F:58:ARG:CG	2.21	0.48
2:J:204:THR:O	2:J:206:ARG:N	2.47	0.48
2:J:236:ARG:NH2	2:J:240:ASN:N	2.54	0.48
1:A:79:GLU:CB	1:A:80:THR:HG23	2.34	0.47
2:B:165:ALA:O	2:B:167:LEU:N	2.47	0.47
2:F:230:MET:C	2:F:232:HIS:N	2.63	0.47
2:B:176:MET:HE2	2:B:176:MET:HB3	1.73	0.47
3:C:57:ILE:HG23	3:C:58:TYR:CD1	2.50	0.47
3:C:192:PHE:HD1	3:C:251:PHE:HZ	1.60	0.47
2:F:58:ARG:HH22	2:F:237:TRP:HZ3	1.56	0.47
2:F:243:PHE:O	2:F:244:LEU:C	2.57	0.47
2:B:42:MET:HG2	2:B:198:ARG:HH21	1.80	0.47
2:B:82:ARG:HH22	2:B:219:PHE:HZ	1.62	0.47
3:G:249:VAL:HG12	3:G:249:VAL:O	2.14	0.47
1:I:318:TYR:CD1	1:I:318:TYR:C	2.93	0.47
1:I:320:ALA:C	1:I:322:VAL:H	2.22	0.47
2:J:76:GLN:NE2	2:J:229:PHE:CZ	2.82	0.47
3:K:93:LEU:O	3:K:96:GLU:HG2	2.14	0.47
3:K:232:THR:HG22	3:K:235:PHE:N	2.22	0.47
1:A:73:VAL:HG23	1:A:118:ILE:HA	1.91	0.47
1:A:225:ASP:O	1:A:226:GLU:C	2.57	0.47
2:B:149:ALA:CB	2:B:232:HIS:CB	2.93	0.47
1:E:60:LYS:O	1:E:63:GLU:HB2	2.14	0.47
1:E:105:ILE:HD13	1:E:105:ILE:HG21	1.58	0.47
1:E:182:ASN:HD22	1:E:183:TYR:N	2.11	0.47
3:G:126:GLU:C	3:G:128:LEU:N	2.70	0.47
3:G:155:GLN:C	3:G:157:GLY:N	2.71	0.47
1:I:322:VAL:HG11	1:I:376:LEU:HD11	1.96	0.47
2:J:125:VAL:O	2:J:126:PRO:C	2.57	0.47
3:C:148:GLY:HA2	3:C:180:SER:OG	2.14	0.47
2:J:55:LYS:HD2	2:J:60:TRP:CZ2	2.50	0.47
2:J:181:ALA:O	2:J:184:GLN:HB2	2.14	0.47
2:F:32:VAL:HG11	3:G:254:LEU:HG	1.96	0.47
1:I:174:THR:HG22	1:I:176:GLN:HG3	1.96	0.47
1:A:258:TYR:CE2	2:B:166:PRO:HG3	2.50	0.47
3:C:194:TYR:O	3:C:198:ARG:HB2	2.14	0.47
3:C:250:ILE:C	3:C:252:GLY:N	2.70	0.47
2:F:47:ASP:CG	2:F:49:ASP:H	2.23	0.47
2:J:42:MET:SD	3:K:154:GLU:HG3	2.54	0.47
2:J:147:VAL:O	2:J:150:MET:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:59:THR:O	3:K:63:LEU:HB2	2.15	0.47
1:E:145:GLN:NE2	1:E:145:GLN:CA	2.72	0.47
1:I:112:ARG:CB	1:I:269:MET:HE3	2.37	0.47
1:I:306:ASN:HD21	1:I:312:ILE:HD13	1.79	0.47
1:A:320:ALA:O	1:A:321:SER:HB2	2.14	0.47
2:F:38:HIS:CD2	2:F:42:MET:HE1	2.50	0.47
2:F:206:ARG:HD3	3:G:185:ILE:HB	1.95	0.47
2:F:228:TYR:C	2:F:230:MET:N	2.71	0.47
1:A:387:PHE:CD2	1:A:388:ALA:N	2.83	0.47
2:B:224:SER:HB3	3:C:256:LEU:CD1	2.44	0.47
3:C:75:SER:O	3:C:76:ALA:CB	2.63	0.47
1:E:305:THR:HB	1:E:359:THR:HB	1.96	0.47
2:F:42:MET:HE3	3:G:153:THR:HG22	1.97	0.47
2:J:117:ASN:HD22	2:J:184:GLN:NE2	2.13	0.47
1:E:182:ASN:C	1:E:182:ASN:ND2	2.67	0.46
2:F:221:ALA:C	2:F:223:MET:N	2.71	0.46
3:G:61:PHE:O	3:G:65:VAL:HG23	2.15	0.46
2:J:228:TYR:C	2:J:230:MET:N	2.72	0.46
1:A:182:ASN:C	1:A:182:ASN:ND2	2.73	0.46
2:B:38:HIS:CE1	3:C:154:GLU:HB2	2.51	0.46
2:B:143:PHE:O	2:B:147:VAL:HG22	2.15	0.46
3:C:167:THR:HB	3:C:169:PHE:H	1.80	0.46
2:F:236:ARG:HH21	2:F:240:ASN:H	1.58	0.46
3:C:144:ALA:HB1	3:C:184:TYR:CB	2.45	0.46
1:E:394:PHE:CD1	1:E:400:ARG:HB3	2.50	0.46
3:K:158:THR:O	3:K:162:THR:CG2	2.63	0.46
2:B:157:TYR:N	2:B:158:PRO:HD2	2.30	0.46
2:B:190:ARG:HH11	2:B:190:ARG:HG2	1.80	0.46
1:E:172:THR:C	1:E:174:THR:N	2.71	0.46
1:I:242:ALA:O	1:I:246:ILE:HG13	2.15	0.46
2:J:58:ARG:HA	2:J:240:ASN:ND2	2.29	0.46
3:C:243:PRO:O	3:C:244:LEU:HB2	2.16	0.46
1:I:245:LEU:HD13	1:I:249:MET:CG	2.45	0.46
2:B:163:ILE:O	2:B:166:PRO:HD2	2.16	0.46
3:C:254:LEU:HA	3:C:254:LEU:HD13	1.34	0.46
2:F:243:PHE:CD1	2:F:243:PHE:C	2.89	0.46
3:K:242:ALA:N	3:K:243:PRO:HD3	2.29	0.46
3:K:246:TYR:O	3:K:247:GLY:C	2.59	0.46
2:B:204:THR:HG22	2:B:205:LEU:N	2.30	0.46
2:F:43:LEU:HG	2:F:196:TYR:OH	2.15	0.46
1:E:59:VAL:O	1:E:159:VAL:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:MET:CE	1:E:272:MET:CA	2.80	0.46
1:A:231:THR:O	1:A:235:VAL:HG23	2.16	0.46
2:B:58:ARG:HH22	2:B:237:TRP:HZ3	1.62	0.46
2:B:243:PHE:CD1	2:B:243:PHE:C	2.88	0.46
1:E:309:ASN:HA	1:E:356:PRO:HB3	1.96	0.46
2:F:57:ARG:O	2:F:240:ASN:ND2	2.48	0.46
1:I:314:LEU:HD13	1:I:346:LEU:HD11	1.98	0.46
2:J:62:THR:O	2:J:66:ILE:HG13	2.15	0.46
2:J:8:VAL:HB	3:K:125:ARG:HH12	1.79	0.46
2:J:97:LEU:HD12	2:J:97:LEU:HA	1.56	0.46
3:K:198:ARG:HB3	3:K:199:LEU:HD12	1.98	0.46
1:A:306:ASN:HD21	1:A:312:ILE:HD13	1.81	0.45
3:C:112:TRP:O	3:C:115:ARG:HB3	2.16	0.45
2:F:222:PHE:HD2	3:G:256:LEU:HD23	1.79	0.45
2:F:224:SER:HB3	3:G:256:LEU:CD1	2.44	0.45
2:J:224:SER:HB3	3:K:256:LEU:CD1	2.46	0.45
1:A:174:THR:HG22	1:A:176:GLN:HG3	1.97	0.45
2:B:206:ARG:HD3	3:C:185:ILE:CG2	2.46	0.45
2:F:207:THR:C	2:F:209:GLY:H	2.24	0.45
3:G:126:GLU:O	3:G:130:ARG:HB2	2.16	0.45
3:G:241:VAL:N	3:G:243:PRO:HD2	2.31	0.45
2:J:90:THR:HA	2:J:128:ALA:HB1	1.97	0.45
1:A:174:THR:O	1:A:174:THR:CG2	2.64	0.45
3:C:248:PHE:O	3:C:248:PHE:CD1	2.69	0.45
1:E:208:ARG:HD2	1:E:208:ARG:HA	1.66	0.45
3:G:132:PHE:O	3:G:133:THR:C	2.60	0.45
1:I:45:ARG:O	1:I:78:PRO:HD3	2.17	0.45
1:I:182:ASN:HD22	1:I:183:TYR:N	2.13	0.45
2:J:71:PHE:O	2:J:75:VAL:HG13	2.17	0.45
2:J:88:GLY:O	2:J:91:VAL:HG12	2.17	0.45
1:A:281:THR:H	1:A:401:GLN:HG2	1.81	0.45
2:B:50:PHE:O	2:B:119:VAL:HA	2.16	0.45
2:B:230:MET:HE3	2:B:231:TRP:HA	1.98	0.45
3:C:246:TYR:O	3:C:247:GLY:C	2.59	0.45
3:C:253:TRP:CE3	3:C:253:TRP:O	2.69	0.45
2:F:38:HIS:CD2	2:F:42:MET:CE	3.00	0.45
1:A:233:ARG:HH12	2:B:137:LEU:HA	1.81	0.45
2:B:58:ARG:HH21	2:B:58:ARG:CG	2.25	0.45
2:J:240:ASN:C	2:J:242:ARG:N	2.73	0.45
1:A:61:ILE:O	1:A:62:ASN:HB2	2.15	0.45
1:A:309:ASN:N	1:A:309:ASN:HD22	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASP:CG	1:E:112:ARG:NH2	2.74	0.45
3:K:234:TRP:HA	3:K:237:GLU:HG2	1.96	0.45
1:A:225:ASP:C	1:A:227:LEU:N	2.71	0.45
1:A:401:GLN:HE21	1:A:401:GLN:HB2	1.43	0.45
3:C:194:TYR:CZ	3:C:198:ARG:HG2	2.51	0.45
3:C:241:VAL:N	3:C:243:PRO:HD2	2.32	0.45
2:F:69:VAL:O	2:F:70:THR:C	2.59	0.45
2:F:100:GLU:O	2:F:104:ARG:HG2	2.17	0.45
2:F:206:ARG:HD3	3:G:185:ILE:CB	2.46	0.45
3:G:177:PHE:O	3:G:182:PRO:HD3	2.17	0.45
1:I:46:THR:HG22	1:I:47:ILE:N	2.22	0.45
2:B:243:PHE:O	2:B:244:LEU:C	2.59	0.45
2:F:157:TYR:HB3	2:F:158:PRO:CD	2.46	0.45
2:J:149:ALA:HB3	2:J:232:HIS:HB2	1.99	0.45
2:J:152:TRP:CD1	2:J:152:TRP:C	2.95	0.45
1:A:413:PHE:CE2	1:E:260:ILE:HG21	2.52	0.45
2:B:197:ILE:O	2:B:199:MET:N	2.49	0.45
3:G:112:TRP:O	3:G:115:ARG:HB3	2.17	0.45
3:G:131:ASN:CB	3:G:199:LEU:HD21	2.38	0.45
1:I:272:MET:CE	1:I:272:MET:CA	2.90	0.45
2:J:118:PHE:CZ	2:J:185:GLY:HA2	2.51	0.45
3:C:242:ALA:N	3:C:243:PRO:HD3	2.32	0.45
1:E:386:ARG:HG2	1:E:408:PRO:HA	1.99	0.45
3:G:192:PHE:HD1	3:G:251:PHE:HZ	1.65	0.45
3:G:242:ALA:N	3:G:243:PRO:HD3	2.31	0.45
2:J:78:TYR:CD1	3:K:253:TRP:CE3	3.05	0.45
2:B:236:ARG:HH21	2:B:240:ASN:H	1.57	0.44
3:C:250:ILE:O	3:C:254:LEU:N	2.50	0.44
1:E:46:THR:HG23	1:E:47:ILE:N	2.31	0.44
1:E:314:LEU:H	1:E:351:ASN:HD21	1.65	0.44
1:E:378:ASP:C	1:E:380:ILE:N	2.73	0.44
2:F:62:THR:O	2:F:66:ILE:HG13	2.17	0.44
2:F:66:ILE:HG23	2:F:233:PHE:HB2	1.99	0.44
2:J:179:SER:OG	2:J:182:ASP:OD1	2.33	0.44
2:B:48:TRP:HA	2:B:54:TRP:HB3	2.00	0.44
1:E:306:ASN:ND2	1:E:312:ILE:HD13	2.32	0.44
1:I:100:ARG:O	2:J:187:ASN:ND2	2.49	0.44
1:I:218:MET:HE2	1:I:226:GLU:OE2	2.17	0.44
3:K:254:LEU:HA	3:K:254:LEU:HD13	1.30	0.44
1:A:208:ARG:HA	1:A:208:ARG:HD2	1.51	0.44
1:A:227:LEU:HD22	1:A:227:LEU:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:239:LEU:O	3:C:240:PHE:CD2	2.70	0.44
3:C:253:TRP:HA	3:C:255:ALA:HB3	1.99	0.44
1:E:229:SER:O	1:E:230:ALA:C	2.58	0.44
2:F:33:ILE:HG22	2:F:34:VAL:N	2.31	0.44
1:I:258:TYR:CE2	2:J:166:PRO:HG3	2.52	0.44
2:J:27:PHE:CE1	3:K:139:VAL:HG13	2.52	0.44
2:J:27:PHE:CE2	2:J:31:PHE:CE2	3.04	0.44
1:A:174:THR:O	1:A:174:THR:HG23	2.17	0.44
2:B:206:ARG:HG2	3:C:184:TYR:OH	2.17	0.44
1:E:231:THR:O	1:E:235:VAL:HG23	2.17	0.44
2:F:32:VAL:HG11	3:G:254:LEU:CD1	2.47	0.44
2:F:240:ASN:O	2:F:241:GLU:C	2.60	0.44
3:K:253:TRP:HA	3:K:255:ALA:HB3	2.00	0.44
2:B:206:ARG:HD3	3:C:185:ILE:HB	2.00	0.44
3:C:80:SER:HA	3:C:85:PHE:CG	2.52	0.44
3:C:132:PHE:HD1	3:C:132:PHE:HA	1.73	0.44
3:C:173:HIS:CD2	3:C:177:PHE:CE1	3.05	0.44
1:I:304:ILE:HG22	1:I:354:LEU:HD23	1.99	0.44
3:K:106:ILE:O	3:K:110:TYR:HB2	2.17	0.44
1:A:120:LYS:HA	1:A:120:LYS:HD3	1.43	0.44
2:B:42:MET:SD	3:C:154:GLU:HG3	2.58	0.44
1:E:304:ILE:HG22	1:E:354:LEU:HD23	2.00	0.44
1:E:350:ASP:OD2	1:E:350:ASP:C	2.60	0.44
1:I:101:LYS:HD2	1:I:101:LYS:HA	1.78	0.44
2:J:106:PHE:N	2:J:106:PHE:HD2	2.16	0.44
2:J:143:PHE:CE1	2:J:147:VAL:HG21	2.53	0.44
2:J:143:PHE:O	2:J:147:VAL:HG22	2.17	0.44
2:J:176:MET:HE2	2:J:176:MET:HB3	1.78	0.44
1:A:51:ASP:O	1:A:69:GLY:HA2	2.17	0.44
1:A:172:THR:HA	2:B:171:VAL:HB	2.00	0.44
3:C:75:SER:O	3:C:76:ALA:HB3	2.18	0.44
1:E:352:SER:HB2	1:E:353:PRO:HD2	1.99	0.44
2:F:21:ILE:O	2:F:22:ASP:C	2.59	0.44
2:F:141:TYR:HB3	2:F:226:LEU:HD21	1.99	0.44
2:F:228:TYR:O	2:F:231:TRP:N	2.50	0.44
1:I:395:ASP:OD2	1:I:395:ASP:C	2.60	0.44
2:J:210:LYS:HE3	3:K:254:LEU:HB3	2.00	0.44
2:B:33:ILE:HG21	2:B:92:CYS:HA	2.00	0.44
2:B:206:ARG:NH2	3:C:188:GLY:HA3	2.33	0.44
1:E:180:LEU:HD11	2:F:180:ILE:HG23	1.99	0.44
1:E:386:ARG:HA	1:E:408:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:204:THR:HG22	2:F:205:LEU:H	1.82	0.44
1:I:230:ALA:HB2	1:I:233:ARG:CG	2.43	0.44
2:J:82:ARG:HH22	2:J:219:PHE:HZ	1.66	0.44
1:A:105:ILE:HD11	1:A:116:LEU:HD11	2.00	0.44
1:A:319:THR:HG23	1:A:320:ALA:N	2.33	0.44
2:B:44:THR:O	2:B:45:MET:HG2	2.17	0.44
3:C:131:ASN:CB	3:C:199:LEU:HD21	2.37	0.44
1:E:101:LYS:HA	1:E:101:LYS:HD2	1.80	0.44
3:G:254:LEU:O	3:G:257:ALA:CB	2.53	0.44
1:I:120:LYS:HA	1:I:120:LYS:HD3	1.63	0.44
1:I:172:THR:C	1:I:174:THR:N	2.76	0.44
1:I:304:ILE:HG22	1:I:354:LEU:CD2	2.47	0.44
3:K:246:TYR:O	3:K:249:VAL:N	2.46	0.44
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.63	0.43
1:I:145:GLN:NE2	1:I:145:GLN:CA	2.76	0.43
1:I:252:SER:HA	1:I:255:ASN:HB2	1.99	0.43
2:J:236:ARG:HH21	2:J:240:ASN:H	1.61	0.43
1:A:273:LYS:HB2	1:A:273:LYS:HZ2	1.81	0.43
2:B:33:ILE:O	2:B:34:VAL:C	2.61	0.43
2:B:75:VAL:HA	3:C:253:TRP:CH2	2.53	0.43
2:B:151:GLY:O	2:B:155:ILE:HG22	2.18	0.43
2:B:207:THR:C	2:B:209:GLY:H	2.26	0.43
3:C:63:LEU:HD12	3:C:63:LEU:HA	1.85	0.43
1:E:213:ILE:N	1:E:214:PRO:HD2	2.33	0.43
2:F:97:LEU:HA	2:F:97:LEU:HD12	1.67	0.43
2:F:135:LEU:O	2:F:139:GLY:HA2	2.19	0.43
1:I:346:LEU:HD21	1:I:364:VAL:HG13	1.99	0.43
1:A:322:VAL:HG11	1:A:376:LEU:HD11	2.00	0.43
1:E:225:ASP:C	1:E:227:LEU:N	2.73	0.43
3:G:243:PRO:O	3:G:244:LEU:HB2	2.19	0.43
2:J:206:ARG:HA	2:J:206:ARG:HD2	1.57	0.43
1:A:183:TYR:CE1	2:B:166:PRO:O	2.71	0.43
3:C:177:PHE:O	3:C:182:PRO:HD3	2.17	0.43
3:C:232:THR:HG22	3:C:234:TRP:CB	2.49	0.43
1:I:300:MET:HE1	1:I:387:PHE:CE2	2.53	0.43
2:J:197:ILE:O	2:J:199:MET:N	2.51	0.43
2:J:206:ARG:O	2:J:206:ARG:HG3	2.18	0.43
2:B:206:ARG:NH2	2:B:210:LYS:HA	2.34	0.43
1:E:108:GLN:HG3	1:E:109:LEU:N	2.33	0.43
2:F:143:PHE:O	2:F:147:VAL:HG22	2.17	0.43
2:F:210:LYS:HE3	3:G:254:LEU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:177:PHE:O	3:K:182:PRO:HD3	2.18	0.43
1:A:189:TYR:O	1:A:190:PHE:C	2.61	0.43
1:A:229:SER:C	1:A:232:ASP:H	2.22	0.43
1:A:304:ILE:HG22	1:A:354:LEU:CD2	2.49	0.43
2:B:58:ARG:HG2	2:B:58:ARG:NH2	2.23	0.43
2:B:206:ARG:HD2	2:B:206:ARG:HA	1.69	0.43
3:C:181:TYR:HA	3:C:184:TYR:CE1	2.54	0.43
3:C:184:TYR:CD2	3:C:184:TYR:C	2.96	0.43
2:F:45:MET:HE3	2:F:47:ASP:OD2	2.19	0.43
1:I:225:ASP:C	1:I:227:LEU:N	2.76	0.43
2:J:101:TRP:O	2:J:102:ILE:C	2.61	0.43
2:J:195:GLU:CG	3:K:160:HIS:CE1	2.84	0.43
2:B:236:ARG:CD	2:B:239:SER:HB3	2.48	0.43
3:C:167:THR:C	3:C:169:PHE:H	2.27	0.43
1:E:229:SER:O	1:E:232:ASP:N	2.34	0.43
2:J:38:HIS:CE1	3:K:154:GLU:HB2	2.53	0.43
2:J:65:PRO:HG2	2:J:236:ARG:HD3	2.00	0.43
3:K:178:TYR:O	3:K:182:PRO:HG2	2.19	0.43
3:K:184:TYR:CD2	3:K:184:TYR:C	2.97	0.43
1:A:137:HIS:CD2	1:A:156:TRP:CE2	3.06	0.43
2:B:39:ILE:O	2:B:43:LEU:HB2	2.18	0.43
2:B:141:TYR:HB3	2:B:226:LEU:HD21	1.99	0.43
2:B:202:LYS:HD3	3:C:181:TYR:CD2	2.54	0.43
3:C:141:TYR:CE1	3:C:188:GLY:CA	3.02	0.43
1:E:35:GLU:HB2	1:E:43:ARG:HD3	2.00	0.43
1:E:90:ASN:HB3	1:E:141:MET:HG3	2.00	0.43
2:F:33:ILE:HG21	2:F:92:CYS:HA	2.00	0.43
3:G:144:ALA:HB1	3:G:184:TYR:HB2	2.01	0.43
1:I:189:TYR:O	1:I:190:PHE:C	2.62	0.43
1:I:243:THR:OG1	2:J:129:ILE:HG21	2.19	0.43
2:B:106:PHE:CD2	2:B:106:PHE:N	2.87	0.43
2:B:222:PHE:HD2	3:C:256:LEU:HD23	1.84	0.43
1:I:195:TRP:HB3	2:J:125:VAL:HB	2.00	0.43
2:J:207:THR:O	2:J:209:GLY:N	2.49	0.43
3:K:241:VAL:N	3:K:243:PRO:HD2	2.34	0.43
1:A:314:LEU:HD23	1:A:314:LEU:HA	1.91	0.43
2:B:238:PHE:O	2:B:240:ASN:N	2.52	0.43
3:C:155:GLN:C	3:C:157:GLY:N	2.77	0.43
3:G:144:ALA:CB	3:G:184:TYR:HB2	2.48	0.43
3:G:254:LEU:HA	3:G:254:LEU:HD13	1.43	0.43
1:I:104:TYR:HA	1:I:108:GLN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:93:VAL:HG21	2:J:128:ALA:HB2	2.01	0.43
2:J:111:TRP:CD1	3:K:74:TRP:HZ3	2.36	0.43
3:C:80:SER:OG	3:C:166:ASP:HB3	2.19	0.42
3:G:130:ARG:C	3:G:132:PHE:H	2.27	0.42
1:I:240:LEU:O	1:I:244:ILE:HG23	2.18	0.42
2:J:204:THR:HG22	2:J:205:LEU:H	1.84	0.42
3:K:115:ARG:HB3	3:K:115:ARG:HE	1.58	0.42
3:K:119:LEU:O	3:K:120:ALA:C	2.62	0.42
3:K:125:ARG:HG2	3:K:129:ARG:HH12	1.84	0.42
3:K:243:PRO:O	3:K:244:LEU:HB2	2.19	0.42
3:K:250:ILE:C	3:K:252:GLY:N	2.69	0.42
1:A:45:ARG:O	1:A:78:PRO:HD3	2.19	0.42
1:A:315:GLY:CA	1:A:329:VAL:HG21	2.49	0.42
2:J:106:PHE:CD2	2:J:106:PHE:N	2.85	0.42
2:J:221:ALA:C	2:J:223:MET:N	2.72	0.42
2:J:236:ARG:O	2:J:239:SER:N	2.51	0.42
1:A:263:PRO:HG3	1:I:381:TYR:O	2.19	0.42
2:B:157:TYR:HB3	2:B:158:PRO:CD	2.50	0.42
3:C:181:TYR:CD1	3:C:184:TYR:HE1	2.37	0.42
1:E:219:VAL:HG22	1:E:224:ALA:HB2	2.01	0.42
1:E:300:MET:HE1	1:E:387:PHE:CE2	2.54	0.42
1:E:336:TYR:CD1	1:E:337:PRO:HD2	2.54	0.42
2:J:21:ILE:HD11	3:K:244:LEU:HD21	2.02	0.42
2:J:41:ALA:O	2:J:45:MET:HG2	2.18	0.42
2:J:50:PHE:O	2:J:119:VAL:HA	2.20	0.42
2:J:206:ARG:HD3	3:K:185:ILE:CB	2.49	0.42
2:B:167:LEU:HB3	2:B:181:ALA:HB2	2.01	0.42
3:C:143:TRP:HA	3:C:143:TRP:CE3	2.54	0.42
3:C:144:ALA:HB1	3:C:184:TYR:HB2	1.99	0.42
1:I:375:ARG:O	1:I:378:ASP:HB2	2.19	0.42
1:A:60:LYS:O	1:A:61:ILE:C	2.62	0.42
1:A:221:ALA:O	1:A:222:GLY:O	2.37	0.42
3:C:93:LEU:O	3:C:96:GLU:HG2	2.19	0.42
2:F:50:PHE:O	2:F:119:VAL:HA	2.20	0.42
1:A:137:HIS:CD2	1:A:156:TRP:CD1	3.07	0.42
2:B:38:HIS:CD2	2:B:42:MET:CE	3.03	0.42
2:B:111:TRP:CZ3	3:C:159:TRP:CE3	3.08	0.42
2:F:103:ASN:CG	3:G:154:GLU:HB3	2.45	0.42
3:G:125:ARG:HG2	3:G:129:ARG:HH12	1.85	0.42
3:G:131:ASN:HB2	3:G:244:LEU:HD12	2.01	0.42
1:I:188:THR:HA	2:J:163:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:231:THR:O	1:I:235:VAL:HG23	2.19	0.42
3:K:194:TYR:CZ	3:K:198:ARG:HG2	2.55	0.42
1:A:270:ARG:HG2	1:A:270:ARG:HH11	1.84	0.42
1:A:355:ALA:HB3	1:A:358:GLU:OE1	2.19	0.42
2:B:68:LEU:HA	2:B:68:LEU:HD12	1.78	0.42
1:E:189:TYR:O	1:E:190:PHE:C	2.62	0.42
1:E:258:TYR:N	1:E:259:PRO:CD	2.82	0.42
1:I:183:TYR:CE1	2:J:166:PRO:O	2.71	0.42
2:J:18:SER:HB2	3:K:236:MET:HE1	2.00	0.42
2:J:98:LEU:O	2:J:102:ILE:HG13	2.19	0.42
3:K:63:LEU:HD12	3:K:63:LEU:HA	1.84	0.42
1:A:209:ARG:HB2	1:A:210:PRO:HD2	2.01	0.42
1:E:162:SER:O	1:E:165:GLU:HB2	2.20	0.42
2:F:39:ILE:HG13	3:G:149:ALA:HB1	2.01	0.42
2:F:206:ARG:HA	2:F:206:ARG:HD2	1.67	0.42
2:J:80:TRP:CZ3	2:J:84:ARG:HG3	2.55	0.42
2:J:222:PHE:HD2	3:K:256:LEU:HD23	1.85	0.42
2:F:78:TYR:CD1	3:G:253:TRP:CE3	3.08	0.42
2:F:83:TYR:OH	3:G:246:TYR:HE2	2.03	0.42
2:F:194:PRO:HD3	3:G:160:HIS:HB3	2.00	0.42
3:G:106:ILE:O	3:G:110:TYR:HB2	2.20	0.42
2:J:167:LEU:O	2:J:180:ILE:HB	2.19	0.42
3:K:145:ILE:HD13	3:K:184:TYR:CE2	2.54	0.42
2:B:8:VAL:HB	3:C:125:ARG:HH12	1.84	0.42
1:E:183:TYR:HE1	2:F:166:PRO:O	2.03	0.42
2:F:143:PHE:CE1	2:F:147:VAL:HG21	2.55	0.42
1:I:245:LEU:O	1:I:249:MET:HG2	2.20	0.42
3:K:248:PHE:O	3:K:248:PHE:CD1	2.73	0.42
1:A:112:ARG:HH22	1:I:384:ASP:CG	2.28	0.41
2:B:55:LYS:HD2	2:B:60:TRP:CZ2	2.55	0.41
3:C:234:TRP:CA	3:C:237:GLU:HG3	2.38	0.41
1:E:314:LEU:HD13	1:E:346:LEU:HD11	2.02	0.41
2:F:55:LYS:HD2	2:F:60:TRP:CZ2	2.55	0.41
1:I:52:LEU:HD22	1:I:69:GLY:HA3	2.02	0.41
1:A:230:ALA:HB2	1:A:233:ARG:CG	2.45	0.41
1:A:292:ARG:HA	1:A:292:ARG:HD2	1.84	0.41
1:E:45:ARG:O	1:E:78:PRO:HD3	2.19	0.41
1:I:386:ARG:HA	1:I:408:PRO:HA	2.02	0.41
1:A:120:LYS:HG3	1:A:274:PRO:CB	2.48	0.41
1:A:348:VAL:HG22	1:A:351:ASN:HB2	2.03	0.41
2:B:194:PRO:HD3	3:C:160:HIS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:ILE:HD11	2:F:21:ILE:HD13	2.01	0.41
2:F:68:LEU:HB3	2:F:152:TRP:HZ2	1.84	0.41
2:F:179:SER:OG	2:F:182:ASP:OD1	2.38	0.41
3:G:131:ASN:ND2	3:G:131:ASN:N	2.62	0.41
1:I:97:VAL:HG21	1:I:136:TRP:CG	2.55	0.41
2:J:151:GLY:O	2:J:155:ILE:HG22	2.20	0.41
2:J:240:ASN:O	2:J:243:PHE:HD1	2.03	0.41
3:K:195:ALA:HB1	3:K:202:PHE:CD1	2.55	0.41
1:A:314:LEU:H	1:A:351:ASN:HD21	1.67	0.41
2:B:55:LYS:HD2	2:B:60:TRP:CE2	2.55	0.41
2:B:66:ILE:HG23	2:B:233:PHE:HB2	2.02	0.41
2:B:240:ASN:O	2:B:243:PHE:HD1	2.04	0.41
3:G:181:TYR:HA	3:G:184:TYR:CD1	2.56	0.41
1:I:314:LEU:HD23	1:I:314:LEU:HA	1.90	0.41
1:I:401:GLN:HE21	1:I:401:GLN:HB2	1.46	0.41
2:J:202:LYS:NZ	2:J:206:ARG:HB3	2.36	0.41
3:K:194:TYR:O	3:K:198:ARG:HB2	2.20	0.41
3:C:55:LEU:HD23	3:C:55:LEU:HA	1.77	0.41
3:C:106:ILE:O	3:C:110:TYR:HB2	2.20	0.41
2:F:71:PHE:O	2:F:75:VAL:HG13	2.20	0.41
3:G:141:TYR:CE1	3:G:188:GLY:CA	3.03	0.41
2:J:206:ARG:NH2	3:K:188:GLY:HA3	2.35	0.41
3:K:239:LEU:O	3:K:240:PHE:CD2	2.74	0.41
1:A:281:THR:HB	1:A:401:GLN:OE1	2.21	0.41
2:F:27:PHE:CE2	2:F:31:PHE:CE2	3.09	0.41
2:J:178:MET:HE2	2:J:178:MET:HB3	1.82	0.41
1:A:114:VAL:O	1:A:114:VAL:HG23	2.18	0.41
3:C:115:ARG:HB3	3:C:115:ARG:HE	1.57	0.41
1:E:100:ARG:O	2:F:187:ASN:ND2	2.52	0.41
1:E:336:TYR:CG	1:E:337:PRO:HD2	2.56	0.41
3:G:57:ILE:HG23	3:G:58:TYR:CD1	2.56	0.41
2:J:58:ARG:HG2	2:J:58:ARG:NH2	2.27	0.41
2:J:231:TRP:O	2:J:231:TRP:HD1	2.04	0.41
1:A:36:LYS:HE2	1:A:373:VAL:O	2.20	0.41
1:A:58:LYS:HG3	1:A:158:THR:HB	2.03	0.41
2:B:43:LEU:HD12	2:B:43:LEU:HA	1.78	0.41
2:B:125:VAL:O	2:B:126:PRO:C	2.61	0.41
2:B:197:ILE:O	2:B:197:ILE:CG1	2.67	0.41
2:B:238:PHE:O	2:B:239:SER:C	2.64	0.41
3:C:134:HIS:CE1	3:C:195:ALA:HB2	2.56	0.41
3:G:80:SER:HA	3:G:85:PHE:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:229:SER:O	1:I:230:ALA:C	2.64	0.41
1:I:391:LEU:HB2	1:I:403:VAL:HG22	2.03	0.41
2:J:69:VAL:HG13	2:J:152:TRP:NE1	2.35	0.41
1:A:218:MET:HE2	1:A:226:GLU:OE2	2.21	0.41
1:A:269:MET:HG3	1:I:386:ARG:NH1	2.34	0.41
2:B:165:ALA:C	2:B:167:LEU:H	2.28	0.41
2:B:202:LYS:NZ	2:B:206:ARG:HB3	2.36	0.41
1:E:225:ASP:O	1:E:226:GLU:C	2.64	0.41
3:G:107:LEU:CD1	3:G:190:ALA:HB2	2.50	0.41
1:I:88:PHE:HD2	1:I:143:ASN:HD22	1.69	0.41
1:I:208:ARG:HA	1:I:208:ARG:HD2	1.65	0.41
1:I:305:THR:HB	1:I:359:THR:CB	2.50	0.41
1:I:348:VAL:HG22	1:I:351:ASN:HB2	2.03	0.41
2:J:141:TYR:O	2:J:142:LEU:C	2.64	0.41
3:K:141:TYR:CD1	3:K:188:GLY:HA2	2.55	0.41
3:K:181:TYR:CD1	3:K:184:TYR:HE1	2.39	0.41
1:A:272:MET:CE	1:A:272:MET:CA	2.97	0.41
2:F:58:ARG:HG2	2:F:58:ARG:NH2	2.21	0.41
2:F:230:MET:HE3	2:F:231:TRP:HA	2.03	0.41
3:G:63:LEU:HD12	3:G:63:LEU:HA	1.89	0.41
2:J:221:ALA:O	2:J:223:MET:N	2.53	0.41
2:B:38:HIS:CD2	2:B:42:MET:HE1	2.55	0.40
2:B:68:LEU:HB3	2:B:152:TRP:HZ2	1.87	0.40
1:E:240:LEU:O	1:E:244:ILE:HG23	2.21	0.40
2:F:116:ILE:C	2:F:118:PHE:H	2.28	0.40
3:G:236:MET:HG3	3:G:237:GLU:N	2.36	0.40
1:I:81:VAL:O	1:I:82:ASP:C	2.64	0.40
1:I:227:LEU:HD22	1:I:227:LEU:H	1.86	0.40
2:J:34:VAL:HG22	2:J:95:GLY:CA	2.51	0.40
3:K:57:ILE:HG23	3:K:58:TYR:CD1	2.56	0.40
2:B:135:LEU:O	2:B:139:GLY:HA2	2.21	0.40
2:F:76:GLN:NE2	2:F:229:PHE:CZ	2.90	0.40
3:G:155:GLN:O	3:G:156:ASP:C	2.63	0.40
3:G:253:TRP:HA	3:G:255:ALA:HB3	2.03	0.40
1:I:270:ARG:HG2	1:I:270:ARG:NH1	2.36	0.40
2:B:69:VAL:O	2:B:70:THR:C	2.64	0.40
1:E:304:ILE:HG22	1:E:354:LEU:CD2	2.52	0.40
2:F:42:MET:SD	3:G:154:GLU:HG3	2.61	0.40
2:J:42:MET:HG2	2:J:198:ARG:NH2	2.31	0.40
3:K:113:LYS:HE3	3:K:113:LYS:HA	2.04	0.40
1:A:112:ARG:NH2	1:I:384:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:GLU:O	2:B:206:ARG:N	2.46	0.40
2:B:228:TYR:C	2:B:230:MET:N	2.79	0.40
1:E:120:LYS:HG3	1:E:274:PRO:CB	2.49	0.40
1:E:245:LEU:HD13	1:E:249:MET:CG	2.52	0.40
1:I:229:SER:O	1:I:232:ASP:N	2.35	0.40
2:B:106:PHE:N	2:B:106:PHE:HD2	2.20	0.40
2:B:111:TRP:O	3:C:74:TRP:CH2	2.75	0.40
2:B:165:ALA:C	2:B:167:LEU:N	2.77	0.40
2:B:240:ASN:O	2:B:241:GLU:C	2.65	0.40
2:F:207:THR:O	2:F:210:LYS:N	2.53	0.40
2:F:210:LYS:HA	2:F:210:LYS:HD2	1.92	0.40
2:J:33:ILE:HG22	2:J:34:VAL:N	2.37	0.40
2:J:181:ALA:O	2:J:182:ASP:C	2.64	0.40
2:J:207:THR:O	2:J:210:LYS:N	2.51	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:HIS:CE1	2:B:11:HIS:NE2[7_556]	2.03	0.17
2:B:11:HIS:NE2	2:B:11:HIS:NE2[7_556]	2.14	0.06
1:A:60:LYS:NZ	1:E:338:GLU:OE2[4_455]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	380/382 (100%)	334 (88%)	34 (9%)	12 (3%)	3	11
1	E	380/382 (100%)	336 (88%)	33 (9%)	11 (3%)	3	13
1	I	380/382 (100%)	327 (86%)	42 (11%)	11 (3%)	3	13
2	B	236/247 (96%)	173 (73%)	42 (18%)	21 (9%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	236/247 (96%)	168 (71%)	44 (19%)	24 (10%)	0	1
2	J	236/247 (96%)	166 (70%)	48 (20%)	22 (9%)	0	1
3	C	184/289 (64%)	147 (80%)	25 (14%)	12 (6%)	1	3
3	G	184/289 (64%)	146 (79%)	27 (15%)	11 (6%)	1	3
3	K	184/289 (64%)	145 (79%)	28 (15%)	11 (6%)	1	3
All	All	2400/2754 (87%)	1942 (81%)	323 (14%)	135 (6%)	1	4

All (135) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	220	ASP
1	A	224	ALA
1	A	225	ASP
1	A	288	ASP
2	B	45	MET
2	B	194	PRO
2	B	196	TYR
2	B	197	ILE
2	B	200	VAL
2	B	205	LEU
2	B	214	PRO
2	B	215	VAL
2	B	218	PHE
2	B	222	PHE
2	B	231	TRP
3	C	46	LEU
3	C	76	ALA
3	C	255	ALA
1	E	220	ASP
1	E	224	ALA
1	E	225	ASP
1	E	288	ASP
2	F	45	MET
2	F	194	PRO
2	F	196	TYR
2	F	197	ILE
2	F	200	VAL
2	F	205	LEU
2	F	214	PRO

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Mol	Chain	Res	Type
2	F	215	VAL
2	F	218	PHE
2	F	222	PHE
2	F	231	TRP
3	G	46	LEU
3	G	76	ALA
3	G	255	ALA
1	I	36	LYS
1	I	220	ASP
1	I	224	ALA
1	I	225	ASP
1	I	288	ASP
2	J	45	MET
2	J	194	PRO
2	J	196	TYR
2	J	197	ILE
2	J	200	VAL
2	J	205	LEU
2	J	214	PRO
2	J	215	VAL
2	J	218	PHE
2	J	222	PHE
2	J	231	TRP
3	K	46	LEU
3	K	76	ALA
3	K	255	ALA
1	A	145	GLN
1	A	147	GLY
1	A	308	GLY
2	B	192	GLY
2	B	239	SER
3	C	235	PHE
1	E	36	LYS
1	E	145	GLN
1	E	147	GLY
2	F	192	GLY
2	F	239	SER
3	G	116	ASP
3	G	123	THR
3	G	127	GLU
3	G	235	PHE
3	G	240	PHE

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Mol	Chain	Res	Type
1	I	145	GLN
1	I	147	GLY
1	I	308	GLY
2	J	239	SER
3	K	235	PHE
3	K	240	PHE
1	A	39	ALA
1	A	222	GLY
2	B	9	ARG
2	B	236	ARG
3	C	116	ASP
3	C	240	PHE
2	F	70	THR
2	F	236	ARG
2	F	237	TRP
3	G	117	ARG
2	J	9	ARG
2	J	229	PHE
2	J	236	ARG
2	J	237	TRP
3	K	116	ASP
3	K	123	THR
1	A	377	SER
2	B	237	TRP
3	C	117	ARG
3	C	127	GLU
1	E	39	ALA
1	E	308	GLY
2	F	9	ARG
2	F	42	MET
3	G	131	ASN
1	I	39	ALA
2	J	70	THR
2	J	192	GLY
3	K	127	GLU
3	K	151	TYR
2	B	206	ARG
2	B	243	PHE
1	E	377	SER
2	F	229	PHE
2	F	230	MET
1	I	310	SER

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Mol	Chain	Res	Type
2	J	42	MET
3	K	117	ARG
3	C	123	THR
3	C	151	TYR
3	C	234	TRP
1	E	310	SER
2	F	34	VAL
2	F	209	GLY
2	J	243	PHE
2	B	193	THR
2	B	203	GLY
2	B	213	ALA
3	C	242	ALA
1	I	222	GLY
2	J	193	THR
2	F	193	THR
3	G	242	ALA
3	K	242	ALA
2	F	203	GLY
2	J	203	GLY
1	A	310	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	323/323 (100%)	245 (76%)	78 (24%)	1	2
1	E	323/323 (100%)	243 (75%)	80 (25%)	1	2
1	I	323/323 (100%)	246 (76%)	77 (24%)	1	3
2	B	203/210 (97%)	153 (75%)	50 (25%)	1	2
2	F	203/210 (97%)	151 (74%)	52 (26%)	0	2
2	J	203/210 (97%)	154 (76%)	49 (24%)	1	2
3	C	161/237 (68%)	118 (73%)	43 (27%)	0	1
3	G	161/237 (68%)	120 (74%)	41 (26%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	161/237 (68%)	118 (73%)	43 (27%)	0	1
All	All	2061/2310 (89%)	1548 (75%)	513 (25%)	0	2

All (513) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	THR
1	A	52	LEU
1	A	56	LYS
1	A	59	VAL
1	A	60	LYS
1	A	64	THR
1	A	65	VAL
1	A	73	VAL
1	A	75	GLU
1	A	80	THR
1	A	86	VAL
1	A	89	LEU
1	A	93	MET
1	A	101	LYS
1	A	105	ILE
1	A	112	ARG
1	A	116	LEU
1	A	117	GLU
1	A	118	ILE
1	A	120	LYS
1	A	121	THR
1	A	135	ASP
1	A	138	VAL
1	A	140	THR
1	A	145	GLN
1	A	164	SER
1	A	174	THR
1	A	176	GLN
1	A	177	THR
1	A	180	LEU
1	A	182	ASN
1	A	185	GLU
1	A	208	ARG
1	A	216	LEU
1	A	219	VAL
1	A	223	ARG

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Mol	Chain	Res	Type
1	A	227	LEU
1	A	228	VAL
1	A	240	LEU
1	A	244	ILE
1	A	245	LEU
1	A	249	MET
1	A	251	MET
1	A	253	SER
1	A	261	THR
1	A	269	MET
1	A	270	ARG
1	A	273	LYS
1	A	276	GLU
1	A	281	THR
1	A	284	VAL
1	A	286	VAL
1	A	287	GLU
1	A	292	ARG
1	A	298	MET
1	A	299	ARG
1	A	305	THR
1	A	307	HIS
1	A	309	ASN
1	A	312	ILE
1	A	314	LEU
1	A	322	VAL
1	A	329	VAL
1	A	331	LYS
1	A	334	THR
1	A	338	GLU
1	A	346	LEU
1	A	348	VAL
1	A	351	ASN
1	A	359	THR
1	A	360	ARG
1	A	362	VAL
1	A	379	ILE
1	A	385	SER
1	A	401	GLN
1	A	402	VAL
1	A	403	VAL
1	A	406	ASP

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Mol	Chain	Res	Type
2	B	11	HIS
2	B	15	VAL
2	B	16	GLN
2	B	21	ILE
2	B	29	VAL
2	B	39	ILE
2	B	43	LEU
2	B	47	ASP
2	B	49	ASP
2	B	58	ARG
2	B	59	LEU
2	B	63	VAL
2	B	68	LEU
2	B	70	THR
2	B	75	VAL
2	B	76	GLN
2	B	84	ARG
2	B	90	THR
2	B	97	LEU
2	B	108	PHE
2	B	116	ILE
2	B	117	ASN
2	B	129	ILE
2	B	135	LEU
2	B	136	MET
2	B	138	SER
2	B	144	THR
2	B	155	ILE
2	B	164	ILE
2	B	169	VAL
2	B	171	VAL
2	B	190	ARG
2	B	197	ILE
2	B	198	ARG
2	B	201	GLU
2	B	202	LYS
2	B	204	THR
2	B	205	LEU
2	B	207	THR
2	B	211	ASP
2	B	214	PRO
2	B	220	SER

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Mol	Chain	Res	Type
2	B	225	ILE
2	B	226	LEU
2	B	228	TYR
2	B	233	PHE
2	B	234	ILE
2	B	236	ARG
2	B	238	PHE
2	B	243	PHE
3	C	47	ASP
3	C	50	TRP
3	C	51	LEU
3	C	60	VAL
3	C	63	LEU
3	C	93	LEU
3	C	94	TYR
3	C	103	THR
3	C	106	ILE
3	C	107	LEU
3	C	113	LYS
3	C	115	ARG
3	C	118	ASN
3	C	122	LEU
3	C	125	ARG
3	C	128	LEU
3	C	129	ARG
3	C	130	ARG
3	C	131	ASN
3	C	132	PHE
3	C	138	LEU
3	C	145	ILE
3	C	158	THR
3	C	162	THR
3	C	163	ILE
3	C	164	VAL
3	C	165	ARG
3	C	180	SER
3	C	183	ILE
3	C	185	ILE
3	C	198	ARG
3	C	232	THR
3	C	235	PHE
3	C	236	MET

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Mol	Chain	Res	Type
3	C	237	GLU
3	C	238	GLU
3	C	239	LEU
3	C	245	HIS
3	C	250	ILE
3	C	254	LEU
3	C	256	LEU
3	C	258	VAL
3	C	259	MET
1	E	46	THR
1	E	52	LEU
1	E	56	LYS
1	E	59	VAL
1	E	60	LYS
1	E	64	THR
1	E	65	VAL
1	E	73	VAL
1	E	75	GLU
1	E	80	THR
1	E	86	VAL
1	E	89	LEU
1	E	93	MET
1	E	105	ILE
1	E	112	ARG
1	E	116	LEU
1	E	117	GLU
1	E	118	ILE
1	E	120	LYS
1	E	121	THR
1	E	135	ASP
1	E	137	HIS
1	E	140	THR
1	E	141	MET
1	E	145	GLN
1	E	164	SER
1	E	174	THR
1	E	176	GLN
1	E	177	THR
1	E	180	LEU
1	E	182	ASN
1	E	185	GLU
1	E	208	ARG

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Mol	Chain	Res	Type
1	E	216	LEU
1	E	219	VAL
1	E	223	ARG
1	E	227	LEU
1	E	228	VAL
1	E	240	LEU
1	E	244	ILE
1	E	245	LEU
1	E	249	MET
1	E	251	MET
1	E	262	ILE
1	E	269	MET
1	E	270	ARG
1	E	272	MET
1	E	273	LYS
1	E	276	GLU
1	E	277	LEU
1	E	281	THR
1	E	284	VAL
1	E	286	VAL
1	E	287	GLU
1	E	292	ARG
1	E	298	MET
1	E	299	ARG
1	E	305	THR
1	E	309	ASN
1	E	312	ILE
1	E	314	LEU
1	E	322	VAL
1	E	329	VAL
1	E	331	LYS
1	E	334	THR
1	E	338	GLU
1	E	346	LEU
1	E	348	VAL
1	E	351	ASN
1	E	359	THR
1	E	360	ARG
1	E	361	THR
1	E	362	VAL
1	E	364	VAL
1	E	379	ILE

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Mol	Chain	Res	Type
1	E	385	SER
1	E	401	GLN
1	E	402	VAL
1	E	403	VAL
1	E	406	ASP
2	F	11	HIS
2	F	15	VAL
2	F	16	GLN
2	F	21	ILE
2	F	29	VAL
2	F	39	ILE
2	F	43	LEU
2	F	47	ASP
2	F	58	ARG
2	F	59	LEU
2	F	63	VAL
2	F	68	LEU
2	F	69	VAL
2	F	70	THR
2	F	75	VAL
2	F	76	GLN
2	F	84	ARG
2	F	90	THR
2	F	97	LEU
2	F	108	PHE
2	F	116	ILE
2	F	117	ASN
2	F	129	ILE
2	F	135	LEU
2	F	137	LEU
2	F	138	SER
2	F	144	THR
2	F	155	ILE
2	F	164	ILE
2	F	169	VAL
2	F	171	VAL
2	F	172	GLU
2	F	189	VAL
2	F	190	ARG
2	F	197	ILE
2	F	198	ARG
2	F	201	GLU

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Mol	Chain	Res	Type
2	F	202	LYS
2	F	204	THR
2	F	205	LEU
2	F	207	THR
2	F	211	ASP
2	F	214	PRO
2	F	220	SER
2	F	225	ILE
2	F	226	LEU
2	F	228	TYR
2	F	233	PHE
2	F	234	ILE
2	F	236	ARG
2	F	238	PHE
2	F	243	PHE
3	G	47	ASP
3	G	50	TRP
3	G	51	LEU
3	G	60	VAL
3	G	63	LEU
3	G	93	LEU
3	G	94	TYR
3	G	103	THR
3	G	106	ILE
3	G	107	LEU
3	G	113	LYS
3	G	115	ARG
3	G	118	ASN
3	G	122	LEU
3	G	125	ARG
3	G	128	LEU
3	G	129	ARG
3	G	131	ASN
3	G	132	PHE
3	G	138	LEU
3	G	145	ILE
3	G	158	THR
3	G	162	THR
3	G	163	ILE
3	G	164	VAL
3	G	165	ARG
3	G	185	ILE

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Mol	Chain	Res	Type
3	G	196	LYS
3	G	198	ARG
3	G	232	THR
3	G	235	PHE
3	G	236	MET
3	G	237	GLU
3	G	238	GLU
3	G	239	LEU
3	G	245	HIS
3	G	250	ILE
3	G	254	LEU
3	G	256	LEU
3	G	258	VAL
3	G	259	MET
1	I	46	THR
1	I	52	LEU
1	I	56	LYS
1	I	59	VAL
1	I	60	LYS
1	I	64	THR
1	I	65	VAL
1	I	73	VAL
1	I	75	GLU
1	I	80	THR
1	I	86	VAL
1	I	89	LEU
1	I	93	MET
1	I	105	ILE
1	I	112	ARG
1	I	116	LEU
1	I	117	GLU
1	I	118	ILE
1	I	120	LYS
1	I	121	THR
1	I	135	ASP
1	I	137	HIS
1	I	138	VAL
1	I	140	THR
1	I	145	GLN
1	I	164	SER
1	I	170	VAL
1	I	174	THR

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Mol	Chain	Res	Type
1	I	176	GLN
1	I	177	THR
1	I	180	LEU
1	I	182	ASN
1	I	185	GLU
1	I	216	LEU
1	I	219	VAL
1	I	223	ARG
1	I	227	LEU
1	I	228	VAL
1	I	240	LEU
1	I	244	ILE
1	I	245	LEU
1	I	249	MET
1	I	251	MET
1	I	261	THR
1	I	269	MET
1	I	270	ARG
1	I	272	MET
1	I	273	LYS
1	I	276	GLU
1	I	277	LEU
1	I	281	THR
1	I	284	VAL
1	I	286	VAL
1	I	287	GLU
1	I	292	ARG
1	I	299	ARG
1	I	305	THR
1	I	307	HIS
1	I	309	ASN
1	I	312	ILE
1	I	314	LEU
1	I	322	VAL
1	I	329	VAL
1	I	331	LYS
1	I	334	THR
1	I	338	GLU
1	I	346	LEU
1	I	348	VAL
1	I	351	ASN
1	I	359	THR

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Mol	Chain	Res	Type
1	I	361	THR
1	I	362	VAL
1	I	379	ILE
1	I	401	GLN
1	I	402	VAL
1	I	403	VAL
1	I	406	ASP
2	J	11	HIS
2	J	15	VAL
2	J	16	GLN
2	J	21	ILE
2	J	29	VAL
2	J	43	LEU
2	J	47	ASP
2	J	58	ARG
2	J	63	VAL
2	J	68	LEU
2	J	69	VAL
2	J	70	THR
2	J	75	VAL
2	J	84	ARG
2	J	90	THR
2	J	97	LEU
2	J	108	PHE
2	J	116	ILE
2	J	126	PRO
2	J	129	ILE
2	J	135	LEU
2	J	136	MET
2	J	138	SER
2	J	144	THR
2	J	152	TRP
2	J	155	ILE
2	J	164	ILE
2	J	169	VAL
2	J	171	VAL
2	J	172	GLU
2	J	190	ARG
2	J	197	ILE
2	J	198	ARG
2	J	201	GLU
2	J	202	LYS

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Mol	Chain	Res	Type
2	J	204	THR
2	J	205	LEU
2	J	207	THR
2	J	211	ASP
2	J	214	PRO
2	J	220	SER
2	J	225	ILE
2	J	226	LEU
2	J	228	TYR
2	J	233	PHE
2	J	234	ILE
2	J	236	ARG
2	J	238	PHE
2	J	243	PHE
3	K	47	ASP
3	K	50	TRP
3	K	51	LEU
3	K	60	VAL
3	K	63	LEU
3	K	93	LEU
3	K	94	TYR
3	K	103	THR
3	K	106	ILE
3	K	107	LEU
3	K	113	LYS
3	K	115	ARG
3	K	118	ASN
3	K	122	LEU
3	K	125	ARG
3	K	128	LEU
3	K	129	ARG
3	K	131	ASN
3	K	132	PHE
3	K	138	LEU
3	K	145	ILE
3	K	158	THR
3	K	162	THR
3	K	163	ILE
3	K	164	VAL
3	K	165	ARG
3	K	180	SER
3	K	183	ILE

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Mol	Chain	Res	Type
3	K	185	ILE
3	K	196	LYS
3	K	198	ARG
3	K	232	THR
3	K	235	PHE
3	K	236	MET
3	K	238	GLU
3	K	239	LEU
3	K	245	HIS
3	K	250	ILE
3	K	251	PHE
3	K	254	LEU
3	K	256	LEU
3	K	258	VAL
3	K	259	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	143	ASN
1	A	145	GLN
1	A	168	ASN
1	A	182	ASN
1	A	192	HIS
1	A	265	GLN
1	A	306	ASN
1	A	309	ASN
1	A	351	ASN
1	A	401	GLN
2	B	76	GLN
2	B	103	ASN
2	B	117	ASN
2	B	187	ASN
3	C	118	ASN
3	C	131	ASN
3	C	155	GLN
1	E	62	ASN
1	E	137	HIS
1	E	143	ASN
1	E	145	GLN
1	E	182	ASN

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Mol	Chain	Res	Type
1	E	187	ASN
1	E	192	HIS
1	E	265	GLN
1	E	306	ASN
1	E	309	ASN
1	E	351	ASN
1	E	401	GLN
2	F	103	ASN
2	F	117	ASN
3	G	118	ASN
3	G	131	ASN
3	G	155	GLN
3	G	231	HIS
1	I	62	ASN
1	I	137	HIS
1	I	143	ASN
1	I	145	GLN
1	I	168	ASN
1	I	182	ASN
1	I	187	ASN
1	I	192	HIS
1	I	265	GLN
1	I	306	ASN
1	I	309	ASN
1	I	351	ASN
1	I	401	GLN
2	J	76	GLN
2	J	103	ASN
2	J	117	ASN
2	J	187	ASN
3	K	131	ASN
3	K	155	GLN
3	K	231	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 11 are monoatomic - leaving 3 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	$\# Z > 2$
6	CUA	A	3	1	0,1,1	-	-	-		
6	CUA	I	600	1	0,1,1	-	-	-		
6	CUA	E	500	1	0,1,1	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	A	382/382 (100%)	0.43	19 (4%) 34 26	65, 70, 73, 76	0
1	E	382/382 (100%)	0.56	25 (6%) 25 18	66, 70, 73, 76	0
1	I	382/382 (100%)	0.70	32 (8%) 17 12	66, 70, 73, 76	0
2	B	238/247 (96%)	1.14	47 (19%) 3 2	66, 70, 74, 78	0
2	F	238/247 (96%)	0.94	33 (13%) 6 5	66, 70, 74, 78	0
2	J	238/247 (96%)	0.94	34 (14%) 6 5	66, 70, 74, 78	0
3	C	188/289 (65%)	1.51	57 (30%) 1 1	67, 70, 72, 73	0
3	G	188/289 (65%)	1.59	61 (32%) 1 1	67, 70, 72, 73	0
3	K	188/289 (65%)	1.50	53 (28%) 1 1	67, 70, 72, 73	0
All	All	2424/2754 (88%)	0.92	361 (14%) 5 4	65, 70, 73, 78	0

All (361) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	203	ALA	10.8
2	F	194	PRO	9.6
3	G	251	PHE	9.5
3	K	251	PHE	9.2
2	B	194	PRO	9.1
1	E	270	ARG	9.0
2	F	200	VAL	8.9
3	C	259	MET	8.9
3	G	203	ALA	8.3
3	C	193	ILE	8.1
3	K	203	ALA	7.9
2	J	194	PRO	7.6
3	C	251	PHE	7.6
1	E	267	GLY	7.4
2	B	109	TRP	7.0

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Mol	Chain	Res	Type	RSRZ
1	E	272	MET	7.0
1	E	275	LEU	6.9
1	E	269	MET	6.5
3	K	258	VAL	6.4
2	J	237	TRP	6.4
3	C	258	VAL	6.3
1	E	274	PRO	6.3
3	K	199	LEU	6.2
1	E	271	GLY	6.2
3	G	233	PHE	6.0
2	B	200	VAL	6.0
2	B	231	TRP	5.8
3	C	235	PHE	5.8
3	K	259	MET	5.7
1	E	266	ALA	5.6
3	K	193	ILE	5.6
3	G	192	PHE	5.4
2	B	244	LEU	5.3
2	B	193	THR	5.3
3	G	241	VAL	5.2
3	K	45	LEU	5.1
1	I	221	ALA	5.0
2	J	48	TRP	5.0
3	K	181	TYR	5.0
3	G	259	MET	4.9
2	J	231	TRP	4.9
2	F	244	LEU	4.8
3	K	84	GLU	4.7
3	G	193	ILE	4.7
2	B	195	GLU	4.6
2	B	196	TYR	4.6
3	C	192	PHE	4.6
3	C	202	PHE	4.5
3	G	256	LEU	4.5
3	C	233	PHE	4.4
1	A	147	GLY	4.4
3	K	241	VAL	4.4
1	E	268	THR	4.4
3	G	258	VAL	4.4
1	I	271	GLY	4.4
2	J	195	GLU	4.3
2	B	113	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
3	K	198	ARG	4.3
2	B	205	LEU	4.3
3	K	195	ALA	4.3
1	E	273	LYS	4.2
3	K	196	LYS	4.2
1	I	210	PRO	4.2
3	G	164	VAL	4.2
3	K	248	PHE	4.1
3	G	73	GLY	4.1
3	G	45	LEU	4.0
3	C	255	ALA	4.0
3	G	156	ASP	3.9
2	F	201	GLU	3.9
2	F	231	TRP	3.9
3	K	192	PHE	3.9
3	C	256	LEU	3.9
3	K	201	PHE	3.9
3	G	172	SER	3.9
3	C	117	ARG	3.8
2	B	218	PHE	3.8
3	G	242	ALA	3.8
3	K	202	PHE	3.8
3	K	172	SER	3.7
3	G	248	PHE	3.7
3	C	159	TRP	3.7
3	G	197	THR	3.7
3	K	233	PHE	3.7
3	C	127	GLU	3.7
1	I	192	HIS	3.6
2	F	138	SER	3.6
3	G	252	GLY	3.6
1	I	381	TYR	3.5
3	K	235	PHE	3.5
2	F	227	ILE	3.5
2	B	198	ARG	3.5
3	G	201	PHE	3.5
2	F	226	LEU	3.5
3	K	244	LEU	3.5
3	G	110	TYR	3.4
3	C	232	THR	3.4
2	F	218	PHE	3.4
2	B	169	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	201	GLU	3.4
1	E	221	ALA	3.4
1	I	307	HIS	3.4
2	J	58	ARG	3.4
3	C	257	ALA	3.4
1	I	326	ASP	3.4
3	G	199	LEU	3.3
3	C	253	TRP	3.3
3	C	241	VAL	3.3
2	B	192	GLY	3.3
3	C	154	GLU	3.3
2	B	186	TYR	3.3
2	J	196	TYR	3.3
3	G	77	GLY	3.3
3	G	173	HIS	3.3
3	G	198	ARG	3.3
2	F	7	ALA	3.3
2	B	226	LEU	3.3
1	I	270	ARG	3.3
2	F	195	GLU	3.2
3	K	191	ALA	3.2
2	J	226	LEU	3.2
3	K	194	TYR	3.2
1	E	148	GLY	3.2
1	I	273	LYS	3.2
3	G	170	THR	3.2
3	C	45	LEU	3.2
2	B	221	ALA	3.2
1	A	297	ALA	3.1
2	F	225	ILE	3.1
2	J	198	ARG	3.1
2	B	203	GLY	3.1
3	C	175	ILE	3.1
3	K	176	GLU	3.1
2	F	193	THR	3.1
3	G	202	PHE	3.0
1	E	414	MET	3.0
2	J	213	ALA	3.0
1	A	212	PHE	3.0
1	I	269	MET	3.0
2	F	223	MET	3.0
3	C	248	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	81	GLU	3.0
1	A	266	ALA	3.0
3	C	164	VAL	3.0
3	C	234	TRP	3.0
2	B	46	GLY	3.0
2	J	46	GLY	3.0
3	G	257	ALA	3.0
3	G	181	TYR	2.9
1	E	230	ALA	2.9
3	K	82	ALA	2.9
3	C	78	LEU	2.9
2	F	46	GLY	2.9
3	G	74	TRP	2.9
3	G	188	GLY	2.9
2	F	15	VAL	2.9
2	J	12	ALA	2.9
1	E	174	THR	2.9
1	A	145	GLN	2.9
3	K	81	PHE	2.9
2	B	227	ILE	2.9
3	G	244	LEU	2.9
1	A	307	HIS	2.8
3	K	182	PRO	2.8
3	G	191	ALA	2.8
3	K	257	ALA	2.8
3	G	175	ILE	2.8
3	G	239	LEU	2.8
1	I	268	THR	2.8
2	B	208	PHE	2.8
3	C	197	THR	2.8
3	G	196	LYS	2.8
3	K	200	PRO	2.8
2	B	206	ARG	2.8
2	B	213	ALA	2.8
3	K	177	PHE	2.8
2	J	174	ASN	2.7
2	J	7	ALA	2.7
3	G	189	PHE	2.7
3	G	194	TYR	2.7
3	C	162	THR	2.7
1	E	233	ARG	2.7
1	I	274	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
3	K	180	SER	2.7
2	J	200	VAL	2.7
2	B	80	TRP	2.7
3	C	87	THR	2.7
2	F	241	GLU	2.7
3	G	179	LEU	2.7
3	G	234	TRP	2.7
3	G	238	GLU	2.7
1	A	256	SER	2.7
2	J	205	LEU	2.7
3	C	199	LEU	2.7
3	K	119	LEU	2.7
2	J	193	THR	2.6
1	A	221	ALA	2.6
2	J	80	TRP	2.6
3	G	184	TYR	2.6
3	C	239	LEU	2.6
1	I	176	GLN	2.6
2	F	213	ALA	2.6
2	B	175	GLY	2.6
2	F	139	GLY	2.6
3	K	179	LEU	2.6
3	C	155	GLN	2.6
2	F	243	PHE	2.6
3	G	171	PRO	2.6
3	C	244	LEU	2.6
3	G	177	PHE	2.6
1	A	371	TRP	2.5
1	I	383	PRO	2.5
1	E	264	LEU	2.5
1	A	211	ILE	2.5
1	I	208	ARG	2.5
3	C	196	LYS	2.5
2	B	185	GLY	2.5
3	K	175	ILE	2.5
3	K	120	ALA	2.5
2	F	198	ARG	2.5
1	I	382	ASP	2.5
3	C	250	ILE	2.5
1	E	206	TRP	2.5
3	K	88	TYR	2.5
1	A	366	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	251	MET	2.5
3	C	172	SER	2.5
2	B	237	TRP	2.5
1	I	177	THR	2.5
1	I	267	GLY	2.4
3	C	130	ARG	2.4
3	C	238	GLU	2.4
1	I	320	ALA	2.4
3	K	122	LEU	2.4
3	G	235	PHE	2.4
3	C	194	TYR	2.4
2	B	44	THR	2.4
1	E	173	LEU	2.4
3	C	57	ILE	2.4
3	K	171	PRO	2.4
2	F	212	VAL	2.4
3	C	249	VAL	2.4
1	A	233	ARG	2.4
2	B	57	ARG	2.4
1	E	212	PHE	2.4
3	G	159	TRP	2.4
3	K	76	ALA	2.4
1	I	231	THR	2.4
3	K	197	THR	2.4
1	I	272	MET	2.4
2	B	116	ILE	2.4
1	I	92	GLY	2.4
2	F	131	LEU	2.4
1	A	210	PRO	2.4
1	E	228	VAL	2.3
2	J	192	GLY	2.3
3	G	195	ALA	2.3
2	B	176	MET	2.3
2	J	223	MET	2.3
3	C	180	SER	2.3
3	C	178	TYR	2.3
3	G	178	TYR	2.3
3	G	232	THR	2.3
3	K	256	LEU	2.3
3	C	113	LYS	2.3
1	I	222	GLY	2.3
1	A	225	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	265	GLN	2.3
1	I	275	LEU	2.3
3	K	46	LEU	2.3
1	A	33	HIS	2.3
3	K	67	TRP	2.3
3	G	246	TYR	2.3
3	K	178	TYR	2.3
2	B	174	ASN	2.3
3	C	254	LEU	2.3
3	K	78	LEU	2.3
2	B	202	LYS	2.3
2	J	197	ILE	2.3
2	F	224	SER	2.3
2	B	15	VAL	2.3
1	I	308	GLY	2.3
1	I	117	GLU	2.2
1	I	309	ASN	2.2
3	G	78	LEU	2.2
3	G	160	HIS	2.2
3	K	74	TRP	2.2
2	B	171	VAL	2.2
3	C	184	TYR	2.2
3	G	88	TYR	2.2
3	K	184	TYR	2.2
2	F	205	LEU	2.2
2	J	201	GLU	2.2
2	J	244	LEU	2.2
3	C	198	ARG	2.2
3	G	253	TRP	2.2
3	K	253	TRP	2.2
3	C	181	TYR	2.2
2	B	219	PHE	2.2
3	K	250	ILE	2.2
1	I	147	GLY	2.2
2	B	220	SER	2.2
3	C	152	PHE	2.2
3	G	174	ILE	2.2
2	B	232	HIS	2.2
2	F	232	HIS	2.2
2	F	20	THR	2.2
2	F	237	TRP	2.2
1	A	189	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	111	LEU	2.2
3	G	180	SER	2.2
1	A	213	ILE	2.1
2	J	227	ILE	2.1
3	C	156	ASP	2.1
3	C	252	GLY	2.1
3	G	87	THR	2.1
3	G	108	TRP	2.1
2	J	113	TYR	2.1
3	C	121	ALA	2.1
1	E	263	PRO	2.1
2	B	125	VAL	2.1
2	B	189	VAL	2.1
2	J	45	MET	2.1
3	G	168	ASP	2.1
3	G	162	THR	2.1
2	F	128	ALA	2.1
3	K	57	ILE	2.1
2	F	238	PHE	2.1
3	C	195	ALA	2.1
2	J	138	SER	2.1
1	A	111	PRO	2.1
3	C	171	PRO	2.1
2	B	233	PHE	2.1
2	J	219	PHE	2.1
3	C	109	GLY	2.1
1	E	261	THR	2.1
1	I	220	ASP	2.1
2	B	207	THR	2.1
2	B	242	ARG	2.1
3	K	47	ASP	2.1
3	K	234	TRP	2.1
1	I	306	ASN	2.0
1	E	147	GLY	2.0
2	J	233	PHE	2.0
2	J	221	ALA	2.0
3	K	190	ALA	2.0
2	F	111	TRP	2.0
3	C	176	GLU	2.0
1	A	137	HIS	2.0
2	J	212	VAL	2.0
2	B	43	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	J	85	LEU	2.0
1	I	299	ARG	2.0
2	F	116	ILE	2.0
3	G	163	ILE	2.0
2	J	217	ALA	2.0
2	J	81	GLU	2.0
3	C	47	ASP	2.0
2	B	173	TYR	2.0
2	F	196	TYR	2.0
3	G	151	TYR	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
5	ZN	E	702	1/1	0.71	0.38	213,213,213,213	0
6	CUA	A	3	2/2	0.93	0.14	74,74,74,82	0
5	ZN	E	701	1/1	0.94	0.10	55,55,55,55	1
6	CUA	I	600	2/2	0.95	0.17	76,76,76,82	0
6	CUA	E	500	2/2	0.96	0.11	75,75,75,82	0
5	ZN	E	900	1/1	0.99	0.05	76,76,76,76	0
4	CU	A	4	1/1	0.99	0.10	61,61,61,61	0
4	CU	E	501	1/1	0.99	0.11	61,61,61,61	0
5	ZN	K	663	1/1	0.99	0.15	60,60,60,60	0
4	CU	I	601	1/1	0.99	0.08	61,61,61,61	0
5	ZN	A	800	1/1	0.99	0.06	77,77,77,77	0
5	ZN	C	661	1/1	0.99	0.12	73,73,73,73	0
5	ZN	C	700	1/1	1.00	0.11	46,46,46,46	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ZN	G	662	1/1	1.00	0.23	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.