



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Sep 17, 2019 – 12:32 PM EDT

PDB ID : 6JSI
EMDB ID: : EMD-9882
Title : Co-purified Fatty Acid Synthase
Authors : Qiu, S.W.; Liu, S.
Deposited on : 2019-04-08
Resolution : 4.70 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

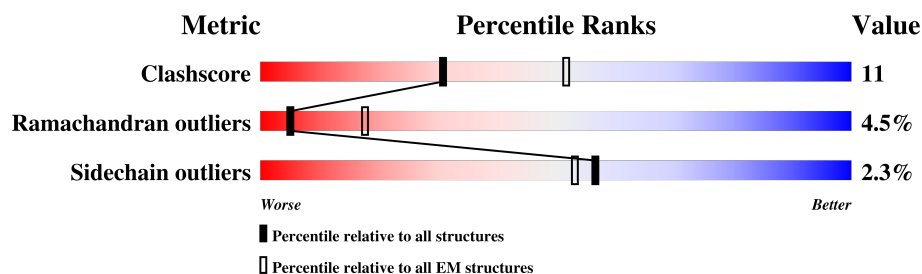
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	2051	
1	F	2051	
1	G	2051	
2	A	1887	
2	D	1887	
2	E	1887	
3	C	71	
3	H	71	
3	I	71	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 62820 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1904	Total	C	N	O	S	0	0
			11746	7280	2144	2306	16		
1	F	1904	Total	C	N	O	S	0	0
			11746	7280	2144	2306	16		
1	G	1904	Total	C	N	O	S	0	0
			11746	7280	2144	2306	16		

- Molecule 2 is a protein called Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1321	Total	C	N	O	S	0	0
			8587	5349	1534	1673	31		
2	D	1321	Total	C	N	O	S	0	0
			8587	5349	1534	1673	31		
2	E	1321	Total	C	N	O	S	0	0
			8587	5349	1534	1673	31		

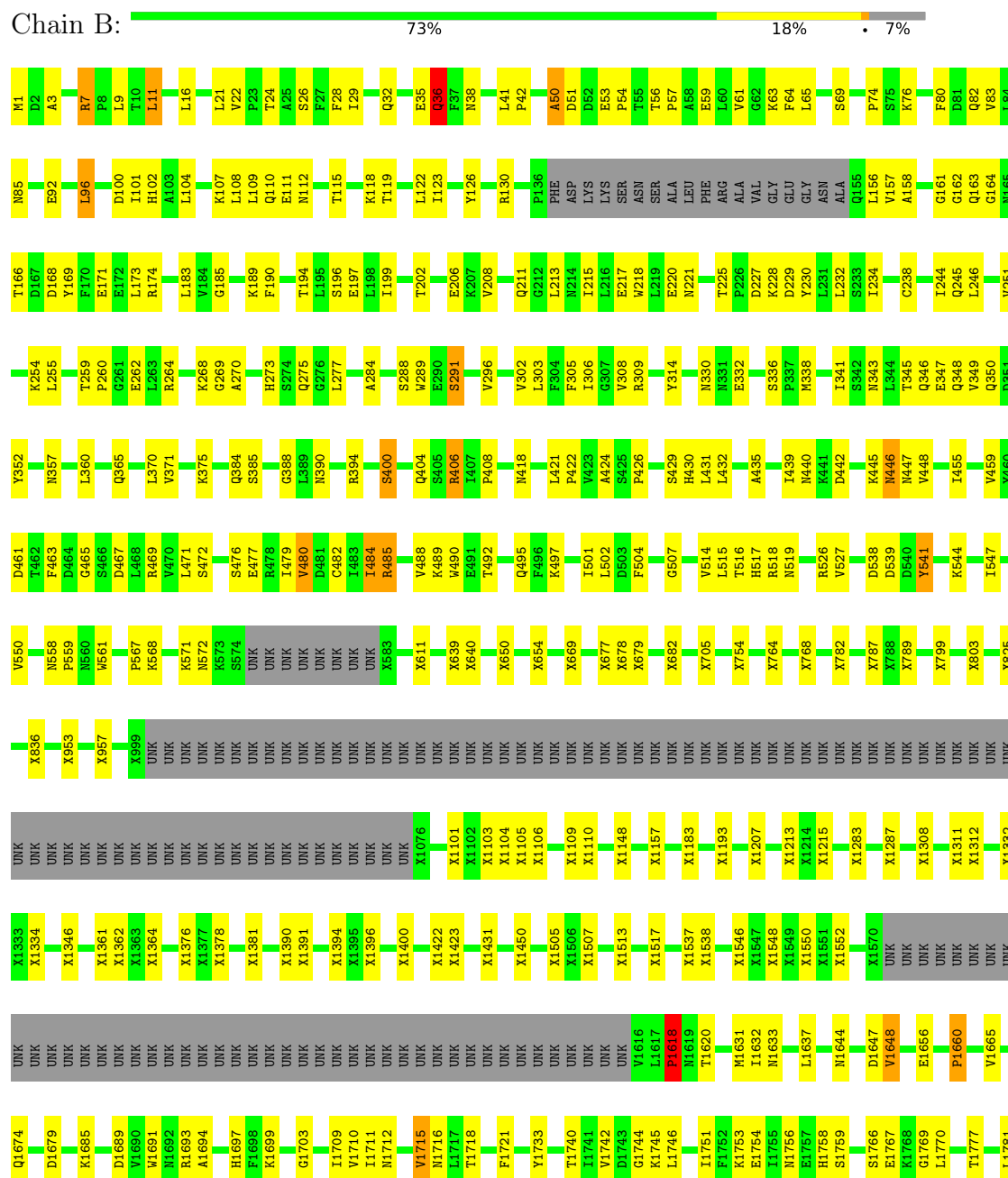
- Molecule 3 is a protein called Fatty acid synthase subunit alpha.

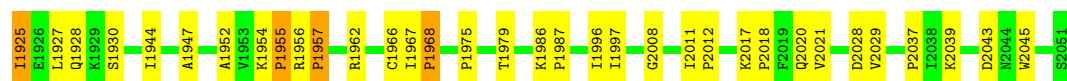
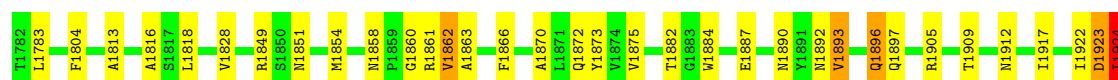
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	71	Total	C	N	O	S	0	0
			607	376	109	121	1		
3	H	71	Total	C	N	O	S	0	0
			607	376	109	121	1		
3	I	71	Total	C	N	O	S	0	0
			607	376	109	121	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

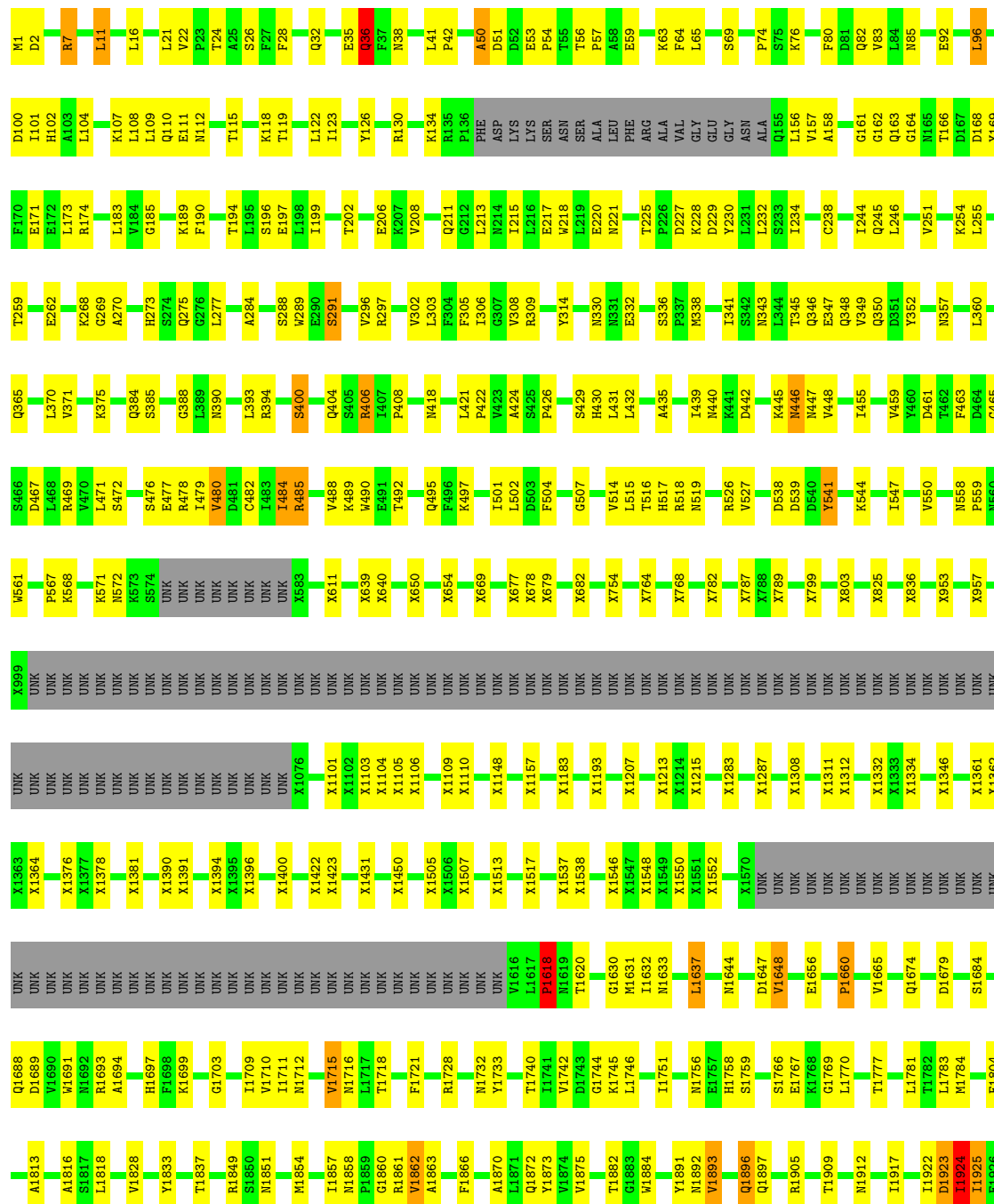
- Molecule 1: Fatty acid synthase subunit beta





• Molecule 1: Fatty acid synthase subunit beta

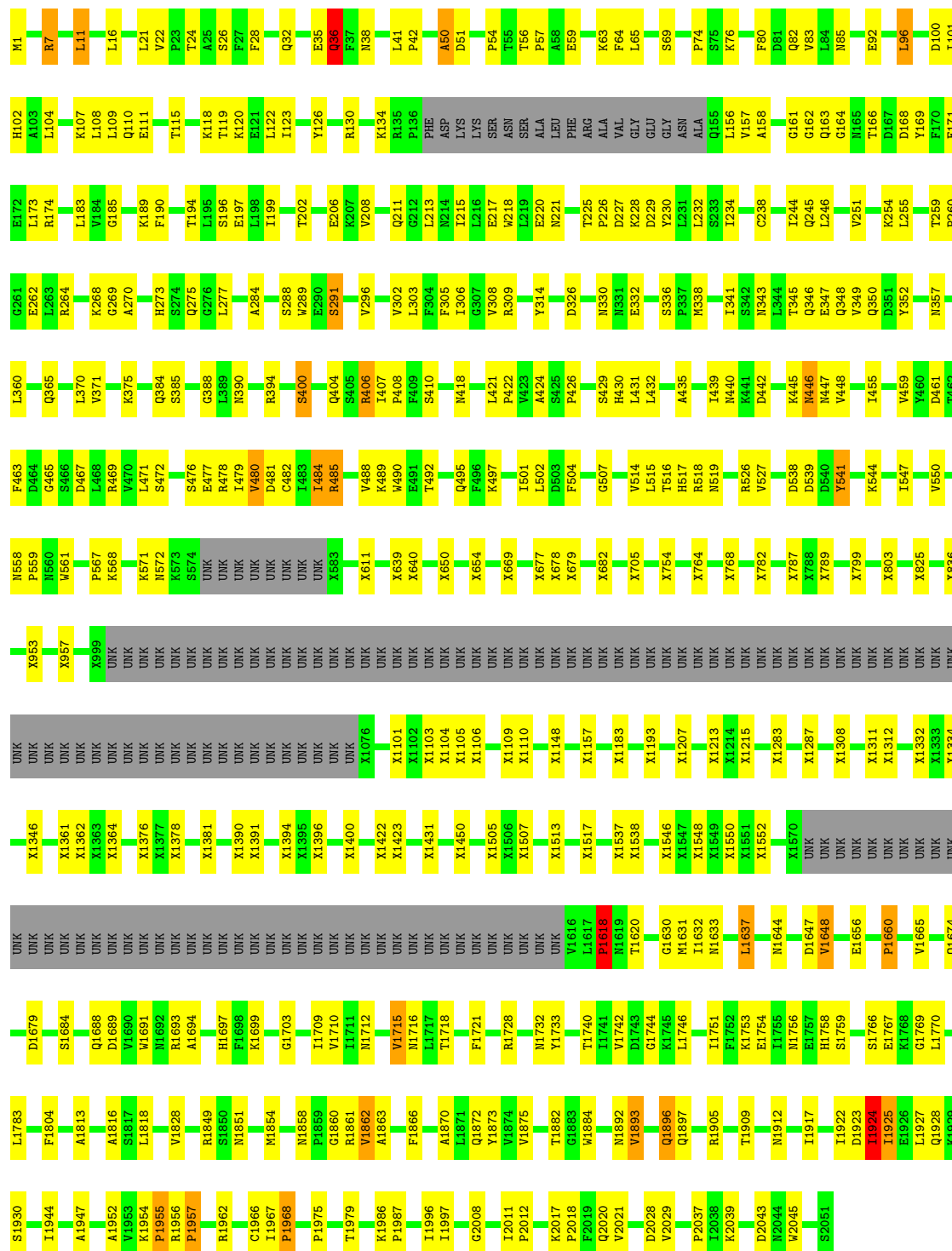
Chain F: 73% 18% 7%





• Molecule 1: Fatty acid synthase subunit beta

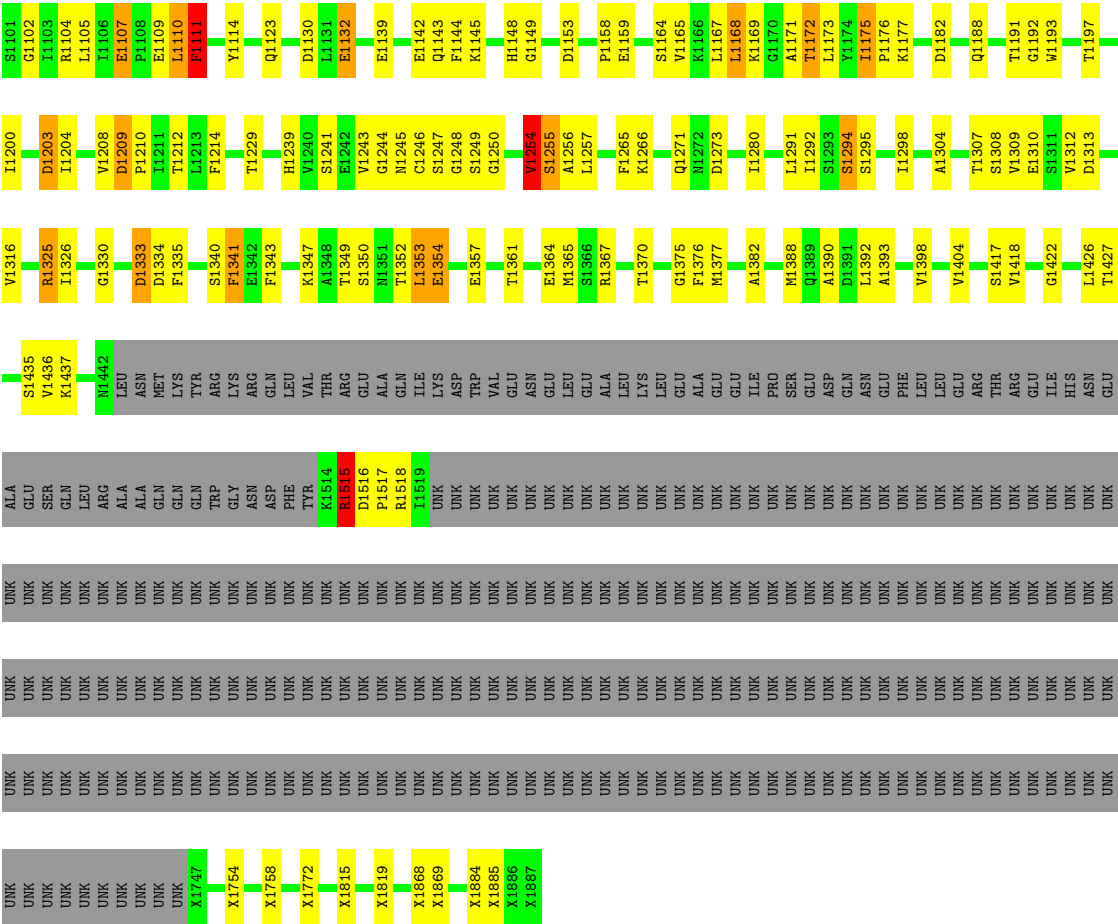
Chain G: 73% 18% 7%



• Molecule 2: Fatty acid synthase subunit alpha







● Molecule 3: Fatty acid synthase subunit alpha



● Molecule 3: Fatty acid synthase subunit alpha



● Molecule 3: Fatty acid synthase subunit alpha



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	3692	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	B	0.39	0/7308	0.74	20/9952 (0.2%)
1	F	0.39	0/7308	0.74	21/9952 (0.2%)
1	G	0.39	0/7308	0.74	21/9952 (0.2%)
2	A	0.46	0/6518	0.80	16/8839 (0.2%)
2	D	0.46	0/6518	0.80	16/8839 (0.2%)
2	E	0.46	0/6518	0.80	15/8839 (0.2%)
3	C	0.40	0/616	0.70	0/828
3	H	0.40	0/616	0.70	0/828
3	I	0.40	0/616	0.70	0/828
All	All	0.42	0/43326	0.77	109/58857 (0.2%)

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	B	0	19
1	F	0	19
1	G	0	19
2	A	0	26
2	D	0	27
2	E	0	27
3	C	0	2
3	H	0	2
3	I	0	2
All	All	0	143

There are no bond length outliers.

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1203	ASP	CB-CG-OD1	8.02	125.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1203	ASP	CB-CG-OD1	8.01	125.51	118.30
2	D	1203	ASP	CB-CG-OD1	7.99	125.49	118.30
1	G	36	GLN	CA-CB-CG	7.75	130.45	113.40
1	F	36	GLN	CA-CB-CG	7.75	130.44	113.40
1	B	36	GLN	CA-CB-CG	7.73	130.41	113.40
2	D	1110	LEU	CA-CB-CG	7.18	131.82	115.30
2	E	1110	LEU	CA-CB-CG	7.17	131.79	115.30
2	A	1110	LEU	CA-CB-CG	7.16	131.76	115.30
2	E	1173	LEU	CA-CB-CG	7.10	131.62	115.30
2	A	1173	LEU	CA-CB-CG	7.09	131.60	115.30
2	D	1173	LEU	CA-CB-CG	7.08	131.59	115.30
1	B	1975	PRO	N-CA-CB	6.90	111.58	103.30
1	G	1975	PRO	N-CA-CB	6.90	111.58	103.30
1	F	1975	PRO	N-CA-CB	6.87	111.54	103.30
2	A	645	PRO	N-CA-CB	6.74	111.39	103.30
2	E	645	PRO	N-CA-CB	6.72	111.36	103.30
2	D	645	PRO	N-CA-CB	6.68	111.32	103.30
1	B	1987	PRO	N-CA-CB	6.67	111.31	103.30
1	F	1987	PRO	N-CA-CB	6.66	111.29	103.30
1	G	1987	PRO	N-CA-CB	6.65	111.28	103.30
1	B	559	PRO	N-CA-CB	6.54	111.14	103.30
1	G	1968	PRO	N-CA-CB	6.53	111.14	103.30
1	B	1968	PRO	N-CA-CB	6.53	111.13	103.30
1	G	559	PRO	N-CA-CB	6.52	111.12	103.30
1	F	559	PRO	N-CA-CB	6.50	111.11	103.30
1	F	1968	PRO	N-CA-CB	6.50	111.10	103.30
1	B	1957	PRO	N-CA-CB	6.38	110.96	103.30
1	F	1957	PRO	N-CA-CB	6.37	110.95	103.30
1	F	2012	PRO	N-CA-CB	6.36	110.93	103.30
1	G	1957	PRO	N-CA-CB	6.36	110.93	103.30
2	A	636	PRO	N-CA-CB	6.35	110.92	103.30
1	G	2012	PRO	N-CA-CB	6.34	110.92	103.30
2	E	636	PRO	N-CA-CB	6.33	110.89	103.30
2	D	636	PRO	N-CA-CB	6.32	110.88	103.30
1	B	2012	PRO	N-CA-CB	6.32	110.88	103.30
1	B	2037	PRO	N-CA-CB	6.24	110.78	103.30
1	G	2037	PRO	N-CA-CB	6.23	110.77	103.30
1	F	2037	PRO	N-CA-CB	6.20	110.74	103.30
2	A	590	PRO	N-CA-CB	6.08	110.60	103.30
1	G	1618	PRO	N-CA-CB	6.08	110.59	103.30
1	F	1618	PRO	N-CA-CB	6.07	110.58	103.30
1	B	1618	PRO	N-CA-CB	6.06	110.57	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	590	PRO	N-CA-CB	6.05	110.56	103.30
2	E	590	PRO	N-CA-CB	6.05	110.56	103.30
2	D	534	PRO	N-CA-CB	5.97	110.46	103.30
2	E	534	PRO	N-CA-CB	5.97	110.46	103.30
2	A	534	PRO	N-CA-CB	5.96	110.45	103.30
1	G	1955	PRO	N-CA-CB	5.93	110.42	103.30
1	B	1955	PRO	N-CA-CB	5.93	110.41	103.30
1	F	109	LEU	CA-CB-CG	5.92	128.91	115.30
1	B	1660	PRO	N-CA-CB	5.91	110.39	103.30
2	D	761	LEU	CA-CB-CG	5.91	128.88	115.30
1	G	2018	PRO	N-CA-CB	5.91	110.39	103.30
1	G	1660	PRO	N-CA-CB	5.90	110.38	103.30
1	B	2018	PRO	N-CA-CB	5.90	110.38	103.30
1	F	1955	PRO	N-CA-CB	5.90	110.38	103.30
1	B	109	LEU	CA-CB-CG	5.90	128.86	115.30
2	E	761	LEU	CA-CB-CG	5.89	128.85	115.30
1	F	1660	PRO	N-CA-CB	5.89	110.36	103.30
1	G	109	LEU	CA-CB-CG	5.89	128.84	115.30
2	A	761	LEU	CA-CB-CG	5.88	128.84	115.30
1	F	2018	PRO	N-CA-CB	5.88	110.36	103.30
1	G	7	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	7	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	F	567	PRO	N-CA-CB	5.79	110.25	103.30
1	G	567	PRO	N-CA-CB	5.78	110.23	103.30
2	E	1175	ILE	C-N-CD	-5.77	107.90	120.60
2	A	1175	ILE	C-N-CD	-5.77	107.91	120.60
2	D	1175	ILE	C-N-CD	-5.75	107.94	120.60
1	B	567	PRO	N-CA-CB	5.75	110.20	103.30
1	F	7	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	406	ARG	CA-CB-CG	5.54	125.60	113.40
2	A	631	PRO	N-CA-CB	5.54	109.95	103.30
1	B	1923	ASP	C-N-CA	5.53	135.53	121.70
1	G	1923	ASP	C-N-CA	5.53	135.53	121.70
1	F	1923	ASP	C-N-CA	5.53	135.52	121.70
2	D	631	PRO	N-CA-CB	5.53	109.93	103.30
1	F	406	ARG	CA-CB-CG	5.52	125.55	113.40
1	G	406	ARG	CA-CB-CG	5.52	125.54	113.40
2	D	541	PRO	N-CA-CB	5.51	109.91	103.30
2	A	541	PRO	N-CA-CB	5.50	109.90	103.30
2	E	631	PRO	N-CA-CB	5.50	109.89	103.30
2	E	541	PRO	N-CA-CB	5.48	109.88	103.30
1	F	476	SER	C-N-CA	5.42	135.24	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	476	SER	C-N-CA	5.41	135.22	121.70
1	B	476	SER	C-N-CA	5.38	135.15	121.70
2	A	617	PRO	N-CA-CB	5.34	109.71	103.30
1	B	1924	ILE	C-N-CA	5.33	135.03	121.70
1	G	1924	ILE	C-N-CA	5.33	135.02	121.70
1	F	1924	ILE	C-N-CA	5.32	134.99	121.70
2	E	617	PRO	N-CA-CB	5.31	109.67	103.30
2	D	617	PRO	N-CA-CB	5.28	109.64	103.30
2	D	1353	LEU	C-N-CA	5.27	134.87	121.70
2	E	1353	LEU	C-N-CA	5.25	134.82	121.70
2	A	1353	LEU	C-N-CA	5.25	134.81	121.70
2	A	1398	VAL	C-N-CD	-5.21	109.14	120.60
2	E	1398	VAL	C-N-CD	-5.20	109.15	120.60
2	D	1056	ILE	CG1-CB-CG2	-5.19	99.99	111.40
2	E	1056	ILE	CG1-CB-CG2	-5.18	100.00	111.40
2	D	1398	VAL	C-N-CD	-5.17	109.22	120.60
2	A	1056	ILE	CG1-CB-CG2	-5.17	100.03	111.40
1	B	16	LEU	CA-CB-CG	5.11	127.04	115.30
1	G	16	LEU	CA-CB-CG	5.09	127.01	115.30
1	F	16	LEU	CA-CB-CG	5.08	126.98	115.30
1	F	478	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	G	478	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	A	1370	THR	C-N-CA	5.01	134.24	121.70
2	D	1158	PRO	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (143) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1046	SER	Peptide
2	A	1070	ARG	Peptide
2	A	1082	GLU	Peptide
2	A	1086	ASP	Peptide
2	A	1087	LYS	Peptide
2	A	1094	GLU	Peptide
2	A	1099	GLU	Peptide
2	A	1107	GLU	Peptide
2	A	1110	LEU	Peptide
2	A	1111	PHE	Peptide
2	A	1132	GLU	Peptide
2	A	1168	LEU	Peptide
2	A	1171	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	A	1177	LYS	Peptide
2	A	1203	ASP	Peptide
2	A	1209	ASP	Peptide
2	A	1244	GLY	Peptide
2	A	1254	VAL	Peptide
2	A	1325	ARG	Peptide
2	A	1341	PHE	Peptide
2	A	1354	GLU	Peptide
2	A	1422	GLY	Peptide
2	A	1515	ARG	Peptide
2	A	684	GLY	Peptide
2	A	786	SER	Peptide
2	A	896	PHE	Peptide
1	B	11	LEU	Peptide
1	B	1207	UNK	Peptide
1	B	1715	VAL	Peptide
1	B	1746	LEU	Peptide
1	B	1756	ASN	Peptide
1	B	1858	ASN	Peptide
1	B	1861	ARG	Peptide
1	B	1862	VAL	Peptide
1	B	1896	GLN	Peptide
1	B	1912	ASN	Peptide
1	B	1922	ILE	Peptide
1	B	1924	ILE	Peptide
1	B	446	ASN	Peptide
1	B	471	LEU	Peptide
1	B	484	ILE	Peptide
1	B	485	ARG	Peptide
1	B	50	ALA	Peptide
1	B	74	PRO	Peptide
1	B	76	LYS	Peptide
3	C	1477	ILE	Peptide
3	C	1478	PRO	Peptide
2	D	1046	SER	Peptide
2	D	1070	ARG	Peptide
2	D	1082	GLU	Peptide
2	D	1086	ASP	Peptide
2	D	1087	LYS	Peptide
2	D	1094	GLU	Peptide
2	D	1099	GLU	Peptide
2	D	1107	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	D	1110	LEU	Peptide
2	D	1111	PHE	Peptide
2	D	1132	GLU	Peptide
2	D	1168	LEU	Peptide
2	D	1171	ALA	Peptide
2	D	1177	LYS	Peptide
2	D	1203	ASP	Peptide
2	D	1209	ASP	Peptide
2	D	1244	GLY	Peptide
2	D	1254	VAL	Peptide
2	D	1292	ILE	Peptide
2	D	1325	ARG	Peptide
2	D	1341	PHE	Peptide
2	D	1354	GLU	Peptide
2	D	1422	GLY	Peptide
2	D	1515	ARG	Peptide
2	D	684	GLY	Peptide
2	D	786	SER	Peptide
2	D	896	PHE	Peptide
2	E	1046	SER	Peptide
2	E	1070	ARG	Peptide
2	E	1082	GLU	Peptide
2	E	1086	ASP	Peptide
2	E	1087	LYS	Peptide
2	E	1094	GLU	Peptide
2	E	1099	GLU	Peptide
2	E	1107	GLU	Peptide
2	E	1110	LEU	Peptide
2	E	1111	PHE	Peptide
2	E	1132	GLU	Peptide
2	E	1168	LEU	Peptide
2	E	1171	ALA	Peptide
2	E	1177	LYS	Peptide
2	E	1203	ASP	Peptide
2	E	1209	ASP	Peptide
2	E	1244	GLY	Peptide
2	E	1254	VAL	Peptide
2	E	1292	ILE	Peptide
2	E	1325	ARG	Peptide
2	E	1341	PHE	Peptide
2	E	1354	GLU	Peptide
2	E	1422	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	E	1515	ARG	Peptide
2	E	684	GLY	Peptide
2	E	786	SER	Peptide
2	E	896	PHE	Peptide
1	F	11	LEU	Peptide
1	F	1207	UNK	Peptide
1	F	1715	VAL	Peptide
1	F	1746	LEU	Peptide
1	F	1756	ASN	Peptide
1	F	1858	ASN	Peptide
1	F	1861	ARG	Peptide
1	F	1862	VAL	Peptide
1	F	1896	GLN	Peptide
1	F	1912	ASN	Peptide
1	F	1922	ILE	Peptide
1	F	1924	ILE	Peptide
1	F	446	ASN	Peptide
1	F	471	LEU	Peptide
1	F	484	ILE	Peptide
1	F	485	ARG	Peptide
1	F	50	ALA	Peptide
1	F	74	PRO	Peptide
1	F	76	LYS	Peptide
1	G	11	LEU	Peptide
1	G	1207	UNK	Peptide
1	G	1715	VAL	Peptide
1	G	1746	LEU	Peptide
1	G	1756	ASN	Peptide
1	G	1858	ASN	Peptide
1	G	1861	ARG	Peptide
1	G	1862	VAL	Peptide
1	G	1896	GLN	Peptide
1	G	1912	ASN	Peptide
1	G	1922	ILE	Peptide
1	G	1924	ILE	Peptide
1	G	446	ASN	Peptide
1	G	471	LEU	Peptide
1	G	484	ILE	Peptide
1	G	485	ARG	Peptide
1	G	50	ALA	Peptide
1	G	74	PRO	Peptide
1	G	76	LYS	Peptide

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Mol	Chain	Res	Type	Group
3	H	1477	ILE	Peptide
3	H	1478	PRO	Peptide
3	I	1477	ILE	Peptide
3	I	1478	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	11746	0	7740	204	0
1	F	11746	0	7741	210	0
1	G	11746	0	7742	206	0
2	A	8587	0	6479	162	0
2	D	8587	0	6479	160	0
2	E	8587	0	6479	164	0
3	C	607	0	580	12	0
3	H	607	0	580	11	0
3	I	607	0	580	11	0
All	All	62820	0	44400	1133	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1133) 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)
1:F:163:GLN:HG2	1:F:275:GLN:HG3	1.74	0.70
1:F:238:CYS:HB2	1:F:303:LEU:HD12	1.74	0.69
1:G:163:GLN:HG2	1:G:275:GLN:HG3	1.74	0.69
1:B:163:GLN:HG2	1:B:275:GLN:HG3	1.74	0.68
1:B:238:CYS:HB2	1:B:303:LEU:HD12	1.74	0.68
1:G:238:CYS:HB2	1:G:303:LEU:HD12	1.74	0.68
1:B:1863:ALA:HA	1:B:1866:PHE:HB2	1.78	0.65
1:B:32:GLN:HA	1:B:35:GLU:HB2	1.79	0.65
1:G:1863:ALA:HA	1:G:1866:PHE:HB2	1.78	0.65
2:A:894:ARG:HE	2:A:895:THR:H	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:GLN:HA	1:G:35:GLU:HB2	1.79	0.64
2:D:1254:VAL:HG23	2:D:1257:LEU:HB3	1.80	0.64
2:E:1175:ILE:HG12	2:E:1176:PRO:HA	1.79	0.64
2:E:1254:VAL:HG23	2:E:1257:LEU:HB3	1.80	0.64
2:E:963:LEU:HA	2:E:966:LYS:HG2	1.80	0.64
2:A:1248:GLY:HA2	2:A:1330:GLY:HA3	1.79	0.64
1:F:32:GLN:HA	1:F:35:GLU:HB2	1.79	0.64
2:D:1248:GLY:HA2	2:D:1330:GLY:HA3	1.79	0.64
1:F:1863:ALA:HA	1:F:1866:PHE:HB2	1.78	0.64
2:D:963:LEU:HA	2:D:966:LYS:HG2	1.80	0.64
2:E:1248:GLY:HA2	2:E:1330:GLY:HA3	1.79	0.63
2:A:1175:ILE:HG12	2:A:1176:PRO:HA	1.80	0.63
2:E:894:ARG:HE	2:E:895:THR:H	1.45	0.63
2:D:894:ARG:HE	2:D:895:THR:H	1.45	0.63
2:D:1197:THR:HG23	2:D:1200:ILE:HG22	1.81	0.63
2:A:1254:VAL:HG23	2:A:1257:LEU:HB3	1.80	0.62
1:B:461:ASP:H	1:B:465:GLY:HA2	1.64	0.62
1:B:38:ASN:HA	1:B:41:LEU:HG	1.82	0.62
2:E:1197:THR:HG23	2:E:1200:ILE:HG22	1.81	0.62
1:F:1860:GLY:H	1:F:1863:ALA:HB2	1.64	0.62
2:A:963:LEU:HA	2:A:966:LYS:HG2	1.80	0.62
2:D:1175:ILE:HG12	2:D:1176:PRO:HA	1.80	0.62
1:G:38:ASN:HA	1:G:41:LEU:HG	1.82	0.62
1:G:1860:GLY:H	1:G:1863:ALA:HB2	1.64	0.62
2:A:1197:THR:HG23	2:A:1200:ILE:HG22	1.81	0.62
1:F:461:ASP:H	1:F:465:GLY:HA2	1.64	0.62
1:F:479:ILE:HG13	1:F:480:VAL:HG12	1.82	0.62
1:G:479:ILE:HG13	1:G:480:VAL:HG12	1.82	0.62
1:G:1546:UNK:O	1:G:1550:UNK:N	2.33	0.61
3:I:1484:GLU:O	3:I:1488:GLU:N	2.33	0.61
1:F:1699:LYS:HA	1:F:1703:GLY:HA2	1.82	0.61
1:B:479:ILE:HG13	1:B:480:VAL:HG12	1.82	0.61
1:F:199:ILE:HG12	1:F:206:GLU:HG3	1.81	0.61
1:B:1699:LYS:HA	1:B:1703:GLY:HA2	1.82	0.61
1:B:517:HIS:NE2	1:B:538:ASP:OD1	2.34	0.61
3:H:1484:GLU:O	3:H:1488:GLU:N	2.33	0.61
1:B:199:ILE:HG12	1:B:206:GLU:HG3	1.81	0.61
2:A:1142:GLU:OE1	2:A:1143:GLN:NE2	2.33	0.61
1:B:1860:GLY:H	1:B:1863:ALA:HB2	1.64	0.61
2:A:863:THR:HG21	2:A:917:CYS:HB3	1.83	0.61
1:G:461:ASP:H	1:G:465:GLY:HA2	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1546:UNK:O	1:F:1550:UNK:N	2.33	0.61
1:F:517:HIS:NE2	1:F:538:ASP:OD1	2.34	0.61
1:B:1546:UNK:O	1:B:1550:UNK:N	2.33	0.61
1:F:38:ASN:HA	1:F:41:LEU:HG	1.81	0.61
1:G:199:ILE:HG12	1:G:206:GLU:HG3	1.81	0.61
3:C:1484:GLU:O	3:C:1488:GLU:N	2.33	0.61
1:G:1699:LYS:HA	1:G:1703:GLY:HA2	1.82	0.61
2:D:1142:GLU:OE1	2:D:1143:GLN:NE2	2.34	0.60
2:E:1142:GLU:OE1	2:E:1143:GLN:NE2	2.34	0.60
1:G:517:HIS:NE2	1:G:538:ASP:OD1	2.34	0.60
2:E:863:THR:HG21	2:E:917:CYS:HB3	1.83	0.60
1:F:126:TYR:OH	1:F:130:ARG:NH1	2.35	0.60
1:G:126:TYR:OH	1:G:130:ARG:NH1	2.35	0.60
1:G:1718:THR:HB	1:G:1770:LEU:HD22	1.83	0.60
1:B:126:TYR:OH	1:B:130:ARG:NH1	2.35	0.60
2:D:863:THR:HG21	2:D:917:CYS:HB3	1.83	0.60
2:D:281:UNK:O	2:D:285:UNK:N	2.35	0.59
1:F:157:VAL:HB	1:F:501:ILE:HG12	1.84	0.59
2:A:281:UNK:O	2:A:285:UNK:N	2.35	0.59
1:B:157:VAL:HB	1:B:501:ILE:HG12	1.84	0.59
2:A:1271:GLN:NE2	2:A:1273:ASP:O	2.36	0.59
2:E:1271:GLN:NE2	2:E:1273:ASP:O	2.36	0.59
2:E:1312:VAL:O	2:E:1316:VAL:N	2.35	0.59
2:E:281:UNK:O	2:E:285:UNK:N	2.35	0.59
1:F:1718:THR:HB	1:F:1770:LEU:HD22	1.83	0.59
1:B:259:THR:HG23	1:B:262:GLU:H	1.67	0.59
2:A:750:GLU:OE2	2:A:809:GLN:NE2	2.36	0.59
1:B:157:VAL:HG13	1:B:269:GLY:HA3	1.84	0.59
1:F:259:THR:HG23	1:F:262:GLU:H	1.67	0.59
1:F:157:VAL:HG13	1:F:269:GLY:HA3	1.84	0.59
1:G:259:THR:HG23	1:G:262:GLU:H	1.67	0.59
1:G:246:LEU:HD11	1:G:296:VAL:HG22	1.85	0.59
1:B:1718:THR:HB	1:B:1770:LEU:HD22	1.84	0.58
2:E:1307:THR:OG1	2:E:1308:SER:N	2.35	0.58
1:G:345:THR:OG1	1:G:348:GLN:NE2	2.36	0.58
1:F:1882:THR:HA	1:F:1893:VAL:HA	1.85	0.58
2:A:1307:THR:OG1	2:A:1308:SER:N	2.35	0.58
2:E:1436:VAL:O	2:E:1518:ARG:NH1	2.36	0.58
1:F:345:THR:OG1	1:F:348:GLN:NE2	2.36	0.58
2:A:1436:VAL:O	2:A:1518:ARG:NH1	2.36	0.58
2:D:1307:THR:OG1	2:D:1308:SER:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:440:ASN:ND2	1:F:477:GLU:OE1	2.36	0.58
1:G:157:VAL:HB	1:G:501:ILE:HG12	1.84	0.58
1:B:343:ASN:HA	1:B:375:LYS:HB3	1.86	0.58
2:E:1868:UNK:HA	2:E:1885:UNK:HA	1.85	0.58
2:D:1094:GLU:H	2:D:1097:ILE:HG22	1.69	0.58
2:E:750:GLU:OE2	2:E:809:GLN:NE2	2.36	0.58
2:D:1271:GLN:NE2	2:D:1273:ASP:O	2.36	0.58
2:A:1294:SER:OG	2:A:1295:SER:N	2.36	0.58
2:A:1868:UNK:HA	2:A:1885:UNK:HA	1.85	0.58
1:G:1742:VAL:HG22	1:G:1744:GLY:H	1.69	0.58
1:B:330:ASN:ND2	1:B:332:GLU:OE2	2.37	0.58
1:B:345:THR:OG1	1:B:348:GLN:NE2	2.36	0.58
1:F:246:LEU:HD11	1:F:296:VAL:HG22	1.86	0.58
1:G:440:ASN:ND2	1:G:477:GLU:OE1	2.36	0.58
2:D:1436:VAL:O	2:D:1518:ARG:NH1	2.36	0.57
1:F:59:GLU:O	1:F:63:LYS:N	2.36	0.57
1:G:467:ASP:OD2	1:G:469:ARG:NH2	2.37	0.57
1:B:246:LEU:HD11	1:B:296:VAL:HG22	1.86	0.57
1:B:440:ASN:ND2	1:B:477:GLU:OE1	2.36	0.57
2:D:1312:VAL:O	2:D:1316:VAL:N	2.35	0.57
1:F:1715:VAL:HA	1:F:1769:GLY:HA2	1.86	0.57
1:B:1390:UNK:O	1:B:1423:UNK:N	2.37	0.57
2:D:1868:UNK:HA	2:D:1885:UNK:HA	1.85	0.57
1:G:1715:VAL:HA	1:G:1769:GLY:HA2	1.86	0.57
1:G:1882:THR:HA	1:G:1893:VAL:HA	1.85	0.57
2:A:1094:GLU:H	2:A:1097:ILE:HG22	1.69	0.57
1:B:1715:VAL:HA	1:B:1769:GLY:HA2	1.86	0.57
1:G:157:VAL:HG13	1:G:269:GLY:HA3	1.84	0.57
1:G:1390:UNK:O	1:G:1423:UNK:N	2.37	0.57
1:B:1882:THR:HA	1:B:1893:VAL:HA	1.85	0.57
1:F:1390:UNK:O	1:F:1423:UNK:N	2.37	0.57
2:E:1094:GLU:H	2:E:1097:ILE:HG22	1.69	0.57
1:F:1742:VAL:HG22	1:F:1744:GLY:H	1.69	0.57
1:G:1740:THR:HB	1:G:1751:ILE:HD12	1.87	0.57
1:B:678:UNK:O	1:B:682:UNK:N	2.38	0.57
1:F:1740:THR:HB	1:F:1751:ILE:HD12	1.87	0.57
1:F:343:ASN:HA	1:F:375:LYS:HB3	1.86	0.57
1:B:232:LEU:HD21	1:B:422:PRO:HB2	1.87	0.57
1:B:59:GLU:O	1:B:63:LYS:N	2.36	0.57
2:E:852:ARG:NH1	2:E:856:GLU:OE1	2.38	0.57
1:F:330:ASN:ND2	1:F:332:GLU:OE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:467:ASP:OD2	1:F:469:ARG:NH2	2.37	0.57
2:A:1312:VAL:O	2:A:1316:VAL:N	2.35	0.56
1:B:467:ASP:OD2	1:B:469:ARG:NH2	2.37	0.56
1:G:343:ASN:HA	1:G:375:LYS:HB3	1.86	0.56
1:B:1538:UNK:O	1:B:1618:PRO:N	2.39	0.56
2:E:1034:ARG:NH2	2:E:1052:GLU:OE2	2.39	0.56
1:G:1422:UNK:O	1:G:1450:UNK:N	2.38	0.56
1:G:400:SER:O	1:G:400:SER:OG	2.23	0.56
1:G:678:UNK:O	1:G:682:UNK:N	2.38	0.56
1:B:1422:UNK:O	1:B:1450:UNK:N	2.38	0.56
1:B:1742:VAL:HG22	1:B:1744:GLY:H	1.69	0.56
1:B:1740:THR:HB	1:B:1751:ILE:HD12	1.87	0.56
2:E:755:THR:HG22	2:E:757:LYS:H	1.71	0.56
1:F:1422:UNK:O	1:F:1450:UNK:N	2.38	0.56
1:F:442:ASP:HA	1:F:445:LYS:HD2	1.88	0.56
1:G:1674:GLN:NE2	1:G:1710:VAL:O	2.39	0.56
2:D:1034:ARG:NH2	2:D:1052:GLU:OE2	2.38	0.56
1:F:1:MET:N	1:F:11:LEU:O	2.38	0.56
1:G:1538:UNK:O	1:G:1618:PRO:N	2.39	0.56
1:G:232:LEU:HD21	1:G:422:PRO:HB2	1.88	0.56
2:A:1034:ARG:NH2	2:A:1052:GLU:OE2	2.39	0.56
1:B:461:ASP:HB2	1:B:465:GLY:HA2	1.88	0.56
2:D:852:ARG:NH1	2:D:856:GLU:OE1	2.38	0.56
2:E:785:ASP:OD1	2:E:785:ASP:N	2.39	0.56
1:F:1538:UNK:O	1:F:1618:PRO:N	2.39	0.56
1:B:1644:ASN:H	1:B:1648:VAL:H	1.54	0.56
1:B:1674:GLN:NE2	1:B:1710:VAL:O	2.39	0.56
1:B:1689:ASP:OD2	1:B:1693:ARG:NH2	2.39	0.56
1:G:1689:ASP:OD2	1:G:1693:ARG:NH2	2.39	0.56
1:G:349:VAL:HA	1:G:352:TYR:HD1	1.71	0.56
1:F:108:LEU:HD13	1:F:119:THR:HG23	1.87	0.56
1:F:232:LEU:HD21	1:F:422:PRO:HB2	1.87	0.56
1:B:115:THR:O	1:B:119:THR:OG1	2.24	0.56
1:F:1644:ASN:H	1:F:1648:VAL:H	1.54	0.56
1:G:115:THR:O	1:G:119:THR:OG1	2.24	0.56
1:G:330:ASN:ND2	1:G:332:GLU:OE2	2.37	0.56
1:B:1311:UNK:HA	1:B:1362:UNK:HA	1.88	0.56
2:D:750:GLU:OE2	2:D:809:GLN:NE2	2.36	0.56
1:F:678:UNK:O	1:F:682:UNK:N	2.38	0.56
1:G:1721:PHE:O	1:G:1733:TYR:OH	2.24	0.56
1:G:59:GLU:O	1:G:63:LYS:N	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:UNK:O	2:D:157:UNK:N	2.39	0.55
1:F:1689:ASP:OD2	1:F:1693:ARG:NH2	2.39	0.55
1:F:461:ASP:HB2	1:F:465:GLY:HA2	1.88	0.55
1:G:1644:ASN:H	1:G:1648:VAL:H	1.54	0.55
2:A:1209:ASP:N	2:A:1209:ASP:OD1	2.39	0.55
1:B:349:VAL:HA	1:B:352:TYR:HD1	1.71	0.55
2:D:755:THR:HG22	2:D:757:LYS:H	1.71	0.55
2:E:1209:ASP:N	2:E:1209:ASP:OD1	2.39	0.55
2:A:373:UNK:O	2:A:377:UNK:N	2.39	0.55
2:A:852:ARG:NH1	2:A:856:GLU:OE1	2.38	0.55
1:B:442:ASP:HA	1:B:445:LYS:HD2	1.88	0.55
2:D:1815:UNK:O	2:D:1819:UNK:N	2.40	0.55
1:F:1674:GLN:NE2	1:F:1710:VAL:O	2.39	0.55
1:F:349:VAL:HA	1:F:352:TYR:HD1	1.71	0.55
1:G:1311:UNK:HA	1:G:1362:UNK:HA	1.89	0.55
1:G:211:GLN:HE22	1:G:230:TYR:HB3	1.71	0.55
1:G:461:ASP:HB2	1:G:465:GLY:HA2	1.88	0.55
1:B:108:LEU:HD13	1:B:119:THR:HG23	1.88	0.55
1:B:1721:PHE:O	1:B:1733:TYR:OH	2.24	0.55
2:E:1073:THR:OG1	2:E:1074:GLY:N	2.40	0.55
1:F:115:THR:O	1:F:119:THR:OG1	2.24	0.55
2:A:755:THR:HG22	2:A:757:LYS:H	1.71	0.55
2:D:1073:THR:OG1	2:D:1074:GLY:N	2.40	0.55
2:D:1209:ASP:OD1	2:D:1209:ASP:N	2.39	0.55
1:G:442:ASP:HA	1:G:445:LYS:HD2	1.88	0.55
1:G:7:ARG:HB3	1:G:54:PRO:HG3	1.89	0.55
1:B:211:GLN:HE22	1:B:230:TYR:HB3	1.71	0.55
1:B:370:LEU:HG	1:B:488:VAL:HB	1.89	0.55
1:B:568:LYS:H	1:B:572:ASN:H	1.55	0.55
2:E:153:UNK:O	2:E:157:UNK:N	2.39	0.55
2:E:1815:UNK:O	2:E:1819:UNK:N	2.40	0.55
1:F:1311:UNK:HA	1:F:1362:UNK:HA	1.89	0.55
1:F:1721:PHE:O	1:F:1733:TYR:OH	2.24	0.55
2:A:1815:UNK:O	2:A:1819:UNK:N	2.40	0.55
1:B:7:ARG:HB3	1:B:54:PRO:HG3	1.89	0.55
2:D:720:SER:O	2:D:724:LYS:N	2.40	0.55
2:D:785:ASP:N	2:D:785:ASP:OD1	2.39	0.55
2:E:896:PHE:HE1	2:E:901:MET:HB3	1.72	0.55
1:F:568:LYS:H	1:F:572:ASN:H	1.55	0.55
2:A:369:UNK:O	2:A:373:UNK:N	2.40	0.55
2:E:373:UNK:O	2:E:377:UNK:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:108:LEU:HD13	1:G:119:THR:HG23	1.88	0.55
1:B:50:ALA:HB2	1:B:118:LYS:HE2	1.89	0.54
2:D:1294:SER:OG	2:D:1295:SER:N	2.36	0.54
2:D:373:UNK:O	2:D:377:UNK:N	2.39	0.54
2:D:786:SER:OG	2:D:787:LYS:N	2.40	0.54
2:E:1294:SER:OG	2:E:1295:SER:N	2.36	0.54
2:E:827:SER:OG	2:E:829:ASN:OD1	2.25	0.54
1:G:370:LEU:HG	1:G:488:VAL:HB	1.89	0.54
2:A:1073:THR:OG1	2:A:1074:GLY:N	2.40	0.54
2:A:786:SER:OG	2:A:787:LYS:N	2.40	0.54
1:F:50:ALA:HB2	1:F:118:LYS:HE2	1.89	0.54
1:F:211:GLN:HE22	1:F:230:TYR:HB3	1.71	0.54
1:F:370:LEU:HG	1:F:488:VAL:HB	1.89	0.54
2:A:153:UNK:O	2:A:157:UNK:N	2.39	0.54
1:B:1758:HIS:CD2	1:B:1759:SER:H	2.26	0.54
1:G:568:LYS:H	1:G:572:ASN:H	1.55	0.54
1:B:480:VAL:O	1:B:484:ILE:N	2.39	0.54
2:D:896:PHE:HE1	2:D:901:MET:HB3	1.72	0.54
2:E:1132:GLU:HB3	2:E:1172:THR:HG23	1.90	0.54
2:E:786:SER:OG	2:E:787:LYS:N	2.40	0.54
1:F:173:LEU:HD12	1:F:244:ILE:HG12	1.90	0.54
1:B:1505:UNK:O	1:B:1507:UNK:N	2.41	0.54
2:D:938:GLU:O	2:D:942:LYS:N	2.40	0.54
2:E:938:GLU:O	2:E:942:LYS:N	2.40	0.54
3:H:1450:ARG:HB3	3:H:1508:TRP:HE1	1.73	0.54
2:A:938:GLU:O	2:A:942:LYS:N	2.40	0.54
2:D:154:UNK:O	2:D:158:UNK:N	2.41	0.54
2:E:369:UNK:O	2:E:373:UNK:N	2.40	0.54
1:F:82:GLN:HE22	1:F:85:ASN:HD22	1.56	0.54
2:A:1145:LYS:O	2:A:1149:GLY:N	2.34	0.54
2:A:27:UNK:O	2:A:58:UNK:N	2.42	0.54
2:A:896:PHE:HE1	2:A:901:MET:HB3	1.72	0.54
2:D:369:UNK:O	2:D:373:UNK:N	2.40	0.54
2:E:1078:SER:OG	2:E:1079:LYS:N	2.41	0.54
1:G:185:GLY:O	1:G:189:LYS:NZ	2.41	0.54
1:B:173:LEU:HD12	1:B:244:ILE:HG12	1.90	0.53
2:D:1333:ASP:N	2:D:1333:ASP:OD1	2.41	0.53
1:F:1505:UNK:O	1:F:1507:UNK:N	2.41	0.53
1:F:7:ARG:HB3	1:F:54:PRO:HG3	1.89	0.53
1:F:1283:UNK:O	1:F:1287:UNK:N	2.41	0.53
1:F:1758:HIS:CD2	1:F:1759:SER:H	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:GLY:O	1:F:189:LYS:NZ	2.41	0.53
2:D:1078:SER:OG	2:D:1079:LYS:N	2.41	0.53
2:D:1061:SER:HB2	2:D:1081:LYS:HD2	1.90	0.53
1:G:173:LEU:HD12	1:G:244:ILE:HG12	1.89	0.53
2:A:1061:SER:HB2	2:A:1081:LYS:HD2	1.90	0.53
2:A:154:UNK:O	2:A:158:UNK:N	2.41	0.53
2:E:1109:GLU:HA	2:E:1188:GLN:HB2	1.90	0.53
2:E:27:UNK:O	2:E:58:UNK:N	2.41	0.53
2:E:1164:SER:OG	2:E:1165:VAL:N	2.41	0.53
2:E:1333:ASP:N	2:E:1333:ASP:OD1	2.41	0.53
2:E:1350:SER:HA	2:E:1375:GLY:HA3	1.89	0.53
1:F:107:LYS:HA	1:F:110:GLN:HE21	1.74	0.53
1:G:50:ALA:HB2	1:G:118:LYS:HE2	1.89	0.53
1:G:480:VAL:O	1:G:484:ILE:N	2.39	0.53
1:G:527:VAL:HG11	1:G:544:LYS:HB2	1.91	0.53
2:A:1350:SER:HA	2:A:1375:GLY:HA3	1.89	0.53
1:B:107:LYS:HA	1:B:110:GLN:HE21	1.74	0.53
1:B:1679:ASP:N	1:B:1679:ASP:OD1	2.41	0.53
1:B:185:GLY:O	1:B:189:LYS:NZ	2.41	0.53
3:C:1450:ARG:HB3	3:C:1508:TRP:HE1	1.73	0.53
2:D:1109:GLU:HA	2:D:1188:GLN:HB2	1.90	0.53
2:E:1100:HIS:O	2:E:1104:ARG:N	2.40	0.53
1:G:1283:UNK:O	1:G:1287:UNK:N	2.41	0.53
1:G:158:ALA:HB3	1:G:270:ALA:HA	1.91	0.53
1:B:1283:UNK:O	1:B:1287:UNK:N	2.41	0.53
1:B:400:SER:O	1:B:400:SER:OG	2.23	0.53
1:B:404:GLN:HA	1:B:408:PRO:HB3	1.90	0.53
2:E:154:UNK:O	2:E:158:UNK:N	2.41	0.53
1:G:107:LYS:HA	1:G:110:GLN:HE21	1.74	0.53
1:G:1758:HIS:CD2	1:G:1759:SER:H	2.26	0.53
1:B:82:GLN:HE22	1:B:85:ASN:HD22	1.56	0.53
1:F:404:GLN:HA	1:F:408:PRO:HB3	1.90	0.53
1:G:1505:UNK:O	1:G:1507:UNK:N	2.41	0.53
1:B:65:LEU:HD21	1:B:83:VAL:HG23	1.91	0.53
1:F:492:THR:HA	1:F:495:GLN:HE21	1.74	0.53
2:A:1078:SER:OG	2:A:1079:LYS:N	2.41	0.53
2:A:827:SER:OG	2:A:829:ASN:OD1	2.25	0.53
1:B:1766:SER:OG	1:B:1767:GLU:N	2.42	0.53
2:D:1164:SER:OG	2:D:1165:VAL:N	2.41	0.53
1:F:527:VAL:HG11	1:F:544:LYS:HB2	1.91	0.53
1:B:273:HIS:O	1:B:277:LEU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:957:VAL:O	2:D:961:THR:OG1	2.25	0.52
2:A:1333:ASP:N	2:A:1333:ASP:OD1	2.41	0.52
1:B:518:ARG:NH2	1:B:519:ASN:OD1	2.41	0.52
3:C:1491:ARG:O	3:C:1495:ASN:ND2	2.42	0.52
2:D:1350:SER:HA	2:D:1375:GLY:HA3	1.89	0.52
1:F:273:HIS:O	1:F:277:LEU:N	2.43	0.52
1:G:1334:UNK:HA	1:G:1381:UNK:HA	1.91	0.52
1:G:492:THR:HA	1:G:495:GLN:HE21	1.74	0.52
3:H:1491:ARG:O	3:H:1495:ASN:ND2	2.42	0.52
2:A:960:GLU:O	2:A:964:GLU:N	2.39	0.52
2:D:786:SER:O	2:D:788:SER:N	2.42	0.52
2:D:827:SER:OG	2:D:829:ASN:OD1	2.25	0.52
1:G:357:ASN:O	1:G:365:GLN:NE2	2.42	0.52
3:I:1491:ARG:O	3:I:1495:ASN:ND2	2.42	0.52
2:D:27:UNK:O	2:D:58:UNK:N	2.42	0.52
1:G:539:ASP:OD1	1:G:539:ASP:N	2.42	0.52
2:A:1132:GLU:HB3	2:A:1172:THR:HG23	1.90	0.52
2:A:1164:SER:OG	2:A:1165:VAL:N	2.41	0.52
2:D:367:UNK:O	2:D:371:UNK:N	2.43	0.52
2:E:720:SER:O	2:E:724:LYS:N	2.40	0.52
2:E:960:GLU:O	2:E:964:GLU:N	2.39	0.52
1:F:1334:UNK:HA	1:F:1381:UNK:HA	1.91	0.52
1:G:404:GLN:HA	1:G:408:PRO:HB3	1.90	0.52
1:G:518:ARG:NH2	1:G:519:ASN:OD1	2.41	0.52
2:D:1132:GLU:HB3	2:D:1172:THR:HG23	1.90	0.52
1:F:539:ASP:OD1	1:F:539:ASP:N	2.42	0.52
1:F:65:LEU:HD21	1:F:83:VAL:HG23	1.91	0.52
1:G:65:LEU:HD21	1:G:83:VAL:HG23	1.91	0.52
2:A:1109:GLU:HA	2:A:1188:GLN:HB2	1.90	0.52
2:E:1061:SER:HB2	2:E:1081:LYS:HD2	1.90	0.52
1:G:1766:SER:OG	1:G:1767:GLU:N	2.42	0.52
1:B:1334:UNK:HA	1:B:1381:UNK:HA	1.91	0.52
1:B:346:GLN:HG2	1:B:347:GLU:HG2	1.92	0.52
1:B:492:THR:HA	1:B:495:GLN:HE21	1.74	0.52
1:B:527:VAL:HG11	1:B:544:LYS:HB2	1.91	0.52
2:E:752:ILE:HG23	2:E:753:TYR:HD1	1.75	0.52
2:E:786:SER:O	2:E:788:SER:N	2.42	0.52
2:A:367:UNK:O	2:A:371:UNK:N	2.43	0.52
2:A:720:SER:O	2:A:724:LYS:N	2.40	0.52
1:B:1332:UNK:HA	1:B:1346:UNK:HA	1.92	0.52
2:E:936:LEU:O	2:E:940:THR:OG1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:273:HIS:O	1:G:277:LEU:N	2.43	0.52
1:G:82:GLN:HE22	1:G:85:ASN:HD22	1.56	0.52
2:A:1515:ARG:HG2	2:A:1516:ASP:H	1.75	0.52
2:A:39:UNK:O	2:A:43:UNK:N	2.43	0.52
2:D:752:ILE:HG23	2:D:753:TYR:HD1	1.75	0.52
2:E:1144:PHE:O	2:E:1148:HIS:N	2.43	0.52
1:G:1679:ASP:OD1	1:G:1679:ASP:N	2.41	0.52
1:G:161:GLY:N	1:G:245:GLN:OE1	2.41	0.52
3:H:1506:GLN:O	3:H:1511:ASP:N	2.43	0.52
2:D:1144:PHE:O	2:D:1148:HIS:N	2.43	0.51
1:F:259:THR:HA	1:F:289:TRP:HE1	1.75	0.51
1:B:158:ALA:HB3	1:B:270:ALA:HA	1.91	0.51
2:D:1100:HIS:O	2:D:1104:ARG:N	2.40	0.51
1:G:1332:UNK:HA	1:G:1346:UNK:HA	1.92	0.51
2:D:39:UNK:O	2:D:43:UNK:N	2.43	0.51
2:E:1111:PHE:HB2	2:E:1114:TYR:HB2	1.92	0.51
2:E:869:ILE:HG22	2:E:926:LEU:HD22	1.93	0.51
1:F:1766:SER:OG	1:F:1767:GLU:N	2.42	0.51
1:F:346:GLN:HG2	1:F:347:GLU:HG2	1.92	0.51
2:A:786:SER:O	2:A:788:SER:N	2.42	0.51
2:A:869:ILE:HG22	2:A:926:LEU:HD22	1.92	0.51
2:E:367:UNK:O	2:E:371:UNK:N	2.43	0.51
1:F:357:ASN:O	1:F:365:GLN:NE2	2.41	0.51
3:I:1450:ARG:HB3	3:I:1508:TRP:HE1	1.73	0.51
1:B:302:VAL:O	1:B:306:ILE:N	2.43	0.51
1:G:1:MET:N	1:G:11:LEU:O	2.38	0.51
2:A:1144:PHE:O	2:A:1148:HIS:N	2.43	0.51
2:A:936:LEU:O	2:A:940:THR:OG1	2.28	0.51
1:B:461:ASP:HB3	1:B:463:PHE:H	1.75	0.51
1:B:539:ASP:OD1	1:B:539:ASP:N	2.42	0.51
2:D:1111:PHE:HB2	2:D:1114:TYR:HB2	1.92	0.51
1:F:158:ALA:HB3	1:F:270:ALA:HA	1.91	0.51
1:G:1213:UNK:O	1:G:1215:UNK:N	2.43	0.51
1:B:1712:ASN:N	1:B:1712:ASN:OD1	2.43	0.51
3:C:1506:GLN:O	3:C:1511:ASP:N	2.43	0.51
1:F:461:ASP:HB3	1:F:463:PHE:H	1.75	0.51
1:G:346:GLN:HG2	1:G:347:GLU:HG2	1.92	0.51
3:I:1506:GLN:O	3:I:1511:ASP:N	2.43	0.51
1:F:1213:UNK:O	1:F:1215:UNK:N	2.43	0.51
1:F:953:UNK:O	1:F:957:UNK:N	2.44	0.51
1:G:1712:ASN:OD1	1:G:1712:ASN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:259:THR:HA	1:G:289:TRP:HE1	1.75	0.51
2:A:1111:PHE:HB2	2:A:1114:TYR:HB2	1.92	0.51
1:B:1213:UNK:O	1:B:1215:UNK:N	2.43	0.51
1:F:347:GLU:HA	1:F:350:GLN:HB3	1.93	0.51
1:G:2039:LYS:O	1:G:2043:ASP:N	2.44	0.51
2:A:1100:HIS:O	2:A:1104:ARG:N	2.40	0.51
1:B:953:UNK:O	1:B:957:UNK:N	2.44	0.51
2:E:1239:HIS:HB2	2:E:1241:SER:H	1.76	0.51
2:E:39:UNK:O	2:E:43:UNK:N	2.43	0.51
1:G:157:VAL:O	1:G:502:LEU:N	2.44	0.51
1:G:347:GLU:HA	1:G:350:GLN:HB3	1.93	0.51
1:B:1106:UNK:O	1:B:1110:UNK:N	2.44	0.50
1:B:1:MET:N	1:B:11:LEU:O	2.38	0.50
2:D:681:THR:HB	2:D:771:PHE:H	1.76	0.50
1:F:480:VAL:O	1:F:484:ILE:N	2.39	0.50
1:G:461:ASP:HB3	1:G:463:PHE:H	1.75	0.50
2:A:752:ILE:HG23	2:A:753:TYR:HD1	1.75	0.50
1:B:259:THR:HA	1:B:289:TRP:HE1	1.75	0.50
2:E:691:GLU:OE1	2:E:694:GLN:NE2	2.44	0.50
1:F:1106:UNK:O	1:F:1110:UNK:N	2.44	0.50
1:F:217:GLU:HA	1:F:220:GLU:HB2	1.93	0.50
2:E:1772:UNK:HA	3:I:1464:GLU:HG2	1.94	0.50
2:A:1326:ILE:HD12	2:A:1388:MET:HG2	1.94	0.50
1:B:104:LEU:HA	1:B:107:LYS:HB2	1.93	0.50
1:B:217:GLU:HA	1:B:220:GLU:HB2	1.93	0.50
2:D:1515:ARG:HG2	2:D:1516:ASP:H	1.75	0.50
2:D:691:GLU:OE1	2:D:694:GLN:NE2	2.44	0.50
1:F:1679:ASP:N	1:F:1679:ASP:OD1	2.41	0.50
1:G:104:LEU:HA	1:G:107:LYS:HB2	1.93	0.50
1:G:390:ASN:O	1:G:394:ARG:N	2.45	0.50
1:G:953:UNK:O	1:G:957:UNK:N	2.44	0.50
2:A:1361:THR:HB	2:A:1364:GLU:HB2	1.93	0.50
1:B:161:GLY:N	1:B:245:GLN:OE1	2.41	0.50
2:D:1361:THR:HB	2:D:1364:GLU:HB2	1.93	0.50
1:F:1394:UNK:O	1:F:1396:UNK:N	2.45	0.50
2:A:1417:SER:OG	2:A:1418:VAL:N	2.45	0.50
1:B:126:TYR:O	1:B:130:ARG:N	2.44	0.50
1:B:1381:UNK:O	1:B:1431:UNK:N	2.45	0.50
1:B:338:MET:HG3	1:B:421:LEU:HD12	1.94	0.50
2:D:1210:PRO:HB2	2:D:1255:SER:HB2	1.94	0.50
2:D:1349:THR:O	2:D:1376:PHE:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:VAL:O	1:F:502:LEU:N	2.44	0.50
1:G:126:TYR:O	1:G:130:ARG:N	2.44	0.50
2:D:1027:VAL:HB	2:D:1382:ALA:HB3	1.94	0.50
1:F:338:MET:HG3	1:F:421:LEU:HD12	1.94	0.50
1:G:217:GLU:HA	1:G:220:GLU:HB2	1.93	0.50
2:A:1239:HIS:HB2	2:A:1241:SER:H	1.76	0.50
1:B:1394:UNK:O	1:B:1396:UNK:N	2.45	0.50
2:D:1340:SER:OG	2:D:1341:PHE:N	2.45	0.50
2:E:1515:ARG:HG2	2:E:1516:ASP:H	1.75	0.50
1:F:1332:UNK:HA	1:F:1346:UNK:HA	1.92	0.50
1:G:1106:UNK:O	1:G:1110:UNK:N	2.44	0.50
2:A:1015:LEU:HD23	3:C:1510:ASN:HD21	1.77	0.50
2:A:1210:PRO:HB2	2:A:1255:SER:HB2	1.94	0.50
1:B:2039:LYS:O	1:B:2043:ASP:N	2.44	0.50
2:E:681:THR:HB	2:E:771:PHE:H	1.76	0.50
1:F:309:ARG:HB3	1:F:435:ALA:HB1	1.94	0.50
2:A:691:GLU:OE1	2:A:694:GLN:NE2	2.44	0.50
2:A:785:ASP:N	2:A:785:ASP:OD1	2.39	0.50
2:D:1239:HIS:HB2	2:D:1241:SER:H	1.76	0.50
1:F:104:LEU:HA	1:F:107:LYS:HB2	1.93	0.50
1:F:518:ARG:NH2	1:F:519:ASN:OD1	2.41	0.50
1:G:338:MET:HG3	1:G:421:LEU:HD12	1.94	0.50
2:A:1027:VAL:HB	2:A:1382:ALA:HB3	1.93	0.49
1:G:1394:UNK:O	1:G:1396:UNK:N	2.45	0.49
1:B:390:ASN:O	1:B:394:ARG:N	2.45	0.49
2:D:1417:SER:OG	2:D:1418:VAL:N	2.45	0.49
2:D:936:LEU:O	2:D:940:THR:OG1	2.28	0.49
2:E:1027:VAL:HB	2:E:1382:ALA:HB3	1.94	0.49
1:F:1381:UNK:O	1:F:1431:UNK:N	2.45	0.49
2:A:1349:THR:O	2:A:1376:PHE:N	2.45	0.49
1:B:357:ASN:O	1:B:365:GLN:NE2	2.42	0.49
1:F:1396:UNK:O	1:F:1400:UNK:N	2.46	0.49
1:G:1381:UNK:O	1:G:1431:UNK:N	2.45	0.49
1:G:164:GLY:O	1:G:169:TYR:OH	2.28	0.49
2:A:1340:SER:OG	2:A:1341:PHE:N	2.45	0.49
1:B:157:VAL:O	1:B:502:LEU:N	2.44	0.49
1:B:347:GLU:HA	1:B:350:GLN:HB3	1.93	0.49
1:B:514:VAL:HG23	1:B:515:LEU:HD12	1.93	0.49
1:B:764:UNK:O	1:B:768:UNK:N	2.46	0.49
2:D:1310:GLU:OE1	2:D:1310:GLU:N	2.45	0.49
2:D:869:ILE:HG22	2:D:926:LEU:HD22	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1245:ASN:HB3	2:E:1298:ILE:HG12	1.94	0.49
1:F:1712:ASN:OD1	1:F:1712:ASN:N	2.43	0.49
1:F:2039:LYS:O	1:F:2043:ASP:N	2.44	0.49
1:F:514:VAL:HG23	1:F:515:LEU:HD12	1.93	0.49
1:G:764:UNK:O	1:G:768:UNK:N	2.46	0.49
2:D:798:ASN:HA	2:D:801:ARG:HH21	1.77	0.49
1:G:330:ASN:HB3	1:G:332:GLU:HG3	1.95	0.49
2:A:1869:UNK:N	2:A:1884:UNK:O	2.46	0.49
2:A:768:ILE:HG22	2:A:770:PRO:HD3	1.95	0.49
1:F:390:ASN:O	1:F:394:ARG:N	2.45	0.49
1:G:1396:UNK:O	1:G:1400:UNK:N	2.46	0.49
1:G:514:VAL:HG23	1:G:515:LEU:HD12	1.93	0.49
2:D:1326:ILE:HD12	2:D:1388:MET:HG2	1.94	0.49
2:E:1326:ILE:HD12	2:E:1388:MET:HG2	1.93	0.49
2:E:798:ASN:HA	2:E:801:ARG:HH21	1.77	0.49
1:F:126:TYR:O	1:F:130:ARG:N	2.44	0.49
1:F:490:TRP:HE1	1:F:516:THR:HG22	1.78	0.49
2:A:1325:ARG:HH11	2:A:1392:LEU:HD11	1.77	0.49
2:A:681:THR:HB	2:A:771:PHE:H	1.77	0.49
1:B:309:ARG:HB3	1:B:435:ALA:HB1	1.94	0.49
2:E:1078:SER:HA	2:E:1088:ASP:HB3	1.95	0.49
2:E:1210:PRO:HB2	2:E:1255:SER:HB2	1.94	0.49
2:E:1340:SER:OG	2:E:1341:PHE:N	2.45	0.49
2:E:692:VAL:HA	2:E:906:LEU:HD21	1.95	0.49
3:H:1509:GLY:H	3:H:1512:PHE:HB2	1.78	0.49
1:B:1396:UNK:O	1:B:1400:UNK:N	2.46	0.49
1:B:330:ASN:HB3	1:B:332:GLU:HG3	1.95	0.49
3:C:1509:GLY:H	3:C:1512:PHE:HB2	1.78	0.49
2:E:1361:THR:HB	2:E:1364:GLU:HB2	1.94	0.49
2:E:1325:ARG:HH11	2:E:1392:LEU:HD11	1.78	0.49
2:E:1417:SER:OG	2:E:1418:VAL:N	2.45	0.49
1:F:302:VAL:O	1:F:306:ILE:N	2.43	0.49
3:I:1509:GLY:H	3:I:1512:PHE:HB2	1.78	0.49
2:A:1078:SER:HA	2:A:1088:ASP:HB3	1.94	0.49
2:D:1869:UNK:N	2:D:1884:UNK:O	2.46	0.49
2:D:692:VAL:HA	2:D:906:LEU:HD21	1.95	0.49
1:F:161:GLY:N	1:F:245:GLN:OE1	2.41	0.49
1:G:1854:MET:HB2	1:G:1952:ALA:HB3	1.95	0.49
3:H:1451:GLN:NE2	3:H:1456:GLU:OE2	2.46	0.49
2:A:692:VAL:HA	2:A:906:LEU:HD21	1.95	0.48
1:F:764:UNK:O	1:F:768:UNK:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1813:ALA:HA	1:G:1816:ALA:HB3	1.95	0.48
2:A:1245:ASN:HB3	2:A:1298:ILE:HG12	1.94	0.48
1:B:1813:ALA:HA	1:B:1816:ALA:HB3	1.95	0.48
2:E:1326:ILE:HG23	2:E:1388:MET:HG2	1.95	0.48
2:E:243:UNK:O	2:E:247:UNK:N	2.46	0.48
1:F:1905:ARG:O	1:F:1909:THR:OG1	2.29	0.48
1:G:490:TRP:HE1	1:G:516:THR:HG22	1.78	0.48
1:B:1884:TRP:H	1:B:1892:ASN:HD22	1.61	0.48
3:C:1451:GLN:NE2	3:C:1456:GLU:OE2	2.46	0.48
2:D:1051:VAL:HA	2:D:1054:ALA:HB3	1.95	0.48
2:D:243:UNK:O	2:D:247:UNK:N	2.46	0.48
2:D:960:GLU:O	2:D:964:GLU:N	2.39	0.48
2:E:1015:LEU:HD23	3:I:1510:ASN:HD21	1.77	0.48
2:E:368:UNK:O	2:E:372:UNK:N	2.47	0.48
2:E:768:ILE:HG22	2:E:770:PRO:HD3	1.94	0.48
1:F:1872:GLN:HA	1:F:1875:VAL:HG22	1.95	0.48
1:G:1872:GLN:HA	1:G:1875:VAL:HG22	1.95	0.48
1:G:50:ALA:HB1	1:G:56:THR:HB	1.95	0.48
2:D:1078:SER:HA	2:D:1088:ASP:HB3	1.95	0.48
2:D:1099:GLU:O	2:D:1102:GLY:N	2.37	0.48
2:D:1245:ASN:HB3	2:D:1298:ILE:HG12	1.94	0.48
2:D:824:LEU:HD21	2:D:846:LEU:HD22	1.96	0.48
2:E:1349:THR:O	2:E:1376:PHE:N	2.45	0.48
1:G:1308:UNK:HA	1:G:1364:UNK:HA	1.96	0.48
1:G:221:ASN:O	1:G:225:THR:OG1	2.26	0.48
1:B:1308:UNK:HA	1:B:1364:UNK:HA	1.96	0.48
1:B:50:ALA:HB1	1:B:56:THR:HB	1.95	0.48
2:D:1145:LYS:O	2:D:1149:GLY:N	2.34	0.48
2:D:644:THR:O	2:D:647:GLY:N	2.47	0.48
2:E:1869:UNK:N	2:E:1884:UNK:O	2.46	0.48
1:F:190:PHE:O	1:F:194:THR:OG1	2.25	0.48
1:F:218:TRP:O	1:F:225:THR:OG1	2.31	0.48
3:I:1451:GLN:NE2	3:I:1456:GLU:OE2	2.46	0.48
2:D:1325:ARG:HH11	2:D:1392:LEU:HD11	1.78	0.48
1:G:309:ARG:HB3	1:G:435:ALA:HB1	1.94	0.48
2:A:368:UNK:O	2:A:372:UNK:N	2.47	0.48
2:A:798:ASN:HA	2:A:801:ARG:HH21	1.77	0.48
1:B:1905:ARG:O	1:B:1909:THR:OG1	2.29	0.48
1:B:640:UNK:H	1:B:669:UNK:HA	1.79	0.48
2:E:1435:SER:OG	2:E:1435:SER:O	2.31	0.48
2:E:644:THR:O	2:E:647:GLY:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1854:MET:HB2	1:F:1952:ALA:HB3	1.95	0.48
1:F:330:ASN:HB3	1:F:332:GLU:HG3	1.95	0.48
1:G:218:TRP:O	1:G:225:THR:OG1	2.31	0.48
2:A:1310:GLU:N	2:A:1310:GLU:OE1	2.45	0.48
2:A:1326:ILE:HG23	2:A:1388:MET:HG2	1.95	0.48
2:A:243:UNK:O	2:A:247:UNK:N	2.46	0.48
2:A:826:MET:HG2	2:A:867:ALA:H	1.79	0.48
1:B:110:GLN:HG3	1:B:111:GLU:HG3	1.96	0.48
1:F:102:HIS:HE1	1:F:123:ILE:HD13	1.79	0.48
1:B:1390:UNK:N	1:B:1423:UNK:O	2.47	0.48
1:B:1854:MET:HB2	1:B:1952:ALA:HB3	1.95	0.48
1:B:56:THR:HA	1:B:122:LEU:HD21	1.96	0.48
2:D:1390:ALA:HA	2:D:1393:ALA:HB3	1.96	0.48
2:D:711:SER:H	2:D:714:VAL:HB	1.79	0.48
2:E:826:MET:HG2	2:E:867:ALA:H	1.78	0.48
1:F:56:THR:HA	1:F:122:LEU:HD21	1.96	0.48
1:B:1537:UNK:O	1:B:1620:THR:N	2.47	0.48
2:D:768:ILE:HG22	2:D:770:PRO:HD3	1.94	0.48
2:E:1065:GLY:HA3	2:E:1068:LYS:NZ	2.29	0.48
2:E:1145:LYS:O	2:E:1149:GLY:N	2.34	0.48
1:F:467:ASP:OD1	1:F:469:ARG:NE	2.47	0.48
1:G:92:GLU:HA	1:G:96:LEU:HD21	1.96	0.48
2:A:957:VAL:O	2:A:961:THR:OG1	2.25	0.47
1:B:490:TRP:HE1	1:B:516:THR:HG22	1.78	0.47
2:E:294:UNK:O	2:E:298:UNK:N	2.47	0.47
1:F:754:UNK:N	1:F:782:UNK:O	2.47	0.47
1:G:1537:UNK:O	1:G:1620:THR:N	2.47	0.47
1:G:183:LEU:HD22	1:G:254:LYS:HB3	1.96	0.47
2:A:644:THR:O	2:A:647:GLY:N	2.47	0.47
1:B:1927:LEU:O	1:B:1930:SER:OG	2.32	0.47
1:B:218:TRP:O	1:B:225:THR:OG1	2.31	0.47
1:B:384:GLN:O	1:B:388:GLY:N	2.47	0.47
1:B:754:UNK:N	1:B:782:UNK:O	2.47	0.47
1:F:110:GLN:HG3	1:F:111:GLU:HG3	1.96	0.47
2:D:1065:GLY:HA3	2:D:1068:LYS:NZ	2.29	0.47
2:E:1130:ASP:OD1	2:E:1130:ASP:N	2.48	0.47
1:F:1537:UNK:O	1:F:1620:THR:N	2.47	0.47
1:F:21:LEU:O	1:F:24:THR:OG1	2.25	0.47
1:G:102:HIS:HE1	1:G:123:ILE:HD13	1.79	0.47
1:G:1390:UNK:N	1:G:1423:UNK:O	2.47	0.47
1:B:1694:ALA:HB1	1:B:1828:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ASP:HA	1:B:57:PRO:HD3	1.96	0.47
1:F:1390:UNK:N	1:F:1423:UNK:O	2.47	0.47
1:F:400:SER:O	1:F:400:SER:OG	2.23	0.47
1:G:110:GLN:HG3	1:G:111:GLU:HG3	1.96	0.47
3:I:1452:LEU:HD23	3:I:1456:GLU:HG3	1.97	0.47
1:B:190:PHE:O	1:B:194:THR:OG1	2.25	0.47
1:F:431:LEU:HG	1:F:432:LEU:HG	1.96	0.47
1:G:1884:TRP:H	1:G:1892:ASN:HD22	1.61	0.47
1:G:467:ASP:OD1	1:G:469:ARG:NE	2.47	0.47
1:G:502:LEU:HD13	1:G:504:PHE:HE2	1.79	0.47
3:H:1452:LEU:HD23	3:H:1456:GLU:HG3	1.97	0.47
2:A:1099:GLU:O	2:A:1102:GLY:N	2.37	0.47
2:A:183:UNK:O	2:A:187:UNK:N	2.48	0.47
1:B:183:LEU:HD22	1:B:254:LYS:HB3	1.95	0.47
2:D:1326:ILE:HG23	2:D:1388:MET:HG2	1.95	0.47
2:E:1390:ALA:HA	2:E:1393:ALA:HB3	1.96	0.47
1:F:1694:ALA:HB1	1:F:1828:VAL:HG21	1.97	0.47
1:F:336:SER:O	1:F:338:MET:N	2.46	0.47
1:F:640:UNK:H	1:F:669:UNK:HA	1.79	0.47
1:G:1694:ALA:HB1	1:G:1828:VAL:HG21	1.97	0.47
1:G:1927:LEU:O	1:G:1930:SER:OG	2.32	0.47
1:B:100:ASP:O	1:B:102:HIS:N	2.48	0.47
1:B:1872:GLN:HA	1:B:1875:VAL:HG22	1.95	0.47
1:B:502:LEU:HD13	1:B:504:PHE:HE2	1.79	0.47
1:B:92:GLU:HA	1:B:96:LEU:HD21	1.96	0.47
2:D:183:UNK:O	2:D:187:UNK:N	2.48	0.47
1:F:1308:UNK:HA	1:F:1364:UNK:HA	1.96	0.47
1:G:1851:ASN:O	1:G:1896:GLN:NE2	2.48	0.47
1:G:190:PHE:O	1:G:194:THR:OG1	2.25	0.47
1:G:640:UNK:H	1:G:669:UNK:HA	1.79	0.47
1:G:677:UNK:O	1:G:679:UNK:N	2.48	0.47
1:B:164:GLY:O	1:B:169:TYR:OH	2.29	0.47
1:B:431:LEU:HG	1:B:432:LEU:HG	1.97	0.47
2:D:368:UNK:O	2:D:372:UNK:N	2.47	0.47
2:E:1354:GLU:H	2:E:1357:GLU:H	1.62	0.47
1:F:164:GLY:O	1:F:169:TYR:OH	2.28	0.47
1:G:56:THR:HA	1:G:122:LEU:HD21	1.96	0.47
2:A:1051:VAL:HA	2:A:1054:ALA:HB3	1.96	0.47
2:D:1354:GLU:H	2:D:1357:GLU:H	1.62	0.47
2:D:294:UNK:O	2:D:298:UNK:N	2.47	0.47
2:D:597:ALA:H	2:D:610:THR:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1105:UNK:O	1:F:1109:UNK:N	2.48	0.47
1:F:1851:ASN:O	1:F:1896:GLN:NE2	2.48	0.47
1:G:100:ASP:O	1:G:102:HIS:N	2.48	0.47
2:A:1130:ASP:N	2:A:1130:ASP:OD1	2.48	0.47
2:A:586:LYS:HA	2:A:671:VAL:H	1.80	0.47
1:B:102:HIS:HE1	1:B:123:ILE:HD13	1.79	0.47
1:B:268:LYS:NZ	1:B:497:LYS:O	2.42	0.47
3:C:1452:LEU:HD23	3:C:1456:GLU:HG3	1.97	0.47
2:D:826:MET:HG2	2:D:867:ALA:H	1.78	0.47
2:E:183:UNK:O	2:E:187:UNK:N	2.48	0.47
1:F:227:ASP:OD1	1:F:227:ASP:N	2.48	0.47
1:F:314:TYR:HB2	1:F:432:LEU:HD21	1.97	0.47
1:F:527:VAL:HG13	1:F:541:TYR:HA	1.97	0.47
1:G:754:UNK:N	1:G:782:UNK:O	2.47	0.47
2:A:1086:ASP:N	2:A:1086:ASP:OD1	2.47	0.47
2:A:294:UNK:O	2:A:298:UNK:N	2.47	0.47
2:A:599:MET:O	2:A:608:ASP:N	2.48	0.47
2:A:640:LEU:HA	2:A:924:ALA:HA	1.97	0.47
2:A:824:LEU:HD21	2:A:846:LEU:HD22	1.96	0.47
2:D:753:TYR:OH	2:D:764:ASP:O	2.33	0.47
2:E:552:LYS:O	2:E:554:ILE:N	2.48	0.47
2:E:711:SER:H	2:E:714:VAL:HB	1.79	0.47
1:F:650:UNK:O	1:F:654:UNK:N	2.48	0.47
2:A:1304:ALA:HA	2:A:1307:THR:HB	1.97	0.46
2:A:661:ASP:O	2:A:665:LYS:N	2.48	0.46
1:B:650:UNK:O	1:B:654:UNK:N	2.48	0.46
2:D:185:UNK:O	2:D:189:UNK:N	2.48	0.46
2:E:1099:GLU:O	2:E:1102:GLY:N	2.37	0.46
2:E:1304:ALA:HA	2:E:1307:THR:HB	1.97	0.46
2:E:957:VAL:O	2:E:961:THR:OG1	2.25	0.46
1:F:100:ASP:O	1:F:102:HIS:N	2.48	0.46
1:F:1884:TRP:H	1:F:1892:ASN:HD22	1.62	0.46
1:F:183:LEU:HD22	1:F:254:LYS:HB3	1.95	0.46
1:F:50:ALA:HB1	1:F:56:THR:HB	1.95	0.46
1:G:51:ASP:HA	1:G:57:PRO:HD3	1.96	0.46
2:A:1214:PHE:HB3	2:A:1382:ALA:HB2	1.98	0.46
1:B:467:ASP:OD1	1:B:469:ARG:NE	2.47	0.46
1:B:527:VAL:HG13	1:B:541:TYR:HA	1.98	0.46
2:D:586:LYS:HA	2:D:671:VAL:H	1.80	0.46
2:D:834:GLY:O	2:D:836:ASP:N	2.48	0.46
2:E:1038:GLU:O	2:E:1042:PHE:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1051:VAL:HA	2:E:1054:ALA:HB3	1.96	0.46
2:E:640:LEU:HA	2:E:924:ALA:HA	1.97	0.46
2:E:824:LEU:HD21	2:E:846:LEU:HD22	1.96	0.46
1:F:502:LEU:HD13	1:F:504:PHE:HE2	1.79	0.46
1:F:51:ASP:HA	1:F:57:PRO:HD3	1.96	0.46
1:G:227:ASP:N	1:G:227:ASP:OD1	2.48	0.46
2:A:1065:GLY:HA3	2:A:1068:LYS:NZ	2.29	0.46
2:A:1070:ARG:O	2:A:1072:TYR:N	2.49	0.46
2:A:1390:ALA:HA	2:A:1393:ALA:HB3	1.96	0.46
1:B:1851:ASN:O	1:B:1896:GLN:NE2	2.48	0.46
2:E:1310:GLU:OE1	2:E:1310:GLU:N	2.45	0.46
2:E:885:ALA:HA	2:E:888:ILE:HD11	1.98	0.46
1:F:1813:ALA:HA	1:F:1816:ALA:HB3	1.95	0.46
2:E:1070:ARG:O	2:E:1072:TYR:N	2.49	0.46
2:E:834:GLY:O	2:E:836:ASP:N	2.48	0.46
1:F:384:GLN:O	1:F:388:GLY:N	2.46	0.46
1:G:1105:UNK:O	1:G:1109:UNK:N	2.48	0.46
1:G:1905:ARG:O	1:G:1909:THR:OG1	2.29	0.46
1:G:430:HIS:O	1:G:485:ARG:NH1	2.48	0.46
2:A:184:UNK:O	2:A:188:UNK:N	2.49	0.46
2:A:185:UNK:O	2:A:189:UNK:N	2.48	0.46
2:E:1214:PHE:HB3	2:E:1382:ALA:HB2	1.98	0.46
2:E:185:UNK:O	2:E:189:UNK:N	2.48	0.46
1:F:677:UNK:O	1:F:679:UNK:N	2.48	0.46
1:F:92:GLU:HA	1:F:96:LEU:HD21	1.96	0.46
1:G:260:PRO:O	1:G:264:ARG:N	2.44	0.46
1:G:341:ILE:HA	1:G:418:ASN:HD22	1.80	0.46
2:A:711:SER:H	2:A:714:VAL:HB	1.79	0.46
1:B:677:UNK:O	1:B:679:UNK:N	2.48	0.46
2:E:184:UNK:O	2:E:188:UNK:N	2.49	0.46
1:F:107:LYS:HA	1:F:110:GLN:HG2	1.97	0.46
1:F:1927:LEU:O	1:F:1930:SER:OG	2.32	0.46
1:G:302:VAL:O	1:G:306:ILE:N	2.43	0.46
1:G:82:GLN:OE1	1:G:134:LYS:NZ	2.45	0.46
2:A:552:LYS:O	2:A:554:ILE:N	2.48	0.46
2:D:1754:UNK:O	2:D:1758:UNK:N	2.49	0.46
1:G:429:SER:H	1:G:484:ILE:HD12	1.80	0.46
1:G:431:LEU:HG	1:G:432:LEU:HG	1.96	0.46
2:A:1354:GLU:H	2:A:1357:GLU:H	1.62	0.46
1:B:227:ASP:OD1	1:B:227:ASP:N	2.48	0.46
2:E:661:ASP:O	2:E:665:LYS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1101:UNK:O	1:F:1103:UNK:N	2.49	0.46
1:F:82:GLN:OE1	1:F:134:LYS:NZ	2.45	0.46
1:B:314:TYR:HB2	1:B:432:LEU:HD21	1.97	0.46
2:D:1304:ALA:HA	2:D:1307:THR:HB	1.97	0.46
2:D:661:ASP:O	2:D:665:LYS:N	2.48	0.46
2:E:1076:VAL:HB	2:E:1087:LYS:HD3	1.98	0.46
2:E:586:LYS:HA	2:E:671:VAL:H	1.80	0.46
2:E:597:ALA:H	2:E:610:THR:HA	1.80	0.46
1:F:341:ILE:HA	1:F:418:ASN:HD22	1.80	0.46
1:G:1101:UNK:O	1:G:1103:UNK:N	2.49	0.46
2:A:1246:CYS:SG	2:A:1247:SER:N	2.89	0.46
2:D:1076:VAL:HB	2:D:1087:LYS:HD3	1.98	0.46
2:D:1130:ASP:OD1	2:D:1130:ASP:N	2.48	0.46
2:D:1214:PHE:HB3	2:D:1382:ALA:HB2	1.98	0.46
2:D:552:LYS:O	2:D:554:ILE:N	2.48	0.46
2:E:1246:CYS:SG	2:E:1247:SER:N	2.89	0.46
1:F:1870:ALA:HA	1:F:1873:TYR:HD2	1.81	0.46
1:F:429:SER:H	1:F:484:ILE:HD12	1.80	0.46
1:G:234:ILE:HG12	1:G:424:ALA:HB3	1.98	0.46
1:G:314:TYR:HB2	1:G:432:LEU:HD21	1.97	0.46
2:A:1754:UNK:O	2:A:1758:UNK:N	2.49	0.45
2:A:597:ALA:H	2:A:610:THR:HA	1.80	0.45
2:A:810:LYS:HG2	2:A:815:ILE:HD11	1.99	0.45
1:B:430:HIS:O	1:B:485:ARG:NH1	2.49	0.45
2:D:184:UNK:O	2:D:188:UNK:N	2.49	0.45
2:D:873:ARG:HG3	2:D:874:GLY:H	1.82	0.45
1:F:430:HIS:O	1:F:485:ARG:NH1	2.49	0.45
1:G:107:LYS:HA	1:G:110:GLN:HG2	1.97	0.45
1:G:650:UNK:O	1:G:654:UNK:N	2.48	0.45
1:B:1105:UNK:O	1:B:1109:UNK:N	2.48	0.45
2:D:1514:LYS:HB3	2:D:1515:ARG:H	1.57	0.45
2:E:1148:HIS:NE2	2:E:1153:ASP:OD1	2.48	0.45
2:E:1280:ILE:HA	2:E:1280:ILE:HD12	1.82	0.45
1:G:336:SER:O	1:G:338:MET:N	2.46	0.45
2:A:1076:VAL:HB	2:A:1087:LYS:HD3	1.98	0.45
2:A:1148:HIS:NE2	2:A:1153:ASP:OD1	2.49	0.45
2:A:1029:PRO:HA	2:A:1193:TRP:HZ2	1.81	0.45
2:E:873:ARG:HG3	2:E:874:GLY:H	1.82	0.45
1:F:22:VAL:O	1:F:26:SER:N	2.50	0.45
1:F:497:LYS:HD3	1:F:497:LYS:HA	1.82	0.45
1:F:825:UNK:N	1:F:836:UNK:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:229:ASP:OD1	1:G:229:ASP:N	2.50	0.45
1:G:825:UNK:N	1:G:836:UNK:O	2.50	0.45
2:A:1309:VAL:O	2:A:1313:ASP:N	2.48	0.45
1:B:429:SER:H	1:B:484:ILE:HD12	1.80	0.45
2:D:1038:GLU:O	2:D:1042:PHE:N	2.45	0.45
1:G:21:LEU:O	1:G:24:THR:OG1	2.25	0.45
1:G:527:VAL:HG13	1:G:541:TYR:HA	1.97	0.45
1:B:107:LYS:HA	1:B:110:GLN:HG2	1.97	0.45
1:B:194:THR:HA	1:B:197:GLU:HB2	1.99	0.45
2:D:1070:ARG:O	2:D:1072:TYR:N	2.49	0.45
2:D:1029:PRO:HA	2:D:1193:TRP:HZ2	1.81	0.45
2:D:599:MET:O	2:D:608:ASP:N	2.48	0.45
2:D:885:ALA:HA	2:D:888:ILE:HD11	1.98	0.45
2:E:1254:VAL:O	2:E:1256:ALA:N	2.35	0.45
2:E:720:SER:HA	2:E:723:ALA:HB3	1.99	0.45
1:F:156:LEU:HD11	1:F:502:LEU:HG	1.99	0.45
1:G:1104:UNK:O	1:G:1106:UNK:N	2.50	0.45
1:G:1513:UNK:O	1:G:1517:UNK:N	2.50	0.45
1:G:1870:ALA:HA	1:G:1873:TYR:HD2	1.81	0.45
2:A:753:TYR:OH	2:A:764:ASP:O	2.33	0.45
1:B:69:SER:OG	1:B:80:PHE:O	2.35	0.45
2:D:640:LEU:HA	2:D:924:ALA:HA	1.97	0.45
1:F:426:PRO:HG2	1:F:432:LEU:HD11	1.99	0.45
1:G:69:SER:OG	1:G:80:PHE:O	2.35	0.45
1:B:1870:ALA:HA	1:B:1873:TYR:HD2	1.81	0.45
2:D:12:UNK:O	2:D:16:UNK:N	2.50	0.45
1:F:1513:UNK:O	1:F:1517:UNK:N	2.50	0.45
1:G:156:LEU:HD11	1:G:502:LEU:HG	1.99	0.45
1:G:799:UNK:O	1:G:803:UNK:N	2.50	0.45
2:A:1123:GLN:N	2:A:1182:ASP:O	2.49	0.45
2:A:885:ALA:HA	2:A:888:ILE:HD11	1.98	0.45
1:B:799:UNK:O	1:B:803:UNK:N	2.50	0.45
2:D:810:LYS:HG2	2:D:815:ILE:HD11	1.99	0.45
1:F:69:SER:OG	1:F:80:PHE:O	2.35	0.45
2:A:873:ARG:HG3	2:A:874:GLY:H	1.82	0.45
1:B:1101:UNK:O	1:B:1103:UNK:N	2.49	0.45
1:B:1513:UNK:O	1:B:1517:UNK:N	2.50	0.45
1:B:260:PRO:O	1:B:264:ARG:N	2.44	0.45
1:B:336:SER:O	1:B:338:MET:N	2.46	0.45
2:D:1015:LEU:HD23	3:H:1510:ASN:HD21	1.82	0.45
2:E:12:UNK:O	2:E:16:UNK:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:753:TYR:OH	2:E:764:ASP:O	2.33	0.45
1:F:1923:ASP:HB3	1:F:1924:ILE:H	1.50	0.45
1:G:120:LYS:HA	1:G:120:LYS:HD2	1.78	0.45
2:A:834:GLY:O	2:A:836:ASP:N	2.48	0.45
1:B:156:LEU:HD11	1:B:502:LEU:HG	1.99	0.45
1:B:221:ASN:O	1:B:225:THR:OG1	2.26	0.45
2:D:1246:CYS:SG	2:D:1247:SER:N	2.89	0.45
2:E:1352:THR:OG1	2:E:1353:LEU:N	2.50	0.45
1:F:284:ALA:HB3	1:F:455:ILE:HG12	1.99	0.45
1:F:799:UNK:O	1:F:803:UNK:N	2.50	0.45
1:G:426:PRO:HG2	1:G:432:LEU:HD11	1.99	0.45
2:A:1352:THR:OG1	2:A:1353:LEU:N	2.50	0.44
2:A:1436:VAL:H	2:A:1518:ARG:HH22	1.65	0.44
1:B:341:ILE:HA	1:B:418:ASN:HD22	1.80	0.44
1:B:426:PRO:HG2	1:B:432:LEU:HD11	1.99	0.44
1:B:284:ALA:HB3	1:B:455:ILE:HG12	1.99	0.44
2:D:1086:ASP:N	2:D:1086:ASP:OD1	2.47	0.44
2:D:1426:LEU:HG	2:D:1427:THR:HG23	1.99	0.44
2:D:1436:VAL:H	2:D:1518:ARG:HH22	1.65	0.44
2:E:1426:LEU:HG	2:E:1427:THR:HG23	1.99	0.44
2:E:599:MET:O	2:E:608:ASP:N	2.48	0.44
1:F:104:LEU:HA	1:F:107:LYS:HD3	1.99	0.44
1:F:1104:UNK:O	1:F:1106:UNK:N	2.50	0.44
1:F:268:LYS:NZ	1:F:497:LYS:O	2.42	0.44
1:G:32:GLN:O	1:G:36:GLN:N	2.39	0.44
1:G:384:GLN:O	1:G:388:GLY:N	2.47	0.44
1:B:309:ARG:HD3	1:B:309:ARG:HA	1.71	0.44
2:E:1029:PRO:HA	2:E:1193:TRP:HZ2	1.81	0.44
2:E:1754:UNK:O	2:E:1758:UNK:N	2.49	0.44
2:E:584:SER:H	2:E:674:LYS:HZ2	1.64	0.44
2:E:810:LYS:HG2	2:E:815:ILE:HD11	1.99	0.44
1:G:1689:ASP:O	1:G:1693:ARG:N	2.51	0.44
2:A:1426:LEU:HG	2:A:1427:THR:HG23	1.99	0.44
2:A:12:UNK:O	2:A:16:UNK:N	2.50	0.44
2:D:1280:ILE:HA	2:D:1280:ILE:HD12	1.82	0.44
1:F:1694:ALA:HA	1:F:1697:HIS:HB3	1.99	0.44
1:B:1104:UNK:O	1:B:1106:UNK:N	2.49	0.44
1:B:1391:UNK:HA	1:B:1422:UNK:HA	1.99	0.44
1:B:1689:ASP:O	1:B:1693:ARG:N	2.50	0.44
1:B:1694:ALA:HA	1:B:1697:HIS:HB3	1.99	0.44
1:B:234:ILE:HG12	1:B:424:ALA:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1745:LYS:HA	1:F:1745:LYS:HD2	1.77	0.44
1:G:1312:UNK:N	1:G:1361:UNK:O	2.51	0.44
2:A:1514:LYS:HB3	2:A:1515:ARG:H	1.57	0.44
1:B:1548:UNK:O	1:B:1552:UNK:N	2.51	0.44
1:B:825:UNK:N	1:B:836:UNK:O	2.49	0.44
2:D:1291:LEU:HA	2:D:1291:LEU:HD23	1.82	0.44
1:F:118:LYS:HD2	1:F:118:LYS:HA	1.90	0.44
2:A:720:SER:HA	2:A:723:ALA:HB3	1.99	0.44
1:B:104:LEU:HA	1:B:107:LYS:HD3	1.99	0.44
2:D:1123:GLN:HB2	2:D:1182:ASP:HB3	2.00	0.44
2:D:1341:PHE:N	2:D:1343:PHE:O	2.48	0.44
2:D:1772:UNK:HA	3:H:1464:GLU:HG2	2.00	0.44
1:F:1183:UNK:HA	1:F:1193:UNK:HA	2.00	0.44
2:A:1099:GLU:HB3	2:A:1100:HIS:H	1.70	0.44
2:D:1265:PHE:HB3	2:D:1266:LYS:HZ2	1.83	0.44
2:E:1436:VAL:H	2:E:1518:ARG:HH22	1.65	0.44
1:F:1391:UNK:HA	1:F:1422:UNK:HA	1.99	0.44
1:F:234:ILE:HG12	1:F:424:ALA:HB3	1.98	0.44
2:A:1191:THR:HB	2:A:1192:GLY:H	1.55	0.44
1:B:22:VAL:O	1:B:26:SER:N	2.50	0.44
1:G:194:THR:HA	1:G:197:GLU:HB2	1.99	0.44
1:B:1884:TRP:O	1:B:1892:ASN:ND2	2.51	0.44
2:D:1204:ILE:HA	2:D:1204:ILE:HD13	1.90	0.44
2:D:1326:ILE:H	2:D:1326:ILE:HG12	1.53	0.44
1:F:1884:TRP:O	1:F:1892:ASN:ND2	2.51	0.44
1:F:194:THR:HA	1:F:197:GLU:HB2	1.99	0.44
1:G:1694:ALA:HA	1:G:1697:HIS:HB3	1.99	0.44
1:G:284:ALA:HB3	1:G:455:ILE:HG12	1.99	0.44
1:G:501:ILE:HB	1:G:526:ARG:HB3	2.00	0.44
2:E:204:UNK:O	2:E:206:UNK:N	2.51	0.43
1:F:446:ASN:O	1:F:448:VAL:N	2.51	0.43
1:B:229:ASP:N	1:B:229:ASP:OD1	2.50	0.43
2:D:1254:VAL:O	2:D:1256:ALA:N	2.35	0.43
2:D:1517:PRO:HG2	2:D:1518:ARG:HE	1.83	0.43
1:F:1548:UNK:O	1:F:1552:UNK:N	2.51	0.43
1:G:1548:UNK:O	1:G:1552:UNK:N	2.51	0.43
1:G:326:ASP:OD2	1:G:394:ARG:NH1	2.42	0.43
1:G:446:ASN:O	1:G:448:VAL:N	2.51	0.43
2:A:1123:GLN:HB2	2:A:1182:ASP:HB3	2.00	0.43
1:B:1312:UNK:N	1:B:1361:UNK:O	2.51	0.43
2:E:1517:PRO:HG2	2:E:1518:ARG:HE	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1689:ASP:O	1:F:1693:ARG:N	2.51	0.43
1:G:104:LEU:HA	1:G:107:LYS:HD3	1.99	0.43
1:B:168:ASP:N	1:B:168:ASP:OD1	2.51	0.43
1:B:288:SER:OG	1:B:291:SER:N	2.42	0.43
3:C:1449:LYS:HE2	3:C:1449:LYS:HB3	1.78	0.43
2:D:1095:THR:HA	2:D:1099:GLU:HG3	2.01	0.43
2:D:644:THR:O	2:D:646:ALA:N	2.51	0.43
1:F:1777:THR:O	1:F:1781:LEU:N	2.48	0.43
1:G:288:SER:OG	1:G:291:SER:N	2.42	0.43
1:G:787:UNK:O	1:G:789:UNK:N	2.52	0.43
3:H:1457:ALA:O	3:H:1461:ASP:N	2.52	0.43
3:I:1457:ALA:O	3:I:1461:ASP:N	2.52	0.43
2:A:644:THR:O	2:A:646:ALA:N	2.51	0.43
2:A:658:LEU:O	2:A:662:GLY:N	2.51	0.43
2:D:1352:THR:OG1	2:D:1353:LEU:N	2.50	0.43
2:D:720:SER:HA	2:D:723:ALA:HB3	1.99	0.43
2:D:801:ARG:HE	2:D:801:ARG:HB2	1.60	0.43
2:E:1060:ILE:HA	2:E:1079:LYS:HA	2.00	0.43
2:E:1079:LYS:HG3	2:E:1080:THR:HG22	2.01	0.43
1:G:1376:UNK:O	1:G:1378:UNK:N	2.52	0.43
2:A:584:SER:H	2:A:674:LYS:HZ2	1.65	0.43
2:A:791:ALA:HA	2:A:794:ILE:HG22	2.01	0.43
1:B:21:LEU:O	1:B:24:THR:OG1	2.25	0.43
1:B:305:PHE:HA	1:B:308:VAL:HG12	2.01	0.43
1:B:501:ILE:HB	1:B:526:ARG:HB3	2.00	0.43
2:D:1148:HIS:NE2	2:D:1153:ASP:OD1	2.48	0.43
2:E:1265:PHE:HB3	2:E:1266:LYS:HZ2	1.84	0.43
1:F:1376:UNK:O	1:F:1378:UNK:N	2.52	0.43
2:D:791:ALA:HA	2:D:794:ILE:HG22	2.01	0.43
2:E:1095:THR:HA	2:E:1099:GLU:HG3	2.01	0.43
2:E:644:THR:O	2:E:646:ALA:N	2.51	0.43
2:E:708:SER:OG	2:E:709:ARG:N	2.52	0.43
2:A:1316:VAL:HG21	2:A:1404:VAL:HG11	2.01	0.43
2:D:204:UNK:O	2:D:206:UNK:N	2.51	0.43
2:D:658:LEU:O	2:D:662:GLY:N	2.51	0.43
2:E:791:ALA:HA	2:E:794:ILE:HG22	2.01	0.43
1:G:1391:UNK:HA	1:G:1422:UNK:HA	1.99	0.43
1:G:309:ARG:HA	1:G:309:ARG:HD3	1.71	0.43
2:A:1095:THR:HA	2:A:1099:GLU:HG3	2.01	0.43
1:B:1376:UNK:O	1:B:1378:UNK:N	2.52	0.43
1:B:254:LYS:HE2	1:B:289:TRP:HH2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ASN:O	1:B:448:VAL:N	2.51	0.43
3:C:1457:ALA:O	3:C:1461:ASP:N	2.52	0.43
2:E:696:LEU:O	2:E:700:GLY:N	2.52	0.43
2:E:826:MET:N	2:E:867:ALA:O	2.37	0.43
1:B:158:ALA:H	1:B:270:ALA:H	1.66	0.43
1:B:208:VAL:HG11	1:B:308:VAL:HG23	2.01	0.43
2:D:1060:ILE:HA	2:D:1079:LYS:HA	2.00	0.43
2:D:1096:SER:H	2:D:1099:GLU:HB2	1.84	0.43
2:E:711:SER:O	2:E:715:THR:OG1	2.30	0.43
1:F:171:GLU:HA	1:F:174:ARG:HB3	2.00	0.43
1:F:305:PHE:HA	1:F:308:VAL:HG12	2.01	0.43
1:F:501:ILE:HB	1:F:526:ARG:HB3	2.00	0.43
1:F:787:UNK:O	1:F:789:UNK:N	2.52	0.43
1:G:171:GLU:HA	1:G:174:ARG:HB3	2.00	0.43
1:G:1884:TRP:O	1:G:1892:ASN:ND2	2.51	0.43
1:G:360:LEU:HD11	1:G:385:SER:HB3	2.01	0.43
2:A:901:MET:H	2:A:901:MET:HG3	1.64	0.42
1:B:787:UNK:O	1:B:789:UNK:N	2.52	0.42
2:D:204:UNK:O	2:D:207:UNK:N	2.52	0.42
2:D:584:SER:H	2:D:674:LYS:HZ2	1.65	0.42
2:E:1123:GLN:HB2	2:E:1182:ASP:HB3	2.00	0.42
2:E:1291:LEU:HD23	2:E:1291:LEU:HA	1.82	0.42
1:G:158:ALA:H	1:G:270:ALA:H	1.66	0.42
1:G:22:VAL:O	1:G:26:SER:N	2.50	0.42
1:G:208:VAL:HG11	1:G:308:VAL:HG23	2.01	0.42
2:A:1060:ILE:HA	2:A:1079:LYS:HA	2.00	0.42
1:B:1685:LYS:HD3	1:B:1685:LYS:HA	1.85	0.42
1:B:196:SER:OG	1:B:213:LEU:O	2.37	0.42
1:B:360:LEU:HD11	1:B:385:SER:HB3	2.01	0.42
2:E:1316:VAL:HG21	2:E:1404:VAL:HG11	2.01	0.42
2:E:1341:PHE:N	2:E:1343:PHE:O	2.48	0.42
2:E:658:LEU:O	2:E:662:GLY:N	2.51	0.42
1:F:309:ARG:HG3	1:F:439:ILE:HB	2.01	0.42
1:G:1183:UNK:HA	1:G:1193:UNK:HA	2.00	0.42
1:G:1699:LYS:HG2	1:G:1699:LYS:H	1.60	0.42
1:G:251:VAL:O	1:G:255:LEU:N	2.51	0.42
1:G:254:LYS:HE2	1:G:289:TRP:HH2	1.84	0.42
1:B:1183:UNK:HA	1:B:1193:UNK:HA	2.00	0.42
1:B:1691:TRP:CE2	1:B:1783:LEU:HG	2.54	0.42
1:B:3:ALA:N	1:B:9:LEU:O	2.50	0.42
2:D:1111:PHE:HD1	2:D:1111:PHE:HA	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1086:ASP:N	2:E:1086:ASP:OD1	2.47	0.42
2:E:1309:VAL:O	2:E:1313:ASP:N	2.48	0.42
1:F:229:ASP:OD1	1:F:229:ASP:N	2.50	0.42
1:G:196:SER:OG	1:G:213:LEU:O	2.37	0.42
1:G:305:PHE:HA	1:G:308:VAL:HG12	2.01	0.42
2:A:1079:LYS:HG3	2:A:1080:THR:HG22	2.01	0.42
2:A:708:SER:OG	2:A:709:ARG:N	2.52	0.42
2:E:1191:THR:HB	2:E:1192:GLY:H	1.55	0.42
1:F:297:ARG:HA	1:F:297:ARG:HD2	1.87	0.42
1:F:393:LEU:HD23	1:F:393:LEU:HA	1.86	0.42
1:G:309:ARG:HG3	1:G:439:ILE:HB	2.01	0.42
1:G:371:VAL:HB	1:G:489:LYS:HA	2.01	0.42
1:G:268:LYS:NZ	1:G:497:LYS:O	2.42	0.42
2:A:1517:PRO:HG2	2:A:1518:ARG:HE	1.83	0.42
1:B:1804:PHE:HE1	1:B:1818:LEU:HG	1.84	0.42
1:B:611:UNK:N	1:B:639:UNK:O	2.53	0.42
2:D:696:LEU:O	2:D:700:GLY:N	2.52	0.42
2:E:204:UNK:O	2:E:207:UNK:N	2.53	0.42
1:F:1312:UNK:N	1:F:1361:UNK:O	2.51	0.42
1:F:158:ALA:H	1:F:270:ALA:H	1.66	0.42
1:F:211:GLN:NE2	1:F:230:TYR:O	2.53	0.42
1:G:1691:TRP:CE2	1:G:1783:LEU:HG	2.55	0.42
2:A:204:UNK:O	2:A:206:UNK:N	2.51	0.42
2:A:696:LEU:O	2:A:700:GLY:N	2.52	0.42
2:A:711:SER:O	2:A:715:THR:OG1	2.30	0.42
1:B:1148:UNK:HA	1:B:1157:UNK:HA	2.02	0.42
1:B:171:GLU:HA	1:B:174:ARG:HB3	2.01	0.42
1:B:309:ARG:HG3	1:B:439:ILE:HB	2.01	0.42
1:F:221:ASN:O	1:F:225:THR:OG1	2.26	0.42
1:G:1148:UNK:HA	1:G:1157:UNK:HA	2.02	0.42
2:A:1413:LYS:HA	2:A:1413:LYS:HD2	1.95	0.42
1:B:1923:ASP:HB3	1:B:1924:ILE:H	1.50	0.42
1:B:32:GLN:O	1:B:36:GLN:N	2.39	0.42
2:D:777:GLN:OE1	2:D:777:GLN:N	2.52	0.42
2:E:1334:ASP:OD1	2:E:1335:PHE:N	2.53	0.42
2:A:204:UNK:O	2:A:207:UNK:N	2.52	0.42
2:A:777:GLN:N	2:A:777:GLN:OE1	2.52	0.42
1:B:1777:THR:O	1:B:1781:LEU:N	2.48	0.42
2:D:708:SER:OG	2:D:709:ARG:N	2.52	0.42
2:E:1096:SER:H	2:E:1099:GLU:HB2	1.84	0.42
2:E:777:GLN:OE1	2:E:777:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:360:LEU:HD11	1:F:385:SER:HB3	2.01	0.42
2:A:1096:SER:H	2:A:1099:GLU:HB2	1.84	0.42
1:B:29:ILE:HA	1:B:29:ILE:HD12	1.89	0.42
1:B:28:PHE:HB3	1:B:64:PHE:HE2	1.85	0.42
2:D:1309:VAL:O	2:D:1313:ASP:N	2.48	0.42
2:E:1249:SER:OG	2:E:1250:GLY:N	2.53	0.42
1:F:196:SER:OG	1:F:213:LEU:O	2.37	0.42
1:F:162:GLY:HA3	1:F:275:GLN:HB2	2.02	0.42
1:F:32:GLN:O	1:F:36:GLN:N	2.39	0.42
1:G:1804:PHE:HE1	1:G:1818:LEU:HG	1.84	0.42
1:B:1745:LYS:HD2	1:B:1745:LYS:HA	1.77	0.42
2:D:1079:LYS:HG3	2:D:1080:THR:HG22	2.01	0.42
2:E:1168:LEU:HG	2:E:1169:LYS:HG2	2.02	0.42
2:E:1204:ILE:HA	2:E:1204:ILE:HD13	1.90	0.42
1:F:168:ASP:OD1	1:F:168:ASP:N	2.51	0.42
1:F:1691:TRP:CE2	1:F:1783:LEU:HG	2.54	0.42
1:F:1833:TYR:O	1:F:1837:THR:OG1	2.28	0.42
1:F:288:SER:OG	1:F:291:SER:N	2.42	0.42
1:F:371:VAL:HB	1:F:489:LYS:HA	2.01	0.42
1:F:502:LEU:HD23	1:F:502:LEU:HA	1.90	0.42
2:A:801:ARG:HB2	2:A:801:ARG:HE	1.60	0.41
2:D:711:SER:O	2:D:715:THR:OG1	2.30	0.41
1:F:1804:PHE:HE1	1:F:1818:LEU:HG	1.84	0.41
1:F:28:PHE:HB3	1:F:64:PHE:HE2	1.85	0.41
1:G:156:LEU:HD12	1:G:156:LEU:HA	1.87	0.41
2:A:1076:VAL:HG11	2:A:1089:VAL:HA	2.02	0.41
2:A:298:UNK:O	2:A:300:UNK:N	2.54	0.41
2:D:1334:ASP:OD1	2:D:1335:PHE:N	2.53	0.41
2:D:1316:VAL:HG21	2:D:1404:VAL:HG11	2.01	0.41
2:E:1076:VAL:HG11	2:E:1089:VAL:HA	2.02	0.41
2:E:1347:LYS:HA	2:E:1347:LYS:HD3	1.93	0.41
1:F:611:UNK:N	1:F:639:UNK:O	2.53	0.41
2:A:1249:SER:OG	2:A:1250:GLY:N	2.53	0.41
2:A:765:LEU:HA	2:A:765:LEU:HD23	1.88	0.41
2:E:1111:PHE:HA	2:E:1111:PHE:HD1	1.72	0.41
1:G:211:GLN:NE2	1:G:230:TYR:O	2.53	0.41
1:G:611:UNK:N	1:G:639:UNK:O	2.53	0.41
2:D:1076:VAL:HG11	2:D:1089:VAL:HA	2.02	0.41
2:D:946:GLU:O	2:D:950:THR:N	2.52	0.41
2:E:1308:SER:OG	2:E:1308:SER:O	2.37	0.41
2:E:1349:THR:HA	2:E:1376:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1925:ILE:HA	1:B:1928:GLN:HB2	2.02	0.41
1:B:251:VAL:O	1:B:255:LEU:N	2.51	0.41
2:D:298:UNK:O	2:D:300:UNK:N	2.54	0.41
2:E:1167:LEU:HA	2:E:1167:LEU:HD23	1.90	0.41
2:E:1869:UNK:O	2:E:1884:UNK:N	2.53	0.41
1:F:1148:UNK:HA	1:F:1157:UNK:HA	2.02	0.41
1:F:254:LYS:HE2	1:F:289:TRP:HH2	1.84	0.41
1:F:208:VAL:HG11	1:F:308:VAL:HG23	2.01	0.41
1:G:162:GLY:HA3	1:G:275:GLN:HB2	2.02	0.41
2:A:826:MET:N	2:A:867:ALA:O	2.37	0.41
1:B:1709:ILE:HD12	1:B:1770:LEU:HD23	2.03	0.41
1:F:53:GLU:HG3	1:F:112:ASN:HB3	2.03	0.41
2:A:394:UNK:O	2:A:396:UNK:N	2.54	0.41
2:D:1168:LEU:HG	2:D:1169:LYS:HG2	2.02	0.41
1:F:1699:LYS:H	1:F:1699:LYS:HG2	1.60	0.41
1:G:485:ARG:HA	1:G:485:ARG:HD2	1.85	0.41
2:A:179:UNK:H	1:G:705:UNK:HA	1.86	0.41
2:A:1308:SER:OG	2:A:1308:SER:O	2.37	0.41
2:A:1869:UNK:O	2:A:1884:UNK:N	2.54	0.41
2:A:946:GLU:O	2:A:950:THR:N	2.52	0.41
1:B:211:GLN:NE2	1:B:230:TYR:O	2.53	0.41
1:B:213:LEU:HA	1:B:213:LEU:HD12	1.94	0.41
1:B:215:ILE:HA	1:B:218:TRP:CD2	2.56	0.41
2:D:1051:VAL:O	2:D:1055:TRP:N	2.54	0.41
2:D:1167:LEU:HD23	2:D:1167:LEU:HA	1.90	0.41
2:D:1349:THR:HA	2:D:1376:PHE:CE1	2.55	0.41
1:F:215:ILE:HA	1:F:218:TRP:CD2	2.56	0.41
1:F:485:ARG:HA	1:F:485:ARG:HD2	1.85	0.41
1:G:28:PHE:HB3	1:G:64:PHE:HE2	1.85	0.41
2:A:1045:PHE:HD1	2:A:1045:PHE:HA	1.78	0.41
2:A:1085:ASP:OD2	2:A:1085:ASP:N	2.50	0.41
2:A:1319:ILE:HD13	2:A:1325:ARG:HA	2.03	0.41
1:B:166:THR:HG21	1:B:507:GLY:HA3	2.02	0.41
3:C:1457:ALA:HA	3:C:1460:LYS:HB3	2.03	0.41
2:D:1748:UNK:O	2:D:1752:UNK:N	2.54	0.41
1:F:1709:ILE:HD12	1:F:1770:LEU:HD23	2.03	0.41
1:F:1728:ARG:HB3	1:F:1732:ASN:HD22	1.85	0.41
1:G:166:THR:HG21	1:G:507:GLY:HA3	2.02	0.41
3:H:1481:ASP:HB3	3:H:1484:GLU:HB3	2.02	0.41
2:A:1748:UNK:O	2:A:1752:UNK:N	2.54	0.41
2:D:1249:SER:OG	2:D:1250:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1630:GLY:N	1:F:1637:LEU:O	2.54	0.41
1:G:1630:GLY:N	1:G:1637:LEU:O	2.54	0.41
1:G:168:ASP:N	1:G:168:ASP:OD1	2.51	0.41
1:G:1925:ILE:HA	1:G:1928:GLN:HB2	2.02	0.41
1:G:407:ILE:HG22	1:G:410:SER:HB2	2.03	0.41
2:A:1038:GLU:O	2:A:1042:PHE:N	2.45	0.41
1:B:29:ILE:HG12	1:B:61:VAL:HG22	2.03	0.41
2:D:1205:ILE:HA	2:D:1208:VAL:HG22	2.03	0.41
2:E:1139:GLU:HB3	2:E:1168:LEU:HD22	2.03	0.41
2:E:298:UNK:O	2:E:300:UNK:N	2.54	0.41
1:F:1857:ILE:HG22	1:F:1891:TYR:HB2	2.03	0.41
1:F:211:GLN:NE2	1:F:230:TYR:HB3	2.36	0.41
1:F:1:MET:HB3	1:F:2:ASP:H	1.70	0.41
1:G:1684:SER:O	1:G:1688:GLN:N	2.54	0.41
1:G:211:GLN:NE2	1:G:230:TYR:HB3	2.36	0.41
3:I:1481:ASP:HB3	3:I:1484:GLU:HB3	2.02	0.41
2:A:1349:THR:HA	2:A:1376:PHE:CE1	2.55	0.40
1:B:53:GLU:HG3	1:B:112:ASN:HB3	2.03	0.40
1:B:162:GLY:HA3	1:B:275:GLN:HB2	2.02	0.40
1:B:1887:GLU:HB2	1:B:1890:ASN:HB3	2.03	0.40
1:B:705:UNK:HA	2:D:179:UNK:H	1.86	0.40
2:E:1208:VAL:O	2:E:1212:THR:OG1	2.28	0.40
1:F:1925:ILE:HA	1:F:1928:GLN:HB2	2.03	0.40
1:G:1709:ILE:HD12	1:G:1770:LEU:HD23	2.03	0.40
1:G:215:ILE:HA	1:G:218:TRP:CD2	2.56	0.40
2:A:1291:LEU:HD23	2:A:1291:LEU:HA	1.82	0.40
1:B:1753:LYS:O	1:B:1754:GLU:HG3	2.21	0.40
1:B:371:VAL:HB	1:B:489:LYS:HA	2.01	0.40
3:C:1481:ASP:HB3	3:C:1484:GLU:HB3	2.02	0.40
2:D:1869:UNK:O	2:D:1884:UNK:N	2.53	0.40
2:E:1326:ILE:HG12	2:E:1326:ILE:H	1.53	0.40
1:F:1691:TRP:HE1	1:F:1784:MET:HA	1.87	0.40
1:F:251:VAL:O	1:F:255:LEU:N	2.51	0.40
1:G:1753:LYS:O	1:G:1754:GLU:HG3	2.21	0.40
2:A:1051:VAL:O	2:A:1055:TRP:N	2.54	0.40
2:E:752:ILE:HD13	2:E:765:LEU:HD11	2.04	0.40
2:E:826:MET:HB2	2:E:868:ILE:HA	2.03	0.40
1:F:174:ARG:NH2	1:F:218:TRP:O	2.49	0.40
1:G:225:THR:HA	1:G:226:PRO:HD3	1.94	0.40
1:G:502:LEU:HD23	1:G:502:LEU:HA	1.90	0.40
2:A:1166:LYS:HA	2:A:1166:LYS:HD2	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1341:PHE:N	2:A:1343:PHE:O	2.48	0.40
2:D:1367:ARG:HB3	2:D:1370:THR:HG21	2.04	0.40
2:D:404:UNK:O	2:D:408:UNK:N	2.55	0.40
2:E:1367:ARG:HB3	2:E:1370:THR:HG21	2.04	0.40
2:E:394:UNK:O	2:E:396:UNK:N	2.54	0.40
1:F:166:THR:HG21	1:F:507:GLY:HA3	2.02	0.40
1:G:1728:ARG:HB3	1:G:1732:ASN:HD22	1.86	0.40
1:G:481:ASP:O	1:G:485:ARG:N	2.55	0.40
2:A:1168:LEU:HG	2:A:1169:LYS:HG2	2.02	0.40
2:A:1334:ASP:OD1	2:A:1335:PHE:N	2.53	0.40
1:B:1674:GLN:NE2	1:B:1711:ILE:O	2.54	0.40
1:B:469:ARG:HD3	1:B:469:ARG:HH11	1.75	0.40
2:E:1051:VAL:O	2:E:1055:TRP:N	2.54	0.40
2:E:1105:LEU:HD23	2:E:1105:LEU:HA	1.87	0.40
1:F:1674:GLN:NE2	1:F:1711:ILE:O	2.54	0.40
1:F:1684:SER:O	1:F:1688:GLN:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	B	986/2051 (48%)	739 (75%)	202 (20%)	45 (5%)	2	27
1	F	986/2051 (48%)	739 (75%)	202 (20%)	45 (5%)	2	27
1	G	986/2051 (48%)	740 (75%)	201 (20%)	45 (5%)	2	27
2	A	879/1887 (47%)	606 (69%)	231 (26%)	42 (5%)	2	26
2	D	879/1887 (47%)	606 (69%)	231 (26%)	42 (5%)	2	26
2	E	879/1887 (47%)	606 (69%)	231 (26%)	42 (5%)	2	26
3	C	69/71 (97%)	53 (77%)	16 (23%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	69/71 (97%)	53 (77%)	16 (23%)	0	100	100
3	I	69/71 (97%)	54 (78%)	15 (22%)	0	100	100
All	All	5802/12027 (48%)	4196 (72%)	1345 (23%)	261 (4%)	5	27

All (261) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	447	ASN
1	B	558	ASN
1	B	1618	PRO
1	B	1862	VAL
1	B	1925	ILE
1	B	1955	PRO
1	B	1956	ARG
1	B	1957	PRO
1	B	1986	LYS
1	B	2011	ILE
1	B	2017	LYS
2	A	617	PRO
2	A	636	PRO
2	A	645	PRO
2	A	787	LYS
2	A	1111	PHE
2	A	1159	GLU
2	A	1255	SER
1	F	447	ASN
1	F	558	ASN
1	F	1618	PRO
1	F	1862	VAL
1	F	1925	ILE
1	F	1955	PRO
1	F	1956	ARG
1	F	1957	PRO
1	F	1986	LYS
1	F	2017	LYS
2	D	617	PRO
2	D	636	PRO
2	D	645	PRO
2	D	787	LYS
2	D	1111	PHE
2	D	1159	GLU

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Mol	Chain	Res	Type
2	D	1255	SER
1	G	447	ASN
1	G	558	ASN
1	G	1618	PRO
1	G	1862	VAL
1	G	1925	ILE
1	G	1955	PRO
1	G	1956	ARG
1	G	1957	PRO
1	G	1986	LYS
1	G	2011	ILE
1	G	2017	LYS
2	E	617	PRO
2	E	636	PRO
2	E	645	PRO
2	E	787	LYS
2	E	1111	PHE
2	E	1159	GLU
2	E	1255	SER
1	B	101	ILE
1	B	547	ILE
1	B	550	VAL
1	B	1632	ILE
1	B	1637	LEU
1	B	1660	PRO
1	B	1924	ILE
1	B	1966	CYS
1	B	1968	PRO
1	B	1996	ILE
1	B	2008	GLY
1	B	2029	VAL
1	B	2045	TRP
2	A	525	TYR
2	A	526	VAL
2	A	552	LYS
2	A	553	ALA
2	A	603	ASP
2	A	605	LEU
2	A	614	ALA
2	A	618	ASN
2	A	648	ASP
2	A	667	ALA

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Mol	Chain	Res	Type
2	A	1092	LYS
2	A	1100	HIS
2	A	1158	PRO
2	A	1172	THR
1	F	101	ILE
1	F	547	ILE
1	F	550	VAL
1	F	1632	ILE
1	F	1637	LEU
1	F	1660	PRO
1	F	1924	ILE
1	F	1966	CYS
1	F	1968	PRO
1	F	1996	ILE
1	F	2008	GLY
1	F	2011	ILE
1	F	2029	VAL
1	F	2045	TRP
2	D	525	TYR
2	D	526	VAL
2	D	552	LYS
2	D	553	ALA
2	D	603	ASP
2	D	605	LEU
2	D	614	ALA
2	D	618	ASN
2	D	648	ASP
2	D	667	ALA
2	D	1092	LYS
2	D	1100	HIS
2	D	1158	PRO
2	D	1172	THR
1	G	101	ILE
1	G	547	ILE
1	G	550	VAL
1	G	1632	ILE
1	G	1637	LEU
1	G	1660	PRO
1	G	1924	ILE
1	G	1966	CYS
1	G	1968	PRO
1	G	1996	ILE

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Mol	Chain	Res	Type
1	G	2008	GLY
1	G	2029	VAL
1	G	2045	TRP
2	E	525	TYR
2	E	526	VAL
2	E	553	ALA
2	E	603	ASP
2	E	605	LEU
2	E	614	ALA
2	E	618	ASN
2	E	648	ASP
2	E	667	ALA
2	E	1092	LYS
2	E	1100	HIS
2	E	1158	PRO
2	E	1172	THR
1	B	571	LYS
1	B	1656	GLU
1	B	1947	ALA
1	B	1954	LYS
1	B	1962	ARG
1	B	2028	ASP
2	A	606	ASP
2	A	612	GLU
2	A	631	PRO
2	A	1083	PRO
2	A	1377	MET
1	F	571	LYS
1	F	1656	GLU
1	F	1947	ALA
1	F	1954	LYS
1	F	1962	ARG
1	F	2028	ASP
2	D	606	ASP
2	D	612	GLU
2	D	631	PRO
2	D	1083	PRO
2	D	1377	MET
1	G	571	LYS
1	G	1656	GLU
1	G	1947	ALA
1	G	1954	LYS

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Mol	Chain	Res	Type
1	G	1962	ARG
1	G	2028	ASP
2	E	552	LYS
2	E	606	ASP
2	E	612	GLU
2	E	631	PRO
2	E	1083	PRO
2	E	1377	MET
1	B	561	TRP
1	B	1631	MET
1	B	1716	ASN
1	B	1979	THR
1	B	2020	GLN
1	B	2021	VAL
2	A	523	SER
2	A	595	GLN
2	A	609	SER
2	A	786	SER
2	A	885	ALA
2	A	1047	LEU
2	A	1080	THR
1	F	561	TRP
1	F	1631	MET
1	F	1716	ASN
1	F	1979	THR
1	F	2020	GLN
1	F	2021	VAL
2	D	523	SER
2	D	595	GLN
2	D	609	SER
2	D	786	SER
2	D	885	ALA
2	D	1047	LEU
2	D	1080	THR
1	G	561	TRP
1	G	1631	MET
1	G	1716	ASN
1	G	1979	THR
1	G	2020	GLN
1	G	2021	VAL
2	E	523	SER
2	E	595	GLN

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Mol	Chain	Res	Type
2	E	608	ASP
2	E	609	SER
2	E	786	SER
2	E	885	ALA
2	E	1047	LEU
2	E	1080	THR
1	B	1633	ASN
1	B	1897	GLN
1	B	1944	ILE
2	A	608	ASP
2	A	613	VAL
2	A	1091	ALA
2	A	1365	MET
1	F	1633	ASN
1	F	1897	GLN
1	F	1944	ILE
2	D	608	ASP
2	D	613	VAL
2	D	1091	ALA
2	D	1365	MET
1	G	1633	ASN
1	G	1897	GLN
1	G	1944	ILE
2	E	613	VAL
2	E	1091	ALA
2	E	1365	MET
1	B	1647	ASP
2	A	581	PHE
2	A	1071	PRO
1	F	1647	ASP
2	D	581	PHE
2	D	1071	PRO
1	G	1647	ASP
2	E	581	PHE
2	E	1071	PRO
1	B	1665	VAL
1	B	1967	ILE
2	A	540	GLN
2	A	1107	GLU
1	F	1665	VAL
1	F	1967	ILE
2	D	540	GLN

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Mol	Chain	Res	Type
2	D	1107	GLU
1	G	1665	VAL
1	G	1967	ILE
2	E	540	GLN
2	E	1107	GLU
1	B	42	PRO
1	B	1648	VAL
1	F	42	PRO
1	F	1648	VAL
1	G	42	PRO
1	G	1648	VAL
1	B	1997	ILE
2	A	601	VAL
1	F	1997	ILE
2	D	601	VAL
1	G	1997	ILE
2	E	601	VAL

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 PDB entries followed by that with respect to all EM entries.

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	B	690/877 (79%)	674 (98%)	16 (2%)	53	76
1	F	690/877 (79%)	674 (98%)	16 (2%)	53	76
1	G	690/877 (79%)	674 (98%)	16 (2%)	53	76
2	A	610/845 (72%)	598 (98%)	12 (2%)	58	79
2	D	610/845 (72%)	598 (98%)	12 (2%)	58	79
2	E	610/845 (72%)	598 (98%)	12 (2%)	58	79
3	C	64/64 (100%)	61 (95%)	3 (5%)	29	60
3	H	64/64 (100%)	61 (95%)	3 (5%)	29	60
3	I	64/64 (100%)	61 (95%)	3 (5%)	29	60
All	All	4092/5358 (76%)	3999 (98%)	93 (2%)	57	76

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	36	GLN
1	B	96	LEU
1	B	202	THR
1	B	228	LYS
1	B	291	SER
1	B	400	SER
1	B	406	ARG
1	B	459	VAL
1	B	472	SER
1	B	480	VAL
1	B	482	CYS
1	B	541	TYR
1	B	1849	ARG
1	B	1893	VAL
1	B	1917	ILE
1	B	1924	ILE
2	A	878	MET
2	A	905	LEU
2	A	943	LEU
2	A	1057	MET
2	A	1068	LYS
2	A	1229	THR
2	A	1243	VAL
2	A	1254	VAL
2	A	1294	SER
2	A	1333	ASP
2	A	1437	LYS
2	A	1515	ARG
3	C	1461	ASP
3	C	1478	PRO
3	C	1499	SER
1	F	36	GLN
1	F	96	LEU
1	F	202	THR
1	F	228	LYS
1	F	291	SER
1	F	400	SER
1	F	406	ARG
1	F	459	VAL
1	F	472	SER
1	F	480	VAL
1	F	482	CYS

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Mol	Chain	Res	Type
1	F	541	TYR
1	F	1849	ARG
1	F	1893	VAL
1	F	1917	ILE
1	F	1924	ILE
2	D	878	MET
2	D	905	LEU
2	D	943	LEU
2	D	1057	MET
2	D	1068	LYS
2	D	1229	THR
2	D	1243	VAL
2	D	1254	VAL
2	D	1294	SER
2	D	1333	ASP
2	D	1437	LYS
2	D	1515	ARG
3	H	1461	ASP
3	H	1478	PRO
3	H	1499	SER
1	G	36	GLN
1	G	96	LEU
1	G	202	THR
1	G	228	LYS
1	G	291	SER
1	G	400	SER
1	G	406	ARG
1	G	459	VAL
1	G	472	SER
1	G	480	VAL
1	G	482	CYS
1	G	541	TYR
1	G	1849	ARG
1	G	1893	VAL
1	G	1917	ILE
1	G	1924	ILE
2	E	878	MET
2	E	905	LEU
2	E	943	LEU
2	E	1057	MET
2	E	1068	LYS
2	E	1229	THR

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Mol	Chain	Res	Type
2	E	1243	VAL
2	E	1254	VAL
2	E	1294	SER
2	E	1333	ASP
2	E	1437	LYS
2	E	1515	ARG
3	I	1461	ASP
3	I	1478	PRO
3	I	1499	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	85	ASN
1	B	110	GLN
1	B	155	GLN
1	B	248	HIS
1	B	348	GLN
1	B	350	GLN
1	B	354	ASN
1	B	418	ASN
1	B	447	ASN
1	B	495	GLN
1	B	1669	GLN
1	B	1674	GLN
1	B	1892	ASN
1	B	1896	GLN
1	B	1939	HIS
2	A	694	GLN
2	A	698	GLN
2	A	860	ASN
3	C	1495	ASN
3	C	1510	ASN
1	F	85	ASN
1	F	110	GLN
1	F	155	GLN
1	F	248	HIS
1	F	348	GLN
1	F	350	GLN
1	F	354	ASN
1	F	418	ASN
1	F	447	ASN

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Mol	Chain	Res	Type
1	F	495	GLN
1	F	1674	GLN
1	F	1892	ASN
1	F	1896	GLN
1	F	1939	HIS
2	D	694	GLN
2	D	698	GLN
2	D	860	ASN
3	H	1495	ASN
3	H	1510	ASN
1	G	85	ASN
1	G	110	GLN
1	G	155	GLN
1	G	248	HIS
1	G	348	GLN
1	G	350	GLN
1	G	354	ASN
1	G	418	ASN
1	G	447	ASN
1	G	495	GLN
1	G	1674	GLN
1	G	1892	ASN
1	G	1896	GLN
1	G	1939	HIS
2	E	694	GLN
2	E	698	GLN
2	E	860	ASN
3	I	1495	ASN
3	I	1510	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.