



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 01:02 PM UTC

PDB ID : 5X5F / pdb_00005x5f
EMDB ID : EMD-6707
Title : Prefusion structure of MERS-CoV spike glycoprotein, conformation 2
Authors : Yuan, Y.; Cao, D.; Zhang, Y.; Ma, J.; Qi, J.; Wang, Q.; Lu, G.; Wu, Y.; Yan, J.; Shi, Y.; Zhang, X.; Gao, G.F.
Deposited on : 2017-02-15
Resolution : 4.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

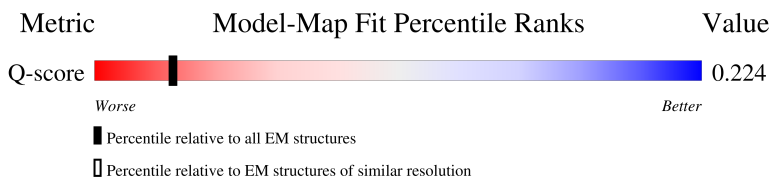
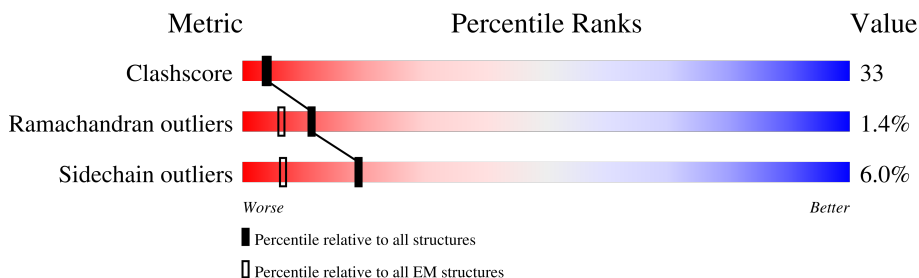
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1323	55% 56% 25% • • 14%
1	B	1323	52% 57% 24% • • 14%
1	C	1323	54% 58% 24% • • 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 26422 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 S protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1141	Total	C	N	O	S	1	0
			8806	5599	1457	1699	51		
1	B	1141	Total	C	N	O	S	1	0
			8806	5599	1457	1699	51		
1	C	1141	Total	C	N	O	S	1	0
			8810	5601	1458	1700	51		

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	751	SER	ARG	engineered mutation	UNP W6A028
A	1020	GLN	ARG	engineered mutation	UNP W6A028
A	1295	GLU	-	expression tag	UNP W6A028
A	1296	PHE	-	expression tag	UNP W6A028
A	1297	ARG	-	expression tag	UNP W6A028
A	1298	LEU	-	expression tag	UNP W6A028
A	1299	VAL	-	expression tag	UNP W6A028
A	1300	PRO	-	expression tag	UNP W6A028
A	1301	ARG	-	expression tag	UNP W6A028
A	1302	GLY	-	expression tag	UNP W6A028
A	1303	SER	-	expression tag	UNP W6A028
A	1304	PRO	-	expression tag	UNP W6A028
A	1305	GLY	-	expression tag	UNP W6A028
A	1306	SER	-	expression tag	UNP W6A028
A	1307	GLY	-	expression tag	UNP W6A028
A	1308	TYR	-	expression tag	UNP W6A028
A	1309	ILE	-	expression tag	UNP W6A028
A	1310	PRO	-	expression tag	UNP W6A028
A	1311	GLU	-	expression tag	UNP W6A028
A	1312	ALA	-	expression tag	UNP W6A028
A	1313	PRO	-	expression tag	UNP W6A028
A	1314	ARG	-	expression tag	UNP W6A028
A	1315	ASP	-	expression tag	UNP W6A028
A	1316	GLY	-	expression tag	UNP W6A028

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1317	GLN	-	expression tag	UNP W6A028
A	1318	ALA	-	expression tag	UNP W6A028
A	1319	TYR	-	expression tag	UNP W6A028
A	1320	VAL	-	expression tag	UNP W6A028
A	1321	ARG	-	expression tag	UNP W6A028
A	1322	LYS	-	expression tag	UNP W6A028
A	1323	ASP	-	expression tag	UNP W6A028
A	1324	GLY	-	expression tag	UNP W6A028
A	1325	GLU	-	expression tag	UNP W6A028
A	1326	TRP	-	expression tag	UNP W6A028
A	1327	VAL	-	expression tag	UNP W6A028
A	1328	LEU	-	expression tag	UNP W6A028
A	1329	LEU	-	expression tag	UNP W6A028
A	1330	SER	-	expression tag	UNP W6A028
A	1331	THR	-	expression tag	UNP W6A028
A	1332	PHE	-	expression tag	UNP W6A028
A	1333	LEU	-	expression tag	UNP W6A028
A	1334	GLY	-	expression tag	UNP W6A028
A	1335	HIS	-	expression tag	UNP W6A028
A	1336	HIS	-	expression tag	UNP W6A028
A	1337	HIS	-	expression tag	UNP W6A028
A	1338	HIS	-	expression tag	UNP W6A028
A	1339	HIS	-	expression tag	UNP W6A028
A	1340	HIS	-	expression tag	UNP W6A028
B	751	SER	ARG	engineered mutation	UNP W6A028
B	1020	GLN	ARG	engineered mutation	UNP W6A028
B	1295	GLU	-	expression tag	UNP W6A028
B	1296	PHE	-	expression tag	UNP W6A028
B	1297	ARG	-	expression tag	UNP W6A028
B	1298	LEU	-	expression tag	UNP W6A028
B	1299	VAL	-	expression tag	UNP W6A028
B	1300	PRO	-	expression tag	UNP W6A028
B	1301	ARG	-	expression tag	UNP W6A028
B	1302	GLY	-	expression tag	UNP W6A028
B	1303	SER	-	expression tag	UNP W6A028
B	1304	PRO	-	expression tag	UNP W6A028
B	1305	GLY	-	expression tag	UNP W6A028
B	1306	SER	-	expression tag	UNP W6A028
B	1307	GLY	-	expression tag	UNP W6A028
B	1308	TYR	-	expression tag	UNP W6A028
B	1309	ILE	-	expression tag	UNP W6A028
B	1310	PRO	-	expression tag	UNP W6A028

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1311	GLU	-	expression tag	UNP W6A028
B	1312	ALA	-	expression tag	UNP W6A028
B	1313	PRO	-	expression tag	UNP W6A028
B	1314	ARG	-	expression tag	UNP W6A028
B	1315	ASP	-	expression tag	UNP W6A028
B	1316	GLY	-	expression tag	UNP W6A028
B	1317	GLN	-	expression tag	UNP W6A028
B	1318	ALA	-	expression tag	UNP W6A028
B	1319	TYR	-	expression tag	UNP W6A028
B	1320	VAL	-	expression tag	UNP W6A028
B	1321	ARG	-	expression tag	UNP W6A028
B	1322	LYS	-	expression tag	UNP W6A028
B	1323	ASP	-	expression tag	UNP W6A028
B	1324	GLY	-	expression tag	UNP W6A028
B	1325	GLU	-	expression tag	UNP W6A028
B	1326	TRP	-	expression tag	UNP W6A028
B	1327	VAL	-	expression tag	UNP W6A028
B	1328	LEU	-	expression tag	UNP W6A028
B	1329	LEU	-	expression tag	UNP W6A028
B	1330	SER	-	expression tag	UNP W6A028
B	1331	THR	-	expression tag	UNP W6A028
B	1332	PHE	-	expression tag	UNP W6A028
B	1333	LEU	-	expression tag	UNP W6A028
B	1334	GLY	-	expression tag	UNP W6A028
B	1335	HIS	-	expression tag	UNP W6A028
B	1336	HIS	-	expression tag	UNP W6A028
B	1337	HIS	-	expression tag	UNP W6A028
B	1338	HIS	-	expression tag	UNP W6A028
B	1339	HIS	-	expression tag	UNP W6A028
B	1340	HIS	-	expression tag	UNP W6A028
C	751	SER	ARG	engineered mutation	UNP W6A028
C	1020	GLN	ARG	engineered mutation	UNP W6A028
C	1295	GLU	-	expression tag	UNP W6A028
C	1296	PHE	-	expression tag	UNP W6A028
C	1297	ARG	-	expression tag	UNP W6A028
C	1298	LEU	-	expression tag	UNP W6A028
C	1299	VAL	-	expression tag	UNP W6A028
C	1300	PRO	-	expression tag	UNP W6A028
C	1301	ARG	-	expression tag	UNP W6A028
C	1302	GLY	-	expression tag	UNP W6A028
C	1303	SER	-	expression tag	UNP W6A028
C	1304	PRO	-	expression tag	UNP W6A028

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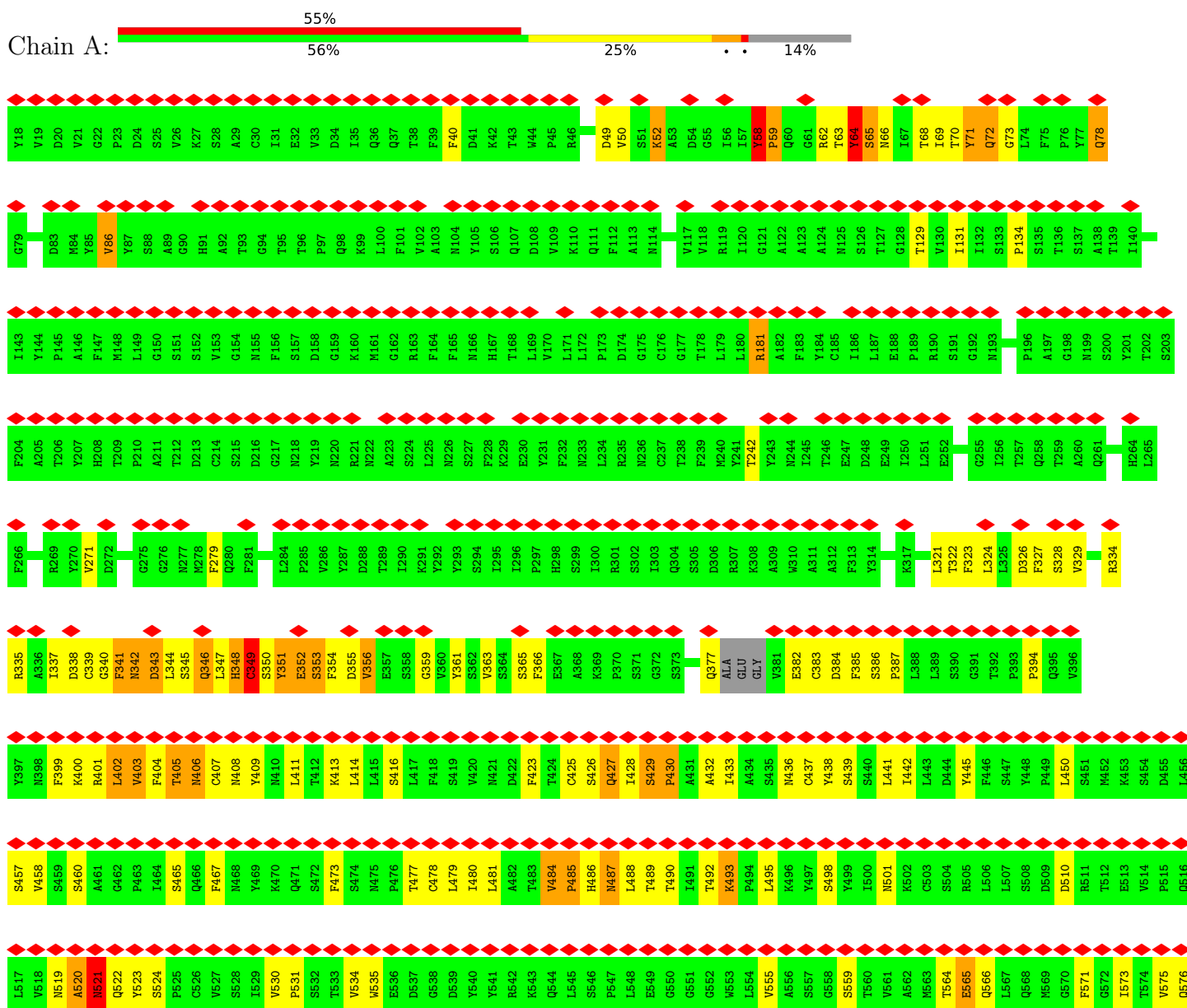
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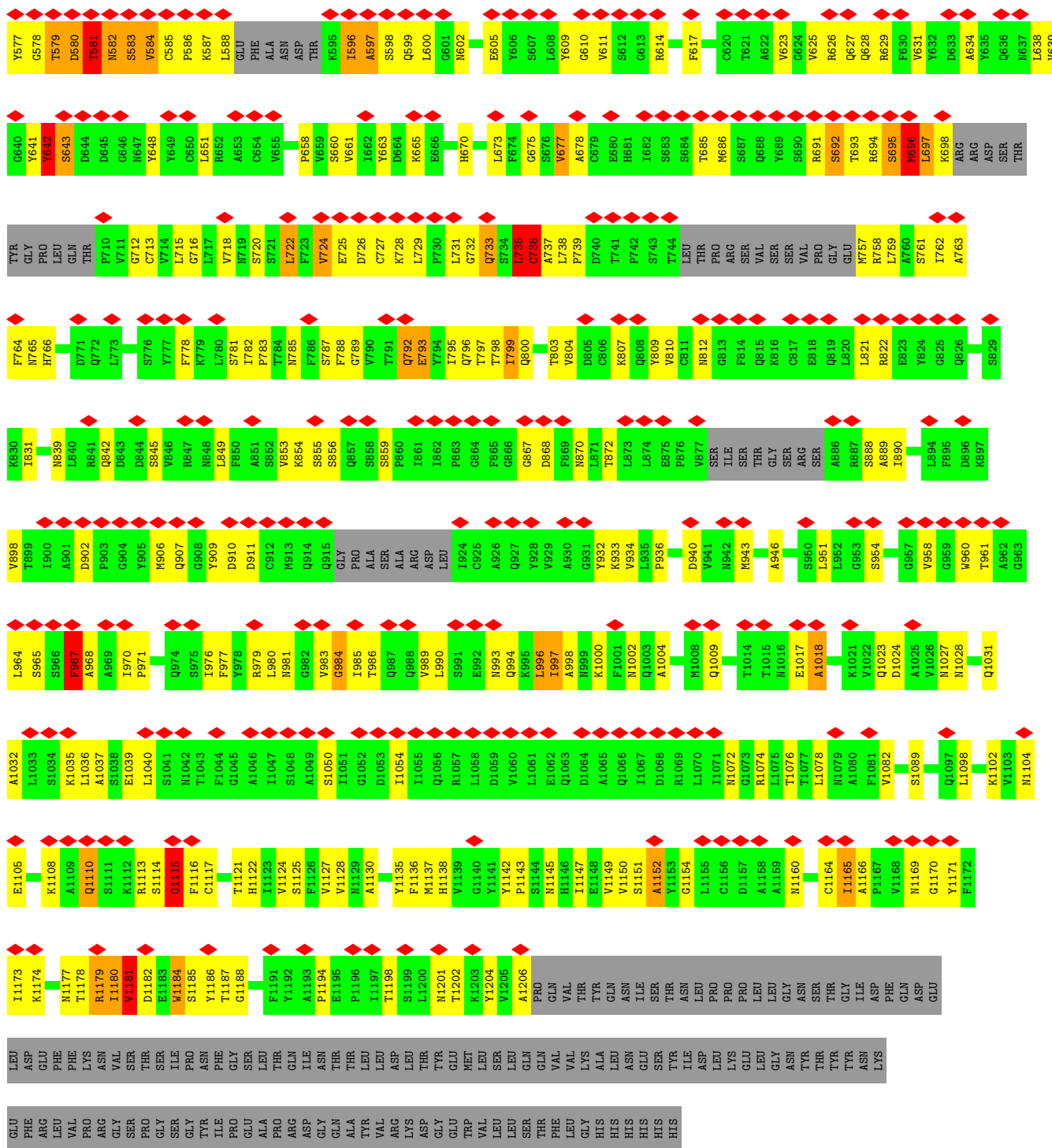
Chain	Residue	Modelled	Actual	Comment	Reference
C	1305	GLY	-	expression tag	UNP W6A028
C	1306	SER	-	expression tag	UNP W6A028
C	1307	GLY	-	expression tag	UNP W6A028
C	1308	TYR	-	expression tag	UNP W6A028
C	1309	ILE	-	expression tag	UNP W6A028
C	1310	PRO	-	expression tag	UNP W6A028
C	1311	GLU	-	expression tag	UNP W6A028
C	1312	ALA	-	expression tag	UNP W6A028
C	1313	PRO	-	expression tag	UNP W6A028
C	1314	ARG	-	expression tag	UNP W6A028
C	1315	ASP	-	expression tag	UNP W6A028
C	1316	GLY	-	expression tag	UNP W6A028
C	1317	GLN	-	expression tag	UNP W6A028
C	1318	ALA	-	expression tag	UNP W6A028
C	1319	TYR	-	expression tag	UNP W6A028
C	1320	VAL	-	expression tag	UNP W6A028
C	1321	ARG	-	expression tag	UNP W6A028
C	1322	LYS	-	expression tag	UNP W6A028
C	1323	ASP	-	expression tag	UNP W6A028
C	1324	GLY	-	expression tag	UNP W6A028
C	1325	GLU	-	expression tag	UNP W6A028
C	1326	TRP	-	expression tag	UNP W6A028
C	1327	VAL	-	expression tag	UNP W6A028
C	1328	LEU	-	expression tag	UNP W6A028
C	1329	LEU	-	expression tag	UNP W6A028
C	1330	SER	-	expression tag	UNP W6A028
C	1331	THR	-	expression tag	UNP W6A028
C	1332	PHE	-	expression tag	UNP W6A028
C	1333	LEU	-	expression tag	UNP W6A028
C	1334	GLY	-	expression tag	UNP W6A028
C	1335	HIS	-	expression tag	UNP W6A028
C	1336	HIS	-	expression tag	UNP W6A028
C	1337	HIS	-	expression tag	UNP W6A028
C	1338	HIS	-	expression tag	UNP W6A028
C	1339	HIS	-	expression tag	UNP W6A028
C	1340	HIS	-	expression tag	UNP W6A028

3 Residue-property plots

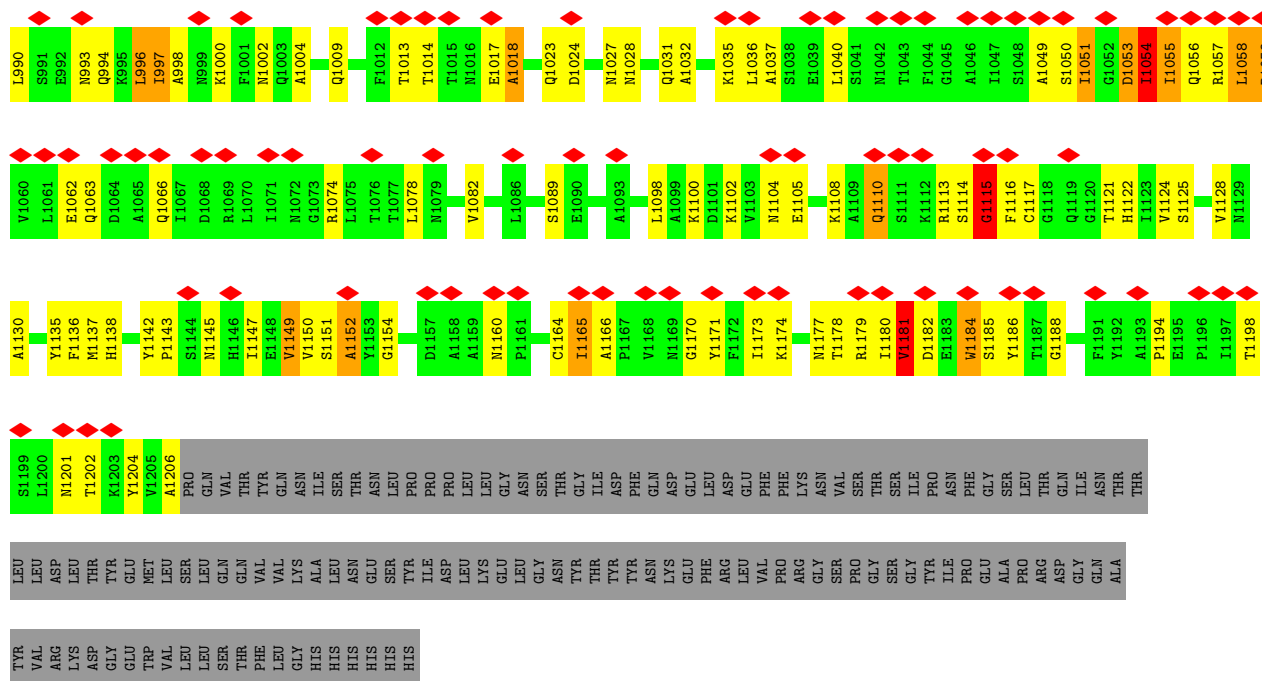
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: S protein

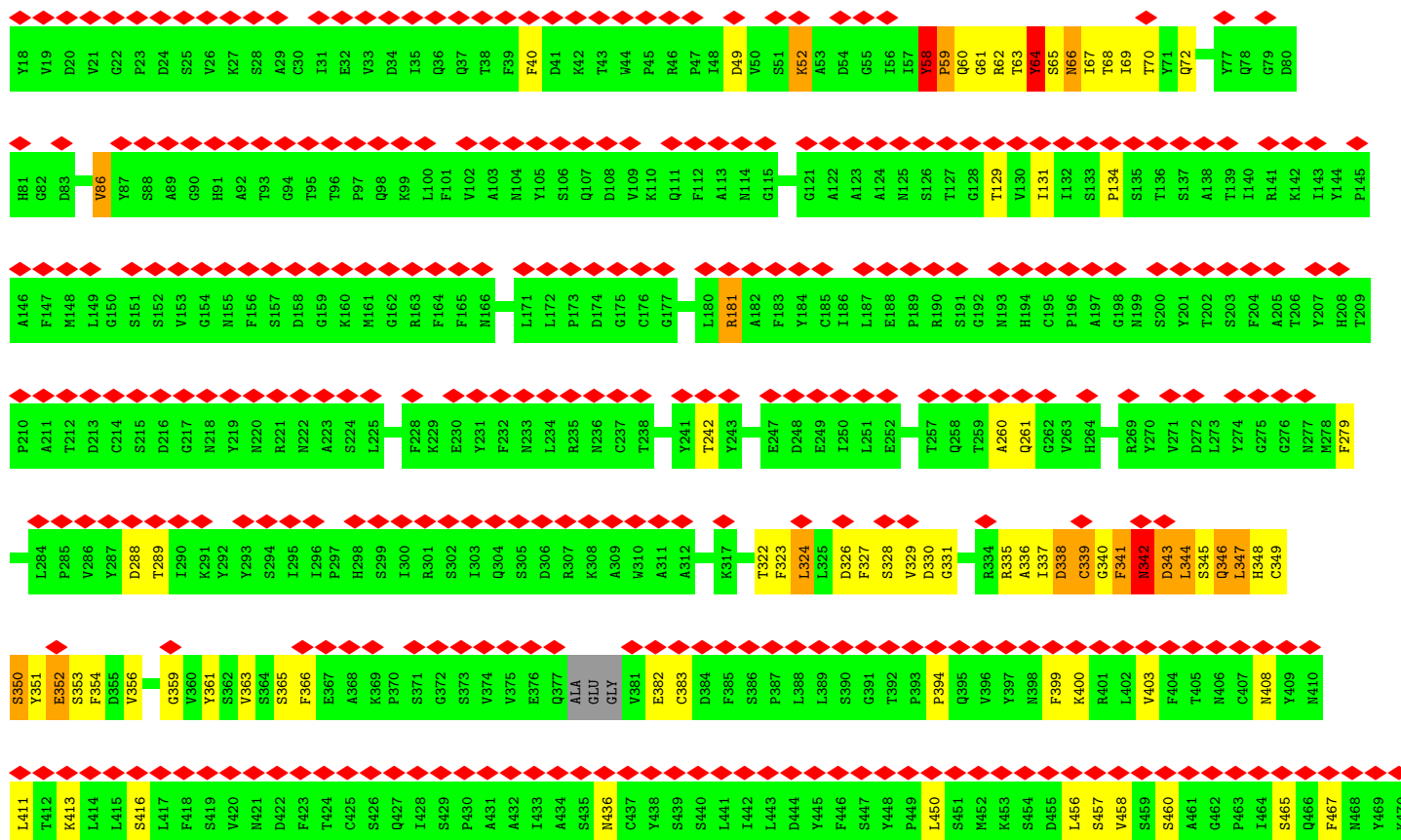








• Molecule 1: S protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	60000	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 ($e^-/\text{\AA}^2$)	8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.179	Depositor
Minimum map value	-0.093	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0595	Depositor
Map size ($\text{\AA}$)	260.0, 260.0, 260.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3, 1.3, 1.3	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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.65	10/9006 (0.1%)	1.07	60/12245 (0.5%)
1	B	0.53	3/9006 (0.0%)	1.05	55/12245 (0.4%)
1	C	0.52	2/9010 (0.0%)	1.01	45/12250 (0.4%)
All	All	0.57	15/27022 (0.1%)	1.04	160/36740 (0.4%)

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	20
1	B	0	20
1	C	0	19
All	All	0	59

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	CYS	N-CA	-25.46	1.16	1.46
1	A	349	CYS	C-O	15.19	1.41	1.24
1	A	696	MET	N-CA	9.09	1.59	1.46
1	A	349	CYS	CA-CB	7.02	1.64	1.53
1	B	822	ARG	N-CA	6.96	1.55	1.46
1	A	349	CYS	C-N	-6.55	1.24	1.33
1	B	58	TYR	C-N	6.47	1.41	1.33
1	C	58	TYR	C-N	6.47	1.41	1.33
1	A	58	TYR	C-N	6.46	1.41	1.33
1	A	696	MET	C-N	6.39	1.42	1.33
1	A	59	PRO	N-CD	5.29	1.55	1.47
1	C	59	PRO	N-CD	5.22	1.55	1.47
1	B	59	PRO	N-CD	5.20	1.55	1.47
1	A	429	SER	C-N	5.15	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	430	PRO	N-CD	5.07	1.54	1.47

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	CYS	O-C-N	-16.59	104.98	122.07
1	A	349	CYS	N-CA-C	-15.09	94.92	111.07
1	A	406	ASN	N-CA-C	-11.54	96.18	113.72
1	A	349	CYS	CA-C-N	10.71	136.82	121.50
1	A	349	CYS	C-N-CA	10.71	136.82	121.50
1	C	1151	SER	CA-C-N	10.27	140.18	121.70
1	C	1151	SER	C-N-CA	10.27	140.18	121.70
1	A	1151	SER	CA-C-N	10.21	140.08	121.70
1	A	1151	SER	C-N-CA	10.21	140.08	121.70
1	B	1151	SER	CA-C-N	10.18	140.03	121.70
1	B	1151	SER	C-N-CA	10.18	140.03	121.70
1	B	663	TYR	N-CA-C	10.10	122.04	111.14
1	A	348	HIS	CA-C-N	10.09	133.56	120.44
1	A	348	HIS	C-N-CA	10.09	133.56	120.44
1	B	261	GLN	N-CA-C	-9.73	100.68	111.28
1	B	347	LEU	CA-C-N	9.42	133.85	120.28
1	B	347	LEU	C-N-CA	9.42	133.85	120.28
1	A	365	SER	CA-C-N	8.99	137.88	121.70
1	A	365	SER	C-N-CA	8.99	137.88	121.70
1	C	1152	ALA	CA-C-N	8.94	137.80	121.70
1	C	1152	ALA	C-N-CA	8.94	137.80	121.70
1	A	1152	ALA	CA-C-N	8.94	137.78	121.70
1	A	1152	ALA	C-N-CA	8.94	137.78	121.70
1	C	365	SER	CA-C-N	8.93	137.77	121.70
1	C	365	SER	C-N-CA	8.93	137.77	121.70
1	B	1152	ALA	CA-C-N	8.90	137.72	121.70
1	B	1152	ALA	C-N-CA	8.90	137.72	121.70
1	B	365	SER	CA-C-N	8.87	137.66	121.70
1	B	365	SER	C-N-CA	8.87	137.66	121.70
1	B	629	ARG	N-CA-C	8.39	123.63	113.23
1	A	997	ILE	N-CA-C	7.62	125.19	109.34
1	B	997	ILE	N-CA-C	7.61	125.17	109.34
1	C	997	ILE	N-CA-C	7.57	125.09	109.34
1	C	735	LEU	CA-CB-CG	7.34	142.00	116.30
1	B	735	LEU	CA-CB-CG	7.32	141.93	116.30
1	A	724	VAL	CA-C-N	7.30	134.83	121.70
1	A	724	VAL	C-N-CA	7.30	134.83	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	735	LEU	CA-CB-CG	7.28	141.78	116.30
1	B	724	VAL	CA-C-N	7.23	134.72	121.70
1	B	724	VAL	C-N-CA	7.23	134.72	121.70
1	C	724	VAL	CA-C-N	7.22	134.71	121.70
1	C	724	VAL	C-N-CA	7.22	134.71	121.70
1	B	1017	GLU	CA-C-N	7.10	134.48	121.70
1	B	1017	GLU	C-N-CA	7.10	134.48	121.70
1	A	1017	GLU	CA-C-N	7.06	134.42	121.70
1	A	1017	GLU	C-N-CA	7.06	134.42	121.70
1	C	1017	GLU	CA-C-N	7.03	134.36	121.70
1	C	1017	GLU	C-N-CA	7.03	134.36	121.70
1	B	261	GLN	CA-C-N	-6.88	112.88	121.83
1	B	261	GLN	C-N-CA	-6.88	112.88	121.83
1	A	1018	ALA	N-CA-C	6.86	130.21	111.00
1	B	1018	ALA	N-CA-C	6.86	130.21	111.00
1	C	1018	ALA	N-CA-C	6.84	130.15	111.00
1	B	348	HIS	CA-C-N	6.76	130.49	122.44
1	B	348	HIS	C-N-CA	6.76	130.49	122.44
1	B	58	TYR	CA-C-N	-6.67	112.90	119.90
1	B	58	TYR	C-N-CA	-6.67	112.90	119.90
1	C	58	TYR	CA-C-N	-6.67	112.90	119.90
1	C	58	TYR	C-N-CA	-6.67	112.90	119.90
1	A	58	TYR	CA-C-N	-6.66	112.91	119.90
1	A	58	TYR	C-N-CA	-6.66	112.91	119.90
1	A	405	THR	N-CA-C	6.61	119.37	108.99
1	A	695	SER	CA-C-N	-6.61	110.90	123.32
1	A	695	SER	C-N-CA	-6.61	110.90	123.32
1	B	643	SER	N-CA-C	6.59	119.20	108.26
1	A	643	SER	N-CA-C	6.59	119.20	108.26
1	C	643	SER	N-CA-C	6.56	119.15	108.26
1	B	793	GLU	CA-C-N	6.52	130.75	121.42
1	B	793	GLU	C-N-CA	6.52	130.75	121.42
1	C	793	GLU	CA-C-N	6.51	130.73	121.42
1	C	793	GLU	C-N-CA	6.51	130.73	121.42
1	A	793	GLU	CA-C-N	6.48	130.69	121.42
1	A	793	GLU	C-N-CA	6.48	130.69	121.42
1	A	582	ASN	N-CA-CB	6.46	121.49	110.50
1	A	580	ASP	N-CA-C	6.37	119.52	108.76
1	A	406	ASN	CA-C-N	-6.36	111.67	122.67
1	A	406	ASN	C-N-CA	-6.36	111.67	122.67
1	C	64	TYR	N-CA-C	6.18	119.09	109.52
1	B	64	TYR	N-CA-C	6.15	119.05	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	822	ARG	N-CA-CB	6.09	120.68	110.32
1	A	64	TYR	N-CA-C	6.08	118.94	109.52
1	A	1184	TRP	CA-C-N	6.01	132.51	121.70
1	A	1184	TRP	C-N-CA	6.01	132.51	121.70
1	B	1184	TRP	CA-C-N	6.00	132.51	121.70
1	B	1184	TRP	C-N-CA	6.00	132.51	121.70
1	C	1184	TRP	CA-C-N	5.98	132.47	121.70
1	C	1184	TRP	C-N-CA	5.98	132.47	121.70
1	C	692	SER	CA-C-N	5.97	132.45	121.70
1	C	692	SER	C-N-CA	5.97	132.45	121.70
1	A	692	SER	CA-C-N	5.96	132.43	121.70
1	A	692	SER	C-N-CA	5.96	132.43	121.70
1	B	692	SER	CA-C-N	5.89	132.31	121.70
1	B	692	SER	C-N-CA	5.89	132.31	121.70
1	B	348	HIS	N-CA-CB	-5.87	101.19	110.22
1	A	1115	GLY	CA-C-N	5.84	132.21	121.70
1	A	1115	GLY	C-N-CA	5.84	132.21	121.70
1	A	1154	GLY	N-CA-C	5.83	119.16	111.52
1	C	1115	GLY	CA-C-N	5.83	132.19	121.70
1	C	1115	GLY	C-N-CA	5.83	132.19	121.70
1	B	1115	GLY	CA-C-N	5.82	132.18	121.70
1	B	1115	GLY	C-N-CA	5.82	132.18	121.70
1	C	1154	GLY	N-CA-C	5.80	119.12	111.52
1	B	1154	GLY	N-CA-C	5.79	119.10	111.52
1	A	429	SER	CA-C-N	-5.73	112.69	119.05
1	A	429	SER	C-N-CA	-5.73	112.69	119.05
1	A	521	ASN	CB-CA-C	5.59	121.54	110.42
1	A	729	LEU	C-N-CD	-5.59	108.31	120.60
1	C	729	LEU	C-N-CD	-5.58	108.32	120.60
1	B	729	LEU	C-N-CD	-5.57	108.34	120.60
1	C	1116	PHE	N-CA-C	5.55	126.54	111.00
1	B	1116	PHE	N-CA-C	5.54	126.51	111.00
1	C	338	ASP	N-CA-C	5.53	117.31	111.28
1	B	854	LYS	CA-C-N	5.52	132.09	121.54
1	B	854	LYS	C-N-CA	5.52	132.09	121.54
1	C	854	LYS	CA-C-N	5.50	132.05	121.54
1	C	854	LYS	C-N-CA	5.50	132.05	121.54
1	A	1116	PHE	N-CA-C	5.50	126.39	111.00
1	C	1054	ILE	CB-CA-C	-5.49	104.73	112.14
1	A	854	LYS	CA-C-N	5.45	131.96	121.54
1	A	854	LYS	C-N-CA	5.45	131.96	121.54
1	B	1202	THR	CA-C-N	5.43	131.91	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1202	THR	C-N-CA	5.43	131.91	121.54
1	C	967	PHE	CA-C-N	5.38	131.39	121.70
1	C	967	PHE	C-N-CA	5.38	131.39	121.70
1	C	1202	THR	CA-C-N	5.38	131.82	121.54
1	C	1202	THR	C-N-CA	5.38	131.82	121.54
1	A	729	LEU	CA-C-N	5.37	139.90	127.00
1	A	729	LEU	C-N-CA	5.37	139.90	127.00
1	A	902	ASP	C-N-CD	-5.37	108.78	120.60
1	A	486	HIS	N-CA-C	-5.37	99.36	110.80
1	C	729	LEU	CA-C-N	5.37	139.88	127.00
1	C	729	LEU	C-N-CA	5.37	139.88	127.00
1	C	486	HIS	N-CA-C	-5.37	99.37	110.80
1	C	902	ASP	C-N-CD	-5.36	108.80	120.60
1	B	729	LEU	CA-C-N	5.36	139.87	127.00
1	B	729	LEU	C-N-CA	5.36	139.87	127.00
1	B	486	HIS	N-CA-C	-5.36	99.38	110.80
1	B	902	ASP	C-N-CD	-5.35	108.83	120.60
1	A	967	PHE	CA-C-N	5.32	131.28	121.70
1	A	967	PHE	C-N-CA	5.32	131.28	121.70
1	A	1202	THR	CA-C-N	5.32	131.70	121.54
1	A	1202	THR	C-N-CA	5.32	131.70	121.54
1	B	967	PHE	CA-C-N	5.32	131.28	121.70
1	B	967	PHE	C-N-CA	5.32	131.28	121.70
1	B	859	SER	CA-C-N	5.29	139.69	127.00
1	B	859	SER	C-N-CA	5.29	139.69	127.00
1	A	1110	GLN	N-CA-C	5.29	119.65	111.56
1	C	1057	ARG	N-CA-C	5.29	119.58	113.18
1	A	859	SER	CA-C-N	5.28	139.68	127.00
1	A	859	SER	C-N-CA	5.28	139.68	127.00
1	C	859	SER	CA-C-N	5.27	139.64	127.00
1	C	859	SER	C-N-CA	5.27	139.64	127.00
1	B	1110	GLN	N-CA-C	5.26	119.60	111.56
1	C	1110	GLN	N-CA-C	5.24	119.58	111.56
1	B	436	ASN	N-CA-C	5.20	117.83	110.50
1	B	259	THR	N-CA-C	-5.18	101.41	109.24
1	A	348	HIS	N-CA-C	5.13	116.56	111.07
1	C	1179	ARG	CA-CB-CG	5.07	124.25	114.10
1	A	1179	ARG	CA-CB-CG	5.05	124.19	114.10
1	B	581	THR	N-CA-C	5.02	116.70	109.07

There are no chirality outliers.

All (59) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1115	GLY	Peptide
1	A	1152	ALA	Peptide
1	A	1170	GLY	Peptide
1	A	1180	ILE	Peptide
1	A	1188	GLY	Peptide
1	A	1204	TYR	Peptide
1	A	520	ALA	Mainchain
1	A	639	VAL	Peptide
1	A	642	TYR	Peptide
1	A	65	SER	Peptide
1	A	733	GLN	Peptide
1	A	736	CYS	Peptide
1	A	788	PHE	Peptide
1	A	792	GLN	Peptide
1	A	795	ILE	Peptide
1	A	809	TYR	Peptide
1	A	856	SER	Peptide
1	A	967	PHE	Peptide
1	A	984	GLY	Peptide
1	A	996	LEU	Peptide
1	B	1115	GLY	Peptide
1	B	1152	ALA	Peptide
1	B	1170	GLY	Peptide
1	B	1180	ILE	Peptide
1	B	1188	GLY	Peptide
1	B	1204	TYR	Peptide
1	B	511	ARG	Peptide
1	B	578	GLY	Peptide
1	B	639	VAL	Peptide
1	B	642	TYR	Peptide
1	B	733	GLN	Peptide
1	B	736	CYS	Peptide
1	B	788	PHE	Peptide
1	B	792	GLN	Peptide
1	B	795	ILE	Peptide
1	B	809	TYR	Peptide
1	B	856	SER	Peptide
1	B	967	PHE	Peptide
1	B	984	GLY	Peptide
1	B	996	LEU	Peptide
1	C	1055	ILE	Peptide
1	C	1115	GLY	Peptide
1	C	1152	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	C	1170	GLY	Peptide
1	C	1180	ILE	Peptide
1	C	1188	GLY	Peptide
1	C	1204	TYR	Peptide
1	C	639	VAL	Peptide
1	C	642	TYR	Peptide
1	C	733	GLN	Peptide
1	C	736	CYS	Peptide
1	C	788	PHE	Peptide
1	C	792	GLN	Peptide
1	C	795	ILE	Peptide
1	C	809	TYR	Peptide
1	C	856	SER	Peptide
1	C	967	PHE	Peptide
1	C	984	GLY	Peptide
1	C	996	LEU	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	A	8806	0	8508	685	0
1	B	8806	0	8504	771	0
1	C	8810	0	8512	587	0
All	All	26422	0	25524	1703	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 33.

All (1703) 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:C:339:CYS:SG	1:C:349:CYS:HB2	1.35	1.62
1:B:344:LEU:CD2	1:B:670:HIS:HB3	1.16	1.61
1:A:583:SER:HB2	1:A:609:TYR:CE1	1.37	1.60
1:C:335:ARG:HB3	1:C:354:PHE:CE2	1.34	1.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LEU:HD22	1:B:670:HIS:CB	1.16	1.58
1:B:347:LEU:CD2	1:B:361:TYR:HB3	1.27	1.57
1:B:335:ARG:CG	1:B:354:PHE:CE2	1.77	1.57
1:B:347:LEU:HD21	1:B:361:TYR:CB	1.18	1.56
1:B:335:ARG:CG	1:B:354:PHE:HE2	1.11	1.54
1:A:429:SER:CB	1:B:1058:LEU:HD22	1.34	1.53
1:A:583:SER:HB2	1:A:609:TYR:CD1	1.38	1.53
1:C:324:LEU:HD11	1:C:354:PHE:CD1	1.37	1.53
1:A:335:ARG:HB2	1:A:354:PHE:CZ	1.42	1.52
1:A:623:VAL:CG1	1:B:65:SER:HB2	1.31	1.51
1:C:1058:LEU:HD11	1:C:1063:GLN:CA	1.37	1.51
1:B:439:SER:CB	1:B:582:ASN:H	1.19	1.49
1:A:429:SER:HB2	1:B:1058:LEU:CD2	1.42	1.49
1:A:335:ARG:CD	1:A:354:PHE:HE2	1.26	1.48
1:A:577:TYR:CD1	1:A:610:GLY:O	1.64	1.48
1:C:1054:ILE:CD1	1:C:1056:GLN:NE2	1.77	1.47
1:A:63:THR:CG2	1:C:628:GLN:HE21	1.27	1.46
1:A:580:ASP:OD2	1:A:628:GLN:CB	1.63	1.46
1:A:335:ARG:HD3	1:A:354:PHE:CE2	1.49	1.45
1:A:343:ASP:CB	1:A:661:VAL:CG2	1.95	1.45
1:A:343:ASP:CB	1:A:661:VAL:HG21	1.47	1.45
1:B:476:PRO:HD2	1:B:577:TYR:CD2	1.48	1.44
1:B:511:ARG:HD2	1:C:436:ASN:ND2	1.16	1.44
1:C:324:LEU:CD1	1:C:354:PHE:HD1	1.31	1.44
1:A:429:SER:CA	1:B:1058:LEU:HD22	1.46	1.43
1:C:339:CYS:SG	1:C:349:CYS:CB	2.06	1.43
1:B:343:ASP:CB	1:B:661:VAL:CG2	1.97	1.42
1:A:623:VAL:CG1	1:B:65:SER:CB	1.98	1.42
1:A:429:SER:CB	1:B:1058:LEU:CD2	1.96	1.41
1:C:1054:ILE:HD12	1:C:1056:GLN:NE2	1.14	1.41
1:A:335:ARG:CB	1:A:354:PHE:CZ	2.02	1.40
1:B:347:LEU:CD2	1:B:361:TYR:CB	1.85	1.40
1:B:348:HIS:HA	1:B:356:VAL:CG2	1.49	1.39
1:B:343:ASP:HB3	1:B:661:VAL:CG2	1.49	1.38
1:A:685:THR:CG2	1:A:697:LEU:HD11	1.54	1.38
1:A:520:ALA:HB1	1:A:521:ASN:ND2	1.31	1.38
1:B:439:SER:HB2	1:B:582:ASN:N	1.09	1.38
1:B:335:ARG:HG3	1:B:354:PHE:CE2	0.87	1.37
1:A:425:CYS:HB3	1:A:428:ILE:CG2	1.50	1.37
1:B:335:ARG:CZ	1:B:354:PHE:HD2	1.36	1.37
1:B:623:VAL:HG13	1:C:329:VAL:O	1.19	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:SER:CB	1:B:582:ASN:N	1.80	1.36
1:A:429:SER:CB	1:B:1058:LEU:HD13	1.54	1.35
1:B:511:ARG:CD	1:C:436:ASN:HD22	1.38	1.34
1:C:343:ASP:CB	1:C:661:VAL:CG2	2.05	1.34
1:C:1054:ILE:CD1	1:C:1056:GLN:HE21	1.37	1.34
1:C:324:LEU:CD1	1:C:354:PHE:CD1	2.07	1.34
1:A:583:SER:CB	1:A:609:TYR:CE1	2.10	1.33
1:A:822:ARG:HG2	1:C:72:GLN:OE1	1.20	1.32
1:C:335:ARG:CB	1:C:354:PHE:HE2	1.42	1.32
1:B:439:SER:CB	1:B:581:THR:HA	1.57	1.31
1:A:271:VAL:HG22	1:C:627:GLN:OE1	1.16	1.31
1:A:377:GLN:OE1	1:A:408:ASN:ND2	1.63	1.31
1:A:63:THR:CB	1:C:625:VAL:HG21	1.59	1.30
1:A:577:TYR:CE2	1:B:1057:ARG:NH2	1.99	1.30
1:A:429:SER:HB3	1:B:1058:LEU:CG	1.60	1.30
1:B:335:ARG:HG3	1:B:354:PHE:CZ	1.67	1.29
1:B:579:THR:C	1:C:61:GLY:HA2	1.56	1.29
1:A:596:ILE:O	1:A:598:SER:N	1.63	1.29
1:A:429:SER:CB	1:B:1058:LEU:CD1	2.11	1.28
1:A:377:GLN:HE21	1:A:585:CYS:CB	1.45	1.28
1:B:582:ASN:HB2	1:B:609:TYR:CD2	1.67	1.28
1:C:1050:SER:O	1:C:1051:ILE:HD13	1.17	1.28
1:B:343:ASP:OD1	1:B:363:VAL:HG11	1.33	1.27
1:A:623:VAL:HG11	1:B:65:SER:CB	1.56	1.27
1:B:439:SER:OG	1:B:581:THR:HA	1.32	1.27
1:B:428:ILE:HD12	1:B:577:TYR:OH	1.34	1.26
1:B:337:ILE:HD11	1:B:348:HIS:CE1	1.71	1.26
1:B:343:ASP:CB	1:B:661:VAL:HG21	1.58	1.26
1:B:625:VAL:CG2	1:C:63:THR:HB	1.64	1.26
1:B:350:SER:O	1:B:351:TYR:HD1	1.18	1.25
1:A:347:LEU:HD21	1:A:361:TYR:CB	1.66	1.25
1:A:521:ASN:HB2	1:B:260:ALA:CB	1.67	1.25
1:B:347:LEU:HD22	1:B:361:TYR:CG	1.72	1.25
1:C:343:ASP:HB2	1:C:661:VAL:CG2	1.62	1.25
1:B:578:GLY:CA	1:B:579:THR:OG1	1.85	1.24
1:B:663:TYR:CE2	1:B:665:LYS:HB3	1.71	1.24
1:C:58:TYR:CD1	1:C:279:PHE:CZ	2.26	1.24
1:B:58:TYR:CD1	1:B:279:PHE:CZ	2.26	1.24
1:B:575:VAL:O	1:B:577:TYR:CD2	1.90	1.24
1:B:428:ILE:HG13	1:C:1056:GLN:O	1.38	1.24
1:B:578:GLY:HA3	1:B:579:THR:OG1	1.16	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:GLN:HA	1:B:577:TYR:CB	1.62	1.23
1:B:576:GLN:CA	1:B:577:TYR:HB2	1.66	1.23
1:B:578:GLY:HA2	1:B:579:THR:CG2	1.68	1.23
1:A:58:TYR:CD1	1:A:279:PHE:CZ	2.26	1.22
1:B:663:TYR:HE2	1:B:665:LYS:CB	1.50	1.22
1:C:812:ASN:HD22	1:C:1051:ILE:CD1	1.53	1.22
1:B:439:SER:CB	1:B:581:THR:CA	2.16	1.22
1:B:347:LEU:CD1	1:B:361:TYR:HB2	1.69	1.22
1:A:347:LEU:O	1:A:350:SER:O	1.55	1.21
1:B:631:VAL:HA	1:C:63:THR:O	1.38	1.21
1:A:63:THR:CG2	1:C:628:GLN:NE2	2.02	1.20
1:A:78:GLN:HB2	1:A:338:ASP:OD2	1.38	1.20
1:B:436:ASN:O	1:B:438:TYR:CE2	1.94	1.20
1:A:385:PHE:CE2	1:A:414:LEU:HB2	1.76	1.20
1:A:425:CYS:HB2	1:A:428:ILE:O	1.38	1.20
1:B:335:ARG:CZ	1:B:354:PHE:CD2	2.25	1.20
1:B:326:ASP:OD2	1:B:335:ARG:HD3	1.40	1.20
1:C:343:ASP:CB	1:C:661:VAL:HG21	1.69	1.20
1:A:429:SER:HB3	1:B:1058:LEU:CD1	1.72	1.20
1:A:63:THR:HG21	1:C:628:GLN:NE2	1.55	1.19
1:B:337:ILE:CD1	1:B:348:HIS:CE1	2.25	1.19
1:B:344:LEU:HD11	1:B:663:TYR:CD1	1.77	1.19
1:B:663:TYR:HE2	1:B:665:LYS:CA	1.54	1.19
1:B:511:ARG:HH22	1:C:575:VAL:HG21	1.04	1.18
1:A:348:HIS:HE1	1:A:356:VAL:CG2	1.57	1.18
1:A:429:SER:CB	1:B:1058:LEU:CG	2.15	1.18
1:A:429:SER:HB3	1:B:1058:LEU:CB	1.72	1.18
1:A:627:GLN:NE2	1:B:271:VAL:HG22	1.57	1.18
1:B:347:LEU:HD13	1:B:361:TYR:CD2	1.77	1.18
1:B:439:SER:HB2	1:B:581:THR:C	1.69	1.18
1:B:1053:ASP:HA	1:B:1057:ARG:CG	1.74	1.18
1:C:1051:ILE:HB	1:C:1054:ILE:HG13	1.26	1.18
1:A:335:ARG:CB	1:A:354:PHE:HZ	1.46	1.18
1:A:338:ASP:O	1:A:345:SER:HB2	1.03	1.18
1:A:425:CYS:CB	1:A:428:ILE:HG23	1.73	1.17
1:A:335:ARG:CB	1:A:354:PHE:CE2	2.27	1.17
1:B:347:LEU:HD22	1:B:361:TYR:CD1	1.80	1.17
1:A:342:ASN:ND2	1:A:344:LEU:HD23	1.56	1.17
1:B:347:LEU:CD2	1:B:361:TYR:CG	2.26	1.17
1:A:377:GLN:NE2	1:A:585:CYS:CB	2.06	1.17
1:A:521:ASN:CB	1:B:260:ALA:CB	2.23	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:ASP:OD2	1:A:628:GLN:HB3	1.43	1.16
1:A:377:GLN:NE2	1:A:585:CYS:HB3	1.59	1.16
1:C:341:PHE:CZ	1:C:696:MET:HG3	1.80	1.16
1:A:348:HIS:CE1	1:A:356:VAL:CG2	2.27	1.16
1:A:521:ASN:CB	1:B:260:ALA:HB1	1.75	1.16
1:B:510:ASP:O	1:B:511:ARG:HD2	1.44	1.16
1:B:623:VAL:CG1	1:C:65:SER:HB2	1.75	1.15
1:A:335:ARG:CD	1:A:354:PHE:CE2	2.17	1.15
1:A:520:ALA:CB	1:A:521:ASN:ND2	2.08	1.15
1:A:271:VAL:CG2	1:C:627:GLN:OE1	1.95	1.15
1:A:344:LEU:HD21	1:A:670:HIS:CB	1.76	1.15
1:A:583:SER:CB	1:A:609:TYR:CD1	2.29	1.15
1:B:575:VAL:O	1:B:577:TYR:HD2	1.24	1.15
1:B:625:VAL:HG21	1:C:63:THR:CB	1.77	1.15
1:A:578:GLY:O	1:A:611:VAL:CG1	1.94	1.15
1:A:623:VAL:HG12	1:B:65:SER:CB	1.69	1.15
1:A:63:THR:HB	1:C:625:VAL:HG21	1.23	1.14
1:C:1053:ASP:HB2	1:C:1058:LEU:HD12	1.23	1.14
1:C:1058:LEU:CD1	1:C:1063:GLN:HA	1.77	1.14
1:B:337:ILE:HD13	1:B:348:HIS:ND1	1.60	1.14
1:B:578:GLY:HA2	1:B:579:THR:HG23	1.16	1.14
1:A:338:ASP:O	1:A:345:SER:CB	1.95	1.14
1:A:66:ASN:HB2	1:A:329:VAL:CA	1.78	1.13
1:A:578:GLY:O	1:A:611:VAL:HG13	1.47	1.13
1:B:350:SER:O	1:B:351:TYR:CD1	2.02	1.13
1:A:521:ASN:HB3	1:B:260:ALA:HB1	1.28	1.13
1:A:437:CYS:HB2	1:A:609:TYR:O	1.47	1.13
1:A:521:ASN:HB2	1:B:260:ALA:HB2	1.17	1.13
1:B:348:HIS:HA	1:B:356:VAL:HG22	1.26	1.13
1:B:377:GLN:HE21	1:B:585:CYS:HB2	1.14	1.12
1:A:520:ALA:C	1:A:521:ASN:HD22	1.55	1.12
1:A:436:ASN:OD1	1:B:1056:GLN:HG2	1.47	1.12
1:A:580:ASP:OD2	1:A:628:GLN:HB2	1.38	1.12
1:B:439:SER:OG	1:B:581:THR:CA	1.98	1.12
1:B:629:ARG:O	1:B:642:TYR:HB2	1.50	1.12
1:B:343:ASP:HB2	1:B:661:VAL:CG2	1.70	1.11
1:A:428:ILE:C	1:B:1058:LEU:HB2	1.75	1.11
1:A:628:GLN:HE21	1:B:63:THR:HG22	1.06	1.11
1:A:335:ARG:HB2	1:A:354:PHE:CE2	1.85	1.11
1:C:343:ASP:HB2	1:C:661:VAL:HG21	1.23	1.11
1:A:580:ASP:CG	1:A:628:GLN:HB2	1.75	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:PRO:CD	1:B:577:TYR:CD2	2.33	1.11
1:B:337:ILE:CD1	1:B:348:HIS:ND1	2.14	1.10
1:A:58:TYR:HD2	1:A:59:PRO:HD2	1.16	1.10
1:A:348:HIS:CE1	1:A:356:VAL:HG22	1.86	1.10
1:A:377:GLN:CG	1:A:585:CYS:HB2	1.82	1.10
1:B:623:VAL:HG11	1:C:65:SER:HB2	1.13	1.10
1:A:685:THR:HG22	1:A:697:LEU:CD1	1.81	1.10
1:A:343:ASP:HB3	1:A:661:VAL:CG2	1.68	1.09
1:B:629:ARG:O	1:B:642:TYR:CB	2.00	1.09
1:A:58:TYR:HD1	1:A:279:PHE:CZ	1.67	1.09
1:A:429:SER:HA	1:B:1058:LEU:HD22	1.22	1.09
1:B:348:HIS:CA	1:B:356:VAL:CG2	2.30	1.09
1:B:632:TYR:CE2	1:C:62:ARG:CB	2.35	1.09
1:A:78:GLN:CB	1:A:338:ASP:OD2	2.01	1.09
1:B:335:ARG:NE	1:B:354:PHE:CD2	2.21	1.09
1:B:1058:LEU:HD12	1:B:1059:ASP:HA	1.25	1.09
1:A:385:PHE:HE2	1:A:414:LEU:HB2	1.02	1.08
1:C:1053:ASP:OD2	1:C:1066:GLN:OE1	1.70	1.08
1:C:1058:LEU:CD1	1:C:1063:GLN:CA	2.30	1.08
1:C:70:THR:HG23	1:C:352:GLU:CG	1.82	1.08
1:B:343:ASP:HB3	1:B:661:VAL:HG23	1.31	1.08
1:B:439:SER:CB	1:B:581:THR:C	2.26	1.08
1:C:812:ASN:HD22	1:C:1051:ILE:HD11	1.00	1.08
1:C:1054:ILE:HD13	1:C:1056:GLN:HE21	1.19	1.08
1:A:692:SER:CB	1:A:696:MET:O	2.02	1.07
1:B:344:LEU:CD1	1:B:663:TYR:CD1	2.36	1.07
1:B:509:ASP:O	1:C:436:ASN:OD1	1.69	1.07
1:B:1051:ILE:HB	1:B:1054:ILE:HG23	1.30	1.07
1:C:58:TYR:HD1	1:C:279:PHE:CZ	1.67	1.07
1:A:343:ASP:HB3	1:A:661:VAL:HG21	1.13	1.07
1:A:347:LEU:HD21	1:A:361:TYR:CG	1.88	1.07
1:A:437:CYS:CB	1:A:609:TYR:O	2.02	1.07
1:C:324:LEU:HG	1:C:354:PHE:HE1	1.14	1.07
1:C:343:ASP:HB3	1:C:661:VAL:CG2	1.80	1.07
1:A:63:THR:OG1	1:C:625:VAL:HG21	1.52	1.07
1:A:436:ASN:ND2	1:B:1056:GLN:O	1.87	1.07
1:B:58:TYR:HD2	1:B:59:PRO:HD2	1.16	1.07
1:A:577:TYR:CD2	1:B:1057:ARG:NH2	2.22	1.07
1:A:685:THR:HA	1:A:697:LEU:HG	1.37	1.07
1:B:58:TYR:HD1	1:B:279:PHE:CZ	1.67	1.07
1:B:377:GLN:OE1	1:B:408:ASN:ND2	1.88	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:LEU:CD1	1:C:337:ILE:HD12	1.85	1.07
1:B:343:ASP:HB3	1:B:661:VAL:HG21	1.14	1.06
1:B:663:TYR:CE2	1:B:665:LYS:CA	2.37	1.06
1:A:377:GLN:HG2	1:A:585:CYS:HB2	1.31	1.06
1:A:63:THR:HG21	1:C:628:GLN:CG	1.86	1.05
1:A:66:ASN:HB2	1:A:329:VAL:HA	1.07	1.05
1:B:511:ARG:HD3	1:C:436:ASN:HB3	1.32	1.05
1:B:582:ASN:HB2	1:B:609:TYR:HD2	0.93	1.05
1:C:58:TYR:HD2	1:C:59:PRO:HD2	1.16	1.05
1:A:63:THR:HG22	1:C:628:GLN:HE21	0.94	1.05
1:C:70:THR:HG23	1:C:352:GLU:HG3	1.06	1.05
1:B:628:GLN:HG2	1:C:63:THR:HG21	1.36	1.05
1:A:63:THR:OG1	1:C:625:VAL:CG2	2.05	1.05
1:A:335:ARG:HB3	1:A:354:PHE:CZ	1.87	1.04
1:A:342:ASN:ND2	1:A:344:LEU:CD2	2.18	1.04
1:A:577:TYR:HD1	1:A:610:GLY:O	1.00	1.04
1:B:347:LEU:HD11	1:B:361:TYR:HB2	1.06	1.04
1:B:511:ARG:HD3	1:C:436:ASN:CB	1.87	1.04
1:B:335:ARG:NE	1:B:354:PHE:HD2	1.54	1.04
1:A:63:THR:HG21	1:C:628:GLN:CD	1.84	1.03
1:A:68:THR:CG2	1:A:326:ASP:HA	1.89	1.03
1:A:343:ASP:HB2	1:A:661:VAL:HG21	1.24	1.03
1:A:520:ALA:CB	1:A:521:ASN:HD22	1.68	1.03
1:C:1058:LEU:HD11	1:C:1063:GLN:HA	1.07	1.03
1:A:623:VAL:HG12	1:B:65:SER:HB3	1.37	1.02
1:A:343:ASP:HB2	1:A:661:VAL:CG2	1.72	1.02
1:C:1051:ILE:HB	1:C:1054:ILE:CG1	1.90	1.02
1:C:1058:LEU:HD21	1:C:1062:GLU:HB2	1.40	1.02
1:A:441:LEU:HD12	1:A:575:VAL:HG12	1.39	1.02
1:C:1058:LEU:HD11	1:C:1063:GLN:CB	1.90	1.02
1:B:511:ARG:CD	1:C:436:ASN:ND2	2.06	1.01
1:A:441:LEU:CD1	1:A:575:VAL:HG12	1.91	1.01
1:B:439:SER:CA	1:B:582:ASN:H	1.71	1.01
1:C:344:LEU:HD21	1:C:670:HIS:CG	1.94	1.01
1:A:70:THR:HB	1:A:323:PHE:O	1.59	1.01
1:B:326:ASP:HB3	1:B:335:ARG:HG2	1.39	1.01
1:C:65:SER:O	1:C:67:ILE:N	1.92	1.01
1:A:627:GLN:HE21	1:B:271:VAL:HG22	1.21	1.01
1:B:65:SER:O	1:B:67:ILE:N	1.92	1.01
1:B:577:TYR:CD1	1:C:1057:ARG:NH1	2.28	1.01
1:A:65:SER:HB2	1:C:623:VAL:CG1	1.91	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:THR:HG22	1:A:324:LEU:HA	1.43	1.00
1:A:685:THR:CB	1:A:697:LEU:HD11	1.90	1.00
1:B:335:ARG:CD	1:B:354:PHE:CE2	2.42	1.00
1:B:663:TYR:CE2	1:B:665:LYS:CB	2.36	1.00
1:B:438:TYR:O	1:B:584:VAL:HB	1.62	1.00
1:B:577:TYR:HD1	1:C:1057:ARG:NH1	1.58	1.00
1:B:1058:LEU:CD1	1:B:1059:ASP:HA	1.92	1.00
1:B:261:GLN:N	1:B:261:GLN:OE1	1.93	0.99
1:A:350:SER:O	1:A:351:TYR:HB2	1.59	0.99
1:B:344:LEU:CD1	1:B:663:TYR:HD1	1.75	0.99
1:C:335:ARG:CB	1:C:354:PHE:CE2	2.29	0.99
1:A:577:TYR:HD1	1:A:610:GLY:C	1.69	0.99
1:A:377:GLN:NE2	1:A:585:CYS:HB2	1.77	0.99
1:A:442:ILE:HD11	1:B:261:GLN:HG3	1.44	0.99
1:B:623:VAL:CG1	1:C:329:VAL:O	2.11	0.99
1:C:1054:ILE:O	1:C:1063:GLN:NE2	1.96	0.99
1:C:323:PHE:CE1	1:C:338:ASP:OD1	2.14	0.98
1:A:344:LEU:HD12	1:A:663:TYR:CE1	1.98	0.98
1:B:401:ARG:HH12	1:C:260:ALA:HB1	1.28	0.98
1:A:337:ILE:HD12	1:A:348:HIS:HB3	1.45	0.98
1:B:428:ILE:HD12	1:B:577:TYR:HH	1.23	0.98
1:A:436:ASN:OD1	1:B:1056:GLN:CG	2.12	0.98
1:C:1054:ILE:HD12	1:C:1054:ILE:H	1.25	0.98
1:A:377:GLN:CD	1:A:585:CYS:HB2	1.89	0.98
1:A:377:GLN:HE21	1:A:585:CYS:HB3	0.83	0.97
1:A:341:PHE:CD1	1:A:696:MET:HB2	1.99	0.97
1:A:583:SER:O	1:A:584:VAL:HG23	1.60	0.97
1:A:429:SER:OG	1:B:1058:LEU:HD13	1.64	0.97
1:B:1051:ILE:CB	1:B:1054:ILE:HG23	1.93	0.97
1:C:343:ASP:HB3	1:C:661:VAL:HG23	1.46	0.97
1:A:63:THR:CG2	1:C:628:GLN:CG	2.43	0.97
1:B:347:LEU:CD1	1:B:361:TYR:CB	2.43	0.97
1:B:377:GLN:HE21	1:B:585:CYS:CB	1.78	0.97
1:A:342:ASN:HD21	1:A:344:LEU:HD23	1.25	0.97
1:B:377:GLN:NE2	1:B:585:CYS:HB2	1.80	0.96
1:B:1053:ASP:HA	1:B:1057:ARG:HG2	1.44	0.96
1:C:70:THR:CG2	1:C:352:GLU:HG3	1.95	0.96
1:B:348:HIS:CA	1:B:356:VAL:HG21	1.94	0.96
1:A:271:VAL:HG22	1:C:627:GLN:CD	1.90	0.96
1:C:1054:ILE:HA	1:C:1063:GLN:HE21	1.27	0.96
1:B:376:GLU:O	1:B:609:TYR:CD1	2.17	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:ILE:HG21	1:C:348:HIS:HB2	1.47	0.96
1:B:347:LEU:HD11	1:B:361:TYR:CB	1.96	0.96
1:A:685:THR:HG22	1:A:697:LEU:HD11	0.98	0.96
1:A:596:ILE:HG22	1:A:597:ALA:H	1.29	0.96
1:A:437:CYS:O	1:A:610:GLY:HA2	1.66	0.96
1:A:628:GLN:NE2	1:B:63:THR:HG22	1.81	0.96
1:C:1058:LEU:HD11	1:C:1063:GLN:N	1.80	0.96
1:A:520:ALA:CA	1:A:521:ASN:HD22	1.79	0.95
1:A:583:SER:O	1:A:584:VAL:CG2	2.14	0.95
1:B:1050:SER:C	1:B:1051:ILE:HD13	1.91	0.95
1:A:68:THR:HG21	1:A:326:ASP:HA	1.48	0.95
1:B:432:ALA:HB2	1:C:1055:ILE:O	1.64	0.95
1:C:343:ASP:CB	1:C:661:VAL:HG23	1.96	0.95
1:C:344:LEU:HD21	1:C:670:HIS:CB	1.96	0.95
1:C:335:ARG:HD2	1:C:354:PHE:CD2	2.02	0.95
1:C:342:ASN:OD1	1:C:344:LEU:N	1.97	0.95
1:B:476:PRO:CG	1:B:577:TYR:CE2	2.50	0.95
1:A:329:VAL:O	1:C:623:VAL:HG13	1.67	0.95
1:A:337:ILE:HD13	1:A:348:HIS:CD2	2.01	0.95
1:B:625:VAL:CG2	1:C:63:THR:CB	2.40	0.95
1:A:596:ILE:C	1:A:598:SER:H	1.75	0.94
1:B:343:ASP:CB	1:B:661:VAL:HG23	1.82	0.94
1:B:428:ILE:CG1	1:C:1056:GLN:O	2.15	0.94
1:C:1053:ASP:CG	1:C:1058:LEU:HB3	1.92	0.94
1:B:261:GLN:O	1:B:287:TYR:HE1	1.51	0.94
1:A:425:CYS:HB3	1:A:428:ILE:HG23	0.95	0.94
1:A:580:ASP:CB	1:A:628:GLN:HB2	1.96	0.94
1:A:822:ARG:CG	1:C:72:GLN:OE1	2.12	0.94
1:B:261:GLN:O	1:B:287:TYR:CE1	2.21	0.94
1:B:343:ASP:OD1	1:B:363:VAL:CG1	2.16	0.94
1:B:441:LEU:HD23	1:B:442:ILE:N	1.83	0.94
1:B:476:PRO:HG2	1:B:577:TYR:CZ	2.03	0.94
1:C:1058:LEU:HD22	1:C:1059:ASP:N	1.83	0.94
1:B:344:LEU:HD12	1:B:663:TYR:HD1	1.31	0.94
1:C:324:LEU:HG	1:C:354:PHE:CE1	2.01	0.93
1:B:349:CYS:O	1:B:351:TYR:N	2.01	0.93
1:B:511:ARG:HH22	1:C:575:VAL:CG2	1.80	0.93
1:B:1053:ASP:HA	1:B:1057:ARG:HG3	1.45	0.93
1:A:579:THR:HB	1:B:61:GLY:O	1.68	0.93
1:A:697:LEU:HD22	1:A:698:LYS:N	1.84	0.93
1:C:1058:LEU:CD2	1:C:1062:GLU:HB2	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:SER:HB2	1:C:623:VAL:HG11	1.50	0.93
1:A:429:SER:CA	1:B:1058:LEU:CD2	2.39	0.93
1:B:663:TYR:CE2	1:B:665:LYS:HA	2.03	0.93
1:A:70:THR:CG2	1:A:324:LEU:HA	1.99	0.93
1:C:1053:ASP:HB3	1:C:1058:LEU:N	1.82	0.93
1:A:523:TYR:HD2	1:B:288:ASP:OD1	1.51	0.93
1:A:685:THR:HA	1:A:697:LEU:CG	1.98	0.93
1:B:441:LEU:HD23	1:B:442:ILE:H	1.33	0.93
1:B:625:VAL:HG21	1:C:63:THR:HB	0.92	0.92
1:B:623:VAL:CG1	1:C:65:SER:CB	2.46	0.92
1:B:634:ALA:HB2	1:C:67:ILE:CD1	2.00	0.92
1:B:1032:ALA:O	1:B:1036:LEU:HB2	1.69	0.92
1:C:58:TYR:CD2	1:C:59:PRO:HD2	2.04	0.92
1:C:1050:SER:O	1:C:1051:ILE:CD1	2.13	0.92
1:A:1032:ALA:O	1:A:1036:LEU:HB2	1.69	0.92
1:B:578:GLY:CA	1:B:579:THR:CB	2.44	0.92
1:B:1058:LEU:HG	1:B:1059:ASP:HB3	1.52	0.92
1:A:66:ASN:O	1:A:327:PHE:O	1.88	0.92
1:C:324:LEU:HD13	1:C:337:ILE:HD12	1.50	0.92
1:C:337:ILE:HD13	1:C:348:HIS:CG	2.03	0.92
1:A:383:CYS:HB3	1:A:404:PHE:CD1	2.05	0.92
1:B:442:ILE:HD11	1:C:261:GLN:HG2	1.52	0.92
1:C:812:ASN:ND2	1:C:1051:ILE:HD11	1.84	0.92
1:A:583:SER:HB2	1:A:609:TYR:HD1	1.27	0.91
1:B:476:PRO:HG2	1:B:577:TYR:CE2	2.05	0.91
1:A:66:ASN:HA	1:A:328:SER:O	1.70	0.91
1:C:1032:ALA:O	1:C:1036:LEU:HB2	1.69	0.91
1:B:58:TYR:CD2	1:B:59:PRO:HD2	2.05	0.91
1:C:341:PHE:CZ	1:C:696:MET:CG	2.53	0.91
1:A:58:TYR:CD2	1:A:59:PRO:HD2	2.05	0.91
1:B:347:LEU:CD1	1:B:361:TYR:CD2	2.53	0.91
1:A:384:ASP:C	1:A:404:PHE:HE1	1.77	0.91
1:A:429:SER:N	1:B:1058:LEU:HB2	1.86	0.91
1:B:634:ALA:HB2	1:C:67:ILE:HD11	1.52	0.91
1:C:812:ASN:ND2	1:C:1051:ILE:CD1	2.34	0.91
1:B:583:SER:H	1:B:609:TYR:CB	1.83	0.90
1:B:476:PRO:HB2	1:B:577:TYR:CE2	2.07	0.90
1:B:376:GLU:O	1:B:609:TYR:HD1	1.55	0.90
1:B:345:SER:O	1:B:348:HIS:HB3	1.72	0.90
1:B:582:ASN:CB	1:B:609:TYR:CD2	2.52	0.90
1:A:344:LEU:HD21	1:A:670:HIS:HB3	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1054:ILE:H	1:C:1056:GLN:HE22	1.11	0.90
1:B:264:HIS:CE1	1:B:283:THR:OG1	2.24	0.90
1:A:66:ASN:CB	1:A:329:VAL:HA	1.98	0.89
1:B:343:ASP:CB	1:B:363:VAL:HG21	2.01	0.89
1:B:439:SER:HG	1:B:581:THR:HA	1.32	0.89
1:B:583:SER:H	1:B:609:TYR:HB2	1.35	0.89
1:C:1054:ILE:N	1:C:1056:GLN:HE22	1.68	0.89
1:A:324:LEU:HB3	1:A:337:ILE:HB	1.55	0.89
1:A:577:TYR:HE2	1:B:1057:ARG:NH2	1.63	0.89
1:C:1062:GLU:O	1:C:1065:ALA:N	2.05	0.89
1:A:63:THR:HG22	1:C:628:GLN:NE2	1.76	0.89
1:A:429:SER:HA	1:B:1058:LEU:CD2	2.00	0.89
1:C:338:ASP:O	1:C:339:CYS:HB2	1.72	0.89
1:B:439:SER:OG	1:B:581:THR:C	2.14	0.89
1:B:476:PRO:HD2	1:B:577:TYR:HD2	1.32	0.89
1:C:347:LEU:HD21	1:C:661:VAL:HG11	1.55	0.89
1:A:335:ARG:CG	1:A:354:PHE:HE2	1.85	0.88
1:B:348:HIS:N	1:B:356:VAL:HG21	1.87	0.88
1:C:341:PHE:CE1	1:C:696:MET:CG	2.56	0.88
1:B:738:LEU:HD11	1:C:943:MET:SD	2.13	0.88
1:C:324:LEU:CD1	1:C:354:PHE:CE1	2.56	0.88
1:B:631:VAL:HG23	1:C:64:TYR:HA	1.54	0.88
1:A:343:ASP:CB	1:A:661:VAL:HG22	2.02	0.88
1:A:943:MET:SD	1:C:738:LEU:HD11	2.13	0.88
1:B:510:ASP:O	1:B:511:ARG:CD	2.18	0.88
1:A:343:ASP:CG	1:A:661:VAL:CG2	2.47	0.88
1:A:583:SER:CB	1:A:609:TYR:HE1	1.69	0.88
1:A:344:LEU:HD21	1:A:670:HIS:CG	2.08	0.88
1:A:347:LEU:CD2	1:A:361:TYR:CB	2.52	0.88
1:B:344:LEU:HD22	1:B:670:HIS:CA	2.04	0.88
1:A:324:LEU:HD11	1:A:353:SER:N	1.88	0.88
1:B:1058:LEU:HG	1:B:1059:ASP:CB	2.04	0.88
1:B:812:ASN:HD22	1:B:1051:ILE:CD1	1.87	0.88
1:A:425:CYS:HB3	1:A:428:ILE:HG22	1.52	0.87
1:C:1055:ILE:H	1:C:1056:GLN:CD	1.82	0.87
1:B:511:ARG:NH2	1:C:575:VAL:HG21	1.89	0.87
1:A:581:THR:CG2	1:A:582:ASN:HA	2.04	0.87
1:A:738:LEU:HD11	1:B:943:MET:SD	2.15	0.87
1:A:583:SER:HB3	1:A:629:ARG:NH2	1.90	0.87
1:B:579:THR:O	1:C:61:GLY:HA2	1.75	0.87
1:C:343:ASP:HB2	1:C:661:VAL:HG22	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:GLY:HA2	1:A:579:THR:OG1	1.74	0.86
1:B:259:THR:OG1	1:B:264:HIS:CD2	2.28	0.86
1:C:323:PHE:HE1	1:C:338:ASP:OD1	1.54	0.86
1:A:429:SER:HB3	1:B:1058:LEU:HD13	1.35	0.86
1:A:596:ILE:HG22	1:A:597:ALA:N	1.87	0.86
1:A:429:SER:HB3	1:B:1058:LEU:HB2	1.57	0.86
1:B:428:ILE:HA	1:C:1057:ARG:C	2.00	0.86
1:B:578:GLY:CA	1:B:579:THR:HG23	2.02	0.86
1:B:623:VAL:HG11	1:C:65:SER:CB	2.03	0.86
1:B:1051:ILE:CG1	1:B:1054:ILE:HG23	2.06	0.86
1:A:677:VAL:HG11	1:B:909:TYR:CE2	2.11	0.86
1:B:347:LEU:CG	1:B:361:TYR:CB	2.53	0.86
1:B:578:GLY:HA2	1:B:579:THR:CB	2.04	0.86
1:A:347:LEU:HD21	1:A:361:TYR:HB3	1.55	0.85
1:A:342:ASN:HD21	1:A:344:LEU:CD2	1.85	0.85
1:A:429:SER:HB2	1:B:1058:LEU:CD1	1.93	0.85
1:B:582:ASN:CB	1:B:609:TYR:HD2	1.85	0.85
1:B:628:GLN:HG2	1:C:63:THR:CG2	2.07	0.85
1:B:677:VAL:HG11	1:C:909:TYR:CE2	2.11	0.85
1:B:812:ASN:HD22	1:B:1051:ILE:HD11	1.41	0.85
1:B:1053:ASP:CA	1:B:1057:ARG:HG3	2.07	0.85
1:B:436:ASN:O	1:B:438:TYR:HE2	1.57	0.85
1:A:628:GLN:HE21	1:B:63:THR:CG2	1.88	0.85
1:C:343:ASP:HB3	1:C:363:VAL:HG21	1.58	0.85
1:B:1053:ASP:CB	1:B:1057:ARG:HG3	2.07	0.85
1:C:337:ILE:HD13	1:C:348:HIS:CB	2.07	0.85
1:B:439:SER:HB3	1:B:581:THR:HA	1.56	0.85
1:B:522:GLN:HG2	1:C:289:THR:HG22	1.59	0.85
1:B:578:GLY:CA	1:B:579:THR:CG2	2.55	0.85
1:B:522:GLN:CD	1:C:289:THR:HG21	2.02	0.84
1:C:341:PHE:O	1:C:342:ASN:ND2	2.10	0.84
1:A:337:ILE:CD1	1:A:348:HIS:HB3	2.07	0.84
1:A:628:GLN:HG2	1:B:63:THR:CG2	2.07	0.84
1:A:627:GLN:HE21	1:B:271:VAL:CG2	1.90	0.84
1:B:377:GLN:CD	1:B:408:ASN:HD21	1.84	0.84
1:C:343:ASP:HB3	1:C:661:VAL:HG21	1.50	0.84
1:C:1054:ILE:CA	1:C:1063:GLN:HE21	1.90	0.84
1:A:340:GLY:O	1:A:696:MET:N	2.10	0.84
1:A:520:ALA:C	1:A:521:ASN:ND2	2.34	0.84
1:B:632:TYR:HB2	1:C:64:TYR:CE1	2.12	0.84
1:A:344:LEU:CD1	1:A:663:TYR:CE1	2.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:SER:HB2	1:B:1058:LEU:HD21	1.58	0.84
1:A:909:TYR:CE2	1:C:677:VAL:HG11	2.13	0.84
1:A:344:LEU:CD1	1:A:663:TYR:CD1	2.61	0.84
1:C:1024:ASP:O	1:C:1028:ASN:HB2	1.78	0.84
1:A:344:LEU:HD11	1:A:663:TYR:CD1	2.13	0.84
1:B:347:LEU:HD21	1:B:361:TYR:HB2	1.56	0.83
1:C:1053:ASP:CB	1:C:1058:LEU:HD12	2.06	0.83
1:C:1058:LEU:CD1	1:C:1063:GLN:CB	2.52	0.83
1:B:1051:ILE:O	1:B:1054:ILE:HG13	1.78	0.83
1:B:522:GLN:HG2	1:C:289:THR:CG2	2.07	0.83
1:B:1024:ASP:O	1:B:1028:ASN:HB2	1.78	0.83
1:A:337:ILE:CD1	1:A:348:HIS:CD2	2.61	0.83
1:A:1024:ASP:O	1:A:1028:ASN:HB2	1.78	0.83
1:B:335:ARG:CB	1:B:354:PHE:HE2	1.91	0.83
1:A:347:LEU:HD21	1:A:361:TYR:HB2	1.61	0.83
1:B:347:LEU:CD1	1:B:361:TYR:CG	2.62	0.83
1:B:348:HIS:HA	1:B:356:VAL:HG21	1.50	0.83
1:A:425:CYS:CB	1:A:428:ILE:O	2.26	0.82
1:B:347:LEU:CG	1:B:361:TYR:HB2	2.08	0.82
1:B:442:ILE:HD11	1:C:261:GLN:CG	2.08	0.82
1:C:337:ILE:HD13	1:C:348:HIS:HB3	1.60	0.82
1:B:343:ASP:HB2	1:B:661:VAL:HG22	1.59	0.82
1:C:324:LEU:HD12	1:C:354:PHE:CD1	2.13	0.82
1:B:439:SER:HB3	1:B:581:THR:HG22	1.59	0.82
1:B:629:ARG:O	1:B:642:TYR:HB3	1.79	0.82
1:B:264:HIS:ND1	1:B:283:THR:OG1	2.13	0.82
1:B:348:HIS:O	1:B:353:SER:O	1.98	0.82
1:A:383:CYS:SG	1:A:404:PHE:HB3	2.19	0.82
1:B:343:ASP:OD2	1:B:363:VAL:HB	1.79	0.82
1:B:349:CYS:O	1:B:352:GLU:N	2.13	0.82
1:A:580:ASP:OD2	1:A:628:GLN:CG	2.26	0.82
1:A:343:ASP:HB2	1:A:661:VAL:HG22	1.58	0.82
1:A:520:ALA:HB1	1:A:521:ASN:HD21	0.99	0.82
1:B:70:THR:HG23	1:B:352:GLU:HG3	1.62	0.82
1:B:264:HIS:CE1	1:B:283:THR:HG1	1.98	0.81
1:A:628:GLN:NE2	1:B:63:THR:CG2	2.43	0.81
1:B:441:LEU:CD2	1:B:442:ILE:N	2.43	0.81
1:B:510:ASP:HB3	1:C:436:ASN:HD21	1.42	0.81
1:C:324:LEU:CG	1:C:354:PHE:CE1	2.63	0.81
1:C:1053:ASP:OD1	1:C:1058:LEU:HB3	1.79	0.81
1:A:430:PRO:O	1:A:433:ILE:HG22	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:TYR:CD1	1:C:279:PHE:HZ	1.99	0.81
1:A:432:ALA:HB1	1:B:1056:GLN:O	1.80	0.81
1:A:628:GLN:CG	1:B:63:THR:CG2	2.57	0.81
1:B:344:LEU:CG	1:B:670:HIS:HB3	2.08	0.81
1:A:343:ASP:OD2	1:A:661:VAL:CG2	2.29	0.81
1:A:343:ASP:OD2	1:A:661:VAL:HG22	1.81	0.81
1:A:377:GLN:HG2	1:A:585:CYS:CB	2.10	0.81
1:A:406:ASN:HA	1:A:583:SER:OG	1.80	0.81
1:A:348:HIS:HE1	1:A:356:VAL:HG23	1.45	0.81
1:B:428:ILE:CD1	1:B:577:TYR:OH	2.24	0.81
1:B:575:VAL:C	1:B:577:TYR:CD2	2.58	0.81
1:B:511:ARG:HD2	1:C:436:ASN:CG	2.04	0.80
1:B:628:GLN:CG	1:C:63:THR:HG21	2.11	0.80
1:C:1054:ILE:HD13	1:C:1056:GLN:NE2	1.76	0.80
1:A:697:LEU:HD13	1:A:697:LEU:O	1.79	0.80
1:B:579:THR:C	1:C:61:GLY:CA	2.49	0.80
1:B:632:TYR:CZ	1:C:62:ARG:CB	2.64	0.80
1:A:521:ASN:HB3	1:B:260:ALA:CB	2.00	0.80
1:C:1050:SER:C	1:C:1051:ILE:HD13	2.05	0.80
1:A:522:GLN:HG2	1:B:289:THR:HG22	1.64	0.80
1:A:677:VAL:HG21	1:B:909:TYR:HD2	1.47	0.80
1:B:511:ARG:CD	1:C:436:ASN:HB3	2.10	0.80
1:B:634:ALA:CB	1:C:67:ILE:HD11	2.11	0.80
1:C:129:THR:HG22	1:C:131:ILE:H	1.47	0.80
1:B:335:ARG:O	1:B:354:PHE:HZ	1.65	0.79
1:B:677:VAL:HG21	1:C:909:TYR:CD2	2.17	0.79
1:C:1054:ILE:C	1:C:1063:GLN:NE2	2.38	0.79
1:B:583:SER:N	1:B:609:TYR:HB2	1.97	0.79
1:B:129:THR:HG22	1:B:131:ILE:H	1.47	0.79
1:B:348:HIS:CA	1:B:356:VAL:HG22	2.06	0.79
1:C:954:SER:O	1:C:958:VAL:HB	1.82	0.79
1:A:954:SER:O	1:A:958:VAL:HB	1.82	0.79
1:B:1051:ILE:HB	1:B:1054:ILE:CG2	2.12	0.79
1:B:476:PRO:CB	1:B:577:TYR:CE2	2.65	0.79
1:A:522:GLN:CD	1:B:289:THR:HG21	2.08	0.79
1:B:677:VAL:HG21	1:C:909:TYR:HD2	1.47	0.79
1:A:63:THR:CB	1:C:625:VAL:CG2	2.52	0.79
1:B:439:SER:HB2	1:B:581:THR:CA	1.96	0.79
1:B:511:ARG:CD	1:C:436:ASN:CB	2.61	0.79
1:C:1054:ILE:HA	1:C:1063:GLN:NE2	1.98	0.79
1:A:436:ASN:OD1	1:B:1056:GLN:CB	2.31	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:SER:HB3	1:C:1059:ASP:HA	1.64	0.79
1:A:523:TYR:CD2	1:B:288:ASP:OD1	2.35	0.78
1:B:628:GLN:CG	1:C:63:THR:CG2	2.61	0.78
1:A:429:SER:HB2	1:B:1058:LEU:CG	1.93	0.78
1:A:583:SER:HB3	1:A:609:TYR:CE1	2.18	0.78
1:A:129:THR:HG22	1:A:131:ILE:H	1.47	0.78
1:B:1053:ASP:HB3	1:B:1057:ARG:HG3	1.64	0.78
1:C:58:TYR:CD1	1:C:279:PHE:CE2	2.71	0.78
1:B:954:SER:O	1:B:958:VAL:HB	1.82	0.78
1:A:344:LEU:HD11	1:A:663:TYR:HD1	1.47	0.78
1:A:909:TYR:HD2	1:C:677:VAL:HG21	1.49	0.78
1:C:324:LEU:CG	1:C:354:PHE:HE1	1.92	0.78
1:A:58:TYR:CD1	1:A:279:PHE:CE2	2.71	0.78
1:B:337:ILE:HD13	1:B:348:HIS:CE1	2.03	0.78
1:B:58:TYR:CD1	1:B:279:PHE:CE2	2.71	0.78
1:A:692:SER:HB2	1:A:696:MET:O	1.84	0.78
1:B:429:SER:HB3	1:C:1059:ASP:CA	2.14	0.78
1:A:405:THR:C	1:A:407:CYS:N	2.38	0.77
1:A:335:ARG:CG	1:A:354:PHE:CE2	2.64	0.77
1:A:403:VAL:HG13	1:A:441:LEU:O	1.84	0.77
1:A:583:SER:C	1:A:584:VAL:HG23	2.09	0.77
1:A:427:GLN:HE21	1:A:427:GLN:HA	1.47	0.77
1:A:677:VAL:HG21	1:B:909:TYR:CD2	2.18	0.77
1:A:343:ASP:CB	1:A:661:VAL:HG23	2.13	0.77
1:A:906:MET:SD	1:C:678:ALA:HA	2.24	0.77
1:A:678:ALA:HA	1:B:906:MET:SD	2.25	0.77
1:B:67:ILE:O	1:B:327:PHE:HD1	1.67	0.77
1:B:343:ASP:CG	1:B:363:VAL:CB	2.58	0.77
1:B:1054:ILE:H	1:B:1054:ILE:HD12	1.48	0.77
1:C:67:ILE:O	1:C:327:PHE:HD1	1.67	0.77
1:C:337:ILE:HG21	1:C:348:HIS:CB	2.13	0.77
1:A:65:SER:HB2	1:C:623:VAL:HG12	1.65	0.77
1:B:623:VAL:HG12	1:C:65:SER:CB	2.14	0.76
1:B:678:ALA:HA	1:C:906:MET:SD	2.25	0.76
1:A:909:TYR:CD2	1:C:677:VAL:HG21	2.20	0.76
1:A:344:LEU:HD12	1:A:663:TYR:HE1	1.47	0.76
1:A:437:CYS:C	1:A:609:TYR:O	2.29	0.76
1:B:439:SER:HB3	1:B:581:THR:CG2	2.15	0.76
1:B:1058:LEU:CG	1:B:1059:ASP:HA	2.15	0.76
1:A:63:THR:CG2	1:C:628:GLN:HG3	2.13	0.76
1:A:63:THR:HG21	1:C:628:GLN:HG2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:GLN:HE21	1:C:1047:ILE:HD11	1.51	0.76
1:A:428:ILE:HG23	1:A:478:CYS:SG	2.26	0.76
1:A:321:LEU:HA	1:B:822:ARG:NH1	2.01	0.76
1:A:628:GLN:HG2	1:B:63:THR:HG21	1.66	0.76
1:B:344:LEU:HD11	1:B:663:TYR:CG	2.21	0.76
1:A:404:PHE:HB3	1:A:407:CYS:SG	2.25	0.76
1:B:335:ARG:CD	1:B:354:PHE:CD2	2.66	0.76
1:A:940:ASP:OD1	1:C:737:ALA:HB1	1.86	0.75
1:B:432:ALA:CB	1:C:1055:ILE:O	2.34	0.75
1:A:58:TYR:CE1	1:A:279:PHE:HZ	2.05	0.75
1:B:326:ASP:CB	1:B:335:ARG:HG2	2.15	0.75
1:B:335:ARG:NE	1:B:354:PHE:CE2	2.53	0.75
1:B:337:ILE:HD11	1:B:348:HIS:HE1	1.45	0.75
1:C:1054:ILE:CA	1:C:1063:GLN:NE2	2.49	0.75
1:A:715:LEU:HD21	1:B:936:PRO:HG2	1.68	0.75
1:B:715:LEU:HD21	1:C:936:PRO:HG2	1.67	0.75
1:C:337:ILE:CD1	1:C:348:HIS:HB3	2.16	0.75
1:A:441:LEU:CD1	1:A:575:VAL:CG1	2.65	0.75
1:C:324:LEU:CD1	1:C:337:ILE:CD1	2.63	0.75
1:B:347:LEU:HD13	1:B:361:TYR:CG	2.19	0.75
1:A:337:ILE:HG21	1:A:348:HIS:HB2	1.69	0.74
1:C:1053:ASP:O	1:C:1063:GLN:HG3	1.87	0.74
1:A:66:ASN:HB2	1:A:329:VAL:N	2.02	0.74
1:A:341:PHE:CD1	1:A:696:MET:CB	2.70	0.74
1:B:343:ASP:HB3	1:B:363:VAL:HG21	1.68	0.74
1:A:634:ALA:HB2	1:B:67:ILE:HD11	1.68	0.74
1:C:58:TYR:CE1	1:C:279:PHE:HZ	2.05	0.74
1:A:337:ILE:CD1	1:A:348:HIS:CB	2.66	0.74
1:A:737:ALA:HB1	1:B:940:ASP:OD1	1.88	0.74
1:A:936:PRO:HG2	1:C:715:LEU:HD21	1.68	0.74
1:B:58:TYR:CE1	1:B:279:PHE:HZ	2.05	0.74
1:A:582:ASN:O	1:A:583:SER:HB3	1.86	0.74
1:C:1058:LEU:HD21	1:C:1062:GLU:CB	2.16	0.74
1:A:343:ASP:HB3	1:A:661:VAL:HG23	1.65	0.74
1:C:341:PHE:CE1	1:C:696:MET:HG2	2.22	0.74
1:A:68:THR:HG21	1:A:326:ASP:CA	2.17	0.74
1:A:1179:ARG:HB2	1:A:1184:TRP:HA	1.70	0.74
1:B:58:TYR:CD1	1:B:279:PHE:HZ	1.99	0.74
1:B:737:ALA:HB1	1:C:940:ASP:OD1	1.88	0.74
1:B:377:GLN:CD	1:B:408:ASN:ND2	2.43	0.73
1:B:1054:ILE:HD12	1:B:1054:ILE:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:HD21	1:A:670:HIS:HB2	1.68	0.73
1:A:583:SER:HB3	1:A:629:ARG:HH21	1.52	0.73
1:B:1179:ARG:HB2	1:B:1184:TRP:HA	1.70	0.73
1:A:337:ILE:HD13	1:A:348:HIS:HD2	1.53	0.73
1:A:1114:SER:HB3	1:B:1104:ASN:HB3	1.70	0.73
1:B:432:ALA:HB1	1:C:1056:GLN:CA	2.18	0.73
1:B:343:ASP:CG	1:B:363:VAL:HB	2.14	0.73
1:B:432:ALA:CB	1:C:1056:GLN:O	2.37	0.73
1:A:337:ILE:HD13	1:A:348:HIS:CG	2.23	0.72
1:A:347:LEU:O	1:A:351:TYR:HB2	1.88	0.72
1:C:324:LEU:HB2	1:C:352:GLU:O	1.89	0.72
1:C:341:PHE:O	1:C:342:ASN:CG	2.32	0.72
1:A:441:LEU:HD12	1:A:575:VAL:CG1	2.17	0.72
1:B:58:TYR:CE1	1:B:279:PHE:CZ	2.77	0.72
1:B:1059:ASP:OD1	1:B:1062:GLU:OE1	2.08	0.72
1:C:324:LEU:HD11	1:C:337:ILE:CD1	2.20	0.72
1:C:1179:ARG:HB2	1:C:1184:TRP:HA	1.70	0.72
1:A:342:ASN:HD22	1:A:344:LEU:H	1.37	0.72
1:C:1058:LEU:HD13	1:C:1058:LEU:C	2.15	0.72
1:A:428:ILE:C	1:B:1058:LEU:CB	2.59	0.72
1:A:63:THR:HG23	1:C:628:GLN:HG3	1.72	0.72
1:C:58:TYR:CE1	1:C:279:PHE:CZ	2.78	0.72
1:A:348:HIS:CE1	1:A:356:VAL:HG21	2.25	0.72
1:B:631:VAL:CA	1:C:63:THR:O	2.30	0.72
1:A:347:LEU:CD2	1:A:361:TYR:HB2	2.18	0.71
1:A:578:GLY:O	1:A:611:VAL:HG11	1.90	0.71
1:A:581:THR:CG2	1:A:582:ASN:ND2	2.53	0.71
1:C:1053:ASP:CB	1:C:1058:LEU:HB3	2.19	0.71
1:A:337:ILE:HD13	1:A:348:HIS:CB	2.21	0.71
1:A:377:GLN:CG	1:A:585:CYS:CB	2.66	0.71
1:B:339:CYS:SG	1:B:349:CYS:CB	2.79	0.71
1:B:1114:SER:HB3	1:C:1104:ASN:HB3	1.71	0.71
1:C:1054:ILE:HD12	1:C:1054:ILE:N	2.03	0.71
1:C:1058:LEU:CD1	1:C:1063:GLN:HB2	2.19	0.71
1:B:343:ASP:C	1:B:661:VAL:HG21	2.14	0.71
1:A:324:LEU:CD1	1:A:353:SER:N	2.52	0.71
1:A:341:PHE:HD1	1:A:696:MET:HB2	1.53	0.71
1:A:385:PHE:CD2	1:A:414:LEU:HD13	2.25	0.71
1:A:581:THR:HG23	1:A:582:ASN:ND2	2.06	0.71
1:A:623:VAL:HG13	1:B:329:VAL:O	1.89	0.71
1:B:337:ILE:HD13	1:B:348:HIS:CG	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:TYR:CE1	1:C:1057:ARG:NH1	2.58	0.71
1:C:339:CYS:SG	1:C:349:CYS:HB3	2.28	0.71
1:A:697:LEU:HD13	1:A:697:LEU:C	2.16	0.70
1:B:344:LEU:HD22	1:B:670:HIS:CG	2.18	0.70
1:B:1051:ILE:HG12	1:B:1054:ILE:HG23	1.72	0.70
1:B:522:GLN:CG	1:C:289:THR:CG2	2.68	0.70
1:A:58:TYR:CE1	1:A:279:PHE:CZ	2.77	0.70
1:A:582:ASN:O	1:A:583:SER:CB	2.39	0.70
1:B:40:PHE:HD1	1:B:86:VAL:HG13	1.57	0.70
1:C:40:PHE:HD1	1:C:86:VAL:HG13	1.57	0.70
1:C:347:LEU:CD2	1:C:661:VAL:HG11	2.21	0.70
1:A:65:SER:CB	1:C:623:VAL:HG12	2.21	0.70
1:A:409:TYR:OH	1:A:433:ILE:O	2.09	0.70
1:B:348:HIS:HA	1:B:356:VAL:HG23	1.69	0.70
1:A:341:PHE:CE1	1:A:696:MET:CB	2.75	0.70
1:C:335:ARG:HB3	1:C:354:PHE:CZ	2.18	0.70
1:B:583:SER:N	1:B:609:TYR:CG	2.58	0.70
1:C:1056:GLN:OE1	1:C:1057:ARG:N	2.23	0.70
1:C:324:LEU:HD11	1:C:354:PHE:HD1	0.60	0.70
1:C:1054:ILE:HD12	1:C:1056:GLN:HE22	0.84	0.70
1:A:63:THR:OG1	1:C:625:VAL:HG23	1.91	0.70
1:A:342:ASN:ND2	1:A:344:LEU:HD22	2.06	0.70
1:A:401:ARG:HH12	1:B:260:ALA:HB1	1.57	0.70
1:A:436:ASN:HD21	1:B:1056:GLN:C	2.00	0.70
1:C:324:LEU:HG	1:C:324:LEU:O	1.92	0.70
1:A:69:ILE:HD12	1:A:69:ILE:C	2.16	0.69
1:A:442:ILE:HD11	1:B:261:GLN:CG	2.22	0.69
1:A:78:GLN:HB3	1:A:338:ASP:OD2	1.90	0.69
1:B:326:ASP:OD2	1:B:335:ARG:CD	2.31	0.69
1:C:1056:GLN:CD	1:C:1057:ARG:H	1.99	0.69
1:A:340:GLY:CA	1:A:695:SER:HB2	2.21	0.69
1:B:343:ASP:CG	1:B:363:VAL:HG11	2.16	0.69
1:C:812:ASN:HD22	1:C:1051:ILE:HD13	1.53	0.69
1:B:476:PRO:CG	1:B:577:TYR:CD2	2.75	0.69
1:A:323:PHE:CE1	1:A:338:ASP:HB2	2.27	0.69
1:A:384:ASP:C	1:A:404:PHE:CE1	2.67	0.69
1:A:1104:ASN:HB3	1:C:1114:SER:HB3	1.72	0.69
1:B:347:LEU:CD2	1:B:361:TYR:CD1	2.63	0.69
1:A:351:TYR:O	1:A:353:SER:OG	2.09	0.69
1:C:67:ILE:O	1:C:327:PHE:CD1	2.46	0.69
1:C:335:ARG:NH1	1:C:354:PHE:HD2	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:ASN:HB3	1:C:587:LYS:HB3	1.75	0.69
1:A:63:THR:HB	1:C:625:VAL:CG2	2.12	0.69
1:A:685:THR:CB	1:A:697:LEU:CD1	2.69	0.69
1:B:339:CYS:SG	1:B:349:CYS:HB2	2.32	0.69
1:B:432:ALA:HB1	1:C:1056:GLN:O	1.92	0.69
1:A:40:PHE:HD1	1:A:86:VAL:HG13	1.57	0.69
1:A:427:GLN:HA	1:A:427:GLN:NE2	2.07	0.69
1:A:432:ALA:O	1:A:436:ASN:ND2	2.26	0.69
1:B:1050:SER:O	1:B:1051:ILE:HD13	1.93	0.69
1:A:581:THR:HG22	1:A:582:ASN:HA	1.72	0.68
1:A:906:MET:SD	1:C:677:VAL:HA	2.33	0.68
1:B:632:TYR:CD2	1:C:62:ARG:CB	2.76	0.68
1:C:1056:GLN:HB2	1:C:1057:ARG:HG2	1.74	0.68
1:B:67:ILE:O	1:B:327:PHE:CD1	2.46	0.68
1:B:343:ASP:CG	1:B:363:VAL:HG21	2.17	0.68
1:B:1058:LEU:HB3	1:B:1059:ASP:OD2	1.93	0.68
1:B:408:ASN:HB3	1:B:587:LYS:HB3	1.74	0.68
1:B:608:LEU:HD22	1:B:630:PHE:HE1	1.58	0.68
1:C:344:LEU:HA	1:C:347:LEU:HD22	1.74	0.68
1:A:405:THR:N	1:A:407:CYS:SG	2.67	0.68
1:A:581:THR:CG2	1:A:582:ASN:HD22	2.06	0.68
1:A:677:VAL:HA	1:B:906:MET:SD	2.34	0.68
1:B:476:PRO:HB2	1:B:577:TYR:HE2	1.58	0.68
1:B:347:LEU:CD2	1:B:361:TYR:HB2	2.05	0.67
1:A:341:PHE:O	1:A:345:SER:HB3	1.95	0.67
1:A:408:ASN:HB3	1:A:587:LYS:HB3	1.75	0.67
1:A:405:THR:C	1:A:407:CYS:H	1.99	0.67
1:B:339:CYS:HB3	1:B:349:CYS:SG	2.34	0.67
1:C:341:PHE:CE1	1:C:696:MET:HG3	2.26	0.67
1:C:337:ILE:HD13	1:C:348:HIS:CD2	2.29	0.67
1:A:425:CYS:CB	1:A:428:ILE:CG2	2.46	0.67
1:B:1031:GLN:O	1:B:1035:LYS:HB2	1.95	0.67
1:C:1031:GLN:O	1:C:1035:LYS:HB2	1.95	0.67
1:B:428:ILE:HA	1:C:1057:ARG:O	1.94	0.67
1:A:66:ASN:CA	1:A:328:SER:O	2.43	0.67
1:A:271:VAL:CG2	1:C:627:GLN:CD	2.60	0.67
1:A:429:SER:CB	1:B:1058:LEU:HB2	2.25	0.67
1:B:1049:ALA:O	1:B:1050:SER:OG	2.13	0.67
1:A:522:GLN:CD	1:B:289:THR:CG2	2.68	0.67
1:B:66:ASN:HB2	1:B:329:VAL:HA	1.77	0.67
1:C:1055:ILE:C	1:C:1056:GLN:OE1	2.38	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:TYR:CE2	1:B:665:LYS:N	2.63	0.66
1:B:677:VAL:HA	1:C:906:MET:SD	2.35	0.66
1:C:493:LYS:NZ	1:C:565:GLU:O	2.29	0.66
1:A:68:THR:CG2	1:A:326:ASP:CA	2.69	0.66
1:A:692:SER:OG	1:A:696:MET:O	2.12	0.66
1:A:764:PHE:CD2	1:B:943:MET:SD	2.89	0.66
1:B:344:LEU:HD12	1:B:663:TYR:CD1	2.17	0.66
1:B:439:SER:CB	1:B:581:THR:HG22	2.25	0.66
1:A:596:ILE:CG2	1:A:597:ALA:H	2.00	0.66
1:B:337:ILE:CD1	1:B:348:HIS:HD1	2.08	0.66
1:B:493:LYS:NZ	1:B:565:GLU:O	2.28	0.66
1:B:335:ARG:NH1	1:B:354:PHE:CD2	2.63	0.66
1:C:324:LEU:HD11	1:C:354:PHE:CE1	2.15	0.66
1:B:406:ASN:HA	1:B:583:SER:HB3	1.76	0.66
1:B:511:ARG:CD	1:C:436:ASN:CG	2.66	0.66
1:A:335:ARG:NE	1:A:354:PHE:CE2	2.64	0.66
1:B:511:ARG:HB2	1:C:436:ASN:HB3	1.78	0.66
1:C:1051:ILE:CB	1:C:1054:ILE:HG13	2.16	0.66
1:A:493:LYS:NZ	1:A:565:GLU:O	2.28	0.65
1:A:1031:GLN:O	1:A:1035:LYS:HB2	1.95	0.65
1:A:337:ILE:CD1	1:A:348:HIS:CG	2.79	0.65
1:A:401:ARG:HH12	1:A:521:ASN:HB3	1.60	0.65
1:B:343:ASP:CA	1:B:661:VAL:HG21	2.25	0.65
1:B:339:CYS:HG	1:B:349:CYS:CB	2.08	0.65
1:A:428:ILE:CG2	1:A:478:CYS:SG	2.85	0.65
1:B:339:CYS:CB	1:B:349:CYS:SG	2.84	0.65
1:B:476:PRO:CD	1:B:577:TYR:CE2	2.76	0.65
1:A:578:GLY:HA2	1:A:579:THR:CB	2.25	0.65
1:B:401:ARG:NH1	1:C:260:ALA:HB1	2.06	0.65
1:B:581:THR:O	1:B:582:ASN:ND2	2.30	0.65
1:B:335:ARG:O	1:B:354:PHE:CZ	2.49	0.65
1:C:66:ASN:HB2	1:C:329:VAL:HA	1.77	0.65
1:C:322:THR:O	1:C:339:CYS:HB2	1.97	0.65
1:C:335:ARG:HD2	1:C:354:PHE:HD2	1.61	0.65
1:A:429:SER:HB2	1:B:1058:LEU:HD22	1.10	0.64
1:B:432:ALA:HB1	1:C:1056:GLN:C	2.22	0.64
1:B:898:VAL:HA	1:B:1023:GLN:HE21	1.62	0.64
1:A:58:TYR:CD1	1:A:279:PHE:HZ	1.98	0.64
1:A:692:SER:HB3	1:A:696:MET:O	1.92	0.64
1:B:347:LEU:HD13	1:B:361:TYR:HD2	1.57	0.64
1:B:510:ASP:CB	1:C:436:ASN:HD21	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1053:ASP:OD2	1:B:1058:LEU:O	2.15	0.64
1:C:595:LYS:HD3	1:C:596:ILE:HG13	1.79	0.64
1:B:634:ALA:CB	1:C:67:ILE:CD1	2.70	0.64
1:C:324:LEU:HD11	1:C:337:ILE:HD12	1.74	0.64
1:A:322:THR:O	1:A:339:CYS:SG	2.56	0.64
1:B:501:ASN:ND2	1:B:559:SER:OG	2.31	0.64
1:B:1053:ASP:CA	1:B:1057:ARG:CG	2.62	0.64
1:B:764:PHE:CD2	1:C:943:MET:SD	2.90	0.64
1:C:70:THR:HG23	1:C:352:GLU:HA	1.79	0.64
1:A:342:ASN:HD22	1:A:344:LEU:CD2	2.06	0.64
1:A:599:GLN:HB3	1:A:600:LEU:HD23	1.80	0.64
1:C:1058:LEU:HD21	1:C:1063:GLN:N	2.12	0.64
1:A:1027:ASN:O	1:A:1031:GLN:HB2	1.98	0.64
1:B:401:ARG:NH1	1:C:260:ALA:O	2.28	0.64
1:B:1027:ASN:O	1:B:1031:GLN:HB2	1.98	0.64
1:B:577:TYR:CE1	1:C:1057:ARG:HD3	2.32	0.64
1:C:340:GLY:O	1:C:695:SER:HB2	1.97	0.64
1:B:259:THR:OG1	1:B:264:HIS:HD2	1.81	0.63
1:C:1053:ASP:HB2	1:C:1058:LEU:CD1	2.15	0.63
1:C:599:GLN:HB3	1:C:600:LEU:HD23	1.80	0.63
1:C:812:ASN:ND2	1:C:1051:ILE:HD13	2.11	0.63
1:C:1027:ASN:O	1:C:1031:GLN:HB2	1.98	0.63
1:C:1110:GLN:O	1:C:1122:HIS:ND1	2.31	0.63
1:A:323:PHE:CE1	1:A:338:ASP:CB	2.80	0.63
1:A:522:GLN:CG	1:B:289:THR:CG2	2.77	0.63
1:B:599:GLN:HB3	1:B:600:LEU:HD23	1.80	0.63
1:C:351:TYR:O	1:C:353:SER:N	2.30	0.63
1:A:432:ALA:HB1	1:B:1056:GLN:C	2.22	0.63
1:A:943:MET:SD	1:C:764:PHE:CD2	2.91	0.63
1:B:510:ASP:O	1:B:511:ARG:CG	2.47	0.63
1:C:1054:ILE:H	1:C:1056:GLN:NE2	1.91	0.63
1:B:339:CYS:CB	1:B:349:CYS:HG	2.12	0.63
1:B:439:SER:HB2	1:B:582:ASN:H	0.69	0.63
1:A:522:GLN:CG	1:B:289:THR:HG22	2.28	0.63
1:A:634:ALA:HB2	1:B:67:ILE:CD1	2.28	0.63
1:B:344:LEU:O	1:B:348:HIS:HB2	1.99	0.63
1:A:579:THR:CB	1:B:61:GLY:O	2.45	0.63
1:B:406:ASN:HA	1:B:583:SER:CB	2.29	0.63
1:B:576:GLN:HA	1:B:577:TYR:HB2	0.75	0.63
1:A:697:LEU:O	1:A:698:LYS:HB3	1.99	0.62
1:B:583:SER:N	1:B:609:TYR:CB	2.60	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:PHE:HB2	1:B:441:LEU:HB3	1.80	0.62
1:C:1058:LEU:HD22	1:C:1059:ASP:H	1.61	0.62
1:A:898:VAL:HA	1:A:1023:GLN:HE21	1.62	0.62
1:C:898:VAL:HA	1:C:1023:GLN:HE21	1.62	0.62
1:A:577:TYR:O	1:A:579:THR:HG23	1.98	0.62
1:C:1055:ILE:N	1:C:1056:GLN:OE1	2.33	0.62
1:A:1110:GLN:O	1:A:1122:HIS:ND1	2.31	0.62
1:B:595:LYS:HD3	1:B:596:ILE:HG13	1.79	0.62
1:C:68:THR:O	1:C:69:ILE:CG2	2.48	0.62
1:A:694:ARG:NH1	1:B:822:ARG:HH21	1.97	0.62
1:A:964:LEU:HD22	1:A:965:SER:HB3	1.82	0.62
1:A:385:PHE:CE2	1:A:414:LEU:CB	2.68	0.62
1:B:68:THR:O	1:B:69:ILE:CG2	2.48	0.62
1:C:351:TYR:HH	1:C:361:TYR:HE1	1.47	0.62
1:A:343:ASP:CG	1:A:661:VAL:HG22	2.18	0.62
1:A:436:ASN:CG	1:B:1056:GLN:HB3	2.25	0.62
1:B:625:VAL:HG23	1:C:63:THR:CB	2.26	0.62
1:A:324:LEU:HD11	1:A:353:SER:CA	2.30	0.61
1:A:685:THR:HB	1:A:697:LEU:HD11	1.79	0.61
1:B:428:ILE:CA	1:C:1058:LEU:HA	2.30	0.61
1:B:1051:ILE:HD13	1:B:1051:ILE:N	2.11	0.61
1:C:964:LEU:HD22	1:C:965:SER:HB3	1.82	0.61
1:B:608:LEU:HD22	1:B:630:PHE:CE1	2.36	0.61
1:B:1110:GLN:O	1:B:1122:HIS:ND1	2.31	0.61
1:C:341:PHE:HZ	1:C:696:MET:HG3	1.58	0.61
1:A:403:VAL:CG1	1:A:441:LEU:O	2.47	0.61
1:B:575:VAL:O	1:B:577:TYR:CG	2.51	0.61
1:A:623:VAL:CG1	1:B:65:SER:HB3	1.98	0.61
1:B:964:LEU:HD22	1:B:965:SER:HB3	1.82	0.61
1:C:351:TYR:CE2	1:C:356:VAL:HG13	2.36	0.61
1:A:405:THR:HA	1:A:584:VAL:HG22	1.82	0.61
1:A:631:VAL:HA	1:B:63:THR:O	2.01	0.61
1:C:343:ASP:CB	1:C:363:VAL:HG21	2.29	0.61
1:B:259:THR:O	1:B:262:GLY:N	2.30	0.61
1:B:343:ASP:CG	1:B:363:VAL:CG2	2.74	0.61
1:C:1054:ILE:N	1:C:1056:GLN:NE2	2.43	0.61
1:A:427:GLN:O	1:B:1057:ARG:HB2	2.00	0.61
1:B:377:GLN:NE2	1:B:585:CYS:CB	2.53	0.61
1:A:581:THR:HG22	1:A:582:ASN:CA	2.31	0.61
1:A:58:TYR:HD2	1:A:59:PRO:CD	2.04	0.60
1:A:344:LEU:CD1	1:A:663:TYR:HD1	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:ASN:ND2	1:A:559:SER:OG	2.30	0.60
1:A:63:THR:CG2	1:C:628:GLN:CD	2.58	0.60
1:A:577:TYR:CE1	1:A:610:GLY:O	2.46	0.60
1:A:577:TYR:OH	1:B:1056:GLN:HB3	2.01	0.60
1:A:582:ASN:C	1:A:629:ARG:HH22	2.08	0.60
1:C:338:ASP:O	1:C:339:CYS:CB	2.45	0.60
1:A:694:ARG:NH1	1:B:822:ARG:NH2	2.50	0.60
1:B:335:ARG:C	1:B:354:PHE:HZ	2.10	0.60
1:C:344:LEU:HD21	1:C:670:HIS:HB2	1.82	0.60
1:A:343:ASP:HB3	1:A:363:VAL:HG21	1.83	0.60
1:A:685:THR:HB	1:A:697:LEU:CD1	2.32	0.60
1:A:812:ASN:ND2	1:A:1050:SER:OG	2.34	0.60
1:C:735:LEU:HD22	1:C:736:CYS:H	1.66	0.60
1:C:1051:ILE:HB	1:C:1054:ILE:HG12	1.83	0.60
1:A:628:GLN:CG	1:B:63:THR:HG21	2.27	0.60
1:B:522:GLN:CG	1:C:289:THR:HG21	2.30	0.60
1:B:68:THR:C	1:B:69:ILE:HG23	2.26	0.60
1:B:346:GLN:O	1:B:350:SER:N	2.34	0.60
1:C:68:THR:C	1:C:69:ILE:HG23	2.27	0.60
1:C:501:ASN:ND2	1:C:559:SER:OG	2.30	0.60
1:B:735:LEU:HD22	1:B:736:CYS:H	1.66	0.60
1:A:402:LEU:HD11	1:A:445:TYR:CE2	2.36	0.59
1:B:441:LEU:HD21	1:B:573:ILE:HG22	1.84	0.59
1:B:582:ASN:HB2	1:B:609:TYR:CE2	2.31	0.59
1:A:68:THR:OG1	1:A:326:ASP:HA	2.02	0.59
1:A:343:ASP:OD2	1:A:661:VAL:HG23	2.02	0.59
1:B:377:GLN:NE2	1:B:408:ASN:ND2	2.50	0.59
1:A:406:ASN:N	1:A:583:SER:O	2.34	0.59
1:B:428:ILE:CA	1:C:1057:ARG:O	2.50	0.59
1:A:735:LEU:HD22	1:A:736:CYS:H	1.66	0.59
1:C:812:ASN:ND2	1:C:1050:SER:OG	2.34	0.59
1:B:625:VAL:HG23	1:C:63:THR:OG1	2.02	0.59
1:C:1058:LEU:HD11	1:C:1063:GLN:HB2	1.80	0.59
1:C:457:SER:HB3	1:C:460:SER:HB3	1.85	0.59
1:B:428:ILE:HA	1:C:1058:LEU:HA	1.84	0.59
1:B:1053:ASP:N	1:B:1053:ASP:OD1	2.34	0.59
1:C:58:TYR:HD2	1:C:59:PRO:CD	2.04	0.59
1:B:439:SER:OG	1:B:582:ASN:N	2.32	0.58
1:A:335:ARG:HB2	1:A:354:PHE:HZ	0.91	0.58
1:A:344:LEU:CD2	1:A:670:HIS:CG	2.84	0.58
1:C:1062:GLU:O	1:C:1063:GLN:C	2.45	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:CYS:HB2	1:A:428:ILE:C	2.24	0.58
1:B:457:SER:HB3	1:B:460:SER:HB3	1.85	0.58
1:A:335:ARG:HB3	1:A:354:PHE:CE2	2.16	0.58
1:B:347:LEU:C	1:B:356:VAL:HG21	2.29	0.58
1:B:432:ALA:HB1	1:C:1056:GLN:HA	1.85	0.58
1:B:476:PRO:HD2	1:B:577:TYR:CG	2.26	0.58
1:C:70:THR:CG2	1:C:352:GLU:CG	2.68	0.58
1:C:602:ASN:ND2	1:C:617:PHE:O	2.37	0.58
1:A:425:CYS:SG	1:A:428:ILE:HG23	2.43	0.58
1:A:428:ILE:O	1:B:1058:LEU:HB2	2.02	0.58
1:A:457:SER:HB3	1:A:460:SER:HB3	1.85	0.58
1:A:783:PRO:HG3	1:A:1143:PRO:HB3	1.86	0.58
1:B:783:PRO:HG3	1:B:1143:PRO:HB3	1.86	0.58
1:A:71:TYR:CE2	1:A:72:GLN:O	2.56	0.58
1:A:623:VAL:CG1	1:B:65:SER:CA	2.81	0.58
1:A:1179:ARG:H	1:A:1186:TYR:H	1.52	0.58
1:B:406:ASN:HA	1:B:583:SER:O	2.04	0.58
1:C:1179:ARG:H	1:C:1186:TYR:H	1.52	0.58
1:B:960:TRP:H	1:B:961:THR:HA	1.68	0.58
1:A:63:THR:CG2	1:C:628:GLN:HG2	2.29	0.58
1:A:602:ASN:ND2	1:A:617:PHE:O	2.37	0.58
1:C:960:TRP:H	1:C:961:THR:HA	1.68	0.58
1:A:343:ASP:CG	1:A:661:VAL:HG23	2.27	0.57
1:A:623:VAL:HG11	1:B:65:SER:HB2	0.62	0.57
1:A:812:ASN:ND2	1:A:1050:SER:O	2.37	0.57
1:A:943:MET:SD	1:C:738:LEU:CD1	2.91	0.57
1:C:783:PRO:HG3	1:C:1143:PRO:HB3	1.85	0.57
1:C:812:ASN:ND2	1:C:1050:SER:O	2.37	0.57
1:B:602:ASN:ND2	1:B:617:PHE:O	2.37	0.57
1:C:605:GLU:HG3	1:C:614:ARG:HG2	1.86	0.57
1:A:577:TYR:CD1	1:A:610:GLY:C	2.56	0.57
1:A:960:TRP:H	1:A:961:THR:HA	1.68	0.57
1:A:1027:ASN:O	1:A:1031:GLN:CB	2.53	0.57
1:B:377:GLN:HA	1:B:609:TYR:CD1	2.39	0.57
1:B:476:PRO:HG2	1:B:577:TYR:CE1	2.39	0.57
1:C:1023:GLN:O	1:C:1027:ASN:HB2	2.04	0.57
1:A:577:TYR:HD1	1:A:610:GLY:CA	2.17	0.57
1:A:738:LEU:HG	1:B:940:ASP:H	1.69	0.57
1:B:428:ILE:HG13	1:C:1056:GLN:C	2.26	0.57
1:B:1027:ASN:O	1:B:1031:GLN:CB	2.53	0.57
1:C:343:ASP:O	1:C:347:LEU:HD13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ASN:HD22	1:A:344:LEU:HD22	1.68	0.57
1:A:341:PHE:CE1	1:A:696:MET:HB3	2.40	0.57
1:A:685:THR:HA	1:A:697:LEU:CD2	2.34	0.57
1:B:582:ASN:OD1	1:B:583:SER:OG	2.16	0.57
1:C:67:ILE:O	1:C:327:PHE:HB2	2.05	0.57
1:C:1027:ASN:O	1:C:1031:GLN:CB	2.53	0.57
1:C:1105:GLU:OE1	1:C:1113:ARG:NH2	2.38	0.57
1:A:351:TYR:O	1:A:352:GLU:C	2.47	0.57
1:A:427:GLN:NE2	1:B:1066:GLN:HE22	2.02	0.57
1:A:78:GLN:HG2	1:A:341:PHE:HD2	1.70	0.57
1:A:344:LEU:H	1:A:344:LEU:HD22	1.69	0.57
1:A:1023:GLN:O	1:A:1027:ASN:HB2	2.04	0.57
1:A:623:VAL:HG12	1:B:65:SER:CA	2.35	0.57
1:A:1105:GLU:OE1	1:A:1113:ARG:NH2	2.38	0.57
1:B:58:TYR:HD2	1:B:59:PRO:CD	2.04	0.57
1:B:577:TYR:HD1	1:C:1057:ARG:HH12	1.52	0.57
1:A:351:TYR:O	1:A:353:SER:N	2.37	0.57
1:B:64:TYR:N	1:B:64:TYR:CD2	2.73	0.57
1:B:738:LEU:CD1	1:C:943:MET:SD	2.92	0.57
1:B:1179:ARG:H	1:B:1186:TYR:H	1.52	0.57
1:C:344:LEU:CD2	1:C:670:HIS:CG	2.80	0.57
1:B:1105:GLU:OE1	1:B:1113:ARG:NH2	2.38	0.56
1:A:65:SER:CB	1:C:623:VAL:CG1	2.74	0.56
1:A:71:TYR:HE2	1:A:73:GLY:HA3	1.70	0.56
1:A:324:LEU:CD1	1:A:353:SER:H	2.18	0.56
1:B:438:TYR:N	1:B:438:TYR:CD2	2.73	0.56
1:B:439:SER:CB	1:B:581:THR:CG2	2.83	0.56
1:C:1059:ASP:OD1	1:C:1062:GLU:HB2	2.04	0.56
1:A:437:CYS:HB3	1:A:609:TYR:O	1.98	0.56
1:B:1023:GLN:O	1:B:1027:ASN:HB2	2.04	0.56
1:C:70:THR:CG2	1:C:352:GLU:HA	2.35	0.56
1:C:399:PHE:O	1:C:523:TYR:OH	2.15	0.56
1:A:64:TYR:N	1:A:64:TYR:CD2	2.73	0.56
1:A:697:LEU:HD22	1:A:697:LEU:C	2.30	0.56
1:B:577:TYR:HE1	1:C:1057:ARG:HD3	1.70	0.56
1:C:64:TYR:N	1:C:64:TYR:CD2	2.73	0.56
1:A:605:GLU:HG3	1:A:614:ARG:HG2	1.87	0.56
1:A:793:GLU:HA	1:A:1018:ALA:HB2	1.88	0.56
1:B:580:ASP:N	1:C:61:GLY:HA2	2.17	0.56
1:B:605:GLU:HG3	1:B:614:ARG:HG2	1.86	0.56
1:B:738:LEU:HG	1:C:940:ASP:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ASN:HA	1:C:328:SER:O	2.06	0.56
1:B:439:SER:CA	1:B:582:ASN:N	2.48	0.56
1:B:511:ARG:NH2	1:C:575:VAL:CG2	2.57	0.56
1:A:787:SER:OG	1:A:1142:TYR:O	2.24	0.56
1:B:259:THR:OG1	1:B:264:HIS:NE2	2.38	0.56
1:B:476:PRO:HD2	1:B:577:TYR:CE2	2.25	0.56
1:A:63:THR:HG23	1:C:628:GLN:CG	2.29	0.56
1:A:628:GLN:HG2	1:B:63:THR:HG23	1.84	0.56
1:B:628:GLN:HE21	1:C:63:THR:HG22	1.71	0.56
1:A:347:LEU:CD2	1:A:361:TYR:CG	2.78	0.55
1:B:67:ILE:O	1:B:327:PHE:HB2	2.05	0.55
1:B:442:ILE:HD11	1:C:261:GLN:HG3	1.89	0.55
1:B:787:SER:H	1:B:1000:LYS:HD3	1.71	0.55
1:B:793:GLU:HA	1:B:1018:ALA:HB2	1.88	0.55
1:B:888:SER:OG	1:B:889:ALA:N	2.39	0.55
1:C:1053:ASP:HB3	1:C:1058:LEU:CB	2.36	0.55
1:A:520:ALA:CA	1:A:521:ASN:ND2	2.53	0.55
1:A:673:LEU:HD13	1:A:735:LEU:HD21	1.88	0.55
1:B:348:HIS:CE1	1:B:354:PHE:O	2.59	0.55
1:B:694:ARG:NH1	1:C:822:ARG:HH21	2.03	0.55
1:B:1102:LYS:HB3	1:B:1136:PHE:HE2	1.71	0.55
1:C:335:ARG:C	1:C:354:PHE:HZ	2.13	0.55
1:A:399:PHE:O	1:A:523:TYR:OH	2.15	0.55
1:A:429:SER:CA	1:B:1058:LEU:HB2	2.35	0.55
1:B:510:ASP:O	1:B:511:ARG:CB	2.53	0.55
1:B:686:MET:SD	1:B:686:MET:N	2.75	0.55
1:B:890:ILE:HD13	1:B:1137:MET:HE2	1.89	0.55
1:C:323:PHE:CE1	1:C:338:ASP:HA	2.41	0.55
1:C:787:SER:H	1:C:1000:LYS:HD3	1.71	0.55
1:C:890:ILE:HD13	1:C:1137:MET:HE2	1.89	0.55
1:B:673:LEU:HD13	1:B:735:LEU:HD21	1.88	0.55
1:A:1102:LYS:HB3	1:A:1136:PHE:HE2	1.71	0.55
1:C:677:VAL:HG22	1:C:678:ALA:HB2	1.89	0.55
1:A:738:LEU:CD1	1:B:943:MET:SD	2.93	0.55
1:A:890:ILE:HD13	1:A:1137:MET:HE2	1.89	0.55
1:B:787:SER:OG	1:B:1142:TYR:O	2.24	0.55
1:C:335:ARG:HD2	1:C:354:PHE:CE2	2.41	0.55
1:B:66:ASN:HA	1:B:328:SER:O	2.06	0.55
1:C:346:GLN:NE2	1:C:346:GLN:HA	2.22	0.55
1:C:793:GLU:HA	1:C:1018:ALA:HB2	1.88	0.55
1:A:697:LEU:HD22	1:A:698:LYS:CA	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:SER:H	1:A:1000:LYS:HD3	1.72	0.55
1:B:663:TYR:C	1:B:663:TYR:CD2	2.84	0.55
1:A:677:VAL:HG11	1:B:909:TYR:CD2	2.41	0.55
1:A:1174:LYS:O	1:A:1177:ASN:ND2	2.40	0.55
1:B:476:PRO:HG2	1:B:577:TYR:CD2	2.41	0.55
1:B:632:TYR:HB2	1:C:64:TYR:CD1	2.42	0.55
1:A:324:LEU:HD11	1:A:353:SER:C	2.32	0.54
1:C:686:MET:SD	1:C:686:MET:N	2.75	0.54
1:C:989:VAL:HB	1:C:1186:TYR:HE1	1.72	0.54
1:C:1058:LEU:HD13	1:C:1058:LEU:O	2.07	0.54
1:A:428:ILE:O	1:B:1058:LEU:CB	2.55	0.54
1:A:765:ASN:HD21	1:B:946:ALA:HB1	1.72	0.54
1:B:70:THR:HG23	1:B:352:GLU:CG	2.35	0.54
1:C:322:THR:O	1:C:339:CYS:CB	2.55	0.54
1:A:68:THR:CB	1:A:326:ASP:HA	2.37	0.54
1:A:940:ASP:H	1:C:738:LEU:HG	1.71	0.54
1:B:624:GLY:O	1:C:330:ASP:O	2.25	0.54
1:B:989:VAL:HB	1:B:1186:TYR:HE1	1.72	0.54
1:C:1102:LYS:HB3	1:C:1136:PHE:HE2	1.71	0.54
1:C:1174:LYS:O	1:C:1177:ASN:ND2	2.40	0.54
1:A:583:SER:O	1:A:584:VAL:HG22	2.03	0.54
1:B:677:VAL:HG22	1:B:678:ALA:HB2	1.89	0.54
1:B:996:LEU:HD23	1:B:998:ALA:HB3	1.89	0.54
1:B:1174:LYS:O	1:B:1177:ASN:ND2	2.41	0.54
1:C:1053:ASP:HB3	1:C:1058:LEU:HB3	1.88	0.54
1:A:71:TYR:C	1:A:71:TYR:CD2	2.86	0.54
1:A:578:GLY:C	1:A:579:THR:HG23	2.33	0.54
1:B:344:LEU:CD2	1:B:670:HIS:CG	2.84	0.54
1:B:376:GLU:C	1:B:609:TYR:CD1	2.85	0.54
1:B:576:GLN:CA	1:B:577:TYR:CB	2.46	0.54
1:C:787:SER:OG	1:C:1142:TYR:O	2.24	0.54
1:A:428:ILE:HG22	1:A:477:THR:O	2.08	0.54
1:A:581:THR:HG23	1:A:582:ASN:HA	1.85	0.54
1:A:989:VAL:HB	1:A:1186:TYR:HE1	1.72	0.54
1:B:663:TYR:CD2	1:B:665:LYS:N	2.76	0.54
1:B:831:ILE:HG23	1:B:1082:VAL:HG21	1.89	0.54
1:A:344:LEU:CD1	1:A:663:TYR:HE1	2.09	0.54
1:B:634:ALA:N	1:C:67:ILE:HD13	2.23	0.54
1:C:343:ASP:HA	1:C:363:VAL:HG11	1.90	0.54
1:C:888:SER:OG	1:C:889:ALA:N	2.40	0.54
1:A:996:LEU:HD23	1:A:998:ALA:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:673:LEU:HD13	1:C:735:LEU:HD21	1.88	0.54
1:C:831:ILE:HG23	1:C:1082:VAL:HG21	1.89	0.54
1:A:677:VAL:HG22	1:A:678:ALA:HB2	1.89	0.54
1:A:909:TYR:CD2	1:C:677:VAL:HG11	2.43	0.54
1:B:1058:LEU:CG	1:B:1059:ASP:CA	2.86	0.54
1:C:335:ARG:CD	1:C:354:PHE:CD2	2.84	0.54
1:C:347:LEU:HD21	1:C:661:VAL:CG1	2.33	0.54
1:B:677:VAL:CG2	1:C:909:TYR:CD2	2.90	0.53
1:A:831:ILE:HG23	1:A:1082:VAL:HG21	1.89	0.53
1:B:343:ASP:CG	1:B:363:VAL:CG1	2.74	0.53
1:C:1053:ASP:HB3	1:C:1058:LEU:CA	2.37	0.53
1:A:271:VAL:CG2	1:C:627:GLN:NE2	2.72	0.53
1:C:337:ILE:HD11	1:C:354:PHE:HA	1.91	0.53
1:C:1053:ASP:CB	1:C:1058:LEU:CB	2.85	0.53
1:A:694:ARG:CZ	1:B:822:ARG:HH21	2.22	0.53
1:B:349:CYS:SG	1:B:350:SER:N	2.81	0.53
1:B:1166:ALA:HB2	1:B:1194:PRO:HD3	1.90	0.53
1:C:351:TYR:CD2	1:C:356:VAL:HG13	2.43	0.53
1:A:888:SER:OG	1:A:889:ALA:N	2.39	0.53
1:B:1059:ASP:OD1	1:B:1062:GLU:CD	2.52	0.53
1:A:628:GLN:CD	1:B:63:THR:CG2	2.81	0.53
1:B:439:SER:CB	1:B:581:THR:CB	2.87	0.53
1:B:523:TYR:HD2	1:C:288:ASP:OD1	1.92	0.53
1:B:579:THR:CA	1:C:61:GLY:HA2	2.36	0.53
1:B:1053:ASP:HB3	1:B:1057:ARG:C	2.33	0.53
1:C:1166:ALA:HB2	1:C:1194:PRO:HD3	1.90	0.53
1:A:436:ASN:OD1	1:B:1056:GLN:HB3	2.09	0.53
1:B:129:THR:HG23	1:B:134:PRO:HA	1.91	0.53
1:B:677:VAL:HG11	1:C:909:TYR:CD2	2.42	0.53
1:C:789:GLY:HA3	1:C:1004:ALA:HB1	1.91	0.53
1:C:996:LEU:HD23	1:C:998:ALA:HB3	1.89	0.53
1:B:326:ASP:HB2	1:B:354:PHE:CZ	2.43	0.53
1:B:429:SER:HB3	1:C:1059:ASP:N	2.24	0.53
1:B:436:ASN:C	1:B:438:TYR:CE2	2.84	0.53
1:B:1053:ASP:HB3	1:B:1057:ARG:O	2.09	0.53
1:A:129:THR:HG23	1:A:134:PRO:HA	1.91	0.52
1:A:344:LEU:HD12	1:A:663:TYR:CD1	2.34	0.52
1:A:480:ILE:HB	1:A:571:PHE:HB2	1.91	0.52
1:A:946:ALA:HB1	1:C:765:ASN:HD21	1.74	0.52
1:B:789:GLY:HA3	1:B:1004:ALA:HB1	1.91	0.52
1:C:697:LEU:HD13	1:C:698:LYS:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1117:CYS:HB3	1:C:1122:HIS:CD2	2.45	0.52
1:A:337:ILE:HG21	1:A:348:HIS:CB	2.37	0.52
1:A:384:ASP:O	1:A:404:PHE:CE1	2.62	0.52
1:C:129:THR:HG23	1:C:134:PRO:HA	1.91	0.52
1:C:335:ARG:C	1:C:354:PHE:CZ	2.87	0.52
1:C:342:ASN:OD1	1:C:343:ASP:N	2.42	0.52
1:A:1166:ALA:HB2	1:A:1194:PRO:HD3	1.90	0.52
1:B:467:PHE:O	1:B:524:SER:HB2	2.10	0.52
1:B:581:THR:O	1:B:582:ASN:CB	2.56	0.52
1:C:977:PHE:O	1:C:981:ASN:HB2	2.10	0.52
1:A:1169:ASN:OD1	1:A:1169:ASN:N	2.43	0.52
1:B:575:VAL:O	1:B:577:TYR:HB2	2.09	0.52
1:B:1051:ILE:HB	1:B:1054:ILE:HA	1.91	0.52
1:B:1117:CYS:HB3	1:B:1122:HIS:CD2	2.44	0.52
1:C:480:ILE:HB	1:C:571:PHE:HB2	1.91	0.52
1:A:324:LEU:HD13	1:A:337:ILE:HD12	1.92	0.52
1:A:977:PHE:O	1:A:981:ASN:HB2	2.10	0.52
1:B:1058:LEU:HD12	1:B:1059:ASP:CA	2.19	0.52
1:A:577:TYR:HE2	1:B:1057:ARG:HH21	1.34	0.52
1:A:628:GLN:CG	1:B:63:THR:HG23	2.37	0.52
1:A:822:ARG:HG2	1:C:72:GLN:CD	2.19	0.52
1:A:1147:ILE:HD12	1:A:1184:TRP:HE1	1.75	0.52
1:C:181:ARG:HG3	1:C:242:THR:HG22	1.92	0.52
1:C:1147:ILE:HD12	1:C:1184:TRP:HE1	1.75	0.52
1:C:1169:ASN:OD1	1:C:1169:ASN:N	2.43	0.52
1:A:789:GLY:HA3	1:A:1004:ALA:HB1	1.92	0.52
1:B:351:TYR:HB3	1:B:353:SER:OG	2.10	0.52
1:C:347:LEU:HD13	1:C:347:LEU:N	2.24	0.52
1:A:677:VAL:CG2	1:B:909:TYR:CD2	2.91	0.52
1:B:1054:ILE:H	1:B:1054:ILE:CD1	2.14	0.52
1:A:1117:CYS:HB3	1:A:1122:HIS:CD2	2.45	0.52
1:B:977:PHE:O	1:B:981:ASN:HB2	2.10	0.52
1:B:1147:ILE:HD12	1:B:1184:TRP:HE1	1.75	0.52
1:C:58:TYR:HD1	1:C:279:PHE:CE1	2.24	0.52
1:C:1054:ILE:C	1:C:1055:ILE:HG13	2.34	0.52
1:C:1059:ASP:O	1:C:1063:GLN:HB2	2.09	0.52
1:A:692:SER:OG	1:A:696:MET:C	2.52	0.51
1:A:909:TYR:CD2	1:C:677:VAL:CG2	2.93	0.51
1:B:1031:GLN:HG2	1:B:1035:LYS:HD3	1.92	0.51
1:B:1058:LEU:HG	1:B:1059:ASP:CA	2.39	0.51
1:B:1165:ILE:HG12	1:C:960:TRP:HH2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ASN:OD1	1:A:328:SER:HA	2.11	0.51
1:A:348:HIS:ND1	1:A:356:VAL:CG2	2.72	0.51
1:A:377:GLN:CD	1:A:408:ASN:ND2	2.59	0.51
1:B:345:SER:O	1:B:348:HIS:CB	2.53	0.51
1:B:523:TYR:CD2	1:C:288:ASP:OD1	2.62	0.51
1:B:1059:ASP:O	1:B:1063:GLN:HB2	2.10	0.51
1:C:1053:ASP:CG	1:C:1066:GLN:OE1	2.50	0.51
1:A:340:GLY:C	1:A:695:SER:HB2	2.35	0.51
1:A:428:ILE:CG2	1:A:477:THR:O	2.58	0.51
1:A:521:ASN:ND2	1:A:521:ASN:N	2.58	0.51
1:A:870:ASN:N	1:A:1002:ASN:OD1	2.43	0.51
1:B:480:ILE:HB	1:B:571:PHE:HB2	1.91	0.51
1:B:629:ARG:HB3	1:B:642:TYR:HB3	1.92	0.51
1:C:1031:GLN:HG2	1:C:1035:LYS:HD3	1.93	0.51
1:C:1058:LEU:HD13	1:C:1063:GLN:HB2	1.90	0.51
1:A:271:VAL:HG22	1:C:627:GLN:NE2	2.26	0.51
1:A:626:ARG:HA	1:A:642:TYR:HE2	1.76	0.51
1:B:799:ILE:HD11	1:B:1089:SER:HA	1.93	0.51
1:A:383:CYS:N	1:A:408:ASN:O	2.44	0.51
1:A:467:PHE:O	1:A:524:SER:HB2	2.10	0.51
1:B:796:GLN:O	1:B:798:THR:N	2.40	0.51
1:A:660:SER:N	1:A:673:LEU:O	2.42	0.51
1:B:181:ARG:HG3	1:B:242:THR:HG22	1.92	0.51
1:B:697:LEU:HD13	1:B:698:LYS:H	1.75	0.51
1:C:467:PHE:O	1:C:524:SER:HB2	2.10	0.51
1:C:799:ILE:HD11	1:C:1089:SER:HA	1.93	0.51
1:A:427:GLN:NE2	1:A:427:GLN:CA	2.73	0.51
1:A:581:THR:HG22	1:A:582:ASN:CB	2.41	0.51
1:C:68:THR:C	1:C:69:ILE:CG2	2.83	0.51
1:C:958:VAL:HG11	1:C:1108:LYS:HD2	1.92	0.51
1:A:324:LEU:HD22	1:A:354:PHE:CD1	2.46	0.51
1:A:428:ILE:HG13	1:A:429:SER:N	2.26	0.51
1:A:958:VAL:HG11	1:A:1108:LYS:HD2	1.92	0.51
1:B:68:THR:C	1:B:69:ILE:CG2	2.83	0.51
1:A:348:HIS:O	1:A:349:CYS:C	2.54	0.51
1:B:439:SER:HB2	1:B:581:THR:CB	2.41	0.51
1:B:626:ARG:HA	1:B:642:TYR:HE2	1.76	0.51
1:B:765:ASN:HD21	1:C:946:ALA:HB1	1.74	0.51
1:C:1062:GLU:O	1:C:1064:ASP:N	2.44	0.51
1:A:181:ARG:HG3	1:A:242:THR:HG22	1.92	0.51
1:B:870:ASN:N	1:B:1002:ASN:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:LEU:CD2	1:A:361:TYR:HB3	2.33	0.50
1:B:347:LEU:CG	1:B:361:TYR:CG	2.93	0.50
1:B:432:ALA:HB3	1:C:1056:GLN:O	2.09	0.50
1:B:660:SER:N	1:B:673:LEU:O	2.42	0.50
1:C:70:THR:CG2	1:C:352:GLU:CD	2.84	0.50
1:C:1130:ALA:HB2	1:C:1135:TYR:HB2	1.93	0.50
1:A:764:PHE:CG	1:B:943:MET:SD	3.05	0.50
1:A:872:THR:OG1	1:A:1009:GLN:NE2	2.39	0.50
1:B:343:ASP:CA	1:B:363:VAL:HG21	2.41	0.50
1:B:377:GLN:HA	1:B:609:TYR:HD1	1.75	0.50
1:A:58:TYR:HD1	1:A:279:PHE:CE1	2.24	0.50
1:A:346:GLN:NE2	1:A:346:GLN:CA	2.73	0.50
1:A:778:PHE:CE1	1:B:971:PRO:HD3	2.47	0.50
1:B:68:THR:HG22	1:B:69:ILE:N	2.26	0.50
1:C:341:PHE:O	1:C:342:ASN:CB	2.59	0.50
1:C:626:ARG:HA	1:C:642:TYR:HE2	1.75	0.50
1:A:628:GLN:CD	1:B:63:THR:HG21	2.36	0.50
1:A:1165:ILE:HG12	1:B:960:TRP:HH2	1.75	0.50
1:B:583:SER:N	1:B:609:TYR:CD2	2.77	0.50
1:B:958:VAL:HG11	1:B:1108:LYS:HD2	1.92	0.50
1:C:351:TYR:OH	1:C:361:TYR:HE1	1.93	0.50
1:C:383:CYS:N	1:C:408:ASN:O	2.44	0.50
1:C:738:LEU:HD13	1:C:762:ILE:HG23	1.94	0.50
1:C:870:ASN:N	1:C:1002:ASN:OD1	2.43	0.50
1:B:428:ILE:HG13	1:C:1057:ARG:HA	1.94	0.50
1:C:68:THR:HG22	1:C:69:ILE:N	2.26	0.50
1:C:343:ASP:O	1:C:347:LEU:HD22	2.11	0.50
1:A:738:LEU:HD13	1:A:762:ILE:HG23	1.94	0.50
1:A:799:ILE:HD11	1:A:1089:SER:HA	1.93	0.50
1:B:725:GLU:OE2	1:B:728:LYS:NZ	2.43	0.50
1:B:872:THR:OG1	1:B:1009:GLN:NE2	2.39	0.50
1:B:1051:ILE:HG12	1:B:1054:ILE:CG2	2.40	0.50
1:C:1053:ASP:HB3	1:C:1058:LEU:H	1.72	0.50
1:A:960:TRP:HH2	1:C:1165:ILE:HG12	1.77	0.50
1:B:623:VAL:HG12	1:C:65:SER:HA	1.94	0.50
1:B:778:PHE:CE1	1:C:971:PRO:HD3	2.47	0.50
1:A:967:PHE:HB3	1:A:968:ALA:HB2	1.94	0.50
1:A:1031:GLN:HG2	1:A:1035:LYS:HD3	1.92	0.50
1:A:1130:ALA:HB2	1:A:1135:TYR:HB2	1.93	0.50
1:B:347:LEU:O	1:B:356:VAL:CG1	2.60	0.50
1:B:625:VAL:CG2	1:C:63:THR:OG1	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:PHE:CZ	1:C:696:MET:CB	2.95	0.50
1:A:66:ASN:HB2	1:A:328:SER:C	2.36	0.49
1:B:49:ASP:HB3	1:B:52:LYS:HD2	1.94	0.49
1:B:347:LEU:C	1:B:356:VAL:HG11	2.37	0.49
1:B:735:LEU:HD12	1:B:739:PRO:HB2	1.94	0.49
1:C:65:SER:C	1:C:67:ILE:H	2.06	0.49
1:B:347:LEU:O	1:B:356:VAL:HG11	2.11	0.49
1:B:377:GLN:HE22	1:B:408:ASN:ND2	2.10	0.49
1:A:341:PHE:HE1	1:A:696:MET:HB3	1.78	0.49
1:A:522:GLN:HG2	1:B:289:THR:CG2	2.37	0.49
1:A:583:SER:OG	1:A:609:TYR:HE1	1.94	0.49
1:B:628:GLN:HG3	1:C:63:THR:CG2	2.40	0.49
1:B:983:VAL:HG12	1:B:1121:THR:HB	1.93	0.49
1:A:324:LEU:CD2	1:A:354:PHE:CD1	2.96	0.49
1:A:1039:GLU:OE2	1:B:830:LYS:NZ	2.28	0.49
1:B:804:VAL:HA	1:B:932:TYR:HA	1.95	0.49
1:C:66:ASN:HA	1:C:327:PHE:O	2.12	0.49
1:C:796:GLN:O	1:C:798:THR:N	2.40	0.49
1:A:804:VAL:HA	1:A:932:TYR:HA	1.94	0.49
1:B:264:HIS:CE1	1:B:283:THR:CG2	2.96	0.49
1:B:335:ARG:C	1:B:354:PHE:CZ	2.90	0.49
1:C:343:ASP:CB	1:C:661:VAL:HG22	2.24	0.49
1:C:1179:ARG:HB2	1:C:1185:SER:HA	1.95	0.49
1:B:582:ASN:CG	1:B:609:TYR:CE2	2.90	0.49
1:C:343:ASP:HB3	1:C:363:VAL:CG2	2.35	0.49
1:A:50:VAL:HG22	1:A:78:GLN:OE1	2.13	0.49
1:A:406:ASN:HA	1:A:583:SER:HG	1.73	0.49
1:A:983:VAL:HG12	1:A:1121:THR:HB	1.94	0.49
1:B:377:GLN:HE21	1:B:585:CYS:HB3	1.74	0.49
1:B:1130:ALA:HB2	1:B:1135:TYR:HB2	1.93	0.49
1:A:337:ILE:HD11	1:A:348:HIS:CD2	2.46	0.49
1:A:519:ASN:HB2	1:A:522:GLN:OE1	2.13	0.49
1:A:577:TYR:HH	1:B:1056:GLN:HB3	1.78	0.49
1:A:796:GLN:O	1:A:798:THR:N	2.40	0.49
1:A:1179:ARG:HB2	1:A:1185:SER:HA	1.95	0.49
1:B:63:THR:C	1:B:64:TYR:CD2	2.91	0.49
1:B:66:ASN:HA	1:B:327:PHE:O	2.11	0.49
1:B:623:VAL:HG12	1:C:65:SER:CA	2.42	0.49
1:C:341:PHE:CE1	1:C:696:MET:HB2	2.48	0.49
1:C:983:VAL:HG12	1:C:1121:THR:HB	1.93	0.49
1:B:68:THR:O	1:B:69:ILE:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:THR:O	1:C:61:GLY:CA	2.53	0.49
1:B:1179:ARG:HB2	1:B:1185:SER:HA	1.95	0.49
1:A:49:ASP:HB3	1:A:52:LYS:HD2	1.95	0.48
1:A:63:THR:C	1:A:64:TYR:CD2	2.91	0.48
1:A:971:PRO:HD3	1:C:778:PHE:CE1	2.48	0.48
1:A:324:LEU:CB	1:A:337:ILE:HB	2.36	0.48
1:A:720:SER:HG	1:A:757:MET:N	2.11	0.48
1:B:519:ASN:HB2	1:B:522:GLN:OE1	2.13	0.48
1:B:764:PHE:CG	1:C:943:MET:SD	3.06	0.48
1:C:63:THR:C	1:C:64:TYR:CD2	2.91	0.48
1:C:660:SER:N	1:C:673:LEU:O	2.42	0.48
1:C:1053:ASP:O	1:C:1063:GLN:NE2	2.46	0.48
1:B:441:LEU:CD2	1:B:441:LEU:C	2.86	0.48
1:B:967:PHE:HB3	1:B:968:ALA:HB2	1.94	0.48
1:C:519:ASN:HB2	1:C:522:GLN:OE1	2.13	0.48
1:A:686:MET:SD	1:A:686:MET:N	2.75	0.48
1:B:68:THR:O	1:B:69:ILE:HG22	2.13	0.48
1:B:70:THR:OG1	1:B:352:GLU:CD	2.57	0.48
1:B:785:ASN:OD1	1:B:1145:ASN:ND2	2.41	0.48
1:C:720:SER:HG	1:C:757:MET:N	2.11	0.48
1:A:735:LEU:HD12	1:A:739:PRO:HB2	1.94	0.48
1:B:344:LEU:CD2	1:B:670:HIS:CB	2.10	0.48
1:B:728:LYS:H	1:B:761:SER:HG	1.61	0.48
1:B:738:LEU:HD13	1:B:762:ILE:HG23	1.94	0.48
1:C:735:LEU:HD12	1:C:739:PRO:HB2	1.94	0.48
1:C:804:VAL:HA	1:C:932:TYR:HA	1.95	0.48
1:A:577:TYR:CE1	1:B:1056:GLN:OE1	2.66	0.48
1:A:990:LEU:HD11	1:A:1179:ARG:HD3	1.96	0.48
1:B:579:THR:O	1:C:61:GLY:O	2.32	0.48
1:A:582:ASN:O	1:A:629:ARG:NH2	2.46	0.48
1:C:68:THR:O	1:C:69:ILE:HG22	2.13	0.48
1:A:725:GLU:OE2	1:A:728:LYS:NZ	2.43	0.48
1:A:728:LYS:H	1:A:761:SER:HG	1.58	0.48
1:A:800:GLN:HE21	1:A:934:VAL:HG11	1.78	0.48
1:B:642:TYR:HA	1:B:643:SER:HA	1.63	0.48
1:C:629:ARG:HB2	1:C:642:TYR:HB3	1.96	0.48
1:A:321:LEU:HD23	1:B:822:ARG:HH12	1.78	0.48
1:B:720:SER:HG	1:B:757:MET:N	2.12	0.48
1:C:967:PHE:HB3	1:C:968:ALA:HB2	1.94	0.48
1:B:625:VAL:CG1	1:C:279:PHE:CE2	2.97	0.48
1:C:49:ASP:HB3	1:C:52:LYS:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:PHE:CD1	1:C:696:MET:HB2	2.49	0.48
1:C:800:GLN:HE21	1:C:934:VAL:HG11	1.78	0.48
1:B:58:TYR:HD1	1:B:279:PHE:CE1	2.24	0.47
1:B:335:ARG:CG	1:B:354:PHE:CZ	2.55	0.47
1:B:440:SER:HB3	1:B:576:GLN:HB2	1.95	0.47
1:B:580:ASP:HB3	1:C:60:GLN:HB3	1.96	0.47
1:C:990:LEU:HD11	1:C:1179:ARG:HD3	1.96	0.47
1:A:804:VAL:HG11	1:A:1078:LEU:HD11	1.96	0.47
1:A:943:MET:SD	1:C:764:PHE:CG	3.07	0.47
1:B:341:PHE:O	1:B:696:MET:O	2.32	0.47
1:B:129:THR:CG2	1:B:131:ILE:H	2.24	0.47
1:B:575:VAL:O	1:B:577:TYR:CB	2.62	0.47
1:B:800:GLN:HE21	1:B:934:VAL:HG11	1.78	0.47
1:B:804:VAL:HG11	1:B:1078:LEU:HD11	1.96	0.47
1:A:405:THR:HA	1:A:584:VAL:CG2	2.43	0.47
1:B:933:LYS:NZ	1:B:934:VAL:O	2.47	0.47
1:C:347:LEU:HD11	1:C:363:VAL:CG2	2.44	0.47
1:C:351:TYR:O	1:C:352:GLU:HB2	2.14	0.47
1:C:798:THR:HB	1:C:842:GLN:HE21	1.80	0.47
1:A:129:THR:CG2	1:A:131:ILE:H	2.24	0.47
1:A:385:PHE:HD2	1:A:414:LEU:HD13	1.78	0.47
1:A:677:VAL:HG21	1:B:910:ASP:OD1	2.14	0.47
1:A:798:THR:HB	1:A:842:GLN:HE21	1.80	0.47
1:A:867:GLY:HA2	1:A:868:ASP:HA	1.63	0.47
1:A:984:GLY:O	1:A:986:THR:N	2.48	0.47
1:A:1160:ASN:HB3	1:A:1198:THR:HG21	1.97	0.47
1:A:425:CYS:CB	1:A:428:ILE:C	2.85	0.47
1:A:629:ARG:HB2	1:A:642:TYR:HB3	1.96	0.47
1:B:343:ASP:HB3	1:B:363:VAL:CG2	2.42	0.47
1:B:344:LEU:CD1	1:B:663:TYR:CB	2.93	0.47
1:B:383:CYS:N	1:B:408:ASN:O	2.44	0.47
1:B:399:PHE:O	1:B:523:TYR:OH	2.15	0.47
1:B:429:SER:CB	1:C:1059:ASP:HA	2.38	0.47
1:B:439:SER:HA	1:B:582:ASN:N	2.28	0.47
1:B:984:GLY:O	1:B:986:THR:N	2.48	0.47
1:C:725:GLU:OE2	1:C:728:LYS:NZ	2.43	0.47
1:A:324:LEU:CD2	1:A:354:PHE:CE1	2.98	0.47
1:A:433:ILE:HA	1:A:438:TYR:OH	2.14	0.47
1:A:579:THR:HA	1:B:61:GLY:O	2.15	0.47
1:B:476:PRO:CD	1:B:577:TYR:CG	2.93	0.47
1:C:129:THR:CG2	1:C:131:ILE:H	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:PRO:O	1:C:566:GLN:HG2	2.15	0.47
1:A:66:ASN:CB	1:A:328:SER:C	2.88	0.47
1:A:324:LEU:HB3	1:A:337:ILE:CB	2.35	0.47
1:A:628:GLN:NE2	1:B:63:THR:HG21	2.28	0.47
1:A:907:GLN:O	1:A:911:ASP:CB	2.63	0.47
1:C:324:LEU:HD12	1:C:352:GLU:O	2.15	0.47
1:C:804:VAL:HG11	1:C:1078:LEU:HD11	1.96	0.47
1:B:1050:SER:OG	1:B:1051:ILE:N	2.47	0.47
1:C:984:GLY:O	1:C:986:THR:N	2.48	0.47
1:A:339:CYS:O	1:A:345:SER:OG	2.30	0.46
1:A:428:ILE:HA	1:B:1058:LEU:H	1.80	0.46
1:C:336:ALA:HA	1:C:354:PHE:HZ	1.81	0.46
1:C:1060:VAL:O	1:C:1063:GLN:HB3	2.15	0.46
1:A:71:TYR:CE2	1:A:72:GLN:C	2.93	0.46
1:B:439:SER:HA	1:B:582:ASN:H	1.72	0.46
1:B:990:LEU:HD11	1:B:1179:ARG:HD3	1.96	0.46
1:A:436:ASN:O	1:A:586:PRO:HD3	2.16	0.46
1:A:437:CYS:CA	1:A:609:TYR:O	2.63	0.46
1:A:485:PRO:O	1:A:566:GLN:HG2	2.15	0.46
1:A:642:TYR:HA	1:A:643:SER:HA	1.64	0.46
1:B:845:SER:O	1:B:849:LEU:HB2	2.15	0.46
1:B:907:GLN:O	1:B:911:ASP:CB	2.63	0.46
1:C:658:PRO:HG2	1:C:675:GLY:HA3	1.98	0.46
1:C:907:GLN:O	1:C:911:ASP:CB	2.63	0.46
1:A:347:LEU:HD11	1:A:361:TYR:HB3	1.97	0.46
1:A:359:GLY:HA2	1:A:733:GLN:HB2	1.97	0.46
1:A:845:SER:O	1:A:849:LEU:HB2	2.15	0.46
1:B:321:LEU:HA	1:C:822:ARG:HH12	1.79	0.46
1:B:798:THR:HB	1:B:842:GLN:HE21	1.80	0.46
1:B:1128:VAL:HG23	1:B:1135:TYR:HB3	1.97	0.46
1:C:845:SER:O	1:C:849:LEU:HB2	2.15	0.46
1:C:872:THR:OG1	1:C:1009:GLN:NE2	2.39	0.46
1:A:66:ASN:HA	1:A:328:SER:C	2.37	0.46
1:A:408:ASN:HA	1:A:585:CYS:O	2.15	0.46
1:A:587:LYS:HB2	1:A:587:LYS:HE3	1.74	0.46
1:B:344:LEU:HA	1:B:661:VAL:HG11	1.97	0.46
1:B:408:ASN:HA	1:B:585:CYS:O	2.15	0.46
1:B:511:ARG:HD2	1:C:436:ASN:HD22	0.65	0.46
1:C:408:ASN:HA	1:C:585:CYS:O	2.15	0.46
1:C:1053:ASP:O	1:C:1063:GLN:CG	2.61	0.46
1:A:334:ARG:C	1:A:335:ARG:HG3	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:LEU:HG	1:A:758:ARG:HA	1.98	0.46
1:A:1072:ASN:O	1:A:1076:THR:OG1	2.28	0.46
1:B:1149:VAL:HG12	1:B:1150:VAL:H	1.81	0.46
1:B:1160:ASN:HB3	1:B:1198:THR:HG21	1.97	0.46
1:C:933:LYS:NZ	1:C:934:VAL:O	2.47	0.46
1:A:807:LYS:HA	1:A:821:LEU:HD13	1.97	0.46
1:A:1181:VAL:HA	1:A:1182:ASP:HA	1.60	0.46
1:B:485:PRO:O	1:B:566:GLN:HG2	2.15	0.46
1:B:658:PRO:HG2	1:B:675:GLY:HA3	1.98	0.46
1:C:68:THR:O	1:C:69:ILE:HG23	2.13	0.46
1:C:335:ARG:CD	1:C:354:PHE:CE2	2.99	0.46
1:C:359:GLY:HA2	1:C:733:GLN:HB2	1.98	0.46
1:A:271:VAL:CG2	1:C:627:GLN:HE22	2.29	0.46
1:A:580:ASP:OD2	1:A:628:GLN:HG3	2.15	0.46
1:C:1128:VAL:HG23	1:C:1135:TYR:HB3	1.98	0.46
1:A:1164:CYS:HA	1:A:1165:ILE:HA	1.69	0.46
1:B:353:SER:C	1:B:355:ASP:N	2.73	0.46
1:C:323:PHE:CD1	1:C:338:ASP:O	2.68	0.46
1:C:1160:ASN:HB3	1:C:1198:THR:HG21	1.97	0.46
1:C:1171:TYR:H	1:C:1178:THR:HG22	1.81	0.46
1:A:340:GLY:HA3	1:A:695:SER:HB2	1.97	0.45
1:A:346:GLN:C	1:A:346:GLN:HE21	2.24	0.45
1:A:433:ILE:CG1	1:A:438:TYR:OH	2.65	0.45
1:A:677:VAL:CB	1:B:909:TYR:CD2	2.99	0.45
1:B:803:THR:HG22	1:B:839:ASN:HD21	1.81	0.45
1:B:807:LYS:HA	1:B:821:LEU:HD13	1.97	0.45
1:C:335:ARG:HH11	1:C:354:PHE:HD2	1.61	0.45
1:C:712:GLY:HA3	1:C:713:CYS:HA	1.67	0.45
1:A:658:PRO:HG2	1:A:675:GLY:HA3	1.98	0.45
1:A:1128:VAL:HG23	1:A:1135:TYR:HB3	1.98	0.45
1:B:339:CYS:HG	1:B:349:CYS:HG	0.92	0.45
1:B:1013:THR:HA	1:B:1014:THR:HA	1.76	0.45
1:C:347:LEU:O	1:C:350:SER:OG	2.28	0.45
1:C:728:LYS:H	1:C:761:SER:HG	1.62	0.45
1:C:807:LYS:HA	1:C:821:LEU:HD13	1.97	0.45
1:A:781:SER:OG	1:B:857:GLN:NE2	2.47	0.45
1:B:511:ARG:NE	1:C:436:ASN:HD22	2.04	0.45
1:B:634:ALA:HB2	1:C:67:ILE:HD13	1.94	0.45
1:B:677:VAL:CB	1:C:909:TYR:CD2	3.00	0.45
1:C:323:PHE:CZ	1:C:338:ASP:OD1	2.67	0.45
1:C:336:ALA:HA	1:C:354:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:PHE:H	1:C:345:SER:CB	2.29	0.45
1:C:803:THR:HG22	1:C:839:ASN:HD21	1.81	0.45
1:C:1149:VAL:HG12	1:C:1150:VAL:H	1.81	0.45
1:A:323:PHE:CZ	1:A:338:ASP:HB3	2.52	0.45
1:A:627:GLN:CD	1:B:271:VAL:HG22	2.36	0.45
1:A:910:ASP:OD1	1:C:677:VAL:HG21	2.17	0.45
1:B:522:GLN:CD	1:C:289:THR:CG2	2.80	0.45
1:B:867:GLY:HA2	1:B:868:ASP:HA	1.63	0.45
1:C:343:ASP:CA	1:C:363:VAL:HG21	2.45	0.45
1:C:1013:THR:HA	1:C:1014:THR:HA	1.76	0.45
1:A:685:THR:CG2	1:A:697:LEU:CD1	2.51	0.45
1:C:498:SER:HB3	1:C:534:VAL:HG23	1.99	0.45
1:A:627:GLN:HE21	1:B:271:VAL:HG13	1.82	0.45
1:A:993:ASN:HA	1:A:994:GLN:HA	1.75	0.45
1:A:1149:VAL:HG12	1:A:1150:VAL:H	1.81	0.45
1:B:722:LEU:HG	1:B:758:ARG:HA	1.98	0.45
1:C:341:PHE:CE1	1:C:696:MET:CB	2.99	0.45
1:A:498:SER:HB3	1:A:534:VAL:HG23	1.99	0.45
1:A:697:LEU:CD2	1:A:698:LYS:N	2.69	0.45
1:B:1051:ILE:CG1	1:B:1054:ILE:CG2	2.86	0.45
1:C:867:GLY:HA2	1:C:868:ASP:HA	1.63	0.45
1:C:1053:ASP:CB	1:C:1058:LEU:CD1	2.85	0.45
1:A:803:THR:HG22	1:A:839:ASN:HD21	1.81	0.45
1:B:349:CYS:C	1:B:351:TYR:N	2.73	0.45
1:C:324:LEU:CD1	1:C:352:GLU:O	2.65	0.45
1:C:993:ASN:HA	1:C:994:GLN:HA	1.75	0.45
1:A:403:VAL:HG22	1:A:442:ILE:HG12	1.99	0.45
1:B:394:PRO:HG3	1:B:400:LYS:HG3	1.99	0.45
1:B:1171:TYR:H	1:B:1178:THR:HG22	1.81	0.45
1:A:66:ASN:CB	1:A:329:VAL:N	2.79	0.45
1:A:1171:TYR:H	1:A:1178:THR:HG22	1.81	0.45
1:C:337:ILE:HD12	1:C:348:HIS:HB3	1.98	0.45
1:A:335:ARG:C	1:A:354:PHE:HZ	2.25	0.44
1:A:346:GLN:NE2	1:A:346:GLN:HA	2.32	0.44
1:A:348:HIS:ND1	1:A:356:VAL:HG22	2.27	0.44
1:B:781:SER:OG	1:C:857:GLN:NE2	2.47	0.44
1:C:792:GLN:HG3	1:C:1138:HIS:HB2	2.00	0.44
1:A:429:SER:HB3	1:B:1058:LEU:CA	2.41	0.44
1:A:577:TYR:CD1	1:A:610:GLY:CA	2.99	0.44
1:A:765:ASN:HB2	1:A:766:HIS:HA	2.00	0.44
1:A:933:LYS:NZ	1:A:934:VAL:O	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1186:TYR:HB3	1:A:1187:THR:H	1.53	0.44
1:B:344:LEU:CD1	1:B:663:TYR:HB2	2.47	0.44
1:B:441:LEU:HD22	1:B:442:ILE:N	2.26	0.44
1:B:501:ASN:HD22	1:B:559:SER:HG	1.60	0.44
1:B:677:VAL:HG21	1:C:910:ASP:OD1	2.17	0.44
1:B:792:GLN:HG3	1:B:1138:HIS:HB2	2.00	0.44
1:C:722:LEU:HG	1:C:758:ARG:HA	1.98	0.44
1:B:68:THR:CG2	1:B:69:ILE:N	2.80	0.44
1:B:377:GLN:HE22	1:B:408:ASN:HD22	1.66	0.44
1:B:498:SER:HB3	1:B:534:VAL:HG23	1.99	0.44
1:B:1164:CYS:HA	1:B:1165:ILE:HA	1.69	0.44
1:A:344:LEU:HD11	1:A:663:TYR:CE1	2.41	0.44
1:C:964:LEU:HA	1:C:965:SER:HA	1.78	0.44
1:A:346:GLN:HG3	1:A:693:THR:OG1	2.18	0.44
1:A:413:LYS:O	1:A:416:SER:OG	2.35	0.44
1:B:712:GLY:HA3	1:B:713:CYS:HA	1.67	0.44
1:C:335:ARG:CG	1:C:354:PHE:CE2	3.00	0.44
1:C:335:ARG:CZ	1:C:354:PHE:HD2	2.30	0.44
1:C:346:GLN:HG2	1:C:693:THR:OG1	2.18	0.44
1:C:394:PRO:HG3	1:C:400:LYS:HG3	1.98	0.44
1:C:577:TYR:O	1:C:577:TYR:CD2	2.70	0.44
1:B:359:GLY:HA2	1:B:733:GLN:HB2	1.98	0.44
1:B:623:VAL:CG1	1:C:65:SER:CA	2.95	0.44
1:C:1062:GLU:C	1:C:1064:ASP:N	2.74	0.44
1:A:423:PHE:CD1	1:A:430:PRO:HG3	2.52	0.44
1:A:964:LEU:HA	1:A:965:SER:HA	1.78	0.44
1:B:344:LEU:CD1	1:B:663:TYR:CG	2.90	0.44
1:B:812:ASN:ND2	1:B:1051:ILE:CD1	2.69	0.44
1:B:1114:SER:OG	1:B:1115:GLY:N	2.51	0.44
1:C:785:ASN:OD1	1:C:1145:ASN:ND2	2.41	0.44
1:A:337:ILE:CD1	1:A:348:HIS:HD2	2.16	0.44
1:A:979:ARG:O	1:A:1110:GLN:NE2	2.51	0.44
1:B:456:LEU:HD12	1:B:456:LEU:HA	1.88	0.44
1:C:68:THR:CG2	1:C:69:ILE:N	2.80	0.44
1:A:394:PRO:HG3	1:A:400:LYS:HG3	1.99	0.44
1:B:326:ASP:CB	1:B:335:ARG:CG	2.93	0.44
1:B:765:ASN:HB2	1:B:766:HIS:HA	2.00	0.44
1:B:979:ARG:O	1:B:1110:GLN:NE2	2.51	0.44
1:C:326:ASP:HB2	1:C:354:PHE:CE2	2.53	0.44
1:C:343:ASP:HA	1:C:363:VAL:HG21	1.99	0.44
1:C:1060:VAL:HA	1:C:1063:GLN:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ILE:HG13	1:A:438:TYR:OH	2.18	0.43
1:A:638:LEU:HG	1:A:651:LEU:HD21	2.00	0.43
1:A:1114:SER:OG	1:A:1115:GLY:N	2.51	0.43
1:B:871:LEU:HA	1:B:871:LEU:HD23	1.84	0.43
1:B:1049:ALA:O	1:B:1050:SER:CB	2.66	0.43
1:C:1037:ALA:HA	1:C:1040:LEU:HD12	2.00	0.43
1:A:909:TYR:CD2	1:C:677:VAL:CB	3.01	0.43
1:B:510:ASP:O	1:B:511:ARG:HB2	2.18	0.43
1:C:484:VAL:HA	1:C:485:PRO:HD3	1.72	0.43
1:B:428:ILE:HA	1:C:1058:LEU:CA	2.49	0.43
1:B:428:ILE:C	1:C:1058:LEU:HA	2.43	0.43
1:B:581:THR:O	1:B:582:ASN:CG	2.62	0.43
1:C:718:VAL:HG11	1:C:759:LEU:HD11	2.00	0.43
1:C:979:ARG:O	1:C:1110:GLN:NE2	2.51	0.43
1:C:1058:LEU:CD1	1:C:1063:GLN:N	2.67	0.43
1:A:792:GLN:HG3	1:A:1138:HIS:HB2	1.99	0.43
1:B:1181:VAL:HA	1:B:1182:ASP:HA	1.60	0.43
1:C:493:LYS:H	1:C:493:LYS:HG2	1.58	0.43
1:C:726:ASP:HB2	1:C:727:CYS:HB3	2.01	0.43
1:A:441:LEU:HD13	1:A:575:VAL:HG12	1.89	0.43
1:B:1173:ILE:HG22	1:B:1174:LYS:H	1.83	0.43
1:C:765:ASN:HB2	1:C:766:HIS:HA	2.00	0.43
1:A:427:GLN:O	1:B:1057:ARG:HD3	2.17	0.43
1:B:726:ASP:HB2	1:B:727:CYS:HB3	2.01	0.43
1:B:1122:HIS:NE2	1:B:1125:SER:HB3	2.34	0.43
1:A:321:LEU:HA	1:B:822:ARG:HH11	1.80	0.43
1:C:638:LEU:HG	1:C:651:LEU:HD21	2.00	0.43
1:C:1114:SER:OG	1:C:1115:GLY:N	2.51	0.43
1:C:1164:CYS:HA	1:C:1165:ILE:HA	1.69	0.43
1:C:346:GLN:NE2	1:C:346:GLN:CA	2.80	0.43
1:A:129:THR:CG2	1:A:134:PRO:HA	2.49	0.43
1:A:625:VAL:HG11	1:B:63:THR:HG21	2.00	0.43
1:A:339:CYS:HA	1:A:345:SER:OG	2.19	0.43
1:A:718:VAL:HG11	1:A:759:LEU:HD11	2.00	0.43
1:C:129:THR:CG2	1:C:134:PRO:HA	2.49	0.43
1:C:335:ARG:NH1	1:C:354:PHE:CD2	2.80	0.43
1:A:68:THR:HG23	1:A:326:ASP:HA	1.89	0.42
1:A:341:PHE:CE1	1:A:696:MET:HB2	2.44	0.42
1:A:428:ILE:HG21	1:A:478:CYS:SG	2.59	0.42
1:A:1173:ILE:HG22	1:A:1174:LYS:H	1.83	0.42
1:C:366:PHE:N	1:C:691:ARG:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:581:THR:O	1:C:583:SER:N	2.47	0.42
1:B:129:THR:CG2	1:B:134:PRO:HA	2.49	0.42
1:B:352:GLU:N	1:B:352:GLU:OE1	2.52	0.42
1:C:1122:HIS:NE2	1:C:1125:SER:HB3	2.34	0.42
1:B:579:THR:O	1:B:581:THR:OG1	2.34	0.42
1:B:638:LEU:HG	1:B:651:LEU:HD21	2.00	0.42
1:B:718:VAL:HG11	1:B:759:LEU:HD11	2.00	0.42
1:B:1054:ILE:HB	1:B:1055:ILE:H	1.65	0.42
1:C:1173:ILE:HG22	1:C:1174:LYS:H	1.83	0.42
1:A:377:GLN:HG2	1:A:585:CYS:SG	2.58	0.42
1:B:347:LEU:HB3	1:B:356:VAL:HG11	2.01	0.42
1:B:511:ARG:HB2	1:C:436:ASN:CB	2.48	0.42
1:B:625:VAL:CG1	1:C:279:PHE:HE2	2.31	0.42
1:B:634:ALA:HB3	1:C:67:ILE:HD11	1.96	0.42
1:B:677:VAL:HA	1:B:678:ALA:HA	1.90	0.42
1:A:377:GLN:NE2	1:A:586:PRO:O	2.42	0.42
1:A:580:ASP:HB2	1:A:628:GLN:HB2	1.91	0.42
1:A:712:GLY:HA3	1:A:713:CYS:HA	1.67	0.42
1:A:1037:ALA:HA	1:A:1040:LEU:HD12	2.00	0.42
1:B:727:CYS:HB2	1:B:763:ALA:HA	2.02	0.42
1:B:993:ASN:HA	1:B:994:GLN:HA	1.75	0.42
1:B:1037:ALA:HA	1:B:1040:LEU:HD12	2.00	0.42
1:C:344:LEU:HD12	1:C:663:TYR:CE1	2.54	0.42
1:B:65:SER:C	1:B:67:ILE:H	2.06	0.42
1:B:587:LYS:HB2	1:B:587:LYS:HE3	1.74	0.42
1:C:1181:VAL:HA	1:C:1182:ASP:HA	1.60	0.42
1:B:511:ARG:HD3	1:C:436:ASN:HB2	1.93	0.42
1:C:727:CYS:HB2	1:C:763:ALA:HA	2.02	0.42
1:A:627:GLN:HE21	1:B:271:VAL:CG1	2.33	0.42
1:A:693:THR:HA	1:A:694:ARG:HA	1.80	0.42
1:A:697:LEU:C	1:A:697:LEU:CD2	2.92	0.42
1:A:716:GLY:HA2	1:B:906:MET:HG2	2.01	0.42
1:A:385:PHE:O	1:A:387:PRO:HD2	2.20	0.42
1:A:423:PHE:CE1	1:A:430:PRO:HG3	2.55	0.42
1:A:583:SER:CA	1:A:609:TYR:CD1	3.00	0.42
1:A:731:LEU:HD22	1:A:732:GLY:H	1.85	0.42
1:A:976:ILE:O	1:A:980:LEU:CB	2.68	0.42
1:B:732:GLY:HA2	1:B:734:SER:HB2	2.02	0.42
1:C:347:LEU:N	1:C:347:LEU:CD1	2.83	0.42
1:C:731:LEU:HD22	1:C:732:GLY:H	1.85	0.42
1:C:976:ILE:O	1:C:980:LEU:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1061:LEU:H	1:C:1061:LEU:HG	1.54	0.42
1:A:726:ASP:HB2	1:A:727:CYS:HB3	2.01	0.42
1:A:1122:HIS:NE2	1:A:1125:SER:HB3	2.34	0.42
1:B:581:THR:O	1:B:582:ASN:HB3	2.20	0.42
1:B:731:LEU:HD22	1:B:732:GLY:H	1.85	0.42
1:C:872:THR:HG1	1:C:1009:GLN:HE21	1.63	0.42
1:C:1056:GLN:OE1	1:C:1056:GLN:N	2.52	0.42
1:B:990:LEU:HD23	1:B:990:LEU:HA	1.86	0.41
1:C:343:ASP:CG	1:C:661:VAL:CG2	2.85	0.41
1:A:341:PHE:HD1	1:A:696:MET:CB	2.24	0.41
1:A:1181:VAL:HB	1:B:967:PHE:CE2	2.54	0.41
1:B:579:THR:CA	1:C:61:GLY:CA	2.98	0.41
1:B:624:GLY:O	1:C:331:GLY:HA3	2.20	0.41
1:B:1201:ASN:HB2	1:B:1206:ALA:HB3	2.02	0.41
1:A:344:LEU:HD22	1:A:344:LEU:N	2.35	0.41
1:A:366:PHE:N	1:A:691:ARG:O	2.51	0.41
1:B:366:PHE:N	1:B:691:ARG:O	2.51	0.41
1:B:436:ASN:HB3	1:B:438:TYR:CZ	2.55	0.41
1:A:401:ARG:NH1	1:B:260:ALA:HB1	2.31	0.41
1:A:429:SER:CB	1:B:1058:LEU:CB	2.59	0.41
1:B:484:VAL:HA	1:B:485:PRO:HD3	1.72	0.41
1:B:976:ILE:O	1:B:980:LEU:CB	2.68	0.41
1:C:351:TYR:C	1:C:353:SER:N	2.78	0.41
1:A:347:LEU:HA	1:A:347:LEU:HD12	1.82	0.41
1:A:785:ASN:OD1	1:A:1145:ASN:ND2	2.41	0.41
1:B:810:VAL:HG22	1:B:1074:ARG:HD2	2.02	0.41
1:C:728:LYS:HA	1:C:729:LEU:HA	1.71	0.41
1:A:69:ILE:C	1:A:69:ILE:CD1	2.86	0.41
1:A:335:ARG:HD3	1:A:354:PHE:CD2	2.32	0.41
1:A:697:LEU:HD22	1:A:698:LYS:CB	2.50	0.41
1:A:1127:VAL:HG13	1:A:1136:PHE:HE1	1.86	0.41
1:C:323:PHE:CD1	1:C:338:ASP:HA	2.55	0.41
1:A:68:THR:HG23	1:A:326:ASP:CA	2.48	0.41
1:A:323:PHE:HA	1:A:337:ILE:O	2.19	0.41
1:A:1201:ASN:HB2	1:A:1206:ALA:HB3	2.02	0.41
1:B:261:GLN:N	1:B:261:GLN:CD	2.73	0.41
1:B:484:VAL:O	1:B:566:GLN:HB3	2.21	0.41
1:B:691:ARG:HB3	1:B:693:THR:HG22	2.03	0.41
1:C:810:VAL:HG22	1:C:1074:ARG:HD2	2.02	0.41
1:A:129:THR:HG22	1:A:131:ILE:N	2.26	0.41
1:A:853:VAL:HG13	1:A:951:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:PHE:CE2	1:C:1181:VAL:HB	2.55	0.41
1:B:609:TYR:OH	1:B:629:ARG:NH2	2.50	0.41
1:C:351:TYR:CD2	1:C:356:VAL:HG22	2.55	0.41
1:C:617:PHE:HB3	1:C:649:TYR:HB3	2.03	0.41
1:C:1054:ILE:CD1	1:C:1054:ILE:H	1.98	0.41
1:A:70:THR:HG22	1:A:324:LEU:CA	2.32	0.41
1:A:778:PHE:CD1	1:B:971:PRO:HD3	2.56	0.41
1:B:641:TYR:CD2	1:B:648:TYR:HA	2.56	0.41
1:B:728:LYS:N	1:B:761:SER:OG	2.45	0.41
1:C:530:VAL:HA	1:C:531:PRO:HD2	1.90	0.41
1:C:764:PHE:HA	1:C:765:ASN:HA	1.81	0.41
1:C:1127:VAL:HG13	1:C:1136:PHE:HE1	1.86	0.41
1:A:341:PHE:O	1:A:342:ASN:CB	2.67	0.41
1:A:401:ARG:HH12	1:B:260:ALA:CB	2.28	0.41
1:A:487:ASN:OD1	1:A:487:ASN:N	2.54	0.41
1:A:641:TYR:CD2	1:A:648:TYR:HA	2.56	0.41
1:B:582:ASN:CB	1:B:609:TYR:CE2	3.00	0.41
1:C:341:PHE:CZ	1:C:696:MET:HB2	2.56	0.41
1:C:484:VAL:O	1:C:566:GLN:HB3	2.21	0.41
1:A:439:SER:OG	1:A:576:GLN:O	2.37	0.40
1:A:530:VAL:HA	1:A:531:PRO:HD2	1.90	0.40
1:A:631:VAL:HG23	1:B:64:TYR:HA	2.03	0.40
1:A:727:CYS:HB2	1:A:763:ALA:HA	2.02	0.40
1:A:733:GLN:H	1:A:733:GLN:HG3	1.64	0.40
1:B:264:HIS:HB3	1:B:280:GLN:OE1	2.21	0.40
1:B:344:LEU:HB2	1:B:670:HIS:CB	2.50	0.40
1:B:504:SER:HB3	1:B:515:PRO:HA	2.03	0.40
1:B:617:PHE:HB3	1:B:649:TYR:HB3	2.03	0.40
1:B:782:ILE:H	1:B:782:ILE:HG13	1.59	0.40
1:C:487:ASN:OD1	1:C:487:ASN:N	2.54	0.40
1:A:62:ARG:CB	1:C:632:TYR:CE2	3.04	0.40
1:A:355:ASP:OD1	1:A:665:LYS:HB2	2.21	0.40
1:A:403:VAL:HG13	1:A:441:LEU:C	2.45	0.40
1:A:426:SER:O	1:A:427:GLN:HB2	2.20	0.40
1:B:428:ILE:HA	1:C:1058:LEU:N	2.34	0.40
1:B:583:SER:HA	1:B:609:TYR:CD1	2.56	0.40
1:B:625:VAL:HG21	1:C:63:THR:CG2	2.46	0.40
1:B:853:VAL:HG13	1:B:951:LEU:HD22	2.03	0.40
1:B:1100:LYS:O	1:B:1104:ASN:ND2	2.54	0.40
1:B:1181:VAL:HB	1:C:967:PHE:CE2	2.56	0.40
1:C:413:LYS:O	1:C:416:SER:OG	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:732:GLY:HA2	1:C:734:SER:HB2	2.02	0.40
1:C:853:VAL:HG13	1:C:951:LEU:HD22	2.03	0.40
1:C:1100:LYS:O	1:C:1104:ASN:ND2	2.54	0.40
1:A:810:VAL:HG22	1:A:1074:ARG:HD2	2.02	0.40
1:B:583:SER:HA	1:B:609:TYR:CG	2.56	0.40
1:C:456:LEU:HD12	1:C:456:LEU:HA	1.88	0.40
1:C:598:SER:OG	1:C:599:GLN:N	2.54	0.40
1:C:1201:ASN:HB2	1:C:1206:ALA:HB3	2.02	0.40
1:A:484:VAL:O	1:A:566:GLN:HB3	2.21	0.40
1:A:906:MET:HG2	1:C:716:GLY:HA2	2.03	0.40
1:B:487:ASN:OD1	1:B:487:ASN:N	2.54	0.40
1:B:716:GLY:HA2	1:C:906:MET:HG2	2.03	0.40
1:A:383:CYS:SG	1:A:404:PHE:CB	3.01	0.40
1:A:423:PHE:CE2	1:A:430:PRO:HB3	2.57	0.40
1:A:726:ASP:OD1	1:A:726:ASP:N	2.52	0.40
1:A:1180:ILE:HG22	1:A:1181:VAL:H	1.87	0.40
1:B:511:ARG:CB	1:C:436:ASN:HB3	2.49	0.40
1:C:493:LYS:NZ	1:C:564:THR:O	2.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	1128/1323 (85%)	964 (86%)	147 (13%)	17 (2%)	8	38
1	B	1128/1323 (85%)	965 (86%)	147 (13%)	16 (1%)	9	39
1	C	1128/1323 (85%)	966 (86%)	147 (13%)	15 (1%)	9	41
All	All	3384/3969 (85%)	2895 (86%)	441 (13%)	48 (1%)	11	39

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	583	SER
1	A	584	VAL
1	A	596	ILE
1	A	597	ALA
1	A	797	THR
1	B	66	ASN
1	B	350	SER
1	B	351	TYR
1	B	511	ARG
1	B	582	ASN
1	B	797	THR
1	B	1054	ILE
1	C	66	ASN
1	C	797	THR
1	C	1056	GLN
1	A	351	TYR
1	A	485	PRO
1	A	997	ILE
1	B	485	PRO
1	B	997	ILE
1	C	342	ASN
1	C	485	PRO
1	C	582	ASN
1	C	997	ILE
1	A	855	SER
1	B	855	SER
1	C	855	SER
1	C	1063	GLN
1	A	382	GLU
1	B	382	GLU
1	C	382	GLU
1	A	386	SER
1	A	581	THR
1	A	642	TYR
1	B	579	THR
1	B	642	TYR
1	B	736	CYS
1	C	642	TYR
1	A	736	CYS
1	C	736	CYS
1	A	1181	VAL
1	B	1181	VAL
1	C	1055	ILE

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Mol	Chain	Res	Type
1	C	1181	VAL
1	A	1054	ILE
1	B	985	ILE
1	C	985	ILE
1	A	985	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	973/1143 (85%)	916 (94%)	57 (6%)	18	41
1	B	973/1143 (85%)	913 (94%)	60 (6%)	16	39
1	C	974/1143 (85%)	916 (94%)	58 (6%)	17	40
All	All	2920/3429 (85%)	2745 (94%)	175 (6%)	19	40

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	58	TYR
1	A	64	TYR
1	A	71	TYR
1	A	72	GLN
1	A	78	GLN
1	A	86	VAL
1	A	181	ARG
1	A	341	PHE
1	A	342	ASN
1	A	343	ASP
1	A	346	GLN
1	A	349	CYS
1	A	352	GLU
1	A	353	SER
1	A	356	VAL
1	A	402	LEU

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Mol	Chain	Res	Type
1	A	403	VAL
1	A	411	LEU
1	A	427	GLN
1	A	450	LEU
1	A	458	VAL
1	A	465	SER
1	A	473	PHE
1	A	479	LEU
1	A	481	LEU
1	A	484	VAL
1	A	487	ASN
1	A	488	LEU
1	A	489	THR
1	A	490	THR
1	A	492	THR
1	A	493	LYS
1	A	495	LEU
1	A	510	ASP
1	A	521	ASN
1	A	535	TRP
1	A	555	VAL
1	A	564	THR
1	A	565	GLU
1	A	573	ILE
1	A	579	THR
1	A	581	THR
1	A	588	LEU
1	A	677	VAL
1	A	696	MET
1	A	697	LEU
1	A	722	LEU
1	A	724	VAL
1	A	735	LEU
1	A	782	ILE
1	A	799	ILE
1	A	970	ILE
1	A	1098	LEU
1	A	1124	VAL
1	A	1165	ILE
1	A	1181	VAL
1	B	52	LYS
1	B	58	TYR

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Mol	Chain	Res	Type
1	B	64	TYR
1	B	86	VAL
1	B	181	ARG
1	B	261	GLN
1	B	349	CYS
1	B	352	GLU
1	B	353	SER
1	B	356	VAL
1	B	403	VAL
1	B	411	LEU
1	B	438	TYR
1	B	441	LEU
1	B	450	LEU
1	B	458	VAL
1	B	465	SER
1	B	473	PHE
1	B	479	LEU
1	B	481	LEU
1	B	484	VAL
1	B	487	ASN
1	B	488	LEU
1	B	489	THR
1	B	490	THR
1	B	492	THR
1	B	493	LYS
1	B	495	LEU
1	B	511	ARG
1	B	535	TRP
1	B	555	VAL
1	B	564	THR
1	B	565	GLU
1	B	573	ILE
1	B	581	THR
1	B	582	ASN
1	B	588	LEU
1	B	608	LEU
1	B	609	TYR
1	B	627	GLN
1	B	629	ARG
1	B	677	VAL
1	B	697	LEU
1	B	722	LEU

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Mol	Chain	Res	Type
1	B	724	VAL
1	B	735	LEU
1	B	782	ILE
1	B	799	ILE
1	B	970	ILE
1	B	1051	ILE
1	B	1053	ASP
1	B	1054	ILE
1	B	1055	ILE
1	B	1058	LEU
1	B	1059	ASP
1	B	1098	LEU
1	B	1124	VAL
1	B	1149	VAL
1	B	1165	ILE
1	B	1181	VAL
1	C	52	LYS
1	C	58	TYR
1	C	64	TYR
1	C	86	VAL
1	C	181	ARG
1	C	324	LEU
1	C	339	CYS
1	C	341	PHE
1	C	342	ASN
1	C	343	ASP
1	C	344	LEU
1	C	346	GLN
1	C	347	LEU
1	C	350	SER
1	C	352	GLU
1	C	403	VAL
1	C	411	LEU
1	C	450	LEU
1	C	458	VAL
1	C	465	SER
1	C	473	PHE
1	C	479	LEU
1	C	481	LEU
1	C	484	VAL
1	C	487	ASN
1	C	488	LEU

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Mol	Chain	Res	Type
1	C	489	THR
1	C	490	THR
1	C	492	THR
1	C	493	LYS
1	C	495	LEU
1	C	510	ASP
1	C	535	TRP
1	C	555	VAL
1	C	564	THR
1	C	565	GLU
1	C	573	ILE
1	C	588	LEU
1	C	677	VAL
1	C	697	LEU
1	C	722	LEU
1	C	724	VAL
1	C	735	LEU
1	C	782	ILE
1	C	799	ILE
1	C	822	ARG
1	C	970	ILE
1	C	1054	ILE
1	C	1055	ILE
1	C	1056	GLN
1	C	1057	ARG
1	C	1058	LEU
1	C	1061	LEU
1	C	1098	LEU
1	C	1124	VAL
1	C	1149	VAL
1	C	1165	ILE
1	C	1181	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	342	ASN
1	A	346	GLN
1	A	348	HIS
1	A	398	ASN
1	A	427	GLN

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Mol	Chain	Res	Type
1	A	466	GLN
1	A	516	GLN
1	A	521	ASN
1	A	566	GLN
1	A	602	ASN
1	A	627	GLN
1	A	628	GLN
1	A	670	HIS
1	A	765	ASN
1	A	800	GLN
1	A	812	ASN
1	A	832	ASN
1	A	839	ASN
1	A	842	GLN
1	A	848	ASN
1	A	870	ASN
1	A	1009	GLN
1	A	1023	GLN
1	A	1028	ASN
1	A	1066	GLN
1	A	1146	HIS
1	B	155	ASN
1	B	377	GLN
1	B	398	ASN
1	B	408	ASN
1	B	427	GLN
1	B	466	GLN
1	B	501	ASN
1	B	516	GLN
1	B	566	GLN
1	B	602	ASN
1	B	765	ASN
1	B	800	GLN
1	B	812	ASN
1	B	832	ASN
1	B	839	ASN
1	B	842	GLN
1	B	848	ASN
1	B	870	ASN
1	B	1009	GLN
1	B	1023	GLN
1	B	1028	ASN

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Mol	Chain	Res	Type
1	B	1066	GLN
1	B	1146	HIS
1	C	155	ASN
1	C	346	GLN
1	C	398	ASN
1	C	436	ASN
1	C	466	GLN
1	C	516	GLN
1	C	566	GLN
1	C	602	ASN
1	C	628	GLN
1	C	765	ASN
1	C	800	GLN
1	C	812	ASN
1	C	832	ASN
1	C	839	ASN
1	C	848	ASN
1	C	870	ASN
1	C	1009	GLN
1	C	1023	GLN
1	C	1028	ASN
1	C	1066	GLN
1	C	1146	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

There are no ligands in this entry.

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.

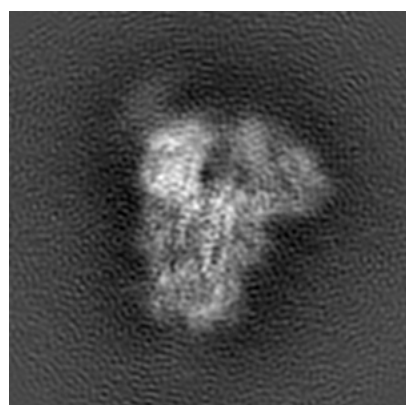
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6707. These allow visual inspection of the internal detail of the map and identification of artifacts.

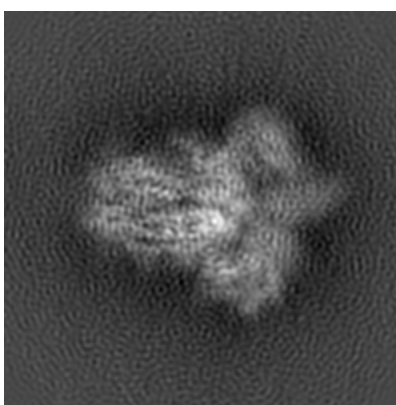
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

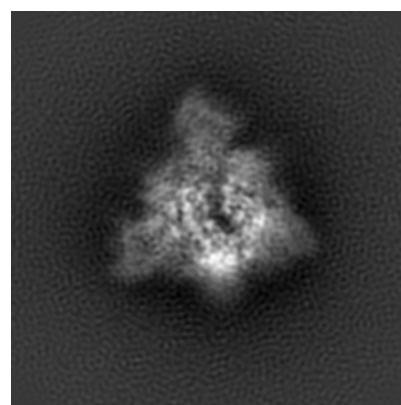
6.1.1 Primary map



X



Y

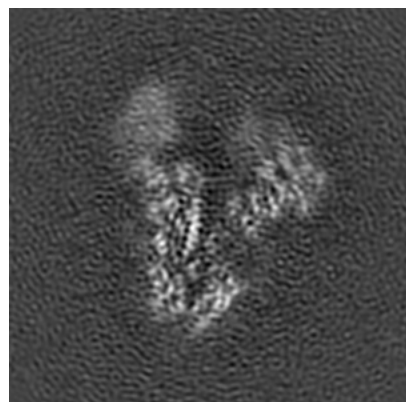


Z

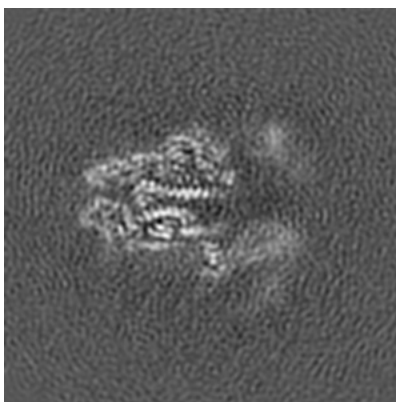
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

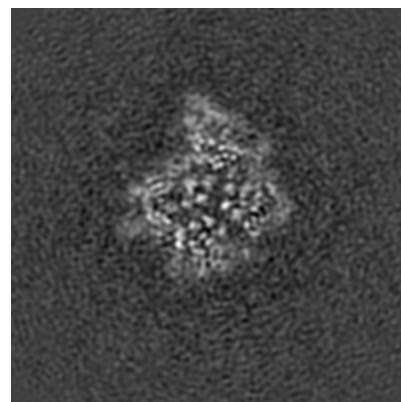
6.2.1 Primary map



X Index: 100



Y Index: 100

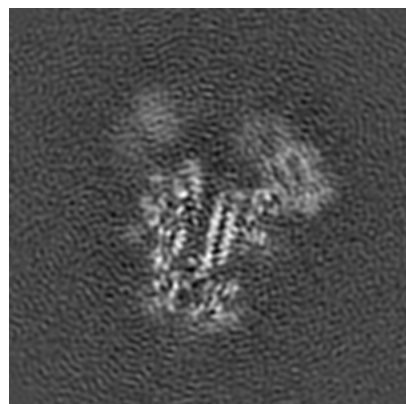


Z Index: 100

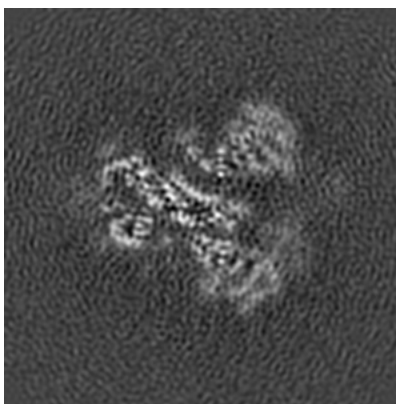
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

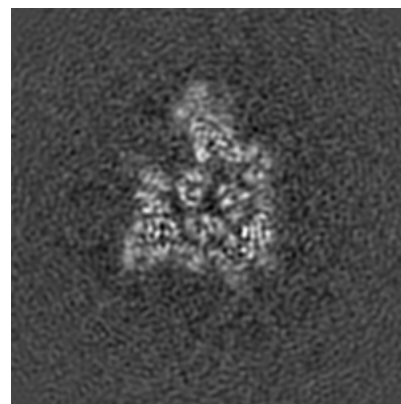
6.3.1 Primary map



X Index: 96



Y Index: 87

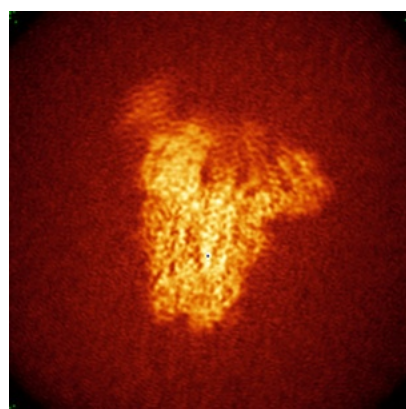


Z Index: 108

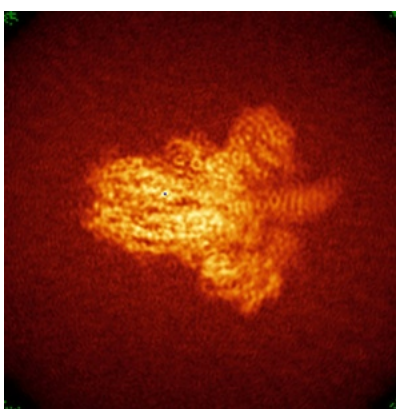
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

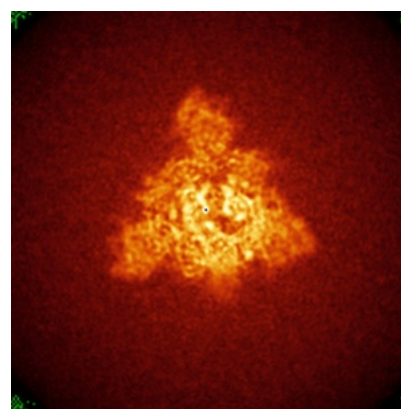
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0595. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

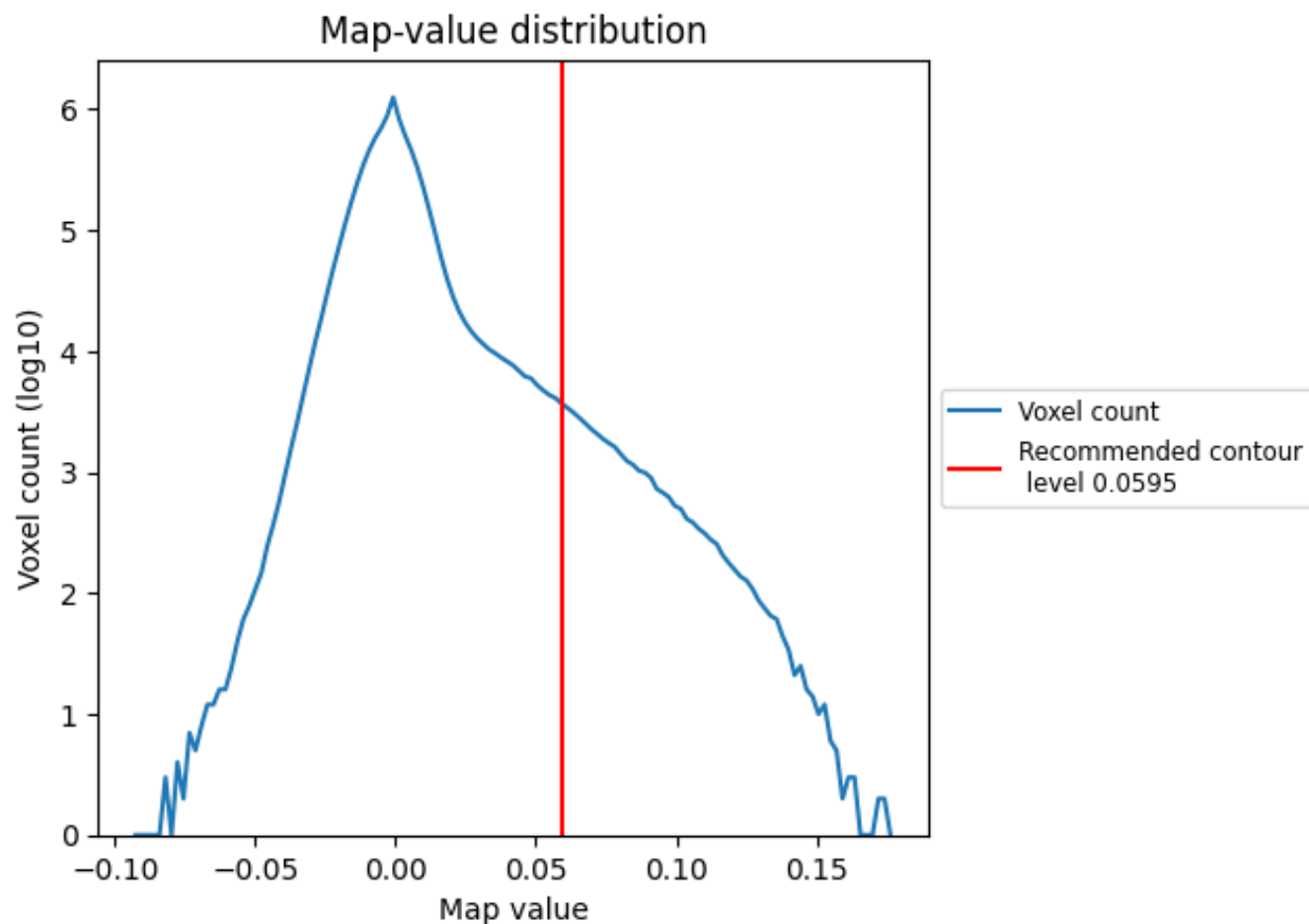
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

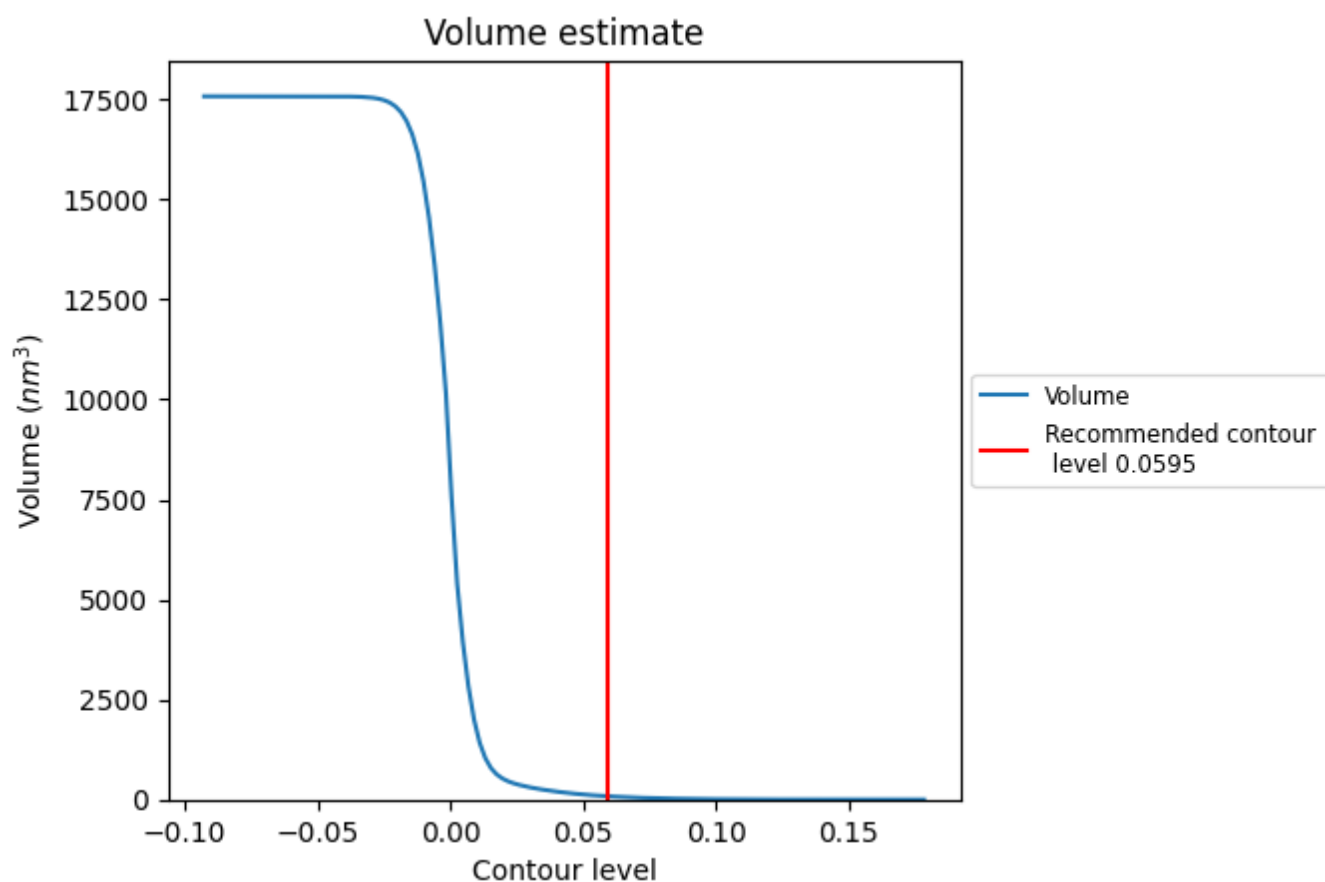
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

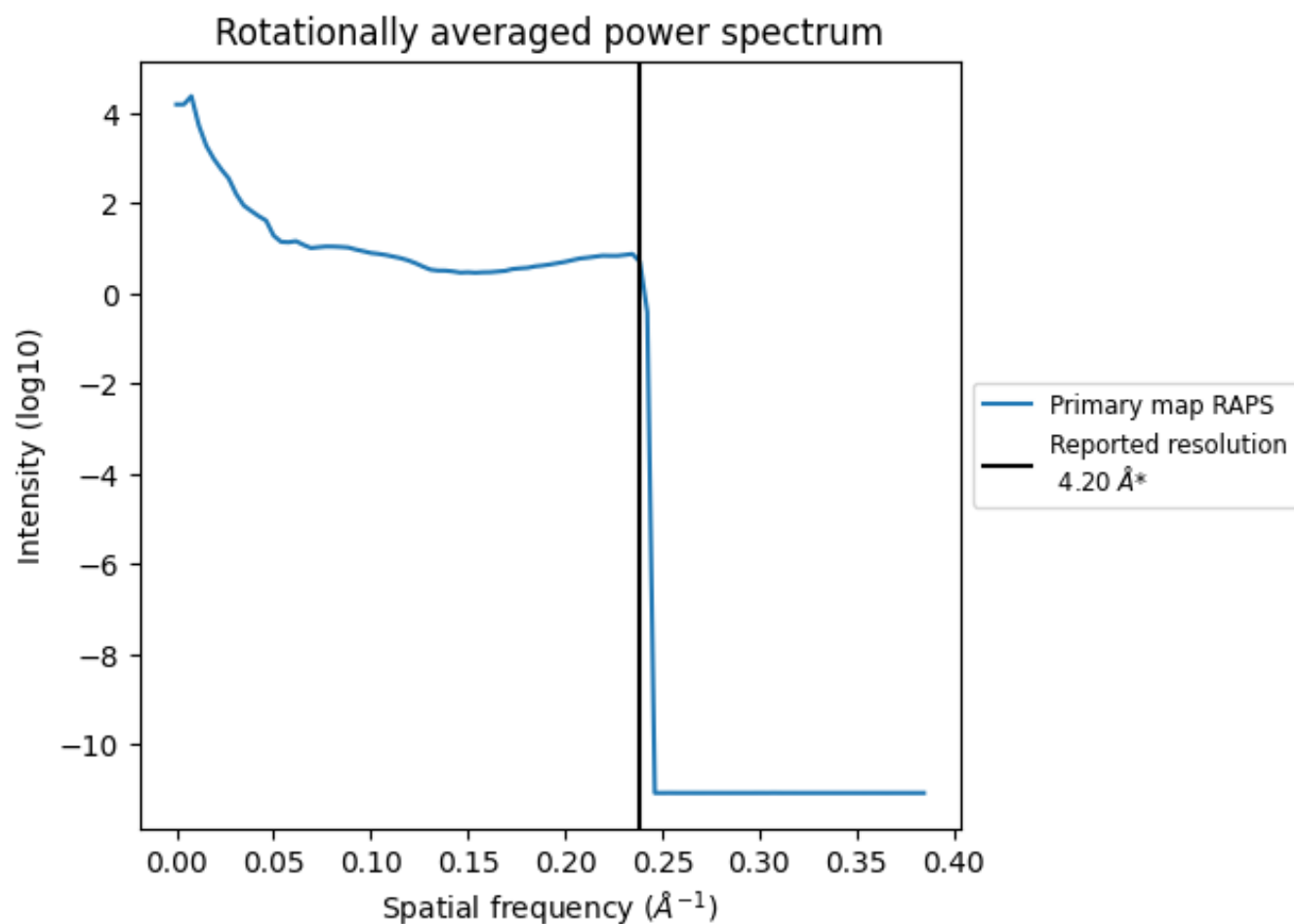
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm³; this corresponds to an approximate mass of 74 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

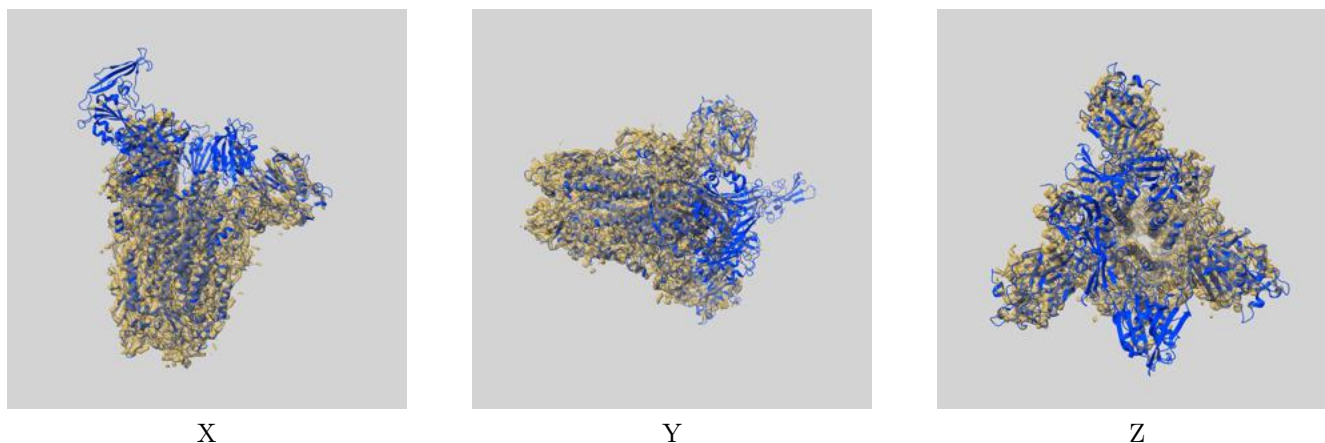
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

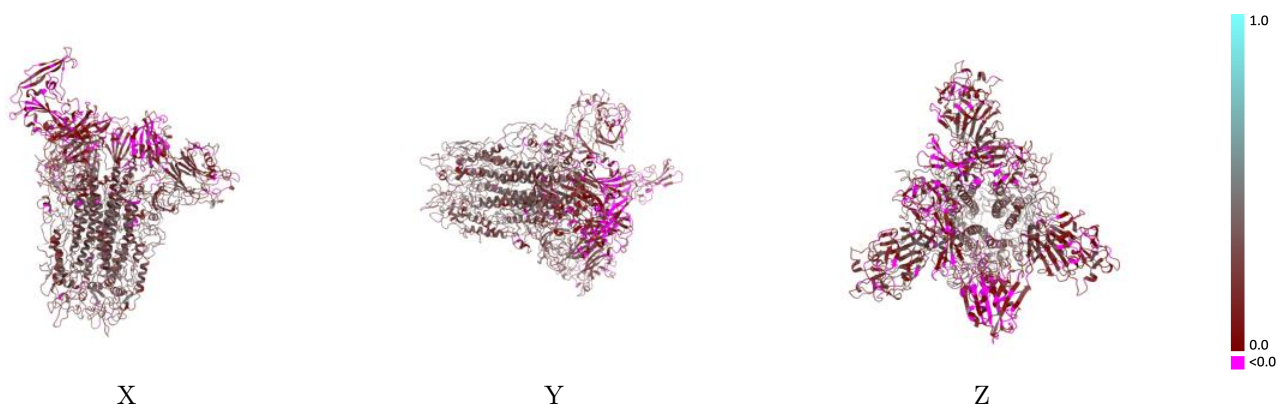
This section contains information regarding the fit between EMDB map EMD-6707 and PDB model 5X5F. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



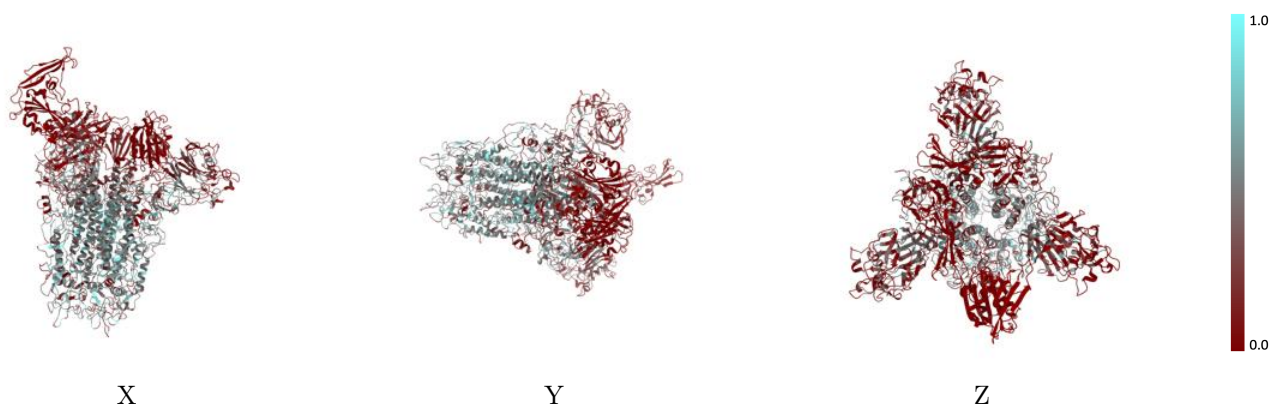
The images above show the 3D surface view of the map at the recommended contour level 0.0595 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



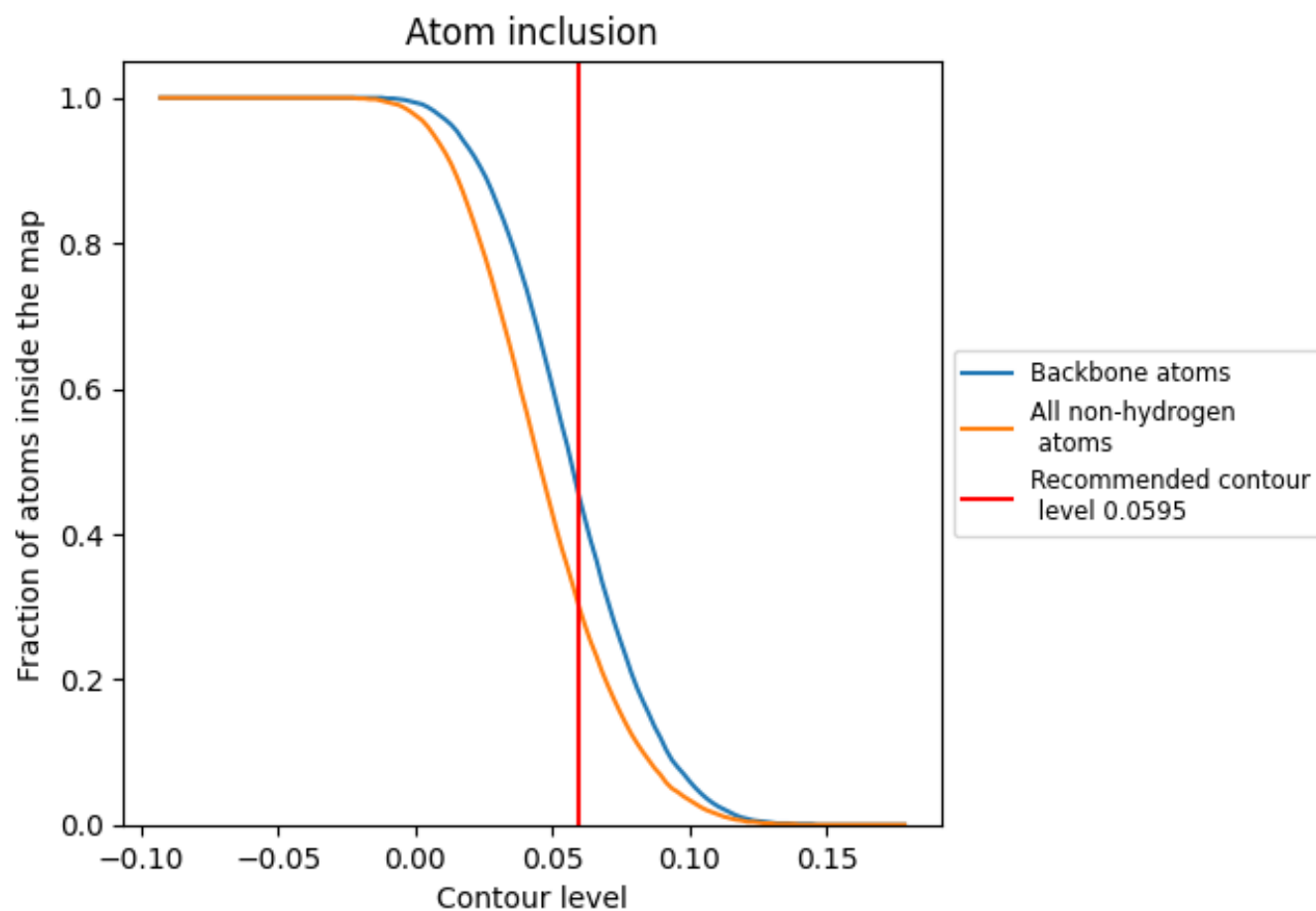
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0595).

9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 30% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0595) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3050	0.2240
A	0.2890	0.2110
B	0.3180	0.2350
C	0.3090	0.2270

