



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:35 PM UTC

PDB ID : 4BOM / pdb_00004bom
EMDB ID : EMD-2380
Title : Structure of herpesvirus fusion glycoprotein B-bilayer complex revealing the protein-membrane and lateral protein-protein interaction
Authors : Maurer, U.E.; Zeev-Ben-Mordehai, Z.; Pandurangan, A.P.; Cairns, T.M.; Hannah, B.P.; Whitbeck, J.C.; Eisenberg, R.J.; Cohen, G.H.; Topf, M.; Huiskonen, J.T.; Grunewald, K.
Deposited on : 2013-05-21
Resolution : 27.00 Å(reported)
Based on initial model : 3NWF

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:

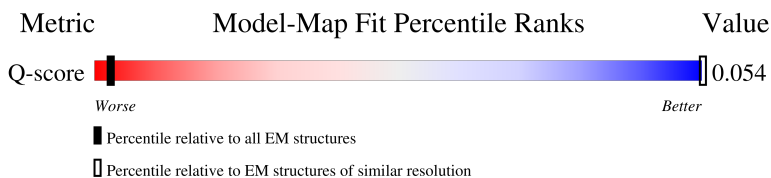
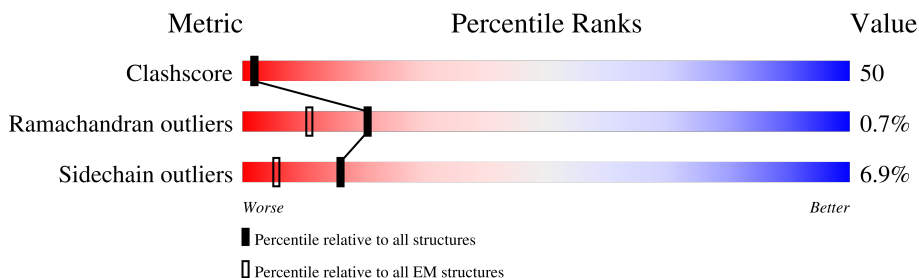
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 27.00 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	6 (26.50 - 27.20)

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	622	 5% 36% 50% 9% ..
1	B	622	 5% 37% 50% 9% ..
1	C	622	 5% 38% 50% 9% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14745 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 ENVELOPE GLYCOPROTEIN B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	608	Total	C	N	O	S	0	1
			4915	3097	869	927	22		
1	B	608	Total	C	N	O	S	0	1
			4915	3097	869	927	22		
1	C	608	Total	C	N	O	S	0	1
			4915	3097	869	927	22		

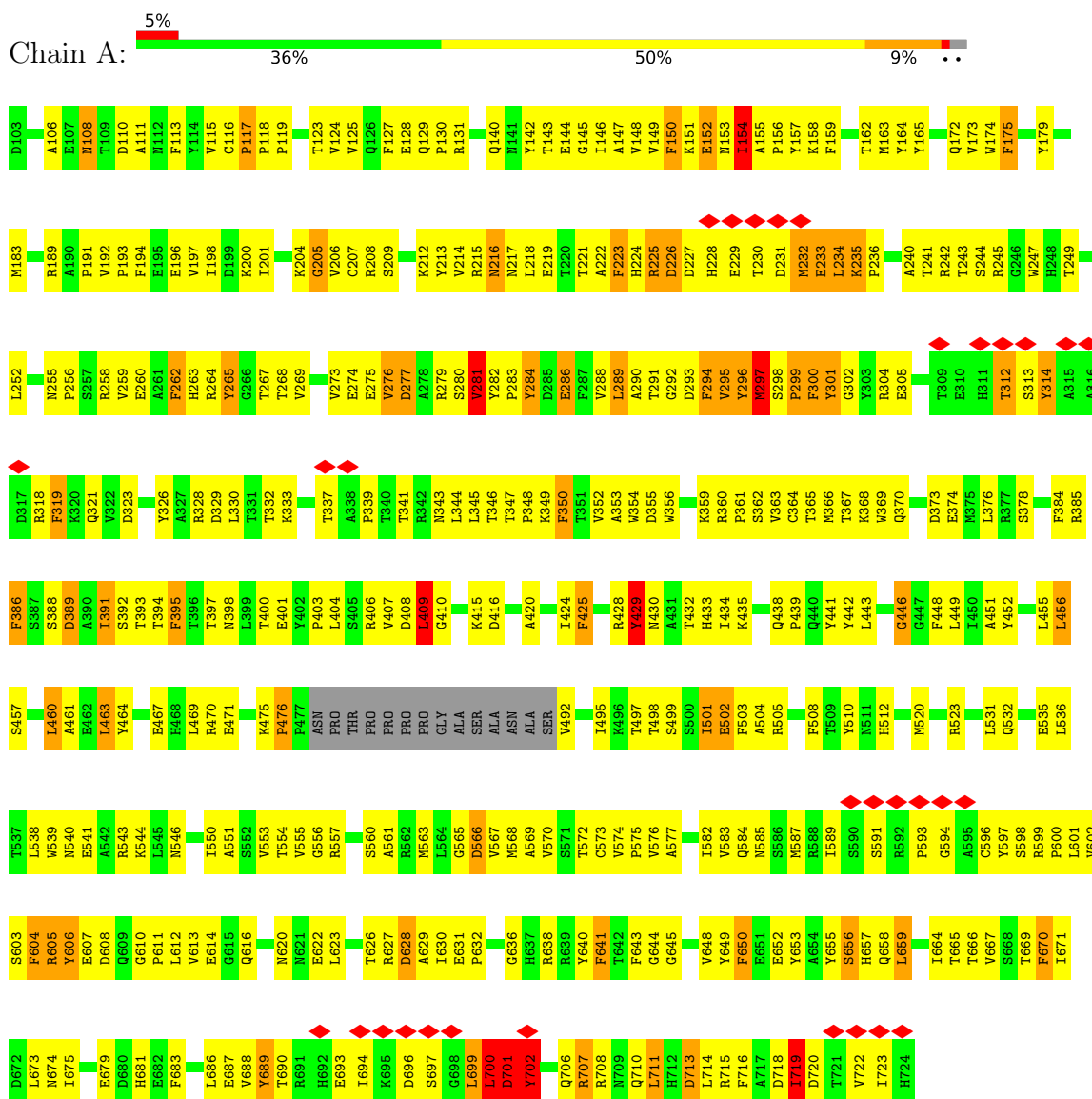
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	313	SER	THR	conflict	UNP P06437
A	443	LEU	GLN	conflict	UNP P06437
B	313	SER	THR	conflict	UNP P06437
B	443	LEU	GLN	conflict	UNP P06437
C	313	SER	THR	conflict	UNP P06437
C	443	LEU	GLN	conflict	UNP P06437

3 Residue-property plots

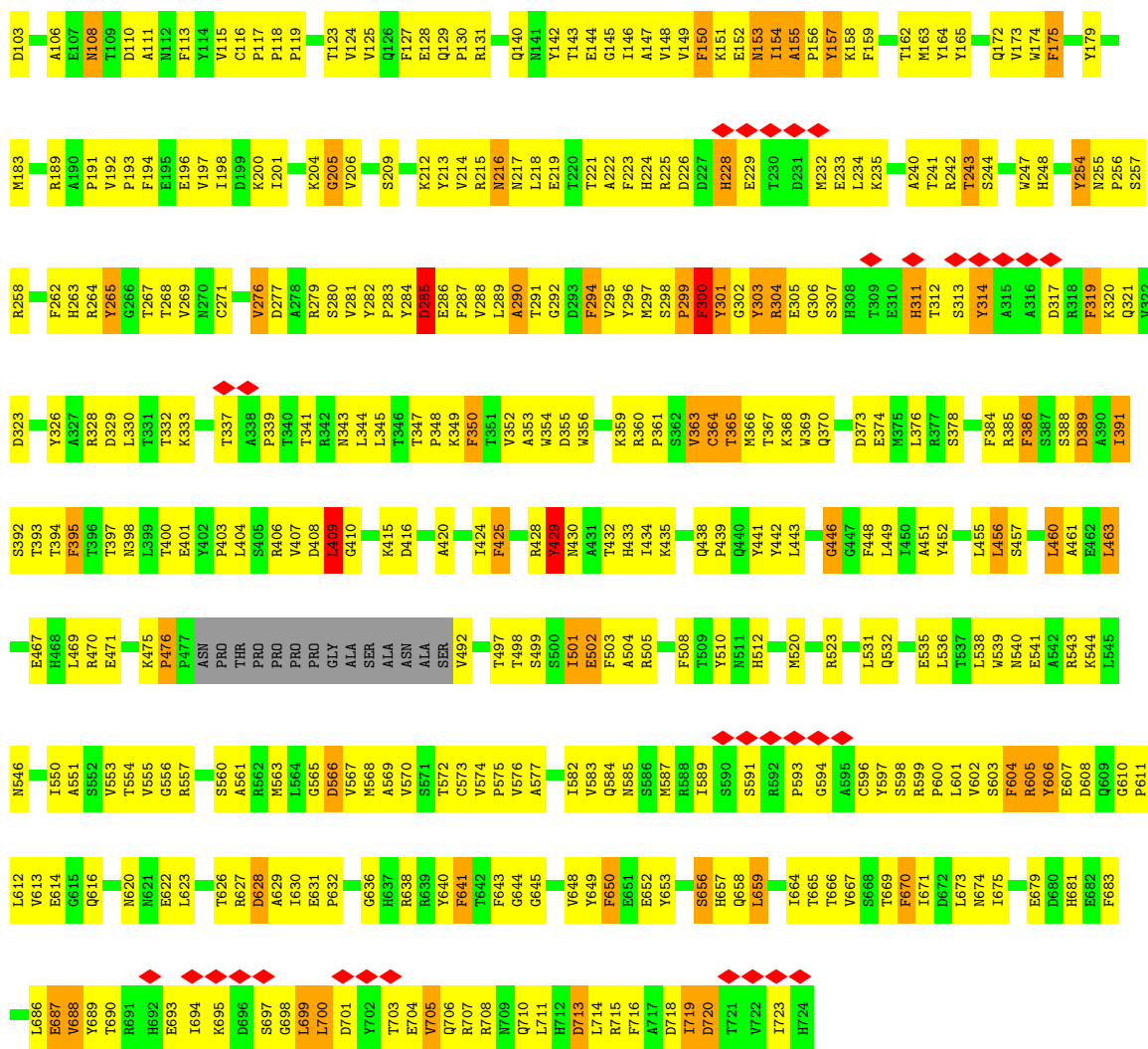
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



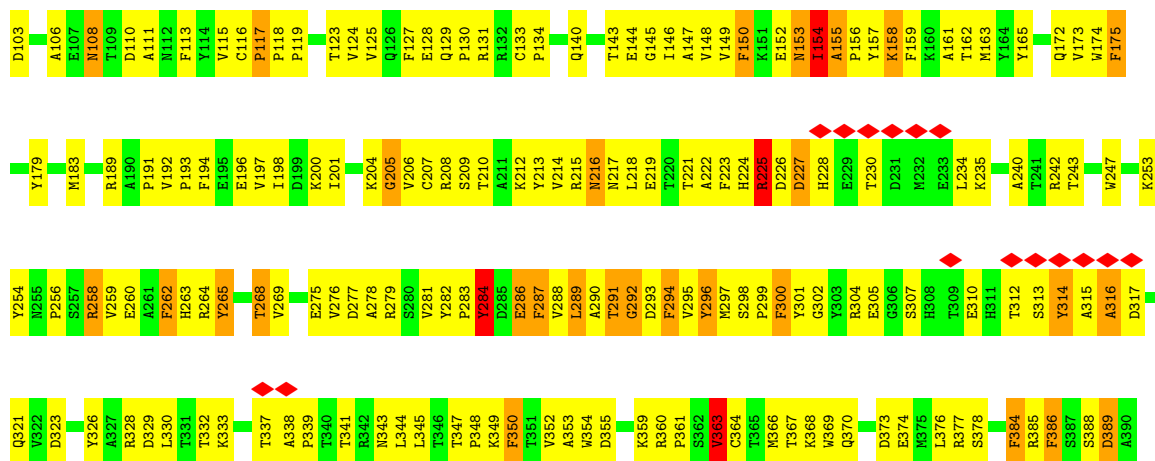
• Molecule 1: ENVELOPE GLYCOPROTEIN B





• Molecule 1: ENVELOPE GLYCOPROTEIN B

Chain C: 5% 38% 50% 9% ..





4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of tilted images used	786	Depositor
Resolution determination method	Not provided	
CTF correction method	LOW PASS FILTER TO THE FIRST ZERO CROSSING OF THE CTF	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	67000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum voxel value	18.674	Depositor
Minimum voxel value	-12.513	Depositor
Average voxel value	0.000	Depositor
Voxel value standard deviation	1.000	Depositor
Recommended contour level	2	Depositor
Tomogram size ($\text{\AA}$)	460.0, 460.0, 460.0	wwPDB
Tomogram dimensions	100, 100, 100	wwPDB
Tomogram angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Grid spacing ($\text{\AA}$)	4.6, 4.6, 4.6	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	1.46	2/5036 (0.0%)	1.58	51/6840 (0.7%)
1	B	1.46	2/5036 (0.0%)	1.57	49/6840 (0.7%)
1	C	1.46	2/5036 (0.0%)	1.58	49/6840 (0.7%)
All	All	1.46	6/15108 (0.0%)	1.58	149/20520 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16
1	B	0	13
1	C	0	12
All	All	0	41

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	656	SER	CA-C	-5.89	1.49	1.52
1	B	656	SER	CA-C	-5.88	1.49	1.52
1	C	656	SER	CA-C	-5.76	1.49	1.52
1	C	476	PRO	C-N	-5.20	1.26	1.34
1	A	476	PRO	C-N	-5.17	1.26	1.34
1	B	476	PRO	C-N	-5.17	1.26	1.34

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	716	PHE	CA-CB-CG	-11.82	101.98	113.80
1	C	716	PHE	CA-CB-CG	-9.53	104.27	113.80
1	B	716	PHE	CA-CB-CG	-9.38	104.42	113.80
1	A	292	GLY	N-CA-C	-8.62	103.71	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	701	ASP	CA-CB-CG	-8.14	104.46	112.60
1	B	604	PHE	CA-CB-CG	-8.02	105.78	113.80
1	C	604	PHE	CA-CB-CG	-8.01	105.79	113.80
1	A	604	PHE	CA-CB-CG	-7.98	105.82	113.80
1	C	641	PHE	CA-CB-CG	-7.84	105.96	113.80
1	B	641	PHE	CA-CB-CG	-7.84	105.96	113.80
1	A	641	PHE	CA-CB-CG	-7.82	105.98	113.80
1	C	300	PHE	CA-CB-CG	-7.59	106.21	113.80
1	A	702	TYR	CA-CB-CG	-7.52	100.36	113.90
1	A	281	VAL	CB-CA-C	-7.50	102.44	111.81
1	B	300	PHE	CA-CB-CG	-7.42	106.38	113.80
1	B	429	TYR	CA-CB-CG	-7.21	100.92	113.90
1	C	429	TYR	CA-CB-CG	-7.20	100.94	113.90
1	B	175	PHE	CA-CB-CG	-7.18	106.62	113.80
1	A	429	TYR	CA-CB-CG	-7.18	100.97	113.90
1	C	292	GLY	N-CA-C	-7.15	105.18	115.27
1	C	175	PHE	CA-CB-CG	-7.13	106.67	113.80
1	A	262	PHE	CA-CB-CG	-7.13	106.67	113.80
1	A	175	PHE	CA-CB-CG	-7.05	106.75	113.80
1	A	295	VAL	CA-C-N	-6.97	112.82	123.14
1	A	295	VAL	C-N-CA	-6.97	112.82	123.14
1	B	262	PHE	CA-CB-CG	-6.81	106.99	113.80
1	C	262	PHE	CA-CB-CG	-6.78	107.02	113.80
1	C	448	PHE	CA-CB-CG	-6.72	107.08	113.80
1	A	448	PHE	CA-CB-CG	-6.71	107.09	113.80
1	B	705	VAL	CB-CA-C	-6.70	103.40	111.97
1	B	448	PHE	CA-CB-CG	-6.68	107.12	113.80
1	A	300	PHE	CA-CB-CG	-6.63	107.17	113.80
1	A	446	GLY	N-CA-C	-6.60	106.63	115.21
1	B	446	GLY	N-CA-C	-6.59	106.64	115.21
1	C	446	GLY	N-CA-C	-6.57	106.67	115.21
1	B	386	PHE	CA-CB-CG	-6.53	107.27	113.80
1	C	386	PHE	CA-CB-CG	-6.53	107.27	113.80
1	C	350	PHE	CA-CB-CG	-6.49	107.31	113.80
1	A	386	PHE	CA-CB-CG	-6.48	107.32	113.80
1	B	350	PHE	CA-CB-CG	-6.46	107.34	113.80
1	A	350	PHE	CA-CB-CG	-6.43	107.37	113.80
1	B	683	PHE	CA-CB-CG	-6.29	107.51	113.80
1	B	155	ALA	CA-C-N	6.28	126.74	120.52
1	B	155	ALA	C-N-CA	6.28	126.74	120.52
1	B	294	PHE	CA-CB-CG	-6.28	107.52	113.80
1	C	153	ASN	CA-CB-CG	-6.28	106.32	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	223	PHE	CA-CB-CG	-6.28	107.52	113.80
1	C	683	PHE	CA-CB-CG	-6.27	107.53	113.80
1	A	205	GLY	N-CA-C	-6.24	107.10	115.21
1	A	683	PHE	CA-CB-CG	-6.22	107.58	113.80
1	C	425	PHE	CA-CB-CG	-6.22	107.58	113.80
1	B	425	PHE	CA-CB-CG	-6.21	107.59	113.80
1	A	425	PHE	CA-CB-CG	-6.21	107.59	113.80
1	A	117	PRO	N-CA-CB	6.14	106.41	103.22
1	C	117	PRO	N-CA-CB	6.10	106.39	103.22
1	A	223	PHE	CA-CB-CG	-6.06	107.74	113.80
1	B	395	PHE	CA-CB-CG	-6.06	107.74	113.80
1	A	395	PHE	CA-CB-CG	-6.04	107.76	113.80
1	C	395	PHE	CA-CB-CG	-6.04	107.76	113.80
1	C	205	GLY	N-CA-C	-6.04	107.36	115.21
1	C	150	PHE	CA-CB-CG	-6.03	107.77	113.80
1	B	153	ASN	CA-CB-CG	-6.03	106.57	112.60
1	B	117	PRO	N-CA-CB	6.01	106.35	103.22
1	B	319	PHE	CA-CB-CG	-5.99	107.81	113.80
1	A	150	PHE	CA-CB-CG	-5.97	107.83	113.80
1	B	150	PHE	CA-CB-CG	-5.97	107.83	113.80
1	B	670	PHE	CA-CB-CG	-5.94	107.86	113.80
1	C	670	PHE	CA-CB-CG	-5.92	107.88	113.80
1	A	670	PHE	CA-CB-CG	-5.91	107.89	113.80
1	A	153	ASN	CA-CB-CG	-5.88	106.72	112.60
1	C	294	PHE	CA-CB-CG	-5.86	107.94	113.80
1	B	108	ASN	CA-CB-CG	-5.84	106.76	112.60
1	C	108	ASN	CA-CB-CG	-5.82	106.78	112.60
1	B	223	PHE	CA-CB-CG	-5.81	107.99	113.80
1	C	155	ALA	CA-C-N	5.80	125.78	120.21
1	C	155	ALA	C-N-CA	5.80	125.78	120.21
1	A	650	PHE	CA-CB-CG	-5.77	108.03	113.80
1	C	650	PHE	CA-CB-CG	-5.73	108.07	113.80
1	A	294	PHE	CA-CB-CG	-5.71	108.09	113.80
1	B	713	ASP	CA-CB-CG	-5.70	106.90	112.60
1	A	299	PRO	N-CA-C	-5.69	105.97	113.65
1	B	650	PHE	CA-CB-CG	-5.68	108.12	113.80
1	C	313	SER	CA-C-N	-5.66	112.96	122.29
1	C	313	SER	C-N-CA	-5.66	112.96	122.29
1	B	290	ALA	N-CA-C	-5.64	105.14	111.28
1	A	108	ASN	CA-CB-CG	-5.61	107.00	112.60
1	A	620	ASN	CA-CB-CG	-5.60	107.00	112.60
1	A	277	ASP	CA-CB-CG	-5.57	107.03	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	PHE	CA-CB-CG	-5.57	108.23	113.80
1	C	287	PHE	CA-CB-CG	-5.56	108.24	113.80
1	C	113	PHE	CA-CB-CG	-5.55	108.25	113.80
1	B	113	PHE	CA-CB-CG	-5.53	108.27	113.80
1	A	127	PHE	CA-CB-CG	-5.52	108.28	113.80
1	B	127	PHE	CA-CB-CG	-5.52	108.28	113.80
1	C	384	PHE	CA-CB-CG	-5.52	108.28	113.80
1	C	127	PHE	CA-CB-CG	-5.52	108.28	113.80
1	C	620	ASN	CA-CB-CG	-5.52	107.08	112.60
1	B	620	ASN	CA-CB-CG	-5.51	107.09	112.60
1	A	713	ASP	CA-CB-CG	-5.51	107.09	112.60
1	B	384	PHE	CA-CB-CG	-5.50	108.30	113.80
1	C	566	ASP	CA-CB-CG	-5.50	107.11	112.60
1	A	384	PHE	CA-CB-CG	-5.46	108.34	113.80
1	A	566	ASP	CA-CB-CG	-5.46	107.14	112.60
1	B	566	ASP	CA-CB-CG	-5.45	107.15	112.60
1	A	319	PHE	CA-CB-CG	-5.44	108.36	113.80
1	B	389	ASP	CA-CB-CG	-5.39	107.21	112.60
1	B	157	TYR	CA-CB-CG	-5.38	104.21	113.90
1	B	636	GLY	N-CA-C	-5.35	106.66	114.90
1	C	389	ASP	CA-CB-CG	-5.35	107.25	112.60
1	A	636	GLY	N-CA-C	-5.34	106.68	114.90
1	A	389	ASP	CA-CB-CG	-5.33	107.27	112.60
1	B	291	THR	N-CA-C	-5.33	105.47	111.28
1	C	157	TYR	CA-CB-CG	-5.32	104.32	113.90
1	C	636	GLY	N-CA-C	-5.32	106.71	114.90
1	B	216	ASN	CA-CB-CG	-5.26	107.34	112.60
1	B	373	ASP	CA-CB-CG	-5.24	107.36	112.60
1	C	373	ASP	CA-CB-CG	-5.24	107.36	112.60
1	A	373	ASP	CA-CB-CG	-5.23	107.37	112.60
1	A	355	ASP	CA-CB-CG	-5.22	107.38	112.60
1	A	701	ASP	N-CA-C	5.21	117.78	109.81
1	B	606	TYR	CA-CB-CG	-5.19	104.55	113.90
1	A	606	TYR	CA-CB-CG	-5.19	104.56	113.90
1	C	216	ASN	CA-CB-CG	-5.18	107.42	112.60
1	C	606	TYR	CA-CB-CG	-5.18	104.58	113.90
1	C	323	ASP	CA-CB-CG	-5.17	107.43	112.60
1	A	323	ASP	CA-CB-CG	-5.15	107.45	112.60
1	C	355	ASP	CA-CB-CG	-5.15	107.45	112.60
1	B	323	ASP	CA-CB-CG	-5.15	107.45	112.60
1	A	216	ASN	CA-CB-CG	-5.14	107.46	112.60
1	C	103	ASP	CA-CB-CG	-5.13	107.47	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	594	GLY	N-CA-C	-5.13	108.24	115.32
1	B	720	ASP	CA-CB-CG	-5.13	107.47	112.60
1	B	205	GLY	N-CA-C	-5.13	107.18	115.08
1	B	103	ASP	CA-CB-CG	-5.12	107.48	112.60
1	A	594	GLY	N-CA-C	-5.11	108.27	115.32
1	B	594	GLY	N-CA-C	-5.11	108.27	115.32
1	A	297	MET	N-CA-C	-5.09	101.67	109.41
1	B	585	ASN	CA-CB-CG	-5.08	107.52	112.60
1	B	416	ASP	CA-CB-CG	-5.07	107.53	112.60
1	A	585	ASN	CA-CB-CG	-5.07	107.53	112.60
1	C	284	TYR	CA-CB-CG	-5.07	104.78	113.90
1	A	718	ASP	CA-CB-CG	-5.06	107.54	112.60
1	A	416	ASP	CA-CB-CG	-5.05	107.55	112.60
1	C	416	ASP	CA-CB-CG	-5.04	107.56	112.60
1	B	355	ASP	CA-CB-CG	-5.04	107.56	112.60
1	C	585	ASN	CA-CB-CG	-5.03	107.58	112.60
1	B	285	ASP	CA-CB-CG	-5.02	107.58	112.60
1	C	702	TYR	N-CA-C	-5.01	105.71	111.07
1	C	643	PHE	CA-CB-CG	-5.01	108.79	113.80

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	ILE	Peptide
1	A	225	ARG	Peptide
1	A	228	HIS	Peptide
1	A	284	TYR	Peptide
1	A	362	SER	Peptide
1	A	363	VAL	Peptide
1	A	365	THR	Peptide
1	A	409	LEU	Peptide
1	A	429	TYR	Peptide
1	A	460	LEU	Peptide
1	A	501	ILE	Peptide
1	A	628	ASP	Peptide
1	A	700	LEU	Peptide
1	A	701	ASP	Peptide
1	A	702	TYR	Peptide
1	A	719	ILE	Peptide
1	B	154	ILE	Peptide
1	B	284	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	B	299	PRO	Peptide
1	B	311	HIS	Peptide
1	B	363	VAL	Peptide
1	B	364	CYS	Peptide
1	B	365	THR	Peptide
1	B	409	LEU	Peptide
1	B	429	TYR	Peptide
1	B	460	LEU	Peptide
1	B	501	ILE	Peptide
1	B	628	ASP	Peptide
1	B	719	ILE	Peptide
1	C	154	ILE	Peptide
1	C	225	ARG	Peptide
1	C	314	TYR	Peptide
1	C	316	ALA	Peptide
1	C	363	VAL	Peptide
1	C	409	LEU	Peptide
1	C	429	TYR	Peptide
1	C	460	LEU	Peptide
1	C	501	ILE	Peptide
1	C	628	ASP	Peptide
1	C	699	LEU	Peptide
1	C	719	ILE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4915	0	4740	569	0
1	B	4915	0	4740	568	0
1	C	4915	0	4740	564	0
All	All	14745	0	14220	1444	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 50.

All (1444) 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:B:699:LEU:HD13	1:C:281:VAL:HG13	1.26	1.14
1:C:408:ASP:HB2	1:C:492:VAL:HG13	1.14	1.14
1:B:706:GLN:HG3	1:C:699:LEU:HD21	1.26	1.13
1:B:700:LEU:HB2	1:C:279:ARG:HG2	1.32	1.11
1:A:397:THR:HG21	1:A:442:TYR:HB3	1.33	1.11
1:B:397:THR:HG21	1:B:442:TYR:HB3	1.33	1.10
1:A:408:ASP:HB2	1:A:492:VAL:HG13	1.19	1.10
1:C:154:ILE:HG13	1:C:155:ALA:HA	1.22	1.10
1:A:700:LEU:HG	1:B:158:LYS:HE3	1.28	1.09
1:C:363:VAL:HG11	1:C:409:LEU:HD13	1.08	1.08
1:B:700:LEU:HG	1:C:158:LYS:HE3	1.36	1.08
1:B:408:ASP:HB2	1:B:492:VAL:HG13	1.16	1.07
1:C:363:VAL:HG13	1:C:364:CYS:HA	1.34	1.07
1:A:699:LEU:HA	1:A:700:LEU:HD13	1.12	1.06
1:B:711:LEU:HD21	1:C:242:ARG:HB2	1.35	1.06
1:C:397:THR:HG21	1:C:442:TYR:HB3	1.33	1.06
1:A:240:ALA:HB3	1:A:243:THR:HG21	1.37	1.05
1:A:701:ASP:H	1:B:158:LYS:HE2	1.14	1.05
1:A:700:LEU:HD21	1:B:156:PRO:HB3	1.40	1.04
1:C:240:ALA:HB3	1:C:243:THR:HG21	1.37	1.04
1:A:154:ILE:HG13	1:A:155:ALA:HA	1.39	1.03
1:A:711:LEU:HD11	1:B:240:ALA:HB3	1.40	1.03
1:C:291:THR:HG23	1:C:293:ASP:H	1.22	1.03
1:A:391:ILE:HG22	1:A:393:THR:HG23	1.41	1.02
1:A:711:LEU:HD21	1:B:240:ALA:HB1	1.42	1.02
1:A:313:SER:HB2	1:A:314:TYR:HA	1.40	1.00
1:B:391:ILE:HG22	1:B:393:THR:HG23	1.41	1.00
1:A:723:ILE:HB	1:C:217:ASN:HB3	1.42	1.00
1:C:391:ILE:HG22	1:C:393:THR:HG23	1.41	1.00
1:C:312:THR:HG23	1:C:314:TYR:HB2	1.44	0.99
1:C:299:PRO:HA	1:C:354:TRP:HE1	1.27	0.99
1:C:286:GLU:HG2	1:C:294:PHE:HD2	1.27	0.99
1:A:707:ARG:HG2	1:B:242:ARG:HG2	1.46	0.98
1:A:209:SER:HB3	1:A:224:HIS:HB3	1.46	0.97
1:C:605:ARG:HD3	1:C:607:GLU:H	1.26	0.96
1:B:688:VAL:HG13	1:C:369:TRP:CH2	2.02	0.95
1:A:298:SER:HB2	1:A:301:TYR:CD1	2.01	0.95
1:A:719:ILE:HG23	1:A:720:ASP:HA	1.48	0.95
1:B:605:ARG:HD3	1:B:607:GLU:H	1.31	0.95
1:C:204:LYS:HB3	1:C:206:VAL:HG22	1.49	0.95
1:C:601:LEU:HD23	1:C:627:ARG:HD3	1.50	0.94
1:A:601:LEU:HD23	1:A:627:ARG:HD3	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:ARG:HD3	1:A:607:GLU:H	1.31	0.94
1:B:601:LEU:HD23	1:B:627:ARG:HD3	1.50	0.93
1:B:700:LEU:CG	1:C:158:LYS:HE3	1.99	0.93
1:A:711:LEU:HD13	1:B:243:THR:HG23	1.51	0.92
1:A:172:GLN:HB2	1:A:183:MET:HB2	1.50	0.92
1:A:699:LEU:HB3	1:A:700:LEU:HD22	1.52	0.91
1:B:708:ARG:HE	1:C:290:ALA:HA	1.34	0.91
1:C:297:MET:HB2	1:C:345:LEU:HD22	1.51	0.91
1:C:299:PRO:HA	1:C:354:TRP:NE1	1.86	0.91
1:A:224:HIS:HB2	1:A:269:VAL:HB	1.53	0.91
1:C:456:LEU:CD2	1:C:461:ALA:HA	2.01	0.91
1:A:298:SER:HB2	1:A:301:TYR:CE1	2.07	0.90
1:B:688:VAL:HG11	1:C:448:PHE:HE2	1.36	0.90
1:A:456:LEU:CD2	1:A:461:ALA:HA	2.01	0.90
1:B:242:ARG:HH12	1:C:284:TYR:HD2	1.20	0.90
1:C:388:SER:HB3	1:C:391:ILE:HB	1.53	0.90
1:B:456:LEU:CD2	1:B:461:ALA:HA	2.01	0.90
1:C:374:GLU:HB2	1:C:428:ARG:HH12	1.37	0.90
1:C:408:ASP:CB	1:C:492:VAL:HG13	2.02	0.90
1:A:408:ASP:CB	1:A:492:VAL:HG13	2.03	0.89
1:C:154:ILE:HG13	1:C:156:PRO:HD3	1.52	0.89
1:B:311:HIS:CE1	1:B:313:SER:HB3	2.08	0.89
1:A:374:GLU:HB2	1:A:428:ARG:HH12	1.37	0.88
1:B:388:SER:HB3	1:B:391:ILE:HB	1.53	0.88
1:B:408:ASP:CB	1:B:492:VAL:HG13	2.02	0.88
1:C:289:LEU:HD22	1:C:290:ALA:H	1.38	0.88
1:A:175:PHE:CD2	1:A:258:ARG:HG3	2.08	0.88
1:A:707:ARG:HG2	1:B:242:ARG:HA	1.54	0.88
1:B:374:GLU:HB2	1:B:428:ARG:HH12	1.37	0.88
1:A:456:LEU:HD21	1:A:461:ALA:HA	1.55	0.88
1:A:388:SER:HB3	1:A:391:ILE:HB	1.53	0.87
1:C:520:MET:HE2	1:C:520:MET:HA	1.56	0.87
1:C:286:GLU:HG2	1:C:294:PHE:CD2	2.09	0.87
1:B:700:LEU:HB3	1:C:279:ARG:NH1	1.90	0.87
1:B:363:VAL:HG21	1:B:409:LEU:HD13	1.57	0.87
1:B:706:GLN:HG3	1:C:699:LEU:CD2	2.03	0.87
1:A:708:ARG:HH11	1:B:244:SER:HB2	1.37	0.87
1:B:456:LEU:HD21	1:B:461:ALA:HA	1.55	0.86
1:C:456:LEU:HD21	1:C:461:ALA:HA	1.55	0.86
1:C:363:VAL:HG13	1:C:364:CYS:CA	2.04	0.86
1:B:520:MET:HE2	1:B:520:MET:HA	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:CYS:HB3	1:B:560:SER:HB2	1.58	0.85
1:A:116:CYS:HB3	1:A:560:SER:HB2	1.58	0.85
1:B:363:VAL:CG2	1:B:409:LEU:HD13	2.06	0.85
1:A:158:LYS:HE3	1:C:700:LEU:HD13	1.58	0.85
1:A:602:VAL:HG21	1:A:623:LEU:HD22	1.59	0.85
1:B:699:LEU:HA	1:C:156:PRO:HB3	1.55	0.85
1:C:116:CYS:HB3	1:C:560:SER:HB2	1.58	0.85
1:C:602:VAL:HG21	1:C:623:LEU:HD22	1.58	0.85
1:A:175:PHE:CZ	1:A:258:ARG:HA	2.11	0.85
1:A:520:MET:HE2	1:A:520:MET:HA	1.57	0.85
1:B:297:MET:HG2	1:B:354:TRP:HH2	1.39	0.84
1:A:699:LEU:CA	1:A:700:LEU:HD13	2.03	0.84
1:B:711:LEU:CD2	1:C:242:ARG:HB2	2.08	0.84
1:B:281:VAL:HG13	1:B:282:TYR:HD1	1.41	0.84
1:C:603:SER:HB3	1:C:612:LEU:HD21	1.58	0.83
1:B:700:LEU:HD21	1:B:704:GLU:CD	2.03	0.83
1:A:708:ARG:NH1	1:B:244:SER:HB2	1.91	0.83
1:A:603:SER:HB3	1:A:612:LEU:HD21	1.58	0.83
1:C:225:ARG:HA	1:C:254:TYR:CD2	2.14	0.83
1:A:328:ARG:NH2	1:A:333:LYS:HD3	1.93	0.83
1:A:397:THR:HG23	1:A:443:LEU:O	1.79	0.83
1:B:603:SER:HB3	1:B:612:LEU:HD21	1.58	0.82
1:B:706:GLN:CG	1:C:699:LEU:HD21	2.06	0.82
1:C:288:VAL:CG1	1:C:292:GLY:HA2	2.09	0.82
1:B:689:TYR:HD2	1:B:694:ILE:HD11	1.44	0.82
1:C:154:ILE:CG1	1:C:155:ALA:HA	2.05	0.82
1:B:602:VAL:HG21	1:B:623:LEU:HD22	1.58	0.82
1:C:328:ARG:NH2	1:C:333:LYS:HD3	1.94	0.82
1:A:699:LEU:HD23	1:A:700:LEU:HD22	1.61	0.82
1:A:616:GLN:CD	1:A:627:ARG:HA	2.05	0.82
1:B:700:LEU:CD1	1:C:158:LYS:HE3	2.10	0.82
1:A:299:PRO:HA	1:A:354:TRP:HE1	1.44	0.81
1:C:286:GLU:HG3	1:C:295:VAL:O	1.80	0.81
1:C:297:MET:HE3	1:C:298:SER:H	1.44	0.81
1:C:298:SER:HB3	1:C:300:PHE:CD2	2.15	0.81
1:A:290:ALA:HB3	1:C:716:PHE:CE2	2.15	0.81
1:B:397:THR:HG23	1:B:443:LEU:O	1.79	0.81
1:C:616:GLN:CD	1:C:627:ARG:HA	2.05	0.81
1:B:688:VAL:HG11	1:C:448:PHE:CE2	2.14	0.81
1:A:714:LEU:HD21	1:C:296:TYR:HB3	1.61	0.81
1:B:699:LEU:HD13	1:C:281:VAL:CG1	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:GLU:OE2	1:C:499:SER:HB2	1.80	0.81
1:A:293:ASP:HA	1:B:713:ASP:OD2	1.81	0.80
1:B:616:GLN:CD	1:B:627:ARG:HA	2.05	0.80
1:B:697:SER:HA	1:C:154:ILE:HG21	1.63	0.80
1:C:159:PHE:CZ	1:C:299:PRO:HG3	2.16	0.80
1:C:397:THR:HG23	1:C:443:LEU:O	1.80	0.80
1:A:700:LEU:HB2	1:B:279:ARG:NH2	1.97	0.80
1:C:616:GLN:OE1	1:C:627:ARG:HA	1.82	0.80
1:A:711:LEU:HD11	1:B:240:ALA:CB	2.11	0.80
1:B:616:GLN:OE1	1:B:627:ARG:HA	1.82	0.80
1:A:616:GLN:OE1	1:A:627:ARG:HA	1.82	0.80
1:B:700:LEU:HD12	1:C:158:LYS:HG2	1.64	0.80
1:A:707:ARG:CG	1:B:242:ARG:HA	2.12	0.79
1:B:305:GLU:HG3	1:B:306:GLY:H	1.45	0.79
1:C:204:LYS:CB	1:C:206:VAL:HG22	2.12	0.79
1:C:286:GLU:CD	1:C:294:PHE:HB3	2.06	0.79
1:C:587:MET:HE1	1:C:598:SER:O	1.83	0.79
1:B:700:LEU:CB	1:C:279:ARG:HG2	2.12	0.79
1:A:279:ARG:NH2	1:C:700:LEU:HD12	1.97	0.79
1:B:601:LEU:HD23	1:B:627:ARG:CD	2.13	0.79
1:A:707:ARG:O	1:B:242:ARG:HB3	1.82	0.78
1:C:601:LEU:HD23	1:C:627:ARG:CD	2.13	0.78
1:B:328:ARG:NH2	1:B:333:LYS:HD3	1.99	0.78
1:A:700:LEU:HG	1:B:158:LYS:CE	2.13	0.78
1:B:687:GLU:OE1	1:B:690:THR:HG22	1.83	0.78
1:A:699:LEU:CB	1:A:700:LEU:HD22	2.13	0.78
1:B:297:MET:HG2	1:B:354:TRP:CH2	2.19	0.78
1:A:699:LEU:HA	1:A:700:LEU:CD1	2.06	0.77
1:A:276:VAL:HG11	1:C:715:ARG:NH1	2.00	0.77
1:A:707:ARG:HG2	1:B:242:ARG:CG	2.14	0.77
1:B:708:ARG:HH21	1:C:290:ALA:HB2	1.49	0.77
1:A:601:LEU:HD23	1:A:627:ARG:CD	2.13	0.77
1:A:719:ILE:HG23	1:A:720:ASP:CA	2.14	0.77
1:B:700:LEU:HD23	1:B:704:GLU:HB3	1.67	0.77
1:C:240:ALA:HB3	1:C:243:THR:CG2	2.15	0.76
1:A:605:ARG:CD	1:A:607:GLU:H	1.99	0.76
1:A:711:LEU:HG	1:B:241:THR:O	1.84	0.76
1:A:543:ARG:HA	1:A:550:ILE:HG12	1.66	0.76
1:A:587:MET:HE1	1:A:598:SER:O	1.85	0.76
1:B:256:PRO:HG3	1:B:265:TYR:C	2.10	0.76
1:B:364:CYS:HB2	1:B:409:LEU:HB3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:ARG:CD	1:B:607:GLU:H	1.99	0.76
1:A:312:THR:HG23	1:A:314:TYR:HB2	1.68	0.76
1:B:209:SER:HB2	1:B:224:HIS:HB3	1.67	0.76
1:B:688:VAL:HG13	1:C:369:TRP:CZ2	2.21	0.76
1:C:253:LYS:HA	1:C:268:THR:HG21	1.65	0.76
1:B:543:ARG:HA	1:B:550:ILE:HG12	1.66	0.76
1:A:499:SER:HB2	1:B:687:GLU:OE2	1.85	0.76
1:B:587:MET:HE1	1:B:598:SER:O	1.84	0.76
1:A:699:LEU:CG	1:A:700:LEU:HD22	2.16	0.76
1:B:708:ARG:NH1	1:C:277:ASP:HB2	2.01	0.76
1:A:425:PHE:CE2	1:A:430:ASN:HA	2.22	0.75
1:A:713:ASP:HB2	1:C:294:PHE:CD1	2.21	0.75
1:C:690:THR:OG1	1:C:693:GLU:HG3	1.85	0.75
1:A:240:ALA:HB3	1:A:243:THR:CG2	2.16	0.75
1:A:256:PRO:HG3	1:A:265:TYR:C	2.12	0.75
1:B:299:PRO:CA	1:B:354:TRP:HE1	2.00	0.75
1:B:551:ALA:O	1:B:555:VAL:HG22	1.87	0.75
1:C:296:TYR:HD1	1:C:296:TYR:H	1.34	0.75
1:A:233:GLU:O	1:A:249:THR:HG22	1.87	0.75
1:C:425:PHE:CE2	1:C:430:ASN:HA	2.22	0.75
1:C:551:ALA:O	1:C:555:VAL:HG22	1.87	0.75
1:B:217:ASN:CG	1:C:723:ILE:HG22	2.12	0.75
1:A:158:LYS:NZ	1:C:700:LEU:HD22	2.03	0.74
1:A:707:ARG:NE	1:B:242:ARG:HA	2.02	0.74
1:A:175:PHE:CE2	1:A:258:ARG:HA	2.21	0.74
1:A:551:ALA:O	1:A:555:VAL:HG22	1.87	0.74
1:A:614:GLU:HG3	1:A:627:ARG:NH2	2.03	0.74
1:C:614:GLU:HG3	1:C:627:ARG:NH2	2.03	0.74
1:C:314:TYR:HB3	1:C:315:ALA:O	1.88	0.74
1:C:543:ARG:HA	1:C:550:ILE:HG12	1.66	0.74
1:B:700:LEU:HB2	1:C:279:ARG:CG	2.16	0.73
1:C:163:MET:HG3	1:C:276:VAL:HG21	1.67	0.73
1:C:695:LYS:NZ	1:C:702:TYR:HB3	2.01	0.73
1:A:700:LEU:HD11	1:B:156:PRO:HG3	1.70	0.73
1:A:242:ARG:O	1:C:711:LEU:HD21	1.87	0.73
1:A:700:LEU:CD2	1:B:156:PRO:HB3	2.18	0.73
1:B:425:PHE:CE2	1:B:430:ASN:HA	2.22	0.73
1:B:614:GLU:HG3	1:B:627:ARG:NH2	2.03	0.73
1:B:707:ARG:HH21	1:C:242:ARG:HG2	1.53	0.73
1:A:154:ILE:CG1	1:A:155:ALA:HA	2.18	0.73
1:A:312:THR:HG23	1:A:314:TYR:CB	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:SER:HB2	1:A:314:TYR:HD1	1.53	0.73
1:C:289:LEU:HD22	1:C:290:ALA:N	2.03	0.73
1:C:286:GLU:CG	1:C:294:PHE:HB3	2.19	0.73
1:A:531:LEU:O	1:A:535:GLU:HG2	1.89	0.73
1:B:531:LEU:O	1:B:535:GLU:HG2	1.89	0.73
1:B:587:MET:HE2	1:B:597:TYR:O	1.89	0.73
1:B:719:ILE:HB	1:B:720:ASP:O	1.87	0.73
1:A:587:MET:HE2	1:A:597:TYR:O	1.90	0.72
1:A:597:TYR:HD1	1:A:599:ARG:H	1.36	0.72
1:B:157:TYR:CE2	1:B:300:PHE:HE1	2.07	0.72
1:C:531:LEU:O	1:C:535:GLU:HG2	1.89	0.72
1:A:289:LEU:HD22	1:A:290:ALA:H	1.54	0.72
1:A:690:THR:OG1	1:A:693:GLU:HG3	1.89	0.72
1:B:605:ARG:NH1	1:B:610:GLY:H	1.88	0.72
1:C:605:ARG:CD	1:C:607:GLU:H	1.99	0.72
1:A:312:THR:CG2	1:A:314:TYR:HB2	2.20	0.72
1:A:605:ARG:NH1	1:A:610:GLY:H	1.87	0.72
1:C:520:MET:HE2	1:C:520:MET:CA	2.19	0.72
1:A:206:VAL:HG12	1:A:233:GLU:OE2	1.90	0.72
1:B:520:MET:HE2	1:B:520:MET:CA	2.19	0.71
1:B:689:TYR:CD2	1:B:694:ILE:HD11	2.24	0.71
1:C:297:MET:CE	1:C:298:SER:H	2.03	0.71
1:C:587:MET:HE2	1:C:597:TYR:O	1.89	0.71
1:A:290:ALA:HB3	1:C:716:PHE:HE2	1.53	0.71
1:C:605:ARG:NH1	1:C:610:GLY:H	1.88	0.71
1:A:297:MET:HG2	1:A:345:LEU:HD22	1.71	0.71
1:A:699:LEU:CD2	1:A:700:LEU:HD22	2.20	0.71
1:B:601:LEU:CD2	1:B:627:ARG:HD3	2.20	0.71
1:B:294:PHE:CZ	1:C:710:GLN:HB3	2.25	0.71
1:B:597:TYR:HD1	1:B:599:ARG:H	1.36	0.71
1:B:193:PRO:O	1:B:197:VAL:HG23	1.91	0.71
1:B:698:GLY:O	1:C:156:PRO:HG3	1.91	0.71
1:C:597:TYR:HD1	1:C:599:ARG:H	1.36	0.71
1:A:520:MET:HE2	1:A:520:MET:CA	2.19	0.71
1:B:172:GLN:HB2	1:B:183:MET:HB2	1.71	0.71
1:B:719:ILE:HB	1:B:720:ASP:C	2.16	0.71
1:C:360:ARG:HB2	1:C:361:PRO:HD3	1.73	0.71
1:A:193:PRO:O	1:A:197:VAL:HG23	1.91	0.70
1:B:175:PHE:CZ	1:B:258:ARG:HA	2.26	0.70
1:A:638:ARG:HG3	1:A:649:TYR:HE1	1.56	0.70
1:A:689:TYR:CD2	1:A:694:ILE:HD11	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:VAL:CG1	1:C:364:CYS:HA	2.19	0.70
1:B:674:ASN:O	1:C:523:ARG:HD2	1.90	0.70
1:A:290:ALA:HB2	1:C:715:ARG:NH2	2.06	0.70
1:A:546:ASN:O	1:A:550:ILE:HD13	1.92	0.70
1:A:674:ASN:O	1:B:523:ARG:HD2	1.90	0.70
1:B:638:ARG:HG3	1:B:649:TYR:HE1	1.56	0.70
1:A:217:ASN:ND2	1:B:723:ILE:H	1.89	0.70
1:B:360:ARG:HB2	1:B:361:PRO:HD3	1.74	0.70
1:A:523:ARG:HD2	1:C:674:ASN:O	1.90	0.70
1:A:707:ARG:HG2	1:B:242:ARG:CA	2.22	0.70
1:B:700:LEU:HB3	1:C:279:ARG:CZ	2.21	0.70
1:B:708:ARG:NH2	1:C:290:ALA:HB2	2.05	0.70
1:B:285:ASP:HA	1:B:298:SER:HB2	1.74	0.70
1:C:546:ASN:O	1:C:550:ILE:HD13	1.92	0.70
1:B:546:ASN:O	1:B:550:ILE:HD13	1.92	0.69
1:C:150:PHE:HB3	1:C:366:MET:HE3	1.74	0.69
1:A:601:LEU:CD2	1:A:627:ARG:HD3	2.20	0.69
1:B:613:VAL:HG12	1:B:614:GLU:O	1.93	0.69
1:C:193:PRO:O	1:C:197:VAL:HG23	1.91	0.69
1:C:156:PRO:HG2	1:C:158:LYS:NZ	2.07	0.69
1:C:601:LEU:CD2	1:C:627:ARG:HD3	2.20	0.69
1:C:638:ARG:HG3	1:C:649:TYR:HE1	1.56	0.69
1:C:329:ASP:HB3	1:C:332:THR:OG1	1.93	0.69
1:A:550:ILE:O	1:A:553:VAL:HG12	1.93	0.69
1:A:329:ASP:HB3	1:A:332:THR:OG1	1.93	0.69
1:C:613:VAL:HG12	1:C:614:GLU:O	1.93	0.69
1:A:613:VAL:HG12	1:A:614:GLU:O	1.92	0.69
1:A:711:LEU:CD1	1:B:243:THR:HG23	2.20	0.69
1:A:715:ARG:HD2	1:B:243:THR:CG2	2.22	0.69
1:C:161:ALA:HB3	1:C:276:VAL:HB	1.75	0.69
1:C:228:HIS:O	1:C:230:THR:HG23	1.93	0.69
1:B:550:ILE:O	1:B:553:VAL:HG12	1.93	0.69
1:C:163:MET:HG3	1:C:276:VAL:CG2	2.22	0.69
1:A:207:CYS:O	1:A:231:ASP:HB2	1.92	0.68
1:A:301:TYR:HD1	1:A:301:TYR:H	1.41	0.68
1:A:723:ILE:CB	1:C:217:ASN:HB3	2.20	0.68
1:B:388:SER:OG	1:B:391:ILE:HG13	1.93	0.68
1:C:550:ILE:O	1:C:553:VAL:HG12	1.93	0.68
1:B:364:CYS:CB	1:B:409:LEU:HB3	2.22	0.68
1:A:289:LEU:HD22	1:A:290:ALA:N	2.09	0.68
1:A:699:LEU:HD23	1:A:700:LEU:CD2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ASP:HB3	1:B:332:THR:OG1	1.93	0.68
1:A:276:VAL:HG11	1:C:715:ARG:CZ	2.24	0.68
1:A:406:ARG:O	1:A:492:VAL:HA	1.93	0.68
1:A:605:ARG:NH2	1:A:611:PRO:HD2	2.09	0.68
1:B:711:LEU:HD21	1:C:242:ARG:CB	2.19	0.68
1:B:281:VAL:HG13	1:B:282:TYR:CD1	2.26	0.68
1:B:605:ARG:NH2	1:B:611:PRO:HD2	2.09	0.68
1:C:603:SER:CB	1:C:612:LEU:HD21	2.24	0.68
1:A:555:VAL:HG23	1:A:557:ARG:H	1.59	0.67
1:B:145:GLY:HA3	1:B:452:TYR:CZ	2.29	0.67
1:C:145:GLY:HA3	1:C:452:TYR:CZ	2.30	0.67
1:C:388:SER:OG	1:C:391:ILE:HG13	1.93	0.67
1:A:194:PHE:O	1:A:198:ILE:HD13	1.95	0.67
1:A:299:PRO:CA	1:A:354:TRP:HE1	2.07	0.67
1:C:297:MET:HE3	1:C:298:SER:N	2.09	0.67
1:B:699:LEU:CA	1:C:156:PRO:HB3	2.25	0.67
1:A:289:LEU:HD13	1:A:290:ALA:N	2.08	0.67
1:A:360:ARG:HB2	1:A:361:PRO:HD3	1.75	0.67
1:A:388:SER:OG	1:A:391:ILE:HG13	1.93	0.67
1:A:603:SER:CB	1:A:612:LEU:HD21	2.25	0.67
1:B:538:LEU:HD21	1:C:539:TRP:CD2	2.30	0.67
1:C:605:ARG:HD2	1:C:607:GLU:O	1.95	0.67
1:A:145:GLY:HA3	1:A:452:TYR:CZ	2.29	0.67
1:A:172:GLN:CB	1:A:183:MET:HB2	2.24	0.67
1:B:603:SER:CB	1:B:612:LEU:HD21	2.24	0.67
1:A:538:LEU:HD21	1:B:539:TRP:CD2	2.30	0.67
1:A:699:LEU:HD12	1:A:699:LEU:H	1.59	0.67
1:B:555:VAL:HG23	1:B:557:ARG:H	1.60	0.67
1:B:700:LEU:H	1:C:279:ARG:CZ	2.06	0.67
1:A:289:LEU:HD13	1:A:290:ALA:H	1.59	0.67
1:C:143:THR:HG22	1:C:144:GLU:O	1.95	0.67
1:C:194:PHE:O	1:C:198:ILE:HD13	1.94	0.67
1:A:701:ASP:H	1:B:158:LYS:CE	2.02	0.66
1:B:700:LEU:CD2	1:B:704:GLU:HB3	2.25	0.66
1:B:143:THR:HG22	1:B:144:GLU:O	1.95	0.66
1:A:539:TRP:CD2	1:C:538:LEU:HD21	2.30	0.66
1:A:707:ARG:CD	1:B:242:ARG:HA	2.24	0.66
1:C:406:ARG:O	1:C:492:VAL:HA	1.94	0.66
1:C:555:VAL:HG23	1:C:557:ARG:H	1.60	0.66
1:A:156:PRO:HG2	1:C:700:LEU:HG	1.76	0.66
1:B:194:PHE:O	1:B:198:ILE:HD13	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:SER:HB2	1:C:687:GLU:OE2	1.95	0.66
1:B:204:LYS:CB	1:B:206:VAL:HG22	2.26	0.66
1:B:224:HIS:HB2	1:B:269:VAL:HB	1.78	0.66
1:C:425:PHE:CE1	1:C:429:TYR:HB3	2.31	0.66
1:B:425:PHE:CE1	1:B:429:TYR:HB3	2.31	0.66
1:B:700:LEU:HD12	1:C:158:LYS:CG	2.25	0.66
1:B:106:ALA:HA	1:B:643:PHE:CE2	2.31	0.66
1:B:297:MET:HB2	1:B:345:LEU:HD22	1.78	0.66
1:B:699:LEU:HB3	1:C:156:PRO:HB3	1.78	0.66
1:B:707:ARG:NH2	1:C:242:ARG:HG2	2.11	0.66
1:C:172:GLN:HB2	1:C:183:MET:HB2	1.78	0.66
1:A:313:SER:CB	1:A:314:TYR:HA	2.14	0.65
1:A:711:LEU:HB2	1:B:242:ARG:O	1.96	0.65
1:B:294:PHE:HZ	1:C:710:GLN:HB3	1.59	0.65
1:A:425:PHE:CE1	1:A:429:TYR:HB3	2.31	0.65
1:A:700:LEU:HB2	1:B:279:ARG:CZ	2.26	0.65
1:A:700:LEU:CG	1:B:158:LYS:HE3	2.16	0.65
1:A:290:ALA:HB2	1:C:715:ARG:CZ	2.26	0.65
1:B:406:ARG:O	1:B:492:VAL:HA	1.95	0.65
1:A:714:LEU:HG	1:C:286:GLU:OE1	1.97	0.65
1:B:700:LEU:HG	1:C:158:LYS:CE	2.22	0.65
1:C:605:ARG:NH2	1:C:611:PRO:HD2	2.12	0.65
1:C:291:THR:HG23	1:C:293:ASP:N	2.03	0.65
1:A:707:ARG:NH1	1:B:243:THR:H	1.95	0.65
1:C:254:TYR:HB2	1:C:268:THR:HG23	1.79	0.65
1:A:106:ALA:HA	1:A:643:PHE:CE2	2.33	0.64
1:A:143:THR:HG22	1:A:144:GLU:O	1.95	0.64
1:B:700:LEU:CD1	1:C:158:LYS:HB3	2.27	0.64
1:A:151:LYS:HD2	1:C:688:VAL:CG1	2.27	0.64
1:A:658:GLN:C	1:A:659:LEU:HD12	2.23	0.64
1:A:321:GLN:HE21	1:A:341:THR:HG21	1.62	0.64
1:B:321:GLN:HE21	1:B:341:THR:HG21	1.62	0.64
1:A:707:ARG:CG	1:B:242:ARG:HG2	2.24	0.64
1:A:713:ASP:OD2	1:C:293:ASP:HA	1.96	0.64
1:B:658:GLN:C	1:B:659:LEU:HD12	2.23	0.64
1:C:106:ALA:HA	1:C:643:PHE:CE2	2.31	0.64
1:C:189:ARG:HH11	1:C:349:LYS:HD3	1.63	0.64
1:A:605:ARG:HD2	1:A:607:GLU:O	1.98	0.64
1:A:659:LEU:HD12	1:A:659:LEU:N	2.13	0.64
1:B:699:LEU:HB3	1:C:156:PRO:HA	1.79	0.64
1:C:701:ASP:O	1:C:705:VAL:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:VAL:HB	1:A:282:TYR:CD2	2.33	0.64
1:A:699:LEU:HB2	1:C:702:TYR:HE2	1.62	0.64
1:B:289:LEU:HB2	1:B:292:GLY:H	1.63	0.64
1:B:605:ARG:HD2	1:B:607:GLU:O	1.98	0.64
1:C:321:GLN:HE21	1:C:341:THR:HG21	1.62	0.64
1:A:158:LYS:HZ1	1:C:700:LEU:HD22	1.63	0.63
1:A:715:ARG:HD2	1:B:243:THR:HG23	1.79	0.63
1:B:189:ARG:HH11	1:B:349:LYS:HD3	1.63	0.63
1:B:321:GLN:NE2	1:B:341:THR:HG21	2.13	0.63
1:B:540:ASN:O	1:B:543:ARG:HG2	1.98	0.63
1:C:256:PRO:HG3	1:C:265:TYR:C	2.23	0.63
1:C:695:LYS:HZ1	1:C:702:TYR:HB3	1.61	0.63
1:A:106:ALA:HA	1:A:643:PHE:HE2	1.62	0.63
1:A:189:ARG:HH11	1:A:349:LYS:HD3	1.63	0.63
1:A:364:CYS:HB2	1:A:409:LEU:HB3	1.79	0.63
1:A:707:ARG:HG2	1:B:242:ARG:CB	2.29	0.63
1:B:156:PRO:HG2	1:B:158:LYS:HZ2	1.63	0.63
1:B:157:TYR:CZ	1:B:300:PHE:HE1	2.17	0.63
1:C:321:GLN:NE2	1:C:341:THR:HG21	2.13	0.63
1:A:540:ASN:O	1:A:543:ARG:HG2	1.98	0.63
1:A:673:LEU:HG	1:A:675:ILE:HG12	1.81	0.63
1:A:714:LEU:HG	1:C:286:GLU:CD	2.23	0.63
1:B:659:LEU:HD12	1:B:659:LEU:N	2.13	0.63
1:B:706:GLN:O	1:B:710:GLN:HG3	1.97	0.63
1:C:540:ASN:O	1:C:543:ARG:HG2	1.98	0.63
1:A:290:ALA:N	1:C:708:ARG:HH21	1.97	0.63
1:A:321:GLN:NE2	1:A:341:THR:HG21	2.13	0.63
1:A:408:ASP:HB2	1:A:492:VAL:CG1	2.13	0.63
1:B:699:LEU:HD12	1:B:699:LEU:H	1.63	0.63
1:C:658:GLN:C	1:C:659:LEU:HD12	2.23	0.63
1:B:225:ARG:HG3	1:B:254:TYR:CE2	2.34	0.62
1:B:311:HIS:HE1	1:B:313:SER:HB3	1.58	0.62
1:A:706:GLN:HA	1:A:706:GLN:OE1	1.99	0.62
1:B:401:GLU:HB2	1:B:476:PRO:HD3	1.81	0.62
1:B:589:ILE:HD11	1:B:630:ILE:HD13	1.82	0.62
1:B:699:LEU:HD22	1:C:281:VAL:O	2.00	0.62
1:C:154:ILE:CG1	1:C:156:PRO:HD3	2.26	0.62
1:C:442:TYR:O	1:C:449:LEU:HD12	1.99	0.62
1:A:401:GLU:HB2	1:A:476:PRO:HD3	1.81	0.62
1:A:591:SER:O	1:A:593:PRO:HD3	1.99	0.62
1:B:442:TYR:O	1:B:449:LEU:HD12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:GLU:HB2	1:C:476:PRO:HD3	1.81	0.62
1:C:572:THR:HG22	1:C:573:CYS:N	2.14	0.62
1:C:659:LEU:HD12	1:C:659:LEU:N	2.13	0.62
1:A:589:ILE:HD11	1:A:630:ILE:HD13	1.82	0.62
1:A:699:LEU:HD12	1:A:699:LEU:N	2.14	0.62
1:A:208:ARG:HA	1:A:231:ASP:HB3	1.82	0.62
1:A:224:HIS:CE1	1:A:225:ARG:HB2	2.35	0.62
1:C:288:VAL:HG11	1:C:292:GLY:HA2	1.80	0.62
1:C:591:SER:O	1:C:593:PRO:HD3	1.99	0.62
1:A:572:THR:HG22	1:A:573:CYS:N	2.14	0.61
1:A:124:VAL:HG13	1:A:568:MET:O	2.01	0.61
1:B:438:GLN:HB3	1:B:439:PRO:HD2	1.82	0.61
1:B:343:ASN:C	1:B:344:LEU:HD12	2.25	0.61
1:B:363:VAL:HG21	1:B:409:LEU:CD1	2.28	0.61
1:B:456:LEU:HD23	1:B:457:SER:O	2.01	0.61
1:B:605:ARG:HG3	1:B:611:PRO:O	2.00	0.61
1:C:673:LEU:HG	1:C:675:ILE:HG12	1.81	0.61
1:A:204:LYS:CB	1:A:206:VAL:HG22	2.31	0.61
1:A:297:MET:CE	1:A:319:PHE:HB2	2.30	0.61
1:B:572:THR:HG22	1:B:573:CYS:N	2.14	0.61
1:B:591:SER:O	1:B:593:PRO:HD3	1.99	0.61
1:B:673:LEU:HG	1:B:675:ILE:HG12	1.81	0.61
1:A:674:ASN:HB3	1:B:523:ARG:HH11	1.65	0.61
1:B:150:PHE:HB3	1:B:366:MET:HE3	1.82	0.61
1:B:189:ARG:NH1	1:B:349:LYS:HD3	2.16	0.61
1:C:614:GLU:HG3	1:C:627:ARG:CZ	2.31	0.61
1:A:442:TYR:O	1:A:449:LEU:HD12	1.99	0.61
1:A:605:ARG:HG3	1:A:611:PRO:O	2.00	0.61
1:A:713:ASP:OD2	1:C:294:PHE:HD1	1.83	0.61
1:A:722:VAL:HA	1:C:217:ASN:ND2	2.16	0.61
1:C:124:VAL:HG13	1:C:568:MET:O	2.01	0.61
1:C:589:ILE:HD11	1:C:630:ILE:HD13	1.82	0.61
1:A:282:TYR:HB2	1:A:283:PRO:HD2	1.83	0.61
1:A:523:ARG:HH11	1:C:674:ASN:HB3	1.65	0.61
1:B:305:GLU:HG3	1:B:306:GLY:N	2.16	0.61
1:B:563:MET:HE1	1:B:566:ASP:O	2.00	0.61
1:C:289:LEU:CD2	1:C:290:ALA:H	2.12	0.61
1:C:343:ASN:C	1:C:344:LEU:HD12	2.25	0.61
1:A:305:GLU:OE1	1:A:359:LYS:HE3	2.01	0.61
1:A:563:MET:HE1	1:A:566:ASP:O	2.00	0.61
1:B:705:VAL:HG23	1:C:279:ARG:HH12	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:GLN:HB3	1:C:439:PRO:HD2	1.83	0.61
1:A:343:ASN:C	1:A:344:LEU:HD12	2.25	0.61
1:B:163:MET:SD	1:B:289:LEU:HD13	2.40	0.61
1:C:563:MET:HE1	1:C:566:ASP:O	2.00	0.61
1:A:260:GLU:O	1:A:262:PHE:HD1	1.83	0.60
1:B:124:VAL:HG13	1:B:568:MET:O	2.01	0.60
1:B:344:LEU:HD12	1:B:344:LEU:N	2.16	0.60
1:C:189:ARG:NH1	1:C:349:LYS:HD3	2.16	0.60
1:C:664:ILE:HG22	1:C:665:THR:O	2.02	0.60
1:A:397:THR:HG22	1:A:398:ASN:N	2.16	0.60
1:A:438:GLN:HB3	1:A:439:PRO:HD2	1.83	0.60
1:C:156:PRO:HG2	1:C:158:LYS:HZ2	1.64	0.60
1:C:344:LEU:HD12	1:C:344:LEU:N	2.16	0.60
1:B:106:ALA:HA	1:B:643:PHE:HE2	1.66	0.60
1:C:106:ALA:HA	1:C:643:PHE:HE2	1.66	0.60
1:C:291:THR:HG21	1:C:293:ASP:HB2	1.82	0.60
1:A:288:VAL:HG12	1:A:289:LEU:O	2.01	0.60
1:B:674:ASN:HB3	1:C:523:ARG:HH11	1.65	0.60
1:C:605:ARG:HG3	1:C:611:PRO:O	2.01	0.60
1:A:456:LEU:HD23	1:A:457:SER:O	2.01	0.60
1:B:204:LYS:HB2	1:B:206:VAL:HG22	1.83	0.60
1:C:368:LYS:O	1:C:368:LYS:HG2	2.01	0.60
1:A:711:LEU:CD2	1:A:714:LEU:HB2	2.32	0.60
1:B:397:THR:HG22	1:B:398:ASN:N	2.17	0.60
1:A:614:GLU:HG3	1:A:627:ARG:CZ	2.31	0.60
1:B:299:PRO:HA	1:B:354:TRP:HE1	1.66	0.60
1:B:614:GLU:HG3	1:B:627:ARG:CZ	2.31	0.60
1:B:688:VAL:HG13	1:C:369:TRP:CZ3	2.37	0.60
1:B:711:LEU:HD11	1:C:242:ARG:HB3	1.84	0.59
1:A:156:PRO:HD2	1:C:700:LEU:CD2	2.31	0.59
1:A:312:THR:HG23	1:A:314:TYR:CG	2.37	0.59
1:B:189:ARG:HD3	1:B:349:LYS:CE	2.33	0.59
1:B:688:VAL:CG1	1:C:448:PHE:HE2	2.12	0.59
1:C:208:ARG:HG2	1:C:210:THR:H	1.66	0.59
1:C:456:LEU:HD23	1:C:457:SER:O	2.01	0.59
1:B:297:MET:O	1:B:298:SER:HB2	2.03	0.59
1:B:502:GLU:HG2	1:C:502:GLU:HG2	1.84	0.59
1:C:115:VAL:HG22	1:C:623:LEU:HB2	1.85	0.59
1:C:189:ARG:HD3	1:C:349:LYS:CE	2.33	0.59
1:A:189:ARG:NH1	1:A:349:LYS:HD3	2.16	0.59
1:B:281:VAL:CG1	1:B:282:TYR:HD1	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:ILE:HG22	1:B:665:THR:O	2.02	0.59
1:A:502:GLU:HG2	1:C:502:GLU:HG2	1.84	0.59
1:A:603:SER:HB3	1:A:612:LEU:CD2	2.33	0.59
1:A:722:VAL:HA	1:C:217:ASN:HD22	1.67	0.59
1:B:706:GLN:HE21	1:C:699:LEU:HD21	1.66	0.59
1:B:129:GLN:HB3	1:B:130:PRO:HD2	1.85	0.59
1:B:280:SER:HB2	1:B:287:PHE:HB3	1.83	0.59
1:B:715:ARG:HG3	1:C:243:THR:HG22	1.85	0.59
1:C:129:GLN:HB3	1:C:130:PRO:HD2	1.85	0.59
1:A:154:ILE:HG13	1:A:155:ALA:CA	2.25	0.59
1:A:502:GLU:HG2	1:B:502:GLU:HG2	1.84	0.59
1:C:224:HIS:HE1	1:C:268:THR:HG22	1.67	0.59
1:A:115:VAL:HG22	1:A:623:LEU:HB2	1.85	0.58
1:A:275:GLU:C	1:A:276:VAL:HG23	2.28	0.58
1:A:289:LEU:CD2	1:A:290:ALA:H	2.15	0.58
1:A:664:ILE:HG22	1:A:665:THR:O	2.02	0.58
1:A:714:LEU:HG	1:C:286:GLU:OE2	2.01	0.58
1:B:688:VAL:HA	1:C:369:TRP:CE2	2.37	0.58
1:C:701:ASP:HB2	1:C:704:GLU:CB	2.33	0.58
1:A:148:VAL:HG13	1:A:370:GLN:O	2.04	0.58
1:A:344:LEU:HD12	1:A:344:LEU:N	2.16	0.58
1:C:288:VAL:HG12	1:C:289:LEU:N	2.18	0.58
1:C:316:ALA:HB3	1:C:317:ASP:HA	1.85	0.58
1:A:129:GLN:HB3	1:A:130:PRO:HD2	1.84	0.58
1:A:189:ARG:HD3	1:A:349:LYS:CE	2.33	0.58
1:C:200:LYS:HE3	1:C:208:ARG:HH21	1.69	0.58
1:A:290:ALA:HB2	1:C:715:ARG:NH1	2.18	0.58
1:A:696:ASP:HA	1:A:701:ASP:OD1	2.04	0.58
1:A:701:ASP:N	1:B:158:LYS:HE2	2.00	0.58
1:A:719:ILE:HG23	1:A:720:ASP:N	2.18	0.58
1:A:711:LEU:HD23	1:A:714:LEU:HB2	1.85	0.58
1:A:232:MET:O	1:A:233:GLU:HG2	2.03	0.58
1:B:163:MET:SD	1:B:276:VAL:HG21	2.44	0.58
1:B:699:LEU:CB	1:C:156:PRO:HB3	2.33	0.58
1:C:189:ARG:HD3	1:C:349:LYS:HD3	1.86	0.58
1:B:276:VAL:HG13	1:B:290:ALA:HB3	1.86	0.58
1:B:695:LYS:HE3	1:B:703:THR:OG1	2.03	0.58
1:B:147:ALA:HA	1:B:451:ALA:O	2.04	0.58
1:B:326:TYR:CZ	1:B:339:PRO:HG3	2.39	0.58
1:C:300:PHE:HB3	1:C:359:LYS:HB2	1.85	0.58
1:C:397:THR:HG22	1:C:398:ASN:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:VAL:HG13	1:B:370:GLN:O	2.03	0.57
1:C:638:ARG:HG3	1:C:649:TYR:CE1	2.39	0.57
1:A:147:ALA:HA	1:A:451:ALA:O	2.04	0.57
1:A:207:CYS:HB2	1:A:234:LEU:CD1	2.34	0.57
1:B:701:ASP:OD1	1:B:704:GLU:HB2	2.04	0.57
1:C:148:VAL:HG13	1:C:370:GLN:O	2.04	0.57
1:A:189:ARG:HD3	1:A:349:LYS:HD3	1.86	0.57
1:A:221:THR:HG22	1:A:222:ALA:N	2.19	0.57
1:A:326:TYR:CZ	1:A:339:PRO:HG3	2.39	0.57
1:B:115:VAL:HG22	1:B:623:LEU:HB2	1.85	0.57
1:B:711:LEU:HD13	1:C:242:ARG:O	2.03	0.57
1:A:638:ARG:HG3	1:A:649:TYR:CE1	2.39	0.57
1:A:700:LEU:HD11	1:B:156:PRO:CG	2.35	0.57
1:B:189:ARG:HD3	1:B:349:LYS:HD3	1.86	0.57
1:B:302:GLY:O	1:B:305:GLU:HB2	2.05	0.57
1:B:288:VAL:CG1	1:B:292:GLY:HA2	2.34	0.57
1:C:147:ALA:HA	1:C:451:ALA:O	2.05	0.57
1:C:221:THR:HG22	1:C:222:ALA:N	2.19	0.57
1:A:108:ASN:HB2	1:A:645:GLY:H	1.69	0.57
1:A:711:LEU:HD12	1:B:242:ARG:O	2.04	0.57
1:A:151:LYS:HD2	1:C:688:VAL:HG13	1.86	0.57
1:A:297:MET:HE3	1:A:319:PHE:HB2	1.86	0.57
1:A:368:LYS:O	1:A:368:LYS:HG2	2.05	0.57
1:C:108:ASN:HB2	1:C:645:GLY:H	1.70	0.57
1:A:706:GLN:O	1:A:710:GLN:HG3	2.05	0.57
1:A:723:ILE:HB	1:C:217:ASN:CB	2.25	0.57
1:B:221:THR:HG22	1:B:222:ALA:N	2.19	0.57
1:C:326:TYR:CZ	1:C:339:PRO:HG3	2.39	0.57
1:A:150:PHE:HB3	1:A:366:MET:HE3	1.87	0.56
1:A:391:ILE:CG2	1:A:393:THR:HG23	2.27	0.56
1:B:287:PHE:HE1	1:B:297:MET:HB3	1.69	0.56
1:C:605:ARG:NH1	1:C:607:GLU:HB3	2.20	0.56
1:A:209:SER:O	1:A:269:VAL:HG11	2.05	0.56
1:B:391:ILE:CG2	1:B:393:THR:HG23	2.27	0.56
1:A:708:ARG:HD2	1:B:244:SER:OG	2.06	0.56
1:A:711:LEU:CD1	1:B:240:ALA:HB3	2.23	0.56
1:B:276:VAL:HG12	1:B:277:ASP:N	2.20	0.56
1:B:281:VAL:HG13	1:B:282:TYR:N	2.20	0.56
1:B:286:GLU:HG2	1:B:296:TYR:CE2	2.41	0.56
1:B:347:THR:HB	1:B:348:PRO:HD2	1.87	0.56
1:B:638:ARG:HG3	1:B:649:TYR:CE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:701:ASP:CG	1:B:704:GLU:HB2	2.30	0.56
1:A:572:THR:HG22	1:A:573:CYS:H	1.71	0.56
1:A:289:LEU:CD1	1:A:290:ALA:H	2.18	0.56
1:A:400:THR:HG22	1:A:401:GLU:N	2.20	0.56
1:A:541:GLU:O	1:A:544:LYS:HB3	2.06	0.56
1:B:108:ASN:HB2	1:B:645:GLY:CA	2.35	0.56
1:A:699:LEU:HD13	1:C:702:TYR:CE2	2.40	0.56
1:B:400:THR:HG22	1:B:401:GLU:N	2.20	0.56
1:B:541:GLU:O	1:B:544:LYS:HB3	2.06	0.56
1:A:291:THR:HG23	1:C:712:HIS:HE1	1.71	0.56
1:B:715:ARG:CG	1:C:243:THR:HG22	2.35	0.56
1:C:541:GLU:O	1:C:544:LYS:HB3	2.06	0.56
1:A:291:THR:HB	1:A:293:ASP:H	1.70	0.56
1:B:108:ASN:HB2	1:B:645:GLY:H	1.70	0.56
1:B:288:VAL:HG12	1:B:289:LEU:N	2.21	0.56
1:C:696:ASP:HA	1:C:701:ASP:OD1	2.05	0.56
1:A:290:ALA:CB	1:C:716:PHE:HE2	2.19	0.56
1:C:347:THR:HB	1:C:348:PRO:HD2	1.87	0.56
1:A:347:THR:HB	1:A:348:PRO:HD2	1.87	0.55
1:B:108:ASN:HB2	1:B:645:GLY:N	2.21	0.55
1:C:108:ASN:HB2	1:C:645:GLY:CA	2.35	0.55
1:C:108:ASN:HB2	1:C:645:GLY:N	2.21	0.55
1:C:400:THR:HG22	1:C:401:GLU:N	2.20	0.55
1:A:108:ASN:HB2	1:A:645:GLY:N	2.21	0.55
1:A:360:ARG:CB	1:A:361:PRO:HD3	2.36	0.55
1:A:582:ILE:HG22	1:A:583:VAL:N	2.21	0.55
1:B:605:ARG:NH1	1:B:607:GLU:HB3	2.21	0.55
1:B:607:GLU:HG2	1:B:608:ASP:N	2.22	0.55
1:A:605:ARG:NH1	1:A:607:GLU:HB3	2.21	0.55
1:B:283:PRO:HA	1:B:300:PHE:CD2	2.41	0.55
1:C:420:ALA:O	1:C:424:ILE:HG13	2.06	0.55
1:B:224:HIS:C	1:B:226:ASP:H	2.15	0.55
1:B:572:THR:HG22	1:B:573:CYS:H	1.71	0.55
1:C:192:VAL:HG13	1:C:193:PRO:HD2	1.88	0.55
1:C:543:ARG:CA	1:C:550:ILE:HG12	2.36	0.55
1:C:601:LEU:HD23	1:C:627:ARG:NE	2.22	0.55
1:A:204:LYS:HB3	1:A:206:VAL:HG22	1.86	0.55
1:B:420:ALA:O	1:B:424:ILE:HG13	2.06	0.55
1:B:719:ILE:N	1:B:720:ASP:HA	2.21	0.55
1:C:175:PHE:HD2	1:C:258:ARG:HH11	1.53	0.55
1:C:360:ARG:CB	1:C:361:PRO:HD3	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:HB2	1:A:645:GLY:CA	2.37	0.55
1:A:420:ALA:O	1:A:424:ILE:HG13	2.06	0.55
1:A:711:LEU:HD22	1:A:715:ARG:HG3	1.89	0.55
1:B:192:VAL:HG13	1:B:193:PRO:HD2	1.88	0.55
1:A:326:TYR:HE1	1:A:337:THR:O	1.90	0.55
1:A:541:GLU:OE2	1:B:546:ASN:HB2	2.07	0.55
1:B:360:ARG:CB	1:B:361:PRO:HD3	2.36	0.55
1:B:649:TYR:CD2	1:B:656:SER:HB3	2.42	0.55
1:A:597:TYR:HD1	1:A:599:ARG:N	2.05	0.55
1:B:157:TYR:CE2	1:B:159:PHE:CD1	2.95	0.55
1:B:388:SER:CB	1:B:391:ILE:HB	2.33	0.55
1:B:541:GLU:OE2	1:C:546:ASN:HB2	2.07	0.55
1:C:175:PHE:CD2	1:C:258:ARG:HG2	2.41	0.55
1:C:649:TYR:CD2	1:C:656:SER:HB3	2.42	0.55
1:A:649:TYR:CD2	1:A:656:SER:HB3	2.42	0.55
1:A:707:ARG:C	1:B:242:ARG:HB3	2.31	0.55
1:B:689:TYR:HD2	1:B:694:ILE:CD1	2.16	0.55
1:C:388:SER:CB	1:C:391:ILE:HB	2.33	0.55
1:C:603:SER:HB3	1:C:612:LEU:CD2	2.32	0.55
1:A:429:TYR:CE2	1:A:455:LEU:HD13	2.43	0.54
1:B:367:THR:HG22	1:B:368:LYS:N	2.22	0.54
1:B:391:ILE:HG22	1:B:393:THR:CG2	2.28	0.54
1:C:326:TYR:HE1	1:C:337:THR:O	1.90	0.54
1:A:299:PRO:HB3	1:A:354:TRP:NE1	2.23	0.54
1:B:600:PRO:HD3	1:B:641:PHE:CE2	2.43	0.54
1:C:297:MET:HG2	1:C:354:TRP:HH2	1.72	0.54
1:C:607:GLU:HG2	1:C:608:ASP:N	2.22	0.54
1:A:652:GLU:OE1	1:A:652:GLU:HA	2.07	0.54
1:A:711:LEU:HD12	1:B:243:THR:CA	2.38	0.54
1:B:157:TYR:CD2	1:B:300:PHE:CE1	2.95	0.54
1:B:217:ASN:ND2	1:C:723:ILE:HG22	2.21	0.54
1:B:242:ARG:NH1	1:C:284:TYR:HD2	1.98	0.54
1:B:543:ARG:CA	1:B:550:ILE:HG12	2.36	0.54
1:B:652:GLU:HA	1:B:652:GLU:OE1	2.07	0.54
1:C:163:MET:CG	1:C:276:VAL:HG21	2.37	0.54
1:A:192:VAL:HG13	1:A:193:PRO:HD2	1.88	0.54
1:C:124:VAL:HG12	1:C:125:VAL:N	2.23	0.54
1:C:553:VAL:HG13	1:C:554:THR:N	2.23	0.54
1:C:600:PRO:HD3	1:C:641:PHE:CE2	2.43	0.54
1:C:652:GLU:HA	1:C:652:GLU:OE1	2.07	0.54
1:A:124:VAL:HG12	1:A:125:VAL:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:VAL:HG23	1:A:264:ARG:HH11	1.73	0.54
1:B:204:LYS:HB3	1:B:206:VAL:HG13	1.89	0.54
1:C:391:ILE:CG2	1:C:393:THR:HG23	2.27	0.54
1:C:429:TYR:CE2	1:C:455:LEU:HD13	2.43	0.54
1:C:582:ILE:HG22	1:C:583:VAL:N	2.22	0.54
1:A:283:PRO:HB3	1:A:300:PHE:HD2	1.73	0.54
1:A:607:GLU:HG2	1:A:608:ASP:N	2.22	0.54
1:B:288:VAL:HG12	1:B:292:GLY:HA2	1.89	0.54
1:B:297:MET:HE2	1:B:319:PHE:CD1	2.43	0.54
1:B:363:VAL:HG23	1:B:364:CYS:HA	1.89	0.54
1:B:432:THR:HG22	1:B:433:HIS:ND1	2.23	0.54
1:A:601:LEU:HD23	1:A:627:ARG:NE	2.22	0.54
1:B:326:TYR:HE1	1:B:337:THR:O	1.90	0.54
1:A:697:SER:CB	1:B:154:ILE:HG13	2.38	0.54
1:B:299:PRO:HG3	1:B:354:TRP:CD1	2.42	0.54
1:B:582:ILE:HG22	1:B:583:VAL:N	2.21	0.54
1:B:601:LEU:HD23	1:B:627:ARG:NE	2.22	0.54
1:B:603:SER:HB3	1:B:612:LEU:CD2	2.32	0.54
1:C:224:HIS:CE1	1:C:268:THR:HG22	2.43	0.54
1:C:701:ASP:HB2	1:C:704:GLU:HB3	1.89	0.54
1:A:156:PRO:HD2	1:C:700:LEU:HD23	1.89	0.54
1:A:275:GLU:O	1:A:276:VAL:HG23	2.08	0.54
1:A:297:MET:CG	1:A:345:LEU:HD22	2.38	0.54
1:A:543:ARG:CA	1:A:550:ILE:HG12	2.36	0.54
1:A:432:THR:HG22	1:A:433:HIS:ND1	2.23	0.53
1:B:429:TYR:CE2	1:B:455:LEU:HD13	2.43	0.53
1:A:128:GLU:HG2	1:A:129:GLN:O	2.08	0.53
1:A:553:VAL:HG13	1:A:554:THR:N	2.22	0.53
1:A:666:THR:HG22	1:A:667:VAL:N	2.22	0.53
1:C:666:THR:HG22	1:C:667:VAL:N	2.22	0.53
1:A:162:THR:HG23	1:A:274:GLU:O	2.08	0.53
1:A:286:GLU:CD	1:A:286:GLU:H	2.17	0.53
1:B:124:VAL:HG12	1:B:125:VAL:N	2.23	0.53
1:C:367:THR:HG22	1:C:368:LYS:N	2.24	0.53
1:A:276:VAL:HG12	1:A:277:ASP:N	2.23	0.53
1:C:591:SER:C	1:C:593:PRO:HD3	2.34	0.53
1:A:546:ASN:HB2	1:C:541:GLU:OE2	2.07	0.53
1:B:162:THR:HG22	1:B:163:MET:N	2.24	0.53
1:B:283:PRO:HA	1:B:300:PHE:CE2	2.44	0.53
1:A:376:LEU:O	1:A:386:PHE:HA	2.09	0.53
1:A:591:SER:C	1:A:593:PRO:HD3	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:PRO:HD3	1:A:641:PHE:CE2	2.43	0.53
1:B:376:LEU:O	1:B:386:PHE:HA	2.09	0.53
1:C:286:GLU:HG2	1:C:294:PHE:HB3	1.90	0.53
1:B:128:GLU:HG2	1:B:129:GLN:O	2.09	0.53
1:B:666:THR:HG22	1:B:667:VAL:N	2.22	0.53
1:C:289:LEU:CD1	1:C:291:THR:HG22	2.39	0.53
1:C:432:THR:HG22	1:C:433:HIS:ND1	2.23	0.53
1:C:572:THR:HG22	1:C:573:CYS:H	1.71	0.53
1:A:321:GLN:HE21	1:A:341:THR:CG2	2.22	0.53
1:A:388:SER:CB	1:A:391:ILE:HB	2.33	0.53
1:A:699:LEU:HB2	1:C:702:TYR:CE2	2.44	0.52
1:A:290:ALA:HB3	1:C:716:PHE:CZ	2.44	0.52
1:A:295:VAL:CG1	1:A:345:LEU:HD23	2.39	0.52
1:A:711:LEU:HD12	1:B:242:ARG:C	2.34	0.52
1:B:368:LYS:HG2	1:B:368:LYS:O	2.09	0.52
1:B:553:VAL:HG13	1:B:554:THR:N	2.23	0.52
1:B:591:SER:C	1:B:593:PRO:HD3	2.34	0.52
1:C:254:TYR:CB	1:C:268:THR:HG23	2.39	0.52
1:C:425:PHE:CD1	1:C:429:TYR:HB3	2.45	0.52
1:C:561:ALA:HB1	1:C:569:ALA:O	2.10	0.52
1:A:561:ALA:HB1	1:A:569:ALA:O	2.10	0.52
1:B:429:TYR:CZ	1:B:455:LEU:HD13	2.44	0.52
1:C:429:TYR:CZ	1:C:455:LEU:HD13	2.44	0.52
1:A:715:ARG:HD2	1:B:243:THR:HG21	1.90	0.52
1:B:520:MET:HE2	1:B:520:MET:N	2.25	0.52
1:B:597:TYR:HD1	1:B:599:ARG:N	2.05	0.52
1:C:376:LEU:O	1:C:386:PHE:HA	2.09	0.52
1:C:701:ASP:HB3	1:C:704:GLU:H	1.74	0.52
1:A:157:TYR:HB3	1:A:280:SER:O	2.09	0.52
1:A:191:PRO:HG3	1:A:348:PRO:O	2.10	0.52
1:A:360:ARG:NH2	1:A:409:LEU:HD23	2.25	0.52
1:A:576:VAL:HG12	1:A:577:ALA:N	2.25	0.52
1:B:217:ASN:CB	1:C:723:ILE:HG22	2.39	0.52
1:B:561:ALA:HB2	1:B:570:VAL:HG12	1.91	0.52
1:A:299:PRO:HB3	1:A:354:TRP:CD1	2.45	0.52
1:A:429:TYR:CZ	1:A:455:LEU:HD13	2.44	0.52
1:A:497:THR:HG22	1:A:498:THR:N	2.25	0.52
1:B:561:ALA:HB1	1:B:569:ALA:O	2.10	0.52
1:A:699:LEU:H	1:A:699:LEU:CD1	2.23	0.52
1:B:217:ASN:ND2	1:C:723:ILE:H	2.07	0.52
1:C:561:ALA:HB2	1:C:570:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:LEU:HD23	1:B:627:ARG:CZ	2.40	0.52
1:B:649:TYR:HB2	1:B:659:LEU:HD11	1.92	0.52
1:C:227:ASP:HB3	1:C:228:HIS:O	2.10	0.52
1:C:276:VAL:HG11	1:C:289:LEU:HD23	1.92	0.52
1:A:520:MET:HE2	1:A:520:MET:N	2.25	0.52
1:B:329:ASP:O	1:B:333:LYS:HA	2.10	0.52
1:A:711:LEU:HD13	1:A:715:ARG:HD2	1.92	0.51
1:B:297:MET:HG3	1:B:298:SER:H	1.76	0.51
1:B:299:PRO:HB3	1:B:354:TRP:CD1	2.45	0.51
1:C:605:ARG:HD3	1:C:607:GLU:N	2.10	0.51
1:A:234:LEU:HD23	1:A:247:TRP:CB	2.40	0.51
1:A:244:SER:HB2	1:A:276:VAL:HG22	1.91	0.51
1:A:391:ILE:HG22	1:A:393:THR:CG2	2.28	0.51
1:A:561:ALA:HB2	1:A:570:VAL:HG12	1.91	0.51
1:B:425:PHE:CD1	1:B:429:TYR:HB3	2.45	0.51
1:C:128:GLU:HG2	1:C:129:GLN:O	2.09	0.51
1:C:329:ASP:O	1:C:333:LYS:HA	2.11	0.51
1:A:208:ARG:HA	1:A:231:ASP:CB	2.41	0.51
1:A:425:PHE:CD1	1:A:429:TYR:HB3	2.44	0.51
1:A:649:TYR:HB2	1:A:659:LEU:HD11	1.92	0.51
1:B:108:ASN:HB2	1:B:645:GLY:HA3	1.92	0.51
1:B:152:GLU:HG2	1:B:153:ASN:N	2.25	0.51
1:C:576:VAL:HG12	1:C:577:ALA:N	2.25	0.51
1:A:567:VAL:HG22	1:B:640:TYR:HB2	1.92	0.51
1:A:640:TYR:HB2	1:C:567:VAL:HG22	1.93	0.51
1:A:670:PHE:HD2	1:C:131:ARG:NH2	2.08	0.51
1:B:321:GLN:HE21	1:B:341:THR:CG2	2.22	0.51
1:C:520:MET:HE2	1:C:520:MET:N	2.25	0.51
1:C:601:LEU:HD23	1:C:627:ARG:CZ	2.40	0.51
1:C:689:TYR:CD2	1:C:694:ILE:HD13	2.44	0.51
1:A:601:LEU:HD23	1:A:627:ARG:CZ	2.40	0.51
1:A:641:PHE:HB2	1:A:648:VAL:CG1	2.40	0.51
1:B:297:MET:HE2	1:B:319:PHE:CE1	2.45	0.51
1:B:701:ASP:OD2	1:B:704:GLU:HB2	2.11	0.51
1:C:497:THR:HG22	1:C:498:THR:N	2.24	0.51
1:C:641:PHE:HB2	1:C:648:VAL:CG1	2.40	0.51
1:C:695:LYS:HZ2	1:C:702:TYR:HB3	1.72	0.51
1:A:329:ASP:O	1:A:333:LYS:HA	2.10	0.51
1:B:175:PHE:CE2	1:B:258:ARG:HA	2.46	0.51
1:B:217:ASN:HB3	1:C:723:ILE:HG22	1.91	0.51
1:A:713:ASP:HB2	1:C:294:PHE:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:VAL:HG12	1:B:149:VAL:N	2.26	0.51
1:B:317:ASP:O	1:B:320:LYS:HE3	2.11	0.51
1:B:576:VAL:HG12	1:B:577:ALA:N	2.25	0.51
1:B:641:PHE:HB2	1:B:648:VAL:CG1	2.40	0.51
1:B:191:PRO:HG3	1:B:348:PRO:O	2.10	0.51
1:C:175:PHE:CE2	1:C:258:ARG:HG2	2.45	0.51
1:C:191:PRO:HG3	1:C:348:PRO:O	2.10	0.51
1:C:631:GLU:HB2	1:C:632:PRO:HD2	1.93	0.51
1:A:131:ARG:NH2	1:B:670:PHE:HD2	2.08	0.51
1:A:471:GLU:HA	1:A:471:GLU:OE1	2.11	0.51
1:B:719:ILE:HB	1:B:720:ASP:CA	2.41	0.51
1:C:145:GLY:HA2	1:C:455:LEU:HG	1.93	0.51
1:C:286:GLU:CG	1:C:294:PHE:HD2	2.11	0.51
1:A:282:TYR:HB2	1:A:283:PRO:CD	2.41	0.50
1:A:605:ARG:HD3	1:A:607:GLU:N	2.14	0.50
1:A:708:ARG:NH2	1:B:276:VAL:HG22	2.27	0.50
1:B:172:GLN:CB	1:B:183:MET:HB2	2.40	0.50
1:C:649:TYR:HB2	1:C:659:LEU:HD11	1.92	0.50
1:A:711:LEU:HD21	1:B:240:ALA:CB	2.27	0.50
1:B:131:ARG:NH2	1:C:670:PHE:HD2	2.08	0.50
1:B:360:ARG:NE	1:B:409:LEU:HD21	2.26	0.50
1:B:605:ARG:HD3	1:B:607:GLU:N	2.14	0.50
1:C:321:GLN:HE21	1:C:341:THR:CG2	2.23	0.50
1:C:471:GLU:HA	1:C:471:GLU:OE1	2.11	0.50
1:A:156:PRO:HB3	1:A:281:VAL:HA	1.94	0.50
1:C:119:PRO:CG	1:C:561:ALA:HA	2.42	0.50
1:C:150:PHE:CE2	1:C:368:LYS:HB2	2.46	0.50
1:C:429:TYR:CE2	1:C:455:LEU:CD1	2.95	0.50
1:C:596:CYS:HB3	1:C:653:TYR:CD1	2.47	0.50
1:A:596:CYS:HB3	1:A:653:TYR:CD1	2.47	0.50
1:A:713:ASP:CG	1:C:294:PHE:HD1	2.19	0.50
1:B:156:PRO:HG2	1:B:158:LYS:NZ	2.27	0.50
1:B:429:TYR:CE2	1:B:455:LEU:CD1	2.95	0.50
1:C:597:TYR:HD1	1:C:599:ARG:N	2.05	0.50
1:A:425:PHE:CD1	1:A:429:TYR:CB	2.95	0.50
1:B:145:GLY:HA2	1:B:455:LEU:HG	1.93	0.50
1:B:567:VAL:HG22	1:C:640:TYR:HB2	1.93	0.50
1:C:159:PHE:CZ	1:C:278:ALA:CB	2.95	0.50
1:C:286:GLU:HA	1:C:295:VAL:O	2.12	0.50
1:C:626:THR:HG22	1:C:627:ARG:N	2.27	0.50
1:A:148:VAL:HG12	1:A:149:VAL:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:GLU:CG	1:B:502:GLU:HG2	2.42	0.50
1:B:204:LYS:HB3	1:B:206:VAL:HG22	1.93	0.50
1:B:631:GLU:HB2	1:B:632:PRO:HD2	1.93	0.50
1:C:108:ASN:HB2	1:C:645:GLY:HA3	1.92	0.50
1:C:152:GLU:HG2	1:C:153:ASN:N	2.25	0.50
1:C:605:ARG:HH11	1:C:607:GLU:C	2.20	0.50
1:C:649:TYR:CD2	1:C:656:SER:CB	2.95	0.50
1:A:290:ALA:HB2	1:C:715:ARG:HH22	1.75	0.50
1:A:502:GLU:HG2	1:C:502:GLU:CG	2.42	0.50
1:B:397:THR:HG22	1:B:398:ASN:O	2.12	0.50
1:B:467:GLU:O	1:B:471:GLU:HG2	2.12	0.50
1:B:681:HIS:HE1	1:C:389:ASP:O	1.95	0.50
1:B:706:GLN:HE21	1:C:699:LEU:CD2	2.25	0.50
1:C:425:PHE:CD1	1:C:429:TYR:CB	2.95	0.50
1:A:119:PRO:CG	1:A:561:ALA:HA	2.42	0.50
1:A:158:LYS:HZ2	1:C:700:LEU:HD22	1.77	0.50
1:B:201:ILE:O	1:B:205:GLY:HA2	2.12	0.50
1:B:596:CYS:HB3	1:B:653:TYR:CD1	2.47	0.50
1:B:626:THR:HG22	1:B:627:ARG:N	2.27	0.50
1:B:471:GLU:OE1	1:B:471:GLU:HA	2.12	0.50
1:B:700:LEU:HD12	1:C:158:LYS:CB	2.42	0.50
1:C:201:ILE:O	1:C:205:GLY:HA2	2.12	0.50
1:A:146:ILE:HG13	1:A:455:LEU:HD11	1.94	0.49
1:A:252:LEU:HD23	1:C:721:THR:HG21	1.94	0.49
1:A:397:THR:HG22	1:A:398:ASN:O	2.12	0.49
1:A:605:ARG:HD3	1:A:606:TYR:N	2.27	0.49
1:B:119:PRO:CG	1:B:561:ALA:HA	2.42	0.49
1:B:276:VAL:HG12	1:B:277:ASP:O	2.12	0.49
1:B:699:LEU:HB3	1:C:156:PRO:CA	2.42	0.49
1:C:401:GLU:CD	1:C:475:LYS:HD3	2.37	0.49
1:A:631:GLU:HB2	1:A:632:PRO:HD2	1.93	0.49
1:A:699:LEU:HB3	1:A:700:LEU:CD2	2.33	0.49
1:B:425:PHE:CD1	1:B:429:TYR:CB	2.95	0.49
1:B:497:THR:HG22	1:B:498:THR:N	2.25	0.49
1:B:649:TYR:CD2	1:B:656:SER:CB	2.95	0.49
1:A:364:CYS:CB	1:A:409:LEU:HB3	2.41	0.49
1:A:429:TYR:CE2	1:A:455:LEU:CD1	2.95	0.49
1:C:397:THR:HG22	1:C:398:ASN:O	2.12	0.49
1:C:467:GLU:O	1:C:471:GLU:HG2	2.12	0.49
1:A:145:GLY:HA2	1:A:455:LEU:HG	1.93	0.49
1:A:467:GLU:O	1:A:471:GLU:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:ARG:HH11	1:B:607:GLU:C	2.20	0.49
1:A:212:LYS:HE2	1:A:219:GLU:OE2	2.12	0.49
1:A:520:MET:HA	1:A:520:MET:CE	2.37	0.49
1:C:689:TYR:CD2	1:C:694:ILE:CD1	2.95	0.49
1:A:719:ILE:HG23	1:A:720:ASP:OD1	2.12	0.49
1:B:146:ILE:HG13	1:B:455:LEU:HD11	1.94	0.49
1:B:297:MET:CE	1:B:319:PHE:CD1	2.95	0.49
1:B:363:VAL:HG23	1:B:364:CYS:CA	2.42	0.49
1:B:543:ARG:HA	1:B:550:ILE:CG1	2.40	0.49
1:C:148:VAL:HG12	1:C:149:VAL:N	2.27	0.49
1:C:205:GLY:O	1:C:234:LEU:HD12	2.12	0.49
1:A:201:ILE:O	1:A:205:GLY:HA2	2.13	0.49
1:A:649:TYR:CD2	1:A:656:SER:CB	2.95	0.49
1:A:707:ARG:CA	1:B:242:ARG:HB3	2.43	0.49
1:C:298:SER:HB3	1:C:300:PHE:CE2	2.48	0.49
1:A:401:GLU:CD	1:A:475:LYS:HD3	2.37	0.49
1:A:626:THR:HG22	1:A:627:ARG:N	2.27	0.49
1:B:233:GLU:HG2	1:B:234:LEU:N	2.28	0.49
1:A:215:ARG:HG3	1:A:216:ASN:OD1	2.13	0.49
1:A:299:PRO:CB	1:A:354:TRP:HE1	2.26	0.49
1:B:501:ILE:HG23	1:B:502:GLU:HA	1.95	0.49
1:B:520:MET:HA	1:B:520:MET:CE	2.37	0.49
1:A:235:LYS:HB2	1:A:236:PRO:HD2	1.95	0.48
1:B:699:LEU:HB3	1:C:156:PRO:CB	2.42	0.48
1:C:456:LEU:HD21	1:C:461:ALA:CA	2.36	0.48
1:A:108:ASN:HB2	1:A:645:GLY:HA3	1.95	0.48
1:A:162:THR:HG22	1:A:163:MET:N	2.27	0.48
1:A:389:ASP:O	1:C:681:HIS:HE1	1.95	0.48
1:B:288:VAL:HG12	1:B:289:LEU:O	2.13	0.48
1:C:162:THR:HG22	1:C:163:MET:N	2.27	0.48
1:C:254:TYR:N	1:C:268:THR:HG23	2.28	0.48
1:A:193:PRO:HD2	1:A:196:GLU:OE1	2.13	0.48
1:B:123:THR:HB	1:B:570:VAL:O	2.14	0.48
1:B:502:GLU:CG	1:C:502:GLU:HG2	2.42	0.48
1:B:699:LEU:CD1	1:C:281:VAL:HG13	2.19	0.48
1:C:146:ILE:HG13	1:C:455:LEU:HD11	1.94	0.48
1:C:193:PRO:HD2	1:C:196:GLU:OE1	2.13	0.48
1:C:291:THR:CG2	1:C:293:ASP:H	2.10	0.48
1:C:501:ILE:HG23	1:C:502:GLU:HA	1.95	0.48
1:A:286:GLU:HA	1:A:296:TYR:HA	1.94	0.48
1:A:722:VAL:HG12	1:A:723:ILE:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:PRO:HD2	1:B:196:GLU:OE1	2.13	0.48
1:C:543:ARG:HA	1:C:550:ILE:CG1	2.40	0.48
1:C:630:ILE:HG22	1:C:631:GLU:N	2.28	0.48
1:A:230:THR:HG22	1:A:231:ASP:N	2.28	0.48
1:A:681:HIS:HE1	1:B:389:ASP:O	1.95	0.48
1:C:599:ARG:HB3	1:C:600:PRO:HD2	1.95	0.48
1:B:225:ARG:HG3	1:B:254:TYR:HE2	1.77	0.48
1:C:215:ARG:HG3	1:C:216:ASN:OD1	2.13	0.48
1:A:605:ARG:HH11	1:A:607:GLU:C	2.21	0.48
1:B:157:TYR:CE2	1:B:300:PHE:CE1	2.95	0.48
1:B:198:ILE:N	1:B:198:ILE:HD12	2.29	0.48
1:B:298:SER:OG	1:B:299:PRO:HD2	2.14	0.48
1:B:401:GLU:CD	1:B:475:LYS:HD3	2.38	0.48
1:B:563:MET:HE3	1:B:565:GLY:O	2.14	0.48
1:B:700:LEU:H	1:C:279:ARG:NH2	2.10	0.48
1:C:159:PHE:CZ	1:C:278:ALA:HB3	2.48	0.48
1:B:173:VAL:HG12	1:B:174:TRP:N	2.29	0.48
1:B:568:MET:HG2	1:B:569:ALA:O	2.14	0.48
1:B:605:ARG:HD3	1:B:606:TYR:N	2.28	0.48
1:B:700:LEU:O	1:B:701:ASP:HB3	2.14	0.48
1:C:123:THR:HB	1:C:570:VAL:O	2.14	0.48
1:A:123:THR:HB	1:A:570:VAL:O	2.14	0.48
1:A:501:ILE:HG23	1:A:502:GLU:HA	1.96	0.48
1:B:287:PHE:CE1	1:B:297:MET:HB3	2.47	0.48
1:B:295:VAL:HG13	1:B:345:LEU:HD23	1.96	0.48
1:B:630:ILE:HG22	1:B:631:GLU:N	2.28	0.48
1:C:260:GLU:O	1:C:262:PHE:HD1	1.97	0.48
1:C:297:MET:HG2	1:C:354:TRP:CH2	2.49	0.48
1:A:198:ILE:HD12	1:A:198:ILE:N	2.29	0.47
1:A:568:MET:HG2	1:A:569:ALA:O	2.14	0.47
1:B:706:GLN:NE2	1:C:699:LEU:HD21	2.27	0.47
1:C:265:TYR:N	1:C:265:TYR:CD1	2.82	0.47
1:A:116:CYS:CB	1:A:560:SER:HB2	2.39	0.47
1:A:630:ILE:HG22	1:A:631:GLU:N	2.28	0.47
1:B:354:TRP:N	1:B:354:TRP:CE3	2.82	0.47
1:A:173:VAL:HG12	1:A:174:TRP:N	2.29	0.47
1:B:599:ARG:HB3	1:B:600:PRO:HD2	1.95	0.47
1:B:604:PHE:N	1:B:604:PHE:CD1	2.83	0.47
1:C:116:CYS:CB	1:C:560:SER:HB2	2.39	0.47
1:C:563:MET:HE3	1:C:565:GLY:O	2.14	0.47
1:A:240:ALA:CB	1:A:243:THR:HG21	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLU:HB3	1:A:295:VAL:O	2.15	0.47
1:A:543:ARG:HA	1:A:550:ILE:CG1	2.40	0.47
1:A:605:ARG:CZ	1:A:611:PRO:HD2	2.45	0.47
1:B:218:LEU:HD23	1:B:219:GLU:C	2.40	0.47
1:B:314:TYR:HD1	1:B:314:TYR:HA	1.37	0.47
1:C:218:LEU:HD23	1:C:219:GLU:C	2.39	0.47
1:C:259:VAL:HG23	1:C:264:ARG:HH11	1.80	0.47
1:A:218:LEU:HD23	1:A:219:GLU:C	2.39	0.47
1:A:289:LEU:CG	1:A:290:ALA:H	2.26	0.47
1:A:297:MET:HE3	1:A:319:PHE:CD1	2.49	0.47
1:A:563:MET:HE3	1:A:565:GLY:O	2.14	0.47
1:B:215:ARG:HG3	1:B:216:ASN:OD1	2.14	0.47
1:B:265:TYR:N	1:B:265:TYR:CD1	2.82	0.47
1:B:605:ARG:CZ	1:B:611:PRO:HD2	2.44	0.47
1:B:708:ARG:CZ	1:C:277:ASP:HB2	2.44	0.47
1:C:198:ILE:N	1:C:198:ILE:HD12	2.29	0.47
1:C:247:TRP:CE3	1:C:330:LEU:HD12	2.50	0.47
1:A:265:TYR:CD1	1:A:265:TYR:N	2.81	0.47
1:A:597:TYR:CD1	1:A:598:SER:N	2.83	0.47
1:B:687:GLU:HG2	1:B:689:TYR:O	2.14	0.47
1:A:165:TYR:CD1	1:A:165:TYR:N	2.83	0.47
1:A:296:TYR:CD1	1:A:296:TYR:N	2.82	0.47
1:A:442:TYR:CD1	1:A:442:TYR:N	2.83	0.47
1:A:599:ARG:HB3	1:A:600:PRO:HD2	1.95	0.47
1:B:295:VAL:CG1	1:B:345:LEU:HD23	2.44	0.47
1:B:365:THR:HG22	1:B:366:MET:N	2.29	0.47
1:B:438:GLN:HB3	1:B:439:PRO:CD	2.45	0.47
1:C:225:ARG:HD2	1:C:254:TYR:CD1	2.49	0.47
1:C:568:MET:HG2	1:C:569:ALA:O	2.14	0.47
1:A:670:PHE:CD1	1:C:532:GLN:HB3	2.50	0.47
1:B:303:TYR:CD1	1:B:304:ARG:N	2.82	0.47
1:B:532:GLN:HB3	1:C:670:PHE:CD1	2.50	0.47
1:C:159:PHE:CD1	1:C:159:PHE:N	2.82	0.47
1:C:276:VAL:HG22	1:C:289:LEU:HD21	1.97	0.47
1:C:354:TRP:N	1:C:354:TRP:CE3	2.83	0.47
1:C:403:PRO:HG2	1:C:406:ARG:HH21	1.80	0.47
1:C:605:ARG:CZ	1:C:611:PRO:HD2	2.44	0.47
1:B:295:VAL:HG12	1:B:296:TYR:N	2.30	0.47
1:B:363:VAL:HG23	1:B:409:LEU:HD13	1.89	0.47
1:B:508:PHE:CE1	1:B:512:HIS:CE1	3.03	0.47
1:C:240:ALA:CB	1:C:243:THR:HG21	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:ILE:HD12	1:C:550:ILE:N	2.30	0.47
1:A:403:PRO:HG2	1:A:406:ARG:HH21	1.80	0.46
1:A:532:GLN:HB3	1:B:670:PHE:CD1	2.50	0.46
1:A:713:ASP:CB	1:C:294:PHE:CD1	2.96	0.46
1:B:697:SER:CA	1:C:154:ILE:HG21	2.39	0.46
1:A:386:PHE:N	1:A:386:PHE:CD1	2.84	0.46
1:B:690:THR:OG1	1:B:693:GLU:HG3	2.16	0.46
1:C:119:PRO:HG3	1:C:561:ALA:HA	1.97	0.46
1:C:391:ILE:HG22	1:C:393:THR:CG2	2.28	0.46
1:A:401:GLU:OE2	1:A:475:LYS:HD3	2.16	0.46
1:B:116:CYS:CB	1:B:560:SER:HB2	2.39	0.46
1:B:165:TYR:N	1:B:165:TYR:CD1	2.83	0.46
1:B:212:LYS:HE2	1:B:219:GLU:OE2	2.15	0.46
1:B:401:GLU:OE2	1:B:475:LYS:HD3	2.16	0.46
1:C:442:TYR:N	1:C:442:TYR:CD1	2.83	0.46
1:A:279:ARG:CZ	1:C:700:LEU:HD12	2.44	0.46
1:A:290:ALA:CA	1:C:708:ARG:HH21	2.27	0.46
1:A:354:TRP:N	1:A:354:TRP:CE3	2.83	0.46
1:A:508:PHE:CE1	1:A:512:HIS:CE1	3.03	0.46
1:A:531:LEU:HD12	1:C:671:ILE:HD13	1.97	0.46
1:A:574:VAL:HG12	1:A:575:PRO:O	2.16	0.46
1:A:604:PHE:CD1	1:A:604:PHE:N	2.83	0.46
1:B:213:TYR:N	1:B:213:TYR:CD1	2.84	0.46
1:C:407:VAL:HG12	1:C:408:ASP:N	2.30	0.46
1:C:408:ASP:OD1	1:C:409:LEU:HG	2.16	0.46
1:C:574:VAL:HG12	1:C:575:PRO:O	2.16	0.46
1:C:597:TYR:CD1	1:C:597:TYR:C	2.94	0.46
1:A:711:LEU:HD23	1:A:714:LEU:HD12	1.98	0.46
1:B:297:MET:SD	1:B:345:LEU:HD13	2.56	0.46
1:B:700:LEU:HD11	1:C:158:LYS:HE3	1.95	0.46
1:C:175:PHE:HD2	1:C:258:ARG:NH1	2.12	0.46
1:C:189:ARG:HD3	1:C:349:LYS:CD	2.45	0.46
1:C:212:LYS:HE2	1:C:219:GLU:OE2	2.16	0.46
1:C:508:PHE:CE1	1:C:512:HIS:CE1	3.03	0.46
1:C:605:ARG:HD3	1:C:606:TYR:N	2.30	0.46
1:A:159:PHE:N	1:A:159:PHE:CD1	2.82	0.46
1:A:196:GLU:OE2	1:A:208:ARG:HG2	2.15	0.46
1:B:247:TRP:CE3	1:B:330:LEU:HD12	2.51	0.46
1:C:165:TYR:N	1:C:165:TYR:CD1	2.83	0.46
1:C:555:VAL:HG23	1:C:556:GLY:N	2.30	0.46
1:C:597:TYR:CD1	1:C:598:SER:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PRO:HG3	1:A:561:ALA:HA	1.97	0.46
1:A:291:THR:HA	1:C:712:HIS:CE1	2.51	0.46
1:B:441:TYR:CD1	1:B:441:TYR:N	2.83	0.46
1:B:463:LEU:HD22	1:B:467:GLU:HG2	1.98	0.46
1:C:604:PHE:N	1:C:604:PHE:CD1	2.83	0.46
1:A:174:TRP:CD1	1:A:263:HIS:CE1	3.04	0.46
1:A:299:PRO:HB3	1:A:354:TRP:HE1	1.81	0.46
1:A:438:GLN:HB3	1:A:439:PRO:CD	2.45	0.46
1:A:441:TYR:CD1	1:A:441:TYR:N	2.83	0.46
1:B:386:PHE:N	1:B:386:PHE:CD1	2.84	0.46
1:B:403:PRO:HG2	1:B:406:ARG:HH21	1.81	0.46
1:B:555:VAL:HG23	1:B:556:GLY:N	2.30	0.46
1:B:574:VAL:HG12	1:B:575:PRO:O	2.16	0.46
1:B:597:TYR:CD1	1:B:598:SER:N	2.83	0.46
1:C:214:VAL:O	1:C:214:VAL:HG13	2.15	0.46
1:C:360:ARG:NH2	1:C:409:LEU:HD23	2.30	0.46
1:C:699:LEU:O	1:C:699:LEU:HG	2.16	0.46
1:A:555:VAL:HG23	1:A:556:GLY:N	2.30	0.46
1:A:671:ILE:HD13	1:B:531:LEU:HD12	1.97	0.46
1:B:407:VAL:HG12	1:B:408:ASP:N	2.30	0.46
1:C:173:VAL:HG12	1:C:174:TRP:N	2.30	0.46
1:B:159:PHE:CD1	1:B:159:PHE:N	2.82	0.46
1:B:214:VAL:O	1:B:214:VAL:HG13	2.15	0.46
1:B:363:VAL:HG23	1:B:364:CYS:N	2.31	0.46
1:C:276:VAL:CG1	1:C:289:LEU:CD2	2.94	0.46
1:A:247:TRP:CE3	1:A:330:LEU:HD12	2.50	0.45
1:A:550:ILE:HD12	1:A:550:ILE:N	2.30	0.45
1:A:699:LEU:HD13	1:C:702:TYR:CD2	2.51	0.45
1:C:386:PHE:N	1:C:386:PHE:CD1	2.84	0.45
1:C:438:GLN:HB3	1:C:439:PRO:CD	2.45	0.45
1:A:189:ARG:HD3	1:A:349:LYS:CD	2.46	0.45
1:A:290:ALA:HA	1:C:708:ARG:NH2	2.31	0.45
1:A:290:ALA:HA	1:C:708:ARG:HH21	1.81	0.45
1:A:688:VAL:HG13	1:B:151:LYS:HD2	1.99	0.45
1:B:174:TRP:CD1	1:B:263:HIS:CE1	3.03	0.45
1:B:597:TYR:CD1	1:B:597:TYR:C	2.94	0.45
1:C:129:GLN:HB3	1:C:130:PRO:CD	2.47	0.45
1:A:300:PHE:N	1:A:300:PHE:CD1	2.82	0.45
1:A:386:PHE:O	1:A:394:THR:HA	2.16	0.45
1:B:189:ARG:HD3	1:B:349:LYS:CD	2.46	0.45
1:B:301:TYR:HB3	1:B:307:SER:OG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:PHE:O	1:B:394:THR:HA	2.16	0.45
1:C:352:VAL:HG22	1:C:353:ALA:N	2.30	0.45
1:A:194:PHE:CD1	1:A:194:PHE:C	2.95	0.45
1:A:213:TYR:N	1:A:213:TYR:CD1	2.84	0.45
1:B:671:ILE:HD13	1:C:531:LEU:HD12	1.98	0.45
1:B:550:ILE:N	1:B:550:ILE:HD12	2.30	0.45
1:A:200:LYS:O	1:A:204:LYS:HB2	2.17	0.45
1:A:289:LEU:CD1	1:C:716:PHE:HZ	2.30	0.45
1:A:349:LYS:HB2	1:A:350:PHE:CD1	2.52	0.45
1:A:475:LYS:HA	1:A:476:PRO:HD3	1.77	0.45
1:A:587:MET:HG3	1:A:650:PHE:CE2	2.52	0.45
1:B:194:PHE:CD1	1:B:194:PHE:C	2.95	0.45
1:B:442:TYR:CD1	1:B:442:TYR:N	2.83	0.45
1:B:705:VAL:HG23	1:C:279:ARG:NH1	2.31	0.45
1:C:291:THR:CG2	1:C:293:ASP:HB2	2.46	0.45
1:A:407:VAL:HG12	1:A:408:ASP:N	2.31	0.45
1:A:510:TYR:CD1	1:A:510:TYR:C	2.95	0.45
1:B:174:TRP:HD1	1:B:263:HIS:CE1	2.35	0.45
1:B:300:PHE:CD2	1:B:359:LYS:HG3	2.52	0.45
1:B:456:LEU:HD21	1:B:461:ALA:CA	2.36	0.45
1:B:503:PHE:CG	1:B:504:ALA:N	2.85	0.45
1:B:587:MET:HG3	1:B:650:PHE:CE2	2.52	0.45
1:B:607:GLU:HG2	1:B:608:ASP:H	1.82	0.45
1:C:284:TYR:HD1	1:C:284:TYR:HA	1.31	0.45
1:C:706:GLN:O	1:C:710:GLN:HG3	2.17	0.45
1:A:150:PHE:CE2	1:A:368:LYS:HB2	2.52	0.45
1:B:256:PRO:HG3	1:B:265:TYR:O	2.17	0.45
1:C:116:CYS:SG	1:C:622:GLU:HG3	2.57	0.45
1:C:209:SER:O	1:C:269:VAL:HG11	2.17	0.45
1:C:276:VAL:CG2	1:C:289:LEU:HD21	2.46	0.45
1:C:510:TYR:CD1	1:C:510:TYR:C	2.95	0.45
1:C:597:TYR:HD1	1:C:598:SER:N	2.14	0.45
1:A:179:TYR:CD1	1:A:179:TYR:C	2.95	0.45
1:A:288:VAL:HG12	1:A:289:LEU:N	2.30	0.45
1:A:463:LEU:HD22	1:A:467:GLU:HG2	1.98	0.45
1:A:689:TYR:CD2	1:A:694:ILE:CD1	2.96	0.45
1:B:129:GLN:HB3	1:B:130:PRO:CD	2.47	0.45
1:B:589:ILE:CD1	1:B:630:ILE:HD13	2.46	0.45
1:B:614:GLU:CG	1:B:627:ARG:CZ	2.95	0.45
1:C:159:PHE:CE1	1:C:278:ALA:HB3	2.52	0.45
1:C:463:LEU:HD22	1:C:467:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:698:GLY:HA2	1:C:699:LEU:HA	1.31	0.45
1:A:129:GLN:HB3	1:A:130:PRO:CD	2.47	0.45
1:B:150:PHE:CB	1:B:366:MET:HE3	2.47	0.45
1:B:157:TYR:CG	1:B:300:PHE:CZ	3.05	0.45
1:B:510:TYR:CD1	1:B:510:TYR:C	2.95	0.45
1:C:289:LEU:HD12	1:C:291:THR:HG22	1.98	0.45
1:C:401:GLU:OE2	1:C:475:LYS:HD3	2.16	0.45
1:C:425:PHE:CD2	1:C:425:PHE:C	2.95	0.45
1:C:614:GLU:CG	1:C:627:ARG:CZ	2.95	0.45
1:A:326:TYR:OH	1:A:339:PRO:HG3	2.17	0.44
1:A:425:PHE:CD2	1:A:425:PHE:C	2.95	0.44
1:C:189:ARG:HB2	1:C:349:LYS:HE2	1.99	0.44
1:C:291:THR:CG2	1:C:293:ASP:CB	2.94	0.44
1:A:116:CYS:SG	1:A:622:GLU:HG3	2.57	0.44
1:A:343:ASN:OD1	1:A:356:TRP:HB2	2.17	0.44
1:A:352:VAL:HG22	1:A:353:ALA:N	2.31	0.44
1:A:700:LEU:CB	1:B:279:ARG:CZ	2.95	0.44
1:B:200:LYS:HB3	1:B:206:VAL:O	2.17	0.44
1:B:686:LEU:HD11	1:C:369:TRP:CZ2	2.53	0.44
1:C:213:TYR:N	1:C:213:TYR:CD1	2.85	0.44
1:C:386:PHE:O	1:C:394:THR:HA	2.16	0.44
1:C:446:GLY:O	1:C:497:THR:HG23	2.17	0.44
1:A:293:ASP:C	1:A:294:PHE:CD1	2.95	0.44
1:A:301:TYR:CD1	1:A:301:TYR:N	2.83	0.44
1:A:597:TYR:HD1	1:A:598:SER:N	2.15	0.44
1:A:597:TYR:CD1	1:A:597:TYR:C	2.94	0.44
1:A:711:LEU:CD2	1:B:240:ALA:HB1	2.31	0.44
1:B:567:VAL:HG21	1:C:640:TYR:CD1	2.53	0.44
1:C:349:LYS:HB2	1:C:350:PHE:CD1	2.52	0.44
1:C:687:GLU:HB3	1:C:689:TYR:O	2.18	0.44
1:A:214:VAL:HG13	1:A:214:VAL:O	2.15	0.44
1:A:241:THR:O	1:A:243:THR:HG23	2.17	0.44
1:A:242:ARG:HA	1:C:707:ARG:HH21	1.82	0.44
1:A:267:THR:HG22	1:A:268:THR:N	2.32	0.44
1:A:293:ASP:C	1:A:294:PHE:HD1	2.24	0.44
1:A:314:TYR:HA	1:A:314:TYR:HD1	1.47	0.44
1:A:649:TYR:HB3	1:A:657:HIS:O	2.18	0.44
1:B:189:ARG:HB2	1:B:349:LYS:HE2	1.99	0.44
1:B:360:ARG:NH2	1:B:409:LEU:HG	2.32	0.44
1:B:425:PHE:CD2	1:B:425:PHE:C	2.95	0.44
1:B:532:GLN:HA	1:B:532:GLN:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:TYR:HD1	1:B:598:SER:N	2.14	0.44
1:C:587:MET:HG3	1:C:650:PHE:CE2	2.52	0.44
1:A:189:ARG:HB2	1:A:349:LYS:HE2	1.99	0.44
1:A:605:ARG:CZ	1:A:607:GLU:HB3	2.48	0.44
1:A:713:ASP:CB	1:C:294:PHE:HB2	2.48	0.44
1:B:116:CYS:SG	1:B:622:GLU:HG3	2.57	0.44
1:B:352:VAL:HG22	1:B:353:ALA:N	2.32	0.44
1:B:360:ARG:O	1:B:363:VAL:HG22	2.18	0.44
1:B:700:LEU:HD21	1:B:704:GLU:OE2	2.17	0.44
1:C:441:TYR:N	1:C:441:TYR:CD1	2.83	0.44
1:A:367:THR:HG22	1:A:368:LYS:N	2.33	0.44
1:B:179:TYR:CD1	1:B:179:TYR:C	2.95	0.44
1:B:369:TRP:C	1:B:370:GLN:HG2	2.43	0.44
1:B:605:ARG:HH12	1:B:610:GLY:H	1.61	0.44
1:B:700:LEU:CD1	1:C:158:LYS:CG	2.95	0.44
1:A:276:VAL:CG1	1:A:277:ASP:N	2.80	0.44
1:A:503:PHE:CG	1:A:504:ALA:N	2.85	0.44
1:A:599:ARG:HA	1:A:600:PRO:HD3	1.76	0.44
1:B:349:LYS:HB2	1:B:350:PHE:CD1	2.52	0.44
1:B:605:ARG:CZ	1:B:607:GLU:HB3	2.48	0.44
1:B:688:VAL:HA	1:C:369:TRP:CZ2	2.53	0.44
1:B:699:LEU:HA	1:B:700:LEU:C	2.42	0.44
1:B:700:LEU:CD1	1:C:158:LYS:CB	2.96	0.44
1:C:108:ASN:CB	1:C:645:GLY:HA3	2.48	0.44
1:C:174:TRP:HD1	1:C:263:HIS:CE1	2.36	0.44
1:C:605:ARG:HB2	1:C:611:PRO:O	2.17	0.44
1:C:701:ASP:CB	1:C:704:GLU:H	2.30	0.44
1:A:589:ILE:CD1	1:A:630:ILE:HD13	2.46	0.44
1:B:538:LEU:HD21	1:C:539:TRP:CE3	2.53	0.44
1:B:649:TYR:HB3	1:B:657:HIS:O	2.17	0.44
1:B:700:LEU:CD2	1:B:704:GLU:CB	2.95	0.44
1:C:194:PHE:CD1	1:C:194:PHE:C	2.95	0.44
1:C:503:PHE:CG	1:C:504:ALA:N	2.85	0.44
1:C:605:ARG:CZ	1:C:607:GLU:HB3	2.48	0.44
1:C:649:TYR:HB3	1:C:657:HIS:O	2.17	0.44
1:A:301:TYR:HA	1:A:302:GLY:HA3	1.78	0.44
1:A:369:TRP:C	1:A:370:GLN:HG2	2.43	0.44
1:A:605:ARG:HH12	1:A:610:GLY:H	1.60	0.44
1:B:119:PRO:HG3	1:B:561:ALA:HA	1.97	0.44
1:B:155:ALA:HA	1:B:156:PRO:HD3	1.63	0.44
1:B:606:TYR:N	1:B:606:TYR:CD1	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:689:TYR:CD2	1:B:694:ILE:CD1	2.95	0.44
1:C:363:VAL:HG13	1:C:364:CYS:N	2.30	0.44
1:A:125:VAL:HG12	1:B:665:THR:OG1	2.18	0.43
1:A:142:TYR:HE1	1:A:378:SER:HG	1.59	0.43
1:A:297:MET:HE3	1:A:319:PHE:CG	2.53	0.43
1:A:313:SER:CB	1:A:314:TYR:CA	2.93	0.43
1:B:299:PRO:CB	1:B:354:TRP:HE1	2.30	0.43
1:B:605:ARG:HB2	1:B:611:PRO:O	2.18	0.43
1:B:708:ARG:NH2	1:C:277:ASP:H	2.15	0.43
1:C:150:PHE:CB	1:C:366:MET:HE3	2.45	0.43
1:A:567:VAL:HG21	1:B:640:TYR:CD1	2.53	0.43
1:A:605:ARG:HB2	1:A:611:PRO:O	2.18	0.43
1:A:607:GLU:HG2	1:A:608:ASP:H	1.82	0.43
1:A:610:GLY:HA3	1:A:611:PRO:HD3	1.44	0.43
1:B:688:VAL:CG1	1:C:369:TRP:CZ2	2.97	0.43
1:B:688:VAL:HG23	1:C:499:SER:O	2.18	0.43
1:C:179:TYR:CD1	1:C:179:TYR:C	2.95	0.43
1:C:253:LYS:CA	1:C:268:THR:HG21	2.43	0.43
1:C:338:ALA:HA	1:C:339:PRO:HD3	1.76	0.43
1:A:156:PRO:HB2	1:C:700:LEU:HD11	1.99	0.43
1:A:294:PHE:CD1	1:A:294:PHE:N	2.85	0.43
1:A:408:ASP:OD1	1:A:409:LEU:HG	2.18	0.43
1:A:501:ILE:HG23	1:A:502:GLU:N	2.33	0.43
1:A:640:TYR:CD1	1:C:567:VAL:HG21	2.53	0.43
1:A:686:LEU:HD11	1:B:369:TRP:CZ2	2.54	0.43
1:B:257:SER:HB3	1:B:264:ARG:HH12	1.83	0.43
1:B:543:ARG:HB3	1:B:550:ILE:HG21	2.00	0.43
1:C:326:TYR:OH	1:C:339:PRO:HG3	2.17	0.43
1:C:563:MET:HE3	1:C:563:MET:HB3	1.84	0.43
1:A:156:PRO:CD	1:C:700:LEU:HD21	2.48	0.43
1:A:614:GLU:CG	1:A:627:ARG:CZ	2.95	0.43
1:B:108:ASN:CB	1:B:645:GLY:HA3	2.48	0.43
1:B:125:VAL:HG12	1:C:665:THR:OG1	2.18	0.43
1:B:397:THR:CG2	1:B:398:ASN:N	2.82	0.43
1:C:610:GLY:HA3	1:C:611:PRO:HD3	1.43	0.43
1:A:152:GLU:HB2	1:A:495:ILE:O	2.19	0.43
1:A:394:THR:HG22	1:A:395:PHE:N	2.33	0.43
1:A:520:MET:CA	1:A:520:MET:CE	2.95	0.43
1:A:532:GLN:HA	1:A:532:GLN:NE2	2.33	0.43
1:A:713:ASP:HB2	1:C:294:PHE:CG	2.53	0.43
1:B:520:MET:CA	1:B:520:MET:CE	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:532:GLN:NE2	1:C:532:GLN:HA	2.33	0.43
1:C:543:ARG:HB3	1:C:550:ILE:HG21	2.00	0.43
1:C:607:GLU:HG2	1:C:608:ASP:H	1.83	0.43
1:A:456:LEU:HD21	1:A:461:ALA:CA	2.36	0.43
1:A:665:THR:OG1	1:C:125:VAL:HG12	2.18	0.43
1:B:146:ILE:HG21	1:B:424:ILE:HD12	2.01	0.43
1:B:434:ILE:HG22	1:B:435:LYS:N	2.34	0.43
1:C:207:CYS:HB2	1:C:234:LEU:HD11	2.00	0.43
1:A:156:PRO:HD2	1:C:700:LEU:HD21	1.99	0.43
1:A:224:HIS:HB2	1:A:269:VAL:CB	2.37	0.43
1:A:284:TYR:HD1	1:A:284:TYR:N	2.16	0.43
1:A:313:SER:HB2	1:A:314:TYR:CD1	2.43	0.43
1:A:543:ARG:HB3	1:A:550:ILE:HG21	2.00	0.43
1:B:142:TYR:HE1	1:B:378:SER:HG	1.59	0.43
1:B:200:LYS:O	1:B:204:LYS:HB2	2.18	0.43
1:B:326:TYR:OH	1:B:339:PRO:HG3	2.17	0.43
1:A:268:THR:HG22	1:A:269:VAL:N	2.33	0.43
1:B:553:VAL:CG1	1:B:554:THR:N	2.82	0.43
1:B:705:VAL:HG12	1:B:706:GLN:N	2.29	0.43
1:C:501:ILE:HG23	1:C:502:GLU:N	2.33	0.43
1:A:434:ILE:HG22	1:A:435:LYS:N	2.34	0.43
1:A:597:TYR:CZ	1:A:629:ALA:O	2.72	0.43
1:C:291:THR:HG21	1:C:293:ASP:CB	2.48	0.43
1:C:404:LEU:HD12	1:C:404:LEU:HA	1.85	0.43
1:C:589:ILE:CD1	1:C:630:ILE:HD13	2.46	0.43
1:A:497:THR:HG22	1:A:498:THR:O	2.19	0.43
1:A:538:LEU:HD21	1:B:539:TRP:CE3	2.53	0.43
1:A:699:LEU:CB	1:C:702:TYR:HE2	2.30	0.43
1:B:393:THR:HG22	1:B:505:ARG:HG2	2.01	0.43
1:C:288:VAL:HG12	1:C:289:LEU:O	2.19	0.43
1:C:384:PHE:HD1	1:C:384:PHE:HA	1.75	0.43
1:A:312:THR:HG23	1:A:313:SER:N	2.34	0.42
1:A:401:GLU:OE1	1:A:475:LYS:HD3	2.19	0.42
1:C:605:ARG:HH12	1:C:610:GLY:H	1.65	0.42
1:A:286:GLU:HG2	1:B:714:LEU:HD21	2.01	0.42
1:B:640:TYR:CD1	1:B:640:TYR:N	2.88	0.42
1:C:254:TYR:N	1:C:268:THR:CG2	2.82	0.42
1:C:305:GLU:OE1	1:C:305:GLU:HA	2.19	0.42
1:C:394:THR:HG22	1:C:395:PHE:N	2.33	0.42
1:C:553:VAL:CG1	1:C:554:THR:N	2.82	0.42
1:C:587:MET:HE1	1:C:598:SER:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:TYR:CD1	1:A:640:TYR:N	2.88	0.42
1:A:701:ASP:HB2	1:B:158:LYS:HZ3	1.84	0.42
1:A:707:ARG:CZ	1:B:242:ARG:H	2.33	0.42
1:B:649:TYR:CD2	1:B:657:HIS:CE1	3.07	0.42
1:C:117:PRO:HA	1:C:118:PRO:HD3	1.90	0.42
1:C:369:TRP:C	1:C:370:GLN:HG2	2.44	0.42
1:A:217:ASN:HB3	1:B:723:ILE:O	2.19	0.42
1:A:467:GLU:CD	1:A:470:ARG:HH12	2.28	0.42
1:A:539:TRP:CE3	1:C:538:LEU:HD21	2.53	0.42
1:B:288:VAL:CG1	1:B:289:LEU:N	2.82	0.42
1:B:394:THR:HG22	1:B:395:PHE:N	2.33	0.42
1:B:475:LYS:HA	1:B:476:PRO:HD3	1.77	0.42
1:B:597:TYR:CZ	1:B:629:ALA:O	2.72	0.42
1:B:688:VAL:N	1:C:369:TRP:CZ2	2.88	0.42
1:C:312:THR:CG2	1:C:314:TYR:HB2	2.30	0.42
1:A:711:LEU:HD13	1:A:715:ARG:CD	2.49	0.42
1:B:360:ARG:CZ	1:B:409:LEU:HD21	2.49	0.42
1:B:446:GLY:O	1:B:497:THR:HG23	2.20	0.42
1:B:467:GLU:CD	1:B:470:ARG:HH12	2.28	0.42
1:C:649:TYR:CD2	1:C:657:HIS:CE1	3.07	0.42
1:C:666:THR:CG2	1:C:667:VAL:N	2.83	0.42
1:A:301:TYR:CD1	1:A:301:TYR:O	2.73	0.42
1:A:553:VAL:CG1	1:A:554:THR:N	2.82	0.42
1:A:715:ARG:CD	1:B:243:THR:HG23	2.46	0.42
1:B:118:PRO:HA	1:B:119:PRO:HD3	1.83	0.42
1:B:150:PHE:CE2	1:B:368:LYS:HB2	2.54	0.42
1:B:401:GLU:OE1	1:B:475:LYS:HD3	2.20	0.42
1:B:501:ILE:HG23	1:B:502:GLU:N	2.33	0.42
1:B:596:CYS:CB	1:B:653:TYR:CE1	3.03	0.42
1:C:301:TYR:HA	1:C:302:GLY:HA3	1.64	0.42
1:C:572:THR:CG2	1:C:573:CYS:N	2.82	0.42
1:C:640:TYR:CD1	1:C:640:TYR:N	2.88	0.42
1:A:366:MET:HE3	1:A:366:MET:HB3	1.89	0.42
1:B:400:THR:CG2	1:B:401:GLU:N	2.83	0.42
1:B:536:LEU:HD13	1:C:669:THR:HG21	2.02	0.42
1:C:401:GLU:OE1	1:C:475:LYS:HD3	2.19	0.42
1:C:434:ILE:HG22	1:C:435:LYS:N	2.34	0.42
1:A:118:PRO:HA	1:A:119:PRO:HD3	1.83	0.42
1:A:124:VAL:CG1	1:A:125:VAL:N	2.83	0.42
1:A:273:VAL:HG12	1:A:274:GLU:N	2.34	0.42
1:A:164:TYR:CD1	1:A:164:TYR:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:TYR:N	1:A:265:TYR:HD1	2.17	0.42
1:A:284:TYR:N	1:A:284:TYR:CD1	2.87	0.42
1:A:397:THR:CG2	1:A:398:ASN:N	2.82	0.42
1:B:378:SER:HB2	1:B:385:ARG:HB2	2.02	0.42
1:A:279:ARG:HH22	1:C:700:LEU:H	1.67	0.42
1:A:576:VAL:CG1	1:A:577:ALA:N	2.83	0.42
1:B:469:LEU:HD22	1:B:469:LEU:HA	1.90	0.42
1:C:111:ALA:HB3	1:C:644:GLY:C	2.45	0.42
1:C:146:ILE:HG21	1:C:424:ILE:HD12	2.01	0.42
1:C:276:VAL:HG13	1:C:289:LEU:CD2	2.50	0.42
1:C:363:VAL:HG13	1:C:364:CYS:SG	2.60	0.42
1:C:367:THR:CG2	1:C:368:LYS:N	2.83	0.42
1:C:550:ILE:N	1:C:550:ILE:CD1	2.83	0.42
1:A:369:TRP:CZ2	1:C:686:LEU:HD11	2.54	0.41
1:A:446:GLY:O	1:A:497:THR:HG23	2.19	0.41
1:A:649:TYR:CD2	1:A:657:HIS:CE1	3.07	0.41
1:A:655:TYR:CE2	1:A:656:SER:O	2.74	0.41
1:B:301:TYR:HA	1:B:359:LYS:HB2	2.02	0.41
1:B:497:THR:HG22	1:B:498:THR:O	2.19	0.41
1:B:550:ILE:N	1:B:550:ILE:CD1	2.83	0.41
1:B:700:LEU:HD11	1:C:158:LYS:HB3	1.98	0.41
1:A:318:ARG:HD2	1:A:346:THR:O	2.20	0.41
1:A:378:SER:HB2	1:A:385:ARG:HB2	2.02	0.41
1:A:536:LEU:CD1	1:B:669:THR:HG21	2.50	0.41
1:A:723:ILE:H	1:C:217:ASN:HB3	1.84	0.41
1:B:124:VAL:CG1	1:B:125:VAL:N	2.83	0.41
1:B:610:GLY:HA3	1:B:611:PRO:HD3	1.44	0.41
1:B:666:THR:CG2	1:B:667:VAL:N	2.83	0.41
1:C:276:VAL:HG12	1:C:277:ASP:N	2.35	0.41
1:C:289:LEU:HD13	1:C:291:THR:HG22	2.02	0.41
1:C:393:THR:HG22	1:C:505:ARG:HG2	2.01	0.41
1:A:108:ASN:CB	1:A:645:GLY:HA3	2.49	0.41
1:A:464:TYR:CD1	1:A:464:TYR:C	2.98	0.41
1:A:536:LEU:HD13	1:B:669:THR:HG21	2.02	0.41
1:A:688:VAL:HA	1:B:369:TRP:CZ2	2.56	0.41
1:A:707:ARG:NH2	1:B:242:ARG:H	2.18	0.41
1:A:711:LEU:CD1	1:B:243:THR:CG2	2.95	0.41
1:B:281:VAL:CG1	1:B:282:TYR:N	2.82	0.41
1:C:296:TYR:HD1	1:C:296:TYR:N	2.10	0.41
1:C:520:MET:CA	1:C:520:MET:CE	2.95	0.41
1:C:576:VAL:CG1	1:C:577:ALA:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:TYR:N	1:C:606:TYR:CD1	2.86	0.41
1:A:146:ILE:HG21	1:A:424:ILE:HD12	2.01	0.41
1:B:157:TYR:CD1	1:B:300:PHE:CZ	3.08	0.41
1:B:283:PRO:O	1:B:300:PHE:HD2	2.02	0.41
1:B:536:LEU:CD1	1:C:669:THR:HG21	2.50	0.41
1:C:288:VAL:CG1	1:C:289:LEU:N	2.82	0.41
1:C:467:GLU:CD	1:C:470:ARG:HH12	2.28	0.41
1:A:111:ALA:HB3	1:A:644:GLY:C	2.45	0.41
1:A:256:PRO:HG3	1:A:265:TYR:O	2.20	0.41
1:B:164:TYR:CD1	1:B:164:TYR:N	2.88	0.41
1:B:276:VAL:CG1	1:B:277:ASP:N	2.82	0.41
1:B:582:ILE:CG2	1:B:583:VAL:N	2.83	0.41
1:B:601:LEU:HD12	1:B:601:LEU:N	2.36	0.41
1:C:124:VAL:CG1	1:C:125:VAL:N	2.83	0.41
1:C:174:TRP:CD1	1:C:263:HIS:CE1	3.08	0.41
1:C:597:TYR:CZ	1:C:629:ALA:O	2.73	0.41
1:A:229:GLU:HG2	1:A:230:THR:N	2.36	0.41
1:A:596:CYS:CB	1:A:653:TYR:CE1	3.03	0.41
1:A:697:SER:OG	1:B:154:ILE:HG13	2.20	0.41
1:B:221:THR:CG2	1:B:222:ALA:N	2.83	0.41
1:B:638:ARG:HH11	1:B:638:ARG:HD2	1.75	0.41
1:C:596:CYS:CB	1:C:653:TYR:CE1	3.03	0.41
1:A:106:ALA:HB2	1:A:643:PHE:CZ	2.55	0.41
1:A:223:PHE:CD1	1:A:223:PHE:N	2.89	0.41
1:A:666:THR:CG2	1:A:667:VAL:N	2.83	0.41
1:A:699:LEU:N	1:A:699:LEU:CD1	2.82	0.41
1:B:154:ILE:HB	1:B:155:ALA:HA	2.02	0.41
1:B:157:TYR:CG	1:B:300:PHE:CE1	3.09	0.41
1:C:172:GLN:CB	1:C:183:MET:HB2	2.48	0.41
1:A:550:ILE:N	1:A:550:ILE:CD1	2.83	0.41
1:A:659:LEU:N	1:A:659:LEU:CD1	2.83	0.41
1:A:667:VAL:HB	1:C:554:THR:CG2	2.51	0.41
1:A:669:THR:HG21	1:C:536:LEU:CD1	2.50	0.41
1:B:576:VAL:CG1	1:B:577:ALA:N	2.83	0.41
1:C:597:TYR:CE2	1:C:629:ALA:O	2.74	0.41
1:A:221:THR:CG2	1:A:222:ALA:N	2.83	0.41
1:A:288:VAL:CG1	1:A:289:LEU:N	2.83	0.41
1:A:400:THR:CG2	1:A:401:GLU:N	2.83	0.41
1:A:582:ILE:CG2	1:A:583:VAL:N	2.83	0.41
1:A:708:ARG:HD2	1:B:244:SER:CB	2.51	0.41
1:B:111:ALA:HB3	1:B:644:GLY:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:HIS:HA	1:B:271:CYS:O	2.20	0.41
1:B:276:VAL:CG1	1:B:290:ALA:H	2.33	0.41
1:B:283:PRO:O	1:B:300:PHE:CD2	2.74	0.41
1:B:332:THR:O	1:B:333:LYS:HB2	2.21	0.41
1:B:554:THR:CG2	1:C:667:VAL:HB	2.51	0.41
1:B:572:THR:CG2	1:B:573:CYS:N	2.82	0.41
1:C:133:CYS:HA	1:C:134:PRO:HD3	1.86	0.41
1:C:221:THR:CG2	1:C:222:ALA:N	2.83	0.41
1:C:287:PHE:CD1	1:C:297:MET:O	2.74	0.41
1:C:378:SER:HB2	1:C:385:ARG:HB2	2.02	0.41
1:A:563:MET:HE3	1:A:563:MET:HB3	1.84	0.41
1:B:267:THR:HG22	1:B:268:THR:N	2.36	0.41
1:B:365:THR:CG2	1:B:366:MET:N	2.84	0.41
1:C:332:THR:O	1:C:333:LYS:HB2	2.21	0.41
1:C:400:THR:CG2	1:C:401:GLU:N	2.83	0.41
1:C:600:PRO:HG3	1:C:641:PHE:CD2	2.56	0.41
1:A:332:THR:O	1:A:333:LYS:HB2	2.21	0.40
1:A:393:THR:HG22	1:A:505:ARG:HG2	2.01	0.40
1:C:283:PRO:HB3	1:C:300:PHE:CZ	2.56	0.40
1:C:655:TYR:CE2	1:C:656:SER:O	2.74	0.40
1:A:276:VAL:HG21	1:C:715:ARG:CZ	2.52	0.40
1:A:700:LEU:HD12	1:B:158:LYS:HZ1	1.86	0.40
1:A:713:ASP:CB	1:C:294:PHE:HD1	2.35	0.40
1:C:175:PHE:CD1	1:C:259:VAL:O	2.74	0.40
1:C:275:GLU:HG2	1:C:276:VAL:N	2.36	0.40
1:C:497:THR:HG22	1:C:498:THR:O	2.21	0.40
1:A:369:TRP:CE2	1:C:688:VAL:HA	2.56	0.40
1:A:554:THR:CG2	1:B:667:VAL:HB	2.51	0.40
1:A:587:MET:HE1	1:A:598:SER:C	2.45	0.40
1:A:597:TYR:CE2	1:A:629:ALA:O	2.74	0.40
1:A:715:ARG:CD	1:B:243:THR:CG2	2.96	0.40
1:B:198:ILE:N	1:B:198:ILE:CD1	2.85	0.40
1:B:597:TYR:CE2	1:B:629:ALA:O	2.74	0.40
1:B:600:PRO:HG3	1:B:641:PHE:CD2	2.56	0.40
1:B:707:ARG:CZ	1:C:242:ARG:HB3	2.51	0.40
1:C:582:ILE:CG2	1:C:583:VAL:N	2.83	0.40
1:C:641:PHE:HB2	1:C:648:VAL:HG12	2.03	0.40
1:A:234:LEU:HD23	1:A:247:TRP:C	2.46	0.40
1:A:469:LEU:HD22	1:A:469:LEU:HA	1.90	0.40
1:A:601:LEU:HD12	1:A:601:LEU:N	2.36	0.40
1:A:669:THR:HG21	1:C:536:LEU:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:THR:HB	1:B:356:TRP:HE3	1.87	0.40
1:B:408:ASP:OD1	1:B:409:LEU:HG	2.21	0.40
1:C:597:TYR:HD1	1:C:597:TYR:C	2.30	0.40
1:A:117:PRO:HA	1:A:118:PRO:HD3	1.90	0.40
1:A:245:ARG:HG3	1:A:275:GLU:OE1	2.22	0.40
1:A:297:MET:HB2	1:A:345:LEU:HD22	2.04	0.40
1:C:224:HIS:HB2	1:C:269:VAL:HB	2.04	0.40
1:C:377:ARG:HA	1:C:385:ARG:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	604/622 (97%)	585 (97%)	14 (2%)	5 (1%)	16	54
1	B	604/622 (97%)	581 (96%)	19 (3%)	4 (1%)	18	56
1	C	604/622 (97%)	588 (97%)	13 (2%)	3 (0%)	24	63
All	All	1812/1866 (97%)	1754 (97%)	46 (2%)	12 (1%)	20	56

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	276	VAL
1	A	409	LEU
1	B	276	VAL
1	B	409	LEU
1	C	226	ASP
1	C	409	LEU
1	A	226	ASP
1	A	233	GLU
1	A	410	GLY

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Mol	Chain	Res	Type
1	B	228	HIS
1	B	410	GLY
1	C	410	GLY

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	530/541 (98%)	489 (92%)	41 (8%)	12	32
1	B	530/541 (98%)	495 (93%)	35 (7%)	15	37
1	C	530/541 (98%)	497 (94%)	33 (6%)	16	38
All	All	1590/1623 (98%)	1481 (93%)	109 (7%)	16	36

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	140	GLN
1	A	152	GLU
1	A	154	ILE
1	A	226	ASP
1	A	227	ASP
1	A	232	MET
1	A	234	LEU
1	A	235	LYS
1	A	255	ASN
1	A	265	TYR
1	A	281	VAL
1	A	286	GLU
1	A	289	LEU
1	A	296	TYR
1	A	297	MET
1	A	301	TYR
1	A	304	ARG
1	A	312	THR

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Mol	Chain	Res	Type
1	A	314	TYR
1	A	391	ILE
1	A	392	SER
1	A	404	LEU
1	A	415	LYS
1	A	456	LEU
1	A	460	LEU
1	A	463	LEU
1	A	502	GLU
1	A	584	GLN
1	A	605	ARG
1	A	628	ASP
1	A	659	LEU
1	A	679	GLU
1	A	689	TYR
1	A	699	LEU
1	A	700	LEU
1	A	701	ASP
1	A	702	TYR
1	A	707	ARG
1	A	711	LEU
1	A	719	ILE
1	B	110	ASP
1	B	140	GLN
1	B	228	HIS
1	B	229	GLU
1	B	232	MET
1	B	235	LYS
1	B	243	THR
1	B	254	TYR
1	B	255	ASN
1	B	265	TYR
1	B	285	ASP
1	B	300	PHE
1	B	301	TYR
1	B	303	TYR
1	B	304	ARG
1	B	312	THR
1	B	314	TYR
1	B	391	ILE
1	B	392	SER
1	B	404	LEU

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Mol	Chain	Res	Type
1	B	415	LYS
1	B	456	LEU
1	B	460	LEU
1	B	463	LEU
1	B	502	GLU
1	B	584	GLN
1	B	605	ARG
1	B	628	ASP
1	B	659	LEU
1	B	679	GLU
1	B	687	GLU
1	B	688	VAL
1	B	699	LEU
1	B	700	LEU
1	B	718	ASP
1	C	110	ASP
1	C	140	GLN
1	C	154	ILE
1	C	158	LYS
1	C	225	ARG
1	C	227	ASP
1	C	235	LYS
1	C	258	ARG
1	C	265	TYR
1	C	268	THR
1	C	282	TYR
1	C	284	TYR
1	C	286	GLU
1	C	289	LEU
1	C	291	THR
1	C	296	TYR
1	C	304	ARG
1	C	307	SER
1	C	310	GLU
1	C	363	VAL
1	C	391	ILE
1	C	392	SER
1	C	404	LEU
1	C	415	LYS
1	C	456	LEU
1	C	460	LEU
1	C	463	LEU

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Mol	Chain	Res	Type
1	C	502	GLU
1	C	584	GLN
1	C	605	ARG
1	C	628	ASP
1	C	659	LEU
1	C	679	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	248	HIS
1	A	321	GLN
1	A	512	HIS
1	A	516	HIS
1	A	580	ASN
1	B	217	ASN
1	B	248	HIS
1	B	255	ASN
1	B	311	HIS
1	B	321	GLN
1	B	512	HIS
1	B	516	HIS
1	B	580	ASN
1	C	217	ASN
1	C	248	HIS
1	C	321	GLN
1	C	512	HIS
1	C	516	HIS
1	C	580	ASN
1	C	712	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

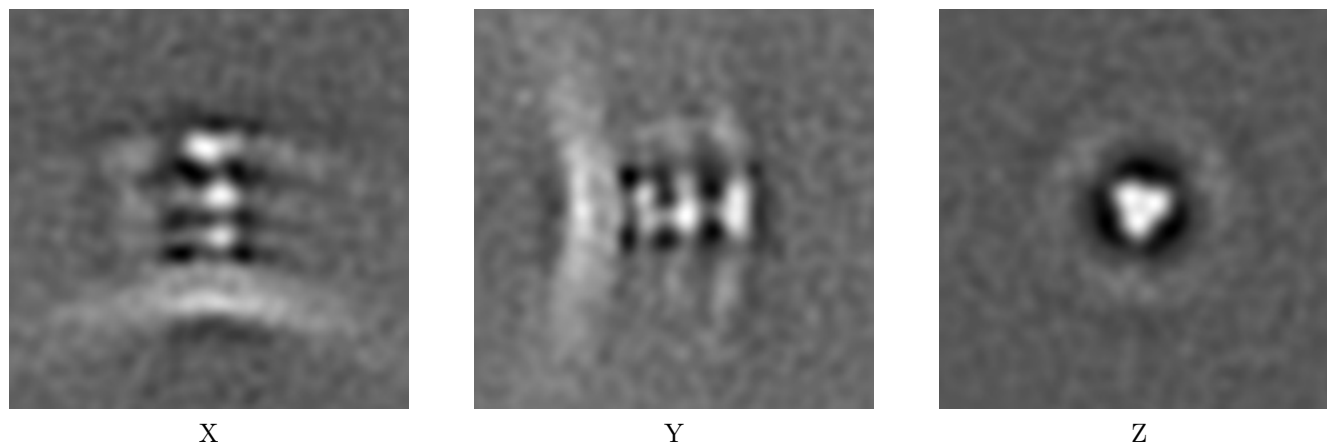
5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Tomogram visualisation [i](#)

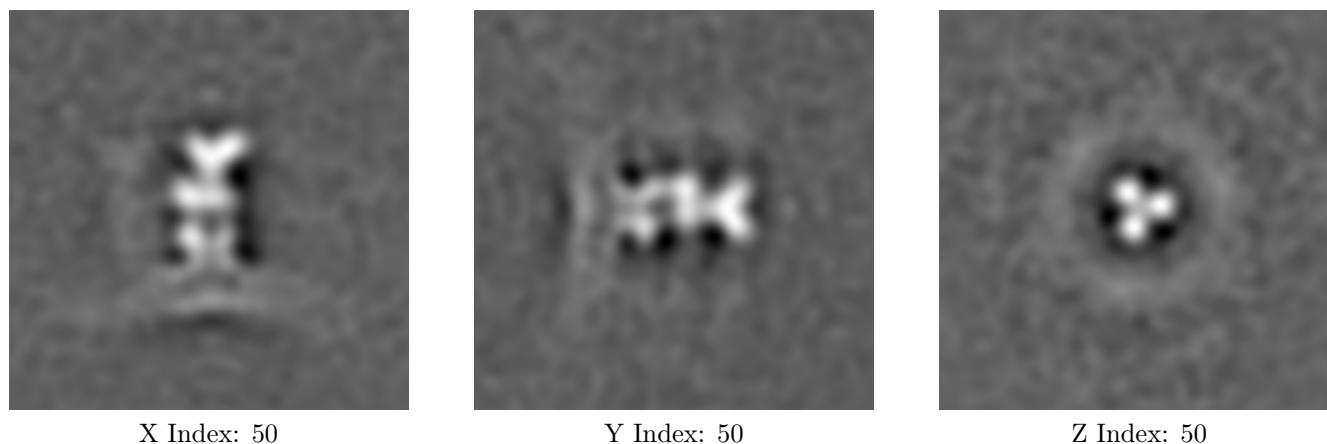
This section contains visualisations of the EMDB entry EMD-2380. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



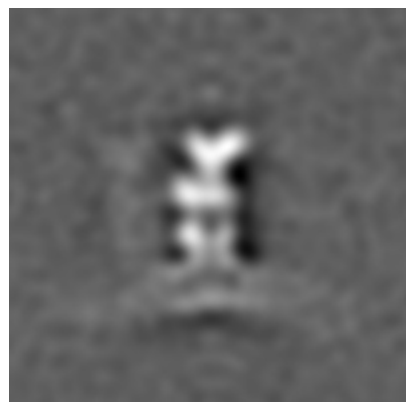
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)

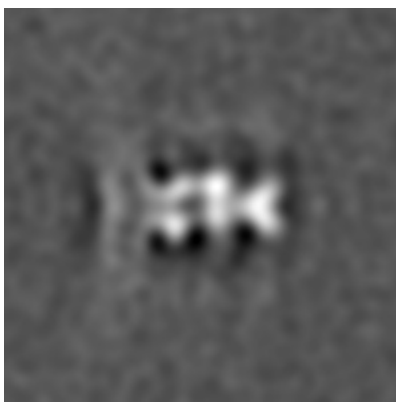


The images above show central slices of the tomogram in three orthogonal directions.

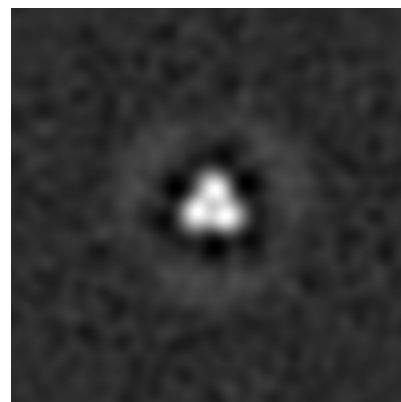
6.3 Largest variance slices [i](#)



X Index: 50



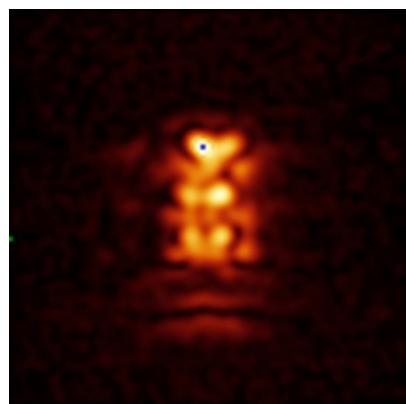
Y Index: 51



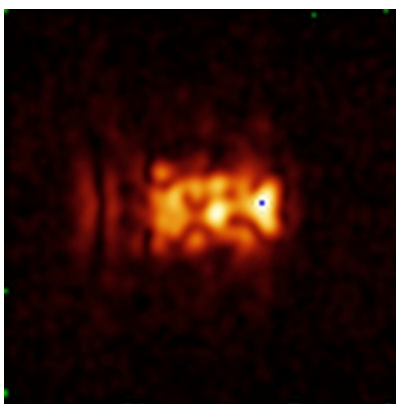
Z Index: 65

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

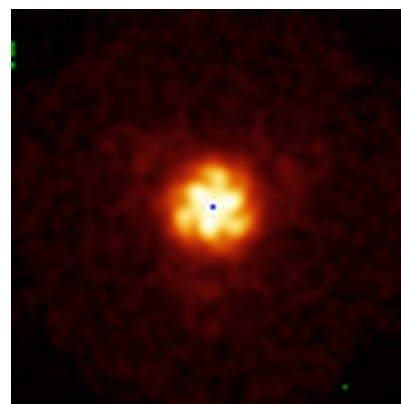
6.4 Orthogonal standard-deviation projections (False-color) [i](#)



X



Y



Z

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

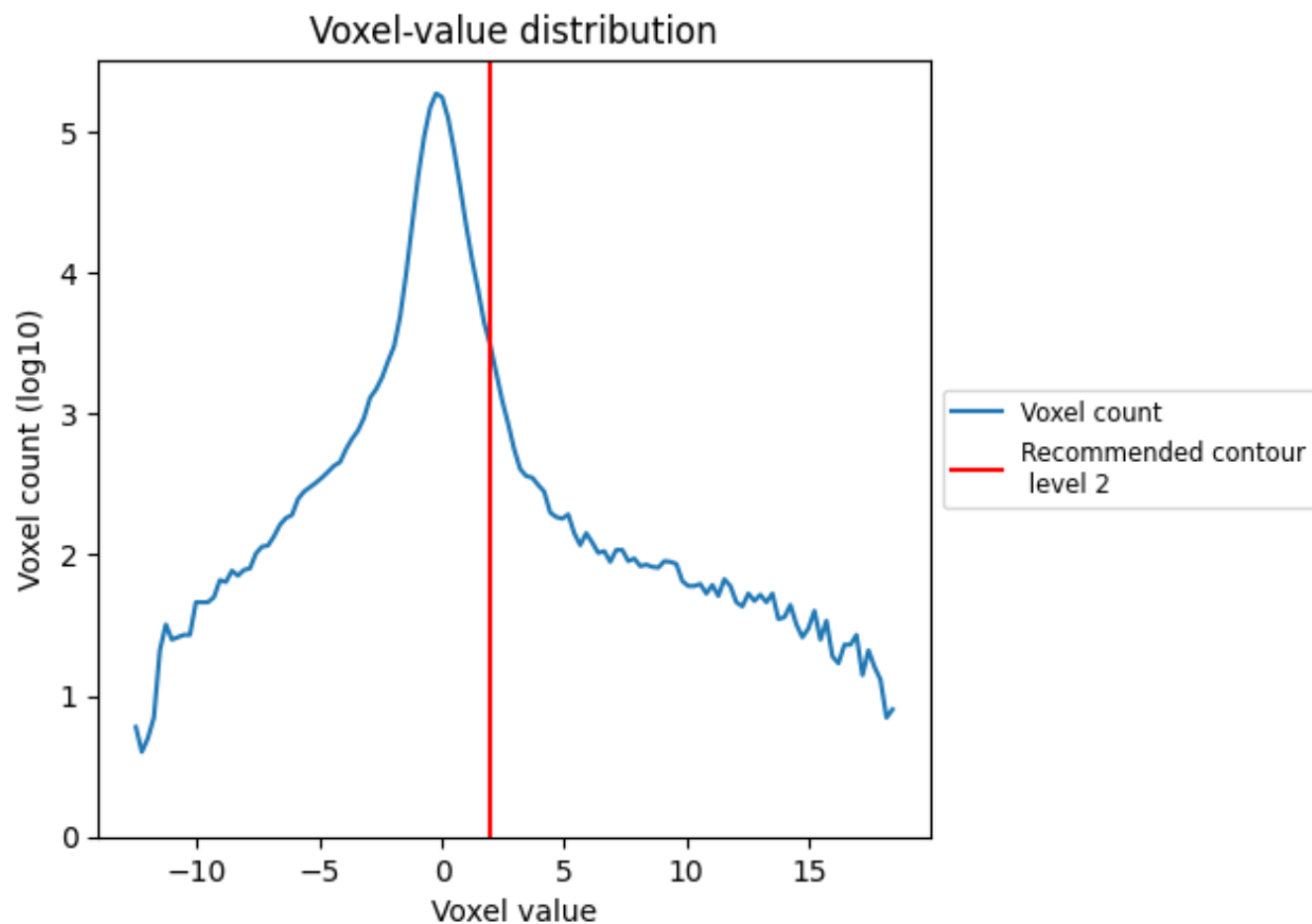
6.5 Mask visualisation [i](#)

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

7 Tomogram analysis [i](#)

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

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

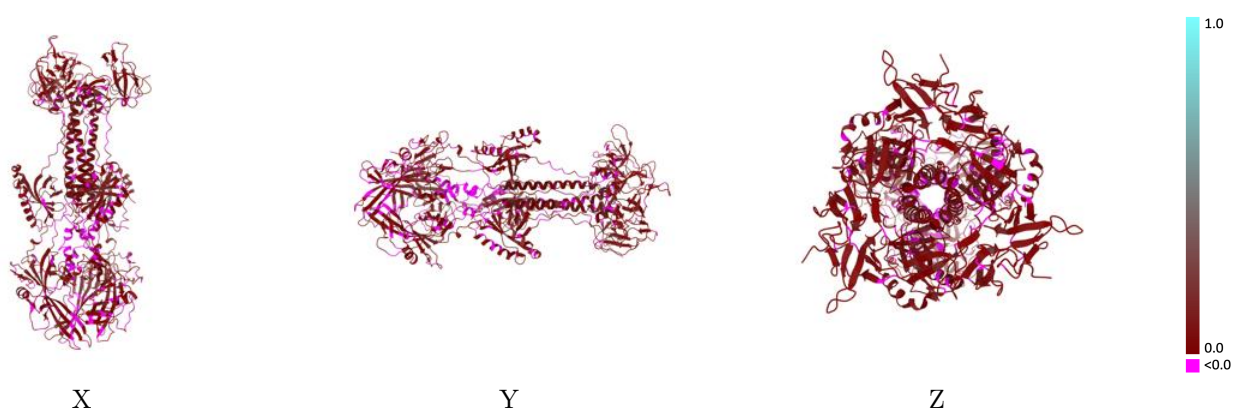
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2380 and PDB model 4BOM. Per-residue inclusion information can be found in section [3](#) on page [4](#).

8.1 Map-model overlay [i](#)

This section was not generated.

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

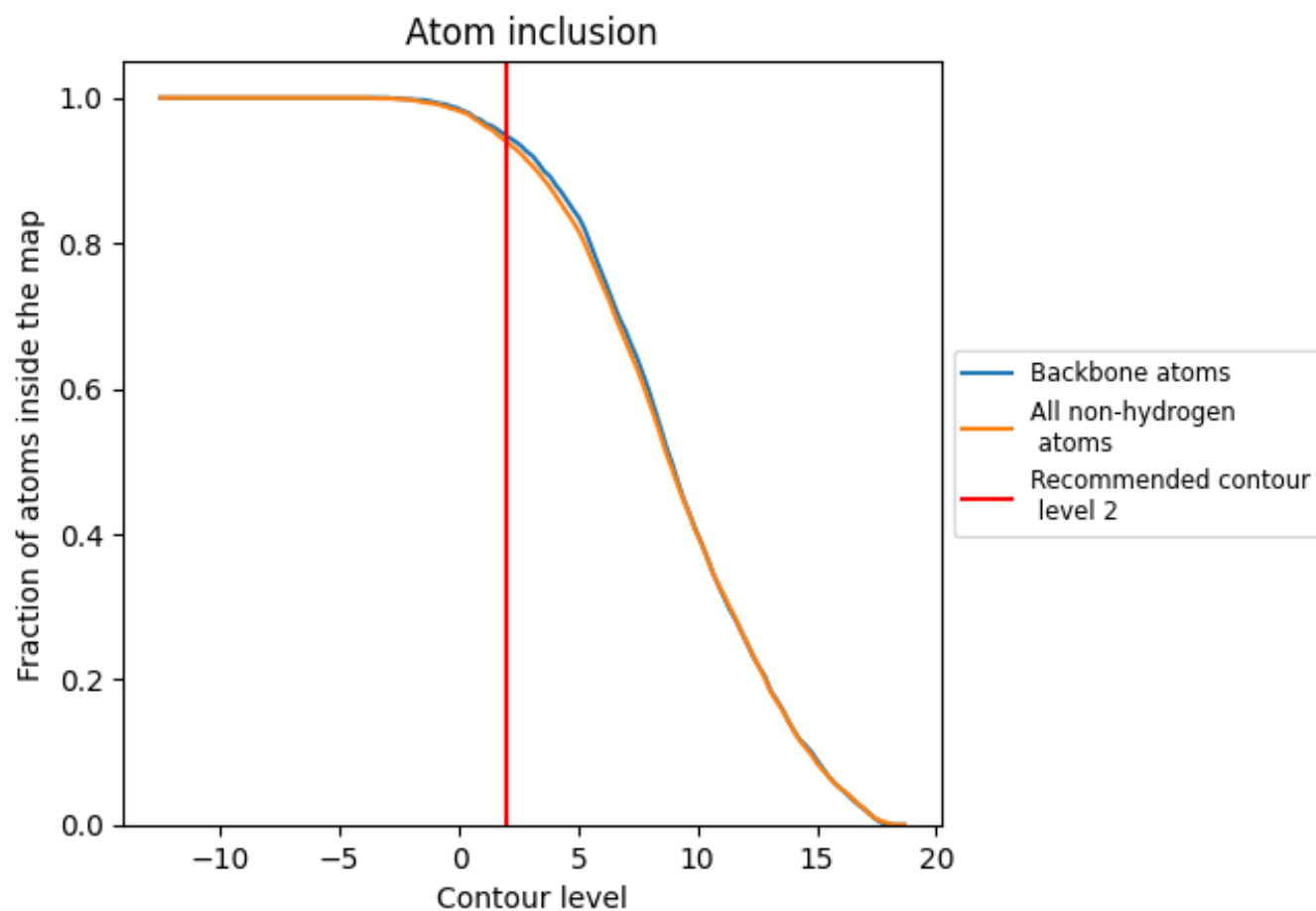


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9390	0.0540
A	0.9370	0.0530
B	0.9400	0.0530
C	0.9400	0.0560

