



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:15 PM UTC

PDB ID : 3J17 / pdb_00003j17
EMDB ID : EMD-5376
Title : Structure of a transcribing cypovirus by cryo-electron microscopy
Authors : Yang, C.; Ji, G.; Liu, H.; Zhang, K.; Liu, G.; Sun, F.; Zhu, P.; Cheng, L.
Deposited on : 2011-12-25
Resolution : 4.10 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
Mogul : 2022.3.0, CSD as543be (2022)
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

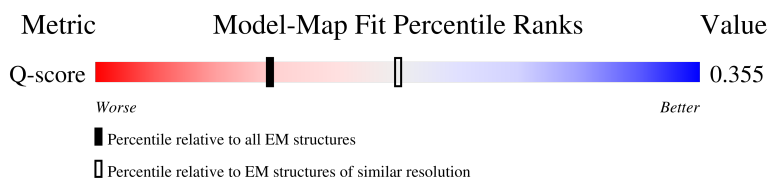
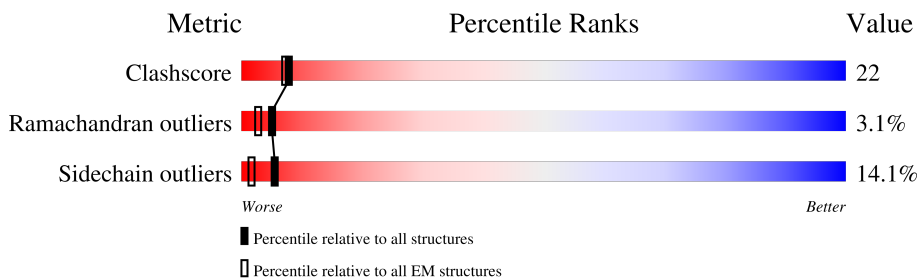
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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	6458 (3.60 - 4.60)

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	1058	
2	B	1333	
2	C	1333	
3	D	448	

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Mol	Chain	Length	Quality of chain
3	E	448	5% 26% 28% 10% 35%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32047 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 Structural protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1047	Total	C	N	O	P	S	
			8372	5304	1444	1579	1	44	0

- Molecule 2 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1180	Total	C	N	O	S		
			9317	5889	1621	1771	36	0	0
2	C	1244	Total	C	N	O	S		
			9806	6191	1704	1873	38	0	0

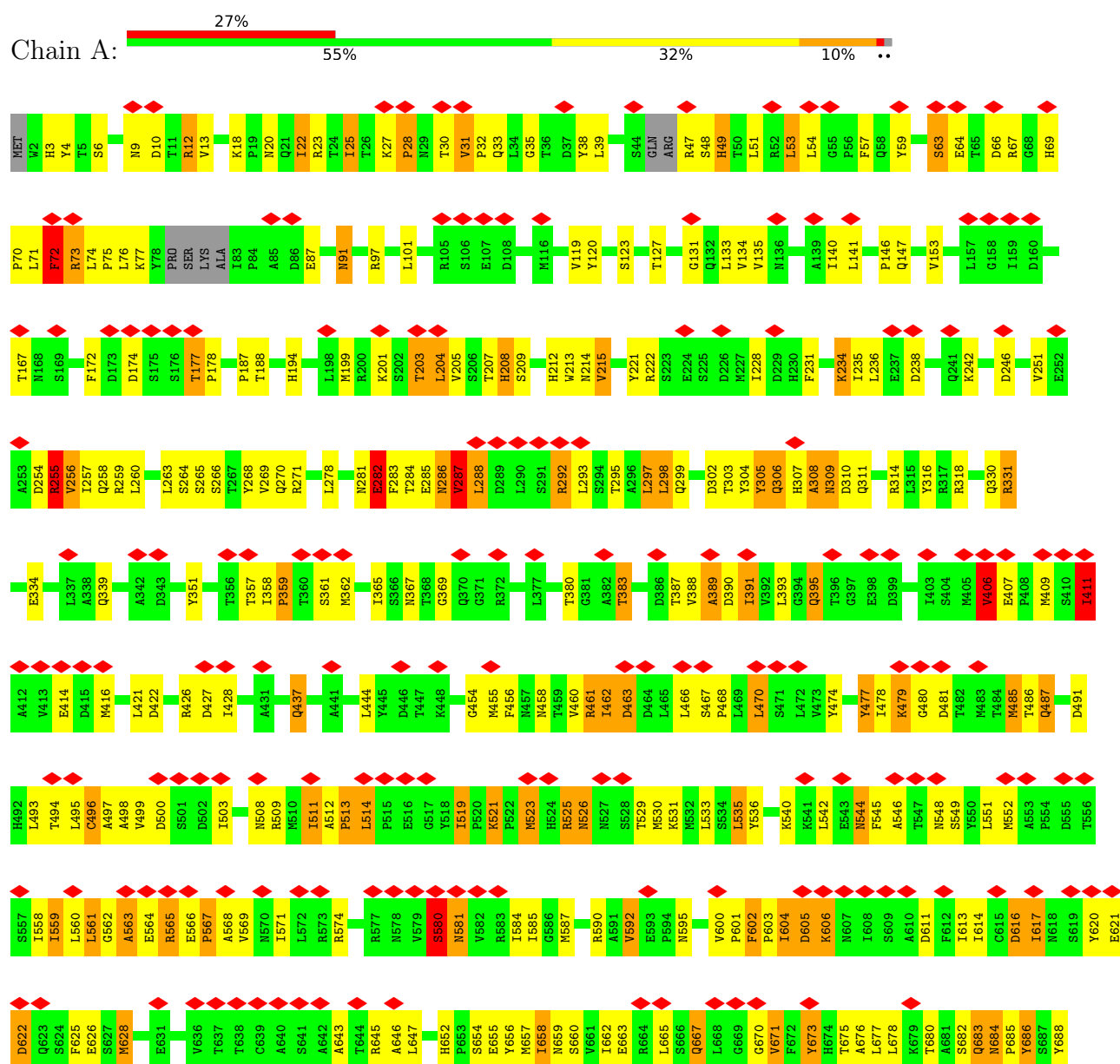
- Molecule 3 is a protein called Structural protein VP5.

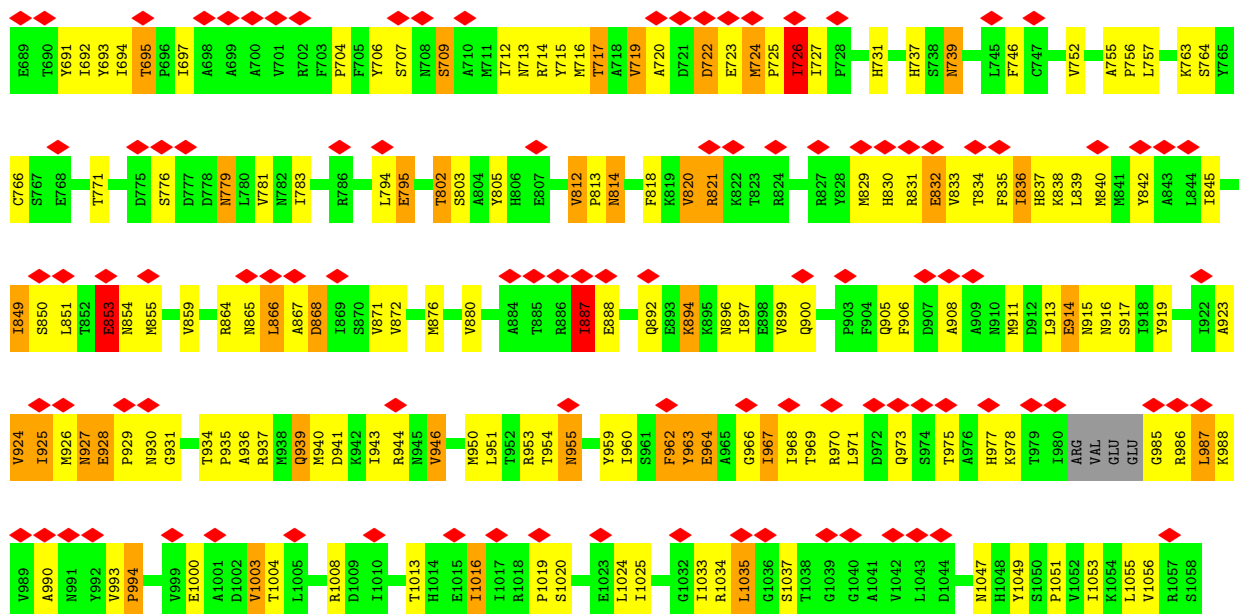
Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	291	Total	C	N	O	S		
			2276	1446	398	424	8	0	0
3	E	291	Total	C	N	O	S		
			2276	1446	398	424	8	0	0

3 Residue-property plots

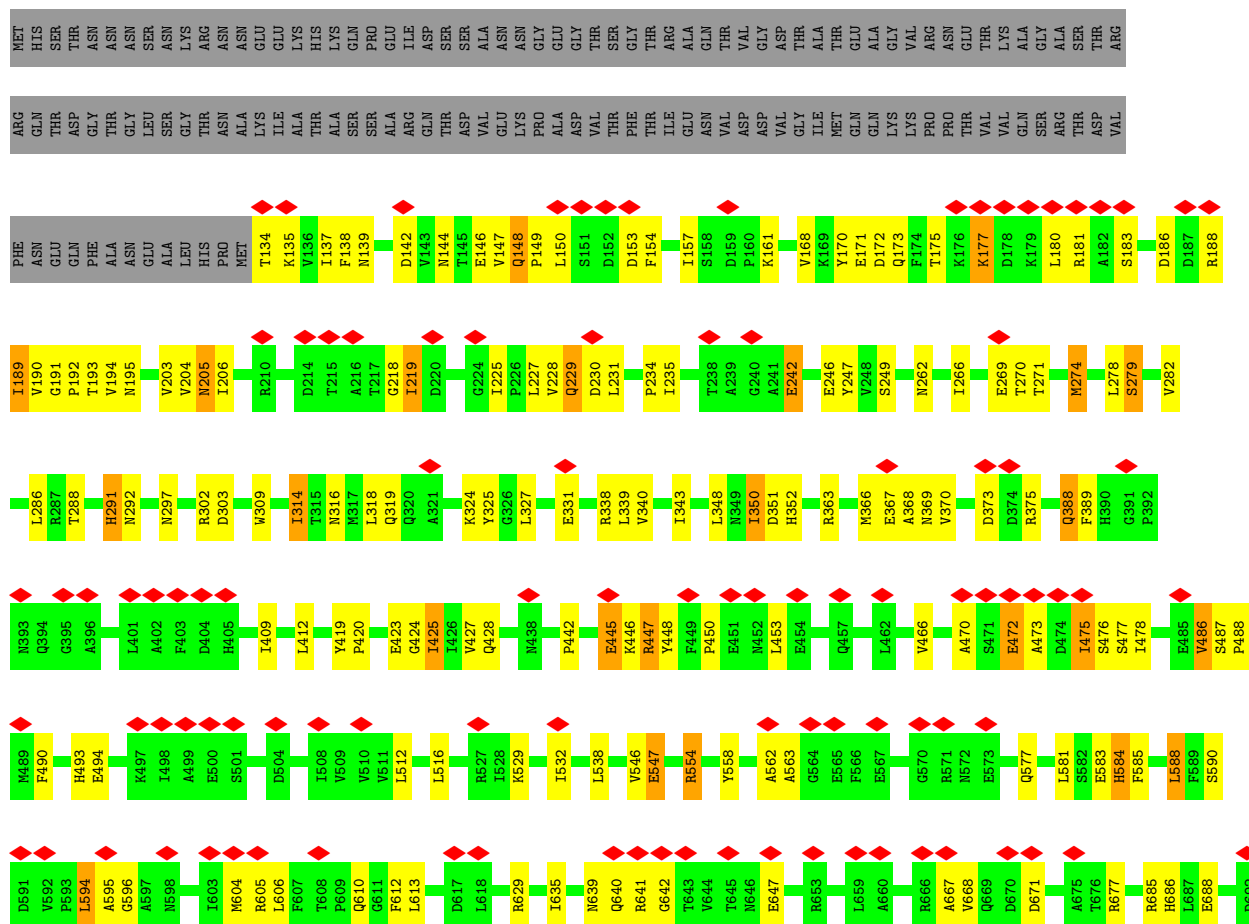
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

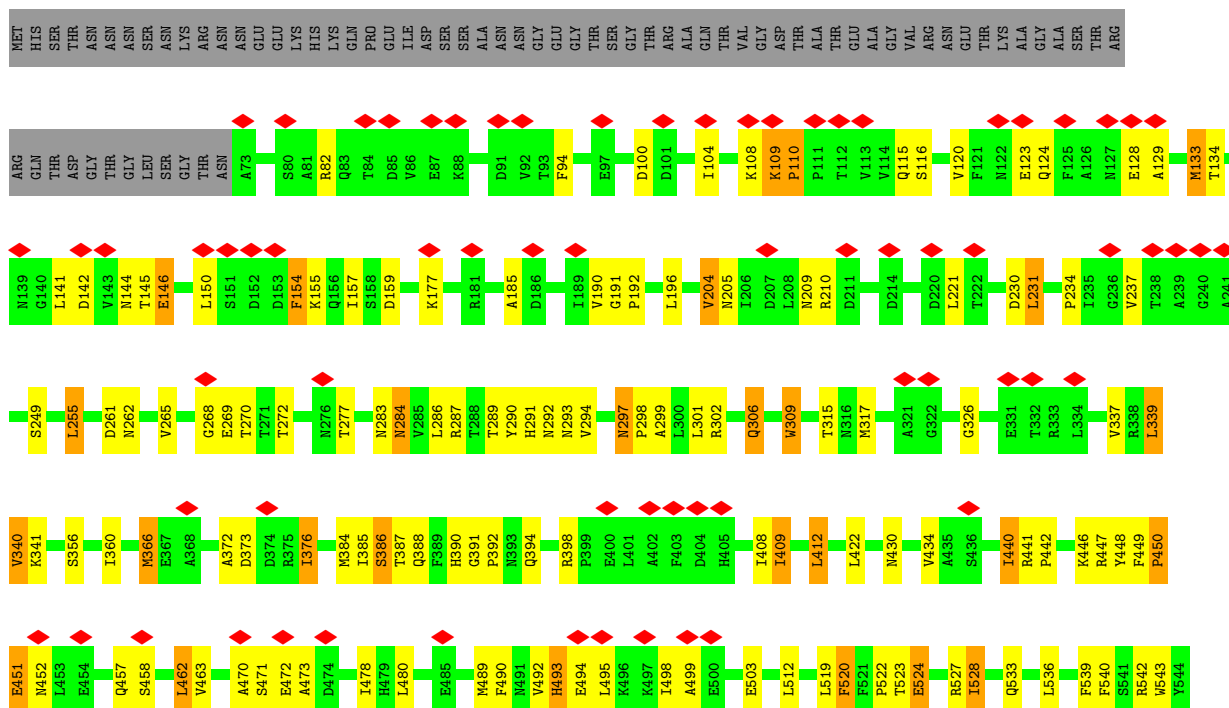
• Molecule 1: Structural protein VP3

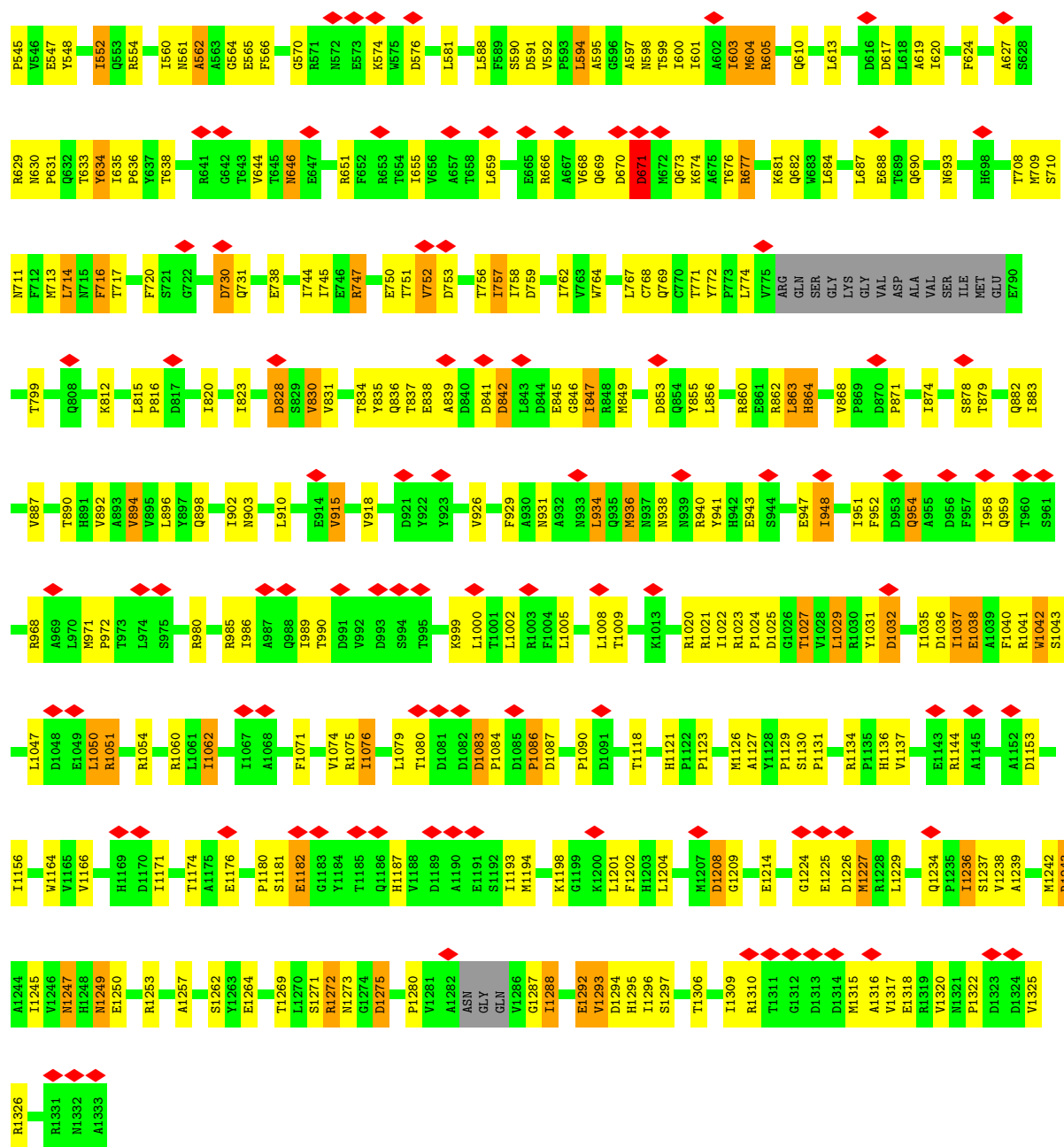




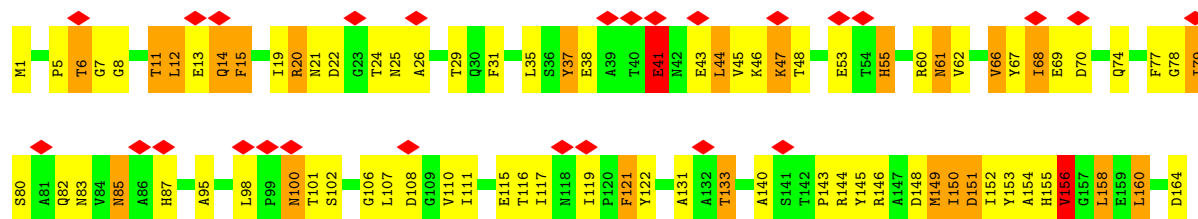
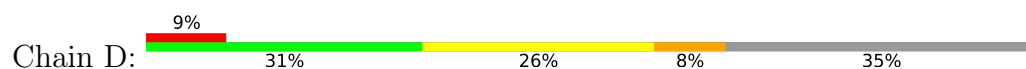
• Molecule 2: VP1

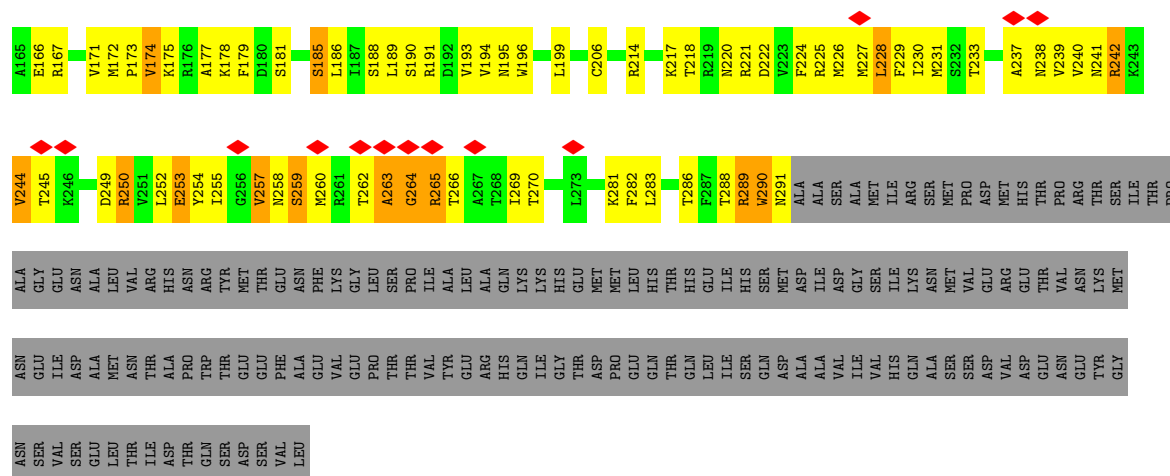




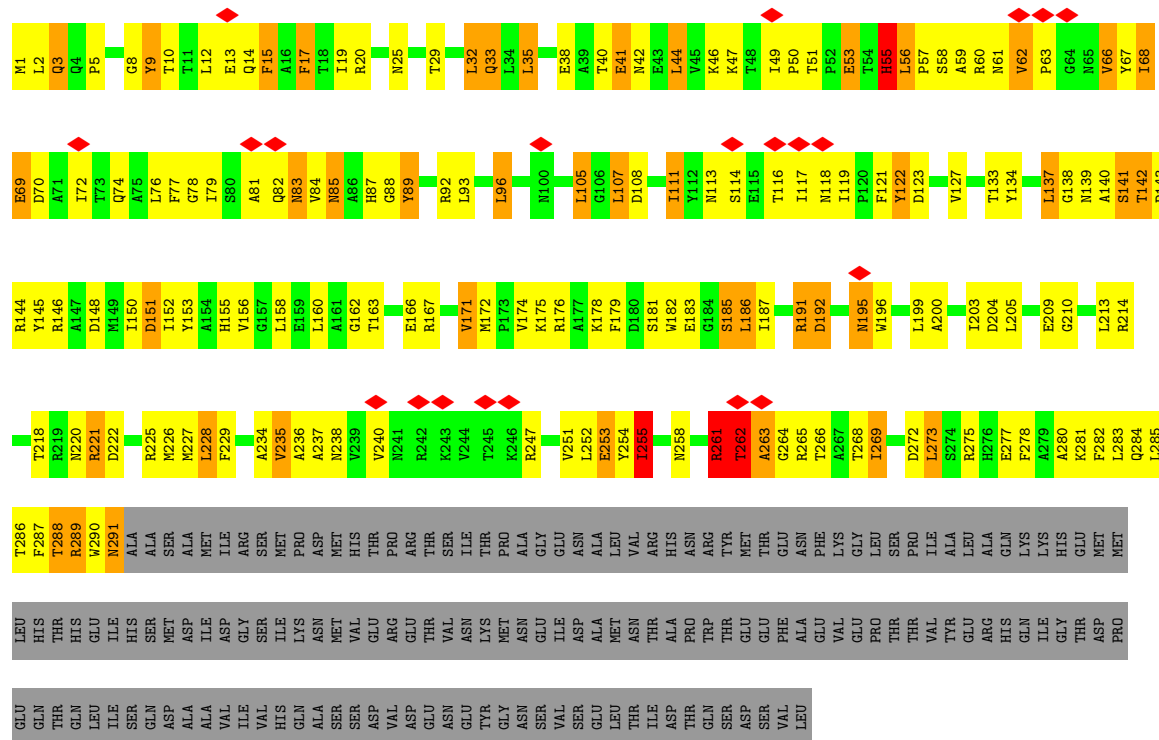
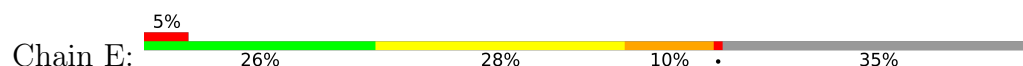


• Molecule 3: Structural protein VP5





• Molecule 3: Structural protein VP5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	8000	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	each image	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	125390	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	15.127	Depositor
Minimum map value	-10.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.002	Depositor
Recommended contour level	2.6	Depositor
Map size ($\text{\AA}$)	861.12, 861.12, 430.56	wwPDB
Map dimensions	720, 720, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.196, 1.196, 1.196	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GPL

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	0.55	0/8520	0.87	11/11599 (0.1%)
2	B	0.48	0/9508	0.82	7/12941 (0.1%)
2	C	0.50	0/10006	0.83	7/13622 (0.1%)
3	D	0.49	0/2322	1.00	14/3156 (0.4%)
3	E	0.51	0/2322	1.22	28/3156 (0.9%)
All	All	0.51	0/32678	0.88	67/44474 (0.2%)

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	235	VAL	N-CA-C	11.79	121.61	110.53
3	E	59	ALA	CB-CA-C	-11.57	92.91	110.26
3	E	253	GLU	N-CA-C	11.50	123.38	111.07
3	E	87	HIS	N-CA-C	10.65	122.89	111.28
3	D	41	GLU	N-CA-C	9.99	125.50	111.52
3	E	57	PRO	CB-CA-C	-9.45	99.63	111.64
3	E	237	ALA	N-CA-C	9.21	121.08	111.14
3	E	60	ARG	N-CA-C	9.18	125.00	113.43
3	E	192	ASP	N-CA-C	9.03	120.89	111.14
3	E	60	ARG	N-CA-CB	-8.16	96.63	110.51
3	E	59	ALA	N-CA-C	7.93	121.24	109.59
3	E	263	ALA	N-CA-C	-7.79	94.91	108.08
3	E	88	GLY	N-CA-C	7.52	121.75	112.73
3	E	96	LEU	N-CA-C	7.33	119.28	111.28
1	A	993	VAL	CA-C-N	7.33	129.01	119.84
1	A	993	VAL	C-N-CA	7.33	129.01	119.84
3	E	261	ARG	N-CA-C	7.23	119.37	107.73
3	E	33	GLN	N-CA-C	7.14	119.06	111.28
2	C	1226	ASP	N-CA-C	7.00	120.64	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	133	THR	N-CA-C	7.00	121.94	113.41
3	D	7	GLY	N-CA-C	-6.99	96.61	113.18
3	E	89	TYR	N-CA-C	6.83	118.72	111.28
2	B	1082	ASP	N-CA-C	6.79	119.97	108.90
3	D	156	VAL	N-CA-C	6.56	117.31	110.62
3	E	141	SER	N-CA-C	6.56	119.42	111.82
1	A	964	GLU	N-CA-C	6.55	118.98	111.11
3	E	58	SER	N-CA-C	6.55	119.02	110.43
3	D	11	THR	N-CA-C	-6.22	106.37	112.97
2	B	1210	LEU	N-CA-C	-6.19	106.37	114.04
3	E	3	GLN	CB-CA-C	-6.11	109.51	116.54
3	E	171	VAL	N-CA-C	6.02	117.68	108.71
2	C	1225	GLU	N-CA-C	5.91	117.62	109.29
3	E	262	THR	N-CA-C	5.84	123.23	110.80
1	A	308	ALA	CA-C-N	5.83	132.19	121.70
1	A	308	ALA	C-N-CA	5.83	132.19	121.70
3	E	181	SER	N-CA-C	5.77	118.05	108.99
3	D	257	VAL	CA-C-N	-5.73	114.82	122.72
3	D	257	VAL	C-N-CA	-5.73	114.82	122.72
3	E	185	SER	N-CA-C	5.71	117.50	111.28
3	D	263	ALA	N-CA-C	-5.66	105.09	112.23
3	D	98	LEU	CA-C-N	5.64	126.90	119.84
3	D	98	LEU	C-N-CA	5.64	126.90	119.84
1	A	208	HIS	N-CA-C	5.61	118.27	107.44
3	D	6	THR	CB-CA-C	-5.60	99.28	110.42
2	B	1122	PRO	N-CA-C	5.58	117.50	110.70
3	D	264	GLY	N-CA-C	5.55	118.94	112.50
3	E	32	LEU	N-CA-C	5.53	118.02	111.33
2	C	110	PRO	N-CA-C	5.52	117.44	110.70
2	C	1083	ASP	CA-C-N	5.50	126.72	119.84
2	C	1083	ASP	C-N-CA	5.50	126.72	119.84
3	E	9	TYR	N-CA-C	-5.50	106.62	113.38
2	C	638	THR	CB-CA-C	-5.43	109.33	115.79
2	B	205	ASN	N-CA-C	5.37	115.63	108.38
3	D	259	SER	N-CA-C	-5.33	101.69	109.63
3	D	185	SER	CB-CA-C	-5.33	109.98	117.23
1	A	72	PHE	N-CA-C	5.32	122.13	110.80
2	B	941	TYR	N-CA-C	-5.28	99.55	110.80
1	A	287	VAL	N-CA-C	5.25	120.26	109.34
3	E	61	ASN	N-CA-C	5.24	118.47	111.24
1	A	766	CYS	N-CA-C	5.14	114.92	108.45
2	B	1255	ARG	CB-CA-C	-5.10	110.68	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	LYS	CA-C-N	5.08	124.25	118.97
1	A	18	LYS	C-N-CA	5.08	124.25	118.97
3	D	151	ASP	N-CA-C	5.07	116.80	111.28
3	E	255	ILE	N-CA-C	5.07	115.79	110.62
2	C	941	TYR	N-CA-C	5.05	116.62	110.41
2	B	668	VAL	N-CA-C	-5.01	107.95	112.96

There are no chirality outliers.

There are no planarity outliers.

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	8372	0	8310	429	0
2	B	9317	0	9234	352	0
2	C	9806	0	9713	347	0
3	D	2276	0	2271	230	0
3	E	2276	0	2277	260	0
All	All	32047	0	31805	1435	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 22.

All (1435) 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:A:194:HIS:CE1	3:D:146:ARG:NH1	1.74	1.53
2:B:271:THR:CG2	2:C:237:VAL:HG23	1.34	1.53
3:E:46:LYS:HD3	3:E:155:HIS:CE1	1.49	1.45
3:E:53:GLU:HG2	3:E:145:TYR:CD1	1.57	1.37
2:B:271:THR:HG21	2:C:237:VAL:CG2	1.54	1.36
2:B:1044:ARG:NH2	3:D:266:THR:HG22	1.42	1.34
2:B:274:MET:CG	2:C:234:PRO:HD3	1.58	1.33
3:E:46:LYS:CD	3:E:155:HIS:HE1	1.40	1.31
3:E:1:MET:HE1	3:E:121:PHE:CE2	1.66	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:253:GLU:OE1	3:D:254:TYR:CE2	1.83	1.30
3:D:253:GLU:HG3	3:D:254:TYR:CD2	1.68	1.29
1:A:194:HIS:CE1	3:D:146:ARG:HH11	1.37	1.29
2:B:271:THR:CG2	2:C:237:VAL:CG2	2.08	1.29
1:A:47:ARG:CZ	2:B:596:GLY:HA2	1.60	1.29
3:D:8:GLY:O	3:D:11:THR:HG22	1.34	1.27
3:D:253:GLU:OE1	3:D:254:TYR:HE2	1.03	1.27
3:E:68:ILE:C	3:E:68:ILE:HD13	1.56	1.26
3:E:32:LEU:O	3:E:35:LEU:CD1	1.84	1.24
1:A:47:ARG:NH2	2:B:596:GLY:CA	2.01	1.23
1:A:47:ARG:NE	2:B:595:ALA:O	1.71	1.23
1:A:47:ARG:HH21	2:B:596:GLY:N	1.35	1.22
1:A:194:HIS:NE2	3:D:146:ARG:NH1	1.88	1.22
3:D:5:PRO:O	3:D:6:THR:CG2	1.90	1.20
2:C:100:ASP:OD1	3:E:82:GLN:NE2	1.73	1.19
3:E:182:TRP:O	3:E:183:GLU:HG2	1.07	1.19
3:E:289:ARG:HD2	3:E:289:ARG:O	1.40	1.19
2:B:137:ILE:HD11	2:C:759:ASP:CG	1.67	1.18
1:A:308:ALA:H	1:A:309:ASN:HB2	1.01	1.18
3:D:45:VAL:HG13	3:D:171:VAL:HG22	1.19	1.18
1:A:724:MET:HB3	1:A:725:PRO:CD	1.71	1.18
1:A:47:ARG:HH21	2:B:596:GLY:CA	1.58	1.17
3:E:55:HIS:HD2	3:E:145:TYR:CE2	1.63	1.17
1:A:47:ARG:NH2	2:B:596:GLY:HA2	1.58	1.17
3:D:5:PRO:O	3:D:6:THR:HG22	1.01	1.16
1:A:307:HIS:CB	1:A:308:ALA:HA	1.70	1.16
2:B:445:GLU:HB3	2:B:446:LYS:HA	1.17	1.15
2:B:388:GLN:OE1	2:C:499:ALA:HB1	1.41	1.15
3:E:137:LEU:HD23	3:E:137:LEU:C	1.72	1.14
3:E:107:LEU:HA	3:E:122:TYR:HE1	1.06	1.14
3:E:158:LEU:O	3:E:162:GLY:HA3	1.48	1.13
1:A:307:HIS:HB2	1:A:308:ALA:CA	1.79	1.12
2:B:1044:ARG:NE	3:D:266:THR:CG2	2.12	1.12
3:E:205:LEU:HD13	3:E:205:LEU:O	1.49	1.12
3:D:217:LYS:HD3	3:D:290:TRP:CH2	1.82	1.12
3:D:149:MET:CE	3:D:260:MET:HE1	1.80	1.11
3:E:175:LYS:HB2	3:E:255:ILE:CD1	1.80	1.11
1:A:308:ALA:N	1:A:309:ASN:HB2	1.66	1.10
3:D:149:MET:HE3	3:D:260:MET:HE1	1.10	1.09
3:E:49:ILE:HG23	3:E:50:PRO:HD2	1.35	1.08
1:A:127:THR:CG2	2:B:640:GLN:H	1.68	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:182:TRP:O	3:E:183:GLU:CG	2.01	1.07
3:D:217:LYS:HD3	3:D:290:TRP:CZ3	1.88	1.06
1:A:461:ARG:HG3	1:A:461:ARG:HH11	1.19	1.06
1:A:928:GLU:HB2	1:A:929:PRO:HD2	1.32	1.06
2:B:1044:ARG:CZ	3:D:266:THR:CG2	2.34	1.06
1:A:127:THR:HG21	2:B:640:GLN:N	1.70	1.05
2:B:338:ARG:HH21	2:C:1002:LEU:HD22	1.21	1.04
2:B:1044:ARG:CZ	3:D:266:THR:HG22	1.84	1.04
3:E:191:ARG:HG3	3:E:191:ARG:NH1	1.60	1.04
3:E:32:LEU:O	3:E:35:LEU:HD12	1.57	1.03
3:E:175:LYS:CB	3:E:255:ILE:HD11	1.86	1.03
3:E:107:LEU:HA	3:E:122:TYR:CE1	1.93	1.03
2:B:274:MET:HG3	2:C:234:PRO:HD3	1.06	1.03
3:D:149:MET:HE3	3:D:260:MET:CE	1.88	1.03
3:E:68:ILE:C	3:E:68:ILE:CD1	2.30	1.03
1:A:47:ARG:HH21	2:B:595:ALA:C	1.66	1.02
2:B:363:ARG:CZ	3:D:80:SER:OG	2.08	1.02
1:A:127:THR:HG21	2:B:640:GLN:H	0.91	1.02
1:A:724:MET:CB	1:A:725:PRO:HD3	1.89	1.02
3:E:32:LEU:O	3:E:35:LEU:HD11	1.57	1.02
3:E:191:ARG:HH11	3:E:191:ARG:CG	1.72	1.01
3:E:53:GLU:CG	3:E:145:TYR:HD1	1.73	1.01
2:C:82:ARG:HH22	2:C:209:ASN:ND2	1.57	1.01
3:E:262:THR:HG22	3:E:263:ALA:O	1.61	1.00
1:A:47:ARG:NE	2:B:596:GLY:HA2	1.75	1.00
1:A:486:THR:O	1:A:487:GLN:HG3	1.61	0.99
3:D:153:TYR:HA	3:D:156:VAL:HG12	1.42	0.99
2:C:337:VAL:HG22	3:E:187:ILE:HD12	1.42	0.99
2:B:271:THR:HG23	2:C:237:VAL:HG23	1.02	0.99
2:B:274:MET:HG3	2:C:234:PRO:CD	1.91	0.99
3:E:127:VAL:HG12	3:E:203:ILE:HD11	1.45	0.99
3:E:158:LEU:O	3:E:162:GLY:CA	2.10	0.98
3:D:253:GLU:CD	3:D:254:TYR:CE2	2.41	0.98
3:D:253:GLU:CG	3:D:254:TYR:CD2	2.46	0.98
1:A:238:ASP:OD2	1:A:259:ARG:HG3	1.62	0.98
3:E:46:LYS:CD	3:E:155:HIS:CE1	2.25	0.98
1:A:174:ASP:HB3	2:B:605:ARG:NH1	1.78	0.98
2:B:137:ILE:CD1	2:C:759:ASP:CG	2.37	0.98
3:E:68:ILE:HD13	3:E:68:ILE:O	1.63	0.97
3:E:1:MET:HE1	3:E:121:PHE:CD2	1.99	0.97
3:E:261:ARG:HH12	3:E:265:ARG:NH2	1.62	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:ARG:NH2	2:C:1002:LEU:HD22	1.80	0.97
3:E:53:GLU:CG	3:E:145:TYR:CD1	2.47	0.97
1:A:47:ARG:CZ	2:B:595:ALA:O	2.13	0.96
3:E:55:HIS:CD2	3:E:145:TYR:CE2	2.53	0.96
2:B:891:HIS:NE2	3:D:240:VAL:HG23	1.80	0.96
2:B:367:GLU:HG3	3:D:82:GLN:OE1	1.65	0.96
1:A:127:THR:CG2	2:B:640:GLN:N	2.28	0.96
1:A:409:MET:HB3	1:A:1034:ARG:HH12	1.31	0.96
2:C:449:PHE:CZ	2:C:463:VAL:HA	2.00	0.95
3:E:261:ARG:HH12	3:E:265:ARG:HH21	1.11	0.95
3:E:68:ILE:HD11	3:E:72:ILE:CD1	1.96	0.95
3:E:107:LEU:HD23	3:E:122:TYR:CE1	2.02	0.95
2:C:1273:ASN:O	3:E:183:GLU:OE1	1.85	0.95
3:D:153:TYR:HA	3:D:156:VAL:CG1	1.96	0.95
2:B:274:MET:HG2	2:C:234:PRO:HD3	1.49	0.94
3:E:53:GLU:HG2	3:E:145:TYR:HD1	0.80	0.94
3:E:191:ARG:HG3	3:E:191:ARG:HH11	0.79	0.94
3:D:262:THR:HG21	3:D:270:THR:HA	1.47	0.94
2:B:891:HIS:HA	3:D:242:ARG:HD2	1.50	0.94
2:B:1044:ARG:HH21	3:D:266:THR:HG22	1.15	0.94
3:E:69:GLU:C	3:E:69:GLU:CD	2.35	0.94
1:A:406:VAL:HB	1:A:407:GLU:HA	1.47	0.94
2:B:445:GLU:HB3	2:B:446:LYS:CA	1.97	0.93
3:E:200:ALA:O	3:E:204:ASP:OD2	1.85	0.93
2:B:1044:ARG:HE	3:D:266:THR:HG21	1.31	0.92
3:E:1:MET:CE	3:E:121:PHE:CE2	2.53	0.92
2:B:748:GLN:O	2:B:748:GLN:HG2	1.69	0.92
2:C:448:TYR:HB3	2:C:768:CYS:SG	2.08	0.92
3:D:253:GLU:HG3	3:D:254:TYR:HD2	1.10	0.92
2:B:1044:ARG:NH2	3:D:266:THR:CG2	2.33	0.92
3:E:289:ARG:HD2	3:E:289:ARG:C	1.87	0.92
2:B:271:THR:HG21	2:C:237:VAL:HG21	1.50	0.91
1:A:481:ASP:HB3	1:A:511:ILE:HG12	1.51	0.91
1:A:310:ASP:CG	1:A:311:GLN:H	1.76	0.91
3:D:214:ARG:O	3:D:218:THR:HG23	1.69	0.91
1:A:724:MET:HB3	1:A:725:PRO:HD3	0.92	0.90
2:B:891:HIS:CD2	3:D:240:VAL:CG2	2.55	0.90
3:D:44:LEU:HD11	3:D:154:ALA:HA	1.50	0.90
1:A:565:ARG:HB3	1:A:592:VAL:N	1.86	0.89
2:B:231:LEU:HB2	2:B:249:SER:HB2	1.52	0.89
2:B:1273:ASN:OD1	3:D:79:ILE:HG21	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:GLN:OE1	2:C:499:ALA:CB	2.20	0.89
2:C:337:VAL:HG22	3:E:187:ILE:CD1	2.02	0.89
3:D:156:VAL:HG23	3:D:228:LEU:CD2	2.02	0.89
3:E:160:LEU:HD11	3:E:229:PHE:HB2	1.55	0.88
1:A:47:ARG:NH2	2:B:595:ALA:C	2.31	0.88
3:D:8:GLY:O	3:D:11:THR:CG2	2.20	0.88
2:C:1273:ASN:HA	3:E:183:GLU:OE1	1.71	0.88
3:D:5:PRO:C	3:D:6:THR:HG22	1.98	0.88
3:E:68:ILE:HD11	3:E:72:ILE:HD12	1.57	0.87
3:E:12:LEU:HG	3:E:14:GLN:HE21	1.38	0.87
1:A:127:THR:HG22	2:B:639:ASN:HB2	1.56	0.86
2:B:939:ASN:O	2:B:940:ARG:HB3	1.73	0.86
2:C:104:ILE:HG23	2:C:1310:ARG:NH2	1.89	0.86
3:E:49:ILE:CG2	3:E:50:PRO:HD2	2.06	0.86
1:A:194:HIS:CG	3:D:146:ARG:HH11	1.94	0.85
1:A:406:VAL:CB	1:A:407:GLU:HA	2.06	0.85
3:E:160:LEU:CD1	3:E:229:PHE:HB2	2.05	0.85
2:B:445:GLU:CB	2:B:446:LYS:HA	2.06	0.85
1:A:59:TYR:HA	1:A:167:THR:HG21	1.57	0.85
3:D:149:MET:CE	3:D:260:MET:CE	2.50	0.85
3:D:153:TYR:O	3:D:156:VAL:HG13	1.74	0.85
3:D:172:MET:HE3	3:D:175:LYS:HG3	1.57	0.85
1:A:914:GLU:HA	1:A:950:MET:HB3	1.59	0.85
1:A:47:ARG:NH2	2:B:596:GLY:N	2.19	0.85
1:A:133:LEU:HD21	2:C:545:PRO:CB	2.06	0.84
1:A:194:HIS:CD2	3:D:146:ARG:NH1	2.44	0.84
1:A:406:VAL:HB	1:A:407:GLU:CA	2.06	0.84
2:B:137:ILE:CD1	2:C:759:ASP:OD1	2.25	0.84
1:A:286:ASN:CG	1:A:287:VAL:H	1.85	0.84
1:A:308:ALA:H	1:A:309:ASN:CB	1.88	0.84
1:A:563:ALA:HA	1:A:564:GLU:HG3	1.58	0.84
1:A:964:GLU:HA	1:A:968:ILE:HD13	1.59	0.84
2:C:1042:TRP:CG	2:C:1043:SER:HA	2.13	0.84
1:A:27:LYS:HB3	1:A:28:PRO:HD3	1.57	0.84
3:E:175:LYS:HB2	3:E:255:ILE:HD11	0.90	0.84
1:A:281:ASN:O	1:A:283:PHE:N	2.11	0.83
3:E:55:HIS:CG	3:E:55:HIS:O	2.30	0.83
2:B:862:ARG:HB3	2:B:952:PHE:CE2	2.13	0.83
3:E:146:ARG:CZ	3:E:277:GLU:OE2	2.26	0.83
1:A:303:THR:HB	1:A:307:HIS:NE2	1.93	0.83
1:A:565:ARG:HB3	1:A:592:VAL:H	1.40	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:448:TYR:C	2:C:450:PRO:HD3	2.04	0.83
2:B:1273:ASN:OD1	3:D:191:ARG:HA	1.79	0.83
2:B:1044:ARG:HE	3:D:266:THR:CG2	1.84	0.83
2:C:104:ILE:HG23	2:C:1310:ARG:HH22	1.43	0.83
1:A:986:ARG:HB3	1:A:994:PRO:CB	2.09	0.82
2:B:135:LYS:CG	2:C:470:ALA:O	2.26	0.82
1:A:48:SER:O	1:A:49:HIS:HB3	1.78	0.82
1:A:222:ARG:HD2	2:B:720:PHE:CZ	2.13	0.82
2:B:475:ILE:O	2:B:478:ILE:HG13	1.80	0.82
3:D:181:SER:HB3	3:D:250:ARG:HG2	1.61	0.82
3:E:69:GLU:HG2	3:E:199:LEU:HB2	1.61	0.82
3:E:79:ILE:HA	3:E:269:ILE:HD13	1.62	0.82
3:E:182:TRP:C	3:E:183:GLU:HG2	2.05	0.82
1:A:135:VAL:HG11	2:C:669:GLN:OE1	1.80	0.82
3:E:137:LEU:C	3:E:137:LEU:CD2	2.49	0.82
1:A:917:SER:HB3	1:A:919:TYR:HE1	1.43	0.81
3:E:166:GLU:OE2	3:E:171:VAL:O	1.97	0.81
2:B:420:PRO:HB2	2:B:748:GLN:OE1	1.81	0.81
3:D:107:LEU:O	3:D:108:ASP:CG	2.23	0.81
3:E:85:ASN:ND2	3:E:141:SER:HB3	1.95	0.81
2:B:642:GLY:HA2	2:C:670:ASP:OD2	1.80	0.81
3:D:100:ASN:H	3:D:100:ASN:HD22	1.24	0.81
1:A:308:ALA:CA	1:A:309:ASN:HB2	2.11	0.81
1:A:222:ARG:HD2	2:B:720:PHE:HZ	1.41	0.81
3:D:258:ASN:OD1	3:D:259:SER:O	1.98	0.81
2:B:891:HIS:CD2	3:D:240:VAL:HG23	2.16	0.81
1:A:318:ARG:NH1	3:D:43:GLU:HG2	1.95	0.80
1:A:670:GLY:O	1:A:671:VAL:HG22	1.81	0.80
2:C:1037:ILE:O	2:C:1038:GLU:HB3	1.79	0.80
1:A:566:GLU:HB2	1:A:567:PRO:HD2	1.60	0.80
2:B:891:HIS:NE2	3:D:240:VAL:CG2	2.44	0.80
3:D:41:GLU:OE1	3:D:41:GLU:HA	1.79	0.80
3:D:264:GLY:O	3:D:266:THR:N	2.14	0.80
3:D:253:GLU:CG	3:D:254:TYR:HD2	1.89	0.80
2:C:1272:ARG:HD2	3:E:247:ARG:HH22	1.44	0.80
1:A:426:ARG:HB2	1:A:707:SER:HB2	1.64	0.80
1:A:565:ARG:HG3	1:A:590:ARG:O	1.81	0.80
3:D:153:TYR:O	3:D:156:VAL:CG1	2.30	0.80
2:B:271:THR:HG23	2:C:237:VAL:CG2	1.93	0.79
2:C:588:LEU:HG	2:C:604:MET:HE3	1.63	0.79
3:E:55:HIS:HD2	3:E:145:TYR:CZ	2.00	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:41:GLU:OE1	3:D:41:GLU:CA	2.30	0.79
3:E:137:LEU:HD23	3:E:137:LEU:O	1.82	0.79
2:C:154:PHE:HB3	2:C:262:ASN:HB2	1.63	0.79
3:E:40:THR:CG2	3:E:41:GLU:OE2	2.30	0.79
3:E:40:THR:HG23	3:E:41:GLU:OE2	1.83	0.79
2:C:1051:ARG:HH11	2:C:1051:ARG:HG2	1.47	0.79
2:B:367:GLU:CG	3:D:82:GLN:OE1	2.31	0.78
1:A:31:VAL:HG23	1:A:32:PRO:HD3	1.63	0.78
3:E:158:LEU:O	3:E:162:GLY:N	2.17	0.78
2:C:1042:TRP:CB	2:C:1043:SER:HA	2.14	0.78
2:B:134:THR:HG22	2:C:472:GLU:OE1	1.84	0.78
3:D:153:TYR:CA	3:D:156:VAL:HG12	2.12	0.78
2:C:141:LEU:HG	2:C:142:ASP:H	1.49	0.78
2:C:292:ASN:O	2:C:293:ASN:HB3	1.82	0.78
2:B:1084:PRO:HB3	2:B:1207:MET:HG3	1.66	0.77
2:C:565:GLU:HG2	2:C:566:PHE:N	1.98	0.77
2:B:1273:ASN:OD1	3:D:79:ILE:CG2	2.32	0.77
3:E:56:LEU:HD23	3:E:56:LEU:H	1.49	0.77
2:B:750:GLU:OE2	2:B:752:VAL:HG13	1.85	0.77
1:A:461:ARG:HG3	1:A:461:ARG:NH1	1.96	0.77
2:C:523:THR:O	2:C:524:GLU:HB3	1.85	0.77
3:D:217:LYS:CD	3:D:290:TRP:CZ3	2.67	0.77
1:A:268:TYR:OH	2:B:562:ALA:HB1	1.84	0.77
2:C:673:GLN:O	2:C:677:ARG:HB2	1.85	0.77
1:A:830:HIS:HD2	1:A:1034:ARG:HH11	1.33	0.77
2:B:137:ILE:HD12	2:C:759:ASP:OD1	1.85	0.76
2:B:1236:ILE:CG1	2:B:1237:SER:H	1.99	0.76
2:C:146:GLU:HB2	2:C:1317:VAL:O	1.84	0.76
2:C:385:ILE:HG13	2:C:708:THR:HG22	1.68	0.76
3:E:68:ILE:HD11	3:E:72:ILE:HD11	1.65	0.76
3:E:107:LEU:HD23	3:E:122:TYR:CZ	2.20	0.76
3:D:45:VAL:HG13	3:D:171:VAL:CG2	2.10	0.76
3:E:262:THR:CG2	3:E:263:ALA:O	2.33	0.76
1:A:725:PRO:O	1:A:726:ILE:HG12	1.86	0.76
2:B:558:TYR:CE2	2:B:590:SER:HB3	2.21	0.76
3:E:42:ASN:HB2	3:E:174:VAL:HB	1.68	0.76
2:B:1044:ARG:NE	3:D:266:THR:HG21	1.89	0.76
2:B:1084:PRO:HG2	2:B:1209:GLY:HA3	1.68	0.76
3:E:68:ILE:HD13	3:E:69:GLU:N	2.00	0.76
2:B:1085:ASP:O	2:B:1208:ASP:HA	1.86	0.76
2:B:950:ASP:CG	2:B:951:ILE:H	1.94	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1180:PRO:HB3	2:C:1209:GLY:HA2	1.69	0.75
2:C:1050:LEU:HD12	2:C:1054:ARG:HH21	1.51	0.75
3:E:69:GLU:CG	3:E:199:LEU:HB2	2.17	0.75
1:A:986:ARG:HB3	1:A:994:PRO:HB3	1.69	0.75
2:B:177:LYS:HE3	2:B:177:LYS:H	1.51	0.75
2:C:442:PRO:HB3	2:C:473:ALA:HB1	1.68	0.75
3:E:192:ASP:OD1	3:E:192:ASP:C	2.30	0.75
1:A:917:SER:HB3	1:A:919:TYR:CE1	2.22	0.74
2:B:1248:HIS:ND1	2:B:1251:VAL:HG22	2.01	0.74
3:E:13:GLU:CD	3:E:13:GLU:O	2.30	0.74
2:B:594:LEU:HD13	2:B:596:GLY:H	1.52	0.74
2:C:408:ILE:O	2:C:412:LEU:HB2	1.87	0.74
2:C:853:ASP:HB2	3:D:117:ILE:HD11	1.69	0.74
3:E:235:VAL:HG13	3:E:258:ASN:HD22	1.51	0.74
2:C:1042:TRP:CD1	2:C:1043:SER:HA	2.21	0.74
2:B:747:ARG:O	2:B:747:ARG:HG3	1.83	0.74
2:C:1273:ASN:CA	3:E:183:GLU:OE1	2.35	0.74
1:A:307:HIS:HB2	1:A:308:ALA:HA	0.82	0.74
2:C:287:ARG:HH21	2:C:326:GLY:HA3	1.52	0.74
3:E:13:GLU:OE1	3:E:13:GLU:C	2.30	0.74
2:C:82:ARG:NH2	2:C:209:ASN:ND2	2.33	0.74
1:A:23:ARG:O	1:A:28:PRO:HD2	1.88	0.73
3:E:69:GLU:CD	3:E:69:GLU:O	2.31	0.73
2:B:183:SER:HB3	2:B:186:ASP:HB2	1.70	0.73
3:D:61:ASN:OD1	3:D:61:ASN:C	2.30	0.73
3:E:156:VAL:HG13	3:E:228:LEU:HD12	1.68	0.73
2:B:1080:THR:HB	2:B:1227:MET:HB3	1.70	0.73
3:D:238:ASN:HB2	3:D:253:GLU:HB2	1.68	0.73
3:D:172:MET:HG3	3:D:173:PRO:HD2	1.69	0.73
2:B:135:LYS:HG2	2:C:470:ALA:O	1.87	0.73
3:D:108:ASP:OD1	3:D:110:VAL:HG23	1.88	0.73
1:A:967:ILE:HD12	1:A:978:LYS:HB2	1.71	0.73
3:E:150:ILE:HG22	3:E:150:ILE:O	1.87	0.73
2:B:1023:ARG:HB2	2:B:1024:PRO:HD2	1.69	0.72
2:C:838:GLU:HG3	2:C:839:ALA:H	1.53	0.72
3:E:214:ARG:O	3:E:218:THR:HG23	1.89	0.72
2:C:376:ILE:HD11	2:C:1317:VAL:HG21	1.71	0.72
2:C:1025:ASP:OD1	3:D:95:ALA:HB1	1.89	0.72
1:A:967:ILE:HG23	1:A:968:ILE:HD12	1.72	0.72
3:D:282:PHE:O	3:D:286:THR:HG22	1.90	0.72
1:A:928:GLU:HB2	1:A:929:PRO:CD	2.17	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:926:VAL:HG21	2:B:936:MET:O	1.89	0.72
2:C:270:THR:HG22	2:C:291:HIS:HA	1.72	0.72
3:D:265:ARG:HA	3:D:265:ARG:NE	2.04	0.72
3:E:137:LEU:HD11	3:E:278:PHE:CZ	2.23	0.72
3:E:253:GLU:OE2	3:E:254:TYR:CZ	2.43	0.72
3:E:53:GLU:HG2	3:E:145:TYR:CE1	2.24	0.72
2:C:750:GLU:HG3	2:C:756:THR:HB	1.72	0.72
1:A:395:GLN:HE21	1:A:395:GLN:HA	1.55	0.72
3:E:139:ASN:C	3:E:139:ASN:OD1	2.33	0.71
2:C:494:GLU:O	2:C:757:ILE:HA	1.90	0.71
2:C:1273:ASN:C	3:E:183:GLU:OE1	2.33	0.71
1:A:544:ASN:HD21	1:A:546:ALA:HB3	1.54	0.71
2:C:1023:ARG:HG2	2:C:1024:PRO:HD2	1.71	0.71
2:C:1042:TRP:HB3	2:C:1043:SER:CA	2.20	0.71
3:D:156:VAL:HG23	3:D:228:LEU:HD21	1.71	0.71
2:C:341:LYS:HG3	2:C:1306:THR:OG1	1.91	0.71
2:C:449:PHE:HE2	2:C:462:LEU:HD13	1.56	0.71
1:A:986:ARG:HB3	1:A:994:PRO:HB2	1.71	0.71
2:B:338:ARG:NH2	2:C:1002:LEU:CD2	2.54	0.71
1:A:47:ARG:CZ	2:B:596:GLY:CA	2.49	0.70
2:B:891:HIS:CD2	3:D:240:VAL:HG21	2.26	0.70
2:B:1288:ILE:HD12	3:D:20:ARG:NH2	2.06	0.70
2:B:186:ASP:HA	2:B:189:ILE:HG22	1.73	0.70
1:A:133:LEU:HD21	2:C:545:PRO:HB3	1.74	0.70
1:A:647:LEU:HD21	1:A:691:TYR:HD2	1.56	0.70
2:B:1273:ASN:CG	3:D:79:ILE:CG2	2.64	0.70
2:B:363:ARG:NH2	3:D:80:SER:OG	2.24	0.70
2:B:1084:PRO:HB2	2:B:1208:ASP:C	2.16	0.70
1:A:559:ILE:HG22	1:A:613:ILE:HG12	1.74	0.70
1:A:928:GLU:CB	1:A:929:PRO:HD2	2.18	0.70
2:C:340:VAL:HG23	2:C:341:LYS:HG2	1.72	0.70
3:E:69:GLU:C	3:E:69:GLU:OE1	2.35	0.70
1:A:174:ASP:O	2:B:605:ARG:HD2	1.91	0.70
3:D:47:LYS:HG3	3:D:48:THR:H	1.57	0.70
1:A:127:THR:CG2	2:B:639:ASN:HB2	2.21	0.70
3:D:85:ASN:C	3:D:85:ASN:HD22	2.00	0.70
2:B:279:SER:HA	2:C:1198:LYS:HE2	1.74	0.69
1:A:254:ASP:O	1:A:255:ARG:HB3	1.92	0.69
2:B:1084:PRO:HB3	2:B:1207:MET:CG	2.23	0.69
2:C:892:VAL:HG13	2:C:894:VAL:H	1.56	0.69
3:E:46:LYS:HD3	3:E:155:HIS:HE1	0.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:ASP:O	1:A:871:VAL:HG23	1.91	0.69
2:C:565:GLU:HG2	2:C:566:PHE:H	1.55	0.69
1:A:383:THR:HG21	1:A:805:TYR:HB3	1.74	0.69
3:E:253:GLU:HG3	3:E:254:TYR:CD2	2.28	0.69
1:A:462:ILE:HG13	1:A:684:ASN:H	1.57	0.69
2:C:82:ARG:NH2	2:C:209:ASN:HD21	1.90	0.69
2:C:838:GLU:HB3	2:C:934:LEU:HB2	1.74	0.69
3:D:55:HIS:ND1	3:D:55:HIS:C	2.50	0.69
3:D:244:VAL:HG12	3:D:245:THR:H	1.57	0.69
2:C:853:ASP:HB2	3:D:117:ILE:CD1	2.23	0.69
2:B:1044:ARG:NE	3:D:266:THR:HG23	2.08	0.68
3:D:22:ASP:C	3:D:22:ASP:OD1	2.36	0.68
3:E:35:LEU:HB3	3:E:179:PHE:HB3	1.75	0.68
2:C:341:LYS:HD2	2:C:1306:THR:HG21	1.75	0.68
2:C:1280:PRO:HB3	2:C:1287:GLY:HA2	1.76	0.68
2:B:147:VAL:HG22	2:B:1315:MET:H	1.59	0.68
1:A:925:ILE:HD11	1:A:930:ASN:HA	1.75	0.67
2:B:446:LYS:HB3	2:B:769:GLN:NE2	2.10	0.67
1:A:764:SER:HA	1:A:795:GLU:HG3	1.76	0.67
2:C:269:GLU:HB3	2:C:292:ASN:CB	2.24	0.67
3:E:56:LEU:H	3:E:56:LEU:CD2	2.08	0.67
1:A:127:THR:HG23	2:B:640:GLN:N	2.10	0.67
1:A:462:ILE:CG1	1:A:684:ASN:H	2.07	0.67
3:E:153:TYR:HD1	3:E:156:VAL:HG21	1.59	0.67
1:A:286:ASN:HB2	1:A:814:ASN:HD21	1.60	0.67
3:D:78:GLY:O	3:D:269:ILE:HD11	1.95	0.67
3:E:68:ILE:CD1	3:E:72:ILE:HD12	2.24	0.67
2:C:841:ASP:O	2:C:842:ASP:HB2	1.93	0.67
3:E:162:GLY:HA2	3:E:172:MET:CE	2.24	0.67
1:A:864:ARG:O	1:A:865:ASN:HB3	1.94	0.67
2:B:1121:HIS:HD2	2:B:1124:THR:HG22	1.60	0.67
2:B:733:VAL:HG21	2:B:741:TYR:CD1	2.31	0.66
1:A:427:ASP:HA	1:A:704:PRO:HD2	1.77	0.66
1:A:562:GLY:HA3	1:A:563:ALA:O	1.96	0.66
3:D:21:ASN:O	3:D:22:ASP:CG	2.39	0.66
2:B:1044:ARG:CZ	3:D:266:THR:HG23	2.24	0.66
3:D:239:VAL:HG12	3:D:250:ARG:HH12	1.61	0.66
1:A:477:TYR:HA	1:A:480:GLY:O	1.94	0.66
3:D:178:LYS:O	3:D:178:LYS:HG3	1.96	0.66
3:E:261:ARG:NH1	3:E:265:ARG:NH2	2.39	0.66
1:A:978:LYS:HG2	1:A:987:LEU:HD13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:ALA:HA	3:D:83:ASN:ND2	2.11	0.65
3:D:100:ASN:H	3:D:100:ASN:ND2	1.94	0.65
3:E:56:LEU:HD23	3:E:56:LEU:N	2.11	0.65
3:E:69:GLU:OE1	3:E:70:ASP:N	2.30	0.65
3:E:247:ARG:HE	3:E:247:ARG:HA	1.62	0.65
1:A:310:ASP:CG	1:A:311:GLN:N	2.49	0.65
1:A:462:ILE:HG12	1:A:684:ASN:HA	1.78	0.65
2:C:272:THR:HB	2:C:289:THR:HG22	1.78	0.65
1:A:71:LEU:HG	1:A:75:PRO:HG2	1.78	0.65
2:B:472:GLU:CD	2:B:472:GLU:H	2.03	0.65
2:C:1021:ARG:HD2	2:C:1032:ASP:HB2	1.79	0.65
3:E:221:ARG:HH11	3:E:225:ARG:HD2	1.60	0.65
1:A:919:TYR:HB2	1:A:955:ASN:HB3	1.79	0.65
3:E:12:LEU:O	3:E:14:GLN:NE2	2.30	0.65
2:C:1051:ARG:HG2	2:C:1051:ARG:NH1	2.05	0.65
2:B:368:ALA:O	3:D:83:ASN:HB2	1.97	0.65
3:D:143:PRO:O	3:D:144:ARG:HB3	1.96	0.65
3:E:134:TYR:OH	3:E:286:THR:HG22	1.97	0.65
2:C:449:PHE:N	2:C:450:PRO:HD3	2.12	0.65
2:B:442:PRO:HG3	2:B:475:ILE:HD12	1.79	0.65
3:E:195:ASN:OD1	3:E:195:ASN:N	2.30	0.65
1:A:667:GLN:H	1:A:667:GLN:NE2	1.94	0.64
2:B:1236:ILE:HG12	2:B:1237:SER:H	1.63	0.64
2:C:1042:TRP:HB3	2:C:1043:SER:HA	1.76	0.64
3:E:53:GLU:N	3:E:53:GLU:OE2	2.30	0.64
1:A:174:ASP:HB3	2:B:605:ARG:HH12	1.58	0.64
2:C:269:GLU:HB3	2:C:292:ASN:HB3	1.78	0.64
2:C:390:HIS:HB2	2:C:1318:GLU:OE2	1.97	0.64
1:A:723:GLU:O	1:A:724:MET:HB2	1.98	0.64
2:B:926:VAL:HG12	2:B:926:VAL:O	1.97	0.64
1:A:174:ASP:HB3	2:B:605:ARG:HH11	1.58	0.64
2:B:1031:TYR:CE2	2:B:1041:ARG:HD3	2.33	0.64
3:D:144:ARG:HD2	3:D:144:ARG:O	1.98	0.64
1:A:47:ARG:NH2	2:B:595:ALA:O	2.27	0.64
1:A:887:ILE:HG22	1:A:888:GLU:H	1.63	0.64
1:A:955:ASN:HD21	1:A:1055:LEU:HB3	1.60	0.64
3:E:191:ARG:NH1	3:E:191:ARG:CG	2.42	0.64
1:A:47:ARG:HE	2:B:595:ALA:C	2.05	0.64
1:A:462:ILE:HG21	1:A:682:SER:HA	1.80	0.64
2:C:838:GLU:HG3	2:C:839:ALA:N	2.12	0.64
2:B:1181:SER:O	2:B:1182:GLU:HG2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:284:GLN:O	3:E:288:THR:HG22	1.96	0.64
2:B:234:PRO:HD2	2:B:242:GLU:HB3	1.80	0.64
2:B:748:GLN:O	2:B:748:GLN:CG	2.45	0.64
3:E:68:ILE:CD1	3:E:69:GLU:N	2.59	0.64
1:A:133:LEU:HD22	2:C:545:PRO:HG3	1.80	0.64
3:D:153:TYR:CA	3:D:156:VAL:CG1	2.72	0.64
3:E:55:HIS:CD2	3:E:145:TYR:CZ	2.85	0.64
3:D:41:GLU:OE1	3:D:41:GLU:N	2.30	0.64
3:E:55:HIS:O	3:E:55:HIS:ND1	2.30	0.64
3:E:262:THR:O	3:E:263:ALA:C	2.41	0.64
2:B:340:VAL:HG21	2:C:1008:LEU:HD23	1.80	0.63
2:C:449:PHE:HE1	2:C:463:VAL:HG22	1.60	0.63
2:C:837:THR:HG22	2:C:934:LEU:HD21	1.78	0.63
3:D:100:ASN:HD22	3:D:100:ASN:N	1.92	0.63
3:E:137:LEU:HD23	3:E:138:GLY:N	2.13	0.63
1:A:962:PHE:CG	1:A:963:TYR:N	2.65	0.63
3:D:82:GLN:OE1	3:D:82:GLN:HA	1.98	0.63
3:E:55:HIS:CD2	3:E:145:TYR:HE2	2.15	0.63
3:D:153:TYR:C	3:D:156:VAL:HG12	2.22	0.63
1:A:486:THR:C	1:A:487:GLN:HG3	2.23	0.63
2:C:1086:PRO:HD3	2:C:1208:ASP:HA	1.80	0.63
3:E:85:ASN:CG	3:E:85:ASN:O	2.41	0.63
2:C:837:THR:HA	2:C:936:MET:HG3	1.80	0.63
2:C:1272:ARG:HD2	3:E:247:ARG:NH2	2.13	0.63
2:C:1243:ARG:NH1	2:C:1243:ARG:HB3	2.14	0.63
2:C:82:ARG:HH22	2:C:209:ASN:HD21	1.39	0.63
3:D:242:ARG:HH11	3:D:242:ARG:CG	2.11	0.63
3:E:234:ALA:O	3:E:263:ALA:HB2	1.98	0.63
2:B:148:GLN:O	2:B:375:ARG:HD3	1.98	0.62
3:E:12:LEU:O	3:E:13:GLU:HB3	1.98	0.62
3:D:35:LEU:HD23	3:D:179:PHE:HB3	1.81	0.62
3:D:237:ALA:HB3	3:D:253:GLU:HG2	1.81	0.62
3:D:253:GLU:CD	3:D:254:TYR:CD2	2.76	0.62
1:A:27:LYS:O	1:A:30:THR:HG23	1.99	0.62
1:A:283:PHE:HA	1:A:284:THR:C	2.24	0.62
2:B:950:ASP:CG	2:B:951:ILE:N	2.57	0.62
2:C:1243:ARG:HB3	2:C:1243:ARG:HH11	1.64	0.62
3:E:77:PHE:CE1	3:E:227:MET:HB2	2.34	0.62
1:A:47:ARG:NE	2:B:596:GLY:CA	2.57	0.62
1:A:935:PRO:O	1:A:939:GLN:N	2.27	0.62
2:C:598:ASN:HA	2:C:601:ILE:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:269:GLU:CB	2:C:292:ASN:HB3	2.30	0.62
1:A:724:MET:CB	1:A:725:PRO:CD	2.60	0.62
3:D:107:LEU:O	3:D:108:ASP:OD2	2.17	0.62
1:A:255:ARG:O	1:A:256:VAL:HG12	2.00	0.62
1:A:286:ASN:O	1:A:288:LEU:N	2.33	0.62
1:A:565:ARG:CB	1:A:592:VAL:HB	2.30	0.62
1:A:955:ASN:ND2	1:A:1055:LEU:HB3	2.15	0.62
3:E:1:MET:O	3:E:2:LEU:HB2	2.00	0.62
3:E:235:VAL:HG13	3:E:258:ASN:ND2	2.14	0.62
3:D:85:ASN:C	3:D:85:ASN:ND2	2.55	0.62
1:A:51:LEU:HB3	1:A:172:PHE:HE1	1.64	0.61
3:E:42:ASN:CB	3:E:174:VAL:HB	2.29	0.61
2:C:449:PHE:CE1	2:C:463:VAL:HG22	2.35	0.61
3:E:209:GLU:O	3:E:213:LEU:HB2	2.00	0.61
1:A:864:ARG:O	1:A:864:ARG:HG2	2.00	0.61
2:B:343:ILE:HD11	2:B:366:MET:HE3	1.83	0.61
2:C:449:PHE:CE1	2:C:463:VAL:HA	2.34	0.61
2:C:671:ASP:HA	2:C:674:LYS:HD3	1.82	0.61
3:E:85:ASN:HD22	3:E:141:SER:HB3	1.65	0.61
2:B:350:ILE:HG22	2:B:351:ASP:H	1.64	0.61
3:E:66:VAL:HG23	3:E:89:TYR:CD2	2.36	0.61
1:A:133:LEU:HD21	2:C:545:PRO:HB2	1.81	0.61
2:C:1042:TRP:HB3	2:C:1043:SER:CB	2.31	0.61
2:B:193:THR:HG23	2:B:297:ASN:H	1.66	0.61
3:D:148:ASP:OD1	3:D:148:ASP:N	2.34	0.61
2:B:1037:ILE:HG12	2:B:1038:GLU:H	1.65	0.61
1:A:308:ALA:HB3	1:A:309:ASN:CG	2.26	0.60
2:B:862:ARG:CB	2:B:952:PHE:CZ	2.84	0.60
2:B:951:ILE:O	2:B:952:PHE:CB	2.49	0.60
2:C:490:PHE:HA	2:C:745:ILE:HG22	1.83	0.60
2:C:520:PHE:HD1	2:C:520:PHE:H	1.49	0.60
2:C:1118:THR:HG22	2:C:1129:PRO:HA	1.82	0.60
3:E:40:THR:CG2	3:E:41:GLU:N	2.63	0.60
1:A:936:ALA:HA	1:A:939:GLN:HE21	1.67	0.60
3:E:40:THR:HG22	3:E:41:GLU:N	2.15	0.60
2:B:427:VAL:HG11	2:B:755:LEU:CD2	2.32	0.60
2:C:231:LEU:CB	2:C:249:SER:HB2	2.32	0.60
2:C:879:THR:O	2:C:883:ILE:HG12	2.01	0.60
3:D:242:ARG:HH11	3:D:242:ARG:HG2	1.66	0.60
1:A:395:GLN:HA	1:A:395:GLN:NE2	2.17	0.60
2:C:269:GLU:HB3	2:C:292:ASN:CG	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:ALA:O	1:A:940:MET:HB3	2.00	0.60
2:B:1276:LEU:HD22	2:B:1300:ASN:HB2	1.83	0.60
2:C:269:GLU:C	2:C:292:ASN:HB2	2.26	0.60
3:E:85:ASN:ND2	3:E:141:SER:CB	2.63	0.60
3:E:85:ASN:C	3:E:85:ASN:OD1	2.44	0.60
1:A:837:HIS:NE2	1:A:1047:ASN:HA	2.17	0.60
2:B:137:ILE:HD11	2:C:759:ASP:CB	2.31	0.60
2:B:1078:TYR:HE2	2:B:1080:THR:HG22	1.67	0.60
2:B:1114:ARG:HD3	2:B:1116:ARG:HH21	1.67	0.60
3:D:217:LYS:CE	3:D:290:TRP:CE3	2.85	0.60
3:E:46:LYS:HD2	3:E:155:HIS:CE1	2.34	0.60
3:E:85:ASN:HD21	3:E:141:SER:CB	2.14	0.60
1:A:561:LEU:HD12	1:A:617:ILE:HD11	1.83	0.60
3:D:37:TYR:HD1	3:D:177:ALA:HB2	1.66	0.60
3:E:209:GLU:HG3	3:E:210:GLY:H	1.66	0.60
1:A:523:MET:HG2	1:A:574:ARG:NH2	2.16	0.60
1:A:911:MET:HE2	1:A:944:ARG:HH22	1.65	0.60
1:A:940:MET:HA	1:A:943:ILE:HG12	1.83	0.59
1:A:71:LEU:HD11	1:A:91:ASN:CG	2.27	0.59
2:C:286:LEU:CD2	2:C:290:TYR:HB3	2.31	0.59
2:C:841:ASP:H	2:C:940:ARG:HH12	1.51	0.59
2:C:1288:ILE:HD13	2:C:1288:ILE:H	1.67	0.59
3:D:224:PHE:O	3:D:228:LEU:HB2	2.02	0.59
2:C:392:PRO:HG2	2:C:1315:MET:HG3	1.84	0.59
2:C:373:ASP:HB2	2:C:394:GLN:HG3	1.83	0.59
3:D:5:PRO:O	3:D:6:THR:CB	2.50	0.59
1:A:831:ARG:HB3	1:A:835:PHE:CE2	2.38	0.59
2:B:1236:ILE:HG12	2:B:1237:SER:N	2.16	0.59
2:C:341:LYS:CD	2:C:1306:THR:HG21	2.32	0.59
1:A:201:LYS:C	2:B:629:ARG:HD3	2.27	0.59
3:D:47:LYS:HG3	3:D:48:THR:N	2.18	0.59
3:E:68:ILE:CD1	3:E:72:ILE:CD1	2.77	0.59
3:E:67:TYR:HB3	3:E:70:ASP:HB3	1.85	0.59
1:A:529:THR:HG22	1:A:568:ALA:HB2	1.84	0.59
1:A:535:LEU:HD11	1:A:614:ILE:HG21	1.85	0.59
2:B:862:ARG:HB3	2:B:952:PHE:CZ	2.37	0.59
2:C:1042:TRP:CB	2:C:1043:SER:CA	2.79	0.59
3:E:13:GLU:CD	3:E:13:GLU:C	2.71	0.59
2:B:752:VAL:CG2	2:B:755:LEU:HB2	2.33	0.58
2:C:1080:THR:HG21	2:C:1227:MET:SD	2.43	0.58
3:D:290:TRP:HE3	3:D:290:TRP:C	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:153:TYR:CD1	3:E:156:VAL:HG21	2.37	0.58
1:A:201:LYS:O	2:B:629:ARG:HG3	2.03	0.58
1:A:717:THR:HG21	1:A:1020:SER:HB2	1.85	0.58
3:D:25:ASN:C	3:D:25:ASN:OD1	2.45	0.58
3:E:1:MET:HE1	3:E:121:PHE:HE2	1.57	0.58
3:E:113:ASN:O	3:E:114:SER:OG	2.16	0.58
1:A:565:ARG:HB2	1:A:592:VAL:HB	1.84	0.58
2:C:356:SER:O	2:C:360:ILE:HG12	2.04	0.58
1:A:549:SER:O	1:A:551:LEU:N	2.33	0.58
2:B:612:PHE:CZ	2:B:635:ILE:HD11	2.39	0.58
2:C:910:LEU:HD13	2:C:915:VAL:HG23	1.86	0.58
3:D:77:PHE:CZ	3:D:227:MET:HB2	2.39	0.58
1:A:268:TYR:CZ	2:B:562:ALA:HB1	2.38	0.58
1:A:519:ILE:HD13	1:A:519:ILE:H	1.69	0.58
2:C:192:PRO:HG3	2:C:294:VAL:HB	1.86	0.58
2:C:1042:TRP:HB3	2:C:1043:SER:HB2	1.86	0.58
3:E:14:GLN:N	3:E:14:GLN:CD	2.61	0.58
1:A:303:THR:HA	1:A:307:HIS:CE1	2.39	0.58
1:A:481:ASP:CB	1:A:511:ILE:HG12	2.30	0.58
2:C:838:GLU:O	2:C:940:ARG:NH1	2.36	0.58
2:C:1273:ASN:O	3:E:183:GLU:CD	2.46	0.58
1:A:667:GLN:CD	1:A:667:GLN:N	2.62	0.58
3:D:217:LYS:CE	3:D:290:TRP:CZ3	2.87	0.58
1:A:499:VAL:HB	1:A:503:ILE:HD11	1.86	0.58
1:A:722:ASP:CG	1:A:723:GLU:H	2.11	0.58
2:B:139:ASN:O	2:C:757:ILE:HG22	2.03	0.57
2:B:872:ILE:HG12	2:B:886:SER:HB2	1.85	0.57
2:B:960:THR:HG23	2:B:965:ARG:HH12	1.68	0.57
2:C:339:LEU:C	2:C:341:LYS:H	2.12	0.57
1:A:286:ASN:CG	1:A:287:VAL:N	2.57	0.57
2:C:841:ASP:CG	2:C:842:ASP:H	2.12	0.57
3:D:217:LYS:HE2	3:D:290:TRP:CE3	2.38	0.57
1:A:47:ARG:NH2	2:B:596:GLY:HA3	2.12	0.57
1:A:64:GLU:HA	1:A:67:ARG:HG2	1.86	0.57
1:A:604:ILE:O	1:A:605:ASP:HB3	2.04	0.57
2:C:673:GLN:HA	2:C:676:THR:HG22	1.84	0.57
1:A:479:LYS:HA	1:A:514:LEU:HD12	1.86	0.57
1:A:318:ARG:HH11	3:D:43:GLU:HG2	1.65	0.57
1:A:318:ARG:HH12	3:D:43:GLU:CD	2.12	0.57
2:C:446:LYS:HA	2:C:769:GLN:NE2	2.19	0.57
2:C:878:SER:HB3	2:C:903:ASN:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1076:ILE:HG23	2:C:1166:VAL:HB	1.87	0.57
1:A:64:GLU:OE1	2:B:647:GLU:OE2	2.23	0.57
1:A:460:VAL:O	1:A:461:ARG:HD3	2.04	0.57
1:A:831:ARG:HB3	1:A:835:PHE:HE2	1.70	0.57
2:B:1228:ARG:HG2	2:B:1231:TYR:CE2	2.39	0.57
3:E:205:LEU:O	3:E:205:LEU:CD1	2.39	0.57
1:A:495:LEU:HG	1:A:503:ILE:HD13	1.87	0.56
1:A:954:THR:HB	1:A:1056:VAL:HG23	1.87	0.56
2:B:338:ARG:NH2	2:C:1005:LEU:HD11	2.20	0.56
2:C:1051:ARG:HH11	2:C:1051:ARG:CG	2.18	0.56
3:D:144:ARG:O	3:D:144:ARG:CD	2.52	0.56
1:A:936:ALA:O	1:A:940:MET:CB	2.53	0.56
1:A:256:VAL:HG13	1:A:257:ILE:HG13	1.88	0.56
1:A:500:ASP:HB2	1:A:521:LYS:O	2.04	0.56
1:A:913:LEU:HD22	1:A:919:TYR:CZ	2.41	0.56
1:A:970:ARG:HH22	1:A:977:HIS:HA	1.70	0.56
2:B:279:SER:OG	2:C:1198:LYS:HE2	2.05	0.56
2:B:352:HIS:HA	2:B:1300:ASN:OD1	2.05	0.56
2:B:1236:ILE:HG13	2:B:1237:SER:H	1.70	0.56
3:E:53:GLU:HB2	3:E:145:TYR:HE1	1.69	0.56
1:A:133:LEU:CD2	2:C:545:PRO:CB	2.82	0.56
1:A:776:SER:HA	1:A:818:PHE:CE1	2.41	0.56
2:C:1271:SER:N	2:C:1275:ASP:O	2.39	0.56
2:B:583:GLU:O	2:B:584:HIS:HB2	2.05	0.56
2:B:1273:ASN:CG	3:D:79:ILE:HG21	2.30	0.56
3:E:44:LEU:HD13	3:E:172:MET:O	2.05	0.56
3:E:235:VAL:CG1	3:E:258:ASN:HA	2.36	0.56
1:A:832:GLU:CD	1:A:833:VAL:H	2.13	0.56
1:A:936:ALA:O	1:A:940:MET:N	2.34	0.56
2:B:368:ALA:O	3:D:83:ASN:CB	2.53	0.56
3:D:153:TYR:C	3:D:156:VAL:CG1	2.79	0.56
3:E:142:THR:HG23	3:E:143:PRO:HD2	1.87	0.56
1:A:494:THR:O	1:A:498:ALA:HB3	2.05	0.56
2:B:1106:PHE:HB3	2:B:1151:VAL:HG21	1.88	0.56
2:C:902:ILE:HB	2:C:929:PHE:HB3	1.88	0.56
3:E:290:TRP:CD1	3:E:290:TRP:C	2.84	0.56
2:C:668:VAL:HG11	2:C:673:GLN:HB2	1.88	0.56
3:D:239:VAL:HG23	3:D:263:ALA:HB1	1.87	0.56
1:A:308:ALA:N	1:A:309:ASN:CB	2.56	0.55
2:B:134:THR:CG2	2:C:472:GLU:CD	2.79	0.55
2:C:1031:TYR:O	2:C:1032:ASP:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:81:ALA:H	3:E:275:ARG:HH21	1.54	0.55
3:E:163:THR:H	3:E:172:MET:HE1	1.71	0.55
1:A:351:TYR:OH	3:D:150:ILE:HB	2.07	0.55
3:E:150:ILE:O	3:E:150:ILE:CG2	2.54	0.55
1:A:283:PHE:CA	1:A:284:THR:C	2.80	0.55
1:A:388:VAL:HG22	1:A:389:ALA:H	1.71	0.55
2:B:191:GLY:HA2	2:B:193:THR:N	2.22	0.55
2:C:154:PHE:HA	2:C:262:ASN:HD22	1.71	0.55
3:E:284:GLN:O	3:E:288:THR:CG2	2.54	0.55
1:A:87:GLU:O	1:A:91:ASN:HB2	2.07	0.55
1:A:486:THR:HA	1:A:491:ASP:OD2	2.07	0.55
1:A:602:PHE:HD1	1:A:602:PHE:H	1.54	0.55
1:A:820:VAL:HG12	1:A:821:ARG:H	1.72	0.55
2:B:142:ASP:HB3	2:B:1318:GLU:HG2	1.89	0.55
2:B:494:GLU:HG2	2:B:577:GLN:HG3	1.88	0.55
2:B:733:VAL:HG21	2:B:741:TYR:HD1	1.70	0.55
2:C:539:PHE:O	2:C:543:TRP:HB3	2.06	0.55
3:E:209:GLU:O	3:E:213:LEU:CB	2.55	0.55
1:A:63:SER:OG	1:A:123:SER:HA	2.07	0.55
1:A:318:ARG:NH1	3:D:43:GLU:CG	2.70	0.55
2:B:1087:ASP:OD2	2:B:1236:ILE:HG23	2.07	0.55
2:C:834:THR:HA	2:C:847:ILE:O	2.07	0.55
2:C:1071:PHE:HD1	2:C:1234:GLN:HG2	1.72	0.55
2:C:1325:VAL:HG12	2:C:1326:ARG:H	1.71	0.55
3:D:290:TRP:CE3	3:D:290:TRP:C	2.85	0.55
1:A:605:ASP:O	1:A:606:LYS:HB2	2.07	0.55
1:A:1024:LEU:HD21	1:A:1035:LEU:HD21	1.89	0.55
3:D:291:ASN:OD1	3:D:291:ASN:C	2.50	0.55
3:E:1:MET:O	3:E:121:PHE:O	2.24	0.55
1:A:562:GLY:HA2	1:A:616:ASP:O	2.07	0.54
2:B:558:TYR:CE2	2:B:585:PHE:HB2	2.42	0.54
2:C:1074:VAL:HG12	2:C:1171:ILE:HG21	1.88	0.54
1:A:523:MET:HG2	1:A:574:ARG:HH22	1.73	0.54
3:E:238:ASN:O	3:E:253:GLU:HB2	2.06	0.54
3:E:285:LEU:O	3:E:288:THR:HG23	2.08	0.54
2:B:1247:ASN:HD22	2:B:1247:ASN:H	1.55	0.54
2:C:1035:ILE:HG22	2:C:1036:ASP:H	1.71	0.54
2:C:1153:ASP:HA	2:C:1156:ILE:HG22	1.90	0.54
3:E:262:THR:HG22	3:E:263:ALA:N	2.21	0.54
2:C:293:ASN:CG	2:C:294:VAL:H	2.16	0.54
2:C:594:LEU:HD12	2:C:597:ALA:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1:MET:O	3:E:2:LEU:CB	2.55	0.54
1:A:467:SER:N	1:A:468:PRO:HD2	2.23	0.54
1:A:667:GLN:H	1:A:667:GLN:CD	2.16	0.54
2:B:1084:PRO:CG	2:B:1209:GLY:HA3	2.35	0.54
1:A:569:VAL:HG11	1:A:595:ASN:HD21	1.73	0.54
3:E:107:LEU:HD23	3:E:122:TYR:HE1	1.70	0.54
3:E:253:GLU:O	3:E:254:TYR:CD1	2.61	0.54
1:A:559:ILE:CG2	1:A:613:ILE:HG12	2.38	0.54
2:B:338:ARG:HH21	2:C:1005:LEU:HD12	1.71	0.54
2:B:862:ARG:CB	2:B:952:PHE:CE2	2.89	0.54
2:C:141:LEU:HD23	2:C:141:LEU:H	1.73	0.54
2:C:440:ILE:HD12	2:C:478:ILE:HG21	1.88	0.54
2:B:1008:LEU:HD13	2:B:1008:LEU:H	1.73	0.54
1:A:531:LYS:HE2	1:A:683:GLN:NE2	2.23	0.54
2:C:129:ALA:HB3	2:C:133:MET:HG2	1.90	0.54
2:C:287:ARG:HH21	2:C:326:GLY:CA	2.18	0.54
2:C:931:ASN:ND2	2:C:934:LEU:O	2.38	0.54
1:A:293:LEU:O	1:A:297:LEU:HB2	2.09	0.53
1:A:719:VAL:HG13	1:A:720:ALA:N	2.23	0.53
2:C:146:GLU:O	2:C:1316:ALA:HA	2.08	0.53
3:D:156:VAL:HG23	3:D:228:LEU:HD23	1.88	0.53
3:D:172:MET:HE3	3:D:175:LYS:CG	2.35	0.53
3:E:229:PHE:CE1	3:E:252:LEU:CD1	2.90	0.53
1:A:236:LEU:HD13	1:A:236:LEU:O	2.08	0.53
2:C:1131:PRO:HA	2:C:1134:ARG:NH1	2.23	0.53
3:D:178:LYS:O	3:D:178:LYS:CG	2.56	0.53
3:D:239:VAL:HG23	3:D:263:ALA:CB	2.38	0.53
1:A:830:HIS:HD2	1:A:1034:ARG:NH1	2.03	0.53
2:B:635:ILE:HG22	2:B:706:TYR:HB3	1.90	0.53
2:B:862:ARG:HB3	2:B:952:PHE:HE2	1.70	0.53
3:E:76:LEU:HD12	3:E:76:LEU:H	1.73	0.53
1:A:194:HIS:CG	3:D:146:ARG:NH1	2.62	0.53
2:C:868:VAL:HB	2:C:890:THR:HA	1.89	0.53
3:E:142:THR:HG22	3:E:144:ARG:H	1.73	0.53
2:C:554:ARG:O	2:C:570:GLY:HA2	2.09	0.53
3:D:242:ARG:HG2	3:D:242:ARG:NH1	2.23	0.53
1:A:426:ARG:HG3	1:A:428:ILE:H	1.74	0.53
2:C:372:ALA:HB1	2:C:1315:MET:HE3	1.89	0.53
1:A:236:LEU:HD13	1:A:236:LEU:C	2.34	0.53
3:E:214:ARG:O	3:E:218:THR:CG2	2.57	0.53
1:A:407:GLU:OE1	1:A:1034:ARG:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:ALA:HA	1:A:564:GLU:CG	2.33	0.53
2:C:716:PHE:CD1	2:C:716:PHE:N	2.76	0.53
2:C:841:ASP:N	2:C:940:ARG:HH12	2.06	0.53
2:C:853:ASP:HB2	3:D:117:ILE:CG1	2.39	0.53
2:C:862:ARG:HG2	2:C:952:PHE:HE1	1.72	0.53
2:B:147:VAL:HG22	2:B:1315:MET:N	2.22	0.53
2:B:546:VAL:HG13	2:B:547:GLU:HG3	1.91	0.53
2:B:1060:ARG:HH12	2:B:1292:GLU:HA	1.74	0.53
2:C:838:GLU:CB	2:C:934:LEU:HB2	2.39	0.53
3:D:172:MET:CE	3:D:175:LYS:HG3	2.33	0.53
1:A:59:TYR:CA	1:A:167:THR:HG21	2.36	0.53
1:A:673:TYR:CD2	1:A:694:ILE:HG23	2.44	0.53
1:A:880:VAL:HB	1:A:899:VAL:HG12	1.91	0.53
1:A:926:MET:HG2	1:A:927:ASN:H	1.74	0.53
2:B:954:GLN:NE2	3:D:240:VAL:CG1	2.71	0.53
2:C:109:LYS:HZ2	2:C:110:PRO:HD2	1.73	0.53
3:E:33:GLN:C	3:E:35:LEU:H	2.17	0.53
3:E:229:PHE:HE1	3:E:252:LEU:HD12	1.73	0.53
1:A:28:PRO:C	1:A:30:THR:H	2.17	0.52
1:A:127:THR:HG23	2:B:641:ARG:H	1.74	0.52
1:A:283:PHE:HA	1:A:285:GLU:N	2.24	0.52
2:C:309:TRP:CD1	2:C:1253:ARG:HB3	2.44	0.52
1:A:53:LEU:HD13	1:A:57:PHE:HB3	1.91	0.52
1:A:407:GLU:CD	1:A:1034:ARG:HG2	2.34	0.52
3:D:111:ILE:O	3:D:111:ILE:HG23	2.07	0.52
1:A:203:THR:H	2:B:629:ARG:HG2	1.73	0.52
1:A:755:ALA:N	1:A:756:PRO:HD2	2.23	0.52
2:C:434:VAL:HG22	2:C:709:MET:HE1	1.90	0.52
3:D:189:LEU:HB3	3:D:230:ILE:HD11	1.91	0.52
2:B:448:TYR:CZ	2:B:470:ALA:HB1	2.45	0.52
1:A:943:ILE:HA	1:A:946:VAL:HB	1.92	0.52
2:C:387:THR:HA	2:C:1322:PRO:HD3	1.92	0.52
3:E:1:MET:CE	3:E:121:PHE:CD2	2.85	0.52
2:C:1087:ASP:HB3	2:C:1236:ILE:HG13	1.92	0.52
1:A:6:SER:HB2	1:A:251:VAL:HG22	1.90	0.52
1:A:474:TYR:O	1:A:477:TYR:HD2	1.92	0.52
1:A:559:ILE:HG12	1:A:585:ILE:HB	1.92	0.52
3:E:74:GLN:O	3:E:78:GLY:HA3	2.10	0.52
3:E:240:VAL:O	3:E:251:VAL:HG22	2.09	0.52
1:A:271:ARG:HG3	1:A:316:TYR:OH	2.10	0.52
1:A:367:ASN:HD22	1:A:369:GLY:H	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:926:MET:HB2	1:A:931:GLY:HA3	1.91	0.52
2:B:138:PHE:O	2:C:759:ASP:OD1	2.27	0.52
2:B:338:ARG:HH21	2:C:1005:LEU:CD1	2.21	0.52
2:B:368:ALA:C	3:D:83:ASN:HD22	2.17	0.52
2:B:1048:ASP:HB3	2:B:1051:ARG:HB2	1.91	0.52
3:E:107:LEU:HD23	3:E:122:TYR:OH	2.09	0.52
3:E:166:GLU:CD	3:E:171:VAL:O	2.53	0.52
1:A:127:THR:HG22	2:B:639:ASN:CB	2.36	0.52
1:A:628:MET:HE3	1:A:657:MET:HE3	1.92	0.52
2:C:520:PHE:CD1	2:C:520:PHE:N	2.78	0.52
3:D:115:GLU:OE2	3:D:115:GLU:N	2.30	0.52
1:A:22:ILE:HG12	1:A:25:ILE:HD11	1.91	0.52
2:B:1118:THR:HG22	2:B:1129:PRO:HA	1.90	0.52
2:C:669:GLN:O	2:C:670:ASP:HB2	2.09	0.52
1:A:282:GLU:O	1:A:285:GLU:HA	2.10	0.51
1:A:731:HIS:HB2	1:A:746:PHE:HB3	1.91	0.51
2:C:828:ASP:O	2:C:948:ILE:HA	2.10	0.51
3:D:217:LYS:HE2	3:D:290:TRP:CZ3	2.45	0.51
1:A:282:GLU:HG3	1:A:286:ASN:OD1	2.11	0.51
1:A:422:ASP:HB3	1:A:677:LEU:HD12	1.93	0.51
3:E:290:TRP:HD1	3:E:291:ASN:HB3	1.75	0.51
1:A:146:PRO:O	1:A:147:GLN:HB3	2.10	0.51
1:A:406:VAL:CB	1:A:407:GLU:CA	2.79	0.51
1:A:723:GLU:O	1:A:724:MET:CB	2.59	0.51
1:A:966:GLY:O	1:A:970:ARG:HD3	2.10	0.51
2:B:338:ARG:NH2	2:C:1005:LEU:CD1	2.73	0.51
2:C:261:ASP:O	2:C:1054:ARG:NH1	2.43	0.51
2:B:368:ALA:CA	3:D:83:ASN:HD22	2.24	0.51
2:C:1264:GLU:HA	2:C:1297:SER:HA	1.93	0.51
1:A:292:ARG:HG2	1:A:295:THR:CG2	2.40	0.51
3:D:44:LEU:HD11	3:D:154:ALA:CA	2.31	0.51
3:D:214:ARG:O	3:D:218:THR:CG2	2.51	0.51
3:E:53:GLU:HB2	3:E:145:TYR:CE1	2.45	0.51
3:E:83:ASN:OD1	3:E:83:ASN:N	2.43	0.51
3:E:262:THR:O	3:E:263:ALA:HB3	2.10	0.51
1:A:201:LYS:HA	2:B:629:ARG:HD3	1.92	0.51
1:A:406:VAL:CG2	1:A:407:GLU:HA	2.40	0.51
1:A:437:GLN:HB3	1:A:656:TYR:HB2	1.92	0.51
1:A:508:ASN:HB2	1:A:509:ARG:HH11	1.74	0.51
1:A:409:MET:HE3	1:A:411:ILE:HD12	1.91	0.51
2:B:153:ASP:HB3	2:B:154:PHE:HD1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:21:ASN:O	3:D:24:THR:O	2.29	0.51
3:E:82:GLN:HG2	3:E:83:ASN:OD1	2.10	0.51
3:E:283:LEU:O	3:E:287:PHE:HB2	2.11	0.51
2:B:269:GLU:O	2:B:291:HIS:CD2	2.63	0.51
2:B:279:SER:CA	2:C:1198:LYS:HE2	2.41	0.51
2:C:255:LEU:HD23	2:C:1062:ILE:HD13	1.93	0.51
2:C:931:ASN:OD1	2:C:934:LEU:HD22	2.11	0.51
3:D:153:TYR:HA	3:D:156:VAL:HG11	1.86	0.51
1:A:59:TYR:HA	1:A:167:THR:CG2	2.38	0.51
1:A:133:LEU:CD2	2:C:545:PRO:HB3	2.41	0.51
2:C:339:LEU:O	2:C:340:VAL:HG22	2.09	0.51
3:E:160:LEU:HD11	3:E:229:PHE:CB	2.36	0.51
1:A:47:ARG:HE	2:B:596:GLY:CA	2.22	0.50
1:A:926:MET:SD	1:A:930:ASN:O	2.69	0.50
3:E:12:LEU:HD23	3:E:15:PHE:CZ	2.46	0.50
1:A:64:GLU:OE1	2:B:647:GLU:CD	2.55	0.50
1:A:605:ASP:O	1:A:606:LYS:CB	2.60	0.50
2:B:368:ALA:O	3:D:83:ASN:ND2	2.41	0.50
3:E:33:GLN:C	3:E:35:LEU:N	2.69	0.50
1:A:255:ARG:HD3	1:A:258:GLN:CD	2.36	0.50
2:C:412:LEU:HD11	2:C:714:LEU:HD23	1.93	0.50
2:C:716:PHE:N	2:C:716:PHE:HD1	2.09	0.50
2:C:871:PRO:HB2	2:C:896:LEU:HD23	1.93	0.50
3:D:250:ARG:HB3	3:D:250:ARG:HH11	1.76	0.50
1:A:567:PRO:O	1:A:568:ALA:HB3	2.12	0.50
1:A:709:SER:HB2	1:A:712:ILE:HB	1.94	0.50
1:A:840:MET:SD	1:A:1019:PRO:HB2	2.51	0.50
3:E:62:VAL:HG23	3:E:63:PRO:HD2	1.93	0.50
2:B:747:ARG:O	2:B:747:ARG:CG	2.58	0.50
2:B:836:GLN:HE22	2:B:844:ASP:HA	1.75	0.50
2:B:926:VAL:O	2:B:926:VAL:CG1	2.59	0.50
2:C:835:TYR:O	2:C:846:GLY:HA3	2.12	0.50
2:C:1126:MET:HG3	2:C:1127:ALA:H	1.76	0.50
3:D:289:ARG:HA	3:D:289:ARG:NE	2.24	0.50
3:E:236:ALA:O	3:E:263:ALA:HA	2.10	0.50
3:E:289:ARG:O	3:E:289:ARG:CD	2.35	0.50
2:B:862:ARG:HH12	2:B:948:ILE:HD13	1.77	0.50
2:B:1263:TYR:CG	2:B:1295:HIS:HD2	2.29	0.50
2:C:520:PHE:HD1	2:C:520:PHE:N	2.10	0.50
3:D:131:ALA:C	3:D:133:THR:H	2.19	0.50
1:A:298:LEU:CD1	2:B:563:ALA:HB3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:941:TYR:O	2:B:941:TYR:CD1	2.65	0.50
2:B:1078:TYR:CE2	2:B:1080:THR:HG22	2.46	0.50
3:E:41:GLU:O	3:E:41:GLU:OE1	2.30	0.50
1:A:208:HIS:HB3	1:A:260:LEU:HA	1.93	0.50
2:B:134:THR:HG22	2:C:472:GLU:CD	2.36	0.50
2:C:298:PRO:O	2:C:299:ALA:HB3	2.12	0.50
2:C:522:PRO:HG3	2:C:636:PRO:HB2	1.94	0.50
3:D:15:PHE:N	3:D:15:PHE:CD1	2.80	0.50
1:A:76:LEU:HB2	1:A:172:PHE:CE2	2.47	0.50
1:A:308:ALA:CB	1:A:309:ASN:HB2	2.41	0.50
2:B:218:GLY:C	2:B:219:ILE:HG12	2.36	0.50
2:C:384:MET:HA	2:C:708:THR:HG21	1.93	0.50
2:C:853:ASP:O	3:D:117:ILE:HD11	2.12	0.50
2:C:1037:ILE:O	2:C:1038:GLU:CB	2.58	0.50
3:D:153:TYR:CE2	3:D:258:ASN:ND2	2.80	0.50
3:E:10:THR:HG23	3:E:17:PHE:HZ	1.77	0.50
3:E:69:GLU:O	3:E:69:GLU:OE2	2.30	0.50
1:A:351:TYR:CE1	3:D:150:ILE:HG21	2.47	0.49
1:A:395:GLN:HE21	1:A:395:GLN:CA	2.20	0.49
1:A:845:ILE:O	1:A:849:ILE:HG12	2.11	0.49
1:A:894:LYS:C	1:A:896:ASN:H	2.19	0.49
2:B:135:LYS:HG3	2:C:470:ALA:O	2.09	0.49
2:B:953:ASP:OD1	3:D:241:ASN:OD1	2.30	0.49
2:B:225:ILE:HG23	2:B:247:TYR:CD2	2.46	0.49
2:B:269:GLU:HB3	2:B:292:ASN:HD22	1.76	0.49
2:B:1276:LEU:HB3	2:B:1290:LYS:HD3	1.95	0.49
2:C:284:ASN:OD1	2:C:284:ASN:N	2.44	0.49
3:E:53:GLU:CD	3:E:53:GLU:O	2.55	0.49
1:A:64:GLU:CG	2:B:647:GLU:OE1	2.60	0.49
1:A:64:GLU:HG3	2:B:647:GLU:OE1	2.12	0.49
1:A:188:THR:HG21	3:D:144:ARG:HG2	1.93	0.49
1:A:416:MET:HG2	1:A:466:LEU:HD21	1.94	0.49
1:A:602:PHE:HD1	1:A:602:PHE:N	2.11	0.49
1:A:662:ILE:HG12	1:A:675:THR:HG21	1.93	0.49
2:B:1078:TYR:C	2:B:1078:TYR:CD2	2.91	0.49
2:C:270:THR:HA	2:C:292:ASN:H	1.77	0.49
2:C:853:ASP:HB2	3:D:117:ILE:HG13	1.93	0.49
2:C:1280:PRO:HB3	2:C:1287:GLY:CA	2.41	0.49
3:D:107:LEU:HD23	3:D:122:TYR:CE1	2.47	0.49
1:A:213:TRP:O	1:A:215:VAL:N	2.36	0.49
1:A:254:ASP:O	1:A:255:ARG:CB	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:THR:HG21	2:C:472:GLU:CD	2.37	0.49
3:E:20:ARG:HD2	3:E:25:ASN:HB3	1.94	0.49
1:A:307:HIS:HD2	1:A:308:ALA:HB2	1.77	0.49
2:B:862:ARG:HB2	2:B:952:PHE:CZ	2.48	0.49
2:C:931:ASN:HB2	2:C:936:MET:SD	2.53	0.49
3:D:21:ASN:O	3:D:22:ASP:OD1	2.31	0.49
3:D:164:ASP:HA	3:D:167:ARG:HG2	1.94	0.49
3:E:84:VAL:HG23	3:E:85:ASN:N	2.28	0.49
1:A:242:LYS:O	1:A:246:ASP:HB2	2.12	0.49
3:E:289:ARG:C	3:E:289:ARG:CD	2.73	0.49
2:B:139:ASN:O	2:C:757:ILE:CG2	2.61	0.49
2:C:1144:ARG:HD2	2:C:1194:MET:HA	1.95	0.49
2:C:1238:VAL:HG23	2:C:1239:ALA:H	1.77	0.49
3:D:172:MET:HG3	3:D:173:PRO:CD	2.42	0.49
3:D:181:SER:HB2	3:D:185:SER:OG	2.13	0.49
3:E:139:ASN:OD1	3:E:139:ASN:O	2.30	0.49
2:C:624:PHE:CE2	2:C:713:MET:HG2	2.48	0.49
2:C:1180:PRO:CB	2:C:1209:GLY:HA2	2.41	0.49
3:E:85:ASN:O	3:E:85:ASN:OD1	2.30	0.49
1:A:503:ILE:N	1:A:503:ILE:HD12	2.28	0.49
3:E:53:GLU:OE2	3:E:53:GLU:O	2.30	0.49
3:E:92:ARG:O	3:E:92:ARG:HD3	2.12	0.49
1:A:351:TYR:CZ	3:D:150:ILE:HG21	2.48	0.48
2:B:234:PRO:HD2	2:B:242:GLU:CB	2.43	0.48
3:E:38:GLU:HB3	3:E:176:ARG:HB3	1.95	0.48
3:E:66:VAL:HG13	3:E:111:ILE:CG2	2.42	0.48
3:E:72:ILE:O	3:E:76:LEU:CD1	2.61	0.48
1:A:409:MET:CB	1:A:1034:ARG:HH12	2.12	0.48
1:A:866:LEU:O	1:A:867:ALA:HB3	2.13	0.48
1:A:840:MET:HE2	1:A:1024:LEU:HD23	1.94	0.48
2:C:528:ILE:HD11	2:C:758:ILE:HD12	1.96	0.48
2:C:533:GLN:HG2	2:C:588:LEU:HD23	1.95	0.48
2:C:878:SER:HB3	2:C:903:ASN:CB	2.43	0.48
3:D:121:PHE:N	3:D:121:PHE:CD1	2.82	0.48
3:E:12:LEU:HG	3:E:14:GLN:HG2	1.95	0.48
3:E:49:ILE:CG2	3:E:50:PRO:CD	2.84	0.48
3:E:162:GLY:HA2	3:E:172:MET:HE2	1.93	0.48
1:A:64:GLU:OE1	2:B:647:GLU:OE1	2.31	0.48
1:A:461:ARG:NH1	1:A:461:ARG:CG	2.73	0.48
1:A:76:LEU:HB2	1:A:172:PHE:CD2	2.48	0.48
2:B:577:GLN:HB2	2:B:747:ARG:HH21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1214:GLU:HB2	2:B:1215:PRO:HD2	1.96	0.48
2:B:1234:GLN:HE21	2:B:1234:GLN:HA	1.79	0.48
2:C:150:LEU:HD12	2:C:150:LEU:H	1.78	0.48
2:C:619:ALA:HB2	2:C:711:ASN:HB2	1.95	0.48
2:C:1025:ASP:OD1	3:D:95:ALA:CB	2.61	0.48
3:E:12:LEU:HG	3:E:14:GLN:NE2	2.18	0.48
3:E:13:GLU:O	3:E:13:GLU:OE1	2.30	0.48
1:A:286:ASN:HB2	1:A:814:ASN:ND2	2.27	0.48
2:B:709:MET:HA	2:B:712:PHE:HD2	1.78	0.48
2:B:836:GLN:NE2	2:B:845:GLU:H	2.11	0.48
3:D:166:GLU:OE2	3:D:166:GLU:HA	2.13	0.48
3:E:122:TYR:N	3:E:122:TYR:CD1	2.82	0.48
1:A:406:VAL:HB	1:A:407:GLU:C	2.39	0.48
1:A:1004:THR:O	1:A:1008:ARG:HG2	2.13	0.48
2:B:751:THR:HG22	2:B:753:ASP:H	1.78	0.48
2:C:210:ARG:O	2:C:210:ARG:HG3	2.13	0.48
2:C:297:ASN:ND2	2:C:298:PRO:O	2.46	0.48
3:E:226:MET:HE3	3:E:226:MET:HA	1.96	0.48
1:A:835:PHE:O	1:A:839:LEU:HG	2.14	0.48
2:B:1077:MET:SD	2:B:1079:LEU:HB2	2.53	0.48
3:D:244:VAL:HG12	3:D:245:THR:N	2.28	0.48
3:D:255:ILE:O	3:D:255:ILE:HG13	2.13	0.48
1:A:12:ARG:O	1:A:12:ARG:HD3	2.14	0.48
3:D:60:ARG:O	3:D:62:VAL:HG23	2.14	0.48
3:D:77:PHE:HE1	3:D:227:MET:O	1.96	0.48
3:E:1:MET:SD	3:E:121:PHE:CZ	3.06	0.48
3:E:5:PRO:HB2	3:E:8:GLY:O	2.14	0.48
1:A:544:ASN:ND2	1:A:546:ALA:HB3	2.24	0.48
1:A:602:PHE:N	1:A:602:PHE:CD1	2.80	0.48
1:A:853:GLU:CD	1:A:854:ASN:H	2.22	0.48
2:B:908:THR:HA	2:B:911:ARG:HE	1.78	0.48
2:C:292:ASN:OD1	2:C:293:ASN:N	2.47	0.48
2:C:772:TYR:C	2:C:774:LEU:H	2.21	0.48
3:D:190:SER:O	3:D:194:VAL:HG23	2.14	0.48
3:D:242:ARG:HH11	3:D:242:ARG:CB	2.27	0.48
3:E:192:ASP:OD1	3:E:192:ASP:O	2.31	0.48
3:E:196:TRP:HH2	3:E:226:MET:HG2	1.79	0.48
1:A:305:TYR:HD2	1:A:316:TYR:HE2	1.62	0.47
2:B:148:GLN:HA	2:B:148:GLN:OE1	2.13	0.47
2:C:385:ILE:O	2:C:386:SER:HB3	2.13	0.47
2:C:855:TYR:HB2	2:C:918:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:937:ARG:O	1:A:941:ASP:HB2	2.13	0.47
1:A:959:TYR:HB2	1:A:1051:PRO:HD2	1.96	0.47
1:A:308:ALA:HB3	1:A:309:ASN:ND2	2.29	0.47
1:A:462:ILE:HG12	1:A:684:ASN:CA	2.44	0.47
1:A:645:ARG:HG3	1:A:695:THR:HG22	1.96	0.47
2:C:492:VAL:HG22	2:C:747:ARG:HA	1.95	0.47
2:C:687:LEU:HD11	2:C:764:TRP:HZ3	1.79	0.47
3:D:152:ILE:O	3:D:155:HIS:HB2	2.14	0.47
3:D:221:ARG:NH1	3:D:225:ARG:HH21	2.12	0.47
3:E:191:ARG:HD2	3:E:191:ARG:HA	1.60	0.47
1:A:302:ASP:O	1:A:305:TYR:HB3	2.14	0.47
1:A:462:ILE:HG22	1:A:463:ASP:N	2.27	0.47
2:B:902:ILE:HD11	2:B:929:PHE:HE1	1.79	0.47
2:B:937:ASN:C	2:B:939:ASN:H	2.22	0.47
2:C:629:ARG:HA	2:C:1037:ILE:HG12	1.95	0.47
3:D:143:PRO:O	3:D:144:ARG:CB	2.63	0.47
3:D:185:SER:O	3:D:188:SER:N	2.43	0.47
1:A:298:LEU:HD13	2:B:563:ALA:HB3	1.95	0.47
1:A:613:ILE:HG13	1:A:643:ALA:HB2	1.96	0.47
1:A:962:PHE:HB3	1:A:1049:TYR:CD1	2.49	0.47
2:B:951:ILE:O	2:B:952:PHE:HB2	2.14	0.47
2:B:1041:ARG:HG3	2:B:1042:TRP:CD1	2.49	0.47
2:B:1263:TYR:CG	2:B:1295:HIS:CD2	3.02	0.47
2:C:268:GLY:O	2:C:269:GLU:HB2	2.14	0.47
2:C:841:ASP:O	2:C:842:ASP:CB	2.61	0.47
1:A:908:ALA:HB2	1:A:943:ILE:HB	1.95	0.47
2:B:424:GLY:O	2:B:428:GLN:HB2	2.15	0.47
2:B:893:ALA:HB1	2:B:915:VAL:HG12	1.95	0.47
2:C:231:LEU:HB2	2:C:249:SER:HB2	1.97	0.47
2:C:523:THR:O	2:C:524:GLU:CB	2.60	0.47
2:C:554:ARG:NH2	2:C:594:LEU:HD23	2.29	0.47
1:A:12:ARG:HD3	1:A:12:ARG:C	2.40	0.47
1:A:467:SER:HA	1:A:470:LEU:HD22	1.96	0.47
1:A:487:GLN:HE22	1:A:548:ASN:HA	1.80	0.47
2:B:427:VAL:HG11	2:B:755:LEU:HD21	1.97	0.47
2:B:961:SER:O	2:B:964:VAL:HG12	2.14	0.47
2:C:836:GLN:HB3	2:C:940:ARG:HH11	1.79	0.47
2:B:765:PRO:HA	2:B:769:GLN:HB2	1.96	0.47
3:D:37:TYR:HD1	3:D:177:ALA:CB	2.28	0.47
1:A:91:ASN:HD22	1:A:91:ASN:HA	1.56	0.47
1:A:409:MET:HB3	1:A:1034:ARG:NH1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:ALA:CA	3:D:83:ASN:ND2	2.78	0.47
2:B:466:VAL:O	2:B:470:ALA:HB2	2.15	0.47
3:E:105:LEU:O	3:E:121:PHE:HB2	2.15	0.47
1:A:667:GLN:NE2	1:A:667:GLN:N	2.62	0.47
2:C:668:VAL:HG22	2:C:669:GLN:H	1.80	0.47
3:E:49:ILE:HG23	3:E:50:PRO:CD	2.24	0.47
3:E:148:ASP:OD1	3:E:151:ASP:HB2	2.15	0.47
3:E:288:THR:HG23	3:E:289:ARG:H	1.80	0.47
1:A:454:GLY:C	1:A:456:PHE:H	2.22	0.46
1:A:833:VAL:O	1:A:837:HIS:N	2.43	0.46
2:C:230:ASP:HB3	2:C:985:ARG:HE	1.79	0.46
3:D:67:TYR:CD1	3:D:110:VAL:HG22	2.50	0.46
1:A:565:ARG:HB3	1:A:592:VAL:HB	1.95	0.46
1:A:567:PRO:O	1:A:568:ALA:CB	2.63	0.46
1:A:580:SER:HB2	1:A:581:ASN:H	1.61	0.46
1:A:834:THR:O	1:A:838:LYS:HG3	2.15	0.46
2:C:449:PHE:CE2	2:C:462:LEU:HD13	2.43	0.46
3:E:53:GLU:OE1	3:E:145:TYR:CD1	2.69	0.46
1:A:303:THR:HB	1:A:307:HIS:CE1	2.50	0.46
1:A:456:PHE:HB3	1:A:686:TYR:HE1	1.79	0.46
1:A:833:VAL:HA	1:A:836:ILE:HB	1.97	0.46
2:B:419:TYR:CE1	2:B:1007:THR:HA	2.51	0.46
2:B:760:THR:C	2:B:762:ILE:H	2.22	0.46
3:D:44:LEU:HB2	3:D:174:VAL:HG23	1.97	0.46
1:A:69:HIS:CB	1:A:70:PRO:HD3	2.45	0.46
1:A:643:ALA:HB3	1:A:646:ALA:HB2	1.97	0.46
1:A:725:PRO:C	1:A:726:ILE:HG12	2.39	0.46
2:B:425:ILE:HD13	2:B:425:ILE:H	1.80	0.46
2:B:748:GLN:HE21	2:B:748:GLN:HB3	1.59	0.46
2:C:552:ILE:HD13	2:C:552:ILE:HA	1.84	0.46
1:A:495:LEU:HA	1:A:503:ILE:HD13	1.97	0.46
1:A:559:ILE:HD11	1:A:587:MET:HG2	1.97	0.46
2:B:667:ALA:HB3	2:B:677:ARG:HD3	1.97	0.46
2:B:935:GLN:O	2:B:940:ARG:NH1	2.49	0.46
2:C:185:ALA:HB3	2:C:277:THR:O	2.15	0.46
1:A:926:MET:HB2	1:A:931:GLY:N	2.30	0.46
3:E:1:MET:SD	3:E:121:PHE:CE2	3.09	0.46
1:A:802:THR:HG23	1:A:803:SER:H	1.80	0.46
2:B:1051:ARG:HG2	2:B:1054:ARG:HH12	1.80	0.46
2:B:1175:ALA:HB2	2:B:1204:LEU:HB2	1.98	0.46
2:B:1242:MET:SD	2:B:1260:PRO:HG3	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:293:ASN:CG	2:C:294:VAL:N	2.73	0.46
3:D:233:THR:HG22	3:D:252:LEU:HD13	1.97	0.46
1:A:560:LEU:HD23	1:A:614:ILE:HB	1.96	0.46
1:A:676:ALA:O	1:A:693:TYR:HB3	2.15	0.46
2:B:581:LEU:HD23	2:B:581:LEU:H	1.81	0.46
2:B:939:ASN:O	2:B:940:ARG:CB	2.56	0.46
2:C:141:LEU:HG	2:C:142:ASP:N	2.26	0.46
2:C:815:LEU:N	2:C:816:PRO:HD2	2.31	0.46
2:C:1075:ARG:HD2	2:C:1090:PRO:HD2	1.97	0.46
3:D:53:GLU:HG2	3:D:145:TYR:HE1	1.81	0.46
1:A:204:LEU:HA	1:A:264:SER:O	2.15	0.46
1:A:285:GLU:HG2	1:A:286:ASN:N	2.31	0.46
1:A:462:ILE:HG12	1:A:685:PRO:HD3	1.97	0.46
1:A:519:ILE:HG12	1:A:519:ILE:O	2.15	0.46
2:B:1277:LEU:HD13	2:B:1287:GLY:HA3	1.96	0.46
2:C:388:GLN:HB3	2:C:1320:VAL:HG23	1.97	0.46
2:C:828:ASP:OD2	2:C:828:ASP:N	2.49	0.46
3:D:66:VAL:O	3:D:111:ILE:HG22	2.16	0.46
1:A:892:GLN:C	1:A:894:LYS:H	2.24	0.46
2:B:154:PHE:CD1	2:B:154:PHE:N	2.84	0.46
2:B:420:PRO:HB2	2:B:748:GLN:CD	2.39	0.46
2:C:231:LEU:HB3	2:C:249:SER:HB2	1.97	0.46
1:A:27:LYS:CB	1:A:28:PRO:HD3	2.39	0.45
1:A:73:ARG:HG3	1:A:74:LEU:HD12	1.97	0.45
2:B:154:PHE:HD1	2:B:154:PHE:N	2.14	0.45
2:B:278:LEU:HB2	2:B:282:VAL:HG13	1.97	0.45
2:B:1084:PRO:HB2	2:B:1209:GLY:N	2.31	0.45
2:B:1321:ASN:C	2:B:1323:ASP:H	2.24	0.45
2:C:302:ARG:HD2	2:C:315:THR:HG22	1.98	0.45
2:C:561:ASN:O	2:C:562:ALA:HB3	2.16	0.45
3:D:217:LYS:O	3:D:221:ARG:HB3	2.15	0.45
1:A:314:ARG:O	1:A:318:ARG:HB2	2.16	0.45
1:A:496:CYS:SG	1:A:497:ALA:N	2.90	0.45
2:B:144:ASN:HB2	2:B:1318:GLU:HA	1.98	0.45
2:B:1273:ASN:ND2	3:D:79:ILE:CG2	2.79	0.45
2:C:144:ASN:HA	2:C:1318:GLU:HB3	1.98	0.45
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.97	0.45
1:A:64:GLU:HA	1:A:67:ARG:CG	2.45	0.45
1:A:456:PHE:HB3	1:A:686:TYR:CE1	2.51	0.45
1:A:491:ASP:OD1	1:A:491:ASP:C	2.60	0.45
1:A:660:SER:HA	1:A:663:GLU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:940:MET:O	1:A:944:ARG:HB2	2.16	0.45
1:A:967:ILE:HB	1:A:978:LYS:HD3	1.98	0.45
2:B:493:HIS:CG	2:B:758:ILE:HD13	2.52	0.45
2:C:94:PHE:HA	2:C:104:ILE:HG21	1.98	0.45
2:C:1060:ARG:HH22	2:C:1292:GLU:HA	1.81	0.45
1:A:600:VAL:HA	1:A:601:PRO:C	2.40	0.45
1:A:673:TYR:CE2	1:A:694:ILE:HG22	2.51	0.45
1:A:934:THR:N	1:A:935:PRO:HD2	2.31	0.45
2:B:862:ARG:C	2:B:952:PHE:HZ	2.24	0.45
2:C:838:GLU:CG	2:C:839:ALA:H	2.23	0.45
2:C:934:LEU:HD13	2:C:934:LEU:H	1.81	0.45
2:C:1027:THR:HG22	3:D:102:SER:OG	2.16	0.45
3:D:140:ALA:HA	3:D:281:LYS:HG3	1.97	0.45
3:D:181:SER:CB	3:D:250:ARG:HG2	2.41	0.45
1:A:308:ALA:HB3	1:A:309:ASN:CB	2.47	0.45
1:A:411:ILE:HD13	1:A:411:ILE:N	2.31	0.45
1:A:658:ILE:HD11	1:A:692:ILE:HD11	1.99	0.45
2:B:763:VAL:HA	2:B:766:ILE:HD12	1.98	0.45
2:C:503:GLU:CD	2:C:542:ARG:HH12	2.25	0.45
2:C:1035:ILE:O	2:C:1036:ASP:HB3	2.17	0.45
2:C:1038:GLU:O	2:C:1041:ARG:HB2	2.17	0.45
3:E:229:PHE:HE1	3:E:252:LEU:CD1	2.29	0.45
1:A:208:HIS:HB3	1:A:260:LEU:HD23	1.99	0.45
3:E:70:ASP:O	3:E:70:ASP:OD2	2.35	0.45
3:E:166:GLU:HG3	3:E:172:MET:SD	2.57	0.45
1:A:752:VAL:HG12	1:A:812:VAL:HG23	1.98	0.45
2:B:1255:ARG:HB3	2:B:1256:GLY:H	1.56	0.45
3:E:70:ASP:OD2	3:E:70:ASP:C	2.60	0.45
1:A:463:ASP:OD2	1:A:530:MET:HB3	2.16	0.45
2:B:180:LEU:HB3	2:B:195:ASN:HD21	1.82	0.45
2:B:279:SER:CB	2:C:1198:LYS:HE2	2.47	0.45
2:B:639:ASN:HB3	2:B:641:ARG:HG3	1.99	0.45
2:C:286:LEU:HD21	2:C:290:TYR:HB3	1.98	0.45
2:C:603:ILE:C	2:C:605:ARG:H	2.25	0.45
3:D:110:VAL:HG12	3:D:111:ILE:N	2.32	0.45
3:D:178:LYS:HD2	3:D:249:ASP:HB3	1.99	0.45
1:A:27:LYS:HB3	1:A:28:PRO:CD	2.36	0.45
1:A:926:MET:HG2	1:A:927:ASN:N	2.31	0.45
2:B:135:LYS:O	2:C:471:SER:HA	2.16	0.45
2:B:147:VAL:HG23	2:B:375:ARG:HH11	1.82	0.45
2:B:835:TYR:CE1	2:B:941:TYR:CD2	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:451:GLU:O	2:C:452:ASN:HB3	2.17	0.45
2:C:627:ALA:H	2:C:716:PHE:HB2	1.82	0.45
2:C:1071:PHE:CD1	2:C:1234:GLN:HG2	2.50	0.45
3:D:106:GLY:HA2	3:D:121:PHE:HB3	1.98	0.45
3:E:148:ASP:O	3:E:280:ALA:HB1	2.16	0.45
1:A:565:ARG:N	1:A:590:ARG:O	2.50	0.45
2:B:472:GLU:CD	2:B:472:GLU:N	2.73	0.45
2:B:884:ALA:O	2:B:888:GLN:HG2	2.16	0.45
2:C:306:GLN:HE21	2:C:306:GLN:N	2.14	0.45
2:C:409:ILE:HD11	2:C:1040:PHE:CZ	2.52	0.45
3:E:53:GLU:CG	3:E:145:TYR:CE1	2.93	0.45
2:B:753:ASP:N	2:B:754:GLY:HA2	2.32	0.44
2:C:447:ARG:C	2:C:450:PRO:HG3	2.42	0.44
2:C:1137:VAL:HG22	2:C:1164:TRP:CE2	2.51	0.44
3:D:185:SER:HB3	3:D:186:LEU:H	1.50	0.44
1:A:308:ALA:HB3	1:A:309:ASN:HB2	1.98	0.44
1:A:331:ARG:HD3	1:A:331:ARG:H	1.82	0.44
1:A:670:GLY:O	1:A:671:VAL:CG2	2.60	0.44
1:A:953:ARG:HH12	1:A:1055:LEU:HD23	1.81	0.44
2:B:348:LEU:HD23	2:B:350:ILE:HD11	1.98	0.44
2:B:583:GLU:HA	2:B:583:GLU:OE1	2.17	0.44
2:B:709:MET:HA	2:B:712:PHE:CD2	2.52	0.44
2:C:863:LEU:HD11	2:C:871:PRO:HD3	1.99	0.44
2:C:980:ARG:HH21	2:C:999:LYS:HE2	1.82	0.44
3:D:221:ARG:HH12	3:D:225:ARG:HH21	1.64	0.44
3:E:116:THR:HG21	3:E:119:ILE:HD12	1.99	0.44
1:A:127:THR:CG2	2:B:639:ASN:CB	2.91	0.44
1:A:222:ARG:NH1	2:B:613:LEU:HD13	2.31	0.44
1:A:358:ILE:HB	1:A:359:PRO:HA	1.99	0.44
1:A:876:MET:HE3	1:A:876:MET:HA	2.00	0.44
1:A:959:TYR:O	1:A:960:ILE:HG13	2.17	0.44
2:B:1298:PHE:O	2:B:1299:SER:OG	2.33	0.44
2:C:751:THR:C	2:C:753:ASP:H	2.24	0.44
3:D:238:ASN:H	3:D:253:GLU:HB3	1.82	0.44
1:A:926:MET:HB2	1:A:931:GLY:CA	2.47	0.44
2:B:888:GLN:NE2	3:D:38:GLU:OE1	2.51	0.44
2:C:192:PRO:HG3	2:C:294:VAL:CG2	2.48	0.44
2:C:385:ILE:O	2:C:386:SER:CB	2.65	0.44
2:C:449:PHE:N	2:C:450:PRO:CD	2.79	0.44
2:C:624:PHE:CD2	2:C:713:MET:HG2	2.53	0.44
2:C:730:ASP:O	2:C:730:ASP:CG	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:149:MET:HE3	3:D:260:MET:SD	2.57	0.44
1:A:127:THR:HG23	2:B:640:GLN:CA	2.47	0.44
1:A:663:GLU:O	1:A:667:GLN:NE2	2.51	0.44
1:A:926:MET:SD	1:A:928:GLU:HG2	2.58	0.44
3:E:42:ASN:HB3	3:E:174:VAL:CG2	2.48	0.44
1:A:351:TYR:CE1	3:D:150:ILE:CG2	3.01	0.44
1:A:470:LEU:HD21	1:A:525:ARG:HD2	1.99	0.44
1:A:526:ASN:OD1	1:A:526:ASN:N	2.49	0.44
1:A:659:ASN:HD21	1:A:706:TYR:H	1.65	0.44
1:A:988:LYS:HD2	1:A:994:PRO:HD3	2.00	0.44
2:C:837:THR:CG2	2:C:934:LEU:HD21	2.46	0.44
3:D:14:GLN:NE2	3:D:107:LEU:HD13	2.32	0.44
3:D:25:ASN:OD1	3:D:26:ALA:N	2.51	0.44
3:D:150:ILE:HG22	3:D:151:ASP:N	2.33	0.44
3:E:33:GLN:O	3:E:35:LEU:N	2.51	0.44
3:E:68:ILE:HD13	3:E:69:GLU:CA	2.47	0.44
1:A:303:THR:CA	1:A:307:HIS:CE1	3.00	0.44
2:B:291:HIS:HB3	2:B:292:ASN:H	1.55	0.44
2:B:473:ALA:HA	2:B:765:PRO:HG3	1.98	0.44
2:B:953:ASP:OD1	2:B:953:ASP:C	2.61	0.44
1:A:525:ARG:HE	1:A:525:ARG:HB2	1.42	0.44
2:B:149:PRO:O	2:B:150:LEU:C	2.60	0.44
2:C:564:GLY:O	2:C:565:GLU:HB3	2.17	0.44
3:D:116:THR:OG1	3:D:119:ILE:HD12	2.18	0.44
3:E:46:LYS:CG	3:E:155:HIS:CE1	3.00	0.44
2:B:146:GLU:OE2	2:B:1314:ASP:HB3	2.18	0.44
2:C:838:GLU:HA	2:C:940:ARG:NE	2.33	0.44
3:E:2:LEU:HD11	3:E:107:LEU:CD1	2.48	0.44
1:A:625:PHE:HA	1:A:628:MET:HB3	2.00	0.43
1:A:842:TYR:HA	1:A:845:ILE:HG22	2.00	0.43
2:B:1306:THR:HG23	2:B:1308:ASN:H	1.83	0.43
3:D:160:LEU:HD23	3:D:229:PHE:HA	2.00	0.43
3:D:255:ILE:O	3:D:255:ILE:CG1	2.65	0.43
1:A:133:LEU:CD2	2:C:545:PRO:HG3	2.48	0.43
1:A:963:TYR:CE2	1:A:985:GLY:HA2	2.53	0.43
2:B:154:PHE:HA	2:B:262:ASN:HD22	1.83	0.43
2:B:172:ASP:HA	2:B:175:THR:HG22	2.00	0.43
2:B:554:ARG:HH21	2:B:594:LEU:HD23	1.83	0.43
2:B:642:GLY:HA2	2:C:670:ASP:CG	2.41	0.43
2:B:862:ARG:NH1	2:B:948:ILE:HD13	2.33	0.43
2:B:883:ILE:HG21	2:B:915:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:204:VAL:CG2	2:C:1242:MET:HG2	2.48	0.43
2:C:772:TYR:C	2:C:774:LEU:N	2.76	0.43
3:D:144:ARG:O	3:D:144:ARG:CG	2.64	0.43
3:E:93:LEU:O	3:E:96:LEU:HB2	2.18	0.43
3:E:186:LEU:HD13	3:E:186:LEU:HA	1.60	0.43
3:E:286:THR:O	3:E:290:TRP:CB	2.65	0.43
2:B:959:GLN:HA	2:B:959:GLN:OE1	2.17	0.43
2:C:390:HIS:O	2:C:1317:VAL:HG23	2.18	0.43
2:C:590:SER:HB2	2:C:592:VAL:HG12	2.00	0.43
2:C:1121:HIS:ND1	2:C:1123:PRO:HD2	2.33	0.43
1:A:318:ARG:NH1	3:D:43:GLU:CD	2.77	0.43
1:A:853:GLU:H	1:A:853:GLU:HG3	1.69	0.43
2:B:1082:ASP:OD2	2:B:1226:ASP:HB2	2.18	0.43
2:B:1083:ASP:OD2	2:B:1083:ASP:N	2.51	0.43
2:C:191:GLY:H	2:C:192:PRO:HD2	1.84	0.43
2:C:627:ALA:HB2	2:C:716:PHE:CD2	2.54	0.43
3:E:122:TYR:CE2	3:E:203:ILE:HG21	2.53	0.43
1:A:265:SER:HB2	1:A:269:VAL:HG21	2.00	0.43
1:A:602:PHE:HB2	1:A:603:PRO:HD2	2.00	0.43
2:B:389:PHE:CE1	2:B:1319:ARG:HG2	2.53	0.43
2:B:938:ASN:C	2:B:940:ARG:H	2.26	0.43
2:C:856:LEU:HD11	3:D:117:ILE:HD12	2.00	0.43
2:C:1293:VAL:O	2:C:1294:ASP:HB2	2.18	0.43
3:E:152:ILE:H	3:E:152:ILE:HD12	1.83	0.43
3:E:253:GLU:HG3	3:E:254:TYR:CE2	2.54	0.43
3:D:46:LYS:HE3	3:D:158:LEU:HD22	2.00	0.43
1:A:131:GLY:O	1:A:134:VAL:HG12	2.19	0.43
1:A:292:ARG:HG2	1:A:295:THR:HG21	2.01	0.43
1:A:512:ALA:HA	1:A:513:PRO:HA	1.74	0.43
2:B:168:VAL:HG23	2:B:204:VAL:HG12	2.00	0.43
2:B:423:GLU:HB3	2:B:490:PHE:CE2	2.53	0.43
3:D:220:ASN:C	3:D:222:ASP:H	2.26	0.43
1:A:282:GLU:O	1:A:283:PHE:CG	2.72	0.43
1:A:977:HIS:O	1:A:988:LYS:HB3	2.19	0.43
2:B:612:PHE:CE1	2:B:635:ILE:HD11	2.53	0.43
2:C:837:THR:HA	2:C:936:MET:HB2	2.00	0.43
2:C:297:ASN:HD22	2:C:298:PRO:N	2.16	0.43
2:C:630:ASN:HA	2:C:631:PRO:HD3	1.87	0.43
3:D:74:GLN:OE1	3:D:74:GLN:HA	2.19	0.43
1:A:535:LEU:HD13	1:A:536:TYR:N	2.34	0.43
1:A:850:SER:HB3	1:A:872:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:115:GLN:HG3	2:C:116:SER:H	1.84	0.43
2:C:450:PRO:HB2	2:C:451:GLU:H	1.59	0.43
2:C:1031:TYR:O	2:C:1032:ASP:CB	2.67	0.43
3:D:14:GLN:HE22	3:D:107:LEU:HD13	1.84	0.43
3:E:282:PHE:CZ	3:E:286:THR:HG21	2.53	0.43
1:A:654:SER:HB3	1:A:715:TYR:HE2	1.84	0.42
1:A:1016:ILE:HD13	1:A:1016:ILE:H	1.84	0.42
2:B:373:ASP:C	2:B:375:ARG:H	2.26	0.42
2:C:391:GLY:HA3	2:C:392:PRO:HD3	1.90	0.42
3:D:53:GLU:CG	3:D:145:TYR:HE1	2.31	0.42
3:D:66:VAL:HG23	3:D:67:TYR:N	2.33	0.42
3:D:241:ASN:HB3	3:D:250:ARG:HD2	2.01	0.42
3:E:162:GLY:O	3:E:167:ARG:NH1	2.48	0.42
3:E:210:GLY:O	3:E:214:ARG:HG3	2.18	0.42
1:A:13:VAL:HG22	1:A:213:TRP:CD1	2.54	0.42
2:B:137:ILE:HB	2:C:471:SER:HB3	2.00	0.42
2:C:860:ARG:O	2:C:864:HIS:HB2	2.19	0.42
3:E:32:LEU:O	3:E:35:LEU:CG	2.58	0.42
1:A:855:MET:HA	1:A:916:ASN:HB3	2.01	0.42
2:B:314:ILE:C	2:B:316:ASN:H	2.28	0.42
2:B:772:TYR:HB3	2:B:773:PRO:HD2	2.01	0.42
2:B:879:THR:C	2:B:881:ASP:H	2.27	0.42
2:C:493:HIS:NE2	2:C:527:ARG:HD2	2.35	0.42
2:C:594:LEU:HD22	2:C:595:ALA:H	1.84	0.42
2:C:855:TYR:CZ	2:C:896:LEU:HD21	2.54	0.42
3:D:60:ARG:O	3:D:61:ASN:C	2.62	0.42
3:E:1:MET:CE	3:E:123:ASP:HA	2.49	0.42
3:E:268:THR:OG1	3:E:269:ILE:N	2.48	0.42
1:A:292:ARG:HG2	1:A:295:THR:HG22	2.02	0.42
1:A:390:ASP:O	1:A:391:ILE:C	2.63	0.42
2:B:318:LEU:HD11	2:B:325:TYR:HB2	1.99	0.42
2:B:604:MET:C	2:B:606:LEU:H	2.26	0.42
2:B:641:ARG:O	2:C:670:ASP:OD2	2.36	0.42
2:C:440:ILE:HD13	2:C:441:ARG:N	2.35	0.42
2:C:1083:ASP:HA	2:C:1084:PRO:HD2	1.75	0.42
2:C:1130:SER:O	2:C:1134:ARG:HD3	2.20	0.42
3:D:217:LYS:HE2	3:D:290:TRP:O	2.18	0.42
1:A:487:GLN:OE1	1:A:548:ASN:HB3	2.19	0.42
1:A:739:ASN:HD22	1:A:739:ASN:HA	1.70	0.42
1:A:752:VAL:HG23	1:A:779:ASN:O	2.20	0.42
1:A:911:MET:HE2	1:A:944:ARG:NH2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:ASN:HD21	1:A:1055:LEU:HD23	1.84	0.42
2:B:1236:ILE:CG1	2:B:1237:SER:N	2.62	0.42
1:A:713:ASN:HA	1:A:716:MET:HB2	2.01	0.42
2:B:153:ASP:HB3	2:B:154:PHE:CD1	2.54	0.42
2:B:172:ASP:O	2:B:173:GLN:HB3	2.19	0.42
2:B:937:ASN:O	2:B:939:ASN:N	2.52	0.42
2:C:952:PHE:C	2:C:954:GLN:N	2.76	0.42
2:C:1020:ARG:HD2	2:C:1031:TYR:HA	2.01	0.42
3:E:32:LEU:HD13	3:E:225:ARG:NH1	2.35	0.42
1:A:147:GLN:HG3	1:A:215:VAL:HG13	2.01	0.42
1:A:199:MET:HG3	1:A:205:VAL:HG21	2.02	0.42
1:A:222:ARG:NH1	2:B:613:LEU:CD1	2.82	0.42
1:A:395:GLN:NE2	1:A:395:GLN:CA	2.79	0.42
2:C:372:ALA:HA	2:C:398:ARG:HD3	2.02	0.42
2:C:540:PHE:O	2:C:548:TYR:HB2	2.19	0.42
2:C:651:ARG:O	2:C:655:ILE:HG12	2.20	0.42
2:C:1035:ILE:HG22	2:C:1036:ASP:N	2.33	0.42
1:A:71:LEU:HB3	1:A:72:PHE:H	1.67	0.42
2:B:188:ARG:NH1	2:C:237:VAL:HG13	2.34	0.42
2:B:363:ARG:NH1	3:D:80:SER:OG	2.50	0.42
3:E:158:LEU:CD2	3:E:172:MET:HB3	2.49	0.42
2:B:274:MET:HG2	2:C:234:PRO:CD	2.35	0.42
2:B:748:GLN:O	2:B:750:GLU:HB3	2.20	0.42
2:C:1036:ASP:O	2:C:1037:ILE:HB	2.19	0.42
2:C:1249:ASN:HA	2:C:1250:GLU:HA	1.48	0.42
3:D:193:VAL:HG11	3:D:230:ILE:HD12	2.02	0.42
3:D:239:VAL:CG1	3:D:250:ARG:HH12	2.30	0.42
1:A:101:LEU:HD21	1:A:119:VAL:HG23	2.02	0.42
1:A:204:LEU:HD13	1:A:221:TYR:HB2	2.02	0.42
1:A:939:GLN:HE21	1:A:939:GLN:HB3	1.66	0.42
1:A:1000:GLU:O	1:A:1003:VAL:HG12	2.20	0.42
2:B:815:LEU:HB3	2:B:816:PRO:HD3	2.01	0.42
2:C:292:ASN:O	2:C:293:ASN:CB	2.58	0.42
2:C:1243:ARG:NH1	2:C:1257:ALA:HA	2.34	0.42
3:E:32:LEU:CD1	3:E:225:ARG:NE	2.83	0.42
3:E:140:ALA:HB1	3:E:281:LYS:HG3	2.02	0.42
3:E:247:ARG:HA	3:E:247:ARG:NE	2.30	0.42
1:A:72:PHE:CD1	1:A:72:PHE:N	2.87	0.41
1:A:208:HIS:NE2	1:A:234:GPL:O1P	2.53	0.41
1:A:306:GLN:HA	1:A:306:GLN:OE1	2.18	0.41
1:A:962:PHE:HE2	1:A:966:GLY:HA3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:835:TYR:CE1	2:B:925:VAL:HG21	2.55	0.41
2:B:1156:ILE:HD11	2:B:1194:MET:HG3	2.02	0.41
2:C:448:TYR:CA	2:C:450:PRO:HD3	2.49	0.41
2:C:1136:HIS:CD2	2:C:1136:HIS:O	2.73	0.41
3:E:220:ASN:C	3:E:222:ASP:N	2.77	0.41
3:E:272:ASP:CG	3:E:273:LEU:H	2.28	0.41
1:A:308:ALA:CA	1:A:309:ASN:CB	2.92	0.41
1:A:566:GLU:HB2	1:A:567:PRO:CD	2.41	0.41
1:A:673:TYR:CE2	1:A:694:ILE:CG2	3.03	0.41
3:E:2:LEU:HD11	3:E:107:LEU:HD11	2.02	0.41
3:E:69:GLU:HG3	3:E:199:LEU:HB2	1.98	0.41
3:E:205:LEU:HD13	3:E:205:LEU:C	2.36	0.41
1:A:1013:THR:O	1:A:1055:LEU:HD12	2.20	0.41
2:C:968:ARG:O	2:C:971:MET:HB2	2.20	0.41
2:C:986:ILE:O	2:C:989:ILE:HG22	2.20	0.41
3:D:12:LEU:HD23	3:D:14:GLN:HB2	2.01	0.41
3:E:72:ILE:O	3:E:76:LEU:HD12	2.20	0.41
3:E:76:LEU:HD21	3:E:282:PHE:CD2	2.55	0.41
1:A:677:LEU:HB3	1:A:692:ILE:HD13	2.02	0.41
1:A:776:SER:HA	1:A:818:PHE:HE1	1.85	0.41
2:B:149:PRO:HB3	2:B:1312:GLY:HA2	2.01	0.41
2:B:150:LEU:O	2:B:804:LEU:HD13	2.20	0.41
2:B:583:GLU:O	2:B:584:HIS:CB	2.69	0.41
2:B:1280:PRO:C	2:B:1282:ALA:H	2.29	0.41
2:C:871:PRO:HG3	2:C:892:VAL:HG11	2.01	0.41
3:D:69:GLU:HB2	3:D:199:LEU:HD11	2.02	0.41
3:E:2:LEU:O	3:E:3:GLN:C	2.61	0.41
3:E:41:GLU:O	3:E:41:GLU:CD	2.64	0.41
1:A:23:ARG:HH21	1:A:27:LYS:HB3	1.85	0.41
1:A:47:ARG:HB2	2:B:595:ALA:O	2.20	0.41
2:B:228:VAL:HG22	2:B:229:GLN:H	1.84	0.41
2:B:838:GLU:HG3	2:B:839:ALA:H	1.84	0.41
2:B:954:GLN:NE2	3:D:240:VAL:HG12	2.35	0.41
2:C:339:LEU:C	2:C:341:LYS:N	2.78	0.41
2:C:451:GLU:O	2:C:452:ASN:CB	2.69	0.41
3:E:205:LEU:CD1	3:E:289:ARG:HG3	2.50	0.41
1:A:49:HIS:NE2	1:A:172:PHE:CD1	2.75	0.41
1:A:665:LEU:N	1:A:667:GLN:HE22	2.17	0.41
2:B:475:ILE:O	2:B:477:SER:N	2.53	0.41
2:B:487:SER:HA	2:B:488:PRO:HD3	1.94	0.41
2:B:871:PRO:HG3	2:B:894:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:908:THR:HA	2:B:911:ARG:HH21	1.85	0.41
3:D:69:GLU:HG3	3:D:199:LEU:HG	2.02	0.41
1:A:203:THR:HG23	1:A:204:LEU:H	1.86	0.41
1:A:361:SER:HB3	1:A:362:MET:H	1.62	0.41
1:A:530:MET:HA	1:A:533:LEU:HB2	2.02	0.41
2:B:588:LEU:HD22	2:B:604:MET:CE	2.51	0.41
2:C:204:VAL:HG23	2:C:1242:MET:HG2	2.02	0.41
3:D:152:ILE:HG21	3:D:283:LEU:HB3	2.01	0.41
2:B:269:GLU:O	2:B:291:HIS:HD2	2.04	0.41
2:B:486:VAL:HG21	2:B:709:MET:HB3	2.03	0.41
2:B:946:LEU:HD22	2:B:947:GLU:H	1.85	0.41
2:B:1023:ARG:O	2:B:1024:PRO:C	2.63	0.41
2:C:926:VAL:CG2	2:C:938:ASN:HB2	2.50	0.41
3:E:182:TRP:CD1	3:E:185:SER:HB3	2.55	0.41
1:A:35:GLY:H	1:A:38:TYR:HE1	1.67	0.41
1:A:71:LEU:O	1:A:73:ARG:N	2.53	0.41
1:A:511:ILE:O	1:A:511:ILE:HD12	2.21	0.41
2:B:228:VAL:O	2:B:246:GLU:HB2	2.20	0.41
2:B:837:THR:O	2:B:838:GLU:CB	2.68	0.41
2:C:82:ARG:CZ	2:C:210:ARG:HB3	2.51	0.41
2:C:597:ALA:O	2:C:600:ILE:HG22	2.20	0.41
2:C:1181:SER:O	2:C:1182:GLU:HB3	2.21	0.41
3:E:66:VAL:HG13	3:E:111:ILE:HG21	2.03	0.41
3:E:140:ALA:CB	3:E:281:LYS:HG3	2.51	0.41
1:A:303:THR:CB	1:A:307:HIS:NE2	2.76	0.41
2:B:1330:ILE:H	2:B:1330:ILE:HD13	1.86	0.41
2:C:633:THR:HG21	2:C:710:SER:OG	2.21	0.41
2:C:1325:VAL:HG12	2:C:1326:ARG:N	2.36	0.41
3:D:258:ASN:OD1	3:D:259:SER:N	2.53	0.41
1:A:194:HIS:ND1	3:D:146:ARG:HD2	2.35	0.40
2:B:445:GLU:HG3	2:B:447:ARG:HG2	2.03	0.40
2:B:450:PRO:HG3	2:B:686:HIS:HB2	2.04	0.40
2:B:612:PHE:CZ	2:B:1331:ARG:HD2	2.56	0.40
2:B:821:ASN:HD22	2:B:821:ASN:HA	1.73	0.40
2:B:941:TYR:O	2:B:941:TYR:HD1	2.04	0.40
2:B:954:GLN:HB3	2:B:956:ASP:O	2.20	0.40
2:C:617:ASP:HA	2:C:620:ILE:HG22	2.03	0.40
2:C:1042:TRP:CE3	2:C:1042:TRP:HA	2.56	0.40
3:D:29:THR:HG22	3:D:222:ASP:OD1	2.21	0.40
1:A:201:LYS:CA	2:B:629:ARG:HD3	2.51	0.40
1:A:406:VAL:HG23	1:A:407:GLU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:PRO:HB2	1:A:514:LEU:H	1.62	0.40
1:A:967:ILE:HA	1:A:970:ARG:HB3	2.02	0.40
2:B:824:LEU:C	2:B:826:GLY:H	2.29	0.40
2:C:317:MET:SD	2:C:1262:SER:HB3	2.61	0.40
2:C:366:MET:HE3	3:E:266:THR:OG1	2.21	0.40
2:C:856:LEU:HA	2:C:860:ARG:HB2	2.03	0.40
2:C:948:ILE:HG22	2:C:948:ILE:O	2.21	0.40
2:C:1247:ASN:HD22	2:C:1247:ASN:C	2.25	0.40
3:D:228:LEU:HA	3:D:231:MET:HE2	2.03	0.40
3:E:209:GLU:CG	3:E:210:GLY:H	2.29	0.40
2:C:159:ASP:OD2	2:C:291:HIS:HE1	2.04	0.40
2:C:835:TYR:HB2	2:C:847:ILE:HD11	2.03	0.40
2:C:999:LYS:HD3	2:C:1009:THR:HG22	2.04	0.40
1:A:177:THR:HA	1:A:178:PRO:HD3	1.95	0.40
2:B:172:ASP:O	2:B:173:GLN:CB	2.70	0.40
2:B:1076:ILE:HB	2:B:1166:VAL:HG23	2.03	0.40
2:B:1078:TYR:C	2:B:1078:TYR:HD2	2.29	0.40
3:D:67:TYR:O	3:D:68:ILE:C	2.64	0.40
3:E:140:ALA:O	3:E:146:ARG:HA	2.22	0.40
3:E:142:THR:HG23	3:E:143:PRO:CD	2.50	0.40
3:E:264:GLY:H	3:E:268:THR:CG2	2.34	0.40
1:A:421:LEU:HD12	1:A:678:LEU:HB3	2.02	0.40
1:A:604:ILE:HD13	1:A:604:ILE:H	1.86	0.40
2:B:192:PRO:C	2:B:194:VAL:H	2.29	0.40
2:B:225:ILE:HG22	2:B:227:LEU:HG	2.04	0.40
2:B:274:MET:CG	2:C:234:PRO:CD	2.55	0.40
2:B:1031:TYR:CD2	2:B:1041:ARG:HD3	2.57	0.40
2:C:177:LYS:H	2:C:177:LYS:HD3	1.86	0.40
2:C:372:ALA:HB1	2:C:1315:MET:CE	2.51	0.40
2:C:447:ARG:HE	2:C:690:GLN:NE2	2.20	0.40
2:C:610:GLN:O	2:C:634:TYR:CE2	2.75	0.40
3:E:53:GLU:CB	3:E:145:TYR:CE1	3.05	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	1038/1058 (98%)	813 (78%)	161 (16%)	64 (6%)	1	15
2	B	1172/1333 (88%)	958 (82%)	186 (16%)	28 (2%)	4	30
2	C	1238/1333 (93%)	1018 (82%)	192 (16%)	28 (2%)	5	31
3	D	289/448 (64%)	253 (88%)	33 (11%)	3 (1%)	12	46
3	E	289/448 (64%)	254 (88%)	34 (12%)	1 (0%)	36	70
All	All	4026/4620 (87%)	3296 (82%)	606 (15%)	124 (3%)	5	25

All (124) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	49	HIS
1	A	72	PHE
1	A	255	ARG
1	A	282	GLU
1	A	287	VAL
1	A	309	ASN
1	A	330	GLN
1	A	359	PRO
1	A	395	GLN
1	A	485	MET
1	A	513	PRO
1	A	724	MET
1	A	813	PRO
1	A	915	ASN
1	A	924	VAL
1	A	962	PHE
2	B	838	GLU
2	B	940	ARG
2	B	1281	VAL
2	C	972	PRO
1	A	187	PRO
1	A	387	THR
1	A	391	ILE
1	A	606	LYS
1	A	697	ILE
1	A	726	ILE

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Mol	Chain	Res	Type
1	A	832	GLU
1	A	923	ALA
1	A	994	PRO
2	B	242	GLU
2	B	279	SER
2	B	749	GLY
2	B	901	VAL
2	B	973	THR
2	B	1299	SER
2	C	340	VAL
2	C	450	PRO
2	C	666	ARG
2	C	752	VAL
2	C	842	ASP
2	C	1032	ASP
2	C	1037	ILE
3	D	244	VAL
1	A	214	ASN
1	A	286	ASN
1	A	305	TYR
1	A	496	CYS
1	A	580	SER
1	A	622	ASP
1	A	671	VAL
1	A	686	TYR
1	A	688	TYR
1	A	802	THR
1	A	853	GLU
1	A	1037	SER
2	B	291	HIS
2	B	584	HIS
2	B	897	TYR
2	B	937	ASN
2	B	952	PHE
2	B	1086	PRO
2	C	386	SER
2	C	948	ILE
2	C	1038	GLU
2	C	1047	LEU
3	D	253	GLU
1	A	28	PRO
1	A	209	SER

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Mol	Chain	Res	Type
1	A	212	HIS
1	A	263	LEU
1	A	684	ASN
1	A	829	MET
1	A	914	GLU
1	A	963	TYR
2	B	229	GLN
2	C	671	ASP
2	C	831	VAL
2	C	1029	LEU
2	C	1208	ASP
2	C	1237	SER
3	D	265	ARG
1	A	203	THR
1	A	266	SER
1	A	304	TYR
1	A	406	VAL
1	A	563	ALA
1	A	709	SER
1	A	722	ASP
1	A	821	ARG
1	A	887	ILE
1	A	990	ALA
2	B	476	SER
2	B	938	ASN
2	B	1234	GLN
2	C	562	ALA
2	C	845	GLU
2	C	951	ILE
2	C	1182	GLU
1	A	389	ALA
1	A	455	MET
1	A	567	PRO
1	A	975	THR
2	B	190	VAL
2	B	840	ASP
2	B	1085	ASP
2	B	1252	ASP
2	C	646	ASN
2	C	757	ILE
3	E	55	HIS
1	A	411	ILE

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Mol	Chain	Res	Type
2	B	830	VAL
2	C	1086	PRO
1	A	25	ILE
2	C	830	VAL
1	A	928	GLU
2	B	880	PRO
2	B	1236	ILE
2	C	1224	GLY
1	A	478	ILE
2	B	1093	PRO
2	C	644	VAL
2	C	1245	ILE
2	B	983	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	932/942 (99%)	779 (84%)	153 (16%)	2	13
2	B	1029/1155 (89%)	912 (89%)	117 (11%)	5	21
2	C	1085/1155 (94%)	941 (87%)	144 (13%)	4	18
3	D	240/379 (63%)	201 (84%)	39 (16%)	2	13
3	E	240/379 (63%)	197 (82%)	43 (18%)	2	11
All	All	3526/4010 (88%)	3030 (86%)	496 (14%)	5	17

All (496) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	TYR
1	A	9	ASN
1	A	10	ASP
1	A	12	ARG
1	A	20	ASN
1	A	22	ILE

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Mol	Chain	Res	Type
1	A	31	VAL
1	A	33	GLN
1	A	39	LEU
1	A	53	LEU
1	A	54	LEU
1	A	63	SER
1	A	66	ASP
1	A	72	PHE
1	A	73	ARG
1	A	77	LYS
1	A	91	ASN
1	A	97	ARG
1	A	120	TYR
1	A	140	ILE
1	A	141	LEU
1	A	153	VAL
1	A	177	THR
1	A	204	LEU
1	A	207	THR
1	A	215	VAL
1	A	228	ILE
1	A	231	PHE
1	A	235	ILE
1	A	255	ARG
1	A	256	VAL
1	A	270	GLN
1	A	278	LEU
1	A	282	GLU
1	A	288	LEU
1	A	292	ARG
1	A	297	LEU
1	A	298	LEU
1	A	299	GLN
1	A	306	GLN
1	A	331	ARG
1	A	334	GLU
1	A	339	GLN
1	A	357	THR
1	A	365	ILE
1	A	380	THR
1	A	383	THR
1	A	393	LEU

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Mol	Chain	Res	Type
1	A	406	VAL
1	A	411	ILE
1	A	414	GLU
1	A	437	GLN
1	A	444	LEU
1	A	458	ASN
1	A	461	ARG
1	A	462	ILE
1	A	463	ASP
1	A	470	LEU
1	A	477	TYR
1	A	479	LYS
1	A	485	MET
1	A	487	GLN
1	A	493	LEU
1	A	511	ILE
1	A	514	LEU
1	A	519	ILE
1	A	521	LYS
1	A	523	MET
1	A	525	ARG
1	A	526	ASN
1	A	535	LEU
1	A	540	LYS
1	A	542	LEU
1	A	544	ASN
1	A	545	PHE
1	A	552	MET
1	A	558	ILE
1	A	559	ILE
1	A	561	LEU
1	A	565	ARG
1	A	571	ILE
1	A	580	SER
1	A	581	ASN
1	A	584	ILE
1	A	592	VAL
1	A	602	PHE
1	A	604	ILE
1	A	605	ASP
1	A	611	ASP
1	A	616	ASP

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Mol	Chain	Res	Type
1	A	617	ILE
1	A	620	TYR
1	A	621	GLU
1	A	622	ASP
1	A	626	GLU
1	A	628	MET
1	A	652	HIS
1	A	655	GLU
1	A	658	ILE
1	A	667	GLN
1	A	673	TYR
1	A	680	THR
1	A	683	GLN
1	A	695	THR
1	A	714	ARG
1	A	717	THR
1	A	719	VAL
1	A	726	ILE
1	A	727	ILE
1	A	737	HIS
1	A	739	ASN
1	A	757	LEU
1	A	763	LYS
1	A	771	THR
1	A	779	ASN
1	A	781	VAL
1	A	783	ILE
1	A	794	LEU
1	A	795	GLU
1	A	812	VAL
1	A	814	ASN
1	A	820	VAL
1	A	836	ILE
1	A	849	ILE
1	A	851	LEU
1	A	853	GLU
1	A	859	VAL
1	A	866	LEU
1	A	868	ASP
1	A	887	ILE
1	A	894	LYS
1	A	897	ILE

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Mol	Chain	Res	Type
1	A	900	GLN
1	A	905	GLN
1	A	906	PHE
1	A	924	VAL
1	A	925	ILE
1	A	927	ASN
1	A	939	GLN
1	A	946	VAL
1	A	951	LEU
1	A	955	ASN
1	A	967	ILE
1	A	969	THR
1	A	971	LEU
1	A	973	GLN
1	A	987	LEU
1	A	1003	VAL
1	A	1016	ILE
1	A	1025	ILE
1	A	1033	ILE
1	A	1035	LEU
1	A	1053	ILE
2	B	148	GLN
2	B	157	ILE
2	B	161	LYS
2	B	170	TYR
2	B	171	GLU
2	B	177	LYS
2	B	181	ARG
2	B	189	ILE
2	B	203	VAL
2	B	205	ASN
2	B	206	ILE
2	B	219	ILE
2	B	230	ASP
2	B	235	ILE
2	B	266	ILE
2	B	270	THR
2	B	274	MET
2	B	286	LEU
2	B	288	THR
2	B	302	ARG
2	B	303	ASP

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Mol	Chain	Res	Type
2	B	309	TRP
2	B	314	ILE
2	B	319	GLN
2	B	324	LYS
2	B	327	LEU
2	B	331	GLU
2	B	339	LEU
2	B	350	ILE
2	B	369	ASN
2	B	370	VAL
2	B	388	GLN
2	B	409	ILE
2	B	412	LEU
2	B	425	ILE
2	B	445	GLU
2	B	447	ARG
2	B	453	LEU
2	B	472	GLU
2	B	475	ILE
2	B	486	VAL
2	B	512	LEU
2	B	516	LEU
2	B	529	LYS
2	B	532	ILE
2	B	538	LEU
2	B	547	GLU
2	B	554	ARG
2	B	588	LEU
2	B	594	LEU
2	B	610	GLN
2	B	671	ASP
2	B	685	ARG
2	B	688	GLU
2	B	694	ILE
2	B	719	ASN
2	B	738	GLU
2	B	747	ARG
2	B	748	GLN
2	B	750	GLU
2	B	758	ILE
2	B	836	GLN
2	B	843	LEU

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Mol	Chain	Res	Type
2	B	850	THR
2	B	856	LEU
2	B	865	ILE
2	B	879	THR
2	B	895	VAL
2	B	897	TYR
2	B	901	VAL
2	B	908	THR
2	B	912	GLU
2	B	922	TYR
2	B	934	LEU
2	B	936	MET
2	B	938	ASN
2	B	940	ARG
2	B	942	HIS
2	B	946	LEU
2	B	953	ASP
2	B	954	GLN
2	B	957	PHE
2	B	964	VAL
2	B	971	MET
2	B	988	GLN
2	B	1008	LEU
2	B	1028	VAL
2	B	1049	GLU
2	B	1050	LEU
2	B	1053	ARG
2	B	1069	ARG
2	B	1075	ARG
2	B	1079	LEU
2	B	1092	VAL
2	B	1103	HIS
2	B	1153	ASP
2	B	1176	GLU
2	B	1182	GLU
2	B	1186	GLN
2	B	1187	HIS
2	B	1202	PHE
2	B	1203	HIS
2	B	1210	LEU
2	B	1211	LEU
2	B	1212	ARG

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Mol	Chain	Res	Type
2	B	1218	PHE
2	B	1227	MET
2	B	1230	ILE
2	B	1242	MET
2	B	1247	ASN
2	B	1252	ASP
2	B	1281	VAL
2	B	1291	LEU
2	B	1300	ASN
2	B	1318	GLU
2	B	1323	ASP
2	B	1330	ILE
2	C	108	LYS
2	C	109	LYS
2	C	120	VAL
2	C	123	GLU
2	C	124	GLN
2	C	128	GLU
2	C	133	MET
2	C	134	THR
2	C	145	THR
2	C	146	GLU
2	C	154	PHE
2	C	155	LYS
2	C	157	ILE
2	C	190	VAL
2	C	196	LEU
2	C	204	VAL
2	C	205	ASN
2	C	221	LEU
2	C	231	LEU
2	C	255	LEU
2	C	265	VAL
2	C	283	ASN
2	C	284	ASN
2	C	297	ASN
2	C	301	LEU
2	C	306	GLN
2	C	309	TRP
2	C	339	LEU
2	C	366	MET
2	C	376	ILE

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Mol	Chain	Res	Type
2	C	409	ILE
2	C	412	LEU
2	C	422	LEU
2	C	430	ASN
2	C	440	ILE
2	C	451	GLU
2	C	457	GLN
2	C	458	SER
2	C	462	LEU
2	C	480	LEU
2	C	489	MET
2	C	493	HIS
2	C	495	LEU
2	C	498	ILE
2	C	512	LEU
2	C	519	LEU
2	C	520	PHE
2	C	524	GLU
2	C	528	ILE
2	C	536	LEU
2	C	547	GLU
2	C	552	ILE
2	C	560	ILE
2	C	574	LYS
2	C	576	ASP
2	C	581	LEU
2	C	591	ASP
2	C	594	LEU
2	C	599	THR
2	C	603	ILE
2	C	604	MET
2	C	605	ARG
2	C	613	LEU
2	C	634	TYR
2	C	635	ILE
2	C	646	ASN
2	C	659	LEU
2	C	671	ASP
2	C	677	ARG
2	C	681	LYS
2	C	682	GLN
2	C	684	LEU

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Mol	Chain	Res	Type
2	C	688	GLU
2	C	693	ASN
2	C	714	LEU
2	C	716	PHE
2	C	717	THR
2	C	720	PHE
2	C	730	ASP
2	C	731	GLN
2	C	738	GLU
2	C	744	ILE
2	C	747	ARG
2	C	752	VAL
2	C	762	ILE
2	C	767	LEU
2	C	771	THR
2	C	799	THR
2	C	812	LYS
2	C	820	ILE
2	C	823	ILE
2	C	828	ASP
2	C	830	VAL
2	C	847	ILE
2	C	849	MET
2	C	863	LEU
2	C	864	HIS
2	C	874	ILE
2	C	882	GLN
2	C	887	VAL
2	C	894	VAL
2	C	898	GLN
2	C	915	VAL
2	C	934	LEU
2	C	936	MET
2	C	943	GLU
2	C	947	GLU
2	C	954	GLN
2	C	958	ILE
2	C	959	GLN
2	C	990	THR
2	C	1000	LEU
2	C	1022	ILE
2	C	1027	THR

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Mol	Chain	Res	Type
2	C	1029	LEU
2	C	1042	TRP
2	C	1050	LEU
2	C	1051	ARG
2	C	1062	ILE
2	C	1076	ILE
2	C	1079	LEU
2	C	1174	THR
2	C	1176	GLU
2	C	1187	HIS
2	C	1193	ILE
2	C	1201	LEU
2	C	1202	PHE
2	C	1204	LEU
2	C	1214	GLU
2	C	1227	MET
2	C	1229	LEU
2	C	1236	ILE
2	C	1243	ARG
2	C	1247	ASN
2	C	1249	ASN
2	C	1269	THR
2	C	1272	ARG
2	C	1275	ASP
2	C	1288	ILE
2	C	1292	GLU
2	C	1293	VAL
2	C	1295	HIS
2	C	1296	ILE
2	C	1309	ILE
3	D	1	MET
3	D	12	LEU
3	D	13	GLU
3	D	14	GLN
3	D	15	PHE
3	D	20	ARG
3	D	37	TYR
3	D	41	GLU
3	D	44	LEU
3	D	47	LYS
3	D	55	HIS
3	D	61	ASN

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Mol	Chain	Res	Type
3	D	66	VAL
3	D	68	ILE
3	D	70	ASP
3	D	79	ILE
3	D	85	ASN
3	D	87	HIS
3	D	100	ASN
3	D	101	THR
3	D	121	PHE
3	D	133	THR
3	D	149	MET
3	D	150	ILE
3	D	156	VAL
3	D	158	LEU
3	D	160	LEU
3	D	174	VAL
3	D	195	ASN
3	D	196	TRP
3	D	206	CYS
3	D	226	MET
3	D	228	LEU
3	D	242	ARG
3	D	250	ARG
3	D	257	VAL
3	D	288	THR
3	D	289	ARG
3	D	290	TRP
3	E	9	TYR
3	E	15	PHE
3	E	17	PHE
3	E	19	ILE
3	E	29	THR
3	E	35	LEU
3	E	41	GLU
3	E	44	LEU
3	E	47	LYS
3	E	51	THR
3	E	53	GLU
3	E	55	HIS
3	E	56	LEU
3	E	62	VAL
3	E	66	VAL

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Mol	Chain	Res	Type
3	E	68	ILE
3	E	69	GLU
3	E	83	ASN
3	E	85	ASN
3	E	105	LEU
3	E	107	LEU
3	E	108	ASP
3	E	111	ILE
3	E	117	ILE
3	E	118	ASN
3	E	122	TYR
3	E	137	LEU
3	E	142	THR
3	E	151	ASP
3	E	178	LYS
3	E	186	LEU
3	E	191	ARG
3	E	195	ASN
3	E	221	ARG
3	E	228	LEU
3	E	255	ILE
3	E	261	ARG
3	E	262	THR
3	E	269	ILE
3	E	273	LEU
3	E	288	THR
3	E	289	ARG
3	E	291	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (133) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	29	ASN
1	A	61	ASN
1	A	91	ASN
1	A	132	GLN
1	A	136	ASN
1	A	241	GLN
1	A	258	GLN
1	A	299	GLN
1	A	321	ASN

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Mol	Chain	Res	Type
1	A	332	HIS
1	A	367	ASN
1	A	395	GLN
1	A	437	GLN
1	A	544	ASN
1	A	548	ASN
1	A	578	ASN
1	A	581	ASN
1	A	595	ASN
1	A	607	ASN
1	A	618	ASN
1	A	623	GLN
1	A	659	ASN
1	A	667	GLN
1	A	674	HIS
1	A	683	GLN
1	A	708	ASN
1	A	737	HIS
1	A	739	ASN
1	A	779	ASN
1	A	801	ASN
1	A	809	GLN
1	A	814	ASN
1	A	830	HIS
1	A	848	GLN
1	A	857	GLN
1	A	905	GLN
1	A	916	ASN
1	A	939	GLN
1	A	955	ASN
1	A	973	GLN
1	A	1048	HIS
2	B	195	ASN
2	B	205	ASN
2	B	291	HIS
2	B	292	ASN
2	B	308	ASN
2	B	319	GLN
2	B	346	HIS
2	B	390	HIS
2	B	394	GLN
2	B	430	ASN

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Mol	Chain	Res	Type
2	B	561	ASN
2	B	610	GLN
2	B	623	ASN
2	B	632	GLN
2	B	646	ASN
2	B	664	ASN
2	B	686	HIS
2	B	690	GLN
2	B	693	ASN
2	B	701	HIS
2	B	715	ASN
2	B	731	GLN
2	B	769	GLN
2	B	802	GLN
2	B	821	ASN
2	B	836	GLN
2	B	858	HIS
2	B	888	GLN
2	B	891	HIS
2	B	935	GLN
2	B	1015	GLN
2	B	1103	HIS
2	B	1121	HIS
2	B	1169	HIS
2	B	1203	HIS
2	B	1205	GLN
2	B	1247	ASN
2	B	1249	ASN
2	B	1295	HIS
2	C	107	GLN
2	C	115	GLN
2	C	122	ASN
2	C	173	GLN
2	C	195	ASN
2	C	205	ASN
2	C	209	ASN
2	C	243	GLN
2	C	262	ASN
2	C	283	ASN
2	C	291	HIS
2	C	297	ASN
2	C	306	GLN

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Mol	Chain	Res	Type
2	C	311	ASN
2	C	320	GLN
2	C	346	HIS
2	C	349	ASN
2	C	394	GLN
2	C	430	ASN
2	C	479	HIS
2	C	491	ASN
2	C	561	ASN
2	C	646	ASN
2	C	682	GLN
2	C	690	GLN
2	C	693	ASN
2	C	711	ASN
2	C	719	ASN
2	C	731	GLN
2	C	836	GLN
2	C	854	GLN
2	C	867	ASN
2	C	882	GLN
2	C	913	ASN
2	C	938	ASN
2	C	954	GLN
2	C	959	GLN
2	C	1136	HIS
2	C	1169	HIS
2	C	1205	GLN
2	C	1247	ASN
2	C	1308	ASN
3	D	3	GLN
3	D	100	ASN
3	D	118	ASN
3	D	238	ASN
3	D	284	GLN
3	E	14	GLN
3	E	55	HIS
3	E	155	HIS
3	E	258	ASN
3	E	291	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GPL	A	234	1	33,34,35	2.11	4 (12%)	43,49,51	2.03	8 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GPL	A	234	1	-	5/19/37/39	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	GPL	P-NZ	10.32	1.74	1.61
1	A	234	GPL	C5-C4	3.11	1.47	1.38
1	A	234	GPL	C6-N1	-2.47	1.34	1.38
1	A	234	GPL	C5-N7	-2.01	1.35	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	GPL	C5-C4-N3	-6.42	118.18	128.39
1	A	234	GPL	P-NZ-CE	-5.12	117.47	124.61
1	A	234	GPL	C2-N3-C4	5.07	121.04	112.30
1	A	234	GPL	N9-C4-N3	4.36	134.67	125.95
1	A	234	GPL	C6-C5-N7	3.42	136.52	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	GPL	C4-C5-N7	-3.00	105.91	110.67
1	A	234	GPL	C3'-C2'-C1'	2.07	105.38	101.46
1	A	234	GPL	C5-C6-N1	2.04	118.44	113.25

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	234	GPL	N-CA-CB-CG
1	A	234	GPL	CG-CD-CE-NZ
1	A	234	GPL	C5'-O5'-P-O1P
1	A	234	GPL	C5'-O5'-P-O2P
1	A	234	GPL	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	234	GPL	1	0

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.

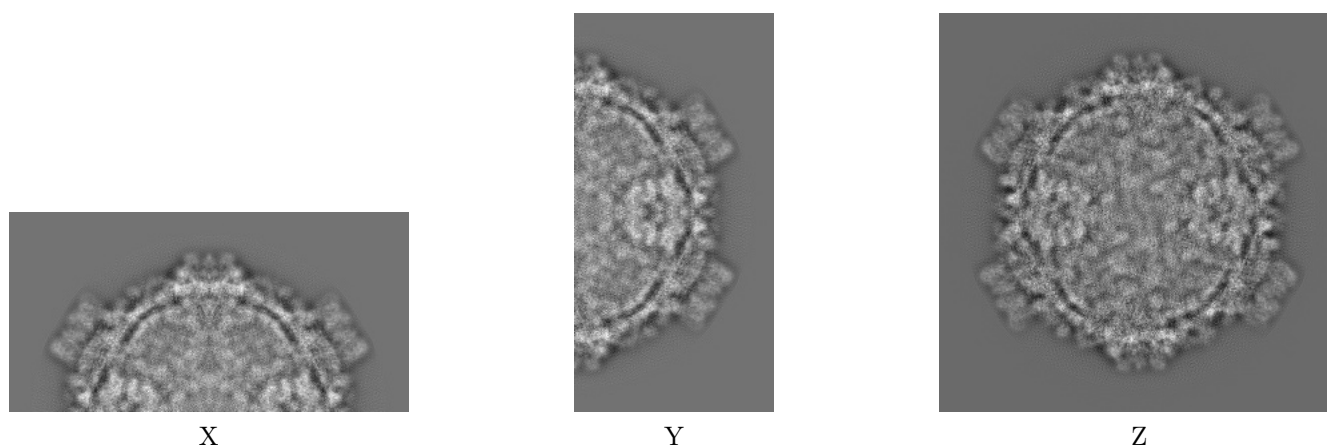
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5376. 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](#)

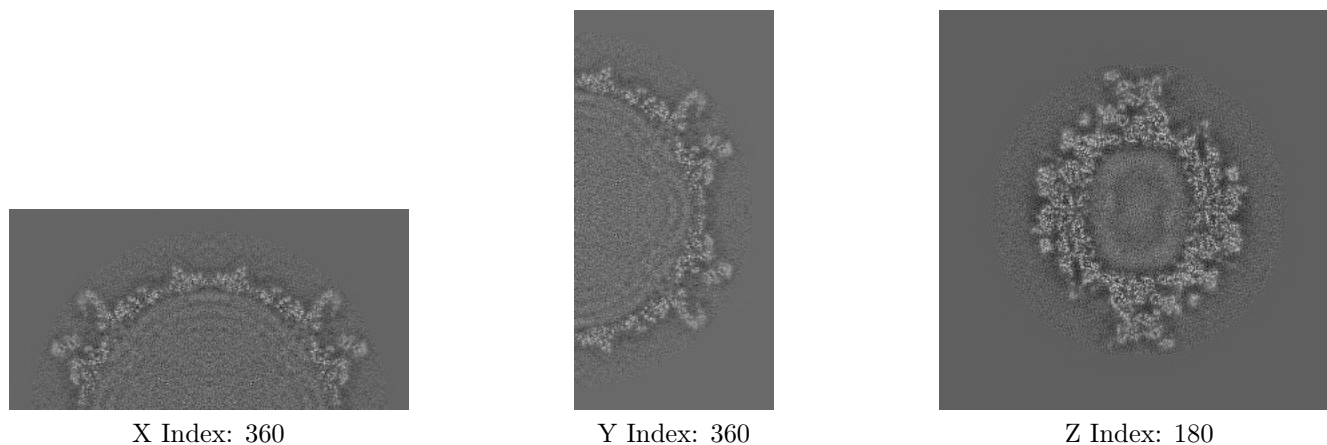
6.1.1 Primary map



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

6.2 Central slices [i](#)

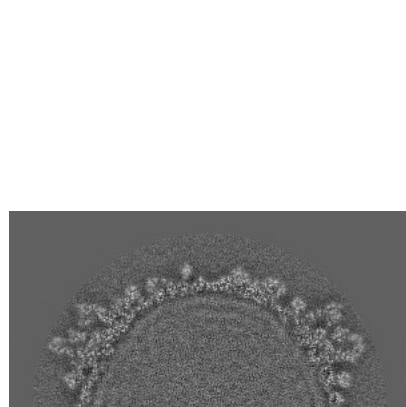
6.2.1 Primary map



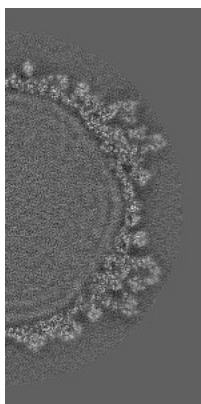
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

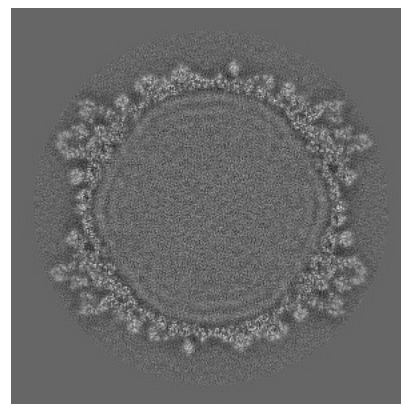
6.3.1 Primary map



X Index: 336



Y Index: 384

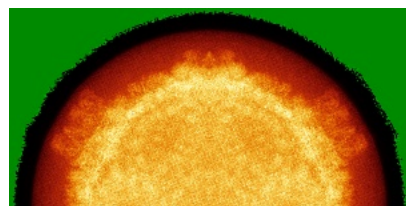


Z Index: 24

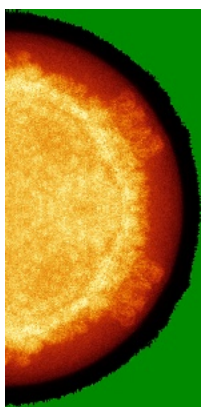
The images above show the largest variance slices of the map in three orthogonal directions.

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

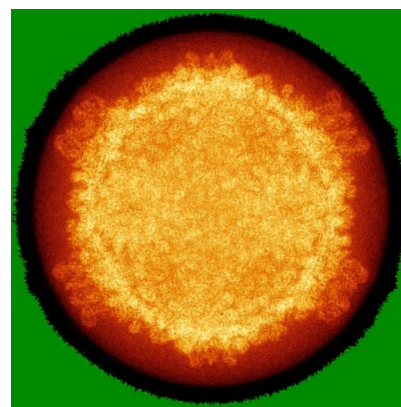
6.4.1 Primary map



X



Y

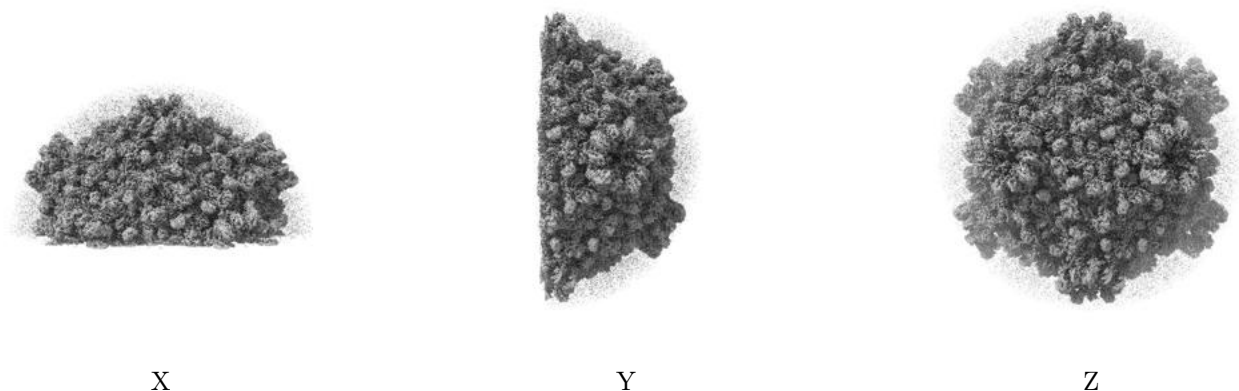


Z

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 2.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

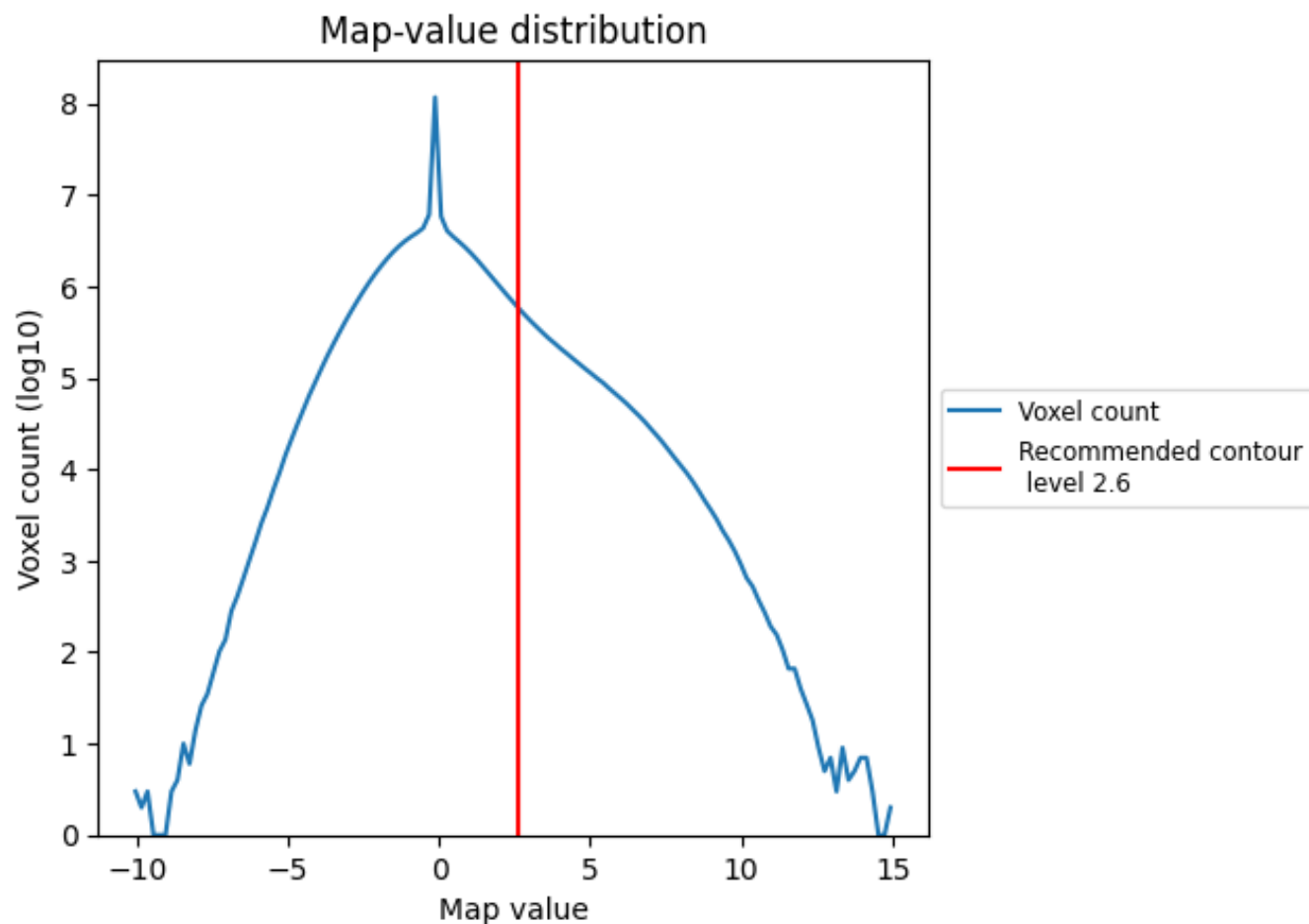
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

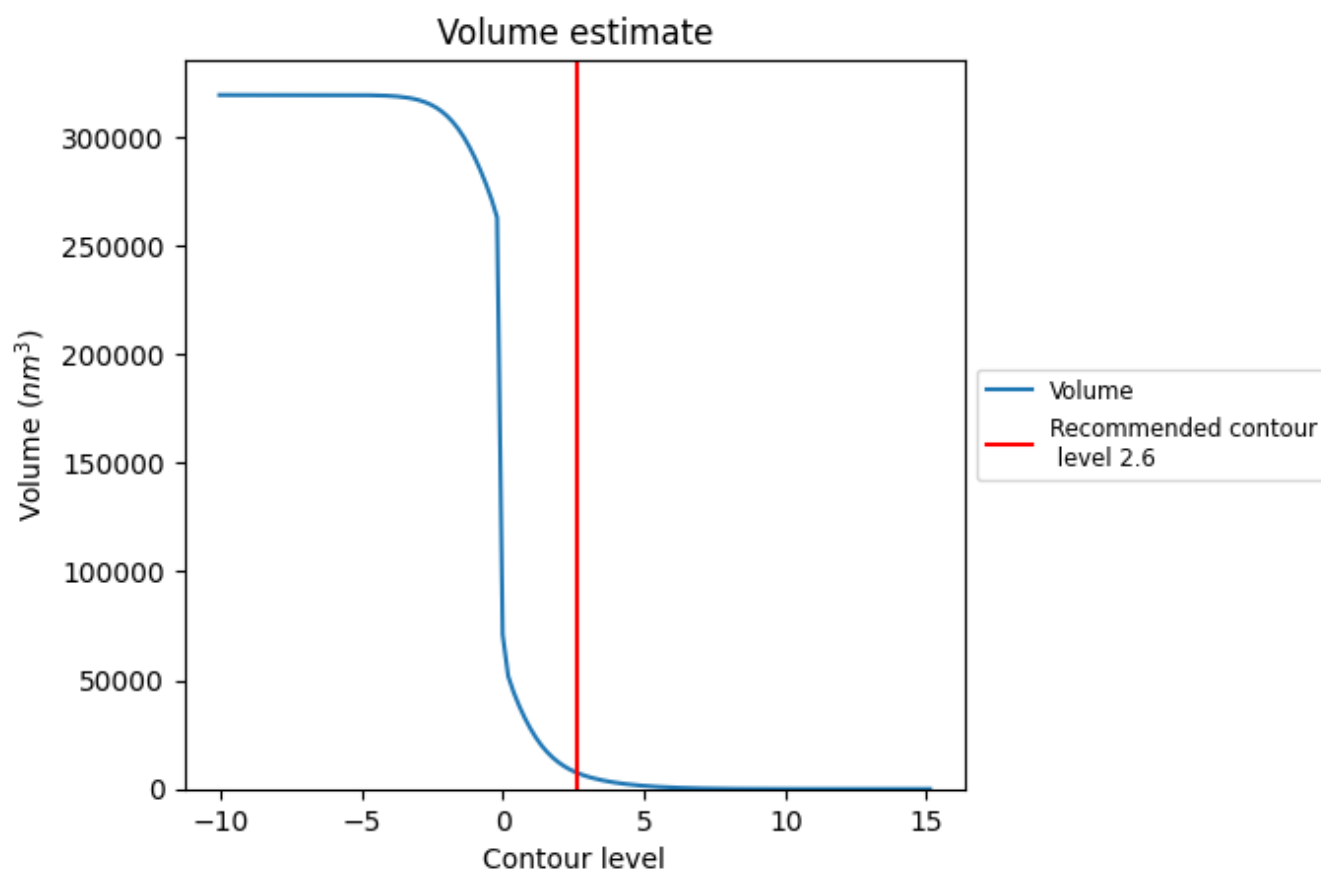
This section contains the results of statistical analysis of the map.

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 7585 nm³; this corresponds to an approximate mass of 6852 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation ⓘ

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

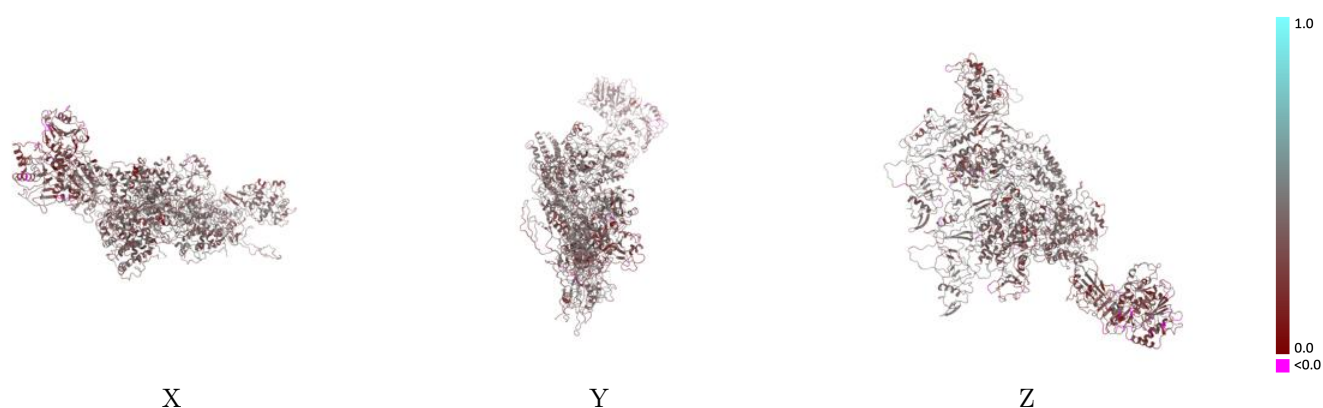
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5376 and PDB model 3J17. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

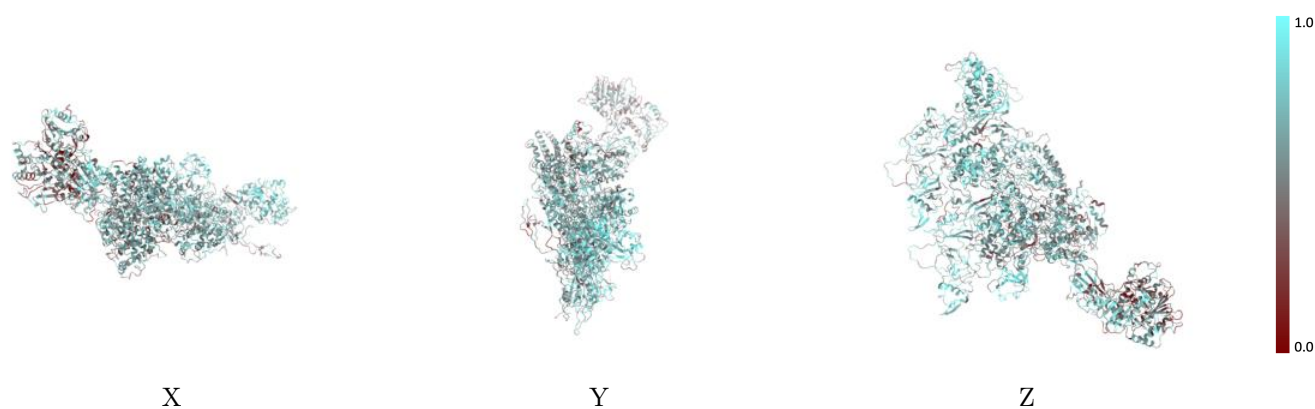
This section was not generated.

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



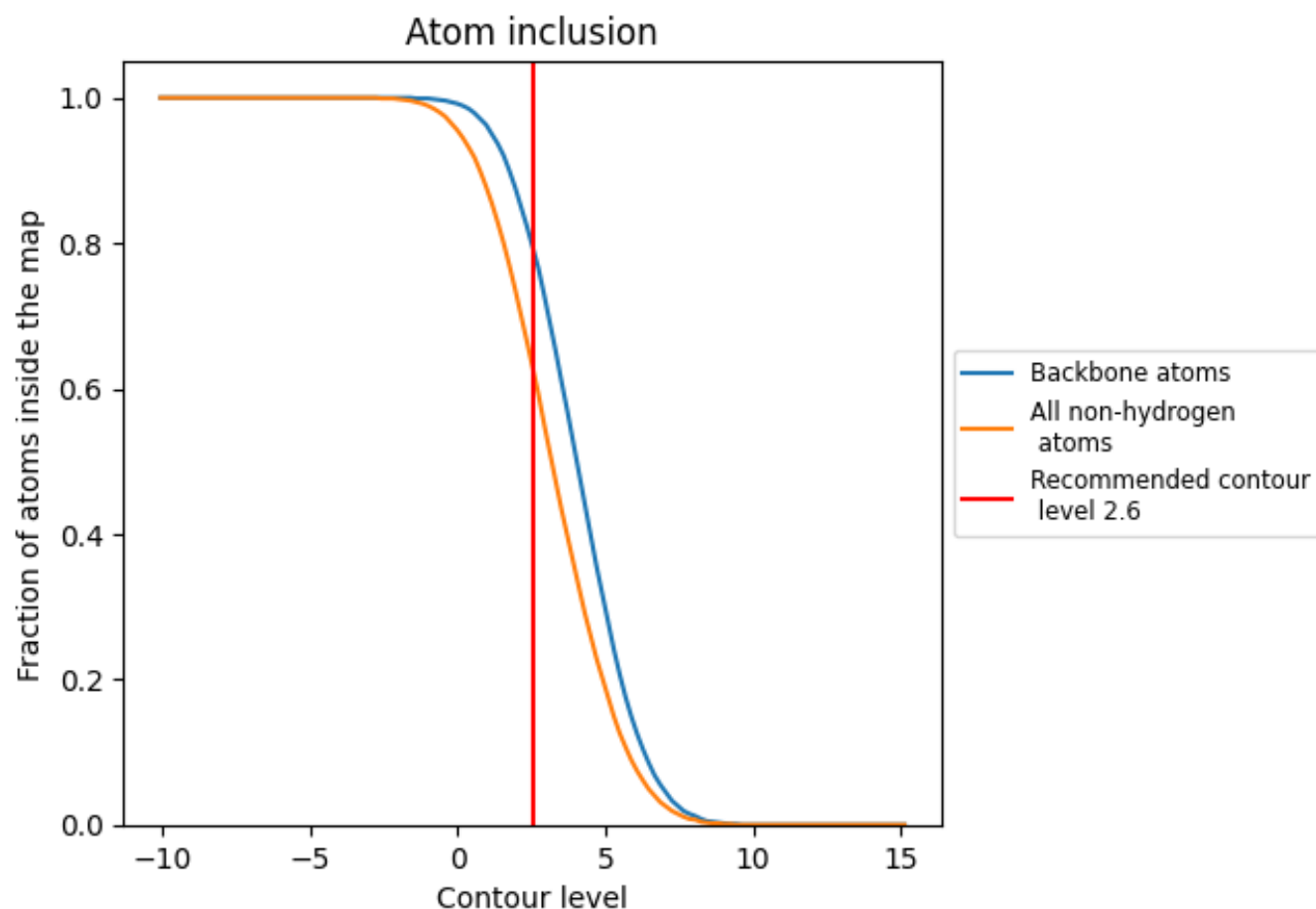
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 62% 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 (2.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6190	0.3550
A	0.5520	0.3190
B	0.6200	0.3700
C	0.6510	0.3760
D	0.6430	0.3500
E	0.7050	0.3340

