



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:57 AM UTC

PDB ID : 3IZ3 / pdb_00003iz3
EMDB ID : EMD-5233
Title : CryoEM structure of cytoplasmic polyhedrosis virus
Authors : Cheng, L.; Sun, J.; Zhang, K.; Mou, Z.; Huang, X.; Ji, G.; Sun, F.; Zhang, J.;
Zhu, P.
Deposited on : 2010-09-14
Resolution : 3.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

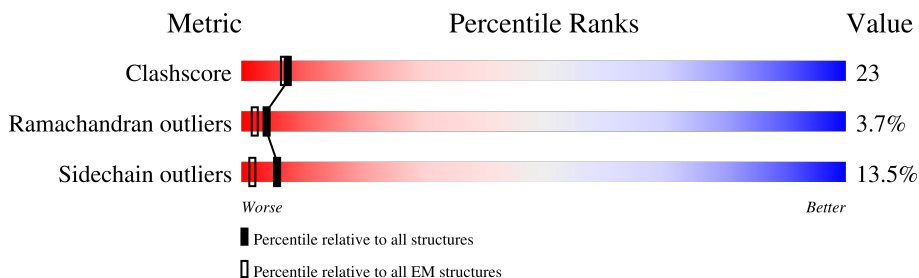
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	93% 55% 34% 9% ..
2	B	1333	79% 56% 27% 5% 11%
2	C	1333	80% 60% 27% 6% 7%
3	D	291	87% 47% 40% 13% .
3	E	291	82% 41% 42% 15% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32024 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	S	0	0
			8349	5294	1439	1572	44		

- Molecule 2 is a protein called Structural protein VP1.

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

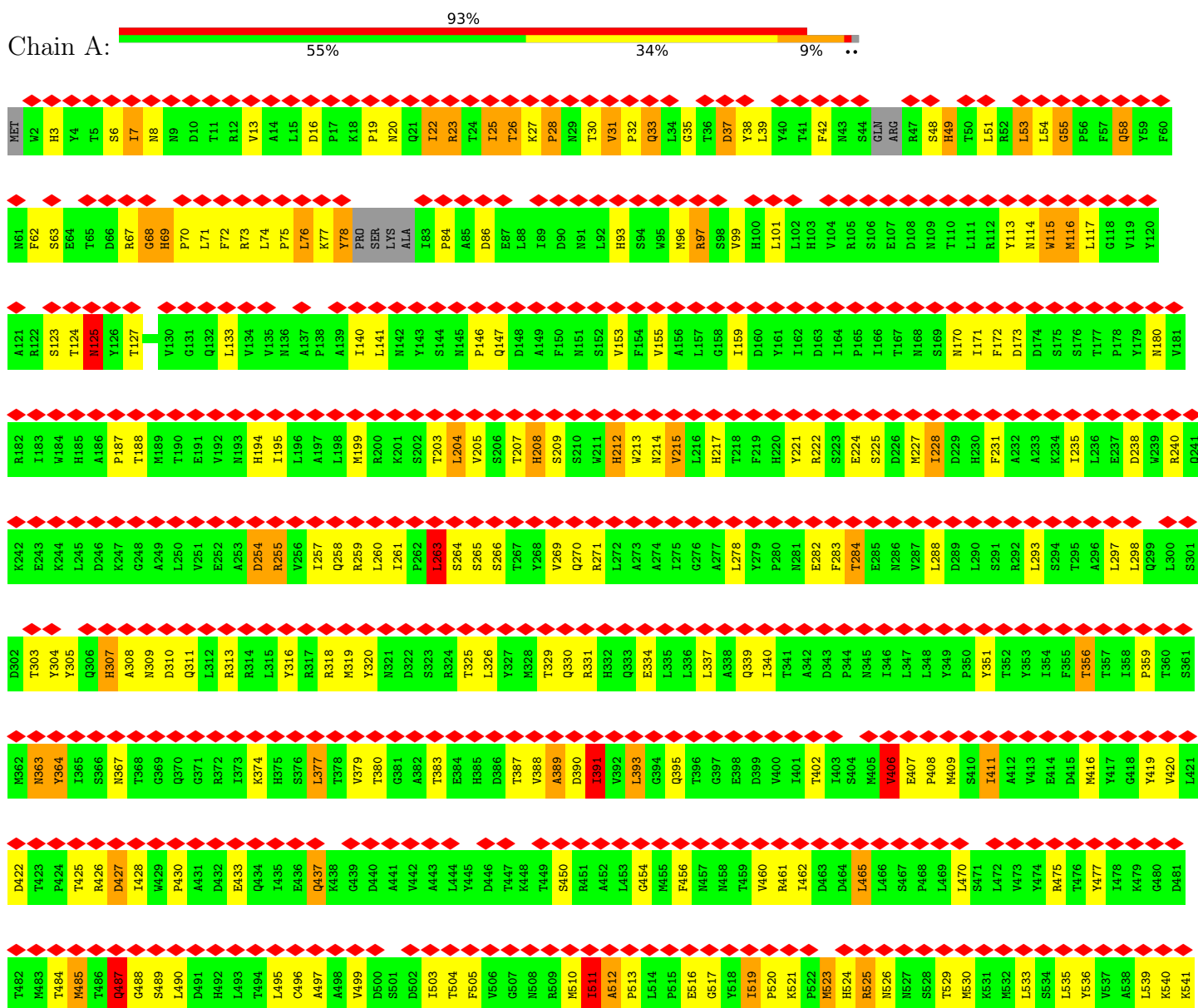
- Molecule 3 is a protein called Viral structural protein 5.

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

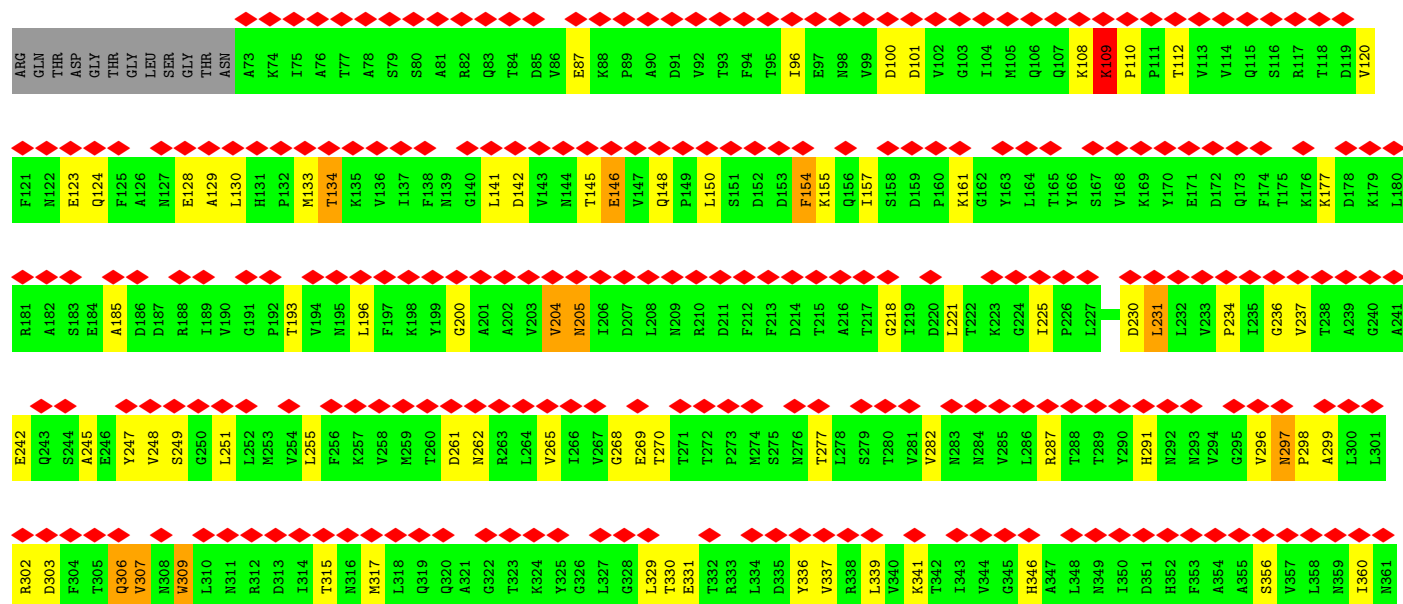
3 Residue-property plots

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.

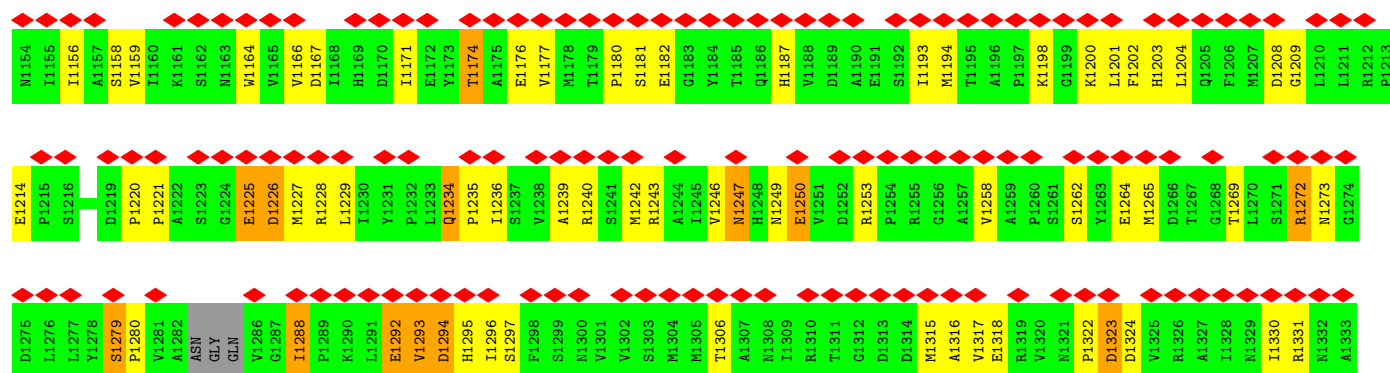
• Molecule 1: Structural protein VP3



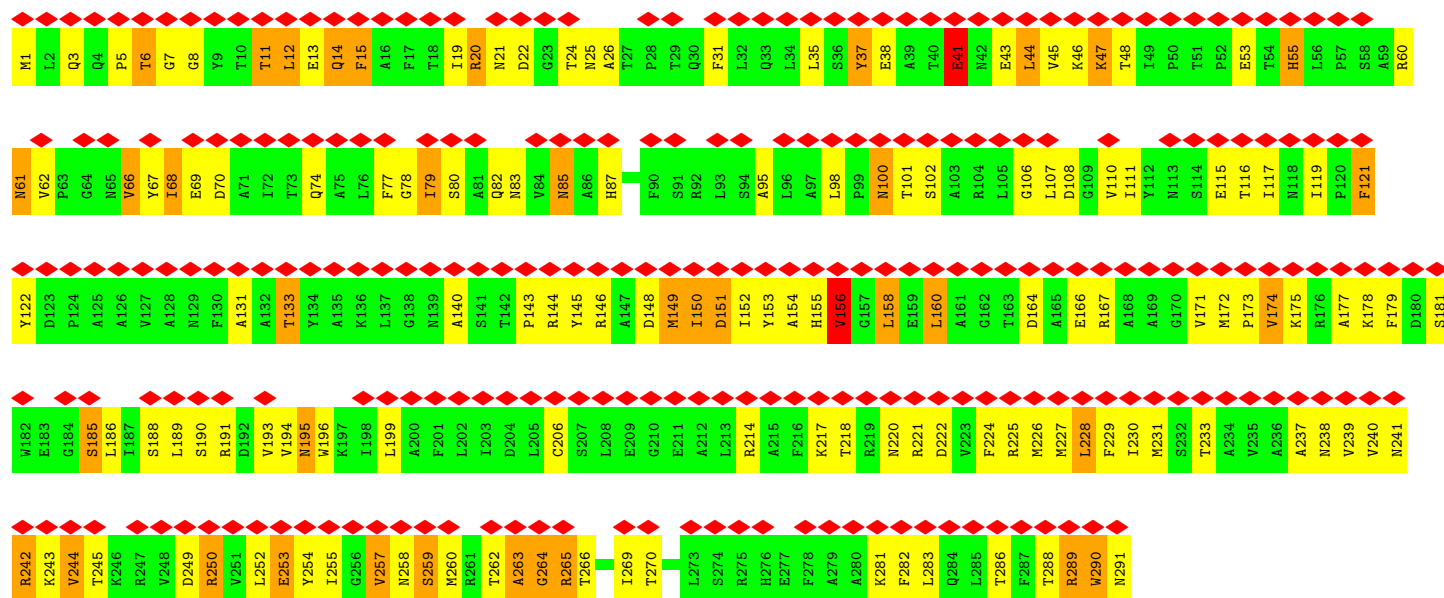
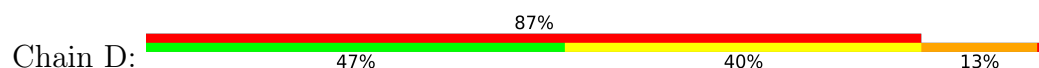
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G846	I847	R848	M849	T850	T851	Y852	D853	Q854	Y855	L856	S857	H858	T859	L860	E861	R862	L863	H864	T865	T866	H867	V868	P869	D870	S871	H872	I873	L874	T875	H876	T877	G878	H879	T880	R881	T882	L883	T884	A885	S886	V887	Q888	A889	T890	H891	Y892	A893	Q894	A895	L896	Y897	Q898	R899	T900	S901	I902	N903	G904	S905
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SER	ILE	MET	GLU	E790	I791	V792	Y793	P794	D795	P796	S797	T798	T799	L800	E801	R802	S803	L804	S805	V806	A807	Q808	H809	L810	S811	K812	L813	T814	L815	P816	D817	A818	D819	N820	R821	R822	L823	L824	S825	G826	G827	D828	S829	V830	H831	R832	R833	T834	Y835	Q836	T837	E838	A839	D840	T841	D842	L843	D844	E845
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R302	D303	F304	T305	Q306	V307	N308	W309	L310	N311	R312	D313	I314	T315	N316	M317	L318	Q319	Q320	A321	G322	T323	K324	Y325	G326	L327	Q328	L329	T330	E331	T332	R333	L334	D335	Y336	V337	R338	L339	V340	K341	T342	I343	F344	G345	H346	A347	L348	N349	I350	D351	H352	F353	A354	A355	V356	A357	L358	N359	I360	N361
L362	R363	A364	L365	M366	E367	A368	N369	V370	T371	R372	D373	E374	R375	I376	K377	A378	L379	Q380	A381	H382	S383	M384	I385	S386	T387	Q388	F389	H390	G391	P392	N393	Q394	G395	A396	L397	R398	S399	E400	L401	A402	F403	D404	H405	D406	H407	I408	I409	R410	C411	L412	M413	L414	A415	A416	A417	M418	Y419	P420	R421
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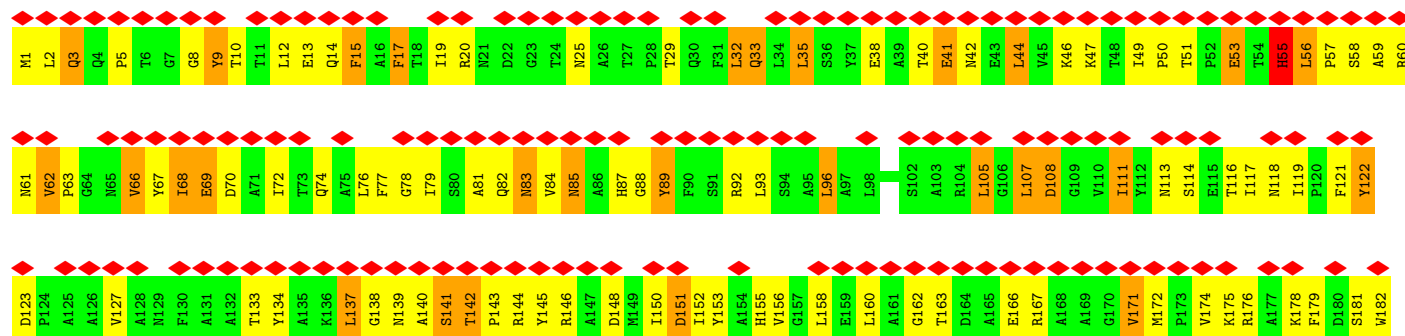
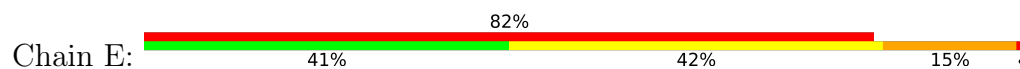
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F1106	Y925	Y925	H865	S805	I745	R685	A622	A562	I440	I376	I376
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E1049	E1049	R928	Y868	W809	G749	T689	R626	F566	Q380	Q380	Q380
L1050	L1050	F929	P869	L810	E750	Q690	A627	F567	A381	A381	A381
R1051	R1051	A930	D870	S811	T751	D692	S628	E507	H382	H382	H382
L1052	L1052	N931	P871	K812	W752	N693	R629	F568	S383	S383	S383
R1053	R1053	A932	T872	L813	D753	T694	M630	G570	M384	M384	M384
R1054	R1054	N933	Y873	T814	Q754	A695	P631	R571	I385	I385	I385
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S1056	S1056	Q935	T875	P816	T756	W696	T633	E513	T387	T387	T387
Y1057	Y1057	M936	G876	D817	I757	A697	Y634	F514	Q388	Q388	Q388
G998	G998	N937	A877	A818	I758	H698	I635	I515	H390	H390	H390
K999	K999	N938	S878	F819	W759	T699	P636	L516	G391	G391	G391
L1000	L1000	N939	T879	T820	D759	W700	Y637	F517	P392	P392	P392
P1122	P1122	R940	P880	N821	T760	H701	T638	A518	Q394	Q394	Q394
P1123	P1123	Y941	P881	M822	S761	L702	N639	F520	G395	G395	G395
T1124	T1124	H942	D882	R823	I762	S703	Y644	F521	A396	A396	A396
G1125	G1125	E943	R883	L824	W763	Y704	T643	F522	L397	L397	L397
M1126	M1126	S944	S825	S825	P765	V705	V644	P523	R398	R398	R398
I1127	I1127	Y945	G826	G826	I766	A706	E647	E524	E400	E400	E400
Y1128	Y1128	L946	A885	G827	L767	T708	F648	F525	H405	H405	H405
P1129	P1129	E947	S886	D828	Q770	M709	S650	N526	D406	D406	D406
S1130	S1130	T948	H887	S829	T771	S710	R651	K529	H407	H407	H407
P1131	P1131	A949	Q888	W830	W772	N711	F652	I528	I408	I408	I408
T1132	T1132	D950	A889	R831	P773	M712	R653	D591	I409	I409	I409
G1133	G1133	P952	H891	R833	L774	L714	T654	Q533	R410	R410	R410
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V1137	V1137	Q1015	H894	R835	W775	F716	R656	L536	L414	L414	L414
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I1141	I1141	I1019	Y897	R839	W775	M718	T658	A471	F420	F420	F420
M1142	M1142	Q959	Q898	A839	W775	M719	L659	E472	R421	R421	R421
E1143	E1143	T960	S899	D840	W775	M719	L659	A468	L422	L422	L422
R1144	R1144	R1021	G900	D841	W775	F720	A660	R469	E423	E423	E423
A1145	A1145	S961	G901	S961	W775	F720	A660	I475	G424	G424	G424
G1146	G1146	D962	Y901	D842	W775	F720	A660	I475	A481	A481	A481
P1086	P1086	A963	I902	L843	W775	G722	V662	S477	I482	I482	I482
D1087	D1087	V964	N903	L843	W775	M723	V663	A483	A483	A483	A483
F1088	F1088	R965	G904	D844	W775	M723	V663	I478	E484	E484	E484
V1089	V1089	Q966	S905	E845	W775	M723	V663	S541	G485	G485	G485
P1090	P1090	L967	A906	E846	W775	M723	V663	F539	E486	E486	E486
K1149	K1149	T1027	S907	T847	W775	M723	V663	S477	E487	E487	E487
A1152	A1152	T1028	A907	E847	W775	M723	V663	I478	E488	E488	E488
D1153	D1153	L1029	T908	R849	W775	M723	V663	S477	E489	E489	E489
		R1030	Y909	T850	W775	M723	V663	S477	E490	E490	E490
		Y1031	L910		W775	M723	V663	S477	E491	E491	E491



• Molecule 3: Viral structural protein 5



• Molecule 3: Viral structural protein 5



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	29000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	0.8	Depositor
Maximum defocus (nm)	2.8	Depositor
Magnification	75000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	18.037	Depositor
Minimum map value	-16.951	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3	Depositor
Map size ($\text{\AA}$)	761.60004, 761.60004, 595.0	wwPDB
Map dimensions	640, 640, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.19, 1.19, 1.19	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/8530	0.87	6/11613 (0.1%)
2	B	0.47	0/9508	0.83	10/12941 (0.1%)
2	C	0.49	0/10006	0.85	11/13622 (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	0.49	0/32688	0.89	69/44488 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	629	ARG	N-CA-C	-12.65	100.20	114.62
3	E	235	VAL	N-CA-C	11.79	121.61	110.53
3	E	59	ALA	CB-CA-C	-11.57	92.90	110.26
3	E	253	GLU	N-CA-C	11.48	123.36	111.07
3	E	87	HIS	N-CA-C	10.67	122.91	111.28
3	D	41	GLU	N-CA-C	10.00	125.52	111.52
3	E	57	PRO	CB-CA-C	-9.45	99.64	111.64
3	E	237	ALA	N-CA-C	9.22	121.10	111.14
3	E	60	ARG	N-CA-C	9.16	124.97	113.43
3	E	192	ASP	N-CA-C	9.01	120.87	111.14
2	C	1226	ASP	N-CA-C	8.96	122.90	110.35
3	E	60	ARG	N-CA-CB	-8.16	96.63	110.51
3	E	59	ALA	N-CA-C	7.94	121.27	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	263	ALA	N-CA-C	-7.77	94.94	108.08
2	C	110	PRO	N-CA-C	7.63	120.00	110.70
1	A	208	HIS	N-CA-C	7.59	119.90	107.23
3	E	88	GLY	N-CA-C	7.55	121.79	112.73
3	E	96	LEU	N-CA-C	7.31	119.25	111.28
3	E	261	ARG	N-CA-C	7.21	119.34	107.73
3	E	33	GLN	N-CA-C	7.12	119.04	111.28
3	E	133	THR	N-CA-C	7.00	121.95	113.41
3	D	7	GLY	N-CA-C	-6.99	96.62	113.18
3	E	89	TYR	N-CA-C	6.86	118.76	111.28
3	E	141	SER	N-CA-C	6.58	119.45	111.82
3	E	58	SER	N-CA-C	6.54	119.00	110.43
3	D	156	VAL	N-CA-C	6.51	117.26	110.62
3	D	11	THR	N-CA-C	-6.21	106.39	112.97
1	A	871	VAL	N-CA-C	-6.21	99.81	108.12
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	B	235	ILE	N-CA-C	6.01	116.67	110.36
3	E	262	THR	N-CA-C	5.83	123.22	110.80
3	E	181	SER	N-CA-C	5.75	118.02	108.99
3	D	257	VAL	CA-C-N	-5.73	114.81	122.72
3	D	257	VAL	C-N-CA	-5.73	114.81	122.72
3	E	185	SER	N-CA-C	5.71	117.51	111.28
2	C	728	LYS	CA-C-N	5.68	125.36	119.05
2	C	728	LYS	C-N-CA	5.68	125.36	119.05
3	D	98	LEU	CA-C-N	5.66	126.91	119.84
3	D	98	LEU	C-N-CA	5.66	126.91	119.84
2	B	1210	LEU	N-CA-C	-5.65	108.18	114.62
2	B	205	ASN	N-CA-C	5.64	115.83	107.88
3	D	263	ALA	N-CA-C	-5.62	105.14	112.23
2	B	1122	PRO	N-CA-C	5.62	117.55	110.70
3	D	6	THR	CB-CA-C	-5.59	99.29	110.42
2	B	931	ASN	N-CA-C	5.56	117.25	108.96
3	D	264	GLY	N-CA-C	5.56	118.95	112.50
3	E	32	LEU	N-CA-C	5.54	118.03	111.33
3	E	9	TYR	N-CA-C	-5.52	106.59	113.38
2	C	1225	GLU	N-CA-C	5.51	119.17	109.80
2	C	635	ILE	N-CA-C	5.42	120.58	108.88
1	A	788	ASP	CA-C-N	5.40	125.07	119.56
1	A	788	ASP	C-N-CA	5.40	125.07	119.56
1	A	33	GLN	N-CA-C	5.38	117.45	107.60
2	B	868	VAL	CA-C-N	5.36	124.82	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	868	VAL	C-N-CA	5.36	124.82	119.24
3	D	259	SER	N-CA-C	-5.35	101.66	109.63
3	D	185	SER	CB-CA-C	-5.33	109.98	117.23
2	B	828	ASP	N-CA-C	5.32	115.38	107.88
2	C	941	TYR	N-CA-C	5.31	116.77	110.19
2	B	471	SER	N-CA-C	5.29	117.13	111.36
2	B	472	GLU	N-CA-C	5.29	116.73	110.97
2	C	109	LYS	CA-C-N	5.23	125.77	120.38
2	C	109	LYS	C-N-CA	5.23	125.77	120.38
3	E	61	ASN	N-CA-C	5.21	118.43	111.24
3	D	151	ASP	N-CA-C	5.12	116.86	111.28
3	E	255	ILE	N-CA-C	5.07	115.79	110.62
1	A	766	CYS	N-CA-C	5.02	115.16	108.23
2	C	561	ASN	N-CA-C	5.00	117.25	109.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1225	GLU	Peptide
2	C	628	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8349	0	8304	341	0
2	B	9317	0	9236	381	0
2	C	9806	0	9713	379	0
3	D	2276	0	2273	293	0
3	E	2276	0	2277	263	0
All	All	32024	0	31803	1456	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 23.

All (1456) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:THR:CG2	2:C:237:VAL:HG23	1.18	1.64
2:B:274:MET:CG	2:C:234:PRO:HD3	1.35	1.51
3:E:46:LYS:HD3	3:E:155:HIS:CE1	1.49	1.45
2:B:1273:ASN:OD1	3:D:79:ILE:CG2	1.68	1.40
2:B:1273:ASN:ND2	3:D:191:ARG:HA	1.38	1.39
2:B:363:ARG:CZ	3:D:80:SER:OG	1.71	1.39
2:B:271:THR:HG21	2:C:237:VAL:CG2	1.52	1.38
3:E:53:GLU:HG2	3:E:145:TYR:CD1	1.57	1.37
2:B:274:MET:HG3	2:C:234:PRO:CD	1.54	1.36
3:E:46:LYS:CD	3:E:155:HIS:HE1	1.41	1.31
3:D:253:GLU:OE1	3:D:254:TYR:CE2	1.83	1.30
3:E:1:MET:HE1	3:E:121:PHE:CE2	1.66	1.30
3:D:253:GLU:HG3	3:D:254:TYR:CD2	1.68	1.29
2:B:891:HIS:CD2	3:D:240:VAL:CG2	2.17	1.28
2:B:954:GLN:CD	3:D:240:VAL:HG12	1.59	1.28
3:D:8:GLY:O	3:D:11:THR:HG22	1.34	1.27
2:B:954:GLN:CD	3:D:240:VAL:CG1	2.09	1.26
3:E:68:ILE:C	3:E:68:ILE:HD13	1.56	1.26
2:C:337:VAL:HG22	3:E:187:ILE:CD1	1.66	1.25
2:B:271:THR:CG2	2:C:237:VAL:CG2	2.09	1.25
3:D:253:GLU:OE1	3:D:254:TYR:HE2	1.03	1.25
3:E:32:LEU:O	3:E:35:LEU:CD1	1.84	1.24
1:A:159:ILE:HD11	2:B:1333:ALA:O	1.32	1.23
2:B:950:ASP:C	3:D:243:LYS:HZ2	1.45	1.21
2:B:950:ASP:HA	3:D:243:LYS:NZ	1.56	1.20
3:D:5:PRO:O	3:D:6:THR:CG2	1.90	1.20
3:E:289:ARG:HD2	3:E:289:ARG:O	1.40	1.19
3:E:182:TRP:O	3:E:183:GLU:HG2	1.08	1.18
3:D:5:PRO:O	3:D:6:THR:HG22	1.01	1.17
3:E:55:HIS:HD2	3:E:145:TYR:CE2	1.63	1.17
3:D:45:VAL:HG13	3:D:171:VAL:HG22	1.19	1.16
2:B:1273:ASN:OD1	3:D:79:ILE:HG22	1.39	1.15
3:E:107:LEU:HA	3:E:122:TYR:HE1	1.06	1.15
2:B:1044:ARG:NH2	3:D:266:THR:HG22	1.59	1.15
2:B:891:HIS:CD2	3:D:240:VAL:HG23	1.82	1.15
2:B:1044:ARG:HH21	3:D:266:THR:HG22	1.01	1.15
3:E:137:LEU:HD23	3:E:137:LEU:C	1.72	1.14
2:B:338:ARG:HH21	2:C:1002:LEU:HD22	0.98	1.14
3:E:158:LEU:O	3:E:162:GLY:HA3	1.48	1.13
1:A:159:ILE:CD1	2:B:1333:ALA:O	1.96	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	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ALA:HB3	1:A:513:PRO:HA	1.27	1.11
3:E:205:LEU:HD13	3:E:205:LEU:O	1.49	1.11
3:E:175:LYS:HB2	3:E:255:ILE:CD1	1.80	1.11
1:A:188:THR:HG21	3:D:144:ARG:HG2	1.34	1.10
2:B:891:HIS:NE2	3:D:240:VAL:HG23	1.67	1.10
2:C:1080:THR:HG21	2:C:1227:MET:SD	1.91	1.10
3:D:149:MET:HE3	3:D:260:MET:HE1	1.10	1.09
2:B:134:THR:HG21	2:C:472:GLU:OE2	1.52	1.09
2:B:271:THR:HG23	2:C:237:VAL:HG23	1.13	1.09
2:B:279:SER:CB	2:C:1198:LYS:HE2	1.83	1.09
2:C:1025:ASP:OD2	3:D:95:ALA:HB2	1.53	1.09
3:E:49:ILE:HG23	3:E:50:PRO:HD2	1.35	1.09
2:C:100:ASP:OD1	3:E:82:GLN:NE2	1.84	1.08
2:C:1273:ASN:O	3:E:183:GLU:OE1	1.70	1.08
1:A:159:ILE:CD1	2:B:1333:ALA:C	2.27	1.08
2:C:878:SER:HB3	2:C:903:ASN:HB2	1.34	1.08
2:B:950:ASP:CA	3:D:243:LYS:NZ	2.16	1.08
2:B:891:HIS:CD2	3:D:240:VAL:HG21	1.84	1.07
1:A:554:PRO:HB3	1:A:580:SER:OG	1.52	1.07
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	1.07
2:B:388:GLN:OE1	2:C:499:ALA:HB1	1.53	1.06
2:C:1273:ASN:HA	3:E:183:GLU:OE1	1.53	1.05
2:B:137:ILE:HD11	2:C:759:ASP:CG	1.81	1.05
3:E:191:ARG:HG3	3:E:191:ARG:NH1	1.60	1.05
1:A:904:PHE:HE2	1:A:906:PHE:HB3	1.16	1.04
2:B:950:ASP:O	3:D:243:LYS:NZ	1.90	1.04
3:E:32:LEU:O	3:E:35:LEU:HD12	1.57	1.04
3:E:175:LYS:CB	3:E:255:ILE:HD11	1.86	1.04
3:E:107:LEU:HA	3:E:122:TYR:CE1	1.93	1.03
2:C:337:VAL:HG22	3:E:187:ILE:HD12	1.06	1.03
2:B:338:ARG:NH2	2:C:1002:LEU:HD22	1.73	1.02
2:B:950:ASP:HA	3:D:243:LYS:HZ1	1.21	1.02
3:D:149:MET:HE3	3:D:260:MET:CE	1.88	1.02
3:E:68:ILE:C	3:E:68:ILE:CD1	2.30	1.02
3:E:53:GLU:CG	3:E:145:TYR:HD1	1.73	1.01
3:E:191:ARG:HH11	3:E:191:ARG:CG	1.72	1.01
3:E:32:LEU:O	3:E:35:LEU:HD11	1.57	1.01
2:C:1051:ARG:HH11	2:C:1051:ARG:HG2	1.24	1.00
3:E:262:THR:HG22	3:E:263:ALA:O	1.61	1.00
1:A:194:HIS:CE1	3:D:146:ARG:NH1	2.30	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:864:HIS:NE2	2:C:1030:ARG:NH2	2.10	0.99
2:C:1050:LEU:HD12	2:C:1054:ARG:HH21	1.23	0.99
3:E:46:LYS:CD	3:E:155:HIS:CE1	2.25	0.99
2:B:1044:ARG:HE	3:D:266:THR:CG2	1.74	0.99
2:B:442:PRO:HG3	2:B:475:ILE:HB	1.40	0.99
2:B:338:ARG:HH21	2:C:1002:LEU:CD2	1.75	0.99
2:B:1044:ARG:NE	3:D:266:THR:CG2	2.26	0.98
3:E:127:VAL:HG12	3:E:203:ILE:HD11	1.44	0.98
3:E:158:LEU:O	3:E:162:GLY:CA	2.10	0.98
3:D:253:GLU:CG	3:D:254:TYR:CD2	2.46	0.98
3:D:153:TYR:HA	3:D:156:VAL:HG12	1.42	0.98
1:A:49:HIS:HE2	1:A:172:PHE:HD1	1.01	0.98
2:B:954:GLN:CG	3:D:240:VAL:HG12	1.93	0.98
3:E:1:MET:HE1	3:E:121:PHE:CD2	1.99	0.97
3:E:68:ILE:HD13	3:E:68:ILE:O	1.62	0.97
3:D:253:GLU:CD	3:D:254:TYR:CE2	2.41	0.97
3:E:261:ARG:HH12	3:E:265:ARG:NH2	1.62	0.97
2:B:1273:ASN:OD1	3:D:79:ILE:HG23	1.64	0.97
2:C:1037:ILE:HG22	2:C:1038:GLU:H	1.27	0.96
2:B:870:ASP:HB3	2:B:871:PRO:HA	1.47	0.96
1:A:194:HIS:NE2	3:D:146:ARG:NH1	2.14	0.96
3:E:55:HIS:CD2	3:E:145:TYR:CE2	2.53	0.96
3:E:53:GLU:CG	3:E:145:TYR:CD1	2.47	0.96
1:A:426:ARG:HB2	1:A:707:SER:HB2	1.47	0.96
3:E:261:ARG:HH12	3:E:265:ARG:HH21	1.11	0.96
2:B:134:THR:CG2	2:C:472:GLU:OE2	2.13	0.96
2:C:146:GLU:HB2	2:C:1317:VAL:O	1.63	0.96
3:D:262:THR:HG21	3:D:270:THR:HA	1.47	0.95
2:C:528:ILE:HD11	2:C:758:ILE:HD12	1.47	0.95
2:B:338:ARG:NH2	2:C:1002:LEU:CD2	2.29	0.95
3:E:53:GLU:HG2	3:E:145:TYR:HD1	0.80	0.95
3:E:68:ILE:HD11	3:E:72:ILE:CD1	1.96	0.95
3:E:289:ARG:HD2	3:E:289:ARG:C	1.87	0.95
1:A:986:ARG:HB3	1:A:994:PRO:HB3	1.44	0.95
2:B:956:ASP:OD1	3:D:266:THR:OG1	1.83	0.95
3:E:107:LEU:HD23	3:E:122:TYR:CE1	2.02	0.95
3:D:153:TYR:HA	3:D:156:VAL:CG1	1.96	0.94
3:E:191:ARG:HG3	3:E:191:ARG:HH11	0.79	0.94
2:B:954:GLN:OE1	3:D:240:VAL:HG12	1.67	0.94
3:E:69:GLU:C	3:E:69:GLU:CD	2.35	0.94
2:B:368:ALA:O	3:D:83:ASN:HB2	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:200:ALA:O	3:E:204:ASP:OD2	1.85	0.93
1:A:225:SER:OG	2:B:563:ALA:HA	1.69	0.93
2:B:891:HIS:NE2	3:D:240:VAL:CG2	2.26	0.93
3:E:1:MET:CE	3:E:121:PHE:CE2	2.53	0.92
2:B:950:ASP:C	3:D:243:LYS:NZ	2.28	0.92
2:C:1273:ASN:CA	3:E:183:GLU:OE1	2.18	0.91
3:D:214:ARG:O	3:D:218:THR:HG23	1.69	0.91
2:B:271:THR:HG21	2:C:237:VAL:HG23	1.01	0.91
2:C:878:SER:HB3	2:C:903:ASN:CB	1.99	0.91
2:C:1025:ASP:OD2	3:D:95:ALA:CB	2.18	0.91
1:A:967:ILE:HG13	1:A:978:LYS:HB2	1.52	0.91
1:A:27:LYS:HB3	1:A:28:PRO:HD3	1.53	0.91
2:B:350:ILE:HG22	2:B:351:ASP:H	1.35	0.91
2:B:279:SER:HB2	2:C:1198:LYS:HE2	1.52	0.90
3:D:44:LEU:HD11	3:D:154:ALA:HA	1.50	0.90
2:C:565:GLU:HG2	2:C:566:PHE:N	1.86	0.90
2:C:1050:LEU:HD12	2:C:1054:ARG:NH2	1.86	0.90
3:D:253:GLU:HG3	3:D:254:TYR:HD2	1.10	0.90
2:B:1273:ASN:HD22	3:D:191:ARG:HA	1.09	0.89
2:B:1273:ASN:HD21	3:D:191:ARG:HA	1.34	0.89
2:B:1288:ILE:HD12	3:D:20:ARG:NH2	1.88	0.89
1:A:406:VAL:CB	1:A:407:GLU:HA	2.03	0.89
1:A:194:HIS:CE1	3:D:146:ARG:HH11	1.88	0.89
2:B:183:SER:HB3	2:B:186:ASP:HB2	1.54	0.89
2:B:956:ASP:CG	3:D:266:THR:OG1	2.15	0.89
2:B:1044:ARG:HE	3:D:266:THR:HG21	1.37	0.89
3:D:156:VAL:HG23	3:D:228:LEU:CD2	2.02	0.89
1:A:406:VAL:HB	1:A:407:GLU:CA	2.03	0.88
2:B:368:ALA:HA	3:D:83:ASN:ND2	1.88	0.88
2:B:231:LEU:HB2	2:B:249:SER:HB2	1.54	0.88
2:B:340:VAL:HG21	2:C:1008:LEU:HD23	1.56	0.88
3:D:5:PRO:C	3:D:6:THR:HG22	1.98	0.88
2:B:279:SER:OG	2:C:1198:LYS:HE2	1.73	0.88
2:C:397:LEU:HD11	3:E:265:ARG:HB3	1.56	0.88
2:B:274:MET:CG	2:C:234:PRO:CD	2.29	0.88
3:E:160:LEU:HD11	3:E:229:PHE:HB2	1.55	0.88
3:D:8:GLY:O	3:D:11:THR:CG2	2.20	0.87
2:B:888:GLN:NE2	3:D:38:GLU:OE1	2.06	0.87
2:C:337:VAL:CG2	3:E:187:ILE:HD12	1.99	0.87
1:A:159:ILE:HD13	2:B:1333:ALA:C	1.98	0.87
1:A:406:VAL:HB	1:A:407:GLU:HA	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1273:ASN:CG	3:D:79:ILE:HG22	1.98	0.87
3:E:12:LEU:HG	3:E:14:GLN:HE21	1.38	0.87
3:E:68:ILE:HD11	3:E:72:ILE:HD12	1.57	0.87
2:B:1023:ARG:HB2	2:B:1024:PRO:HD2	1.55	0.87
1:A:970:ARG:HH22	1:A:977:HIS:HA	1.38	0.87
2:B:1248:HIS:ND1	2:B:1251:VAL:HG22	1.90	0.87
2:B:891:HIS:HD2	3:D:240:VAL:CG2	1.85	0.87
2:B:954:GLN:CD	3:D:240:VAL:HG13	1.97	0.86
2:C:638:THR:HB	2:C:1331:ARG:HH21	1.41	0.86
2:C:1273:ASN:C	3:E:183:GLU:OE1	2.19	0.86
1:A:868:ASP:O	1:A:871:VAL:HG23	1.75	0.86
3:D:153:TYR:O	3:D:156:VAL:HG13	1.74	0.86
1:A:194:HIS:CD2	3:D:146:ARG:NH1	2.44	0.86
1:A:512:ALA:CB	1:A:513:PRO:HA	2.06	0.86
2:B:1273:ASN:CG	3:D:79:ILE:CG2	2.47	0.86
3:E:49:ILE:CG2	3:E:50:PRO:HD2	2.06	0.86
2:B:1273:ASN:ND2	3:D:191:ARG:CA	2.33	0.85
2:C:1023:ARG:HG2	2:C:1024:PRO:HD2	1.56	0.85
2:B:950:ASP:CA	3:D:243:LYS:HZ2	1.80	0.85
3:E:160:LEU:CD1	3:E:229:PHE:HB2	2.05	0.85
1:A:31:VAL:HG23	1:A:32:PRO:HD3	1.59	0.85
2:B:186:ASP:HA	2:B:189:ILE:HG22	1.57	0.85
3:D:172:MET:HE3	3:D:175:LYS:HG3	1.58	0.85
3:D:149:MET:CE	3:D:260:MET:CE	2.50	0.84
3:E:175:LYS:HB2	3:E:255:ILE:HD11	0.90	0.84
2:C:1071:PHE:HB3	2:C:1234:GLN:HG3	1.58	0.84
3:E:146:ARG:CZ	3:E:277:GLU:OE2	2.26	0.84
2:B:274:MET:HG2	2:C:234:PRO:HD3	1.54	0.84
3:E:55:HIS:CG	3:E:55:HIS:O	2.30	0.84
1:A:49:HIS:NE2	1:A:172:PHE:HD1	1.76	0.83
1:A:76:LEU:O	1:A:78:TYR:N	2.10	0.83
2:C:619:ALA:HB2	2:C:711:ASN:HB2	1.60	0.83
2:C:1050:LEU:CD1	2:C:1054:ARG:HH21	1.92	0.83
1:A:904:PHE:CE2	1:A:906:PHE:HB3	2.08	0.83
2:B:870:ASP:HB3	2:B:871:PRO:CA	2.09	0.82
3:D:181:SER:HB3	3:D:250:ARG:HG2	1.62	0.82
3:E:69:GLU:HG2	3:E:199:LEU:HB2	1.61	0.82
1:A:406:VAL:HG21	1:A:408:PRO:HD3	1.59	0.82
3:E:137:LEU:C	3:E:137:LEU:CD2	2.49	0.82
3:E:182:TRP:C	3:E:183:GLU:HG2	2.04	0.82
2:C:449:PHE:N	2:C:450:PRO:HD3	1.95	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ASP:HA	1:A:704:PRO:HD2	1.61	0.82
2:B:363:ARG:NE	3:D:80:SER:OG	2.13	0.82
2:B:954:GLN:OE1	3:D:240:VAL:CG1	2.24	0.82
3:E:79:ILE:HA	3:E:269:ILE:HD13	1.62	0.82
1:A:188:THR:HG21	3:D:144:ARG:CG	2.09	0.82
3:D:100:ASN:H	3:D:100:ASN:HD22	1.24	0.82
3:E:166:GLU:OE2	3:E:171:VAL:O	1.97	0.82
3:D:258:ASN:OD1	3:D:259:SER:O	1.98	0.82
1:A:978:LYS:HG2	1:A:987:LEU:HD13	1.62	0.81
1:A:124:THR:O	1:A:125:ASN:HB2	1.79	0.81
2:B:954:GLN:HG2	3:D:240:VAL:HG12	1.61	0.81
3:E:85:ASN:ND2	3:E:141:SER:HB3	1.95	0.81
2:B:1044:ARG:NH2	3:D:266:THR:CG2	2.43	0.81
3:D:107:LEU:O	3:D:108:ASP:CG	2.23	0.81
2:B:219:ILE:HG22	2:B:220:ASP:H	1.45	0.81
2:C:450:PRO:C	2:C:452:ASN:H	1.86	0.81
1:A:597:ARG:HH11	1:A:597:ARG:HG3	1.45	0.80
3:D:41:GLU:OE1	3:D:41:GLU:HA	1.79	0.80
2:C:443:VAL:HG22	2:C:444:SER:H	1.46	0.80
1:A:864:ARG:HG3	1:A:866:LEU:H	1.46	0.80
2:B:1263:TYR:CG	2:B:1295:HIS:HD2	1.99	0.80
3:D:264:GLY:O	3:D:266:THR:N	2.14	0.80
2:B:442:PRO:HD3	2:B:475:ILE:HD12	1.62	0.80
2:C:1051:ARG:HG2	2:C:1051:ARG:NH1	1.88	0.80
2:C:154:PHE:HB3	2:C:262:ASN:HB2	1.62	0.80
3:D:153:TYR:O	3:D:156:VAL:CG1	2.30	0.80
1:A:27:LYS:O	1:A:30:THR:HG23	1.82	0.80
3:D:253:GLU:CG	3:D:254:TYR:HD2	1.89	0.79
3:E:55:HIS:HD2	3:E:145:TYR:CZ	2.00	0.79
2:B:733:VAL:HG21	2:B:741:TYR:CD1	2.18	0.79
2:B:956:ASP:CG	3:D:266:THR:HG1	1.90	0.79
1:A:406:VAL:CG2	1:A:407:GLU:HA	2.13	0.79
2:B:1234:GLN:HE21	2:B:1234:GLN:HA	1.47	0.79
2:B:1274:GLY:CA	3:D:191:ARG:HG3	2.12	0.79
2:C:864:HIS:CE1	2:C:1030:ARG:NH2	2.50	0.79
3:E:137:LEU:HD23	3:E:137:LEU:O	1.82	0.79
1:A:55:GLY:H	1:A:58:GLN:HG2	1.47	0.79
2:B:1044:ARG:CZ	3:D:266:THR:CG2	2.60	0.79
3:D:41:GLU:OE1	3:D:41:GLU:CA	2.30	0.79
2:B:368:ALA:O	3:D:83:ASN:CB	2.31	0.79
2:C:1042:TRP:CG	2:C:1043:SER:HA	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:40:THR:CG2	3:E:41:GLU:OE2	2.30	0.79
1:A:648:VAL:HG22	1:A:649:LYS:N	1.99	0.78
3:D:153:TYR:CA	3:D:156:VAL:HG12	2.12	0.78
3:E:40:THR:HG23	3:E:41:GLU:OE2	1.83	0.78
2:C:750:GLU:HB3	2:C:757:ILE:HD13	1.63	0.78
2:B:1037:ILE:HG12	2:B:1038:GLU:H	1.48	0.78
2:C:291:HIS:HD2	2:C:346:HIS:CD2	2.01	0.78
2:C:385:ILE:HG13	2:C:708:THR:HG22	1.65	0.78
3:E:158:LEU:O	3:E:162:GLY:N	2.16	0.78
1:A:48:SER:O	1:A:49:HIS:HB3	1.83	0.78
2:C:565:GLU:HG2	2:C:566:PHE:H	1.45	0.78
3:E:56:LEU:HD23	3:E:56:LEU:H	1.49	0.77
1:A:730:ILE:HG22	1:A:731:HIS:H	1.48	0.77
2:B:363:ARG:NH2	3:D:80:SER:OG	2.16	0.77
1:A:717:THR:HG21	1:A:1020:SER:HB2	1.67	0.77
2:C:141:LEU:HG	2:C:142:ASP:H	1.50	0.77
3:D:217:LYS:CD	3:D:290:TRP:CZ3	2.67	0.77
3:D:45:VAL:HG13	3:D:171:VAL:CG2	2.10	0.76
3:E:68:ILE:HD11	3:E:72:ILE:HD11	1.64	0.76
2:C:1051:ARG:HH11	2:C:1051:ARG:CG	1.98	0.76
3:E:262:THR:CG2	3:E:263:ALA:O	2.33	0.76
2:B:137:ILE:CD1	2:C:759:ASP:CG	2.59	0.76
1:A:228:ILE:HD12	2:B:563:ALA:HB1	1.67	0.76
3:E:42:ASN:HB2	3:E:174:VAL:HB	1.68	0.76
3:E:107:LEU:HD23	3:E:122:TYR:CZ	2.20	0.76
2:C:638:THR:HB	2:C:1331:ARG:NH2	2.00	0.75
3:E:68:ILE:HD13	3:E:69:GLU:N	2.00	0.75
2:C:838:GLU:HB3	2:C:934:LEU:HB2	1.68	0.75
1:A:560:LEU:HD12	1:A:569:VAL:HG23	1.67	0.75
2:B:137:ILE:CD1	2:C:759:ASP:OD1	2.34	0.75
2:B:1272:ARG:HH12	3:D:69:GLU:CD	1.93	0.75
3:E:69:GLU:CG	3:E:199:LEU:HB2	2.17	0.75
2:B:271:THR:HA	2:C:236:GLY:HA3	1.67	0.75
2:C:841:ASP:CG	2:C:842:ASP:H	1.94	0.75
3:E:235:VAL:HG13	3:E:258:ASN:HD22	1.51	0.75
1:A:194:HIS:CG	3:D:146:ARG:HH11	2.05	0.75
2:B:620:ILE:HG21	2:B:631:PRO:HG3	1.69	0.75
3:E:192:ASP:OD1	3:E:192:ASP:C	2.30	0.74
2:B:1044:ARG:NE	3:D:266:THR:HG23	2.02	0.74
3:E:13:GLU:CD	3:E:13:GLU:O	2.30	0.74
2:B:1044:ARG:CZ	3:D:266:THR:HG22	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1156:ILE:HD11	2:B:1194:MET:HG3	1.68	0.74
2:C:390:HIS:HB2	2:C:1318:GLU:OE2	1.87	0.74
3:D:238:ASN:HB2	3:D:253:GLU:HB2	1.68	0.74
2:C:963:ALA:HB3	2:C:1059:LEU:CD2	2.18	0.74
3:E:156:VAL:HG13	3:E:228:LEU:HD12	1.68	0.74
2:B:956:ASP:OD2	3:D:266:THR:OG1	2.06	0.74
2:C:841:ASP:O	2:C:842:ASP:HB2	1.87	0.74
3:E:13:GLU:OE1	3:E:13:GLU:C	2.30	0.74
3:D:61:ASN:OD1	3:D:61:ASN:C	2.30	0.73
2:B:177:LYS:HE3	2:B:177:LYS:H	1.51	0.73
2:C:639:ASN:H	2:C:1331:ARG:NH2	1.85	0.73
3:D:108:ASP:OD1	3:D:110:VAL:HG23	1.88	0.73
3:E:69:GLU:CD	3:E:69:GLU:O	2.31	0.73
2:B:1273:ASN:HB2	3:D:194:VAL:HG11	1.69	0.73
2:B:960:THR:HG23	2:B:965:ARG:HH12	1.52	0.73
2:B:234:PRO:HD2	2:B:242:GLU:HB3	1.70	0.73
2:B:363:ARG:NH1	3:D:80:SER:OG	2.20	0.73
3:E:150:ILE:HG22	3:E:150:ILE:O	1.87	0.73
3:D:172:MET:HG3	3:D:173:PRO:HD2	1.69	0.72
3:E:137:LEU:HD11	3:E:278:PHE:CZ	2.23	0.72
3:E:214:ARG:O	3:E:218:THR:HG23	1.89	0.72
1:A:406:VAL:HG23	1:A:407:GLU:HA	1.71	0.72
2:B:891:HIS:HA	3:D:242:ARG:HD2	1.71	0.72
2:B:1121:HIS:HD2	2:B:1124:THR:HG22	1.55	0.72
1:A:97:ARG:HH11	1:A:97:ARG:HB2	1.54	0.72
2:B:836:GLN:O	2:B:935:GLN:HB3	1.89	0.72
3:E:53:GLU:HG2	3:E:145:TYR:CE1	2.24	0.72
3:E:253:GLU:OE2	3:E:254:TYR:CZ	2.43	0.72
3:D:282:PHE:O	3:D:286:THR:HG22	1.90	0.72
3:E:139:ASN:C	3:E:139:ASN:OD1	2.33	0.72
2:B:1263:TYR:CG	2:B:1295:HIS:CD2	2.78	0.71
3:D:265:ARG:HA	3:D:265:ARG:NE	2.05	0.71
1:A:406:VAL:CG2	1:A:408:PRO:HD3	2.21	0.71
3:D:156:VAL:HG23	3:D:228:LEU:HD21	1.71	0.71
2:C:440:ILE:HD12	2:C:478:ILE:HG21	1.72	0.71
2:B:137:ILE:HD11	2:C:759:ASP:OD1	1.91	0.71
2:C:628:SER:O	2:C:1037:ILE:HD11	1.90	0.71
1:A:420:VAL:HG12	1:A:970:ARG:HG3	1.71	0.71
2:C:449:PHE:HB2	2:C:683:TRP:CD1	2.26	0.71
2:C:898:GLN:OE1	3:D:3:GLN:NE2	2.24	0.70
1:A:648:VAL:HG22	1:A:649:LYS:H	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:954:GLN:CG	3:D:240:VAL:CG1	2.63	0.70
3:D:47:LYS:HG3	3:D:48:THR:H	1.57	0.69
3:E:69:GLU:C	3:E:69:GLU:OE1	2.35	0.69
1:A:963:TYR:HE2	1:A:978:LYS:HB3	1.57	0.69
3:D:85:ASN:C	3:D:85:ASN:HD22	2.00	0.69
1:A:764:SER:HA	1:A:795:GLU:HG3	1.74	0.69
1:A:887:ILE:HG22	1:A:888:GLU:H	1.56	0.69
2:C:270:THR:HG22	2:C:291:HIS:HA	1.74	0.69
2:C:528:ILE:O	2:C:528:ILE:HG22	1.90	0.69
1:A:925:ILE:HD13	1:A:937:ARG:HH12	1.56	0.69
1:A:928:GLU:HG3	1:A:929:PRO:HD2	1.73	0.69
2:C:376:ILE:HD11	2:C:1317:VAL:HG21	1.75	0.69
2:C:963:ALA:HB3	2:C:1059:LEU:HD21	1.75	0.69
3:E:46:LYS:HD3	3:E:155:HIS:HE1	0.56	0.69
3:E:253:GLU:HG3	3:E:254:TYR:CD2	2.28	0.69
1:A:19:PRO:O	1:A:22:ILE:HG22	1.93	0.69
2:B:1271:SER:OG	3:D:195:ASN:OD1	2.11	0.69
1:A:842:TYR:HA	1:A:845:ILE:HG22	1.74	0.69
3:D:22:ASP:C	3:D:22:ASP:OD1	2.36	0.68
1:A:406:VAL:HB	1:A:407:GLU:C	2.17	0.68
3:D:244:VAL:HG12	3:D:245:THR:H	1.57	0.68
2:C:1166:VAL:HG12	2:C:1167:ASP:H	1.57	0.68
3:E:35:LEU:HB3	3:E:179:PHE:HB3	1.75	0.68
1:A:23:ARG:O	1:A:28:PRO:HD2	1.93	0.68
1:A:658:ILE:HD11	1:A:692:ILE:HD11	1.75	0.68
2:B:1272:ARG:NH1	3:D:69:GLU:OE1	2.27	0.68
1:A:713:ASN:HA	1:A:716:MET:HB2	1.74	0.68
2:B:368:ALA:CA	3:D:83:ASN:HD22	2.06	0.68
2:B:737:PRO:HA	2:B:861:GLU:HG2	1.75	0.68
2:B:1306:THR:HG23	2:B:1308:ASN:H	1.59	0.68
3:D:55:HIS:ND1	3:D:55:HIS:C	2.50	0.68
2:B:486:VAL:HG21	2:B:709:MET:HB3	1.76	0.68
2:C:146:GLU:O	2:C:1316:ALA:HA	1.93	0.68
1:A:926:MET:HG3	1:A:928:GLU:H	1.57	0.68
1:A:1034:ARG:HA	1:A:1034:ARG:NE	2.09	0.68
2:C:540:PHE:HB3	2:C:600:ILE:HD11	1.75	0.68
1:A:73:ARG:O	1:A:75:PRO:HD3	1.94	0.67
1:A:377:LEU:HD12	1:A:377:LEU:H	1.59	0.67
1:A:76:LEU:C	1:A:78:TYR:H	2.00	0.67
1:A:659:ASN:HD21	1:A:706:TYR:H	1.40	0.67
2:C:853:ASP:HB2	3:D:117:ILE:CD1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:733:VAL:HG21	2:B:741:TYR:HD1	1.59	0.67
2:B:1051:ARG:HG2	2:B:1054:ARG:HH12	1.58	0.67
3:D:78:GLY:O	3:D:269:ILE:HD11	1.95	0.67
3:E:56:LEU:H	3:E:56:LEU:CD2	2.08	0.67
3:E:153:TYR:HD1	3:E:156:VAL:HG21	1.59	0.67
3:E:162:GLY:HA2	3:E:172:MET:CE	2.24	0.67
2:C:1072:ASP:O	2:C:1234:GLN:NE2	2.28	0.67
2:C:1042:TRP:CD1	2:C:1043:SER:HA	2.30	0.67
3:E:68:ILE:CD1	3:E:72:ILE:HD12	2.24	0.67
2:B:1289:PRO:HD2	3:D:20:ARG:CD	2.25	0.67
2:C:841:ASP:N	2:C:940:ARG:HH12	1.93	0.67
1:A:238:ASP:OD2	1:A:259:ARG:HG3	1.95	0.66
1:A:962:PHE:CG	1:A:963:TYR:N	2.64	0.66
2:C:1076:ILE:HG23	2:C:1166:VAL:HB	1.77	0.66
3:E:261:ARG:NH1	3:E:265:ARG:NH2	2.39	0.66
1:A:523:MET:HG3	1:A:524:HIS:H	1.59	0.66
1:A:203:THR:H	2:B:629:ARG:HG2	1.61	0.66
2:C:853:ASP:HB2	3:D:117:ILE:HG13	1.78	0.66
2:C:879:THR:O	2:C:883:ILE:HG12	1.94	0.66
3:D:239:VAL:HG12	3:D:250:ARG:HH12	1.61	0.66
2:B:954:GLN:NE2	3:D:240:VAL:HG13	2.10	0.66
3:D:21:ASN:O	3:D:22:ASP:CG	2.39	0.66
2:B:1180:PRO:HA	2:B:1207:MET:HE1	1.78	0.66
3:D:178:LYS:O	3:D:178:LYS:HG3	1.96	0.66
2:C:414:LEU:HB2	2:C:1045:TYR:HE2	1.61	0.66
2:C:910:LEU:HD13	2:C:915:VAL:HG23	1.77	0.65
3:D:100:ASN:H	3:D:100:ASN:ND2	1.94	0.65
3:E:221:ARG:HH11	3:E:225:ARG:HD2	1.60	0.65
1:A:512:ALA:HB3	1:A:513:PRO:CA	2.16	0.65
2:C:450:PRO:C	2:C:452:ASN:N	2.53	0.65
2:C:902:ILE:HB	2:C:929:PHE:HB3	1.78	0.65
1:A:1039:GLY:O	1:A:1043:LEU:HB2	1.96	0.65
2:B:368:ALA:HA	3:D:83:ASN:HD22	1.61	0.65
3:E:247:ARG:HE	3:E:247:ARG:HA	1.62	0.65
3:E:69:GLU:OE1	3:E:70:ASP:N	2.30	0.65
3:E:12:LEU:O	3:E:14:GLN:NE2	2.30	0.65
3:E:56:LEU:HD23	3:E:56:LEU:N	2.11	0.65
2:B:956:ASP:OD2	3:D:266:THR:CG2	2.44	0.65
1:A:484:THR:HB	1:A:511:ILE:HG21	1.76	0.65
2:C:837:THR:HA	2:C:936:MET:HG3	1.77	0.65
2:B:1060:ARG:HH12	2:B:1292:GLU:HA	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:134:TYR:OH	3:E:286:THR:HG22	1.97	0.65
3:E:53:GLU:N	3:E:53:GLU:OE2	2.30	0.65
2:B:956:ASP:OD2	3:D:266:THR:HG23	1.96	0.64
2:C:309:TRP:CD1	2:C:1253:ARG:HB3	2.32	0.64
3:D:153:TYR:CA	3:D:156:VAL:CG1	2.72	0.64
2:C:523:THR:O	2:C:524:GLU:HB3	1.95	0.64
3:E:195:ASN:OD1	3:E:195:ASN:N	2.30	0.64
1:A:93:HIS:HE1	1:A:97:ARG:HH12	1.45	0.64
1:A:555:ASP:HA	1:A:583:ARG:HH22	1.61	0.64
3:D:144:ARG:HD2	3:D:144:ARG:O	1.98	0.64
1:A:559:ILE:HG22	1:A:613:ILE:HG12	1.79	0.64
1:A:963:TYR:HE2	1:A:978:LYS:CB	2.10	0.64
2:C:373:ASP:HB2	2:C:394:GLN:HG3	1.79	0.64
3:E:284:GLN:O	3:E:288:THR:HG22	1.96	0.64
1:A:416:MET:HE1	1:A:470:LEU:HD21	1.79	0.64
2:B:269:GLU:HB3	2:B:292:ASN:HD22	1.61	0.64
2:B:274:MET:HG3	2:C:234:PRO:HD3	0.66	0.64
3:E:68:ILE:CD1	3:E:69:GLU:N	2.59	0.64
2:B:1106:PHE:HB3	2:B:1151:VAL:HG21	1.79	0.64
2:C:291:HIS:CD2	2:C:346:HIS:CD2	2.86	0.64
3:D:143:PRO:O	3:D:144:ARG:HB3	1.96	0.64
2:C:449:PHE:N	2:C:450:PRO:CD	2.61	0.64
3:D:82:GLN:HA	3:D:82:GLN:OE1	1.98	0.64
2:B:1273:ASN:OD1	3:D:79:ILE:HG21	1.89	0.64
3:E:262:THR:O	3:E:263:ALA:C	2.41	0.64
2:B:271:THR:HG21	2:C:237:VAL:HG21	1.72	0.63
2:C:1042:TRP:HB3	2:C:1043:SER:HB2	1.79	0.63
3:D:153:TYR:C	3:D:156:VAL:HG12	2.22	0.63
3:E:137:LEU:HD23	3:E:138:GLY:N	2.13	0.63
1:A:470:LEU:HB3	1:A:497:ALA:HB1	1.81	0.63
2:C:440:ILE:HD11	2:C:770:CYS:HB2	1.80	0.63
2:C:878:SER:CB	2:C:903:ASN:CB	2.76	0.63
2:C:931:ASN:ND2	2:C:934:LEU:O	2.29	0.63
3:E:55:HIS:CD2	3:E:145:TYR:HE2	2.15	0.63
3:E:55:HIS:O	3:E:55:HIS:ND1	2.30	0.63
1:A:426:ARG:HG3	1:A:428:ILE:H	1.62	0.63
2:B:271:THR:HG23	2:C:237:VAL:CG2	2.01	0.63
2:B:279:SER:OG	2:C:1198:LYS:CE	2.46	0.63
2:B:924:ASP:HA	2:B:938:ASN:ND2	2.14	0.63
3:D:100:ASN:HD22	3:D:100:ASN:N	1.92	0.63
2:B:147:VAL:HG22	2:B:1315:MET:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:856:LEU:HD11	3:D:117:ILE:HD12	1.81	0.63
1:A:926:MET:HB3	1:A:931:GLY:H	1.64	0.63
2:C:528:ILE:CD1	2:C:758:ILE:HD12	2.25	0.63
3:D:41:GLU:OE1	3:D:41:GLU:N	2.30	0.63
3:E:85:ASN:CG	3:E:85:ASN:O	2.41	0.63
2:B:489:MET:HE1	2:B:492:VAL:HA	1.81	0.63
2:B:954:GLN:NE2	3:D:240:VAL:CG1	2.61	0.63
2:B:1273:ASN:CB	3:D:194:VAL:HG11	2.28	0.63
3:D:242:ARG:HH11	3:D:242:ARG:CG	2.11	0.63
1:A:194:HIS:CD2	3:D:146:ARG:HH11	2.13	0.63
3:D:253:GLU:CD	3:D:254:TYR:CD2	2.76	0.63
2:C:1153:ASP:HA	2:C:1156:ILE:HG22	1.81	0.63
3:E:234:ALA:O	3:E:263:ALA:HB2	1.98	0.63
3:E:12:LEU:O	3:E:13:GLU:HB3	1.98	0.62
2:B:368:ALA:CA	3:D:83:ASN:ND2	2.61	0.62
2:B:635:ILE:HG22	2:B:706:TYR:HB3	1.81	0.62
3:D:35:LEU:HD23	3:D:179:PHE:HB3	1.81	0.62
3:E:77:PHE:CE1	3:E:227:MET:HB2	2.34	0.62
1:A:846:ARG:HA	1:A:849:ILE:HD11	1.80	0.62
2:B:950:ASP:O	3:D:243:LYS:CE	2.46	0.62
2:C:148:GLN:HE21	2:C:379:LEU:HD11	1.63	0.62
1:A:904:PHE:HE2	1:A:906:PHE:CB	2.02	0.62
3:D:237:ALA:HB3	3:D:253:GLU:HG2	1.81	0.62
1:A:845:ILE:O	1:A:849:ILE:HG12	1.99	0.62
2:B:838:GLU:O	2:B:935:GLN:HG3	2.00	0.62
2:C:853:ASP:HB2	3:D:117:ILE:HD11	1.80	0.62
2:B:388:GLN:OE1	2:C:499:ALA:CB	2.41	0.62
2:C:231:LEU:CB	2:C:249:SER:HB2	2.30	0.62
2:C:864:HIS:NE2	2:C:1030:ARG:CZ	2.62	0.62
2:B:271:THR:HG23	2:C:237:VAL:N	2.14	0.62
3:D:85:ASN:C	3:D:85:ASN:ND2	2.55	0.62
2:B:148:GLN:O	2:B:375:ARG:HD3	2.00	0.62
2:C:1037:ILE:HG22	2:C:1038:GLU:N	2.09	0.62
3:E:209:GLU:O	3:E:213:LEU:HB2	2.00	0.62
1:A:155:VAL:O	2:C:548:TYR:HE1	1.83	0.61
3:E:235:VAL:HG13	3:E:258:ASN:ND2	2.14	0.61
3:E:1:MET:O	3:E:2:LEU:HB2	2.00	0.61
3:E:42:ASN:CB	3:E:174:VAL:HB	2.29	0.61
1:A:648:VAL:CG2	1:A:649:LYS:H	2.13	0.61
2:C:112:THR:HG22	2:C:134:THR:HB	1.82	0.61
2:C:1042:TRP:CB	2:C:1043:SER:HA	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:VAL:HG11	1:A:1034:ARG:HD2	1.83	0.61
3:D:107:LEU:O	3:D:108:ASP:OD2	2.17	0.61
3:E:66:VAL:HG23	3:E:89:TYR:CD2	2.36	0.61
3:E:85:ASN:HD22	3:E:141:SER:HB3	1.65	0.61
2:C:1240:ARG:HD3	2:C:1258:VAL:HG21	1.81	0.61
1:A:731:HIS:HB2	1:A:746:PHE:HB3	1.82	0.61
2:C:539:PHE:O	2:C:543:TRP:HB3	2.00	0.61
2:B:629:ARG:HD2	2:B:1034:GLN:O	2.01	0.61
2:B:956:ASP:CG	3:D:266:THR:CG2	2.73	0.61
2:C:841:ASP:CG	2:C:842:ASP:N	2.59	0.61
2:C:853:ASP:HB2	3:D:117:ILE:CG1	2.31	0.61
2:B:935:GLN:HG2	2:B:940:ARG:NE	2.16	0.61
2:C:494:GLU:O	2:C:757:ILE:HA	2.00	0.61
3:D:148:ASP:OD1	3:D:148:ASP:N	2.34	0.61
3:E:40:THR:CG2	3:E:41:GLU:N	2.63	0.61
3:E:46:LYS:HD2	3:E:155:HIS:CE1	2.34	0.61
1:A:648:VAL:CG2	1:A:649:LYS:N	2.63	0.60
1:A:866:LEU:O	1:A:867:ALA:HB3	2.01	0.60
3:E:55:HIS:CD2	3:E:145:TYR:CZ	2.84	0.60
2:C:302:ARG:HG3	2:C:303:ASP:OD1	2.01	0.60
2:C:1323:ASP:CG	2:C:1324:ASP:H	2.08	0.60
3:E:40:THR:HG22	3:E:41:GLU:N	2.15	0.60
1:A:892:GLN:C	1:A:894:LYS:H	2.09	0.60
2:B:1288:ILE:HD12	3:D:20:ARG:HH22	1.66	0.60
2:C:853:ASP:O	3:D:117:ILE:HD11	2.00	0.60
1:A:659:ASN:ND2	1:A:706:TYR:H	1.97	0.60
2:C:540:PHE:O	2:C:548:TYR:HB2	2.00	0.60
2:C:1288:ILE:HG13	2:C:1293:VAL:HG21	1.83	0.60
3:D:217:LYS:CE	3:D:290:TRP:CE3	2.85	0.60
2:C:397:LEU:CD1	3:E:265:ARG:HB3	2.31	0.60
3:D:37:TYR:HD1	3:D:177:ALA:HB2	1.66	0.60
3:E:85:ASN:ND2	3:E:141:SER:CB	2.63	0.60
1:A:379:VAL:HG13	1:A:791:ARG:HH21	1.67	0.60
1:A:393:LEU:HD13	1:A:748:GLY:HA3	1.83	0.60
1:A:561:LEU:HD22	1:A:587:MET:HB2	1.83	0.60
1:A:749:CYS:HA	1:A:782:ASN:HA	1.84	0.60
2:B:1214:GLU:HB2	2:B:1215:PRO:HD2	1.84	0.60
2:B:1273:ASN:HD21	3:D:79:ILE:HG21	1.67	0.60
3:E:85:ASN:C	3:E:85:ASN:OD1	2.44	0.60
3:E:85:ASN:HD21	3:E:141:SER:CB	2.14	0.60
2:B:1274:GLY:HA2	3:D:191:ARG:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:209:GLU:HG3	3:E:210:GLY:H	1.66	0.60
1:A:717:THR:HG21	1:A:1020:SER:CB	2.31	0.60
2:B:1181:SER:O	2:B:1182:GLU:HB3	2.00	0.60
2:C:112:THR:HG22	2:C:134:THR:CB	2.32	0.60
3:D:242:ARG:HH11	3:D:242:ARG:HG2	1.66	0.60
2:B:148:GLN:C	2:B:150:LEU:H	2.09	0.59
2:B:614:ARG:O	2:B:633:THR:HG22	2.02	0.59
1:A:49:HIS:HB3	1:A:76:LEU:HD11	1.83	0.59
1:A:796:PHE:O	1:A:874:LEU:HD12	2.01	0.59
2:B:1273:ASN:HD22	3:D:191:ARG:CA	2.01	0.59
2:C:230:ASP:HB3	2:C:985:ARG:HE	1.67	0.59
2:C:522:PRO:HG3	2:C:636:PRO:HB2	1.84	0.59
1:A:566:GLU:OE2	1:A:569:VAL:HG12	2.01	0.59
1:A:597:ARG:HG3	1:A:597:ARG:NH1	2.17	0.59
2:B:1273:ASN:HD21	3:D:191:ARG:CA	2.08	0.59
3:D:224:PHE:O	3:D:228:LEU:HB2	2.02	0.59
1:A:42:PHE:HA	1:A:49:HIS:HA	1.85	0.59
1:A:96:MET:O	1:A:99:VAL:HG12	2.03	0.59
2:B:547:GLU:HB2	2:B:597:ALA:HB2	1.83	0.59
2:C:1042:TRP:HB3	2:C:1043:SER:CA	2.32	0.59
2:B:604:MET:C	2:B:606:LEU:H	2.10	0.59
2:B:1079:LEU:HD12	2:B:1090:PRO:HB3	1.83	0.59
3:D:5:PRO:O	3:D:6:THR:CB	2.50	0.59
3:D:47:LYS:HG3	3:D:48:THR:N	2.18	0.59
1:A:880:VAL:HB	1:A:899:VAL:HG12	1.83	0.59
2:C:448:TYR:HA	2:C:768:CYS:SG	2.43	0.59
1:A:560:LEU:HD23	1:A:614:ILE:HB	1.85	0.59
2:B:954:GLN:HG2	3:D:240:VAL:CG1	2.29	0.59
2:C:838:GLU:CB	2:C:934:LEU:HB2	2.33	0.59
3:E:13:GLU:CD	3:E:13:GLU:C	2.71	0.59
3:E:67:TYR:HB3	3:E:70:ASP:HB3	1.85	0.59
1:A:35:GLY:H	1:A:38:TYR:HE1	1.51	0.59
2:C:1045:TYR:O	2:C:1046:PHE:CD1	2.56	0.59
2:B:338:ARG:NH2	2:C:1002:LEU:HD21	2.18	0.59
2:C:1234:GLN:HB2	2:C:1235:PRO:C	2.28	0.59
3:D:290:TRP:HE3	3:D:290:TRP:C	2.11	0.59
2:C:449:PHE:H	2:C:450:PRO:HD3	1.68	0.58
2:C:1054:ARG:HG2	2:C:1054:ARG:HH11	1.68	0.58
3:D:25:ASN:C	3:D:25:ASN:OD1	2.45	0.58
3:E:153:TYR:CD1	3:E:156:VAL:HG21	2.37	0.58
3:E:14:GLN:N	3:E:14:GLN:CD	2.61	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:68:ILE:CD1	3:E:72:ILE:CD1	2.77	0.58
1:A:569:VAL:HG22	1:A:584:ILE:HG22	1.85	0.58
2:B:459:ALA:HB2	2:B:679:CYS:HB3	1.85	0.58
3:D:217:LYS:HE2	3:D:290:TRP:CE3	2.38	0.58
1:A:70:PRO:HA	1:A:73:ARG:HB3	1.85	0.58
1:A:409:MET:HE3	1:A:411:ILE:HD12	1.86	0.58
3:D:77:PHE:CZ	3:D:227:MET:HB2	2.39	0.58
1:A:820:VAL:HG12	1:A:821:ARG:H	1.69	0.58
2:B:191:GLY:HA2	2:B:193:THR:N	2.19	0.58
3:E:1:MET:HE1	3:E:121:PHE:HE2	1.57	0.58
1:A:49:HIS:NE2	1:A:172:PHE:CD1	2.63	0.58
1:A:407:GLU:OE1	1:A:1034:ARG:HB3	2.04	0.58
2:B:205:ASN:HB2	2:B:1239:ALA:HB1	1.85	0.58
2:C:469:ARG:HH12	2:C:498:ILE:HD13	1.69	0.58
3:E:113:ASN:O	3:E:114:SER:OG	2.16	0.58
1:A:730:ILE:HG22	1:A:731:HIS:N	2.18	0.58
2:C:356:SER:O	2:C:360:ILE:HG12	2.04	0.58
3:D:217:LYS:CE	3:D:290:TRP:CZ3	2.87	0.58
1:A:934:THR:HG23	1:A:935:PRO:HD3	1.86	0.58
2:B:179:LYS:HG3	2:B:181:ARG:HE	1.68	0.58
2:B:835:TYR:CZ	2:B:925:VAL:HG21	2.39	0.58
1:A:228:ILE:CD1	2:B:563:ALA:HB1	2.32	0.57
2:B:924:ASP:HA	2:B:938:ASN:HD21	1.68	0.57
3:E:205:LEU:O	3:E:205:LEU:CD1	2.39	0.57
1:A:27:LYS:HB3	1:A:28:PRO:CD	2.31	0.57
2:B:817:ASP:HA	2:B:983:ILE:HG21	1.86	0.57
2:B:935:GLN:HG2	2:B:940:ARG:CZ	2.34	0.57
2:C:297:ASN:HD22	2:C:298:PRO:HD2	1.68	0.57
1:A:894:LYS:C	1:A:896:ASN:H	2.12	0.57
2:C:878:SER:CB	2:C:903:ASN:HB2	2.23	0.57
2:C:1072:ASP:H	2:C:1234:GLN:NE2	2.02	0.57
2:B:1274:GLY:HA3	3:D:191:ARG:HG3	1.87	0.57
1:A:28:PRO:C	1:A:30:THR:H	2.11	0.57
2:C:741:TYR:OH	2:C:1022:ILE:HD11	2.05	0.57
2:C:1272:ARG:HD2	3:E:247:ARG:HH22	1.69	0.57
2:B:1242:MET:HG3	2:B:1245:ILE:HD11	1.87	0.57
2:C:434:VAL:HG22	2:C:709:MET:HE1	1.87	0.57
2:B:143:VAL:HG12	2:B:1316:ALA:HB1	1.86	0.57
2:C:874:ILE:HG21	2:C:897:TYR:HD1	1.70	0.57
2:C:1273:ASN:O	3:E:183:GLU:CD	2.45	0.57
3:D:144:ARG:O	3:D:144:ARG:CD	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:543:TRP:HD1	2:C:544:TYR:HD1	1.53	0.57
2:B:137:ILE:HD12	2:C:759:ASP:OD1	2.04	0.56
2:C:109:LYS:HZ2	2:C:109:LYS:HB3	1.70	0.56
2:C:129:ALA:O	2:C:130:LEU:HB2	2.03	0.56
2:C:385:ILE:O	2:C:386:SER:HB3	2.04	0.56
2:C:565:GLU:CG	2:C:566:PHE:N	2.66	0.56
2:C:1079:LEU:HD23	2:C:1081:ASP:OD2	2.05	0.56
1:A:159:ILE:CD1	2:B:1333:ALA:OXT	2.51	0.56
2:B:817:ASP:HA	2:B:983:ILE:CG2	2.35	0.56
2:B:956:ASP:OD1	3:D:266:THR:CB	2.52	0.56
2:B:1288:ILE:CD1	3:D:20:ARG:NH2	2.66	0.56
2:B:148:GLN:O	2:B:150:LEU:N	2.39	0.56
2:B:902:ILE:HD11	2:B:929:PHE:HE1	1.70	0.56
2:B:1263:TYR:CD1	2:B:1295:HIS:CD2	2.93	0.56
2:C:1033:ASP:O	2:C:1034:GLN:HB2	2.06	0.56
2:C:1322:PRO:O	2:C:1323:ASP:CB	2.53	0.56
2:B:350:ILE:HG22	2:B:351:ASP:N	2.14	0.56
2:C:1072:ASP:N	2:C:1234:GLN:NE2	2.53	0.56
3:E:53:GLU:HB2	3:E:145:TYR:HE1	1.69	0.56
2:B:1273:ASN:ND2	3:D:79:ILE:HG21	2.21	0.56
2:C:1042:TRP:HB3	2:C:1043:SER:CB	2.35	0.56
2:C:141:LEU:HD23	2:C:141:LEU:H	1.71	0.56
2:C:1250:GLU:OE1	2:C:1250:GLU:HA	2.05	0.56
3:D:239:VAL:HG23	3:D:263:ALA:HB1	1.87	0.56
3:E:44:LEU:HD13	3:E:172:MET:O	2.05	0.56
1:A:238:ASP:HB2	1:A:258:GLN:HB2	1.88	0.56
3:E:108:ASP:OD2	3:E:108:ASP:N	2.30	0.56
3:E:235:VAL:CG1	3:E:258:ASN:HA	2.35	0.56
1:A:686:TYR:HD2	1:A:686:TYR:O	1.89	0.56
2:B:1289:PRO:CD	3:D:20:ARG:HD2	2.36	0.56
2:C:261:ASP:O	2:C:1054:ARG:NH1	2.39	0.56
2:C:291:HIS:HD2	2:C:346:HIS:HD2	1.49	0.56
3:E:142:THR:HG23	3:E:143:PRO:HD2	1.87	0.56
1:A:484:THR:O	1:A:485:MET:HG3	2.05	0.56
1:A:986:ARG:HB3	1:A:994:PRO:CB	2.29	0.56
2:B:709:MET:HA	2:B:712:PHE:HD2	1.70	0.56
2:C:407:HIS:CD2	2:C:1047:LEU:HA	2.40	0.56
2:C:833:ARG:HB2	2:C:942:HIS:HB2	1.88	0.56
2:C:1288:ILE:HD13	2:C:1288:ILE:H	1.69	0.56
2:C:1322:PRO:O	2:C:1323:ASP:CG	2.48	0.56
3:E:290:TRP:CD1	3:E:290:TRP:C	2.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ILE:HG12	1:A:25:ILE:HD11	1.86	0.56
3:E:163:THR:H	3:E:172:MET:HE1	1.71	0.56
1:A:407:GLU:HG3	1:A:829:MET:O	2.05	0.55
1:A:919:TYR:HB2	1:A:955:ASN:HB3	1.86	0.55
2:B:494:GLU:HG2	2:B:577:GLN:HG3	1.87	0.55
3:E:150:ILE:O	3:E:150:ILE:CG2	2.54	0.55
3:E:81:ALA:H	3:E:275:ARG:HH21	1.54	0.55
3:D:153:TYR:C	3:D:156:VAL:CG1	2.79	0.55
2:B:709:MET:HA	2:B:712:PHE:CD2	2.42	0.55
3:E:49:ILE:CG2	3:E:50:PRO:CD	2.84	0.55
2:B:895:VAL:HG22	2:B:915:VAL:HG22	1.88	0.55
2:C:185:ALA:HB3	2:C:277:THR:O	2.07	0.55
3:E:209:GLU:O	3:E:213:LEU:CB	2.55	0.55
3:E:284:GLN:O	3:E:288:THR:CG2	2.54	0.55
2:C:337:VAL:CG2	3:E:187:ILE:CD1	2.62	0.55
2:C:734:ILE:HG23	2:C:1017:ALA:HB1	1.88	0.55
2:C:864:HIS:CE1	2:C:1030:ARG:HH21	2.18	0.55
3:D:290:TRP:CE3	3:D:290:TRP:C	2.85	0.55
2:B:1274:GLY:HA3	3:D:191:ARG:CG	2.36	0.55
1:A:849:ILE:HD12	1:A:872:VAL:HG12	1.89	0.55
2:B:134:THR:CG2	2:C:472:GLU:CD	2.79	0.55
2:B:1048:ASP:HB3	2:B:1051:ARG:HB2	1.87	0.55
1:A:180:ASN:CG	1:A:222:ARG:HH22	2.15	0.55
2:B:144:ASN:HB2	2:B:1318:GLU:HA	1.88	0.55
2:B:926:VAL:HG12	2:B:926:VAL:O	2.07	0.55
1:A:63:SER:HB3	1:A:123:SER:HA	1.87	0.55
1:A:913:LEU:HB2	1:A:950:MET:HE2	1.89	0.55
2:B:612:PHE:CZ	2:B:1331:ARG:HD2	2.42	0.55
2:C:1074:VAL:HG12	2:C:1171:ILE:HG21	1.88	0.55
3:E:1:MET:O	3:E:121:PHE:O	2.24	0.55
1:A:967:ILE:HG23	1:A:968:ILE:H	1.72	0.54
2:B:960:THR:HG23	2:B:965:ARG:NH1	2.19	0.54
3:D:291:ASN:OD1	3:D:291:ASN:C	2.50	0.54
2:B:147:VAL:HG12	2:B:379:LEU:HD22	1.89	0.54
3:E:107:LEU:HD23	3:E:122:TYR:HE1	1.70	0.54
2:C:407:HIS:CE1	2:C:1047:LEU:HD12	2.42	0.54
3:E:1:MET:O	3:E:2:LEU:CB	2.55	0.54
3:E:285:LEU:O	3:E:288:THR:HG23	2.08	0.54
1:A:484:THR:CB	1:A:511:ILE:HG21	2.37	0.54
2:C:390:HIS:O	2:C:1317:VAL:HG23	2.08	0.54
1:A:146:PRO:O	1:A:147:GLN:HB3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:ALA:N	1:A:756:PRO:HD2	2.22	0.54
1:A:963:TYR:CE2	1:A:978:LYS:HB3	2.41	0.54
2:C:1181:SER:O	2:C:1182:GLU:HB3	2.07	0.54
3:E:253:GLU:O	3:E:254:TYR:CD1	2.61	0.54
1:A:409:MET:HG2	1:A:465:LEU:HD22	1.90	0.54
1:A:628:MET:HE3	1:A:657:MET:HE3	1.89	0.54
2:B:255:LEU:HD12	2:B:1062:ILE:HG21	1.89	0.54
2:B:862:ARG:HH12	2:B:948:ILE:HD13	1.73	0.54
3:E:238:ASN:O	3:E:253:GLU:HB2	2.06	0.54
2:B:1273:ASN:CG	3:D:79:ILE:HG21	2.32	0.54
2:C:793:TYR:OH	2:C:1323:ASP:O	2.15	0.54
3:E:229:PHE:CE1	3:E:252:LEU:CD1	2.90	0.54
1:A:383:THR:HG21	1:A:805:TYR:HB3	1.88	0.54
1:A:194:HIS:CD2	3:D:146:ARG:HH12	2.19	0.54
1:A:600:VAL:HG12	1:A:601:PRO:HA	1.88	0.54
2:B:1111:ALA:HB3	2:B:1116:ARG:HD2	1.90	0.54
3:D:172:MET:HE3	3:D:175:LYS:CG	2.35	0.54
3:E:262:THR:HG22	3:E:263:ALA:N	2.22	0.54
1:A:69:HIS:CD2	1:A:71:LEU:H	2.27	0.53
1:A:208:HIS:HB3	1:A:260:LEU:HD23	1.90	0.53
2:B:833:ARG:HG2	2:B:922:TYR:OH	2.07	0.53
2:C:372:ALA:HA	2:C:398:ARG:HD3	1.90	0.53
2:C:1037:ILE:HD13	2:C:1040:PHE:HE1	1.73	0.53
2:C:1126:MET:HG3	2:C:1127:ALA:H	1.73	0.53
1:A:1034:ARG:NH2	1:A:1035:LEU:HB2	2.23	0.53
2:C:547:GLU:HG3	2:C:597:ALA:HA	1.91	0.53
2:C:838:GLU:HA	2:C:940:ARG:CZ	2.38	0.53
2:C:892:VAL:HG13	2:C:894:VAL:H	1.73	0.53
2:B:639:ASN:HB3	2:B:641:ARG:HG3	1.89	0.53
2:B:953:ASP:O	3:D:241:ASN:OD1	2.26	0.53
2:B:1076:ILE:HB	2:B:1166:VAL:HG23	1.91	0.53
3:E:142:THR:HG22	3:E:144:ARG:H	1.73	0.53
1:A:495:LEU:HA	1:A:503:ILE:HD13	1.91	0.53
2:C:469:ARG:HE	2:C:469:ARG:HA	1.73	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
3:E:76:LEU:HD12	3:E:76:LEU:H	1.73	0.53
2:C:148:GLN:NE2	2:C:379:LEU:HD11	2.24	0.53
1:A:38:TYR:HA	1:A:53:LEU:HA	1.89	0.53
1:A:406:VAL:HG21	1:A:826:PHE:CD1	2.44	0.53
1:A:636:VAL:HG22	1:A:648:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1180:PRO:HB3	2:C:1209:GLY:HA2	1.89	0.53
1:A:78:TYR:N	1:A:78:TYR:CD2	2.76	0.53
2:B:884:ALA:O	2:B:888:GLN:HG2	2.08	0.53
2:C:384:MET:HA	2:C:708:THR:HG21	1.91	0.53
2:C:822:MET:HG3	2:C:1044:ARG:HD2	1.90	0.53
3:D:115:GLU:OE2	3:D:115:GLU:N	2.30	0.53
3:E:214:ARG:O	3:E:218:THR:CG2	2.57	0.53
1:A:195:ILE:O	1:A:199:MET:HB2	2.08	0.53
2:B:368:ALA:C	3:D:83:ASN:HB2	2.33	0.53
2:C:385:ILE:O	2:C:386:SER:CB	2.57	0.53
1:A:23:ARG:HH21	1:A:27:LYS:HB3	1.73	0.53
1:A:228:ILE:HD12	2:B:563:ALA:CB	2.38	0.53
2:B:234:PRO:HD2	2:B:242:GLU:CB	2.39	0.53
2:B:1289:PRO:CD	3:D:20:ARG:CD	2.87	0.53
2:C:565:GLU:CG	2:C:566:PHE:H	2.18	0.53
1:A:853:GLU:CD	1:A:854:ASN:H	2.17	0.53
2:B:232:LEU:HD22	2:B:974:LEU:HD21	1.91	0.53
2:B:1044:ARG:CZ	3:D:266:THR:HG23	2.37	0.53
3:D:111:ILE:O	3:D:111:ILE:HG23	2.07	0.53
3:D:189:LEU:HB3	3:D:230:ILE:HD11	1.91	0.53
3:D:242:ARG:HG2	3:D:242:ARG:NH1	2.23	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:282:GLU:HB2	1:A:363:ASN:HB2	1.90	0.52
2:B:180:LEU:HB3	2:B:195:ASN:HD21	1.74	0.52
2:C:1042:TRP:CB	2:C:1043:SER:CA	2.87	0.52
1:A:204:LEU:HA	1:A:264:SER:O	2.09	0.52
2:B:1103:HIS:H	2:B:1103:HIS:CD2	2.26	0.52
2:B:1118:THR:HG22	2:B:1129:PRO:HA	1.90	0.52
2:C:1293:VAL:O	2:C:1294:ASP:HB2	2.08	0.52
1:A:213:TRP:O	1:A:215:VAL:N	2.41	0.52
2:B:142:ASP:HB3	2:B:1318:GLU:HG2	1.91	0.52
2:C:154:PHE:HA	2:C:262:ASN:HD22	1.74	0.52
2:C:524:GLU:OE1	2:C:758:ILE:HG21	2.09	0.52
2:C:1027:THR:HG22	3:D:102:SER:OG	2.09	0.52
2:B:980:ARG:HH22	2:B:1011:SER:HA	1.74	0.52
2:C:828:ASP:O	2:C:948:ILE:HA	2.09	0.52
3:D:172:MET:CE	3:D:175:LYS:HG3	2.33	0.52
3:E:1:MET:CE	3:E:121:PHE:CD2	2.85	0.52
1:A:55:GLY:N	1:A:58:GLN:HG2	2.20	0.52
2:B:281:VAL:CG1	2:B:302:ARG:HD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1264:GLU:HA	2:C:1297:SER:HA	1.91	0.52
1:A:406:VAL:CG2	1:A:826:PHE:CD1	2.92	0.52
2:C:306:GLN:HE21	2:C:306:GLN:N	2.08	0.52
3:D:156:VAL:HG23	3:D:228:LEU:HD23	1.88	0.52
1:A:450:SER:H	1:A:718:ALA:HB1	1.74	0.52
1:A:766:CYS:HB3	1:A:786:ARG:O	2.10	0.52
2:B:546:VAL:HG13	2:B:547:GLU:HG3	1.92	0.52
3:E:166:GLU:CD	3:E:171:VAL:O	2.53	0.52
2:B:1175:ALA:HB2	2:B:1204:LEU:HB2	1.91	0.52
2:C:112:THR:HG22	2:C:134:THR:OG1	2.10	0.52
3:E:74:GLN:O	3:E:78:GLY:HA3	2.10	0.52
1:A:261:ILE:HD11	1:A:326:LEU:HB3	1.91	0.52
1:A:856:THR:H	1:A:916:ASN:HB3	1.74	0.52
2:B:837:THR:O	2:B:838:GLU:HB2	2.09	0.52
3:E:240:VAL:O	3:E:251:VAL:HG22	2.09	0.52
2:B:1087:ASP:OD2	2:B:1235:PRO:HB2	2.09	0.52
3:D:217:LYS:HE2	3:D:290:TRP:CZ3	2.45	0.52
3:E:107:LEU:HD23	3:E:122:TYR:OH	2.09	0.52
1:A:613:ILE:HG13	1:A:643:ALA:HB2	1.93	0.51
1:A:963:TYR:CE2	1:A:967:ILE:HG21	2.45	0.51
2:B:405:HIS:CD2	2:B:623:ASN:HD21	2.27	0.51
3:E:290:TRP:HD1	3:E:291:ASN:HB3	1.75	0.51
1:A:26:THR:HG23	1:A:27:LYS:H	1.76	0.51
1:A:388:VAL:HG22	1:A:389:ALA:H	1.75	0.51
1:A:495:LEU:HD13	1:A:575:PHE:HA	1.90	0.51
2:B:891:HIS:HD2	3:D:240:VAL:CB	2.22	0.51
2:B:1273:ASN:ND2	3:D:79:ILE:CG2	2.73	0.51
2:C:1077:MET:SD	2:C:1079:LEU:HD12	2.50	0.51
1:A:27:LYS:CB	1:A:28:PRO:HD3	2.34	0.51
1:A:756:PRO:HB3	1:A:809:GLN:HA	1.92	0.51
1:A:954:THR:HB	1:A:1056:VAL:HG23	1.92	0.51
2:C:847:ILE:HD12	2:C:936:MET:HE2	1.92	0.51
2:C:1042:TRP:HA	2:C:1042:TRP:CE3	2.45	0.51
2:C:1081:ASP:O	2:C:1082:ASP:HB2	2.11	0.51
2:C:443:VAL:HG22	2:C:444:SER:N	2.20	0.51
3:D:44:LEU:HD11	3:D:154:ALA:CA	2.31	0.51
3:E:53:GLU:HB2	3:E:145:TYR:CE1	2.45	0.51
1:A:925:ILE:HA	1:A:937:ARG:HH22	1.75	0.51
1:A:962:PHE:HB3	1:A:1049:TYR:CD2	2.44	0.51
1:A:986:ARG:CB	1:A:994:PRO:HB3	2.30	0.51
2:B:442:PRO:HG3	2:B:475:ILE:CB	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:528:ILE:HG12	2:B:758:ILE:HG21	1.91	0.51
2:B:649:ALA:HB2	2:B:695:ALA:HB2	1.91	0.51
2:B:685:ARG:HH11	2:B:685:ARG:HA	1.75	0.51
2:C:414:LEU:HB2	2:C:1045:TYR:CE2	2.42	0.51
2:C:1085:ASP:HB3	2:C:1243:ARG:HH22	1.76	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
1:A:1034:ARG:HA	1:A:1034:ARG:HE	1.74	0.51
3:D:214:ARG:O	3:D:218:THR:CG2	2.51	0.51
1:A:62:PHE:HZ	1:A:171:ILE:HD12	1.76	0.51
1:A:422:ASP:HB3	1:A:677:LEU:HD12	1.91	0.51
2:C:815:LEU:N	2:C:816:PRO:HD2	2.26	0.51
2:C:838:GLU:O	2:C:940:ARG:NH1	2.44	0.51
3:E:262:THR:O	3:E:263:ALA:HB3	2.11	0.51
3:E:289:ARG:O	3:E:289:ARG:CD	2.35	0.51
3:E:83:ASN:OD1	3:E:83:ASN:N	2.43	0.51
1:A:925:ILE:HA	1:A:937:ARG:NH2	2.26	0.51
1:A:955:ASN:HD21	1:A:1055:LEU:HB3	1.75	0.51
2:B:847:ILE:HD11	2:B:911:ARG:HE	1.76	0.51
2:C:1131:PRO:HA	2:C:1134:ARG:NH1	2.26	0.51
3:E:12:LEU:HD23	3:E:15:PHE:CZ	2.46	0.51
1:A:561:LEU:HB3	1:A:615:CYS:HA	1.92	0.50
2:C:840:ASP:O	2:C:841:ASP:OD1	2.28	0.50
2:C:855:TYR:HB2	2:C:918:VAL:HG11	1.92	0.50
3:D:21:ASN:O	3:D:24:THR:O	2.29	0.50
3:E:236:ALA:O	3:E:263:ALA:HA	2.10	0.50
1:A:69:HIS:HD2	1:A:71:LEU:H	1.59	0.50
1:A:560:LEU:O	1:A:586:GLY:HA2	2.11	0.50
2:B:824:LEU:C	2:B:826:GLY:H	2.19	0.50
2:B:1023:ARG:HB2	2:B:1024:PRO:CD	2.35	0.50
3:D:289:ARG:HA	3:D:289:ARG:NE	2.24	0.50
2:B:910:LEU:HD23	2:B:915:VAL:HG13	1.92	0.50
2:C:408:ILE:O	2:C:412:LEU:HB2	2.10	0.50
3:D:250:ARG:HB3	3:D:250:ARG:HH11	1.76	0.50
3:E:33:GLN:C	3:E:35:LEU:N	2.69	0.50
3:E:62:VAL:HG23	3:E:63:PRO:HD2	1.93	0.50
3:E:191:ARG:NH1	3:E:191:ARG:CG	2.42	0.50
1:A:13:VAL:HG22	1:A:213:TRP:CD1	2.47	0.50
2:B:134:THR:HG22	2:C:472:GLU:CD	2.36	0.50
2:B:272:THR:HG22	2:B:289:THR:HB	1.93	0.50
2:B:343:ILE:HD11	2:B:366:MET:HE3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:956:ASP:OD1	3:D:266:THR:HG21	2.11	0.50
2:C:841:ASP:H	2:C:940:ARG:HH12	1.58	0.50
3:E:160:LEU:HD11	3:E:229:PHE:CB	2.36	0.50
1:A:643:ALA:HB3	1:A:646:ALA:HB2	1.93	0.50
2:B:956:ASP:CG	3:D:266:THR:HG21	2.35	0.50
2:B:959:GLN:HG3	2:B:964:VAL:HG11	1.94	0.50
2:C:1279:SER:HB3	2:C:1280:PRO:C	2.36	0.50
1:A:28:PRO:C	1:A:30:THR:N	2.67	0.50
1:A:437:GLN:HG3	1:A:655:GLU:OE1	2.12	0.50
2:C:772:TYR:C	2:C:774:LEU:H	2.19	0.50
3:D:107:LEU:HD23	3:D:122:TYR:CE1	2.47	0.50
3:E:41:GLU:O	3:E:41:GLU:OE1	2.30	0.50
1:A:68:GLY:O	1:A:69:HIS:O	2.30	0.50
1:A:265:SER:HB2	1:A:269:VAL:HG21	1.93	0.50
1:A:536:TYR:CG	1:A:572:LEU:HD11	2.46	0.50
2:C:931:ASN:HB2	2:C:936:MET:SD	2.52	0.50
2:C:1174:THR:HG23	2:C:1203:HIS:HB3	1.93	0.50
3:E:10:THR:HG23	3:E:17:PHE:HZ	1.77	0.50
1:A:308:ALA:HB1	1:A:313:ARG:N	2.26	0.50
1:A:959:TYR:HB2	1:A:1051:PRO:HD2	1.93	0.50
2:B:280:THR:HG23	2:B:281:VAL:H	1.76	0.50
2:B:871:PRO:HG3	2:B:894:VAL:HG13	1.93	0.50
2:C:1036:ASP:C	2:C:1037:ILE:HD12	2.37	0.50
2:C:1121:HIS:CD2	2:C:1135:PRO:HD2	2.47	0.50
3:D:15:PHE:N	3:D:15:PHE:CD1	2.80	0.50
3:E:69:GLU:O	3:E:69:GLU:OE2	2.30	0.50
1:A:304:TYR:HD1	1:A:364:TYR:HE2	1.60	0.49
1:A:487:GLN:HG3	1:A:488:GLY:N	2.27	0.49
1:A:505:PHE:CE1	1:A:511:ILE:HG22	2.47	0.49
2:B:772:TYR:HB3	2:B:773:PRO:HD2	1.95	0.49
2:C:204:VAL:CG2	2:C:1242:MET:HG3	2.42	0.49
3:E:53:GLU:CD	3:E:53:GLU:O	2.55	0.49
2:B:1080:THR:HA	2:B:1228:ARG:H	1.77	0.49
3:D:131:ALA:C	3:D:133:THR:H	2.19	0.49
3:D:153:TYR:HA	3:D:156:VAL:HG11	1.86	0.49
3:D:153:TYR:CE2	3:D:258:ASN:ND2	2.80	0.49
1:A:967:ILE:HG23	1:A:968:ILE:N	2.26	0.49
1:A:512:ALA:CB	1:A:513:PRO:CA	2.80	0.49
2:B:360:ILE:HD11	2:B:1057:VAL:HG21	1.94	0.49
2:B:363:ARG:CZ	3:D:80:SER:CB	2.84	0.49
2:B:935:GLN:HA	2:B:940:ARG:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:528:ILE:O	2:C:528:ILE:CG2	2.60	0.49
3:D:172:MET:HG3	3:D:173:PRO:CD	2.42	0.49
3:E:20:ARG:HD2	3:E:25:ASN:HB3	1.94	0.49
1:A:318:ARG:CZ	3:D:43:GLU:HG2	2.43	0.49
2:B:1149:LYS:HG3	2:B:1195:THR:HG21	1.95	0.49
2:C:926:VAL:CG2	2:C:938:ASN:HB2	2.42	0.49
2:B:193:THR:HG23	2:B:297:ASN:H	1.76	0.49
2:C:1272:ARG:HD2	3:E:247:ARG:NH2	2.28	0.49
3:E:84:VAL:HG23	3:E:85:ASN:N	2.28	0.49
3:E:85:ASN:O	3:E:85:ASN:OD1	2.30	0.49
2:B:451:GLU:C	2:B:453:LEU:H	2.19	0.49
2:C:372:ALA:HB1	2:C:1315:MET:HE3	1.94	0.49
3:D:21:ASN:O	3:D:22:ASP:OD1	2.31	0.49
3:D:181:SER:HB2	3:D:185:SER:OG	2.13	0.49
2:B:950:ASP:CG	3:D:243:LYS:HZ3	2.20	0.49
2:C:200:GLY:HA2	2:C:1246:VAL:HG22	1.94	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
2:C:838:GLU:HA	2:C:940:ARG:NE	2.28	0.49
3:D:164:ASP:HA	3:D:167:ARG:HG2	1.94	0.49
3:E:66:VAL:HG13	3:E:111:ILE:CG2	2.42	0.49
1:A:204:LEU:HD13	1:A:221:TYR:HB2	1.95	0.49
1:A:516:GLU:OE1	1:A:516:GLU:HA	2.12	0.49
2:B:389:PHE:CE1	2:B:1319:ARG:HG2	2.48	0.49
2:B:529:LYS:HA	2:B:532:ILE:HG22	1.94	0.49
3:E:12:LEU:HG	3:E:14:GLN:HG2	1.95	0.49
2:B:424:GLY:O	2:B:428:GLN:HB2	2.13	0.48
2:C:231:LEU:HB3	2:C:249:SER:HB2	1.93	0.48
2:C:302:ARG:HD2	2:C:315:THR:HG22	1.95	0.48
3:D:255:ILE:O	3:D:255:ILE:HG13	2.13	0.48
3:E:72:ILE:O	3:E:76:LEU:CD1	2.61	0.48
3:E:139:ASN:OD1	3:E:139:ASN:O	2.30	0.48
1:A:857:GLN:HE22	1:A:917:SER:HA	1.78	0.48
2:B:235:ILE:HG23	2:B:978:GLN:HG2	1.93	0.48
2:C:449:PHE:HE2	2:C:463:VAL:HG22	1.78	0.48
3:E:13:GLU:O	3:E:13:GLU:OE1	2.30	0.48
3:E:38:GLU:HB3	3:E:176:ARG:HB3	1.95	0.48
1:A:724:MET:SD	1:A:725:PRO:HD3	2.53	0.48
1:A:1037:SER:O	1:A:1039:GLY:N	2.46	0.48
2:B:1206:PHE:HE1	2:B:1232:PRO:HG3	1.79	0.48
2:C:841:ASP:O	2:C:842:ASP:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1027:THR:CG2	3:D:102:SER:OG	2.61	0.48
3:D:121:PHE:N	3:D:121:PHE:CD1	2.82	0.48
3:D:185:SER:O	3:D:188:SER:N	2.43	0.48
3:E:162:GLY:HA2	3:E:172:MET:HE2	1.93	0.48
1:A:271:ARG:HG3	1:A:316:TYR:OH	2.12	0.48
2:B:837:THR:O	2:B:838:GLU:CB	2.61	0.48
2:C:268:GLY:O	2:C:269:GLU:HB2	2.11	0.48
1:A:562:GLY:O	1:A:588:GLY:HA3	2.14	0.48
1:A:797:ARG:HH12	1:A:871:VAL:HG11	1.77	0.48
1:A:159:ILE:HD12	2:B:1333:ALA:OXT	2.14	0.48
2:B:147:VAL:HG22	2:B:1315:MET:N	2.28	0.48
2:B:204:VAL:CG2	2:B:1242:MET:HG2	2.44	0.48
2:C:860:ARG:O	2:C:864:HIS:HB2	2.14	0.48
2:C:1037:ILE:CG2	2:C:1038:GLU:H	2.09	0.48
3:E:122:TYR:N	3:E:122:TYR:CD1	2.82	0.48
3:E:226:MET:HE3	3:E:226:MET:HA	1.96	0.48
2:C:1144:ARG:HD2	2:C:1194:MET:HA	1.96	0.48
3:D:166:GLU:OE2	3:D:166:GLU:HA	2.13	0.48
3:E:12:LEU:HG	3:E:14:GLN:NE2	2.18	0.48
3:E:196:TRP:HH2	3:E:226:MET:HG2	1.79	0.48
1:A:51:LEU:O	1:A:171:ILE:HG12	2.13	0.48
2:B:265:VAL:HG12	2:B:1304:MET:HE3	1.95	0.48
2:B:1247:ASN:HD22	2:B:1247:ASN:H	1.61	0.48
3:D:60:ARG:O	3:D:62:VAL:HG23	2.14	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
3:E:191:ARG:HD2	3:E:191:ARG:HA	1.60	0.48
1:A:133:LEU:HD21	2:C:545:PRO:HG3	1.96	0.48
1:A:866:LEU:O	1:A:867:ALA:CB	2.62	0.48
3:D:190:SER:O	3:D:194:VAL:HG23	2.14	0.47
3:E:192:ASP:OD1	3:E:192:ASP:O	2.31	0.47
1:A:254:ASP:O	1:A:255:ARG:HB2	2.13	0.47
2:C:242:GLU:O	2:C:1200:LYS:HG2	2.14	0.47
2:C:1046:PHE:HE2	2:C:1055:LEU:HD22	1.78	0.47
2:C:1159:VAL:HG23	2:C:1164:TRP:O	2.14	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
1:A:124:THR:O	1:A:125:ASN:CB	2.57	0.47
1:A:462:ILE:HA	1:A:465:LEU:HB2	1.96	0.47
2:C:871:PRO:HB2	2:C:896:LEU:HD23	1.96	0.47
3:D:77:PHE:HE1	3:D:227:MET:O	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:LEU:HD21	2:C:545:PRO:CG	2.45	0.47
1:A:1019:PRO:HB2	1:A:1047:ASN:HD21	1.79	0.47
2:B:419:TYR:CE1	2:B:1007:THR:HA	2.49	0.47
1:A:377:LEU:HD23	1:A:759:LEU:O	2.15	0.47
1:A:496:CYS:SG	1:A:497:ALA:N	2.87	0.47
2:B:612:PHE:CE1	2:B:1331:ARG:HD2	2.48	0.47
2:B:893:ALA:HB1	2:B:915:VAL:HA	1.96	0.47
3:D:143:PRO:O	3:D:144:ARG:CB	2.63	0.47
1:A:93:HIS:HE1	1:A:97:ARG:NH1	2.12	0.47
1:A:454:GLY:C	1:A:456:PHE:H	2.23	0.47
2:C:1087:ASP:HB3	2:C:1236:ILE:HG13	1.97	0.47
3:D:244:VAL:HG12	3:D:245:THR:N	2.28	0.47
1:A:337:LEU:HA	1:A:340:ILE:HG22	1.97	0.47
1:A:959:TYR:O	1:A:960:ILE:HG13	2.14	0.47
2:B:452:ASN:C	2:B:454:GLU:H	2.22	0.47
2:B:956:ASP:OD1	3:D:266:THR:CG2	2.63	0.47
2:C:1087:ASP:HB2	2:C:1235:PRO:HB2	1.97	0.47
3:D:242:ARG:HH11	3:D:242:ARG:CB	2.27	0.47
1:A:212:HIS:HD2	1:A:217:HIS:NE2	2.13	0.47
2:B:815:LEU:HB3	2:B:816:PRO:HD3	1.96	0.47
2:B:1134:ARG:NH2	2:B:1154:ASN:OD1	2.48	0.47
2:C:1071:PHE:HB3	2:C:1234:GLN:CG	2.40	0.47
3:D:37:TYR:HD1	3:D:177:ALA:CB	2.28	0.47
2:C:948:ILE:HG12	2:C:962:ASP:HB2	1.96	0.47
3:D:44:LEU:HB2	3:D:174:VAL:HG23	1.97	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
2:B:891:HIS:HD2	3:D:240:VAL:HB	1.80	0.47
3:E:105:LEU:O	3:E:121:PHE:HB2	2.15	0.47
1:A:487:GLN:HE22	1:A:548:ASN:HA	1.79	0.46
1:A:600:VAL:CG1	1:A:601:PRO:HA	2.45	0.46
2:B:340:VAL:HG21	2:C:1008:LEU:CD2	2.37	0.46
1:A:967:ILE:C	1:A:969:THR:H	2.23	0.46
3:E:49:ILE:HG23	3:E:50:PRO:CD	2.24	0.46
1:A:97:ARG:HB2	1:A:97:ARG:NH1	2.26	0.46
1:A:955:ASN:ND2	1:A:1055:LEU:HB3	2.31	0.46
2:B:230:ASP:O	2:B:985:ARG:HG2	2.16	0.46
2:B:950:ASP:OD2	3:D:243:LYS:NZ	2.37	0.46
2:C:193:THR:HA	2:C:296:VAL:HG12	1.97	0.46
2:C:360:ILE:HD12	2:C:1053:ARG:NH2	2.31	0.46
2:C:764:TRP:N	2:C:765:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1208:ASP:CG	2:C:1209:GLY:H	2.23	0.46
3:E:53:GLU:OE1	3:E:145:TYR:CD1	2.69	0.46
2:B:1112:ASN:CG	2:B:1113:LYS:H	2.23	0.46
2:B:1276:LEU:HB3	2:B:1290:LYS:HG2	1.96	0.46
2:C:1323:ASP:CG	2:C:1324:ASP:N	2.73	0.46
1:A:93:HIS:CE1	1:A:97:ARG:HH12	2.28	0.46
1:A:411:ILE:HD13	1:A:411:ILE:N	2.31	0.46
1:A:510:MET:O	1:A:511:ILE:HG13	2.16	0.46
1:A:929:PRO:O	1:A:993:VAL:HG12	2.15	0.46
2:B:274:MET:HG2	2:C:234:PRO:CD	2.27	0.46
3:D:53:GLU:HG2	3:D:145:TYR:HE1	1.81	0.46
3:D:67:TYR:CD1	3:D:110:VAL:HG22	2.50	0.46
1:A:747:CYS:HB3	1:A:784:ILE:HD13	1.97	0.46
2:C:306:GLN:HE21	2:C:306:GLN:H	1.62	0.46
2:C:337:VAL:HA	3:E:187:ILE:HD13	1.97	0.46
2:C:772:TYR:C	2:C:774:LEU:N	2.74	0.46
2:C:177:LYS:H	2:C:177:LYS:HD3	1.80	0.46
2:C:330:THR:HG22	2:C:331:GLU:N	2.30	0.46
3:D:217:LYS:O	3:D:221:ARG:HB3	2.15	0.46
1:A:62:PHE:CZ	1:A:171:ILE:HG23	2.50	0.46
2:B:1037:ILE:HG12	2:B:1038:GLU:N	2.24	0.46
2:C:87:GLU:OE2	2:C:161:LYS:HB2	2.16	0.46
2:C:341:LYS:HG3	2:C:1306:THR:HB	1.98	0.46
2:C:561:ASN:O	2:C:562:ALA:HB3	2.15	0.46
3:E:1:MET:SD	3:E:121:PHE:CE2	3.09	0.46
1:A:591:ALA:HB1	1:A:595:ASN:HB2	1.97	0.46
2:B:649:ALA:HB2	2:B:695:ALA:CB	2.46	0.46
2:C:329:LEU:HD23	2:C:346:HIS:CE1	2.51	0.46
3:D:233:THR:HG22	3:D:252:LEU:HD13	1.97	0.46
1:A:653:PRO:O	1:A:712:ILE:HG23	2.15	0.46
2:C:96:ILE:HD11	2:C:101:ASP:HB3	1.98	0.46
2:C:829:SER:CB	2:C:965:ARG:HD2	2.46	0.46
2:C:856:LEU:HA	2:C:860:ARG:HB2	1.98	0.46
2:C:898:GLN:OE1	3:D:3:GLN:CD	2.59	0.46
2:C:1080:THR:HB	2:C:1226:ASP:O	2.16	0.46
3:D:66:VAL:O	3:D:111:ILE:HG22	2.16	0.46
3:D:140:ALA:HA	3:D:281:LYS:HG3	1.97	0.46
1:A:557:SER:HB3	1:A:583:ARG:HE	1.82	0.45
2:B:1080:THR:HG22	2:B:1227:MET:HB3	1.98	0.45
2:B:1276:LEU:HB3	2:B:1290:LYS:CG	2.46	0.45
2:C:883:ILE:O	2:C:887:VAL:HB	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:185:SER:HB3	3:D:186:LEU:H	1.50	0.45
2:C:443:VAL:HG12	2:C:769:GLN:HA	1.98	0.45
2:C:878:SER:HB3	2:C:903:ASN:CG	2.40	0.45
1:A:631:GLU:O	1:A:635:VAL:HG23	2.17	0.45
2:B:228:VAL:HG21	2:B:253:MET:HG3	1.98	0.45
2:B:1168:ILE:HG21	2:B:1171:ILE:HD12	1.97	0.45
2:C:730:ASP:O	2:C:730:ASP:CG	2.59	0.45
3:E:53:GLU:CG	3:E:145:TYR:CE1	2.93	0.45
1:A:284:THR:HG23	1:A:367:ASN:HB3	1.97	0.45
1:A:496:CYS:HB2	1:A:571:ILE:HG23	1.97	0.45
2:B:765:PRO:HA	2:B:769:GLN:HB2	1.97	0.45
2:B:1008:LEU:HD13	2:B:1008:LEU:H	1.81	0.45
2:C:141:LEU:HG	2:C:142:ASP:N	2.27	0.45
2:C:413:MET:HG2	2:C:1019:ILE:HD13	1.98	0.45
2:C:514:PHE:CD2	2:C:532:ILE:HD11	2.51	0.45
2:C:878:SER:C	2:C:880:PRO:HD3	2.42	0.45
1:A:38:TYR:O	1:A:38:TYR:CG	2.70	0.45
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.97	0.45
1:A:938:MET:O	1:A:942:LYS:HB2	2.16	0.45
2:B:330:THR:HG23	2:B:331:GLU:HG3	1.98	0.45
2:C:231:LEU:HB2	2:C:249:SER:HB2	1.98	0.45
2:C:841:ASP:CA	2:C:940:ARG:HH12	2.30	0.45
2:C:1137:VAL:HG22	2:C:1164:TRP:CE2	2.52	0.45
3:D:106:GLY:HA2	3:D:121:PHE:HB3	1.98	0.45
3:E:70:ASP:OD2	3:E:70:ASP:C	2.60	0.45
3:E:166:GLU:HG3	3:E:172:MET:SD	2.57	0.45
3:E:229:PHE:HE1	3:E:252:LEU:CD1	2.29	0.45
1:A:559:ILE:CG2	1:A:613:ILE:HG12	2.46	0.45
3:E:70:ASP:OD2	3:E:70:ASP:O	2.35	0.45
3:E:148:ASP:O	3:E:280:ALA:HB1	2.16	0.45
1:A:6:SER:O	1:A:7:ILE:HB	2.16	0.45
1:A:565:ARG:O	1:A:566:GLU:HB3	2.17	0.45
2:C:523:THR:O	2:C:524:GLU:CB	2.63	0.45
2:C:997:TYR:C	2:C:999:LYS:H	2.25	0.45
3:D:110:VAL:HG12	3:D:111:ILE:N	2.32	0.45
3:D:144:ARG:CG	3:D:144:ARG:O	2.64	0.45
1:A:908:ALA:HB2	1:A:943:ILE:HB	1.99	0.45
2:B:291:HIS:HB3	2:B:292:ASN:H	1.54	0.45
2:C:330:THR:HG22	2:C:331:GLU:H	1.81	0.45
2:C:614:ARG:HB3	2:C:635:ILE:HD11	1.98	0.45
2:B:184:GLU:C	2:B:186:ASP:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:635:ILE:H	2:C:636:PRO:HA	1.82	0.45
2:C:986:ILE:O	2:C:989:ILE:HG22	2.17	0.45
2:C:999:LYS:HB3	2:C:1009:THR:HG22	1.98	0.45
1:A:617:ILE:HD11	1:A:635:VAL:HG11	1.98	0.44
1:A:914:GLU:HG2	1:A:950:MET:HE3	1.99	0.44
2:B:204:VAL:HG22	2:B:1242:MET:HG2	1.98	0.44
2:B:1084:PRO:HG3	2:B:1212:ARG:HH11	1.82	0.44
2:C:413:MET:HG2	2:C:1019:ILE:CD1	2.47	0.44
2:C:442:PRO:HB3	2:C:473:ALA:HB1	1.99	0.44
3:D:221:ARG:HH12	3:D:225:ARG:HH21	1.63	0.44
3:E:116:THR:HG21	3:E:119:ILE:HD12	1.99	0.44
1:A:16:ASP:HB3	1:A:113:TYR:O	2.17	0.44
1:A:303:THR:HG21	1:A:813:PRO:HD3	1.99	0.44
1:A:525:ARG:H	1:A:525:ARG:HD3	1.82	0.44
1:A:775:ASP:O	1:A:777:ASP:N	2.50	0.44
2:B:916:LEU:H	2:B:916:LEU:HD23	1.83	0.44
2:B:924:ASP:O	2:B:928:ARG:NH2	2.46	0.44
2:B:1147:MET:HB3	2:B:1152:ALA:HB2	1.97	0.44
2:C:1060:ARG:HH22	2:C:1292:GLU:HA	1.81	0.44
2:C:1134:ARG:H	2:C:1135:PRO:HA	1.81	0.44
2:C:1220:PRO:HA	2:C:1221:PRO:HD3	1.80	0.44
3:D:255:ILE:O	3:D:255:ILE:CG1	2.65	0.44
2:B:350:ILE:CG2	2:B:351:ASP:H	2.17	0.44
2:B:1075:ARG:HG3	2:B:1075:ARG:O	2.17	0.44
2:B:1112:ASN:ND2	2:B:1113:LYS:H	2.16	0.44
2:B:1121:HIS:CD2	2:B:1124:THR:HG22	2.43	0.44
2:C:770:CYS:O	2:C:770:CYS:SG	2.75	0.44
2:C:957:PHE:O	2:C:958:ILE:HG12	2.18	0.44
2:C:1042:TRP:HB3	2:C:1043:SER:HA	1.95	0.44
2:C:1049:GLU:CD	2:C:1053:ARG:HG3	2.42	0.44
3:D:178:LYS:HD2	3:D:249:ASP:HB3	1.99	0.44
1:A:37:ASP:CG	1:A:38:TYR:H	2.26	0.44
1:A:923:ALA:C	1:A:925:ILE:H	2.25	0.44
2:B:172:ASP:O	2:B:173:GLN:HB3	2.17	0.44
2:B:367:GLU:HG3	3:D:82:GLN:HA	2.00	0.44
2:B:923:TYR:CE1	2:B:924:ASP:HB3	2.53	0.44
3:D:14:GLN:NE2	3:D:107:LEU:HD13	2.32	0.44
3:E:186:LEU:HD13	3:E:186:LEU:HA	1.60	0.44
2:B:425:ILE:HD13	2:B:425:ILE:H	1.81	0.44
2:B:1079:LEU:O	2:B:1081:ASP:N	2.50	0.44
2:C:298:PRO:O	2:C:299:ALA:HB3	2.17	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
3:D:160:LEU:HD23	3:D:229:PHE:HA	1.99	0.44
1:A:766:CYS:CB	1:A:786:ARG:O	2.65	0.44
1:A:1034:ARG:CZ	1:A:1035:LEU:H	2.31	0.44
2:B:1289:PRO:HD2	3:D:20:ARG:NE	2.33	0.44
2:C:652:PHE:HE1	2:C:688:GLU:HA	1.82	0.44
3:D:181:SER:CB	3:D:250:ARG:HG2	2.41	0.44
3:E:2:LEU:HD11	3:E:107:LEU:CD1	2.48	0.44
3:E:68:ILE:HD13	3:E:69:GLU:CA	2.47	0.44
1:A:539:LEU:HD11	1:A:612:PHE:HB3	2.00	0.44
1:A:562:GLY:O	1:A:588:GLY:CA	2.66	0.44
1:A:864:ARG:HG3	1:A:865:ASN:N	2.33	0.44
1:A:914:GLU:HA	1:A:950:MET:HB3	2.00	0.44
2:B:191:GLY:HA2	2:B:192:PRO:C	2.43	0.44
2:B:1280:PRO:O	2:B:1281:VAL:HG12	2.18	0.44
2:B:1298:PHE:O	2:B:1299:SER:HB3	2.18	0.44
3:E:33:GLN:O	3:E:35:LEU:N	2.51	0.44
3:E:42:ASN:HB3	3:E:174:VAL:CG2	2.48	0.44
3:E:286:THR:O	3:E:290:TRP:CB	2.65	0.44
1:A:732:THR:O	1:A:733:VAL:HB	2.17	0.44
1:A:971:LEU:HD23	1:A:971:LEU:O	2.18	0.44
2:C:1118:THR:HG22	2:C:1129:PRO:HA	2.00	0.44
3:D:25:ASN:OD1	3:D:26:ALA:N	2.51	0.44
3:D:116:THR:OG1	3:D:119:ILE:HD12	2.18	0.44
3:D:150:ILE:HG22	3:D:151:ASP:N	2.33	0.44
3:D:238:ASN:H	3:D:253:GLU:HB3	1.82	0.44
3:E:46:LYS:CG	3:E:155:HIS:CE1	3.00	0.44
1:A:759:LEU:C	1:A:761:GLN:H	2.26	0.43
1:A:1034:ARG:NH1	1:A:1035:LEU:HD23	2.32	0.43
2:B:1255:ARG:HB3	2:B:1256:GLY:H	1.57	0.43
2:B:1315:MET:C	2:B:1317:VAL:H	2.25	0.43
2:C:544:TYR:HA	2:C:545:PRO:HD3	1.74	0.43
1:A:504:THR:O	1:A:512:ALA:HA	2.18	0.43
1:A:654:SER:HB3	1:A:715:TYR:HE2	1.83	0.43
2:B:138:PHE:O	2:C:759:ASP:OD1	2.35	0.43
2:B:870:ASP:CB	2:B:871:PRO:CA	2.90	0.43
2:B:1263:TYR:C	2:B:1265:MET:H	2.25	0.43
2:C:317:MET:SD	2:C:1262:SER:HB3	2.58	0.43
2:C:709:MET:HA	2:C:712:PHE:CE1	2.54	0.43
1:A:203:THR:HG23	1:A:204:LEU:H	1.82	0.43
1:A:224:GLU:O	1:A:227:MET:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:THR:O	1:A:683:GLN:HG3	2.19	0.43
2:B:225:ILE:HG23	2:B:247:TYR:CD2	2.52	0.43
2:B:291:HIS:CE1	2:B:1304:MET:HE1	2.53	0.43
3:E:32:LEU:O	3:E:35:LEU:CG	2.58	0.43
3:E:93:LEU:O	3:E:96:LEU:HB2	2.18	0.43
1:A:959:TYR:HB3	1:A:960:ILE:H	1.70	0.43
2:B:192:PRO:C	2:B:194:VAL:H	2.25	0.43
2:B:210:ARG:HH21	2:B:215:THR:HG21	1.83	0.43
2:B:449:PHE:HA	2:B:450:PRO:HD2	1.83	0.43
2:C:526:ASN:HB2	2:C:721:SER:HB2	1.99	0.43
3:D:220:ASN:C	3:D:222:ASP:H	2.26	0.43
1:A:30:THR:HG22	1:A:97:ARG:HD3	2.00	0.43
1:A:580:SER:HB2	1:A:581:ASN:H	1.67	0.43
1:A:684:ASN:O	1:A:685:PRO:C	2.61	0.43
2:B:241:ALA:O	2:B:242:GLU:HG3	2.19	0.43
2:B:1103:HIS:CD2	2:B:1103:HIS:N	2.85	0.43
2:C:855:TYR:CZ	2:C:896:LEU:HD21	2.53	0.43
2:C:1322:PRO:O	2:C:1323:ASP:HB3	2.17	0.43
3:E:152:ILE:H	3:E:152:ILE:HD12	1.83	0.43
1:A:530:MET:HE3	1:A:530:MET:HA	2.00	0.43
1:A:713:ASN:OD1	1:A:713:ASN:C	2.61	0.43
3:E:122:TYR:CE2	3:E:203:ILE:HG21	2.53	0.43
1:A:535:LEU:HD12	1:A:614:ILE:HG12	2.00	0.43
2:C:392:PRO:HG2	2:C:1315:MET:HG3	2.00	0.43
2:C:449:PHE:HB2	2:C:683:TRP:HD1	1.78	0.43
2:C:509:VAL:HG12	2:C:509:VAL:O	2.19	0.43
2:C:617:ASP:HA	2:C:620:ILE:HG22	2.00	0.43
2:C:853:ASP:C	3:D:117:ILE:HD11	2.44	0.43
3:D:46:LYS:HE3	3:D:158:LEU:HD22	2.00	0.43
3:E:253:GLU:HG3	3:E:254:TYR:CE2	2.54	0.43
3:E:282:PHE:CZ	3:E:286:THR:HG21	2.53	0.43
1:A:941:ASP:HA	1:A:944:ARG:HB3	2.00	0.43
2:B:551:PHE:C	2:B:553:GLN:H	2.25	0.43
2:B:1289:PRO:HD2	3:D:20:ARG:HD2	1.97	0.43
2:C:816:PRO:O	2:C:820:ILE:HG22	2.19	0.43
2:C:837:THR:HA	2:C:936:MET:HB2	2.01	0.43
2:C:874:ILE:HG21	2:C:897:TYR:CD1	2.53	0.43
3:D:66:VAL:HG23	3:D:67:TYR:N	2.33	0.43
3:D:241:ASN:HB3	3:D:250:ARG:HD2	2.01	0.43
3:E:162:GLY:O	3:E:167:ARG:NH1	2.48	0.43
1:A:67:ARG:O	1:A:72:PHE:HD1	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LEU:HB3	1:A:264:SER:H	1.68	0.43
1:A:685:PRO:O	1:A:686:TYR:CD2	2.72	0.43
2:B:879:THR:C	2:B:881:ASP:H	2.27	0.43
1:A:437:GLN:HE21	1:A:437:GLN:CA	2.32	0.43
1:A:730:ILE:CG2	1:A:731:HIS:H	2.26	0.43
1:A:873:PRO:HD2	1:A:876:MET:HB2	1.99	0.43
2:B:832:MET:HE2	2:B:946:LEU:HG	2.00	0.43
2:C:1072:ASP:H	2:C:1234:GLN:HE22	1.66	0.43
3:D:14:GLN:HE22	3:D:107:LEU:HD13	1.84	0.43
2:B:280:THR:HG23	2:B:281:VAL:HG23	2.01	0.42
2:B:406:ASP:HA	2:B:409:ILE:HG22	1.99	0.42
2:C:733:VAL:HG11	2:C:1022:ILE:HG13	2.01	0.42
2:C:1121:HIS:ND1	2:C:1123:PRO:HD2	2.34	0.42
3:D:60:ARG:O	3:D:61:ASN:C	2.62	0.42
3:D:217:LYS:HE2	3:D:290:TRP:O	2.18	0.42
1:A:437:GLN:HE21	1:A:437:GLN:N	2.16	0.42
1:A:526:ASN:OD1	1:A:529:THR:HG23	2.20	0.42
2:B:141:LEU:HG	2:B:142:ASP:H	1.83	0.42
2:B:1083:ASP:O	2:B:1084:PRO:C	2.63	0.42
2:C:837:THR:HG22	2:C:934:LEU:HD21	2.00	0.42
3:E:210:GLY:O	3:E:214:ARG:HG3	2.18	0.42
1:A:496:CYS:SG	1:A:533:LEU:HD11	2.59	0.42
1:A:961:SER:HA	1:A:997:THR:OG1	2.20	0.42
2:B:587:ALA:C	2:B:589:PHE:H	2.27	0.42
2:B:701:HIS:C	2:B:703:SER:H	2.28	0.42
2:C:627:ALA:H	2:C:716:PHE:HB2	1.84	0.42
2:C:751:THR:C	2:C:753:ASP:H	2.28	0.42
2:C:1027:THR:HG22	3:D:102:SER:HG	1.84	0.42
3:D:74:GLN:OE1	3:D:74:GLN:HA	2.19	0.42
3:E:1:MET:CE	3:E:123:ASP:HA	2.49	0.42
1:A:84:PRO:C	1:A:86:ASP:H	2.26	0.42
1:A:114:ASN:HD21	1:A:117:LEU:HB3	1.85	0.42
1:A:305:TYR:CE1	1:A:313:ARG:HG3	2.54	0.42
1:A:590:ARG:HA	1:A:597:ARG:HH12	1.84	0.42
1:A:850:SER:HB3	1:A:872:VAL:HG21	2.01	0.42
2:B:267:VAL:HG12	2:B:1306:THR:HA	2.01	0.42
2:B:274:MET:HE1	2:C:972:PRO:HG2	2.02	0.42
2:B:983:ILE:HG22	2:B:983:ILE:O	2.19	0.42
2:C:543:TRP:CD1	2:C:544:TYR:HD1	2.33	0.42
2:C:738:GLU:HB3	2:C:1015:GLN:HG3	2.02	0.42
2:C:817:ASP:O	2:C:821:ASN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:53:GLU:CG	3:D:145:TYR:HE1	2.31	0.42
1:A:752:VAL:HG12	1:A:812:VAL:HG23	2.01	0.42
1:A:828:TYR:HA	1:A:1032:GLY:O	2.20	0.42
2:B:193:THR:O	2:B:193:THR:HG22	2.20	0.42
2:B:935:GLN:OE1	2:B:940:ARG:HB3	2.19	0.42
2:C:341:LYS:CG	2:C:1306:THR:HB	2.50	0.42
2:C:852:TYR:CE2	2:C:856:LEU:HD23	2.55	0.42
2:C:1134:ARG:NH1	2:C:1158:SER:OG	2.52	0.42
1:A:555:ASP:OD1	1:A:555:ASP:N	2.53	0.42
2:B:426:ILE:HA	2:B:429:ILE:HG22	2.02	0.42
2:C:863:LEU:HD11	2:C:871:PRO:HD3	2.02	0.42
1:A:93:HIS:CE1	1:A:97:ARG:NH1	2.87	0.42
1:A:311:GLN:NE2	1:A:359:PRO:HG3	2.34	0.42
1:A:519:ILE:HA	1:A:520:PRO:HD2	1.96	0.42
2:B:402:ALA:HB2	3:D:83:ASN:ND2	2.34	0.42
2:B:588:LEU:HD22	2:B:604:MET:HE2	2.02	0.42
2:B:635:ILE:HD12	2:B:635:ILE:O	2.18	0.42
2:B:733:VAL:HG22	2:B:741:TYR:HB2	2.01	0.42
2:B:956:ASP:OD2	3:D:266:THR:CB	2.67	0.42
2:B:1080:THR:HA	2:B:1227:MET:HA	2.02	0.42
2:C:336:TYR:CE1	3:E:191:ARG:HG2	2.54	0.42
2:C:554:ARG:HD3	2:C:568:PHE:CD1	2.55	0.42
2:C:564:GLY:O	2:C:565:GLU:HB3	2.20	0.42
2:C:843:LEU:HD11	2:C:943:GLU:HB3	2.02	0.42
2:C:1136:HIS:HA	2:C:1164:TRP:CD1	2.54	0.42
3:E:69:GLU:HG3	3:E:199:LEU:HB2	1.98	0.42
3:E:247:ARG:HA	3:E:247:ARG:NE	2.30	0.42
1:A:377:LEU:H	1:A:377:LEU:CD1	2.30	0.42
1:A:566:GLU:CD	1:A:570:ASN:HB2	2.45	0.42
2:B:302:ARG:HD3	2:B:315:THR:HG22	2.01	0.42
2:B:598:ASN:HA	2:B:601:ILE:HG22	2.02	0.42
2:C:309:TRP:CD1	2:C:1253:ARG:HE	2.37	0.42
2:C:1023:ARG:HG2	2:C:1024:PRO:CD	2.40	0.42
3:E:32:LEU:HD13	3:E:225:ARG:NH1	2.35	0.42
3:E:158:LEU:CD2	3:E:172:MET:HB3	2.49	0.42
3:E:268:THR:OG1	3:E:269:ILE:N	2.48	0.42
2:B:862:ARG:NH1	2:B:948:ILE:HD13	2.35	0.42
2:C:526:ASN:HB2	2:C:721:SER:CB	2.50	0.42
2:C:822:MET:CG	2:C:1044:ARG:HD2	2.50	0.42
2:C:1126:MET:HB3	2:C:1128:TYR:CE2	2.54	0.42
3:D:239:VAL:CG1	3:D:250:ARG:HH12	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:GLY:O	2:B:553:GLN:HB2	2.19	0.42
2:B:836:GLN:HG2	2:B:941:TYR:HA	2.02	0.42
2:C:931:ASN:OD1	2:C:934:LEU:HD22	2.19	0.42
1:A:127:THR:CG2	2:B:639:ASN:HB2	2.49	0.41
1:A:488:GLY:C	1:A:490:LEU:N	2.78	0.41
1:A:496:CYS:HB2	1:A:571:ILE:CG2	2.50	0.41
1:A:549:SER:C	1:A:551:LEU:H	2.27	0.41
1:A:690:THR:C	1:A:691:TYR:HD2	2.28	0.41
2:B:493:HIS:CG	2:B:758:ILE:HD13	2.55	0.41
2:B:1071:PHE:HB3	2:B:1234:GLN:HG3	2.01	0.41
2:B:1140:THR:HA	2:B:1167:ASP:HB2	2.02	0.41
2:B:1236:ILE:CG1	2:B:1237:SER:H	2.33	0.41
2:B:1249:ASN:O	2:C:1109:SER:HA	2.19	0.41
2:B:1271:SER:OG	3:D:195:ASN:CG	2.63	0.41
2:C:633:THR:HG21	2:C:710:SER:OG	2.20	0.41
2:C:835:TYR:HB2	2:C:847:ILE:HD11	2.03	0.41
3:D:152:ILE:HG21	3:D:283:LEU:HB3	2.01	0.41
3:E:2:LEU:HD11	3:E:107:LEU:HD11	2.02	0.41
3:E:32:LEU:CD1	3:E:225:ARG:NE	2.83	0.41
3:E:72:ILE:O	3:E:76:LEU:HD12	2.20	0.41
1:A:686:TYR:HE1	1:A:1034:ARG:NH1	2.18	0.41
2:B:1263:TYR:CD1	2:B:1295:HIS:HD2	2.32	0.41
2:C:375:ARG:HG2	2:C:398:ARG:HH21	1.86	0.41
2:C:443:VAL:CG2	2:C:444:SER:H	2.26	0.41
3:E:140:ALA:HB1	3:E:281:LYS:HG3	2.02	0.41
3:E:220:ASN:C	3:E:222:ASP:N	2.77	0.41
1:A:828:TYR:O	1:A:1033:ILE:HA	2.19	0.41
1:A:1016:ILE:HD13	1:A:1016:ILE:H	1.84	0.41
2:B:722:GLY:O	2:B:723:ASN:HB3	2.20	0.41
2:C:245:ALA:C	2:C:247:TYR:H	2.28	0.41
2:C:898:GLN:OE1	3:D:3:GLN:OE1	2.39	0.41
3:D:193:VAL:HG11	3:D:230:ILE:HD12	2.02	0.41
3:E:272:ASP:CG	3:E:273:LEU:H	2.28	0.41
1:A:240:ARG:HH21	1:A:288:LEU:HD23	1.84	0.41
1:A:525:ARG:HD3	1:A:525:ARG:N	2.35	0.41
2:B:760:THR:C	2:B:762:ILE:H	2.28	0.41
3:D:12:LEU:HD23	3:D:14:GLN:HB2	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
3:E:205:LEU:CD1	3:E:289:ARG:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:TYR:HD2	1:A:51:LEU:HD11	1.85	0.41
1:A:541:LYS:HG2	1:A:971:LEU:HD22	2.02	0.41
1:A:653:PRO:O	1:A:654:SER:C	2.63	0.41
1:A:968:ILE:H	1:A:968:ILE:HG13	1.69	0.41
2:B:196:LEU:HD22	2:B:296:VAL:HG11	2.02	0.41
2:B:373:ASP:C	2:B:375:ARG:H	2.27	0.41
3:D:69:GLU:HG3	3:D:199:LEU:HG	2.02	0.41
2:B:164:LEU:HD22	2:B:1296:ILE:HD13	2.02	0.41
2:B:609:PRO:HD3	2:B:724:HIS:NE2	2.35	0.41
2:B:1292:GLU:OE1	2:B:1293:VAL:HG13	2.20	0.41
2:C:478:ILE:HD12	2:C:766:ILE:HG23	2.02	0.41
2:C:704:VAL:HG22	2:C:1330:ILE:HD11	2.03	0.41
2:C:1236:ILE:HG13	2:C:1236:ILE:H	1.76	0.41
3:E:76:LEU:HD21	3:E:282:PHE:CD2	2.55	0.41
1:A:170:ASN:HB3	1:A:173:ASP:HB2	2.02	0.41
1:A:475:ARG:C	1:A:477:TYR:H	2.29	0.41
1:A:496:CYS:SG	1:A:533:LEU:CD1	3.09	0.41
1:A:543:GLU:HA	1:A:645:ARG:HH22	1.84	0.41
1:A:559:ILE:HG12	1:A:585:ILE:HB	2.03	0.41
1:A:797:ARG:HH22	1:A:878:TYR:HB2	1.86	0.41
2:B:485:GLU:OE1	2:B:521:PHE:HB3	2.21	0.41
2:B:583:GLU:O	2:B:584:HIS:HB2	2.21	0.41
2:B:879:THR:HA	2:B:880:PRO:HD3	1.95	0.41
2:C:299:ALA:HB2	2:C:1265:MET:SD	2.61	0.41
2:C:454:GLU:C	2:C:456:ASN:H	2.27	0.41
2:C:612:PHE:O	2:C:635:ILE:HD13	2.19	0.41
2:C:958:ILE:O	2:C:958:ILE:HG13	2.20	0.41
2:C:1087:ASP:HB2	2:C:1235:PRO:CB	2.51	0.41
3:E:205:LEU:HD13	3:E:205:LEU:C	2.36	0.41
1:A:155:VAL:HG12	2:C:548:TYR:CE1	2.56	0.41
1:A:390:ASP:O	1:A:391:ILE:C	2.63	0.41
2:B:850:THR:HG22	2:B:851:THR:H	1.86	0.41
2:B:1102:ALA:O	2:B:1105:LEU:HG	2.21	0.41
2:B:1263:TYR:CD2	2:B:1295:HIS:CD2	3.09	0.41
2:C:651:ARG:O	2:C:655:ILE:HG12	2.21	0.41
2:C:868:VAL:HB	2:C:890:THR:HA	2.02	0.41
2:C:1029:LEU:HB3	2:C:1030:ARG:H	1.63	0.41
3:E:182:TRP:CD1	3:E:185:SER:HB3	2.55	0.41
1:A:325:THR:HG22	1:A:351:TYR:HB3	2.03	0.41
1:A:383:THR:HG21	1:A:805:TYR:CB	2.51	0.41
1:A:411:ILE:HD13	1:A:411:ILE:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:TYR:O	1:A:686:TYR:CD2	2.71	0.41
2:B:219:ILE:HG22	2:B:220:ASP:N	2.24	0.41
2:B:297:ASN:C	2:B:299:ALA:H	2.29	0.41
2:B:876:GLY:HA2	2:B:902:ILE:CG2	2.50	0.41
2:B:1031:TYR:CE2	2:B:1041:ARG:HD3	2.56	0.41
2:C:218:GLY:HA3	2:C:989:ILE:HD11	2.03	0.41
2:C:547:GLU:HG2	2:C:599:THR:HG23	2.02	0.41
2:C:624:PHE:CD2	2:C:713:MET:HA	2.56	0.41
2:C:887:VAL:HA	2:C:890:THR:HG22	2.02	0.41
2:C:926:VAL:HG22	2:C:938:ASN:HB2	2.03	0.41
3:D:258:ASN:OD1	3:D:259:SER:N	2.53	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:309:ASN:O	1:A:311:GLN:N	2.53	0.41
2:B:268:GLY:O	2:B:269:GLU:HB2	2.21	0.41
2:B:363:ARG:NE	3:D:80:SER:CB	2.83	0.41
2:C:524:GLU:OE2	2:C:758:ILE:HD13	2.21	0.41
2:C:547:GLU:HB3	2:C:600:ILE:HD12	2.01	0.41
2:C:687:LEU:HD11	2:C:764:TRP:HZ3	1.86	0.41
3:D:67:TYR:O	3:D:68:ILE:C	2.64	0.41
1:A:115:TRP:O	1:A:116:MET:C	2.64	0.40
1:A:329:THR:O	1:A:331:ARG:N	2.54	0.40
1:A:731:HIS:HB2	1:A:746:PHE:HD2	1.86	0.40
1:A:868:ASP:O	1:A:869:ILE:C	2.64	0.40
2:B:980:ARG:NH2	2:B:1010:ARG:O	2.53	0.40
2:B:1084:PRO:HB2	2:B:1209:GLY:HA3	2.02	0.40
2:B:1114:ARG:HG3	2:B:1116:ARG:HH21	1.85	0.40
2:C:205:ASN:HB2	2:C:1239:ALA:HB1	2.02	0.40
2:C:225:ILE:HG23	2:C:247:TYR:HD2	1.86	0.40
3:D:239:VAL:HG12	3:D:250:ARG:NH1	2.33	0.40
1:A:75:PRO:HD2	1:A:76:LEU:H	1.86	0.40
1:A:188:THR:CG2	3:D:144:ARG:CG	2.91	0.40
1:A:278:LEU:HD23	1:A:319:MET:HE1	2.03	0.40
1:A:872:VAL:HA	1:A:873:PRO:HA	1.84	0.40
1:A:967:ILE:HB	1:A:978:LYS:HD3	2.03	0.40
2:B:1298:PHE:O	2:B:1299:SER:CB	2.68	0.40
2:C:1247:ASN:C	2:C:1247:ASN:HD22	2.27	0.40
1:A:407:GLU:CG	1:A:829:MET:O	2.69	0.40
1:A:430:PRO:HB2	1:A:433:GLU:HG3	2.03	0.40
1:A:484:THR:N	1:A:511:ILE:HG21	2.36	0.40
1:A:939:GLN:O	1:A:943:ILE:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1013:THR:O	1:A:1055:LEU:HD12	2.21	0.40
2:B:934:LEU:O	2:B:935:GLN:HB2	2.21	0.40
2:B:1205:GLN:C	2:B:1206:PHE:HD2	2.29	0.40
2:B:1236:ILE:HG12	2:B:1237:SER:H	1.85	0.40
2:C:838:GLU:HG3	2:C:839:ALA:N	2.36	0.40
2:C:1076:ILE:HD13	2:C:1159:VAL:HG21	2.02	0.40
2:C:1097:VAL:HG13	2:C:1137:VAL:HG12	2.03	0.40
3:D:228:LEU:HA	3:D:231:MET:HE2	2.03	0.40
3:E:140:ALA:O	3:E:146:ARG:HA	2.22	0.40
1:A:199:MET:HE3	1:A:205:VAL:HG11	2.04	0.40
2:B:281:VAL:HG11	2:B:302:ARG:HD2	2.03	0.40
2:B:1321:ASN:C	2:B:1323:ASP:H	2.29	0.40
2:C:493:HIS:HB3	2:C:756:THR:HA	2.02	0.40
2:C:1086:PRO:HG3	2:C:1177:VAL:HG12	2.03	0.40
1:A:419:TYR:HB3	1:A:680:THR:HG23	2.03	0.40
2:B:172:ASP:O	2:B:173:GLN:CB	2.70	0.40
2:B:733:VAL:HA	2:B:743:PRO:HA	2.04	0.40
2:C:490:PHE:HA	2:C:745:ILE:HG22	2.04	0.40
3:E:53:GLU:CB	3:E:145:TYR:CE1	3.05	0.40
3:E:261:ARG:O	3:E:262:THR:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1039/1058 (98%)	775 (75%)	180 (17%)	84 (8%)	1	11
2	B	1172/1333 (88%)	915 (78%)	219 (19%)	38 (3%)	3	25
2	C	1238/1333 (93%)	974 (79%)	240 (19%)	24 (2%)	6	33
3	D	289/291 (99%)	253 (88%)	33 (11%)	3 (1%)	12	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	289/291 (99%)	254 (88%)	34 (12%)	1 (0%)	36	69
All	All	4027/4306 (94%)	3171 (79%)	706 (18%)	150 (4%)	4	22

All (150) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	25	ILE
1	A	49	HIS
1	A	55	GLY
1	A	69	HIS
1	A	76	LEU
1	A	77	LYS
1	A	125	ASN
1	A	255	ARG
1	A	330	GLN
1	A	364	TYR
1	A	391	ILE
1	A	485	MET
1	A	487	GLN
1	A	511	ILE
1	A	549	SER
1	A	580	SER
1	A	608	ILE
1	A	776	SER
1	A	813	PRO
1	A	853	GLU
1	A	924	VAL
1	A	962	PHE
1	A	964	GLU
1	A	1035	LEU
1	A	1038	THR
2	B	280	THR
2	B	616	ASP
2	B	838	GLU
2	B	870	ASP
2	B	1080	THR
2	B	1281	VAL
2	B	1299	SER
2	C	628	SER
2	C	842	ASP
2	C	1037	ILE

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Mol	Chain	Res	Type
2	C	1323	ASP
1	A	3	HIS
1	A	116	MET
1	A	187	PRO
1	A	212	HIS
1	A	263	LEU
1	A	284	THR
1	A	395	GLN
1	A	499	VAL
1	A	512	ALA
1	A	671	VAL
1	A	688	TYR
1	A	697	ILE
1	A	733	VAL
1	A	851	LEU
1	A	915	ASN
1	A	926	MET
1	A	990	ALA
2	B	149	PRO
2	B	150	LEU
2	B	671	ASP
2	B	897	TYR
2	B	901	VAL
2	B	914	GLU
2	C	1294	ASP
3	D	244	VAL
1	A	209	SER
1	A	214	ASN
1	A	266	SER
1	A	387	THR
1	A	389	ALA
1	A	519	ILE
1	A	655	GLU
1	A	686	TYR
1	A	829	MET
1	A	888	GLU
2	B	229	GLN
2	B	291	HIS
2	B	339	LEU
2	B	753	ASP
2	B	973	THR
2	C	386	SER

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Mol	Chain	Res	Type
2	C	450	PRO
2	C	992	VAL
2	C	1234	GLN
3	D	253	GLU
1	A	37	ASP
1	A	380	THR
1	A	406	VAL
1	A	566	GLU
1	A	684	ASN
1	A	740	THR
1	A	893	GLU
1	A	894	LYS
1	A	960	ILE
2	B	193	THR
2	B	451	GLU
2	B	1112	ASN
2	B	1234	GLN
2	C	666	ARG
2	C	1249	ASN
3	D	265	ARG
1	A	115	TRP
1	A	307	HIS
1	A	310	ASP
1	A	363	ASN
1	A	523	MET
1	A	623	GLN
1	A	760	SER
1	A	821	ARG
1	A	968	ILE
2	B	190	VAL
2	B	307	VAL
2	B	438	ASN
2	B	452	ASN
2	C	545	PRO
2	C	591	ASP
2	C	831	VAL
2	C	948	ILE
1	A	28	PRO
1	A	74	LEU
1	A	356	THR
1	A	489	SER
1	A	517	GLY

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Mol	Chain	Res	Type
1	A	802	THR
1	A	815	GLY
2	B	840	ASP
2	B	915	VAL
2	C	757	ILE
2	C	830	VAL
2	C	838	GLU
2	C	938	ASN
3	E	55	HIS
1	A	68	GLY
1	A	929	PRO
2	B	983	ILE
2	C	762	ILE
2	C	1279	SER
2	B	749	GLY
2	B	830	VAL
2	C	1086	PRO
1	A	602	PHE
1	A	704	PRO
2	B	157	ILE
2	B	219	ILE
2	B	1037	ILE
1	A	887	ILE
2	B	194	VAL
1	A	925	ILE
2	B	1084	PRO
2	B	1180	PRO
2	C	307	VAL
2	C	644	VAL
2	B	192	PRO

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	933/943 (99%)	804 (86%)	129 (14%)	3 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	1029/1155 (89%)	907 (88%)	122 (12%)	5	21
2	C	1085/1155 (94%)	942 (87%)	143 (13%)	4	19
3	D	240/240 (100%)	201 (84%)	39 (16%)	2	14
3	E	240/240 (100%)	197 (82%)	43 (18%)	2	12
All	All	3527/3733 (94%)	3051 (86%)	476 (14%)	6	18

All (476) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	20	ASN
1	A	22	ILE
1	A	23	ARG
1	A	26	THR
1	A	31	VAL
1	A	33	GLN
1	A	39	LEU
1	A	53	LEU
1	A	54	LEU
1	A	58	GLN
1	A	78	TYR
1	A	97	ARG
1	A	101	LEU
1	A	125	ASN
1	A	140	ILE
1	A	141	LEU
1	A	153	VAL
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	254	ASP
1	A	257	ILE
1	A	263	LEU
1	A	270	GLN
1	A	283	PHE
1	A	293	LEU
1	A	297	LEU
1	A	298	LEU

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Mol	Chain	Res	Type
1	A	307	HIS
1	A	320	TYR
1	A	334	GLU
1	A	339	GLN
1	A	356	THR
1	A	374	LYS
1	A	377	LEU
1	A	391	ILE
1	A	393	LEU
1	A	402	THR
1	A	406	VAL
1	A	411	ILE
1	A	425	THR
1	A	427	ASP
1	A	437	GLN
1	A	461	ARG
1	A	465	LEU
1	A	487	GLN
1	A	511	ILE
1	A	521	LYS
1	A	525	ARG
1	A	540	LYS
1	A	542	LEU
1	A	555	ASP
1	A	558	ILE
1	A	559	ILE
1	A	561	LEU
1	A	565	ARG
1	A	569	VAL
1	A	578	ASN
1	A	581	ASN
1	A	582	VAL
1	A	584	ILE
1	A	608	ILE
1	A	611	ASP
1	A	617	ILE
1	A	628	MET
1	A	652	HIS
1	A	655	GLU
1	A	658	ILE
1	A	662	ILE
1	A	667	GLN

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Mol	Chain	Res	Type
1	A	677	LEU
1	A	692	ILE
1	A	695	THR
1	A	697	ILE
1	A	708	ASN
1	A	713	ASN
1	A	714	ARG
1	A	717	THR
1	A	724	MET
1	A	737	HIS
1	A	739	ASN
1	A	757	LEU
1	A	763	LYS
1	A	771	THR
1	A	773	ARG
1	A	781	VAL
1	A	783	ILE
1	A	788	ASP
1	A	794	LEU
1	A	795	GLU
1	A	802	THR
1	A	809	GLN
1	A	812	VAL
1	A	814	ASN
1	A	820	VAL
1	A	823	THR
1	A	832	GLU
1	A	833	VAL
1	A	841	MET
1	A	849	ILE
1	A	851	LEU
1	A	859	VAL
1	A	868	ASP
1	A	874	LEU
1	A	876	MET
1	A	887	ILE
1	A	894	LYS
1	A	897	ILE
1	A	905	GLN
1	A	906	PHE
1	A	939	GLN
1	A	955	ASN

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Mol	Chain	Res	Type
1	A	960	ILE
1	A	967	ILE
1	A	968	ILE
1	A	969	THR
1	A	973	GLN
1	A	987	LEU
1	A	988	LYS
1	A	1016	ILE
1	A	1025	ILE
1	A	1033	ILE
1	A	1034	ARG
1	A	1053	ILE
1	A	1054	LYS
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	237	VAL
2	B	266	ILE
2	B	270	THR
2	B	274	MET
2	B	278	LEU
2	B	286	LEU
2	B	291	HIS
2	B	302	ARG
2	B	303	ASP
2	B	309	TRP
2	B	314	ILE
2	B	316	ASN
2	B	319	GLN
2	B	324	LYS
2	B	327	LEU
2	B	331	GLU

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Mol	Chain	Res	Type
2	B	339	LEU
2	B	388	GLN
2	B	409	ILE
2	B	412	LEU
2	B	423	GLU
2	B	425	ILE
2	B	434	VAL
2	B	446	LYS
2	B	448	TYR
2	B	453	LEU
2	B	458	SER
2	B	463	VAL
2	B	469	ARG
2	B	482	ILE
2	B	486	VAL
2	B	496	LYS
2	B	512	LEU
2	B	516	LEU
2	B	529	LYS
2	B	547	GLU
2	B	554	ARG
2	B	588	LEU
2	B	599	THR
2	B	604	MET
2	B	610	GLN
2	B	617	ASP
2	B	618	LEU
2	B	640	GLN
2	B	659	LEU
2	B	680	THR
2	B	685	ARG
2	B	688	GLU
2	B	694	ILE
2	B	719	ASN
2	B	738	GLU
2	B	748	GLN
2	B	752	VAL
2	B	758	ILE
2	B	821	ASN
2	B	841	ASP
2	B	850	THR
2	B	856	LEU

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Mol	Chain	Res	Type
2	B	865	ILE
2	B	879	THR
2	B	895	VAL
2	B	897	TYR
2	B	901	VAL
2	B	910	LEU
2	B	917	VAL
2	B	922	TYR
2	B	934	LEU
2	B	942	HIS
2	B	946	LEU
2	B	954	GLN
2	B	960	THR
2	B	971	MET
2	B	985	ARG
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	1082	ASP
2	B	1092	VAL
2	B	1103	HIS
2	B	1113	LYS
2	B	1114	ARG
2	B	1134	ARG
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	1212	ARG
2	B	1218	PHE
2	B	1230	ILE
2	B	1234	GLN
2	B	1240	ARG

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Mol	Chain	Res	Type
2	B	1247	ASN
2	B	1251	VAL
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	150	LEU
2	C	154	PHE
2	C	155	LYS
2	C	157	ILE
2	C	196	LEU
2	C	204	VAL
2	C	205	ASN
2	C	221	LEU
2	C	231	LEU
2	C	248	VAL
2	C	251	LEU
2	C	255	LEU
2	C	265	VAL
2	C	282	VAL
2	C	287	ARG
2	C	297	ASN
2	C	306	GLN
2	C	307	VAL
2	C	309	TRP
2	C	339	LEU
2	C	366	MET
2	C	376	ILE
2	C	409	ILE

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Mol	Chain	Res	Type
2	C	412	LEU
2	C	422	LEU
2	C	430	ASN
2	C	440	ILE
2	C	441	ARG
2	C	448	TYR
2	C	469	ARG
2	C	472	GLU
2	C	475	ILE
2	C	480	LEU
2	C	489	MET
2	C	493	HIS
2	C	494	GLU
2	C	495	LEU
2	C	498	ILE
2	C	512	LEU
2	C	524	GLU
2	C	536	LEU
2	C	547	GLU
2	C	560	ILE
2	C	561	ASN
2	C	574	LYS
2	C	576	ASP
2	C	577	GLN
2	C	581	LEU
2	C	591	ASP
2	C	594	LEU
2	C	599	THR
2	C	600	ILE
2	C	613	LEU
2	C	635	ILE
2	C	637	TYR
2	C	659	LEU
2	C	669	GLN
2	C	681	LYS
2	C	682	GLN
2	C	684	LEU
2	C	688	GLU
2	C	693	ASN
2	C	720	PHE
2	C	730	ASP
2	C	731	GLN

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Mol	Chain	Res	Type
2	C	738	GLU
2	C	746	GLU
2	C	748	GLN
2	C	753	ASP
2	C	756	THR
2	C	762	ILE
2	C	767	LEU
2	C	812	LYS
2	C	813	LEU
2	C	820	ILE
2	C	823	ILE
2	C	830	VAL
2	C	841	ASP
2	C	847	ILE
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	910	LEU
2	C	918	VAL
2	C	928	ARG
2	C	934	LEU
2	C	936	MET
2	C	937	ASN
2	C	943	GLU
2	C	945	VAL
2	C	947	GLU
2	C	948	ILE
2	C	959	GLN
2	C	970	LEU
2	C	1000	LEU
2	C	1019	ILE
2	C	1021	ARG
2	C	1022	ILE
2	C	1025	ASP
2	C	1037	ILE
2	C	1042	TRP
2	C	1046	PHE
2	C	1050	LEU

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Mol	Chain	Res	Type
2	C	1051	ARG
2	C	1062	ILE
2	C	1076	ILE
2	C	1079	LEU
2	C	1083	ASP
2	C	1110	LEU
2	C	1112	ASN
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	1228	ARG
2	C	1229	LEU
2	C	1247	ASN
2	C	1250	GLU
2	C	1269	THR
2	C	1272	ARG
2	C	1288	ILE
2	C	1292	GLU
2	C	1293	VAL
2	C	1295	HIS
2	C	1296	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
3	D	66	VAL
3	D	68	ILE
3	D	70	ASP
3	D	79	ILE

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Mol	Chain	Res	Type
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
3	E	68	ILE
3	E	69	GLU
3	E	83	ASN
3	E	85	ASN

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Mol	Chain	Res	Type
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	8	ASN
1	A	20	ASN
1	A	29	ASN
1	A	43	ASN
1	A	61	ASN
1	A	69	HIS
1	A	91	ASN
1	A	93	HIS
1	A	114	ASN
1	A	125	ASN
1	A	132	GLN
1	A	136	ASN
1	A	151	ASN
1	A	168	ASN

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Mol	Chain	Res	Type
1	A	212	HIS
1	A	281	ASN
1	A	311	GLN
1	A	321	ASN
1	A	437	GLN
1	A	487	GLN
1	A	544	ASN
1	A	548	ASN
1	A	578	ASN
1	A	581	ASN
1	A	651	ASN
1	A	659	ASN
1	A	674	HIS
1	A	708	ASN
1	A	737	HIS
1	A	739	ASN
1	A	782	ASN
1	A	848	GLN
1	A	857	GLN
1	A	915	ASN
1	A	916	ASN
1	A	930	ASN
1	A	939	GLN
1	A	955	ASN
1	A	991	ASN
1	A	1047	ASN
1	A	1048	HIS
2	B	195	ASN
2	B	205	ASN
2	B	283	ASN
2	B	292	ASN
2	B	293	ASN
2	B	319	GLN
2	B	346	HIS
2	B	369	ASN
2	B	394	GLN
2	B	430	ASN
2	B	561	ASN
2	B	577	GLN
2	B	610	GLN
2	B	623	ASN
2	B	632	GLN

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Mol	Chain	Res	Type
2	B	646	ASN
2	B	664	ASN
2	B	693	ASN
2	B	701	HIS
2	B	723	ASN
2	B	731	GLN
2	B	748	GLN
2	B	769	GLN
2	B	802	GLN
2	B	821	ASN
2	B	836	GLN
2	B	858	HIS
2	B	891	HIS
2	B	931	ASN
2	B	933	ASN
2	B	935	GLN
2	B	938	ASN
2	B	1015	GLN
2	B	1103	HIS
2	B	1121	HIS
2	B	1203	HIS
2	B	1205	GLN
2	B	1247	ASN
2	B	1308	ASN
2	B	1321	ASN
2	B	1332	ASN
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
2	C	320	GLN
2	C	346	HIS
2	C	349	ASN

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Mol	Chain	Res	Type
2	C	382	HIS
2	C	394	GLN
2	C	407	HIS
2	C	430	ASN
2	C	491	ASN
2	C	561	ASN
2	C	577	GLN
2	C	646	ASN
2	C	693	ASN
2	C	719	ASN
2	C	724	HIS
2	C	731	GLN
2	C	748	GLN
2	C	769	GLN
2	C	854	GLN
2	C	867	ASN
2	C	882	GLN
2	C	913	ASN
2	C	954	GLN
2	C	959	GLN
2	C	1018	GLN
2	C	1112	ASN
2	C	1169	HIS
2	C	1205	GLN
2	C	1234	GLN
2	C	1247	ASN
3	D	83	ASN
3	D	100	ASN
3	D	118	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

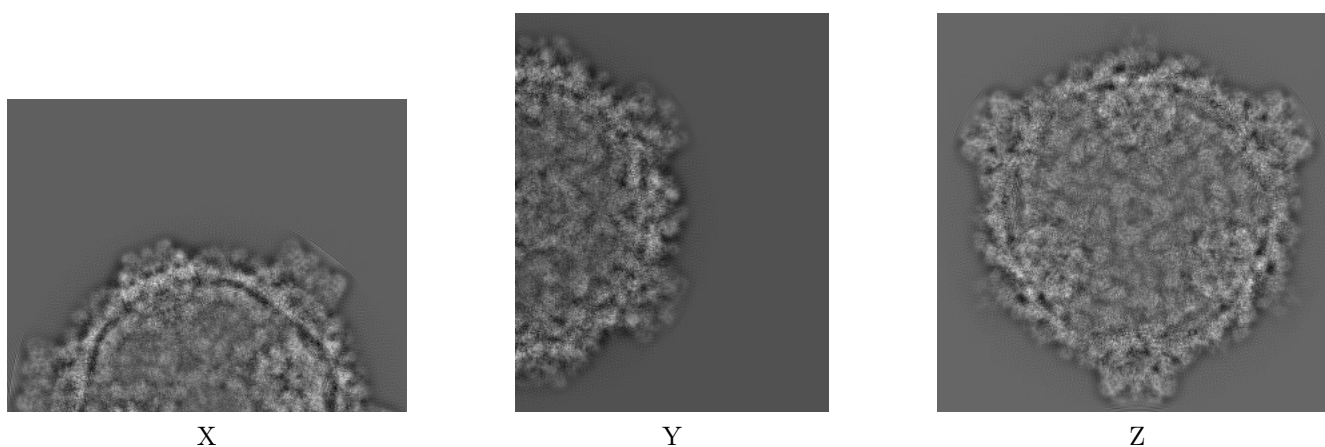
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5233. 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](#)

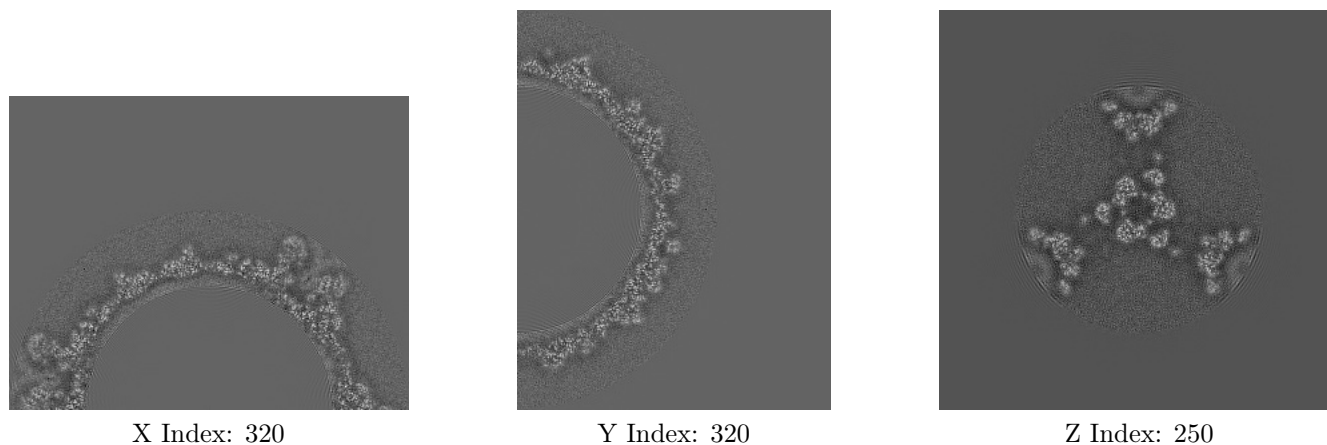
6.1.1 Primary map



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

6.2 Central slices [i](#)

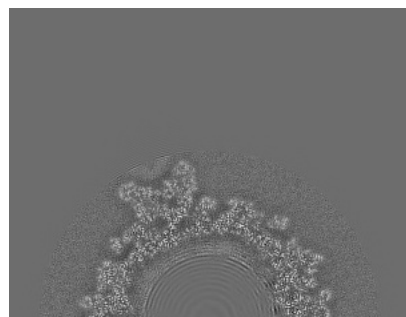
6.2.1 Primary map



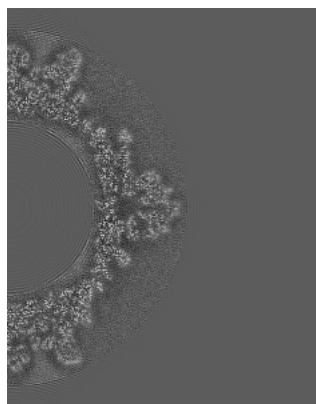
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

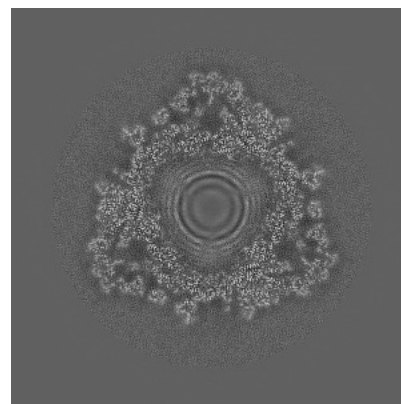
6.3.1 Primary map



X Index: 486



Y Index: 460

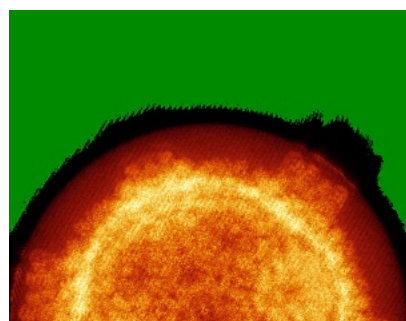


Z Index: 189

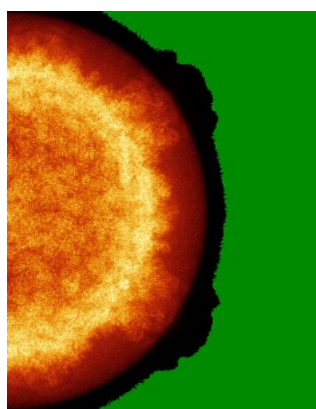
The images above show the largest variance slices of the map in three orthogonal directions.

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

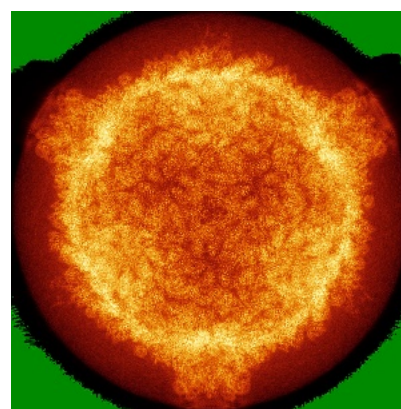
6.4.1 Primary map



X



Y

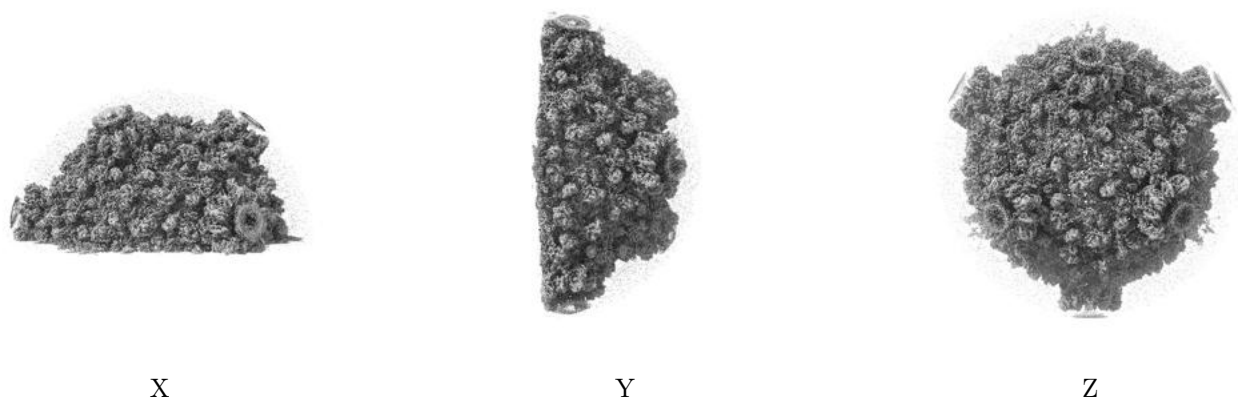


Z

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

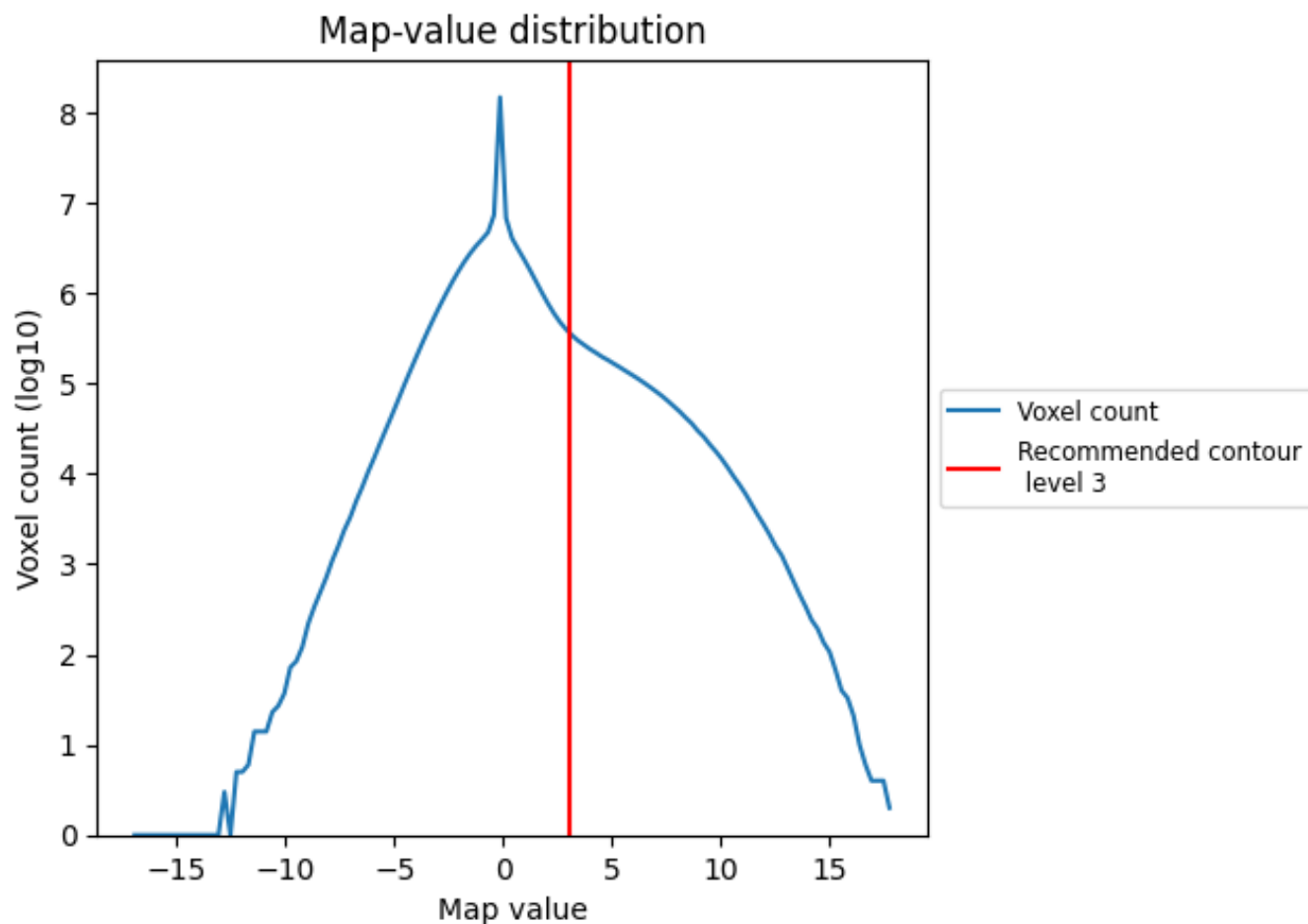
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

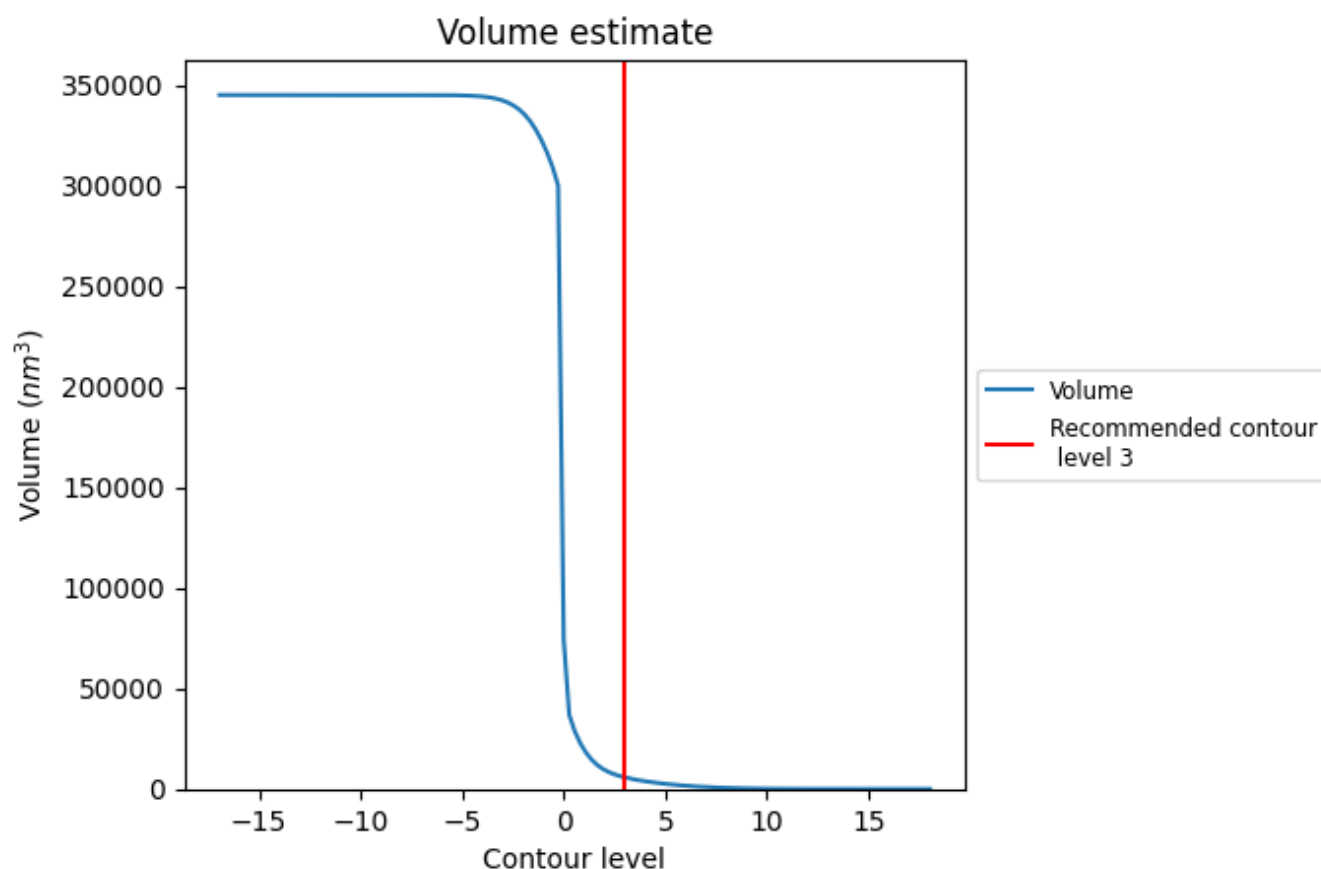
This section contains the results of statistical analysis of the map.

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 5776 nm³; this corresponds to an approximate mass of 5218 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 ⓘ

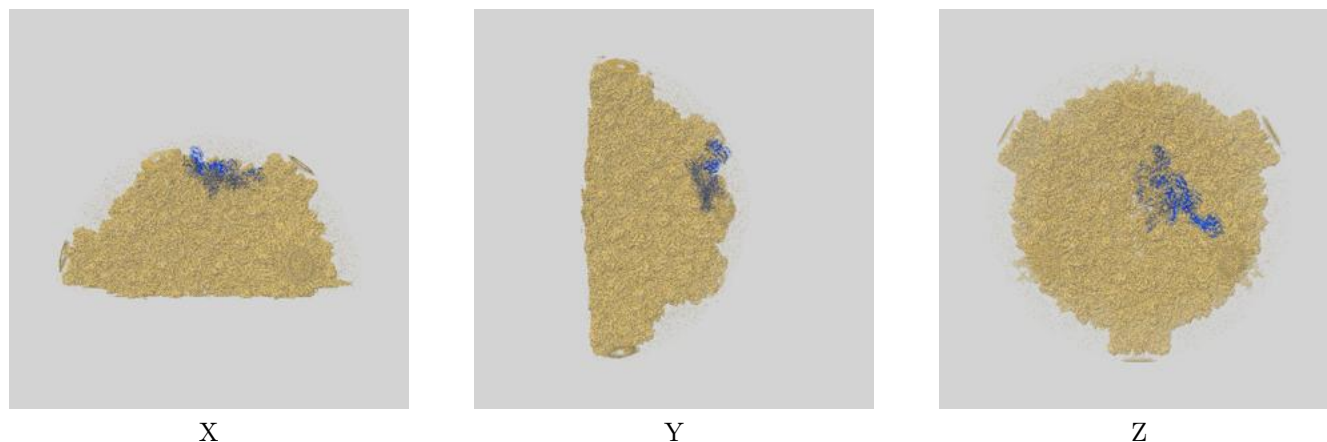
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-5233 and PDB model 3IZ3. Per-residue inclusion information can be found in section 3 on page 4.

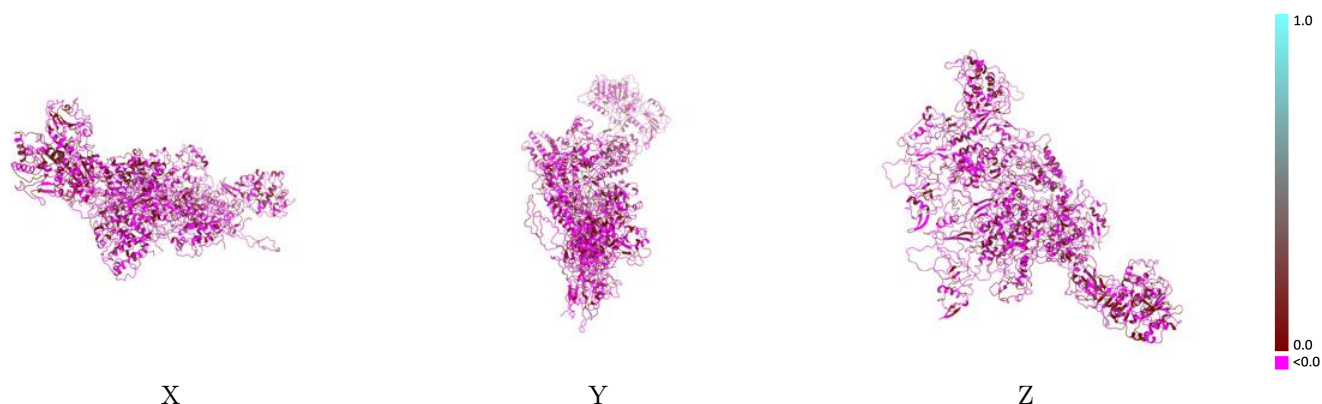
9.1 Map-model overlays

9.1.1 Map-model overlay ⓘ



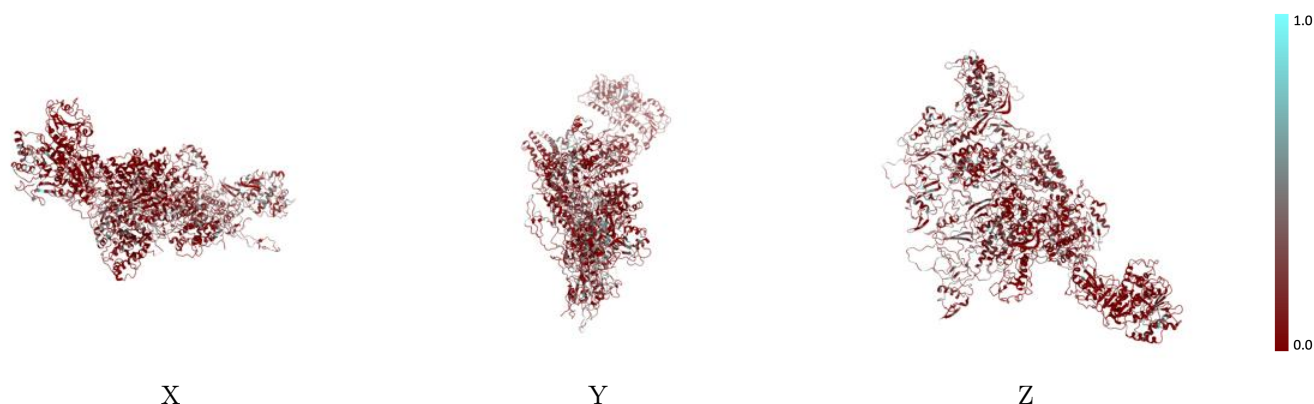
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



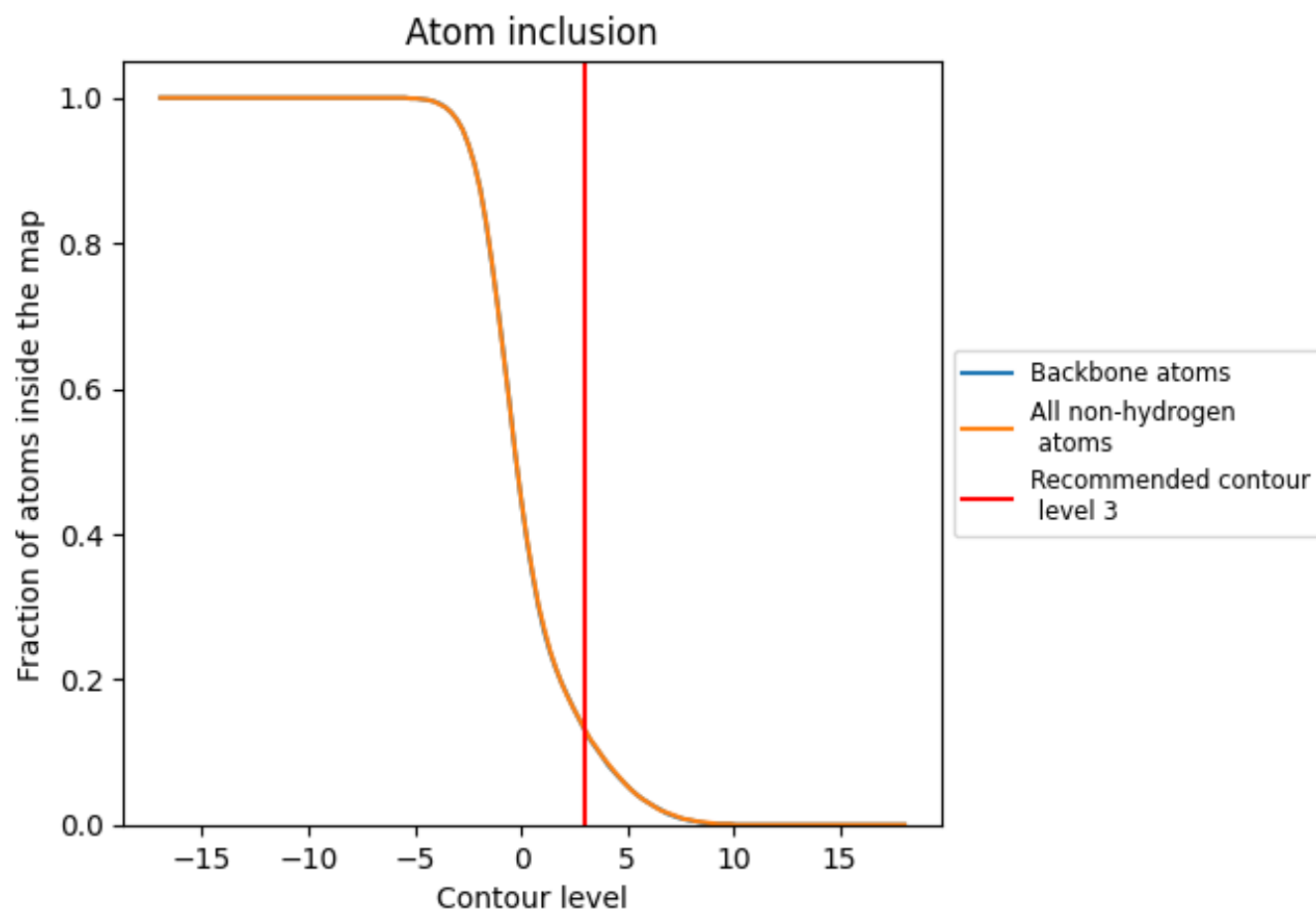
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 13% of all backbone atoms, 13% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1310	-0.0110
A	0.0690	0.0000
B	0.1390	-0.0140
C	0.1650	-0.0200
D	0.1160	-0.0100
E	0.1940	-0.0040

