



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:51 PM UTC

PDB ID : 8CVR / pdb_00008cvr
EMDB ID : EMD-27013
Title : Human 20S proteasome with MG-132
Authors : Zhao, J.
Deposited on : 2022-05-18
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

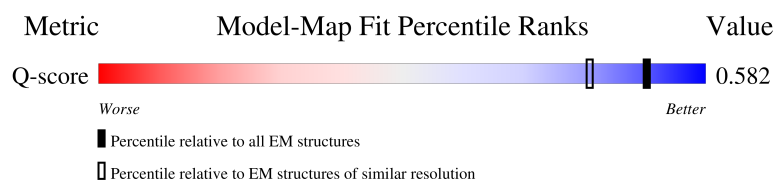
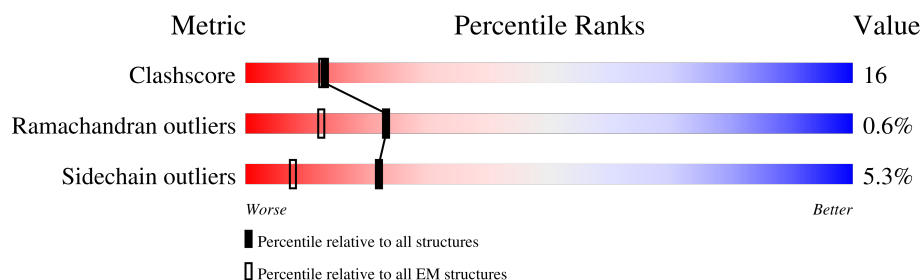
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	246	
1	O	246	
2	B	234	
2	P	234	

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Mol	Chain	Length	Quality of chain
3	C	261	
3	Q	261	
4	D	248	
4	R	248	
5	E	241	
5	S	241	
6	F	263	
6	T	263	
7	G	255	
7	U	255	
8	H	205	
8	V	205	
9	I	234	
9	W	234	
10	J	205	
10	X	205	
11	K	201	
11	Y	201	
12	L	204	
12	Z	204	
13	M	241	
13	a	241	
14	N	264	
14	b	264	

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 45586 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 Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	240	Total	C	N	O	S	0	0
			1738	1106	304	316	12		
1	O	240	Total	C	N	O	S	0	0
			1734	1104	304	314	12		

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1662	1080	288	288	6		
2	P	229	Total	C	N	O	S	0	0
			1662	1080	288	288	6		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	247	Total	C	N	O	S	0	0
			1786	1143	320	313	10		
3	Q	247	Total	C	N	O	S	0	0
			1786	1143	320	313	10		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	232	Total	C	N	O	S	0	0
			1633	1038	306	284	5		
4	R	232	Total	C	N	O	S	0	0
			1633	1038	306	284	5		

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	233	Total	C	N	O	S	0	0
			1660	1056	287	306	11		
5	S	233	Total	C	N	O	S	0	0
			1660	1056	287	306	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	233	Total	C	N	O	S	0	0
			1704	1087	315	293	9		
6	T	233	Total	C	N	O	S	0	0
			1707	1089	315	293	10		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1760	1131	308	311	10		
7	U	239	Total	C	N	O	S	0	0
			1760	1131	308	311	10		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	202	Total	C	N	O	S	0	0
			1469	928	257	272	12		
8	V	202	Total	C	N	O	S	0	0
			1465	926	256	271	12		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	220	Total	C	N	O	S	0	0
			1580	1005	272	294	9		
9	W	220	Total	C	N	O	S	0	0
			1576	1003	272	292	9		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total	C	N	O	S	0	0
			1546	992	262	273	19		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	204	Total	C	N	O	S	0	0
			1534	987	262	267	18		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	196	Total	C	N	O	S	0	0
			1509	974	259	268	8		
11	Y	196	Total	C	N	O	S	0	0
			1506	973	259	266	8		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	200	Total	C	N	O	S	0	0
			1504	957	271	267	9		
12	Z	200	Total	C	N	O	S	0	0
			1500	954	270	267	9		

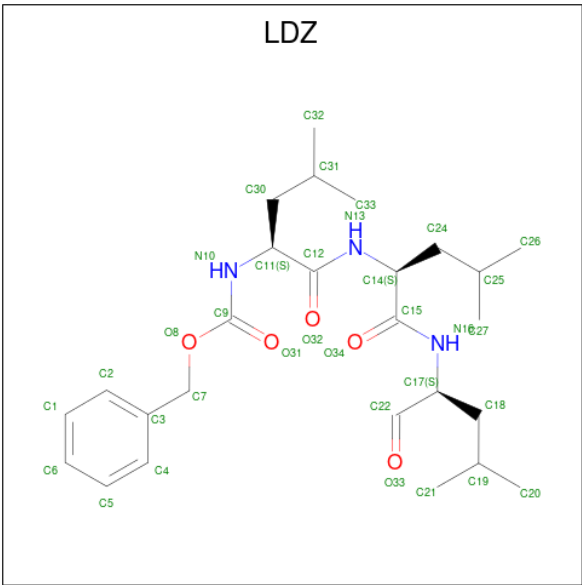
- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	212	Total	C	N	O	S	0	0
			1584	1016	279	279	10		
13	a	212	Total	C	N	O	S	0	0
			1584	1016	279	279	10		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	212	Total	C	N	O	S	0	0
			1568	998	279	280	11		
14	b	212	Total	C	N	O	S	0	0
			1572	1000	279	282	11		

- Molecule 15 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-4-methyl-1-oxopentan-2-yl]-L-leucinamide (CCD ID: LDZ) (formula: C₂₆H₄₁N₃O₅) (labeled as "Ligand of Interest" by depositor).

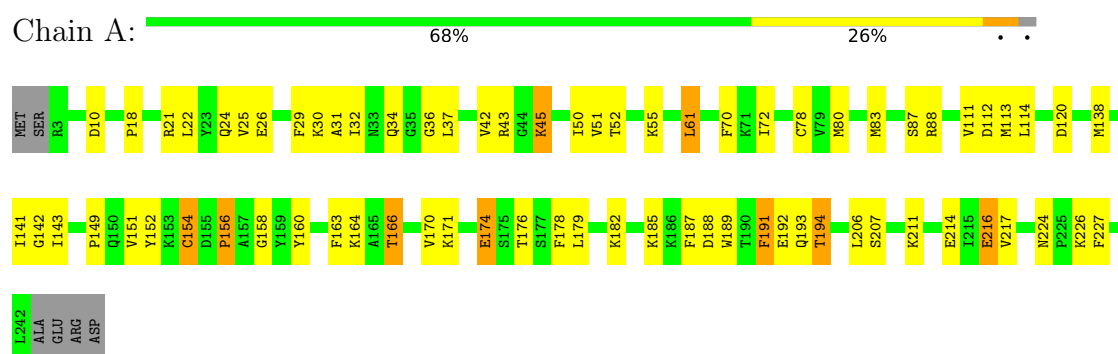


Mol	Chain	Residues	Atoms				AltConf
15	H	1	Total	C	N	O	0
			34	26	3	5	
15	I	1	Total	C	N	O	0
			34	26	3	5	
15	L	1	Total	C	N	O	0
			34	26	3	5	
15	V	1	Total	C	N	O	0
			34	26	3	5	
15	W	1	Total	C	N	O	0
			34	26	3	5	
15	Z	1	Total	C	N	O	0
			34	26	3	5	

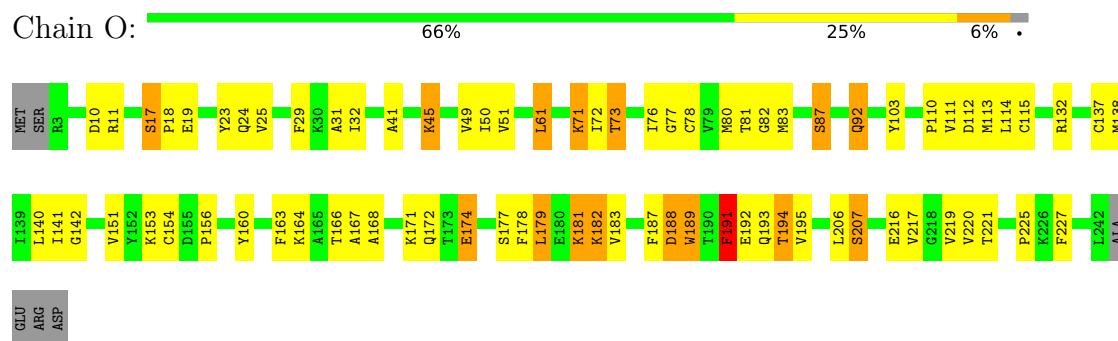
3 Residue-property plots

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.

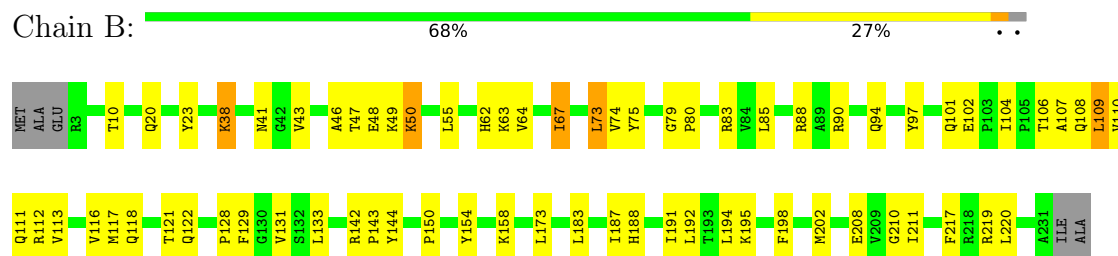
• Molecule 1: Proteasome subunit alpha type-6



• Molecule 1: Proteasome subunit alpha type-6



• Molecule 2: Proteasome subunit alpha type-2



• Molecule 2: Proteasome subunit alpha type-2

Met	Ala	GLU	R3	P14	I21	Y23	A24	L25	V28	K38	N41	E48	K49	K50	K69	H70	L73	V74	M78	G79	P80	R83	R88	K91	L92	Q95	P105	T106	A107	Q108	L109	V110	Q111	R112	V116	F129	G130	V131	S132	L133	L134	T135
C136	G137	P143	P150	S151	Y154	K158	M162	L173	L183	I187	H188	I191	L192	M202	I207	E208	I211	C212	R219	L220	T223	K226	A231	I236	ALA																	

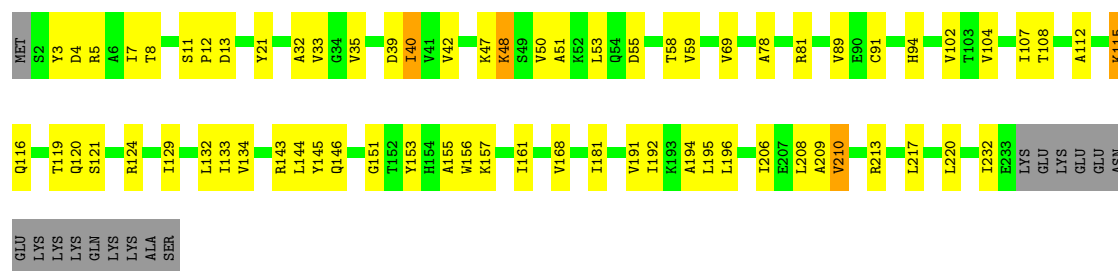
A208	A94	ME1
T215	Q95	S2
L216	Q100	R3
V224	Q109	D6
K229	T112	S7
V233	L114	R8
I237	R128	P14
E248	L135	V21
ARG	G138	A24
GLU	Y143	M25
LYS	Q146	E26
GLU	L147	A27
GLY	P152	I28
LYS	G158	T33
GLU	W159	C34
GLY	K160	L35
GLN	A161	D41
LYS	T162	G42
GLU	C163	V43
GLU	I164	L44
LYS	S168	L45
LYS	A171	A46
ASP	V172	A47
ASP	S173	H53
LYS	M174	L56
LYS	L175	D57
LYS	K176	E58
LYS	K180	Y59
LYS	M184	F60
GLU	T185	F61
GLU	L186	K64
GLY	K187	I65
LYS	L190	Y66
LYS	V196	K67
LYS	K199	L68
LYS	T200	N69
LYS	M201	M72
LYS	D202	A73
LYS	S204	C74
LYS	S207	S75
LYS	L232	V76
LYS	L233	S81
LYS	L234	D82
LYS	L235	A83
LYS	L236	L90
LYS	L237	R91
LYS	L238	L92
LYS	L239	L93

V224	Q119	ME1
I225	S2	R3
V233	G131	T9
I237	V132	P14
E248	S133	Q20
ARG	L134	Y23
GLU	I136	A24
GLU	I137	M25
LYS	G138	E26
LYS	K141	A27
GLU	F145	I28
LYS	Q146	T33
GLU	L147	C34
ASP	G157	L35
LYS	G158	V43
	V159	L44
	K160	L45
	A161	A46
	T162	A47
	C163	E48
	I164	F61
	A171	K64
	M174	L68
	L175	D71
	K176	M72
	Q177	A73
	K180	C74
	M184	S75
	K187	V76
	S188	E89
	A189	L90
	L190	R91
	I194	L92
	K195	I93
	V196	R96
	L197	Y97
	N198	L98
	K199	X101
	T200	Q102
	V203	Q109
	L206	T112
	S207	A113
	A208	L114
	L216	C115

L208	A209	V210	M211	R212	R213	L217	R218	I219	L220	E233	LYS	GLU	LYS	LYS	GLU	GLY	ASN	GLU	LYS	LYS	LYS	GLN	LYS	ALA	SER																	
T108	R109	K115	T119	Q120	S121	R124	I129	L132	I133	V134	G135	F136	G140	T141	P142	R143	L144	Y145	Y153	H154	A155	M156	K157	I161	G162	R163	V168	L172	I181	D184	T187	I188	I192	R193	A194	L195	L196	V199	G202	G203	L206	E207
MET	S2	R5	S11	P12	D13	G14	H15	Y21	E24	K27	A32	V33	R36	V41	V42	K47	K48	L53	Q54	D55	T58	V59	C63	V69	C70	A80	R81	I84	V89	F90	C91	H94	R95	L96	T97	V98	V102	T103	V104	T107		

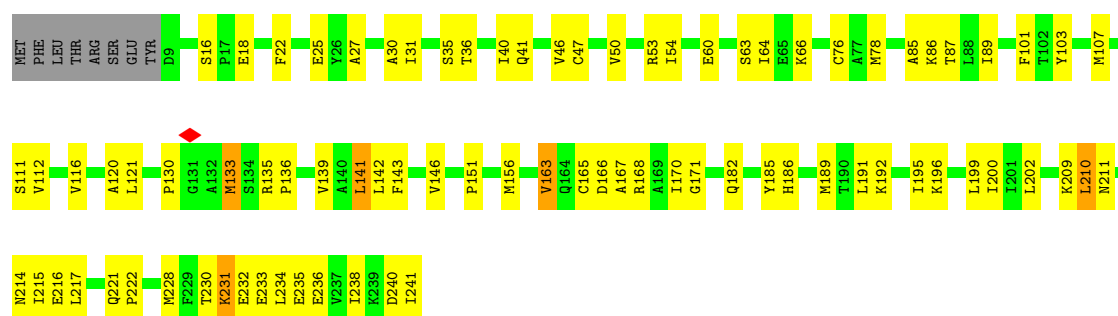
WORLDWIDE
 PDB
PROTEIN DATA BANK

Chain R:  66% 26% 6%



• Molecule 5: Proteasome subunit alpha type-5

Chain E:  62% 32% 6%



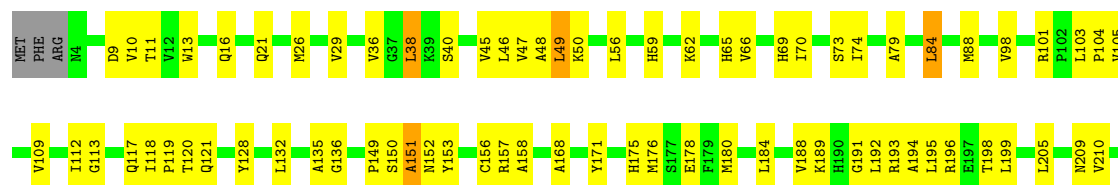
• Molecule 5: Proteasome subunit alpha type-5

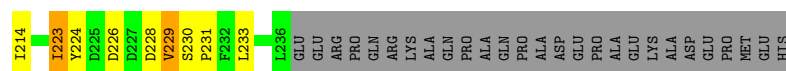
Chain S:  67% 27% 6%



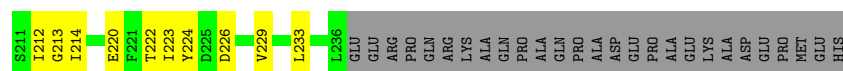
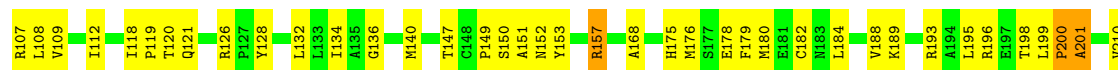
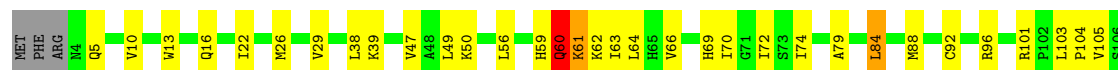
• Molecule 6: Proteasome subunit alpha type-1

Chain F:  57% 29% 11%

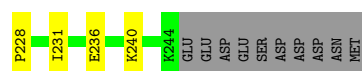
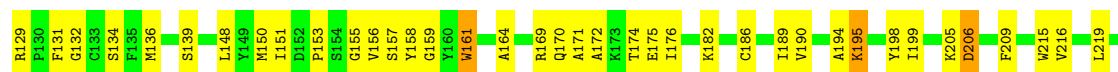




• Molecule 6: Proteasome subunit alpha type-1



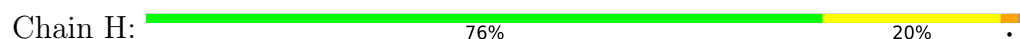
• Molecule 7: Proteasome subunit alpha type-3



• Molecule 7: Proteasome subunit alpha type-3



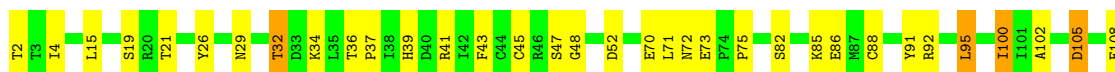
• Molecule 8: Proteasome subunit beta type-6





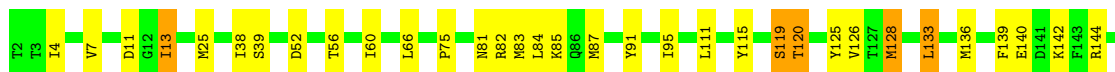
• Molecule 8: Proteasome subunit beta type-6

Chain V: 70% 27% ..



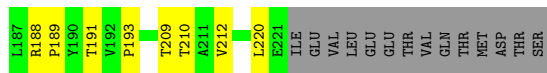
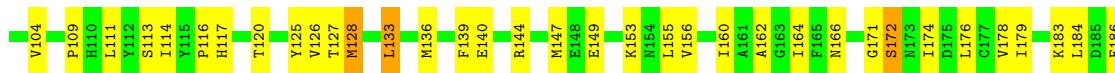
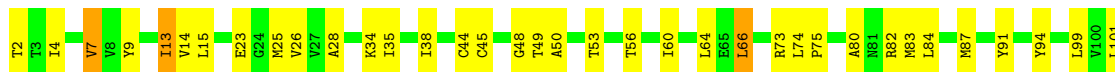
• Molecule 9: Proteasome subunit beta type-7

Chain I: 70% 20% • 6%



• Molecule 9: Proteasome subunit beta type-7

Chain W: 60% 31% • 6%



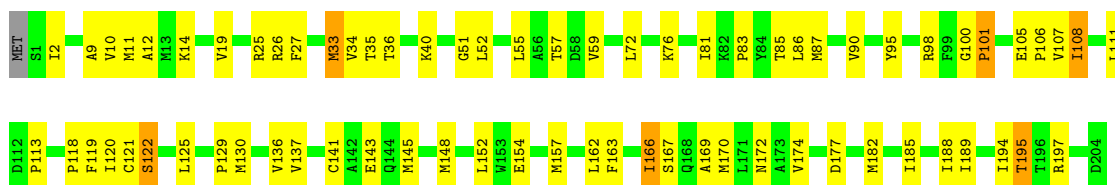
• Molecule 10: Proteasome subunit beta type-3

Chain J: 68% 29% •

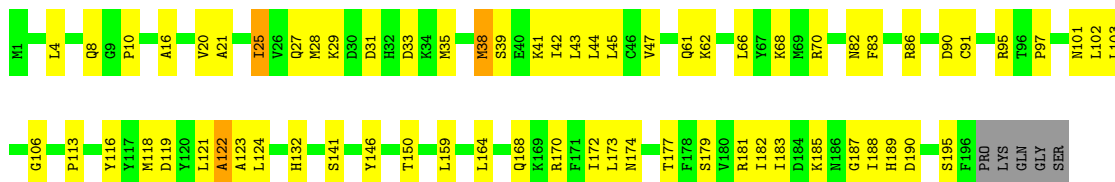


• Molecule 10: Proteasome subunit beta type-3

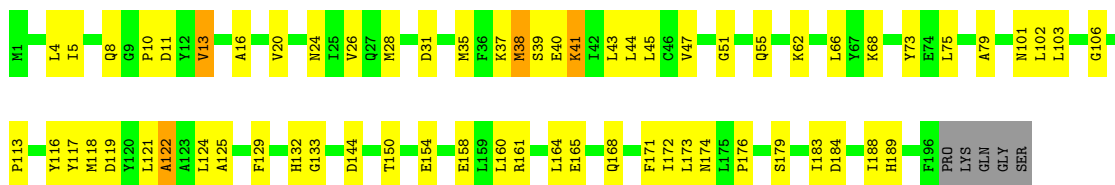
Chain X: 65% 32% •



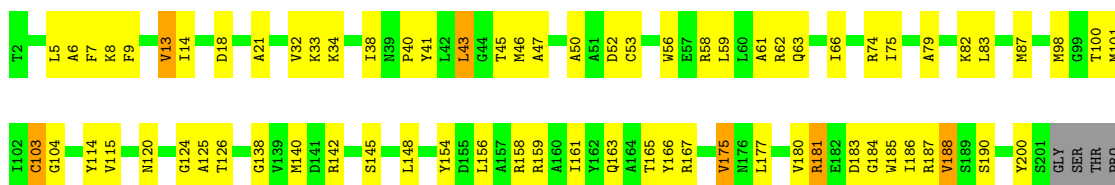
- Molecule 11: Proteasome subunit beta type-2



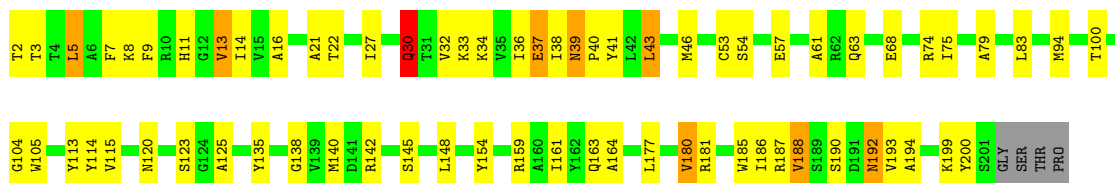
- Molecule 11: Proteasome subunit beta type-2



- Molecule 12: Proteasome subunit beta type-5

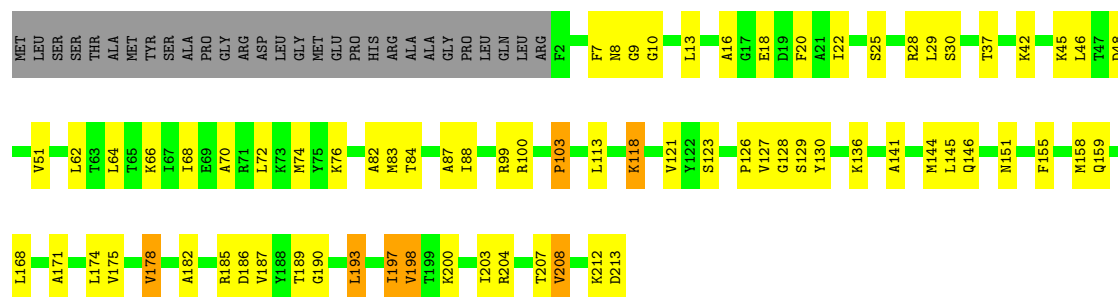


- Molecule 12: Proteasome subunit beta type-5



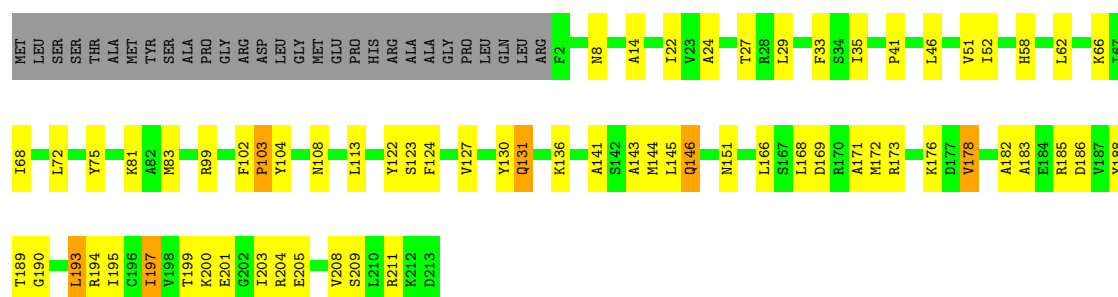
- Molecule 13: Proteasome subunit beta type-1





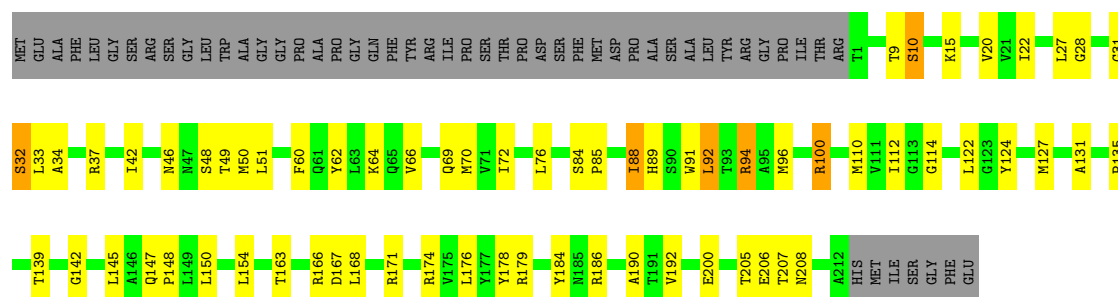
• Molecule 13: Proteasome subunit beta type-1

Chain a: 60% 25% 12%



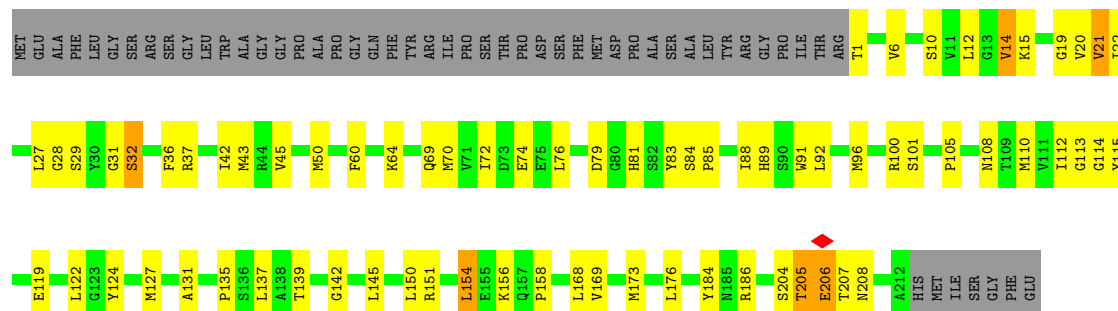
• Molecule 14: Proteasome subunit beta type-4

Chain N: 55% 23% 20%



• Molecule 14: Proteasome subunit beta type-4

Chain b: 53% 25% 20%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	214790	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.788	Depositor
Minimum map value	-0.318	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.93	0/1767	1.21	1/2398 (0.0%)
1	O	0.93	0/1763	1.19	2/2393 (0.1%)
2	B	0.92	0/1701	1.18	2/2318 (0.1%)
2	P	0.92	0/1701	1.18	2/2318 (0.1%)
3	C	0.93	0/1815	1.19	1/2466 (0.0%)
3	Q	0.93	0/1815	1.18	1/2466 (0.0%)
4	D	0.95	0/1657	1.20	2/2261 (0.1%)
4	R	0.95	0/1657	1.19	1/2261 (0.0%)
5	E	0.95	0/1686	1.17	0/2290
5	S	0.94	0/1686	1.16	1/2290 (0.0%)
6	F	0.93	0/1738	1.17	1/2364 (0.0%)
6	T	0.93	0/1741	1.18	2/2367 (0.1%)
7	G	0.92	0/1795	1.17	1/2434 (0.0%)
7	U	0.92	0/1795	1.17	1/2434 (0.0%)
8	H	0.91	0/1495	1.17	0/2026
8	V	0.90	0/1491	1.20	0/2021
9	I	0.91	0/1607	1.21	1/2185 (0.0%)
9	W	0.92	0/1603	1.20	1/2180 (0.0%)
10	J	0.89	0/1575	1.20	4/2128 (0.2%)
10	X	0.89	0/1563	1.21	4/2113 (0.2%)
11	K	0.88	0/1541	1.14	0/2092
11	Y	0.89	0/1538	1.15	1/2088 (0.0%)
12	L	0.88	0/1535	1.14	0/2080
12	Z	0.88	0/1531	1.15	1/2076 (0.0%)
13	M	0.89	0/1614	1.19	1/2178 (0.0%)
13	a	0.90	0/1614	1.18	2/2178 (0.1%)
14	N	0.89	0/1598	1.17	0/2170
14	b	0.90	0/1602	1.18	1/2175 (0.0%)
All	All	0.91	0/46224	1.18	34/62750 (0.1%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	38	ILE	N-CA-C	-7.93	105.47	111.90
9	W	38	ILE	N-CA-C	-7.55	105.32	111.81
2	B	158	LYS	N-CA-C	-7.14	104.69	113.41
2	P	158	LYS	N-CA-C	-7.08	104.77	113.41
3	C	160	LYS	N-CA-C	-6.69	105.24	113.41
7	U	161	TRP	N-CA-C	-6.41	105.62	113.50
6	F	66	VAL	N-CA-C	-6.37	106.59	112.96
14	b	205	THR	N-CA-C	-6.35	105.59	113.15
10	J	34	VAL	N-CA-C	-6.29	106.40	111.81
13	M	103	PRO	N-CA-C	6.04	120.81	111.21
11	Y	133	GLY	CA-C-O	-5.99	118.00	122.37
2	P	69	LYS	N-CA-C	-5.92	106.67	114.31
2	B	67	ILE	N-CA-C	-5.88	105.35	111.58
7	G	161	TRP	N-CA-C	-5.86	105.96	113.23
1	A	194	THR	N-CA-C	-5.82	105.44	112.54
1	O	194	THR	N-CA-C	-5.79	106.06	113.01
10	J	183	GLY	CA-C-O	-5.76	118.48	122.22
10	X	101	PRO	N-CA-C	5.75	120.31	111.57
13	a	103	PRO	N-CA-C	5.66	120.11	111.34
10	J	40	LYS	N-CA-C	-5.58	106.36	114.12
6	T	66	VAL	N-CA-C	-5.56	107.39	111.90
10	X	2	ILE	N-CA-C	-5.54	106.40	113.22
6	T	157	ARG	N-CA-C	-5.48	105.33	112.23
4	D	157	LYS	N-CA-C	-5.46	105.75	112.90
5	S	70	ILE	N-CA-C	-5.45	105.80	111.58
10	J	101	PRO	N-CA-C	5.37	120.73	111.77
3	Q	160	LYS	N-CA-C	-5.29	105.97	112.90
12	Z	30	GLN	N-CA-C	-5.24	105.22	113.02
10	X	40	LYS	N-CA-C	-5.12	107.70	114.31
10	X	34	VAL	N-CA-C	-5.11	107.76	111.90
4	D	98	VAL	N-CA-C	-5.09	108.01	112.90
4	R	157	LYS	N-CA-C	-5.07	105.45	111.69
1	O	164	LYS	N-CA-C	-5.07	105.84	111.36
13	a	131	GLN	CB-CA-C	-5.03	99.73	109.68

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1738	0	1656	58	0
1	O	1734	0	1652	63	0
2	B	1662	0	1590	52	0
2	P	1662	0	1590	49	0
3	C	1786	0	1717	66	0
3	Q	1786	0	1717	52	0
4	D	1633	0	1518	58	0
4	R	1633	0	1518	54	0
5	E	1660	0	1589	59	0
5	S	1660	0	1589	58	0
6	F	1704	0	1638	71	0
6	T	1707	0	1645	64	0
7	G	1760	0	1680	59	0
7	U	1760	0	1680	58	0
8	H	1469	0	1422	42	0
8	V	1465	0	1416	54	0
9	I	1580	0	1559	54	0
9	W	1576	0	1555	70	0
10	J	1546	0	1552	59	0
10	X	1534	0	1539	56	0
11	K	1509	0	1477	49	0
11	Y	1506	0	1475	48	0
12	L	1504	0	1449	57	0
12	Z	1500	0	1438	65	0
13	M	1584	0	1579	57	0
13	a	1584	0	1579	58	0
14	N	1568	0	1513	53	0
14	b	1572	0	1517	58	0
15	H	34	0	41	3	0
15	I	34	0	41	3	0
15	L	34	0	41	12	0
15	V	34	0	41	9	0
15	W	34	0	41	9	0
15	Z	34	0	41	11	0
All	All	45586	0	44095	1466	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 16.

All (1466) 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)
15:Z:301:LDZ:C6	13:a:131:GLN:HB2	1.81	1.11
3:Q:158:GLY:H	4:R:58:THR:HG21	1.16	1.09
3:C:158:GLY:H	4:D:58:THR:HG21	1.03	1.07
8:V:45:CYS:HB2	8:V:100:ILE:HG23	1.43	1.00
9:I:188:ARG:HB3	9:I:189:PRO:HD3	1.46	0.96
2:P:73:LEU:HD11	2:P:133:LEU:HB3	1.46	0.94
6:T:50:LYS:HB3	6:T:59:HIS:HB3	1.48	0.94
1:O:183:VAL:HA	1:O:187:PHE:HA	1.48	0.93
15:W:301:LDZ:H3	10:X:125:LEU:HD21	1.49	0.93
3:C:158:GLY:N	4:D:58:THR:HG21	1.84	0.93
5:S:31:ILE:HD13	5:S:140:ALA:HB2	1.54	0.89
5:E:146:VAL:HG11	5:E:222:PRO:HA	1.56	0.88
2:P:202:MET:HE3	2:P:207:ILE:HG21	1.56	0.88
6:T:47:VAL:HG12	6:T:195:LEU:HD22	1.56	0.87
10:J:148:MET:HG2	10:J:169:ALA:HA	1.56	0.86
13:M:144:MET:HE1	13:M:185:ARG:HB2	1.56	0.85
12:Z:192:ASN:HD22	12:Z:194:ALA:H	1.22	0.85
10:X:148:MET:HG2	10:X:169:ALA:HA	1.56	0.85
15:Z:301:LDZ:C5	13:a:131:GLN:HB2	2.05	0.84
3:Q:158:GLY:N	4:R:58:THR:HG21	1.92	0.84
1:A:52:THR:HG23	1:A:216:GLU:HG3	1.58	0.84
12:Z:13:VAL:HG13	12:Z:180:VAL:HB	1.59	0.84
2:B:118:GLN:HG3	3:C:81:SER:HB2	1.59	0.84
10:J:117:LYS:HD2	10:J:118:PRO:HD2	1.60	0.83
13:a:186:ASP:HB3	13:a:189:THR:HG22	1.60	0.83
8:V:139:TYR:O	8:V:143:THR:HG22	1.79	0.83
13:M:186:ASP:HB3	13:M:189:THR:HG22	1.59	0.82
12:L:13:VAL:HG13	12:L:180:VAL:HB	1.61	0.82
13:M:145:LEU:HD21	13:M:182:ALA:HB2	1.62	0.81
14:N:145:LEU:HD21	14:N:179:ARG:HB2	1.60	0.81
10:J:11:MET:HE2	10:J:166:ILE:HG13	1.63	0.81
13:a:145:LEU:HD21	13:a:182:ALA:HB2	1.62	0.81
12:L:47:ALA:HA	15:L:301:LDZ:H20	1.62	0.81
8:H:88:CYS:SG	8:H:119:GLY:HA2	2.21	0.80
8:V:52:ASP:HB3	8:V:95:LEU:HD13	1.61	0.80
3:Q:76:VAL:HG12	3:Q:134:LEU:HD22	1.63	0.80
6:T:50:LYS:HB3	6:T:59:HIS:CB	2.13	0.79
8:H:139:TYR:O	8:H:143:THR:HG22	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:188:ARG:HB3	9:W:189:PRO:HD3	1.65	0.79
15:Z:301:LDZ:H5	13:a:131:GLN:CD	2.08	0.79
10:J:11:MET:HG3	10:J:137:VAL:HG12	1.65	0.79
8:V:143:THR:HG23	8:V:156:PHE:CE1	2.18	0.78
2:P:88:ARG:HH11	2:P:88:ARG:HB3	1.48	0.78
7:U:99:ARG:HH11	14:b:69:GLN:HE22	1.32	0.78
14:b:22:ILE:HG23	14:b:50:MET:HE3	1.66	0.78
12:Z:7:PHE:HB3	12:Z:140:MET:HE2	1.66	0.78
7:G:117:MET:HA	7:G:117:MET:HE2	1.67	0.77
9:W:50:ALA:HA	15:W:301:LDZ:H19	1.66	0.77
3:C:44:LEU:HD22	3:C:190:LEU:HD12	1.64	0.77
9:I:52:ASP:HB3	9:I:95:ILE:HG23	1.65	0.77
1:O:61:LEU:HD21	7:U:158:TYR:HB3	1.66	0.76
1:O:78:CYS:SG	1:O:138:MET:HG3	2.25	0.76
6:T:49:LEU:HB2	6:T:195:LEU:HD11	1.67	0.76
1:O:72:ILE:HG21	1:O:114:LEU:HD21	1.68	0.76
10:X:19:VAL:HG23	10:X:189:ILE:HB	1.67	0.76
6:F:26:MET:HA	6:F:149:PRO:HG2	1.67	0.75
8:H:143:THR:HG23	8:H:156:PHE:CE1	2.21	0.75
13:a:145:LEU:HD22	13:a:178:VAL:HG22	1.66	0.75
8:H:29:ASN:HB2	15:H:301:LDZ:H4	1.69	0.75
2:P:110:VAL:HG22	2:P:135:ILE:HD12	1.68	0.75
8:V:143:THR:HG23	8:V:156:PHE:HE1	1.52	0.74
1:A:24:GLN:NE2	7:G:14:PHE:H	1.85	0.74
3:Q:194:ILE:HG23	3:Q:206:LEU:HD12	1.70	0.74
15:I:301:LDZ:H3	10:J:125:LEU:HD21	1.70	0.74
8:V:82:SER:O	8:V:86:GLU:HG2	1.88	0.74
14:N:150:LEU:HD23	14:N:168:LEU:HG	1.68	0.73
5:S:54:ILE:HD13	5:S:64:ILE:HD12	1.70	0.73
9:I:13:ILE:HG23	9:I:179:ILE:HB	1.70	0.73
11:K:39:SER:HB2	11:K:42:ILE:HG12	1.70	0.73
12:L:21:ALA:HB2	12:L:32:VAL:HG21	1.69	0.73
9:I:164:ILE:HG23	9:I:171:GLY:HA2	1.71	0.73
9:W:164:ILE:HG23	9:W:171:GLY:HA2	1.69	0.73
2:P:73:LEU:HD13	2:P:135:ILE:HG12	1.71	0.73
12:L:50:ALA:HA	15:L:301:LDZ:H19	1.71	0.73
8:H:45:CYS:HB2	8:H:100:ILE:CG1	2.19	0.72
9:W:153:LYS:HD3	9:W:178:VAL:HG21	1.69	0.72
4:R:89:VAL:HG22	11:Y:66:LEU:HD21	1.69	0.72
15:Z:301:LDZ:H5	13:a:131:GLN:OE1	1.89	0.72
10:X:26:ARG:HB2	10:X:182:MET:HB2	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:55:ASP:O	4:D:58:THR:HG22	1.88	0.72
10:X:188:ILE:HB	10:X:195:THR:HG23	1.70	0.72
4:R:55:ASP:O	4:R:58:THR:HG22	1.89	0.71
7:G:99:ARG:HH11	14:N:69:GLN:HE22	1.38	0.71
3:Q:44:LEU:HD22	3:Q:190:LEU:HD12	1.71	0.71
2:P:80:PRO:HA	2:P:83:ARG:HE	1.56	0.71
3:C:43:VAL:HG23	3:C:216:LEU:HB3	1.70	0.71
9:I:81:ASN:HD21	9:I:120:THR:HG21	1.55	0.71
6:T:60:GLN:O	6:T:61:LYS:HB3	1.91	0.71
13:a:186:ASP:HB3	13:a:189:THR:CG2	2.21	0.70
15:V:301:LDZ:H2	9:W:117:HIS:HD2	1.55	0.70
3:C:53:HIS:H	3:C:56:LEU:HD12	1.57	0.70
6:F:152:ASN:HA	7:G:85:ARG:HH22	1.55	0.70
8:V:88:CYS:SG	8:V:119:GLY:HA2	2.31	0.70
11:Y:4:LEU:HD22	11:Y:45:LEU:HB3	1.73	0.70
3:C:171:ALA:HB2	3:C:200:THR:HG21	1.73	0.70
6:T:103:LEU:HD12	6:T:104:PRO:HD2	1.74	0.70
12:Z:36:ILE:HD11	12:Z:46:MET:HE3	1.73	0.70
2:P:28:VAL:HG11	2:P:132:SER:HB2	1.73	0.70
14:N:60:PHE:CE2	14:N:64:LYS:HD2	2.26	0.70
1:O:183:VAL:HA	1:O:187:PHE:CA	2.20	0.70
1:A:111:VAL:HG21	1:A:142:GLY:HA3	1.74	0.69
8:V:52:ASP:HB3	8:V:95:LEU:CD1	2.21	0.69
1:A:224:ASN:HD21	1:A:226:LYS:HG2	1.57	0.69
5:E:103:TYR:CD1	13:M:83:MET:HE3	2.27	0.69
10:J:11:MET:CE	10:J:166:ILE:HG13	2.22	0.69
14:N:10:SER:HB3	14:N:139:THR:O	1.93	0.69
1:O:171:LYS:HD2	1:O:174:GLU:HG3	1.74	0.69
1:A:191:PHE:CD1	1:A:193:GLN:HB2	2.27	0.69
9:W:220:LEU:HD11	10:X:194:ILE:HG12	1.74	0.69
7:U:108:LEU:HD21	7:U:137:LEU:HB3	1.75	0.69
14:b:92:LEU:O	14:b:96:MET:HG2	1.93	0.69
10:X:11:MET:HE2	10:X:170:MET:HG2	1.74	0.69
11:Y:35:MET:HG2	11:Y:45:LEU:HG	1.73	0.69
9:W:9:TYR:CE2	9:W:149:GLU:HG2	2.28	0.69
11:K:35:MET:HB2	11:K:181:ARG:HH21	1.57	0.69
12:Z:39:ASN:HB2	12:Z:41:TYR:CD1	2.28	0.69
5:E:166:ASP:HB3	5:E:185:TYR:CZ	2.27	0.68
7:U:213:LEU:HD12	7:U:232:ARG:HG3	1.74	0.68
15:V:301:LDZ:H1	9:W:116:PRO:HD2	1.74	0.68
8:V:85:LYS:HA	8:V:88:CYS:SG	2.34	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:150:LEU:HD23	14:b:168:LEU:HG	1.76	0.68
8:V:116:PRO:HD2	8:V:120:MET:O	1.92	0.68
10:J:202:ARG:HH22	12:Z:192:ASN:HD21	1.41	0.68
12:Z:43:LEU:HD21	12:Z:180:VAL:HG22	1.76	0.68
14:b:70:MET:HE1	14:b:91:TRP:CE2	2.29	0.68
12:Z:38:ILE:HG23	12:Z:61:ALA:HA	1.75	0.68
8:H:85:LYS:HD2	8:H:121:MET:HE2	1.76	0.67
4:R:40:ILE:HG13	4:R:210:VAL:HG13	1.76	0.67
14:N:96:MET:HE3	14:N:127:MET:HA	1.76	0.67
15:Z:301:LDZ:H5	13:a:131:GLN:HB2	1.71	0.67
7:U:117:MET:HA	7:U:117:MET:HE2	1.77	0.67
2:B:118:GLN:CG	3:C:81:SER:HB2	2.24	0.67
13:M:123:SER:HB3	13:M:136:LYS:HG2	1.76	0.67
13:a:99:ARG:HD3	13:a:104:TYR:CZ	2.30	0.67
7:U:134:SER:OG	7:U:153:PRO:HD3	1.94	0.67
11:K:28:MET:HE1	12:L:114:TYR:CE2	2.30	0.67
12:Z:21:ALA:HB2	12:Z:32:VAL:HG21	1.75	0.67
1:O:188:ASP:O	1:O:189:TRP:C	2.37	0.66
6:F:121:GLN:HG3	7:G:129:ARG:HG2	1.76	0.66
6:F:196:ARG:HG3	6:F:199:LEU:HD12	1.77	0.66
11:K:35:MET:HG2	11:K:45:LEU:HG	1.78	0.66
13:M:186:ASP:HB3	13:M:189:THR:CG2	2.25	0.66
6:F:152:ASN:HA	7:G:85:ARG:NH2	2.11	0.66
4:R:91:CYS:HA	4:R:102:VAL:HG11	1.78	0.66
13:a:169:ASP:O	13:a:173:ARG:HG3	1.95	0.66
12:L:38:ILE:HG23	12:L:61:ALA:HA	1.77	0.66
3:Q:158:GLY:H	4:R:58:THR:CG2	2.01	0.66
1:A:24:GLN:HE21	7:G:14:PHE:H	1.43	0.66
6:F:152:ASN:HD22	7:G:85:ARG:HH22	1.44	0.66
1:A:31:ALA:HB1	1:A:83:MET:HE3	1.78	0.65
15:I:301:LDZ:H5	10:J:98:ARG:HH12	1.59	0.65
15:V:301:LDZ:C1	9:W:116:PRO:HD2	2.25	0.65
14:b:96:MET:HE3	14:b:127:MET:HA	1.77	0.65
9:I:60:ILE:HD12	9:I:83:MET:HB3	1.79	0.65
5:E:54:ILE:HD13	5:E:64:ILE:HD12	1.78	0.65
1:A:191:PHE:CE1	1:A:193:GLN:HB2	2.31	0.65
12:L:34:LYS:HE2	15:L:301:LDZ:H23	1.78	0.65
6:T:59:HIS:O	6:T:60:GLN:HB2	1.96	0.65
11:K:164:LEU:O	11:K:168:GLN:HG2	1.96	0.65
5:S:203:LYS:HE3	5:S:210:LEU:HB3	1.79	0.65
4:D:135:GLY:HA2	4:D:211:MET:HE1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:159:ARG:HH21	12:L:163:GLN:NE2	1.95	0.64
6:F:121:GLN:HG3	7:G:129:ARG:CG	2.27	0.64
9:I:111:LEU:HD21	9:I:126:VAL:HG22	1.78	0.64
3:Q:174:MET:HE1	3:Q:199:LYS:HB2	1.78	0.64
14:b:205:THR:O	14:b:207:THR:N	2.30	0.64
4:D:192:ILE:O	4:D:196:LEU:HG	1.96	0.64
5:S:31:ILE:HD11	5:S:158:PRO:CG	2.26	0.64
13:a:75:TYR:CG	13:a:83:MET:HG2	2.33	0.64
1:A:224:ASN:ND2	1:A:226:LYS:HG2	2.13	0.64
4:D:94:HIS:HB3	4:D:102:VAL:HG12	1.79	0.64
6:F:176:MET:HE3	7:G:57:LEU:HD23	1.78	0.64
5:S:50:VAL:HG12	5:S:216:GLU:HB3	1.78	0.64
1:O:24:GLN:HE21	7:U:14:PHE:H	1.44	0.64
3:Q:35:LEU:HG	3:Q:46:ALA:HB3	1.80	0.64
6:T:128:TYR:O	6:T:149:PRO:HB3	1.97	0.64
5:S:22:PHE:O	5:S:25:GLU:HG2	1.98	0.64
12:Z:43:LEU:HD21	12:Z:180:VAL:CG2	2.28	0.64
7:G:131:PHE:O	7:G:153:PRO:HB3	1.97	0.63
12:L:5:LEU:HD11	12:L:140:MET:SD	2.37	0.63
13:M:29:LEU:HB3	13:M:37:THR:HG22	1.80	0.63
2:B:64:VAL:HG12	2:B:217:PHE:HZ	1.63	0.63
6:F:105:VAL:O	6:F:109:VAL:HG23	1.97	0.63
12:L:41:TYR:CE1	12:L:74:ARG:HD3	2.33	0.63
12:Z:5:LEU:CD2	12:Z:16:ALA:HB3	2.28	0.63
3:C:147:LEU:HD21	3:C:162:THR:HG22	1.80	0.63
12:L:45:THR:HG21	12:L:101:MET:HE3	1.79	0.63
6:T:152:ASN:ND2	7:U:85:ARG:HH21	1.96	0.63
12:L:180:VAL:HA	12:L:185:TRP:HA	1.80	0.63
13:a:41:PRO:HB3	13:a:194:ARG:HG3	1.80	0.63
5:E:116:VAL:HB	5:E:156:MET:HE1	1.81	0.63
5:S:20:ARG:O	5:S:21:LEU:HB2	1.98	0.63
3:C:202:ASP:O	3:C:203:VAL:C	2.42	0.63
10:X:83:PRO:HD3	10:X:113:PRO:HD3	1.81	0.63
11:Y:38:MET:HE3	11:Y:44:LEU:HB2	1.81	0.63
10:J:26:ARG:HB2	10:J:182:MET:HB2	1.80	0.62
1:A:72:ILE:HG21	1:A:114:LEU:HD21	1.80	0.62
1:A:80:MET:HB3	1:A:87:SER:HB2	1.81	0.62
4:R:42:VAL:HG22	4:R:210:VAL:HG22	1.81	0.62
9:I:81:ASN:ND2	9:I:120:THR:HG21	2.15	0.62
2:B:183:LEU:O	2:B:187:ILE:HG13	2.00	0.62
1:O:81:THR:HB	1:O:137:CYS:SG	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:56:THR:HG23	9:I:87:MET:HE3	1.80	0.62
4:R:47:LYS:O	4:R:48:LYS:C	2.42	0.62
5:E:103:TYR:HD1	13:M:83:MET:HE3	1.63	0.62
12:L:187:ARG:HH22	12:L:190:SER:HB2	1.65	0.62
2:P:79:GLY:N	2:P:80:PRO:HD2	2.14	0.62
4:D:80:ALA:HA	4:D:129:ILE:HD13	1.80	0.62
8:V:188:GLN:HE21	8:V:190:LEU:HD21	1.63	0.62
10:X:148:MET:HE3	10:X:152:LEU:HD11	1.81	0.62
14:N:92:LEU:O	14:N:96:MET:HG2	2.00	0.62
2:B:85:LEU:HD13	2:B:133:LEU:HD11	1.82	0.62
3:C:174:MET:HE3	3:C:196:VAL:HA	1.81	0.62
6:F:175:HIS:O	6:F:178:GLU:HG2	2.00	0.62
8:H:4:ILE:HD12	8:H:100:ILE:HG12	1.82	0.62
8:H:116:PRO:HD2	8:H:120:MET:O	2.00	0.62
8:V:48:GLY:O	15:V:301:LDZ:H23	2.00	0.62
13:a:46:LEU:HD11	13:a:52:ILE:HB	1.81	0.62
4:D:91:CYS:HA	4:D:102:VAL:HG11	1.81	0.61
13:M:198:VAL:HG13	13:M:203:ILE:HG12	1.82	0.61
12:Z:39:ASN:HB2	12:Z:41:TYR:HD1	1.62	0.61
4:D:24:GLU:HA	4:D:27:LYS:HE2	1.81	0.61
13:a:193:LEU:HB3	13:a:208:VAL:HG12	1.82	0.61
3:Q:112:THR:HG23	4:R:81:ARG:HD2	1.83	0.61
12:L:43:LEU:HD21	12:L:180:VAL:CG2	2.30	0.61
12:L:43:LEU:HD23	12:L:43:LEU:N	2.15	0.61
2:P:108:GLN:HE21	2:P:112:ARG:HH12	1.47	0.61
4:R:208:LEU:HD23	4:R:209:ALA:N	2.16	0.61
3:C:138:GLY:HA2	3:C:216:LEU:HD13	1.81	0.61
6:F:119:PRO:HG2	6:F:128:TYR:CE1	2.35	0.61
8:H:85:LYS:HG3	8:H:119:GLY:O	2.01	0.61
4:R:35:VAL:HG22	4:R:191:VAL:HG23	1.82	0.61
8:V:100:ILE:CD1	8:V:112:VAL:HG13	2.31	0.61
13:M:187:VAL:HG21	9:W:25:MET:HE3	1.83	0.61
9:W:111:LEU:HD21	9:W:126:VAL:HG22	1.81	0.61
12:Z:7:PHE:HB3	12:Z:140:MET:CE	2.30	0.61
2:B:67:ILE:HD11	2:B:73:LEU:HD21	1.83	0.60
10:X:10:VAL:HG11	10:X:51:GLY:HA3	1.81	0.60
11:Y:164:LEU:O	11:Y:168:GLN:HG2	2.01	0.60
15:L:301:LDZ:H1	13:M:126:PRO:HB2	1.83	0.60
12:Z:30:GLN:HE21	12:Z:30:GLN:HA	1.65	0.60
8:H:135:TYR:HA	8:V:134:SER:O	2.01	0.60
9:I:153:LYS:HD3	9:I:178:VAL:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:43:LEU:N	12:Z:43:LEU:HD23	2.16	0.60
8:H:143:THR:HG23	8:H:156:PHE:HE1	1.62	0.60
8:V:43:PHE:CZ	8:V:185:VAL:HG11	2.37	0.60
3:Q:44:LEU:HD23	3:Q:189:ALA:HB1	1.84	0.60
1:A:45:LYS:HB2	1:A:45:LYS:NZ	2.16	0.60
8:H:20:ARG:HG2	8:H:22:THR:HG23	1.82	0.60
2:P:106:THR:O	2:P:110:VAL:HG23	2.02	0.60
2:P:183:LEU:O	2:P:187:ILE:HG13	2.02	0.60
5:E:107:MET:HG2	5:E:111:SER:OG	2.02	0.60
8:H:45:CYS:HB2	8:H:100:ILE:HG13	1.84	0.60
12:L:138:GLY:O	12:L:142:ARG:HG2	2.02	0.59
1:O:103:TYR:O	9:W:82:ARG:HD3	2.02	0.59
6:T:226:ASP:O	6:T:229:VAL:HG22	2.02	0.59
7:U:175:GLU:HA	7:U:178:LYS:HE2	1.84	0.59
13:a:22:ILE:HD11	13:a:168:LEU:HD12	1.84	0.59
6:F:119:PRO:HG2	6:F:128:TYR:HE1	1.67	0.59
10:J:148:MET:HE3	10:J:152:LEU:HD11	1.84	0.59
11:Y:116:TYR:HB3	11:Y:124:LEU:HD11	1.84	0.59
3:C:95:GLN:HG3	10:J:72:LEU:HD13	1.83	0.59
11:Y:103:LEU:HG	11:Y:132:HIS:HD2	1.67	0.59
5:S:120:ALA:O	5:S:121:LEU:HB2	2.02	0.59
5:S:133:MET:HE3	5:S:133:MET:HA	1.82	0.59
7:U:81:LEU:O	7:U:85:ARG:HG3	2.02	0.59
15:L:301:LDZ:O8	15:L:301:LDZ:H35	2.02	0.59
3:C:174:MET:HE1	3:C:199:LYS:HB2	1.85	0.59
4:D:168:VAL:HG13	4:D:194:ALA:HB1	1.85	0.59
5:E:66:LYS:HA	5:E:78:MET:HE2	1.84	0.59
4:R:94:HIS:CG	4:R:102:VAL:HG12	2.37	0.59
8:V:45:CYS:HB2	8:V:100:ILE:CG2	2.25	0.59
9:W:156:VAL:O	9:W:160:ILE:HG12	2.03	0.59
3:Q:135:LEU:HG	3:Q:164:ILE:HD13	1.83	0.59
13:a:27:THR:CG2	13:a:194:ARG:HG2	2.33	0.59
2:B:129:PHE:O	2:B:150:PRO:HB3	2.03	0.59
3:Q:43:VAL:HG22	3:Q:145:PHE:HB3	1.85	0.59
14:b:108:ASN:HB3	14:b:110:MET:SD	2.43	0.59
4:D:69:VAL:HG11	4:D:107:ILE:HG21	1.83	0.58
5:E:133:MET:HE3	5:E:133:MET:HA	1.85	0.58
14:N:70:MET:HE1	14:N:91:TRP:CE2	2.38	0.58
12:Z:36:ILE:HD11	12:Z:46:MET:SD	2.43	0.58
1:O:50:ILE:HD11	1:O:227:PHE:CE1	2.38	0.58
1:O:177:SER:O	1:O:181:LYS:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:50:VAL:HG11	5:S:66:LYS:HB2	1.85	0.58
13:a:194:ARG:HH21	13:a:205:GLU:HB3	1.67	0.58
11:K:101:ASN:HD22	11:K:119:ASP:HA	1.68	0.58
6:T:200:PRO:O	6:T:201:ALA:C	2.45	0.58
6:F:196:ARG:O	6:F:199:LEU:HB2	2.03	0.58
11:K:10:PRO:HG3	11:K:150:THR:HA	1.85	0.58
12:Z:46:MET:HE1	12:Z:54:SER:HA	1.85	0.58
9:I:214:THR:HG23	10:J:198:THR:HB	1.85	0.58
10:X:25:ARG:HD3	10:X:185:ILE:HB	1.86	0.58
7:G:52:LEU:HD23	7:G:209:PHE:HB3	1.83	0.58
1:O:191:PHE:O	1:O:194:THR:HG23	2.04	0.58
12:Z:36:ILE:N	12:Z:36:ILE:HD12	2.18	0.58
2:B:88:ARG:HB3	2:B:88:ARG:NH1	2.18	0.58
12:L:159:ARG:HH21	12:L:163:GLN:HE21	1.52	0.58
8:V:145:ARG:O	8:V:148:MET:HG3	2.03	0.58
9:W:127:THR:OG1	9:W:136:MET:HG2	2.03	0.58
14:b:92:LEU:HD23	14:b:112:ILE:HD11	1.84	0.58
3:C:8:ARG:HH21	4:D:5:ARG:NE	2.02	0.58
4:D:199:VAL:HG11	4:D:206:ILE:HG22	1.84	0.58
10:J:10:VAL:HG11	10:J:51:GLY:HA3	1.85	0.58
1:A:138:MET:HB3	1:A:154:CYS:SG	2.44	0.58
3:C:21:VAL:O	3:C:25:MET:HG3	2.03	0.58
9:I:13:ILE:HD13	9:I:111:LEU:HD13	1.85	0.58
11:K:41:LYS:HD3	11:K:187:GLY:HA2	1.86	0.58
12:L:21:ALA:HB1	15:L:301:LDZ:H38	1.86	0.58
9:I:136:MET:HE2	9:I:140:GLU:HG2	1.86	0.58
14:N:22:ILE:HG23	14:N:50:MET:HE3	1.84	0.58
11:Y:184:ASP:OD1	11:Y:189:HIS:HE1	1.87	0.58
3:C:3:ARG:O	3:C:8:ARG:NH2	2.33	0.57
7:G:164:ALA:O	7:G:169:ARG:HG3	2.04	0.57
12:L:104:GLY:HA2	12:L:180:VAL:HG11	1.85	0.57
6:T:175:HIS:O	6:T:178:GLU:HG2	2.04	0.57
14:N:9:THR:HG23	14:N:10:SER:H	1.68	0.57
12:Z:36:ILE:CD1	12:Z:46:MET:HE3	2.34	0.57
9:I:125:TYR:CD2	9:I:136:MET:HE1	2.39	0.57
1:A:32:ILE:HD11	1:A:156:PRO:CG	2.34	0.57
11:K:181:ARG:HG2	11:K:190:ASP:HA	1.85	0.57
1:O:206:LEU:O	1:O:207:SER:C	2.47	0.57
3:C:8:ARG:HH21	4:D:5:ARG:HE	1.52	0.57
7:U:52:LEU:HD23	7:U:209:PHE:HB3	1.84	0.57
13:a:68:ILE:O	13:a:72:LEU:HG	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:121:LEU:HD12	6:F:79:ALA:HB3	1.87	0.57
6:F:26:MET:HG2	6:F:149:PRO:HD2	1.86	0.57
4:R:4:ASP:O	5:S:125:GLU:HB2	2.04	0.57
10:X:148:MET:CG	10:X:169:ALA:HA	2.32	0.57
6:T:64:LEU:CD1	6:T:74:ILE:HD11	2.34	0.57
2:B:79:GLY:N	2:B:80:PRO:HD2	2.20	0.57
14:N:31:GLY:O	14:N:32:SER:HB3	2.05	0.57
7:U:15:SER:C	7:U:17:ASP:H	2.13	0.57
12:Z:36:ILE:HD11	12:Z:46:MET:CE	2.34	0.57
9:I:188:ARG:CB	9:I:189:PRO:HD3	2.29	0.57
12:L:75:ILE:HG12	12:L:79:ALA:HB3	1.86	0.57
2:B:80:PRO:HA	2:B:83:ARG:HE	1.70	0.57
8:H:19:SER:C	8:H:32:THR:HG23	2.30	0.57
5:S:200:ILE:O	5:S:204:GLN:HG3	2.05	0.57
6:F:65:HIS:NE2	6:F:223:ILE:HD12	2.20	0.56
11:K:66:LEU:HG	11:K:70:ARG:HD2	1.86	0.56
13:M:136:LYS:HA	13:M:146:GLN:OE1	2.04	0.56
15:Z:301:LDZ:C6	13:a:131:GLN:CB	2.70	0.56
4:D:134:VAL:HG12	4:D:144:LEU:HD13	1.87	0.56
1:O:115:CYS:SG	1:O:160:TYR:HB2	2.45	0.56
5:S:146:VAL:HG11	5:S:222:PRO:HA	1.87	0.56
5:E:50:VAL:HG12	5:E:216:GLU:HB3	1.87	0.56
8:H:134:SER:O	8:V:135:TYR:HA	2.06	0.56
1:O:10:ASP:OD2	1:O:18:PRO:HD3	2.06	0.56
1:O:178:PHE:HD1	1:O:179:LEU:HD13	1.69	0.56
2:P:74:VAL:HG12	2:P:134:LEU:HB2	1.87	0.56
3:Q:147:LEU:HD21	3:Q:162:THR:HG22	1.86	0.56
10:X:27:PHE:HB3	10:X:35:THR:OG1	2.04	0.56
13:a:99:ARG:O	13:a:103:PRO:HA	2.06	0.56
1:A:42:VAL:HG13	1:A:194:THR:HG22	1.86	0.56
14:N:9:THR:HG23	14:N:10:SER:N	2.21	0.56
3:Q:119:GLN:HG3	4:R:78:ALA:HB1	1.88	0.56
7:U:75:MET:HE3	7:U:135:PHE:CG	2.41	0.56
1:O:73:THR:HG23	1:O:76:ILE:HB	1.87	0.56
5:S:107:MET:HG2	5:S:111:SER:OG	2.06	0.56
6:T:13:TRP:CH2	7:U:132:GLY:HA3	2.39	0.56
14:b:85:PRO:HB3	14:b:114:GLY:HA3	1.86	0.56
14:b:205:THR:C	14:b:207:THR:N	2.62	0.56
7:G:49:VAL:HG11	7:G:65:ARG:HB2	1.87	0.56
10:J:185:ILE:HD11	10:J:196:THR:HG22	1.87	0.56
12:L:43:LEU:HD21	12:L:180:VAL:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:20:PHE:HB2	13:M:197:ILE:HD11	1.88	0.56
7:U:196:ILE:O	7:U:199:ILE:HG22	2.05	0.56
11:Y:154:GLU:O	11:Y:158:GLU:HG3	2.05	0.56
12:Z:14:ILE:HG23	12:Z:177:LEU:HD11	1.88	0.56
1:A:143:ILE:HD13	1:A:149:PRO:HA	1.88	0.56
10:J:52:LEU:HB2	10:J:59:VAL:HG13	1.87	0.56
1:O:191:PHE:O	1:O:194:THR:N	2.37	0.56
9:W:125:TYR:HE2	9:W:136:MET:HE1	1.71	0.56
15:Z:301:LDZ:H5	13:a:131:GLN:CB	2.36	0.56
1:A:21:ARG:O	1:A:22:LEU:HB2	2.04	0.56
5:E:86:LYS:O	5:E:89:ILE:HG12	2.05	0.56
14:N:205:THR:C	14:N:207:THR:H	2.14	0.56
6:T:150:SER:O	6:T:151:ALA:HB3	2.06	0.56
9:W:60:ILE:HG13	9:W:84:LEU:HG	1.88	0.56
2:B:74:VAL:HG22	2:B:75:TYR:H	1.71	0.56
10:J:33:MET:HG3	10:J:33:MET:O	2.05	0.56
1:O:11:ARG:HG2	1:O:23:TYR:CD2	2.41	0.56
5:S:31:ILE:HD11	5:S:158:PRO:CD	2.36	0.56
7:G:151:ILE:HG13	7:G:157:SER:HB3	1.88	0.55
12:L:100:THR:HG22	12:L:115:VAL:O	2.07	0.55
13:M:8:ASN:HA	13:M:30:SER:O	2.05	0.55
2:P:78:MET:H	2:P:131:VAL:HG13	1.71	0.55
2:B:88:ARG:HB3	2:B:88:ARG:HH11	1.71	0.55
5:E:50:VAL:HG11	5:E:66:LYS:HB2	1.88	0.55
1:O:141:ILE:HG22	1:O:151:VAL:HG22	1.88	0.55
11:K:95:ARG:C	11:K:97:PRO:HD3	2.32	0.55
1:O:31:ALA:HB1	1:O:83:MET:HE3	1.88	0.55
3:Q:180:LYS:O	3:Q:184:MET:HG2	2.06	0.55
8:V:21:THR:CG2	15:V:301:LDZ:H34	2.36	0.55
9:W:220:LEU:HD11	10:X:194:ILE:CG1	2.36	0.55
11:Y:101:ASN:HB3	11:Y:132:HIS:CE1	2.42	0.55
13:a:172:MET:HE3	13:a:195:ILE:HG21	1.88	0.55
3:C:64:LYS:O	3:C:75:SER:HA	2.07	0.55
3:C:160:LYS:N	4:D:53:LEU:O	2.39	0.55
6:F:189:LYS:O	6:F:193:ARG:HG3	2.06	0.55
1:O:29:PHE:CE2	1:O:156:PRO:HD2	2.41	0.55
7:U:184:MET:HE1	7:U:192:GLU:HG3	1.87	0.55
3:C:6:ASP:HB3	3:C:8:ARG:NH2	2.21	0.55
13:M:22:ILE:HD11	13:M:168:LEU:HD12	1.87	0.55
4:D:209:ALA:HB1	4:D:217:LEU:HD22	1.89	0.55
14:N:15:LYS:HG2	14:N:135:PRO:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:68:LEU:HD11	3:Q:74:CYS:HB3	1.88	0.55
7:U:40:ARG:O	7:U:181:MET:HB2	2.06	0.55
9:W:23:GLU:O	9:W:26:VAL:HG12	2.07	0.55
1:A:176:THR:HG23	2:B:55:LEU:HD12	1.88	0.55
10:J:10:VAL:HG23	10:J:53:ALA:HB2	1.89	0.55
13:a:123:SER:O	13:a:130:TYR:HA	2.07	0.55
2:B:38:LYS:HG3	2:B:43:VAL:HG22	1.88	0.55
9:W:191:THR:O	9:W:193:PRO:HD3	2.07	0.55
12:L:181:ARG:HG2	12:L:184:GLY:O	2.06	0.54
1:O:61:LEU:HD23	7:U:159:GLY:O	2.08	0.54
6:T:121:GLN:HG3	7:U:129:ARG:HG3	1.89	0.54
8:V:26:TYR:CE1	9:W:133:LEU:HD22	2.42	0.54
4:D:120:GLN:HG2	5:E:133:MET:HG3	1.88	0.54
1:A:171:LYS:HE2	1:A:174:GLU:HG3	1.88	0.54
14:N:27:LEU:HD23	14:N:37:ARG:HG2	1.88	0.54
14:N:51:LEU:HD21	14:N:110:MET:HG2	1.89	0.54
9:I:136:MET:HE3	9:I:136:MET:HA	1.90	0.54
12:Z:39:ASN:CG	12:Z:41:TYR:HE1	2.16	0.54
14:b:22:ILE:HD11	14:b:42:ILE:HG23	1.88	0.54
5:E:167:ALA:HB3	6:F:56:LEU:HD13	1.90	0.54
14:N:142:GLY:HA2	14:N:176:LEU:HD21	1.88	0.54
5:S:179:SER:O	5:S:182:GLN:HG2	2.08	0.54
11:Y:118:MET:HE2	11:Y:124:LEU:HD13	1.90	0.54
7:G:236:GLU:HB3	7:G:240:LYS:NZ	2.22	0.54
3:Q:171:ALA:HB2	3:Q:200:THR:HG21	1.90	0.54
15:V:301:LDZ:H2	9:W:117:HIS:CD2	2.41	0.54
12:Z:181:ARG:HH21	12:Z:186:ILE:HG21	1.73	0.54
13:a:141:ALA:O	13:a:145:LEU:HG	2.07	0.54
4:R:108:THR:HG21	4:R:145:TYR:HB3	1.89	0.54
4:R:32:ALA:HB3	4:R:161:ILE:HG12	1.89	0.54
9:I:214:THR:CG2	10:J:198:THR:HB	2.38	0.54
4:R:192:ILE:O	4:R:196:LEU:HG	2.08	0.54
10:X:170:MET:O	10:X:174:VAL:HG22	2.07	0.54
13:a:144:MET:HE1	13:a:185:ARG:HB2	1.90	0.54
8:H:66:PHE:O	8:H:70:GLU:HG3	2.08	0.53
7:U:198:TYR:HE1	7:U:211:LEU:HD22	1.73	0.53
9:I:149:GLU:O	9:I:153:LYS:HG3	2.09	0.53
2:P:191:ILE:HG23	2:P:202:MET:HE1	1.90	0.53
3:Q:34:CYS:SG	3:Q:75:SER:HB3	2.48	0.53
11:Y:5:ILE:CG2	11:Y:16:ALA:HB3	2.39	0.53
10:J:200:LYS:HB3	10:J:200:LYS:NZ	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:60:PHE:O	14:N:64:LYS:HG3	2.09	0.53
2:P:208:GLU:OE2	2:P:219:ARG:HD2	2.07	0.53
5:S:141:LEU:HD23	5:S:143:PHE:CZ	2.44	0.53
9:W:144:ARG:O	9:W:147:MET:HG3	2.07	0.53
11:Y:75:LEU:HD22	11:Y:79:ALA:HB1	1.89	0.53
2:B:48:GLU:OE2	2:B:50:LYS:HE3	2.09	0.53
13:M:197:ILE:HG23	13:M:204:ARG:HB3	1.90	0.53
4:R:121:SER:HB2	4:R:124:ARG:HD2	1.90	0.53
12:Z:159:ARG:HH21	12:Z:163:GLN:HE21	1.57	0.53
1:A:61:LEU:HD23	7:G:159:GLY:O	2.08	0.53
2:P:73:LEU:CD1	2:P:135:ILE:HG12	2.39	0.53
8:V:100:ILE:HD11	8:V:102:ALA:HB2	1.89	0.53
10:X:108:ILE:HD11	10:X:119:PHE:CD1	2.42	0.53
5:E:195:ILE:HG23	5:E:217:LEU:HD11	1.91	0.53
6:F:49:LEU:O	6:F:50:LYS:C	2.52	0.53
10:J:14:LYS:HE2	10:J:133:ASP:HA	1.90	0.53
13:a:75:TYR:CD1	13:a:83:MET:HG2	2.44	0.53
13:M:62:LEU:O	13:M:66:LYS:HG3	2.09	0.53
5:S:146:VAL:HG23	5:S:220:VAL:HG12	1.91	0.53
12:Z:9:PHE:CE1	12:Z:14:ILE:HG12	2.43	0.53
1:A:192:GLU:C	1:A:194:THR:H	2.16	0.53
5:E:76:CYS:SG	5:E:141:LEU:HG	2.49	0.53
7:G:172:ALA:O	7:G:176:ILE:HG13	2.08	0.53
1:O:50:ILE:HG23	1:O:141:ILE:HG21	1.91	0.53
5:S:210:LEU:HG	5:S:215:ILE:HG21	1.91	0.53
15:Z:301:LDZ:H25	15:Z:301:LDZ:H39	1.90	0.53
8:H:191:LEU:HD12	8:H:194:GLN:NE2	2.24	0.53
6:T:121:GLN:HG3	7:U:129:ARG:CG	2.39	0.53
7:U:135:PHE:CZ	7:U:151:ILE:HD12	2.44	0.53
10:X:36:THR:HG22	10:X:182:MET:HB3	1.91	0.53
3:C:186:LEU:HD21	3:C:215:THR:HB	1.91	0.53
15:I:301:LDZ:C4	10:J:125:LEU:HD21	2.38	0.53
11:K:116:TYR:HB3	11:K:124:LEU:HD11	1.90	0.53
1:A:10:ASP:OD2	1:A:18:PRO:HD3	2.10	0.52
10:J:21:ILE:HG23	10:J:41:ILE:HD13	1.90	0.52
5:S:50:VAL:CG1	5:S:216:GLU:HB3	2.39	0.52
10:X:111:LEU:HD23	10:X:118:PRO:HA	1.91	0.52
11:K:38:MET:HE3	11:K:61:GLN:N	2.24	0.52
5:S:78:MET:HE2	5:S:82:ILE:HD12	1.91	0.52
11:Y:13:VAL:HG23	11:Y:183:ILE:HB	1.91	0.52
14:b:45:VAL:HG11	14:b:88:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLY:HA2	1:A:170:VAL:HG21	1.92	0.52
6:F:10:VAL:HG21	6:F:120:THR:HA	1.91	0.52
6:F:49:LEU:HB2	6:F:195:LEU:HD11	1.92	0.52
14:N:145:LEU:HD13	9:W:133:LEU:HB3	1.91	0.52
3:Q:197:LEU:HB3	3:Q:206:LEU:HD21	1.92	0.52
2:B:191:ILE:HG23	2:B:202:MET:HE2	1.90	0.52
4:D:104:VAL:HG13	4:D:133:ILE:HG22	1.92	0.52
12:L:41:TYR:CD1	12:L:74:ARG:HD3	2.44	0.52
13:M:128:GLY:O	13:M:129:SER:C	2.52	0.52
1:O:49:VAL:HG22	1:O:219:VAL:HG12	1.92	0.52
1:O:77:GLY:HA3	1:O:227:PHE:CD1	2.45	0.52
8:V:100:ILE:HD13	8:V:112:VAL:HG13	1.90	0.52
8:V:188:GLN:NE2	8:V:190:LEU:HD21	2.24	0.52
12:L:115:VAL:HA	12:L:120:ASN:O	2.10	0.52
1:O:137:CYS:SG	1:O:168:ALA:HB1	2.50	0.52
2:P:88:ARG:HD3	2:P:116:VAL:HG11	1.90	0.52
6:T:184:LEU:HD21	6:T:214:ILE:HG21	1.91	0.52
6:T:213:GLY:HA2	6:T:222:THR:O	2.10	0.52
3:Q:35:LEU:C	3:Q:35:LEU:HD12	2.35	0.52
5:S:167:ALA:HB3	6:T:56:LEU:HD13	1.91	0.52
9:W:34:LYS:HZ3	15:W:301:LDZ:H23	1.74	0.52
10:X:52:LEU:HB2	10:X:59:VAL:HG13	1.92	0.52
11:Y:10:PRO:HG3	11:Y:150:THR:HA	1.92	0.52
5:E:116:VAL:CG1	5:E:156:MET:HE1	2.39	0.52
12:L:21:ALA:HB1	15:L:301:LDZ:C32	2.39	0.52
12:L:83:LEU:O	12:L:87:MET:HG3	2.10	0.52
13:M:99:ARG:HH12	14:N:100:ARG:HH22	1.57	0.52
7:G:205:LYS:O	7:G:206:ASP:C	2.53	0.52
13:M:155:PHE:HA	13:M:158:MET:HE2	1.92	0.52
2:P:183:LEU:HD21	2:P:211:ILE:HB	1.92	0.52
5:S:121:LEU:HD12	6:T:79:ALA:HB3	1.92	0.52
2:B:41:ASN:OD1	2:B:183:LEU:N	2.43	0.51
2:P:108:GLN:HB3	2:P:112:ARG:NH1	2.25	0.51
8:V:2:THR:O	8:V:130:GLY:HA3	2.10	0.51
12:L:145:SER:O	12:L:148:LEU:HB2	2.09	0.51
15:L:301:LDZ:N10	15:L:301:LDZ:H26	2.26	0.51
1:O:192:GLU:O	1:O:195:VAL:HG23	2.10	0.51
7:G:69:VAL:HA	7:G:92:ARG:HG2	1.92	0.51
6:T:107:ARG:NH2	14:b:74:GLU:HG2	2.25	0.51
9:W:56:THR:HG23	9:W:87:MET:HE3	1.92	0.51
2:B:38:LYS:HD2	2:B:143:PRO:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:GLN:HG2	2:B:154:TYR:CZ	2.46	0.51
11:K:38:MET:HB2	11:K:42:ILE:HG13	1.92	0.51
14:N:205:THR:C	14:N:207:THR:N	2.68	0.51
2:B:10:THR:HG23	2:B:20:GLN:HB2	1.91	0.51
5:E:22:PHE:O	5:E:25:GLU:HG2	2.11	0.51
8:H:145:ARG:HG2	8:H:148:MET:HG3	1.92	0.51
13:M:136:LYS:HD2	13:M:146:GLN:OE1	2.10	0.51
4:R:156:TRP:CZ2	5:S:59:MET:HE2	2.46	0.51
6:F:48:ALA:HB1	6:F:62:LYS:HE3	1.93	0.51
4:R:32:ALA:HB3	4:R:161:ILE:CG1	2.41	0.51
5:S:182:GLN:HA	6:T:56:LEU:HD11	1.92	0.51
6:T:132:LEU:HB2	6:T:147:THR:OG1	2.11	0.51
7:U:110:HIS:O	7:U:114:ARG:HG3	2.11	0.51
9:W:60:ILE:HG13	9:W:84:LEU:CD2	2.41	0.51
4:D:89:VAL:HG22	11:K:66:LEU:HD21	1.93	0.51
1:O:138:MET:HB3	1:O:154:CYS:SG	2.51	0.51
3:Q:33:THR:HG23	3:Q:163:CYS:SG	2.51	0.51
11:Y:28:MET:HE1	12:Z:114:TYR:CE2	2.46	0.51
12:Z:113:TYR:CE2	12:Z:123:SER:HB2	2.46	0.51
3:C:69:ASN:ND2	3:C:94:ALA:HB1	2.25	0.51
4:D:212:ARG:O	4:D:213:ARG:C	2.52	0.51
5:E:215:ILE:HD11	5:E:238:ILE:HD11	1.93	0.51
6:F:49:LEU:HD11	6:F:199:LEU:HG	1.93	0.51
14:N:89:HIS:HD2	14:N:112:ILE:HD13	1.74	0.51
8:V:26:TYR:OH	9:W:136:MET:HG3	2.11	0.51
11:Y:38:MET:HE3	11:Y:44:LEU:CB	2.40	0.51
12:Z:39:ASN:HB3	12:Z:40:PRO:HD2	1.93	0.51
12:Z:199:LYS:HE3	12:Z:200:TYR:CE1	2.46	0.51
13:a:122:TYR:HA	13:a:131:GLN:O	2.10	0.51
10:J:48:LEU:HD12	10:J:110:GLY:HA3	1.93	0.50
12:L:62:ARG:O	12:L:66:ILE:HG13	2.09	0.50
8:V:71:LEU:O	8:V:73:GLU:N	2.43	0.50
9:W:91:TYR:O	9:W:94:TYR:HD2	1.93	0.50
6:F:205:LEU:HA	6:F:209:ASN:HD21	1.77	0.50
10:J:106:PRO:HD2	10:J:123:LEU:HB2	1.91	0.50
5:S:12:VAL:HG11	5:S:134:SER:O	2.10	0.50
6:T:184:LEU:O	6:T:188:VAL:HG23	2.11	0.50
7:U:37:ILE:HD11	7:U:193:VAL:HG13	1.93	0.50
10:X:95:TYR:CE1	10:X:98:ARG:HG3	2.46	0.50
6:T:39:LYS:HG3	6:T:180:MET:HE1	1.94	0.50
6:T:92:CYS:O	6:T:96:ARG:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:29:ASN:HB3	8:V:32:THR:HG22	1.93	0.50
8:V:150:LYS:HE2	8:V:179:ALA:CB	2.40	0.50
4:D:121:SER:HB2	4:D:124:ARG:HD2	1.92	0.50
1:O:61:LEU:HG	7:U:160:TYR:CE2	2.46	0.50
2:P:38:LYS:HD2	2:P:143:PRO:O	2.11	0.50
7:U:50:GLU:HB2	7:U:197:ILE:HG23	1.92	0.50
10:X:9:ALA:HB2	10:X:141:CYS:SG	2.52	0.50
5:E:209:LYS:O	5:E:214:ASN:ND2	2.44	0.50
7:G:41:CYS:HB3	7:G:189:ILE:HG13	1.93	0.50
7:G:195:LYS:HD2	7:G:199:ILE:HD11	1.93	0.50
10:J:9:ALA:HB2	10:J:141:CYS:SG	2.51	0.50
1:O:29:PHE:CZ	1:O:156:PRO:HD2	2.46	0.50
9:W:13:ILE:HG23	9:W:179:ILE:HB	1.92	0.50
14:b:27:LEU:HD11	14:b:29:SER:OG	2.11	0.50
3:C:6:ASP:HB3	3:C:8:ARG:CZ	2.41	0.50
12:L:59:LEU:HD12	12:L:62:ARG:HD3	1.92	0.50
2:P:136:CYS:SG	2:P:212:CYS:HB2	2.52	0.50
6:T:152:ASN:HD21	7:U:85:ARG:HH21	1.60	0.50
1:A:141:ILE:HG22	1:A:151:VAL:HG22	1.94	0.50
5:S:195:ILE:HG23	5:S:217:LEU:HD11	1.94	0.50
6:F:36:VAL:HB	6:F:47:VAL:CG2	2.40	0.50
8:H:15:LEU:HD12	8:H:15:LEU:N	2.27	0.50
13:M:83:MET:HE2	13:M:87:ALA:C	2.37	0.50
5:S:85:ALA:HB2	5:S:139:VAL:HG11	1.93	0.50
3:C:41:ASP:CG	3:C:186:LEU:H	2.20	0.50
5:E:186:HIS:CE1	5:E:189:MET:HA	2.46	0.50
6:F:69:HIS:CD2	6:F:70:ILE:HG13	2.46	0.49
7:G:55:SER:HB3	7:G:58:TYR:CD2	2.47	0.49
7:G:134:SER:OG	7:G:153:PRO:HD3	2.12	0.49
14:N:184:TYR:HE2	14:N:186:ARG:HH11	1.60	0.49
2:B:208:GLU:OE2	2:B:219:ARG:HD2	2.12	0.49
5:E:35:SER:HB3	5:E:53:ARG:HD2	1.93	0.49
6:F:113:GLY:O	6:F:151:ALA:HB1	2.11	0.49
6:F:158:ALA:HB3	7:G:57:LEU:HD22	1.94	0.49
11:K:103:LEU:HG	11:K:132:HIS:HD2	1.76	0.49
2:P:41:ASN:OD1	2:P:183:LEU:N	2.45	0.49
9:W:179:ILE:HG12	9:W:184:LEU:HD23	1.94	0.49
11:Y:75:LEU:HD22	11:Y:79:ALA:CB	2.41	0.49
14:b:14:VAL:HG13	14:b:21:VAL:HG13	1.92	0.49
2:B:107:ALA:O	2:B:111:GLN:HG3	2.11	0.49
4:R:168:VAL:HG13	4:R:194:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:21:THR:OG1	8:V:32:THR:HG21	2.13	0.49
13:a:8:ASN:HB3	13:a:29:LEU:CD1	2.43	0.49
2:B:211:ILE:HG12	2:B:220:LEU:HD21	1.94	0.49
3:C:180:LYS:O	3:C:184:MET:HG2	2.12	0.49
4:D:33:VAL:HG13	4:D:172:LEU:HD11	1.94	0.49
14:N:167:ASP:O	14:N:171:ARG:HG3	2.13	0.49
7:G:72:HIS:CE1	7:G:105:ASN:HB3	2.46	0.49
1:O:50:ILE:HD11	1:O:227:PHE:HE1	1.77	0.49
2:P:211:ILE:HG12	2:P:220:LEU:HD21	1.95	0.49
7:U:171:ALA:O	7:U:175:GLU:HG2	2.13	0.49
9:W:188:ARG:CB	9:W:189:PRO:HD3	2.40	0.49
1:A:191:PHE:CD1	1:A:191:PHE:N	2.79	0.49
3:C:90:LEU:HG	3:C:114:LEU:HD13	1.95	0.49
15:H:301:LDZ:H6	9:I:115:TYR:CD1	2.48	0.49
13:a:193:LEU:HD22	13:a:195:ILE:HG12	1.95	0.49
7:G:28:LYS:HB3	7:G:28:LYS:NZ	2.28	0.49
13:M:28:ARG:HH22	13:M:213:ASP:H	1.59	0.49
2:P:21:ILE:HG21	2:P:151:SER:HB3	1.94	0.49
4:R:35:VAL:CG2	4:R:191:VAL:HG23	2.42	0.49
5:E:101:PHE:CD2	12:L:58:ARG:HG2	2.47	0.49
11:K:121:LEU:O	11:K:122:ALA:HB3	2.13	0.49
13:M:99:ARG:O	13:M:103:PRO:HA	2.13	0.49
5:S:31:ILE:HD11	5:S:158:PRO:HD3	1.95	0.49
7:U:172:ALA:O	7:U:176:ILE:HG13	2.13	0.49
10:J:11:MET:HE1	10:J:169:ALA:HB3	1.95	0.49
14:N:145:LEU:CD1	9:W:133:LEU:HB3	2.43	0.49
2:P:70:HIS:O	2:P:212:CYS:SG	2.71	0.49
2:P:91:LYS:NZ	2:P:91:LYS:HB2	2.27	0.49
11:Y:161:ARG:O	11:Y:165:GLU:HG3	2.12	0.49
6:F:176:MET:CE	7:G:57:LEU:HD23	2.41	0.49
7:G:186:CYS:O	7:G:190:VAL:HG23	2.12	0.49
8:H:191:LEU:HD12	8:H:194:GLN:HE22	1.77	0.49
11:K:182:ILE:HG22	11:K:189:HIS:HB2	1.95	0.49
12:L:7:PHE:HA	12:L:125:ALA:O	2.13	0.49
2:P:91:LYS:O	2:P:95:GLN:HG3	2.13	0.49
2:P:105:PRO:HB2	2:P:108:GLN:HG2	1.95	0.49
2:P:111:GLN:HG2	2:P:154:TYR:CZ	2.48	0.49
6:T:26:MET:O	6:T:29:VAL:HG22	2.12	0.49
7:U:187:ARG:NH1	7:U:219:LEU:HD13	2.28	0.49
7:G:195:LYS:O	7:G:199:ILE:HG13	2.13	0.48
9:I:188:ARG:HB3	9:I:189:PRO:CD	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:24:GLN:NE2	7:U:14:PHE:H	2.10	0.48
9:W:179:ILE:HG12	9:W:184:LEU:CD2	2.43	0.48
10:X:35:THR:HG21	11:Y:125:ALA:HB1	1.95	0.48
13:a:200:LYS:HG2	13:a:201:GLU:CD	2.38	0.48
14:b:70:MET:HG2	14:b:83:TYR:CE2	2.48	0.48
2:B:49:LYS:HZ1	2:B:62:HIS:HA	1.78	0.48
3:C:95:GLN:CG	10:J:72:LEU:HD13	2.43	0.48
4:D:133:ILE:HD12	4:D:133:ILE:H	1.79	0.48
6:F:103:LEU:HD12	6:F:104:PRO:HD2	1.95	0.48
8:H:35:LEU:HB2	8:H:187:ARG:NH2	2.28	0.48
1:O:141:ILE:HD12	1:O:220:VAL:HG22	1.95	0.48
14:b:150:LEU:HA	14:b:168:LEU:HD21	1.94	0.48
2:B:108:GLN:HB3	2:B:112:ARG:NH1	2.27	0.48
4:D:36:ARG:NH2	4:D:157:LYS:HG2	2.28	0.48
7:G:151:ILE:HG13	7:G:157:SER:CB	2.43	0.48
11:K:118:MET:HA	11:K:123:ALA:O	2.13	0.48
13:M:145:LEU:HD22	13:M:178:VAL:HG22	1.94	0.48
3:Q:171:ALA:HB2	3:Q:200:THR:CG2	2.42	0.48
9:W:60:ILE:HD12	9:W:83:MET:HB3	1.94	0.48
10:X:121:CYS:SG	10:X:122:SER:N	2.86	0.48
11:Y:38:MET:HE2	11:Y:38:MET:N	2.29	0.48
14:b:60:PHE:CZ	14:b:64:LYS:HD3	2.48	0.48
5:E:85:ALA:O	5:E:89:ILE:HG23	2.13	0.48
10:J:125:LEU:HD23	10:J:125:LEU:H	1.77	0.48
1:O:51:VAL:HG22	1:O:217:VAL:HG22	1.94	0.48
12:L:50:ALA:HA	15:L:301:LDZ:C20	2.43	0.48
2:P:14:PRO:HA	3:Q:23:TYR:CD1	2.49	0.48
9:W:104:VAL:HG22	9:W:109:PRO:HB3	1.96	0.48
13:a:75:TYR:HE1	13:a:81:LYS:HG3	1.78	0.48
5:E:40:ILE:HB	5:E:47:CYS:SG	2.54	0.48
7:G:171:ALA:O	7:G:175:GLU:HG2	2.13	0.48
8:H:45:CYS:HB2	8:H:100:ILE:HG12	1.94	0.48
10:J:111:LEU:HD23	10:J:118:PRO:HA	1.94	0.48
12:L:181:ARG:HD3	12:L:186:ILE:HG23	1.96	0.48
1:O:71:LYS:NZ	1:O:71:LYS:HB3	2.29	0.48
15:V:301:LDZ:H23	15:V:301:LDZ:H11	1.96	0.48
9:W:56:THR:HG22	9:W:84:LEU:HD23	1.95	0.48
3:C:187:LYS:NZ	3:C:187:LYS:HB3	2.29	0.48
3:C:203:VAL:O	3:C:204:SER:C	2.56	0.48
4:D:195:LEU:O	4:D:199:VAL:N	2.39	0.48
6:F:150:SER:O	6:F:152:ASN:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:200:LYS:HB3	10:J:200:LYS:HZ3	1.78	0.48
14:b:27:LEU:HD22	14:b:28:GLY:N	2.28	0.48
6:F:184:LEU:HD11	6:F:214:ILE:HG21	1.96	0.48
4:R:134:VAL:HG12	4:R:144:LEU:HD13	1.95	0.48
9:W:28:ALA:O	10:X:130:MET:HE1	2.14	0.48
11:Y:121:LEU:O	11:Y:122:ALA:HB3	2.13	0.48
6:F:74:ILE:HG13	6:F:132:LEU:CD2	2.43	0.48
8:H:26:TYR:CZ	9:I:133:LEU:HD22	2.49	0.48
11:K:41:LYS:O	11:K:106:GLY:HA2	2.14	0.48
1:O:221:THR:O	1:O:225:PRO:HA	2.14	0.48
2:P:70:HIS:O	2:P:137:GLY:HA2	2.14	0.48
6:T:119:PRO:HG2	6:T:128:TYR:CE2	2.49	0.48
7:U:87:LEU:HD12	7:U:133:CYS:SG	2.54	0.48
9:W:162:ALA:O	9:W:166:ASN:HB2	2.14	0.48
13:a:193:LEU:CB	13:a:208:VAL:HG12	2.44	0.48
6:F:88:MET:HE3	6:F:112:ILE:HD11	1.96	0.48
9:I:82:ARG:HA	9:I:85:LYS:HG2	1.96	0.48
9:I:125:TYR:HD2	9:I:136:MET:HE1	1.79	0.48
9:I:136:MET:HE3	9:I:139:PHE:HB2	1.96	0.48
10:J:148:MET:CG	10:J:169:ALA:HA	2.37	0.48
10:X:11:MET:HG3	10:X:137:VAL:HG12	1.96	0.48
14:b:184:TYR:CE2	14:b:186:ARG:HB2	2.49	0.48
9:I:220:LEU:HD11	10:J:194:ILE:HG12	1.95	0.47
13:M:20:PHE:HB2	13:M:197:ILE:CD1	2.44	0.47
7:U:169:ARG:HB2	7:U:173:LYS:HE3	1.95	0.47
12:Z:53:CYS:O	12:Z:57:GLU:HG3	2.14	0.47
13:a:124:PHE:CD2	13:a:130:TYR:HB3	2.49	0.47
8:H:43:PHE:CZ	8:H:185:VAL:HG11	2.49	0.47
10:X:188:ILE:HB	10:X:195:THR:CG2	2.41	0.47
12:Z:22:THR:O	15:Z:301:LDZ:N13	2.45	0.47
14:b:15:LYS:HD2	14:b:135:PRO:HA	1.96	0.47
1:A:43:ARG:CG	1:A:149:PRO:HB2	2.44	0.47
5:E:240:ASP:O	5:E:241:ILE:C	2.57	0.47
6:F:171:TYR:CD1	6:F:194:ALA:HB2	2.49	0.47
9:I:220:LEU:HD11	10:J:194:ILE:CG1	2.45	0.47
10:J:38:PHE:CZ	10:J:56:ALA:HB1	2.49	0.47
14:N:60:PHE:CZ	14:N:64:LYS:HD2	2.49	0.47
7:U:109:LYS:HG2	7:U:149:TYR:OH	2.14	0.47
7:U:236:GLU:HB3	7:U:240:LYS:NZ	2.29	0.47
9:W:50:ALA:HB2	15:W:301:LDZ:H14	1.96	0.47
12:Z:145:SER:O	12:Z:148:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:117:LYS:HD2	10:J:118:PRO:CD	2.38	0.47
12:L:161:ILE:O	12:L:165:THR:HG23	2.14	0.47
8:V:4:ILE:HD13	8:V:47:SER:HB3	1.95	0.47
10:X:11:MET:CE	10:X:170:MET:HG2	2.44	0.47
10:X:87:MET:SD	10:X:129:PRO:HB3	2.54	0.47
1:A:174:GLU:CD	1:A:174:GLU:H	2.21	0.47
2:B:50:LYS:HD3	2:B:198:PHE:CE2	2.49	0.47
3:C:92:LEU:HD23	10:J:72:LEU:HD21	1.97	0.47
6:F:69:HIS:O	6:F:136:GLY:HA2	2.14	0.47
10:J:141:CYS:O	10:J:145:MET:HG3	2.15	0.47
12:L:13:VAL:HG21	12:L:103:CYS:HB3	1.97	0.47
13:M:10:GLY:HA2	13:M:42:LYS:HE2	1.96	0.47
3:Q:197:LEU:HB2	3:Q:206:LEU:HD11	1.96	0.47
5:S:186:HIS:CE1	5:S:189:MET:HA	2.49	0.47
7:U:211:LEU:HD23	7:U:236:GLU:HG2	1.95	0.47
8:V:105:ASP:OD1	8:V:108:GLU:N	2.38	0.47
13:a:72:LEU:HD23	13:a:83:MET:SD	2.55	0.47
4:D:41:VAL:HG22	4:D:136:PHE:CE1	2.50	0.47
6:F:46:LEU:HG	6:F:135:ALA:HB2	1.97	0.47
6:F:158:ALA:O	7:G:57:LEU:HB3	2.14	0.47
9:I:13:ILE:CD1	9:I:111:LEU:HD13	2.45	0.47
10:J:185:ILE:HD11	10:J:196:THR:CG2	2.44	0.47
3:Q:101:TYR:CE1	11:Y:75:LEU:HD11	2.50	0.47
1:A:160:TYR:O	1:A:160:TYR:CD2	2.67	0.47
3:C:35:LEU:C	3:C:35:LEU:HD12	2.39	0.47
4:D:140:GLY:O	4:D:213:ARG:NH2	2.47	0.47
8:H:136:ILE:O	8:H:140:VAL:HG22	2.15	0.47
11:K:16:ALA:HA	11:K:179:SER:O	2.14	0.47
11:K:27:GLN:HE22	11:K:174:ASN:HB3	1.80	0.47
1:O:191:PHE:O	1:O:191:PHE:HD1	1.97	0.47
2:P:25:LEU:HD21	2:P:150:PRO:HD2	1.95	0.47
3:Q:3:ARG:HB3	4:R:5:ARG:HH21	1.79	0.47
9:W:9:TYR:CZ	9:W:149:GLU:HG2	2.49	0.47
11:Y:171:PHE:CE2	11:Y:173:LEU:HB2	2.50	0.47
1:A:50:ILE:HD11	1:A:227:PHE:CE1	2.50	0.47
3:C:14:PRO:HA	4:D:21:TYR:CE1	2.49	0.47
3:C:25:MET:HA	3:C:28:ILE:HD13	1.97	0.47
13:M:7:PHE:CZ	13:M:9:GLY:HA2	2.50	0.47
3:Q:114:LEU:HD23	3:Q:136:TYR:OH	2.14	0.47
6:T:176:MET:HA	6:T:179:PHE:CD2	2.50	0.47
9:W:49:THR:O	9:W:53:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:113:SER:O	9:W:120:THR:HA	2.14	0.47
1:A:18:PRO:HA	2:B:23:TYR:CE1	2.50	0.47
6:F:226:ASP:O	6:F:229:VAL:HG22	2.15	0.47
9:I:195:LYS:HD2	9:I:196:LYS:O	2.14	0.47
10:J:204:ASP:HB3	12:Z:193:VAL:HG11	1.97	0.47
12:L:34:LYS:HA	12:L:46:MET:HE2	1.96	0.47
2:P:173:LEU:HD12	2:P:173:LEU:HA	1.75	0.47
4:R:42:VAL:HG13	4:R:208:LEU:HD21	1.96	0.47
5:S:230:THR:N	5:S:233:GLU:HG3	2.30	0.47
7:U:111:LEU:O	7:U:115:VAL:HG23	2.14	0.47
3:C:24:ALA:O	3:C:27:ALA:HB3	2.14	0.47
3:C:172:VAL:O	3:C:176:LYS:HG3	2.15	0.47
9:I:133:LEU:HD23	9:I:133:LEU:N	2.30	0.47
13:M:22:ILE:HD11	13:M:168:LEU:CD1	2.46	0.47
14:N:20:VAL:HG11	14:N:122:LEU:HD13	1.97	0.47
3:Q:115:CYS:SG	3:Q:156:TYR:HB3	2.55	0.47
10:X:86:LEU:O	10:X:90:VAL:HG23	2.15	0.47
9:I:220:LEU:HD11	10:J:194:ILE:HD11	1.97	0.46
14:N:22:ILE:HD11	14:N:42:ILE:HG23	1.96	0.46
14:N:84:SER:O	14:N:88:ILE:HD12	2.15	0.46
1:A:50:ILE:HG23	1:A:141:ILE:HG21	1.96	0.46
3:C:25:MET:HE3	3:C:152:PRO:HD2	1.97	0.46
3:C:201:MET:O	3:C:202:ASP:C	2.57	0.46
5:E:135:ARG:HB2	5:E:136:PRO:HD2	1.96	0.46
7:G:228:PRO:HD2	7:G:231:ILE:HD12	1.96	0.46
11:K:25:ILE:HA	11:Y:172:ILE:HG12	1.96	0.46
11:K:43:LEU:HG	11:K:188:ILE:HD13	1.96	0.46
13:M:70:ALA:O	13:M:74:MET:HG3	2.15	0.46
5:S:191:LEU:O	5:S:195:ILE:HG13	2.16	0.46
2:B:106:THR:O	2:B:110:VAL:HG23	2.16	0.46
3:C:76:VAL:HG11	3:C:83:ALA:HB1	1.98	0.46
4:D:42:VAL:HG22	4:D:210:VAL:HG22	1.96	0.46
4:D:70:CYS:SG	4:D:211:MET:HE2	2.54	0.46
3:Q:160:LYS:HG3	4:R:53:LEU:C	2.41	0.46
6:T:64:LEU:HD11	6:T:74:ILE:HD11	1.97	0.46
6:T:189:LYS:O	6:T:193:ARG:HG3	2.16	0.46
10:X:100:GLY:H	10:X:101:PRO:HD3	1.80	0.46
1:A:111:VAL:CG2	1:A:142:GLY:HA3	2.44	0.46
7:G:34:SER:OG	7:G:65:ARG:NH1	2.48	0.46
9:I:139:PHE:CE1	9:I:155:LEU:HG	2.51	0.46
12:L:41:TYR:CE1	12:L:74:ARG:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:84:THR:O	13:M:88:ILE:HG13	2.15	0.46
1:O:174:GLU:CD	1:O:174:GLU:H	2.23	0.46
2:P:79:GLY:O	2:P:83:ARG:HG3	2.14	0.46
6:F:9:ASP:OD2	6:F:11:THR:OG1	2.34	0.46
6:F:176:MET:HE1	7:G:57:LEU:HA	1.98	0.46
9:I:179:ILE:HG23	9:I:184:LEU:HD23	1.97	0.46
10:J:188:ILE:HB	10:J:195:THR:HG23	1.97	0.46
11:K:21:ALA:HB3	11:K:29:LYS:HB3	1.96	0.46
11:K:90:ASP:OD1	11:K:91:CYS:N	2.48	0.46
14:N:15:LYS:HD2	14:N:135:PRO:HA	1.98	0.46
14:N:33:LEU:HD13	8:V:135:TYR:CE1	2.51	0.46
6:T:152:ASN:HD22	6:T:153:TYR:H	1.64	0.46
9:W:80:ALA:HB3	9:W:101:LEU:HD21	1.96	0.46
12:Z:37:GLU:H	12:Z:37:GLU:HG2	1.55	0.46
1:A:80:MET:HE2	1:A:87:SER:HA	1.97	0.46
5:E:232:GLU:O	5:E:236:GLU:HG3	2.15	0.46
6:F:168:ALA:HB2	6:F:198:THR:CG2	2.45	0.46
8:H:13:VAL:HG21	8:H:102:ALA:HB1	1.96	0.46
11:K:170:ARG:O	11:Y:26:VAL:HA	2.15	0.46
12:L:158:ARG:HA	12:L:175:VAL:HG21	1.97	0.46
3:Q:90:LEU:HD11	3:Q:114:LEU:HD22	1.96	0.46
7:U:71:ARG:HH11	14:b:72:ILE:HD13	1.80	0.46
9:W:56:THR:HG22	9:W:84:LEU:CD2	2.46	0.46
10:X:108:ILE:O	10:X:108:ILE:HG13	2.14	0.46
11:Y:160:LEU:O	11:Y:164:LEU:HG	2.14	0.46
4:D:163:ARG:O	4:D:163:ARG:HG2	2.15	0.46
5:E:116:VAL:CB	5:E:156:MET:HE1	2.46	0.46
6:F:223:ILE:HD13	6:F:223:ILE:H	1.81	0.46
7:G:110:HIS:O	7:G:114:ARG:HG2	2.16	0.46
13:M:141:ALA:O	13:M:145:LEU:HG	2.15	0.46
13:M:159:GLN:HG2	9:W:209:THR:O	2.15	0.46
13:M:193:LEU:O	13:M:207:THR:HA	2.16	0.46
14:N:206:GLU:C	14:N:208:ASN:H	2.23	0.46
5:S:38:ILE:HG23	5:S:181:LEU:HD11	1.97	0.46
9:W:48:GLY:O	15:W:301:LDZ:H18	2.16	0.46
10:X:19:VAL:CG2	10:X:189:ILE:HB	2.41	0.46
10:X:141:CYS:O	10:X:145:MET:HG3	2.15	0.46
14:b:50:MET:HG2	14:b:113:GLY:O	2.15	0.46
14:b:205:THR:C	14:b:207:THR:H	2.23	0.46
1:A:160:TYR:O	1:A:160:TYR:CG	2.69	0.46
2:B:94:GLN:HG3	9:I:66:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:73:SER:C	6:F:74:ILE:HD12	2.41	0.46
14:N:166:ARG:HH12	14:N:200:GLU:HG3	1.80	0.46
3:Q:176:LYS:HA	4:R:53:LEU:HD11	1.98	0.46
3:Q:198:ASN:OD1	3:Q:206:LEU:HG	2.16	0.46
4:R:133:ILE:HD12	4:R:133:ILE:H	1.81	0.46
6:T:179:PHE:O	6:T:182:CYS:HB2	2.16	0.46
13:a:24:ALA:HB1	13:a:193:LEU:HD21	1.97	0.46
2:B:47:THR:HB	2:B:74:VAL:HG21	1.97	0.46
4:D:132:LEU:HG	4:D:161:ILE:HD13	1.97	0.46
5:E:112:VAL:O	5:E:116:VAL:HG23	2.15	0.46
5:E:234:LEU:O	5:E:238:ILE:HG13	2.16	0.46
6:F:228:ASP:O	6:F:231:PRO:HD2	2.15	0.46
7:G:111:LEU:O	7:G:115:VAL:HG23	2.15	0.46
12:L:41:TYR:CZ	12:L:74:ARG:HB3	2.50	0.46
14:N:62:TYR:O	14:N:66:VAL:HG23	2.16	0.46
1:O:187:PHE:O	1:O:189:TRP:N	2.48	0.46
5:S:166:ASP:HB3	5:S:185:TYR:CZ	2.50	0.46
6:T:107:ARG:NE	14:b:79:ASP:OD2	2.49	0.46
7:U:34:SER:OG	7:U:65:ARG:NH1	2.48	0.46
7:U:232:ARG:O	7:U:236:GLU:HG3	2.16	0.46
8:V:120:MET:HG2	8:V:121:MET:N	2.31	0.46
12:Z:75:ILE:HG12	12:Z:79:ALA:HB3	1.98	0.46
1:A:70:PHE:HB2	1:A:78:CYS:SG	2.56	0.46
9:I:144:ARG:O	9:I:147:MET:HG3	2.16	0.46
14:N:27:LEU:HD21	14:N:34:ALA:HB1	1.98	0.46
14:N:184:TYR:CE2	14:N:186:ARG:HB2	2.51	0.46
1:O:112:ASP:CG	9:W:73:ARG:HH22	2.23	0.46
3:Q:138:GLY:HA2	3:Q:216:LEU:HD13	1.97	0.46
5:S:13:ASN:HB3	6:T:126:ARG:HB3	1.98	0.46
9:W:149:GLU:O	9:W:153:LYS:HG3	2.15	0.46
14:b:14:VAL:HG13	14:b:21:VAL:CG1	2.46	0.46
1:A:25:VAL:O	1:A:29:PHE:HD1	1.99	0.45
3:C:112:THR:HG23	4:D:81:ARG:HD2	1.96	0.45
13:M:212:LYS:O	13:M:213:ASP:C	2.59	0.45
14:N:27:LEU:HD22	14:N:28:GLY:N	2.31	0.45
14:N:174:ARG:HD3	14:N:207:THR:O	2.16	0.45
8:V:4:ILE:HD12	8:V:100:ILE:HG22	1.97	0.45
8:V:39:HIS:CG	8:V:75:PRO:HG3	2.51	0.45
14:b:27:LEU:HD23	14:b:37:ARG:HG2	1.98	0.45
1:A:191:PHE:C	1:A:193:GLN:N	2.74	0.45
3:C:138:GLY:HA2	3:C:216:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:94:HIS:CG	4:D:102:VAL:HG12	2.52	0.45
6:F:118:ILE:HB	6:F:119:PRO:HD3	1.97	0.45
10:J:108:ILE:HG23	10:J:121:CYS:SG	2.56	0.45
13:M:51:VAL:CG2	13:M:203:ILE:HD13	2.46	0.45
13:M:145:LEU:HD22	13:M:178:VAL:HG13	1.97	0.45
6:T:223:ILE:O	6:T:223:ILE:HG13	2.16	0.45
7:U:239:ALA:O	7:U:243:LEU:HD13	2.17	0.45
12:Z:34:LYS:HA	12:Z:46:MET:HG3	1.99	0.45
1:A:29:PHE:CE2	1:A:156:PRO:HD2	2.51	0.45
6:F:230:SER:HB2	6:F:231:PRO:HD3	1.99	0.45
9:I:25:MET:HG3	13:a:188:TYR:CE2	2.51	0.45
9:I:171:GLY:O	9:I:172:SER:HB2	2.15	0.45
2:P:202:MET:CE	2:P:207:ILE:HG21	2.38	0.45
7:U:120:HIS:CE1	7:U:124:LEU:HD11	2.51	0.45
10:X:162:LEU:O	10:X:166:ILE:HG22	2.16	0.45
12:Z:187:ARG:HH22	12:Z:190:SER:HB2	1.81	0.45
1:A:43:ARG:HG3	1:A:149:PRO:HB2	1.99	0.45
11:K:35:MET:HB2	11:K:181:ARG:NH2	2.30	0.45
10:X:11:MET:HE1	10:X:169:ALA:HB3	1.97	0.45
12:Z:192:ASN:ND2	12:Z:194:ALA:H	2.01	0.45
2:B:90:ARG:HB3	9:I:66:LEU:HD11	1.98	0.45
7:G:116:ALA:HB1	7:G:155:GLY:O	2.16	0.45
8:H:26:TYR:CE1	9:I:133:LEU:HD22	2.51	0.45
9:I:25:MET:HE3	13:a:188:TYR:OH	2.17	0.45
11:K:4:LEU:HD11	11:K:47:VAL:HG13	1.98	0.45
13:M:123:SER:O	13:M:130:TYR:HA	2.16	0.45
7:U:74:GLY:HA3	7:U:224:HIS:CD2	2.52	0.45
7:U:99:ARG:NH1	14:b:69:GLN:HE22	2.07	0.45
12:Z:33:LYS:HD2	12:Z:33:LYS:N	2.32	0.45
14:b:122:LEU:HG	14:b:137:LEU:HD12	1.98	0.45
1:A:61:LEU:HD21	7:G:158:TYR:HB3	1.99	0.45
3:C:69:ASN:HD21	3:C:94:ALA:HB1	1.81	0.45
3:C:171:ALA:HB2	3:C:200:THR:CG2	2.46	0.45
4:D:11:SER:O	4:D:12:PRO:C	2.59	0.45
4:D:36:ARG:HD2	4:D:142:PRO:O	2.15	0.45
5:E:16:SER:C	5:E:18:GLU:H	2.24	0.45
7:G:109:LYS:HE3	7:G:109:LYS:HB2	1.79	0.45
8:H:116:PRO:HG2	8:H:120:MET:CG	2.46	0.45
9:I:167:ASP:OD1	13:a:33:PHE:HB3	2.17	0.45
11:K:39:SER:CB	11:K:42:ILE:HG12	2.42	0.45
5:S:24:VAL:O	5:S:28:ILE:HD13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:168:ALA:HB2	6:T:198:THR:CG2	2.47	0.45
9:W:7:VAL:O	9:W:13:ILE:HD12	2.16	0.45
9:W:34:LYS:O	9:W:45:CYS:HA	2.17	0.45
11:Y:101:ASN:HD22	11:Y:119:ASP:HA	1.81	0.45
12:Z:38:ILE:CG2	12:Z:61:ALA:HA	2.44	0.45
13:a:183:ALA:HB1	13:a:211:ARG:HG2	1.98	0.45
14:b:1:THR:N	14:b:105:PRO:O	2.45	0.45
3:C:60:PHE:O	3:C:61:PHE:C	2.58	0.45
7:G:65:ARG:HH21	7:G:78:ALA:HA	1.81	0.45
10:J:176:ARG:NH1	12:Z:27:ILE:O	2.46	0.45
11:K:141:SER:OG	12:Z:135:TYR:HB3	2.17	0.45
1:O:191:PHE:C	1:O:193:GLN:N	2.72	0.45
5:S:107:MET:HE2	5:S:111:SER:HB2	1.98	0.45
5:S:230:THR:H	5:S:233:GLU:HG3	1.82	0.45
6:T:84:LEU:O	6:T:88:MET:HG3	2.15	0.45
10:X:130:MET:HE3	10:X:130:MET:HB2	1.90	0.45
2:B:195:LYS:HE2	2:B:202:MET:HG3	1.99	0.45
7:G:52:LEU:HD22	7:G:206:ASP:HB3	1.98	0.45
10:J:10:VAL:O	10:J:145:MET:HE1	2.17	0.45
12:L:8:LYS:HE2	12:L:124:GLY:O	2.17	0.45
5:S:52:LYS:HE2	5:S:64:ILE:O	2.17	0.45
5:S:86:LYS:O	5:S:89:ILE:HG12	2.16	0.45
6:T:22:ILE:HD11	6:T:120:THR:HB	1.99	0.45
11:Y:103:LEU:HD23	11:Y:117:TYR:HA	1.99	0.45
14:b:204:SER:C	14:b:206:GLU:H	2.25	0.45
7:G:15:SER:C	7:G:17:ASP:H	2.25	0.45
1:O:17:SER:HB2	1:O:23:TYR:CE2	2.52	0.45
1:O:178:PHE:O	1:O:182:LYS:HG2	2.17	0.45
13:a:14:ALA:HA	13:a:22:ILE:O	2.17	0.45
13:a:29:LEU:HD11	13:a:58:HIS:HB2	1.98	0.45
13:a:197:ILE:HD11	13:a:199:THR:HG23	1.99	0.45
2:B:191:ILE:HG23	2:B:202:MET:CE	2.47	0.45
4:D:208:LEU:HD22	4:D:220:LEU:HD12	1.98	0.45
5:E:36:THR:HA	5:E:171:GLY:HA3	1.97	0.45
5:E:230:THR:OG1	5:E:233:GLU:HG3	2.16	0.45
6:F:109:VAL:HG12	6:F:153:TYR:CG	2.52	0.45
7:G:219:LEU:HD23	7:G:219:LEU:N	2.32	0.45
8:H:115:VAL:HA	8:H:120:MET:O	2.17	0.45
12:L:177:LEU:O	12:L:188:VAL:HG13	2.16	0.45
2:P:92:LEU:HD13	2:P:112:ARG:HB3	1.99	0.45
4:R:195:LEU:HD13	4:R:206:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:157:ARG:HG3	7:U:59:GLU:HG2	1.98	0.45
9:W:44:CYS:SG	9:W:99:LEU:HB3	2.57	0.45
10:X:11:MET:HB2	10:X:145:MET:CE	2.47	0.45
10:X:81:ILE:HD11	10:X:85:THR:HG22	1.98	0.45
11:Y:43:LEU:HD12	11:Y:183:ILE:HD11	1.99	0.45
13:a:197:ILE:HG23	13:a:204:ARG:HB3	1.99	0.45
3:C:44:LEU:HD12	3:C:44:LEU:C	2.42	0.44
3:C:65:ILE:O	3:C:74:CYS:O	2.35	0.44
8:H:43:PHE:CE1	8:H:185:VAL:HG21	2.52	0.44
4:R:116:GLN:HG3	5:S:83:ALA:HB1	1.98	0.44
9:W:133:LEU:N	9:W:133:LEU:HD23	2.33	0.44
10:X:189:ILE:HG23	10:X:194:ILE:CD1	2.47	0.44
2:B:50:LYS:HD3	2:B:198:PHE:CZ	2.52	0.44
7:G:219:LEU:HD23	7:G:219:LEU:H	1.83	0.44
15:L:301:LDZ:H29	15:L:301:LDZ:H11	1.71	0.44
14:N:150:LEU:HD23	14:N:168:LEU:CG	2.43	0.44
12:Z:9:PHE:CE2	12:Z:11:HIS:HB2	2.51	0.44
14:b:43:MET:HE2	14:b:45:VAL:HA	1.99	0.44
1:A:26:GLU:O	1:A:30:LYS:HG3	2.17	0.44
1:A:112:ASP:HB3	1:A:152:TYR:CZ	2.52	0.44
1:A:113:MET:HA	1:A:113:MET:HE2	1.98	0.44
2:B:104:ILE:HD13	2:B:109:LEU:HD23	1.99	0.44
11:K:101:ASN:HB3	11:K:132:HIS:CE1	2.53	0.44
11:K:177:THR:HG22	11:K:195:SER:HB3	1.99	0.44
13:M:83:MET:HE2	13:M:87:ALA:O	2.18	0.44
1:O:80:MET:HE2	1:O:87:SER:HA	1.98	0.44
9:W:2:THR:OG1	15:W:301:LDZ:O33	2.35	0.44
10:X:108:ILE:HD11	10:X:119:PHE:HD1	1.80	0.44
12:Z:3:THR:HG21	12:Z:164:ALA:CB	2.47	0.44
13:a:22:ILE:HD11	13:a:168:LEU:CD1	2.48	0.44
14:b:206:GLU:C	14:b:208:ASN:H	2.23	0.44
9:I:140:GLU:OE1	9:I:140:GLU:HA	2.18	0.44
2:P:48:GLU:OE2	2:P:50:LYS:HD3	2.17	0.44
2:P:74:VAL:CG1	2:P:134:LEU:HB2	2.47	0.44
2:P:188:HIS:O	2:P:192:LEU:HG	2.18	0.44
6:T:10:VAL:HG21	6:T:120:THR:HA	1.98	0.44
14:b:84:SER:HB2	14:b:85:PRO:HD2	1.98	0.44
14:b:96:MET:CE	14:b:127:MET:HA	2.47	0.44
1:A:51:VAL:HG22	1:A:217:VAL:HG22	2.00	0.44
2:B:202:MET:HE3	2:B:202:MET:HB3	1.91	0.44
3:C:229:LYS:HB2	3:C:229:LYS:NZ	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:192:LEU:HD13	6:F:233:LEU:HD23	2.00	0.44
10:J:148:MET:HE1	13:a:151:ASN:CB	2.48	0.44
12:L:6:ALA:HA	12:L:14:ILE:O	2.18	0.44
5:S:123:PHE:CZ	5:S:136:PRO:HG3	2.53	0.44
7:U:27:MET:HE2	7:U:27:MET:HB3	1.86	0.44
1:A:178:PHE:O	1:A:182:LYS:HG2	2.18	0.44
2:B:142:ARG:HD3	2:B:144:TYR:CZ	2.52	0.44
6:F:84:LEU:HD12	6:F:84:LEU:HA	1.83	0.44
7:G:161:TRP:CZ3	7:G:182:LYS:HG2	2.53	0.44
15:V:301:LDZ:H19	15:V:301:LDZ:H13	1.74	0.44
4:D:80:ALA:O	4:D:84:ILE:HG13	2.18	0.44
5:E:231:LYS:HE2	5:E:235:GLU:OE2	2.18	0.44
12:L:18:ASP:CG	12:L:34:LYS:HZ2	2.26	0.44
2:P:108:GLN:HE22	10:X:76:LYS:HG2	1.83	0.44
8:V:91:TYR:O	8:V:95:LEU:HB2	2.16	0.44
10:X:12:ALA:HB3	10:X:136:VAL:CG2	2.48	0.44
11:Y:41:LYS:O	11:Y:106:GLY:HA2	2.18	0.44
14:b:142:GLY:HA2	14:b:176:LEU:HD21	2.00	0.44
3:C:28:ILE:HD12	3:C:28:ILE:H	1.83	0.44
11:K:33:ASP:CG	11:K:181:ARG:HH22	2.25	0.44
11:K:38:MET:CB	11:K:42:ILE:HG13	2.48	0.44
12:L:159:ARG:O	12:L:163:GLN:HG2	2.18	0.44
13:M:16:ALA:HB2	13:M:121:VAL:HG23	2.00	0.44
13:M:123:SER:CB	13:M:136:LYS:HG2	2.47	0.44
5:S:196:LYS:O	5:S:200:ILE:HG13	2.18	0.44
7:U:135:PHE:CE2	7:U:151:ILE:HD12	2.53	0.44
12:Z:68:GLU:HG2	12:Z:74:ARG:HA	2.00	0.44
3:C:207:SER:O	3:C:208:ALA:HB3	2.18	0.44
4:D:13:ASP:O	4:D:15:HIS:HD2	2.01	0.44
4:D:94:HIS:CB	4:D:102:VAL:HG12	2.46	0.44
6:F:40:SER:HA	6:F:180:MET:HA	1.99	0.44
10:J:202:ARG:NH2	12:Z:192:ASN:HD21	2.12	0.44
12:L:167:ARG:CZ	10:X:33:MET:HE3	2.48	0.44
4:R:133:ILE:HD12	4:R:133:ILE:N	2.32	0.44
4:R:146:GLN:O	4:R:153:TYR:HA	2.18	0.44
6:T:101:ARG:HH11	14:b:83:TYR:HE1	1.66	0.44
8:V:2:THR:HG23	8:V:34:LYS:HZ2	1.81	0.44
10:X:107:VAL:HG12	10:X:122:SER:OG	2.18	0.44
12:Z:7:PHE:HD2	12:Z:140:MET:HE3	1.83	0.44
1:A:120:ASP:OD1	2:B:83:ARG:NH1	2.51	0.43
4:D:135:GLY:HA2	4:D:211:MET:CE	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:125:TYR:CE2	9:I:136:MET:HE1	2.53	0.43
12:L:40:PRO:HD2	12:L:74:ARG:NH1	2.33	0.43
5:E:186:HIS:NE2	5:E:189:MET:HG3	2.32	0.43
5:E:191:LEU:CD2	5:E:221:GLN:HG2	2.48	0.43
6:F:38:LEU:HD11	6:F:191:GLY:HA3	2.00	0.43
13:M:76:LYS:HE2	13:M:82:ALA:HA	1.99	0.43
14:N:147:GLN:N	14:N:148:PRO:CD	2.81	0.43
3:Q:14:PRO:HA	4:R:21:TYR:CE1	2.52	0.43
3:Q:187:LYS:HE2	3:Q:187:LYS:HA	2.00	0.43
4:R:112:ALA:HB1	4:R:151:GLY:O	2.18	0.43
5:S:192:LYS:NZ	5:S:192:LYS:HB3	2.33	0.43
9:W:74:LEU:CD2	9:W:75:PRO:HD2	2.48	0.43
13:a:51:VAL:CG2	13:a:203:ILE:HD13	2.48	0.43
1:A:43:ARG:NH2	1:A:164:LYS:HG2	2.34	0.43
2:B:46:ALA:HB1	2:B:194:LEU:HD11	2.00	0.43
3:C:33:THR:HG23	3:C:163:CYS:SG	2.58	0.43
3:C:168:SER:O	3:C:172:VAL:HG23	2.18	0.43
10:J:92:ASN:O	10:J:96:GLU:HG3	2.18	0.43
14:N:27:LEU:HD22	14:N:28:GLY:H	1.83	0.43
3:Q:71:ASP:O	3:Q:216:LEU:HD11	2.18	0.43
11:Y:129:PHE:HZ	11:Y:144:ASP:OD1	2.00	0.43
12:Z:5:LEU:HD23	12:Z:5:LEU:O	2.18	0.43
2:B:63:LYS:N	2:B:208:GLU:OE1	2.48	0.43
2:B:188:HIS:O	2:B:192:LEU:HG	2.17	0.43
6:F:224:TYR:O	6:F:229:VAL:HG12	2.18	0.43
12:L:52:ASP:O	12:L:56:TRP:HD1	2.01	0.43
12:L:159:ARG:HG2	12:L:200:TYR:CZ	2.54	0.43
13:M:193:LEU:CB	13:M:208:VAL:HG22	2.48	0.43
4:R:58:THR:HG23	4:R:59:VAL:HG13	2.00	0.43
4:R:107:ILE:HD12	4:R:107:ILE:HA	1.88	0.43
9:W:56:THR:O	9:W:60:ILE:HG12	2.18	0.43
11:Y:68:LYS:HA	11:Y:73:TYR:O	2.17	0.43
1:A:52:THR:CG2	1:A:216:GLU:HG3	2.40	0.43
10:J:19:VAL:HG13	10:J:118:PRO:HB3	2.00	0.43
12:L:140:MET:HA	12:L:156:LEU:HD11	2.00	0.43
2:P:202:MET:HE2	2:P:207:ILE:HD13	2.00	0.43
4:R:3:TYR:HE2	4:R:7:ILE:HD11	1.83	0.43
6:T:220:GLU:O	6:T:222:THR:HG23	2.17	0.43
4:D:155:ALA:H	5:E:63:SER:CB	2.32	0.43
4:D:199:VAL:HG12	4:D:202:GLY:H	1.84	0.43
8:H:136:ILE:CG2	8:H:164:ALA:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:39:SER:HB2	9:I:75:PRO:HG3	2.00	0.43
13:M:10:GLY:CA	13:M:42:LYS:HE2	2.48	0.43
14:N:46:ASN:OD1	14:N:49:THR:N	2.51	0.43
14:N:48:SER:O	14:N:114:GLY:HA2	2.17	0.43
14:N:50:MET:HE2	14:N:192:VAL:HG12	2.01	0.43
14:N:91:TRP:CE3	14:N:92:LEU:HD22	2.54	0.43
8:V:21:THR:HG23	15:V:301:LDZ:H34	2.00	0.43
8:V:39:HIS:CD2	8:V:75:PRO:HG3	2.53	0.43
14:b:124:TYR:O	14:b:131:ALA:HA	2.17	0.43
3:C:53:HIS:HB3	3:C:56:LEU:HG	2.01	0.43
4:D:94:HIS:HB3	4:D:102:VAL:CG1	2.48	0.43
6:F:117:GLN:HB2	6:F:151:ALA:CB	2.48	0.43
9:I:39:SER:CB	9:I:75:PRO:HG3	2.48	0.43
13:M:13:LEU:HD12	13:M:136:LYS:O	2.19	0.43
13:M:151:ASN:O	13:M:155:PHE:HA	2.18	0.43
1:O:167:ALA:O	1:O:172:GLN:HG3	2.19	0.43
2:P:134:LEU:HG	2:P:162:MET:SD	2.59	0.43
7:U:99:ARG:O	7:U:103:GLY:HA2	2.18	0.43
9:W:4:ILE:HD11	9:W:128:MET:HB2	2.00	0.43
9:W:35:ILE:HB	9:W:186:PHE:HE1	1.84	0.43
10:X:105:GLU:HA	10:X:106:PRO:HD3	1.83	0.43
12:Z:104:GLY:HA2	12:Z:180:VAL:HG11	1.99	0.43
14:b:6:VAL:HG21	14:b:36:PHE:HE2	1.83	0.43
1:A:37:LEU:HD21	1:A:55:LYS:HG3	2.00	0.43
6:F:84:LEU:O	6:F:88:MET:HG3	2.17	0.43
6:F:184:LEU:HD11	6:F:214:ILE:HD13	2.01	0.43
6:F:205:LEU:HB3	6:F:210:VAL:HG21	2.01	0.43
14:N:124:TYR:O	14:N:131:ALA:HA	2.19	0.43
3:Q:233:VAL:O	3:Q:237:ILE:HG13	2.19	0.43
6:T:118:ILE:HB	6:T:119:PRO:HD3	2.01	0.43
8:V:15:LEU:HD23	8:V:45:CYS:SG	2.59	0.43
8:V:165:MET:SD	8:V:175:ILE:HG12	2.58	0.43
11:Y:101:ASN:HB3	11:Y:132:HIS:ND1	2.34	0.43
12:Z:138:GLY:O	12:Z:142:ARG:HG2	2.18	0.43
13:a:35:ILE:O	14:b:151:ARG:NH2	2.47	0.43
4:D:217:LEU:HD23	4:D:217:LEU:HA	1.85	0.43
5:E:214:ASN:OD1	5:E:215:ILE:HG23	2.19	0.43
10:J:144:GLN:HA	13:a:143:ALA:O	2.19	0.43
14:N:85:PRO:CG	14:N:114:GLY:HA3	2.49	0.43
4:R:50:VAL:O	4:R:51:ALA:HB3	2.19	0.43
4:R:104:VAL:HG21	4:R:143:ARG:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:181:MET:HG2	7:U:182:LYS:N	2.34	0.43
8:V:4:ILE:HD12	8:V:100:ILE:CG2	2.49	0.43
8:V:71:LEU:HD12	8:V:71:LEU:N	2.34	0.43
11:Y:37:LYS:HA	11:Y:43:LEU:HD23	2.00	0.43
13:a:172:MET:O	13:a:176:LYS:HG3	2.19	0.43
14:b:31:GLY:O	14:b:32:SER:CB	2.67	0.43
1:A:192:GLU:C	1:A:194:THR:N	2.77	0.43
3:C:160:LYS:HG2	4:D:53:LEU:O	2.19	0.43
6:F:205:LEU:HD22	6:F:210:VAL:CG2	2.48	0.43
11:K:146:TYR:HB2	11:K:159:LEU:HD13	2.01	0.43
15:L:301:LDZ:H2	13:M:126:PRO:HD2	2.01	0.43
1:O:138:MET:HG2	1:O:140:LEU:HG	2.01	0.43
2:P:88:ARG:HB3	2:P:88:ARG:NH1	2.25	0.43
5:S:31:ILE:C	5:S:33:LEU:H	2.27	0.43
8:V:145:ARG:NH1	8:V:148:MET:HG2	2.34	0.43
10:X:141:CYS:HB3	10:X:177:ASP:HB2	2.00	0.43
3:C:233:VAL:O	3:C:237:ILE:HG13	2.19	0.42
4:D:54:GLN:NE2	4:D:59:VAL:HG11	2.34	0.42
5:E:166:ASP:HB3	5:E:185:TYR:CE2	2.53	0.42
7:G:89:ASP:O	7:G:93:GLU:HG3	2.18	0.42
9:I:179:ILE:HG12	9:I:184:LEU:CD2	2.49	0.42
13:M:45:LYS:HE3	13:M:48:ASP:HA	2.00	0.42
4:R:35:VAL:HG22	4:R:191:VAL:CG2	2.49	0.42
4:R:155:ALA:H	5:S:63:SER:CB	2.32	0.42
6:T:5:GLN:OE1	6:T:5:GLN:N	2.46	0.42
6:T:69:HIS:CD2	6:T:70:ILE:HG13	2.54	0.42
9:W:15:LEU:HB3	9:W:45:CYS:SG	2.58	0.42
9:W:64:LEU:HD23	9:W:64:LEU:HA	1.85	0.42
11:Y:174:ASN:O	11:Y:176:PRO:HD3	2.19	0.42
12:Z:43:LEU:HD22	12:Z:185:TRP:CD1	2.54	0.42
14:b:20:VAL:HG11	14:b:122:LEU:HD13	2.01	0.42
7:G:15:SER:C	7:G:17:ASP:N	2.76	0.42
7:G:76:ALA:HB3	7:G:136:MET:HE3	2.00	0.42
10:J:5:TYR:CE2	11:K:121:LEU:HD12	2.54	0.42
11:K:8:GLN:HG3	11:K:113:PRO:HB2	2.00	0.42
1:O:111:VAL:HG21	1:O:142:GLY:HA3	2.01	0.42
8:V:145:ARG:CZ	8:V:148:MET:HG2	2.49	0.42
10:X:163:PHE:CE1	10:X:197:ARG:HD2	2.55	0.42
13:a:51:VAL:HG23	13:a:203:ILE:HD13	2.00	0.42
2:B:122:GLN:HG3	3:C:128:ARG:HG2	2.00	0.42
3:C:47:ALA:HB1	3:C:64:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:90:LEU:HD11	3:C:114:LEU:HD22	2.01	0.42
4:D:108:THR:HG21	4:D:145:TYR:HB3	2.00	0.42
6:F:121:GLN:HG3	7:G:129:ARG:HG3	1.99	0.42
6:F:209:ASN:OD1	6:F:210:VAL:HG23	2.19	0.42
8:H:20:ARG:HG3	8:H:27:ILE:HG23	2.00	0.42
8:H:128:ILE:HD11	8:H:137:TYR:CE1	2.54	0.42
9:I:182:ASN:O	9:I:183:LYS:HB2	2.20	0.42
1:O:18:PRO:HA	2:P:23:TYR:CE1	2.54	0.42
1:O:132:ARG:CZ	7:U:124:LEU:HD23	2.49	0.42
7:U:30:VAL:HG11	7:U:134:SER:HB2	2.01	0.42
2:B:121:THR:HG22	2:B:128:PRO:HB3	2.02	0.42
7:G:139:SER:HA	7:G:216:VAL:HG11	2.02	0.42
9:I:91:TYR:CB	9:I:95:ILE:HD13	2.49	0.42
10:J:12:ALA:HB3	10:J:136:VAL:CG2	2.50	0.42
10:J:34:VAL:HG12	10:J:35:THR:HG23	2.01	0.42
14:N:22:ILE:HG12	14:N:190:ALA:HB3	2.01	0.42
3:Q:44:LEU:CD2	3:Q:189:ALA:HB1	2.48	0.42
6:T:69:HIS:O	6:T:136:GLY:HA2	2.20	0.42
6:T:212:ILE:O	6:T:224:TYR:N	2.41	0.42
7:U:192:GLU:O	7:U:196:ILE:HG13	2.20	0.42
8:V:41:ARG:O	8:V:180:ILE:HG21	2.18	0.42
8:V:100:ILE:HD11	8:V:112:VAL:HG13	2.00	0.42
10:X:14:LYS:HE3	10:X:120:ILE:HG12	2.01	0.42
12:Z:46:MET:HE1	12:Z:54:SER:CA	2.49	0.42
13:a:102:PHE:HE2	14:b:101:SER:HA	1.84	0.42
5:E:143:PHE:HE1	5:E:156:MET:HE3	1.83	0.42
5:E:186:HIS:O	5:E:189:MET:HB2	2.20	0.42
7:G:151:ILE:HD12	7:G:151:ILE:N	2.34	0.42
8:H:88:CYS:HG	8:H:119:GLY:HA2	1.83	0.42
9:I:60:ILE:HG13	9:I:84:LEU:CD2	2.49	0.42
2:P:129:PHE:O	2:P:150:PRO:HB3	2.19	0.42
5:S:234:LEU:O	5:S:238:ILE:HG13	2.20	0.42
6:T:210:VAL:HG11	6:T:233:LEU:HD11	2.01	0.42
10:X:55:LEU:HG	10:X:57:THR:HG22	2.01	0.42
12:Z:39:ASN:HB2	12:Z:41:TYR:CE1	2.53	0.42
12:Z:154:TYR:HA	12:Z:177:LEU:HD21	2.00	0.42
13:a:8:ASN:HB3	13:a:29:LEU:HD11	2.01	0.42
14:b:19:GLY:HA2	14:b:115:TYR:CD1	2.54	0.42
3:C:143:TYR:HB2	3:C:146:GLN:NE2	2.34	0.42
5:E:16:SER:C	5:E:18:GLU:N	2.76	0.42
8:H:52:ASP:O	8:H:56:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:48:LEU:HD12	10:J:48:LEU:HA	1.90	0.42
12:L:9:PHE:CE1	12:L:14:ILE:HG12	2.54	0.42
1:O:41:ALA:HB2	1:O:50:ILE:HG22	2.01	0.42
4:R:120:GLN:HG2	5:S:133:MET:HG3	2.02	0.42
5:S:22:PHE:HA	5:S:25:GLU:CD	2.44	0.42
5:S:210:LEU:HA	5:S:214:ASN:HD21	1.85	0.42
6:T:5:GLN:HG2	7:U:9:LEU:HD21	2.00	0.42
6:T:49:LEU:HD11	6:T:199:LEU:CD2	2.49	0.42
8:V:134:SER:HA	8:V:137:TYR:HD2	1.85	0.42
10:X:9:ALA:CB	10:X:141:CYS:SG	3.08	0.42
14:b:206:GLU:C	14:b:208:ASN:N	2.78	0.42
2:B:88:ARG:HD3	2:B:116:VAL:HG11	2.01	0.42
10:J:14:LYS:HG2	10:J:120:ILE:HG23	2.00	0.42
11:K:45:LEU:N	11:K:45:LEU:HD12	2.34	0.42
11:K:177:THR:HG22	11:K:195:SER:CB	2.50	0.42
14:N:72:ILE:O	14:N:76:LEU:HG	2.19	0.42
2:P:223:THR:O	2:P:226:LYS:HB3	2.19	0.42
4:R:39:ASP:HA	4:R:213:ARG:HH11	1.84	0.42
4:R:115:LYS:HE3	4:R:129:ILE:O	2.19	0.42
12:Z:159:ARG:HD2	12:Z:163:GLN:HE21	1.83	0.42
1:A:111:VAL:HG21	1:A:142:GLY:CA	2.47	0.42
10:J:125:LEU:HD23	10:J:125:LEU:N	2.34	0.42
13:M:171:ALA:O	13:M:175:VAL:HG23	2.19	0.42
3:Q:199:LYS:NZ	3:Q:199:LYS:HB3	2.34	0.42
6:T:108:LEU:O	6:T:112:ILE:HG13	2.19	0.42
12:Z:41:TYR:CE1	12:Z:74:ARG:HG2	2.54	0.42
15:Z:301:LDZ:H11	15:Z:301:LDZ:H9	1.63	0.42
11:K:118:MET:HE2	11:K:124:LEU:HD13	2.02	0.42
3:Q:73:ALA:HB2	3:Q:225:ILE:HD13	2.02	0.42
8:V:36:THR:HA	8:V:37:PRO:HD3	1.90	0.42
8:V:139:TYR:CE2	8:V:143:THR:HG21	2.54	0.42
14:b:27:LEU:HD22	14:b:28:GLY:H	1.85	0.42
2:B:49:LYS:O	2:B:49:LYS:HG2	2.20	0.42
6:F:11:THR:HA	7:G:129:ARG:HB3	2.02	0.42
7:G:190:VAL:HG21	7:G:215:TRP:CZ3	2.55	0.42
12:L:154:TYR:HA	12:L:177:LEU:HD21	2.02	0.42
13:M:100:ARG:O	13:M:100:ARG:HD3	2.20	0.42
1:O:110:PRO:HD2	1:O:113:MET:HB2	2.00	0.42
5:S:50:VAL:HG21	5:S:66:LYS:HB3	2.01	0.42
6:T:105:VAL:O	6:T:109:VAL:HG23	2.20	0.42
12:Z:16:ALA:HB2	12:Z:177:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:136:LYS:HA	13:a:146:GLN:OE1	2.19	0.42
1:A:158:GLY:O	2:B:83:ARG:NH2	2.53	0.41
2:B:64:VAL:HG11	2:B:210:GLY:HA3	2.02	0.41
3:C:135:LEU:HG	3:C:164:ILE:HD13	2.01	0.41
13:M:25:SER:O	13:M:193:LEU:HD23	2.20	0.41
1:O:92:GLN:NE2	8:V:70:GLU:HG2	2.35	0.41
3:Q:24:ALA:O	3:Q:27:ALA:HB3	2.19	0.41
3:Q:174:MET:HE3	3:Q:196:VAL:HA	2.02	0.41
6:T:72:ILE:HG22	6:T:134:ILE:HG13	2.02	0.41
8:V:180:ILE:HG23	8:V:185:VAL:HG22	2.02	0.41
9:W:66:LEU:HD12	9:W:66:LEU:HA	1.73	0.41
15:W:301:LDZ:H11	15:W:301:LDZ:H32	1.62	0.41
11:Y:11:ASP:OD1	11:Y:11:ASP:N	2.52	0.41
4:D:115:LYS:O	4:D:119:THR:HG23	2.20	0.41
5:E:163:VAL:HG23	6:F:59:HIS:O	2.19	0.41
8:H:197:LYS:HB2	8:H:197:LYS:NZ	2.34	0.41
10:J:98:ARG:HD2	10:J:99:PHE:CZ	2.55	0.41
1:O:32:ILE:HA	1:O:82:GLY:HA2	2.01	0.41
4:R:132:LEU:HG	4:R:161:ILE:HD13	2.01	0.41
9:W:212:VAL:HG11	10:X:197:ARG:HD3	2.00	0.41
1:A:163:PHE:CD2	1:A:166:THR:HG23	2.55	0.41
1:A:187:PHE:O	1:A:188:ASP:C	2.63	0.41
3:C:100:GLN:HE21	11:K:83:PHE:HE1	1.66	0.41
4:D:109:ARG:HG3	4:D:153:TYR:OH	2.21	0.41
5:E:41:GLN:NE2	5:E:151:PRO:O	2.53	0.41
5:E:202:LEU:HD23	5:E:202:LEU:HA	1.88	0.41
6:F:157:ARG:HD3	6:F:176:MET:HE2	2.02	0.41
13:M:193:LEU:HB2	13:M:208:VAL:HG22	2.02	0.41
8:V:115:VAL:HA	8:V:120:MET:O	2.20	0.41
10:X:55:LEU:HD12	10:X:55:LEU:HA	1.95	0.41
11:Y:8:GLN:HE21	11:Y:113:PRO:HB2	1.85	0.41
14:b:150:LEU:HD23	14:b:168:LEU:CG	2.48	0.41
2:B:142:ARG:HD3	2:B:144:TYR:CE2	2.56	0.41
3:C:174:MET:CE	3:C:196:VAL:HA	2.48	0.41
5:E:210:LEU:HD23	5:E:238:ILE:HG23	2.03	0.41
8:H:143:THR:CG2	8:H:156:PHE:HE1	2.32	0.41
10:J:154:GLU:O	10:J:157:MET:HG3	2.19	0.41
13:M:200:LYS:HB2	13:M:200:LYS:NZ	2.36	0.41
14:N:112:ILE:HD12	14:N:112:ILE:N	2.35	0.41
1:O:191:PHE:O	1:O:192:GLU:C	2.63	0.41
4:R:209:ALA:HB1	4:R:217:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:13:ASN:HB3	6:T:126:ARG:HD3	2.03	0.41
6:T:5:GLN:CG	7:U:9:LEU:HD21	2.50	0.41
9:W:174:ILE:HG22	9:W:176:LEU:CD2	2.51	0.41
9:W:184:LEU:C	9:W:184:LEU:HD13	2.46	0.41
11:Y:16:ALA:HB2	11:Y:160:LEU:HD21	2.02	0.41
12:Z:8:LYS:HE2	12:Z:125:ALA:HA	2.02	0.41
13:a:166:LEU:HG	13:a:171:ALA:HB2	2.01	0.41
14:b:89:HIS:HD2	14:b:112:ILE:HD13	1.86	0.41
14:b:205:THR:O	14:b:206:GLU:C	2.63	0.41
2:B:64:VAL:CG1	2:B:217:PHE:HZ	2.31	0.41
3:C:201:MET:HE2	3:C:201:MET:HB3	1.89	0.41
6:F:98:VAL:HA	14:N:94:ARG:HG3	2.01	0.41
9:I:133:LEU:O	14:b:145:LEU:HD23	2.20	0.41
6:T:63:ILE:O	6:T:64:LEU:HD23	2.20	0.41
7:U:109:LYS:HG2	7:U:149:TYR:CZ	2.56	0.41
12:Z:115:VAL:HA	12:Z:120:ASN:O	2.21	0.41
14:b:110:MET:HE2	14:b:110:MET:HB2	1.89	0.41
14:b:156:LYS:O	14:b:158:PRO:HD3	2.19	0.41
1:A:211:LYS:HG2	1:A:214:GLU:CD	2.46	0.41
2:B:113:VAL:O	2:B:117:MET:HG3	2.21	0.41
4:D:47:LYS:O	4:D:48:LYS:C	2.64	0.41
4:D:199:VAL:HG11	4:D:206:ILE:CG2	2.49	0.41
5:E:196:LYS:O	5:E:200:ILE:HG13	2.21	0.41
5:E:228:MET:HE2	5:E:228:MET:HB2	1.90	0.41
6:F:128:TYR:O	6:F:149:PRO:HB3	2.21	0.41
7:G:170:GLN:O	7:G:174:THR:HG23	2.20	0.41
9:I:156:VAL:O	9:I:160:ILE:HG12	2.20	0.41
3:Q:98:LEU:O	3:Q:102:GLN:HA	2.21	0.41
5:S:166:ASP:HB3	5:S:185:TYR:OH	2.21	0.41
5:S:179:SER:HA	5:S:182:GLN:NE2	2.36	0.41
9:W:34:LYS:HG2	15:W:301:LDZ:H22	2.03	0.41
10:X:148:MET:HE2	10:X:172:ASN:HD22	1.85	0.41
12:Z:7:PHE:HA	12:Z:125:ALA:O	2.21	0.41
12:Z:13:VAL:HG13	12:Z:180:VAL:CB	2.41	0.41
15:Z:301:LDZ:O34	15:Z:301:LDZ:H27	2.21	0.41
14:b:12:LEU:HD12	14:b:173:MET:CE	2.50	0.41
1:A:45:LYS:HB2	1:A:45:LYS:HZ3	1.82	0.41
4:D:181:ILE:HA	4:D:187:THR:HG22	2.03	0.41
4:D:184:ASP:O	4:D:188:ILE:HG13	2.21	0.41
7:G:194:ALA:O	7:G:198:TYR:HD1	2.04	0.41
10:J:13:MET:SD	10:J:153:TRP:HD1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:72:LEU:HD12	10:J:72:LEU:HA	1.80	0.41
14:N:178:TYR:OH	14:N:208:ASN:HA	2.21	0.41
1:O:25:VAL:O	1:O:29:PHE:HD1	2.03	0.41
4:R:12:PRO:O	4:R:13:ASP:CB	2.69	0.41
4:R:120:GLN:HG3	5:S:135:ARG:HG3	2.03	0.41
4:R:208:LEU:HD22	4:R:220:LEU:HD12	2.01	0.41
5:S:31:ILE:C	5:S:33:LEU:N	2.77	0.41
7:U:44:GLY:HA2	7:U:146:ALA:HB2	2.02	0.41
9:W:136:MET:CE	9:W:140:GLU:HG2	2.51	0.41
13:a:62:LEU:O	13:a:66:LYS:HG3	2.21	0.41
6:F:16:GLN:HE21	6:F:16:GLN:HB2	1.68	0.41
6:F:152:ASN:HD22	6:F:153:TYR:H	1.69	0.41
9:I:184:LEU:HD13	9:I:184:LEU:C	2.46	0.41
12:L:34:LYS:CE	15:L:301:LDZ:H23	2.50	0.41
12:L:53:CYS:SG	12:L:98:MET:HG3	2.60	0.41
13:M:144:MET:HE2	13:M:144:MET:HB3	1.86	0.41
1:O:45:LYS:NZ	1:O:45:LYS:HB2	2.36	0.41
1:O:153:LYS:HB3	1:O:163:PHE:CE1	2.56	0.41
3:Q:92:LEU:O	3:Q:96:ARG:HG3	2.21	0.41
4:R:33:VAL:CG2	4:R:168:VAL:HG11	2.51	0.41
15:W:301:LDZ:H42	15:W:301:LDZ:H9	1.86	0.41
10:X:154:GLU:O	10:X:157:MET:HG3	2.21	0.41
11:Y:43:LEU:HG	11:Y:188:ILE:HD13	2.03	0.41
12:Z:94:MET:HE2	12:Z:94:MET:HB3	1.96	0.41
13:a:123:SER:HB3	13:a:136:LYS:HG2	2.03	0.41
2:B:97:TYR:O	2:B:101:GLN:HA	2.20	0.41
3:C:24:ALA:O	3:C:28:ILE:HD12	2.21	0.41
3:C:35:LEU:HG	3:C:46:ALA:HB3	2.02	0.41
3:C:72:MET:HE2	3:C:72:MET:HB3	1.97	0.41
5:E:41:GLN:HA	5:E:46:VAL:HG12	2.03	0.41
5:E:116:VAL:HB	5:E:156:MET:CE	2.49	0.41
5:E:211:ASN:OD1	5:E:214:ASN:N	2.54	0.41
5:E:236:GLU:HG3	5:E:236:GLU:H	1.75	0.41
6:F:45:VAL:HG11	6:F:188:VAL:HG22	2.03	0.41
7:G:151:ILE:HA	7:G:156:VAL:O	2.21	0.41
8:H:136:ILE:HG23	8:H:164:ALA:HB2	2.03	0.41
9:I:85:LYS:HB2	9:I:85:LYS:HE3	1.88	0.41
12:L:7:PHE:HB2	12:L:126:THR:HG22	2.02	0.41
1:O:182:LYS:NZ	1:O:182:LYS:HB3	2.36	0.41
2:P:191:ILE:HG23	2:P:202:MET:CE	2.51	0.41
3:Q:9:THR:HB	3:Q:20:GLN:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:89:GLU:O	3:Q:93:ILE:HG13	2.20	0.41
5:S:228:MET:HE2	5:S:228:MET:HB2	1.89	0.41
6:T:134:ILE:HD12	6:T:134:ILE:N	2.36	0.41
6:T:196:ARG:O	6:T:199:LEU:HB2	2.21	0.41
7:U:69:VAL:HG23	7:U:73:VAL:HB	2.02	0.41
8:V:19:SER:O	8:V:32:THR:HG23	2.20	0.41
11:Y:5:ILE:HG22	11:Y:16:ALA:HB3	2.03	0.41
12:Z:135:TYR:HB2	12:Z:164:ALA:HA	2.02	0.41
14:b:10:SER:HB3	14:b:139:THR:O	2.20	0.41
1:A:31:ALA:HA	1:A:34:GLN:HG2	2.02	0.41
5:E:31:ILE:HD12	5:E:31:ILE:N	2.36	0.41
5:E:120:ALA:O	5:E:121:LEU:HB2	2.20	0.41
5:E:195:ILE:HG23	5:E:217:LEU:CD1	2.51	0.41
11:K:172:ILE:HD13	11:Y:24:ASN:O	2.21	0.41
13:M:46:LEU:HB3	13:M:72:LEU:HD11	2.03	0.41
3:Q:207:SER:O	3:Q:208:ALA:HB3	2.21	0.41
4:R:8:THR:HB	4:R:119:THR:O	2.21	0.41
9:W:171:GLY:O	9:W:172:SER:HB2	2.21	0.41
11:Y:4:LEU:HD11	11:Y:47:VAL:HG13	2.02	0.41
11:Y:39:SER:OG	11:Y:40:GLU:N	2.53	0.41
4:D:32:ALA:HB3	4:D:161:ILE:HG12	2.04	0.40
5:E:27:ALA:O	5:E:30:ALA:HB3	2.21	0.40
8:H:15:LEU:HD21	8:H:102:ALA:HB3	2.02	0.40
8:H:110:GLY:C	8:H:111:GLN:HG3	2.46	0.40
11:K:31:ASP:N	11:K:31:ASP:OD1	2.55	0.40
11:K:82:ASN:O	11:K:86:ARG:HG2	2.21	0.40
12:L:14:ILE:HG23	12:L:177:LEU:HD11	2.02	0.40
12:L:166:TYR:CD2	10:X:33:MET:HE2	2.56	0.40
1:O:78:CYS:SG	1:O:80:MET:SD	3.19	0.40
1:O:132:ARG:HD3	7:U:11:ALA:O	2.21	0.40
2:P:202:MET:CE	2:P:207:ILE:HD13	2.51	0.40
11:Y:16:ALA:HA	11:Y:179:SER:O	2.21	0.40
12:Z:5:LEU:HD22	12:Z:161:ILE:HD11	2.02	0.40
14:b:154:LEU:HD12	14:b:154:LEU:HA	1.75	0.40
2:B:117:MET:HE2	2:B:150:PRO:HA	2.02	0.40
4:D:94:HIS:C	4:D:96:LEU:N	2.78	0.40
11:K:27:GLN:NE2	11:K:174:ASN:HB3	2.35	0.40
13:M:18:GLU:O	13:M:118:LYS:HG3	2.22	0.40
3:Q:44:LEU:C	3:Q:44:LEU:HD12	2.46	0.40
3:Q:101:TYR:O	3:Q:102:GLN:HB2	2.22	0.40
9:W:139:PHE:CE1	9:W:155:LEU:HG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:51:GLY:O	11:Y:55:GLN:HG2	2.21	0.40
12:Z:177:LEU:HD23	12:Z:188:VAL:HG21	2.03	0.40
1:A:206:LEU:O	1:A:207:SER:C	2.65	0.40
5:E:142:LEU:HG	5:E:170:ILE:HD13	2.04	0.40
8:H:180:ILE:HG23	8:H:185:VAL:HG22	2.04	0.40
15:H:301:LDZ:H2	9:I:119:SER:HB2	2.03	0.40
3:Q:45:LEU:HG	3:Q:137:ILE:HG21	2.03	0.40
4:R:11:SER:O	4:R:12:PRO:C	2.62	0.40
6:T:50:LYS:HA	6:T:62:LYS:HD3	2.03	0.40
6:T:140:MET:HG2	14:b:81:HIS:CE1	2.55	0.40
3:C:229:LYS:O	3:C:233:VAL:HG23	2.21	0.40
6:F:175:HIS:HB3	6:F:178:GLU:OE2	2.21	0.40
9:I:4:ILE:HD11	9:I:128:MET:HB2	2.02	0.40
11:K:43:LEU:HB2	11:K:183:ILE:HD11	2.02	0.40
11:K:173:LEU:HD23	11:Y:173:LEU:HD23	2.03	0.40
13:M:64:LEU:O	13:M:68:ILE:HG13	2.20	0.40
2:P:107:ALA:O	2:P:111:GLN:HG3	2.21	0.40
6:T:49:LEU:HB2	6:T:195:LEU:CD1	2.45	0.40
9:W:14:VAL:CG1	9:W:176:LEU:HD12	2.51	0.40
9:W:210:THR:HG21	10:X:167:SER:HB2	2.03	0.40
14:b:72:ILE:O	14:b:76:LEU:HG	2.21	0.40
4:D:63:CYS:SG	4:D:84:ILE:HD13	2.61	0.40
6:F:13:TRP:CH2	7:G:132:GLY:HA3	2.56	0.40
6:F:199:LEU:HD11	6:F:205:LEU:HD23	2.03	0.40
8:H:15:LEU:HD23	8:H:45:CYS:SG	2.62	0.40
11:K:38:MET:HE2	11:K:44:LEU:HD22	2.02	0.40
14:N:92:LEU:HD13	14:N:92:LEU:HA	1.77	0.40
1:O:138:MET:HB3	1:O:154:CYS:HG	1.87	0.40
3:Q:28:ILE:HD11	3:Q:131:GLY:C	2.46	0.40
3:Q:48:GLU:O	3:Q:64:LYS:NZ	2.55	0.40
4:R:120:GLN:HG3	5:S:135:ARG:CG	2.51	0.40
9:W:74:LEU:HD23	9:W:75:PRO:HD2	2.04	0.40
11:Y:31:ASP:OD1	11:Y:31:ASP:N	2.55	0.40
13:a:208:VAL:HG22	13:a:209:SER:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	238/246 (97%)	223 (94%)	12 (5%)	3 (1%)	9	25
1	O	238/246 (97%)	221 (93%)	13 (6%)	4 (2%)	7	19
2	B	227/234 (97%)	222 (98%)	5 (2%)	0	100	100
2	P	227/234 (97%)	224 (99%)	3 (1%)	0	100	100
3	C	245/261 (94%)	231 (94%)	9 (4%)	5 (2%)	6	16
3	Q	245/261 (94%)	240 (98%)	4 (2%)	1 (0%)	30	54
4	D	230/248 (93%)	219 (95%)	9 (4%)	2 (1%)	14	35
4	R	230/248 (93%)	220 (96%)	7 (3%)	3 (1%)	9	25
5	E	231/241 (96%)	219 (95%)	11 (5%)	1 (0%)	30	54
5	S	231/241 (96%)	221 (96%)	9 (4%)	1 (0%)	30	54
6	F	231/263 (88%)	217 (94%)	13 (6%)	1 (0%)	30	54
6	T	231/263 (88%)	220 (95%)	7 (3%)	4 (2%)	7	19
7	G	237/255 (93%)	228 (96%)	9 (4%)	0	100	100
7	U	237/255 (93%)	230 (97%)	5 (2%)	2 (1%)	16	37
8	H	200/205 (98%)	195 (98%)	5 (2%)	0	100	100
8	V	200/205 (98%)	191 (96%)	8 (4%)	1 (0%)	24	48
9	I	218/234 (93%)	211 (97%)	5 (2%)	2 (1%)	14	35
9	W	218/234 (93%)	210 (96%)	7 (3%)	1 (0%)	24	48
10	J	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
10	X	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
11	K	194/201 (96%)	187 (96%)	5 (3%)	2 (1%)	12	32
11	Y	194/201 (96%)	187 (96%)	6 (3%)	1 (0%)	24	48
12	L	198/204 (97%)	190 (96%)	8 (4%)	0	100	100
12	Z	198/204 (97%)	192 (97%)	6 (3%)	0	100	100
13	M	210/241 (87%)	200 (95%)	9 (4%)	1 (0%)	24	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	210/241 (87%)	202 (96%)	7 (3%)	1 (0%)	24	48
14	N	210/264 (80%)	194 (92%)	15 (7%)	1 (0%)	24	48
14	b	210/264 (80%)	197 (94%)	11 (5%)	2 (1%)	12	32
All	All	6142/6604 (93%)	5883 (96%)	220 (4%)	39 (1%)	23	44

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	203	VAL
11	K	25	ILE
1	O	191	PHE
4	R	48	LYS
4	R	181	ILE
6	T	60	GLN
6	T	201	ALA
14	b	206	GLU
1	A	185	LYS
9	I	172	SER
1	O	188	ASP
1	O	189	TRP
1	O	207	SER
7	U	207	LYS
8	V	72	ASN
9	W	172	SER
3	C	61	PHE
4	D	213	ARG
13	M	190	GLY
14	N	32	SER
6	T	61	LYS
11	Y	122	ALA
1	A	189	TRP
3	C	66	TYR
3	C	202	ASP
14	b	32	SER
5	E	130	PRO
11	K	122	ALA
4	R	232	ILE
6	T	200	PRO
3	C	204	SER
4	D	203	GLY
6	F	151	ALA

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Mol	Chain	Res	Type
9	I	188	ARG
7	U	16	PRO
13	a	190	GLY
3	Q	203	VAL
1	A	156	PRO
5	S	176	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	164/210 (78%)	155 (94%)	9 (6%)	19	45
1	O	163/210 (78%)	148 (91%)	15 (9%)	8	22
2	B	150/191 (78%)	143 (95%)	7 (5%)	23	51
2	P	150/191 (78%)	145 (97%)	5 (3%)	33	63
3	C	160/221 (72%)	154 (96%)	6 (4%)	29	58
3	Q	160/221 (72%)	151 (94%)	9 (6%)	19	44
4	D	136/211 (64%)	130 (96%)	6 (4%)	25	53
4	R	136/211 (64%)	132 (97%)	4 (3%)	37	67
5	E	158/203 (78%)	145 (92%)	13 (8%)	10	27
5	S	158/203 (78%)	148 (94%)	10 (6%)	16	39
6	F	160/224 (71%)	151 (94%)	9 (6%)	19	44
6	T	161/224 (72%)	157 (98%)	4 (2%)	42	71
7	G	162/212 (76%)	154 (95%)	8 (5%)	22	49
7	U	162/212 (76%)	153 (94%)	9 (6%)	19	44
8	H	141/159 (89%)	135 (96%)	6 (4%)	26	54
8	V	140/159 (88%)	133 (95%)	7 (5%)	22	48
9	I	158/195 (81%)	145 (92%)	13 (8%)	10	27
9	W	157/195 (80%)	150 (96%)	7 (4%)	24	52
10	J	159/174 (91%)	152 (96%)	7 (4%)	25	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	X	155/174 (89%)	148 (96%)	7 (4%)	24	52
11	K	149/171 (87%)	143 (96%)	6 (4%)	28	56
11	Y	148/171 (86%)	142 (96%)	6 (4%)	27	56
12	L	139/159 (87%)	129 (93%)	10 (7%)	13	32
12	Z	138/159 (87%)	124 (90%)	14 (10%)	7	18
13	M	158/199 (79%)	149 (94%)	9 (6%)	18	43
13	a	158/199 (79%)	151 (96%)	7 (4%)	25	53
14	N	149/215 (69%)	142 (95%)	7 (5%)	23	51
14	b	150/215 (70%)	144 (96%)	6 (4%)	28	56
All	All	4279/5488 (78%)	4053 (95%)	226 (5%)	22	46

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	61	LEU
1	A	88	ARG
1	A	154	CYS
1	A	166	THR
1	A	174	GLU
1	A	179	LEU
1	A	191	PHE
1	A	216	GLU
2	B	38	LYS
2	B	50	LYS
2	B	73	LEU
2	B	102	GLU
2	B	109	LEU
2	B	131	VAL
2	B	173	LEU
3	C	43	VAL
3	C	58	GLU
3	C	67	LYS
3	C	109	GLN
3	C	224	VAL
3	C	229	LYS
4	D	59	VAL
4	D	102	VAL
4	D	163	ARG

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Mol	Chain	Res	Type
4	D	206	ILE
4	D	211	MET
4	D	219	ILE
5	E	60	GLU
5	E	87	THR
5	E	133	MET
5	E	139	VAL
5	E	141	LEU
5	E	163	VAL
5	E	165	CYS
5	E	168	ARG
5	E	182	GLN
5	E	192	LYS
5	E	199	LEU
5	E	210	LEU
5	E	231	LYS
6	F	21	GLN
6	F	29	VAL
6	F	38	LEU
6	F	49	LEU
6	F	84	LEU
6	F	101	ARG
6	F	156	CYS
6	F	223	ILE
6	F	229	VAL
7	G	17	ASP
7	G	53	VAL
7	G	108	LEU
7	G	109	LYS
7	G	148	LEU
7	G	150	MET
7	G	195	LYS
7	G	206	ASP
8	H	32	THR
8	H	88	CYS
8	H	122	VAL
8	H	145	ARG
8	H	191	LEU
8	H	197	LYS
9	I	7	VAL
9	I	11	ASP
9	I	13	ILE

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Mol	Chain	Res	Type
9	I	119	SER
9	I	120	THR
9	I	128	MET
9	I	133	LEU
9	I	142	LYS
9	I	175	ASP
9	I	183	LYS
9	I	195	LYS
9	I	212	VAL
9	I	214	THR
10	J	33	MET
10	J	72	LEU
10	J	108	ILE
10	J	114	LYS
10	J	176	ARG
10	J	193	LYS
10	J	200	LYS
11	K	20	VAL
11	K	38	MET
11	K	62	LYS
11	K	68	LYS
11	K	102	LEU
11	K	185	LYS
12	L	13	VAL
12	L	33	LYS
12	L	43	LEU
12	L	63	GLN
12	L	82	LYS
12	L	103	CYS
12	L	175	VAL
12	L	181	ARG
12	L	183	ASP
12	L	188	VAL
13	M	113	LEU
13	M	118	LYS
13	M	127	VAL
13	M	174	LEU
13	M	178	VAL
13	M	193	LEU
13	M	197	ILE
13	M	198	VAL
13	M	208	VAL

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Mol	Chain	Res	Type
14	N	10	SER
14	N	88	ILE
14	N	92	LEU
14	N	94	ARG
14	N	100	ARG
14	N	154	LEU
14	N	163	THR
1	O	17	SER
1	O	19	GLU
1	O	45	LYS
1	O	61	LEU
1	O	71	LYS
1	O	73	THR
1	O	87	SER
1	O	92	GLN
1	O	166	THR
1	O	174	GLU
1	O	179	LEU
1	O	181	LYS
1	O	182	LYS
1	O	191	PHE
1	O	216	GLU
2	P	88	ARG
2	P	91	LYS
2	P	131	VAL
2	P	135	ILE
2	P	173	LEU
3	Q	25	MET
3	Q	43	VAL
3	Q	61	PHE
3	Q	109	GLN
3	Q	132	VAL
3	Q	141	LYS
3	Q	177	GLN
3	Q	199	LYS
3	Q	224	VAL
4	R	40	ILE
4	R	69	VAL
4	R	115	LYS
4	R	210	VAL
5	S	52	LYS
5	S	78	MET

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Mol	Chain	Res	Type
5	S	121	LEU
5	S	133	MET
5	S	139	VAL
5	S	163	VAL
5	S	196	LYS
5	S	199	LEU
5	S	221	GLN
5	S	233	GLU
6	T	16	GLN
6	T	38	LEU
6	T	60	GLN
6	T	84	LEU
7	U	53	VAL
7	U	69	VAL
7	U	93	GLU
7	U	108	LEU
7	U	148	LEU
7	U	156	VAL
7	U	170	GLN
7	U	195	LYS
7	U	219	LEU
8	V	32	THR
8	V	92	ARG
8	V	95	LEU
8	V	100	ILE
8	V	105	ASP
8	V	111	GLN
8	V	197	LYS
9	W	7	VAL
9	W	13	ILE
9	W	66	LEU
9	W	114	ILE
9	W	128	MET
9	W	133	LEU
9	W	183	LYS
10	X	33	MET
10	X	72	LEU
10	X	108	ILE
10	X	122	SER
10	X	143	GLU
10	X	166	ILE
10	X	195	THR

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Mol	Chain	Res	Type
11	Y	13	VAL
11	Y	20	VAL
11	Y	38	MET
11	Y	41	LYS
11	Y	62	LYS
11	Y	102	LEU
12	Z	2	THR
12	Z	5	LEU
12	Z	13	VAL
12	Z	30	GLN
12	Z	37	GLU
12	Z	39	ASN
12	Z	43	LEU
12	Z	63	GLN
12	Z	83	LEU
12	Z	100	THR
12	Z	105	TRP
12	Z	180	VAL
12	Z	188	VAL
12	Z	192	ASN
13	a	108	ASN
13	a	113	LEU
13	a	127	VAL
13	a	146	GLN
13	a	178	VAL
13	a	193	LEU
13	a	197	ILE
14	b	14	VAL
14	b	21	VAL
14	b	100	ARG
14	b	119	GLU
14	b	154	LEU
14	b	169	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	34	GLN
1	A	224	ASN
2	B	108	GLN
3	C	102	GLN

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Mol	Chain	Res	Type
3	C	109	GLN
3	C	142	HIS
3	C	146	GLN
3	C	167	ASN
3	C	198	ASN
4	D	15	HIS
4	D	54	GLN
4	D	122	ASN
5	E	41	GLN
5	E	97	GLN
5	E	204	GLN
5	E	225	ASN
5	E	227	HIS
6	F	16	GLN
6	F	43	HIS
6	F	60	GLN
6	F	143	HIS
6	F	152	ASN
7	G	110	HIS
7	G	147	GLN
7	G	180	GLN
8	H	107	GLN
8	H	124	GLN
8	H	194	GLN
11	K	63	ASN
11	K	82	ASN
11	K	101	ASN
11	K	132	HIS
11	K	189	HIS
12	L	163	GLN
13	M	77	HIS
13	M	131	GLN
13	M	163	HIS
14	N	65	GLN
14	N	69	GLN
14	N	89	HIS
14	N	188	GLN
1	O	24	GLN
1	O	53	GLN
1	O	75	ASN
1	O	193	GLN
2	P	94	GLN

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Mol	Chain	Res	Type
2	P	108	GLN
2	P	188	HIS
3	Q	30	HIS
3	Q	40	ASN
3	Q	102	GLN
3	Q	109	GLN
3	Q	167	ASN
3	Q	177	GLN
3	Q	240	HIS
5	S	41	GLN
5	S	152	GLN
5	S	155	HIS
5	S	164	GLN
5	S	186	HIS
5	S	225	ASN
6	T	16	GLN
6	T	43	HIS
6	T	152	ASN
7	U	110	HIS
8	V	188	GLN
9	W	117	HIS
9	W	166	ASN
10	X	32	GLN
10	X	172	ASN
11	Y	8	GLN
11	Y	63	ASN
11	Y	82	ASN
11	Y	87	ASN
11	Y	101	ASN
11	Y	132	HIS
11	Y	189	HIS
12	Z	163	GLN
12	Z	192	ASN
13	a	157	ASN
13	a	163	HIS
14	b	69	GLN
14	b	89	HIS
14	b	188	GLN

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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	LDZ	Z	301	-	33,34,34	1.73	7 (21%)	42,44,44	1.16	5 (11%)
15	LDZ	V	301	-	33,34,34	1.80	7 (21%)	42,44,44	1.39	4 (9%)
15	LDZ	I	301	-	33,34,34	1.81	7 (21%)	42,44,44	1.34	6 (14%)
15	LDZ	L	301	-	33,34,34	1.85	7 (21%)	42,44,44	1.53	8 (19%)
15	LDZ	W	301	-	33,34,34	1.76	7 (21%)	42,44,44	1.17	2 (4%)
15	LDZ	H	301	-	33,34,34	1.76	7 (21%)	42,44,44	1.22	4 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	LDZ	Z	301	-	-	10/38/39/39	0/1/1/1
15	LDZ	V	301	-	-	13/38/39/39	0/1/1/1
15	LDZ	I	301	-	-	9/38/39/39	0/1/1/1
15	LDZ	L	301	-	-	23/38/39/39	0/1/1/1
15	LDZ	W	301	-	-	17/38/39/39	0/1/1/1
15	LDZ	H	301	-	-	15/38/39/39	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	301	LDZ	C15-N16	5.55	1.45	1.34
15	I	301	LDZ	C12-N13	5.52	1.45	1.34
15	L	301	LDZ	C12-N13	5.52	1.45	1.34
15	L	301	LDZ	C15-N16	5.45	1.45	1.34
15	W	301	LDZ	C15-N16	5.29	1.45	1.34
15	I	301	LDZ	C15-N16	5.27	1.45	1.34
15	V	301	LDZ	C12-N13	5.18	1.45	1.34
15	H	301	LDZ	C12-N13	5.17	1.45	1.34
15	H	301	LDZ	C15-N16	5.11	1.45	1.34
15	W	301	LDZ	C12-N13	5.07	1.44	1.34
15	Z	301	LDZ	C12-N13	4.88	1.44	1.34
15	Z	301	LDZ	C15-N16	4.71	1.44	1.34
15	L	301	LDZ	C9-N10	4.51	1.45	1.34
15	I	301	LDZ	C9-N10	4.34	1.45	1.34
15	Z	301	LDZ	C9-N10	4.32	1.45	1.34
15	W	301	LDZ	C9-N10	4.16	1.45	1.34
15	V	301	LDZ	C9-N10	4.15	1.45	1.34
15	H	301	LDZ	C9-N10	4.15	1.45	1.34
15	H	301	LDZ	O8-C7	-2.67	1.40	1.45
15	H	301	LDZ	O32-C12	-2.65	1.18	1.23
15	H	301	LDZ	O34-C15	-2.65	1.18	1.23
15	W	301	LDZ	O8-C7	-2.64	1.40	1.45
15	L	301	LDZ	O34-C15	-2.63	1.18	1.23
15	Z	301	LDZ	O34-C15	-2.63	1.18	1.23
15	V	301	LDZ	O34-C15	-2.61	1.18	1.23
15	L	301	LDZ	O32-C12	-2.59	1.18	1.23
15	Z	301	LDZ	O8-C7	-2.58	1.40	1.45
15	I	301	LDZ	O8-C7	-2.58	1.40	1.45
15	L	301	LDZ	O8-C9	2.56	1.40	1.35
15	L	301	LDZ	O8-C7	-2.56	1.40	1.45
15	W	301	LDZ	O34-C15	-2.54	1.18	1.23
15	V	301	LDZ	O8-C7	-2.53	1.40	1.45
15	V	301	LDZ	O32-C12	-2.53	1.18	1.23
15	Z	301	LDZ	O8-C9	2.52	1.40	1.35
15	I	301	LDZ	O8-C9	2.50	1.40	1.35
15	I	301	LDZ	O34-C15	-2.49	1.18	1.23
15	Z	301	LDZ	O32-C12	-2.48	1.18	1.23
15	W	301	LDZ	O32-C12	-2.47	1.18	1.23
15	W	301	LDZ	O8-C9	2.46	1.40	1.35
15	I	301	LDZ	O32-C12	-2.46	1.18	1.23
15	V	301	LDZ	O8-C9	2.40	1.40	1.35
15	H	301	LDZ	O8-C9	2.16	1.39	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	301	LDZ	O8-C9-N10	5.23	121.64	110.45
15	I	301	LDZ	O8-C9-N10	4.54	120.15	110.45
15	H	301	LDZ	O8-C9-N10	4.27	119.58	110.45
15	V	301	LDZ	O8-C9-N10	4.15	119.33	110.45
15	Z	301	LDZ	O8-C9-N10	4.03	119.07	110.45
15	W	301	LDZ	O8-C9-N10	3.94	118.89	110.45
15	V	301	LDZ	C14-C15-N16	3.77	124.67	116.63
15	L	301	LDZ	C11-C12-N13	3.49	124.08	116.63
15	L	301	LDZ	O31-C9-N10	-3.44	119.23	124.86
15	I	301	LDZ	O31-C9-N10	-3.10	119.78	124.86
15	V	301	LDZ	O34-C15-N16	-3.06	117.47	122.96
15	V	301	LDZ	O31-C9-N10	-2.87	120.16	124.86
15	W	301	LDZ	O31-C9-N10	-2.82	120.24	124.86
15	L	301	LDZ	O32-C12-N13	-2.77	118.00	122.96
15	I	301	LDZ	C11-C12-N13	2.76	122.51	116.63
15	H	301	LDZ	O31-C9-N10	-2.70	120.44	124.86
15	L	301	LDZ	O8-C9-O31	-2.68	119.12	124.26
15	L	301	LDZ	C18-C17-N16	2.60	114.61	110.69
15	Z	301	LDZ	O8-C9-O31	-2.30	119.84	124.26
15	Z	301	LDZ	O31-C9-N10	-2.30	121.09	124.86
15	H	301	LDZ	O8-C9-O31	-2.23	119.98	124.26
15	I	301	LDZ	O8-C9-O31	-2.18	120.07	124.26
15	L	301	LDZ	O33-C22-C17	-2.18	119.17	124.77
15	I	301	LDZ	O33-C22-C17	-2.16	119.21	124.77
15	I	301	LDZ	O32-C12-N13	-2.10	119.20	122.96
15	Z	301	LDZ	O34-C15-N16	-2.10	119.20	122.96
15	Z	301	LDZ	C22-C17-N16	-2.08	105.47	109.50
15	L	301	LDZ	C14-N13-C12	2.07	126.10	121.65
15	H	301	LDZ	C14-C15-N16	2.01	120.92	116.63

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	H	301	LDZ	C22-C17-C18-C19
15	I	301	LDZ	C18-C17-C22-O33
15	I	301	LDZ	C22-C17-C18-C19
15	V	301	LDZ	O31-C9-O8-C7
15	V	301	LDZ	N10-C9-O8-C7
15	W	301	LDZ	C22-C17-C18-C19
15	Z	301	LDZ	O31-C9-O8-C7

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Mol	Chain	Res	Type	Atoms
15	Z	301	LDZ	N10-C9-O8-C7
15	H	301	LDZ	O8-C9-N10-C11
15	H	301	LDZ	O31-C9-O8-C7
15	I	301	LDZ	C15-C14-C24-C25
15	Z	301	LDZ	C12-C11-C30-C31
15	H	301	LDZ	N10-C9-O8-C7
15	L	301	LDZ	N10-C9-O8-C7
15	H	301	LDZ	O31-C9-N10-C11
15	L	301	LDZ	O31-C9-N10-C11
15	L	301	LDZ	O31-C9-O8-C7
15	L	301	LDZ	O8-C9-N10-C11
15	W	301	LDZ	N10-C11-C30-C31
15	W	301	LDZ	N13-C14-C24-C25
15	W	301	LDZ	C12-C11-C30-C31
15	W	301	LDZ	O8-C9-N10-C11
15	I	301	LDZ	N16-C17-C18-C19
15	H	301	LDZ	N10-C11-C30-C31
15	Z	301	LDZ	N16-C17-C18-C19
15	H	301	LDZ	C12-C11-C30-C31
15	W	301	LDZ	C15-C14-C24-C25
15	W	301	LDZ	N10-C9-O8-C7
15	H	301	LDZ	N16-C17-C18-C19
15	Z	301	LDZ	N10-C11-C30-C31
15	I	301	LDZ	C11-C12-N13-C14
15	L	301	LDZ	C11-C12-N13-C14
15	Z	301	LDZ	C11-C12-N13-C14
15	H	301	LDZ	C17-C18-C19-C20
15	V	301	LDZ	C14-C24-C25-C27
15	H	301	LDZ	C17-C18-C19-C21
15	Z	301	LDZ	C14-C24-C25-C26
15	I	301	LDZ	O32-C12-N13-C14
15	L	301	LDZ	O32-C12-N13-C14
15	V	301	LDZ	O34-C15-N16-C17
15	Z	301	LDZ	O32-C12-N13-C14
15	Z	301	LDZ	C14-C24-C25-C27
15	V	301	LDZ	C14-C15-N16-C17
15	V	301	LDZ	C14-C24-C25-C26
15	W	301	LDZ	O31-C9-O8-C7
15	W	301	LDZ	N16-C17-C18-C19
15	W	301	LDZ	O31-C9-N10-C11
15	H	301	LDZ	C14-C24-C25-C26
15	L	301	LDZ	C15-C14-C24-C25

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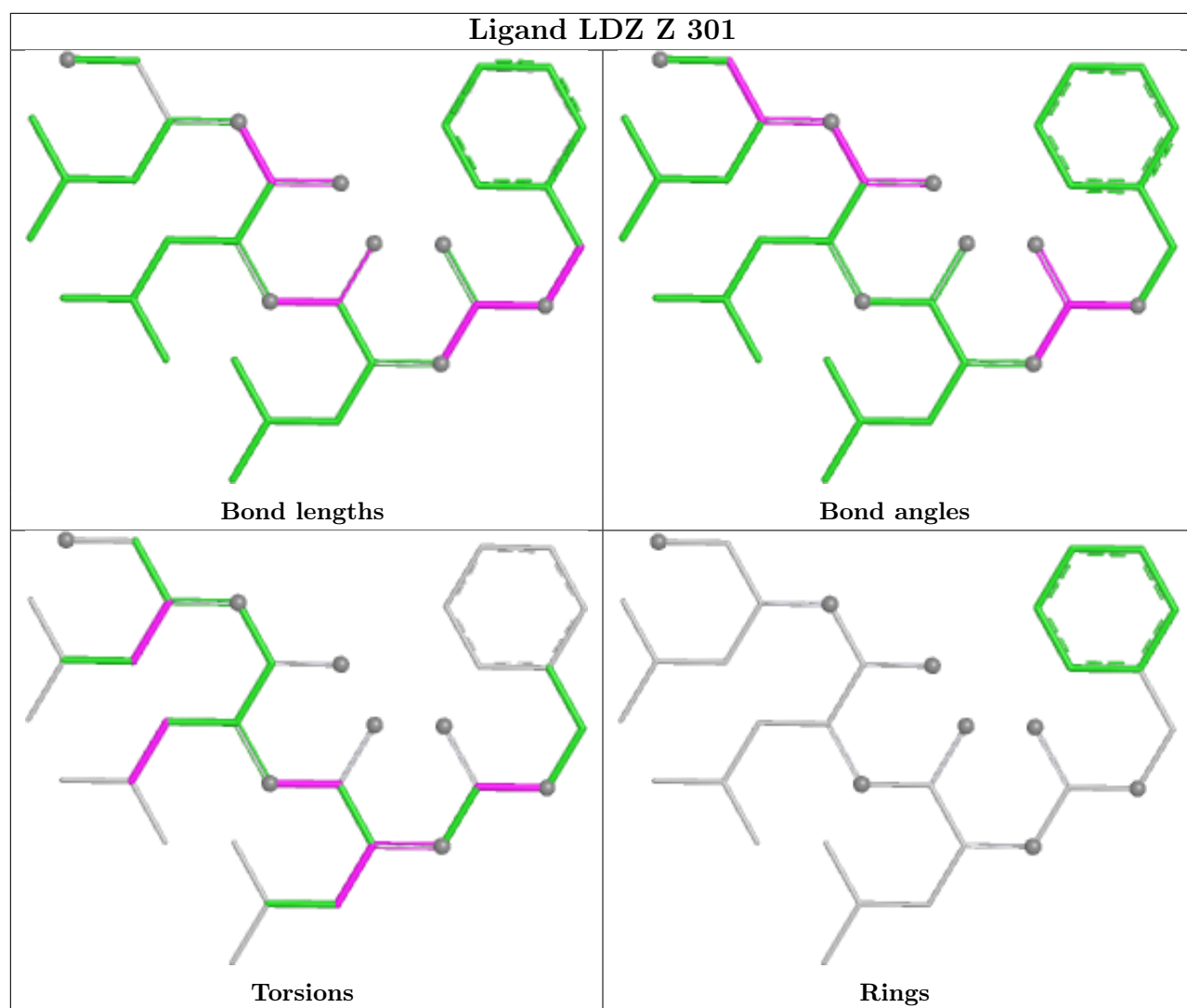
Mol	Chain	Res	Type	Atoms
15	L	301	LDZ	C30-C11-N10-C9
15	H	301	LDZ	C14-C24-C25-C27
15	W	301	LDZ	N13-C14-C15-N16
15	W	301	LDZ	N13-C14-C15-O34
15	W	301	LDZ	C22-C17-N16-C15
15	W	301	LDZ	C14-C24-C25-C27
15	L	301	LDZ	N10-C11-C12-O32
15	H	301	LDZ	C18-C17-N16-C15
15	W	301	LDZ	C18-C17-N16-C15
15	L	301	LDZ	N13-C14-C24-C25
15	L	301	LDZ	C17-C18-C19-C21
15	L	301	LDZ	N10-C11-C12-N13
15	V	301	LDZ	N13-C14-C24-C25
15	V	301	LDZ	N16-C17-C18-C19
15	L	301	LDZ	C17-C18-C19-C20
15	I	301	LDZ	N13-C14-C24-C25
15	H	301	LDZ	C22-C17-N16-C15
15	L	301	LDZ	C22-C17-N16-C15
15	V	301	LDZ	C22-C17-N16-C15
15	L	301	LDZ	N13-C14-C15-O34
15	L	301	LDZ	C3-C7-O8-C9
15	I	301	LDZ	N13-C14-C15-O34
15	V	301	LDZ	N10-C11-C12-O32
15	V	301	LDZ	C17-C18-C19-C20
15	L	301	LDZ	C18-C17-N16-C15
15	V	301	LDZ	C18-C17-N16-C15
15	V	301	LDZ	N10-C11-C12-N13
15	L	301	LDZ	C24-C14-C15-O34
15	I	301	LDZ	N13-C14-C15-N16
15	H	301	LDZ	C30-C11-C12-O32
15	Z	301	LDZ	C30-C11-N10-C9
15	L	301	LDZ	N13-C14-C15-N16
15	W	301	LDZ	C24-C14-C15-O34
15	L	301	LDZ	C24-C14-N13-C12
15	L	301	LDZ	C30-C11-C12-O32
15	W	301	LDZ	C24-C14-C15-N16
15	L	301	LDZ	N10-C11-C30-C31
15	L	301	LDZ	C24-C14-C15-N16

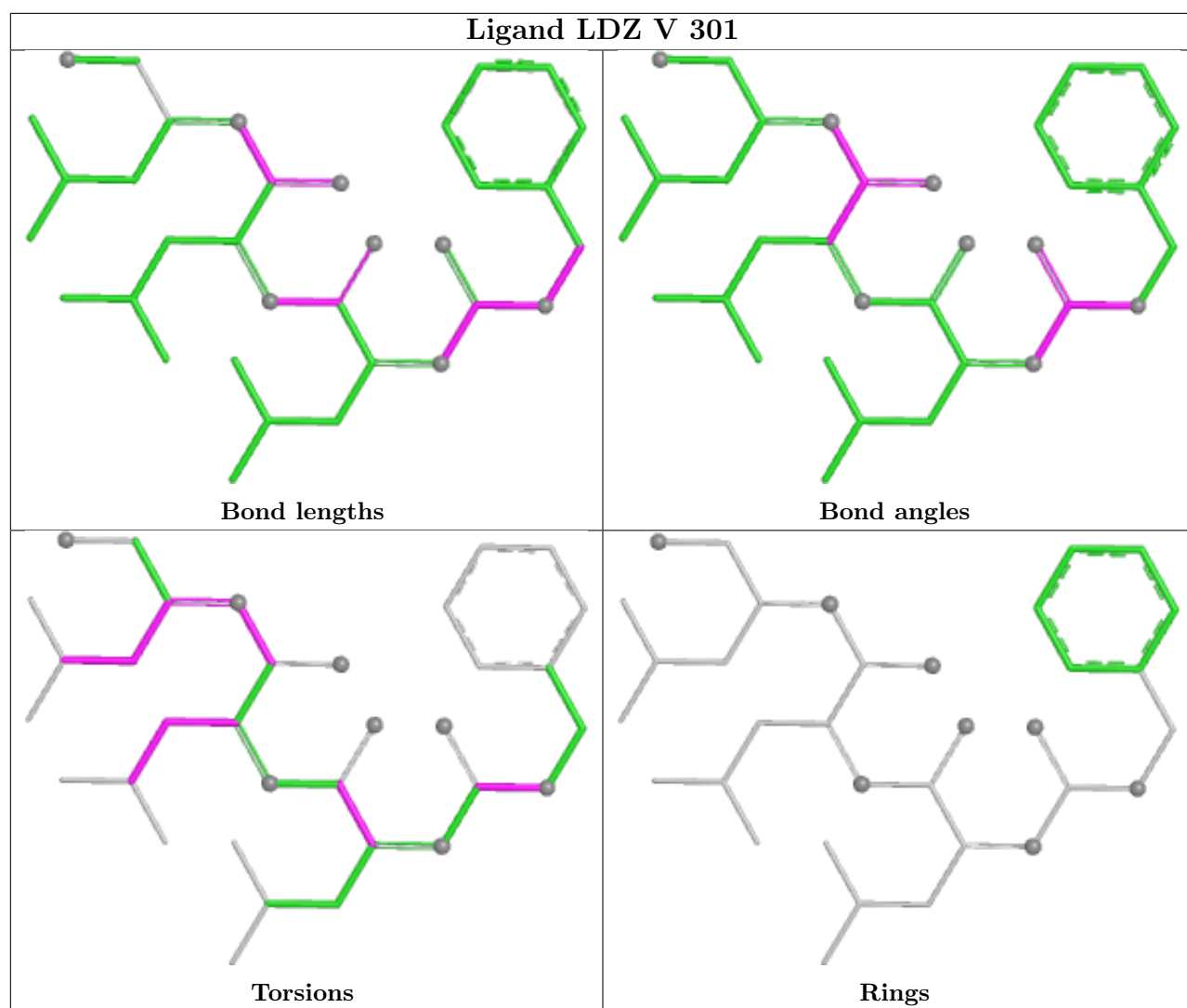
There are no ring outliers.

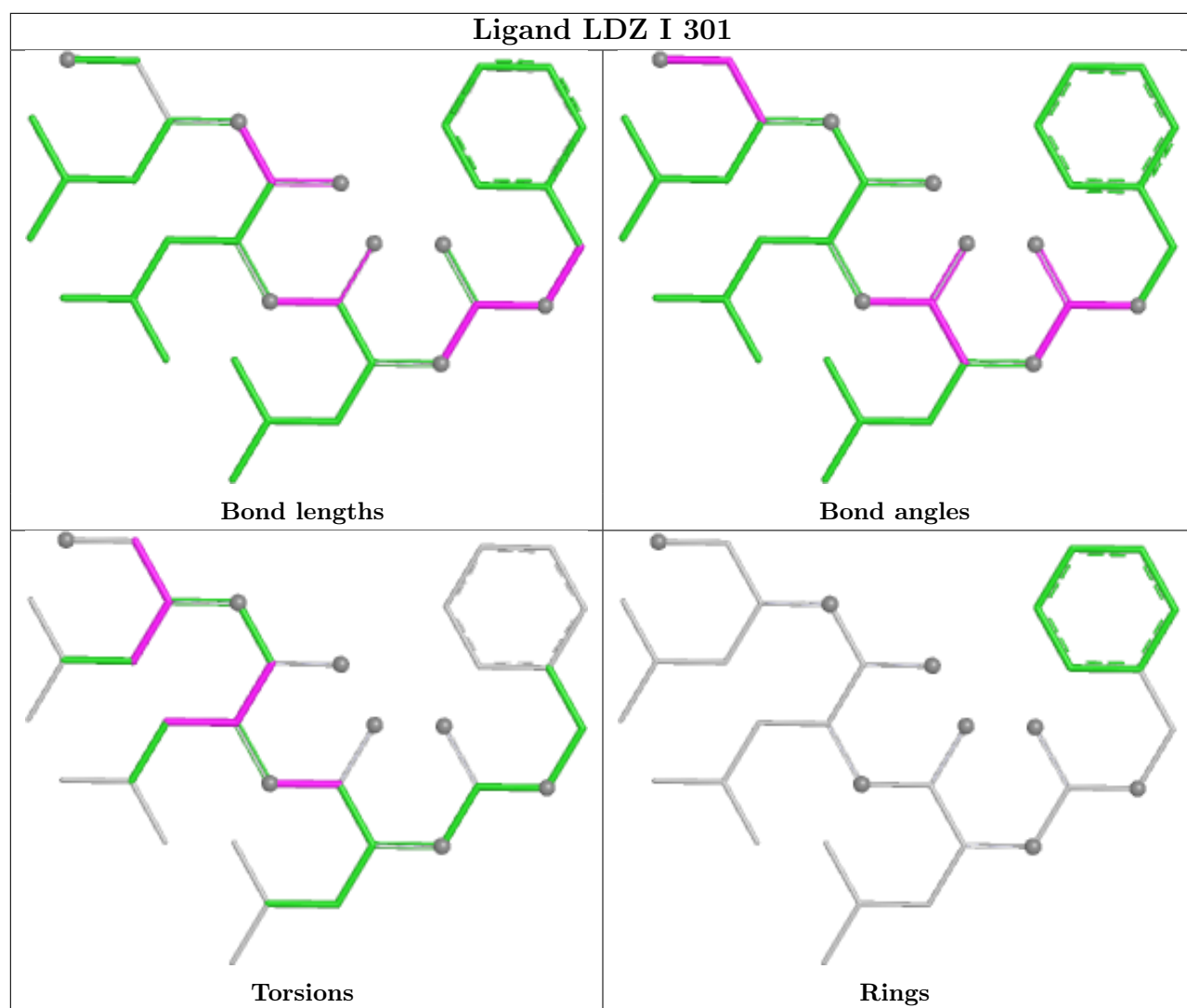
6 monomers are involved in 47 short contacts:

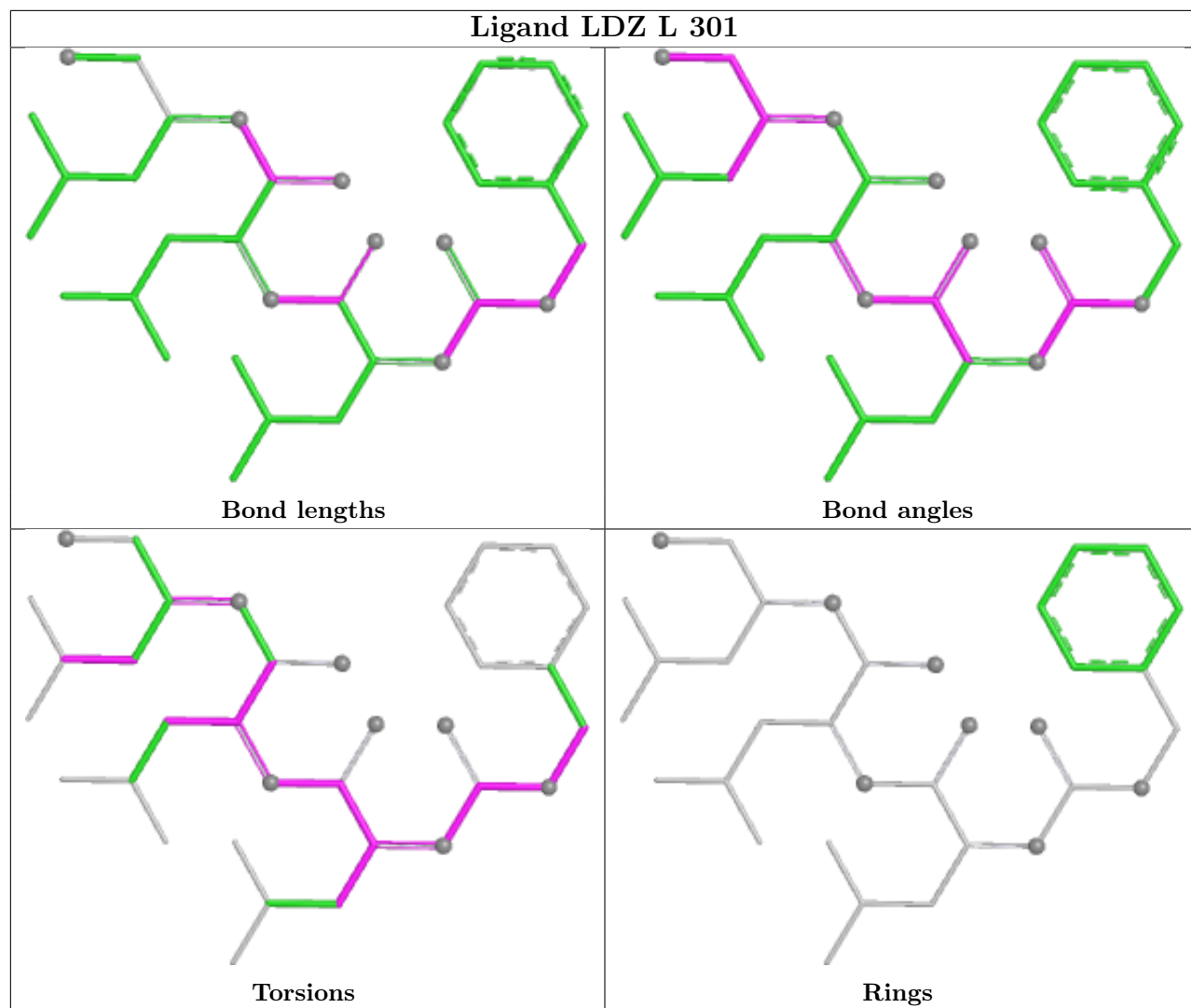
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Z	301	LDZ	11	0
15	V	301	LDZ	9	0
15	I	301	LDZ	3	0
15	L	301	LDZ	12	0
15	W	301	LDZ	9	0
15	H	301	LDZ	3	0

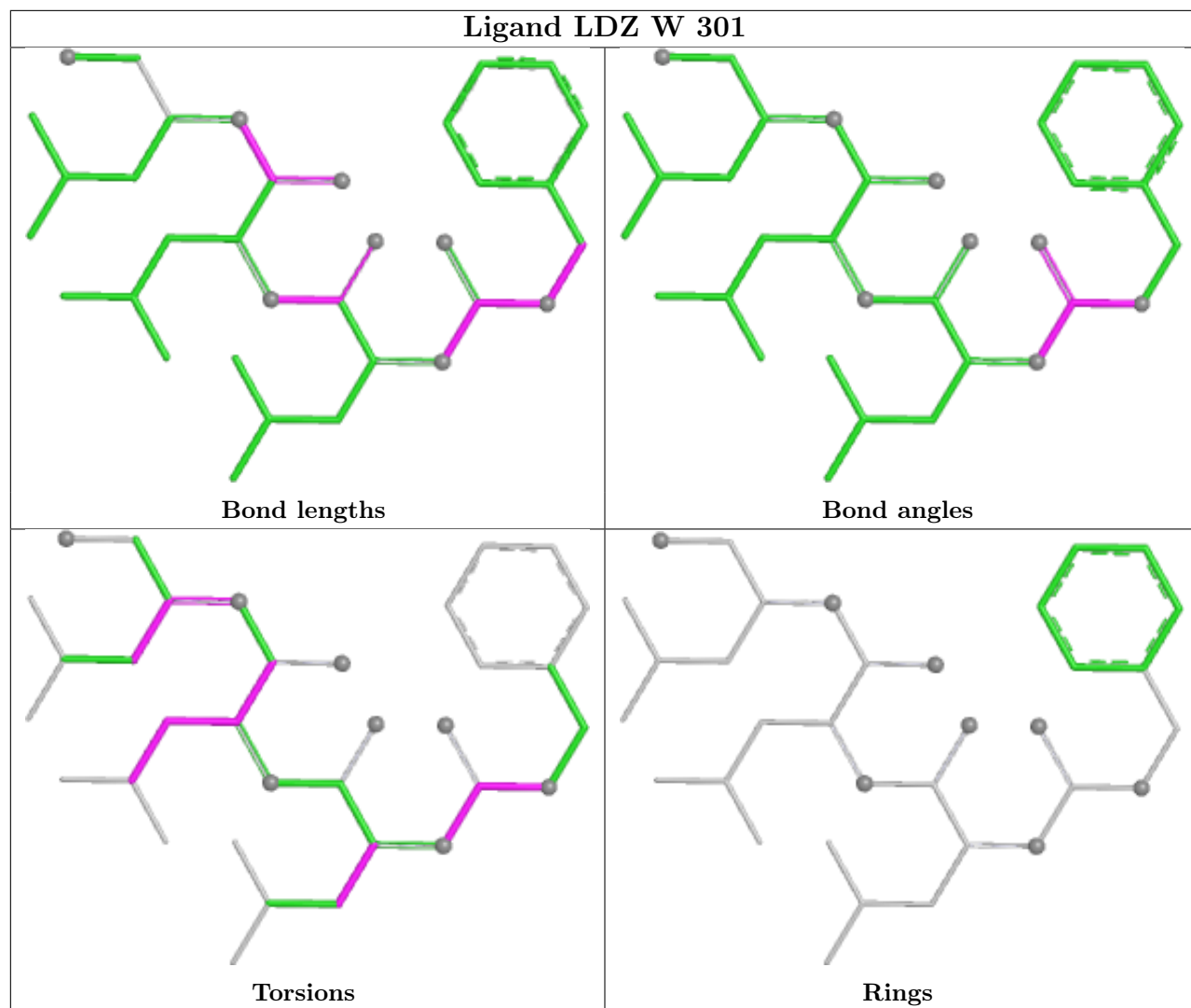
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

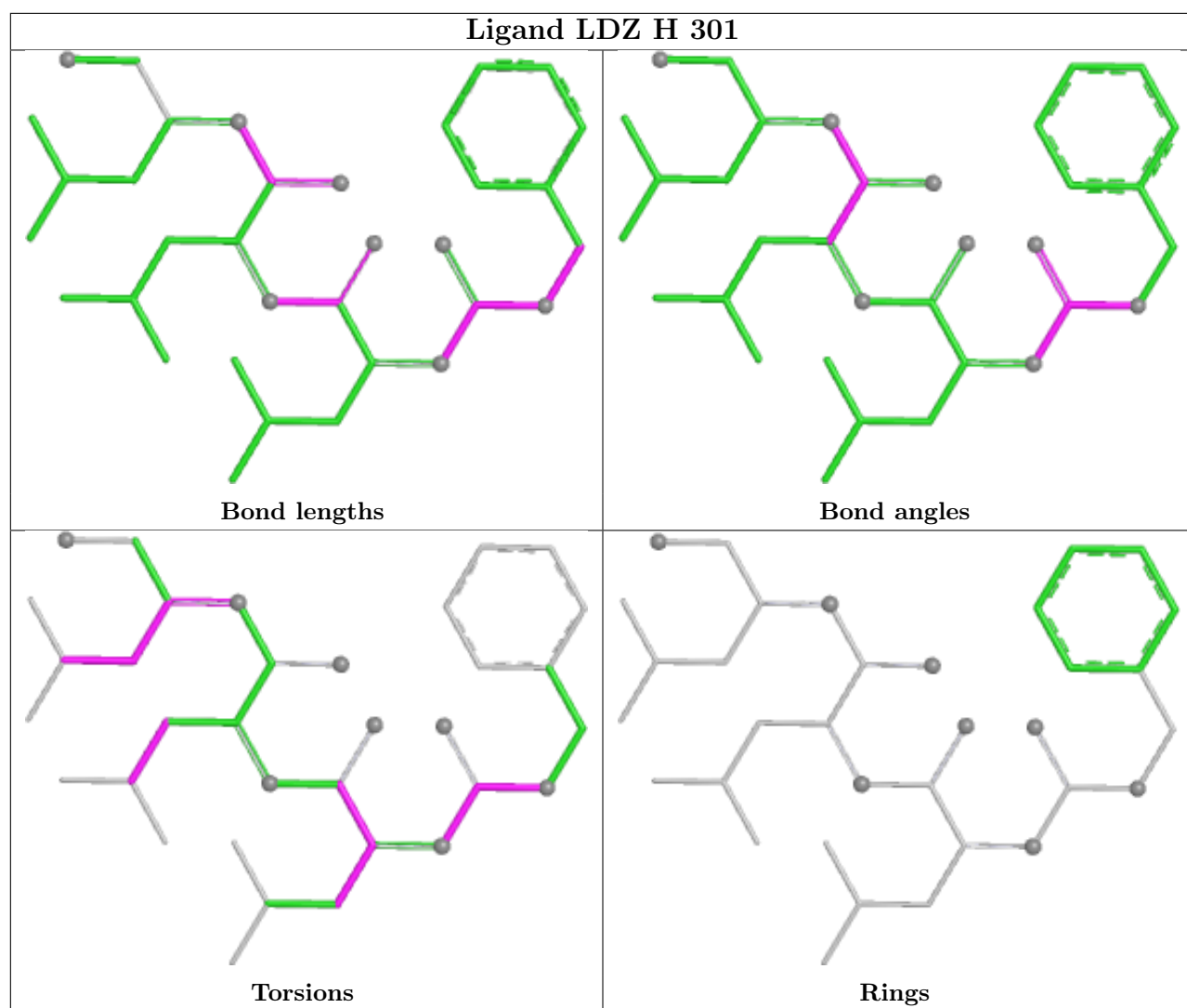












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

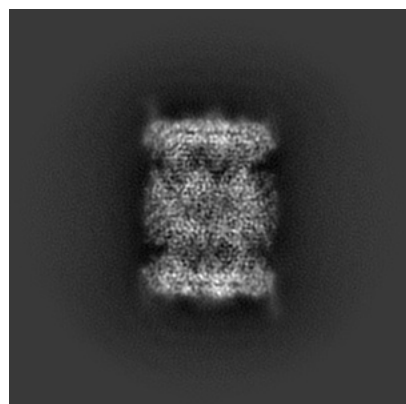
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27013. These allow visual inspection of the internal detail of the map and identification of artifacts.

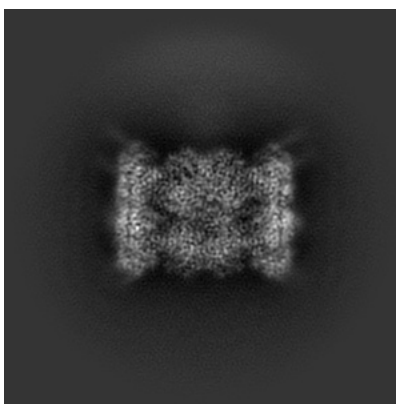
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

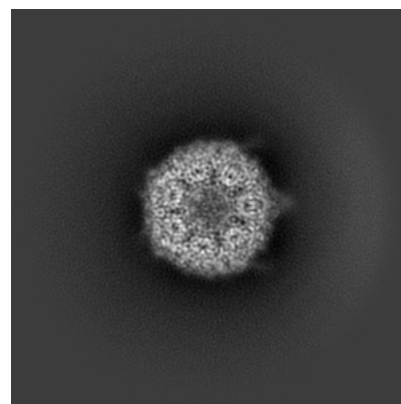
6.1.1 Primary map



X

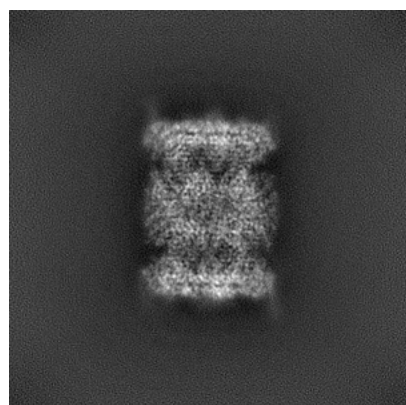


Y

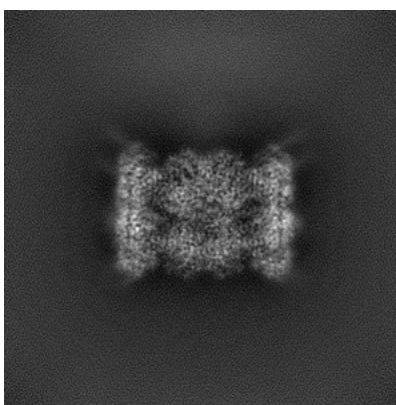


Z

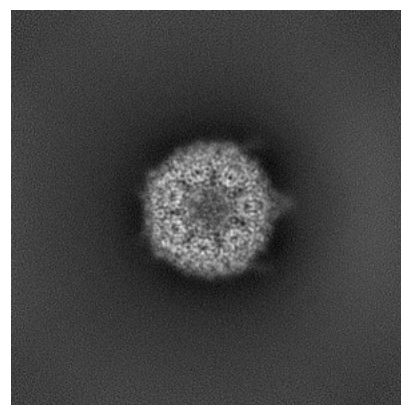
6.1.2 Raw map



X



Y

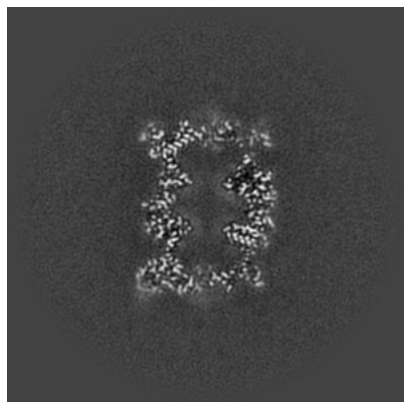


Z

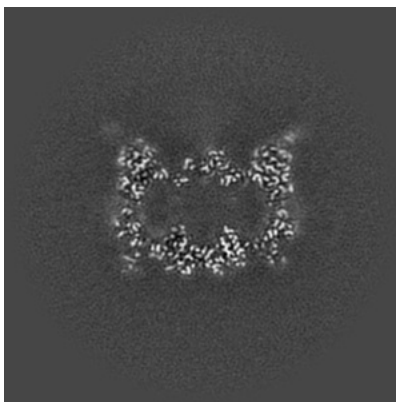
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

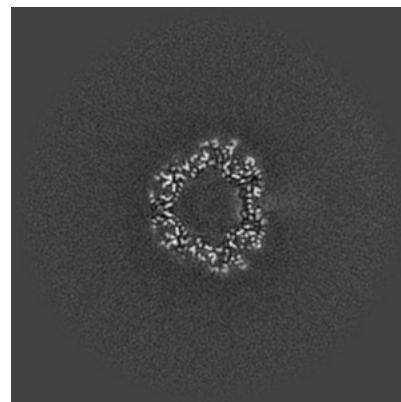
6.2.1 Primary map



X Index: 160

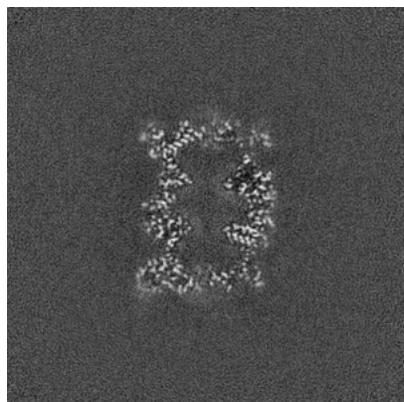


Y Index: 160

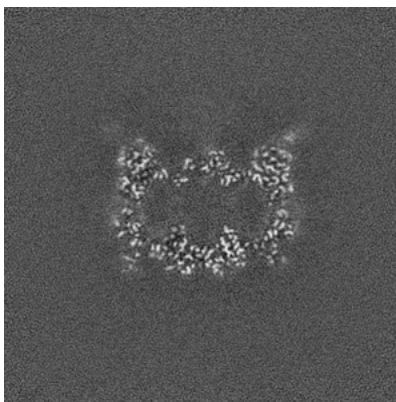


Z Index: 160

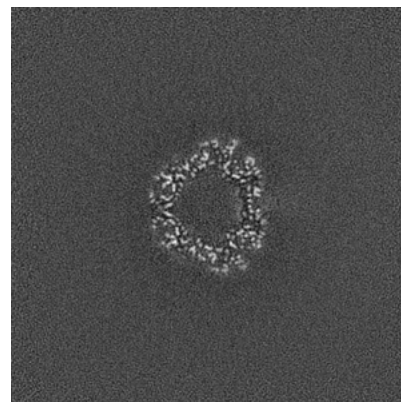
6.2.2 Raw map



X Index: 160



Y Index: 160

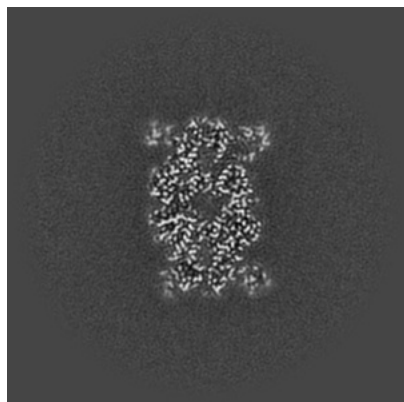


Z Index: 160

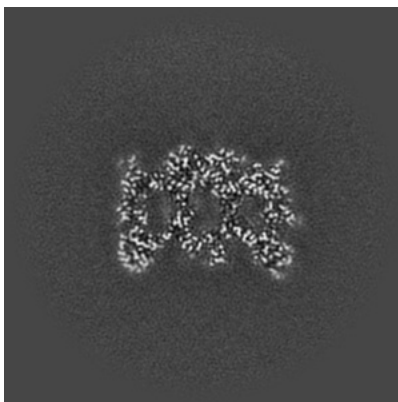
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

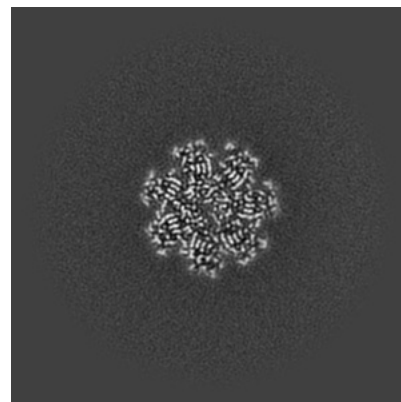
6.3.1 Primary map



X Index: 135

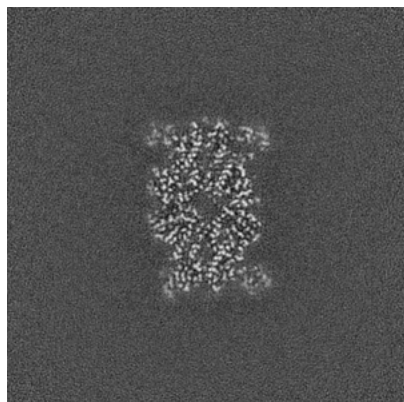


Y Index: 140

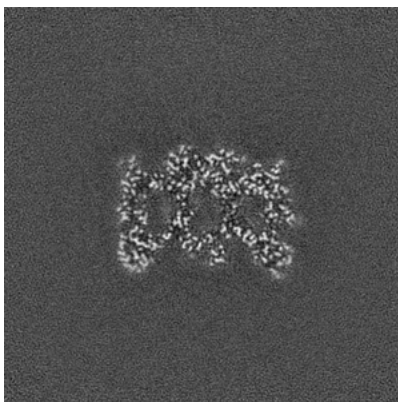


Z Index: 106

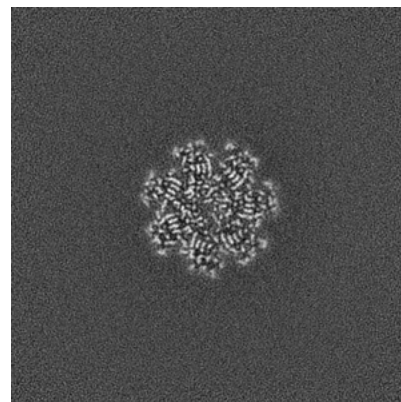
6.3.2 Raw map



X Index: 134



Y Index: 140

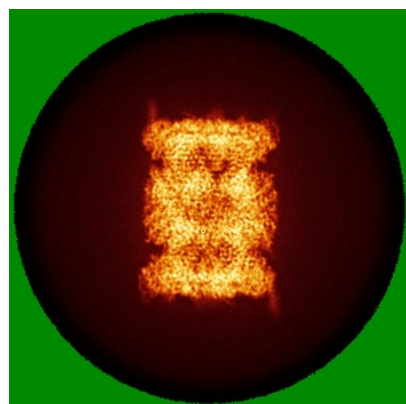


Z Index: 106

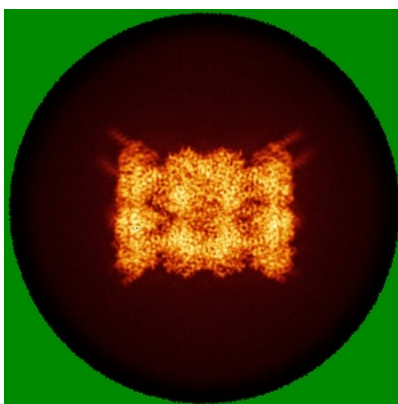
The images above show the largest variance slices of the map in three orthogonal directions.

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

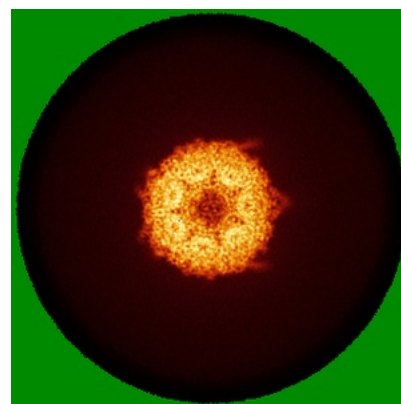
6.4.1 Primary map



X

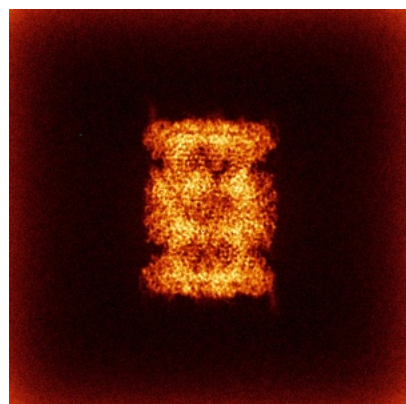


Y

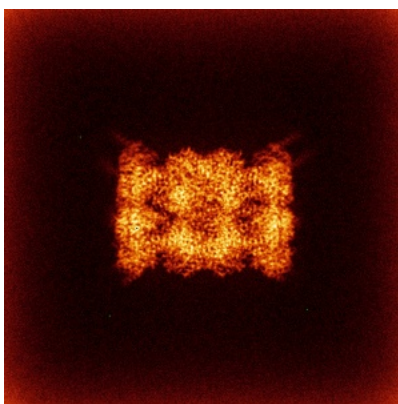


Z

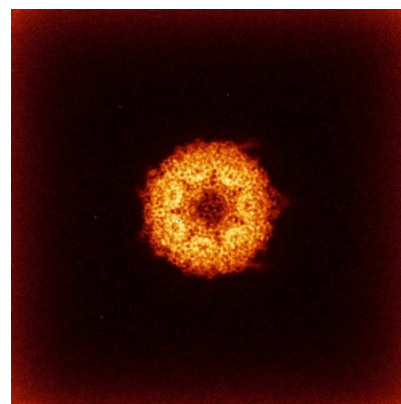
6.4.2 Raw map



X



Y

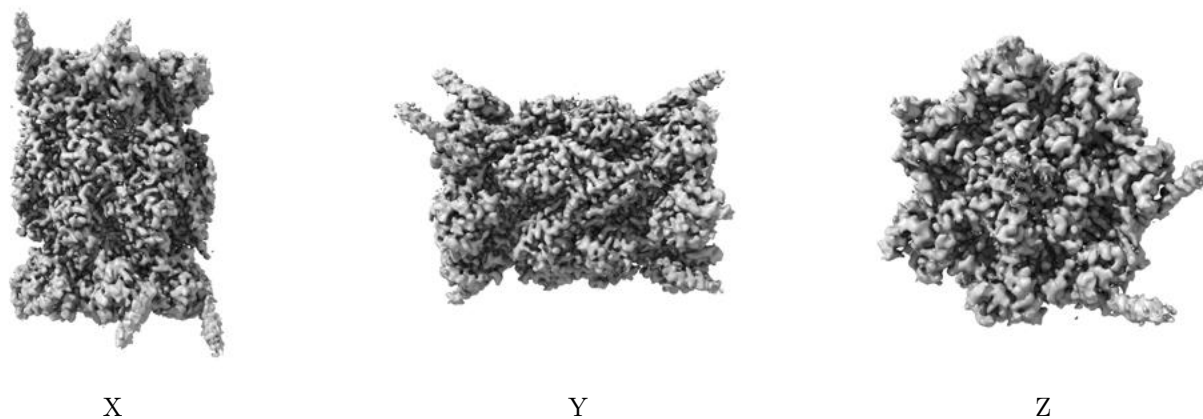


Z

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

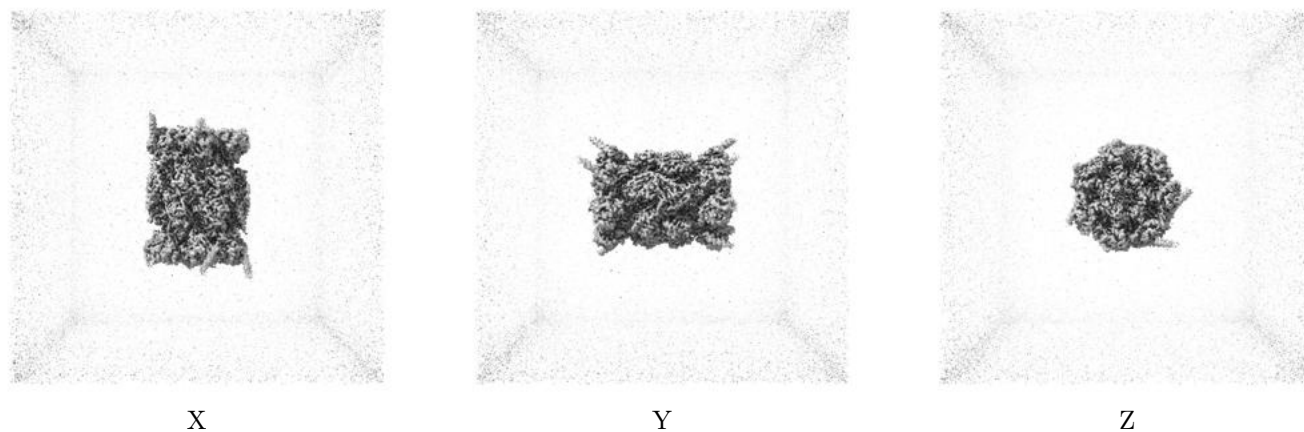
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

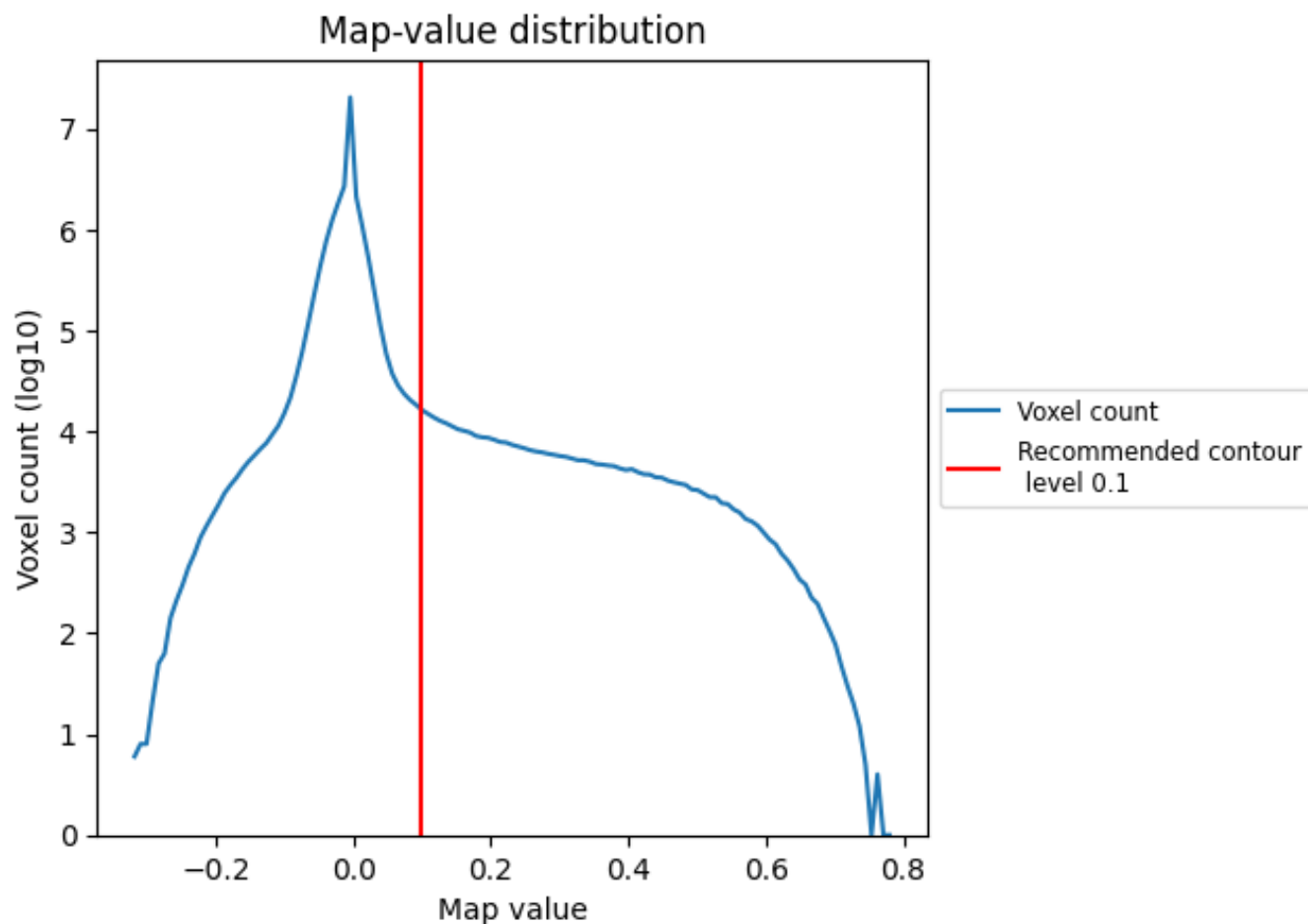
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

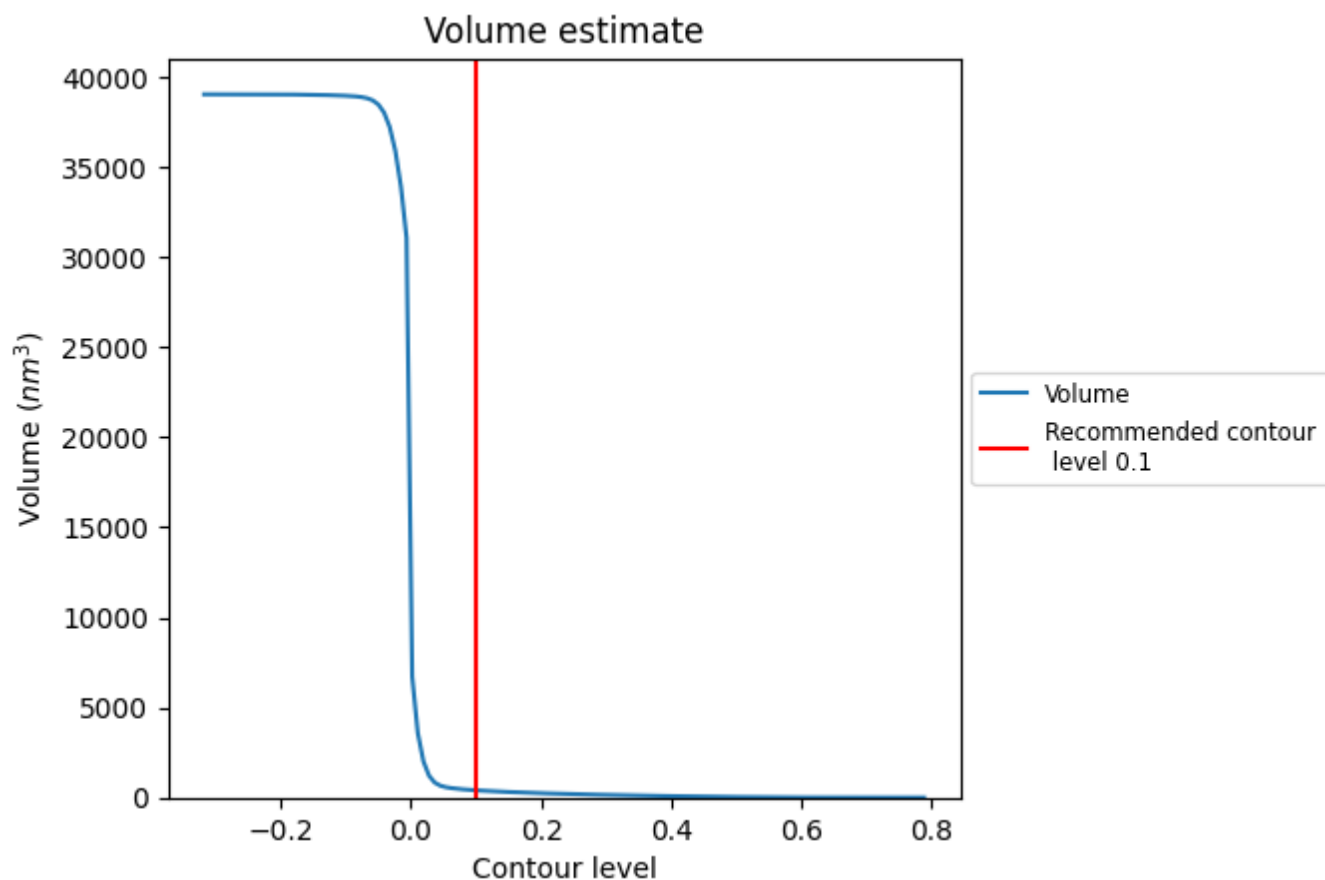
This section contains the results of statistical analysis of the map.

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.

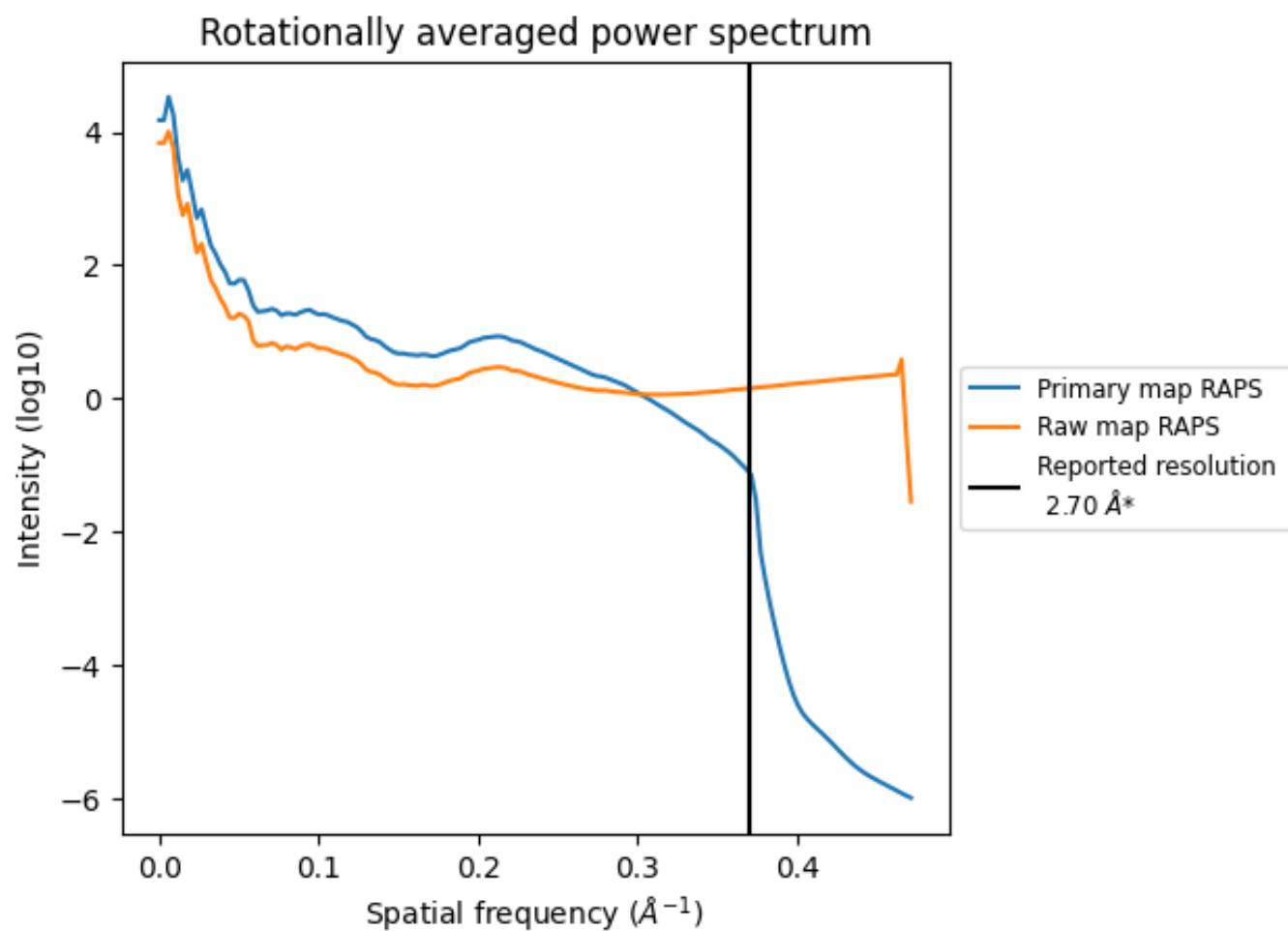
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 403 nm^3 ; this corresponds to an approximate mass of 364 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

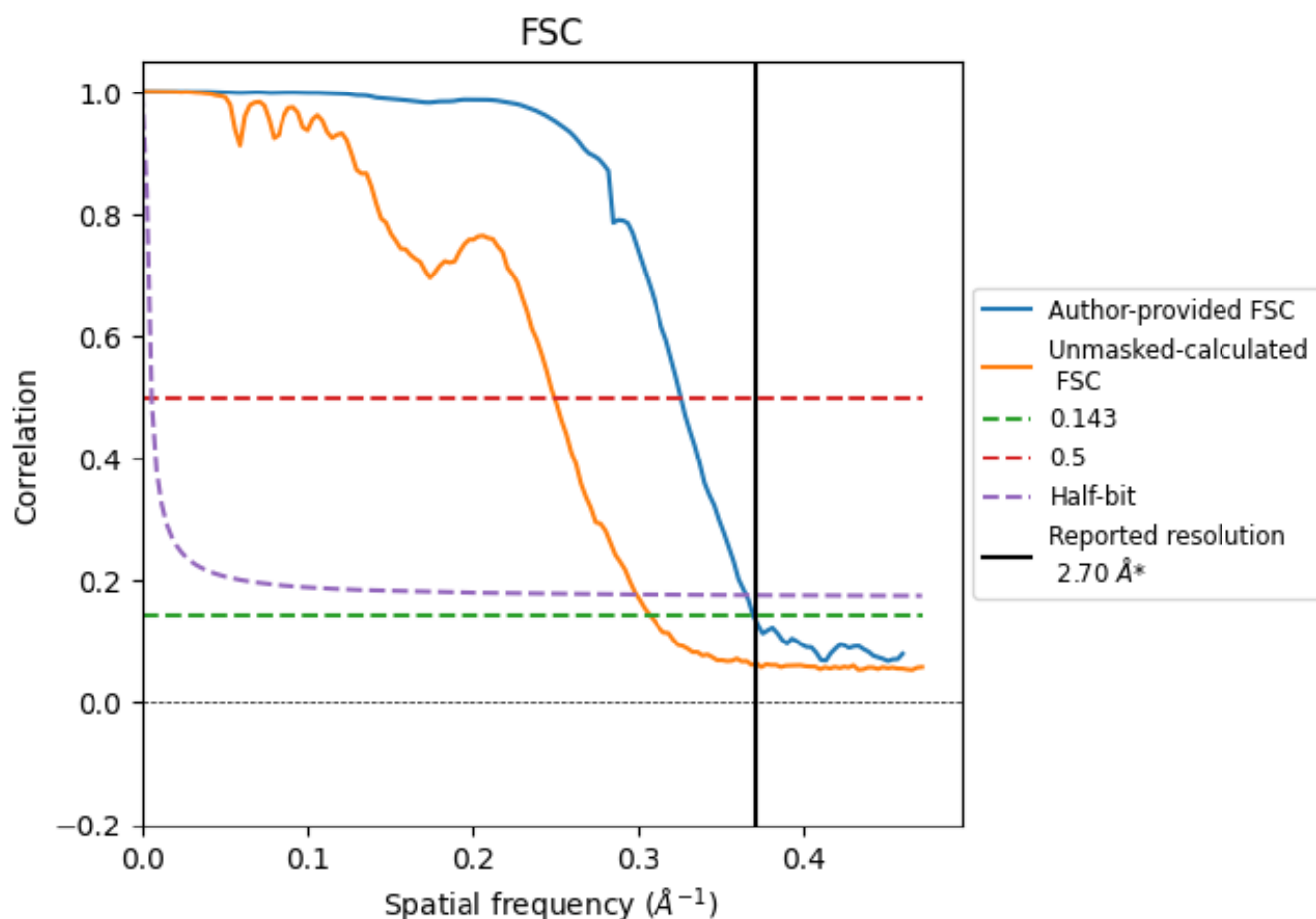


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

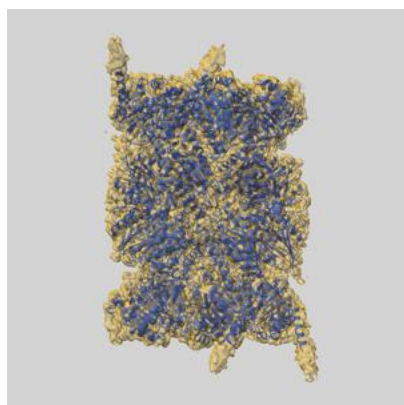
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.71	3.07	2.74
Unmasked-calculated*	3.26	4.01	3.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.26 differs from the reported value 2.7 by more than 10 %

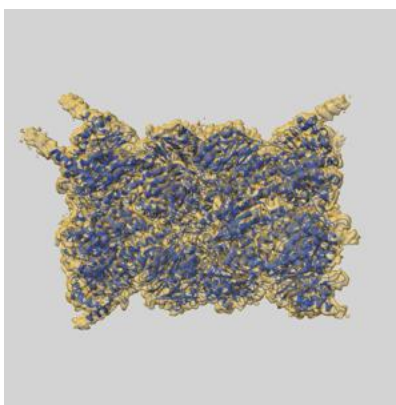
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27013 and PDB model 8CVR. Per-residue inclusion information can be found in section [3](#) on page [8](#).

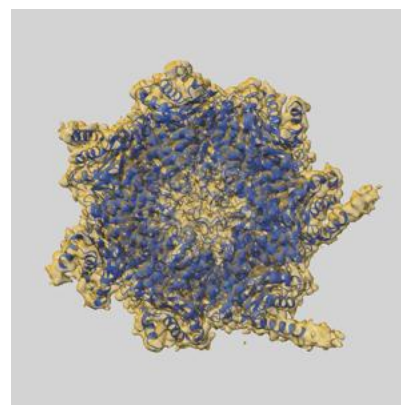
9.1 Map-model overlay [i](#)



X



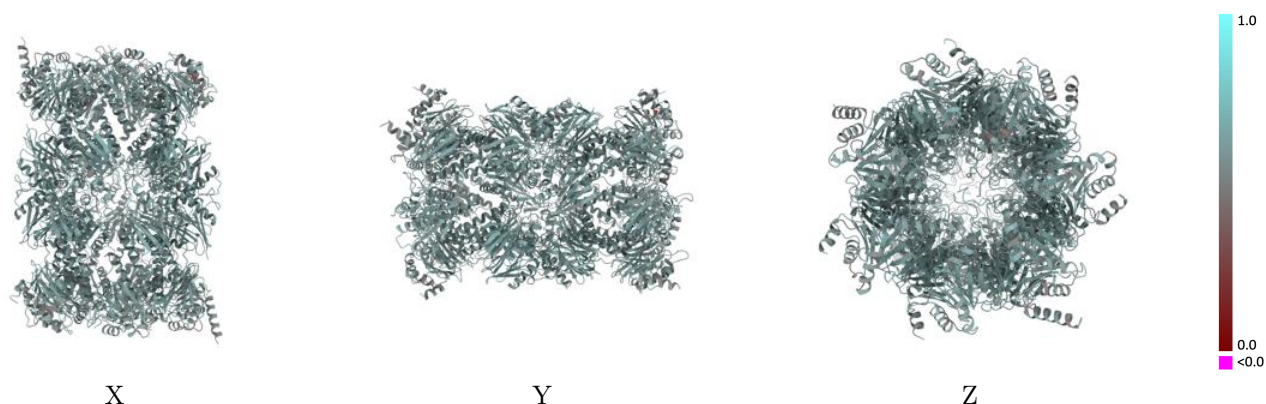
Y



Z

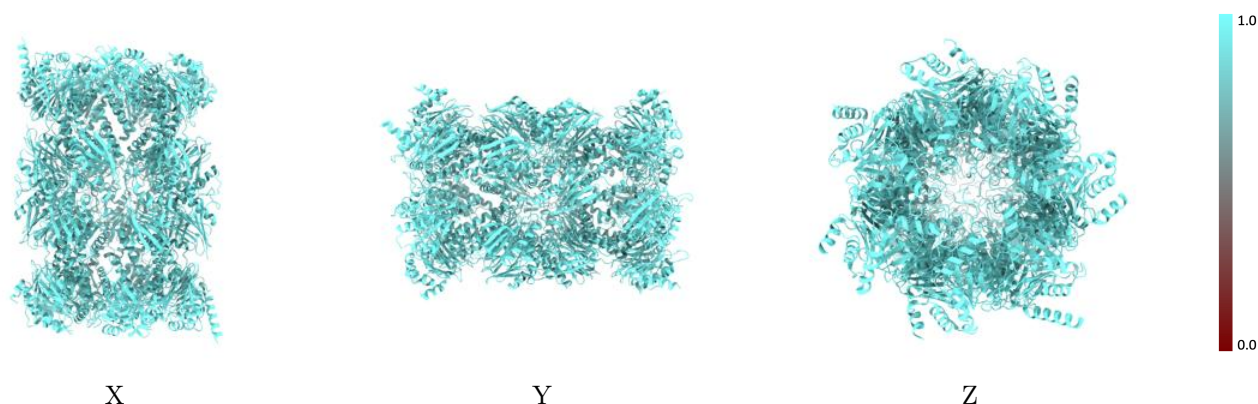
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



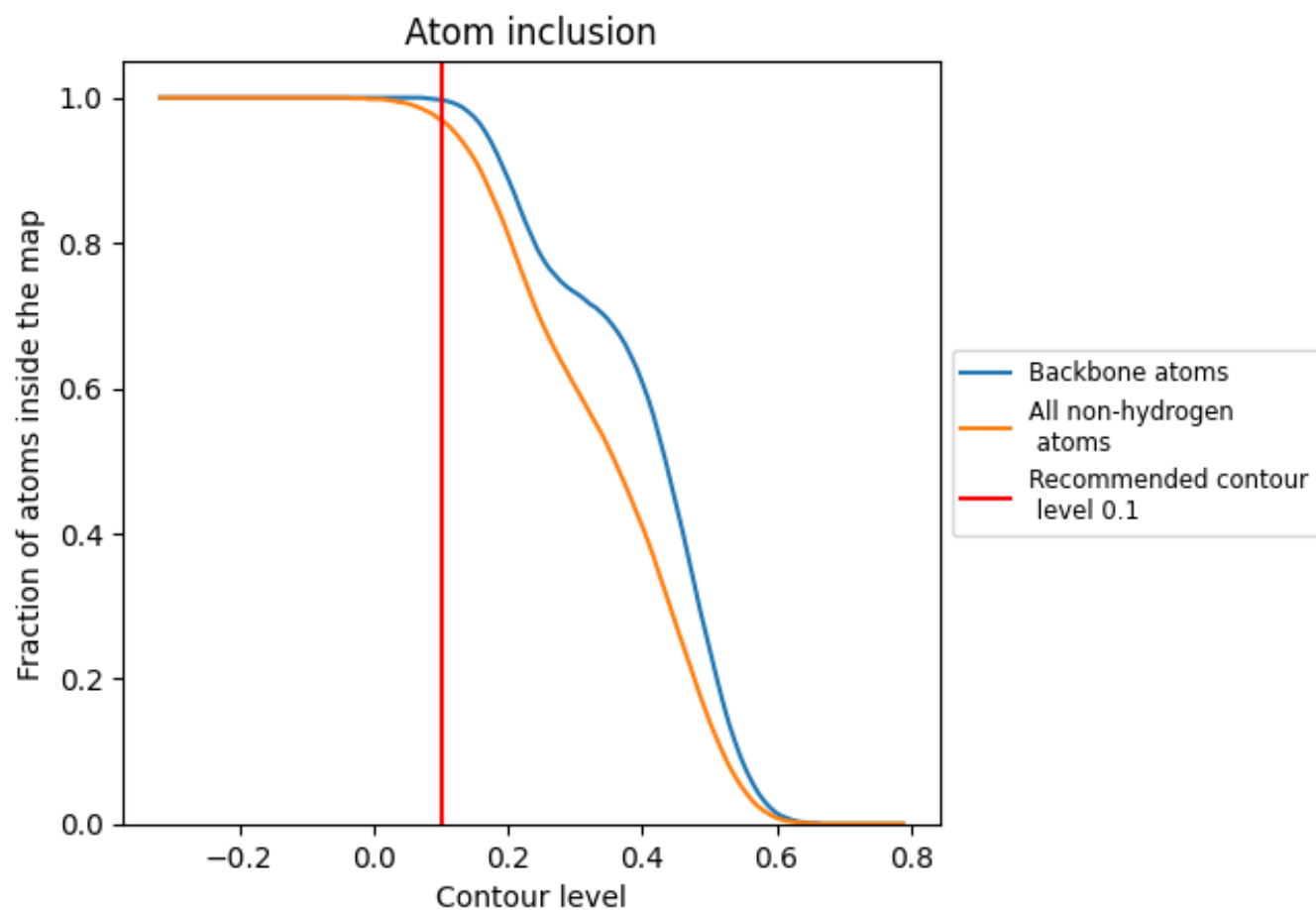
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9690	 0.5820
A	 0.9760	 0.5720
B	 0.9800	 0.5820
C	 0.9710	 0.5700
D	 0.9720	 0.5680
E	 0.9540	 0.5720
F	 0.9690	 0.5710
G	 0.9760	 0.5750
H	 0.9570	 0.5940
I	 0.9680	 0.5880
J	 0.9700	 0.5930
K	 0.9660	 0.5950
L	 0.9600	 0.5880
M	 0.9740	 0.5970
N	 0.9800	 0.5950
O	 0.9770	 0.5760
P	 0.9810	 0.5810
Q	 0.9650	 0.5710
R	 0.9680	 0.5670
S	 0.9600	 0.5660
T	 0.9720	 0.5720
U	 0.9710	 0.5720
V	 0.9590	 0.5900
W	 0.9700	 0.5920
X	 0.9730	 0.5970
Y	 0.9650	 0.5930
Z	 0.9630	 0.5880
a	 0.9730	 0.5910
b	 0.9720	 0.5950

