



Full wwPDB EM Validation Report ⓘ

Nov 27, 2022 – 04:13 PM EST

PDB ID : 6X5Z
EMDB ID : EMD-22067
Title : Bovine Cardiac Myosin in Complex with Chicken Skeletal Actin and Human Cardiac Tropomyosin in the Rigor State
Authors : Doran, M.H.; Lehman, W.; Rynkiewicz, M.J.; Bullitt, E.
Deposited on : 2020-05-27
Resolution : 4.24 Å (reported)
Based on initial models : 3I5G, 6KN8

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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

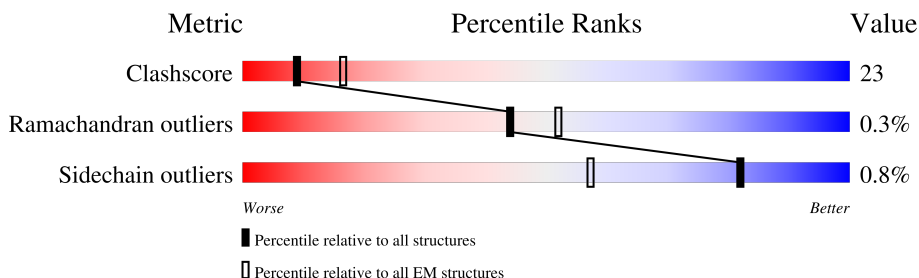
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.24 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	377	
1	B	377	
1	C	377	
2	O	284	
2	P	284	
3	D	850	
3	G	850	
3	J	850	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 28416 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	369	Total	C	N	O	S	0	0
			2880	1823	487	549	21		
1	A	369	Total	C	N	O	S	0	0
			2880	1823	487	549	21		
1	C	369	Total	C	N	O	S	0	0
			2880	1823	487	549	21		

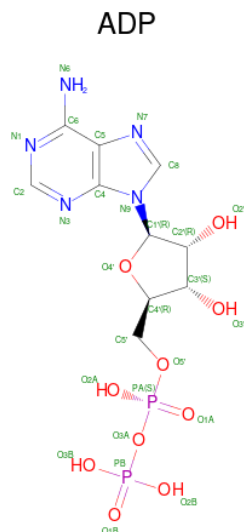
- Molecule 2 is a protein called Tropomyosin alpha-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	166	Total	C	N	O	S	0	0
			1326	806	230	287	3		
2	P	166	Total	C	N	O	S	0	0
			1326	806	230	287	3		

- Molecule 3 is a protein called Myosin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	705	Total	C	N	O	S	0	0
			5680	3636	958	1056	30		
3	D	705	Total	C	N	O	S	0	0
			5680	3636	958	1056	30		
3	J	705	Total	C	N	O	S	0	0
			5680	3636	958	1056	30		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total 27	C 10	N 5	O 10	P 2	0
4	A	1	Total 27	C 10	N 5	O 10	P 2	0
4	C	1	Total 27	C 10	N 5	O 10	P 2	0

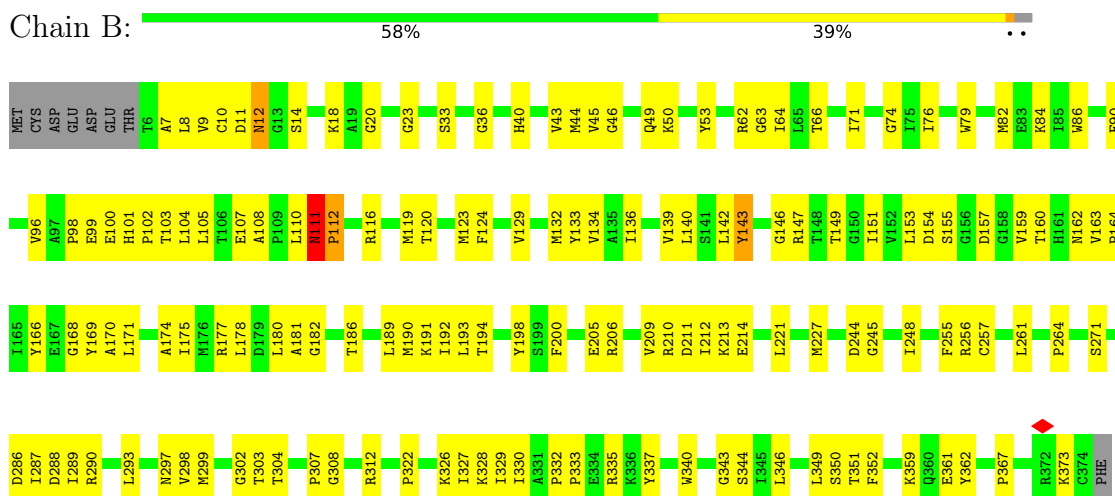
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total Mg 1 1	0
5	A	1	Total Mg 1 1	0
5	C	1	Total Mg 1 1	0

3 Residue-property plots [i](#)

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: Actin, alpha skeletal muscle

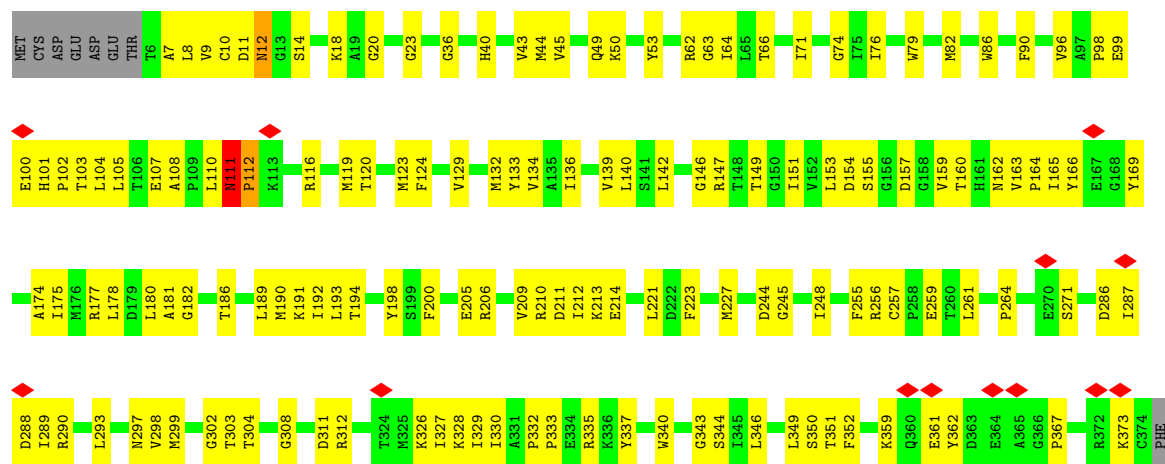


- Molecule 1: Actin, alpha skeletal muscle

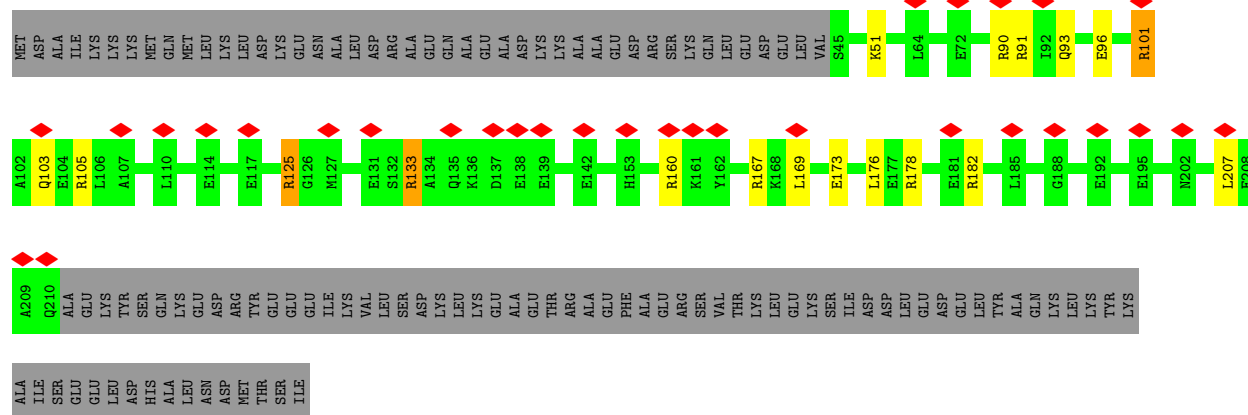


- Molecule 1: Actin, alpha skeletal muscle

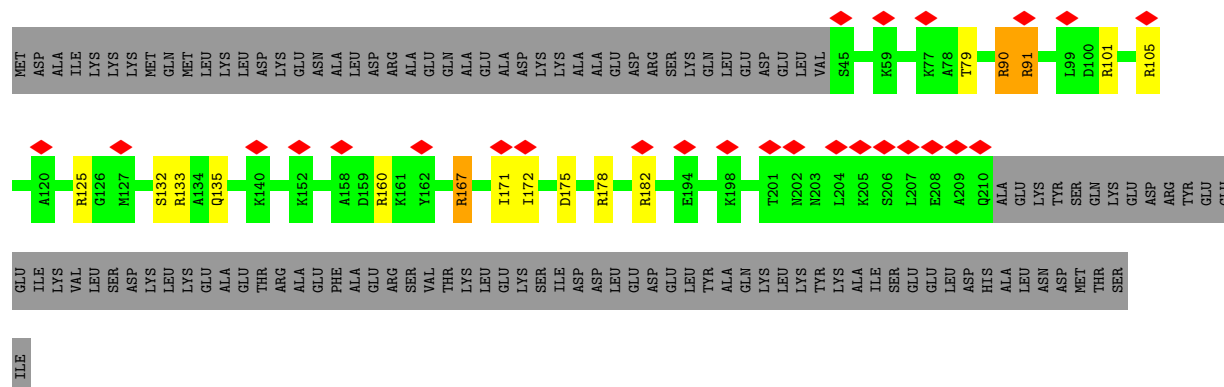




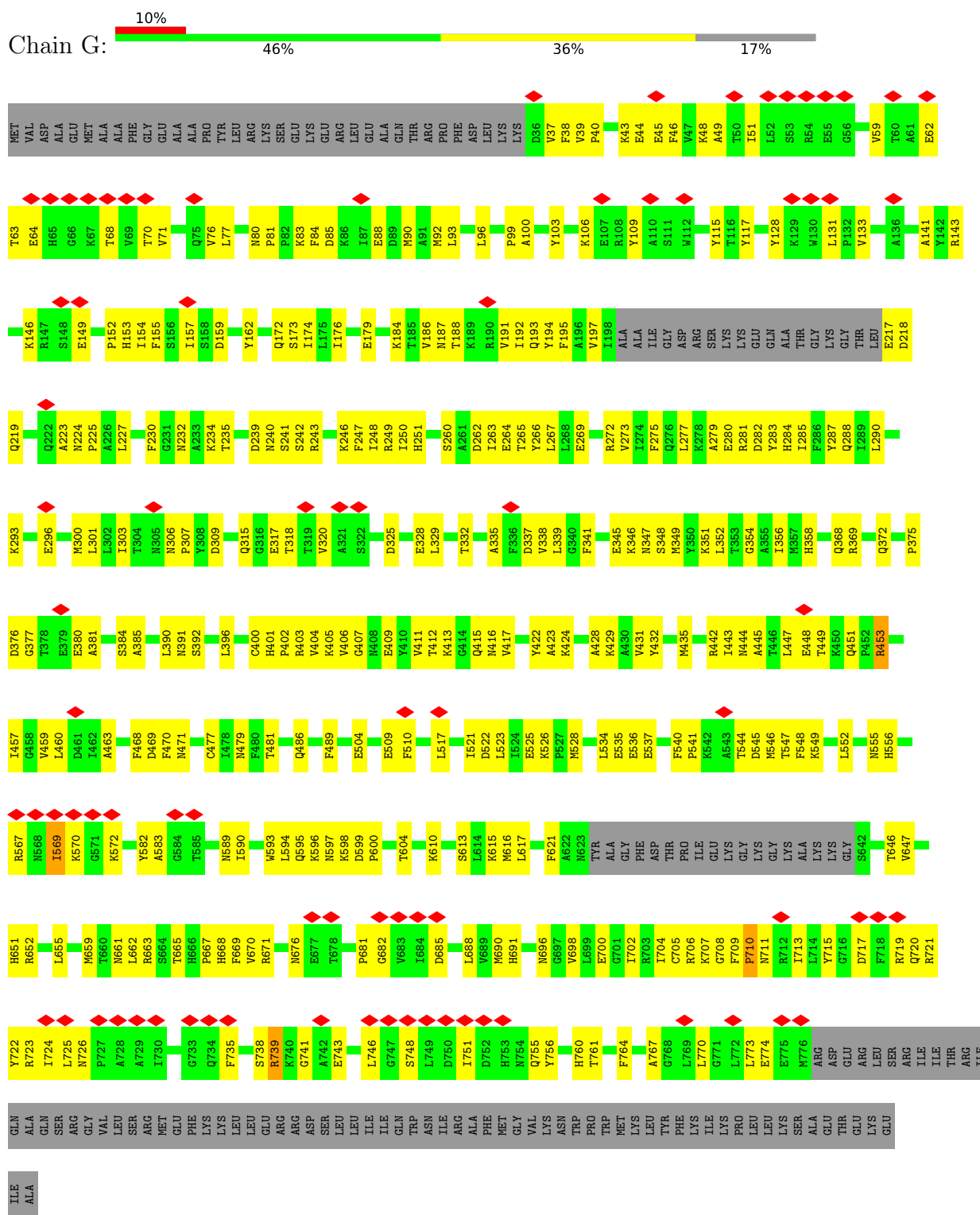
• Molecule 2: Tropomyosin alpha-1 chain



• Molecule 2: Tropomyosin alpha-1 chain



• Molecule 3: Myosin-7



• Molecule 3: Myosin-7



MET	GLU	PHE	LYS	LYS	LEU	LEU	GLU	ARG	ARG	ASP	SER	LEU	LEU	ILE	ILE	GLN	TRP	ASN	ILE	ARG	ALA	PHE	MET	GLY	VAL	LYS	ASN	TRP	PRO	TRP	LYS	LEU	TYR	PHE	LYS	ILE	LYS	PRO	LEU	LEU	LYS	LEU	SER	ALA	GLU	THR	GLU	LYS	GLU	ILE	ALA								
D737	S738	R739	K740	G741	A742	E743	K744	L745	L746	G747	S748	L749	D750	I751	D752	H753	N754	Q755	Y756	G759	H760	T761	K762	V763	F764	A767	G768	L769	L770	G771	L772	L773	E774	E775	H776	ARG	ASP	GLU	THR	GLU	LYS	GLU	ARG	LEU	SER	ARG	ILE	ALA											
R671	S738	N676	E677	T678	K679	S680	P681	G682	V683	I684	D685	N686	P687	L688	V689	M690	H691	N696	G697	V698	L699	E700	G701	I702	R703	I704	C705	R706	G707	G708	F709	P710	N711	R712	I713	L714	Y715	G716	D717	F718	R719	Q720	R721	Y722	R723	I724	L725	N726	F727	A728	A729	I730	F731	E732	G733	Q734	F735	I736	
Q595	K596	N597	K598	D599	P600	T604	K610	E611	S613	L614	K615	M616	L617	F621	A622	N623	TYR	ALA	PHE	ASP	THR	PRO	ILE	GLU	LYS	LYS	LYS	LYS	ALA	LYS	S560	S561	Q564	K565	P566	R567	N568	I569	K570	G571	K572	L580	H581	Y582	A583	G584	T585	V586	D587	Y588	N589	L590	M593	L594					
I621	D522	E525	K526	P527	M528	L534	E535	E536	E537	F540	P541	K542	A543	T544	D545	M546	T547	F548	K549	A550	R551	L552	F553	D554	N555	H556	L557	G558	K559	S560	S561	Q564	K565	P566	R567	N568	I569	K570	G571	K572	L580	H581	Y582	A583	G584	T585	V586	D587	Y588	N589	L590	M593	L594						
A428	K429	A430	V431	Y432	M435	R442	I443	N444	A445	T446	L447	E448	T449	K450	Q451	P452	R453	I457	G458	V459	L460	A463	E466	I467	F468	D469	F470	N471	C477	I478	N479	T481	Q486	F489	K502	K503	E504	G505	I506	E507	M508	E509	F510	I511	D512	D516	L517												
K351	L352	T353	G354	A355	I356	M357	H358	F364	K365	L366	K367	Q368	R369	E370	E371	Q372	P375	D376	G377	T378	E379	E380	A381	D382	K383	S384	A385	L390	N391	S392	L396	H401	P402	R403	V404	K405	V406	G407	R408	E409	Y410	V411	T412	K413	G414	Q415	N416	V417	Q418	Y422	A423	K424							
T285	F286	Y287	Q288	I289	L290	S291	N292	K293	K294	P295	E296	M300	L301	L302	I303	T304	N305	N306	P307	Y308	D309	S314	Q315	G316	E317	T318	T319	V320	A321	S322	I323	D324	D325	A326	E327	E328	E329	L329	M330	A331	T332	D333	N334	A335	F336	D337	V338	L339	G340	F341	E344	E345	K346	N347	S348	M349	Y350		
THR	LEU	E217	D218	Q219		A223	R147	P225	A226	L227		F230	G231	N232	K233	K234	T235	V236	R237	N238	D239	N240	S241	S242	R243		K246	F247	T248	R249	T250	H251		K257		S260	K261	Q193	T194	F195	A196	V197	I198	ALA	ALA	ILE	GLY	ASP	ARG	SER	LYS	LYS	GLN	GLU	THR	R281	D282	Y283	H284
E137		A141	Y142	R143		K146	R147	S148	E149			P152	H153	F155	S156	I157	S158	D159		Y162		Q172	S173	I174	L175	I176		E179	K184	T185	V186	N187	T188			V191	I192	Q193	T194	F195	A196	V197	I198	ALA	ALA	ILE	GLY	ASP	ARG	SER	LYS	LYS	GLN	GLU	THR	R281	D282	Y283	H284

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.4°, rise=27.5 Å, axial sym=C1	Depositor
Number of segments used	32158	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 ($e^-/\text{Å}^2$)	53	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	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: MG, ADP

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	0.45	0/2942	0.54	0/3986
1	B	0.45	0/2942	0.54	0/3986
1	C	0.45	0/2942	0.54	0/3986
2	O	0.64	0/1328	0.97	10/1770 (0.6%)
2	P	0.64	0/1328	0.97	10/1770 (0.6%)
3	D	0.33	0/5803	0.53	0/7825
3	G	0.33	0/5803	0.53	0/7825
3	J	0.33	0/5803	0.53	0/7825
All	All	0.41	0/28891	0.59	20/38973 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
3	D	0	2
3	G	0	2
3	J	0	2
All	All	0	12

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	178	ARG	NE-CZ-NH1	7.41	124.00	120.30
2	P	182	ARG	NE-CZ-NH1	6.99	123.80	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	101	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	P	90	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	O	182	ARG	NE-CZ-NH1	6.71	123.66	120.30
2	P	167	ARG	NE-CZ-NH1	6.67	123.64	120.30
2	O	91	ARG	NE-CZ-NH2	6.55	123.57	120.30
2	O	167	ARG	NE-CZ-NH2	6.53	123.56	120.30
2	O	160	ARG	NE-CZ-NH1	6.42	123.51	120.30
2	P	160	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	O	178	ARG	NE-CZ-NH1	6.26	123.43	120.30
2	P	105	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	P	91	ARG	NE-CZ-NH2	6.00	123.30	120.30
2	P	101	ARG	NE-CZ-NH1	5.90	123.25	120.30
2	O	90	ARG	NE-CZ-NH2	5.85	123.22	120.30
2	O	125	ARG	NE-CZ-NH1	5.69	123.14	120.30
2	O	105	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	P	133	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	O	133	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	P	125	ARG	NE-CZ-NH1	5.54	123.07	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	LEU	Peptide
1	A	111	ASN	Peptide
1	B	110	LEU	Peptide
1	B	111	ASN	Peptide
1	C	110	LEU	Peptide
1	C	111	ASN	Peptide
3	D	569	ILE	Peptide
3	D	726	ASN	Peptide
3	G	569	ILE	Peptide
3	G	726	ASN	Peptide
3	J	569	ILE	Peptide
3	J	726	ASN	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2880	0	2852	205	0
1	B	2880	0	2852	245	0
1	C	2880	0	2853	179	0
2	O	1326	0	1330	45	0
2	P	1326	0	1332	63	0
3	D	5680	0	5633	272	0
3	G	5680	0	5633	259	0
3	J	5680	0	5635	269	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
All	All	28416	0	28156	1311	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (1311) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:GLY:HA2	1:C:44:MET:CE	1.30	1.59
1:B:170:ALA:HB3	1:C:43:VAL:CG1	1.29	1.56
1:B:170:ALA:CB	1:C:43:VAL:HG11	1.28	1.55
1:B:205:GLU:CD	1:A:287:ILE:HD13	1.17	1.55
1:B:205:GLU:CD	1:A:287:ILE:CD1	1.81	1.46
1:B:307:PRO:HB2	2:O:125:ARG:NH1	1.20	1.41
1:B:308:GLY:CA	2:O:125:ARG:NH2	1.81	1.41
1:B:287:ILE:HD13	1:C:205:GLU:CD	1.44	1.37
1:B:64:ILE:CD1	1:A:169:TYR:CD1	2.07	1.35
1:B:307:PRO:CB	2:O:125:ARG:HH12	1.49	1.25
1:B:62:ARG:HG3	1:A:288:ASP:OD2	1.31	1.25
1:B:308:GLY:N	2:O:125:ARG:HH22	1.36	1.23
1:B:169:TYR:CD1	1:C:64:ILE:HD13	1.75	1.22
1:B:308:GLY:HA3	2:O:125:ARG:NH2	1.39	1.21
2:P:91:ARG:NH1	1:A:311:ASP:HB2	1.55	1.20
1:B:169:TYR:CD1	1:C:64:ILE:CD1	2.25	1.20
2:P:171:ILE:HD13	1:C:311:ASP:OD1	1.42	1.18
1:B:168:GLY:CA	1:C:44:MET:CE	2.23	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:90:ARG:CD	1:A:221:LEU:HD23	1.75	1.16
1:B:63:GLY:HA3	1:A:289:ILE:CD1	1.76	1.15
1:B:308:GLY:CA	2:O:125:ARG:HH22	1.45	1.14
1:B:168:GLY:HA2	1:C:44:MET:HE3	1.19	1.14
1:B:44:MET:CE	1:A:168:GLY:HA2	1.77	1.14
1:B:287:ILE:CD1	1:C:205:GLU:CD	2.16	1.13
1:B:40:HIS:CE1	1:A:171:LEU:HD11	1.85	1.12
1:B:205:GLU:OE1	1:A:287:ILE:CD1	1.97	1.11
1:B:170:ALA:N	1:C:43:VAL:HG21	1.66	1.11
1:B:64:ILE:HD13	1:A:169:TYR:CD1	1.77	1.10
2:P:171:ILE:HD13	1:C:311:ASP:CG	1.72	1.10
1:B:205:GLU:CG	1:A:287:ILE:HD13	1.80	1.10
1:B:63:GLY:CA	1:A:289:ILE:HD11	1.81	1.09
1:B:289:ILE:HD11	1:C:63:GLY:HA3	1.31	1.09
1:B:168:GLY:HA2	1:C:44:MET:HE2	1.17	1.07
2:P:91:ARG:CZ	1:A:311:ASP:HB2	1.84	1.07
1:B:168:GLY:CA	1:C:44:MET:HE3	1.83	1.06
1:B:307:PRO:CB	2:O:125:ARG:NH1	2.13	1.04
2:P:90:ARG:HD2	1:A:221:LEU:HD23	1.33	1.04
2:P:90:ARG:HD2	1:A:221:LEU:CD2	1.88	1.04
2:O:173:GLU:HG2	2:P:172:ILE:HD13	1.41	1.02
1:B:205:GLU:OE2	1:A:287:ILE:HD13	1.58	1.02
2:P:91:ARG:NH2	1:A:311:ASP:OD1	1.94	1.01
2:P:171:ILE:CD1	1:C:311:ASP:CG	2.28	1.01
1:B:170:ALA:HB2	1:C:43:VAL:CB	1.92	0.99
1:B:170:ALA:N	1:C:43:VAL:CG2	2.25	0.99
1:B:308:GLY:N	2:O:125:ARG:NH2	2.01	0.99
1:B:44:MET:HE2	1:A:168:GLY:HA2	1.41	0.98
2:O:133:ARG:HB3	3:G:369:ARG:HH22	1.26	0.98
1:B:288:ASP:OD2	1:C:62:ARG:HG3	1.64	0.97
1:B:307:PRO:C	2:O:125:ARG:HH22	1.68	0.97
2:P:91:ARG:CZ	1:A:311:ASP:OD1	2.13	0.96
2:O:169:LEU:CD2	2:O:173:GLU:OE2	2.14	0.95
1:B:169:TYR:CE1	1:C:64:ILE:CD1	2.50	0.95
2:O:173:GLU:HG2	2:P:172:ILE:CD1	1.95	0.95
1:B:170:ALA:CB	1:C:43:VAL:HG21	1.95	0.94
1:B:170:ALA:CB	1:C:43:VAL:CB	2.45	0.94
1:B:308:GLY:CA	2:O:125:ARG:HH21	1.75	0.94
1:B:205:GLU:OE2	1:A:287:ILE:CD1	2.13	0.94
1:B:205:GLU:CD	1:A:287:ILE:HD11	1.87	0.94
1:B:170:ALA:CA	1:C:43:VAL:HG21	1.99	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ALA:HB2	1:C:43:VAL:HG21	1.50	0.92
2:O:93:GLN:CA	3:D:368:GLN:HE22	1.80	0.92
1:C:142:LEU:HD12	1:C:165:ILE:HD12	1.50	0.92
1:B:287:ILE:HD13	1:C:205:GLU:OE2	1.69	0.91
1:B:64:ILE:CD1	1:A:169:TYR:CE1	2.53	0.91
1:B:244:ASP:OD1	1:A:287:ILE:O	1.88	0.91
2:P:91:ARG:CZ	1:A:311:ASP:CB	2.47	0.91
1:B:169:TYR:CE1	1:C:64:ILE:HD11	2.05	0.91
2:O:93:GLN:HA	3:D:368:GLN:HE22	1.34	0.90
1:B:170:ALA:HB2	1:C:43:VAL:CG2	2.00	0.90
1:B:205:GLU:OE1	1:A:287:ILE:HD11	1.69	0.90
1:B:308:GLY:HA3	2:O:125:ARG:HH21	1.27	0.90
2:P:91:ARG:NH1	1:A:311:ASP:CB	2.34	0.90
3:D:290:LEU:HD21	3:D:307:PRO:HB3	1.53	0.89
1:B:46:GLY:HA3	3:D:540:PHE:CE1	2.07	0.89
1:B:64:ILE:HD11	1:A:169:TYR:CD1	2.08	0.88
1:B:44:MET:HE3	1:A:168:GLY:HA2	1.55	0.88
3:G:290:LEU:HD21	3:G:307:PRO:HB3	1.52	0.88
1:B:64:ILE:HD12	1:A:169:TYR:CD1	2.08	0.88
3:J:290:LEU:HD21	3:J:307:PRO:HB3	1.52	0.88
3:J:569:ILE:HD12	3:J:572:LYS:HG3	1.56	0.87
3:G:368:GLN:HE22	2:P:135:GLN:HB3	1.39	0.87
3:G:569:ILE:HD12	3:G:572:LYS:HG3	1.56	0.87
3:J:174:ILE:HG13	3:J:668:HIS:HE1	1.39	0.87
3:D:569:ILE:HD12	3:D:572:LYS:HG3	1.56	0.87
3:G:174:ILE:HG13	3:G:668:HIS:HE1	1.39	0.86
3:G:723:ARG:HE	3:G:735:PHE:HB2	1.41	0.86
3:D:723:ARG:HE	3:D:735:PHE:HB2	1.41	0.86
2:P:90:ARG:HD2	1:A:221:LEU:CG	2.04	0.86
1:B:287:ILE:CD1	1:C:205:GLU:OE1	2.24	0.86
3:J:723:ARG:HE	3:J:735:PHE:HB2	1.41	0.86
3:D:174:ILE:HG13	3:D:668:HIS:HE1	1.39	0.85
1:B:170:ALA:CB	1:C:43:VAL:CG1	2.09	0.84
1:B:307:PRO:HB2	2:O:125:ARG:HH11	1.40	0.84
1:B:64:ILE:HD11	1:A:169:TYR:CE1	2.14	0.83
1:B:170:ALA:CB	1:C:43:VAL:CG2	2.56	0.83
1:B:245:GLY:HA3	1:A:322:PRO:CG	2.09	0.82
1:B:170:ALA:H	1:C:43:VAL:CG2	1.88	0.82
3:G:288:GLN:NE2	3:G:332:THR:OG1	2.13	0.82
2:P:172:ILE:HA	3:J:369:ARG:HH22	1.41	0.82
3:J:288:GLN:NE2	3:J:332:THR:OG1	2.13	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:VAL:CG2	1:A:170:ALA:N	2.42	0.82
3:D:288:GLN:NE2	3:D:332:THR:OG1	2.12	0.81
1:A:143:TYR:OH	3:D:540:PHE:CE1	2.34	0.81
1:A:107:GLU:HG2	1:A:116:ARG:HE	1.46	0.80
1:C:107:GLU:HG2	1:C:116:ARG:HE	1.46	0.80
2:P:79:THR:HG22	1:A:238:LYS:HZ1	1.47	0.79
1:B:107:GLU:HG2	1:B:116:ARG:HE	1.46	0.79
1:B:245:GLY:HA3	1:A:322:PRO:HG3	1.65	0.79
1:B:46:GLY:C	3:D:540:PHE:CZ	2.56	0.79
1:B:40:HIS:CE1	1:A:171:LEU:CD1	2.64	0.79
1:B:123:MET:HE1	1:B:132:MET:HG3	1.66	0.78
3:D:719:ARG:HG3	3:D:738:SER:HA	1.65	0.78
1:B:43:VAL:HG21	1:A:170:ALA:N	1.99	0.77
3:G:719:ARG:HG3	3:G:738:SER:HA	1.65	0.77
2:O:173:GLU:HB3	3:J:368:GLN:HE22	1.49	0.76
3:J:719:ARG:HG3	3:J:738:SER:HA	1.65	0.76
2:P:79:THR:HG22	1:A:238:LYS:NZ	2.00	0.76
2:O:173:GLU:CG	2:P:172:ILE:HD13	2.16	0.76
1:B:40:HIS:CG	1:A:171:LEU:HD12	2.21	0.75
1:B:170:ALA:H	1:C:43:VAL:HG22	1.50	0.75
1:B:43:VAL:HG21	1:A:170:ALA:CA	2.16	0.75
2:P:175:ASP:HB2	3:J:369:ARG:NH2	2.01	0.75
2:O:93:GLN:CB	3:D:368:GLN:HE22	2.00	0.74
1:B:63:GLY:HA3	1:A:289:ILE:HD11	0.85	0.74
1:B:64:ILE:HD13	1:A:169:TYR:HD1	1.44	0.74
3:D:234:LYS:HG3	3:D:239:ASP:HB2	1.69	0.74
3:J:449:THR:OG1	3:J:451:GLN:OE1	2.06	0.73
1:B:287:ILE:HD13	1:C:205:GLU:CG	2.18	0.73
1:B:308:GLY:HA2	2:O:125:ARG:NH2	1.96	0.73
1:B:205:GLU:HG2	1:A:287:ILE:HD13	1.71	0.73
1:C:149:THR:HG23	1:C:166:TYR:HA	1.70	0.73
1:C:123:MET:HE1	1:C:132:MET:HG3	1.68	0.73
1:B:149:THR:HG23	1:B:166:TYR:HA	1.70	0.72
3:D:449:THR:OG1	3:D:451:GLN:OE1	2.06	0.72
1:B:169:TYR:CG	1:C:64:ILE:HD13	2.24	0.72
3:G:234:LYS:HG3	3:G:239:ASP:HB2	1.69	0.72
1:B:45:VAL:O	3:D:540:PHE:CE1	2.43	0.72
1:A:123:MET:HE1	1:A:132:MET:HG3	1.69	0.72
1:A:149:THR:HG23	1:A:166:TYR:HA	1.70	0.72
2:O:93:GLN:HA	3:D:368:GLN:NE2	2.04	0.72
3:G:449:THR:OG1	3:G:451:GLN:OE1	2.06	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:128:TYR:HD2	3:G:681:PRO:HG3	1.55	0.72
2:P:172:ILE:HG13	3:J:369:ARG:NH2	2.04	0.72
3:J:128:TYR:HD2	3:J:681:PRO:HG3	1.55	0.72
1:A:8:LEU:HD22	1:A:103:THR:HG23	1.72	0.72
1:B:8:LEU:HD22	1:B:103:THR:HG23	1.72	0.72
3:J:234:LYS:HG3	3:J:239:ASP:HB2	1.69	0.72
3:G:535:GLU:OE1	3:G:646:THR:OG1	2.08	0.71
3:D:128:TYR:HD2	3:D:681:PRO:HG3	1.55	0.71
1:C:8:LEU:HD22	1:C:103:THR:HG23	1.72	0.71
3:D:720:GLN:O	3:D:723:ARG:NH2	2.24	0.71
1:B:143:TYR:OH	1:C:45:VAL:O	2.08	0.71
1:B:169:TYR:CD1	1:C:64:ILE:HD11	2.22	0.71
3:G:720:GLN:O	3:G:723:ARG:NH2	2.24	0.71
1:B:163:VAL:HG12	1:B:175:ILE:HG12	1.72	0.71
1:A:163:VAL:HG12	1:A:175:ILE:HG12	1.72	0.71
3:D:192:ILE:HD11	3:D:250:ILE:HG21	1.72	0.70
1:C:111:ASN:OD1	1:C:177:ARG:NH1	2.21	0.70
1:C:163:VAL:HG12	1:C:175:ILE:HG12	1.72	0.70
3:J:100:ALA:HA	3:J:103:TYR:CE1	2.26	0.70
2:P:90:ARG:NH1	1:A:221:LEU:HD23	2.06	0.70
3:D:235:THR:HG21	3:D:243:ARG:HH11	1.56	0.70
3:J:235:THR:HG21	3:J:243:ARG:HH11	1.56	0.70
2:P:172:ILE:HA	3:J:369:ARG:NH2	2.07	0.70
3:D:37:VAL:HG21	3:D:51:ILE:HG23	1.73	0.70
3:J:720:GLN:O	3:J:723:ARG:NH2	2.24	0.70
3:J:535:GLU:OE1	3:J:646:THR:OG1	2.08	0.70
3:G:100:ALA:HA	3:G:103:TYR:CE1	2.26	0.70
3:G:192:ILE:HD11	3:G:250:ILE:HG21	1.72	0.70
3:D:535:GLU:OE1	3:D:646:THR:OG1	2.08	0.70
3:G:235:THR:HG21	3:G:243:ARG:HH11	1.56	0.70
3:D:725:LEU:HD11	3:D:773:LEU:HD13	1.74	0.70
2:P:90:ARG:NE	1:A:221:LEU:HD23	2.06	0.69
3:G:37:VAL:HG21	3:G:51:ILE:HG23	1.73	0.69
2:P:79:THR:CG2	1:A:238:LYS:NZ	2.55	0.69
3:J:192:ILE:HD11	3:J:250:ILE:HG21	1.72	0.69
1:B:180:LEU:HD21	1:B:261:LEU:HA	1.74	0.69
2:P:90:ARG:CZ	1:A:221:LEU:HD23	2.21	0.69
1:A:180:LEU:HD21	1:A:261:LEU:HA	1.74	0.69
3:D:100:ALA:HA	3:D:103:TYR:CE1	2.26	0.69
1:C:180:LEU:HD21	1:C:261:LEU:HA	1.74	0.69
3:G:725:LEU:HD11	3:G:773:LEU:HD13	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:37:VAL:HG21	3:J:51:ILE:HG23	1.73	0.69
1:B:45:VAL:O	3:D:540:PHE:HE1	1.75	0.69
1:B:170:ALA:HB2	1:C:43:VAL:HB	1.71	0.69
2:P:79:THR:CG2	1:A:238:LYS:HZ1	2.05	0.69
2:P:132:SER:O	2:P:135:GLN:HG2	1.93	0.69
2:O:103:GLN:OE1	1:A:326:LYS:NZ	2.19	0.69
3:G:155:PHE:HB3	3:G:194:TYR:CZ	2.29	0.68
3:D:155:PHE:HB3	3:D:194:TYR:CZ	2.29	0.68
3:J:725:LEU:HD11	3:J:773:LEU:HD13	1.74	0.68
3:J:155:PHE:HB3	3:J:194:TYR:CZ	2.29	0.68
1:B:111:ASN:OD1	1:B:177:ARG:NH1	2.21	0.68
1:B:40:HIS:ND1	1:A:171:LEU:CD1	2.57	0.68
1:B:168:GLY:CA	1:C:44:MET:HE2	2.08	0.68
2:O:133:ARG:HB3	3:G:369:ARG:NH2	2.05	0.68
1:A:142:LEU:HD12	1:A:165:ILE:HD12	1.76	0.68
1:C:11:ASP:OD1	1:C:12:ASN:N	2.27	0.68
2:P:90:ARG:HD2	1:A:221:LEU:HG	1.73	0.67
1:A:11:ASP:OD1	1:A:12:ASN:N	2.27	0.67
1:B:11:ASP:OD1	1:B:12:ASN:N	2.27	0.67
1:B:43:VAL:HG22	1:A:170:ALA:N	2.09	0.67
2:O:93:GLN:CB	3:D:368:GLN:NE2	2.57	0.67
1:C:11:ASP:OD2	1:C:18:LYS:NZ	2.27	0.67
1:A:11:ASP:OD2	1:A:18:LYS:NZ	2.27	0.67
1:B:11:ASP:OD2	1:B:18:LYS:NZ	2.27	0.67
3:G:172:GLN:HB2	3:G:457:ILE:HG23	1.77	0.67
2:P:91:ARG:CZ	1:A:311:ASP:CG	2.62	0.67
2:P:175:ASP:OD2	3:J:369:ARG:NH2	2.28	0.67
3:D:153:HIS:CE1	3:D:155:PHE:HB2	2.30	0.67
3:D:445:ALA:HA	3:D:448:GLU:HG3	1.77	0.67
3:J:172:GLN:HB2	3:J:457:ILE:HG23	1.77	0.67
1:A:350:SER:OG	3:D:536:GLU:OE1	2.10	0.67
3:D:184:LYS:NZ	3:D:188:THR:OG1	2.26	0.67
3:G:301:LEU:HD11	3:G:354:GLY:HA3	1.77	0.66
1:A:297:ASN:HB3	1:A:329:ILE:HG22	1.77	0.66
3:D:172:GLN:HB2	3:D:457:ILE:HG23	1.77	0.66
3:J:301:LEU:HD11	3:J:354:GLY:HA3	1.77	0.66
1:A:111:ASN:OD1	1:A:177:ARG:NH1	2.21	0.66
3:D:281:ARG:HH11	3:D:320:VAL:HG11	1.61	0.66
1:B:40:HIS:ND1	1:A:171:LEU:HD11	2.09	0.66
1:B:44:MET:HE3	1:A:168:GLY:CA	2.24	0.66
1:B:308:GLY:HA3	2:O:125:ARG:HH22	1.18	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:301:LEU:HD11	3:D:354:GLY:HA3	1.77	0.66
3:J:153:HIS:CE1	3:J:155:PHE:HB2	2.30	0.66
3:J:281:ARG:HH11	3:J:320:VAL:HG11	1.61	0.66
1:B:350:SER:OG	3:G:536:GLU:OE1	2.10	0.66
3:G:153:HIS:CE1	3:G:155:PHE:HB2	2.30	0.66
3:G:445:ALA:HA	3:G:448:GLU:HG3	1.77	0.66
1:B:297:ASN:HB3	1:B:329:ILE:HG22	1.77	0.66
3:G:293:LYS:HB3	3:G:329:LEU:HD21	1.78	0.66
3:J:293:LYS:HB3	3:J:329:LEU:HD21	1.78	0.66
3:G:184:LYS:NZ	3:G:188:THR:OG1	2.26	0.65
3:J:176:ILE:HG21	3:J:184:LYS:HE3	1.79	0.65
3:G:176:ILE:HG21	3:G:184:LYS:HE3	1.79	0.65
3:D:293:LYS:HB3	3:D:329:LEU:HD21	1.78	0.65
3:D:39:VAL:HG23	3:D:71:VAL:HG11	1.79	0.65
3:D:176:ILE:HG21	3:D:184:LYS:HE3	1.79	0.65
1:C:297:ASN:HB3	1:C:329:ILE:HG22	1.77	0.65
3:J:39:VAL:HG23	3:J:71:VAL:HG11	1.79	0.65
3:J:184:LYS:NZ	3:J:188:THR:OG1	2.26	0.65
1:C:142:LEU:CD1	1:C:165:ILE:HD12	2.24	0.65
3:G:39:VAL:HG23	3:G:71:VAL:HG11	1.79	0.65
2:P:171:ILE:CD1	1:C:311:ASP:OD1	2.29	0.65
3:D:143:ARG:NH1	3:D:159:ASP:OD1	2.29	0.65
3:J:445:ALA:HA	3:J:448:GLU:HG3	1.77	0.65
3:D:486:GLN:HG2	3:D:517:LEU:HD11	1.79	0.65
3:G:143:ARG:NH1	3:G:159:ASP:OD1	2.29	0.65
3:G:281:ARG:HH11	3:G:320:VAL:HG11	1.61	0.65
3:D:709:PHE:O	3:D:711:ASN:N	2.30	0.65
3:J:143:ARG:NH1	3:J:159:ASP:OD1	2.29	0.65
3:J:477:CYS:SG	3:J:651:HIS:NE2	2.70	0.65
3:G:486:GLN:HG2	3:G:517:LEU:HD11	1.79	0.64
1:B:287:ILE:CD1	1:C:205:GLU:OE2	2.36	0.64
1:B:290:ARG:HD2	1:C:244:ASP:OD1	1.97	0.64
3:G:468:PHE:O	3:G:471:ASN:ND2	2.30	0.64
3:G:709:PHE:O	3:G:711:ASN:N	2.30	0.64
1:C:350:SER:OG	3:J:536:GLU:OE1	2.10	0.64
3:J:724:ILE:HD12	3:J:774:GLU:HA	1.79	0.64
1:B:304:THR:O	1:B:335:ARG:NH2	2.29	0.64
3:D:468:PHE:O	3:D:471:ASN:ND2	2.30	0.64
3:G:724:ILE:HD12	3:G:774:GLU:HA	1.79	0.64
3:D:162:TYR:HB2	3:D:195:PHE:CE1	2.33	0.64
3:D:174:ILE:HG13	3:D:668:HIS:CE1	2.28	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:477:CYS:SG	3:G:651:HIS:NE2	2.70	0.64
3:D:275:PHE:HD2	3:D:596:LYS:HE3	1.62	0.64
3:J:486:GLN:HG2	3:J:517:LEU:HD11	1.79	0.64
1:B:64:ILE:CD1	1:A:169:TYR:HD1	1.99	0.64
3:D:477:CYS:SG	3:D:651:HIS:NE2	2.70	0.64
3:J:723:ARG:NE	3:J:735:PHE:HB2	2.12	0.64
3:J:709:PHE:O	3:J:711:ASN:N	2.30	0.64
1:B:170:ALA:N	1:C:43:VAL:HG22	2.09	0.64
1:B:307:PRO:HB2	2:O:125:ARG:HH12	0.82	0.64
3:J:46:PHE:HD2	3:J:99:PRO:HG3	1.63	0.64
2:O:169:LEU:O	2:O:173:GLU:HG3	1.98	0.64
2:P:171:ILE:HD11	1:C:311:ASP:CG	2.15	0.64
3:D:717:ASP:HB3	3:D:721:ARG:NH1	2.13	0.64
3:D:724:ILE:HD12	3:D:774:GLU:HA	1.79	0.64
3:G:717:ASP:HB3	3:G:721:ARG:NH1	2.13	0.63
1:B:171:LEU:HD11	1:C:40:HIS:CE1	2.32	0.63
3:G:174:ILE:HB	3:G:459:VAL:HA	1.79	0.63
1:A:304:THR:O	1:A:335:ARG:NH2	2.29	0.63
3:G:162:TYR:HB2	3:G:195:PHE:CE1	2.33	0.63
1:B:307:PRO:CA	2:O:125:ARG:HH12	2.11	0.63
3:G:266:TYR:OH	3:G:661:ASN:ND2	2.30	0.63
3:J:266:TYR:OH	3:J:661:ASN:ND2	2.30	0.63
3:G:174:ILE:HG13	3:G:668:HIS:CE1	2.28	0.63
3:G:723:ARG:NE	3:G:735:PHE:HB2	2.12	0.63
1:C:304:THR:O	1:C:335:ARG:NH2	2.29	0.63
3:G:247:PHE:HD1	3:G:460:LEU:HB3	1.63	0.63
3:G:275:PHE:HD2	3:G:596:LYS:HE3	1.62	0.63
3:J:275:PHE:HD2	3:J:596:LYS:HE3	1.62	0.63
1:B:23:GLY:N	1:B:344:SER:OG	2.32	0.63
3:J:162:TYR:HB2	3:J:195:PHE:CE1	2.32	0.63
3:J:717:ASP:HB3	3:J:721:ARG:NH1	2.13	0.63
2:O:169:LEU:HD23	2:O:173:GLU:OE2	1.99	0.63
3:D:266:TYR:OH	3:D:661:ASN:ND2	2.30	0.63
1:C:23:GLY:N	1:C:344:SER:OG	2.32	0.63
3:G:46:PHE:HD2	3:G:99:PRO:HG3	1.62	0.62
3:D:723:ARG:NE	3:D:735:PHE:HB2	2.12	0.62
1:A:23:GLY:N	1:A:344:SER:OG	2.32	0.62
3:D:162:TYR:HB2	3:D:195:PHE:HE1	1.64	0.62
3:D:174:ILE:HB	3:D:459:VAL:HA	1.79	0.62
1:B:64:ILE:HD13	1:A:169:TYR:CG	2.33	0.62
3:J:174:ILE:HB	3:J:459:VAL:HA	1.79	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:HB2	1:B:134:VAL:HG12	1.82	0.62
1:A:105:LEU:HB2	1:A:134:VAL:HG12	1.82	0.62
3:J:174:ILE:HG13	3:J:668:HIS:CE1	2.28	0.62
3:G:162:TYR:HB2	3:G:195:PHE:HE1	1.64	0.62
3:J:162:TYR:HB2	3:J:195:PHE:HE1	1.64	0.62
1:B:64:ILE:CD1	1:A:169:TYR:CG	2.78	0.62
3:G:470:PHE:HD2	3:G:589:ASN:HD21	1.47	0.62
3:D:46:PHE:HD2	3:D:99:PRO:HG3	1.62	0.62
3:D:470:PHE:HD2	3:D:589:ASN:HD21	1.47	0.61
3:J:247:PHE:HD1	3:J:460:LEU:HB3	1.63	0.61
3:J:470:PHE:HD2	3:J:589:ASN:HD21	1.47	0.61
1:C:105:LEU:HB2	1:C:134:VAL:HG12	1.82	0.61
3:G:406:VAL:HG12	3:G:407:GLY:H	1.66	0.61
3:D:247:PHE:HD1	3:D:460:LEU:HB3	1.63	0.61
3:D:719:ARG:NE	3:D:741:GLY:HA3	2.15	0.61
3:J:406:VAL:HG12	3:J:407:GLY:H	1.66	0.61
3:J:599:ASP:OD1	3:J:646:THR:HA	2.01	0.61
3:J:719:ARG:NE	3:J:741:GLY:HA3	2.15	0.61
2:P:90:ARG:NH1	1:A:221:LEU:CD2	2.63	0.61
3:D:406:VAL:HG12	3:D:407:GLY:H	1.66	0.61
1:A:157:ASP:O	1:A:182:GLY:N	2.32	0.61
3:G:599:ASP:OD1	3:G:646:THR:HA	2.01	0.61
3:G:534:LEU:HD23	3:G:597:ASN:HD22	1.66	0.61
1:B:157:ASP:O	1:B:182:GLY:N	2.32	0.60
1:B:168:GLY:HA2	1:C:44:MET:HE1	1.65	0.60
3:G:719:ARG:NE	3:G:741:GLY:HA3	2.15	0.60
3:G:715:TYR:OH	3:G:719:ARG:NH1	2.34	0.60
3:J:755:GLN:HG3	3:J:756:TYR:HD1	1.66	0.60
2:P:90:ARG:CD	1:A:221:LEU:CD2	2.57	0.60
1:A:189:LEU:HA	1:A:192:ILE:HG22	1.84	0.60
3:J:715:TYR:OH	3:J:719:ARG:NH1	2.34	0.60
3:G:676:ASN:HA	3:G:688:LEU:HD22	1.84	0.60
1:C:98:PRO:HB2	1:C:129:VAL:HG12	1.84	0.60
3:J:534:LEU:HD23	3:J:597:ASN:HD22	1.66	0.60
3:J:676:ASN:HA	3:J:688:LEU:HD22	1.84	0.60
2:O:169:LEU:HD22	2:O:173:GLU:OE2	2.00	0.60
3:D:676:ASN:HA	3:D:688:LEU:HD22	1.84	0.60
3:J:288:GLN:NE2	3:J:329:LEU:HA	2.17	0.60
3:D:715:TYR:OH	3:D:719:ARG:NH1	2.34	0.60
1:A:98:PRO:HB2	1:A:129:VAL:HG12	1.84	0.60
1:A:143:TYR:OH	3:D:540:PHE:CZ	2.55	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:375:PRO:HG3	3:J:396:LEU:HD13	1.84	0.60
1:B:189:LEU:HA	1:B:192:ILE:HG22	1.84	0.60
3:G:288:GLN:NE2	3:G:329:LEU:HA	2.17	0.60
3:J:416:ASN:OD1	3:J:417:VAL:N	2.35	0.60
3:G:416:ASN:OD1	3:G:417:VAL:N	2.35	0.59
2:P:175:ASP:HB2	3:J:369:ARG:HH22	1.66	0.59
1:C:189:LEU:HA	1:C:192:ILE:HG22	1.84	0.59
3:J:356:ILE:HD13	3:J:432:TYR:HB2	1.84	0.59
1:B:98:PRO:HB2	1:B:129:VAL:HG12	1.84	0.59
3:G:375:PRO:HG3	3:G:396:LEU:HD13	1.84	0.59
3:D:534:LEU:HD23	3:D:597:ASN:HD22	1.66	0.59
3:D:599:ASP:OD1	3:D:646:THR:HA	2.01	0.59
1:C:157:ASP:O	1:C:182:GLY:N	2.32	0.59
3:G:671:ARG:HG2	3:G:696:ASN:HD21	1.67	0.59
3:G:356:ILE:HD13	3:G:432:TYR:HB2	1.84	0.59
3:G:755:GLN:HG3	3:G:756:TYR:HD1	1.66	0.59
1:A:124:PHE:HZ	1:A:359:LYS:HA	1.67	0.59
3:D:375:PRO:HG3	3:D:396:LEU:HD13	1.84	0.59
3:D:288:GLN:NE2	3:D:329:LEU:HA	2.17	0.59
1:C:124:PHE:HZ	1:C:359:LYS:HA	1.67	0.59
3:J:671:ARG:HG2	3:J:696:ASN:HD21	1.67	0.59
1:B:40:HIS:CG	1:A:171:LEU:CD1	2.86	0.59
1:B:124:PHE:HZ	1:B:359:LYS:HA	1.67	0.59
3:D:188:THR:HA	3:D:191:VAL:HB	1.85	0.59
3:D:671:ARG:HG2	3:D:696:ASN:HD21	1.67	0.59
2:P:91:ARG:NE	1:A:311:ASP:OD1	2.35	0.59
3:D:504:GLU:HG3	3:D:760:HIS:HB2	1.85	0.59
3:J:468:PHE:O	3:J:471:ASN:ND2	2.30	0.59
1:A:50:LYS:HB2	1:A:53:TYR:CZ	2.38	0.59
1:A:209:VAL:O	1:A:212:ILE:HG22	2.02	0.59
3:D:416:ASN:OD1	3:D:417:VAL:N	2.35	0.59
1:B:209:VAL:O	1:B:212:ILE:HG22	2.02	0.59
2:O:169:LEU:HD23	2:O:173:GLU:CD	2.23	0.59
3:J:153:HIS:HE1	3:J:155:PHE:CD2	2.21	0.59
2:O:93:GLN:HB3	3:D:368:GLN:NE2	2.18	0.59
3:G:153:HIS:HE1	3:G:155:PHE:CD2	2.21	0.58
3:G:504:GLU:HG3	3:G:760:HIS:HB2	1.85	0.58
3:D:356:ILE:HD13	3:D:432:TYR:HB2	1.84	0.58
1:C:142:LEU:HD12	1:C:165:ILE:CD1	2.30	0.58
1:C:209:VAL:O	1:C:212:ILE:HG22	2.03	0.58
1:B:44:MET:CE	1:A:168:GLY:CA	2.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:91:ARG:NH1	1:A:311:ASP:CA	2.66	0.58
1:C:155:SER:HA	1:C:160:THR:HA	1.85	0.58
1:B:155:SER:HA	1:B:160:THR:HA	1.85	0.58
3:D:755:GLN:HG3	3:D:756:TYR:HD1	1.66	0.58
1:B:50:LYS:HB2	1:B:53:TYR:CZ	2.38	0.58
3:G:146:LYS:N	3:G:149:GLU:OE2	2.37	0.58
3:G:188:THR:HA	3:G:191:VAL:HB	1.85	0.58
2:P:91:ARG:CD	1:A:311:ASP:OD1	2.51	0.58
1:A:264:PRO:HG3	1:A:271:SER:O	2.04	0.58
1:C:210:ARG:NH1	1:C:214:GLU:OE2	2.37	0.58
1:A:155:SER:HA	1:A:160:THR:HA	1.85	0.58
1:B:307:PRO:C	2:O:125:ARG:HH12	2.06	0.58
3:J:504:GLU:HG3	3:J:760:HIS:HB2	1.85	0.58
1:B:264:PRO:HG3	1:B:271:SER:O	2.04	0.58
1:A:210:ARG:NH1	1:A:214:GLU:OE2	2.37	0.58
1:C:50:LYS:HB2	1:C:53:TYR:CZ	2.38	0.58
1:B:210:ARG:NH1	1:B:214:GLU:OE2	2.37	0.58
2:P:90:ARG:HH11	1:A:221:LEU:HD23	1.67	0.58
3:D:81:PRO:O	3:D:85:ASP:N	2.36	0.58
3:D:153:HIS:HE1	3:D:155:PHE:CD2	2.21	0.58
3:J:188:THR:HA	3:J:191:VAL:HB	1.85	0.58
1:B:287:ILE:HD11	1:C:205:GLU:OE1	2.03	0.57
3:D:146:LYS:N	3:D:149:GLU:OE2	2.37	0.57
3:J:81:PRO:O	3:J:85:ASP:N	2.36	0.57
1:B:307:PRO:C	2:O:125:ARG:NH2	2.47	0.57
3:G:534:LEU:HA	3:G:548:PHE:HE2	1.70	0.57
3:D:545:ASP:OD1	3:D:546:MET:N	2.37	0.57
1:C:264:PRO:HG3	1:C:271:SER:O	2.04	0.57
3:J:352:LEU:HD21	3:J:616:MET:HG2	1.87	0.57
2:P:91:ARG:HD3	1:A:311:ASP:OD1	2.05	0.57
3:J:545:ASP:OD1	3:J:546:MET:N	2.37	0.57
1:B:168:GLY:HA3	1:C:44:MET:HE3	1.79	0.57
2:P:175:ASP:CB	3:J:369:ARG:NH2	2.65	0.57
3:J:77:LEU:HD12	3:J:99:PRO:HG2	1.87	0.57
3:G:352:LEU:HD21	3:G:616:MET:HG2	1.87	0.57
3:D:352:LEU:HD21	3:D:616:MET:HG2	1.87	0.57
1:B:290:ARG:CD	1:C:244:ASP:OD1	2.53	0.57
3:G:77:LEU:HD12	3:G:99:PRO:HG2	1.86	0.57
3:G:405:LYS:HA	3:G:409:GLU:HG3	1.87	0.56
3:G:713:ILE:HG23	3:G:721:ARG:HH22	1.70	0.56
3:D:154:ILE:HG12	3:D:670:VAL:HG22	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:405:LYS:HA	3:D:409:GLU:HG3	1.87	0.56
3:D:713:ILE:HG23	3:D:721:ARG:HH22	1.70	0.56
3:J:37:VAL:HG23	3:J:49:ALA:HB3	1.88	0.56
3:J:154:ILE:HG12	3:J:670:VAL:HG22	1.88	0.56
1:B:64:ILE:HD12	1:A:169:TYR:CE1	2.35	0.56
3:G:37:VAL:HG23	3:G:49:ALA:HB3	1.87	0.56
3:G:154:ILE:HG12	3:G:670:VAL:HG22	1.88	0.56
3:J:534:LEU:HA	3:J:548:PHE:HE2	1.70	0.56
3:D:77:LEU:HD12	3:D:99:PRO:HG2	1.86	0.56
3:J:713:ILE:HG23	3:J:721:ARG:HH22	1.70	0.56
3:G:545:ASP:OD1	3:G:546:MET:N	2.37	0.56
1:A:151:ILE:HD11	1:A:293:LEU:HB3	1.87	0.56
3:D:37:VAL:HG23	3:D:49:ALA:HB3	1.87	0.56
1:C:151:ILE:HD11	1:C:293:LEU:HB3	1.87	0.56
1:B:308:GLY:HA2	2:O:125:ARG:HH21	1.64	0.55
2:P:167:ARG:NH2	1:C:308:GLY:HA3	2.21	0.55
3:D:234:LYS:HA	3:D:240:ASN:H	1.71	0.55
3:D:247:PHE:HE2	3:D:249:ARG:HD3	1.71	0.55
3:D:534:LEU:HA	3:D:548:PHE:HE2	1.70	0.55
3:G:232:ASN:HA	3:G:242:SER:HA	1.89	0.55
3:G:234:LYS:HA	3:G:240:ASN:H	1.71	0.55
1:B:82:MET:SD	1:B:86:TRP:NE1	2.80	0.55
3:G:247:PHE:HE2	3:G:249:ARG:HD3	1.71	0.55
2:P:171:ILE:CD1	1:C:311:ASP:OD2	2.54	0.55
3:D:232:ASN:HA	3:D:242:SER:HA	1.89	0.55
1:B:151:ILE:HD11	1:B:293:LEU:HB3	1.87	0.55
3:J:391:ASN:OD1	3:J:392:SER:N	2.40	0.55
1:B:205:GLU:OE2	1:A:287:ILE:HD11	2.01	0.55
3:J:146:LYS:N	3:J:149:GLU:OE2	2.37	0.55
3:J:232:ASN:HA	3:J:242:SER:HA	1.88	0.55
3:J:405:LYS:HA	3:J:409:GLU:HG3	1.87	0.55
1:B:169:TYR:CG	1:C:64:ILE:CD1	2.86	0.55
3:G:325:ASP:HA	3:G:328:GLU:HB2	1.88	0.55
3:D:738:SER:HB2	3:D:739:ARG:NH2	2.22	0.55
1:C:74:GLY:O	1:C:111:ASN:ND2	2.40	0.55
3:J:247:PHE:HE2	3:J:249:ARG:HD3	1.71	0.55
1:B:74:GLY:O	1:B:111:ASN:ND2	2.40	0.55
2:O:176:LEU:CD2	3:J:369:ARG:HH21	2.20	0.55
3:G:81:PRO:O	3:G:85:ASP:N	2.36	0.55
3:G:391:ASN:OD1	3:G:392:SER:N	2.40	0.55
2:P:90:ARG:NH2	1:A:311:ASP:HB3	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:184:LYS:HG2	3:G:187:ASN:HD22	1.71	0.55
2:P:90:ARG:CZ	1:A:221:LEU:CD2	2.84	0.55
1:C:82:MET:SD	1:C:86:TRP:NE1	2.80	0.55
3:J:184:LYS:HG2	3:J:187:ASN:HD22	1.71	0.55
3:J:325:ASP:HA	3:J:328:GLU:HB2	1.88	0.55
3:J:738:SER:HB2	3:J:739:ARG:NH2	2.22	0.55
1:B:186:THR:HG23	1:B:209:VAL:HG13	1.89	0.55
1:A:186:THR:HG23	1:A:209:VAL:HG13	1.89	0.55
3:G:347:ASN:O	3:G:351:LYS:HG3	2.07	0.54
3:G:738:SER:HB2	3:G:739:ARG:NH2	2.22	0.54
3:D:391:ASN:OD1	3:D:392:SER:N	2.40	0.54
1:C:186:THR:HG23	1:C:209:VAL:HG13	1.89	0.54
1:A:82:MET:SD	1:A:86:TRP:NE1	2.80	0.54
3:D:39:VAL:HG11	3:D:63:THR:HG22	1.89	0.54
3:D:184:LYS:HG2	3:D:187:ASN:HD22	1.71	0.54
3:D:325:ASP:HA	3:D:328:GLU:HB2	1.88	0.54
3:G:368:GLN:NE2	2:P:135:GLN:HB3	2.16	0.54
3:J:234:LYS:HA	3:J:240:ASN:H	1.71	0.54
1:B:46:GLY:CA	3:D:540:PHE:CZ	2.90	0.54
3:D:287:TYR:HA	3:D:290:LEU:HB2	1.90	0.54
3:J:293:LYS:HG3	3:J:329:LEU:HD11	1.89	0.54
3:J:347:ASN:O	3:J:351:LYS:HG3	2.07	0.54
3:J:447:LEU:HD23	3:J:447:LEU:O	2.08	0.54
1:B:40:HIS:CD2	1:A:171:LEU:HD12	2.41	0.54
1:A:103:THR:O	1:A:132:MET:HA	2.08	0.54
1:C:11:ASP:HB3	1:C:18:LYS:HG2	1.90	0.54
1:C:103:THR:O	1:C:132:MET:HA	2.08	0.54
3:G:447:LEU:HD23	3:G:447:LEU:O	2.08	0.54
1:A:74:GLY:O	1:A:111:ASN:ND2	2.40	0.54
1:A:79:TRP:HH2	1:A:119:MET:HB2	1.73	0.54
1:C:9:VAL:HG13	1:C:340:TRP:NE1	2.23	0.54
1:B:11:ASP:HB3	1:B:18:LYS:HG2	1.90	0.54
1:B:103:THR:O	1:B:132:MET:HA	2.08	0.54
3:G:39:VAL:HG11	3:G:63:THR:HG22	1.89	0.54
3:G:287:TYR:HA	3:G:290:LEU:HB2	1.90	0.54
3:G:293:LYS:HG3	3:G:329:LEU:HD11	1.89	0.54
3:G:671:ARG:HG2	3:G:696:ASN:ND2	2.23	0.54
2:O:169:LEU:HD23	2:O:173:GLU:HG3	1.89	0.54
3:D:192:ILE:HD11	3:D:250:ILE:HD13	1.90	0.54
3:D:447:LEU:O	3:D:447:LEU:HD23	2.08	0.54
3:J:403:ARG:NH1	3:J:409:GLU:O	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:96:GLU:OE1	3:D:368:GLN:HB3	2.08	0.53
2:O:173:GLU:HB3	3:J:368:GLN:NE2	2.20	0.53
3:G:192:ILE:HD11	3:G:250:ILE:HD13	1.91	0.53
3:D:347:ASN:O	3:D:351:LYS:HG3	2.07	0.53
1:B:43:VAL:HG22	1:A:170:ALA:H	1.72	0.53
3:G:404:VAL:O	3:G:412:THR:OG1	2.25	0.53
1:A:11:ASP:HB3	1:A:18:LYS:HG2	1.90	0.53
3:J:192:ILE:HD11	3:J:250:ILE:HD13	1.90	0.53
3:J:287:TYR:HA	3:J:290:LEU:HB2	1.90	0.53
3:J:422:TYR:HE2	3:J:598:LYS:HD2	1.73	0.53
1:B:79:TRP:HH2	1:B:119:MET:HB2	1.73	0.53
3:G:422:TYR:HE2	3:G:598:LYS:HD2	1.73	0.53
3:G:755:GLN:HG3	3:G:756:TYR:CD1	2.43	0.53
3:D:59:VAL:N	3:D:71:VAL:O	2.34	0.53
3:D:293:LYS:HG3	3:D:329:LEU:HD11	1.89	0.53
3:D:422:TYR:HE2	3:D:598:LYS:HD2	1.73	0.53
3:D:705:CYS:HA	3:D:710:PRO:HG2	1.90	0.53
3:J:39:VAL:HG11	3:J:63:THR:HG22	1.89	0.53
3:J:59:VAL:N	3:J:71:VAL:O	2.34	0.53
3:G:403:ARG:NH1	3:G:409:GLU:O	2.40	0.53
3:D:248:ILE:O	3:D:459:VAL:N	2.42	0.53
3:D:403:ARG:NH1	3:D:409:GLU:O	2.40	0.53
3:D:755:GLN:HG3	3:D:756:TYR:CD1	2.44	0.53
3:J:671:ARG:HG2	3:J:696:ASN:ND2	2.23	0.53
3:J:755:GLN:HG3	3:J:756:TYR:CD1	2.43	0.53
3:D:404:VAL:O	3:D:412:THR:OG1	2.25	0.53
1:C:198:TYR:CZ	1:C:248:ILE:HG13	2.44	0.53
2:O:169:LEU:HD23	2:O:173:GLU:CG	2.39	0.53
3:G:131:LEU:O	3:G:133:VAL:N	2.40	0.53
2:P:175:ASP:OD2	3:J:369:ARG:CZ	2.57	0.53
1:A:9:VAL:HG13	1:A:340:TRP:NE1	2.23	0.53
1:A:198:TYR:CZ	1:A:248:ILE:HG13	2.44	0.53
3:D:88:GLU:HB2	3:D:152:PRO:HG3	1.89	0.53
3:J:406:VAL:HG12	3:J:407:GLY:N	2.23	0.53
1:B:198:TYR:CZ	1:B:248:ILE:HG13	2.44	0.53
3:G:179:GLU:OE2	3:G:241:SER:OG	2.27	0.53
3:D:179:GLU:OE2	3:D:241:SER:OG	2.27	0.53
3:D:671:ARG:HG2	3:D:696:ASN:ND2	2.23	0.53
3:J:88:GLU:HB2	3:J:152:PRO:HG3	1.89	0.53
3:G:406:VAL:HG12	3:G:407:GLY:N	2.24	0.53
3:J:179:GLU:OE2	3:J:241:SER:OG	2.27	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:403:ARG:NH1	3:J:409:GLU:HG2	2.24	0.53
3:J:509:GLU:HG3	3:J:510:PHE:H	1.74	0.53
3:J:555:ASN:HB3	3:J:556:HIS:ND1	2.24	0.53
1:B:9:VAL:HG13	1:B:340:TRP:NE1	2.23	0.53
3:G:80:ASN:ND2	3:G:93:LEU:HB3	2.24	0.53
3:G:403:ARG:NH1	3:G:409:GLU:HG2	2.24	0.53
1:A:20:GLY:HA3	1:A:340:TRP:CZ2	2.44	0.53
3:D:509:GLU:HG3	3:D:510:PHE:H	1.74	0.53
1:A:8:LEU:HD23	1:A:9:VAL:N	2.24	0.53
3:D:80:ASN:ND2	3:D:93:LEU:HB3	2.24	0.53
1:C:157:ASP:O	1:C:181:ALA:HB1	2.09	0.53
1:C:326:LYS:HB3	1:C:328:LYS:HZ3	1.74	0.53
1:B:157:ASP:O	1:B:181:ALA:HB1	2.09	0.52
2:P:91:ARG:HH11	1:A:311:ASP:HB2	1.61	0.52
3:D:306:ASN:HB3	3:D:309:ASP:OD2	2.09	0.52
3:D:403:ARG:NH1	3:D:409:GLU:HG2	2.24	0.52
1:C:8:LEU:HD23	1:C:9:VAL:N	2.24	0.52
3:J:306:ASN:HB3	3:J:309:ASP:OD2	2.09	0.52
1:B:20:GLY:HA3	1:B:340:TRP:CZ2	2.44	0.52
1:B:44:MET:HE3	1:A:148:THR:OG1	2.09	0.52
1:B:290:ARG:HD2	1:C:244:ASP:CG	2.29	0.52
3:G:217:GLU:HG2	3:G:218:ASP:N	2.25	0.52
3:G:306:ASN:HB3	3:G:309:ASP:OD2	2.09	0.52
3:D:548:PHE:CE1	3:D:552:LEU:HD11	2.45	0.52
3:J:705:CYS:HA	3:J:710:PRO:HG2	1.90	0.52
1:B:8:LEU:HD23	1:B:9:VAL:N	2.24	0.52
3:G:88:GLU:HB2	3:G:152:PRO:HG3	1.89	0.52
3:G:548:PHE:CE1	3:G:552:LEU:HD11	2.45	0.52
2:P:167:ARG:HH21	1:C:308:GLY:HA3	1.75	0.52
3:D:217:GLU:HG2	3:D:218:ASP:N	2.25	0.52
1:C:20:GLY:HA3	1:C:340:TRP:CZ2	2.44	0.52
3:J:80:ASN:ND2	3:J:93:LEU:HB3	2.24	0.52
3:D:406:VAL:HG12	3:D:407:GLY:N	2.23	0.52
3:D:555:ASN:HB3	3:D:556:HIS:ND1	2.24	0.52
3:J:217:GLU:HG2	3:J:218:ASP:N	2.25	0.52
1:B:132:MET:SD	1:B:133:TYR:N	2.82	0.52
3:G:509:GLU:HG3	3:G:510:PHE:H	1.74	0.52
1:A:140:LEU:HD11	1:A:343:GLY:HA2	1.91	0.52
1:C:79:TRP:HH2	1:C:119:MET:HB2	1.73	0.52
3:G:109:TYR:OH	3:G:682:GLY:N	2.34	0.52
3:G:555:ASN:HB3	3:G:556:HIS:ND1	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:403:ARG:HE	3:G:411:VAL:HA	1.75	0.52
1:A:157:ASP:O	1:A:181:ALA:HB1	2.09	0.52
3:D:109:TYR:OH	3:D:682:GLY:N	2.34	0.52
3:J:403:ARG:HE	3:J:411:VAL:HA	1.75	0.52
2:P:172:ILE:HG13	3:J:369:ARG:CZ	2.40	0.52
1:C:132:MET:SD	1:C:133:TYR:N	2.82	0.52
1:C:287:ILE:HG13	1:C:290:ARG:NH2	2.25	0.52
2:P:171:ILE:HG21	1:C:311:ASP:OD1	2.09	0.52
2:O:93:GLN:HB3	3:D:368:GLN:HE22	1.75	0.52
3:G:705:CYS:HA	3:G:710:PRO:HG2	1.90	0.52
3:J:277:LEU:HG	3:J:279:ALA:H	1.75	0.52
3:J:548:PHE:CE1	3:J:552:LEU:HD11	2.45	0.52
1:B:46:GLY:CA	3:D:540:PHE:CE1	2.88	0.51
1:B:287:ILE:HG13	1:B:290:ARG:NH2	2.25	0.51
3:D:277:LEU:HG	3:D:279:ALA:H	1.75	0.51
3:G:277:LEU:HG	3:G:279:ALA:H	1.75	0.51
1:A:132:MET:SD	1:A:133:TYR:N	2.82	0.51
1:C:140:LEU:HD11	1:C:343:GLY:HA2	1.91	0.51
1:C:142:LEU:HD22	1:C:147:ARG:O	2.10	0.51
3:J:103:TYR:HA	3:J:106:LYS:HE2	1.91	0.51
3:D:48:LYS:HB3	3:D:64:GLU:OE1	2.10	0.51
1:B:71:ILE:HD11	1:B:82:MET:HG3	1.93	0.51
1:B:90:PHE:CE2	1:B:98:PRO:HB3	2.46	0.51
3:G:48:LYS:HB3	3:G:64:GLU:OE1	2.09	0.51
3:D:103:TYR:HA	3:D:106:LYS:HE2	1.91	0.51
3:J:48:LYS:HB3	3:J:64:GLU:OE1	2.09	0.51
1:A:71:ILE:HD11	1:A:82:MET:HG3	1.93	0.51
3:D:403:ARG:HE	3:D:411:VAL:HA	1.75	0.51
1:C:190:MET:HE1	1:C:206:ARG:HA	1.93	0.51
3:G:103:TYR:HA	3:G:106:LYS:HE2	1.91	0.51
3:G:704:ILE:HD13	3:G:707:LYS:HZ3	1.75	0.51
1:C:71:ILE:HD11	1:C:82:MET:HG3	1.92	0.51
1:C:90:PHE:CE2	1:C:98:PRO:HB3	2.46	0.51
1:B:190:MET:HE1	1:B:206:ARG:HA	1.93	0.51
1:A:90:PHE:CE2	1:A:98:PRO:HB3	2.46	0.51
3:J:528:MET:HG2	3:J:528:MET:O	2.10	0.51
1:B:289:ILE:HG22	1:B:293:LEU:HG	1.93	0.51
3:G:528:MET:O	3:G:528:MET:HG2	2.10	0.51
1:A:287:ILE:HG13	1:A:290:ARG:NH2	2.25	0.51
3:D:337:ASP:OD1	3:D:346:LYS:HG3	2.11	0.51
3:D:381:ALA:O	3:D:384:SER:OG	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:HD11	1:B:343:GLY:HA2	1.91	0.51
1:A:289:ILE:HG22	1:A:293:LEU:HG	1.93	0.51
3:D:423:ALA:HA	3:D:600:PRO:HD2	1.93	0.51
3:G:423:ALA:HA	3:G:600:PRO:HD2	1.93	0.51
3:G:534:LEU:CD2	3:G:597:ASN:HD22	2.24	0.51
3:D:528:MET:O	3:D:528:MET:HG2	2.10	0.51
3:D:348:SER:HA	3:D:351:LYS:HG3	1.92	0.50
3:D:717:ASP:HB3	3:D:721:ARG:HH12	1.75	0.50
3:J:248:ILE:O	3:J:459:VAL:N	2.41	0.50
1:B:14:SER:OG	1:B:157:ASP:OD1	2.29	0.50
3:G:348:SER:HA	3:G:351:LYS:HG3	1.92	0.50
1:A:116:ARG:HD3	1:A:134:VAL:HG21	1.93	0.50
3:D:534:LEU:CD2	3:D:597:ASN:HD22	2.24	0.50
3:J:534:LEU:CD2	3:J:597:ASN:HD22	2.24	0.50
3:D:93:LEU:O	3:D:96:LEU:HD22	2.11	0.50
3:G:93:LEU:O	3:G:96:LEU:HD22	2.11	0.50
1:A:111:ASN:HB3	1:A:112:PRO:HD3	1.93	0.50
1:A:190:MET:HE1	1:A:206:ARG:HA	1.93	0.50
3:D:131:LEU:O	3:D:133:VAL:N	2.40	0.50
1:C:289:ILE:HG22	1:C:293:LEU:HG	1.93	0.50
3:J:93:LEU:O	3:J:96:LEU:HD22	2.11	0.50
3:J:401:HIS:HD2	3:J:413:LYS:HB3	1.77	0.50
3:J:423:ALA:HA	3:J:600:PRO:HD2	1.93	0.50
3:G:337:ASP:OD1	3:G:346:LYS:HG3	2.11	0.50
3:D:287:TYR:HD1	3:D:290:LEU:HD22	1.77	0.50
3:D:243:ARG:HB3	3:D:269:GLU:OE1	2.11	0.50
3:J:337:ASP:OD1	3:J:346:LYS:HG3	2.11	0.50
3:G:243:ARG:HB3	3:G:269:GLU:OE1	2.11	0.50
3:G:287:TYR:HD1	3:G:290:LEU:HD22	1.77	0.50
3:G:401:HIS:HD2	3:G:413:LYS:HB3	1.77	0.50
3:G:597:ASN:OD1	3:G:647:VAL:N	2.45	0.50
1:C:116:ARG:HD3	1:C:134:VAL:HG21	1.93	0.50
3:J:348:SER:HA	3:J:351:LYS:HG3	1.92	0.50
3:J:597:ASN:OD1	3:J:647:VAL:N	2.45	0.50
3:J:613:SER:HB3	3:J:616:MET:HE3	1.94	0.50
1:B:111:ASN:HB3	1:B:112:PRO:HD3	1.93	0.50
1:B:116:ARG:HD3	1:B:134:VAL:HG21	1.93	0.50
3:G:154:ILE:HD12	3:G:157:ILE:HB	1.94	0.50
1:C:153:LEU:HD13	1:C:162:ASN:OD1	2.12	0.50
3:J:287:TYR:HD1	3:J:290:LEU:HD22	1.77	0.50
1:A:20:GLY:HA3	1:A:340:TRP:HZ2	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:HD13	1:A:162:ASN:OD1	2.12	0.50
1:A:227:MET:HA	1:A:255:PHE:CZ	2.47	0.50
3:D:597:ASN:OD1	3:D:647:VAL:N	2.45	0.50
1:C:146:GLY:HA2	3:J:541:PRO:HB3	1.94	0.50
3:J:288:GLN:HE21	3:J:329:LEU:HA	1.76	0.50
3:J:243:ARG:HB3	3:J:269:GLU:OE1	2.11	0.49
3:G:59:VAL:N	3:G:71:VAL:O	2.34	0.49
3:G:613:SER:HB3	3:G:616:MET:HE3	1.93	0.49
1:A:326:LYS:HB3	1:A:328:LYS:HZ3	1.76	0.49
3:D:288:GLN:HE21	3:D:329:LEU:HA	1.76	0.49
3:D:613:SER:HB3	3:D:616:MET:HE3	1.93	0.49
1:C:221:LEU:HD13	1:C:312:ARG:HD2	1.94	0.49
3:J:153:HIS:HE1	3:J:155:PHE:HB2	1.77	0.49
3:G:345:GLU:O	3:G:349:MET:HG2	2.13	0.49
1:C:111:ASN:HB3	1:C:112:PRO:HD3	1.93	0.49
1:B:146:GLY:HA2	3:G:541:PRO:HB3	1.94	0.49
1:A:146:GLY:HA2	3:D:541:PRO:HB3	1.94	0.49
3:J:720:GLN:HA	3:J:723:ARG:NH1	2.27	0.49
1:B:227:MET:HA	1:B:255:PHE:CZ	2.47	0.49
3:G:717:ASP:HB3	3:G:721:ARG:HH12	1.75	0.49
3:D:401:HIS:HD2	3:D:413:LYS:HB3	1.77	0.49
3:D:720:GLN:HA	3:D:723:ARG:NH1	2.27	0.49
1:C:227:MET:HA	1:C:255:PHE:HZ	1.78	0.49
1:B:221:LEU:HD13	1:B:312:ARG:HD2	1.94	0.49
3:G:720:GLN:HA	3:G:723:ARG:NH1	2.27	0.49
1:A:227:MET:HA	1:A:255:PHE:HZ	1.78	0.49
1:C:20:GLY:HA3	1:C:340:TRP:HZ2	1.76	0.49
1:C:227:MET:HA	1:C:255:PHE:CZ	2.47	0.49
1:A:221:LEU:HD13	1:A:312:ARG:HD2	1.94	0.49
3:D:345:GLU:O	3:D:349:MET:HG2	2.13	0.49
3:J:154:ILE:HD12	3:J:157:ILE:HB	1.94	0.49
1:B:64:ILE:HD12	1:A:169:TYR:CG	2.47	0.49
3:D:128:TYR:CD2	3:D:681:PRO:HG3	2.43	0.49
3:D:296:GLU:O	3:D:300:MET:HG2	2.13	0.49
3:D:509:GLU:HG3	3:D:510:PHE:N	2.28	0.49
1:C:14:SER:OG	1:C:157:ASP:OD1	2.29	0.49
3:J:193:GLN:O	3:J:197:VAL:HG23	2.12	0.49
1:B:49:GLN:OE1	1:B:49:GLN:N	2.46	0.49
3:G:509:GLU:HG3	3:G:510:PHE:N	2.28	0.49
3:G:741:GLY:O	3:G:743:GLU:HG3	2.13	0.49
3:D:741:GLY:O	3:D:743:GLU:HG3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:GLY:HA3	1:B:340:TRP:HZ2	1.76	0.48
1:B:63:GLY:HA3	1:A:289:ILE:CG1	2.41	0.48
3:D:62:GLU:HA	3:D:68:THR:HA	1.95	0.48
3:J:131:LEU:O	3:J:133:VAL:N	2.40	0.48
3:J:345:GLU:O	3:J:349:MET:HG2	2.13	0.48
3:J:509:GLU:HG3	3:J:510:PHE:N	2.28	0.48
1:B:153:LEU:HD13	1:B:162:ASN:OD1	2.12	0.48
1:A:7:ALA:O	1:A:8:LEU:HB2	2.13	0.48
3:D:154:ILE:HD12	3:D:157:ILE:HB	1.94	0.48
3:D:540:PHE:CG	3:D:541:PRO:HD2	2.49	0.48
3:J:717:ASP:HB3	3:J:721:ARG:HH12	1.75	0.48
3:G:193:GLN:O	3:G:197:VAL:HG23	2.12	0.48
3:G:540:PHE:CG	3:G:541:PRO:HD2	2.48	0.48
3:D:193:GLN:O	3:D:197:VAL:HG23	2.12	0.48
3:D:469:ASP:HA	3:D:572:LYS:HE3	1.94	0.48
2:P:132:SER:O	2:P:135:GLN:CG	2.61	0.48
3:D:722:TYR:OH	3:D:770:LEU:HA	2.14	0.48
3:J:741:GLY:O	3:J:743:GLU:HG3	2.13	0.48
2:O:173:GLU:HG2	2:P:172:ILE:HD11	1.91	0.48
3:G:62:GLU:HA	3:G:68:THR:HA	1.95	0.48
1:C:142:LEU:HD11	1:C:165:ILE:HB	1.94	0.48
1:C:349:LEU:HD22	3:J:536:GLU:HG3	1.95	0.48
3:J:296:GLU:O	3:J:300:MET:HG2	2.13	0.48
1:B:256:ARG:HG2	1:B:256:ARG:O	2.14	0.48
1:B:349:LEU:HD22	3:G:536:GLU:HG3	1.95	0.48
3:G:381:ALA:O	3:G:384:SER:OG	2.28	0.48
3:J:62:GLU:HA	3:J:68:THR:HA	1.95	0.48
3:J:281:ARG:NH1	3:J:320:VAL:HG11	2.28	0.48
3:G:610:LYS:HD2	3:G:610:LYS:N	2.29	0.48
3:G:711:ASN:HD22	3:G:767:ALA:HB2	1.79	0.48
3:D:690:MET:SD	3:D:691:HIS:N	2.87	0.48
3:D:722:TYR:OH	3:D:773:LEU:HD12	2.14	0.48
3:J:540:PHE:CG	3:J:541:PRO:HD2	2.48	0.48
3:G:248:ILE:HB	3:G:459:VAL:HG13	1.96	0.48
3:G:296:GLU:O	3:G:300:MET:HG2	2.13	0.48
1:C:256:ARG:O	1:C:256:ARG:HG2	2.14	0.48
3:J:548:PHE:HE1	3:J:552:LEU:HD11	1.79	0.48
3:J:690:MET:SD	3:J:691:HIS:N	2.87	0.48
1:B:200:PHE:HD1	1:B:205:GLU:HB3	1.79	0.48
3:G:248:ILE:O	3:G:459:VAL:N	2.42	0.48
3:G:690:MET:SD	3:G:691:HIS:N	2.87	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LEU:HD22	3:D:536:GLU:HG3	1.95	0.48
3:J:469:ASP:HA	3:J:572:LYS:HE3	1.94	0.48
1:B:7:ALA:O	1:B:8:LEU:HB2	2.14	0.47
3:G:722:TYR:OH	3:G:770:LEU:HA	2.14	0.47
1:A:14:SER:OG	1:A:157:ASP:OD1	2.29	0.47
3:D:248:ILE:HB	3:D:459:VAL:HG13	1.96	0.47
1:C:7:ALA:O	1:C:8:LEU:HB2	2.14	0.47
1:C:49:GLN:N	1:C:49:GLN:OE1	2.46	0.47
3:G:288:GLN:HE21	3:G:329:LEU:HA	1.77	0.47
1:A:71:ILE:CD1	1:A:76:ILE:HG12	2.44	0.47
1:A:71:ILE:HD12	1:A:76:ILE:HG12	1.96	0.47
1:A:256:ARG:O	1:A:256:ARG:HG2	2.14	0.47
1:A:351:THR:HG23	3:D:536:GLU:OE1	2.14	0.47
3:D:669:PHE:HB3	3:D:671:ARG:NH1	2.29	0.47
3:D:704:ILE:HD13	3:D:707:LYS:NZ	2.28	0.47
1:C:120:THR:O	1:C:124:PHE:CB	2.62	0.47
1:C:333:PRO:HG2	3:J:413:LYS:O	2.15	0.47
3:J:404:VAL:O	3:J:412:THR:OG1	2.25	0.47
1:B:120:THR:O	1:B:124:PHE:CB	2.63	0.47
1:B:333:PRO:HG2	3:G:413:LYS:O	2.15	0.47
3:G:184:LYS:O	3:G:186:VAL:N	2.47	0.47
3:G:230:PHE:HE1	3:G:285:ILE:HG12	1.80	0.47
3:G:469:ASP:HA	3:G:572:LYS:HE3	1.94	0.47
1:A:120:THR:O	1:A:124:PHE:CB	2.63	0.47
1:A:361:GLU:OE2	1:A:373:LYS:NZ	2.47	0.47
3:D:358:HIS:HE1	3:D:380:GLU:O	1.98	0.47
3:D:711:ASN:HD22	3:D:767:ALA:HB2	1.79	0.47
3:J:248:ILE:HB	3:J:459:VAL:HG13	1.96	0.47
3:J:704:ILE:HD13	3:J:707:LYS:NZ	2.28	0.47
3:J:722:TYR:OH	3:J:770:LEU:HA	2.14	0.47
1:B:71:ILE:HD12	1:B:76:ILE:HG12	1.96	0.47
1:B:227:MET:HA	1:B:255:PHE:HZ	1.78	0.47
3:G:669:PHE:HB3	3:G:671:ARG:NH1	2.29	0.47
3:G:704:ILE:HD13	3:G:707:LYS:NZ	2.28	0.47
1:A:49:GLN:N	1:A:49:GLN:OE1	2.46	0.47
3:D:128:TYR:H	3:D:681:PRO:HB3	1.80	0.47
3:D:184:LYS:HG2	3:D:187:ASN:ND2	2.29	0.47
3:D:610:LYS:N	3:D:610:LYS:HD2	2.29	0.47
1:C:79:TRP:CH2	1:C:119:MET:HB2	2.50	0.47
1:C:96:VAL:HG21	1:C:101:HIS:NE2	2.30	0.47
1:C:154:ASP:OD1	1:C:155:SER:N	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:GLU:OE2	1:C:373:LYS:NZ	2.47	0.47
3:J:128:TYR:H	3:J:681:PRO:HB3	1.80	0.47
3:J:610:LYS:HD2	3:J:610:LYS:N	2.29	0.47
3:G:548:PHE:HE1	3:G:552:LEU:HD11	1.79	0.47
3:G:722:TYR:OH	3:G:773:LEU:HD12	2.14	0.47
1:C:288:ASP:OD1	1:C:289:ILE:HG12	2.14	0.47
1:B:71:ILE:CD1	1:B:76:ILE:HG12	2.44	0.47
1:B:96:VAL:HG21	1:B:101:HIS:NE2	2.30	0.47
1:B:361:GLU:OE2	1:B:373:LYS:NZ	2.47	0.47
2:O:176:LEU:HD22	3:J:369:ARG:HH21	1.80	0.47
3:D:570:LYS:HE2	3:D:570:LYS:HA	1.96	0.47
1:C:209:VAL:HA	1:C:212:ILE:HG22	1.95	0.47
3:J:128:TYR:CD2	3:J:681:PRO:HG3	2.43	0.47
1:B:79:TRP:CH2	1:B:119:MET:HB2	2.50	0.47
1:B:154:ASP:OD1	1:B:155:SER:N	2.47	0.47
1:B:205:GLU:OE1	1:A:287:ILE:HD12	2.07	0.47
1:B:209:VAL:HA	1:B:212:ILE:HG22	1.95	0.47
1:B:351:THR:HG23	3:G:536:GLU:OE1	2.14	0.47
3:G:184:LYS:HG2	3:G:187:ASN:ND2	2.29	0.47
3:G:709:PHE:O	3:G:764:PHE:HB3	2.15	0.47
2:P:79:THR:HG21	1:A:238:LYS:NZ	2.30	0.47
3:D:184:LYS:O	3:D:186:VAL:N	2.47	0.47
3:D:546:MET:O	3:D:549:LYS:HG2	2.14	0.47
3:D:548:PHE:HE1	3:D:552:LEU:HD11	1.79	0.47
3:J:275:PHE:HA	3:J:315:GLN:HE22	1.80	0.47
3:J:546:MET:O	3:J:549:LYS:HG2	2.14	0.47
3:J:669:PHE:HB3	3:J:671:ARG:NH1	2.29	0.47
3:J:709:PHE:O	3:J:764:PHE:HB3	2.15	0.47
3:G:275:PHE:HA	3:G:315:GLN:HE22	1.80	0.47
3:G:281:ARG:NH1	3:G:320:VAL:HG11	2.28	0.47
3:D:230:PHE:HE1	3:D:285:ILE:HG12	1.79	0.47
3:D:248:ILE:HG23	3:D:263:ILE:HG22	1.96	0.47
1:C:71:ILE:CD1	1:C:76:ILE:HG12	2.44	0.47
3:J:184:LYS:HG2	3:J:187:ASN:ND2	2.29	0.47
3:J:381:ALA:O	3:J:384:SER:OG	2.28	0.47
3:J:711:ASN:HD22	3:J:767:ALA:HB2	1.79	0.47
3:G:546:MET:O	3:G:549:LYS:HG2	2.14	0.47
1:A:288:ASP:OD1	1:A:289:ILE:HG12	2.15	0.47
3:J:230:PHE:HE1	3:J:285:ILE:HG12	1.80	0.47
3:J:249:ARG:HG2	3:J:262:ASP:O	2.15	0.47
3:J:722:TYR:OH	3:J:773:LEU:HD12	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:GLY:HA3	1:A:322:PRO:HG2	1.93	0.47
3:G:176:ILE:CG2	3:G:184:LYS:HE3	2.45	0.47
3:G:358:HIS:HE1	3:G:380:GLU:O	1.98	0.47
1:A:96:VAL:HG21	1:A:101:HIS:NE2	2.30	0.47
3:D:709:PHE:O	3:D:764:PHE:HB3	2.15	0.47
1:B:322:PRO:HG3	1:C:245:GLY:HA3	1.97	0.46
3:G:517:LEU:O	3:G:521:ILE:HG12	2.15	0.46
1:A:209:VAL:HA	1:A:212:ILE:HG22	1.96	0.46
1:A:333:PRO:HG2	3:D:413:LYS:O	2.15	0.46
3:D:275:PHE:HA	3:D:315:GLN:HE22	1.80	0.46
3:D:282:ASP:HB2	3:D:287:TYR:OH	2.15	0.46
3:J:477:CYS:SG	3:J:651:HIS:CD2	3.08	0.46
1:B:288:ASP:OD1	1:B:289:ILE:HG12	2.15	0.46
3:G:570:LYS:HE2	3:G:570:LYS:HA	1.96	0.46
1:A:136:ILE:HG13	1:A:139:VAL:HG22	1.98	0.46
1:A:164:PRO:HG2	1:A:174:ALA:HB3	1.97	0.46
1:A:200:PHE:HD1	1:A:205:GLU:HB3	1.79	0.46
3:D:176:ILE:CG2	3:D:184:LYS:HE3	2.45	0.46
3:D:273:VAL:HB	3:D:429:LYS:HG2	1.97	0.46
1:C:351:THR:HG23	3:J:536:GLU:OE1	2.15	0.46
1:C:362:TYR:CE1	1:C:367:PRO:HA	2.50	0.46
3:J:176:ILE:CG2	3:J:184:LYS:HE3	2.45	0.46
3:J:451:GLN:OE1	3:J:451:GLN:N	2.49	0.46
3:G:451:GLN:OE1	3:G:451:GLN:N	2.49	0.46
3:G:544:THR:OG1	3:G:547:THR:OG1	2.29	0.46
3:D:423:ALA:HB2	3:D:600:PRO:HG2	1.97	0.46
3:J:184:LYS:O	3:J:186:VAL:N	2.47	0.46
1:B:136:ILE:HG13	1:B:139:VAL:HG22	1.98	0.46
1:B:164:PRO:HG2	1:B:174:ALA:HB3	1.97	0.46
1:B:332:PRO:O	1:B:335:ARG:HG3	2.16	0.46
3:G:273:VAL:HB	3:G:429:LYS:HG2	1.97	0.46
1:A:332:PRO:O	1:A:335:ARG:HG3	2.16	0.46
3:J:570:LYS:HA	3:J:570:LYS:HE2	1.96	0.46
1:B:177:ARG:HG2	1:B:178:LEU:N	2.31	0.46
1:B:362:TYR:CE1	1:B:367:PRO:HA	2.50	0.46
3:G:248:ILE:HG23	3:G:263:ILE:HG22	1.96	0.46
3:G:282:ASP:HB2	3:G:287:TYR:OH	2.15	0.46
1:A:154:ASP:OD1	1:A:155:SER:N	2.47	0.46
1:A:177:ARG:HG2	1:A:178:LEU:N	2.31	0.46
1:B:287:ILE:HD11	1:C:205:GLU:CD	2.24	0.46
3:G:249:ARG:HG2	3:G:262:ASP:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:TYR:CD2	1:A:289:ILE:HG23	2.51	0.46
1:A:362:TYR:CE1	1:A:367:PRO:HA	2.51	0.46
3:D:100:ALA:HA	3:D:103:TYR:HE1	1.79	0.46
1:C:136:ILE:HG13	1:C:139:VAL:HG22	1.98	0.46
1:C:191:LYS:O	1:C:194:THR:HG22	2.16	0.46
1:C:200:PHE:HD1	1:C:205:GLU:HB3	1.79	0.46
3:J:248:ILE:HG23	3:J:263:ILE:HG22	1.96	0.46
3:J:335:ALA:HA	3:J:338:VAL:HG22	1.98	0.46
3:J:704:ILE:HD13	3:J:707:LYS:HZ3	1.81	0.46
3:G:153:HIS:HE1	3:G:155:PHE:HB2	1.77	0.46
3:G:335:ALA:HA	3:G:338:VAL:HG22	1.98	0.46
2:P:91:ARG:NE	1:A:311:ASP:HB2	2.29	0.46
3:J:385:ALA:HB1	3:J:390:LEU:O	2.16	0.46
3:J:423:ALA:HB2	3:J:600:PRO:HG2	1.97	0.46
3:G:128:TYR:H	3:G:681:PRO:HB3	1.80	0.46
3:G:232:ASN:O	3:G:284:HIS:HD2	1.99	0.46
3:G:262:ASP:OD1	3:G:444:ASN:ND2	2.49	0.46
1:A:107:GLU:OE1	1:A:111:ASN:ND2	2.49	0.46
3:D:288:GLN:HG3	3:D:329:LEU:HB3	1.98	0.46
1:C:164:PRO:HG2	1:C:174:ALA:HB3	1.97	0.46
1:C:166:TYR:CD2	1:C:289:ILE:HG23	2.51	0.46
1:C:332:PRO:O	1:C:335:ARG:HG3	2.16	0.46
3:J:282:ASP:HB2	3:J:287:TYR:OH	2.15	0.46
3:J:358:HIS:HE1	3:J:380:GLU:O	1.98	0.46
1:B:107:GLU:OE1	1:B:111:ASN:ND2	2.49	0.46
1:B:166:TYR:CD2	1:B:289:ILE:HG23	2.51	0.46
1:B:191:LYS:O	1:B:194:THR:HG22	2.16	0.46
3:G:423:ALA:HB2	3:G:600:PRO:HG2	1.97	0.46
3:G:477:CYS:SG	3:G:651:HIS:CD2	3.08	0.46
1:A:79:TRP:CH2	1:A:119:MET:HB2	2.50	0.46
3:D:335:ALA:HA	3:D:338:VAL:HG22	1.98	0.46
1:C:177:ARG:HG2	1:C:178:LEU:N	2.31	0.46
3:J:273:VAL:HB	3:J:429:LYS:HG2	1.97	0.46
3:D:38:PHE:O	3:D:76:VAL:HG13	2.16	0.46
3:D:81:PRO:HD2	3:D:84:PHE:HB2	1.98	0.46
3:D:385:ALA:HB1	3:D:390:LEU:O	2.16	0.46
3:D:451:GLN:OE1	3:D:451:GLN:N	2.49	0.46
3:D:517:LEU:O	3:D:521:ILE:HG12	2.15	0.46
1:C:107:GLU:OE1	1:C:111:ASN:ND2	2.49	0.46
3:J:232:ASN:O	3:J:284:HIS:HD2	1.99	0.46
3:J:288:GLN:HG3	3:J:329:LEU:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:700:GLU:O	3:J:704:ILE:HG12	2.16	0.46
3:G:81:PRO:HD2	3:G:84:PHE:HB2	1.98	0.45
3:G:288:GLN:HG3	3:G:329:LEU:HB3	1.98	0.45
3:D:700:GLU:O	3:D:704:ILE:HG12	2.16	0.45
1:C:71:ILE:HD12	1:C:76:ILE:HG12	1.96	0.45
3:J:517:LEU:O	3:J:521:ILE:HG12	2.15	0.45
3:J:549:LYS:HB3	3:J:590:ILE:HD11	1.97	0.45
3:J:262:ASP:OD1	3:J:444:ASN:ND2	2.49	0.45
3:G:549:LYS:HB3	3:G:590:ILE:HD11	1.97	0.45
1:A:166:TYR:O	1:A:169:TYR:N	2.48	0.45
3:D:90:MET:HG2	3:D:117:TYR:O	2.17	0.45
3:D:249:ARG:HG2	3:D:262:ASP:O	2.15	0.45
3:D:477:CYS:SG	3:D:651:HIS:CD2	3.08	0.45
3:J:81:PRO:HD2	3:J:84:PHE:HB2	1.98	0.45
3:J:90:MET:HG2	3:J:117:TYR:O	2.17	0.45
3:J:402:PRO:HG3	3:J:415:GLN:HE21	1.82	0.45
3:G:38:PHE:O	3:G:76:VAL:HG13	2.16	0.45
3:D:262:ASP:OD1	3:D:444:ASN:ND2	2.49	0.45
1:B:335:ARG:C	1:B:337:TYR:H	2.20	0.45
3:G:83:LYS:HD3	3:G:721:ARG:HG2	1.99	0.45
3:D:402:PRO:HG3	3:D:415:GLN:HE21	1.82	0.45
3:D:549:LYS:HB3	3:D:590:ILE:HD11	1.97	0.45
1:A:335:ARG:C	1:A:337:TYR:H	2.20	0.45
3:D:83:LYS:HD3	3:D:721:ARG:HG2	1.99	0.45
3:D:281:ARG:NH1	3:D:320:VAL:HG11	2.28	0.45
1:A:191:LYS:O	1:A:194:THR:HG22	2.16	0.45
1:C:256:ARG:HH11	1:C:256:ARG:HG3	1.81	0.45
1:B:18:LYS:HD2	1:B:340:TRP:HB2	1.99	0.45
3:G:385:ALA:HB1	3:G:390:LEU:O	2.16	0.45
3:G:700:GLU:O	3:G:704:ILE:HG12	2.16	0.45
1:A:287:ILE:O	1:A:287:ILE:HG22	2.17	0.45
3:D:232:ASN:O	3:D:284:HIS:HD2	1.99	0.45
3:D:301:LEU:HG	3:D:303:ILE:HG12	1.99	0.45
3:D:402:PRO:HA	3:D:604:THR:HG21	1.99	0.45
1:C:7:ALA:HA	1:C:102:PRO:HD2	1.99	0.45
3:J:567:ARG:HD2	3:J:567:ARG:HA	1.74	0.45
1:B:7:ALA:HA	1:B:102:PRO:HD2	1.99	0.45
1:B:244:ASP:OD1	1:A:287:ILE:C	2.54	0.45
3:J:38:PHE:O	3:J:76:VAL:HG13	2.16	0.45
1:B:62:ARG:CG	1:A:288:ASP:OD2	2.27	0.45
3:G:435:MET:HG3	3:G:615:LYS:NZ	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:155:PHE:HE1	3:J:191:VAL:HG22	1.82	0.45
3:J:555:ASN:HB3	3:J:556:HIS:CE1	2.52	0.45
1:B:46:GLY:O	3:D:540:PHE:CZ	2.70	0.44
1:B:287:ILE:CG2	1:C:244:ASP:HB2	2.47	0.44
3:G:155:PHE:HE1	3:G:191:VAL:HG22	1.82	0.44
3:G:251:HIS:HB3	3:G:453:ARG:HB2	1.99	0.44
3:D:555:ASN:HB3	3:D:556:HIS:CE1	2.52	0.44
3:D:659:MET:O	3:D:663:ARG:N	2.45	0.44
3:J:153:HIS:O	3:J:156:SER:OG	2.19	0.44
1:B:351:THR:H	3:G:536:GLU:CD	2.21	0.44
3:G:402:PRO:HA	3:G:604:THR:HG21	1.99	0.44
2:P:171:ILE:HD11	1:C:311:ASP:OD2	2.16	0.44
1:A:7:ALA:HA	1:A:102:PRO:HD2	1.99	0.44
1:C:107:GLU:HG3	1:C:108:ALA:O	2.18	0.44
3:J:402:PRO:HA	3:J:604:THR:HG21	1.99	0.44
1:B:99:GLU:HB2	1:B:100:GLU:OE1	2.17	0.44
3:G:248:ILE:N	3:G:459:VAL:O	2.41	0.44
3:G:555:ASN:HB3	3:G:556:HIS:CE1	2.52	0.44
1:A:351:THR:H	3:D:536:GLU:CD	2.21	0.44
3:D:77:LEU:HD23	3:D:77:LEU:HA	1.83	0.44
3:D:155:PHE:HE1	3:D:191:VAL:HG22	1.82	0.44
3:D:251:HIS:HB3	3:D:453:ARG:HB2	1.99	0.44
3:D:704:ILE:HD13	3:D:707:LYS:HZ3	1.81	0.44
1:C:99:GLU:HB2	1:C:100:GLU:OE1	2.17	0.44
1:C:189:LEU:HD12	1:C:257:CYS:SG	2.58	0.44
3:J:251:HIS:HB3	3:J:453:ARG:HB2	1.99	0.44
1:B:46:GLY:HA3	3:D:540:PHE:CZ	2.48	0.44
1:B:107:GLU:HG3	1:B:108:ALA:O	2.17	0.44
1:B:287:ILE:HG22	1:B:287:ILE:O	2.17	0.44
3:G:301:LEU:HG	3:G:303:ILE:HG12	1.99	0.44
3:G:567:ARG:HD2	3:G:567:ARG:HA	1.74	0.44
1:A:99:GLU:HB2	1:A:100:GLU:OE1	2.17	0.44
1:A:107:GLU:HG3	1:A:108:ALA:O	2.17	0.44
3:J:100:ALA:HA	3:J:103:TYR:HE1	1.79	0.44
3:J:217:GLU:HG2	3:J:218:ASP:H	1.82	0.44
3:J:301:LEU:HG	3:J:303:ILE:HG12	1.99	0.44
3:J:676:ASN:HB3	3:J:685:ASP:HB2	2.00	0.44
3:D:269:GLU:HG2	3:D:269:GLU:O	2.17	0.44
3:D:435:MET:HG3	3:D:615:LYS:NZ	2.32	0.44
1:C:351:THR:H	3:J:536:GLU:CD	2.21	0.44
1:B:189:LEU:HD12	1:B:257:CYS:SG	2.58	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:90:MET:HG2	3:G:117:TYR:O	2.17	0.44
1:A:7:ALA:HB1	1:A:102:PRO:HB2	2.00	0.44
1:A:18:LYS:HD2	1:A:340:TRP:HB2	1.99	0.44
3:D:219:GLN:HG3	3:D:447:LEU:HD12	2.00	0.44
3:D:594:LEU:HD12	3:D:595:GLN:N	2.33	0.44
3:D:698:VAL:O	3:D:702:ILE:HG12	2.18	0.44
3:J:115:TYR:CE1	3:J:154:ILE:HG22	2.53	0.44
1:B:45:VAL:O	3:D:540:PHE:CZ	2.70	0.44
3:G:269:GLU:O	3:G:269:GLU:HG2	2.17	0.44
3:J:435:MET:HG3	3:J:615:LYS:NZ	2.32	0.44
1:B:10:CYS:SG	1:B:86:TRP:HZ3	2.41	0.44
1:B:256:ARG:HG3	1:B:256:ARG:HH11	1.81	0.44
1:A:193:LEU:HD12	1:A:193:LEU:HA	1.86	0.44
3:J:83:LYS:HD3	3:J:721:ARG:HG2	1.99	0.44
3:J:281:ARG:HH22	3:J:284:HIS:CD2	2.36	0.44
1:B:7:ALA:HB1	1:B:102:PRO:HB2	2.00	0.44
1:B:151:ILE:HD11	1:B:293:LEU:HD22	1.99	0.44
3:G:217:GLU:HG2	3:G:218:ASP:H	1.82	0.44
3:G:594:LEU:HD12	3:G:595:GLN:N	2.33	0.44
1:A:286:ASP:O	1:A:290:ARG:NE	2.51	0.44
1:C:287:ILE:O	1:C:287:ILE:HG22	2.17	0.44
3:J:219:GLN:HG3	3:J:447:LEU:HD12	2.00	0.44
3:J:540:PHE:CD2	3:J:541:PRO:HD2	2.53	0.44
3:J:617:LEU:O	3:J:621:PHE:HB2	2.18	0.44
3:G:115:TYR:CE1	3:G:154:ILE:HG22	2.53	0.43
3:G:219:GLN:HG3	3:G:447:LEU:HD12	2.00	0.43
3:G:376:ASP:OD1	3:G:377:GLY:N	2.51	0.43
3:G:402:PRO:HG3	3:G:415:GLN:HE21	1.82	0.43
3:G:540:PHE:CD2	3:G:541:PRO:HD2	2.53	0.43
1:A:189:LEU:HD12	1:A:257:CYS:SG	2.58	0.43
3:D:217:GLU:HG2	3:D:218:ASP:H	1.82	0.43
1:C:166:TYR:O	1:C:169:TYR:N	2.48	0.43
3:J:376:ASP:OD1	3:J:377:GLY:N	2.51	0.43
3:G:676:ASN:HB3	3:G:685:ASP:HB2	2.00	0.43
1:A:10:CYS:SG	1:A:86:TRP:HZ3	2.41	0.43
1:A:147:ARG:NE	1:A:330:ILE:HG21	2.33	0.43
1:A:256:ARG:HG3	1:A:256:ARG:HH11	1.81	0.43
3:D:260:SER:HB2	3:D:449:THR:HB	2.00	0.43
3:D:281:ARG:HH22	3:D:284:HIS:CD2	2.36	0.43
3:D:746:LEU:HD12	3:D:751:ILE:O	2.19	0.43
1:C:120:THR:O	1:C:124:PHE:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ARG:NE	1:B:330:ILE:HG21	2.34	0.43
3:G:128:TYR:CD2	3:G:681:PRO:HG3	2.43	0.43
3:G:617:LEU:O	3:G:621:PHE:HB2	2.18	0.43
1:A:84:LYS:HE3	1:A:84:LYS:HB2	1.82	0.43
3:D:376:ASP:OD1	3:D:377:GLY:N	2.51	0.43
3:J:223:ALA:HB1	3:J:227:LEU:HD23	2.00	0.43
3:J:230:PHE:CE1	3:J:285:ILE:HG12	2.54	0.43
3:J:260:SER:HB2	3:J:449:THR:HB	2.00	0.43
3:J:594:LEU:HD12	3:J:595:GLN:N	2.33	0.43
1:B:12:ASN:O	1:B:12:ASN:ND2	2.51	0.43
1:B:166:TYR:O	1:B:169:TYR:N	2.48	0.43
1:B:289:ILE:CD1	1:C:63:GLY:HA3	2.23	0.43
1:B:322:PRO:CG	1:C:245:GLY:HA3	2.48	0.43
1:C:18:LYS:HD2	1:C:340:TRP:HB2	1.99	0.43
1:C:159:VAL:HG21	1:C:177:ARG:CZ	2.48	0.43
3:J:269:GLU:O	3:J:269:GLU:HG2	2.17	0.43
3:J:698:VAL:O	3:J:702:ILE:HG12	2.17	0.43
3:J:709:PHE:N	3:J:710:PRO:HD2	2.34	0.43
1:B:33:SER:O	1:B:33:SER:OG	2.34	0.43
3:G:260:SER:HB2	3:G:449:THR:HB	2.01	0.43
3:D:676:ASN:HB3	3:D:685:ASP:HB2	2.00	0.43
1:C:147:ARG:NE	1:C:330:ILE:HG21	2.33	0.43
1:C:286:ASP:O	1:C:290:ARG:NE	2.51	0.43
3:J:277:LEU:HB3	3:J:280:GLU:HG2	2.01	0.43
1:B:120:THR:O	1:B:124:PHE:HB2	2.18	0.43
1:B:159:VAL:HG21	1:B:177:ARG:CZ	2.48	0.43
1:B:286:ASP:O	1:B:290:ARG:NE	2.51	0.43
3:G:267:LEU:HD21	3:G:655:LEU:HB2	2.00	0.43
3:G:746:LEU:HD12	3:G:751:ILE:O	2.19	0.43
2:P:90:ARG:NE	1:A:221:LEU:CD2	2.79	0.43
3:D:230:PHE:CE1	3:D:285:ILE:HG12	2.53	0.43
1:C:7:ALA:HB1	1:C:102:PRO:HB2	2.00	0.43
1:C:10:CYS:SG	1:C:86:TRP:HZ3	2.41	0.43
1:C:335:ARG:C	1:C:337:TYR:H	2.20	0.43
3:J:192:ILE:CD1	3:J:250:ILE:HD13	2.48	0.43
3:G:277:LEU:HB3	3:G:280:GLU:HG2	2.01	0.43
1:A:159:VAL:HG21	1:A:177:ARG:CZ	2.48	0.43
1:A:346:LEU:HG	1:A:352:PHE:CE2	2.54	0.43
3:D:115:TYR:CE1	3:D:154:ILE:HG22	2.53	0.43
3:D:267:LEU:HD21	3:D:655:LEU:HB2	2.00	0.43
3:J:269:GLU:OE2	3:J:269:GLU:N	2.37	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:223:ALA:HB1	3:G:227:LEU:HD23	2.00	0.43
3:G:709:PHE:N	3:G:710:PRO:HD2	2.34	0.43
3:D:277:LEU:HB3	3:D:280:GLU:HG2	2.01	0.43
3:D:540:PHE:CD2	3:D:541:PRO:HD2	2.53	0.43
3:D:617:LEU:O	3:D:621:PHE:HB2	2.18	0.43
1:C:151:ILE:HD11	1:C:293:LEU:HD22	1.99	0.43
1:C:346:LEU:HG	1:C:352:PHE:CE2	2.54	0.43
3:J:428:ALA:O	3:J:431:VAL:HG12	2.19	0.43
1:B:346:LEU:HG	1:B:352:PHE:CE2	2.54	0.43
3:G:230:PHE:CE1	3:G:285:ILE:HG12	2.54	0.43
1:A:12:ASN:O	1:A:12:ASN:ND2	2.51	0.43
3:D:192:ILE:CD1	3:D:250:ILE:HD13	2.48	0.43
3:D:223:ALA:HB1	3:D:227:LEU:HD23	2.00	0.43
3:D:709:PHE:N	3:D:710:PRO:HD2	2.34	0.43
1:C:36:GLY:HA2	1:C:66:THR:O	2.19	0.43
3:G:525:GLU:CD	3:G:652:ARG:HE	2.21	0.43
3:G:698:VAL:O	3:G:702:ILE:HG12	2.18	0.43
3:D:173:SER:OG	3:D:667:PRO:HA	2.19	0.43
3:J:525:GLU:CD	3:J:652:ARG:HE	2.21	0.43
1:B:36:GLY:HA2	1:B:66:THR:O	2.19	0.42
3:G:428:ALA:O	3:G:431:VAL:HG12	2.19	0.42
1:A:151:ILE:HD11	1:A:293:LEU:HD22	1.99	0.42
3:D:567:ARG:HD2	3:D:567:ARG:HA	1.74	0.42
3:G:443:ILE:HD13	3:G:443:ILE:HA	1.89	0.42
3:G:659:MET:O	3:G:663:ARG:N	2.45	0.42
1:A:198:TYR:CE1	1:A:248:ILE:HG13	2.55	0.42
3:D:249:ARG:HH12	3:D:264:GLU:N	2.18	0.42
3:D:269:GLU:OE2	3:D:269:GLU:N	2.37	0.42
3:J:141:ALA:O	3:J:143:ARG:N	2.52	0.42
3:J:267:LEU:HD21	3:J:655:LEU:HB2	2.00	0.42
1:B:151:ILE:HG23	1:B:163:VAL:O	2.20	0.42
3:G:281:ARG:HH22	3:G:284:HIS:CD2	2.36	0.42
3:G:372:GLN:OE1	3:G:401:HIS:NE2	2.51	0.42
1:A:120:THR:O	1:A:124:PHE:HB2	2.18	0.42
3:D:141:ALA:O	3:D:143:ARG:N	2.52	0.42
3:D:522:ASP:HA	3:D:526:LYS:HB2	2.01	0.42
1:C:12:ASN:O	1:C:12:ASN:ND2	2.51	0.42
3:J:659:MET:O	3:J:663:ARG:N	2.45	0.42
1:A:142:LEU:HD23	1:A:142:LEU:HA	1.87	0.42
3:D:246:LYS:O	3:D:248:ILE:HG12	2.19	0.42
3:D:428:ALA:O	3:D:431:VAL:HG12	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:173:SER:OG	3:J:667:PRO:HA	2.19	0.42
3:J:372:GLN:OE1	3:J:401:HIS:NE2	2.52	0.42
3:J:477:CYS:HG	3:J:651:HIS:CE1	2.37	0.42
1:B:108:ALA:HB3	1:B:111:ASN:HD21	1.85	0.42
1:B:198:TYR:CE1	1:B:248:ILE:HG13	2.55	0.42
3:G:37:VAL:HG21	3:G:51:ILE:CG2	2.46	0.42
3:G:272:ARG:HB3	3:G:283:TYR:OH	2.19	0.42
1:A:36:GLY:HA2	1:A:66:THR:O	2.19	0.42
3:D:272:ARG:HB3	3:D:283:TYR:OH	2.20	0.42
3:D:372:GLN:OE1	3:D:401:HIS:NE2	2.51	0.42
3:D:525:GLU:CD	3:D:652:ARG:HE	2.21	0.42
3:J:249:ARG:HH12	3:J:264:GLU:N	2.17	0.42
3:J:522:ASP:HA	3:J:526:LYS:HB2	2.01	0.42
3:J:746:LEU:HD12	3:J:751:ILE:O	2.19	0.42
1:B:193:LEU:HD12	1:B:193:LEU:HA	1.86	0.42
3:G:173:SER:OG	3:G:667:PRO:HA	2.19	0.42
3:G:192:ILE:CD1	3:G:250:ILE:HD13	2.49	0.42
3:G:269:GLU:OE2	3:G:269:GLU:N	2.37	0.42
1:C:198:TYR:CE1	1:C:248:ILE:HG13	2.55	0.42
3:J:272:ARG:HB3	3:J:283:TYR:OH	2.20	0.42
3:G:246:LYS:O	3:G:248:ILE:HG12	2.19	0.42
2:P:79:THR:HG21	1:A:238:LYS:HZ2	1.85	0.42
3:D:59:VAL:HG21	3:D:76:VAL:HG21	2.01	0.42
3:D:725:LEU:HB3	3:D:748:SER:OG	2.19	0.42
1:C:108:ALA:HB3	1:C:111:ASN:HD21	1.85	0.42
3:J:59:VAL:O	3:J:70:THR:HA	2.20	0.42
3:J:262:ASP:OD1	3:J:263:ILE:N	2.53	0.42
3:J:761:THR:HG22	3:J:761:THR:O	2.20	0.42
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.75	0.42
1:B:327:ILE:HG22	1:B:327:ILE:O	2.20	0.42
3:G:249:ARG:HH12	3:G:264:GLU:N	2.17	0.42
3:D:224:ASN:N	3:D:225:PRO:HD2	2.35	0.42
1:C:213:LYS:HZ2	1:C:213:LYS:HG2	1.59	0.42
3:J:569:ILE:CD1	3:J:572:LYS:HG3	2.40	0.42
3:G:59:VAL:HG21	3:G:76:VAL:HG21	2.01	0.42
3:G:141:ALA:O	3:G:143:ARG:N	2.52	0.42
3:G:725:LEU:HB3	3:G:748:SER:OG	2.19	0.42
1:A:76:ILE:HG21	1:A:82:MET:HE2	2.02	0.42
1:A:104:LEU:O	1:A:105:LEU:HD23	2.20	0.42
1:A:200:PHE:CD1	1:A:205:GLU:HB3	2.55	0.42
1:C:76:ILE:HG21	1:C:82:MET:HE2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:320:VAL:HG13	3:J:320:VAL:O	2.20	0.42
1:B:104:LEU:O	1:B:105:LEU:HD23	2.20	0.42
1:B:210:ARG:HG3	1:B:211:ASP:N	2.35	0.42
3:G:761:THR:HG22	3:G:761:THR:O	2.20	0.42
1:A:151:ILE:HG23	1:A:163:VAL:O	2.19	0.42
1:A:206:ARG:O	1:A:209:VAL:HG12	2.20	0.42
3:D:335:ALA:O	3:D:339:LEU:HG	2.20	0.42
1:C:327:ILE:O	1:C:327:ILE:HG22	2.20	0.42
1:B:298:VAL:HG22	1:B:299:MET:O	2.20	0.41
3:G:320:VAL:HG13	3:G:320:VAL:O	2.20	0.41
3:G:662:LEU:HA	3:G:665:THR:OG1	2.20	0.41
2:P:167:ARG:HH21	1:C:308:GLY:CA	2.32	0.41
1:A:327:ILE:HG22	1:A:327:ILE:O	2.20	0.41
3:D:663:ARG:HD3	3:D:663:ARG:HA	1.85	0.41
3:J:662:LEU:HA	3:J:665:THR:OG1	2.20	0.41
1:B:200:PHE:CD1	1:B:205:GLU:HB3	2.55	0.41
3:G:179:GLU:CD	3:G:463:ALA:HA	2.41	0.41
3:G:262:ASP:OD1	3:G:263:ILE:N	2.53	0.41
1:A:108:ALA:HB3	1:A:111:ASN:HD21	1.85	0.41
3:D:40:PRO:HA	3:D:45:GLU:HA	2.03	0.41
3:D:320:VAL:O	3:D:320:VAL:HG13	2.20	0.41
3:D:477:CYS:O	3:D:481:THR:HG23	2.21	0.41
1:C:298:VAL:HG22	1:C:299:MET:O	2.20	0.41
3:J:246:LYS:HA	3:J:265:THR:HA	2.02	0.41
3:J:335:ALA:O	3:J:339:LEU:HG	2.20	0.41
1:B:213:LYS:HZ2	1:B:213:LYS:HG2	1.59	0.41
3:G:477:CYS:HG	3:G:651:HIS:CE1	2.38	0.41
3:D:153:HIS:O	3:D:156:SER:OG	2.19	0.41
3:D:179:GLU:CD	3:D:463:ALA:HA	2.41	0.41
3:D:537:GLU:HG2	3:D:548:PHE:HD2	1.85	0.41
3:J:59:VAL:HG21	3:J:76:VAL:HG21	2.01	0.41
3:J:224:ASN:N	3:J:225:PRO:HD2	2.35	0.41
3:J:246:LYS:O	3:J:248:ILE:HG12	2.19	0.41
3:J:477:CYS:O	3:J:481:THR:HG23	2.20	0.41
1:B:76:ILE:HG21	1:B:82:MET:HE2	2.02	0.41
3:G:59:VAL:O	3:G:70:THR:HA	2.20	0.41
3:G:77:LEU:HD23	3:G:77:LEU:HA	1.83	0.41
3:G:224:ASN:N	3:G:225:PRO:HD2	2.35	0.41
1:A:298:VAL:HG22	1:A:299:MET:O	2.20	0.41
3:D:422:TYR:CE2	3:D:598:LYS:HD2	2.53	0.41
3:J:537:GLU:HG2	3:J:548:PHE:HD2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:725:LEU:HB3	3:J:748:SER:OG	2.20	0.41
1:B:206:ARG:O	1:B:209:VAL:HG12	2.20	0.41
3:G:40:PRO:HA	3:G:45:GLU:HA	2.03	0.41
3:G:247:PHE:HA	3:G:460:LEU:HA	2.03	0.41
1:A:108:ALA:HB3	1:A:111:ASN:ND2	2.36	0.41
1:A:133:TYR:CD2	1:A:352:PHE:HZ	2.38	0.41
3:D:43:LYS:HB3	3:D:44:GLU:OE1	2.20	0.41
3:D:153:HIS:CE1	3:D:155:PHE:CD2	3.06	0.41
3:D:184:LYS:HD3	3:D:184:LYS:C	2.41	0.41
3:D:662:LEU:HA	3:D:665:THR:OG1	2.20	0.41
1:C:200:PHE:CD1	1:C:205:GLU:HB3	2.55	0.41
3:J:40:PRO:HA	3:J:45:GLU:HA	2.02	0.41
3:J:109:TYR:OH	3:J:682:GLY:N	2.34	0.41
3:J:184:LYS:HD3	3:J:184:LYS:C	2.41	0.41
3:J:481:THR:HG22	3:J:655:LEU:HD12	2.02	0.41
3:J:544:THR:OG1	3:J:547:THR:OG1	2.29	0.41
1:B:326:LYS:HD3	1:B:328:LYS:HZ1	1.84	0.41
3:G:335:ALA:O	3:G:339:LEU:HG	2.20	0.41
3:G:422:TYR:CE2	3:G:598:LYS:HD2	2.53	0.41
3:D:481:THR:HG22	3:D:655:LEU:HD12	2.02	0.41
3:D:761:THR:O	3:D:761:THR:HG22	2.20	0.41
1:C:104:LEU:O	1:C:105:LEU:HD23	2.20	0.41
1:C:151:ILE:HG23	1:C:163:VAL:O	2.19	0.41
3:J:317:GLU:O	3:J:318:THR:HG22	2.21	0.41
1:B:133:TYR:CD2	1:B:352:PHE:HZ	2.38	0.41
1:B:326:LYS:HB3	1:B:328:LYS:HZ3	1.86	0.41
3:G:184:LYS:C	3:G:184:LYS:HD3	2.41	0.41
3:G:522:ASP:HA	3:G:526:LYS:HB2	2.01	0.41
1:A:210:ARG:HG3	1:A:211:ASP:N	2.35	0.41
3:D:262:ASP:OD1	3:D:263:ILE:N	2.53	0.41
3:D:403:ARG:CZ	3:D:411:VAL:HG22	2.51	0.41
1:C:206:ARG:O	1:C:209:VAL:HG12	2.20	0.41
3:J:179:GLU:CD	3:J:463:ALA:HA	2.41	0.41
1:B:84:LYS:HE3	1:B:84:LYS:HB2	1.82	0.41
1:B:302:GLY:O	1:B:303:THR:HG22	2.21	0.41
3:G:317:GLU:O	3:G:318:THR:HG22	2.21	0.41
3:D:246:LYS:HA	3:D:265:THR:HA	2.03	0.41
3:D:544:THR:OG1	3:D:547:THR:OG1	2.29	0.41
1:C:210:ARG:HG3	1:C:211:ASP:N	2.35	0.41
3:J:77:LEU:HD23	3:J:77:LEU:HA	1.83	0.41
3:J:247:PHE:HA	3:J:460:LEU:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:341:PHE:CE1	3:J:442:ARG:HG2	2.56	0.41
3:G:43:LYS:HB3	3:G:44:GLU:OE1	2.20	0.41
3:G:341:PHE:CE1	3:G:442:ARG:HG2	2.56	0.41
3:G:400:CYS:SG	3:G:401:HIS:ND1	2.73	0.41
2:P:175:ASP:CG	3:J:369:ARG:NH2	2.74	0.41
1:A:302:GLY:O	1:A:303:THR:HG22	2.21	0.41
3:D:59:VAL:O	3:D:70:THR:HA	2.20	0.41
3:D:115:TYR:CD1	3:D:153:HIS:HA	2.56	0.41
3:D:153:HIS:HE1	3:D:155:PHE:HB2	1.77	0.41
3:D:281:ARG:HH22	3:D:284:HIS:CG	2.39	0.41
3:D:341:PHE:CE1	3:D:442:ARG:HG2	2.56	0.41
3:D:489:PHE:HD1	3:D:669:PHE:CZ	2.39	0.41
3:D:590:ILE:HA	3:D:593:TRP:NE1	2.36	0.41
1:C:108:ALA:HB3	1:C:111:ASN:ND2	2.36	0.41
1:C:193:LEU:HD12	1:C:193:LEU:HA	1.86	0.41
3:J:715:TYR:CZ	3:J:719:ARG:NH1	2.89	0.41
3:G:281:ARG:HH22	3:G:284:HIS:CG	2.39	0.41
3:G:403:ARG:CZ	3:G:411:VAL:HG22	2.51	0.41
3:G:489:PHE:HD1	3:G:669:PHE:CZ	2.39	0.41
3:G:590:ILE:HA	3:G:593:TRP:NE1	2.36	0.41
3:D:92:MET:O	3:D:93:LEU:HG	2.21	0.41
1:C:302:GLY:O	1:C:303:THR:HG22	2.21	0.41
3:J:281:ARG:HH22	3:J:284:HIS:CG	2.39	0.41
3:J:590:ILE:HA	3:J:593:TRP:NE1	2.36	0.41
3:G:92:MET:O	3:G:93:LEU:HG	2.21	0.40
3:G:246:LYS:HA	3:G:265:THR:HA	2.03	0.40
3:G:537:GLU:HG2	3:G:548:PHE:HD2	1.85	0.40
3:D:247:PHE:HA	3:D:460:LEU:HA	2.03	0.40
3:D:522:ASP:OD2	3:D:523:LEU:N	2.54	0.40
3:D:708:GLY:C	3:D:710:PRO:HD2	2.42	0.40
1:C:223:PHE:HB2	1:C:259:GLU:OE2	2.21	0.40
3:J:422:TYR:CE2	3:J:598:LYS:HD2	2.53	0.40
3:J:582:TYR:CG	3:J:583:ALA:N	2.89	0.40
3:G:477:CYS:O	3:G:481:THR:HG23	2.20	0.40
3:G:481:THR:HG22	3:G:655:LEU:HD12	2.02	0.40
3:G:522:ASP:OD2	3:G:523:LEU:N	2.54	0.40
3:G:708:GLY:C	3:G:710:PRO:HD2	2.42	0.40
3:D:248:ILE:N	3:D:459:VAL:O	2.41	0.40
3:J:115:TYR:HB3	3:J:152:PRO:O	2.22	0.40
3:G:39:VAL:HB	3:G:49:ALA:HB2	2.03	0.40
3:G:115:TYR:CD1	3:G:153:HIS:HA	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PHE:HB2	1:A:259:GLU:OE2	2.21	0.40
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.94	0.40
1:C:133:TYR:CD2	1:C:352:PHE:HZ	2.38	0.40
3:J:325:ASP:O	3:J:329:LEU:N	2.54	0.40
3:J:412:THR:C	3:J:413:LYS:HG3	2.42	0.40
3:J:478:ILE:O	3:J:481:THR:OG1	2.33	0.40
3:J:489:PHE:HD1	3:J:669:PHE:CZ	2.39	0.40
3:G:154:ILE:HD12	3:G:154:ILE:HA	1.91	0.40
1:A:24:ASP:OD1	1:A:25:ASP:N	2.55	0.40
3:D:317:GLU:O	3:D:318:THR:HG22	2.21	0.40
3:J:39:VAL:HB	3:J:49:ALA:HB2	2.03	0.40
3:J:708:GLY:C	3:J:710:PRO:HD2	2.42	0.40
1:B:108:ALA:HB3	1:B:111:ASN:ND2	2.36	0.40
3:G:412:THR:C	3:G:413:LYS:HG3	2.42	0.40
3:G:582:TYR:CG	3:G:583:ALA:N	2.89	0.40
2:P:90:ARG:HH22	1:A:308:GLY:HA2	1.87	0.40
3:D:39:VAL:HB	3:D:49:ALA:HB2	2.03	0.40
3:D:412:THR:C	3:D:413:LYS:HG3	2.42	0.40
1:C:327:ILE:O	1:C:329:ILE:HG23	2.22	0.40
3:J:43:LYS:HB3	3:J:44:GLU:OE1	2.21	0.40
3:J:403:ARG:CZ	3:J:411:VAL:HG22	2.51	0.40
3:J:738:SER:HB2	3:J:739:ARG:HH21	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	367/377 (97%)	324 (88%)	41 (11%)	2 (0%)	29	68
1	B	367/377 (97%)	324 (88%)	41 (11%)	2 (0%)	29	68
1	C	367/377 (97%)	324 (88%)	41 (11%)	2 (0%)	29	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	164/284 (58%)	164 (100%)	0	0	100	100
2	P	164/284 (58%)	164 (100%)	0	0	100	100
3	D	699/850 (82%)	618 (88%)	80 (11%)	1 (0%)	51	85
3	G	699/850 (82%)	618 (88%)	80 (11%)	1 (0%)	51	85
3	J	699/850 (82%)	618 (88%)	80 (11%)	1 (0%)	51	85
All	All	3526/4249 (83%)	3154 (89%)	363 (10%)	9 (0%)	44	76

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	111	ASN
3	G	710	PRO
1	A	111	ASN
3	D	710	PRO
1	C	111	ASN
3	J	710	PRO
1	B	112	PRO
1	A	112	PRO
1	C	112	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/320 (98%)	310 (99%)	2 (1%)	86	92
1	B	312/320 (98%)	310 (99%)	2 (1%)	86	92
1	C	312/320 (98%)	311 (100%)	1 (0%)	92	95
2	O	141/245 (58%)	138 (98%)	3 (2%)	53	72
2	P	141/245 (58%)	141 (100%)	0	100	100
3	D	616/736 (84%)	611 (99%)	5 (1%)	81	89
3	G	616/736 (84%)	611 (99%)	5 (1%)	81	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	616/736 (84%)	611 (99%)	5 (1%)	81	89
All	All	3066/3658 (84%)	3043 (99%)	23 (1%)	82	89

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	12	ASN
1	B	143	TYR
2	O	51	LYS
2	O	101	ARG
2	O	207	LEU
3	G	424	LYS
3	G	453	ARG
3	G	479	ASN
3	G	706	ARG
3	G	739	ARG
1	A	12	ASN
1	A	143	TYR
3	D	424	LYS
3	D	453	ARG
3	D	479	ASN
3	D	706	ARG
3	D	739	ARG
1	C	12	ASN
3	J	424	LYS
3	J	453	ARG
3	J	479	ASN
3	J	706	ARG
3	J	739	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	354	GLN
3	G	126	ASN
3	G	153	HIS
3	G	187	ASN
3	G	284	HIS
3	G	288	GLN
3	G	358	HIS
3	G	368	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	372	GLN
3	G	492	HIS
3	G	661	ASN
3	G	668	HIS
1	A	354	GLN
3	D	126	ASN
3	D	153	HIS
3	D	187	ASN
3	D	251	HIS
3	D	284	HIS
3	D	288	GLN
3	D	358	HIS
3	D	368	GLN
3	D	372	GLN
3	D	492	HIS
3	D	661	ASN
3	D	668	HIS
1	C	246	GLN
1	C	354	GLN
3	J	126	ASN
3	J	153	HIS
3	J	187	ASN
3	J	251	HIS
3	J	284	HIS
3	J	288	GLN
3	J	358	HIS
3	J	372	GLN
3	J	492	HIS
3	J	661	ASN
3	J	668	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
4	ADP	A	401	5	24,29,29	0.94	1 (4%)	29,45,45	1.42	4 (13%)
4	ADP	C	401	5	24,29,29	0.94	1 (4%)	29,45,45	1.42	4 (13%)
4	ADP	B	401	5	24,29,29	0.93	1 (4%)	29,45,45	1.42	4 (13%)

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
4	ADP	A	401	5	-	7/12/32/32	0/3/3/3
4	ADP	C	401	5	-	7/12/32/32	0/3/3/3
4	ADP	B	401	5	-	7/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	ADP	C5-C4	2.17	1.46	1.40
4	A	401	ADP	C5-C4	2.15	1.46	1.40
4	B	401	ADP	C5-C4	2.14	1.46	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	ADP	PA-O3A-PB	-4.04	118.97	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	ADP	PA-O3A-PB	-4.03	118.99	132.83
4	A	401	ADP	PA-O3A-PB	-4.03	119.00	132.83
4	A	401	ADP	N3-C2-N1	-3.14	123.77	128.68
4	B	401	ADP	N3-C2-N1	-3.12	123.80	128.68
4	C	401	ADP	N3-C2-N1	-3.08	123.86	128.68
4	A	401	ADP	C4-C5-N7	-2.97	106.30	109.40
4	B	401	ADP	C4-C5-N7	-2.95	106.32	109.40
4	C	401	ADP	C4-C5-N7	-2.94	106.34	109.40
4	A	401	ADP	C3'-C2'-C1'	2.55	104.82	100.98
4	B	401	ADP	C3'-C2'-C1'	2.55	104.82	100.98
4	C	401	ADP	C3'-C2'-C1'	2.55	104.81	100.98

There are no chirality outliers.

All (21) torsion outliers are listed below:

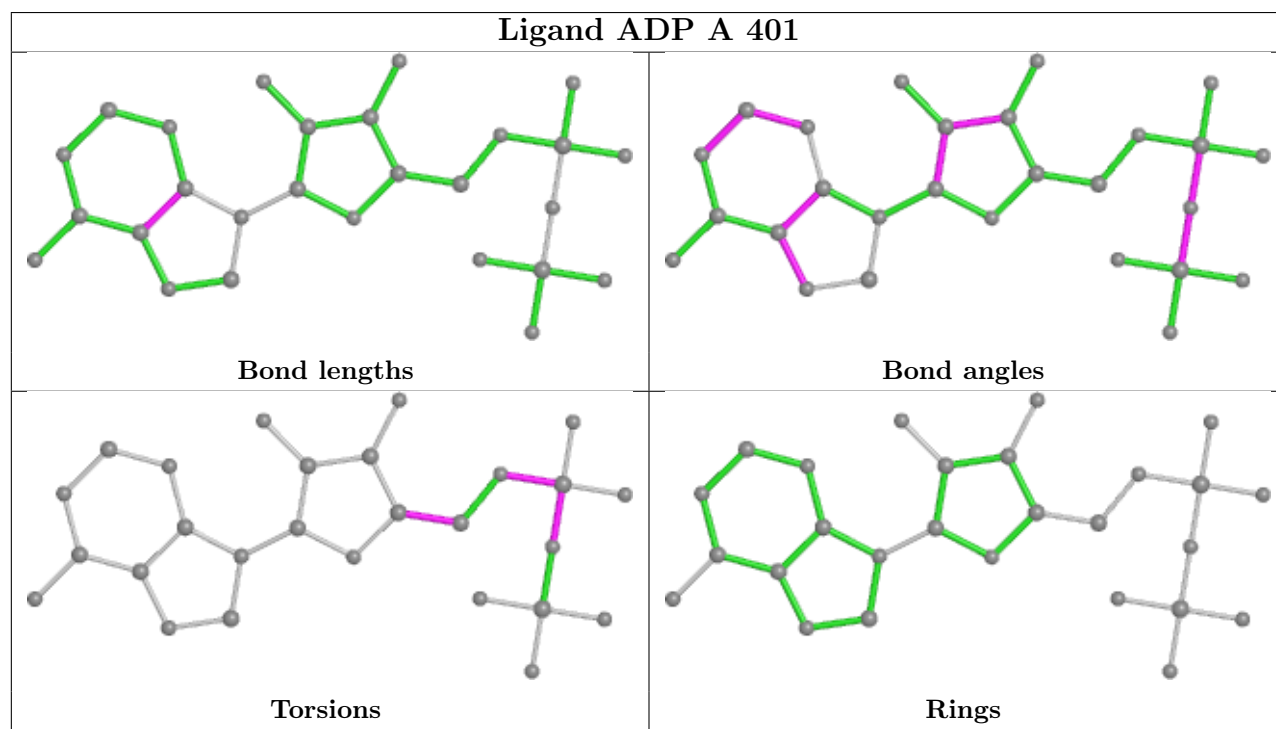
Mol	Chain	Res	Type	Atoms
4	B	401	ADP	C5'-O5'-PA-O1A
4	B	401	ADP	C3'-C4'-C5'-O5'
4	A	401	ADP	C5'-O5'-PA-O1A
4	A	401	ADP	C3'-C4'-C5'-O5'
4	C	401	ADP	C5'-O5'-PA-O1A
4	C	401	ADP	C3'-C4'-C5'-O5'
4	B	401	ADP	O4'-C4'-C5'-O5'
4	A	401	ADP	O4'-C4'-C5'-O5'
4	C	401	ADP	O4'-C4'-C5'-O5'
4	B	401	ADP	C5'-O5'-PA-O3A
4	A	401	ADP	C5'-O5'-PA-O3A
4	C	401	ADP	C5'-O5'-PA-O3A
4	B	401	ADP	C5'-O5'-PA-O2A
4	A	401	ADP	C5'-O5'-PA-O2A
4	C	401	ADP	C5'-O5'-PA-O2A
4	B	401	ADP	PB-O3A-PA-O1A
4	A	401	ADP	PB-O3A-PA-O1A
4	C	401	ADP	PB-O3A-PA-O1A
4	B	401	ADP	PB-O3A-PA-O2A
4	A	401	ADP	PB-O3A-PA-O2A
4	C	401	ADP	PB-O3A-PA-O2A

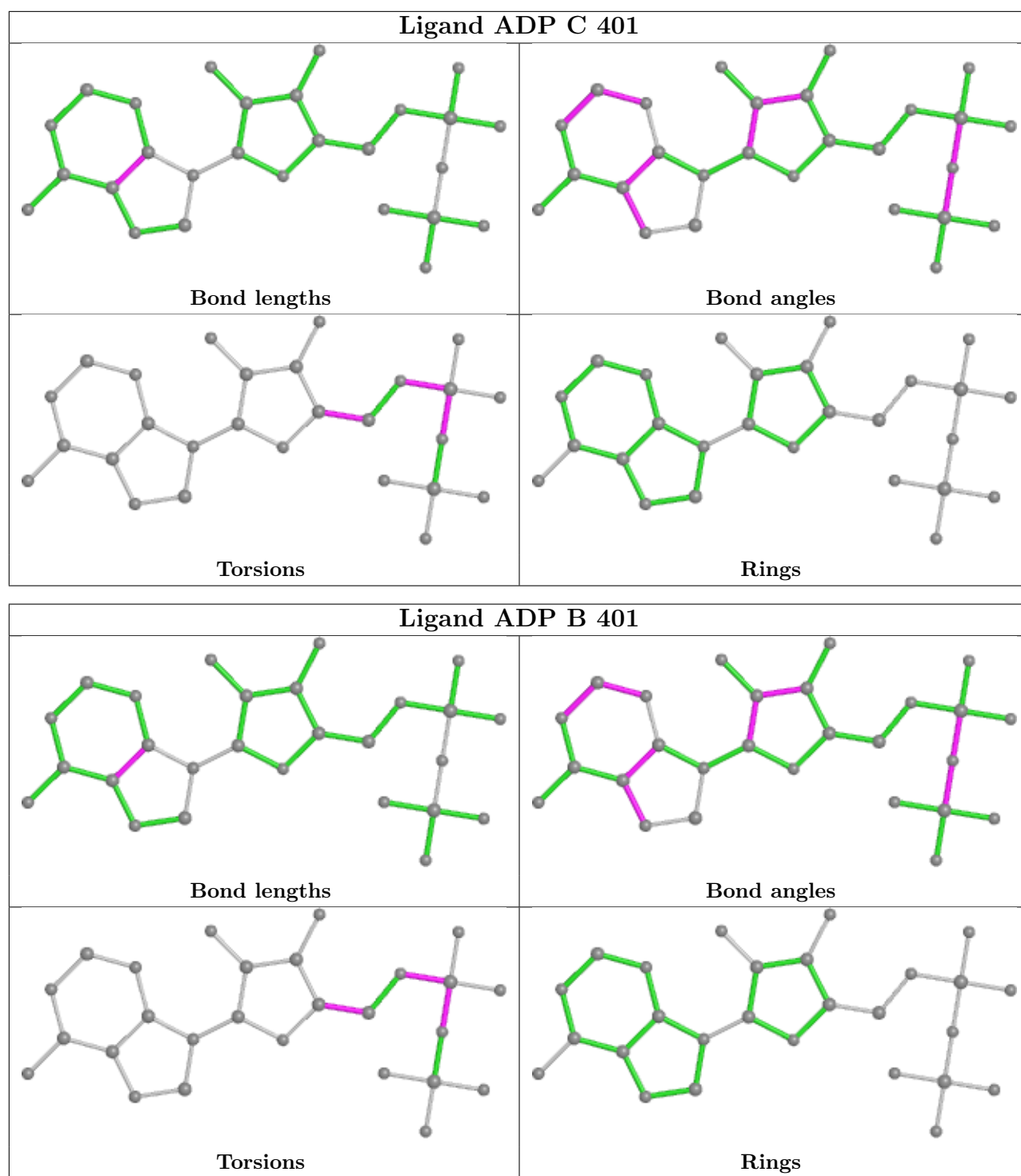
There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

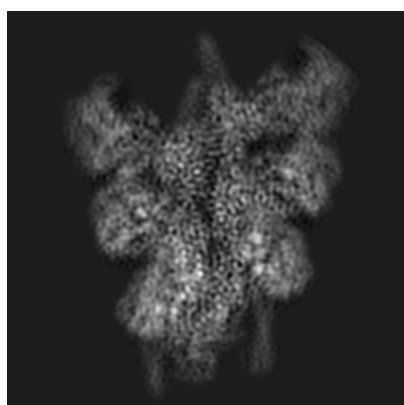
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22067. These allow visual inspection of the internal detail of the map and identification of artifacts.

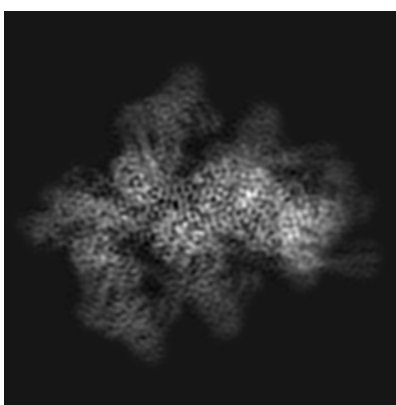
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

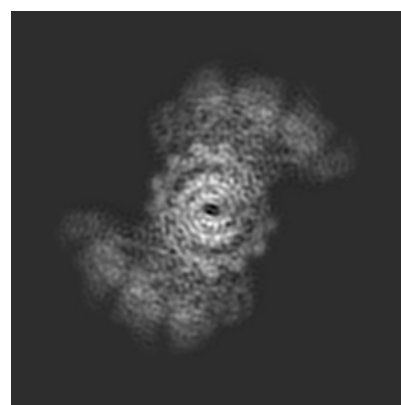
6.1.1 Primary map



X



Y



Z

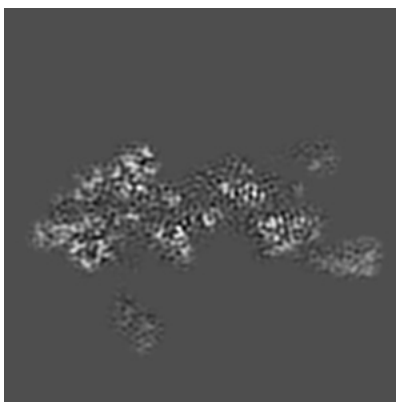
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

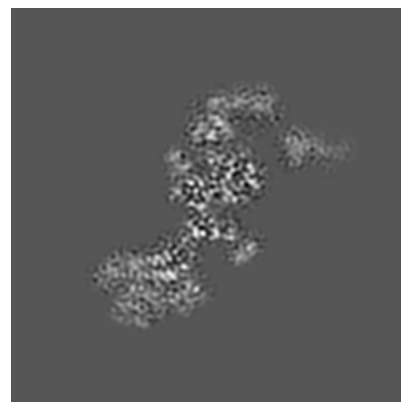
6.2.1 Primary map



X Index: 128



Y Index: 128

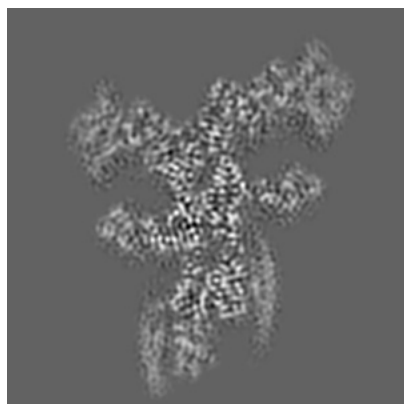


Z Index: 128

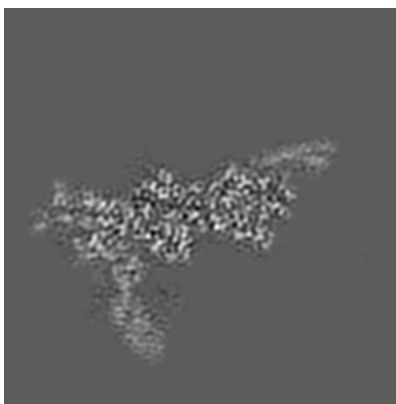
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

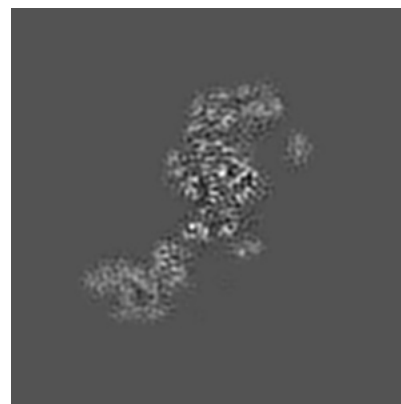
6.3.1 Primary map



X Index: 122



Y Index: 116

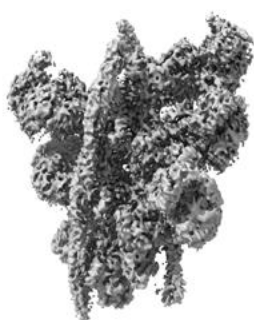


Z Index: 136

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

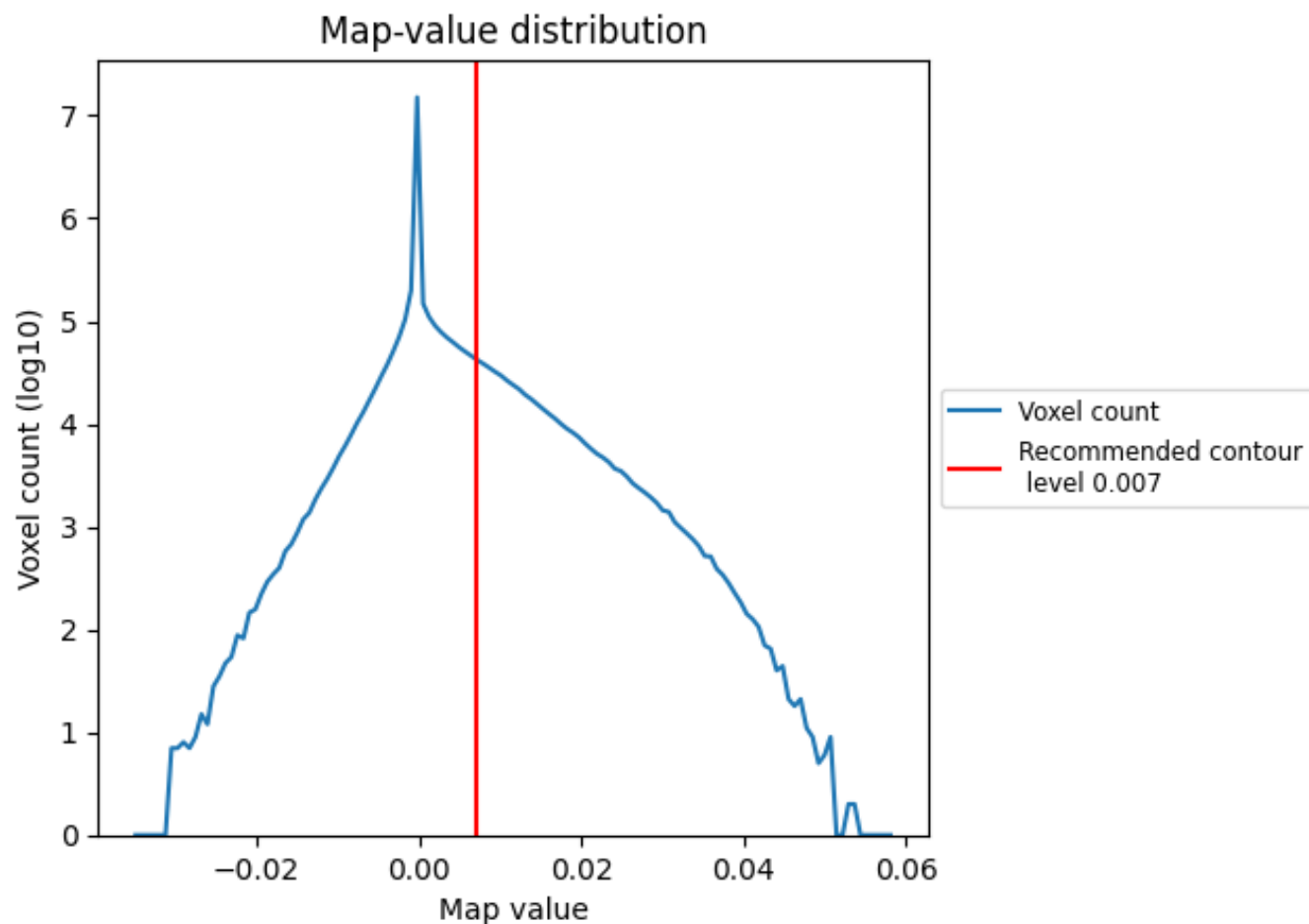
6.5 Mask visualisation

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

7 Map analysis [i](#)

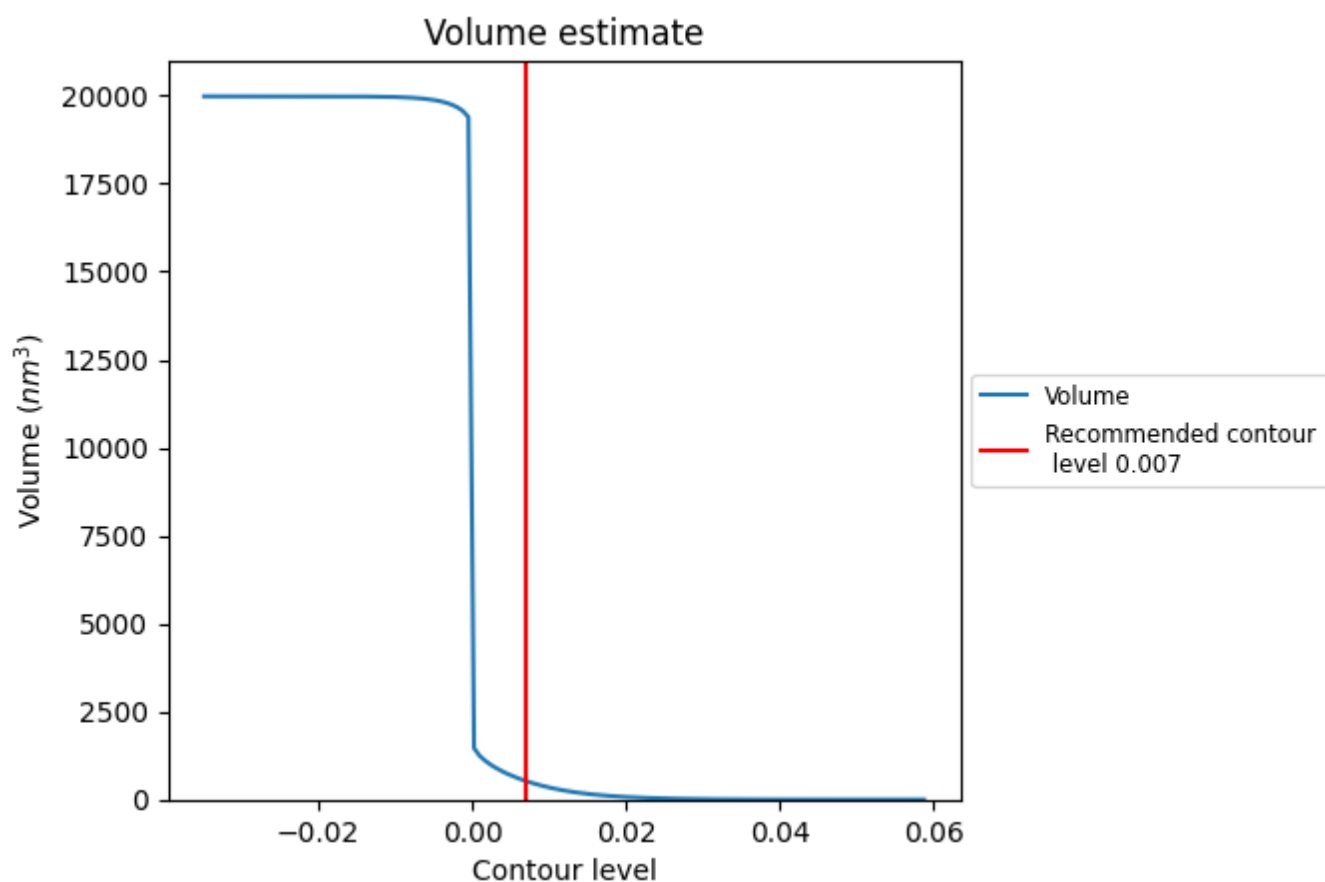
This section contains the results of statistical analysis of the map.

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.

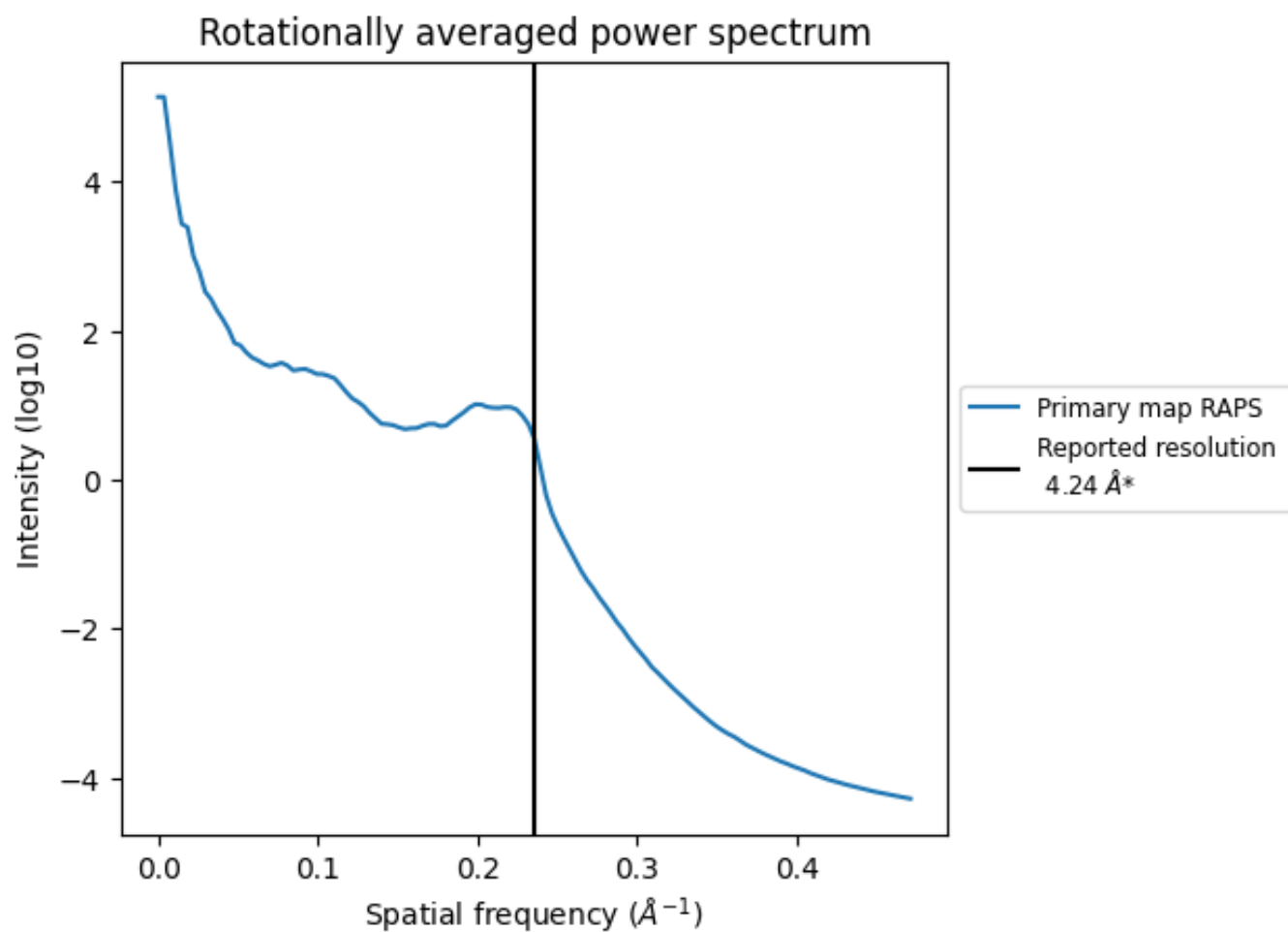
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 528 nm³; this corresponds to an approximate mass of 477 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 ⓘ

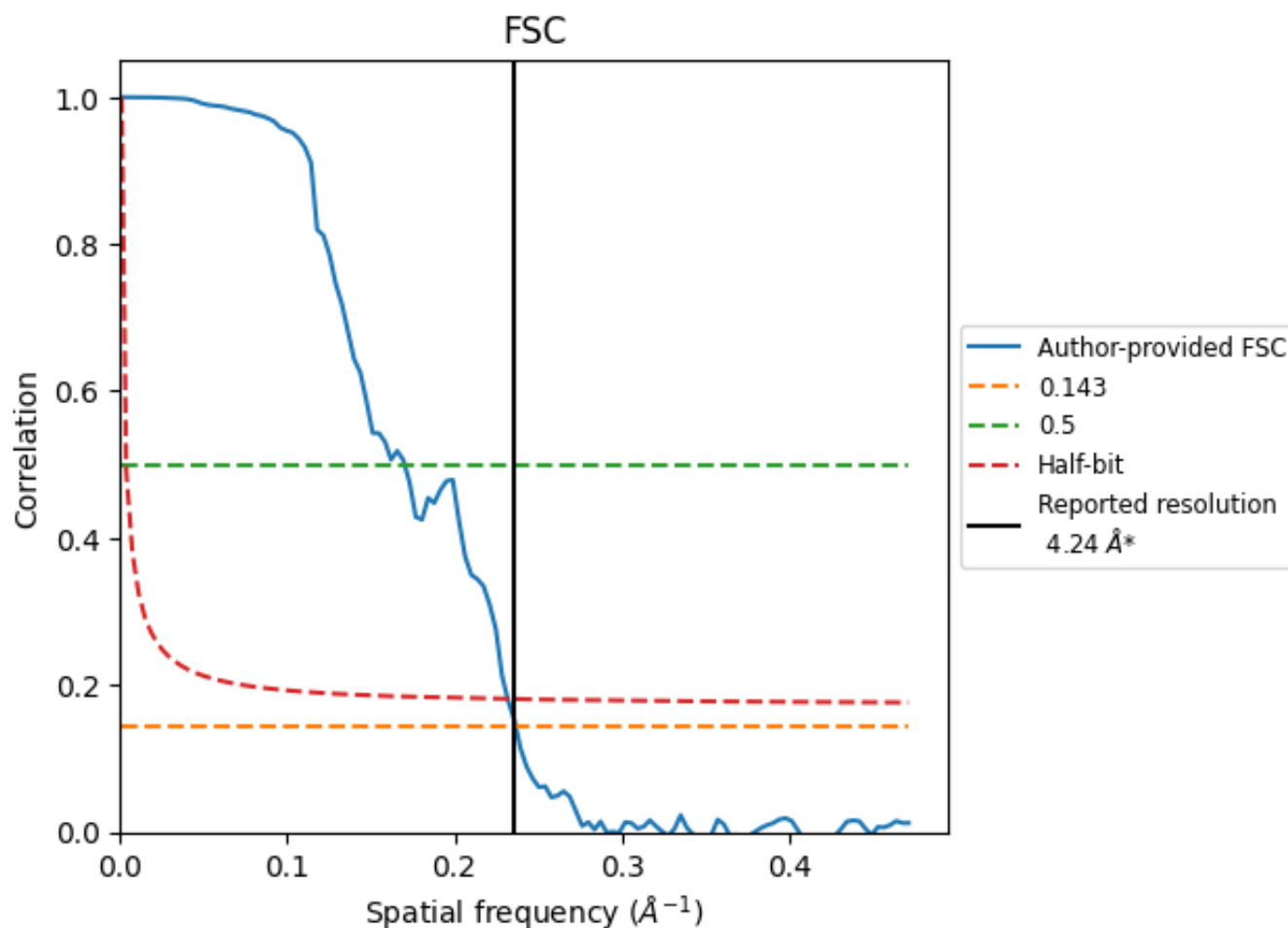


*Reported resolution corresponds to spatial frequency of 0.236 Å⁻¹

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 0.236 Å⁻¹

8.2 Resolution estimates [i](#)

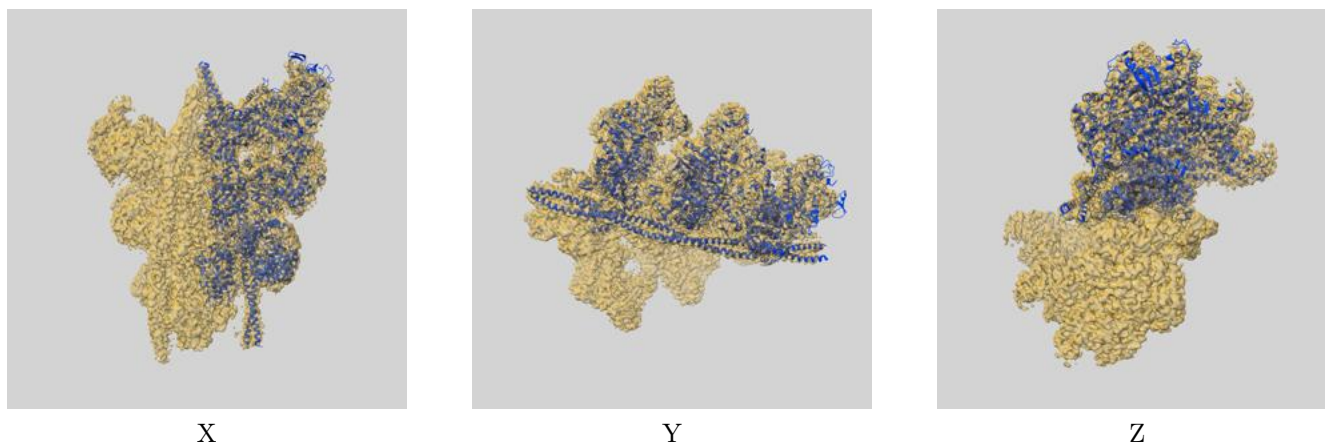
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.24	-	-
Author-provided FSC curve	4.22	5.88	4.31
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

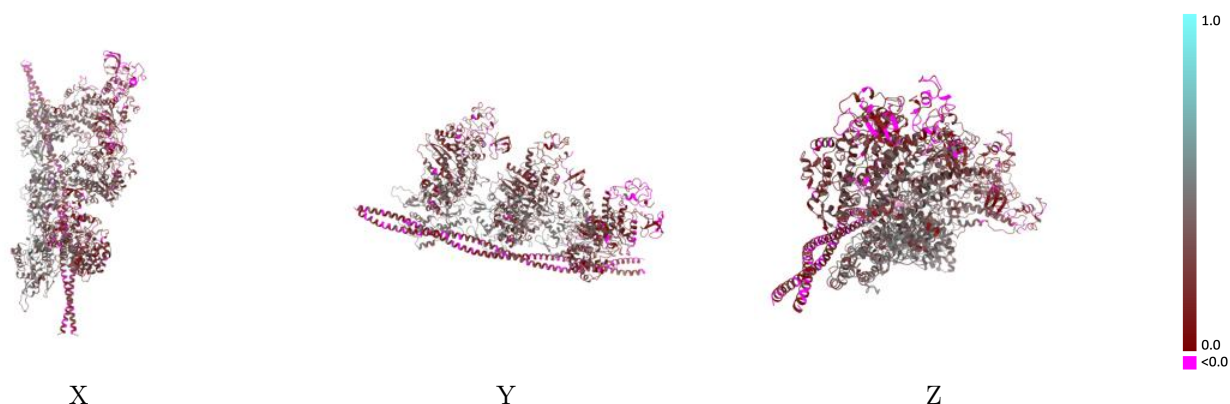
This section contains information regarding the fit between EMDB map EMD-22067 and PDB model 6X5Z. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



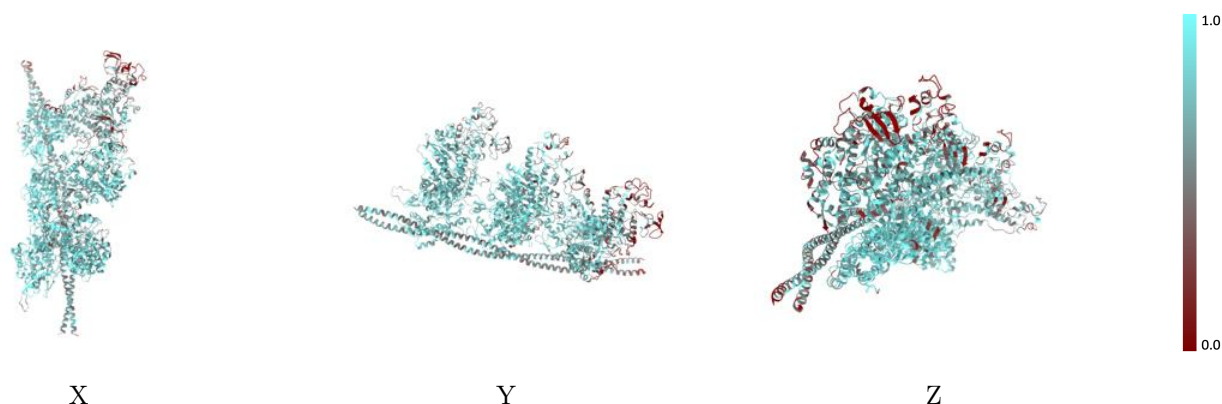
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



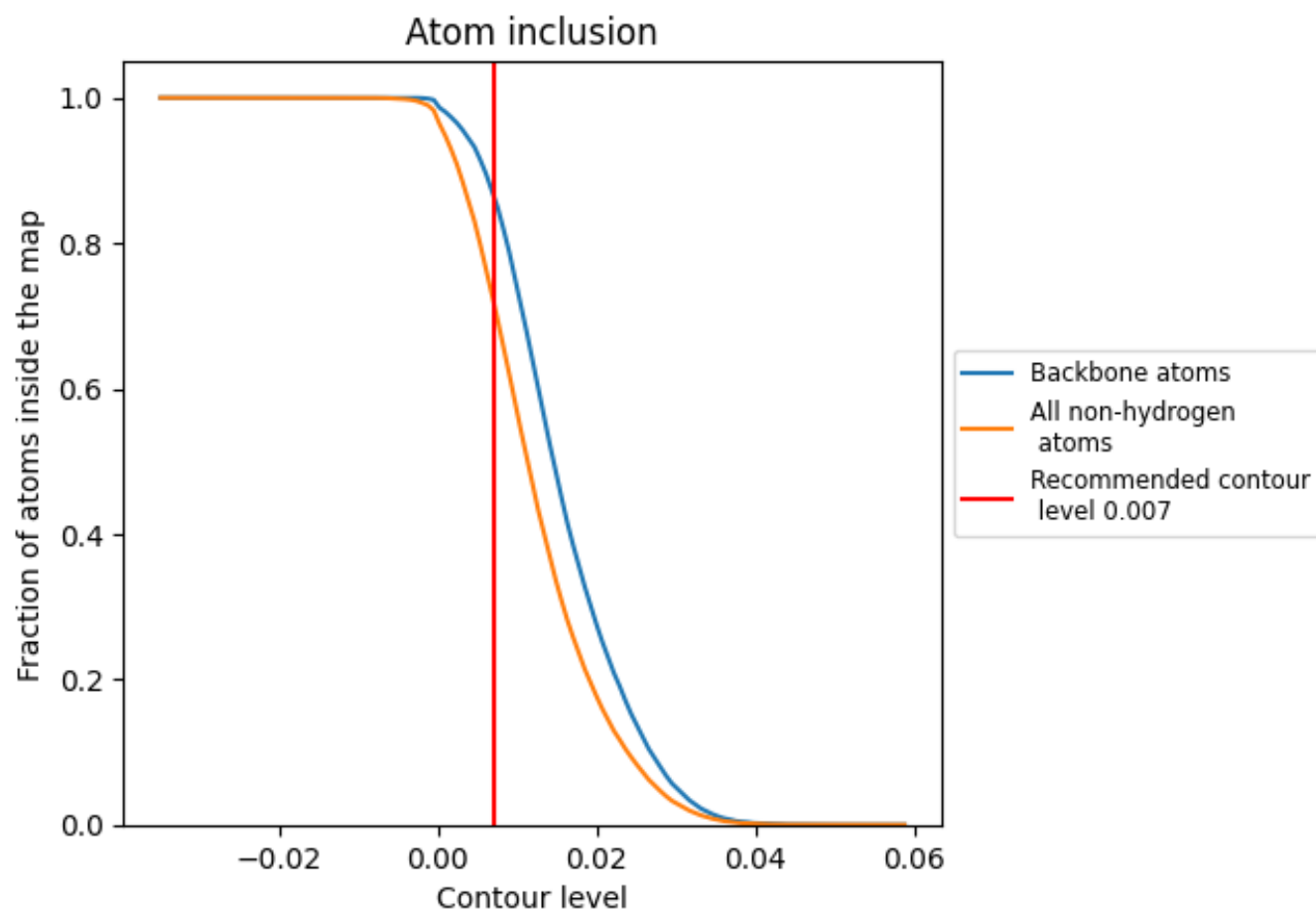
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 72% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7226	<div></div> 0.2870
A	<div></div> 0.8633	<div></div> 0.4140
B	<div></div> 0.8990	<div></div> 0.4410
C	<div></div> 0.8198	<div></div> 0.3960
D	<div></div> 0.7195	<div></div> 0.2510
G	<div></div> 0.7337	<div></div> 0.3010
J	<div></div> 0.5659	<div></div> 0.2000
O	<div></div> 0.5790	<div></div> 0.0850
P	<div></div> 0.5966	<div></div> 0.1040

