



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:23 PM UTC

PDB ID : 7BWA / pdb_00007bwa
EMDB ID : EMD-30231
Title : Cryo-EM Structure for the Ectodomain of the Full-length Human Insulin Receptor in Complex with 2 Insulin
Authors : Yu, D.; Zhang, X.; Sun, J.; Li, X.; Wu, Z.; Han, X.; Fan, C.; Ma, Y.; Ouyang, Q.; Wang, T.
Deposited on : 2020-04-14
Resolution : 4.90 Å (reported)
Based on initial model : 6PXV

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

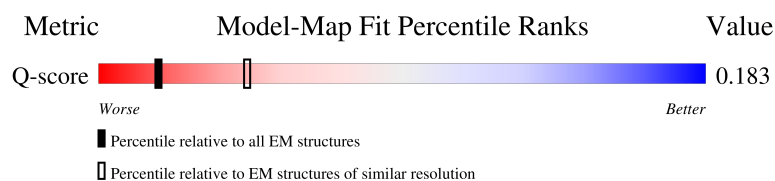
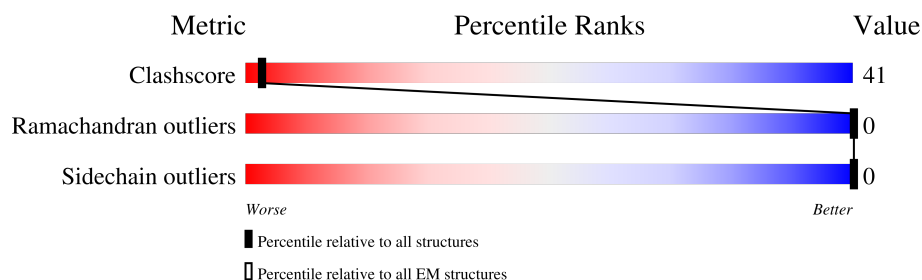
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1274 (4.40 - 5.40)

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	1355	12% 18% 32% 50%
1	C	1355	14% 18% 32% 50%
2	D	74	22% 35% 30% 35%
2	E	74	20% 35% 30% 35%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11670 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 Insulin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	674	Total	C	N	O	S	0	0
			5459	3472	938	1008	41		
1	C	674	Total	C	N	O	S	0	0
			5459	3472	938	1008	41		

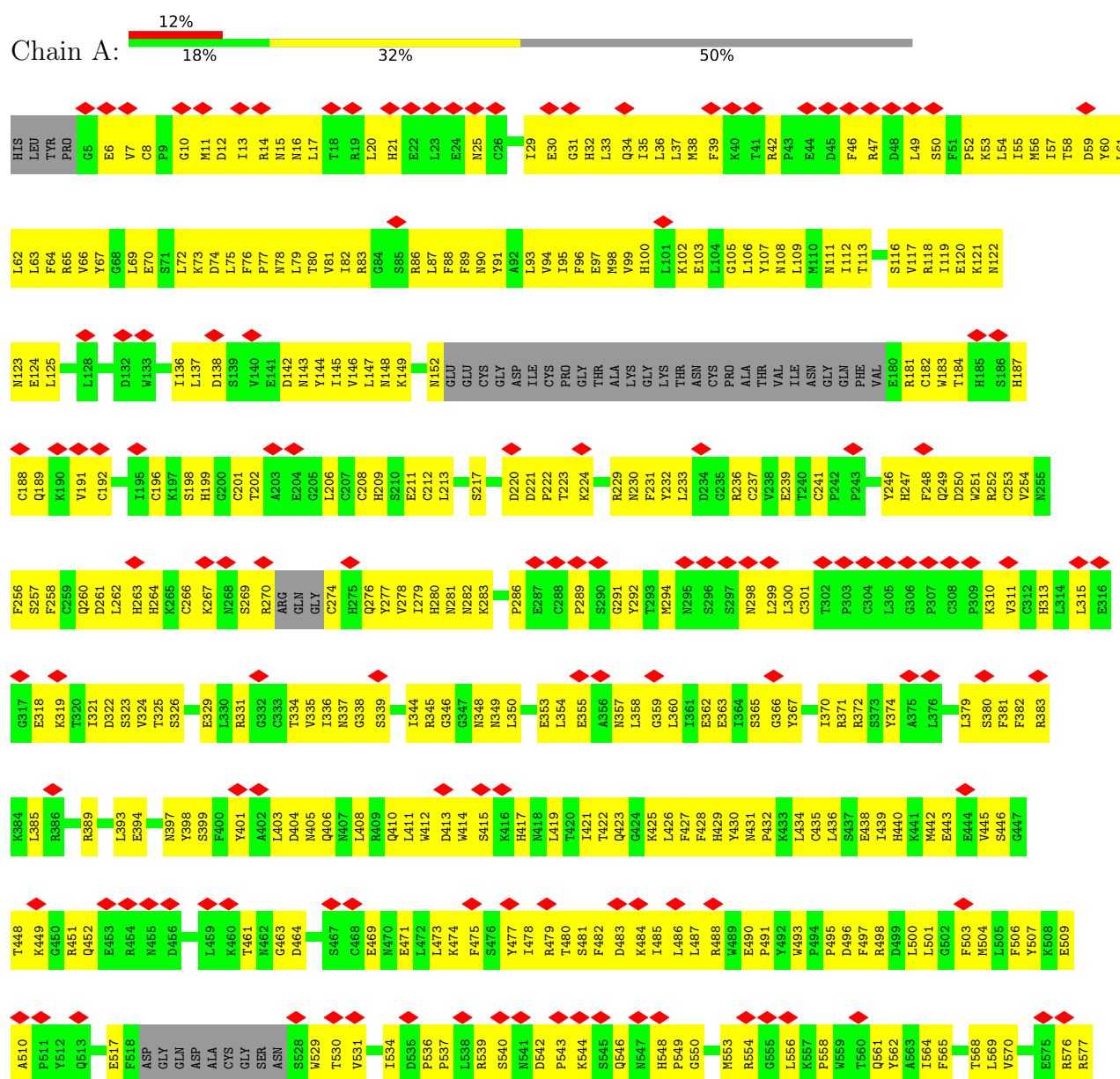
- Molecule 2 is a protein called Insulin fusion.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	48	Total	C	N	O	S	0	0
			376	238	61	71	6		
2	E	48	Total	C	N	O	S	0	0
			376	238	61	71	6		

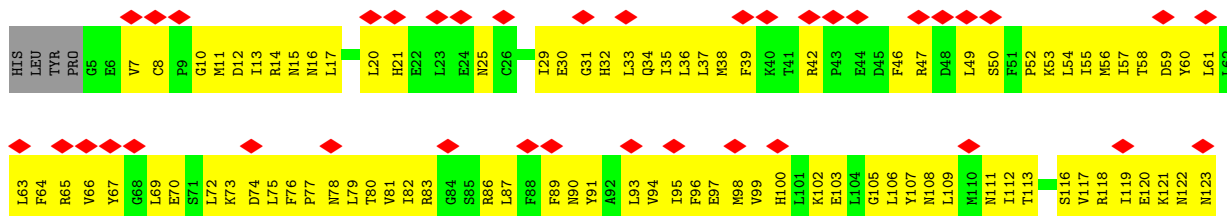
3 Residue-property plots

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: Insulin receptor



- Molecule 1: Insulin receptor



GLY	SER	ILE	ARG	ILE	D813	SER	T704	LEU	G580	A510	E444	R383	L315	V254	S186	E124
PRO	GLU	VAL	LEU	TYR	A581	ASP	F705	ASP	A581	G384	V445	K384	E316	M255	H187	L125
GLU	GLY	GLY	GLY	CYS	K582	TYR	E706	TYR	K582	L385	S446	L385	G317	F256	C188	L128
HIS	LEU	PRO	LEU	LEU	S583	LEU	D707	LEU	S583	R386	G447	L387	E318	S257	Q189	A129
ARG	PRO	VAL	ARG	GLY	D584	GLY	H708	GLY	D584	I388	T448	I388	K319	F258	K190	T130
P758	H710	THR	P758	ASP	I585	LEU	H710	ASP	I585	R389	K449	R389	I321	C259	V191	D132
F759	N711	HIS	F759	GLY	I586	LEU	N711	GLY	I586	G450	G450	G390	D322	Q260	C192	I131
E760	W712	LEU	E760	GLN	V587	LEU	W712	GLN	V587	R451	R451	G390	D322	D261	P193	T130
K761	F713	LEU	K761	ASP	V588	LEU	F713	ASP	V588	Q452	Q452	G390	S323	L262	T194	D132
V762	F714	PRO	V762	ALA	Q589	PRO	F714	ALA	Q589	E391	E391	G390	S323	H263	I195	I136
F763	V715	SER	F763	CYS	T590	ARG	V715	CYS	T590	T392	E453	T392	T325	H264	C196	R135
N764	W715	ARG	N764	GLY	D591	THR	W715	GLY	D591	L393	R454	L393	S326	K265	L137	I136
K765	P716	THR	K765	SER	P591	THR	P716	SER	P591	E394	N455	E394	E329	K197	L137	L137
E766	R717	TRP	E766	ASN	N594	TRP	R717	ASN	N594	N397	L459	N397	L330	K267	L138	D138
S767	L717	PRO	S767	LEU	S595	PRO	L717	LEU	S595	Y398	K460	Y398	R331	M268	S139	S139
L768	THR	PRO	L768	PRO	S596	PRO	THR	PRO	S596	S399	L460	S399	R331	G200	V140	V140
V769	THR	SER	V769	PRO	L599	SER	V769	PRO	L599	F400	T461	F400	T334	S269	E201	E141
I770	GLY	SER	I770	GLY	V531	PHE	I770	GLY	V531	Y401	G462	Y401	T335	T202	T202	D142
S771	THR	GLY	S771	THR	P601	GLY	S771	THR	P601	A402	G463	A402	I336	A203	A203	N143
G772	ALA	GLY	G772	GLY	D602	ASP	G772	GLY	D602	L403	D464	L403	I337	E204	E204	Y144
L773	ASP	ALA	L773	ASP	I602	GLY	L773	ASP	I602	D404	D464	D404	G338	G205	G205	I145
H774	PRO	GLY	H774	SER	V604	GLY	H774	SER	V604	N405	C468	N405	S339	L206	L206	V146
R775	ASN	GLY	R775	SER	S605	GLY	R775	SER	S605	A406	E469	A406	I340	C207	C207	L147
F776	PRO	ASN	F776	LYS	N606	LYS	F776	ASN	N606	M407	N470	M407	I341	C208	H209	N148
T777	ARG	ASN	T777	ASN	S607	ASN	T777	ASN	S607	L408	E471	L408	T344	Y277	Y277	K149
G778	PRO	GLY	G778	GLY	Q610	GLY	G778	GLY	Q610	R409	L472	R409	T344	V278	S210	D150
Y779	LEU	LEU	Y779	SER	I611	LEU	Y779	SER	I611	Q410	L473	Q410	R345	E211	E211	D151
R780	THR	ILE	R780	ARG	L612	THR	R780	ARG	L612	L411	L473	L411	G346	C212	C212	N152
I781	VAL	VAL	I781	LYS	L613	VAL	I781	LYS	L613	W412	K474	W412	G347	G214	G214	GLU
E782	LEU	LEU	E782	GLY	M614	LEU	E782	GLY	M614	D413	F475	D413	N348	N215	N215	GLU
L783	TYR	TYR	L783	ASP	N615	TYR	L783	ASP	N615	W414	F475	W414	N349	C216	C216	GLU
Q784	GLY	GLY	Q784	LEU	K616	GLY	Q784	LEU	K616	S415	L478	S415	L350	S217	S217	GLU
A785	VAL	SER	A785	VAL	P617	VAL	A785	SER	P617	R416	T479	R416	E353	D220	D220	GLU
C786	ASN	TYR	C786	SER	S618	TYR	C786	SER	S618	H417	T480	H417	L354	D221	D221	GLU
ASN	GLN	TYR	ASN	GLY	H548	GLY	ASN	GLY	H548	M418	S481	M418	E355	D222	D222	CYS
GLN	ASP	TYR	GLN	GLY	P618	GLY	GLN	GLY	P618	L419	F482	L419	A356	D223	D223	ASP
ASP	ASP	ARG	ASP	GLY	G550	ASP	ASP	GLY	G550	T420	K483	T420	N357	K224	K224	ASP
GLY	GLY	GLY	GLY	CYS	M553	CYS	GLY	CYS	M553	I421	L485	I421	L358	D229	D229	GLY
PRO	PRO	GLY	PRO	SER	R554	SER	PRO	SER	R554	T422	L486	T422	G359	G291	G291	PRO
GLU	GLU	ASP	GLU	CYS	G555	CYS	GLU	CYS	G555	Q423	L487	Q423	L360	C291	C291	THR
GLU	VAL	GLY	GLU	LYS	L556	LYS	GLU	LYS	L556	G424	R488	G424	I361	Y292	Y292	LYS
ALA	ALA	VAL	ALA	THR	G623	THR	ALA	THR	G623	K425	W489	K425	I361	T293	T293	GLY
VAL	VAL	LEU	VAL	ASP	K557	ASP	VAL	ASP	K557	L426	E490	L426	E362	M294	M294	LYS
THR	THR	THR	THR	SER	P558	SER	THR	SER	P558	F427	P491	F427	E363	N295	N295	THR
VAL	VAL	VAL	VAL	SER	T526	SER	VAL	SER	T526	F428	Y492	F428	I364	S296	S296	ASN
ALA	ALA	VAL	ALA	VAL	Q561	VAL	ALA	VAL	Q561	H429	W493	H429	S365	S297	S297	CYS
ALA	ALA	VAL	ALA	VAL	Y562	VAL	ALA	VAL	Y562	Y430	D496	Y430	S366	N298	N298	PRO
ALA	ALA	VAL	ALA	VAL	I564	VAL	ALA	VAL	I564	N431	F497	N431	G366	C237	C237	ALA
PRO	PRO	VAL	PRO	VAL	F565	VAL	PRO	VAL	F565	P432	R498	P432	Y367	V238	V238	THR
ASN	ASN	THR	ASN	THR	T568	THR	ASN	THR	T568	L434	D499	L434	I370	E239	E239	VAL
THR	THR	THR	THR	THR	G632	THR	THR	THR	G632	K433	L500	K433	R371	C240	C240	ILE
ALA	ALA	THR	ALA	THR	S633	THR	ALA	THR	S633	L436	L501	L436	R372	C241	C241	ASN
LEU	LEU	THR	LEU	THR	H634	THR	LEU	THR	H634	S437	G502	S437	Y374	Y246	Y246	GLN
SER	SER	SER	SER	SER	D574	SER	SER	SER	D574	E438	F503	E438	L379	H247	H247	PHE
LEU	LEU	THR	LEU	THR	E575	THR	LEU	THR	E575	I439	L505	I439	L379	F248	F248	VAL
GLY	GLY	VAL	GLY	VAL	R576	VAL	GLY	VAL	R576	H440	F506	H440	S380	Q249	Q249	THR
VAL	VAL	PRO	VAL	PRO	R577	PRO	VAL	PRO	R577	K441	Y507	K441	F381	D250	D250	THR
THR	THR	THR	THR	THR	T578	THR	THR	THR	T578	M442	K508	M442	F382	W251	W251	C182
GLY	GLY	THR	GLY	THR	Y579	THR	GLY	THR	Y579	E443	E509	E443	F382	R252	R252	T184
GLY	GLY	THR	GLY	THR	GLU	THR	GLY	THR	GLU					C253	C253	H185

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	368511	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 ($e^-/\text{\AA}^2$)	50.0	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	43796	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.098	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	219.2, 219.2, 219.2	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.22	0/5589	0.46	0/7569
1	C	0.22	0/5589	0.46	0/7569
2	D	0.22	0/383	0.41	0/518
2	E	0.22	0/383	0.41	0/518
All	All	0.22	0/11944	0.46	0/16174

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5459	0	5329	462	0
1	C	5459	0	5329	466	0
2	D	376	0	346	26	0
2	E	376	0	346	25	0
All	All	11670	0	11350	946	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 41.

All (946) 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:C:436:LEU:HD21	1:C:577:ARG:CD	1.74	1.16
1:A:576:ARG:HD3	1:A:579:TYR:CE1	1.89	1.08
1:A:484:LYS:HA	1:A:553:MET:O	1.57	1.02
1:C:484:LYS:HA	1:C:553:MET:O	1.57	1.01
1:C:469:GLU:HA	1:C:577:ARG:HH12	1.21	0.99
1:A:37:LEU:HD21	2:D:24:PHE:HB2	1.44	0.99
1:C:469:GLU:O	1:C:577:ARG:NH2	1.97	0.97
1:A:562:TYR:O	1:A:587:TYR:HA	1.66	0.95
1:C:562:TYR:O	1:C:587:TYR:HA	1.66	0.95
1:A:564:ILE:O	1:A:585:ILE:HA	1.69	0.93
1:C:436:LEU:HD21	1:C:577:ARG:HD2	1.49	0.93
1:C:564:ILE:O	1:C:585:ILE:HA	1.69	0.92
1:C:470:ASN:ND2	1:C:577:ARG:NH2	2.19	0.91
1:A:576:ARG:CZ	1:A:579:TYR:CD1	2.54	0.90
1:C:313:HIS:HB2	1:C:337:ASN:HB3	1.57	0.87
1:A:313:HIS:HB2	1:A:337:ASN:HB3	1.57	0.87
1:A:783:LEU:HB3	1:A:799:ALA:HB3	1.61	0.83
1:A:88:PHE:HZ	1:C:712:VAL:HG21	1.43	0.82
1:C:436:LEU:HD21	1:C:577:ARG:HD3	1.62	0.82
1:A:576:ARG:CD	1:A:579:TYR:CE1	2.62	0.82
2:E:18:VAL:HG11	2:E:71:LEU:HG	1.62	0.81
1:A:17:LEU:HD22	1:A:20:LEU:HD22	1.63	0.81
1:C:783:LEU:HB3	1:C:799:ALA:HB3	1.61	0.81
1:C:601:PRO:HA	1:C:614:LYS:O	1.81	0.81
1:C:10:GLY:HA2	1:C:32:HIS:O	1.81	0.80
1:A:10:GLY:HA2	1:A:32:HIS:O	1.82	0.80
1:A:601:PRO:HA	1:A:614:LYS:O	1.81	0.80
2:D:18:VAL:HG11	2:D:71:LEU:HG	1.63	0.80
1:C:17:LEU:HD22	1:C:20:LEU:HD22	1.63	0.80
1:A:576:ARG:HD3	1:A:579:TYR:HE1	1.43	0.80
1:C:469:GLU:HA	1:C:577:ARG:NH1	1.96	0.78
1:C:470:ASN:HD21	1:C:577:ARG:NH2	1.82	0.77
1:A:183:TRP:HE1	1:A:189:GLN:HG3	1.50	0.77
1:A:213:LEU:HB2	1:A:229:ARG:HA	1.68	0.76
1:C:488:ARG:HD2	1:C:550:GLY:HA3	1.67	0.76
1:C:183:TRP:HE1	1:C:189:GLN:HG3	1.50	0.76
1:A:631:PHE:O	1:A:781:ILE:HA	1.86	0.75
1:C:213:LEU:HB2	1:C:229:ARG:HA	1.68	0.75
1:A:448:THR:HB	1:A:451:ARG:HB2	1.68	0.75
1:A:506:PHE:HB3	1:A:529:TRP:HB3	1.68	0.75
1:C:448:THR:HB	1:C:451:ARG:HB2	1.68	0.75
1:C:25:ASN:HD22	1:C:53:LYS:HE3	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:631:PHE:O	1:C:781:ILE:HA	1.86	0.74
1:A:488:ARG:HD2	1:A:550:GLY:HA3	1.67	0.74
1:C:506:PHE:HB3	1:C:529:TRP:HB3	1.68	0.74
1:A:25:ASN:HD22	1:A:53:LYS:HE3	1.52	0.74
1:C:436:LEU:O	1:C:440:HIS:ND1	2.20	0.73
1:C:470:ASN:ND2	1:C:577:ARG:CZ	2.51	0.73
1:A:576:ARG:NH2	1:A:579:TYR:HA	2.03	0.73
1:C:247:HIS:HB2	1:C:283:LYS:HG2	1.71	0.73
1:C:436:LEU:HD21	1:C:577:ARG:CG	2.19	0.73
1:C:615:TRP:CE2	1:C:766:GLU:HA	2.24	0.72
1:C:10:GLY:CA	1:C:32:HIS:O	2.37	0.72
1:C:706:GLU:O	1:C:710:HIS:ND1	2.17	0.72
1:C:63:LEU:O	1:C:95:ILE:HA	1.89	0.72
1:A:632:TRP:NE1	1:A:771:SER:O	2.23	0.72
1:A:565:PHE:HB3	1:A:585:ILE:HG13	1.71	0.72
1:A:615:TRP:CE2	1:A:766:GLU:HA	2.24	0.72
1:C:565:PHE:HB3	1:C:585:ILE:HG13	1.71	0.72
1:A:436:LEU:O	1:A:440:HIS:ND1	2.20	0.71
1:A:10:GLY:CA	1:A:32:HIS:O	2.37	0.71
1:A:247:HIS:HB2	1:A:283:LYS:HG2	1.70	0.71
1:A:249:GLN:HB2	1:A:251:TRP:CD1	2.25	0.71
2:E:22:ARG:NH2	2:E:75:CYS:SG	2.63	0.71
1:A:29:ILE:HB	1:A:57:ILE:HG23	1.73	0.71
2:D:22:ARG:NH2	2:D:75:CYS:SG	2.63	0.71
1:A:63:LEU:O	1:A:95:ILE:HA	1.89	0.71
1:C:249:GLN:HB2	1:C:251:TRP:CD1	2.25	0.71
1:C:29:ILE:HB	1:C:57:ILE:HG23	1.73	0.71
1:C:497:PHE:HD2	1:C:539:ARG:HE	1.39	0.70
1:C:422:THR:HG22	1:C:423:GLN:HG3	1.74	0.70
1:C:632:TRP:NE1	1:C:771:SER:O	2.23	0.70
1:C:313:HIS:ND1	1:C:337:ASN:O	2.24	0.70
1:A:313:HIS:ND1	1:A:337:ASN:O	2.24	0.70
1:C:77:PRO:O	1:C:108:ASN:ND2	2.22	0.70
1:C:59:ASP:OD2	1:C:86:ARG:NH1	2.25	0.69
1:A:59:ASP:OD2	1:A:86:ARG:NH1	2.25	0.69
1:C:208:CYS:HA	1:C:220:ASP:H	1.58	0.69
1:C:354:LEU:O	1:C:358:LEU:N	2.26	0.69
1:A:497:PHE:HD2	1:A:539:ARG:HE	1.39	0.69
2:D:13:GLU:O	2:D:17:LEU:HD12	1.93	0.69
1:A:192:CYS:SG	1:A:201:CYS:N	2.65	0.69
1:C:498:ARG:HB2	1:C:703:LYS:HZ2	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:ARG:NH1	1:A:579:TYR:CD1	2.61	0.68
1:A:398:TYR:OH	1:C:454:ARG:NH2	2.24	0.68
1:C:470:ASN:HD21	1:C:577:ARG:CZ	2.06	0.68
1:A:717:ARG:NH1	2:E:75:CYS:O	2.26	0.68
1:A:77:PRO:O	1:A:108:ASN:ND2	2.22	0.68
1:A:706:GLU:O	1:A:710:HIS:ND1	2.17	0.68
1:C:576:ARG:CB	1:C:579:TYR:OH	2.42	0.68
1:A:354:LEU:O	1:A:358:LEU:N	2.26	0.68
1:A:422:THR:HG22	1:A:423:GLN:HG3	1.74	0.68
1:A:509:GLU:HG3	1:A:556:LEU:HD22	1.75	0.67
2:D:57:ILE:HD12	2:D:74:TYR:HE1	1.58	0.67
2:E:13:GLU:O	2:E:17:LEU:HD12	1.93	0.67
1:A:208:CYS:HA	1:A:220:ASP:H	1.58	0.67
1:A:89:PHE:HB2	1:C:708:TYR:HE2	1.59	0.67
1:C:639:SER:HA	1:C:642:PHE:HD2	1.59	0.67
1:C:509:GLU:HG3	1:C:556:LEU:HD22	1.75	0.67
1:C:576:ARG:CZ	1:C:579:TYR:CE1	2.78	0.67
1:A:221:ASP:OD1	1:A:223:THR:OG1	2.12	0.67
1:A:627:HIS:HA	1:A:764:ASN:H	1.58	0.67
1:A:87:LEU:HB3	1:A:90:ASN:HA	1.76	0.67
1:C:87:LEU:HB3	1:C:90:ASN:HA	1.76	0.67
2:E:57:ILE:HD12	2:E:74:TYR:HE1	1.58	0.67
1:A:47:ARG:NH1	1:A:74:ASP:OD2	2.28	0.66
1:A:414:TRP:HA	1:A:417:HIS:HB3	1.77	0.66
1:A:595:PRO:HB2	1:A:796:SER:HB2	1.76	0.66
1:C:576:ARG:CZ	1:C:579:TYR:CD1	2.78	0.66
1:C:414:TRP:HA	1:C:417:HIS:HB3	1.77	0.66
1:A:498:ARG:HB2	1:A:703:LYS:HZ2	1.59	0.66
1:C:576:ARG:HD3	1:C:579:TYR:CE1	2.30	0.66
1:C:120:GLU:HG3	1:C:121:LYS:HG2	1.77	0.66
1:C:595:PRO:HB2	1:C:796:SER:HB2	1.76	0.66
1:A:57:ILE:HG22	1:A:58:THR:H	1.61	0.66
1:A:120:GLU:HG3	1:A:121:LYS:HG2	1.77	0.66
1:A:241:CYS:HB2	1:A:282:ASN:HD21	1.61	0.66
1:C:47:ARG:NH1	1:C:74:ASP:OD2	2.28	0.66
1:C:394:GLU:HB2	1:C:398:TYR:HB2	1.78	0.66
1:C:192:CYS:SG	1:C:201:CYS:N	2.65	0.66
1:A:394:GLU:HB2	1:A:398:TYR:HB2	1.78	0.65
1:C:241:CYS:HB2	1:C:282:ASN:HD21	1.61	0.65
1:C:627:HIS:HA	1:C:764:ASN:H	1.58	0.65
1:A:639:SER:HA	1:A:642:PHE:HD2	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ILE:N	1:A:299:LEU:O	2.29	0.65
1:C:631:PHE:HA	1:C:759:PHE:HB2	1.79	0.65
1:C:279:ILE:N	1:C:299:LEU:O	2.29	0.65
1:C:380:SER:O	1:C:383:ARG:NH1	2.20	0.65
1:C:611:ILE:HB	1:C:770:ILE:HB	1.77	0.65
1:A:93:LEU:H	1:A:117:VAL:HG12	1.61	0.65
1:A:611:ILE:HB	1:A:770:ILE:HB	1.78	0.65
1:C:568:THR:HG21	1:C:580:GLY:HA3	1.79	0.65
1:C:93:LEU:H	1:C:117:VAL:HG12	1.61	0.64
1:A:277:TYR:HA	1:A:286:PRO:HA	1.80	0.64
1:A:717:ARG:HH22	2:E:75:CYS:H	1.46	0.64
1:C:57:ILE:HG22	1:C:58:THR:H	1.61	0.64
1:A:509:GLU:HA	1:A:562:TYR:HA	1.78	0.64
1:A:148:ASN:O	1:A:152:ASN:N	2.31	0.64
1:C:617:PRO:HD3	1:C:766:GLU:HG2	1.80	0.64
1:C:561:GLN:HA	1:C:589:GLN:HG2	1.80	0.64
1:A:631:PHE:HA	1:A:759:PHE:HB2	1.79	0.64
1:C:221:ASP:OD1	1:C:223:THR:OG1	2.12	0.64
1:A:380:SER:O	1:A:383:ARG:NH1	2.20	0.63
1:C:509:GLU:HA	1:C:562:TYR:HA	1.78	0.63
1:A:568:THR:HB	1:A:581:ALA:H	1.63	0.63
1:C:568:THR:HB	1:C:581:ALA:H	1.63	0.63
1:A:785:ALA:H	1:A:796:SER:H	1.47	0.63
1:C:785:ALA:H	1:C:796:SER:H	1.47	0.63
1:A:404:ASP:OD1	1:A:406:GLN:NE2	2.32	0.63
1:C:209:HIS:HD2	1:C:211:GLU:HB2	1.64	0.63
1:C:277:TYR:HA	1:C:286:PRO:HA	1.80	0.63
1:C:404:ASP:OD1	1:C:406:GLN:NE2	2.32	0.63
1:A:209:HIS:HD2	1:A:211:GLU:HB2	1.64	0.62
1:C:222:PRO:HB2	1:C:236:ARG:HB2	1.81	0.62
1:A:120:GLU:O	1:A:122:ASN:ND2	2.32	0.62
1:C:329:GLU:OE1	1:C:329:GLU:N	2.23	0.62
1:A:617:PRO:HD3	1:A:766:GLU:HG2	1.80	0.62
1:C:148:ASN:O	1:C:152:ASN:N	2.31	0.62
1:C:350:LEU:HD12	1:C:354:LEU:HB2	1.80	0.62
1:A:222:PRO:HB2	1:A:236:ARG:HB2	1.81	0.62
1:A:570:VAL:HG11	1:A:579:TYR:C	2.24	0.62
1:C:232:TYR:HA	1:C:237:CYS:HA	1.81	0.62
1:A:90:ASN:H	1:A:325:THR:HG23	1.65	0.62
1:A:181:ARG:HH11	1:A:191:VAL:HG11	1.64	0.62
1:C:448:THR:OG1	1:C:452:GLN:NE2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:HD12	1:A:354:LEU:HB2	1.80	0.62
1:A:448:THR:OG1	1:A:452:GLN:NE2	2.33	0.62
1:C:120:GLU:O	1:C:122:ASN:ND2	2.32	0.62
1:C:181:ARG:HH11	1:C:191:VAL:HG11	1.64	0.62
1:A:469:GLU:O	1:A:577:ARG:CZ	2.48	0.62
1:C:613:LEU:HD13	1:C:801:VAL:HG21	1.82	0.62
1:A:782:GLU:OE2	1:A:784:GLN:NE2	2.33	0.61
1:C:318:GLU:O	1:C:319:LYS:NZ	2.30	0.61
1:C:576:ARG:HB2	1:C:579:TYR:OH	2.00	0.61
1:A:561:GLN:HA	1:A:589:GLN:HG2	1.80	0.61
1:C:96:PHE:CD1	1:C:120:GLU:HB3	2.36	0.61
1:A:613:LEU:HD13	1:A:801:VAL:HG21	1.82	0.61
1:A:616:LYS:HD2	1:A:617:PRO:HD2	1.82	0.61
1:A:232:TYR:HA	1:A:237:CYS:HA	1.82	0.61
1:C:782:GLU:OE2	1:C:784:GLN:NE2	2.33	0.61
1:C:263:HIS:CD2	1:C:267:LYS:HD2	2.35	0.61
1:A:96:PHE:CD1	1:A:120:GLU:HB3	2.36	0.61
1:C:90:ASN:H	1:C:325:THR:HG23	1.64	0.61
1:C:111:ASN:HA	1:C:136:ILE:HG13	1.83	0.61
1:A:73:LYS:HD2	1:A:187:HIS:CE1	2.36	0.60
1:A:481:SER:N	1:A:484:LYS:O	2.34	0.60
1:A:103:GLU:OE2	1:A:105:GLY:N	2.34	0.60
1:A:576:ARG:NE	1:A:579:TYR:CE1	2.70	0.60
2:D:56:GLY:N	2:D:59:GLU:OE2	2.35	0.60
1:A:14:ARG:HB3	1:A:37:LEU:HD23	1.83	0.60
1:A:318:GLU:O	1:A:319:LYS:NZ	2.30	0.60
2:E:56:GLY:N	2:E:59:GLU:OE2	2.35	0.60
1:C:298:ASN:OD1	1:C:299:LEU:N	2.34	0.60
1:C:616:LYS:HD2	1:C:617:PRO:HD2	1.82	0.60
1:A:55:ILE:O	1:A:80:THR:N	2.34	0.60
1:A:98:MET:N	1:A:122:ASN:OD1	2.33	0.60
1:A:263:HIS:CD2	1:A:267:LYS:HD2	2.35	0.60
1:C:55:ILE:O	1:C:80:THR:N	2.34	0.60
1:A:94:VAL:HA	1:A:118:ARG:O	2.02	0.60
1:A:576:ARG:NH1	1:A:579:TYR:HD1	2.00	0.60
1:A:34:GLN:NE2	1:A:60:TYR:OH	2.31	0.60
1:A:507:TYR:HB2	1:A:564:ILE:HG13	1.84	0.60
1:A:298:ASN:OD1	1:A:299:LEU:N	2.34	0.60
1:C:73:LYS:HD2	1:C:187:HIS:CE1	2.36	0.60
1:C:80:THR:HG22	1:C:81:VAL:HG23	1.83	0.60
1:C:184:THR:HB	1:C:187:HIS:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:SER:N	1:C:484:LYS:O	2.34	0.60
1:C:497:PHE:HZ	2:D:8:GLY:HA3	1.65	0.60
1:C:50:SER:HA	1:C:75:LEU:HA	1.84	0.60
1:C:94:VAL:HA	1:C:118:ARG:O	2.02	0.60
1:C:103:GLU:OE2	1:C:105:GLY:N	2.34	0.60
1:C:507:TYR:HB2	1:C:564:ILE:HG13	1.84	0.59
1:C:603:SER:HB2	1:C:613:LEU:HD13	1.84	0.59
1:A:50:SER:HA	1:A:75:LEU:HA	1.84	0.59
1:C:541:ASN:ND2	2:D:10:HIS:HB2	2.16	0.59
1:A:111:ASN:HA	1:A:136:ILE:HG13	1.83	0.59
1:C:246:TYR:HE2	1:C:256:PHE:HB3	1.67	0.59
1:A:576:ARG:HD3	1:A:579:TYR:CZ	2.36	0.59
1:C:363:GLU:HG2	1:C:389:ARG:HD3	1.85	0.59
1:A:184:THR:HB	1:A:187:HIS:H	1.66	0.59
1:A:80:THR:HG22	1:A:81:VAL:HG23	1.83	0.59
1:C:11:MET:HG3	1:C:12:ASP:H	1.67	0.59
1:C:443:GLU:OE1	1:C:452:GLN:NE2	2.36	0.59
1:C:436:LEU:HD21	1:C:577:ARG:HG3	1.85	0.59
1:A:329:GLU:OE1	1:A:329:GLU:N	2.23	0.58
1:A:717:ARG:HH22	2:E:75:CYS:N	2.00	0.58
2:D:15:LEU:HA	2:D:18:VAL:HG12	1.85	0.58
1:A:488:ARG:HA	1:A:550:GLY:HA3	1.85	0.58
1:A:11:MET:HG3	1:A:12:ASP:H	1.67	0.58
1:A:65:ARG:CZ	2:D:12:VAL:HG11	2.33	0.58
1:C:34:GLN:NE2	1:C:60:TYR:OH	2.31	0.58
1:C:83:ARG:NH2	1:C:250:ASP:O	2.37	0.58
1:C:107:TYR:HA	1:C:183:TRP:CD1	2.38	0.58
1:A:95:ILE:O	1:A:119:ILE:HA	2.03	0.58
1:A:107:TYR:HA	1:A:183:TRP:CD1	2.38	0.58
1:A:426:LEU:HB3	1:A:428:PHE:CZ	2.38	0.58
1:C:411:LEU:HB2	1:C:442:MET:HE3	1.86	0.58
1:C:426:LEU:HB3	1:C:428:PHE:CZ	2.38	0.58
1:A:83:ARG:NH2	1:A:250:ASP:O	2.37	0.58
1:A:443:GLU:OE1	1:A:452:GLN:NE2	2.36	0.58
1:C:12:ASP:OD2	1:C:14:ARG:NH2	2.37	0.58
1:C:14:ARG:HB3	1:C:37:LEU:HD23	1.83	0.58
1:C:98:MET:N	1:C:122:ASN:OD1	2.33	0.58
1:A:12:ASP:OD2	1:A:14:ARG:NH2	2.37	0.58
1:A:16:ASN:HA	1:A:38:MET:HE3	1.85	0.58
1:A:246:TYR:HE2	1:A:256:PHE:HB3	1.67	0.58
1:A:411:LEU:HB2	1:A:442:MET:HE3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HD11	1:A:106:LEU:HD21	1.85	0.58
1:A:785:ALA:O	1:A:796:SER:N	2.37	0.58
1:C:72:LEU:HD11	1:C:106:LEU:HD21	1.85	0.58
1:A:603:SER:HB2	1:A:613:LEU:HD13	1.84	0.58
1:C:488:ARG:HA	1:C:550:GLY:HA3	1.85	0.58
1:A:469:GLU:O	1:A:577:ARG:NH1	2.37	0.58
1:A:30:GLU:OE1	1:A:252:ARG:NH2	2.37	0.57
1:A:363:GLU:HG2	1:A:389:ARG:HD3	1.85	0.57
1:A:374:TYR:HD1	1:A:406:GLN:HG3	1.69	0.57
1:A:410:GLN:NE2	1:A:412:TRP:O	2.36	0.57
1:C:436:LEU:HA	1:C:439:ILE:HD12	1.86	0.57
1:C:473:LEU:HB2	1:C:583:SER:HB2	1.86	0.57
1:C:576:ARG:HB3	1:C:579:TYR:CZ	2.38	0.57
1:C:95:ILE:O	1:C:119:ILE:HA	2.03	0.57
1:A:116:SER:HG	1:A:117:VAL:H	1.53	0.57
1:A:183:TRP:NE1	1:A:189:GLN:HG3	2.19	0.57
1:A:196:CYS:HB2	1:A:199:HIS:HD2	1.68	0.57
1:A:698:GLU:OE1	1:A:698:GLU:N	2.28	0.57
1:C:30:GLU:OE1	1:C:252:ARG:NH2	2.37	0.57
2:E:15:LEU:HA	2:E:18:VAL:HG12	1.85	0.57
1:C:431:ASN:HB3	1:C:434:LEU:HB3	1.87	0.57
1:C:438:GLU:OE1	1:C:438:GLU:N	2.25	0.57
1:C:629:LEU:HD13	1:C:761:LYS:HE2	1.87	0.57
1:A:473:LEU:HB2	1:A:583:SER:HB2	1.86	0.57
1:A:70:GLU:HB3	1:A:102:LYS:HB3	1.87	0.57
1:C:374:TYR:HD1	1:C:406:GLN:HG3	1.69	0.57
1:C:504:MET:HE2	1:C:569:LEU:HD13	1.87	0.57
1:A:39:PHE:O	1:A:42:ARG:NH2	2.28	0.57
1:A:436:LEU:HA	1:A:439:ILE:HD12	1.86	0.57
1:C:315:LEU:O	1:C:319:LYS:NZ	2.37	0.57
1:C:692:ILE:HG13	1:C:693:LEU:H	1.70	0.57
1:A:57:ILE:HG12	1:A:79:LEU:HD11	1.87	0.56
1:A:355:GLU:HG2	1:A:381:PHE:HB2	1.88	0.56
1:A:429:HIS:HB3	1:A:430:TYR:CD2	2.40	0.56
1:C:196:CYS:HB2	1:C:199:HIS:HD2	1.68	0.56
1:C:310:LYS:H	1:C:334:THR:HG1	1.53	0.56
1:C:501:LEU:HB2	1:C:569:LEU:HG	1.87	0.56
1:C:785:ALA:O	1:C:796:SER:N	2.37	0.56
1:A:501:LEU:HB2	1:A:569:LEU:HG	1.87	0.56
1:A:709:LEU:O	1:A:713:VAL:HG23	2.06	0.56
1:C:429:HIS:HB3	1:C:430:TYR:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:576:ARG:NE	1:C:579:TYR:CE1	2.73	0.56
2:E:57:ILE:HB	2:E:74:TYR:OH	2.05	0.56
1:A:125:LEU:O	1:A:149:LYS:HB3	2.05	0.56
1:C:16:ASN:HA	1:C:38:MET:HE3	1.85	0.56
1:C:541:ASN:HD22	2:D:10:HIS:HB2	1.70	0.56
1:A:692:ILE:HG13	1:A:693:LEU:H	1.70	0.56
1:C:70:GLU:HB3	1:C:102:LYS:HB3	1.87	0.56
1:C:709:LEU:O	1:C:713:VAL:HG23	2.06	0.56
1:C:90:ASN:HB3	1:C:324:VAL:HB	1.88	0.56
1:A:36:LEU:HG	1:A:37:LEU:HB2	1.87	0.56
1:A:323:SER:OG	1:A:324:VAL:N	2.38	0.56
1:A:349:ASN:OD1	1:A:350:LEU:N	2.39	0.56
1:A:539:ARG:HB2	1:A:546:GLN:HE22	1.72	0.56
1:A:629:LEU:HD13	1:A:761:LYS:HE2	1.87	0.56
1:C:36:LEU:HG	1:C:37:LEU:HB2	1.87	0.56
1:C:349:ASN:OD1	1:C:350:LEU:N	2.39	0.56
1:C:183:TRP:NE1	1:C:189:GLN:HG3	2.19	0.55
1:C:610:GLN:HE22	1:C:771:SER:HB2	1.71	0.55
1:C:774:ARG:O	1:C:779:TYR:OH	2.23	0.55
2:D:57:ILE:HB	2:D:74:TYR:OH	2.05	0.55
1:A:469:GLU:CB	1:A:581:ALA:HA	2.36	0.55
1:A:474:LYS:HB2	1:A:490:GLU:HB3	1.89	0.55
1:A:481:SER:OG	1:A:484:LYS:N	2.39	0.55
1:A:576:ARG:CZ	1:A:579:TYR:CE1	2.89	0.55
1:C:57:ILE:HG12	1:C:79:LEU:HD11	1.86	0.55
1:C:355:GLU:HG2	1:C:381:PHE:HB2	1.88	0.55
1:A:431:ASN:HB3	1:A:434:LEU:HB3	1.87	0.55
1:A:484:LYS:HD3	1:A:486:LEU:HG	1.89	0.55
1:A:702:ARG:NH2	1:A:706:GLU:OE2	2.40	0.55
1:C:497:PHE:CZ	2:D:8:GLY:HA3	2.40	0.55
1:C:507:TYR:HB3	1:C:564:ILE:HG23	1.89	0.55
1:C:605:SER:HA	1:C:611:ILE:HA	1.88	0.55
1:C:481:SER:OG	1:C:484:LYS:N	2.39	0.55
1:A:504:MET:HE2	1:A:569:LEU:HD13	1.87	0.55
1:C:125:LEU:O	1:C:149:LYS:HB3	2.05	0.55
1:C:484:LYS:HD3	1:C:486:LEU:HG	1.89	0.55
1:A:507:TYR:HB3	1:A:564:ILE:HG23	1.89	0.55
1:A:610:GLN:HE22	1:A:771:SER:HB2	1.71	0.55
1:C:323:SER:OG	1:C:324:VAL:N	2.38	0.55
1:C:698:GLU:OE1	1:C:698:GLU:N	2.28	0.55
1:A:697:GLU:N	1:A:697:GLU:OE1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:SER:HG	1:C:117:VAL:H	1.56	0.54
1:C:263:HIS:CE1	1:C:276:GLN:HB3	2.42	0.54
1:C:708:TYR:O	1:C:711:ASN:HB3	2.06	0.54
1:A:57:ILE:O	1:A:82:ILE:HA	2.08	0.54
1:A:99:VAL:HG12	1:A:100:HIS:CD2	2.43	0.54
1:A:708:TYR:O	1:A:711:ASN:HB3	2.06	0.54
1:C:510:ALA:N	1:C:561:GLN:O	2.36	0.54
1:C:702:ARG:NH2	1:C:706:GLU:OE2	2.40	0.54
1:A:209:HIS:CD2	1:A:211:GLU:HB2	2.43	0.54
1:A:605:SER:HA	1:A:611:ILE:HA	1.88	0.54
1:C:474:LYS:HB2	1:C:490:GLU:HB3	1.89	0.54
1:A:717:ARG:HB3	2:E:25:PHE:CE2	2.41	0.54
1:C:57:ILE:O	1:C:82:ILE:HA	2.08	0.54
1:C:628:TYR:OH	1:C:766:GLU:OE2	2.14	0.54
1:C:411:LEU:HD11	1:C:434:LEU:HD21	1.90	0.54
1:C:540:SER:OG	1:C:542:ASP:OD1	2.26	0.54
1:C:697:GLU:OE1	1:C:697:GLU:N	2.38	0.54
1:A:628:TYR:OH	1:A:766:GLU:OE2	2.14	0.54
1:A:263:HIS:CE1	1:A:276:GLN:HB3	2.42	0.54
1:A:469:GLU:O	1:A:577:ARG:NH2	2.41	0.54
1:A:540:SER:OG	1:A:542:ASP:OD1	2.26	0.54
1:A:90:ASN:HB3	1:A:324:VAL:HB	1.88	0.54
1:A:471:GLU:HB2	1:A:581:ALA:HB2	1.88	0.54
1:A:506:PHE:HE1	1:A:531:VAL:HG12	1.73	0.54
1:A:615:TRP:CD1	1:A:766:GLU:HG3	2.43	0.54
1:A:117:VAL:N	1:A:143:ASN:OD1	2.37	0.54
1:A:264:HIS:ND1	1:A:267:LYS:HD3	2.22	0.54
1:A:323:SER:N	1:A:326:SER:OG	2.37	0.54
1:C:264:HIS:ND1	1:C:267:LYS:HD3	2.22	0.53
1:A:331:ARG:HG3	1:A:357:ASN:HA	1.91	0.53
1:C:506:PHE:HE1	1:C:531:VAL:HG12	1.73	0.53
1:A:15:ASN:HD21	2:D:24:PHE:HD2	1.57	0.53
1:A:64:PHE:HD1	1:A:96:PHE:HB3	1.73	0.53
1:A:543:PRO:HA	1:A:546:GLN:HG2	1.91	0.53
1:C:99:VAL:HG12	1:C:100:HIS:CD2	2.43	0.53
1:C:209:HIS:CD2	1:C:211:GLU:HB2	2.43	0.53
1:C:413:ASP:OD2	1:C:415:SER:OG	2.25	0.53
1:C:500:LEU:HD13	1:C:537:PRO:HD2	1.90	0.53
1:C:506:PHE:CE1	1:C:531:VAL:HG12	2.43	0.53
1:A:701:PHE:HE1	1:C:89:PHE:HZ	1.56	0.53
1:C:480:THR:HA	1:C:485:ILE:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:57:ILE:HD12	2:E:74:TYR:CE1	2.40	0.53
1:A:233:LEU:HB3	1:A:236:ARG:NH1	2.24	0.53
1:A:471:GLU:HG2	1:A:577:ARG:NH2	2.23	0.53
1:C:410:GLN:NE2	1:C:412:TRP:O	2.36	0.53
1:C:615:TRP:CD1	1:C:766:GLU:HG3	2.43	0.53
1:C:715:VAL:HG11	2:D:27:THR:H	1.72	0.53
1:A:379:LEU:HA	1:A:381:PHE:CE1	2.44	0.53
1:A:480:THR:HA	1:A:485:ILE:HG12	1.91	0.53
1:C:233:LEU:HB3	1:C:236:ARG:NH1	2.24	0.53
1:C:439:ILE:O	1:C:443:GLU:HG2	2.09	0.53
1:C:539:ARG:HB2	1:C:546:GLN:HE22	1.72	0.53
1:A:506:PHE:CE1	1:A:531:VAL:HG12	2.44	0.53
2:D:57:ILE:HD12	2:D:74:TYR:CE1	2.40	0.53
1:A:344:ILE:O	1:A:346:GLY:N	2.43	0.52
1:A:439:ILE:O	1:A:443:GLU:HG2	2.09	0.52
1:A:717:ARG:NH2	2:E:73:ASN:O	2.41	0.52
1:C:379:LEU:HA	1:C:381:PHE:CE1	2.44	0.52
1:A:372:ARG:HA	1:A:404:ASP:HB3	1.91	0.52
1:A:401:TYR:HE2	1:A:403:LEU:HB2	1.75	0.52
1:A:411:LEU:HD11	1:A:434:LEU:HD21	1.90	0.52
1:C:372:ARG:HA	1:C:404:ASP:HB3	1.91	0.52
1:A:500:LEU:HD13	1:A:537:PRO:HD2	1.90	0.52
1:C:64:PHE:HD1	1:C:96:PHE:HB3	1.73	0.52
1:A:315:LEU:O	1:A:319:LYS:NZ	2.37	0.52
1:A:616:LYS:HD2	1:A:617:PRO:CD	2.39	0.52
1:A:397:ASN:HB3	1:A:425:LYS:HG2	1.92	0.52
1:C:616:LYS:HD2	1:C:617:PRO:CD	2.39	0.52
1:A:605:SER:OG	1:A:607:SER:O	2.28	0.52
1:C:331:ARG:HG3	1:C:357:ASN:HA	1.90	0.52
1:C:576:ARG:CD	1:C:579:TYR:CE1	2.93	0.52
1:C:543:PRO:HA	1:C:546:GLN:HG2	1.91	0.52
1:C:401:TYR:HE2	1:C:403:LEU:HB2	1.75	0.52
1:C:464:ASP:OD1	1:C:464:ASP:N	2.41	0.52
1:C:119:ILE:O	1:C:145:ILE:HA	2.10	0.52
1:C:564:ILE:N	1:C:585:ILE:HG23	2.25	0.52
1:C:605:SER:OG	1:C:607:SER:O	2.28	0.52
1:A:119:ILE:O	1:A:145:ILE:HA	2.10	0.52
1:A:774:ARG:O	1:A:779:TYR:OH	2.23	0.52
1:A:464:ASP:N	1:A:464:ASP:OD1	2.41	0.51
1:A:620:ASP:OD2	1:A:622:ASN:ND2	2.43	0.51
1:C:620:ASP:OD2	1:C:622:ASN:ND2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:ASN:HB3	1:C:425:LYS:HG2	1.92	0.51
1:C:482:PHE:HE1	1:C:558:PRO:HG3	1.75	0.51
1:A:510:ALA:N	1:A:561:GLN:O	2.36	0.51
1:C:280:HIS:HB2	1:C:301:CYS:HB2	1.90	0.51
1:A:15:ASN:HD21	1:A:37:LEU:HG	1.76	0.51
1:A:280:HIS:HB2	1:A:301:CYS:HB2	1.90	0.51
1:A:475:PHE:HD1	1:A:478:ILE:HD11	1.76	0.51
1:A:564:ILE:N	1:A:585:ILE:HG23	2.25	0.51
1:A:783:LEU:O	1:A:799:ALA:N	2.44	0.51
1:C:379:LEU:HD11	1:C:408:LEU:HD11	1.92	0.51
1:A:7:VAL:O	1:A:29:ILE:HA	2.11	0.51
1:A:311:VAL:HA	1:A:335:VAL:HB	1.93	0.51
1:A:438:GLU:OE1	1:A:438:GLU:N	2.25	0.51
1:C:435:CYS:SG	1:C:463:GLY:HA3	2.51	0.51
1:C:701:PHE:O	1:C:704:THR:OG1	2.28	0.51
1:C:15:ASN:HD21	1:C:37:LEU:HG	1.76	0.51
2:D:11:LEU:HD11	2:D:57:ILE:HD11	1.93	0.51
1:A:339:SER:HA	1:A:366:GLY:HA3	1.93	0.51
1:A:413:ASP:OD2	1:A:415:SER:OG	2.25	0.51
1:A:630:VAL:O	1:A:759:PHE:HB2	2.11	0.51
1:C:7:VAL:O	1:C:29:ILE:HA	2.11	0.51
1:C:630:VAL:O	1:C:759:PHE:HB2	2.11	0.51
1:A:257:SER:O	1:A:260:GLN:HG3	2.12	0.50
1:A:379:LEU:HD11	1:A:408:LEU:HD11	1.91	0.50
1:A:482:PHE:HE1	1:A:558:PRO:HG3	1.75	0.50
1:A:142:ASP:OD1	1:A:348:ASN:ND2	2.36	0.50
1:A:97:GLU:HA	1:A:121:LYS:O	2.12	0.50
1:C:311:VAL:HA	1:C:335:VAL:HB	1.93	0.50
1:C:475:PHE:HD1	1:C:478:ILE:HD11	1.76	0.50
1:A:66:VAL:N	1:A:98:MET:SD	2.83	0.50
1:C:123:ASN:C	1:C:149:LYS:HB2	2.37	0.50
1:C:323:SER:N	1:C:326:SER:OG	2.37	0.50
1:C:344:ILE:O	1:C:346:GLY:N	2.43	0.50
1:C:611:ILE:HD13	1:C:803:ALA:HB3	1.94	0.50
1:C:783:LEU:O	1:C:799:ALA:N	2.44	0.50
1:A:123:ASN:C	1:A:149:LYS:HB2	2.37	0.50
1:C:29:ILE:HG12	1:C:57:ILE:HD12	1.94	0.50
1:C:38:MET:HB2	1:C:66:VAL:HG22	1.93	0.50
1:A:611:ILE:HD13	1:A:803:ALA:HB3	1.94	0.50
1:C:337:ASN:HA	1:C:365:SER:HB2	1.94	0.50
1:C:564:ILE:H	1:C:585:ILE:HG23	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ILE:HG12	1:A:57:ILE:HD12	1.94	0.50
1:A:435:CYS:SG	1:A:463:GLY:HA3	2.51	0.50
1:A:615:TRP:NE1	1:A:766:GLU:HA	2.26	0.50
1:A:771:SER:OG	1:A:772:GLY:N	2.45	0.50
1:C:46:PHE:CD1	1:C:69:LEU:HD22	2.46	0.50
1:C:783:LEU:N	1:C:799:ALA:O	2.45	0.50
1:A:568:THR:HG21	1:A:580:GLY:HA3	1.94	0.50
1:A:701:PHE:O	1:A:704:THR:OG1	2.28	0.50
1:C:97:GLU:HA	1:C:121:LYS:O	2.12	0.50
2:E:11:LEU:HD11	2:E:57:ILE:HD11	1.93	0.50
1:A:310:LYS:H	1:A:334:THR:HG1	1.54	0.49
1:A:783:LEU:N	1:A:799:ALA:O	2.45	0.49
1:C:611:ILE:HD11	1:C:779:TYR:HD1	1.77	0.49
2:D:15:LEU:HG	2:D:24:PHE:CE1	2.47	0.49
1:A:46:PHE:CD1	1:A:69:LEU:HD22	2.46	0.49
1:A:701:PHE:HE1	1:C:89:PHE:CZ	2.29	0.49
1:C:96:PHE:HD1	1:C:120:GLU:HB3	1.77	0.49
1:C:257:SER:O	1:C:260:GLN:HG3	2.12	0.49
1:A:138:ASP:N	1:A:138:ASP:OD1	2.45	0.49
1:A:198:SER:OG	1:A:229:ARG:NH1	2.45	0.49
1:A:611:ILE:HD11	1:A:779:TYR:HD1	1.77	0.49
1:C:83:ARG:O	1:C:113:THR:HB	2.13	0.49
1:C:339:SER:HA	1:C:366:GLY:HA3	1.93	0.49
1:C:615:TRP:NE1	1:C:766:GLU:HA	2.26	0.49
2:D:11:LEU:HD21	2:D:57:ILE:HD13	1.94	0.49
1:C:198:SER:OG	1:C:229:ARG:NH1	2.45	0.49
1:A:83:ARG:O	1:A:113:THR:HB	2.13	0.49
1:A:471:GLU:CB	1:A:581:ALA:HB2	2.43	0.49
1:C:500:LEU:HD21	1:C:539:ARG:CZ	2.43	0.49
1:C:705:PHE:O	1:C:709:LEU:HG	2.13	0.49
1:A:337:ASN:HA	1:A:365:SER:HB2	1.94	0.49
1:A:38:MET:HB2	1:A:66:VAL:HG22	1.93	0.49
1:C:39:PHE:O	1:C:42:ARG:NH2	2.28	0.49
1:A:370:ILE:HG22	1:A:405:ASN:OD1	2.13	0.49
1:C:529:TRP:CD2	1:C:565:PHE:HE1	2.31	0.49
1:A:231:PHE:CE1	1:A:247:HIS:HB3	2.48	0.48
1:C:79:LEU:HD21	1:C:82:ILE:HD11	1.95	0.48
1:C:370:ILE:HG22	1:C:405:ASN:OD1	2.13	0.48
1:A:496:ASP:OD1	1:A:498:ARG:NH2	2.47	0.48
1:A:564:ILE:H	1:A:585:ILE:HG23	1.77	0.48
1:A:610:GLN:HE21	1:A:769:VAL:HG12	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:TYR:HB3	1:C:117:VAL:HA	1.95	0.48
1:C:142:ASP:OD1	1:C:348:ASN:ND2	2.36	0.48
1:C:771:SER:OG	1:C:772:GLY:N	2.45	0.48
1:A:785:ALA:H	1:A:796:SER:N	2.11	0.48
1:C:63:LEU:HB2	1:C:95:ILE:HG13	1.96	0.48
1:C:596:SER:OG	1:C:620:ASP:OD1	2.30	0.48
2:E:11:LEU:HD21	2:E:57:ILE:HD13	1.95	0.48
2:E:15:LEU:HG	2:E:24:PHE:CE1	2.47	0.48
1:A:88:PHE:CZ	1:C:712:VAL:HG21	2.34	0.48
1:A:310:LYS:N	1:A:334:THR:OG1	2.29	0.48
1:A:500:LEU:HD21	1:A:539:ARG:CZ	2.43	0.48
1:A:89:PHE:HB2	1:C:708:TYR:CE2	2.44	0.48
1:C:66:VAL:N	1:C:98:MET:SD	2.83	0.48
1:A:116:SER:OG	1:A:117:VAL:N	2.47	0.48
1:A:469:GLU:HA	1:A:577:ARG:NH1	2.28	0.48
1:A:596:SER:OG	1:A:620:ASP:OD1	2.30	0.48
1:A:338:GLY:O	1:A:366:GLY:N	2.47	0.48
1:C:102:LYS:O	1:C:125:LEU:HD12	2.14	0.48
1:C:233:LEU:HB2	1:C:253:CYS:HB2	1.95	0.48
1:C:496:ASP:OD1	1:C:498:ARG:NH2	2.46	0.48
1:C:575:GLU:OE1	1:C:579:TYR:OH	2.23	0.48
1:A:529:TRP:CD2	1:A:565:PHE:HE1	2.31	0.48
1:C:91:TYR:HD1	1:C:116:SER:HB3	1.78	0.48
1:C:438:GLU:H	1:C:438:GLU:CD	2.19	0.48
1:A:63:LEU:HB2	1:A:95:ILE:HG13	1.95	0.48
1:A:241:CYS:HB2	1:A:282:ASN:ND2	2.29	0.48
1:A:91:TYR:HB3	1:A:117:VAL:HA	1.95	0.47
1:A:102:LYS:O	1:A:125:LEU:HD12	2.14	0.47
1:C:116:SER:OG	1:C:117:VAL:N	2.47	0.47
1:C:117:VAL:N	1:C:143:ASN:OD1	2.37	0.47
1:A:233:LEU:HB2	1:A:253:CYS:HB2	1.95	0.47
1:A:717:ARG:HB3	2:E:25:PHE:CD2	2.50	0.47
1:A:479:ARG:O	1:A:485:ILE:HA	2.15	0.47
1:A:695:GLU:HA	1:A:698:GLU:OE2	2.15	0.47
1:A:705:PHE:O	1:A:709:LEU:HG	2.13	0.47
1:C:231:PHE:CE1	1:C:247:HIS:HB3	2.49	0.47
1:A:79:LEU:HD21	1:A:82:ILE:HD11	1.95	0.47
1:A:91:TYR:HD1	1:A:116:SER:HB3	1.78	0.47
1:A:322:ASP:N	1:A:326:SER:OG	2.45	0.47
1:A:408:LEU:HD22	1:A:434:LEU:HD22	1.97	0.47
1:A:700:SER:O	1:A:704:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:SER:OG	1:C:224:LYS:O	2.23	0.47
1:C:338:GLY:O	1:C:366:GLY:N	2.47	0.47
1:C:404:ASP:O	1:C:406:GLN:NE2	2.47	0.47
1:C:691:GLN:N	1:C:694:LYS:HB2	2.30	0.47
1:A:70:GLU:HA	1:A:102:LYS:H	1.80	0.47
1:A:497:PHE:O	1:A:539:ARG:NH2	2.48	0.47
1:C:13:ILE:HD11	1:C:35:ILE:HG12	1.96	0.47
1:C:322:ASP:N	1:C:326:SER:OG	2.45	0.47
1:C:497:PHE:O	1:C:539:ARG:NH2	2.48	0.47
1:C:517:GLU:OE1	1:C:517:GLU:N	2.47	0.47
1:C:700:SER:O	1:C:704:THR:HG23	2.15	0.47
1:A:8:CYS:O	1:A:29:ILE:HG23	2.15	0.47
1:A:67:TYR:HD2	1:A:99:VAL:HB	1.79	0.47
1:A:65:ARG:NH2	2:D:12:VAL:HG11	2.29	0.47
1:A:95:ILE:HB	1:A:119:ILE:HG12	1.97	0.47
1:A:109:LEU:HD12	1:A:112:ILE:HD11	1.96	0.47
1:A:542:ASP:OD1	1:A:542:ASP:N	2.48	0.47
1:C:109:LEU:HD12	1:C:112:ILE:HD11	1.96	0.47
1:C:118:ARG:HG3	1:C:144:TYR:HB3	1.97	0.47
1:C:138:ASP:N	1:C:138:ASP:OD1	2.45	0.47
1:C:498:ARG:NH2	2:D:62:CYS:SG	2.82	0.47
1:A:21:HIS:CG	1:A:49:LEU:HD11	2.50	0.47
1:A:517:GLU:N	1:A:517:GLU:OE1	2.47	0.47
1:C:610:GLN:HE21	1:C:769:VAL:HG12	1.79	0.47
1:A:181:ARG:HB2	1:A:189:GLN:HB3	1.97	0.46
1:A:270:ARG:O	1:A:274:CYS:N	2.48	0.46
1:A:358:LEU:HG	1:A:359:GLY:H	1.80	0.46
1:C:67:TYR:HD2	1:C:99:VAL:HB	1.79	0.46
1:C:781:ILE:HB	1:C:801:VAL:HG22	1.97	0.46
1:A:13:ILE:HD11	1:A:35:ILE:HG12	1.96	0.46
1:A:144:TYR:O	1:A:145:ILE:HD13	2.15	0.46
1:C:8:CYS:O	1:C:29:ILE:HG23	2.15	0.46
1:C:21:HIS:CG	1:C:49:LEU:HD11	2.50	0.46
1:C:144:TYR:O	1:C:145:ILE:HD13	2.14	0.46
1:C:506:PHE:HB2	1:C:565:PHE:CE1	2.50	0.46
1:A:506:PHE:HB2	1:A:565:PHE:CE1	2.50	0.46
1:A:691:GLN:N	1:A:694:LYS:HB2	2.30	0.46
1:C:54:LEU:HG	1:C:79:LEU:HD13	1.98	0.46
1:C:57:ILE:HB	1:C:82:ILE:HD12	1.96	0.46
1:C:70:GLU:HA	1:C:102:LYS:H	1.80	0.46
1:C:695:GLU:HA	1:C:698:GLU:OE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:LEU:H	2:D:6:LEU:HD12	1.81	0.46
1:A:96:PHE:HD1	1:A:120:GLU:HB3	1.77	0.46
1:C:436:LEU:CD2	1:C:577:ARG:HD2	2.33	0.46
1:C:632:TRP:CE3	1:C:770:ILE:HG12	2.51	0.46
1:A:54:LEU:HG	1:A:79:LEU:HD13	1.98	0.46
1:A:57:ILE:HB	1:A:82:ILE:HD12	1.96	0.46
1:A:632:TRP:CE3	1:A:770:ILE:HG12	2.50	0.46
1:C:358:LEU:HG	1:C:359:GLY:H	1.80	0.46
1:C:509:GLU:HG2	1:C:562:TYR:CD1	2.51	0.46
1:C:785:ALA:H	1:C:796:SER:N	2.12	0.46
1:A:95:ILE:HB	1:A:119:ILE:HG23	1.97	0.46
1:A:393:LEU:HD13	1:A:397:ASN:OD1	2.16	0.46
1:C:258:PHE:CZ	1:C:262:LEU:HD11	2.51	0.46
1:C:479:ARG:O	1:C:485:ILE:HA	2.15	0.46
1:C:632:TRP:CH2	1:C:760:GLU:HB2	2.51	0.46
1:C:116:SER:HG	1:C:143:ASN:CG	2.19	0.46
2:E:6:LEU:HD13	2:E:66:CYS:HB3	1.98	0.46
1:A:79:LEU:O	1:A:109:LEU:HD22	2.16	0.46
1:A:404:ASP:O	1:A:406:GLN:NE2	2.47	0.46
1:C:95:ILE:HB	1:C:119:ILE:HG23	1.97	0.46
1:C:181:ARG:HB2	1:C:189:GLN:HB3	1.97	0.46
2:E:19:CYS:HB3	2:E:75:CYS:HB3	1.73	0.46
1:A:509:GLU:HG2	1:A:562:TYR:CD1	2.51	0.46
1:A:616:LYS:HD2	1:A:617:PRO:N	2.31	0.46
1:C:430:TYR:HA	1:C:461:THR:HB	1.97	0.46
1:C:606:ASN:ND2	1:C:612:ILE:HB	2.31	0.46
1:A:116:SER:HG	1:A:143:ASN:CG	2.20	0.46
1:A:258:PHE:CZ	1:A:262:LEU:HD11	2.51	0.46
1:A:471:GLU:HG2	1:A:577:ARG:HH22	1.81	0.46
1:A:480:THR:HB	1:A:588:VAL:CG2	2.46	0.46
1:A:632:TRP:CH2	1:A:760:GLU:HB2	2.51	0.46
1:C:270:ARG:O	1:C:274:CYS:N	2.48	0.46
1:C:421:ILE:HG12	1:C:451:ARG:HH12	1.81	0.46
1:A:118:ARG:HG3	1:A:144:TYR:HB3	1.97	0.45
1:C:21:HIS:ND1	1:C:49:LEU:HD11	2.31	0.45
1:C:249:GLN:HB2	1:C:251:TRP:HD1	1.80	0.45
1:A:414:TRP:HH2	1:A:419:LEU:HB3	1.81	0.45
1:A:430:TYR:HA	1:A:461:THR:HB	1.97	0.45
1:A:495:PRO:O	2:E:5:HIS:CE1	2.69	0.45
1:A:634:ARG:HG3	1:A:777:THR:HG21	1.98	0.45
2:D:6:LEU:HD13	2:D:66:CYS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:LEU:HD12	2:E:6:LEU:H	1.81	0.45
1:A:281:ASN:HB3	1:A:283:LYS:HE3	1.98	0.45
1:A:606:ASN:ND2	1:A:612:ILE:HB	2.31	0.45
1:A:716:PRO:HB3	2:E:74:TYR:HE2	1.81	0.45
1:A:762:VAL:HG21	1:A:768:LEU:HB2	1.98	0.45
1:A:781:ILE:HB	1:A:801:VAL:HG22	1.97	0.45
1:C:762:VAL:HG21	1:C:768:LEU:HB2	1.98	0.45
1:A:196:CYS:SG	1:A:199:HIS:HB2	2.56	0.45
1:A:381:PHE:O	1:A:383:ARG:N	2.49	0.45
1:A:488:ARG:HA	1:A:550:GLY:CA	2.46	0.45
1:A:594:ASN:OD1	1:A:797:VAL:HG13	2.16	0.45
1:C:196:CYS:SG	1:C:199:HIS:HB2	2.56	0.45
1:C:350:LEU:HA	1:C:353:GLU:CD	2.42	0.45
1:C:488:ARG:HA	1:C:550:GLY:CA	2.46	0.45
1:A:345:ARG:HD2	1:C:704:THR:HG21	1.98	0.45
1:A:613:LEU:HG	1:A:615:TRP:CE3	2.52	0.45
1:A:615:TRP:HH2	1:A:762:VAL:HG21	1.82	0.45
1:C:230:ASN:HD22	1:C:239:GLU:HG3	1.82	0.45
1:C:291:GLY:H	1:C:310:LYS:NZ	2.14	0.45
1:C:616:LYS:HD2	1:C:617:PRO:N	2.31	0.45
1:A:121:LYS:HB3	1:A:121:LYS:HE3	1.64	0.45
1:A:217:SER:OG	1:A:224:LYS:O	2.23	0.45
1:A:701:PHE:CE1	1:C:89:PHE:CZ	3.04	0.45
1:C:95:ILE:HB	1:C:119:ILE:HG12	1.97	0.45
1:C:98:MET:HE3	1:C:98:MET:HB3	1.86	0.45
1:C:358:LEU:HD21	1:C:382:PHE:CE1	2.52	0.45
1:C:414:TRP:HH2	1:C:419:LEU:HB3	1.81	0.45
1:C:594:ASN:OD1	1:C:797:VAL:HG13	2.16	0.45
1:C:344:ILE:HG21	1:C:350:LEU:CD2	2.47	0.45
1:C:542:ASP:OD1	1:C:542:ASP:N	2.48	0.45
1:A:291:GLY:H	1:A:310:LYS:NZ	2.14	0.45
1:A:484:LYS:HE3	1:A:484:LYS:HB3	1.84	0.45
1:C:50:SER:HA	1:C:75:LEU:HD23	1.99	0.45
1:C:79:LEU:O	1:C:109:LEU:HD22	2.16	0.45
1:A:358:LEU:HD21	1:A:382:PHE:CE1	2.52	0.45
1:A:600:ASP:O	1:A:615:TRP:HA	2.17	0.45
1:C:491:PRO:HD2	1:C:548:HIS:ND1	2.32	0.45
1:C:600:ASP:O	1:C:615:TRP:HA	2.17	0.45
1:C:613:LEU:HG	1:C:615:TRP:CZ3	2.52	0.45
1:A:196:CYS:HB2	1:A:199:HIS:CD2	2.51	0.45
1:A:613:LEU:HG	1:A:615:TRP:CZ3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ASN:ND2	1:C:37:LEU:HG	2.32	0.45
1:C:73:LYS:HB2	1:C:105:GLY:HA3	1.99	0.45
1:C:281:ASN:HB3	1:C:283:LYS:HE3	1.98	0.45
1:C:393:LEU:HD13	1:C:397:ASN:OD1	2.16	0.45
1:C:408:LEU:HD22	1:C:434:LEU:HD22	1.97	0.45
1:C:480:THR:HB	1:C:588:VAL:CG2	2.46	0.45
1:C:634:ARG:HG3	1:C:777:THR:HG21	1.98	0.45
1:C:702:ARG:HA	1:C:702:ARG:HH11	1.82	0.45
1:C:783:LEU:H	1:C:799:ALA:H	1.64	0.45
1:A:21:HIS:ND1	1:A:49:LEU:HD11	2.31	0.44
1:A:96:PHE:HA	1:A:122:ASN:HD21	1.81	0.44
1:A:350:LEU:HA	1:A:353:GLU:CD	2.42	0.44
1:A:606:ASN:HD21	1:A:769:VAL:HG13	1.82	0.44
1:C:8:CYS:HB2	1:C:29:ILE:HD12	1.99	0.44
1:C:96:PHE:HA	1:C:122:ASN:HD21	1.81	0.44
1:C:121:LYS:HE3	1:C:121:LYS:HB3	1.64	0.44
1:C:493:TRP:CE3	1:C:493:TRP:HA	2.52	0.44
1:C:606:ASN:HD21	1:C:769:VAL:HG13	1.82	0.44
1:A:73:LYS:HB2	1:A:105:GLY:HA3	1.99	0.44
1:A:230:ASN:HD22	1:A:239:GLU:HG3	1.82	0.44
1:A:434:LEU:O	1:A:463:GLY:N	2.51	0.44
1:A:471:GLU:O	1:A:581:ALA:HB1	2.17	0.44
1:A:78:ASN:HA	1:A:108:ASN:ND2	2.33	0.44
1:A:248:PHE:HB2	1:A:254:VAL:HG22	2.00	0.44
1:A:421:ILE:HG12	1:A:451:ARG:HH12	1.81	0.44
1:A:427:PHE:HE1	1:C:454:ARG:NH1	2.16	0.44
1:A:782:GLU:HG3	1:A:798:ALA:HB1	1.99	0.44
1:C:119:ILE:HD12	1:C:145:ILE:HD12	2.00	0.44
1:C:434:LEU:O	1:C:463:GLY:N	2.51	0.44
1:A:231:PHE:HA	1:A:251:TRP:O	2.18	0.44
1:A:344:ILE:HG21	1:A:350:LEU:CD2	2.47	0.44
1:A:371:ARG:HG2	1:A:372:ARG:NH1	2.32	0.44
1:A:632:TRP:NE1	1:A:758:PRO:HG2	2.33	0.44
1:C:371:ARG:HG2	1:C:372:ARG:NH1	2.32	0.44
1:C:544:LYS:H	1:C:544:LYS:HG3	1.59	0.44
1:A:414:TRP:CD2	1:A:445:VAL:HG21	2.53	0.44
1:A:491:PRO:HD2	1:A:548:HIS:ND1	2.32	0.44
1:C:209:HIS:ND1	1:C:222:PRO:HD3	2.32	0.44
1:A:209:HIS:ND1	1:A:222:PRO:HD3	2.33	0.44
1:A:367:TYR:HB2	1:A:399:SER:O	2.18	0.44
1:C:260:GLN:NE2	1:C:261:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:637:GLU:OE2	1:C:804:ARG:NH2	2.51	0.44
1:A:209:HIS:HB3	1:A:212:CYS:SG	2.58	0.44
1:C:209:HIS:HB3	1:C:212:CYS:SG	2.58	0.44
1:C:362:GLU:HA	1:C:385:LEU:HA	2.00	0.44
1:C:381:PHE:O	1:C:383:ARG:N	2.49	0.44
1:A:72:LEU:HD13	1:A:76:PHE:HD1	1.83	0.44
1:A:291:GLY:H	1:A:310:LYS:HZ1	1.64	0.44
1:A:544:LYS:H	1:A:544:LYS:HG3	1.59	0.44
1:C:480:THR:OG1	1:C:481:SER:N	2.51	0.44
1:A:50:SER:HA	1:A:75:LEU:HD23	1.99	0.44
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.89	0.44
1:A:119:ILE:HD12	1:A:145:ILE:HD12	2.00	0.44
1:A:700:SER:OG	1:C:345:ARG:HD3	2.17	0.44
1:C:231:PHE:HA	1:C:251:TRP:O	2.18	0.44
1:C:321:ILE:HA	1:C:326:SER:HB2	2.00	0.44
1:C:613:LEU:HG	1:C:615:TRP:CE3	2.52	0.44
1:C:615:TRP:HH2	1:C:762:VAL:HG21	1.82	0.44
1:C:782:GLU:HG3	1:C:798:ALA:HB1	1.99	0.44
1:A:260:GLN:NE2	1:A:261:ASP:OD1	2.51	0.43
1:A:702:ARG:HH11	1:A:702:ARG:HA	1.82	0.43
1:A:783:LEU:H	1:A:799:ALA:H	1.64	0.43
1:C:196:CYS:HB2	1:C:199:HIS:CD2	2.51	0.43
1:C:401:TYR:HA	1:C:427:PHE:HB3	2.00	0.43
1:C:470:ASN:HD21	1:C:577:ARG:HH21	1.63	0.43
1:C:506:PHE:HA	1:C:530:THR:O	2.18	0.43
1:A:73:LYS:HB2	1:A:105:GLY:CA	2.48	0.43
1:C:38:MET:O	1:C:66:VAL:HA	2.19	0.43
1:C:248:PHE:HB2	1:C:254:VAL:HG22	2.00	0.43
1:C:529:TRP:CE3	1:C:529:TRP:HA	2.53	0.43
1:C:599:LEU:O	1:C:616:LYS:HB3	2.18	0.43
1:C:692:ILE:HG13	1:C:693:LEU:N	2.32	0.43
1:A:8:CYS:HB2	1:A:29:ILE:HD12	1.99	0.43
1:A:599:LEU:O	1:A:616:LYS:HB3	2.18	0.43
1:C:367:TYR:HB2	1:C:399:SER:O	2.18	0.43
1:C:484:LYS:HB3	1:C:484:LYS:HE3	1.84	0.43
1:C:484:LYS:CA	1:C:553:MET:O	2.48	0.43
1:C:607:SER:HB3	1:C:610:GLN:HB2	2.00	0.43
1:C:632:TRP:NE1	1:C:758:PRO:HG2	2.33	0.43
1:A:401:TYR:HA	1:A:427:PHE:HB3	2.00	0.43
1:A:404:ASP:C	1:A:406:GLN:HE21	2.26	0.43
1:A:448:THR:HG1	1:A:452:GLN:NE2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:TRP:HA	1:A:529:TRP:CE3	2.53	0.43
1:A:601:PRO:HB3	1:A:615:TRP:HB3	2.01	0.43
1:C:78:ASN:HA	1:C:108:ASN:ND2	2.33	0.43
1:C:112:ILE:HB	1:C:137:LEU:HD11	2.01	0.43
1:C:146:VAL:HG12	1:C:147:LEU:N	2.33	0.43
1:A:37:LEU:HD12	1:A:39:PHE:CE2	2.53	0.43
1:A:479:ARG:HB3	1:A:486:LEU:HB2	2.00	0.43
1:A:480:THR:OG1	1:A:481:SER:N	2.51	0.43
1:A:781:ILE:O	1:A:800:TYR:HA	2.19	0.43
1:C:72:LEU:HD13	1:C:76:PHE:HD1	1.83	0.43
1:C:241:CYS:HB2	1:C:282:ASN:ND2	2.29	0.43
1:C:781:ILE:O	1:C:800:TYR:HA	2.19	0.43
1:A:52:PRO:HB2	1:A:78:ASN:ND2	2.33	0.43
1:C:73:LYS:HB2	1:C:105:GLY:CA	2.48	0.43
1:C:414:TRP:CD2	1:C:445:VAL:HG21	2.53	0.43
1:A:241:CYS:O	1:A:282:ASN:ND2	2.52	0.43
1:A:429:HIS:HB3	1:A:430:TYR:HD2	1.83	0.43
1:A:493:TRP:HA	1:A:493:TRP:CE3	2.53	0.43
1:C:52:PRO:HB2	1:C:78:ASN:ND2	2.33	0.43
1:C:500:LEU:O	1:C:501:LEU:HD23	2.19	0.43
1:C:503:PHE:H	1:C:534:ILE:HB	1.84	0.43
1:C:576:ARG:HD3	1:C:579:TYR:HE1	1.83	0.43
1:A:15:ASN:ND2	1:A:37:LEU:HG	2.32	0.43
1:A:33:LEU:O	1:A:61:LEU:HD23	2.19	0.43
1:A:38:MET:O	1:A:66:VAL:HA	2.19	0.43
1:A:80:THR:HA	1:A:109:LEU:HA	2.01	0.43
1:A:321:ILE:HA	1:A:326:SER:HB2	2.00	0.43
1:A:615:TRP:HZ2	1:A:762:VAL:HB	1.84	0.43
1:A:632:TRP:HA	1:A:780:ARG:O	2.19	0.43
1:A:637:GLU:OE2	1:A:804:ARG:NH2	2.51	0.43
1:A:701:PHE:CE1	1:C:89:PHE:HZ	2.36	0.43
1:C:37:LEU:HD12	1:C:39:PHE:CE2	2.53	0.43
1:C:291:GLY:H	1:C:310:LYS:HZ1	1.67	0.43
1:A:432:PRO:HA	1:A:464:ASP:OD1	2.19	0.43
1:A:692:ILE:HG13	1:A:693:LEU:N	2.32	0.43
1:C:80:THR:HA	1:C:109:LEU:HA	2.01	0.43
1:C:632:TRP:HA	1:C:780:ARG:O	2.18	0.43
1:A:96:PHE:CE1	1:A:120:GLU:HB3	2.54	0.43
1:A:146:VAL:HG12	1:A:147:LEU:N	2.32	0.43
1:A:362:GLU:HA	1:A:385:LEU:HA	2.00	0.43
1:A:449:LYS:HA	1:A:449:LYS:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:LEU:CD1	1:A:536:PRO:HB3	2.49	0.43
1:A:506:PHE:HA	1:A:530:THR:O	2.18	0.43
1:C:10:GLY:HA3	1:C:32:HIS:O	2.18	0.43
1:C:247:HIS:CE1	1:C:282:ASN:HD22	2.37	0.43
1:C:500:LEU:CD1	1:C:536:PRO:HB3	2.49	0.43
1:A:249:GLN:HB2	1:A:251:TRP:NE1	2.34	0.42
1:C:33:LEU:O	1:C:61:LEU:HD23	2.19	0.42
1:C:298:ASN:HD21	1:C:300:LEU:HD23	1.84	0.42
1:C:334:THR:HA	1:C:360:LEU:O	2.19	0.42
1:C:432:PRO:HA	1:C:464:ASP:OD1	2.19	0.42
1:C:479:ARG:HB3	1:C:486:LEU:HB2	2.00	0.42
1:A:12:ASP:OD1	1:A:13:ILE:N	2.52	0.42
1:A:298:ASN:HD21	1:A:300:LEU:HD23	1.84	0.42
1:A:397:ASN:HD22	1:A:425:LYS:HG2	1.84	0.42
1:A:487:LEU:HD23	1:A:487:LEU:HA	1.81	0.42
1:C:120:GLU:OE2	1:C:147:LEU:HB2	2.19	0.42
1:C:241:CYS:O	1:C:282:ASN:ND2	2.52	0.42
1:C:709:LEU:O	1:C:712:VAL:HG22	2.19	0.42
1:A:31:GLY:O	1:A:59:ASP:HB2	2.19	0.42
1:A:503:PHE:H	1:A:534:ILE:HB	1.84	0.42
1:A:607:SER:HB3	1:A:610:GLN:HB2	2.00	0.42
1:A:702:ARG:HH12	1:A:705:PHE:HB3	1.84	0.42
1:C:12:ASP:OD1	1:C:13:ILE:N	2.52	0.42
1:C:93:LEU:HB2	1:C:117:VAL:CG1	2.50	0.42
1:C:231:PHE:HB3	1:C:253:CYS:SG	2.60	0.42
1:C:397:ASN:HD22	1:C:425:LYS:HG2	1.84	0.42
1:A:278:VAL:HA	1:A:299:LEU:HB3	2.02	0.42
1:A:336:ILE:N	1:A:363:GLU:OE1	2.48	0.42
1:A:784:GLN:HB3	1:A:796:SER:O	2.20	0.42
1:C:280:HIS:O	1:C:283:LYS:HB2	2.20	0.42
1:C:404:ASP:C	1:C:406:GLN:HE21	2.26	0.42
1:C:436:LEU:CD2	1:C:577:ARG:HD3	2.43	0.42
1:A:120:GLU:OE2	1:A:147:LEU:HB2	2.19	0.42
1:A:247:HIS:CE1	1:A:282:ASN:HD22	2.37	0.42
1:A:500:LEU:O	1:A:501:LEU:HD23	2.19	0.42
1:C:35:ILE:HB	1:C:63:LEU:HD23	2.01	0.42
1:C:56:MET:HE3	1:C:56:MET:HB2	1.91	0.42
1:C:601:PRO:HB3	1:C:615:TRP:HB3	2.01	0.42
1:C:630:VAL:HA	1:C:782:GLU:O	2.20	0.42
1:A:35:ILE:HB	1:A:63:LEU:HD23	2.01	0.42
1:A:781:ILE:HB	1:A:801:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:LEU:HG	1:C:38:MET:HE1	2.02	0.42
1:C:692:ILE:HG13	1:C:693:LEU:HG	2.01	0.42
2:D:21:GLU:H	2:D:21:GLU:CD	2.28	0.42
1:A:38:MET:HE2	1:A:38:MET:HB3	1.90	0.42
1:A:112:ILE:HB	1:A:137:LEU:HD11	2.01	0.42
1:A:266:CYS:HA	1:A:269:SER:H	1.85	0.42
1:A:710:HIS:HB3	1:A:714:PHE:HE2	1.85	0.42
1:C:89:PHE:HB3	1:C:91:TYR:CE2	2.55	0.42
1:C:96:PHE:CE1	1:C:120:GLU:HB3	2.54	0.42
1:C:487:LEU:HD23	1:C:487:LEU:HA	1.81	0.42
1:C:781:ILE:HB	1:C:801:VAL:CG2	2.50	0.42
1:A:613:LEU:HD22	1:A:781:ILE:HG21	2.02	0.41
1:A:779:TYR:O	1:A:802:SER:HA	2.20	0.41
1:C:38:MET:HE2	1:C:38:MET:HB3	1.90	0.41
1:C:702:ARG:HH12	1:C:705:PHE:HB3	1.84	0.41
1:A:39:PHE:HE1	1:A:65:ARG:HB3	1.85	0.41
1:A:52:PRO:O	1:A:78:ASN:ND2	2.46	0.41
1:A:93:LEU:HB2	1:A:117:VAL:CG1	2.50	0.41
1:A:231:PHE:HB3	1:A:253:CYS:SG	2.60	0.41
1:A:401:TYR:CE2	1:A:403:LEU:HB2	2.55	0.41
1:A:709:LEU:O	1:A:712:VAL:HG22	2.20	0.41
1:C:31:GLY:O	1:C:59:ASP:HB2	2.19	0.41
1:C:496:ASP:CG	1:C:498:ARG:HH21	2.28	0.41
1:A:89:PHE:HB3	1:A:91:TYR:CE2	2.55	0.41
1:A:280:HIS:O	1:A:283:LYS:HB2	2.20	0.41
1:A:692:ILE:HG13	1:A:693:LEU:HG	2.01	0.41
1:C:89:PHE:N	1:C:325:THR:HG21	2.35	0.41
1:C:97:GLU:OE1	1:C:121:LYS:HB3	2.20	0.41
1:C:350:LEU:CD1	1:C:354:LEU:HB2	2.48	0.41
1:C:440:HIS:HA	1:C:443:GLU:HG2	2.03	0.41
1:A:34:GLN:HA	1:A:62:LEU:HB3	2.03	0.41
1:A:100:HIS:HA	1:A:124:GLU:HG3	2.02	0.41
1:C:610:GLN:NE2	1:C:771:SER:HB2	2.36	0.41
1:C:697:GLU:HG2	1:C:698:GLU:OE1	2.20	0.41
1:C:784:GLN:HB3	1:C:796:SER:O	2.20	0.41
1:A:56:MET:HE3	1:A:56:MET:HB2	1.91	0.41
1:A:89:PHE:N	1:A:325:THR:HG21	2.35	0.41
1:A:97:GLU:OE1	1:A:121:LYS:HB3	2.19	0.41
1:A:246:TYR:HD1	1:A:282:ASN:HA	1.86	0.41
1:A:334:THR:HA	1:A:360:LEU:O	2.20	0.41
1:A:350:LEU:CD1	1:A:354:LEU:HB2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:HIS:HA	1:A:443:GLU:HG2	2.03	0.41
1:A:697:GLU:HG2	1:A:698:GLU:OE1	2.21	0.41
1:C:56:MET:O	1:C:57:ILE:HD13	2.21	0.41
1:C:146:VAL:HG12	1:C:147:LEU:CD2	2.51	0.41
1:A:182:CYS:HA	1:A:188:CYS:HA	2.03	0.41
1:A:289:PRO:HG2	1:A:292:TYR:CD2	2.56	0.41
1:A:630:VAL:HA	1:A:782:GLU:O	2.20	0.41
1:A:714:PHE:CD2	2:E:57:ILE:HG21	2.56	0.41
1:C:199:HIS:HA	1:C:212:CYS:O	2.21	0.41
1:C:249:GLN:HB2	1:C:251:TRP:NE1	2.34	0.41
1:C:576:ARG:NH2	1:C:579:TYR:HA	2.36	0.41
1:C:710:HIS:HB3	1:C:714:PHE:HE2	1.85	0.41
2:E:8:GLY:O	2:E:12:VAL:HG23	2.21	0.41
1:A:17:LEU:HG	1:A:38:MET:HE1	2.02	0.41
1:A:322:ASP:H	1:A:326:SER:CB	2.34	0.41
1:A:436:LEU:HA	1:A:439:ILE:HB	2.03	0.41
1:A:442:MET:O	1:A:446:SER:N	2.54	0.41
1:C:266:CYS:HA	1:C:269:SER:H	1.84	0.41
1:C:289:PRO:HG2	1:C:292:TYR:CD2	2.56	0.41
1:C:796:SER:OG	1:C:797:VAL:N	2.54	0.41
1:C:69:LEU:HD12	1:C:70:GLU:H	1.86	0.41
1:C:576:ARG:HD3	1:C:579:TYR:CZ	2.55	0.41
2:D:8:GLY:O	2:D:12:VAL:HG23	2.21	0.41
1:A:6:GLU:HB3	1:A:8:CYS:SG	2.60	0.41
1:A:247:HIS:ND1	1:A:282:ASN:O	2.54	0.41
1:A:496:ASP:CG	1:A:498:ARG:HH21	2.29	0.41
1:C:37:LEU:HD12	1:C:39:PHE:HE2	1.86	0.41
1:C:106:LEU:HD23	1:C:106:LEU:HA	1.72	0.41
1:C:121:LYS:HD2	1:C:147:LEU:HG	2.03	0.41
1:C:202:THR:HG23	1:C:206:LEU:O	2.21	0.41
1:C:213:LEU:HD13	1:C:229:ARG:HD3	2.03	0.41
1:C:278:VAL:HA	1:C:299:LEU:HB3	2.02	0.41
1:C:280:HIS:ND1	1:C:289:PRO:HG3	2.36	0.41
1:C:442:MET:O	1:C:446:SER:N	2.54	0.41
1:C:469:GLU:CA	1:C:577:ARG:HH12	2.11	0.41
1:C:613:LEU:HD22	1:C:781:ILE:HG21	2.02	0.41
2:E:21:GLU:H	2:E:21:GLU:CD	2.28	0.41
1:A:56:MET:O	1:A:57:ILE:HD13	2.21	0.41
1:A:199:HIS:HA	1:A:212:CYS:O	2.20	0.41
1:A:294:MET:H	1:A:294:MET:HG3	1.68	0.41
1:A:576:ARG:HH22	1:A:579:TYR:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:GLN:NE2	1:A:771:SER:HB2	2.36	0.41
1:A:796:SER:OG	1:A:797:VAL:N	2.54	0.41
1:C:100:HIS:HA	1:C:124:GLU:HG3	2.03	0.41
1:C:261:ASP:O	1:C:265:LYS:HG3	2.21	0.41
1:C:290:SER:HA	1:C:310:LYS:HZ3	1.85	0.41
1:C:585:ILE:HD12	1:C:585:ILE:H	1.86	0.41
1:C:599:LEU:HB2	1:C:616:LYS:HG3	2.03	0.41
1:C:779:TYR:O	1:C:802:SER:HA	2.20	0.41
2:D:57:ILE:O	2:D:61:CYS:N	2.47	0.41
1:A:146:VAL:HG12	1:A:147:LEU:CD2	2.51	0.40
1:A:632:TRP:CD1	1:A:758:PRO:HG2	2.57	0.40
1:C:39:PHE:HE1	1:C:65:ARG:HB3	1.85	0.40
1:C:52:PRO:O	1:C:78:ASN:ND2	2.46	0.40
1:C:322:ASP:H	1:C:326:SER:CB	2.34	0.40
1:A:89:PHE:HD1	1:C:708:TYR:CE2	2.39	0.40
1:A:121:LYS:HD2	1:A:147:LEU:HG	2.03	0.40
1:A:208:CYS:CA	1:A:220:ASP:H	2.30	0.40
1:A:427:PHE:HE1	1:C:454:ARG:HH12	1.69	0.40
1:A:537:PRO:HB3	1:A:549:PRO:HB3	2.04	0.40
1:C:436:LEU:HA	1:C:439:ILE:HB	2.03	0.40
1:C:438:GLU:HA	1:C:441:LYS:HB3	2.03	0.40
1:C:615:TRP:HZ2	1:C:762:VAL:HB	1.84	0.40
1:C:705:PHE:CE1	1:C:709:LEU:HD21	2.56	0.40
1:A:280:HIS:ND1	1:A:289:PRO:HG3	2.36	0.40
1:A:354:LEU:HD12	1:A:357:ASN:HD21	1.86	0.40
1:A:477:TYR:HB2	1:A:488:ARG:HB2	2.04	0.40
1:A:702:ARG:HH12	1:A:705:PHE:HD2	1.70	0.40
1:C:182:CYS:HA	1:C:188:CYS:HA	2.03	0.40
1:C:315:LEU:HG	1:C:316:GLU:HG3	2.03	0.40
1:C:449:LYS:HA	1:C:449:LYS:HD2	1.82	0.40
1:C:776:PHE:HD1	1:C:807:PRO:HB3	1.87	0.40
1:C:786:CYS:SG	1:C:795:CYS:N	2.94	0.40
1:A:483:ASP:O	1:A:554:ARG:HA	2.21	0.40
1:A:599:LEU:HB2	1:A:616:LYS:HG3	2.03	0.40
1:C:483:ASP:O	1:C:554:ARG:HA	2.21	0.40
1:A:202:THR:HG23	1:A:206:LEU:O	2.21	0.40
1:A:335:VAL:HG13	1:A:363:GLU:HB3	2.03	0.40
1:C:73:LYS:HE2	1:C:184:THR:OG1	2.21	0.40
1:C:247:HIS:ND1	1:C:282:ASN:O	2.54	0.40
1:C:436:LEU:HD11	1:C:577:ARG:HG3	2.03	0.40
1:C:508:LYS:HE3	1:C:508:LYS:HB3	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:510:ALA:HB3	1:C:561:GLN:CB	2.51	0.40
1:C:632:TRP:CD1	1:C:758:PRO:HG2	2.56	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	660/1355 (49%)	571 (86%)	89 (14%)	0	100	100
1	C	660/1355 (49%)	571 (86%)	89 (14%)	0	100	100
2	D	44/74 (60%)	39 (89%)	5 (11%)	0	100	100
2	E	44/74 (60%)	39 (89%)	5 (11%)	0	100	100
All	All	1408/2858 (49%)	1220 (87%)	188 (13%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	618/1212 (51%)	618 (100%)	0	100	100
1	C	618/1212 (51%)	618 (100%)	0	100	100
2	D	43/65 (66%)	43 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	43/65 (66%)	43 (100%)	0	100	100
All	All	1322/2554 (52%)	1322 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	25	ASN
1	A	90	ASN
1	A	199	HIS
1	A	209	HIS
1	A	263	HIS
1	A	276	GLN
1	A	282	ASN
1	A	337	ASN
1	A	397	ASN
1	A	452	GLN
1	A	610	GLN
1	A	627	HIS
1	C	15	ASN
1	C	25	ASN
1	C	90	ASN
1	C	199	HIS
1	C	263	HIS
1	C	276	GLN
1	C	282	ASN
1	C	337	ASN
1	C	397	ASN
1	C	423	GLN
1	C	452	GLN
1	C	470	ASN
1	C	541	ASN
1	C	610	GLN
1	C	627	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

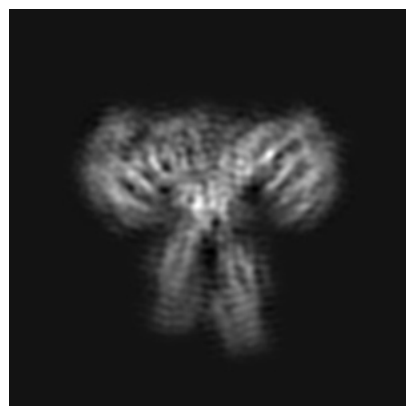
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30231. These allow visual inspection of the internal detail of the map and identification of artifacts.

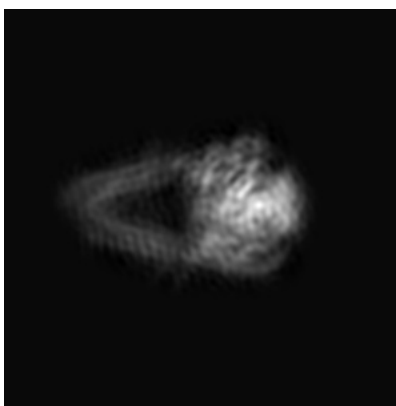
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

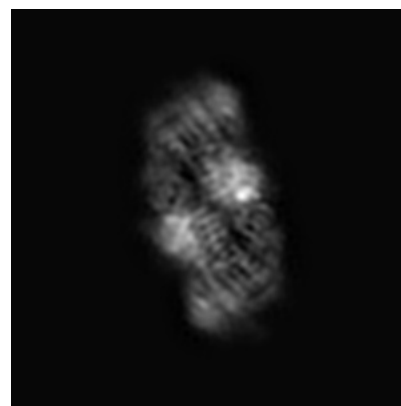
6.1.1 Primary map



X

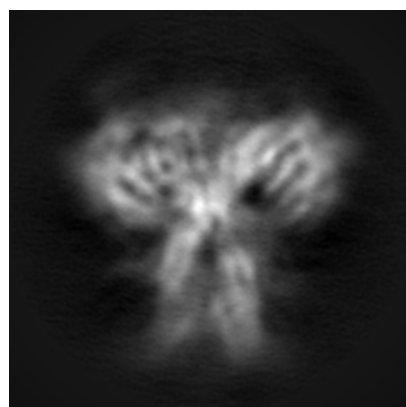


Y

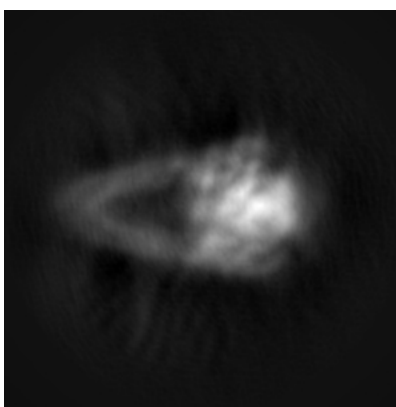


Z

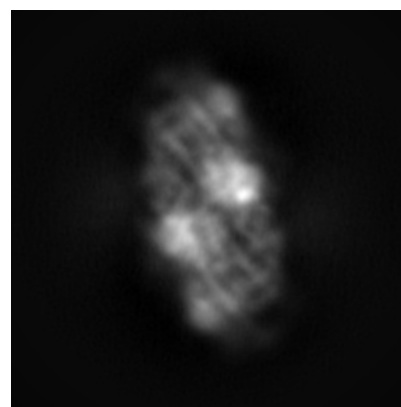
6.1.2 Raw map



X



Y

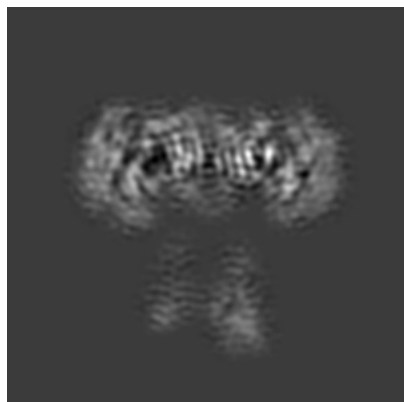


Z

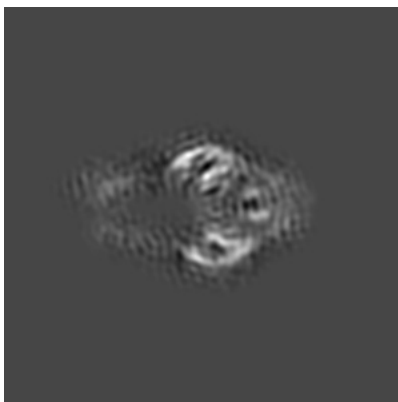
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

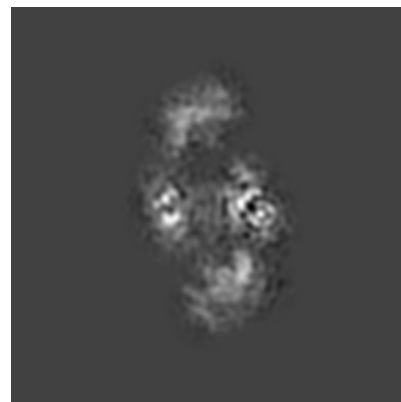
6.2.1 Primary map



X Index: 80

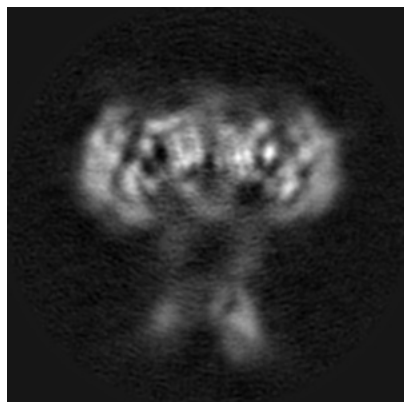


Y Index: 80

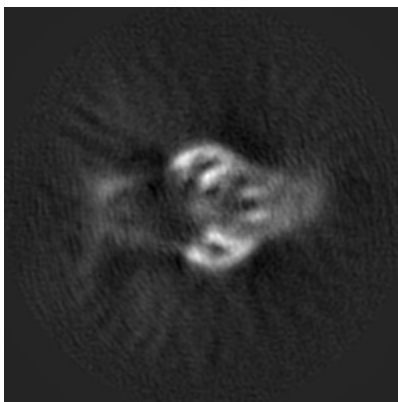


Z Index: 80

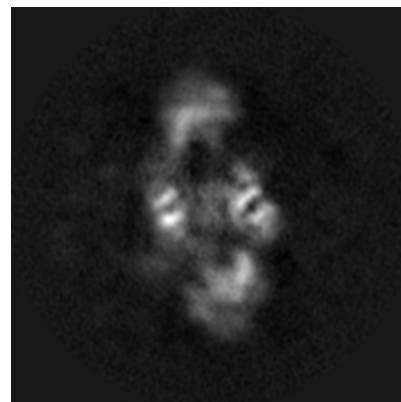
6.2.2 Raw map



X Index: 80



Y Index: 80

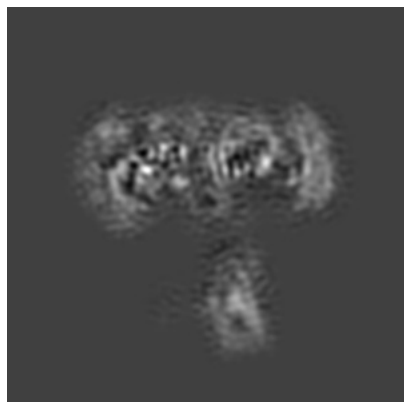


Z Index: 80

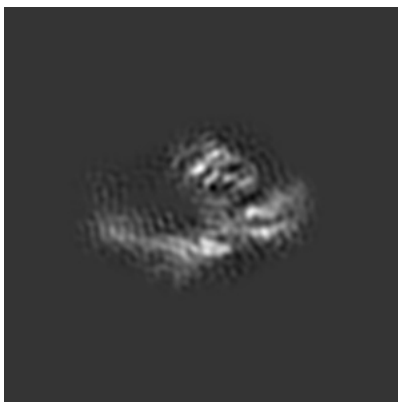
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 85

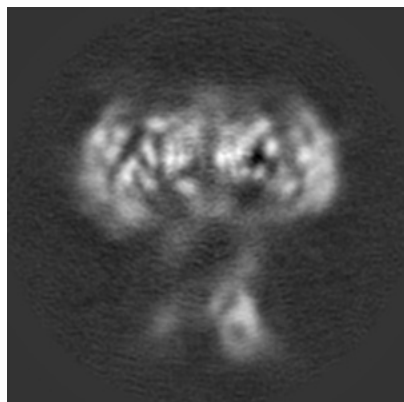


Y Index: 75

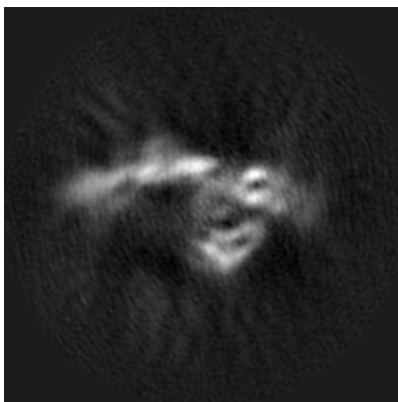


Z Index: 98

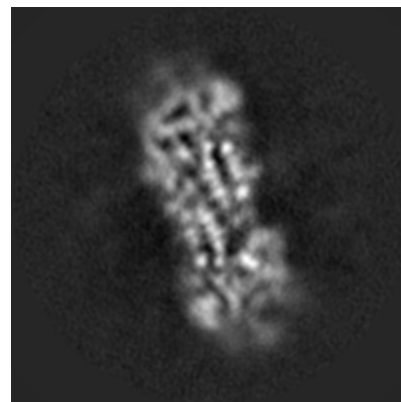
6.3.2 Raw map



X Index: 82



Y Index: 86



Z Index: 98

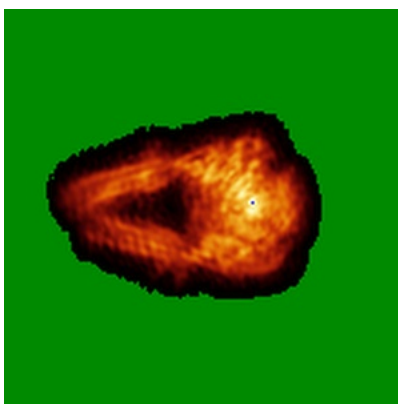
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

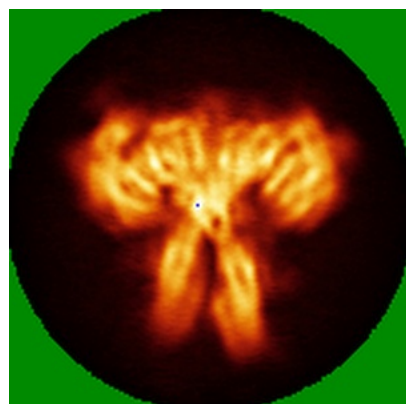


Y

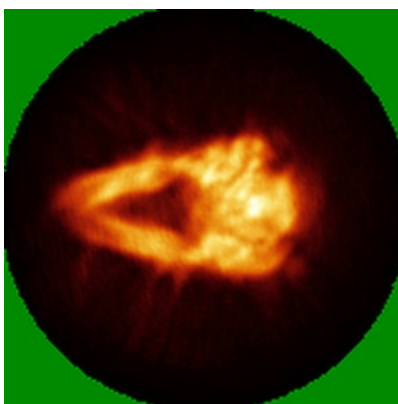


Z

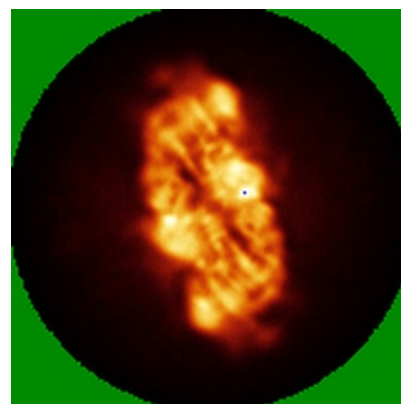
6.4.2 Raw map



X



Y

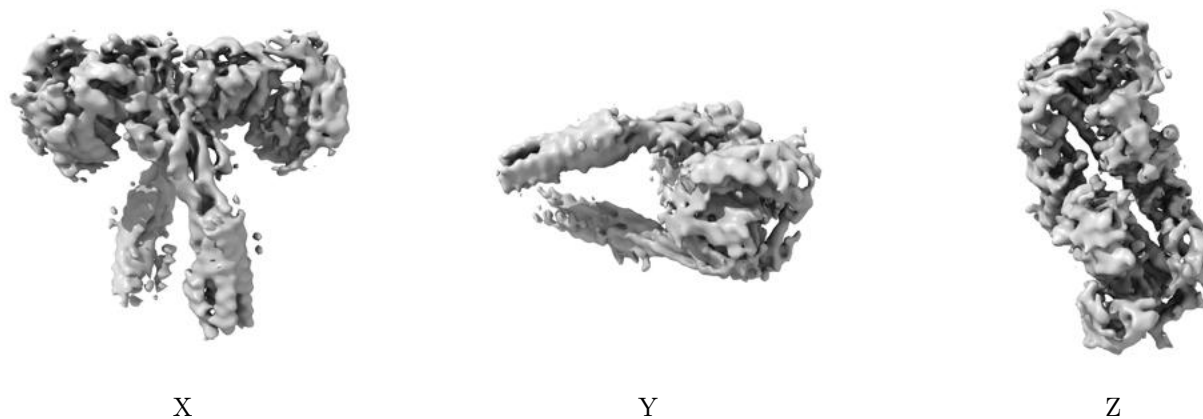


Z

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 0.023. 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.

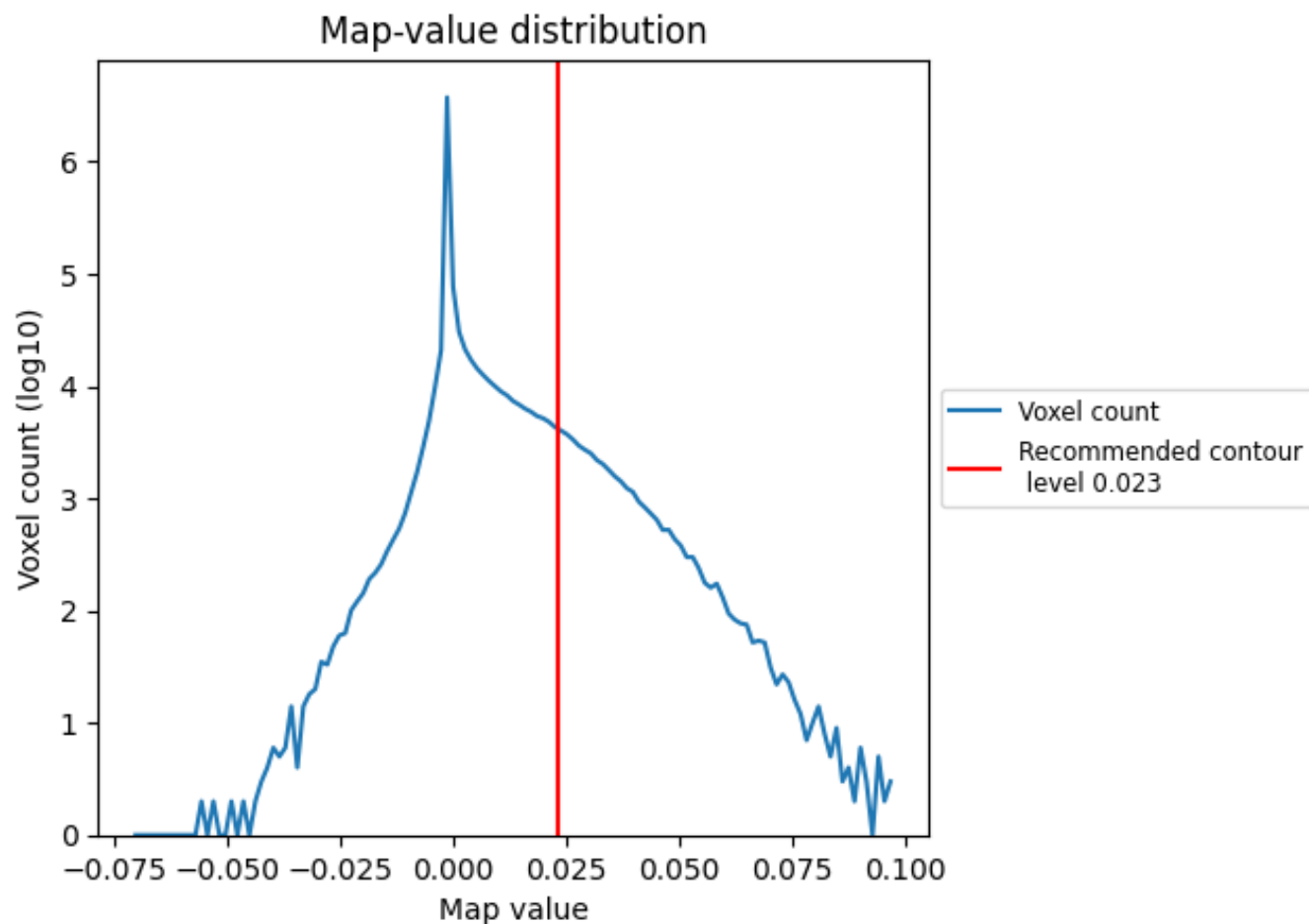
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

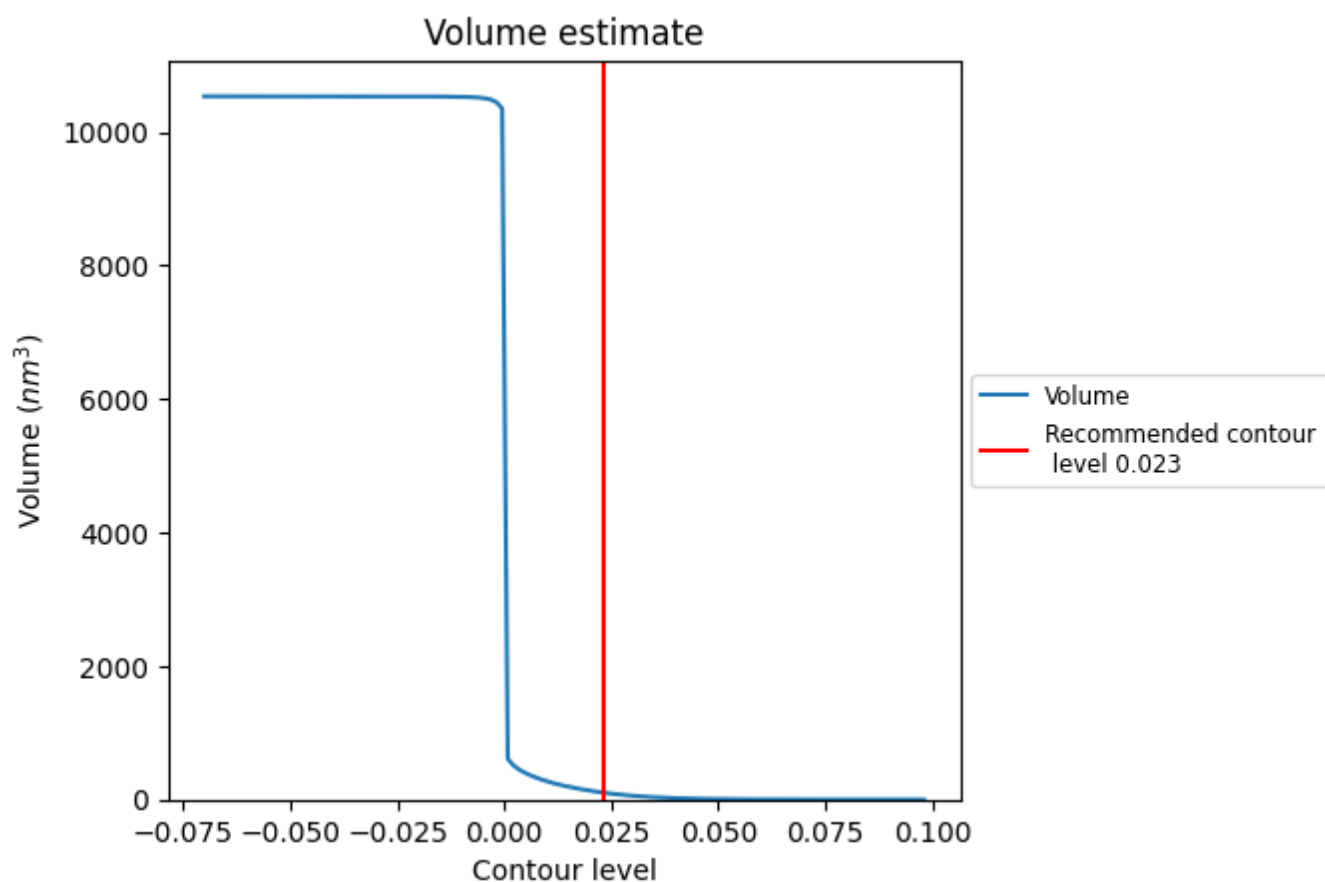
This section contains the results of statistical analysis of the map.

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.

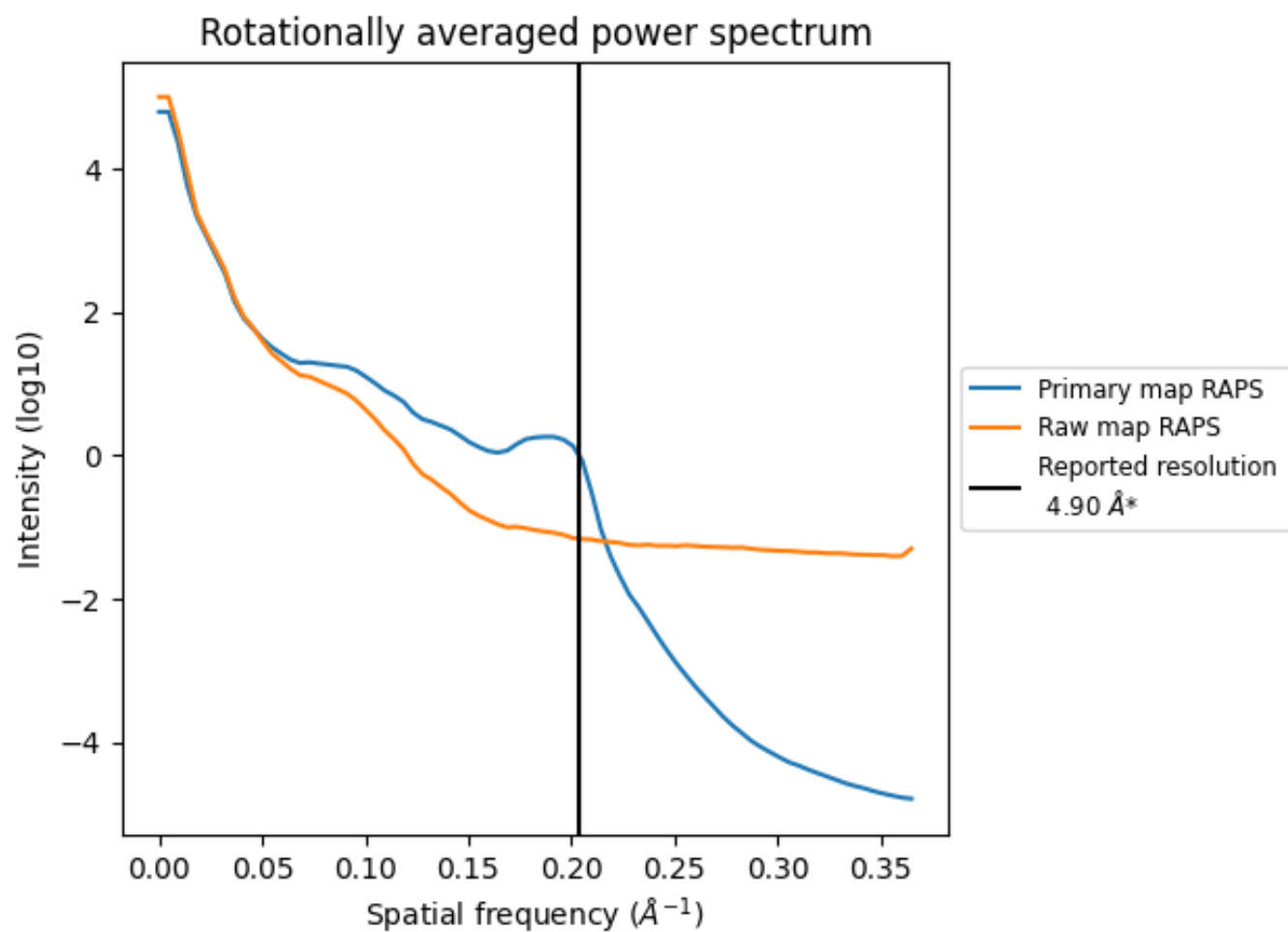
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 105 nm³; this corresponds to an approximate mass of 95 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 ⓘ

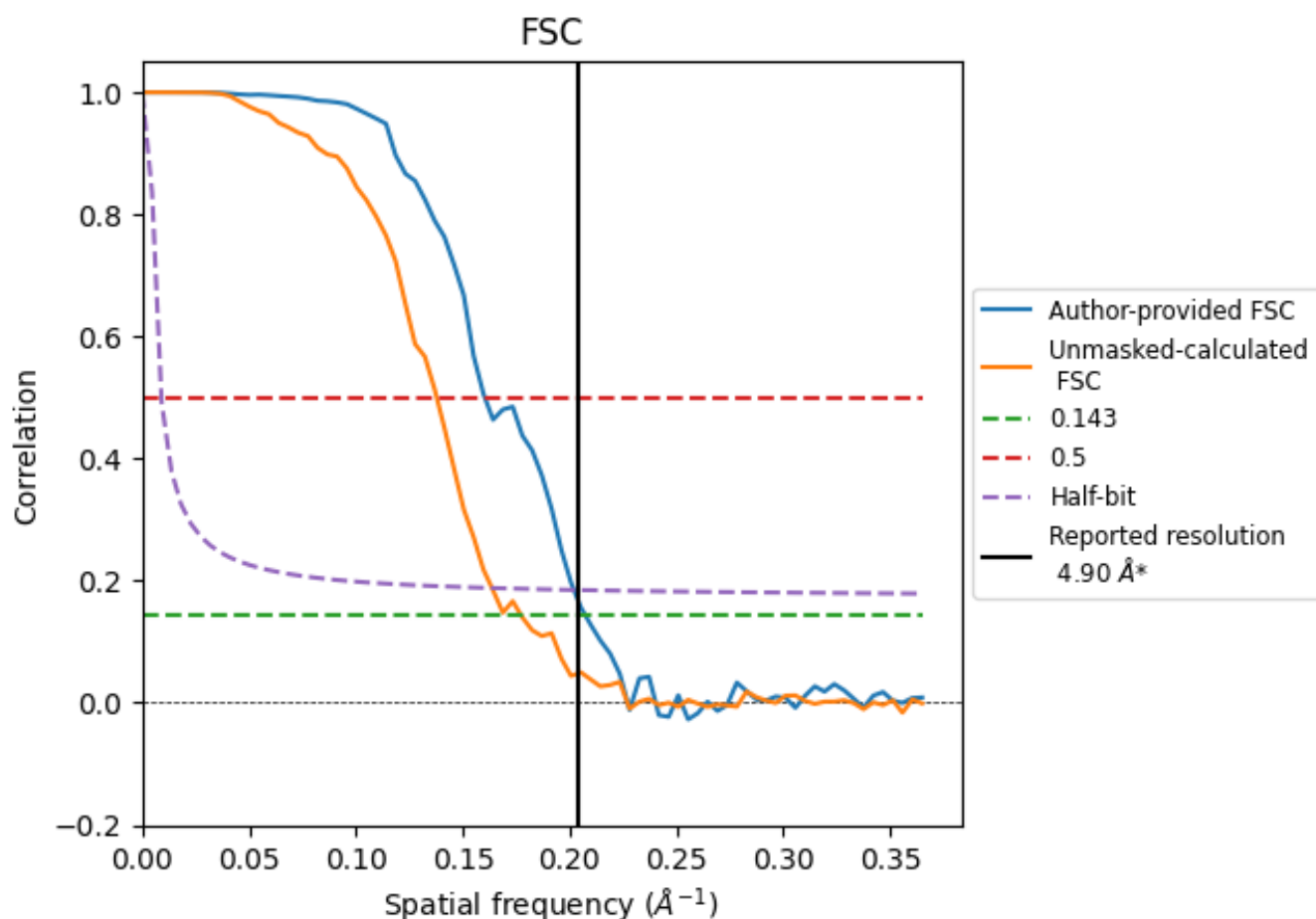


*Reported resolution corresponds to spatial frequency of 0.204 $\text{\AA}^{-1}$

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 0.204 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

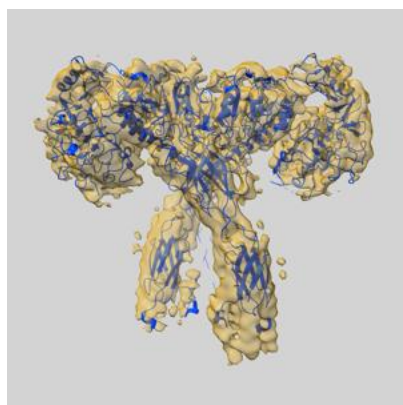
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.90	-	-
Author-provided FSC curve	4.82	6.24	4.95
Unmasked-calculated*	5.64	7.26	6.11

*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 5.64 differs from the reported value 4.9 by more than 10 %

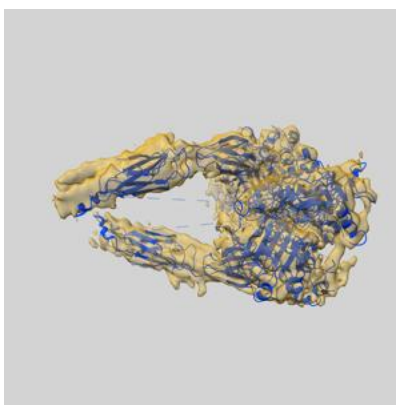
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30231 and PDB model 7BWA. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

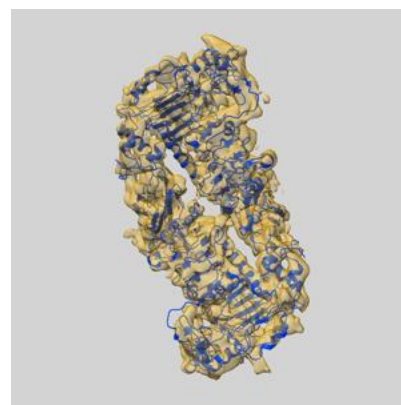
9.1 Map-model overlay [i](#)



X



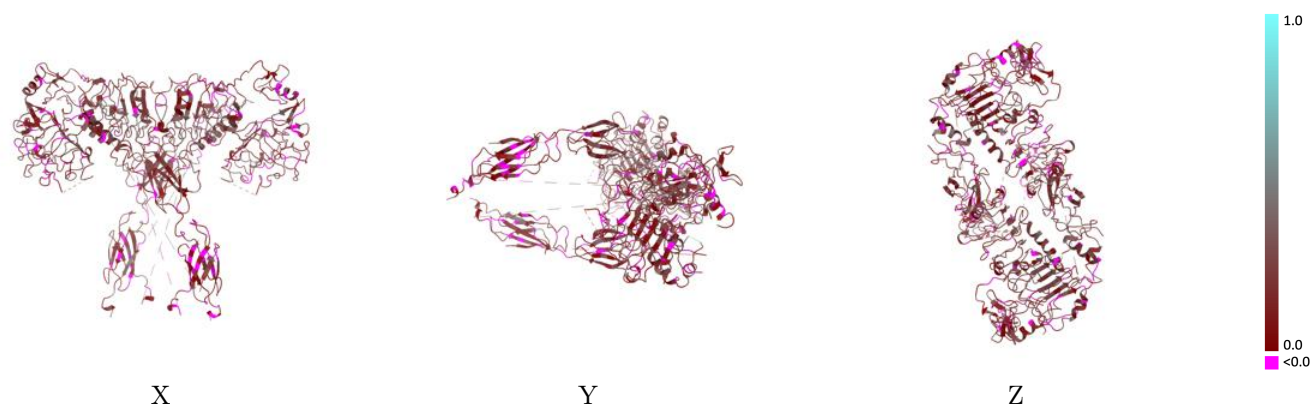
Y



Z

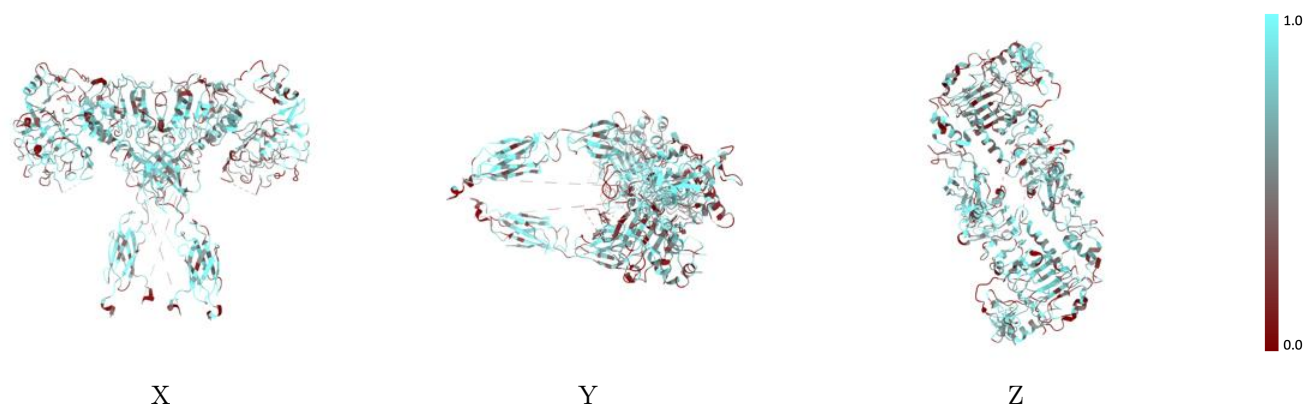
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



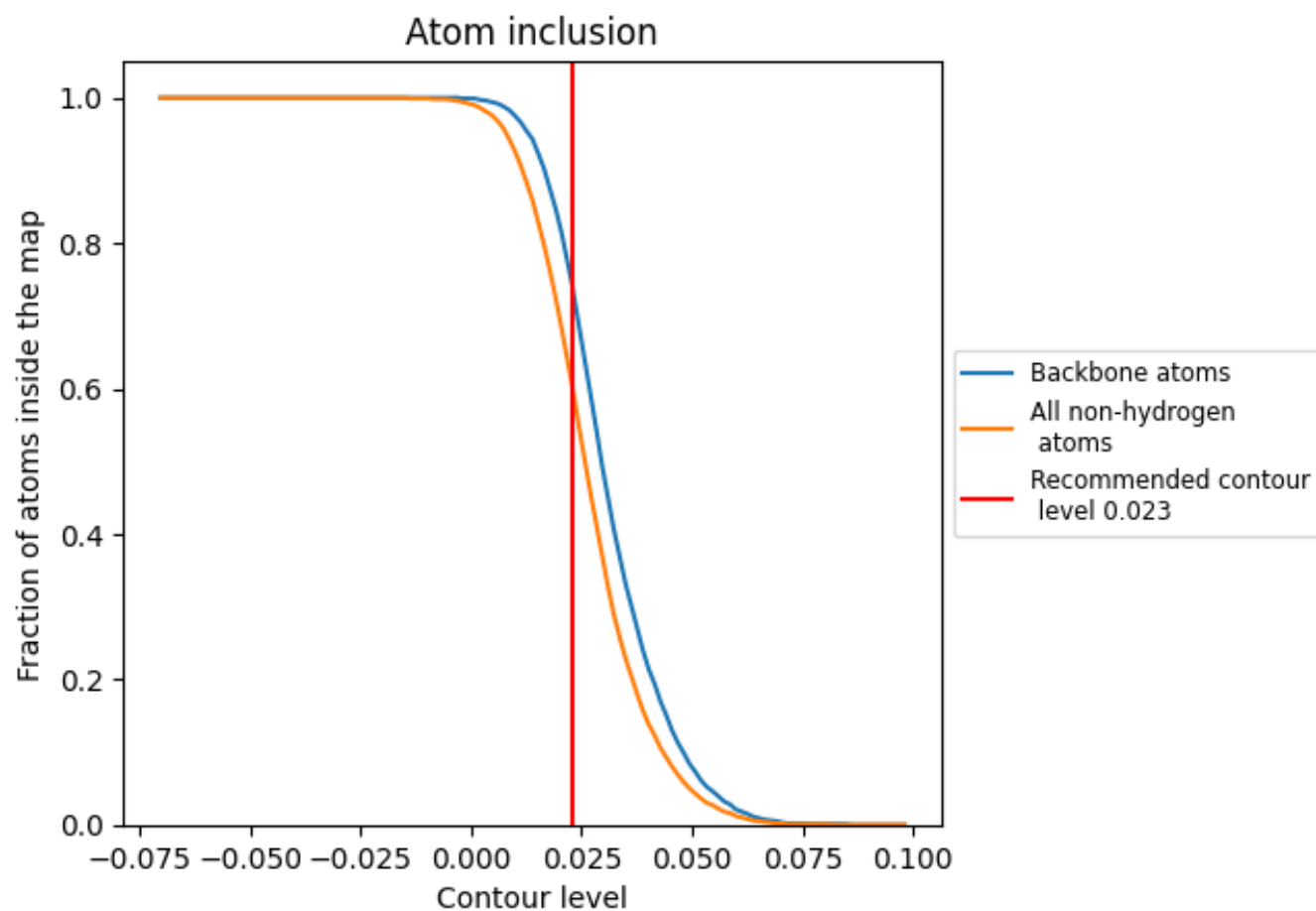
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 60% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6020	0.1830
A	0.6180	0.1890
C	0.5900	0.1740
D	0.6080	0.2270
E	0.5220	0.1820

