



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 02:15 AM UTC

PDB ID : 2NSU / pdb_00002nsu
EMDB ID : EMD-1288
Title : Crystal structure of the ectodomain of human transferrin receptor fitted into a cryo-EM reconstruction of canine parvovirus and feline transferrin receptor complex
Authors : Hafenstein, S.; Kostyuchenko, V.A.; Rossmann, M.G.
Deposited on : 2006-11-06
Resolution : 27.00 Å(reported)
Based on initial model : 1CX8

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

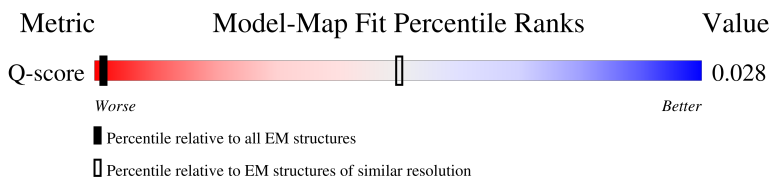
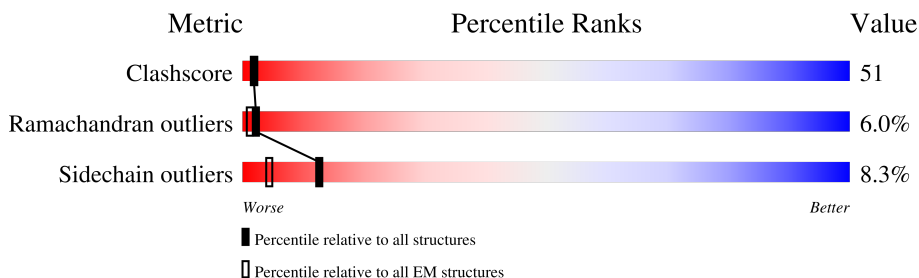
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 27.00 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	6 (26.50 - 27.20)

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

Mol	Chain	Length	Quality of chain
1	A	639	
1	B	639	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10112 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 Transferrin receptor protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	639	Total	C	N	O	S	0	0
			5056	3244	846	952	14		
1	B	639	Total	C	N	O	S	0	0
			5056	3244	846	952	14		

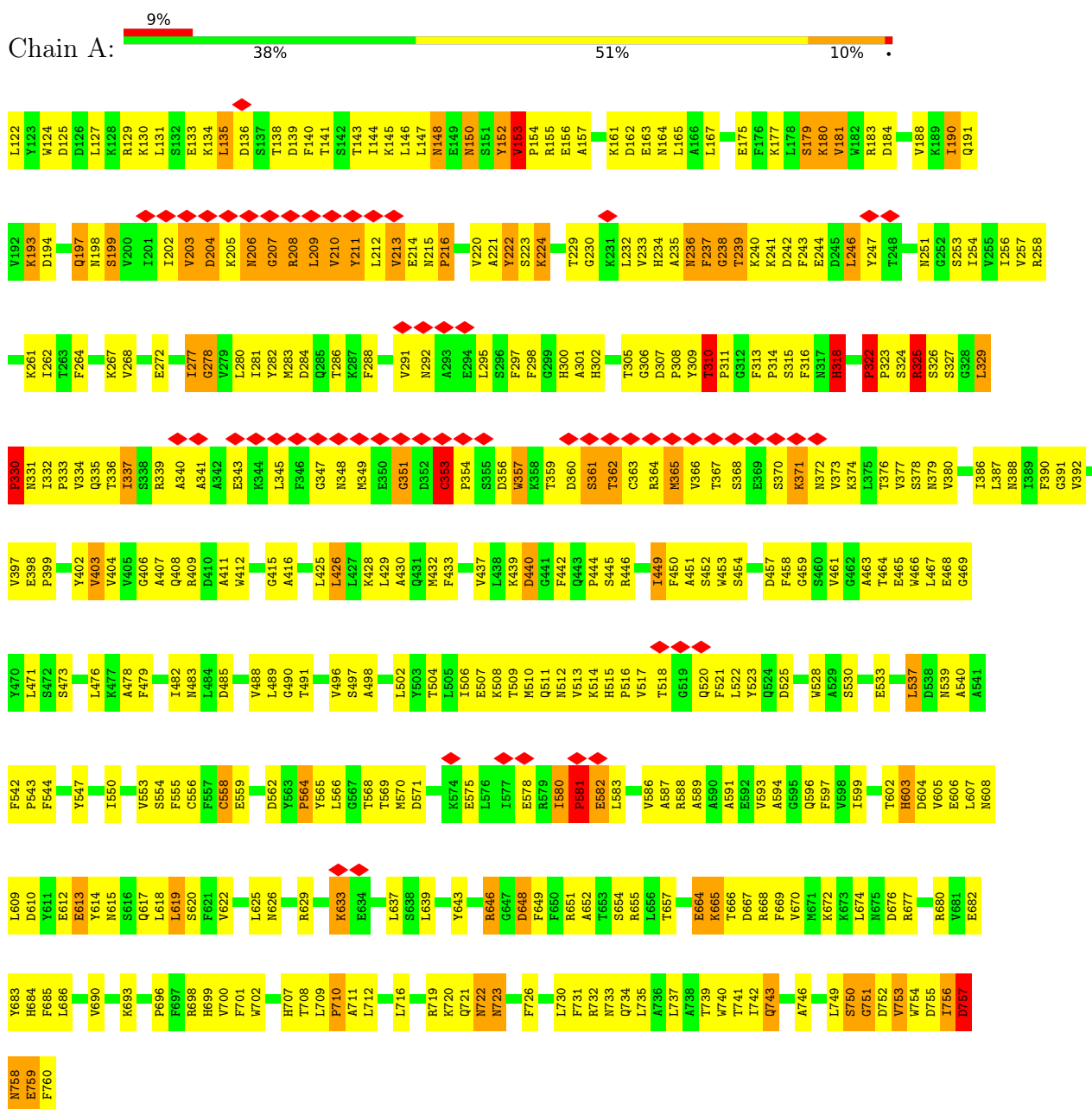
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	SER	GLY	variant	UNP P02786
A	172	GLU	GLN	SEE REMARK 999	UNP P02786
A	613	GLU	ARG	SEE REMARK 999	UNP P02786
B	142	SER	GLY	variant	UNP P02786
B	172	GLU	GLN	SEE REMARK 999	UNP P02786
B	613	GLU	ARG	SEE REMARK 999	UNP P02786

3 Residue-property plots

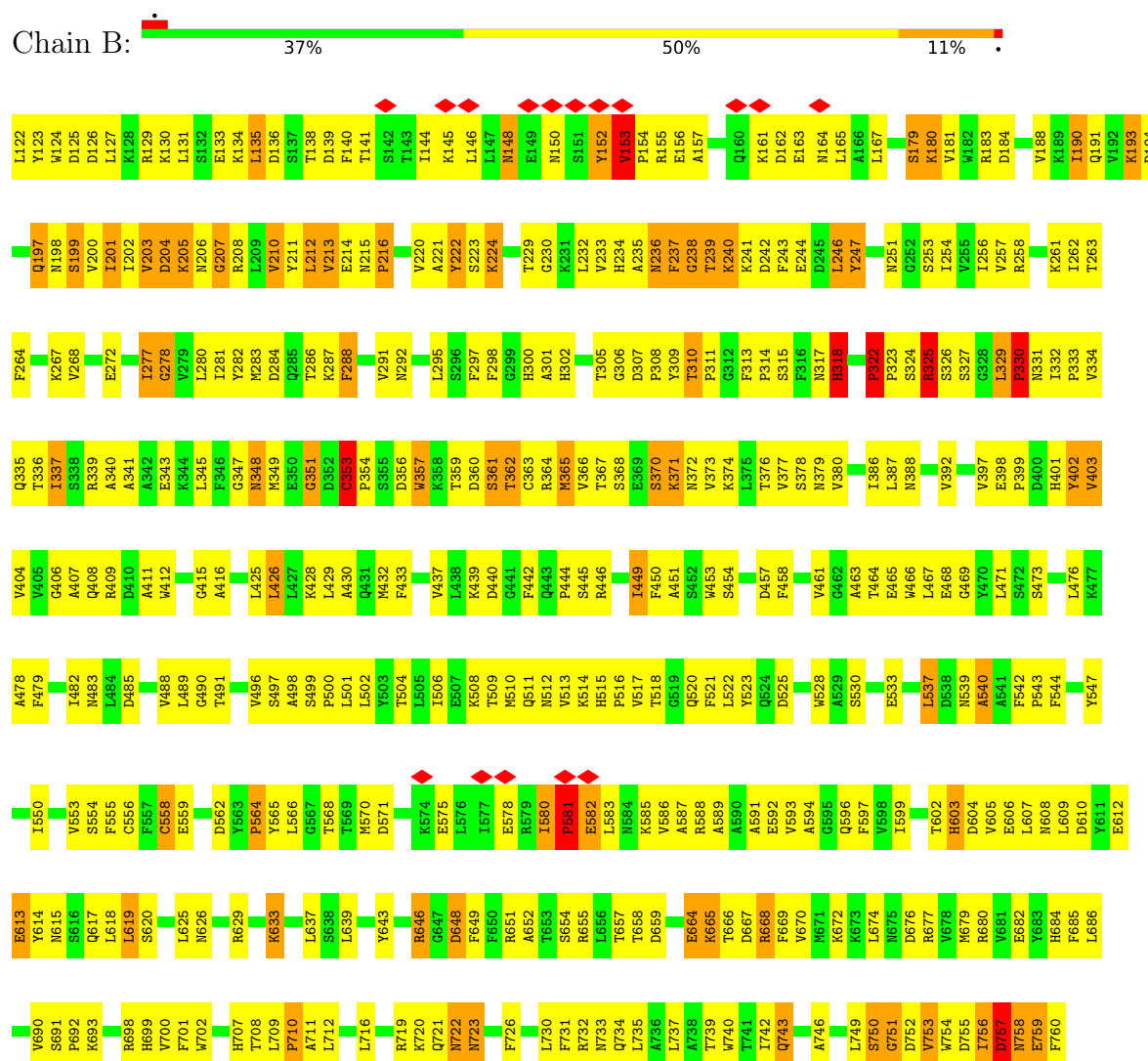
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Transferrin receptor protein 1



• Molecule 1: Transferrin receptor protein 1

Chain B:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	8566	Depositor
Resolution determination method	Not provided	
CTF correction method	CTF correction of each particle	Depositor
Microscope	FEI/PHILIPS CM200FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25.96	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3900	Depositor
Magnification	54000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	9.013	Depositor
Minimum map value	-3.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size ($\text{\AA}$)	665.6, 665.6, 665.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing ($\text{\AA}$)	2.6, 2.6, 2.6	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	0.43	0/5177	0.97	26/7021 (0.4%)
1	B	0.45	0/5177	0.96	22/7021 (0.3%)
All	All	0.44	0/10354	0.96	48/14042 (0.3%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	751	GLY	N-CA-C	-10.27	100.12	115.32
1	A	751	GLY	N-CA-C	-10.18	100.25	115.32
1	B	318	HIS	N-CA-C	-9.61	101.69	113.41
1	B	580	ILE	CA-C-N	7.94	129.77	119.84
1	B	580	ILE	C-N-CA	7.94	129.77	119.84
1	A	318	HIS	N-CA-C	-7.86	101.52	112.45
1	A	466	TRP	N-CA-C	-7.23	103.34	111.14
1	A	329	LEU	CA-C-N	7.21	128.85	119.84
1	A	329	LEU	C-N-CA	7.21	128.85	119.84
1	B	329	LEU	CA-C-N	7.10	128.72	119.84
1	B	329	LEU	C-N-CA	7.10	128.72	119.84
1	A	528	TRP	N-CA-C	-7.05	104.16	114.39
1	A	353	CYS	CA-C-N	7.00	126.96	120.03
1	A	353	CYS	C-N-CA	7.00	126.96	120.03
1	B	322	PRO	N-CA-C	6.87	119.08	110.70
1	B	528	TRP	N-CA-C	-6.87	104.57	114.12
1	A	615	ASN	N-CA-C	-6.79	103.80	111.07
1	A	580	ILE	CA-C-N	6.77	128.30	119.84
1	A	580	ILE	C-N-CA	6.77	128.30	119.84
1	A	322	PRO	N-CA-C	6.57	118.71	110.70
1	B	356	ASP	N-CA-C	-6.51	103.29	111.11
1	B	353	CYS	CA-C-N	6.45	126.42	120.03
1	B	353	CYS	C-N-CA	6.45	126.42	120.03
1	B	757	ASP	N-CA-C	-6.37	102.63	110.65
1	A	578	GLU	N-CA-C	-6.36	105.01	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	466	TRP	N-CA-C	-6.24	104.40	111.14
1	A	356	ASP	N-CA-C	-6.15	103.73	111.11
1	B	615	ASN	N-CA-C	-6.02	104.64	111.14
1	A	403	VAL	CB-CA-C	-5.99	105.18	111.23
1	A	757	ASP	N-CA-C	-5.93	103.18	110.65
1	A	153	VAL	CA-C-N	-5.85	110.81	120.88
1	A	153	VAL	C-N-CA	-5.85	110.81	120.88
1	B	578	GLU	N-CA-C	-5.78	105.72	112.89
1	B	608	ASN	N-CA-C	5.76	118.58	108.56
1	A	608	ASN	N-CA-C	5.66	118.40	108.56
1	A	310	THR	CA-C-N	5.55	126.78	119.84
1	A	310	THR	C-N-CA	5.55	126.78	119.84
1	A	440	ASP	N-CA-C	5.53	119.87	113.18
1	A	199	SER	N-CA-C	5.41	117.07	108.79
1	B	403	VAL	CB-CA-C	-5.35	105.82	111.23
1	B	439	LYS	N-CA-C	5.28	117.84	111.40
1	A	288	PHE	CA-C-N	5.18	126.31	119.84
1	A	288	PHE	C-N-CA	5.18	126.31	119.84
1	B	199	SER	N-CA-C	5.10	116.59	108.79
1	B	402	TYR	N-CA-C	5.08	117.97	110.46
1	A	439	LYS	N-CA-C	5.04	117.55	111.40
1	B	288	PHE	CA-C-N	5.03	126.13	119.84
1	B	288	PHE	C-N-CA	5.03	126.13	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5056	0	4982	526	0
1	B	5056	0	4982	511	0
All	All	10112	0	9964	1020	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 51.

All (1020) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:HG13	1:A:154:PRO:HD3	1.20	1.17
1:B:153:VAL:HG13	1:B:154:PRO:HD3	1.21	1.09
1:B:210:VAL:HG13	1:B:211:TYR:H	1.22	1.05
1:B:359:THR:HG22	1:B:360:ASP:H	1.22	1.04
1:A:359:THR:HG22	1:A:360:ASP:H	1.25	0.99
1:B:348:ASN:HB3	1:B:371:LYS:HE3	1.47	0.96
1:A:203:VAL:HB	1:A:208:ARG:HA	1.49	0.94
1:B:306:GLY:HA2	1:B:461:VAL:HA	1.50	0.94
1:B:184:ASP:HB3	1:B:388:ASN:HB2	1.46	0.94
1:A:348:ASN:HB3	1:A:371:LYS:HE3	1.49	0.93
1:B:708:THR:HG22	1:B:711:ALA:H	1.31	0.93
1:A:209:LEU:HG	1:A:210:VAL:H	1.35	0.92
1:A:354:PRO:HD3	1:A:365:MET:SD	2.09	0.92
1:A:130:LYS:HE3	1:A:134:LYS:HD3	1.51	0.90
1:A:349:MET:HB2	1:A:364:ARG:HG3	1.54	0.90
1:A:140:PHE:HE1	1:A:588:ARG:HA	1.36	0.90
1:B:130:LYS:HE3	1:B:134:LYS:HD3	1.54	0.89
1:B:349:MET:HB2	1:B:364:ARG:HG3	1.54	0.89
1:A:161:LYS:HA	1:A:164:ASN:HD22	1.37	0.89
1:A:184:ASP:HB3	1:A:388:ASN:HB2	1.52	0.89
1:B:444:PRO:HB3	1:B:602:THR:HG21	1.56	0.88
1:A:153:VAL:HG13	1:A:154:PRO:CD	2.04	0.88
1:B:161:LYS:HA	1:B:164:ASN:HD22	1.39	0.88
1:B:300:HIS:HE1	1:B:302:HIS:HB3	1.39	0.88
1:A:239:THR:HB	1:A:244:GLU:HG2	1.55	0.88
1:B:354:PRO:HD3	1:B:365:MET:SD	2.14	0.87
1:A:465:GLU:OE2	1:A:468:GLU:CD	2.17	0.87
1:B:153:VAL:CG1	1:B:154:PRO:HD3	2.05	0.87
1:A:353:CYS:HA	1:A:365:MET:SD	2.15	0.86
1:B:140:PHE:HE1	1:B:588:ARG:HA	1.38	0.86
1:B:667:ASP:HB3	1:B:670:VAL:HG22	1.57	0.86
1:A:708:THR:HG22	1:A:711:ALA:H	1.39	0.85
1:B:239:THR:HB	1:B:244:GLU:HG2	1.57	0.85
1:A:153:VAL:CG1	1:A:154:PRO:HD3	2.03	0.85
1:B:426:LEU:HD21	1:B:450:PHE:HB3	1.58	0.85
1:B:465:GLU:OE2	1:B:468:GLU:CD	2.19	0.85
1:B:353:CYS:HA	1:B:365:MET:SD	2.16	0.84
1:B:708:THR:HG23	1:B:710:PRO:HD2	1.59	0.84
1:A:667:ASP:HB3	1:A:670:VAL:HG22	1.57	0.84
1:B:201:ILE:HD11	1:B:208:ARG:HB2	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:LEU:HD21	1:A:450:PHE:HB3	1.59	0.83
1:A:306:GLY:HA2	1:A:461:VAL:HA	1.59	0.83
1:A:442:PHE:CZ	1:A:444:PRO:HG3	2.13	0.83
1:A:708:THR:HG23	1:A:710:PRO:HD2	1.59	0.83
1:B:646:ARG:HG2	1:B:646:ARG:HH11	1.42	0.83
1:A:758:ASN:HB2	1:B:183:ARG:O	1.79	0.83
1:B:442:PHE:CZ	1:B:444:PRO:HG3	2.14	0.83
1:B:310:THR:OG1	1:B:468:GLU:OE1	1.96	0.82
1:B:300:HIS:CE1	1:B:302:HIS:HB3	2.14	0.82
1:B:153:VAL:HG13	1:B:154:PRO:CD	2.06	0.82
1:A:300:HIS:CE1	1:A:302:HIS:HB3	2.14	0.81
1:B:280:LEU:HD12	1:B:337:ILE:HD13	1.61	0.81
1:A:300:HIS:HE1	1:A:302:HIS:HB3	1.42	0.81
1:A:140:PHE:CE1	1:A:588:ARG:HA	2.17	0.80
1:A:310:THR:OG1	1:A:468:GLU:OE1	1.98	0.80
1:A:444:PRO:HB3	1:A:602:THR:HG21	1.64	0.80
1:A:465:GLU:CD	1:A:468:GLU:OE2	2.25	0.79
1:B:150:ASN:HA	1:B:153:VAL:HG12	1.64	0.79
1:A:646:ARG:HH11	1:A:646:ARG:HG2	1.46	0.79
1:B:199:SER:HB2	1:B:212:LEU:HD11	1.63	0.79
1:B:310:THR:HG21	1:B:315:SER:HB3	1.63	0.79
1:A:465:GLU:OE2	1:A:468:GLU:OE2	2.01	0.79
1:B:210:VAL:HG13	1:B:211:TYR:N	1.97	0.79
1:B:685:PHE:O	1:B:700:VAL:HG22	1.84	0.78
1:B:465:GLU:OE2	1:B:468:GLU:OE1	2.01	0.78
1:A:208:ARG:HD2	1:A:208:ARG:O	1.83	0.78
1:B:309:TYR:HE2	1:B:325:ARG:HA	1.47	0.78
1:B:140:PHE:CE1	1:B:588:ARG:HA	2.18	0.78
1:A:310:THR:HG21	1:A:315:SER:HB3	1.66	0.77
1:A:397:VAL:C	1:A:399:PRO:HD3	2.09	0.77
1:B:496:VAL:HG11	1:B:506:ILE:HG21	1.65	0.77
1:A:496:VAL:HG11	1:A:506:ILE:HG21	1.65	0.77
1:A:188:VAL:CG2	1:A:386:ILE:HD11	2.14	0.76
1:A:280:LEU:HD12	1:A:337:ILE:HD13	1.65	0.76
1:B:238:GLY:HA3	1:B:267:LYS:HG2	1.67	0.76
1:B:191:GLN:HE22	1:B:223:SER:H	1.33	0.76
1:B:232:LEU:HD22	1:B:373:VAL:HG11	1.68	0.75
1:A:150:ASN:HA	1:A:153:VAL:HG12	1.68	0.75
1:A:310:THR:O	1:A:468:GLU:OE1	2.04	0.75
1:B:465:GLU:CD	1:B:468:GLU:OE2	2.29	0.75
1:B:518:THR:HG22	1:B:520:GLN:H	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:TYR:HE2	1:A:325:ARG:HA	1.50	0.75
1:A:220:VAL:HG21	1:A:334:VAL:HG12	1.69	0.75
1:B:397:VAL:C	1:B:399:PRO:HD3	2.12	0.75
1:A:278:GLY:H	1:A:332:ILE:HG23	1.53	0.74
1:B:204:ASP:C	1:B:206:ASN:H	1.95	0.74
1:B:278:GLY:H	1:B:332:ILE:HG23	1.53	0.73
1:B:318:HIS:O	1:B:322:PRO:HB3	1.88	0.73
1:A:183:ARG:O	1:B:758:ASN:HB2	1.87	0.73
1:A:188:VAL:HG21	1:A:386:ILE:HD11	1.70	0.73
1:A:191:GLN:HE22	1:A:223:SER:H	1.34	0.73
1:A:232:LEU:HD22	1:A:373:VAL:HG11	1.70	0.73
1:A:229:THR:HB	1:A:374:LYS:HG3	1.71	0.72
1:B:295:LEU:HD21	1:B:568:THR:HG21	1.70	0.72
1:B:398:GLU:HB2	1:B:446:ARG:HG2	1.72	0.72
1:A:310:THR:OG1	1:A:310:THR:O	2.00	0.72
1:B:183:ARG:NH1	1:B:387:LEU:HD21	2.04	0.72
1:B:310:THR:OG1	1:B:310:THR:O	2.03	0.72
1:A:740:TRP:CZ2	1:B:314:PRO:HB2	2.25	0.72
1:A:518:THR:HG22	1:A:520:GLN:H	1.54	0.72
1:B:407:ALA:HB3	1:B:426:LEU:HD12	1.70	0.72
1:B:305:THR:HG23	1:B:464:THR:HG21	1.71	0.72
1:A:685:PHE:O	1:A:700:VAL:HG22	1.90	0.71
1:A:407:ALA:HB3	1:A:426:LEU:HD12	1.72	0.71
1:A:295:LEU:HD21	1:A:568:THR:HG21	1.70	0.71
1:B:359:THR:HG22	1:B:360:ASP:N	2.03	0.71
1:A:515:HIS:HD2	1:A:517:VAL:H	1.37	0.71
1:B:229:THR:HB	1:B:374:LYS:CG	2.21	0.71
1:B:188:VAL:CG2	1:B:386:ILE:HD11	2.21	0.70
1:A:212:LEU:HD21	1:A:215:ASN:HD21	1.55	0.70
1:B:229:THR:HB	1:B:374:LYS:HG3	1.70	0.70
1:B:341:ALA:O	1:B:345:LEU:HD23	1.91	0.70
1:A:318:HIS:O	1:A:322:PRO:HB3	1.90	0.70
1:A:130:LYS:HE2	1:A:440:ASP:OD1	1.92	0.70
1:A:229:THR:HB	1:A:374:LYS:CG	2.21	0.70
1:B:297:PHE:O	1:B:336:THR:HG21	1.90	0.70
1:B:238:GLY:HA3	1:B:267:LYS:CG	2.22	0.70
1:A:664:GLU:H	1:A:664:GLU:CD	2.00	0.70
1:A:708:THR:CG2	1:A:710:PRO:HD2	2.21	0.70
1:B:625:LEU:HD21	1:B:639:LEU:HD11	1.73	0.70
1:B:732:ARG:HH11	1:B:732:ARG:HG3	1.55	0.70
1:A:239:THR:HB	1:A:244:GLU:CG	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ASN:HA	1:B:153:VAL:CG1	2.22	0.69
1:A:626:ASN:HB3	1:A:629:ARG:HH21	1.58	0.69
1:B:664:GLU:CD	1:B:664:GLU:H	2.01	0.69
1:A:183:ARG:NH1	1:A:387:LEU:HD21	2.08	0.69
1:A:732:ARG:HG3	1:A:732:ARG:HH11	1.58	0.69
1:A:349:MET:HG2	1:A:367:THR:HA	1.73	0.69
1:B:506:ILE:O	1:B:510:MET:HG3	1.93	0.69
1:A:214:GLU:O	1:A:216:PRO:HD3	1.94	0.68
1:A:488:VAL:C	1:A:489:LEU:HD12	2.18	0.68
1:B:515:HIS:HD2	1:B:517:VAL:H	1.38	0.68
1:B:213:VAL:HG11	1:B:345:LEU:HD21	1.74	0.68
1:A:130:LYS:HE2	1:A:440:ASP:CG	2.19	0.68
1:B:307:ASP:HB3	1:B:465:GLU:OE1	1.94	0.68
1:A:300:HIS:HD1	1:A:302:HIS:H	1.41	0.68
1:A:398:GLU:HB2	1:A:446:ARG:HG2	1.75	0.68
1:B:220:VAL:HG21	1:B:334:VAL:HG12	1.75	0.68
1:B:239:THR:HB	1:B:244:GLU:CG	2.24	0.68
1:B:349:MET:HG2	1:B:367:THR:HA	1.76	0.68
1:B:351:GLY:O	1:B:364:ARG:HD3	1.93	0.68
1:B:208:ARG:HG2	1:B:208:ARG:O	1.93	0.68
1:B:300:HIS:HD1	1:B:302:HIS:H	1.40	0.68
1:A:297:PHE:O	1:A:336:THR:HG21	1.94	0.68
1:B:309:TYR:CE2	1:B:325:ARG:HA	2.28	0.68
1:B:330:PRO:O	1:B:331:ASN:HB3	1.94	0.68
1:B:254:ILE:HA	1:B:277:ILE:O	1.94	0.68
1:B:313:PHE:O	1:B:468:GLU:OE1	2.12	0.68
1:B:542:PHE:HB3	1:B:543:PRO:HD3	1.75	0.68
1:B:232:LEU:HB3	1:B:367:THR:HG23	1.76	0.67
1:B:310:THR:O	1:B:468:GLU:OE1	2.11	0.67
1:A:140:PHE:O	1:A:144:ILE:HG13	1.94	0.67
1:A:240:LYS:C	1:A:242:ASP:H	2.00	0.67
1:A:254:ILE:HA	1:A:277:ILE:O	1.95	0.67
1:B:167:LEU:HD22	1:B:183:ARG:HH22	1.58	0.67
1:B:337:ILE:HG23	1:B:341:ALA:HB3	1.77	0.67
1:A:490:GLY:HA3	1:A:559:GLU:HG2	1.76	0.67
1:A:359:THR:HG22	1:A:360:ASP:N	2.06	0.67
1:A:341:ALA:O	1:A:345:LEU:HD23	1.95	0.67
1:A:204:ASP:C	1:A:206:ASN:H	2.02	0.67
1:A:351:GLY:O	1:A:364:ARG:HD3	1.95	0.67
1:A:488:VAL:O	1:A:489:LEU:HD12	1.94	0.67
1:A:330:PRO:O	1:A:331:ASN:HB3	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:VAL:HG21	1:B:386:ILE:HD11	1.76	0.66
1:B:465:GLU:OE2	1:B:468:GLU:OE2	2.11	0.66
1:A:309:TYR:CE2	1:A:325:ARG:HA	2.30	0.66
1:A:337:ILE:HG23	1:A:341:ALA:HB3	1.76	0.66
1:B:240:LYS:C	1:B:242:ASP:H	2.04	0.66
1:B:238:GLY:C	1:B:240:LYS:H	2.02	0.66
1:B:183:ARG:HH12	1:B:387:LEU:HD21	1.58	0.66
1:A:150:ASN:HA	1:A:153:VAL:CG1	2.26	0.66
1:A:311:PRO:O	1:A:693:LYS:HA	1.96	0.65
1:A:209:LEU:CG	1:A:210:VAL:H	2.07	0.65
1:B:686:LEU:HD23	1:B:699:HIS:CA	2.26	0.65
1:A:246:LEU:HD12	1:A:247:TYR:N	2.12	0.65
1:B:140:PHE:O	1:B:144:ILE:HG13	1.96	0.65
1:A:155:ARG:HH21	1:A:165:LEU:HD22	1.60	0.65
1:A:686:LEU:HD23	1:A:699:HIS:CA	2.25	0.65
1:B:353:CYS:HB2	1:B:363:CYS:O	1.96	0.65
1:B:626:ASN:HB3	1:B:629:ARG:HH21	1.62	0.65
1:B:359:THR:CG2	1:B:360:ASP:H	2.02	0.65
1:B:349:MET:HB2	1:B:364:ARG:CG	2.27	0.65
1:A:238:GLY:HA3	1:A:267:LYS:HG2	1.80	0.64
1:A:353:CYS:HB2	1:A:363:CYS:O	1.97	0.64
1:B:139:ASP:OD1	1:B:141:THR:HG22	1.97	0.64
1:B:229:THR:HB	1:B:374:LYS:CB	2.28	0.64
1:B:488:VAL:C	1:B:489:LEU:HD12	2.23	0.64
1:A:232:LEU:HD11	1:A:256:ILE:HG13	1.80	0.64
1:A:625:LEU:HD21	1:A:639:LEU:HD11	1.79	0.64
1:A:686:LEU:HD23	1:A:699:HIS:HA	1.79	0.64
1:A:758:ASN:N	1:A:758:ASN:HD22	1.96	0.64
1:B:238:GLY:O	1:B:240:LYS:N	2.31	0.64
1:B:191:GLN:NE2	1:B:223:SER:H	1.96	0.64
1:B:349:MET:HB3	1:B:366:VAL:O	1.98	0.64
1:A:542:PHE:HB3	1:A:543:PRO:HD3	1.80	0.64
1:B:130:LYS:HE2	1:B:440:ASP:CG	2.23	0.64
1:A:238:GLY:C	1:A:240:LYS:H	2.04	0.64
1:A:654:SER:O	1:A:657:THR:HG22	1.98	0.64
1:B:716:LEU:HD13	1:B:731:PHE:CE1	2.33	0.64
1:A:238:GLY:O	1:A:240:LYS:N	2.29	0.63
1:B:220:VAL:CG1	1:B:301:ALA:HB2	2.28	0.63
1:A:183:ARG:HH12	1:A:387:LEU:HD21	1.61	0.63
1:B:625:LEU:CD2	1:B:639:LEU:HD11	2.28	0.63
1:B:155:ARG:HH21	1:B:165:LEU:HD22	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LEU:HB3	1:A:367:THR:HG23	1.78	0.63
1:B:200:VAL:HG23	1:B:213:VAL:HB	1.79	0.63
1:B:646:ARG:HG2	1:B:646:ARG:NH1	2.11	0.63
1:B:664:GLU:C	1:B:666:THR:H	2.07	0.63
1:B:156:GLU:HG2	1:B:157:ALA:H	1.64	0.63
1:B:130:LYS:HE2	1:B:440:ASP:OD1	1.97	0.63
1:A:232:LEU:HD21	1:A:256:ILE:HD11	1.79	0.63
1:A:349:MET:HB2	1:A:364:ARG:CG	2.27	0.63
1:A:349:MET:HB3	1:A:366:VAL:O	1.99	0.63
1:B:446:ARG:HD2	1:B:479:PHE:CE2	2.34	0.63
1:A:167:LEU:HD22	1:A:183:ARG:HH22	1.63	0.63
1:A:465:GLU:OE2	1:A:468:GLU:OE1	2.16	0.63
1:B:324:SER:HB3	1:B:325:ARG:HE	1.64	0.63
1:B:488:VAL:O	1:B:489:LEU:HD12	1.99	0.63
1:B:690:VAL:HG23	1:B:698:ARG:HG2	1.81	0.63
1:A:555:PHE:CE2	1:A:593:VAL:HG23	2.34	0.62
1:A:664:GLU:OE1	1:A:667:ASP:HB2	1.98	0.62
1:B:152:TYR:HA	1:B:161:LYS:HE2	1.82	0.62
1:A:539:ASN:HD22	1:A:540:ALA:N	1.97	0.62
1:A:515:HIS:CD2	1:A:517:VAL:H	2.16	0.62
1:B:348:ASN:N	1:B:348:ASN:HD22	1.97	0.62
1:A:229:THR:HB	1:A:374:LYS:CB	2.30	0.62
1:B:191:GLN:HE22	1:B:223:SER:N	1.98	0.62
1:B:201:ILE:HD13	1:B:212:LEU:HA	1.80	0.62
1:A:278:GLY:H	1:A:332:ILE:CG2	2.12	0.62
1:A:664:GLU:C	1:A:666:THR:H	2.08	0.62
1:A:506:ILE:O	1:A:510:MET:HG3	2.00	0.62
1:A:210:VAL:HG22	1:A:211:TYR:H	1.63	0.62
1:A:313:PHE:O	1:A:468:GLU:OE1	2.18	0.62
1:B:167:LEU:CD2	1:B:183:ARG:HH22	2.11	0.62
1:A:191:GLN:HE22	1:A:223:SER:N	1.98	0.62
1:B:239:THR:C	1:B:241:LYS:H	2.08	0.62
1:B:708:THR:CG2	1:B:710:PRO:HD2	2.27	0.62
1:A:191:GLN:NE2	1:A:223:SER:H	1.97	0.62
1:A:446:ARG:HD2	1:A:479:PHE:CE2	2.34	0.62
1:B:664:GLU:OE1	1:B:667:ASP:HB2	1.99	0.62
1:A:156:GLU:HG2	1:A:157:ALA:H	1.64	0.61
1:B:278:GLY:HA2	1:B:333:PRO:O	2.00	0.61
1:A:238:GLY:HA3	1:A:267:LYS:CG	2.29	0.61
1:A:349:MET:HA	1:A:367:THR:HA	1.83	0.61
1:B:194:ASP:HB3	1:B:378:SER:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LEU:HD12	1:B:247:TYR:N	2.16	0.61
1:B:490:GLY:HA3	1:B:559:GLU:HG2	1.82	0.61
1:A:446:ARG:H	1:A:602:THR:CG2	2.13	0.61
1:B:236:ASN:OD1	1:B:258:ARG:HD3	2.00	0.61
1:A:238:GLY:H	1:A:257:VAL:HB	1.65	0.61
1:B:686:LEU:HD23	1:B:699:HIS:HA	1.82	0.61
1:A:236:ASN:OD1	1:A:258:ARG:HD3	2.00	0.61
1:A:307:ASP:HB3	1:A:465:GLU:OE1	2.01	0.61
1:A:605:VAL:HG11	1:A:665:LYS:HB3	1.83	0.61
1:B:280:LEU:HD12	1:B:337:ILE:CD1	2.30	0.61
1:B:758:ASN:N	1:B:758:ASN:HD22	1.96	0.61
1:A:220:VAL:CG1	1:A:301:ALA:HB2	2.31	0.60
1:B:349:MET:HA	1:B:367:THR:HA	1.84	0.60
1:B:295:LEU:HD11	1:B:568:THR:OG1	2.01	0.60
1:B:368:SER:OG	1:B:371:LYS:HE2	2.01	0.60
1:A:139:ASP:OD1	1:A:141:THR:HG22	2.01	0.60
1:A:167:LEU:CD2	1:A:183:ARG:HH22	2.15	0.60
1:A:655:ARG:NH1	1:A:751:GLY:HA2	2.16	0.60
1:B:515:HIS:CD2	1:B:517:VAL:H	2.18	0.60
1:B:131:LEU:O	1:B:135:LEU:HD23	2.00	0.60
1:B:188:VAL:HG21	1:B:461:VAL:HG11	1.82	0.60
1:A:336:THR:O	1:A:337:ILE:HD12	2.01	0.60
1:B:654:SER:O	1:B:657:THR:HG22	2.01	0.60
1:A:152:TYR:HA	1:A:161:LYS:HE2	1.84	0.60
1:A:210:VAL:HG13	1:A:211:TYR:O	2.01	0.60
1:A:690:VAL:HG23	1:A:698:ARG:HG2	1.82	0.60
1:A:220:VAL:HG12	1:A:301:ALA:HB2	1.82	0.59
1:B:130:LYS:O	1:B:134:LYS:HG2	2.02	0.59
1:B:310:THR:OG1	1:B:465:GLU:OE2	2.20	0.59
1:A:131:LEU:O	1:A:135:LEU:HD23	2.02	0.59
1:A:348:ASN:HD22	1:A:348:ASN:N	2.00	0.59
1:A:368:SER:OG	1:A:371:LYS:HE2	2.01	0.59
1:A:209:LEU:HG	1:A:210:VAL:N	2.11	0.59
1:A:314:PRO:HB2	1:B:740:TRP:CZ2	2.37	0.59
1:A:324:SER:HB3	1:A:325:ARG:HE	1.68	0.59
1:A:298:PHE:HB2	1:A:412:TRP:CD2	2.38	0.59
1:B:167:LEU:HD22	1:B:183:ARG:NH2	2.17	0.59
1:B:324:SER:CB	1:B:325:ARG:HE	2.15	0.59
1:A:237:PHE:CD2	1:A:258:ARG:HB2	2.38	0.59
1:A:345:LEU:O	1:A:349:MET:HG3	2.03	0.59
1:B:214:GLU:O	1:B:216:PRO:HD3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASP:H	1:A:461:VAL:HG13	1.68	0.59
1:A:719:ARG:HG3	1:A:719:ARG:HH11	1.68	0.59
1:B:588:ARG:HG3	1:B:588:ARG:HH11	1.67	0.59
1:A:347:GLY:C	1:A:348:ASN:HD22	2.11	0.59
1:A:515:HIS:CD2	1:A:516:PRO:HD2	2.38	0.58
1:A:654:SER:C	1:A:657:THR:HG22	2.28	0.58
1:B:403:VAL:HG22	1:B:479:PHE:CZ	2.37	0.58
1:B:220:VAL:HG12	1:B:301:ALA:HB2	1.85	0.58
1:B:237:PHE:HB2	1:B:243:PHE:HE1	1.67	0.58
1:B:268:VAL:HG21	1:B:334:VAL:HG21	1.86	0.58
1:A:300:HIS:O	1:A:301:ALA:HB3	2.02	0.58
1:B:655:ARG:NH1	1:B:751:GLY:HA2	2.18	0.58
1:A:280:LEU:HD12	1:A:337:ILE:CD1	2.33	0.58
1:A:625:LEU:CD2	1:A:639:LEU:HD11	2.33	0.58
1:A:202:ILE:HB	1:A:210:VAL:HG11	1.86	0.58
1:B:238:GLY:O	1:B:262:ILE:HD11	2.04	0.58
1:B:278:GLY:H	1:B:332:ILE:CG2	2.16	0.58
1:A:264:PHE:CE2	1:A:281:ILE:HG21	2.39	0.57
1:A:446:ARG:H	1:A:602:THR:HG23	1.68	0.57
1:A:238:GLY:O	1:A:262:ILE:HD11	2.04	0.57
1:A:699:HIS:HD2	1:A:702:TRP:H	1.51	0.57
1:B:442:PHE:CE2	1:B:444:PRO:HG3	2.38	0.57
1:B:555:PHE:CE2	1:B:593:VAL:HG23	2.39	0.57
1:A:749:LEU:O	1:A:750:SER:CB	2.53	0.57
1:B:719:ARG:HD3	1:B:726:PHE:CD2	2.40	0.57
1:A:239:THR:C	1:A:241:LYS:H	2.11	0.57
1:A:433:PHE:O	1:A:437:VAL:HG23	2.04	0.57
1:A:672:LYS:HD3	1:A:676:ASP:OD2	2.05	0.57
1:A:670:VAL:O	1:A:674:LEU:HG	2.05	0.57
1:A:758:ASN:HD22	1:A:758:ASN:H	1.50	0.57
1:A:453:TRP:CD2	1:A:463:ALA:HB2	2.40	0.57
1:B:212:LEU:O	1:B:213:VAL:C	2.47	0.57
1:B:272:GLU:OE2	1:B:330:PRO:O	2.23	0.57
1:B:426:LEU:CD2	1:B:450:PHE:HB3	2.31	0.57
1:A:496:VAL:HG11	1:A:506:ILE:CG2	2.35	0.57
1:B:347:GLY:C	1:B:348:ASN:HD22	2.11	0.57
1:A:403:VAL:HG22	1:A:479:PHE:CZ	2.40	0.57
1:B:756:ILE:HG22	1:B:756:ILE:O	2.04	0.57
1:A:298:PHE:HE2	1:A:457:ASP:HB3	1.70	0.57
1:B:336:THR:O	1:B:337:ILE:HD12	2.05	0.56
1:B:496:VAL:HG11	1:B:506:ILE:CG2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ASP:HB3	1:A:378:SER:O	2.05	0.56
1:B:758:ASN:HD22	1:B:758:ASN:H	1.52	0.56
1:A:167:LEU:HD22	1:A:183:ARG:NH2	2.20	0.56
1:A:272:GLU:OE2	1:A:330:PRO:O	2.23	0.56
1:B:237:PHE:CD2	1:B:258:ARG:HB2	2.40	0.56
1:B:680:ARG:HB3	1:B:684:HIS:HD2	1.71	0.56
1:A:237:PHE:HB2	1:A:243:PHE:HE1	1.69	0.56
1:A:339:ARG:O	1:A:343:GLU:HG2	2.05	0.56
1:A:398:GLU:N	1:A:399:PRO:HD3	2.21	0.56
1:B:345:LEU:O	1:B:349:MET:HG3	2.04	0.56
1:A:238:GLY:N	1:A:257:VAL:HB	2.20	0.56
1:A:453:TRP:CG	1:A:463:ALA:HB2	2.41	0.56
1:A:719:ARG:HD3	1:A:726:PHE:CD2	2.41	0.56
1:B:286:THR:CG2	1:B:360:ASP:HB2	2.35	0.56
1:B:300:HIS:O	1:B:301:ALA:HB3	2.06	0.56
1:B:719:ARG:HG3	1:B:719:ARG:HH11	1.70	0.56
1:A:442:PHE:CE2	1:A:444:PRO:HG3	2.40	0.56
1:B:232:LEU:HB3	1:B:367:THR:CG2	2.35	0.56
1:B:618:LEU:HD11	1:B:742:ILE:HD13	1.87	0.56
1:B:756:ILE:H	1:B:756:ILE:HD12	1.71	0.56
1:A:539:ASN:O	1:A:542:PHE:N	2.38	0.56
1:A:680:ARG:HB3	1:A:684:HIS:HD2	1.71	0.56
1:A:286:THR:CG2	1:A:360:ASP:HB2	2.36	0.55
1:B:539:ASN:HD22	1:B:540:ALA:N	2.04	0.55
1:B:676:ASP:O	1:B:680:ARG:HG3	2.06	0.55
1:B:759:GLU:HG3	1:B:760:PHE:N	2.21	0.55
1:A:539:ASN:HD22	1:A:539:ASN:C	2.15	0.55
1:A:654:SER:HA	1:A:657:THR:HG22	1.89	0.55
1:A:756:ILE:HG22	1:A:756:ILE:O	2.05	0.55
1:A:759:GLU:O	1:A:760:PHE:C	2.49	0.55
1:B:239:THR:C	1:B:241:LYS:N	2.64	0.55
1:B:565:TYR:CE1	1:B:575:GLU:HB3	2.41	0.55
1:A:426:LEU:CD2	1:A:450:PHE:HB3	2.34	0.55
1:A:565:TYR:CE1	1:A:575:GLU:HB3	2.42	0.55
1:A:607:LEU:CD1	1:A:609:LEU:HG	2.37	0.55
1:B:204:ASP:C	1:B:206:ASN:N	2.63	0.55
1:B:446:ARG:H	1:B:602:THR:HG23	1.70	0.55
1:B:752:ASP:O	1:B:753:VAL:HB	2.06	0.55
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.88	0.55
1:A:156:GLU:HG2	1:A:157:ALA:N	2.22	0.55
1:A:349:MET:HE2	1:A:367:THR:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:GLU:N	1:B:399:PRO:HD3	2.22	0.55
1:A:237:PHE:CD1	1:A:261:LYS:HG3	2.42	0.55
1:A:619:LEU:HD23	1:A:620:SER:N	2.22	0.55
1:B:699:HIS:HD2	1:B:702:TRP:H	1.55	0.55
1:A:306:GLY:HA2	1:A:461:VAL:CA	2.34	0.55
1:A:471:LEU:HD13	1:A:547:TYR:OH	2.07	0.55
1:B:654:SER:C	1:B:657:THR:HG22	2.32	0.55
1:A:324:SER:CB	1:A:325:ARG:HE	2.19	0.54
1:B:618:LEU:HD13	1:B:701:PHE:HZ	1.72	0.54
1:A:232:LEU:HB3	1:A:367:THR:CG2	2.36	0.54
1:A:239:THR:HB	1:A:244:GLU:CD	2.33	0.54
1:A:425:LEU:HD22	1:A:591:ALA:HB2	1.88	0.54
1:B:197:GLN:HE21	1:B:215:ASN:HB3	1.71	0.54
1:B:446:ARG:H	1:B:602:THR:CG2	2.20	0.54
1:B:222:TYR:HB3	1:B:329:LEU:HD23	1.89	0.54
1:A:335:GLN:NE2	1:A:336:THR:HG22	2.23	0.54
1:A:155:ARG:HA	1:A:161:LYS:HB2	1.90	0.54
1:A:268:VAL:HG21	1:A:334:VAL:HG21	1.87	0.54
1:B:190:ILE:HG13	1:B:458:PHE:CD2	2.43	0.54
1:B:238:GLY:H	1:B:257:VAL:HB	1.72	0.54
1:B:502:LEU:O	1:B:506:ILE:HG13	2.08	0.54
1:B:135:LEU:HD22	1:B:432:MET:SD	2.47	0.54
1:A:278:GLY:HA2	1:A:333:PRO:O	2.07	0.54
1:A:488:VAL:HG13	1:A:586:VAL:HG11	1.90	0.54
1:A:758:ASN:CB	1:B:183:ARG:O	2.55	0.54
1:B:232:LEU:HD11	1:B:256:ILE:HG13	1.90	0.54
1:B:237:PHE:CD1	1:B:261:LYS:HG3	2.43	0.54
1:B:471:LEU:HD13	1:B:547:TYR:OH	2.08	0.54
1:B:515:HIS:CD2	1:B:516:PRO:HD2	2.43	0.54
1:B:672:LYS:HD3	1:B:676:ASP:OD2	2.08	0.54
1:A:212:LEU:HD21	1:A:215:ASN:ND2	2.23	0.53
1:A:540:ALA:O	1:A:543:PRO:HD2	2.08	0.53
1:A:588:ARG:HG3	1:A:588:ARG:HH11	1.73	0.53
1:B:311:PRO:O	1:B:693:LYS:HA	2.08	0.53
1:B:749:LEU:O	1:B:750:SER:CB	2.55	0.53
1:A:131:LEU:HD22	1:A:599:ILE:HD11	1.89	0.53
1:A:513:VAL:HG21	1:A:593:VAL:HG12	1.89	0.53
1:B:756:ILE:HD12	1:B:756:ILE:N	2.23	0.53
1:A:667:ASP:OD1	1:A:669:PHE:HB3	2.09	0.53
1:B:156:GLU:HG2	1:B:157:ALA:N	2.22	0.53
1:B:201:ILE:HB	1:B:212:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:SER:HA	1:B:657:THR:HG22	1.89	0.53
1:A:496:VAL:CG1	1:A:506:ILE:HD13	2.39	0.53
1:A:646:ARG:HG2	1:A:646:ARG:NH1	2.17	0.53
1:A:743:GLN:O	1:A:746:ALA:HB3	2.08	0.53
1:B:146:LEU:HD23	1:B:146:LEU:C	2.32	0.53
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.91	0.53
1:A:232:LEU:CD2	1:A:256:ILE:HD11	2.38	0.53
1:B:240:LYS:HA	1:B:262:ILE:HD13	1.90	0.53
1:A:236:ASN:HB2	1:A:357:TRP:CD1	2.44	0.53
1:B:236:ASN:HB2	1:B:357:TRP:CD1	2.44	0.53
1:B:712:LEU:C	1:B:712:LEU:HD23	2.34	0.53
1:B:719:ARG:HH11	1:B:719:ARG:CG	2.22	0.53
1:A:197:GLN:HE21	1:A:215:ASN:HB3	1.74	0.52
1:A:295:LEU:HD11	1:A:568:THR:OG1	2.08	0.52
1:A:712:LEU:HD23	1:A:712:LEU:C	2.33	0.52
1:A:719:ARG:HH11	1:A:719:ARG:CG	2.22	0.52
1:B:239:THR:HB	1:B:244:GLU:CD	2.34	0.52
1:A:145:LYS:O	1:A:148:ASN:HB2	2.09	0.52
1:A:361:SER:O	1:A:362:THR:CB	2.58	0.52
1:A:135:LEU:HD22	1:A:432:MET:SD	2.49	0.52
1:B:199:SER:CB	1:B:212:LEU:HD11	2.38	0.52
1:B:540:ALA:O	1:B:543:PRO:HD2	2.10	0.52
1:B:619:LEU:HD23	1:B:620:SER:N	2.23	0.52
1:A:239:THR:C	1:A:241:LYS:N	2.65	0.52
1:A:515:HIS:CD2	1:A:516:PRO:CD	2.92	0.52
1:B:206:ASN:O	1:B:207:GLY:O	2.26	0.52
1:B:580:ILE:HG23	1:B:580:ILE:O	2.08	0.52
1:B:698:ARG:HA	1:B:707:HIS:NE2	2.24	0.52
1:A:473:SER:O	1:A:476:LEU:HB2	2.09	0.52
1:B:201:ILE:HD12	1:B:202:ILE:N	2.25	0.52
1:B:298:PHE:HE2	1:B:457:ASP:HB3	1.74	0.52
1:B:523:TYR:HE1	1:B:530:SER:OG	1.91	0.52
1:B:759:GLU:O	1:B:760:PHE:C	2.52	0.52
1:A:648:ASP:OD2	1:A:757:ASP:OD2	2.28	0.52
1:A:752:ASP:O	1:A:753:VAL:HB	2.09	0.52
1:B:201:ILE:HD13	1:B:212:LEU:CA	2.40	0.52
1:A:212:LEU:CD2	1:A:215:ASN:HD21	2.21	0.52
1:A:618:LEU:HD11	1:A:742:ILE:HD13	1.92	0.52
1:A:668:ARG:HD2	1:B:669:PHE:CD2	2.45	0.52
1:B:339:ARG:O	1:B:343:GLU:HG2	2.09	0.52
1:B:433:PHE:O	1:B:437:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:ALA:HB2	1:B:553:VAL:HA	1.91	0.52
1:A:124:TRP:HH2	1:A:596:GLN:HG2	1.75	0.52
1:A:163:GLU:O	1:A:167:LEU:HG	2.10	0.52
1:A:188:VAL:HG21	1:A:461:VAL:HG11	1.92	0.52
1:B:409:ARG:NH2	1:B:454:SER:HB2	2.24	0.52
1:B:553:VAL:HG22	1:B:554:SER:N	2.25	0.52
1:B:564:PRO:HG2	1:B:565:TYR:H	1.74	0.52
1:B:754:TRP:O	1:B:755:ASP:C	2.53	0.52
1:A:453:TRP:CE3	1:A:463:ALA:HA	2.44	0.52
1:B:146:LEU:HD23	1:B:146:LEU:O	2.10	0.52
1:B:335:GLN:NE2	1:B:336:THR:HG22	2.25	0.52
1:A:188:VAL:HG22	1:A:386:ILE:HD11	1.90	0.51
1:A:280:LEU:C	1:A:281:ILE:HD12	2.35	0.51
1:B:513:VAL:HG21	1:B:593:VAL:HG12	1.90	0.51
1:A:664:GLU:CD	1:A:664:GLU:N	2.69	0.51
1:A:676:ASP:O	1:A:680:ARG:HG3	2.10	0.51
1:B:198:ASN:OD1	1:B:378:SER:N	2.43	0.51
1:B:232:LEU:HD21	1:B:256:ILE:HD11	1.91	0.51
1:A:502:LEU:O	1:A:506:ILE:HG13	2.10	0.51
1:B:453:TRP:CG	1:B:463:ALA:HB2	2.45	0.51
1:B:607:LEU:CD1	1:B:609:LEU:HG	2.40	0.51
1:B:238:GLY:HA3	1:B:267:LYS:CD	2.41	0.51
1:B:238:GLY:N	1:B:257:VAL:HB	2.26	0.51
1:B:282:TYR:HE1	1:B:284:ASP:HB3	1.76	0.51
1:B:286:THR:HG21	1:B:360:ASP:HB2	1.93	0.51
1:A:210:VAL:HG22	1:A:211:TYR:N	2.25	0.51
1:A:498:ALA:HB2	1:A:553:VAL:HA	1.92	0.51
1:B:127:LEU:N	1:B:127:LEU:HD22	2.25	0.51
1:B:749:LEU:O	1:B:750:SER:HB3	2.11	0.51
1:A:199:SER:O	1:A:376:THR:HG22	2.11	0.51
1:A:232:LEU:HD11	1:A:256:ILE:CG1	2.40	0.51
1:A:349:MET:HA	1:A:368:SER:N	2.26	0.51
1:A:483:ASN:HD21	1:A:540:ALA:HB3	1.75	0.51
1:B:155:ARG:HA	1:B:161:LYS:HB2	1.91	0.51
1:B:750:SER:OG	1:B:751:GLY:N	2.42	0.51
1:A:130:LYS:O	1:A:134:LYS:HG2	2.10	0.51
1:A:316:PHE:CZ	1:B:740:TRP:NE1	2.75	0.51
1:A:425:LEU:O	1:A:429:LEU:HB2	2.11	0.51
1:A:582:GLU:CD	1:A:582:GLU:H	2.18	0.51
1:A:618:LEU:HD21	1:A:742:ILE:HG23	1.92	0.51
1:A:716:LEU:HD13	1:A:731:PHE:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:VAL:HG11	1:B:665:LYS:HB3	1.92	0.51
1:A:146:LEU:C	1:A:146:LEU:HD23	2.36	0.51
1:A:669:PHE:CD2	1:B:668:ARG:HD2	2.46	0.51
1:B:199:SER:O	1:B:376:THR:HG22	2.11	0.51
1:B:401:HIS:ND1	1:B:679:MET:HE1	2.26	0.51
1:A:700:VAL:HG23	1:A:701:PHE:CD1	2.46	0.51
1:B:145:LYS:O	1:B:148:ASN:HB2	2.11	0.51
1:B:307:ASP:H	1:B:461:VAL:HG13	1.76	0.51
1:B:361:SER:O	1:B:362:THR:CB	2.59	0.51
1:B:667:ASP:OD1	1:B:669:PHE:HB3	2.12	0.51
1:B:682:GLU:OE2	1:B:699:HIS:CE1	2.64	0.50
1:A:537:LEU:HD22	1:A:542:PHE:CE2	2.46	0.50
1:B:256:ILE:CD1	1:B:349:MET:HE1	2.41	0.50
1:B:539:ASN:O	1:B:542:PHE:N	2.39	0.50
1:B:655:ARG:HH11	1:B:751:GLY:HA2	1.77	0.50
1:A:446:ARG:HH12	1:A:602:THR:HA	1.76	0.50
1:A:677:ARG:NE	1:A:750:SER:HB2	2.26	0.50
1:B:278:GLY:HA2	1:B:333:PRO:HG2	1.93	0.50
1:A:224:LYS:HE3	1:A:224:LYS:HA	1.94	0.50
1:A:553:VAL:HG22	1:A:554:SER:N	2.27	0.50
1:B:349:MET:HA	1:B:368:SER:N	2.26	0.50
1:B:568:THR:HG23	1:B:570:MET:H	1.76	0.50
1:A:240:LYS:O	1:A:240:LYS:HG2	2.12	0.50
1:A:731:PHE:O	1:A:732:ARG:C	2.54	0.50
1:B:291:VAL:HG13	1:B:292:ASN:N	2.27	0.50
1:B:453:TRP:CD2	1:B:463:ALA:HB2	2.47	0.50
1:B:648:ASP:OD2	1:B:757:ASP:OD2	2.29	0.50
1:A:238:GLY:HA3	1:A:267:LYS:HD3	1.94	0.50
1:A:307:ASP:N	1:A:461:VAL:HG13	2.26	0.50
1:A:392:VAL:HG12	1:A:449:ILE:HB	1.94	0.50
1:B:197:GLN:NE2	1:B:215:ASN:HB3	2.27	0.50
1:B:224:LYS:HB3	1:B:332:ILE:C	2.37	0.50
1:B:565:TYR:HE1	1:B:575:GLU:HB3	1.75	0.50
1:A:222:TYR:HB3	1:A:329:LEU:HD23	1.93	0.50
1:A:282:TYR:HE1	1:A:284:ASP:HB3	1.77	0.50
1:A:283:MET:HE2	1:A:297:PHE:CD1	2.46	0.50
1:A:224:LYS:HB3	1:A:332:ILE:C	2.37	0.50
1:A:238:GLY:HA3	1:A:267:LYS:CD	2.42	0.50
1:A:483:ASN:ND2	1:A:540:ALA:HB3	2.27	0.50
1:A:655:ARG:HH11	1:A:751:GLY:HA2	1.76	0.50
1:A:667:ASP:HB3	1:A:670:VAL:CG2	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LYS:HE3	1:B:224:LYS:HA	1.93	0.50
1:B:539:ASN:HD22	1:B:539:ASN:C	2.19	0.50
1:A:305:THR:HG23	1:A:464:THR:HG21	1.93	0.49
1:A:553:VAL:HG21	1:A:597:PHE:CE2	2.46	0.49
1:A:754:TRP:O	1:A:755:ASP:C	2.55	0.49
1:B:556:CYS:C	1:B:558:CYS:H	2.19	0.49
1:B:667:ASP:HB3	1:B:670:VAL:CG2	2.37	0.49
1:A:278:GLY:HA2	1:A:333:PRO:HG2	1.94	0.49
1:A:408:GLN:HB3	1:A:485:ASP:OD1	2.12	0.49
1:A:409:ARG:HB2	1:A:452:SER:OG	2.11	0.49
1:A:618:LEU:HD13	1:A:701:PHE:HZ	1.76	0.49
1:A:759:GLU:HG3	1:A:760:PHE:N	2.27	0.49
1:A:349:MET:HE2	1:A:367:THR:CG2	2.42	0.49
1:A:496:VAL:HG11	1:A:506:ILE:HD13	1.94	0.49
1:A:238:GLY:HA2	1:A:257:VAL:HG11	1.95	0.49
1:A:286:THR:HG21	1:A:360:ASP:HB2	1.94	0.49
1:A:556:CYS:C	1:A:558:CYS:H	2.21	0.49
1:A:682:GLU:OE2	1:A:699:HIS:CE1	2.65	0.49
1:B:496:VAL:CG1	1:B:506:ILE:HD13	2.42	0.49
1:B:618:LEU:HD21	1:B:742:ILE:HG23	1.94	0.49
1:B:670:VAL:O	1:B:674:LEU:HG	2.12	0.49
1:A:180:LYS:HD2	1:A:180:LYS:N	2.28	0.49
1:A:213:VAL:O	1:A:214:GLU:HB2	2.13	0.49
1:A:238:GLY:C	1:A:240:LYS:N	2.70	0.49
1:A:523:TYR:HE1	1:A:530:SER:OG	1.95	0.49
1:B:210:VAL:CG1	1:B:211:TYR:N	2.69	0.49
1:B:349:MET:HE2	1:B:367:THR:HG23	1.94	0.49
1:B:411:ALA:HA	1:B:457:ASP:OD2	2.13	0.49
1:A:197:GLN:NE2	1:A:215:ASN:HB3	2.28	0.49
1:A:240:LYS:HA	1:A:262:ILE:HD13	1.95	0.49
1:A:756:ILE:N	1:A:756:ILE:HD12	2.27	0.49
1:B:497:SER:OG	1:B:533:GLU:HB3	2.12	0.49
1:A:568:THR:HG23	1:A:570:MET:H	1.77	0.49
1:A:756:ILE:HD12	1:A:756:ILE:H	1.77	0.49
1:B:733:ASN:O	1:B:734:GLN:C	2.56	0.49
1:A:209:LEU:O	1:A:210:VAL:HG12	2.13	0.49
1:A:297:PHE:CD1	1:A:297:PHE:N	2.81	0.49
1:B:237:PHE:HB2	1:B:243:PHE:CE1	2.46	0.49
1:B:256:ILE:HD11	1:B:349:MET:HE1	1.94	0.49
1:B:361:SER:O	1:B:362:THR:HB	2.13	0.49
1:A:467:LEU:HD21	1:A:544:PHE:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:ASN:O	1:A:734:GLN:C	2.55	0.49
1:A:361:SER:O	1:A:362:THR:HB	2.12	0.48
1:B:264:PHE:CE2	1:B:281:ILE:HG21	2.47	0.48
1:A:580:ILE:HG23	1:A:580:ILE:O	2.13	0.48
1:A:237:PHE:HB2	1:A:243:PHE:CE1	2.47	0.48
1:A:603:HIS:CD2	1:A:603:HIS:C	2.91	0.48
1:B:163:GLU:O	1:B:167:LEU:HG	2.12	0.48
1:B:240:LYS:O	1:B:241:LYS:HB3	2.13	0.48
1:B:325:ARG:HG2	1:B:326:SER:N	2.28	0.48
1:B:664:GLU:CD	1:B:664:GLU:N	2.70	0.48
1:B:680:ARG:HB3	1:B:684:HIS:CD2	2.47	0.48
1:B:731:PHE:O	1:B:732:ARG:C	2.56	0.48
1:A:240:LYS:O	1:A:241:LYS:HB3	2.13	0.48
1:B:677:ARG:NE	1:B:750:SER:HB2	2.27	0.48
1:A:133:GLU:HA	1:A:136:ASP:HB2	1.96	0.48
1:A:203:VAL:HG23	1:A:206:ASN:O	2.14	0.48
1:A:735:LEU:HD23	1:A:735:LEU:C	2.38	0.48
1:A:749:LEU:O	1:A:750:SER:HB3	2.14	0.48
1:B:232:LEU:HD13	1:B:254:ILE:HG22	1.96	0.48
1:A:131:LEU:HD22	1:A:599:ILE:CD1	2.43	0.48
1:A:680:ARG:HB3	1:A:684:HIS:CD2	2.48	0.48
1:A:699:HIS:CD2	1:A:701:PHE:HB2	2.49	0.48
1:A:700:VAL:HG23	1:A:701:PHE:HD1	1.79	0.48
1:A:721:GLN:C	1:A:723:ASN:H	2.22	0.48
1:B:386:ILE:CG2	1:B:454:SER:HB3	2.43	0.48
1:B:408:GLN:HB3	1:B:485:ASP:OD1	2.14	0.48
1:B:504:THR:OG1	1:B:610:ASP:OD2	2.30	0.48
1:A:153:VAL:HG22	1:A:154:PRO:CD	2.43	0.48
1:A:198:ASN:OD1	1:A:378:SER:N	2.44	0.48
1:A:232:LEU:HB2	1:A:373:VAL:CG1	2.44	0.48
1:A:305:THR:HG23	1:A:305:THR:O	2.13	0.48
1:A:430:ALA:HA	1:A:450:PHE:CZ	2.49	0.48
1:B:305:THR:HG23	1:B:305:THR:O	2.13	0.48
1:B:753:VAL:HG12	1:B:754:TRP:CG	2.48	0.48
1:A:237:PHE:HD2	1:A:258:ARG:HB2	1.78	0.48
1:A:677:ARG:HE	1:A:750:SER:HB2	1.78	0.48
1:B:152:TYR:HA	1:B:161:LYS:HB3	1.95	0.48
1:B:211:TYR:CG	1:B:212:LEU:N	2.81	0.48
1:B:297:PHE:N	1:B:297:PHE:CD1	2.82	0.48
1:B:582:GLU:CD	1:B:582:GLU:H	2.21	0.48
1:B:735:LEU:C	1:B:735:LEU:HD23	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:O	1:A:213:VAL:C	2.55	0.48
1:A:236:ASN:O	1:A:243:PHE:HD1	1.97	0.48
1:B:343:GLU:OE2	1:B:362:THR:HG21	2.14	0.48
1:B:425:LEU:HD22	1:B:591:ALA:HB2	1.96	0.48
1:B:453:TRP:CE3	1:B:463:ALA:HA	2.49	0.48
1:B:537:LEU:HD22	1:B:542:PHE:CE2	2.48	0.48
1:A:146:LEU:C	1:A:148:ASN:H	2.22	0.48
1:A:386:ILE:CG2	1:A:454:SER:HB3	2.44	0.48
1:A:565:TYR:HE1	1:A:575:GLU:HB3	1.78	0.48
1:B:146:LEU:C	1:B:148:ASN:H	2.22	0.48
1:B:230:GLY:O	1:B:372:ASN:HB2	2.13	0.48
1:B:306:GLY:HA2	1:B:461:VAL:CA	2.32	0.48
1:B:515:HIS:CD2	1:B:516:PRO:CD	2.97	0.48
1:B:161:LYS:O	1:B:164:ASN:HB2	2.14	0.47
1:B:425:LEU:O	1:B:429:LEU:HB2	2.12	0.47
1:A:161:LYS:O	1:A:164:ASN:HB2	2.14	0.47
1:B:244:GLU:HA	1:B:244:GLU:OE1	2.14	0.47
1:A:180:LYS:HD2	1:A:180:LYS:H	1.80	0.47
1:A:357:TRP:O	1:A:359:THR:N	2.43	0.47
1:B:409:ARG:HG2	1:B:409:ARG:HH11	1.79	0.47
1:B:698:ARG:HA	1:B:707:HIS:HE2	1.78	0.47
1:A:213:VAL:HG11	1:A:345:LEU:CD2	2.44	0.47
1:A:256:ILE:CD1	1:A:349:MET:HE1	2.45	0.47
1:A:300:HIS:NE2	1:A:458:PHE:C	2.73	0.47
1:B:430:ALA:HA	1:B:450:PHE:CZ	2.50	0.47
1:B:651:ARG:HH11	1:B:651:ARG:HG2	1.79	0.47
1:A:152:TYR:HA	1:A:161:LYS:HB3	1.96	0.47
1:A:179:SER:O	1:A:180:LYS:C	2.58	0.47
1:A:478:ALA:O	1:A:550:ILE:HD12	2.14	0.47
1:B:222:TYR:CE2	1:B:308:PRO:HG3	2.50	0.47
1:B:239:THR:O	1:B:243:PHE:HB2	2.15	0.47
1:A:239:THR:O	1:A:243:PHE:HB2	2.15	0.47
1:A:409:ARG:HG2	1:A:409:ARG:HH11	1.78	0.47
1:B:180:LYS:HD2	1:B:180:LYS:N	2.30	0.47
1:A:324:SER:O	1:A:325:ARG:HB3	2.14	0.47
1:A:465:GLU:HA	1:A:468:GLU:HB2	1.95	0.47
1:A:497:SER:OG	1:A:533:GLU:HB3	2.14	0.47
1:A:720:LYS:C	1:A:722:ASN:H	2.22	0.47
1:B:203:VAL:HB	1:B:208:ARG:HA	1.97	0.47
1:B:236:ASN:O	1:B:243:PHE:HD1	1.96	0.47
1:B:330:PRO:O	1:B:331:ASN:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:LEU:C	1:A:469:GLY:N	2.70	0.47
1:B:153:VAL:HG22	1:B:154:PRO:CD	2.45	0.47
1:B:759:GLU:HG3	1:B:760:PHE:H	1.80	0.47
1:A:183:ARG:O	1:B:758:ASN:CB	2.58	0.47
1:A:619:LEU:HD23	1:A:619:LEU:C	2.40	0.47
1:A:683:TYR:CD1	1:A:686:LEU:HD12	2.50	0.47
1:A:244:GLU:OE1	1:A:244:GLU:HA	2.15	0.47
1:A:446:ARG:NH1	1:A:602:THR:HA	2.30	0.47
1:A:553:VAL:HG21	1:A:597:PHE:HE2	1.79	0.47
1:B:188:VAL:HG22	1:B:386:ILE:HD11	1.97	0.47
1:B:473:SER:O	1:B:476:LEU:HB2	2.15	0.47
1:A:204:ASP:C	1:A:206:ASN:N	2.71	0.46
1:A:353:CYS:HA	1:A:354:PRO:HD3	1.75	0.46
1:A:564:PRO:HG2	1:A:565:TYR:H	1.80	0.46
1:B:239:THR:O	1:B:241:LYS:N	2.48	0.46
1:B:639:LEU:HD23	1:B:643:TYR:HE1	1.80	0.46
1:A:134:LYS:O	1:A:138:THR:HG23	2.14	0.46
1:A:188:VAL:HG23	1:A:190:ILE:HD13	1.98	0.46
1:A:491:THR:HB	1:A:517:VAL:HG21	1.98	0.46
1:B:237:PHE:O	1:B:238:GLY:C	2.59	0.46
1:B:240:LYS:O	1:B:240:LYS:HG2	2.15	0.46
1:B:553:VAL:HG21	1:B:597:PHE:CE2	2.51	0.46
1:B:743:GLN:O	1:B:746:ALA:HB3	2.15	0.46
1:A:325:ARG:HG2	1:A:326:SER:N	2.29	0.46
1:A:580:ILE:N	1:A:581:PRO:HD3	2.31	0.46
1:A:730:LEU:HG	1:A:734:GLN:OE1	2.15	0.46
1:B:194:ASP:HB2	1:B:380:VAL:HG13	1.96	0.46
1:B:229:THR:HB	1:B:374:LYS:HB2	1.96	0.46
1:B:357:TRP:HE1	1:B:365:MET:CE	2.28	0.46
1:A:281:ILE:HD12	1:A:281:ILE:N	2.30	0.46
1:A:568:THR:C	1:A:570:MET:H	2.23	0.46
1:A:654:SER:CA	1:A:657:THR:HG22	2.45	0.46
1:A:753:VAL:HG11	1:B:402:TYR:CE1	2.50	0.46
1:B:238:GLY:HA3	1:B:267:LYS:HD3	1.98	0.46
1:B:446:ARG:HH12	1:B:602:THR:HA	1.80	0.46
1:B:721:GLN:C	1:B:723:ASN:H	2.23	0.46
1:A:190:ILE:HG13	1:A:458:PHE:CD2	2.50	0.46
1:B:307:ASP:N	1:B:461:VAL:HG13	2.30	0.46
1:B:580:ILE:N	1:B:581:PRO:HD3	2.30	0.46
1:B:700:VAL:HG23	1:B:701:PHE:CD1	2.51	0.46
1:B:198:ASN:OD1	1:B:377:VAL:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:GLY:HA2	1:B:571:ASP:CG	2.40	0.46
1:A:190:ILE:CG2	1:A:191:GLN:N	2.78	0.46
1:A:232:LEU:CD1	1:A:256:ILE:HG13	2.45	0.46
1:A:409:ARG:NH2	1:A:454:SER:HB2	2.31	0.46
1:A:618:LEU:O	1:A:622:VAL:HG23	2.16	0.46
1:A:340:ALA:O	1:A:343:GLU:HB2	2.16	0.46
1:B:467:LEU:C	1:B:469:GLY:N	2.73	0.46
1:B:664:GLU:C	1:B:666:THR:N	2.73	0.46
1:A:127:LEU:N	1:A:127:LEU:HD22	2.31	0.46
1:A:348:ASN:HB3	1:A:371:LYS:CE	2.35	0.46
1:A:508:LYS:O	1:A:512:ASN:ND2	2.49	0.46
1:A:698:ARG:HA	1:A:707:HIS:NE2	2.31	0.46
1:B:134:LYS:O	1:B:138:THR:HG23	2.16	0.46
1:B:253:SER:C	1:B:277:ILE:HD12	2.41	0.46
1:B:720:LYS:C	1:B:722:ASN:H	2.24	0.46
1:A:553:VAL:HG11	1:A:597:PHE:CD2	2.51	0.45
1:B:122:LEU:HD12	1:B:122:LEU:N	2.30	0.45
1:B:201:ILE:HD13	1:B:211:TYR:C	2.41	0.45
1:B:445:SER:N	1:B:602:THR:HG22	2.31	0.45
1:B:732:ARG:HG3	1:B:732:ARG:NH1	2.27	0.45
1:B:348:ASN:HB3	1:B:371:LYS:CE	2.33	0.45
1:A:555:PHE:HZ	1:A:594:ALA:HB2	1.81	0.45
1:A:750:SER:OG	1:A:751:GLY:N	2.48	0.45
1:A:607:LEU:HD11	1:A:609:LEU:HG	1.98	0.45
1:A:639:LEU:HD23	1:A:643:TYR:HE1	1.79	0.45
1:B:124:TRP:HH2	1:B:596:GLN:HG2	1.82	0.45
1:B:232:LEU:HB2	1:B:373:VAL:CG1	2.47	0.45
1:B:237:PHE:HD2	1:B:258:ARG:HB2	1.81	0.45
1:B:283:MET:HE2	1:B:297:PHE:CD1	2.51	0.45
1:A:233:VAL:HG12	1:A:234:HIS:N	2.32	0.45
1:A:509:THR:C	1:A:511:GLN:H	2.24	0.45
1:A:699:HIS:CD2	1:A:702:TRP:H	2.32	0.45
1:B:240:LYS:C	1:B:242:ASP:N	2.72	0.45
1:B:496:VAL:HG11	1:B:506:ILE:HD13	1.99	0.45
1:A:390:PHE:CD2	1:A:449:ILE:HD11	2.51	0.45
1:B:664:GLU:O	1:B:666:THR:N	2.50	0.45
1:A:291:VAL:HG13	1:A:292:ASN:N	2.31	0.45
1:B:357:TRP:O	1:B:359:THR:N	2.43	0.45
1:B:588:ARG:HG3	1:B:588:ARG:NH1	2.31	0.45
1:A:648:ASP:CG	1:A:757:ASP:OD2	2.60	0.45
1:A:753:VAL:HG12	1:A:754:TRP:CG	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:LYS:HA	1:B:428:LYS:HD3	1.79	0.45
1:A:700:VAL:HG11	1:A:741:THR:HG21	1.97	0.45
1:A:721:GLN:O	1:A:723:ASN:N	2.50	0.45
1:B:211:TYR:CE1	1:B:212:LEU:O	2.69	0.45
1:B:568:THR:C	1:B:570:MET:H	2.25	0.45
1:A:161:LYS:HA	1:A:164:ASN:ND2	2.19	0.45
1:A:194:ASP:HB2	1:A:380:VAL:HG13	1.99	0.45
1:A:740:TRP:CD2	1:B:314:PRO:HD2	2.52	0.45
1:B:465:GLU:HA	1:B:468:GLU:HB2	1.99	0.45
1:A:235:ALA:O	1:A:236:ASN:C	2.59	0.44
1:A:646:ARG:HH11	1:A:646:ARG:CG	2.24	0.44
1:B:193:LYS:HA	1:B:379:ASN:OD1	2.17	0.44
1:B:197:GLN:OE1	1:B:197:GLN:HA	2.16	0.44
1:B:201:ILE:HD13	1:B:212:LEU:N	2.32	0.44
1:B:699:HIS:CD2	1:B:702:TRP:CD1	3.05	0.44
1:A:197:GLN:HA	1:A:197:GLN:OE1	2.17	0.44
1:A:221:ALA:O	1:A:223:SER:N	2.50	0.44
1:A:237:PHE:O	1:A:238:GLY:C	2.59	0.44
1:A:238:GLY:HA2	1:A:257:VAL:HB	1.99	0.44
1:A:690:VAL:CG2	1:A:698:ARG:HG2	2.47	0.44
1:B:340:ALA:O	1:B:343:GLU:HB2	2.17	0.44
1:B:610:ASP:HB3	1:B:613:GLU:CG	2.47	0.44
1:A:143:THR:O	1:A:147:LEU:HG	2.17	0.44
1:A:307:ASP:OD1	1:A:309:TYR:N	2.48	0.44
1:B:348:ASN:N	1:B:348:ASN:ND2	2.65	0.44
1:A:256:ILE:HD11	1:A:349:MET:HE1	2.00	0.44
1:A:349:MET:CG	1:A:367:THR:HA	2.45	0.44
1:A:547:TYR:HD1	1:A:696:PRO:O	1.99	0.44
1:A:580:ILE:HG23	1:A:583:LEU:HB2	1.99	0.44
1:B:233:VAL:HG12	1:B:234:HIS:N	2.33	0.44
1:B:263:THR:O	1:B:264:PHE:C	2.59	0.44
1:B:677:ARG:HE	1:B:750:SER:HB2	1.83	0.44
1:A:122:LEU:N	1:A:122:LEU:HD12	2.32	0.44
1:A:306:GLY:HA2	1:A:461:VAL:HG22	1.99	0.44
1:A:612:GLU:O	1:A:614:TYR:N	2.50	0.44
1:B:281:ILE:HD12	1:B:281:ILE:N	2.32	0.44
1:B:404:VAL:HA	1:B:449:ILE:HG23	2.00	0.44
1:B:619:LEU:HD23	1:B:619:LEU:C	2.42	0.44
1:B:669:PHE:CD1	1:B:669:PHE:C	2.95	0.44
1:A:262:ILE:HD11	1:A:267:LYS:HG2	1.98	0.44
1:A:357:TRP:HE1	1:A:365:MET:CE	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:VAL:HG12	1:B:449:ILE:HG13	1.99	0.44
1:B:654:SER:CA	1:B:657:THR:HG22	2.47	0.44
1:A:229:THR:HB	1:A:374:LYS:HB2	1.99	0.44
1:A:240:LYS:C	1:A:242:ASP:N	2.69	0.44
1:A:343:GLU:OE2	1:A:362:THR:HG21	2.18	0.44
1:A:349:MET:HG2	1:A:367:THR:HG22	2.00	0.44
1:A:637:LEU:CD1	1:A:731:PHE:HE2	2.31	0.44
1:B:133:GLU:HA	1:B:136:ASP:HB2	2.00	0.44
1:B:508:LYS:O	1:B:512:ASN:ND2	2.51	0.44
1:B:603:HIS:CD2	1:B:603:HIS:C	2.95	0.44
1:B:690:VAL:CG2	1:B:698:ARG:HG2	2.47	0.44
1:A:146:LEU:HD23	1:A:146:LEU:O	2.17	0.44
1:A:300:HIS:O	1:A:301:ALA:CB	2.66	0.44
1:A:488:VAL:HG21	1:A:587:ALA:HA	2.00	0.44
1:B:280:LEU:C	1:B:281:ILE:HD12	2.42	0.44
1:B:309:TYR:HE2	1:B:325:ARG:CA	2.21	0.44
1:A:651:ARG:HG2	1:A:651:ARG:HH11	1.83	0.44
1:B:633:LYS:O	1:B:633:LYS:HD3	2.18	0.44
1:B:637:LEU:CD1	1:B:731:PHE:HE2	2.30	0.44
1:B:737:LEU:C	1:B:739:THR:N	2.75	0.44
1:A:222:TYR:CE2	1:A:308:PRO:HG3	2.53	0.43
1:A:392:VAL:HG12	1:A:449:ILE:CB	2.49	0.43
1:A:415:GLY:HA2	1:A:571:ASP:CG	2.42	0.43
1:A:614:TYR:HA	1:A:617:GLN:HB2	1.99	0.43
1:A:603:HIS:ND1	1:A:604:ASP:OD1	2.52	0.43
1:A:654:SER:HA	1:A:657:THR:CG2	2.48	0.43
1:B:180:LYS:HD2	1:B:180:LYS:H	1.83	0.43
1:B:188:VAL:HB	1:B:307:ASP:HB2	2.00	0.43
1:B:235:ALA:O	1:B:236:ASN:C	2.60	0.43
1:B:478:ALA:O	1:B:550:ILE:HD12	2.19	0.43
1:A:488:VAL:HG13	1:A:586:VAL:CG1	2.49	0.43
1:A:633:LYS:O	1:A:633:LYS:HD3	2.18	0.43
1:B:499:SER:O	1:B:501:LEU:N	2.50	0.43
1:B:565:TYR:HB3	1:B:570:MET:HB3	1.99	0.43
1:A:190:ILE:HG23	1:A:191:GLN:N	2.32	0.43
1:A:482:ILE:HG22	1:A:483:ASN:N	2.33	0.43
1:A:669:PHE:CD1	1:A:669:PHE:C	2.96	0.43
1:B:513:VAL:HB	1:B:522:LEU:HD12	2.00	0.43
1:A:239:THR:O	1:A:241:LYS:N	2.51	0.43
1:B:402:TYR:HB3	1:B:449:ILE:HG22	2.00	0.43
1:B:513:VAL:HG22	1:B:592:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:HIS:CD2	1:B:701:PHE:HB2	2.53	0.43
1:B:732:ARG:NH1	1:B:732:ARG:CG	2.82	0.43
1:A:330:PRO:O	1:A:331:ASN:CB	2.62	0.43
1:A:359:THR:CG2	1:A:360:ASP:H	2.04	0.43
1:A:564:PRO:HG2	1:A:565:TYR:CD2	2.54	0.43
1:A:664:GLU:C	1:A:666:THR:N	2.74	0.43
1:B:204:ASP:OD2	1:B:370:SER:O	2.36	0.43
1:B:565:TYR:N	1:B:565:TYR:CD2	2.83	0.43
1:B:723:ASN:C	1:B:723:ASN:HD22	2.25	0.43
1:A:202:ILE:C	1:A:203:VAL:HG12	2.42	0.43
1:A:206:ASN:O	1:A:207:GLY:C	2.62	0.43
1:A:392:VAL:HG12	1:A:449:ILE:HG13	2.00	0.43
1:B:467:LEU:HD21	1:B:544:PHE:CZ	2.54	0.43
1:B:499:SER:O	1:B:500:PRO:C	2.59	0.43
1:B:667:ASP:CG	1:B:670:VAL:HG13	2.44	0.43
1:A:124:TRP:CH2	1:A:596:GLN:HG2	2.54	0.43
1:A:737:LEU:C	1:A:739:THR:N	2.74	0.43
1:A:737:LEU:HD11	1:B:693:LYS:HE2	2.00	0.43
1:B:221:ALA:O	1:B:301:ALA:HB3	2.19	0.43
1:A:327:SER:N	1:A:329:LEU:HD12	2.34	0.43
1:A:565:TYR:CD2	1:A:565:TYR:N	2.86	0.43
1:B:201:ILE:HD12	1:B:202:ILE:H	1.81	0.43
1:B:283:MET:HG3	1:B:297:PHE:CE1	2.54	0.43
1:B:318:HIS:C	1:B:318:HIS:HD1	2.27	0.43
1:B:324:SER:O	1:B:325:ARG:HB3	2.19	0.43
1:B:540:ALA:C	1:B:543:PRO:HD2	2.44	0.43
1:A:175:GLU:C	1:A:177:LYS:N	2.76	0.43
1:A:639:LEU:O	1:A:643:TYR:CD1	2.72	0.43
1:B:179:SER:O	1:B:180:LYS:C	2.60	0.43
1:B:488:VAL:HG13	1:B:586:VAL:HG11	2.01	0.43
1:B:603:HIS:ND1	1:B:604:ASP:OD1	2.52	0.43
1:A:610:ASP:HB3	1:A:613:GLU:CG	2.49	0.42
1:A:749:LEU:O	1:A:749:LEU:HG	2.19	0.42
1:B:232:LEU:CD2	1:B:256:ILE:HD11	2.49	0.42
1:B:730:LEU:HG	1:B:734:GLN:OE1	2.19	0.42
1:A:181:VAL:HA	1:A:391:GLY:HA2	2.00	0.42
1:A:214:GLU:OE1	1:A:341:ALA:HB2	2.19	0.42
1:A:221:ALA:O	1:A:301:ALA:HB3	2.18	0.42
1:A:230:GLY:O	1:A:372:ASN:HB2	2.19	0.42
1:A:309:TYR:HE2	1:A:325:ARG:CA	2.24	0.42
1:A:348:ASN:N	1:A:348:ASN:ND2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:THR:HG23	1:A:376:THR:O	2.18	0.42
1:A:509:THR:C	1:A:511:GLN:N	2.76	0.42
1:B:588:ARG:HD3	1:B:589:ALA:N	2.34	0.42
1:B:646:ARG:NH1	1:B:646:ARG:CG	2.77	0.42
1:A:402:TYR:CD1	1:A:402:TYR:N	2.87	0.42
1:B:131:LEU:HD22	1:B:599:ILE:HD11	2.01	0.42
1:B:308:PRO:HB2	1:B:329:LEU:HD11	2.01	0.42
1:B:482:ILE:HG22	1:B:483:ASN:N	2.34	0.42
1:B:716:LEU:HD13	1:B:731:PHE:CZ	2.54	0.42
1:A:175:GLU:C	1:A:177:LYS:H	2.26	0.42
1:A:238:GLY:HA2	1:A:257:VAL:CG1	2.49	0.42
1:A:283:MET:HG3	1:A:297:PHE:CE1	2.55	0.42
1:A:588:ARG:HD3	1:A:589:ALA:N	2.34	0.42
1:A:649:PHE:O	1:A:652:ALA:HB3	2.20	0.42
1:B:204:ASP:OD1	1:B:205:LYS:N	2.43	0.42
1:B:213:VAL:HG11	1:B:345:LEU:CD2	2.47	0.42
1:B:238:GLY:HA2	1:B:257:VAL:HB	2.01	0.42
1:B:317:ASN:HD22	1:B:317:ASN:HA	1.69	0.42
1:A:198:ASN:OD1	1:A:377:VAL:HA	2.19	0.42
1:A:202:ILE:HG13	1:A:213:VAL:HG21	2.01	0.42
1:A:406:GLY:HA2	1:A:451:ALA:O	2.19	0.42
1:A:513:VAL:HB	1:A:522:LEU:HD12	2.00	0.42
1:A:588:ARG:HD3	1:A:588:ARG:C	2.45	0.42
1:A:754:TRP:HE3	1:A:754:TRP:HA	1.84	0.42
1:B:201:ILE:HB	1:B:212:LEU:CD1	2.49	0.42
1:B:318:HIS:C	1:B:318:HIS:ND1	2.77	0.42
1:B:488:VAL:HG11	1:B:583:LEU:HD12	2.02	0.42
1:B:509:THR:C	1:B:511:GLN:H	2.27	0.42
1:B:539:ASN:C	1:B:539:ASN:ND2	2.78	0.42
1:B:564:PRO:HG2	1:B:565:TYR:CD2	2.55	0.42
1:A:411:ALA:HA	1:A:457:ASP:OD2	2.19	0.42
1:A:428:LYS:HD3	1:A:428:LYS:HA	1.83	0.42
1:A:467:LEU:O	1:A:468:GLU:C	2.62	0.42
1:A:669:PHE:CE2	1:B:668:ARG:HD2	2.55	0.42
1:B:353:CYS:HA	1:B:354:PRO:HD3	1.75	0.42
1:B:402:TYR:N	1:B:402:TYR:CD1	2.88	0.42
1:A:213:VAL:HG11	1:A:345:LEU:HD21	2.01	0.42
1:A:759:GLU:HG3	1:A:760:PHE:H	1.85	0.42
1:B:721:GLN:O	1:B:723:ASN:N	2.53	0.42
1:A:193:LYS:HA	1:A:379:ASN:OD1	2.20	0.42
1:A:264:PHE:O	1:A:268:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASP:HB3	1:A:310:THR:HG23	2.01	0.42
1:A:326:SER:N	1:A:329:LEU:HD13	2.34	0.42
1:A:514:LYS:HA	1:A:521:PHE:HA	2.00	0.42
1:A:686:LEU:HD23	1:A:699:HIS:N	2.34	0.42
1:B:376:THR:HG23	1:B:376:THR:O	2.19	0.42
1:B:648:ASP:CG	1:B:757:ASP:OD2	2.63	0.42
1:B:667:ASP:C	1:B:669:PHE:N	2.78	0.42
1:A:161:LYS:O	1:A:162:ASP:C	2.63	0.42
1:A:402:TYR:CE1	1:B:753:VAL:HG11	2.55	0.42
1:A:612:GLU:C	1:A:614:TYR:N	2.78	0.42
1:B:370:SER:OG	1:B:371:LYS:HG3	2.20	0.42
1:B:553:VAL:HG11	1:B:597:PHE:CD2	2.54	0.42
1:B:754:TRP:HA	1:B:754:TRP:HE3	1.84	0.42
1:A:335:GLN:NE2	1:A:336:THR:H	2.18	0.42
1:A:402:TYR:HB3	1:A:449:ILE:HG22	2.01	0.42
1:A:488:VAL:HG11	1:A:583:LEU:HD12	2.02	0.42
1:B:238:GLY:HA2	1:B:257:VAL:HG11	2.02	0.42
1:B:360:ASP:O	1:B:361:SER:O	2.38	0.42
1:B:406:GLY:HA2	1:B:451:ALA:O	2.20	0.42
1:A:145:LYS:O	1:A:148:ASN:N	2.52	0.41
1:A:232:LEU:HD13	1:A:254:ILE:HG22	2.00	0.41
1:A:253:SER:C	1:A:277:ILE:HD12	2.45	0.41
1:A:504:THR:OG1	1:A:610:ASP:OD2	2.37	0.41
1:A:614:TYR:O	1:A:618:LEU:HB2	2.20	0.41
1:A:723:ASN:N	1:A:723:ASN:HD22	2.17	0.41
1:B:193:LYS:NZ	1:B:193:LYS:HB2	2.35	0.41
1:B:349:MET:HB2	1:B:364:ARG:CB	2.50	0.41
1:A:349:MET:HB2	1:A:364:ARG:CB	2.51	0.41
1:A:349:MET:HA	1:A:367:THR:CA	2.50	0.41
1:A:555:PHE:CZ	1:A:594:ALA:HB2	2.55	0.41
1:A:754:TRP:NE1	1:B:449:ILE:HD12	2.35	0.41
1:B:123:TYR:O	1:B:126:ASP:HB2	2.20	0.41
1:B:221:ALA:O	1:B:223:SER:N	2.52	0.41
1:B:326:SER:N	1:B:329:LEU:HD13	2.35	0.41
1:B:667:ASP:O	1:B:669:PHE:N	2.54	0.41
1:B:699:HIS:CD2	1:B:702:TRP:H	2.36	0.41
1:A:148:ASN:HD21	1:A:416:ALA:HB2	1.86	0.41
1:A:308:PRO:HB2	1:A:329:LEU:HD11	2.01	0.41
1:A:540:ALA:C	1:A:543:PRO:HD2	2.45	0.41
1:B:327:SER:N	1:B:329:LEU:HD12	2.35	0.41
1:B:654:SER:HA	1:B:657:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LYS:H	1:A:180:LYS:CD	2.34	0.41
1:A:208:ARG:O	1:A:208:ARG:CD	2.63	0.41
1:A:565:TYR:HB3	1:A:570:MET:HB3	2.03	0.41
1:B:154:PRO:HD2	1:B:161:LYS:HZ3	1.84	0.41
1:B:386:ILE:HG22	1:B:454:SER:HB3	2.02	0.41
1:B:491:THR:HB	1:B:517:VAL:HG21	2.02	0.41
1:A:238:GLY:HA2	1:A:257:VAL:CB	2.50	0.41
1:A:308:PRO:HG3	1:A:329:LEU:HD21	2.03	0.41
1:A:322:PRO:O	1:A:323:PRO:C	2.64	0.41
1:B:509:THR:C	1:B:511:GLN:N	2.77	0.41
1:B:686:LEU:HD23	1:B:699:HIS:N	2.35	0.41
1:A:154:PRO:HD2	1:A:161:LYS:HZ3	1.84	0.41
1:A:667:ASP:C	1:A:669:PHE:N	2.78	0.41
1:A:668:ARG:HD2	1:B:669:PHE:CG	2.55	0.41
1:A:732:ARG:HG3	1:A:732:ARG:NH1	2.28	0.41
1:B:153:VAL:O	1:B:155:ARG:N	2.50	0.41
1:B:612:GLU:C	1:B:614:TYR:N	2.78	0.41
1:B:709:LEU:CB	1:B:710:PRO:HD3	2.51	0.41
1:A:278:GLY:N	1:A:332:ILE:CG2	2.82	0.41
1:A:398:GLU:N	1:A:399:PRO:CD	2.84	0.41
1:A:740:TRP:CH2	1:B:314:PRO:HB2	2.55	0.41
1:B:208:ARG:H	1:B:208:ARG:HD3	1.84	0.41
1:A:188:VAL:HB	1:A:307:ASP:HB2	2.03	0.41
1:A:723:ASN:HD22	1:A:723:ASN:C	2.29	0.41
1:A:730:LEU:O	1:A:734:GLN:HG3	2.21	0.41
1:B:262:ILE:HD11	1:B:267:LYS:HG2	2.02	0.41
1:A:310:THR:OG1	1:A:465:GLU:OE2	2.38	0.41
1:A:351:GLY:O	1:A:364:ARG:HB3	2.21	0.41
1:A:732:ARG:NH1	1:A:732:ARG:CG	2.84	0.41
1:A:753:VAL:HG12	1:A:754:TRP:N	2.35	0.41
1:B:156:GLU:O	1:B:162:ASP:HB2	2.21	0.41
1:B:188:VAL:HG23	1:B:190:ILE:HD13	2.02	0.41
1:B:222:TYR:CD2	1:B:308:PRO:HG3	2.56	0.41
1:B:287:LYS:HB3	1:B:288:PHE:CD1	2.56	0.41
1:B:300:HIS:NE2	1:B:458:PHE:C	2.79	0.41
1:B:377:VAL:O	1:B:377:VAL:HG23	2.21	0.41
1:B:398:GLU:N	1:B:399:PRO:CD	2.84	0.41
1:B:458:PHE:HB2	1:B:461:VAL:HG21	2.02	0.41
1:B:467:LEU:O	1:B:468:GLU:C	2.63	0.41
1:B:499:SER:C	1:B:501:LEU:N	2.79	0.41
1:B:585:LYS:O	1:B:588:ARG:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:ARG:HD3	1:B:588:ARG:C	2.46	0.41
1:B:658:THR:O	1:B:659:ASP:C	2.64	0.41
1:B:691:SER:HA	1:B:692:PRO:HD3	1.98	0.41
1:B:754:TRP:HA	1:B:754:TRP:CE3	2.56	0.41
1:A:238:GLY:CA	1:A:257:VAL:HB	2.51	0.41
1:A:306:GLY:N	1:A:459:GLY:O	2.53	0.41
1:B:498:ALA:CB	1:B:553:VAL:HA	2.50	0.41
1:B:649:PHE:O	1:B:652:ALA:HB3	2.21	0.41
1:A:357:TRP:HE1	1:A:365:MET:HE2	1.86	0.40
1:A:360:ASP:O	1:A:361:SER:O	2.39	0.40
1:B:148:ASN:HD21	1:B:416:ALA:HB2	1.85	0.40
1:B:190:ILE:HG23	1:B:191:GLN:N	2.36	0.40
1:B:322:PRO:O	1:B:323:PRO:C	2.63	0.40
1:B:514:LYS:HA	1:B:521:PHE:HA	2.02	0.40
1:B:614:TYR:HA	1:B:617:GLN:HB2	2.04	0.40
1:A:318:HIS:ND1	1:A:318:HIS:C	2.79	0.40
1:B:127:LEU:N	1:B:127:LEU:CD2	2.85	0.40
1:B:307:ASP:HB3	1:B:310:THR:HG23	2.02	0.40
1:B:444:PRO:CB	1:B:602:THR:HG21	2.37	0.40
1:B:488:VAL:HG21	1:B:587:ALA:HA	2.02	0.40
1:A:280:LEU:N	1:A:280:LEU:HD22	2.36	0.40
1:A:430:ALA:HA	1:A:450:PHE:CE2	2.56	0.40
1:A:516:PRO:HG3	1:A:586:VAL:HA	2.02	0.40
1:B:349:MET:CG	1:B:367:THR:HA	2.48	0.40
1:B:351:GLY:O	1:B:364:ARG:HB3	2.20	0.40
1:B:555:PHE:HZ	1:B:594:ALA:HB2	1.87	0.40
1:A:335:GLN:NE2	1:A:336:THR:N	2.68	0.40
1:A:404:VAL:HA	1:A:449:ILE:HG23	2.03	0.40
1:A:637:LEU:HD21	1:A:732:ARG:HE	1.85	0.40
1:B:190:ILE:CG2	1:B:191:GLN:N	2.84	0.40
1:B:298:PHE:HB2	1:B:412:TRP:CD2	2.57	0.40
1:B:719:ARG:CG	1:B:719:ARG:NH1	2.80	0.40
1:B:723:ASN:HD22	1:B:723:ASN:N	2.19	0.40
1:A:445:SER:N	1:A:602:THR:HG22	2.36	0.40
1:B:278:GLY:N	1:B:332:ILE:CG2	2.84	0.40
1:B:446:ARG:NH1	1:B:602:THR:HA	2.36	0.40
1:B:698:ARG:HA	1:B:707:HIS:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	637/639 (100%)	497 (78%)	102 (16%)	38 (6%)	1	13
1	B	637/639 (100%)	498 (78%)	100 (16%)	39 (6%)	1	13
All	All	1274/1278 (100%)	995 (78%)	202 (16%)	77 (6%)	2	13

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	210	VAL
1	A	251	ASN
1	A	330	PRO
1	A	361	SER
1	A	362	THR
1	A	722	ASN
1	A	750	SER
1	A	753	VAL
1	A	759	GLU
1	B	179	SER
1	B	207	GLY
1	B	210	VAL
1	B	251	ASN
1	B	361	SER
1	B	362	THR
1	B	722	ASN
1	B	750	SER
1	B	753	VAL
1	B	759	GLU
1	A	179	SER
1	A	207	GLY
1	A	209	LEU
1	A	222	TYR
1	A	236	ASN

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Mol	Chain	Res	Type
1	A	613	GLU
1	B	213	VAL
1	B	222	TYR
1	B	236	ASN
1	B	238	GLY
1	B	278	GLY
1	B	330	PRO
1	B	665	LYS
1	A	208	ARG
1	A	237	PHE
1	A	238	GLY
1	A	239	THR
1	A	278	GLY
1	A	322	PRO
1	A	325	ARG
1	A	370	SER
1	A	558	CYS
1	A	581	PRO
1	A	665	LYS
1	B	237	PHE
1	B	322	PRO
1	B	325	ARG
1	B	581	PRO
1	A	180	LYS
1	A	566	LEU
1	B	212	LEU
1	B	239	THR
1	B	558	CYS
1	B	566	LEU
1	B	613	GLU
1	B	668	ARG
1	A	213	VAL
1	A	507	GLU
1	B	180	LYS
1	B	204	ASP
1	B	205	LYS
1	B	240	LYS
1	B	370	SER
1	B	540	ALA
1	A	153	VAL
1	A	205	LYS
1	A	569	THR

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Mol	Chain	Res	Type
1	B	153	VAL
1	B	247	TYR
1	B	351	GLY
1	B	216	PRO
1	A	216	PRO
1	B	564	PRO
1	A	351	GLY
1	A	564	PRO
1	A	756	ILE
1	B	756	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	548/548 (100%)	502 (92%)	46 (8%)	10	30
1	B	548/548 (100%)	503 (92%)	45 (8%)	10	31
All	All	1096/1096 (100%)	1005 (92%)	91 (8%)	12	30

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	ASP
1	A	129	ARG
1	A	135	LEU
1	A	148	ASN
1	A	150	ASN
1	A	152	TYR
1	A	153	VAL
1	A	181	VAL
1	A	190	ILE
1	A	193	LYS
1	A	197	GLN
1	A	203	VAL
1	A	204	ASP

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Mol	Chain	Res	Type
1	A	211	TYR
1	A	224	LYS
1	A	246	LEU
1	A	277	ILE
1	A	310	THR
1	A	318	HIS
1	A	322	PRO
1	A	325	ARG
1	A	330	PRO
1	A	337	ILE
1	A	353	CYS
1	A	357	TRP
1	A	365	MET
1	A	371	LYS
1	A	426	LEU
1	A	449	ILE
1	A	525	ASP
1	A	537	LEU
1	A	562	ASP
1	A	581	PRO
1	A	582	GLU
1	A	603	HIS
1	A	606	GLU
1	A	619	LEU
1	A	633	LYS
1	A	646	ARG
1	A	648	ASP
1	A	664	GLU
1	A	710	PRO
1	A	723	ASN
1	A	743	GLN
1	A	757	ASP
1	A	758	ASN
1	B	125	ASP
1	B	129	ARG
1	B	135	LEU
1	B	148	ASN
1	B	152	TYR
1	B	153	VAL
1	B	181	VAL
1	B	190	ILE
1	B	193	LYS

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Mol	Chain	Res	Type
1	B	197	GLN
1	B	201	ILE
1	B	203	VAL
1	B	224	LYS
1	B	246	LEU
1	B	277	ILE
1	B	310	THR
1	B	318	HIS
1	B	322	PRO
1	B	325	ARG
1	B	330	PRO
1	B	337	ILE
1	B	348	ASN
1	B	353	CYS
1	B	357	TRP
1	B	365	MET
1	B	371	LYS
1	B	426	LEU
1	B	449	ILE
1	B	525	ASP
1	B	537	LEU
1	B	562	ASP
1	B	581	PRO
1	B	582	GLU
1	B	603	HIS
1	B	606	GLU
1	B	619	LEU
1	B	633	LYS
1	B	646	ARG
1	B	648	ASP
1	B	664	GLU
1	B	710	PRO
1	B	723	ASN
1	B	743	GLN
1	B	757	ASP
1	B	758	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	160	GLN

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Mol	Chain	Res	Type
1	A	164	ASN
1	A	191	GLN
1	A	215	ASN
1	A	270	ASN
1	A	275	ASN
1	A	317	ASN
1	A	335	GLN
1	A	348	ASN
1	A	408	GLN
1	A	431	GLN
1	A	443	GLN
1	A	515	HIS
1	A	527	ASN
1	A	539	ASN
1	A	603	HIS
1	A	617	GLN
1	A	662	ASN
1	A	684	HIS
1	A	699	HIS
1	A	723	ASN
1	A	758	ASN
1	B	148	ASN
1	B	160	GLN
1	B	164	ASN
1	B	191	GLN
1	B	197	GLN
1	B	270	ASN
1	B	275	ASN
1	B	317	ASN
1	B	335	GLN
1	B	348	ASN
1	B	408	GLN
1	B	431	GLN
1	B	443	GLN
1	B	515	HIS
1	B	539	ASN
1	B	617	GLN
1	B	662	ASN
1	B	684	HIS
1	B	699	HIS
1	B	721	GLN
1	B	723	ASN

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Mol	Chain	Res	Type
1	B	758	ASN

5.3.3 RNA [i](#)

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.

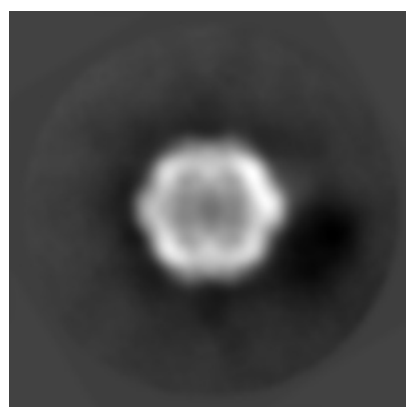
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1288. These allow visual inspection of the internal detail of the map and identification of artifacts.

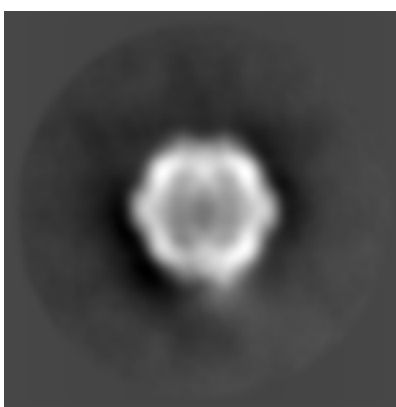
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

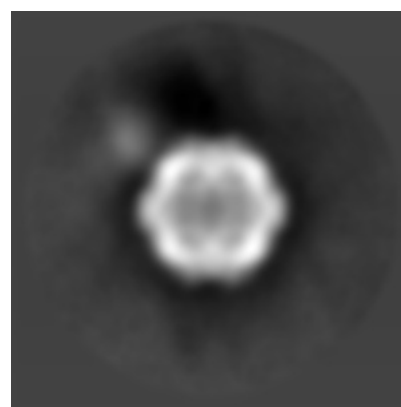
6.1.1 Primary map



X



Y

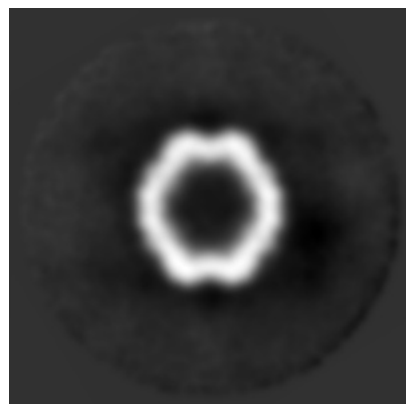


Z

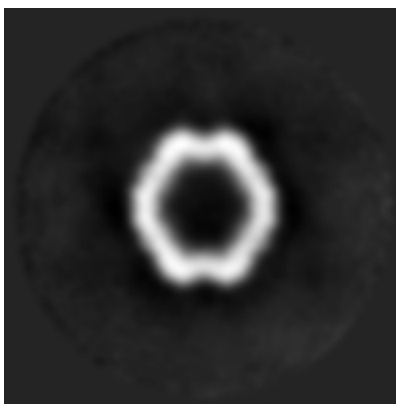
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

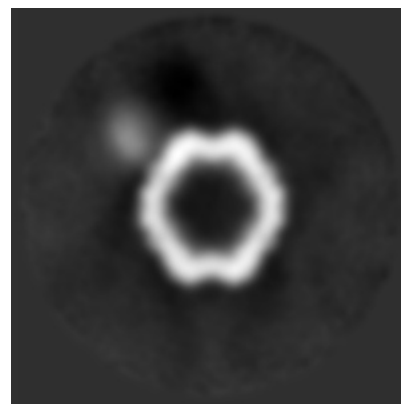
6.2.1 Primary map



X Index: 128



Y Index: 128

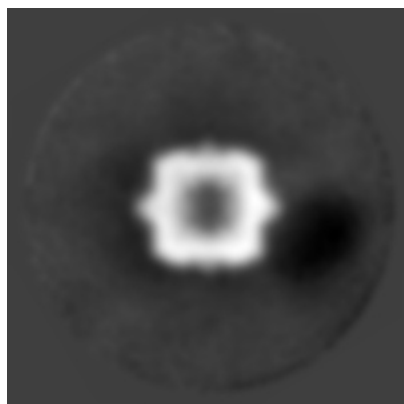


Z Index: 128

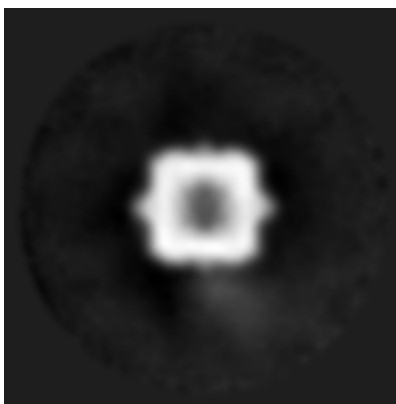
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

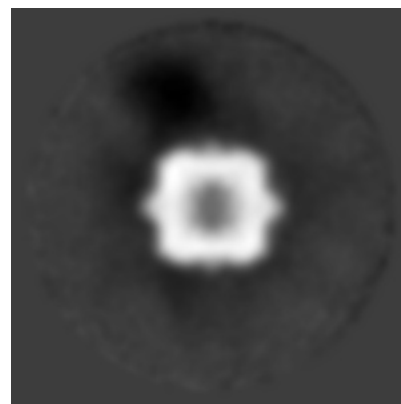
6.3.1 Primary map



X Index: 103



Y Index: 155

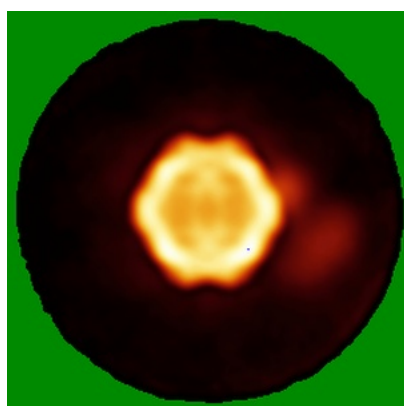


Z Index: 101

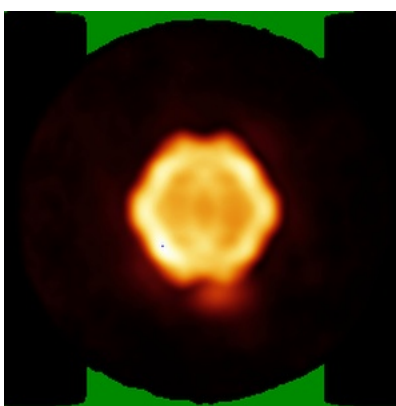
The images above show the largest variance slices of the map in three orthogonal directions.

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

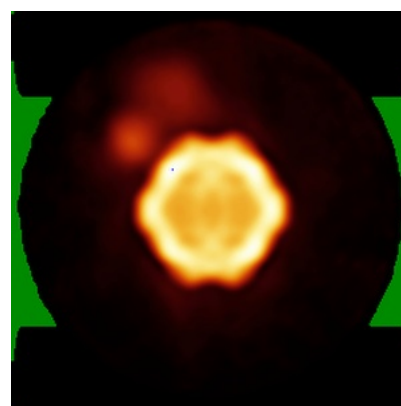
6.4.1 Primary map



X



Y

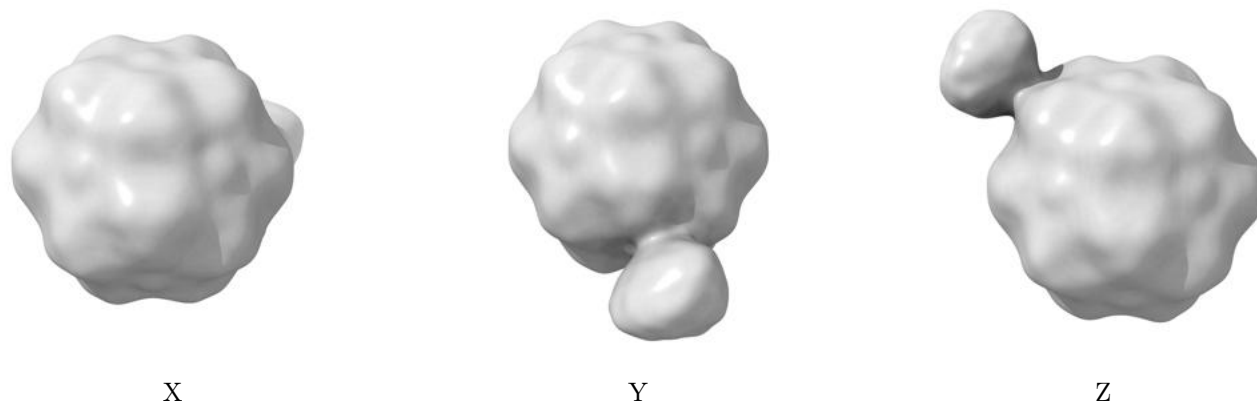


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

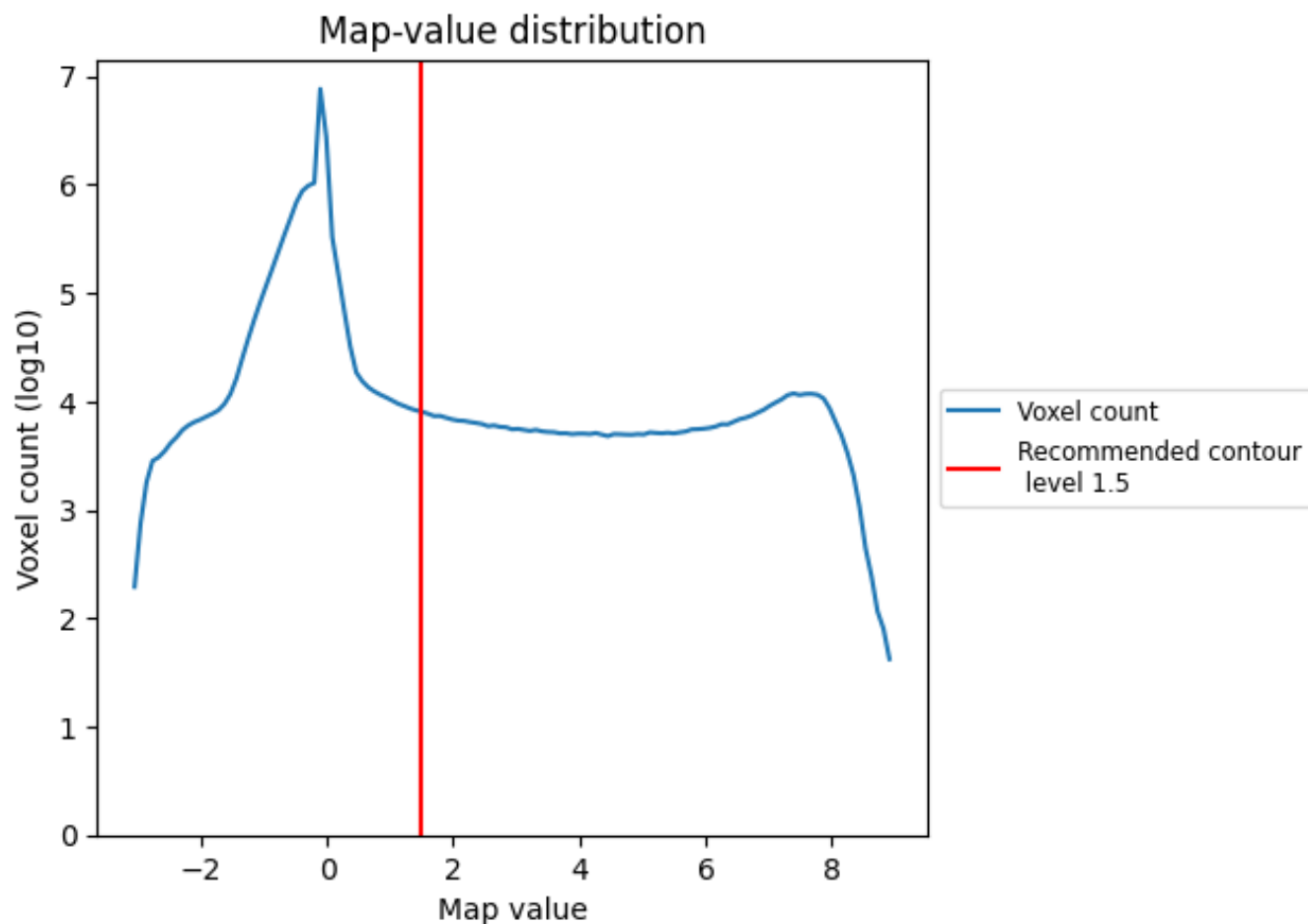
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

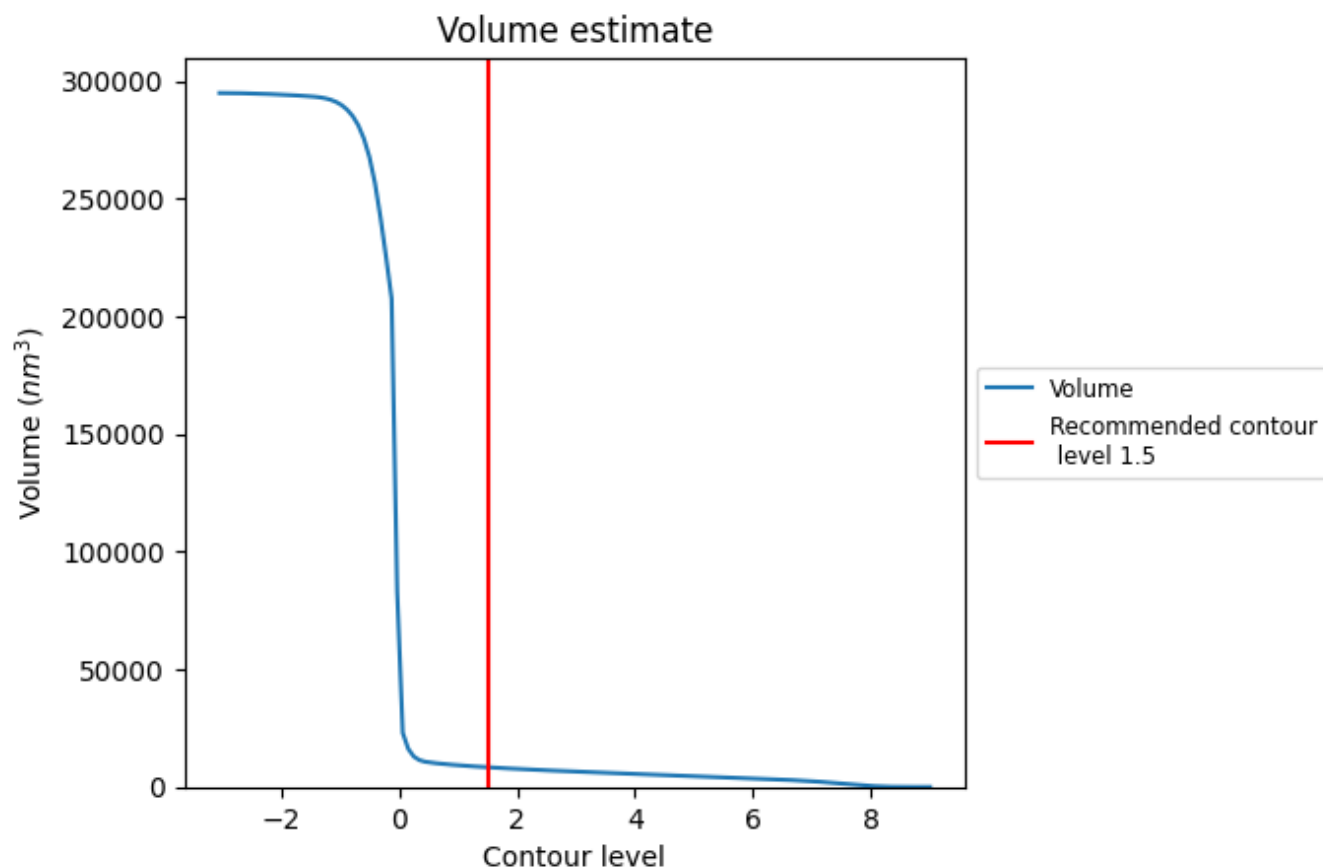
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

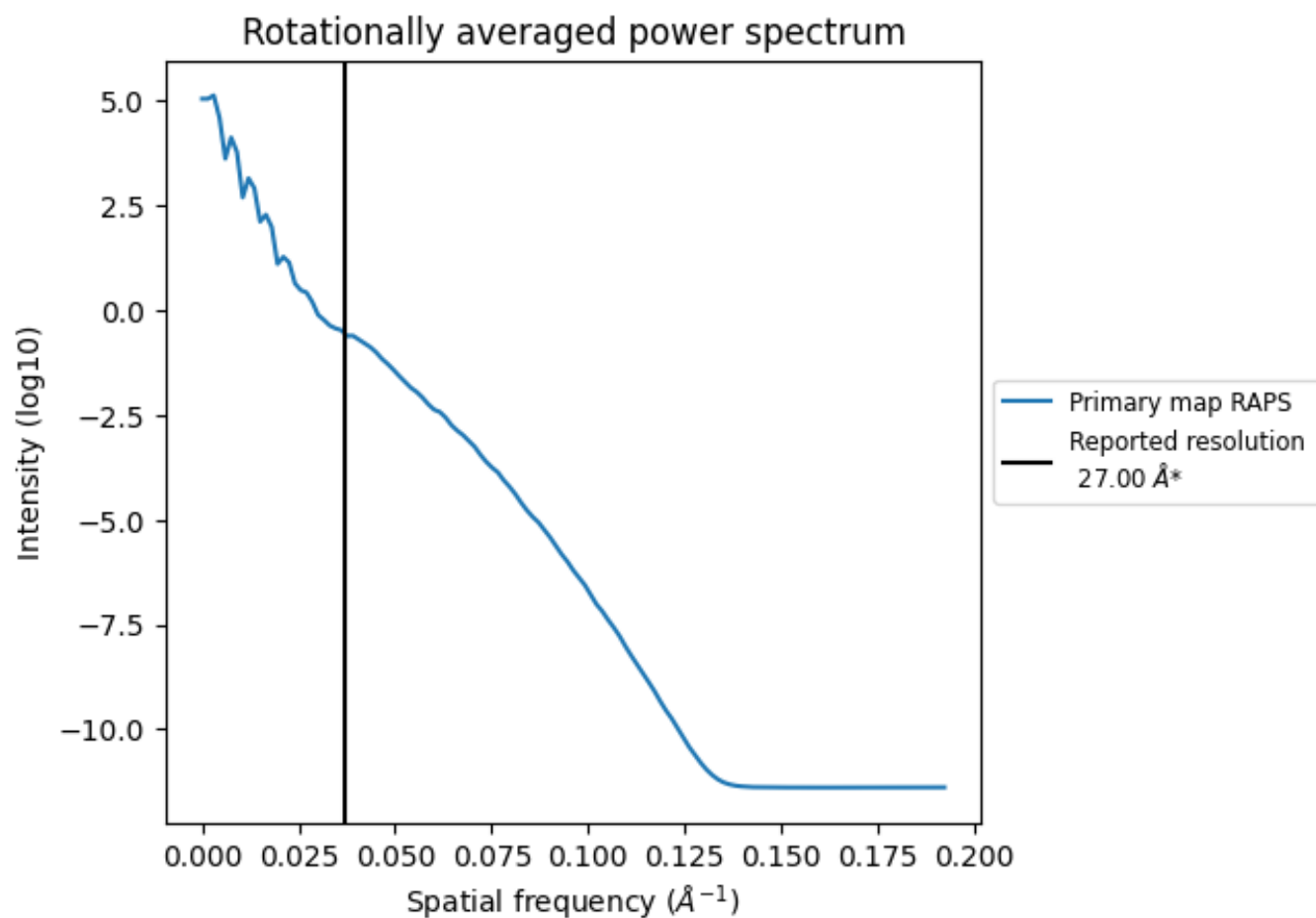
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 8371 nm^3 ; this corresponds to an approximate mass of 7561 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 0.037 Å⁻¹

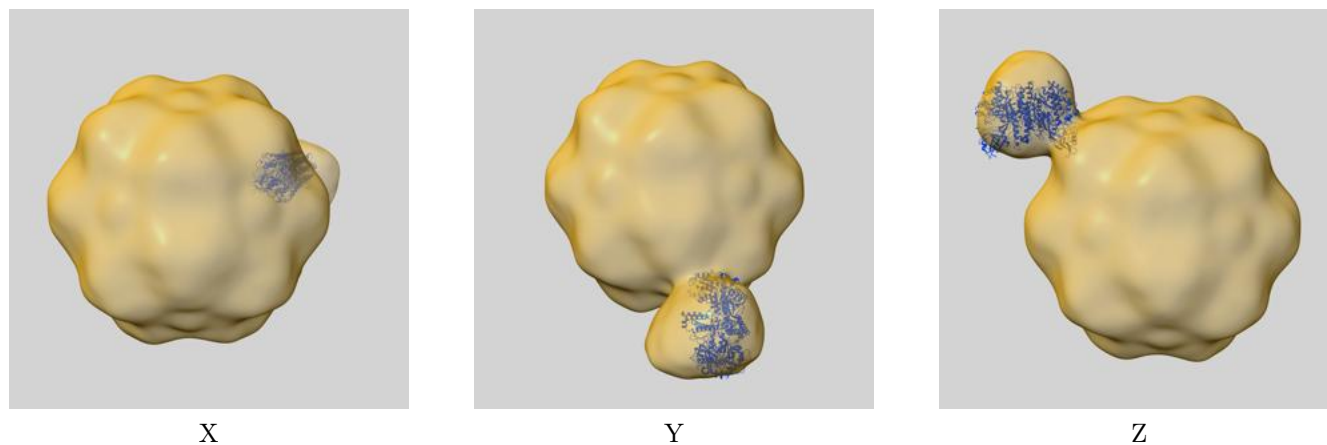
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

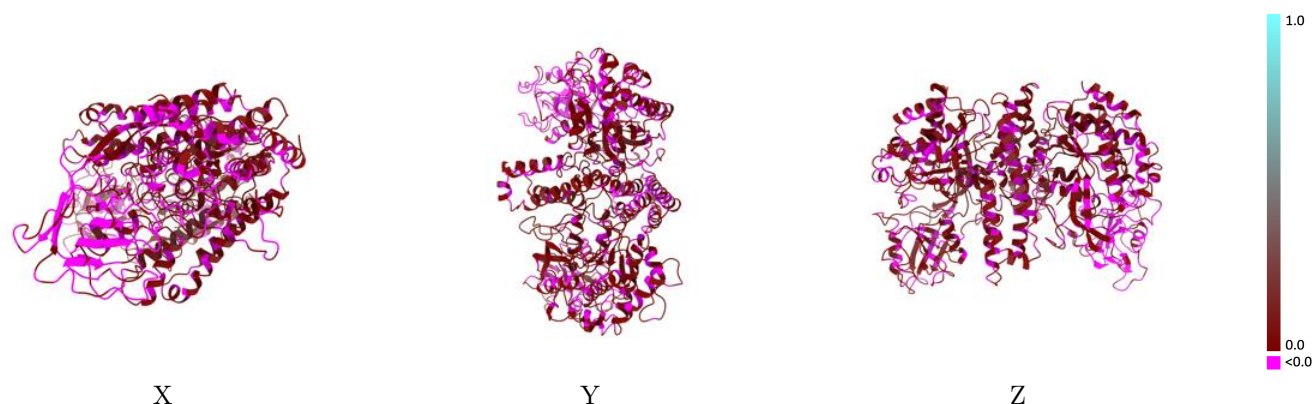
This section contains information regarding the fit between EMDB map EMD-1288 and PDB model 2NSU. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



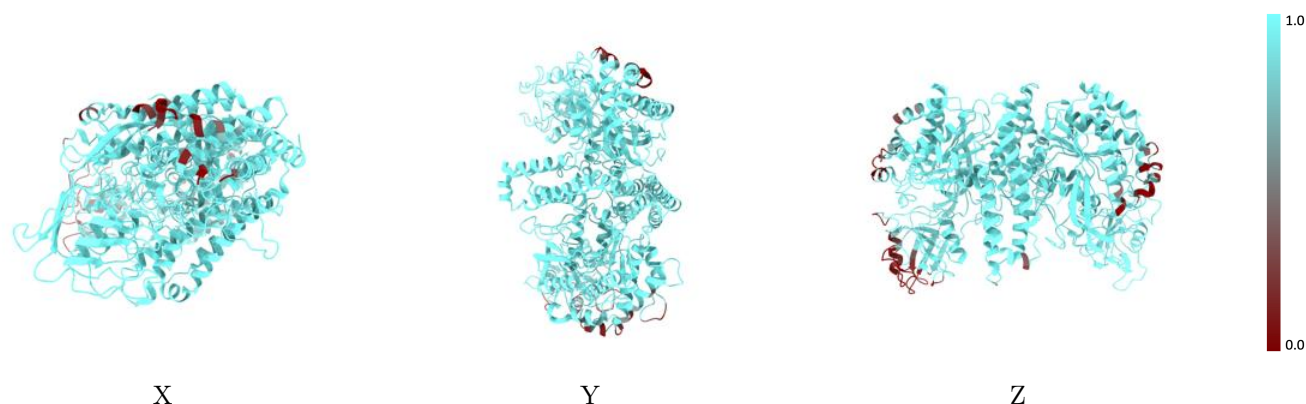
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



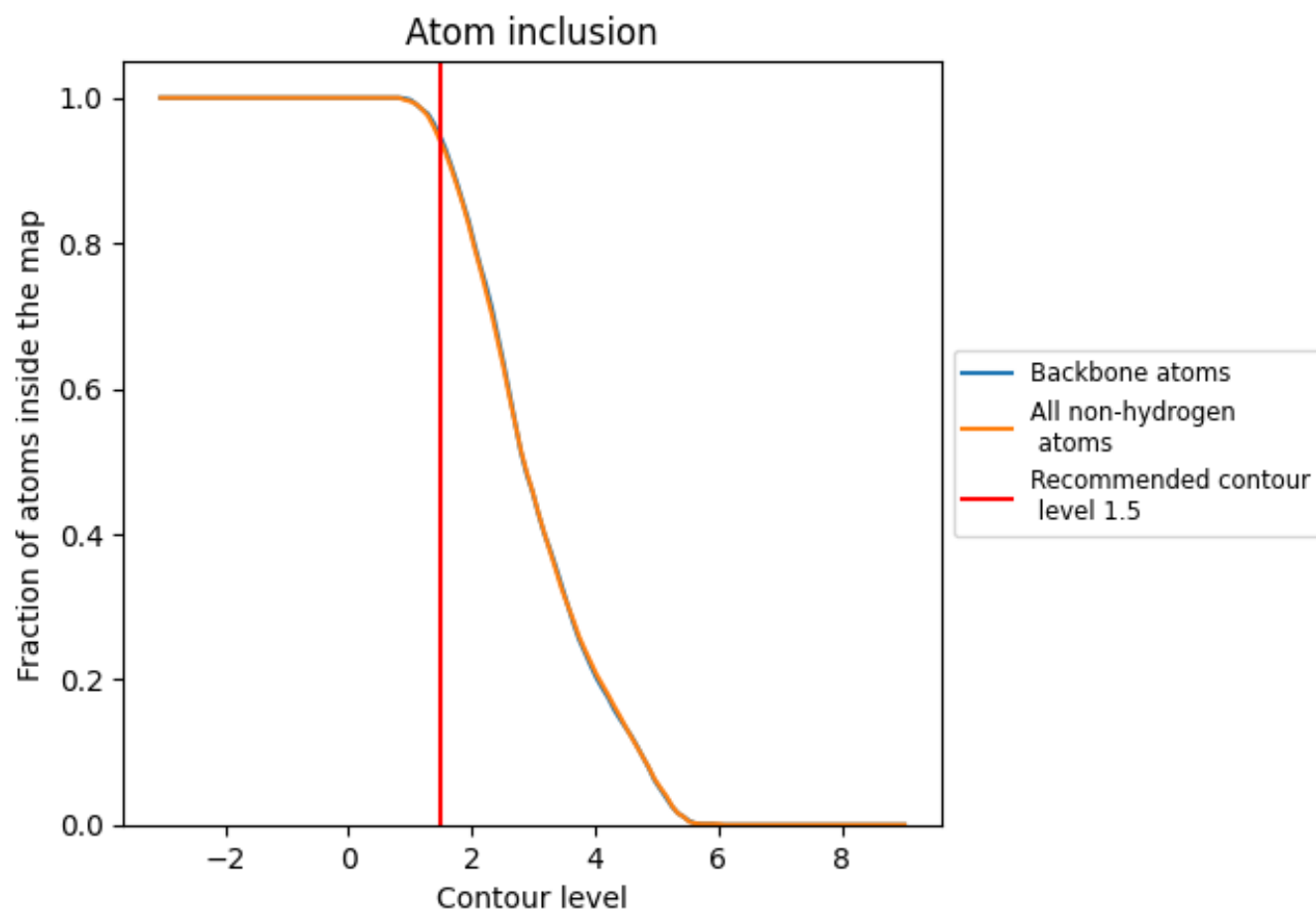
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9380	0.0280
A	0.9020	0.0330
B	0.9740	0.0230

