



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 04:58 PM UTC

PDB ID : 6YRF / pdb_00006yrf
EMDB ID : EMD-10888
Title : Vip3Bc1 tetramer
Authors : Thompson, R.F.; Byrne, M.J.; Iadanza, M.I.; Arribas Perez, M.; Maskell, D.P.; George, R.M.; Hesketh, E.L.; Beales, P.A.; Zack, M.D.; Berry, C.
Deposited on : 2020-04-20
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

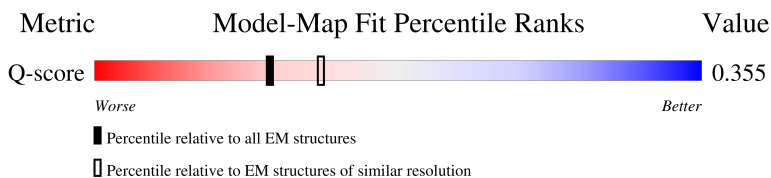
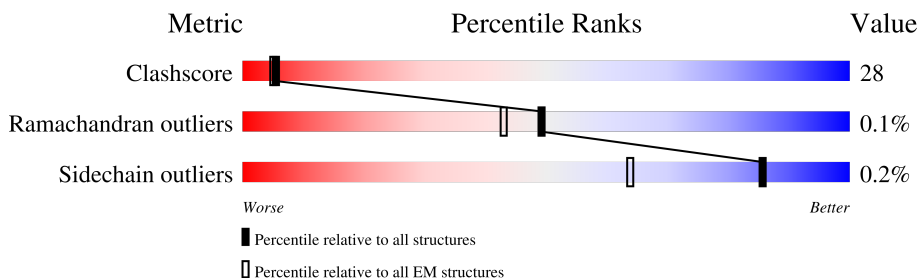
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	803	 44% 52%
1	B	803	 46% 50%
1	C	803	 44% 52%
1	D	803	 47% 49%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24828 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.

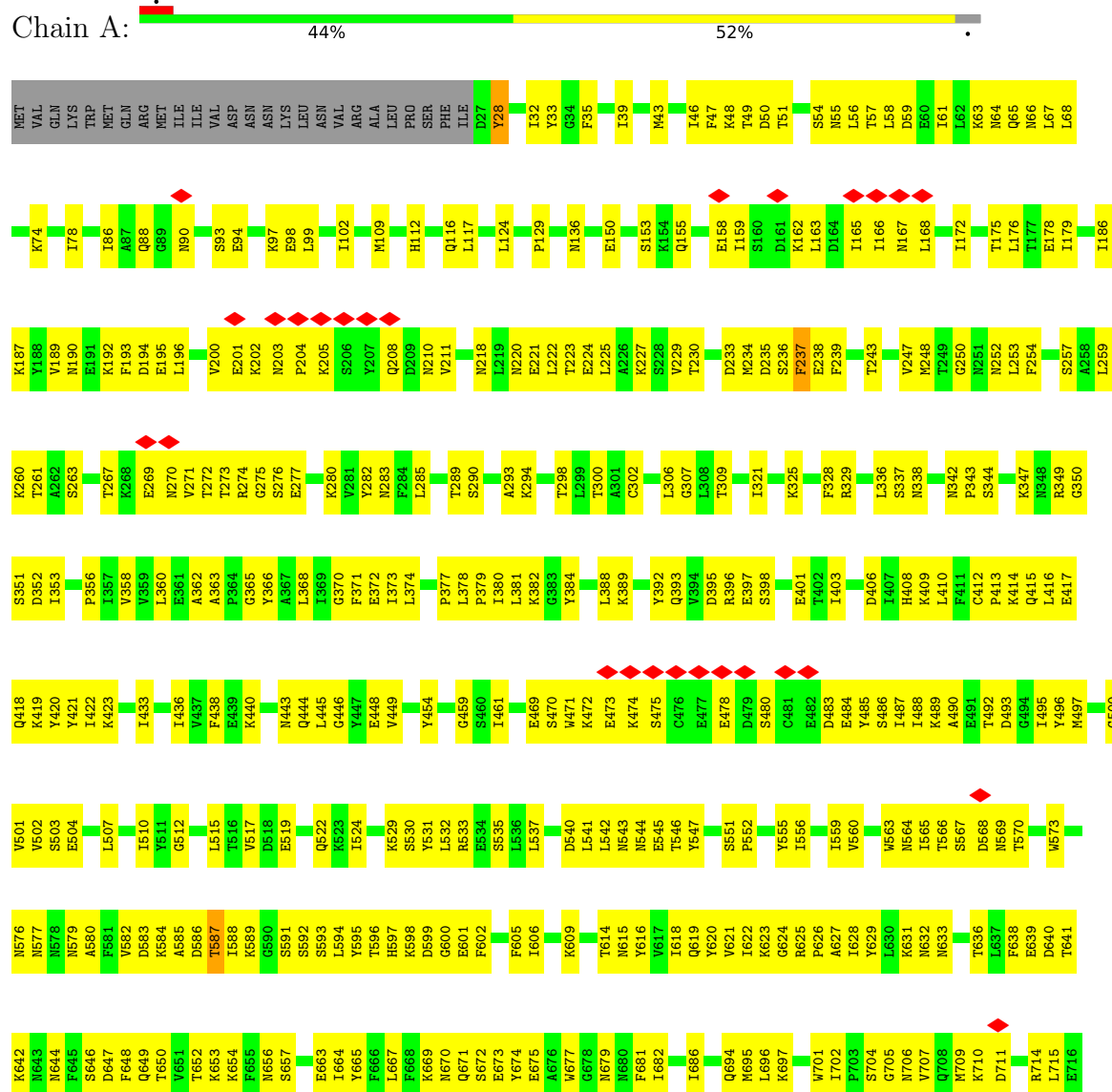
- Molecule 1 is a protein called Vegetative insecticidal protein.

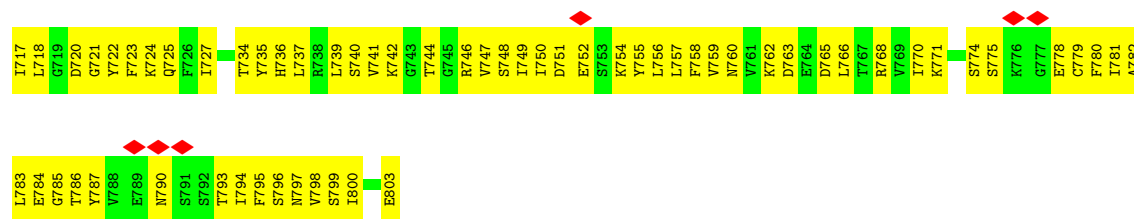
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	777	Total	C	N	O	S	0	0
			6207	3950	1009	1231	17		
1	B	777	Total	C	N	O	S	0	0
			6207	3950	1009	1231	17		
1	C	777	Total	C	N	O	S	0	0
			6207	3950	1009	1231	17		
1	D	777	Total	C	N	O	S	0	0
			6207	3950	1009	1231	17		

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.

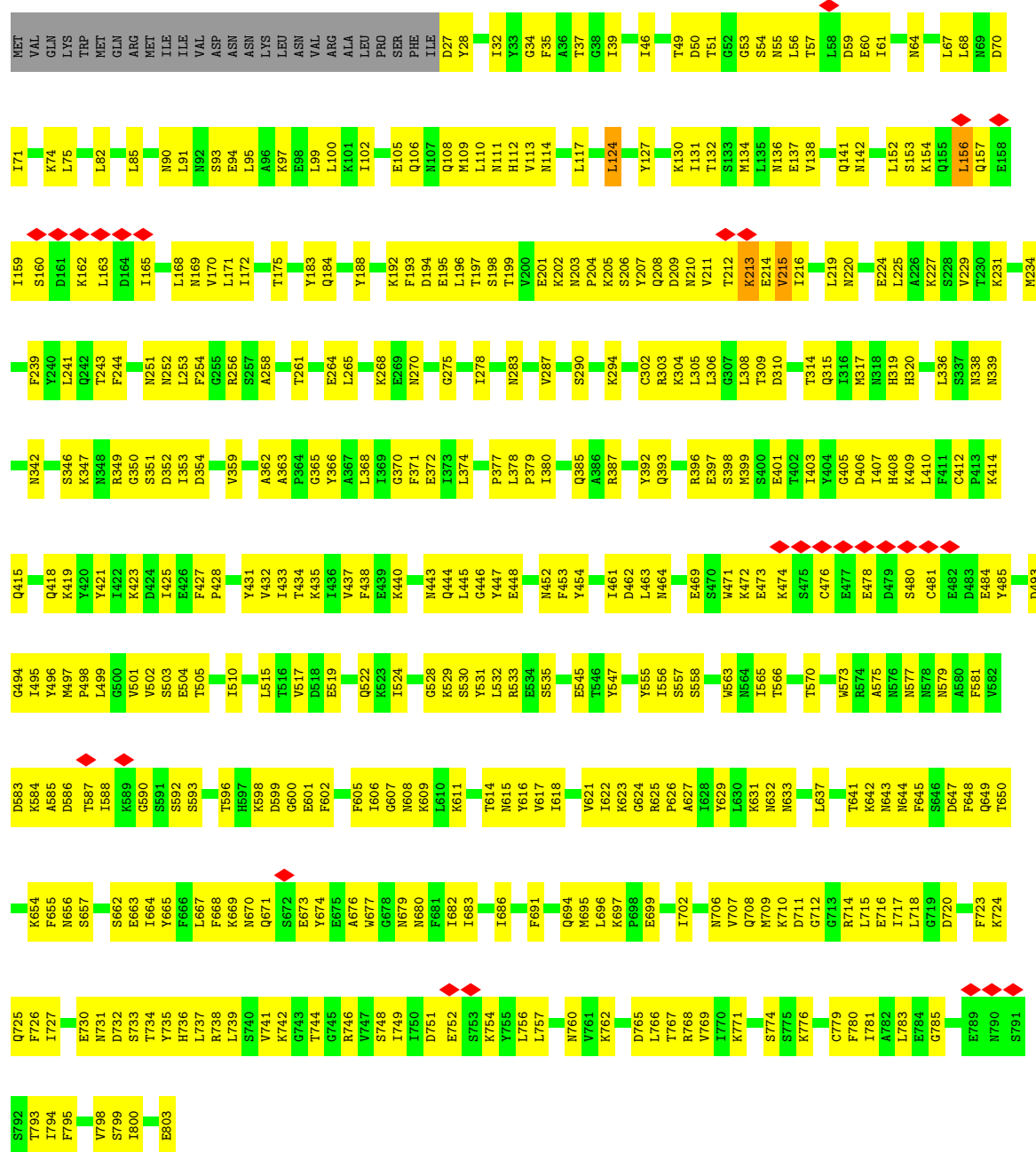
• Molecule 1: Vegetative insecticidal protein





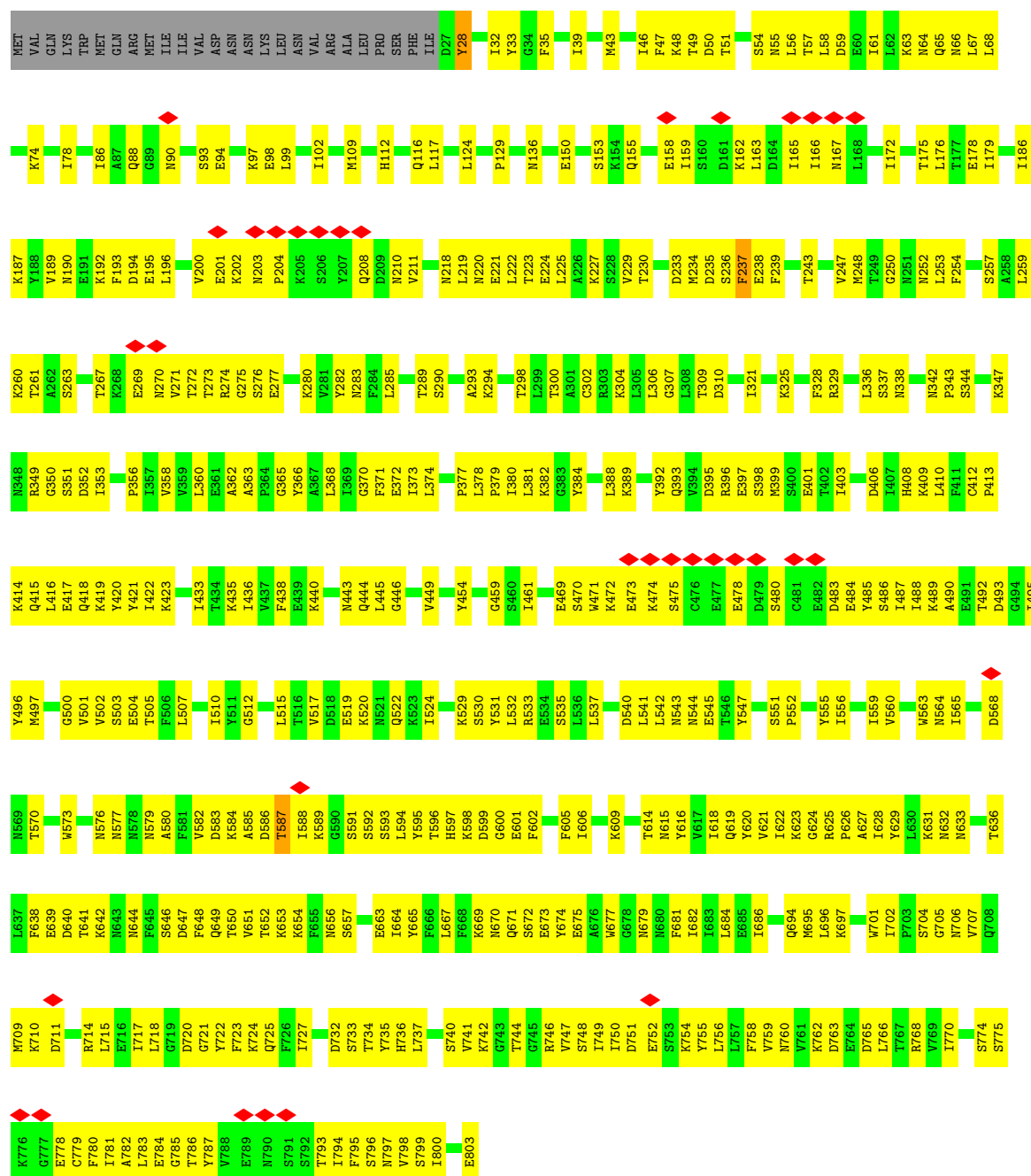
- Molecule 1: Vegetative insecticidal protein

Chain B: 46% 50%



- Molecule 1: Vegetative insecticidal protein

Chain C:  44% 52%



• Molecule 1: Vegetative insecticidal protein

Chain D:  47% 49%



L85	V170	N252	D352	P428	H597	N670	L739
N90	L171	L253	I353	Y431	K598	Q671	S740
L91	I172	F254	D354	V432	D599	S672	V741
N92	T175	G255	V359	T516	G600	E673	K742
S93	L176	R256	T359	T434	E601	G743	G743
E94	Y183	S257	A362	K435	F602	E675	T744
L95	Q184	A258	A363	T436	F605	A676	G745
A96	Y188	T261	A364	V437	I606	W677	R746
K97	Y192	E264	G365	F438	G607	G678	V747
I102	L265	Y366	Y366	E439	N608	I749	S748
E105	K192	L265	A367	K440	K609	F681	I750
Q106	F193	L368	L368	M443	K611	I682	D751
M107	F193	K268	F371	Q444	T614	I683	E752
M108	D194	E269	E372	L445	N615	I686	S753
Q109	E195	N270	I373	G446	Y616	K687	K754
M110	L196	G275	L374	Y447	L532	F691	Y755
M111	T197	I278	P379	E448	R533	I618	L756
H112	S198	V200	I380	M452	E534	Q694	L757
V113	T199	E201	I380	F453	S535	M695	N760
M114	K202	K202	Q385	Y454	E545	L696	V761
L117	N203	N203	A386	I461	T546	K697	K762
L124	P204	P204	E387	D462	Y547	E699	D765
Y127	K205	S290	Y392	L463	Y555	I702	L766
K130	S206	K294	Q393	M464	I556	N706	L767
T131	Y207	C302	R396	E469	S557	V707	I770
T132	D209	R303	E397	S470	S558	Q708	K771
S133	N210	K304	S398	W471	W563	W709	S774
M134	V211	L305	M399	K472	N564	K710	S775
L135	T212	L308	S400	E473	I565	D711	K776
N136	K213	T309	E401	K474	T570	G712	C779
E137	E214	D310	I403	S475	W573	G713	F780
V138	V215	T314	Y404	C476	R574	R714	L781
Q141	I216	Q315	G405	E477	A575	L715	L782
N142	L219	I316	I407	E478	N576	E716	L783
L152	N220	H408	H408	D479	N577	L717	E784
S153	E224	N318	K409	S480	N578	L718	G785
K154	L225	H319	L410	C481	N579	G719	D789
Q155	A226	H320	F411	E482	A580	F723	N789
L156	S227	I321	C412	D483	F581	K724	M790
Q157	V229	L336	P413	E484	V582	Q725	S791
E158	T230	S337	K414	Y485	K584	F726	S792
I159	K231	N338	Q415	D493	A585	I727	I793
S160	M234	N339	Q418	G494	D586	E730	I794
D161	F239	N342	K419	T495	T587	N731	F795
K162	Y240	S346	Y421	Y496	I588	D732	V798
L163	L241	K347	I422	M497	K589	S733	S799
D164	Q242	N348	K423	P498	G590	T734	I800
I165	T243	R349	D424	L499	S591	Y735	E803
L168	F244	G350	I425	G500	S592	H736	
M169	N251	S351	E426	V501	S593	L737	
			F427	V502	T596	R738	
				E504	T505		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	1414999	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 ($e^-/\text{\AA}^2$)	76.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	4.103	Depositor
Minimum map value	-1.650	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.171	Depositor
Recommended contour level	0.83	Depositor
Map size (Å)	281.16, 281.16, 281.16	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	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	0.28	0/6317	0.49	0/8542
1	B	0.29	0/6317	0.45	0/8542
1	C	0.28	0/6317	0.49	0/8542
1	D	0.29	0/6317	0.45	0/8542
All	All	0.28	0/25268	0.47	0/34168

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	D	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	213	LYS	Peptide
1	B	215	VAL	Peptide
1	D	213	LYS	Peptide
1	D	215	VAL	Peptide

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	6207	0	6174	358	0
1	B	6207	0	6174	352	0
1	C	6207	0	6174	358	0
1	D	6207	0	6174	352	0
All	All	24828	0	24696	1375	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 28.

All (1375) 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:229:VAL:HG23	1:C:302:CYS:HB3	1.57	0.86
1:A:229:VAL:HG23	1:A:302:CYS:HB3	1.57	0.85
1:C:631:LYS:HG3	1:C:633:ASN:H	1.41	0.84
1:A:631:LYS:HG3	1:A:633:ASN:H	1.41	0.84
1:C:165:ILE:HD12	1:C:269:GLU:HB3	1.61	0.82
1:A:165:ILE:HD12	1:A:269:GLU:HB3	1.61	0.82
1:D:175:THR:HG21	1:D:261:THR:HG21	1.62	0.81
1:B:175:THR:HG21	1:B:261:THR:HG21	1.62	0.80
1:C:625:ARG:HG3	1:C:644:ASN:HB3	1.63	0.78
1:D:211:VAL:HG22	1:D:212:THR:HG22	1.66	0.78
1:A:625:ARG:HG3	1:A:644:ASN:HB3	1.63	0.77
1:B:51:THR:HG23	1:B:53:GLY:H	1.49	0.77
1:B:211:VAL:HG22	1:B:212:THR:HG22	1.66	0.77
1:D:51:THR:HG23	1:D:53:GLY:H	1.49	0.77
1:B:169:ASN:H	1:B:172:ILE:HD13	1.49	0.77
1:D:647:ASP:OD1	1:D:649:GLN:NE2	2.19	0.76
1:D:169:ASN:H	1:D:172:ILE:HD13	1.49	0.76
1:A:583:ASP:HB2	1:A:595:TYR:HB2	1.69	0.75
1:B:647:ASP:OD1	1:B:649:GLN:NE2	2.19	0.75
1:A:277:GLU:OE1	1:A:337:SER:N	2.20	0.74
1:C:623:LYS:HG3	1:C:647:ASP:HA	1.69	0.74
1:B:629:TYR:HB2	1:B:667:LEU:HB2	1.69	0.74
1:D:419:LYS:HB3	1:D:444:GLN:HA	1.68	0.74
1:B:303:ARG:NH2	1:B:309:THR:OG1	2.21	0.74
1:C:583:ASP:HB2	1:C:595:TYR:HB2	1.69	0.74
1:A:413:PRO:HG2	1:A:490:ALA:HB2	1.69	0.74
1:B:419:LYS:HB3	1:B:444:GLN:HA	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:LYS:HD2	1:C:221:GLU:HB3	1.70	0.74
1:A:623:LYS:HG3	1:A:647:ASP:HA	1.69	0.73
1:C:371:PHE:HB2	1:C:502:VAL:HB	1.71	0.73
1:A:78:ILE:HD13	1:B:106:GLN:HG2	1.70	0.73
1:A:352:ASP:OD1	1:A:443:ASN:ND2	2.22	0.73
1:D:629:TYR:HB2	1:D:667:LEU:HB2	1.69	0.73
1:C:488:ILE:HD11	1:C:517:VAL:HG21	1.71	0.73
1:C:352:ASP:OD1	1:C:443:ASN:ND2	2.22	0.72
1:A:488:ILE:HD11	1:A:517:VAL:HG21	1.71	0.72
1:D:303:ARG:NH2	1:D:309:THR:OG1	2.21	0.72
1:D:393:GLN:HE22	1:D:547:TYR:HD1	1.37	0.72
1:A:202:LYS:HD2	1:A:221:GLU:HB3	1.70	0.72
1:C:413:PRO:HG2	1:C:490:ALA:HB2	1.69	0.72
1:A:565:ILE:HB	1:A:592:SER:HB3	1.71	0.72
1:D:201:GLU:O	1:D:207:TYR:OH	2.03	0.72
1:A:379:PRO:HB3	1:A:497:MET:HE1	1.72	0.72
1:A:746:ARG:HA	1:A:760:ASN:HA	1.72	0.72
1:A:371:PHE:HB2	1:A:502:VAL:HB	1.71	0.72
1:C:565:ILE:HB	1:C:592:SER:HB3	1.71	0.72
1:D:593:SER:HA	1:D:679:ASN:HB3	1.72	0.72
1:D:742:LYS:N	1:D:794:ILE:O	2.21	0.72
1:C:454:TYR:HB2	1:C:461:ILE:HG22	1.72	0.71
1:B:56:LEU:HB2	1:B:127:TYR:HE2	1.55	0.71
1:C:379:PRO:HB3	1:C:497:MET:HE1	1.72	0.71
1:C:489:LYS:NZ	1:C:490:ALA:O	2.23	0.71
1:D:615:ASN:HA	1:D:656:ASN:HA	1.72	0.71
1:A:57:THR:HG22	1:A:58:LEU:H	1.55	0.71
1:C:57:THR:HG22	1:C:58:LEU:H	1.55	0.71
1:C:78:ILE:HD13	1:D:106:GLN:HG2	1.73	0.71
1:B:201:GLU:O	1:B:207:TYR:OH	2.03	0.71
1:B:349:ARG:HH22	1:B:415:GLN:HG3	1.55	0.71
1:A:621:VAL:HA	1:A:650:THR:HA	1.73	0.71
1:A:454:TYR:HB2	1:A:461:ILE:HG22	1.72	0.70
1:C:746:ARG:HA	1:C:760:ASN:HA	1.72	0.70
1:D:769:VAL:O	1:D:771:LYS:NZ	2.24	0.70
1:B:593:SER:HA	1:B:679:ASN:HB3	1.72	0.70
1:C:395:ASP:OD2	1:C:398:SER:N	2.25	0.70
1:C:621:VAL:HA	1:C:650:THR:HA	1.73	0.70
1:D:56:LEU:HB2	1:D:127:TYR:HE2	1.55	0.70
1:D:349:ARG:HH22	1:D:415:GLN:HG3	1.55	0.70
1:A:670:ASN:ND2	1:A:674:TYR:O	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:LYS:N	1:B:794:ILE:O	2.21	0.70
1:A:542:LEU:O	1:A:544:ASN:ND2	2.25	0.70
1:C:401:GLU:OE2	1:C:556:ILE:N	2.24	0.70
1:C:277:GLU:OE1	1:C:337:SER:N	2.20	0.69
1:B:336:LEU:O	1:B:533:ARG:NH1	2.24	0.69
1:B:393:GLN:HE22	1:B:547:TYR:HD1	1.37	0.69
1:B:615:ASN:HA	1:B:656:ASN:HA	1.72	0.69
1:D:336:LEU:O	1:D:533:ARG:NH1	2.24	0.69
1:C:670:ASN:ND2	1:C:674:TYR:O	2.25	0.69
1:D:697:LYS:H	1:D:725:GLN:HE22	1.41	0.69
1:C:579:ASN:ND2	1:C:597:HIS:O	2.26	0.69
1:A:401:GLU:OE2	1:A:556:ILE:N	2.24	0.69
1:A:489:LYS:NZ	1:A:490:ALA:O	2.23	0.69
1:A:579:ASN:ND2	1:A:597:HIS:O	2.26	0.69
1:B:608:ASN:OD1	1:B:609:LYS:NZ	2.25	0.69
1:B:769:VAL:O	1:B:771:LYS:NZ	2.25	0.69
1:C:542:LEU:O	1:C:544:ASN:ND2	2.25	0.69
1:C:706:ASN:ND2	1:C:718:LEU:O	2.26	0.69
1:D:94:GLU:OE2	1:D:94:GLU:N	2.22	0.69
1:D:352:ASP:O	1:D:738:ARG:NH1	2.26	0.69
1:B:352:ASP:O	1:B:738:ARG:NH1	2.26	0.69
1:C:596:THR:O	1:C:670:ASN:ND2	2.25	0.69
1:A:395:ASP:OD2	1:A:398:SER:N	2.25	0.69
1:B:75:LEU:HB3	1:B:110:LEU:HD13	1.76	0.68
1:A:596:THR:O	1:A:670:ASN:ND2	2.25	0.68
1:A:192:LYS:O	1:A:195:GLU:HG3	1.93	0.68
1:B:372:GLU:HG2	1:B:501:VAL:HA	1.75	0.68
1:B:697:LYS:H	1:B:725:GLN:HE22	1.41	0.68
1:D:608:ASN:OD1	1:D:609:LYS:NZ	2.25	0.68
1:B:641:THR:HB	1:B:671:GLN:HE22	1.59	0.68
1:A:706:ASN:ND2	1:A:718:LEU:O	2.26	0.68
1:A:419:LYS:HB3	1:A:444:GLN:HA	1.75	0.68
1:B:162:LYS:NZ	1:B:270:ASN:O	2.27	0.68
1:B:203:ASN:O	1:B:206:SER:OG	2.11	0.68
1:C:336:LEU:O	1:C:533:ARG:NH1	2.27	0.68
1:C:243:THR:OG1	1:D:184:GLN:NE2	2.27	0.68
1:D:162:LYS:NZ	1:D:270:ASN:O	2.27	0.68
1:A:336:LEU:O	1:A:533:ARG:NH1	2.27	0.68
1:C:694:GLN:O	1:C:697:LYS:NZ	2.22	0.68
1:D:621:VAL:HG22	1:D:650:THR:HB	1.76	0.68
1:A:194:ASP:OD1	1:A:195:GLU:N	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:LYS:O	1:C:195:GLU:HG3	1.93	0.68
1:B:352:ASP:H	1:B:414:LYS:NZ	1.92	0.67
1:B:621:VAL:HG22	1:B:650:THR:HB	1.76	0.67
1:D:352:ASP:H	1:D:414:LYS:NZ	1.92	0.67
1:A:243:THR:OG1	1:B:184:GLN:NE2	2.28	0.67
1:A:478:GLU:HG3	1:A:480:SER:H	1.58	0.67
1:D:203:ASN:O	1:D:206:SER:OG	2.11	0.67
1:D:393:GLN:OE1	1:D:547:TYR:N	2.27	0.67
1:C:194:ASP:OD1	1:C:195:GLU:N	2.27	0.67
1:C:478:GLU:HG3	1:C:480:SER:H	1.58	0.67
1:A:723:PHE:O	1:A:783:LEU:N	2.28	0.67
1:B:716:GLU:HB2	1:B:794:ILE:HG23	1.76	0.67
1:D:75:LEU:HB3	1:D:110:LEU:HD13	1.76	0.67
1:B:474:LYS:HG3	1:B:484:GLU:HG2	1.77	0.67
1:C:419:LYS:HB3	1:C:444:GLN:HA	1.75	0.67
1:A:697:LYS:H	1:A:725:GLN:HE22	1.43	0.66
1:B:710:LYS:HB2	1:B:714:ARG:HB2	1.76	0.66
1:D:27:ASP:HA	1:D:396:ARG:HD3	1.77	0.66
1:D:372:GLU:HG2	1:D:501:VAL:HA	1.75	0.66
1:A:641:THR:H	1:A:642:LYS:HZ2	1.43	0.66
1:B:627:ALA:HA	1:B:641:THR:HG22	1.77	0.66
1:A:694:GLN:O	1:A:697:LYS:NZ	2.22	0.66
1:D:641:THR:HB	1:D:671:GLN:HE22	1.59	0.66
1:A:253:LEU:HD23	1:A:254:PHE:HB3	1.78	0.66
1:C:723:PHE:O	1:C:783:LEU:N	2.28	0.66
1:D:474:LYS:HG3	1:D:484:GLU:HG2	1.77	0.66
1:D:716:GLU:HB2	1:D:794:ILE:HG23	1.76	0.66
1:C:329:ARG:HH11	1:C:541:LEU:HB3	1.60	0.66
1:B:707:VAL:HG12	1:B:717:ILE:HA	1.78	0.66
1:D:710:LYS:HB2	1:D:714:ARG:HB2	1.76	0.66
1:A:436:ILE:HG12	1:A:449:VAL:HG22	1.78	0.65
1:C:419:LYS:N	1:C:443:ASN:O	2.27	0.65
1:D:708:GLN:NE2	1:D:709:MET:O	2.26	0.65
1:A:329:ARG:HH11	1:A:541:LEU:HB3	1.60	0.65
1:B:708:GLN:NE2	1:B:709:MET:O	2.26	0.65
1:C:436:ILE:HG12	1:C:449:VAL:HG22	1.78	0.65
1:D:707:VAL:HG12	1:D:717:ILE:HA	1.77	0.65
1:B:742:LYS:HB2	1:B:794:ILE:HB	1.79	0.65
1:C:159:ILE:HG22	1:C:163:LEU:HD23	1.79	0.65
1:A:274:ARG:NH1	1:A:551:SER:OG	2.30	0.65
1:B:27:ASP:HA	1:B:396:ARG:HD3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:GLU:OE2	1:B:94:GLU:N	2.22	0.65
1:C:282:TYR:OH	1:C:540:ASP:OD2	2.14	0.65
1:D:744:THR:HA	1:D:762:LYS:HA	1.79	0.65
1:C:519:GLU:O	1:C:522:GLN:NE2	2.30	0.65
1:A:282:TYR:OH	1:A:540:ASP:OD2	2.14	0.65
1:D:627:ALA:HA	1:D:641:THR:HG22	1.78	0.64
1:C:236:SER:O	1:C:239:PHE:N	2.30	0.64
1:C:752:GLU:HB3	1:C:778:GLU:HB3	1.79	0.64
1:D:742:LYS:HB2	1:D:794:ILE:HB	1.79	0.64
1:A:727:ILE:HG12	1:A:800:ILE:HD13	1.78	0.64
1:C:697:LYS:H	1:C:725:GLN:HE22	1.43	0.64
1:C:727:ILE:HG12	1:C:800:ILE:HD13	1.79	0.64
1:D:453:PHE:HB3	1:D:462:ASP:HB3	1.78	0.64
1:A:64:ASN:ND2	1:B:64:ASN:OD1	2.30	0.64
1:B:746:ARG:NH2	1:B:785:GLY:O	2.31	0.64
1:C:274:ARG:NH1	1:C:551:SER:OG	2.30	0.64
1:C:641:THR:H	1:C:642:LYS:HZ1	1.44	0.64
1:B:744:THR:HA	1:B:762:LYS:HA	1.79	0.64
1:C:253:LEU:HD23	1:C:254:PHE:HB3	1.78	0.64
1:A:159:ILE:HG22	1:A:163:LEU:HD23	1.79	0.64
1:A:519:GLU:O	1:A:522:GLN:NE2	2.30	0.64
1:D:618:ILE:HD11	1:D:655:PHE:HD1	1.63	0.64
1:D:746:ARG:NH2	1:D:785:GLY:O	2.31	0.64
1:A:710:LYS:HB2	1:A:714:ARG:HB2	1.80	0.63
1:D:446:GLY:HA3	1:D:472:LYS:HE3	1.80	0.63
1:A:752:GLU:HB3	1:A:778:GLU:HB3	1.79	0.63
1:B:201:GLU:OE1	1:B:202:LYS:N	2.31	0.63
1:B:352:ASP:H	1:B:414:LYS:HZ3	1.46	0.63
1:C:342:ASN:ND2	1:C:344:SER:O	2.31	0.63
1:A:236:SER:O	1:A:239:PHE:N	2.30	0.63
1:A:696:LEU:HD13	1:A:798:VAL:HB	1.80	0.63
1:B:393:GLN:OE1	1:B:547:TYR:N	2.27	0.63
1:C:28:TYR:CE1	1:C:547:TYR:HB3	2.33	0.63
1:C:155:GLN:OE1	1:C:283:ASN:ND2	2.32	0.63
1:A:418:GLN:HA	1:A:443:ASN:HB3	1.81	0.63
1:B:408:HIS:O	1:B:412:CYS:N	2.32	0.63
1:B:453:PHE:HB3	1:B:462:ASP:HB3	1.78	0.63
1:C:64:ASN:ND2	1:D:64:ASN:OD1	2.31	0.63
1:C:584:LYS:HG3	1:C:585:ALA:N	2.14	0.63
1:A:342:ASN:ND2	1:A:344:SER:O	2.31	0.63
1:B:446:GLY:HA3	1:B:472:LYS:HE3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:742:LYS:N	1:C:794:ILE:O	2.26	0.63
1:D:408:HIS:O	1:D:412:CYS:N	2.32	0.63
1:B:618:ILE:HD11	1:B:655:PHE:HD1	1.63	0.63
1:C:88:GLN:O	1:C:90:ASN:ND2	2.32	0.63
1:D:602:PHE:HB2	1:D:668:PHE:HB3	1.81	0.63
1:A:155:GLN:OE1	1:A:283:ASN:ND2	2.32	0.62
1:B:421:TYR:CD1	1:B:485:TYR:HB3	2.34	0.62
1:B:462:ASP:OD1	1:B:464:ASN:ND2	2.32	0.62
1:C:696:LEU:HD13	1:C:798:VAL:HB	1.80	0.62
1:A:269:GLU:HG2	1:A:270:ASN:HD22	1.64	0.62
1:C:710:LYS:HB2	1:C:714:ARG:HB2	1.80	0.62
1:D:314:THR:OG1	1:D:315:GLN:NE2	2.33	0.62
1:A:28:TYR:CE1	1:A:547:TYR:HB3	2.33	0.62
1:D:156:LEU:HA	1:D:159:ILE:HD12	1.81	0.62
1:B:737:LEU:HD22	1:B:749:ILE:HD11	1.81	0.62
1:B:453:PHE:O	1:B:462:ASP:N	2.33	0.62
1:B:90:ASN:H	1:D:90:ASN:H	1.47	0.62
1:B:419:LYS:N	1:B:443:ASN:O	2.28	0.62
1:D:201:GLU:OE1	1:D:202:LYS:N	2.31	0.62
1:D:421:TYR:CD1	1:D:485:TYR:HB3	2.34	0.62
1:D:462:ASP:OD1	1:D:464:ASN:ND2	2.32	0.62
1:A:260:LYS:O	1:A:263:SER:OG	2.18	0.62
1:D:419:LYS:N	1:D:443:ASN:O	2.28	0.62
1:A:88:GLN:O	1:A:90:ASN:ND2	2.32	0.62
1:D:28:TYR:CE2	1:D:547:TYR:HB3	2.35	0.62
1:B:156:LEU:HA	1:B:159:ILE:HD12	1.81	0.62
1:B:656:ASN:ND2	1:B:657:SER:O	2.33	0.62
1:B:314:THR:OG1	1:B:315:GLN:NE2	2.32	0.61
1:B:454:TYR:HB2	1:B:461:ILE:HG22	1.82	0.61
1:B:752:GLU:HB2	1:B:776:LYS:HE2	1.82	0.61
1:A:419:LYS:N	1:A:443:ASN:O	2.27	0.61
1:C:269:GLU:HG2	1:C:270:ASN:HD22	1.64	0.61
1:D:716:GLU:HG2	1:D:718:LEU:HD12	1.82	0.61
1:B:624:GLY:N	1:B:645:PHE:O	2.19	0.61
1:B:716:GLU:HG2	1:B:718:LEU:HD12	1.82	0.61
1:C:418:GLN:HA	1:C:443:ASN:HB3	1.81	0.61
1:A:372:GLU:HG2	1:A:501:VAL:HG12	1.83	0.61
1:D:454:TYR:HB2	1:D:461:ILE:HG22	1.81	0.61
1:C:372:GLU:HG2	1:C:501:VAL:HG12	1.82	0.61
1:D:519:GLU:O	1:D:522:GLN:NE2	2.33	0.61
1:D:656:ASN:ND2	1:D:657:SER:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:GLN:NE2	1:A:765:ASP:OD2	2.34	0.61
1:A:584:LYS:HG3	1:A:585:ALA:N	2.14	0.61
1:D:737:LEU:HD22	1:D:749:ILE:HD11	1.81	0.61
1:A:742:LYS:N	1:A:794:ILE:O	2.26	0.61
1:C:641:THR:H	1:C:642:LYS:NZ	1.99	0.61
1:B:28:TYR:CE2	1:B:547:TYR:HB3	2.35	0.61
1:D:453:PHE:O	1:D:462:ASP:N	2.33	0.61
1:B:519:GLU:O	1:B:522:GLN:NE2	2.33	0.61
1:B:602:PHE:HB2	1:B:668:PHE:HB3	1.81	0.61
1:D:374:LEU:O	1:D:380:ILE:N	2.27	0.60
1:D:752:GLU:HB2	1:D:776:LYS:HE2	1.82	0.60
1:B:374:LEU:O	1:B:380:ILE:N	2.27	0.60
1:D:702:ILE:N	1:D:724:LYS:O	2.34	0.60
1:C:415:GLN:NE2	1:C:765:ASP:OD2	2.34	0.60
1:D:275:GLY:HA2	1:D:504:GLU:HA	1.83	0.60
1:B:401:GLU:OE1	1:B:557:SER:N	2.25	0.60
1:D:231:LYS:HG3	1:D:234:MET:HE1	1.83	0.60
1:D:406:ASP:HB3	1:D:409:LYS:HG3	1.83	0.60
1:A:627:ALA:HB3	1:A:669:LYS:HB2	1.84	0.60
1:B:108:GLN:CD	1:D:111:ASN:HD22	2.10	0.60
1:B:111:ASN:HD22	1:D:108:GLN:CD	2.10	0.60
1:B:231:LYS:HG3	1:B:234:MET:HE1	1.83	0.60
1:B:278:ILE:HD11	1:B:533:ARG:HH11	1.67	0.60
1:B:418:GLN:HE22	1:B:440:LYS:HE3	1.67	0.59
1:B:588:ILE:HG23	1:B:590:GLY:H	1.67	0.59
1:D:727:ILE:HG12	1:D:780:PHE:HA	1.85	0.59
1:A:32:ILE:HD13	1:A:325:LYS:HD3	1.83	0.59
1:A:352:ASP:H	1:A:414:LYS:NZ	2.00	0.59
1:A:641:THR:H	1:A:642:LYS:NZ	1.99	0.59
1:D:278:ILE:HD11	1:D:533:ARG:HH11	1.67	0.59
1:B:670:ASN:ND2	1:B:674:TYR:O	2.36	0.59
1:B:702:ILE:N	1:B:724:LYS:O	2.34	0.59
1:C:78:ILE:HG23	1:D:102:ILE:HG23	1.84	0.59
1:D:211:VAL:HG13	1:D:212:THR:H	1.66	0.59
1:A:711:ASP:OD1	1:A:714:ARG:NH2	2.35	0.59
1:C:260:LYS:O	1:C:263:SER:OG	2.18	0.59
1:D:418:GLN:HE22	1:D:440:LYS:HE3	1.67	0.59
1:B:211:VAL:HG13	1:B:212:THR:H	1.66	0.59
1:A:584:LYS:HB3	1:A:589:LYS:HB3	1.84	0.59
1:B:581:PHE:HD2	1:B:583:ASP:HB2	1.68	0.59
1:B:710:LYS:NZ	1:B:716:GLU:OE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:ASP:H	1:C:414:LYS:NZ	2.00	0.59
1:C:371:PHE:N	1:C:502:VAL:O	2.35	0.59
1:B:170:VAL:HG21	1:C:172:ILE:HG13	1.85	0.59
1:C:627:ALA:HB3	1:C:669:LYS:HB2	1.84	0.59
1:A:377:PRO:O	1:A:654:LYS:NZ	2.28	0.59
1:B:275:GLY:HA2	1:B:504:GLU:HA	1.83	0.59
1:B:406:ASP:HB3	1:B:409:LYS:HG3	1.83	0.59
1:A:474:LYS:HG2	1:A:478:GLU:HB3	1.85	0.58
1:B:727:ILE:HG12	1:B:780:PHE:HA	1.85	0.58
1:C:584:LYS:HB3	1:C:589:LYS:HB3	1.85	0.58
1:C:61:ILE:O	1:C:65:GLN:HB2	2.03	0.58
1:C:474:LYS:HG2	1:C:478:GLU:HB3	1.85	0.58
1:D:625:ARG:NE	1:D:642:LYS:O	2.36	0.58
1:A:172:ILE:HG13	1:D:170:VAL:HG21	1.85	0.58
1:B:605:PHE:HB2	1:B:665:TYR:CZ	2.38	0.58
1:C:32:ILE:HD13	1:C:325:LYS:HD3	1.83	0.58
1:C:711:ASP:OD1	1:C:714:ARG:NH2	2.35	0.58
1:B:379:PRO:HB3	1:B:497:MET:HE1	1.85	0.58
1:C:338:ASN:HB2	1:C:530:SER:H	1.68	0.58
1:D:379:PRO:HB3	1:D:497:MET:HE1	1.85	0.58
1:D:588:ILE:HG23	1:D:590:GLY:H	1.67	0.58
1:A:61:ILE:O	1:A:65:GLN:HB2	2.03	0.58
1:A:78:ILE:HG23	1:B:102:ILE:HG23	1.84	0.58
1:C:275:GLY:HA2	1:C:504:GLU:HA	1.86	0.58
1:A:338:ASN:HB2	1:A:530:SER:H	1.68	0.58
1:B:50:ASP:OD2	1:B:130:LYS:NZ	2.36	0.58
1:B:319:HIS:CD2	1:B:320:HIS:HD2	2.21	0.58
1:A:579:ASN:ND2	1:A:599:ASP:OD1	2.34	0.58
1:A:632:ASN:HB2	1:A:663:GLU:HB2	1.84	0.57
1:B:419:LYS:HG3	1:B:485:TYR:CD1	2.39	0.57
1:D:224:GLU:O	1:D:227:LYS:HG2	2.04	0.57
1:D:627:ALA:HB3	1:D:669:LYS:HB2	1.85	0.57
1:D:319:HIS:CD2	1:D:320:HIS:HD2	2.21	0.57
1:D:754:LYS:HE3	1:D:776:LYS:HZ2	1.70	0.57
1:B:596:THR:O	1:B:670:ASN:ND2	2.37	0.57
1:D:371:PHE:HB2	1:D:502:VAL:HB	1.86	0.57
1:A:755:TYR:HD2	1:A:758:PHE:HB2	1.69	0.57
1:B:371:PHE:HB2	1:B:502:VAL:HB	1.86	0.57
1:C:632:ASN:HB2	1:C:663:GLU:HB2	1.84	0.57
1:B:46:ILE:O	1:B:304:LYS:NZ	2.37	0.57
1:B:627:ALA:HB3	1:B:669:LYS:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:717:ILE:HB	1:C:793:THR:HB	1.87	0.57
1:D:50:ASP:OD2	1:D:130:LYS:NZ	2.36	0.57
1:A:347:LYS:HD2	1:A:496:TYR:CZ	2.40	0.57
1:C:347:LYS:HD2	1:C:496:TYR:CZ	2.40	0.57
1:C:353:ILE:HD13	1:C:797:ASN:HD22	1.70	0.57
1:C:748:SER:OG	1:C:782:ALA:O	2.23	0.57
1:D:46:ILE:O	1:D:304:LYS:NZ	2.37	0.57
1:D:670:ASN:ND2	1:D:674:TYR:O	2.36	0.57
1:B:224:GLU:O	1:B:227:LYS:HG2	2.04	0.57
1:B:421:TYR:HB3	1:B:472:LYS:HB2	1.87	0.57
1:C:352:ASP:H	1:C:414:LYS:HZ3	1.52	0.57
1:C:615:ASN:HA	1:C:656:ASN:HA	1.87	0.57
1:D:736:HIS:CD2	1:D:803:GLU:HB2	2.40	0.57
1:B:201:GLU:HB3	1:B:207:TYR:HE1	1.70	0.57
1:D:419:LYS:HG3	1:D:485:TYR:CD1	2.39	0.57
1:D:581:PHE:HD2	1:D:583:ASP:HB2	1.68	0.57
1:D:709:MET:HB3	1:D:715:LEU:HD23	1.87	0.57
1:A:401:GLU:CD	1:A:556:ILE:H	2.12	0.57
1:A:737:LEU:HD22	1:A:749:ILE:HD11	1.86	0.57
1:C:748:SER:HB2	1:C:750:ILE:HD11	1.87	0.57
1:C:755:TYR:HD2	1:C:758:PHE:HB2	1.70	0.57
1:A:275:GLY:HA2	1:A:504:GLU:HA	1.86	0.56
1:A:353:ILE:HD13	1:A:797:ASN:HD22	1.70	0.56
1:A:717:ILE:HB	1:A:793:THR:HB	1.87	0.56
1:B:736:HIS:CD2	1:B:803:GLU:HB2	2.40	0.56
1:D:596:THR:O	1:D:670:ASN:ND2	2.38	0.56
1:D:605:PHE:HB2	1:D:665:TYR:CZ	2.39	0.56
1:B:579:ASN:HD22	1:B:599:ASP:CG	2.12	0.56
1:D:49:THR:OG1	1:D:50:ASP:N	2.38	0.56
1:D:710:LYS:NZ	1:D:716:GLU:OE1	2.35	0.56
1:A:368:LEU:HD23	1:A:371:PHE:HE1	1.70	0.56
1:C:274:ARG:O	1:C:280:LYS:NZ	2.38	0.56
1:D:201:GLU:HB3	1:D:207:TYR:HE1	1.70	0.56
1:D:421:TYR:HB3	1:D:472:LYS:HB2	1.87	0.56
1:D:739:LEU:O	1:D:766:LEU:N	2.34	0.56
1:C:368:LEU:HD23	1:C:371:PHE:HE1	1.70	0.56
1:C:737:LEU:HD22	1:C:749:ILE:HD11	1.86	0.56
1:A:274:ARG:O	1:A:280:LYS:NZ	2.38	0.56
1:B:579:ASN:ND2	1:B:599:ASP:OD1	2.32	0.56
1:C:401:GLU:CD	1:C:556:ILE:H	2.12	0.56
1:D:392:TYR:O	1:D:535:SER:OG	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ILE:HG22	1:A:167:ASN:H	1.70	0.56
1:A:393:GLN:OE1	1:A:547:TYR:N	2.39	0.56
1:A:615:ASN:HA	1:A:656:ASN:HA	1.86	0.56
1:D:579:ASN:HD22	1:D:599:ASP:CG	2.12	0.56
1:A:579:ASN:HB2	1:A:597:HIS:CE1	2.41	0.56
1:A:748:SER:HB2	1:A:750:ILE:HD11	1.87	0.56
1:B:49:THR:OG1	1:B:50:ASP:N	2.38	0.56
1:B:392:TYR:O	1:B:535:SER:OG	2.22	0.56
1:A:472:LYS:HB3	1:A:475:SER:HB2	1.88	0.56
1:B:225:LEU:O	1:B:229:VAL:HG22	2.06	0.56
1:B:709:MET:HB3	1:B:715:LEU:HD23	1.87	0.56
1:C:166:ILE:HG22	1:C:167:ASN:H	1.70	0.56
1:D:225:LEU:O	1:D:229:VAL:HG22	2.06	0.56
1:D:352:ASP:H	1:D:414:LYS:HZ3	1.53	0.56
1:A:227:LYS:O	1:A:230:THR:OG1	2.22	0.56
1:B:418:GLN:OE1	1:B:443:ASN:ND2	2.37	0.56
1:C:393:GLN:OE1	1:C:547:TYR:N	2.39	0.56
1:C:495:ILE:HG23	1:C:522:GLN:HB3	1.87	0.56
1:C:749:ILE:HG12	1:C:781:ILE:HB	1.88	0.56
1:A:309:THR:OG1	1:B:220:ASN:ND2	2.39	0.55
1:A:352:ASP:H	1:A:414:LYS:HZ3	1.54	0.55
1:B:194:ASP:O	1:B:197:THR:OG1	2.24	0.55
1:B:625:ARG:NE	1:B:642:LYS:O	2.36	0.55
1:D:350:GLY:HA3	1:D:412:CYS:HB2	1.87	0.55
1:A:418:GLN:OE1	1:A:443:ASN:ND2	2.38	0.55
1:B:350:GLY:HA3	1:B:412:CYS:HB2	1.87	0.55
1:B:739:LEU:O	1:B:766:LEU:N	2.34	0.55
1:D:111:ASN:HA	1:D:114:ASN:HD21	1.71	0.55
1:D:132:THR:HG21	1:D:203:ASN:N	2.21	0.55
1:C:736:HIS:HD2	1:C:803:GLU:HB2	1.72	0.55
1:D:418:GLN:OE1	1:D:443:ASN:ND2	2.37	0.55
1:C:50:ASP:OD1	1:C:51:THR:N	2.34	0.55
1:C:150:GLU:O	1:C:153:SER:OG	2.25	0.55
1:D:194:ASP:O	1:D:197:THR:OG1	2.24	0.55
1:A:736:HIS:HD2	1:A:803:GLU:HB2	1.72	0.55
1:A:749:ILE:HG12	1:A:781:ILE:HB	1.88	0.55
1:D:624:GLY:N	1:D:645:PHE:O	2.19	0.55
1:A:234:MET:H	1:B:227:LYS:NZ	2.05	0.55
1:B:203:ASN:N	1:B:204:PRO:HD2	2.22	0.55
1:C:373:ILE:N	1:C:500:GLY:O	2.29	0.55
1:C:377:PRO:O	1:C:654:LYS:NZ	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASN:HA	1:B:114:ASN:HD21	1.71	0.55
1:A:50:ASP:OD1	1:A:51:THR:N	2.34	0.55
1:A:252:ASN:OD1	1:A:253:LEU:N	2.35	0.55
1:A:349:ARG:NH2	1:A:414:LYS:HB2	2.22	0.55
1:B:310:ASP:OD1	1:B:310:ASP:N	2.38	0.55
1:B:749:ILE:N	1:B:757:LEU:O	2.38	0.55
1:C:349:ARG:NH2	1:C:414:LYS:HB2	2.22	0.55
1:A:495:ILE:HG23	1:A:522:GLN:HB3	1.87	0.55
1:C:418:GLN:OE1	1:C:443:ASN:ND2	2.38	0.55
1:C:570:THR:HB	1:C:573:TRP:HD1	1.72	0.55
1:C:579:ASN:HB2	1:C:597:HIS:CE1	2.41	0.55
1:A:406:ASP:HB2	1:A:408:HIS:NE2	2.22	0.54
1:A:570:THR:HB	1:A:573:TRP:HD1	1.72	0.54
1:C:309:THR:OG1	1:D:220:ASN:ND2	2.40	0.54
1:D:310:ASP:OD1	1:D:310:ASP:N	2.38	0.54
1:D:695:MET:HB2	1:D:800:ILE:HG23	1.89	0.54
1:A:614:THR:N	1:A:657:SER:OG	2.33	0.54
1:B:577:ASN:ND2	1:B:599:ASP:OD2	2.40	0.54
1:C:227:LYS:O	1:C:230:THR:OG1	2.22	0.54
1:D:203:ASN:N	1:D:204:PRO:HD2	2.22	0.54
1:C:406:ASP:HB2	1:C:408:HIS:NE2	2.22	0.54
1:D:208:GLN:C	1:D:210:ASN:H	2.14	0.54
1:A:371:PHE:N	1:A:502:VAL:O	2.35	0.54
1:B:183:TYR:HB2	1:B:244:PHE:HE2	1.72	0.54
1:B:229:VAL:HG12	1:B:302:CYS:SG	2.48	0.54
1:B:696:LEU:HD13	1:B:798:VAL:HB	1.90	0.54
1:D:363:ALA:HB3	1:D:366:TYR:CG	2.42	0.54
1:A:606:ILE:HG12	1:A:665:TYR:HA	1.90	0.54
1:B:132:THR:HG21	1:B:203:ASN:N	2.21	0.54
1:B:208:GLN:C	1:B:210:ASN:H	2.14	0.54
1:C:598:LYS:HD3	1:C:673:GLU:HB2	1.89	0.54
1:B:342:ASN:HD22	1:B:498:PRO:HB3	1.73	0.54
1:B:565:ILE:O	1:B:592:SER:HB2	2.08	0.54
1:C:472:LYS:HB3	1:C:475:SER:HB2	1.88	0.54
1:D:696:LEU:HD13	1:D:798:VAL:HB	1.90	0.54
1:B:754:LYS:HE3	1:B:776:LYS:HZ2	1.73	0.54
1:C:234:MET:H	1:D:227:LYS:NZ	2.06	0.54
1:C:570:THR:O	1:C:573:TRP:N	2.41	0.54
1:D:229:VAL:HG12	1:D:302:CYS:SG	2.48	0.54
1:B:717:ILE:HB	1:B:793:THR:HB	1.89	0.54
1:C:252:ASN:OD1	1:C:253:LEU:N	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:717:ILE:HB	1:D:793:THR:HB	1.89	0.54
1:A:580:ALA:HB2	1:A:600:GLY:HA2	1.89	0.54
1:A:584:LYS:HG3	1:A:585:ALA:H	1.73	0.54
1:C:606:ILE:HG12	1:C:665:TYR:HA	1.90	0.54
1:C:707:VAL:HG12	1:C:717:ILE:HA	1.89	0.54
1:D:579:ASN:ND2	1:D:599:ASP:OD1	2.32	0.54
1:B:695:MET:HB2	1:B:800:ILE:HG23	1.89	0.53
1:C:580:ALA:HB2	1:C:600:GLY:HA2	1.89	0.53
1:D:55:ASN:O	1:D:57:THR:N	2.41	0.53
1:D:598:LYS:HA	1:D:673:GLU:HA	1.90	0.53
1:A:570:THR:O	1:A:573:TRP:N	2.41	0.53
1:B:251:ASN:O	1:C:187:LYS:NZ	2.42	0.53
1:B:314:THR:HA	1:B:317:MET:HE3	1.90	0.53
1:C:421:TYR:HB2	1:C:446:GLY:HA2	1.90	0.53
1:C:579:ASN:ND2	1:C:599:ASP:OD1	2.34	0.53
1:D:183:TYR:HB2	1:D:244:PHE:HE2	1.72	0.53
1:D:423:LYS:HB2	1:D:472:LYS:C	2.34	0.53
1:A:748:SER:OG	1:A:782:ALA:O	2.23	0.53
1:C:321:ILE:HG22	1:C:325:LYS:HE2	1.90	0.53
1:B:423:LYS:HB2	1:B:472:LYS:C	2.34	0.53
1:B:623:LYS:HB3	1:B:677:TRP:HB2	1.89	0.53
1:C:598:LYS:NZ	1:C:673:GLU:O	2.31	0.53
1:D:342:ASN:HD22	1:D:498:PRO:HB3	1.73	0.53
1:D:623:LYS:HB3	1:D:677:TRP:HB2	1.89	0.53
1:A:598:LYS:HD3	1:A:673:GLU:HB2	1.89	0.53
1:A:601:GLU:HG3	1:A:669:LYS:HG2	1.90	0.53
1:B:55:ASN:O	1:B:57:THR:N	2.41	0.53
1:B:618:ILE:HD11	1:B:655:PHE:CD1	2.43	0.53
1:B:741:VAL:C	1:B:742:LYS:HZ2	2.15	0.53
1:D:401:GLU:OE1	1:D:557:SER:N	2.25	0.53
1:C:601:GLU:HG3	1:C:669:LYS:HG2	1.90	0.53
1:D:563:TRP:HE3	1:D:680:ASN:HA	1.74	0.53
1:A:419:LYS:HE2	1:A:485:TYR:CE2	2.44	0.53
1:D:749:ILE:N	1:D:757:LEU:O	2.38	0.53
1:A:469:GLU:N	1:A:469:GLU:OE1	2.42	0.53
1:B:363:ALA:HB3	1:B:366:TYR:CG	2.43	0.53
1:B:598:LYS:HA	1:B:673:GLU:HA	1.90	0.53
1:C:599:ASP:OD1	1:C:599:ASP:N	2.41	0.53
1:C:623:LYS:HB2	1:C:648:PHE:H	1.74	0.53
1:A:285:LEU:O	1:A:289:THR:HG22	2.09	0.53
1:B:419:LYS:HE2	1:B:485:TYR:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:LEU:O	1:C:289:THR:HG22	2.09	0.53
1:C:419:LYS:HE2	1:C:485:TYR:CE2	2.44	0.53
1:A:93:SER:O	1:A:97:LYS:N	2.32	0.52
1:D:206:SER:HB2	1:D:208:GLN:CD	2.35	0.52
1:D:618:ILE:HD11	1:D:655:PHE:CD1	2.43	0.52
1:A:421:TYR:HB2	1:A:446:GLY:HA2	1.90	0.52
1:D:565:ILE:O	1:D:592:SER:HB2	2.08	0.52
1:A:599:ASP:OD1	1:A:599:ASP:N	2.41	0.52
1:B:437:VAL:O	1:B:448:GLU:N	2.38	0.52
1:C:362:ALA:HB2	1:C:368:LEU:HD12	1.91	0.52
1:C:384:TYR:CE1	1:C:401:GLU:HG2	2.45	0.52
1:C:584:LYS:HG3	1:C:585:ALA:H	1.73	0.52
1:C:741:VAL:HA	1:C:795:PHE:HA	1.91	0.52
1:A:321:ILE:HG22	1:A:325:LYS:HE2	1.90	0.52
1:A:564:ASN:O	1:A:565:ILE:HG13	2.09	0.52
1:B:192:LYS:O	1:B:195:GLU:HG3	2.09	0.52
1:B:256:ARG:HH21	1:B:261:THR:HA	1.74	0.52
1:C:469:GLU:OE1	1:C:469:GLU:N	2.42	0.52
1:D:577:ASN:ND2	1:D:599:ASP:OD2	2.40	0.52
1:A:627:ALA:HB1	1:A:629:TYR:HE2	1.74	0.52
1:A:707:VAL:HG12	1:A:717:ILE:HA	1.89	0.52
1:B:751:ASP:HB2	1:B:756:LEU:HG	1.92	0.52
1:D:59:ASP:OD1	1:D:60:GLU:N	2.43	0.52
1:A:109:MET:HE1	1:B:71:ILE:HA	1.92	0.52
1:A:504:GLU:HG2	1:A:532:LEU:HD22	1.92	0.52
1:B:447:TYR:O	1:B:472:LYS:HD2	2.09	0.52
1:B:496:TYR:HB2	1:B:522:GLN:O	2.10	0.52
1:C:276:SER:H	1:C:504:GLU:CD	2.18	0.52
1:D:192:LYS:O	1:D:195:GLU:HG3	2.09	0.52
1:D:751:ASP:HB2	1:D:756:LEU:HG	1.92	0.52
1:A:384:TYR:CE1	1:A:401:GLU:HG2	2.45	0.52
1:D:111:ASN:HA	1:D:114:ASN:ND2	2.25	0.52
1:D:447:TYR:O	1:D:472:LYS:HD2	2.09	0.52
1:A:187:LYS:NZ	1:D:251:ASN:O	2.42	0.52
1:A:623:LYS:HB2	1:A:648:PHE:H	1.74	0.52
1:A:741:VAL:HA	1:A:795:PHE:HA	1.91	0.52
1:B:111:ASN:HA	1:B:114:ASN:ND2	2.25	0.52
1:B:731:ASN:HB2	1:B:774:SER:HB2	1.92	0.52
1:C:614:THR:N	1:C:657:SER:OG	2.33	0.52
1:A:74:LYS:HB2	1:B:109:MET:HE2	1.92	0.52
1:B:563:TRP:HE3	1:B:680:ASN:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:LYS:O	1:B:614:THR:OG1	2.28	0.52
1:D:699:GLU:N	1:D:699:GLU:OE1	2.42	0.52
1:A:362:ALA:HB2	1:A:368:LEU:HD12	1.92	0.52
1:C:627:ALA:HB1	1:C:629:TYR:HE2	1.74	0.52
1:A:150:GLU:O	1:A:153:SER:OG	2.25	0.51
1:A:486:SER:OG	1:A:519:GLU:OE2	2.27	0.51
1:A:559:ILE:HG23	1:A:609:LYS:HD2	1.92	0.51
1:A:568:ASP:OD2	1:A:585:ALA:HB1	2.10	0.51
1:B:338:ASN:HB2	1:B:530:SER:H	1.74	0.51
1:C:744:THR:HA	1:C:762:LYS:HA	1.93	0.51
1:B:165:ILE:HG22	1:B:168:LEU:HB3	1.91	0.51
1:B:425:ILE:HG23	1:B:469:GLU:HG3	1.93	0.51
1:C:504:GLU:HG2	1:C:532:LEU:HD22	1.92	0.51
1:C:559:ILE:HG23	1:C:609:LYS:HD2	1.92	0.51
1:D:314:THR:HA	1:D:317:MET:HE3	1.90	0.51
1:D:419:LYS:HE2	1:D:485:TYR:CZ	2.44	0.51
1:B:670:ASN:HD21	1:B:674:TYR:C	2.18	0.51
1:C:397:GLU:OE1	1:C:397:GLU:N	2.29	0.51
1:C:564:ASN:O	1:C:565:ILE:HG13	2.09	0.51
1:D:165:ILE:HG22	1:D:168:LEU:HB3	1.91	0.51
1:A:392:TYR:O	1:A:535:SER:OG	2.26	0.51
1:D:670:ASN:HD21	1:D:674:TYR:C	2.18	0.51
1:B:699:GLU:N	1:B:699:GLU:OE1	2.42	0.51
1:C:78:ILE:HD11	1:D:105:GLU:HG2	1.91	0.51
1:D:437:VAL:O	1:D:448:GLU:N	2.38	0.51
1:D:570:THR:HB	1:D:573:TRP:HB2	1.93	0.51
1:A:172:ILE:HA	1:A:175:THR:HG22	1.92	0.51
1:B:206:SER:HB2	1:B:208:GLN:CD	2.35	0.51
1:C:28:TYR:HE1	1:C:547:TYR:HB3	1.73	0.51
1:C:614:THR:HB	1:C:616:TYR:HE2	1.76	0.51
1:D:256:ARG:HH21	1:D:261:THR:HA	1.74	0.51
1:A:370:GLY:HA3	1:A:503:SER:OG	2.11	0.51
1:A:605:PHE:HA	1:A:665:TYR:CB	2.41	0.51
1:C:568:ASP:OD2	1:C:585:ALA:HB1	2.10	0.51
1:D:338:ASN:HB2	1:D:530:SER:H	1.74	0.51
1:D:425:ILE:HG23	1:D:469:GLU:HG3	1.93	0.51
1:C:605:PHE:HA	1:C:665:TYR:CB	2.41	0.51
1:C:704:SER:OG	1:C:722:TYR:O	2.25	0.51
1:D:362:ALA:HB2	1:D:368:LEU:HD22	1.93	0.51
1:A:48:LYS:HD2	1:A:48:LYS:O	2.11	0.51
1:A:276:SER:H	1:A:504:GLU:CD	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ASP:OD1	1:B:60:GLU:N	2.43	0.51
1:B:362:ALA:HB2	1:B:368:LEU:HD22	1.93	0.51
1:C:172:ILE:HA	1:C:175:THR:HG22	1.92	0.51
1:D:709:MET:HA	1:D:715:LEU:HA	1.93	0.51
1:C:486:SER:OG	1:C:519:GLU:OE2	2.27	0.51
1:D:611:LYS:O	1:D:614:THR:OG1	2.28	0.51
1:A:744:THR:HA	1:A:762:LYS:HA	1.93	0.50
1:C:744:THR:HG22	1:C:786:THR:HG21	1.93	0.50
1:A:515:LEU:HD21	1:A:524:ILE:HG23	1.93	0.50
1:A:747:VAL:N	1:A:759:VAL:O	2.44	0.50
1:B:616:TYR:HB2	1:B:655:PHE:CE1	2.46	0.50
1:C:351:SER:O	1:C:440:LYS:NZ	2.41	0.50
1:D:410:LEU:HD21	1:D:438:PHE:HD2	1.76	0.50
1:A:750:ILE:HG22	1:A:751:ASP:O	2.12	0.50
1:C:48:LYS:HD2	1:C:48:LYS:O	2.11	0.50
1:C:370:GLY:HA3	1:C:503:SER:OG	2.11	0.50
1:D:496:TYR:HB2	1:D:522:GLN:O	2.10	0.50
1:D:731:ASN:HB2	1:D:774:SER:HB2	1.92	0.50
1:D:783:LEU:HD22	1:D:795:PHE:CE2	2.46	0.50
1:A:48:LYS:O	1:A:49:THR:OG1	2.26	0.50
1:B:403:ILE:HD11	1:B:555:TYR:HE1	1.77	0.50
1:B:671:GLN:HG2	1:B:674:TYR:CD2	2.46	0.50
1:C:515:LEU:HD21	1:C:524:ILE:HG23	1.93	0.50
1:C:749:ILE:HG22	1:C:756:LEU:HB2	1.93	0.50
1:D:707:VAL:HB	1:D:723:PHE:CE1	2.47	0.50
1:A:614:THR:HB	1:A:616:TYR:HE2	1.76	0.50
1:B:454:TYR:HA	1:B:461:ILE:HA	1.92	0.50
1:B:711:ASP:OD1	1:B:712:GLY:N	2.43	0.50
1:C:109:MET:HE1	1:D:71:ILE:HA	1.93	0.50
1:C:496:TYR:HB2	1:C:522:GLN:O	2.12	0.50
1:D:319:HIS:CD2	1:D:320:HIS:CD2	3.00	0.50
1:D:403:ILE:HD11	1:D:555:TYR:HE1	1.77	0.50
1:A:702:ILE:HD12	1:A:724:LYS:HG3	1.94	0.50
1:B:157:GLN:O	1:B:160:SER:OG	2.26	0.50
1:B:275:GLY:HA3	1:B:505:THR:HG23	1.94	0.50
1:B:570:THR:HB	1:B:573:TRP:HB2	1.93	0.50
1:C:702:ILE:HD12	1:C:724:LYS:HG3	1.94	0.50
1:C:750:ILE:HG22	1:C:751:ASP:O	2.12	0.50
1:B:209:ASP:OD1	1:B:209:ASP:N	2.45	0.50
1:B:303:ARG:HH21	1:B:309:THR:HG1	1.59	0.50
1:D:616:TYR:HB2	1:D:655:PHE:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:SER:O	1:A:440:LYS:NZ	2.40	0.50
1:A:373:ILE:N	1:A:500:GLY:O	2.29	0.50
1:B:601:GLU:HG3	1:B:669:LYS:HG2	1.94	0.50
1:A:28:TYR:HE1	1:A:547:TYR:HB3	1.73	0.49
1:A:709:MET:HG2	1:A:715:LEU:HD23	1.94	0.49
1:C:747:VAL:N	1:C:759:VAL:O	2.44	0.49
1:A:176:LEU:HA	1:A:179:ILE:HG22	1.94	0.49
1:B:171:LEU:HG	1:B:256:ARG:HG2	1.94	0.49
1:C:74:LYS:HB2	1:D:109:MET:HE2	1.94	0.49
1:C:454:TYR:CE1	1:C:459:GLY:HA2	2.48	0.49
1:D:432:VAL:O	1:D:434:THR:HG23	2.12	0.49
1:D:671:GLN:HG2	1:D:674:TYR:CD2	2.46	0.49
1:D:741:VAL:C	1:D:742:LYS:HZ2	2.20	0.49
1:B:583:ASP:HB3	1:B:586:ASP:OD1	2.12	0.49
1:D:264:GLU:O	1:D:268:LYS:HG2	2.13	0.49
1:D:454:TYR:HA	1:D:461:ILE:HA	1.93	0.49
1:A:78:ILE:HD11	1:B:105:GLU:HG2	1.93	0.49
1:A:372:GLU:N	1:A:382:LYS:O	2.45	0.49
1:B:462:ASP:OD1	1:B:463:LEU:N	2.45	0.49
1:C:372:GLU:HG2	1:C:501:VAL:HA	1.95	0.49
1:B:432:VAL:O	1:B:434:THR:HG23	2.12	0.49
1:B:709:MET:HA	1:B:715:LEU:HA	1.93	0.49
1:C:48:LYS:O	1:C:49:THR:OG1	2.26	0.49
1:D:702:ILE:HB	1:D:724:LYS:HG3	1.95	0.49
1:A:234:MET:HA	1:B:227:LYS:HZ3	1.78	0.49
1:A:372:GLU:HG2	1:A:501:VAL:HA	1.95	0.49
1:A:744:THR:HG22	1:A:786:THR:HG21	1.93	0.49
1:B:783:LEU:HD22	1:B:795:PHE:CE2	2.46	0.49
1:C:395:ASP:HB3	1:C:398:SER:HB3	1.95	0.49
1:B:410:LEU:HD21	1:B:438:PHE:HD2	1.76	0.49
1:B:734:THR:HB	1:B:803:GLU:HB3	1.95	0.49
1:C:709:MET:HG2	1:C:715:LEU:HD23	1.94	0.49
1:D:694:GLN:OE1	1:D:799:SER:HA	2.12	0.49
1:C:576:ASN:OD1	1:C:577:ASN:ND2	2.45	0.49
1:A:397:GLU:OE1	1:A:397:GLU:N	2.29	0.49
1:B:264:GLU:O	1:B:268:LYS:HG2	2.13	0.49
1:D:631:LYS:HG2	1:D:633:ASN:H	1.78	0.49
1:A:263:SER:O	1:A:267:THR:HG22	2.13	0.49
1:A:347:LYS:HA	1:A:495:ILE:O	2.13	0.49
1:A:749:ILE:HG22	1:A:756:LEU:HB2	1.93	0.49
1:B:319:HIS:CD2	1:B:320:HIS:CD2	3.00	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:TYR:O	1:B:531:TYR:OH	2.29	0.49
1:B:702:ILE:HB	1:B:724:LYS:HG3	1.95	0.49
1:C:252:ASN:CG	1:C:253:LEU:H	2.21	0.49
1:C:570:THR:HB	1:C:573:TRP:CD1	2.48	0.49
1:B:694:GLN:OE1	1:B:799:SER:HA	2.12	0.48
1:B:707:VAL:HB	1:B:723:PHE:CE1	2.47	0.48
1:D:196:LEU:HD11	1:D:224:GLU:HG2	1.95	0.48
1:A:454:TYR:CE1	1:A:459:GLY:HA2	2.48	0.48
1:A:566:THR:OG1	1:A:567:SER:N	2.33	0.48
1:A:695:MET:HE1	1:A:735:TYR:CE2	2.49	0.48
1:D:91:LEU:HD21	1:D:95:LEU:HD22	1.94	0.48
1:A:576:ASN:OD1	1:A:577:ASN:ND2	2.45	0.48
1:A:624:GLY:O	1:A:644:ASN:HA	2.13	0.48
1:A:746:ARG:NH2	1:A:784:GLU:OE1	2.46	0.48
1:C:176:LEU:HA	1:C:179:ILE:HG22	1.93	0.48
1:C:271:VAL:O	1:C:273:THR:HG23	2.14	0.48
1:C:672:SER:HB3	1:C:674:TYR:CE2	2.48	0.48
1:D:275:GLY:HA3	1:D:505:THR:HG23	1.94	0.48
1:D:339:ASN:HA	1:D:528:GLY:O	2.12	0.48
1:D:462:ASP:OD1	1:D:463:LEU:N	2.45	0.48
1:D:473:GLU:HG2	1:D:476:CYS:H	1.78	0.48
1:A:235:ASP:HB3	1:B:231:LYS:HD2	1.96	0.48
1:A:711:ASP:OD1	1:A:711:ASP:N	2.47	0.48
1:B:697:LYS:HB3	1:B:699:GLU:CD	2.39	0.48
1:C:178:GLU:OE1	1:C:247:VAL:HG21	2.14	0.48
1:C:235:ASP:HB3	1:D:231:LYS:HD2	1.95	0.48
1:C:347:LYS:HA	1:C:495:ILE:O	2.13	0.48
1:C:372:GLU:N	1:C:382:LYS:O	2.45	0.48
1:C:746:ARG:NH2	1:C:784:GLU:OE1	2.46	0.48
1:D:723:PHE:O	1:D:783:LEU:N	2.43	0.48
1:A:178:GLU:OE1	1:A:247:VAL:HG21	2.13	0.48
1:A:395:ASP:HB3	1:A:398:SER:HB3	1.95	0.48
1:A:496:TYR:HB2	1:A:522:GLN:O	2.12	0.48
1:A:672:SER:HB3	1:A:674:TYR:CE2	2.48	0.48
1:B:196:LEU:HD11	1:B:224:GLU:HG2	1.95	0.48
1:D:583:ASP:HB3	1:D:586:ASP:OD1	2.12	0.48
1:D:601:GLU:HG3	1:D:669:LYS:HG2	1.94	0.48
1:D:697:LYS:HB3	1:D:699:GLU:CD	2.39	0.48
1:A:193:PHE:HA	1:A:196:LEU:HB3	1.95	0.48
1:B:308:LEU:O	1:B:309:THR:OG1	2.24	0.48
1:B:339:ASN:HA	1:B:528:GLY:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:716:GLU:HA	1:B:794:ILE:HA	1.96	0.48
1:B:726:PHE:HA	1:B:780:PHE:HB3	1.96	0.48
1:B:736:HIS:NE2	1:B:803:GLU:OE2	2.33	0.48
1:C:234:MET:HA	1:D:227:LYS:HZ3	1.78	0.48
1:D:171:LEU:HG	1:D:256:ARG:HG2	1.94	0.48
1:A:271:VAL:O	1:A:273:THR:HG23	2.14	0.48
1:B:425:ILE:HD12	1:B:447:TYR:HE2	1.79	0.48
1:D:157:GLN:O	1:D:160:SER:OG	2.26	0.48
1:D:198:SER:OG	1:D:199:THR:N	2.46	0.48
1:A:196:LEU:O	1:A:200:VAL:HG23	2.14	0.48
1:A:707:VAL:HB	1:A:723:PHE:CE2	2.49	0.48
1:B:723:PHE:O	1:B:783:LEU:N	2.43	0.48
1:C:483:ASP:OD1	1:C:484:GLU:N	2.36	0.48
1:C:742:LYS:O	1:C:794:ILE:N	2.44	0.48
1:D:726:PHE:HA	1:D:780:PHE:HB3	1.96	0.48
1:A:605:PHE:HA	1:A:665:TYR:HB3	1.95	0.48
1:B:637:LEU:HD13	1:B:655:PHE:HE2	1.79	0.48
1:C:165:ILE:HA	1:C:269:GLU:OE1	2.14	0.48
1:D:716:GLU:HA	1:D:794:ILE:HA	1.96	0.48
1:D:732:ASP:OD1	1:D:732:ASP:N	2.43	0.48
1:D:734:THR:HB	1:D:803:GLU:HB3	1.95	0.48
1:A:218:ASN:O	1:A:222:LEU:HD22	2.14	0.48
1:B:91:LEU:HD21	1:B:95:LEU:HD22	1.94	0.48
1:B:198:SER:OG	1:B:199:THR:N	2.46	0.48
1:B:359:VAL:HG23	1:B:437:VAL:HG22	1.96	0.48
1:B:473:GLU:HG2	1:B:476:CYS:H	1.78	0.48
1:B:575:ALA:HB2	1:B:602:PHE:CE1	2.49	0.48
1:C:136:ASN:OD1	1:C:200:VAL:HG13	2.14	0.48
1:C:193:PHE:HA	1:C:196:LEU:HB3	1.95	0.48
1:C:236:SER:O	1:C:238:GLU:N	2.47	0.48
1:C:263:SER:O	1:C:267:THR:HG22	2.13	0.48
1:B:211:VAL:HG13	1:B:212:THR:N	2.28	0.47
1:C:493:ASP:OD2	1:C:493:ASP:N	2.47	0.47
1:C:695:MET:HE1	1:C:735:TYR:CE2	2.49	0.47
1:D:421:TYR:CB	1:D:472:LYS:HB2	2.43	0.47
1:D:637:LEU:HD13	1:D:655:PHE:HE2	1.79	0.47
1:B:616:TYR:HE2	1:B:657:SER:HB3	1.79	0.47
1:B:631:LYS:HG2	1:B:633:ASN:H	1.78	0.47
1:C:512:GLY:HA3	1:C:529:LYS:HB2	1.96	0.47
1:C:605:PHE:HA	1:C:665:TYR:HB3	1.95	0.47
1:D:632:ASN:N	1:D:664:ILE:HD13	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:THR:HB	1:A:573:TRP:CD1	2.48	0.47
1:B:421:TYR:CB	1:B:472:LYS:HB2	2.44	0.47
1:C:162:LYS:HD3	1:C:271:VAL:O	2.15	0.47
1:D:349:ARG:NH2	1:D:415:GLN:HG3	2.26	0.47
1:A:162:LYS:HD3	1:A:271:VAL:O	2.15	0.47
1:C:93:SER:O	1:C:97:LYS:N	2.32	0.47
1:C:248:MET:O	1:C:257:SER:OG	2.20	0.47
1:D:575:ALA:HB2	1:D:602:PHE:CE1	2.49	0.47
1:D:616:TYR:HE2	1:D:657:SER:HB3	1.79	0.47
1:B:53:GLY:C	1:B:55:ASN:H	2.22	0.47
1:D:625:ARG:NH1	1:D:644:ASN:HB2	2.29	0.47
1:A:136:ASN:OD1	1:A:200:VAL:HG13	2.14	0.47
1:A:220:ASN:HA	1:A:223:THR:HG23	1.97	0.47
1:A:704:SER:OG	1:A:722:TYR:O	2.25	0.47
1:B:645:PHE:CD2	1:B:649:GLN:HB2	2.50	0.47
1:C:196:LEU:O	1:C:200:VAL:HG23	2.14	0.47
1:D:446:GLY:CA	1:D:472:LYS:HE3	2.45	0.47
1:A:742:LYS:O	1:A:794:ILE:N	2.44	0.47
1:B:229:VAL:HG11	1:B:305:LEU:HD23	1.97	0.47
1:B:440:LYS:HB2	1:B:445:LEU:HD13	1.97	0.47
1:B:447:TYR:H	1:B:472:LYS:HD2	1.79	0.47
1:B:631:LYS:O	1:B:665:TYR:N	2.34	0.47
1:C:55:ASN:HA	1:D:216:ILE:HD12	1.96	0.47
1:C:234:MET:H	1:D:227:LYS:HZ3	1.62	0.47
1:C:350:GLY:HA3	1:C:412:CYS:HB3	1.97	0.47
1:C:619:GLN:HG3	1:C:652:THR:HG22	1.96	0.47
1:C:624:GLY:O	1:C:644:ASN:HA	2.13	0.47
1:D:351:SER:HA	1:D:414:LYS:HG2	1.96	0.47
1:D:447:TYR:H	1:D:472:LYS:HD2	1.79	0.47
1:D:607:GLY:N	1:D:664:ILE:O	2.48	0.47
1:A:165:ILE:HA	1:A:269:GLU:OE1	2.14	0.47
1:A:233:ASP:HB3	1:B:227:LYS:HE2	1.97	0.47
1:A:239:PHE:HB2	1:B:188:TYR:CE1	2.50	0.47
1:B:625:ARG:NH1	1:B:644:ASN:HB2	2.29	0.47
1:B:632:ASN:N	1:B:664:ILE:HD13	2.29	0.47
1:C:94:GLU:OE1	1:C:94:GLU:N	2.44	0.47
1:C:129:PRO:HB3	1:C:210:ASN:ND2	2.30	0.47
1:C:360:LEU:HD21	1:C:381:LEU:HD21	1.96	0.47
1:C:629:TYR:HB2	1:C:667:LEU:HB2	1.97	0.47
1:D:440:LYS:HB2	1:D:445:LEU:HD13	1.97	0.47
1:D:583:ASP:O	1:D:586:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:645:PHE:CD2	1:D:649:GLN:HB2	2.50	0.47
1:D:711:ASP:OD1	1:D:712:GLY:N	2.43	0.47
1:A:68:LEU:HG	1:A:117:LEU:HD12	1.97	0.47
1:A:740:SER:O	1:A:796:SER:N	2.48	0.47
1:B:346:SER:O	1:B:497:MET:N	2.39	0.47
1:D:211:VAL:HG13	1:D:212:THR:N	2.28	0.47
1:A:236:SER:O	1:A:238:GLU:N	2.47	0.47
1:A:625:ARG:HB3	1:A:671:GLN:HB3	1.96	0.47
1:D:425:ILE:HD12	1:D:447:TYR:HE2	1.79	0.47
1:A:39:ILE:HG13	1:A:293:ALA:HB1	1.97	0.46
1:A:129:PRO:HB3	1:A:210:ASN:ND2	2.30	0.46
1:C:224:GLU:H	1:C:224:GLU:CD	2.23	0.46
1:C:584:LYS:HB2	1:C:589:LYS:H	1.80	0.46
1:C:638:PHE:CE1	1:C:653:LYS:HD2	2.50	0.46
1:C:707:VAL:HB	1:C:723:PHE:CE2	2.49	0.46
1:A:224:GLU:H	1:A:224:GLU:CD	2.23	0.46
1:A:419:LYS:HE2	1:A:485:TYR:CZ	2.50	0.46
1:C:218:ASN:O	1:C:222:LEU:HD22	2.14	0.46
1:B:56:LEU:HD12	1:B:127:TYR:CE2	2.51	0.46
1:B:252:ASN:OD1	1:B:253:LEU:HD23	2.16	0.46
1:B:627:ALA:HB1	1:B:629:TYR:HE2	1.80	0.46
1:C:68:LEU:HG	1:C:117:LEU:HD12	1.97	0.46
1:C:220:ASN:HA	1:C:223:THR:HG23	1.97	0.46
1:A:55:ASN:HA	1:B:216:ILE:HD12	1.96	0.46
1:A:594:LEU:HD22	1:A:602:PHE:CZ	2.51	0.46
1:A:766:LEU:HD21	1:A:768:ARG:HG2	1.98	0.46
1:B:35:PHE:CE1	1:B:290:SER:HA	2.51	0.46
1:B:347:LYS:HG3	1:B:496:TYR:CD1	2.51	0.46
1:B:349:ARG:NH2	1:B:415:GLN:HG3	2.26	0.46
1:B:584:LYS:HA	1:B:592:SER:OG	2.15	0.46
1:D:359:VAL:HG23	1:D:437:VAL:HG22	1.96	0.46
1:A:638:PHE:CE1	1:A:653:LYS:HD2	2.50	0.46
1:B:112:HIS:CE1	1:B:113:VAL:HG23	2.50	0.46
1:B:583:ASP:O	1:B:586:ASP:N	2.47	0.46
1:A:66:ASN:OD1	1:A:67:LEU:N	2.49	0.46
1:A:483:ASP:OD1	1:A:484:GLU:N	2.36	0.46
1:A:545:GLU:HB3	1:A:547:TYR:CZ	2.51	0.46
1:C:625:ARG:HB3	1:C:671:GLN:HB3	1.96	0.46
1:C:711:ASP:OD1	1:C:711:ASP:N	2.47	0.46
1:D:353:ILE:HG12	1:D:414:LYS:HZ1	1.80	0.46
1:A:350:GLY:HA3	1:A:412:CYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:LEU:HD21	1:A:381:LEU:HD21	1.96	0.46
1:A:374:LEU:O	1:A:380:ILE:N	2.37	0.46
1:A:584:LYS:HB2	1:A:589:LYS:H	1.80	0.46
1:A:619:GLN:HG3	1:A:652:THR:HG22	1.96	0.46
1:A:621:VAL:HG22	1:A:650:THR:HB	1.98	0.46
1:C:374:LEU:O	1:C:380:ILE:N	2.37	0.46
1:A:403:ILE:HD11	1:A:555:TYR:HE1	1.81	0.46
1:A:512:GLY:HA3	1:A:529:LYS:HB2	1.96	0.46
1:A:629:TYR:HB2	1:A:667:LEU:HB2	1.97	0.46
1:B:339:ASN:ND2	1:B:529:LYS:HG2	2.31	0.46
1:B:517:VAL:HB	1:B:524:ILE:HG23	1.98	0.46
1:C:372:GLU:O	1:C:382:LYS:N	2.24	0.46
1:C:419:LYS:HE2	1:C:485:TYR:CZ	2.50	0.46
1:C:545:GLU:HB3	1:C:547:TYR:CZ	2.51	0.46
1:C:627:ALA:HB1	1:C:629:TYR:CE2	2.51	0.46
1:D:53:GLY:C	1:D:55:ASN:H	2.22	0.46
1:D:347:LYS:HG3	1:D:496:TYR:CD1	2.51	0.46
1:D:584:LYS:HA	1:D:592:SER:OG	2.15	0.46
1:B:351:SER:HA	1:B:414:LYS:HG2	1.97	0.46
1:B:607:GLY:N	1:B:664:ILE:O	2.48	0.46
1:C:219:LEU:HD13	1:C:219:LEU:HA	1.70	0.46
1:C:388:LEU:HD23	1:C:388:LEU:HA	1.81	0.46
1:C:403:ILE:HG21	1:C:686:ILE:HG12	1.97	0.46
1:D:35:PHE:CE1	1:D:290:SER:HA	2.51	0.46
1:D:112:HIS:CE1	1:D:113:VAL:HG23	2.50	0.46
1:D:229:VAL:HG11	1:D:305:LEU:HD23	1.97	0.46
1:D:587:THR:HG21	1:D:648:PHE:HE2	1.80	0.46
1:D:627:ALA:HB1	1:D:629:TYR:HE2	1.80	0.46
1:A:701:TRP:CH2	1:A:783:LEU:HG	2.51	0.46
1:B:387:ARG:NH1	1:B:387:ARG:HB2	2.31	0.46
1:B:587:THR:HG21	1:B:648:PHE:HE2	1.81	0.46
1:C:343:PRO:HD3	1:C:501:VAL:O	2.16	0.46
1:C:740:SER:O	1:C:796:SER:N	2.48	0.46
1:D:339:ASN:ND2	1:D:529:LYS:HG2	2.31	0.46
1:A:94:GLU:OE1	1:A:94:GLU:N	2.44	0.45
1:A:252:ASN:CG	1:A:253:LEU:H	2.21	0.45
1:A:343:PRO:HD3	1:A:501:VAL:O	2.16	0.45
1:B:377:PRO:O	1:B:654:LYS:NZ	2.46	0.45
1:C:98:GLU:OE1	1:D:85:LEU:HD13	2.16	0.45
1:C:392:TYR:O	1:C:535:SER:OG	2.26	0.45
1:C:594:LEU:HD22	1:C:602:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:705:GLY:O	1:C:721:GLY:HA3	2.17	0.45
1:D:75:LEU:HD12	1:D:75:LEU:HA	1.78	0.45
1:A:389:LYS:HB2	1:A:393:GLN:HB2	1.98	0.45
1:A:656:ASN:OD1	1:A:657:SER:N	2.48	0.45
1:A:706:ASN:O	1:A:718:LEU:HB2	2.17	0.45
1:C:596:THR:HB	1:C:600:GLY:HA3	1.97	0.45
1:C:656:ASN:OD1	1:C:657:SER:N	2.48	0.45
1:D:110:LEU:O	1:D:114:ASN:ND2	2.49	0.45
1:B:137:GLU:OE1	1:B:141:GLN:NE2	2.50	0.45
1:C:584:LYS:HE3	1:C:592:SER:HA	1.98	0.45
1:C:621:VAL:HG22	1:C:650:THR:HB	1.98	0.45
1:D:136:ASN:HA	1:D:202:LYS:HZ3	1.82	0.45
1:D:727:ILE:HG13	1:D:779:CYS:SG	2.57	0.45
1:A:403:ILE:HG21	1:A:686:ILE:HG12	1.97	0.45
1:A:584:LYS:HE3	1:A:592:SER:HA	1.98	0.45
1:A:632:ASN:N	1:A:664:ILE:HD13	2.31	0.45
1:B:354:ASP:HB3	1:B:691:PHE:CE1	2.52	0.45
1:C:66:ASN:OD1	1:C:67:LEU:N	2.49	0.45
1:C:239:PHE:HB2	1:D:188:TYR:CE1	2.51	0.45
1:C:294:LYS:HE3	1:C:294:LYS:HB2	1.69	0.45
1:C:583:ASP:CG	1:C:677:TRP:HE1	2.24	0.45
1:C:646:SER:OG	1:C:647:ASP:N	2.50	0.45
1:C:766:LEU:HD21	1:C:768:ARG:HG2	1.98	0.45
1:D:601:GLU:HA	1:D:669:LYS:HA	1.98	0.45
1:A:201:GLU:O	1:A:204:PRO:HD2	2.17	0.45
1:A:493:ASP:OD2	1:A:493:ASP:N	2.47	0.45
1:B:405:GLY:O	1:B:407:ILE:N	2.48	0.45
1:C:196:LEU:HD13	1:C:225:LEU:HD21	1.99	0.45
1:C:584:LYS:C	1:C:586:ASP:H	2.24	0.45
1:A:799:SER:O	1:A:799:SER:OG	2.35	0.45
1:B:110:LEU:O	1:B:114:ASN:ND2	2.49	0.45
1:B:188:TYR:OH	1:B:192:LYS:NZ	2.50	0.45
1:C:201:GLU:O	1:C:204:PRO:HD2	2.17	0.45
1:C:632:ASN:N	1:C:664:ILE:HD13	2.31	0.45
1:D:352:ASP:H	1:D:414:LYS:HZ2	1.65	0.45
1:D:387:ARG:HB2	1:D:387:ARG:NH1	2.31	0.45
1:D:405:GLY:O	1:D:407:ILE:N	2.48	0.45
1:A:46:ILE:HG13	1:A:47:PHE:N	2.32	0.45
1:A:583:ASP:CG	1:A:677:TRP:HE1	2.25	0.45
1:A:596:THR:HB	1:A:600:GLY:HA3	1.97	0.45
1:A:640:ASP:OD1	1:A:642:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LYS:HB2	1:B:205:LYS:HE2	1.66	0.45
1:B:437:VAL:HB	1:B:448:GLU:HB3	1.99	0.45
1:B:601:GLU:HA	1:B:669:LYS:HA	1.99	0.45
1:C:39:ILE:HG13	1:C:293:ALA:HB1	1.97	0.45
1:C:701:TRP:CH2	1:C:783:LEU:HG	2.51	0.45
1:D:137:GLU:OE1	1:D:141:GLN:NE2	2.50	0.45
1:D:471:TRP:C	1:D:472:LYS:HD3	2.42	0.45
1:A:196:LEU:HD13	1:A:225:LEU:HD21	1.99	0.45
1:B:278:ILE:HG13	1:B:336:LEU:HB2	1.98	0.45
1:C:186:ILE:O	1:C:190:ASN:ND2	2.33	0.45
1:C:489:LYS:HA	1:C:489:LYS:HD2	1.82	0.45
1:C:595:TYR:CE2	1:C:675:GLU:HB3	2.52	0.45
1:D:56:LEU:HD12	1:D:127:TYR:CE2	2.51	0.45
1:A:358:VAL:HG21	1:A:410:LEU:HD22	1.99	0.45
1:A:374:LEU:N	1:A:380:ILE:O	2.43	0.45
1:A:413:PRO:HB3	1:A:418:GLN:HB2	1.99	0.45
1:A:566:THR:O	1:A:567:SER:OG	2.33	0.45
1:B:90:ASN:ND2	1:D:90:ASN:HA	2.32	0.45
1:B:365:GLY:C	1:B:461:ILE:HD11	2.42	0.45
1:C:233:ASP:HB3	1:D:227:LYS:HE2	1.98	0.45
1:C:403:ILE:HG22	1:C:686:ILE:HG23	1.99	0.45
1:C:626:PRO:O	1:C:671:GLN:HB2	2.17	0.45
1:D:252:ASN:OD1	1:D:253:LEU:HD23	2.16	0.45
1:D:596:THR:HB	1:D:670:ASN:HB2	1.99	0.45
1:A:186:ILE:O	1:A:190:ASN:ND2	2.33	0.45
1:A:423:LYS:HE2	1:A:473:GLU:HB3	1.99	0.45
1:B:53:GLY:O	1:B:55:ASN:N	2.49	0.45
1:B:339:ASN:OD1	1:B:529:LYS:NZ	2.50	0.45
1:B:707:VAL:HB	1:B:723:PHE:CZ	2.52	0.45
1:B:746:ARG:HG2	1:B:760:ASN:HA	1.99	0.45
1:D:354:ASP:HB3	1:D:691:PHE:CE1	2.52	0.45
1:D:671:GLN:HG2	1:D:674:TYR:HD2	1.81	0.45
1:A:582:VAL:HB	1:A:585:ALA:HB2	1.99	0.44
1:C:57:THR:HG22	1:C:58:LEU:N	2.29	0.44
1:C:640:ASP:OD1	1:C:642:LYS:HG2	2.17	0.44
1:D:347:LYS:NZ	1:D:493:ASP:OD2	2.36	0.44
1:D:437:VAL:HB	1:D:448:GLU:HB3	1.99	0.44
1:D:558:SER:OG	1:D:682:ILE:HA	2.16	0.44
1:D:616:TYR:CE2	1:D:657:SER:HB3	2.52	0.44
1:A:626:PRO:O	1:A:671:GLN:HB2	2.17	0.44
1:A:646:SER:OG	1:A:647:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ASP:OD1	1:B:28:TYR:N	2.50	0.44
1:B:93:SER:OG	1:B:97:LYS:NZ	2.41	0.44
1:B:239:PHE:O	1:B:243:THR:HG23	2.17	0.44
1:B:446:GLY:CA	1:B:472:LYS:HE3	2.45	0.44
1:B:476:CYS:SG	1:B:480:SER:HA	2.57	0.44
1:B:515:LEU:HD23	1:B:517:VAL:H	1.82	0.44
1:B:671:GLN:HG2	1:B:674:TYR:HD2	1.81	0.44
1:C:349:ARG:NH1	1:C:492:THR:O	2.50	0.44
1:C:403:ILE:HD11	1:C:555:TYR:HE1	1.81	0.44
1:A:470:SER:OG	1:A:471:TRP:N	2.50	0.44
1:A:533:ARG:O	1:A:537:LEU:HB2	2.18	0.44
1:B:153:SER:O	1:B:157:GLN:HG3	2.18	0.44
1:B:558:SER:OG	1:B:682:ILE:HA	2.17	0.44
1:C:356:PRO:HG3	1:C:409:LYS:O	2.18	0.44
1:D:631:LYS:O	1:D:665:TYR:N	2.34	0.44
1:B:90:ASN:HA	1:D:90:ASN:ND2	2.32	0.44
1:B:124:LEU:HA	1:B:124:LEU:HD22	1.71	0.44
1:B:471:TRP:C	1:B:472:LYS:HD3	2.42	0.44
1:C:46:ILE:HG13	1:C:47:PHE:N	2.32	0.44
1:C:112:HIS:CE1	1:C:116:GLN:HE21	2.36	0.44
1:C:533:ARG:O	1:C:537:LEU:HB2	2.18	0.44
1:D:27:ASP:OD1	1:D:28:TYR:N	2.50	0.44
1:D:152:LEU:HB3	1:D:283:ASN:OD1	2.18	0.44
1:D:278:ILE:HG13	1:D:336:LEU:HB2	1.98	0.44
1:D:346:SER:O	1:D:497:MET:N	2.39	0.44
1:D:515:LEU:HD23	1:D:517:VAL:H	1.82	0.44
1:D:517:VAL:HB	1:D:524:ILE:HG23	1.98	0.44
1:B:258:ALA:HA	1:B:261:THR:HG22	1.99	0.44
1:B:414:LYS:HE2	1:B:765:ASP:OD2	2.18	0.44
1:B:596:THR:HB	1:B:670:ASN:HB2	1.99	0.44
1:B:626:PRO:HB3	1:B:676:ALA:HB1	2.00	0.44
1:B:727:ILE:HG13	1:B:779:CYS:SG	2.57	0.44
1:C:389:LYS:HB2	1:C:393:GLN:HB2	1.98	0.44
1:C:413:PRO:HB3	1:C:418:GLN:HB2	1.99	0.44
1:C:470:SER:OG	1:C:471:TRP:N	2.50	0.44
1:C:531:TYR:O	1:C:535:SER:N	2.39	0.44
1:C:706:ASN:O	1:C:718:LEU:HB2	2.17	0.44
1:D:176:LEU:HD12	1:D:176:LEU:HA	1.85	0.44
1:D:339:ASN:OD1	1:D:529:LYS:NZ	2.50	0.44
1:D:347:LYS:HE3	1:D:496:TYR:CE2	2.53	0.44
1:D:707:VAL:HB	1:D:723:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:HIS:CE1	1:A:116:GLN:HE21	2.36	0.44
1:A:248:MET:O	1:A:257:SER:OG	2.20	0.44
1:A:363:ALA:HB3	1:A:366:TYR:CD2	2.53	0.44
1:A:638:PHE:HE1	1:A:653:LYS:HD2	1.82	0.44
1:C:365:GLY:C	1:C:461:ILE:HD11	2.42	0.44
1:C:624:GLY:O	1:C:626:PRO:HD3	2.17	0.44
1:C:638:PHE:HE1	1:C:653:LYS:HD2	1.82	0.44
1:D:209:ASP:N	1:D:209:ASP:OD1	2.45	0.44
1:D:401:GLU:CD	1:D:556:ILE:H	2.26	0.44
1:A:584:LYS:C	1:A:586:ASP:H	2.24	0.44
1:B:749:ILE:O	1:B:756:LEU:N	2.50	0.44
1:C:269:GLU:O	1:C:270:ASN:ND2	2.51	0.44
1:C:423:LYS:HE2	1:C:473:GLU:HB3	1.99	0.44
1:C:727:ILE:HG22	1:C:780:PHE:HA	2.00	0.44
1:D:239:PHE:O	1:D:243:THR:HG23	2.17	0.44
1:D:476:CYS:SG	1:D:480:SER:HA	2.57	0.44
1:D:746:ARG:HG2	1:D:760:ASN:HA	1.99	0.44
1:A:269:GLU:O	1:A:270:ASN:ND2	2.51	0.44
1:A:349:ARG:NH1	1:A:492:THR:O	2.50	0.44
1:A:358:VAL:HB	1:A:438:PHE:HB2	2.00	0.44
1:A:365:GLY:C	1:A:461:ILE:HD11	2.42	0.44
1:A:737:LEU:HD12	1:A:799:SER:O	2.18	0.44
1:B:163:LEU:HD13	1:B:265:LEU:HD21	2.00	0.44
1:B:353:ILE:HG12	1:B:414:LYS:HZ1	1.82	0.44
1:B:606:ILE:HA	1:B:609:LYS:HZ1	1.83	0.44
1:B:625:ARG:HD2	1:B:674:TYR:CD2	2.53	0.44
1:C:737:LEU:HD12	1:C:799:SER:O	2.18	0.44
1:D:153:SER:OG	1:D:154:LYS:N	2.51	0.44
1:D:365:GLY:C	1:D:461:ILE:HD11	2.42	0.44
1:D:403:ILE:HG22	1:D:686:ILE:HA	2.00	0.44
1:D:414:LYS:HE2	1:D:765:ASP:OD2	2.18	0.44
1:D:599:ASP:OD1	1:D:599:ASP:N	2.51	0.44
1:A:378:LEU:HB2	1:A:654:LYS:HD3	2.00	0.44
1:A:593:SER:HA	1:A:679:ASN:HB3	2.00	0.44
1:A:595:TYR:CE2	1:A:675:GLU:HB3	2.52	0.44
1:A:624:GLY:O	1:A:626:PRO:HD3	2.17	0.44
1:A:705:GLY:O	1:A:721:GLY:HA3	2.17	0.44
1:B:156:LEU:HG	1:B:287:VAL:HG21	1.98	0.44
1:B:616:TYR:CE2	1:B:657:SER:HB3	2.52	0.44
1:C:358:VAL:HG21	1:C:410:LEU:HD22	1.99	0.44
1:D:53:GLY:O	1:D:55:ASN:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:LEU:HD13	1:D:265:LEU:HD21	2.00	0.44
1:D:410:LEU:HD11	1:D:438:PHE:HB3	2.00	0.44
1:D:606:ILE:HA	1:D:609:LYS:HZ1	1.82	0.44
1:D:625:ARG:HD2	1:D:674:TYR:CD2	2.53	0.44
1:A:43:MET:HG2	1:A:300:THR:HG21	2.00	0.43
1:A:531:TYR:O	1:A:535:SER:N	2.39	0.43
1:B:378:LEU:HB3	1:B:654:LYS:HZ1	1.83	0.43
1:B:410:LEU:HD11	1:B:438:PHE:HB3	2.00	0.43
1:C:582:VAL:HB	1:C:585:ALA:HB2	1.99	0.43
1:A:56:LEU:HD13	1:B:212:THR:OG1	2.17	0.43
1:A:618:ILE:HD12	1:A:682:ILE:O	2.18	0.43
1:C:175:THR:HG21	1:C:261:THR:HG21	2.00	0.43
1:C:358:VAL:HB	1:C:438:PHE:HB2	2.00	0.43
1:C:418:GLN:NE2	1:C:420:TYR:OH	2.50	0.43
1:D:67:LEU:HD23	1:D:68:LEU:HD23	2.01	0.43
1:D:153:SER:O	1:D:157:GLN:HG3	2.18	0.43
1:A:98:GLU:OE1	1:B:85:LEU:HD13	2.18	0.43
1:A:403:ILE:HG22	1:A:686:ILE:HG23	1.99	0.43
1:A:586:ASP:O	1:A:588:ILE:N	2.52	0.43
1:B:152:LEU:HB3	1:B:283:ASN:OD1	2.18	0.43
1:B:599:ASP:OD1	1:B:599:ASP:N	2.51	0.43
1:C:363:ALA:HB3	1:C:366:TYR:CD2	2.53	0.43
1:D:258:ALA:HA	1:D:261:THR:HG22	1.99	0.43
1:D:585:ALA:HA	1:D:588:ILE:O	2.19	0.43
1:D:749:ILE:O	1:D:756:LEU:N	2.51	0.43
1:A:351:SER:HA	1:A:414:LYS:CG	2.48	0.43
1:A:727:ILE:HG22	1:A:780:PHE:HA	2.00	0.43
1:B:70:ASP:O	1:B:74:LYS:HG2	2.18	0.43
1:B:347:LYS:HE3	1:B:496:TYR:CE2	2.53	0.43
1:B:401:GLU:CD	1:B:556:ILE:H	2.26	0.43
1:B:585:ALA:HA	1:B:588:ILE:O	2.18	0.43
1:B:767:THR:H	1:B:768:ARG:NH1	2.16	0.43
1:D:205:LYS:HB2	1:D:205:LYS:HE2	1.67	0.43
1:D:643:ASN:OD1	1:D:643:ASN:N	2.50	0.43
1:A:372:GLU:OE1	1:A:374:LEU:HG	2.19	0.43
1:A:672:SER:OG	1:A:673:GLU:OE1	2.29	0.43
1:A:757:LEU:HD23	1:A:757:LEU:HA	1.89	0.43
1:B:403:ILE:HG22	1:B:686:ILE:HA	2.00	0.43
1:B:435:LYS:HE2	1:B:435:LYS:HB3	1.72	0.43
1:B:545:GLU:HB3	1:B:547:TYR:CE1	2.54	0.43
1:C:102:ILE:HG21	1:D:82:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:GLN:H	1:C:208:GLN:CD	2.27	0.43
1:C:351:SER:HA	1:C:414:LYS:CG	2.48	0.43
1:C:372:GLU:OE1	1:C:374:LEU:HG	2.19	0.43
1:C:593:SER:HA	1:C:679:ASN:HB3	2.00	0.43
1:C:620:TYR:HD2	1:C:622:ILE:HG23	1.83	0.43
1:C:694:GLN:OE1	1:C:696:LEU:HB2	2.18	0.43
1:D:767:THR:H	1:D:768:ARG:NH1	2.17	0.43
1:A:175:THR:HG21	1:A:261:THR:HG21	2.00	0.43
1:A:203:ASN:HB3	1:A:204:PRO:HD3	2.01	0.43
1:A:418:GLN:NE2	1:A:420:TYR:OH	2.50	0.43
1:A:627:ALA:HB1	1:A:629:TYR:CE2	2.51	0.43
1:C:419:LYS:HA	1:C:487:ILE:HG12	2.01	0.43
1:D:156:LEU:HG	1:D:287:VAL:HG21	1.98	0.43
1:A:636:THR:HG21	1:A:639:GLU:HB2	2.01	0.43
1:A:694:GLN:OE1	1:A:696:LEU:HB2	2.18	0.43
1:B:142:ASN:HD21	1:B:294:LYS:HE3	1.84	0.43
1:D:736:HIS:NE2	1:D:803:GLU:OE2	2.33	0.43
1:A:189:VAL:HG21	1:A:237:PHE:CD1	2.54	0.43
1:A:423:LYS:HG2	1:A:473:GLU:OE1	2.19	0.43
1:A:620:TYR:HD2	1:A:622:ILE:HG23	1.83	0.43
1:C:56:LEU:HD13	1:D:212:THR:OG1	2.18	0.43
1:C:61:ILE:HG21	1:C:124:LEU:HB3	2.00	0.43
1:C:586:ASP:O	1:C:588:ILE:N	2.52	0.43
1:D:56:LEU:HB2	1:D:127:TYR:CE2	2.45	0.43
1:D:372:GLU:OE1	1:D:374:LEU:HG	2.19	0.43
1:A:57:THR:HG22	1:A:58:LEU:N	2.29	0.43
1:A:422:ILE:O	1:A:422:ILE:HG13	2.19	0.43
1:A:642:LYS:HE3	1:A:642:LYS:HB3	1.90	0.43
1:B:153:SER:OG	1:B:154:LYS:N	2.51	0.43
1:B:428:PRO:HG2	1:B:431:TYR:CD2	2.54	0.43
1:C:189:VAL:HG21	1:C:237:PHE:CD1	2.54	0.43
1:C:620:TYR:HB3	1:C:681:PHE:HA	2.01	0.43
1:D:142:ASN:HD21	1:D:294:LYS:HE3	1.84	0.43
1:D:253:LEU:HG	1:D:254:PHE:CD1	2.54	0.43
1:D:545:GLU:HB3	1:D:547:TYR:CE1	2.54	0.43
1:D:617:VAL:O	1:D:683:ILE:HA	2.19	0.43
1:A:54:SER:HA	1:A:57:THR:HB	2.00	0.43
1:A:59:ASP:HB2	1:A:307:GLY:N	2.34	0.43
1:A:275:GLY:O	1:A:280:LYS:NZ	2.52	0.43
1:A:419:LYS:HA	1:A:487:ILE:HG12	2.01	0.43
1:A:736:HIS:CD2	1:A:803:GLU:HB2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:GLN:OE1	1:C:208:GLN:N	2.50	0.43
1:C:250:GLY:HA3	1:C:257:SER:HB2	2.01	0.43
1:D:61:ILE:H	1:D:61:ILE:HD12	1.83	0.43
1:A:414:LYS:O	1:A:415:GLN:HG2	2.19	0.42
1:B:214:GLU:OE2	1:B:215:VAL:HG22	2.19	0.42
1:B:570:THR:HB	1:B:573:TRP:CB	2.49	0.42
1:C:43:MET:HG2	1:C:300:THR:HG21	2.00	0.42
1:D:342:ASN:HD22	1:D:498:PRO:CB	2.32	0.42
1:A:356:PRO:HG3	1:A:409:LYS:O	2.18	0.42
1:A:734:THR:HG23	1:A:770:ILE:O	2.19	0.42
1:C:86:ILE:HD11	1:C:99:LEU:HB3	2.01	0.42
1:C:435:LYS:HE2	1:C:435:LYS:HB3	1.82	0.42
1:C:584:LYS:HE3	1:C:591:SER:C	2.44	0.42
1:D:317:MET:HE3	1:D:317:MET:HB3	1.91	0.42
1:D:674:TYR:HD1	1:D:674:TYR:HA	1.76	0.42
1:D:706:ASN:HB3	1:D:720:ASP:O	2.20	0.42
1:A:61:ILE:HG21	1:A:124:LEU:HB3	2.00	0.42
1:A:102:ILE:HG21	1:B:82:LEU:HD12	2.00	0.42
1:A:351:SER:HA	1:A:414:LYS:HG2	2.01	0.42
1:A:771:LYS:HD2	1:A:771:LYS:HA	1.84	0.42
1:B:61:ILE:HD12	1:B:61:ILE:H	1.83	0.42
1:C:59:ASP:HB2	1:C:307:GLY:N	2.34	0.42
1:C:203:ASN:HB3	1:C:204:PRO:HD3	2.01	0.42
1:C:597:HIS:HA	1:C:670:ASN:HD22	1.85	0.42
1:D:51:THR:O	1:D:54:SER:OG	2.33	0.42
1:D:70:ASP:O	1:D:74:LYS:HG2	2.18	0.42
1:D:214:GLU:OE2	1:D:215:VAL:HG22	2.19	0.42
1:D:570:THR:HB	1:D:573:TRP:CB	2.49	0.42
1:D:626:PRO:HB3	1:D:676:ALA:HB1	2.00	0.42
1:D:632:ASN:HB2	1:D:663:GLU:HB2	2.00	0.42
1:A:86:ILE:HD11	1:A:99:LEU:HB3	2.01	0.42
1:A:433:ILE:HD12	1:A:510:ILE:HG13	2.02	0.42
1:C:54:SER:HA	1:C:57:THR:HB	2.00	0.42
1:C:644:ASN:OD1	1:C:644:ASN:N	2.53	0.42
1:C:734:THR:HG23	1:C:770:ILE:O	2.19	0.42
1:D:215:VAL:HG12	1:D:219:LEU:CD2	2.49	0.42
1:D:428:PRO:HG2	1:D:431:TYR:CD2	2.54	0.42
1:A:35:PHE:CE1	1:A:290:SER:HA	2.55	0.42
1:B:131:ILE:HD13	1:B:131:ILE:HA	1.87	0.42
1:B:215:VAL:HG12	1:B:219:LEU:CD2	2.49	0.42
1:B:397:GLU:O	1:B:398:SER:OG	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:PHE:HB3	1:B:428:PRO:HD2	2.01	0.42
1:B:632:ASN:HB2	1:B:663:GLU:HB2	2.00	0.42
1:C:378:LEU:HB2	1:C:654:LYS:HD3	2.00	0.42
1:C:422:ILE:HG13	1:C:422:ILE:O	2.19	0.42
1:C:618:ILE:HD12	1:C:682:ILE:O	2.18	0.42
1:D:427:PHE:HB3	1:D:428:PRO:HD2	2.01	0.42
1:D:730:GLU:N	1:D:735:TYR:OH	2.50	0.42
1:A:541:LEU:HD13	1:A:541:LEU:HA	1.88	0.42
1:B:136:ASN:HA	1:B:202:LYS:HZ3	1.85	0.42
1:B:317:MET:HE3	1:B:317:MET:HB3	1.91	0.42
1:B:347:LYS:HG3	1:B:496:TYR:CE1	2.55	0.42
1:B:643:ASN:OD1	1:B:643:ASN:N	2.50	0.42
1:C:414:LYS:O	1:C:415:GLN:HG2	2.19	0.42
1:C:419:LYS:HD3	1:C:444:GLN:HG2	2.02	0.42
1:C:560:VAL:HG12	1:C:563:TRP:HA	2.02	0.42
1:C:622:ILE:O	1:C:649:GLN:N	2.53	0.42
1:D:504:GLU:HG2	1:D:532:LEU:HD22	2.02	0.42
1:A:250:GLY:HA3	1:A:257:SER:HB2	2.01	0.42
1:A:395:ASP:OD2	1:A:397:GLU:N	2.53	0.42
1:A:597:HIS:HA	1:A:670:ASN:HD22	1.85	0.42
1:B:34:GLY:O	1:B:37:THR:OG1	2.32	0.42
1:B:67:LEU:HD23	1:B:68:LEU:HD23	2.01	0.42
1:B:99:LEU:HD23	1:B:99:LEU:HA	1.82	0.42
1:B:474:LYS:O	1:B:478:GLU:HG3	2.19	0.42
1:B:645:PHE:CG	1:B:649:GLN:HB2	2.55	0.42
1:B:732:ASP:OD1	1:B:732:ASP:N	2.43	0.42
1:C:395:ASP:OD2	1:C:397:GLU:N	2.53	0.42
1:C:636:THR:HG21	1:C:639:GLU:HB2	2.01	0.42
1:A:158:GLU:OE2	1:A:273:THR:HB	2.20	0.42
1:A:211:VAL:HG23	1:A:211:VAL:O	2.20	0.42
1:A:694:GLN:NE2	1:A:798:VAL:O	2.53	0.42
1:B:39:ILE:HD12	1:B:39:ILE:HA	1.86	0.42
1:B:346:SER:HB2	1:B:499:LEU:HD22	2.02	0.42
1:C:642:LYS:HE3	1:C:642:LYS:HB3	1.90	0.42
1:C:736:HIS:CD2	1:C:803:GLU:HB2	2.51	0.42
1:D:474:LYS:O	1:D:478:GLU:HG3	2.19	0.42
1:D:600:GLY:O	1:D:670:ASN:N	2.53	0.42
1:A:419:LYS:HD3	1:A:444:GLN:HG2	2.02	0.42
1:B:372:GLU:OE1	1:B:374:LEU:HG	2.19	0.42
1:D:347:LYS:HG3	1:D:496:TYR:CE1	2.55	0.42
1:D:581:PHE:CD2	1:D:583:ASP:HB2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:GLU:O	1:A:382:LYS:N	2.24	0.42
1:A:507:LEU:HD21	1:A:552:PRO:HD2	2.02	0.42
1:B:241:LEU:HD12	1:B:241:LEU:HA	1.90	0.42
1:B:306:LEU:HD13	1:B:306:LEU:HA	1.89	0.42
1:B:765:ASP:OD1	1:B:765:ASP:N	2.47	0.42
1:C:33:TYR:CD1	1:C:543:ASN:HB3	2.55	0.42
1:C:372:GLU:CG	1:C:501:VAL:HG12	2.50	0.42
1:C:684:LEU:HD23	1:C:684:LEU:HA	1.90	0.42
1:C:694:GLN:NE2	1:C:798:VAL:O	2.53	0.42
1:D:473:GLU:OE2	1:D:476:CYS:HB2	2.20	0.42
1:A:380:ILE:CG2	1:A:403:ILE:HG23	2.50	0.41
1:A:417:GLU:HA	1:A:489:LYS:HA	2.02	0.41
1:A:620:TYR:HB3	1:A:681:PHE:HA	2.01	0.41
1:A:751:ASP:OD1	1:A:752:GLU:N	2.44	0.41
1:A:785:GLY:HA2	1:A:793:THR:HG21	2.02	0.41
1:B:253:LEU:HG	1:B:254:PHE:CD1	2.54	0.41
1:B:617:VAL:O	1:B:683:ILE:HA	2.19	0.41
1:C:399:MET:HE2	1:C:399:MET:HB3	1.82	0.41
1:C:507:LEU:HD21	1:C:552:PRO:HD2	2.02	0.41
1:C:584:LYS:NZ	1:C:587:THR:H	2.18	0.41
1:D:193:PHE:O	1:D:197:THR:HG23	2.19	0.41
1:A:208:GLN:H	1:A:208:GLN:CD	2.27	0.41
1:A:208:GLN:OE1	1:A:208:GLN:N	2.50	0.41
1:A:754:LYS:HZ3	1:A:756:LEU:HG	1.84	0.41
1:B:32:ILE:HD12	1:B:32:ILE:HA	1.87	0.41
1:B:270:ASN:OD1	1:B:270:ASN:C	2.63	0.41
1:C:352:ASP:OD2	1:C:416:LEU:HB2	2.20	0.41
1:C:762:LYS:HE3	1:C:763:ASP:OD2	2.21	0.41
1:D:397:GLU:C	1:D:399:MET:H	2.28	0.41
1:A:205:LYS:HE2	1:A:205:LYS:HB3	1.94	0.41
1:A:350:GLY:HA3	1:A:412:CYS:O	2.21	0.41
1:A:584:LYS:HE3	1:A:591:SER:C	2.45	0.41
1:B:134:MET:O	1:B:138:VAL:HG23	2.21	0.41
1:B:342:ASN:HD22	1:B:498:PRO:CB	2.32	0.41
1:C:35:PHE:CE1	1:C:290:SER:HA	2.55	0.41
1:C:194:ASP:OD1	1:C:194:ASP:C	2.63	0.41
1:C:304:LYS:NZ	1:C:310:ASP:OD1	2.46	0.41
1:C:417:GLU:HA	1:C:489:LYS:HA	2.02	0.41
1:C:423:LYS:HG2	1:C:473:GLU:OE1	2.19	0.41
1:D:134:MET:O	1:D:138:VAL:HG23	2.21	0.41
1:D:308:LEU:O	1:D:309:THR:OG1	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:LEU:HD13	1:D:368:LEU:HA	1.94	0.41
1:A:622:ILE:O	1:A:649:GLN:N	2.53	0.41
1:B:28:TYR:HE2	1:B:547:TYR:HB3	1.84	0.41
1:B:193:PHE:O	1:B:197:THR:HG23	2.19	0.41
1:B:434:THR:HG21	1:B:452:ASN:CG	2.45	0.41
1:B:706:ASN:HB3	1:B:720:ASP:O	2.19	0.41
1:C:158:GLU:OE2	1:C:273:THR:HB	2.20	0.41
1:C:380:ILE:HG21	1:C:403:ILE:HG23	2.03	0.41
1:C:628:ILE:O	1:C:639:GLU:HA	2.21	0.41
1:D:270:ASN:OD1	1:D:270:ASN:C	2.63	0.41
1:D:346:SER:HB2	1:D:499:LEU:HD22	2.02	0.41
1:D:645:PHE:CG	1:D:649:GLN:HB2	2.55	0.41
1:A:294:LYS:HE3	1:A:294:LYS:HB2	1.69	0.41
1:A:352:ASP:OD2	1:A:416:LEU:HB2	2.20	0.41
1:B:353:ILE:HG22	1:B:738:ARG:HB3	2.03	0.41
1:C:28:TYR:CE2	1:C:396:ARG:HB2	2.56	0.41
1:C:350:GLY:HA3	1:C:412:CYS:O	2.20	0.41
1:C:351:SER:HA	1:C:414:LYS:HG2	2.01	0.41
1:D:93:SER:OG	1:D:97:LYS:NZ	2.41	0.41
1:D:213:LYS:O	1:D:213:LYS:HD3	2.21	0.41
1:D:627:ALA:O	1:D:669:LYS:N	2.52	0.41
1:D:711:ASP:OD1	1:D:714:ARG:NE	2.52	0.41
1:A:33:TYR:CD1	1:A:543:ASN:HB3	2.55	0.41
1:A:162:LYS:NZ	1:A:272:THR:HB	2.36	0.41
1:A:168:LEU:HD12	1:A:168:LEU:HA	1.85	0.41
1:A:762:LYS:HE3	1:A:763:ASP:OD2	2.21	0.41
1:B:56:LEU:HB2	1:B:127:TYR:CE2	2.45	0.41
1:B:600:GLY:O	1:B:670:ASN:N	2.53	0.41
1:C:627:ALA:HB2	1:C:671:GLN:HA	2.03	0.41
1:D:434:THR:HG21	1:D:452:ASN:CG	2.45	0.41
1:D:625:ARG:HH22	1:D:644:ASN:ND2	2.19	0.41
1:D:751:ASP:OD1	1:D:775:SER:OG	2.25	0.41
1:A:540:ASP:OD1	1:A:546:THR:HG21	2.21	0.41
1:A:567:SER:C	1:A:569:ASN:N	2.79	0.41
1:A:584:LYS:CB	1:A:589:LYS:H	2.34	0.41
1:A:644:ASN:OD1	1:A:644:ASN:N	2.53	0.41
1:B:566:THR:HA	1:B:592:SER:OG	2.21	0.41
1:B:607:GLY:O	1:B:662:SER:HA	2.21	0.41
1:B:751:ASP:HA	1:B:779:CYS:CB	2.51	0.41
1:C:233:ASP:O	1:C:236:SER:HB2	2.21	0.41
1:C:584:LYS:CB	1:C:589:LYS:H	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:LEU:CB	1:D:117:LEU:HD12	2.51	0.41
1:D:744:THR:O	1:D:793:THR:OG1	2.31	0.41
1:A:163:LEU:O	1:A:165:ILE:HG12	2.20	0.41
1:A:259:LEU:HD21	1:A:328:PHE:HB2	2.03	0.41
1:A:360:LEU:HD23	1:A:371:PHE:CE1	2.56	0.41
1:A:489:LYS:HA	1:A:489:LYS:HD2	1.82	0.41
1:B:370:GLY:HA3	1:B:503:SER:OG	2.21	0.41
1:B:730:GLU:HB2	1:B:733:SER:OG	2.21	0.41
1:C:193:PHE:CZ	1:C:298:THR:HG23	2.56	0.41
1:C:754:LYS:HE3	1:C:774:SER:OG	2.20	0.41
1:D:433:ILE:HD12	1:D:510:ILE:HG13	2.02	0.41
1:D:607:GLY:O	1:D:662:SER:HA	2.21	0.41
1:D:617:VAL:HB	1:D:686:ILE:HD11	2.02	0.41
1:D:751:ASP:OD2	1:D:776:LYS:HG2	2.21	0.41
1:D:751:ASP:HA	1:D:779:CYS:CB	2.51	0.41
1:A:380:ILE:HG21	1:A:403:ILE:HG23	2.02	0.41
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.81	0.41
1:A:419:LYS:O	1:A:445:LEU:N	2.54	0.41
1:A:584:LYS:NZ	1:A:587:THR:H	2.18	0.41
1:A:768:ARG:HA	1:A:768:ARG:HD3	1.77	0.41
1:B:100:LEU:HD12	1:B:100:LEU:HA	1.85	0.41
1:B:473:GLU:HB2	1:B:484:GLU:HB3	2.03	0.41
1:B:504:GLU:HG2	1:B:532:LEU:HD22	2.02	0.41
1:B:627:ALA:O	1:B:669:LYS:N	2.52	0.41
1:C:163:LEU:O	1:C:165:ILE:HG12	2.20	0.41
1:C:211:VAL:HG23	1:C:211:VAL:O	2.20	0.41
1:C:360:LEU:HD23	1:C:371:PHE:CE1	2.56	0.41
1:C:403:ILE:HD11	1:C:555:TYR:CE1	2.56	0.41
1:C:433:ILE:HD12	1:C:510:ILE:HG13	2.02	0.41
1:C:625:ARG:HG2	1:C:671:GLN:CD	2.46	0.41
1:C:737:LEU:HA	1:C:799:SER:O	2.21	0.41
1:C:775:SER:OG	1:C:779:CYS:SG	2.61	0.41
1:D:64:ASN:HB3	1:D:67:LEU:HB3	2.03	0.41
1:D:241:LEU:HD12	1:D:241:LEU:HA	1.90	0.41
1:D:435:LYS:HB3	1:D:435:LYS:HE2	1.72	0.41
1:D:792:SER:O	1:D:792:SER:OG	2.32	0.41
1:A:193:PHE:HA	1:A:193:PHE:HD1	1.69	0.41
1:A:448:GLU:HA	1:A:470:SER:HA	2.03	0.41
1:A:560:VAL:HG12	1:A:563:TRP:HA	2.02	0.41
1:A:627:ALA:HB2	1:A:671:GLN:HA	2.03	0.41
1:B:68:LEU:CB	1:B:117:LEU:HD12	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:HIS:HD2	1:B:320:HIS:CD2	2.39	0.41
1:B:473:GLU:OE2	1:B:476:CYS:HB2	2.20	0.41
1:B:625:ARG:HH22	1:B:644:ASN:ND2	2.19	0.41
1:B:748:SER:O	1:B:781:ILE:HD12	2.21	0.41
1:C:349:ARG:HD2	1:C:492:THR:O	2.21	0.41
1:C:419:LYS:O	1:C:445:LEU:N	2.54	0.41
1:C:619:GLN:HA	1:C:651:VAL:O	2.21	0.41
1:C:768:ARG:HA	1:C:768:ARG:HD3	1.77	0.41
1:D:28:TYR:HE2	1:D:547:TYR:HB3	1.84	0.41
1:D:557:SER:OG	1:D:558:SER:N	2.54	0.41
1:A:28:TYR:CE2	1:A:396:ARG:HB2	2.56	0.40
1:A:193:PHE:CZ	1:A:298:THR:HG23	2.56	0.40
1:A:194:ASP:OD1	1:A:194:ASP:C	2.63	0.40
1:A:594:LEU:HD13	1:A:602:PHE:CG	2.56	0.40
1:A:754:LYS:HE3	1:A:774:SER:OG	2.20	0.40
1:A:783:LEU:HB3	1:A:795:PHE:CE2	2.56	0.40
1:B:397:GLU:C	1:B:399:MET:H	2.28	0.40
1:B:433:ILE:HD12	1:B:510:ILE:HG13	2.02	0.40
1:B:476:CYS:HA	1:B:481:CYS:H	1.86	0.40
1:B:730:GLU:N	1:B:735:TYR:OH	2.50	0.40
1:C:39:ILE:HA	1:C:39:ILE:HD13	1.88	0.40
1:C:162:LYS:NZ	1:C:272:THR:HB	2.36	0.40
1:C:275:GLY:O	1:C:280:LYS:NZ	2.52	0.40
1:D:473:GLU:HB2	1:D:484:GLU:HB3	2.03	0.40
1:D:584:LYS:HZ2	1:D:591:SER:HA	1.86	0.40
1:D:748:SER:O	1:D:781:ILE:HD12	2.21	0.40
1:A:63:LYS:HA	1:A:66:ASN:ND2	2.37	0.40
1:A:625:ARG:HG2	1:A:671:GLN:CD	2.46	0.40
1:A:720:ASP:OD1	1:A:787:TYR:HA	2.22	0.40
1:A:790:ASN:OD1	1:A:790:ASN:N	2.54	0.40
1:B:202:LYS:HA	1:B:202:LYS:HD3	1.85	0.40
1:B:213:LYS:O	1:B:213:LYS:HD3	2.21	0.40
1:B:493:ASP:OD1	1:B:494:GLY:N	2.54	0.40
1:B:617:VAL:HB	1:B:686:ILE:HD11	2.02	0.40
1:B:629:TYR:CE2	1:B:669:LYS:HE2	2.56	0.40
1:C:63:LYS:HE2	1:C:63:LYS:HB2	1.87	0.40
1:C:275:GLY:HA3	1:C:505:THR:HG23	2.03	0.40
1:C:520:LYS:HB2	1:C:520:LYS:HE2	1.92	0.40
1:C:597:HIS:HA	1:C:670:ASN:ND2	2.37	0.40
1:C:605:PHE:HA	1:C:665:TYR:HB2	2.03	0.40
1:C:702:ILE:N	1:C:724:LYS:O	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:783:LEU:HB3	1:C:795:PHE:CE2	2.56	0.40
1:D:219:LEU:HA	1:D:219:LEU:HD13	1.85	0.40
1:D:404:TYR:CE1	1:D:687:LYS:HD2	2.57	0.40
1:D:407:ILE:HD12	1:D:407:ILE:HA	1.90	0.40
1:D:431:TYR:O	1:D:531:TYR:OH	2.29	0.40
1:D:622:ILE:HG13	1:D:645:PHE:HD2	1.86	0.40
1:A:233:ASP:O	1:A:236:SER:HB2	2.21	0.40
1:A:410:LEU:HD21	1:A:438:PHE:HB3	2.03	0.40
1:B:362:ALA:HA	1:B:385:GLN:OE1	2.21	0.40
1:C:259:LEU:HD21	1:C:328:PHE:HB2	2.03	0.40
1:C:380:ILE:CG2	1:C:403:ILE:HG23	2.50	0.40
1:C:785:GLY:HA2	1:C:793:THR:HG21	2.02	0.40
1:D:321:ILE:HD13	1:D:321:ILE:HA	1.89	0.40
1:D:362:ALA:HA	1:D:385:GLN:OE1	2.21	0.40
1:D:476:CYS:HA	1:D:481:CYS:H	1.86	0.40
1:D:493:ASP:OD1	1:D:494:GLY:N	2.54	0.40
1:D:730:GLU:HB2	1:D:733:SER:OG	2.21	0.40
1:A:229:VAL:HG11	1:A:306:LEU:HB2	2.04	0.40
1:A:628:ILE:O	1:A:639:GLU:HA	2.21	0.40
1:A:746:ARG:O	1:A:784:GLU:HG3	2.21	0.40
1:A:775:SER:OG	1:A:779:CYS:SG	2.61	0.40
1:B:751:ASP:OD2	1:B:776:LYS:HG2	2.21	0.40
1:C:732:ASP:OD1	1:C:733:SER:N	2.55	0.40
1:D:353:ILE:HG22	1:D:738:ARG:HB3	2.03	0.40
1:D:479:ASP:HB3	1:D:481:CYS:SG	2.62	0.40
1:D:629:TYR:CE2	1:D:669:LYS:HE2	2.56	0.40
1:A:353:ILE:HD11	1:A:739:LEU:HA	2.03	0.40
1:B:51:THR:O	1:B:54:SER:OG	2.33	0.40
1:B:347:LYS:HA	1:B:495:ILE:O	2.22	0.40
1:B:622:ILE:HG13	1:B:645:PHE:HD2	1.86	0.40
1:B:674:TYR:HD1	1:B:674:TYR:HA	1.76	0.40
1:B:742:LYS:HA	1:B:742:LYS:HD3	1.99	0.40
1:C:63:LYS:HA	1:C:66:ASN:ND2	2.36	0.40
1:C:229:VAL:HG11	1:C:306:LEU:HB2	2.04	0.40
1:C:234:MET:N	1:D:227:LYS:HZ3	2.20	0.40
1:C:720:ASP:OD1	1:C:787:TYR:HA	2.22	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	775/803 (96%)	675 (87%)	98 (13%)	2 (0%)	36	69
1	B	775/803 (96%)	675 (87%)	100 (13%)	0	100	100
1	C	775/803 (96%)	675 (87%)	98 (13%)	2 (0%)	36	69
1	D	775/803 (96%)	675 (87%)	100 (13%)	0	100	100
All	All	3100/3212 (96%)	2700 (87%)	396 (13%)	4 (0%)	49	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	PHE
1	C	237	PHE
1	A	587	THR
1	C	587	THR

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	705/730 (97%)	704 (100%)	1 (0%)	88	89
1	B	705/730 (97%)	703 (100%)	2 (0%)	86	85
1	C	705/730 (97%)	704 (100%)	1 (0%)	88	89
1	D	705/730 (97%)	703 (100%)	2 (0%)	86	85
All	All	2820/2920 (97%)	2814 (100%)	6 (0%)	85	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	TYR
1	B	124	LEU
1	B	156	LEU
1	C	28	TYR
1	D	124	LEU
1	D	156	LEU

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

Mol	Chain	Res	Type
1	A	30	ASN
1	A	90	ASN
1	A	92	ASN
1	A	107	ASN
1	A	111	ASN
1	A	116	GLN
1	A	118	ASN
1	A	203	ASN
1	A	210	ASN
1	A	270	ASN
1	A	319	HIS
1	A	342	ASN
1	A	577	ASN
1	A	619	GLN
1	A	725	GLN
1	A	797	ASN
1	B	30	ASN
1	B	90	ASN
1	B	106	GLN
1	B	107	ASN
1	B	111	ASN
1	B	114	ASN
1	B	142	ASN
1	B	155	GLN
1	B	173	ASN
1	B	184	GLN
1	B	218	ASN
1	B	220	ASN
1	B	232	ASN
1	B	245	HIS
1	B	315	GLN

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Mol	Chain	Res	Type
1	B	319	HIS
1	B	320	HIS
1	B	348	ASN
1	B	418	GLN
1	B	443	ASN
1	B	464	ASN
1	B	562	ASN
1	B	644	ASN
1	B	656	ASN
1	B	671	GLN
1	B	706	ASN
1	B	725	GLN
1	B	772	ASN
1	C	90	ASN
1	C	92	ASN
1	C	107	ASN
1	C	111	ASN
1	C	116	GLN
1	C	118	ASN
1	C	203	ASN
1	C	210	ASN
1	C	270	ASN
1	C	319	HIS
1	C	342	ASN
1	C	577	ASN
1	C	619	GLN
1	C	725	GLN
1	C	797	ASN
1	D	30	ASN
1	D	90	ASN
1	D	106	GLN
1	D	107	ASN
1	D	111	ASN
1	D	114	ASN
1	D	155	GLN
1	D	173	ASN
1	D	184	GLN
1	D	218	ASN
1	D	220	ASN
1	D	232	ASN
1	D	315	GLN
1	D	319	HIS

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Mol	Chain	Res	Type
1	D	320	HIS
1	D	348	ASN
1	D	418	GLN
1	D	443	ASN
1	D	464	ASN
1	D	562	ASN
1	D	644	ASN
1	D	656	ASN
1	D	671	GLN
1	D	706	ASN
1	D	725	GLN
1	D	772	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.

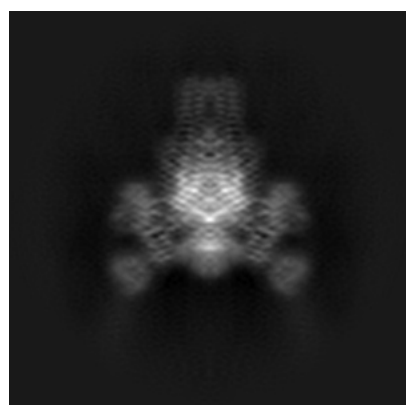
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10888. These allow visual inspection of the internal detail of the map and identification of artifacts.

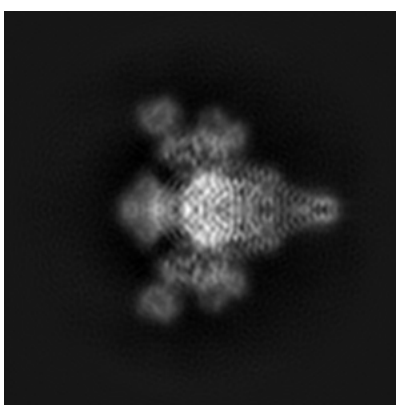
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

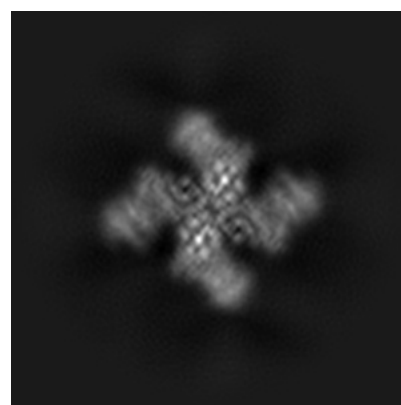
6.1.1 Primary map



X



Y

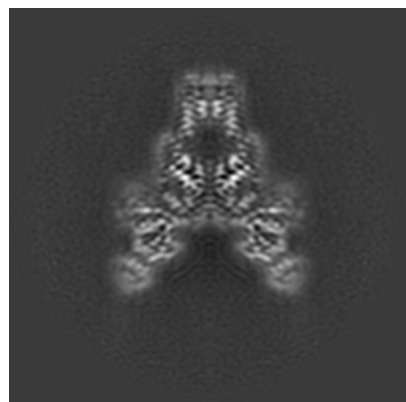


Z

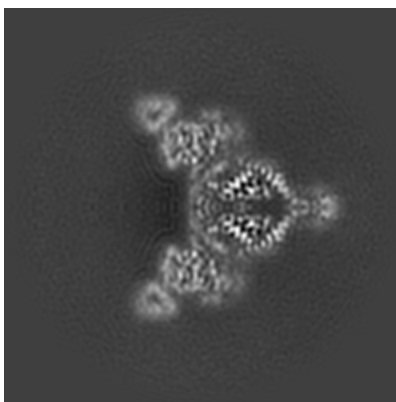
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

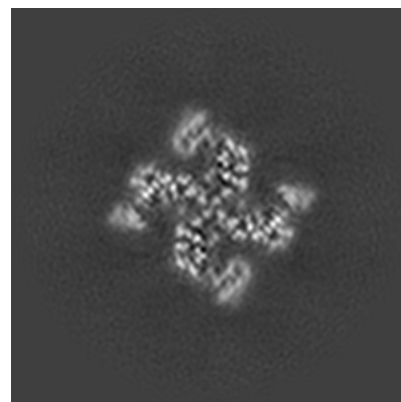
6.2.1 Primary map



X Index: 132



Y Index: 132

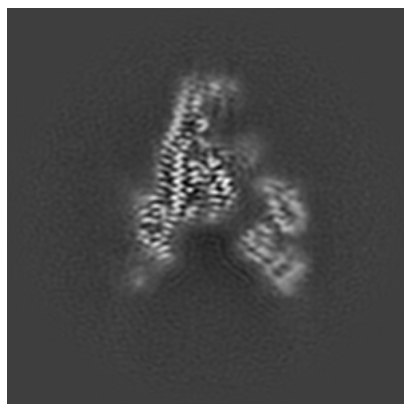


Z Index: 132

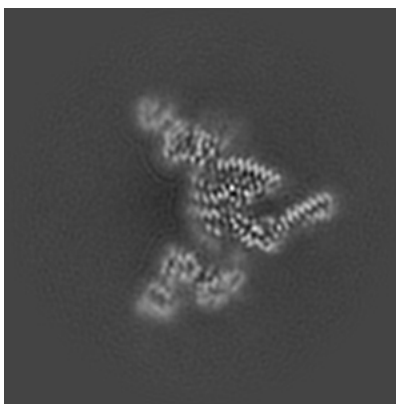
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

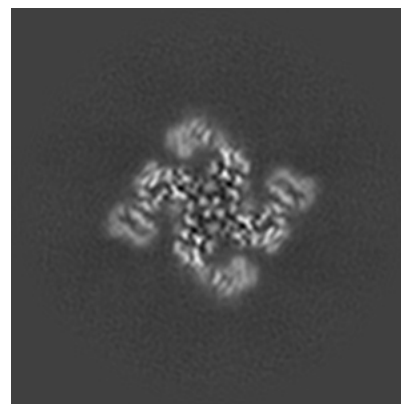
6.3.1 Primary map



X Index: 124



Y Index: 128

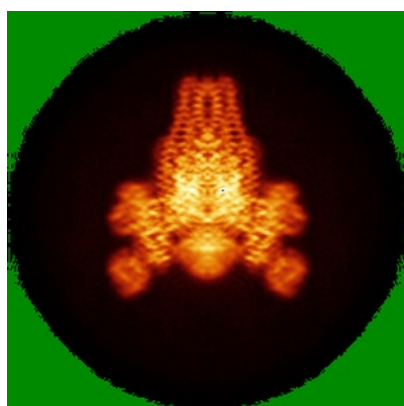


Z Index: 138

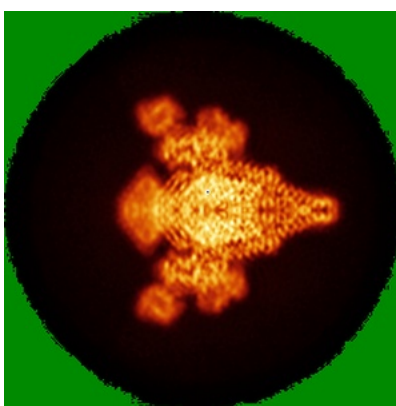
The images above show the largest variance slices of the map in three orthogonal directions.

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

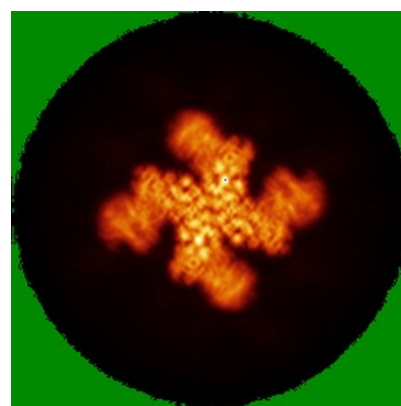
6.4.1 Primary map



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

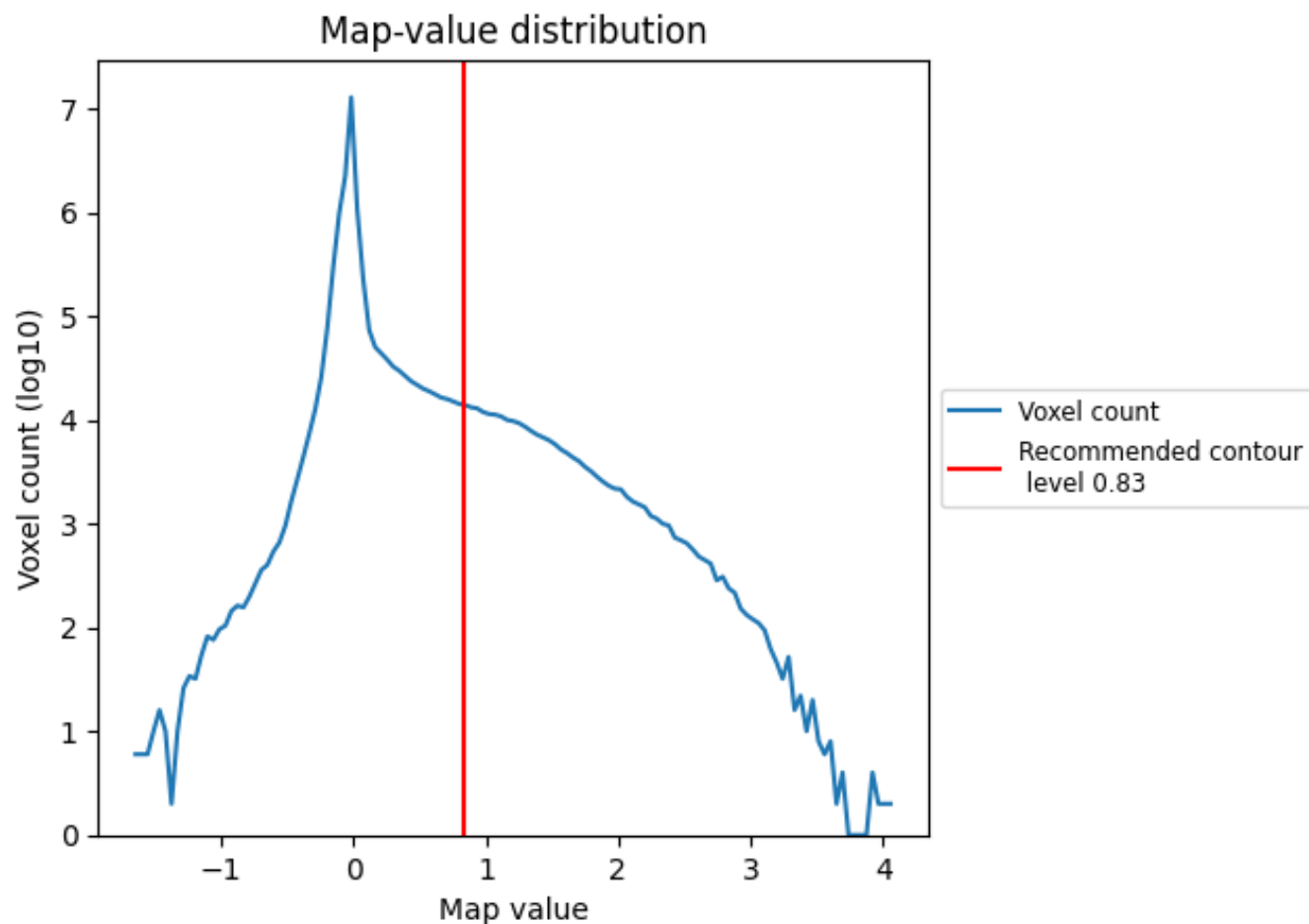
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

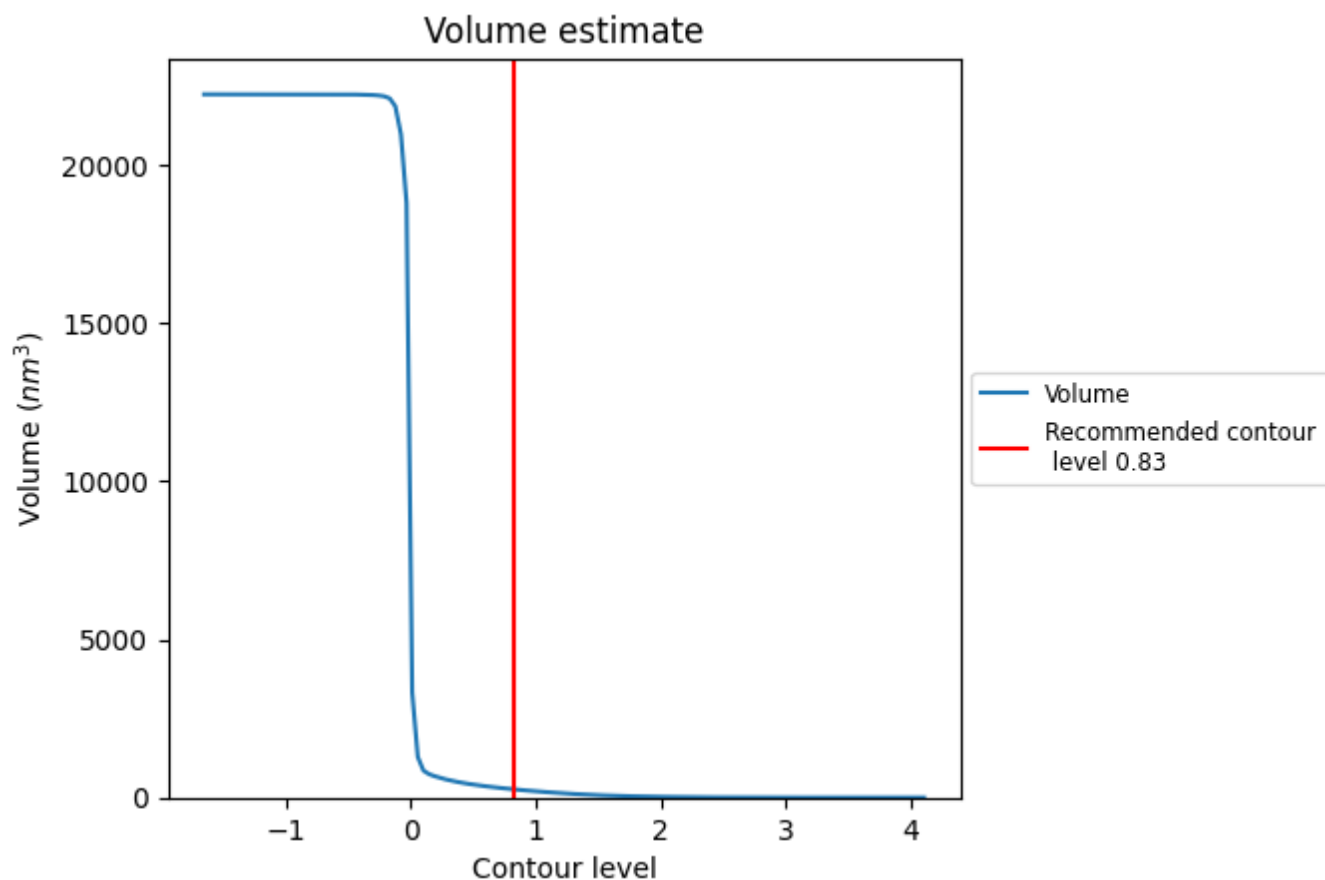
This section contains the results of statistical analysis of the map.

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.

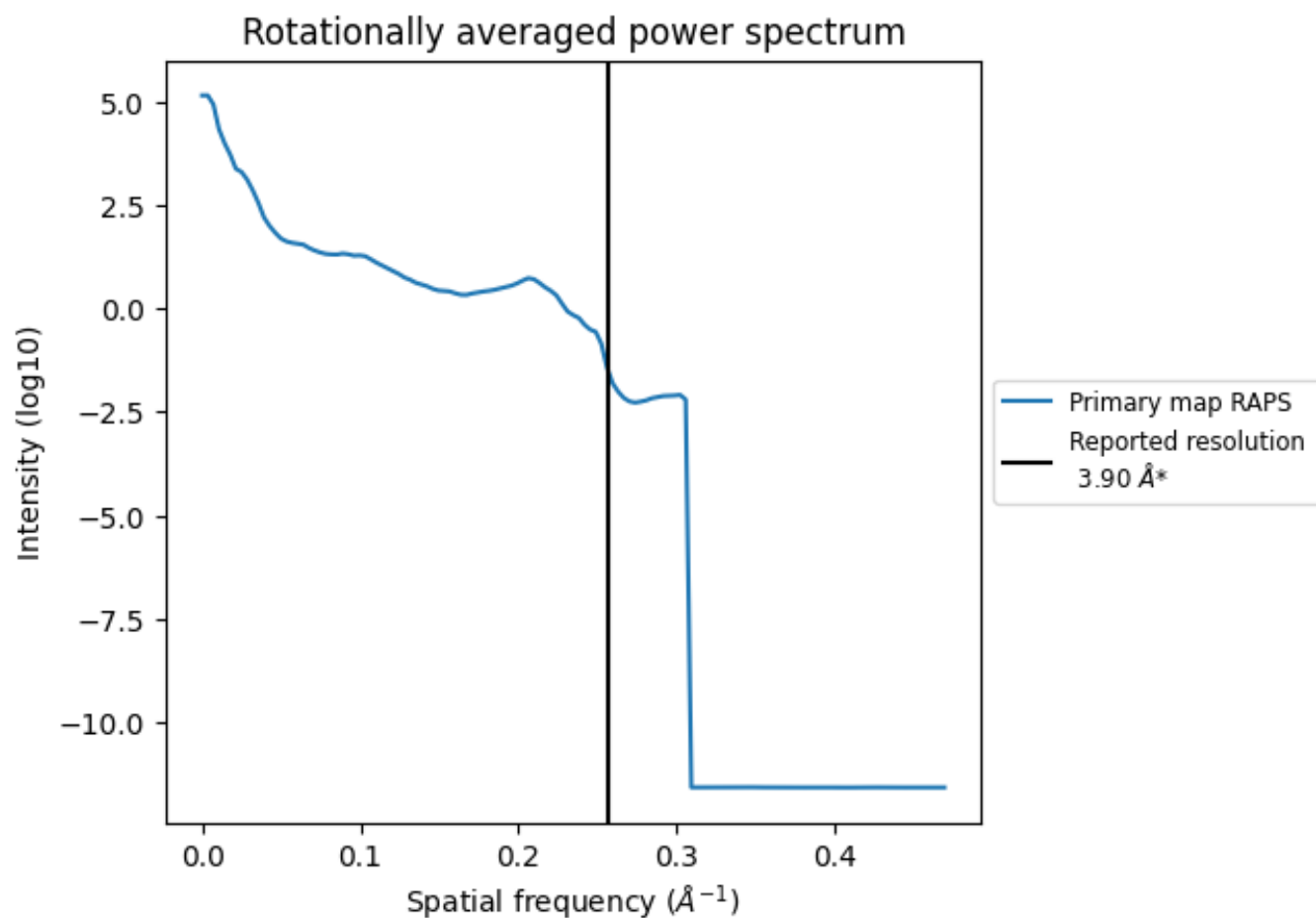
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 259 nm³; this corresponds to an approximate mass of 234 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 ⓘ

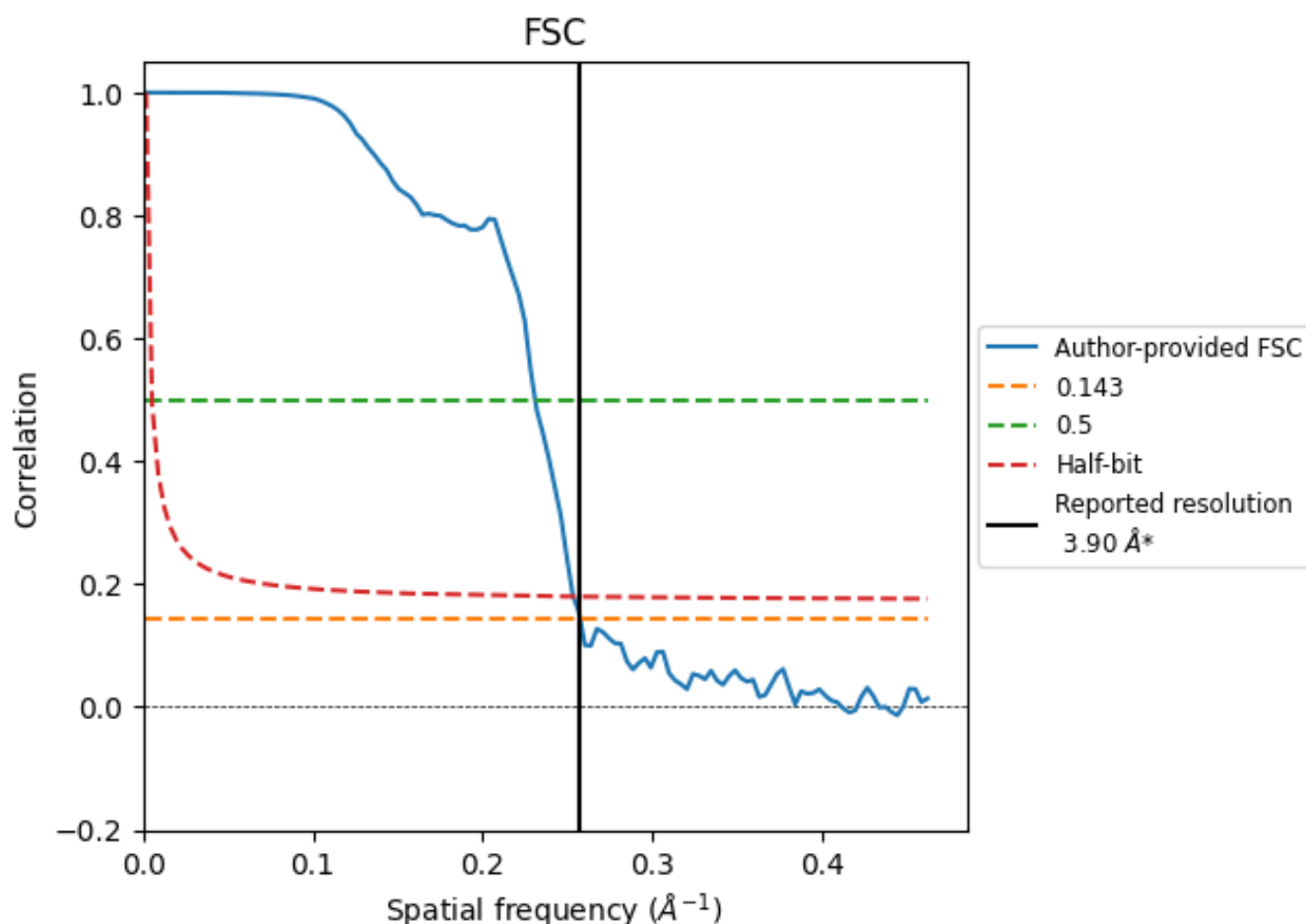


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

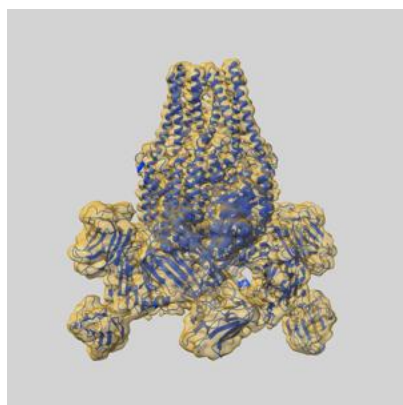
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.89	4.33	3.95
Unmasked-calculated*	-	-	-

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

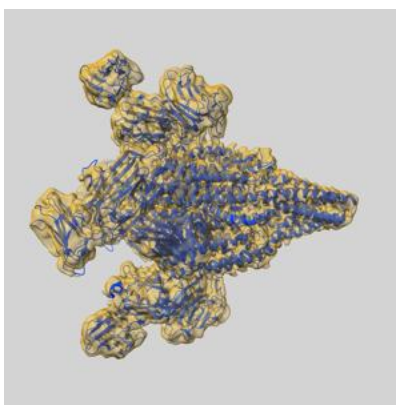
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10888 and PDB model 6YRF. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

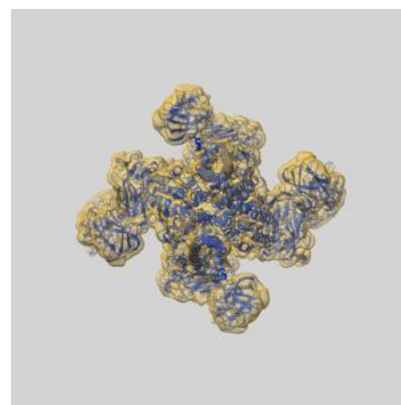
9.1 Map-model overlay [i](#)



X



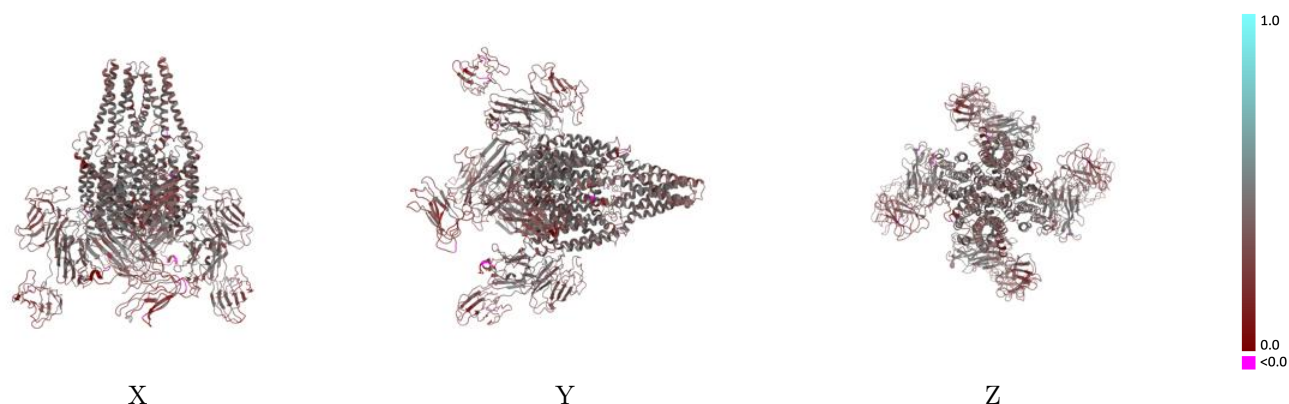
Y



Z

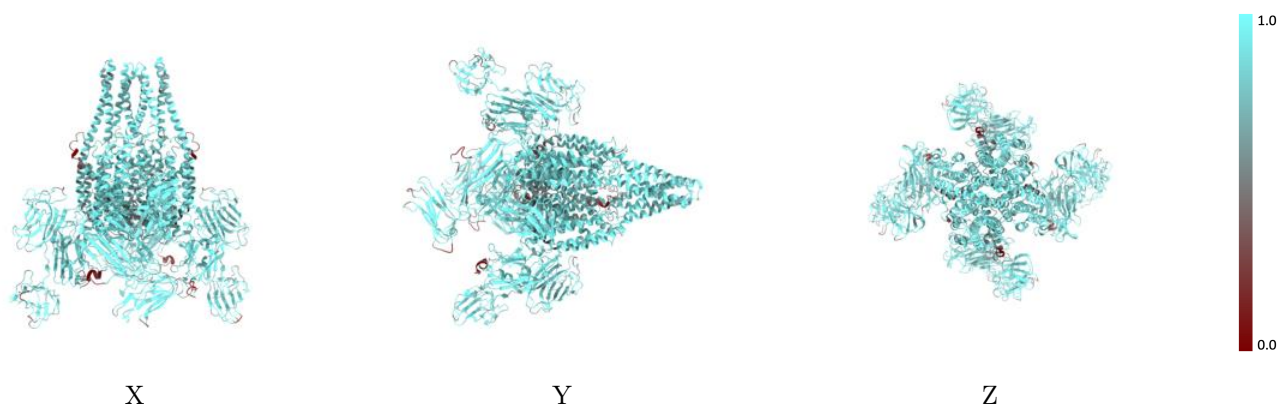
The images above show the 3D surface view of the map at the recommended contour level 0.83 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



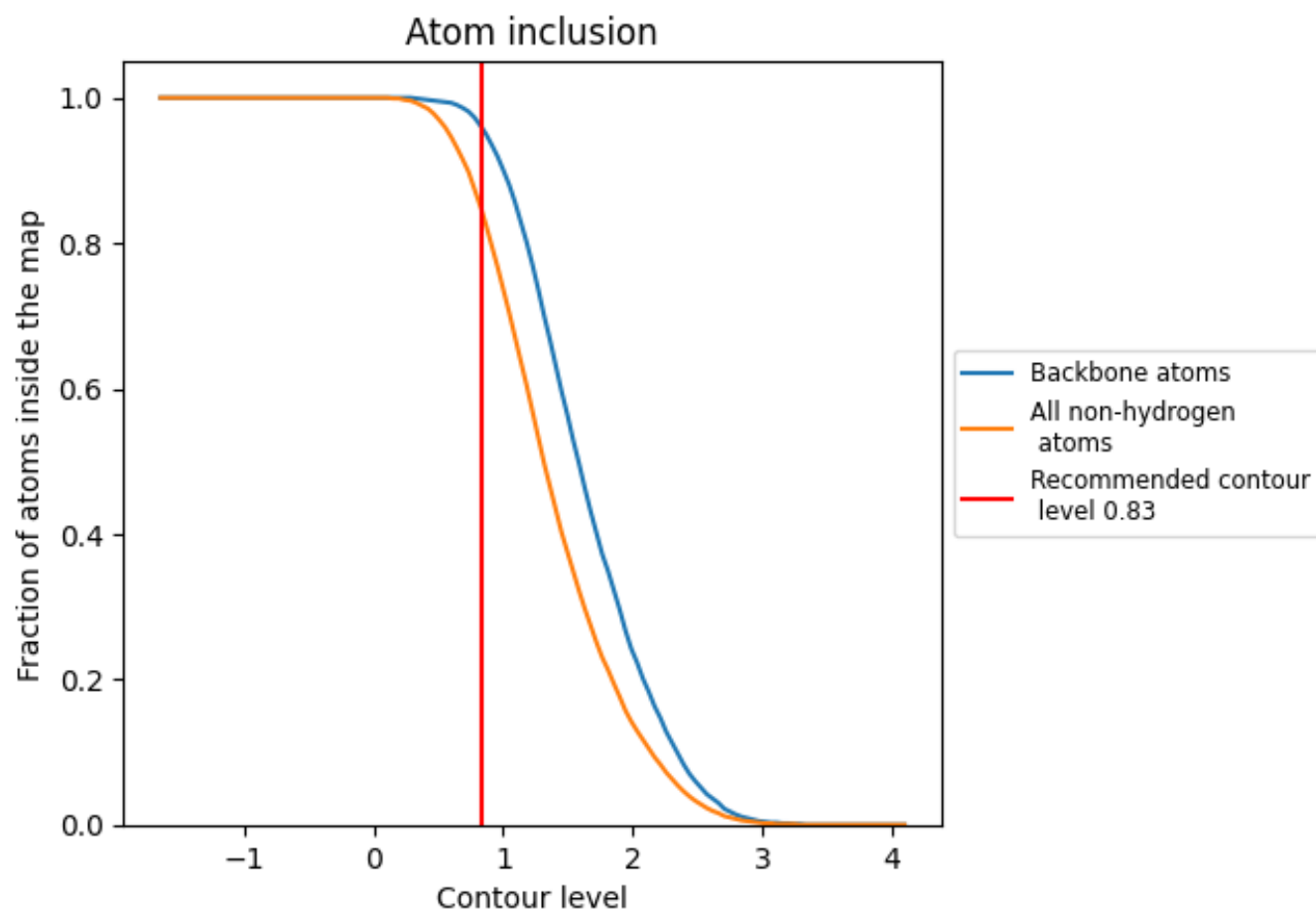
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.83).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 85% 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 (0.83) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8470	0.3550
A	0.8380	0.3540
B	0.8560	0.3560
C	0.8380	0.3530
D	0.8560	0.3560

