



## Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 02:45 AM UTC

PDB ID : 9CMO / pdb\_00009cmo  
EMDB ID : EMD-45751  
Title : Cryo-EM model derived from localized reconstruction of Ad657-hexon-FII complex at 4.14Å resolution  
Authors : Reddy, V.S.; Ma, O.X.  
Deposited on : 2024-07-15  
Resolution : 4.17 Å(reported)  
Based on initial model : 6BIT

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

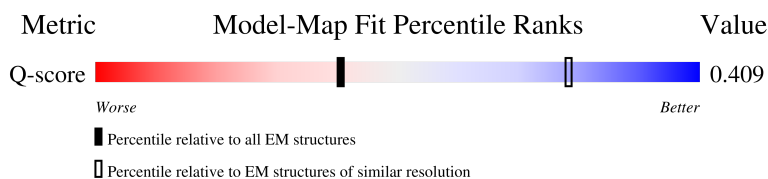
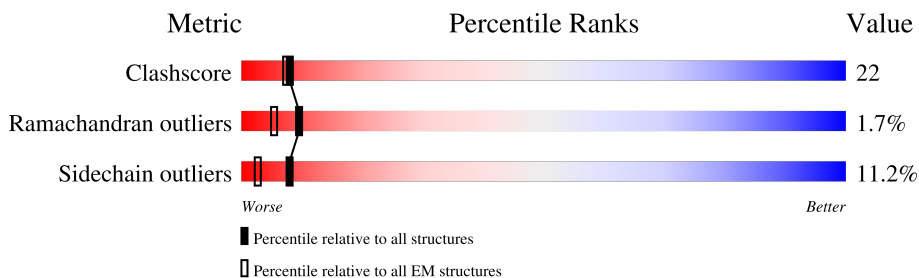
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.17 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	5438 ( 3.67 - 4.67 )

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  $\geq 3$ , 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	J	959	<p>54% 35% 7% ..</p>
1	K	959	<p>55% 34% 7% ..</p>
1	L	959	<p>56% 32% 7% ..</p>
2	Z	622	<p>85% 56% 33% . 7%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	CGU	Z	19	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 26791 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 Hexon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	J	931	7402	4685	1259	1420	38	0	0
1	K	929	7393	4680	1258	1417	38	0	0
1	L	927	7374	4670	1252	1414	38	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	291	LEU	VAL	conflict	UNP A0A348FV85
J	827	ILE	LEU	conflict	UNP A0A348FV85
J	853	VAL	PHE	conflict	UNP A0A348FV85
K	291	LEU	VAL	conflict	UNP A0A348FV85
K	827	ILE	LEU	conflict	UNP A0A348FV85
K	853	VAL	PHE	conflict	UNP A0A348FV85
L	291	LEU	VAL	conflict	UNP A0A348FV85
L	827	ILE	LEU	conflict	UNP A0A348FV85
L	853	VAL	PHE	conflict	UNP A0A348FV85

- Molecule 2 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Z	579	4615	2868	805	910	32	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	L	1	Total	Ca	0
			1	1	

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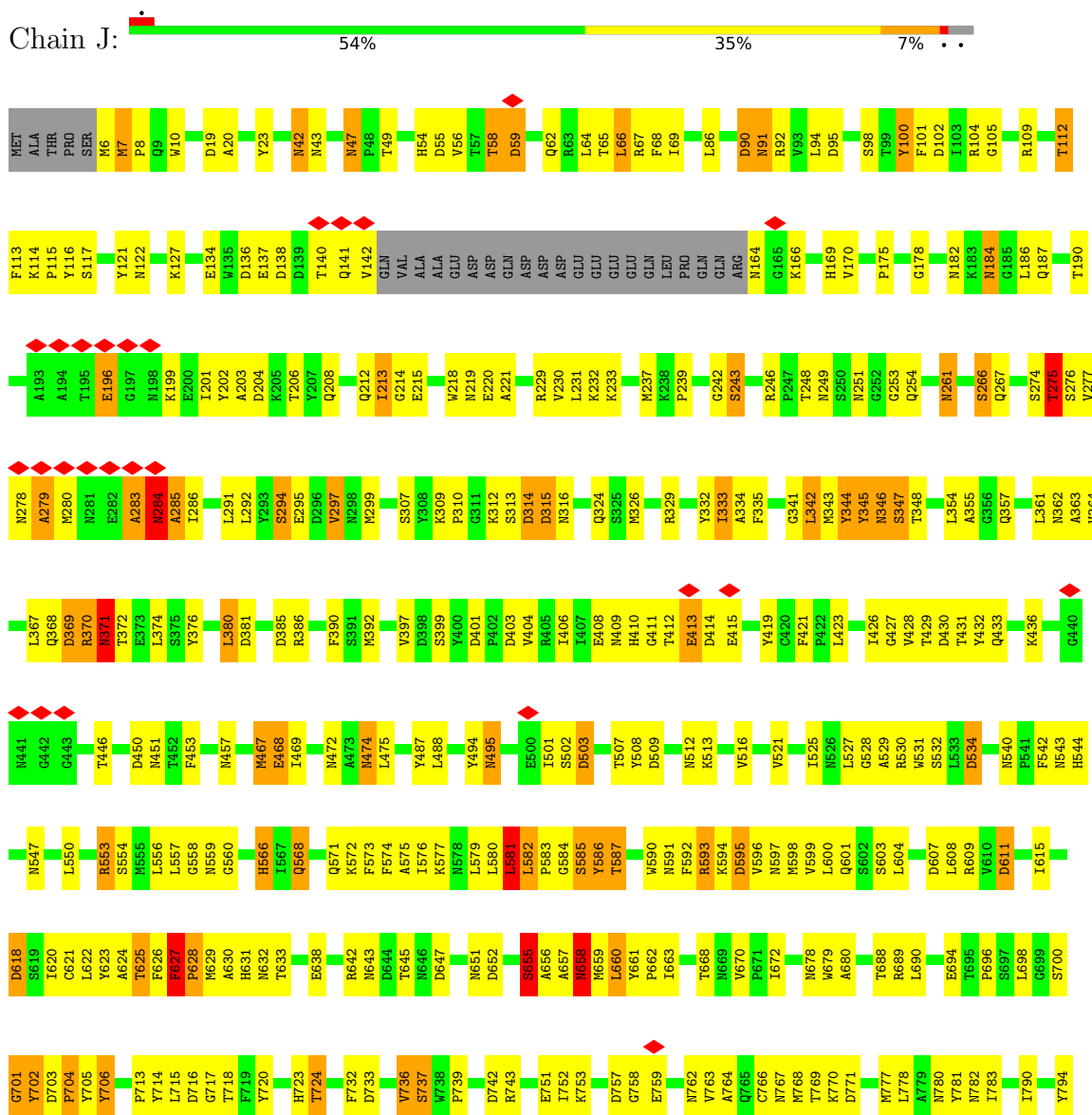
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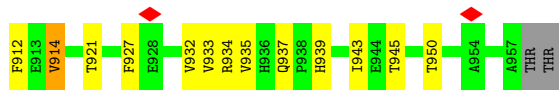
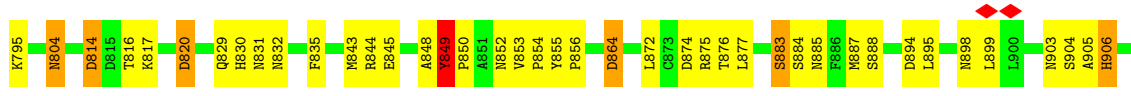
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
3	Z	6	6	6	0

### 3 Residue-property plots

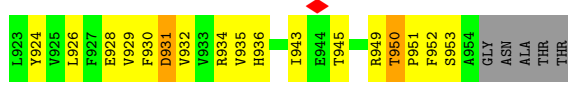
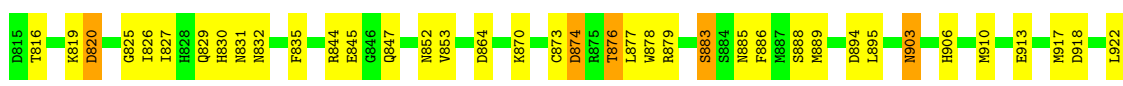
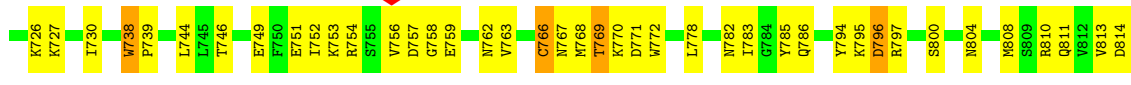
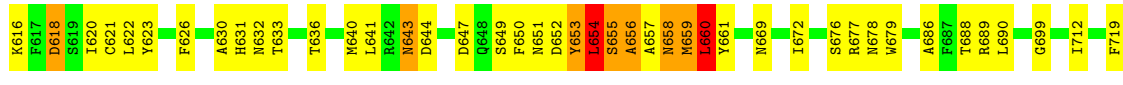
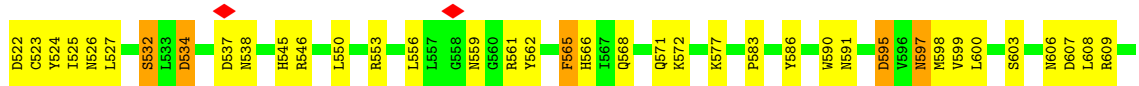
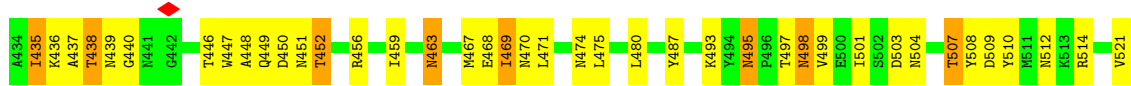
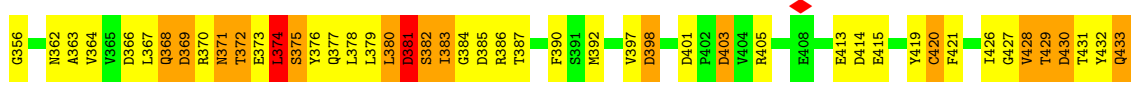
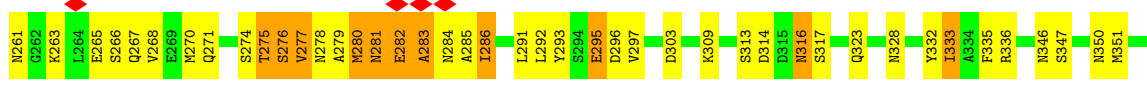
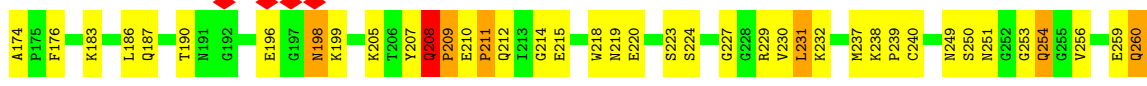
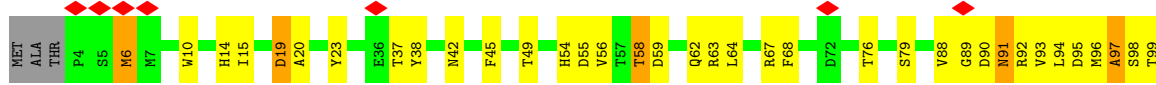
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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





• Molecule 1: Hexon protein





T561	H562	V563	F564	R565	L566	K567	X568	Y569	I570	S571	P572	D573	E574	G575	H576	K577	F578	E579
P441	D442	R443	F444	T445	A446	A447	S448	L449	V450	K451	A452	G453	A454	K455	G456	R457	V458	T459
I501	T502	D503	N504	M505	F506	C507	A508	G509	V510	K511	P512	D513	E514	G515	H516	K517	F518	D519
A520	C521	E522	G523	D524	S525	G526	G527	P528	F529	V530	M531	K532	S533	P534	F535	N536	M537	R538
W539	Y540	Q541	M542	G543	T544	V545	S546	M547	G548	V549	L540	A541	A542	V543	A544	L545	L546	S547
L548	L549	L548	E489	G550	C551	D552	R553	D554	K555	L556	F557	F558	G559	K560	L561	L562	L563	L564
L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583
L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602
L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621
L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640
L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659
L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678
L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697
L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716
L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735
L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754
L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773
L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792
L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811
L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830
L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849
L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868
L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887
L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906
L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925
L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944
L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963
L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982
L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000	L1001
L1002	L1003	L1004	L1005	L1006	L1007	L1008	L1009	L1010	L1011	L1012	L1013	L1014	L1015	L1016	L1017	L1018	L1019	L1020
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L1629	L1630	L1631	L1632	L1633	L1634	L1635	L1636	L1637	L1638	L1639	L1640	L1641	L1642	L1643	L1644	L1645	L1646	L1647
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L1762	L1763	L1764	L1765	L1766	L1767	L1768	L1769	L1770	L1771	L1772	L1773	L1774	L1775	L1776	L1777	L1778	L1779	L1780
L1781	L1782	L1783	L1784	L1785	L1786	L1787	L1788	L1789	L1790	L1791	L1792	L1793	L1794	L1795	L1796	L1797	L1798	L1799
L1800	L1801	L1802	L1803	L1804	L1805	L1806	L1807	L1808	L1809	L1810	L1811	L1812	L1813	L1814	L1815	L1816	L1817	L1818
L1819	L1820	L1821	L1822	L1823	L1824	L1825	L1826	L1827	L1828	L1829	L1830	L1831	L1832	L1833	L1834	L1835	L1836	L1837

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	4635	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	81	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.029	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size ( $\text{\AA}$ )	129.536, 211.2, 112.64	wwPDB
Map dimensions	150, 80, 92	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.408, 1.408, 1.408	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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	J	0.52	1/7595 (0.0%)	0.55	3/10330 (0.0%)
1	K	0.48	2/7587 (0.0%)	0.56	6/10318 (0.1%)
1	L	0.52	4/7568 (0.1%)	0.58	9/10294 (0.1%)
2	Z	0.17	0/4597	0.46	0/6220
All	All	0.47	7/27347 (0.0%)	0.55	18/37162 (0.0%)

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	J	0	1
1	K	0	2
1	L	0	2
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	847	GLN	CA-C	-7.75	1.49	1.53
1	L	696	PRO	CA-C	-6.84	1.44	1.52
1	J	627	PHE	C-O	-5.51	1.20	1.25
1	L	380	LEU	CA-C	-5.33	1.46	1.52
1	K	381	ASP	CA-C	-5.20	1.45	1.52
1	L	948	LEU	CA-C	-5.08	1.46	1.52
1	K	371	ASN	CA-C	-5.02	1.47	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	276	SER	N-CA-C	-12.12	97.59	112.38
1	L	697	SER	N-CA-C	-9.75	98.42	110.41
1	K	380	LEU	N-CA-C	-8.64	101.56	110.97
1	L	849	TYR	CA-C-N	-6.80	113.68	120.21
1	L	849	TYR	C-N-CA	-6.80	113.68	120.21
1	L	380	LEU	N-CA-C	-6.70	102.85	111.02
1	L	847	GLN	CB-CA-C	-6.17	108.18	117.07
1	K	382	SER	N-CA-C	6.15	118.91	111.40
1	J	279	ALA	N-CA-C	-5.82	104.31	111.75
1	L	344	TYR	N-CA-C	-5.66	103.45	110.41
1	L	695	THR	CA-C-N	-5.57	114.21	119.89
1	L	695	THR	C-N-CA	-5.57	114.21	119.89
1	J	849	TYR	CA-C-N	-5.48	114.61	120.03
1	J	849	TYR	C-N-CA	-5.48	114.61	120.03
1	K	275	THR	N-CA-C	5.43	116.97	109.15
1	K	374	LEU	N-CA-C	-5.17	105.13	111.75
1	L	376	TYR	N-CA-C	-5.12	105.20	111.75
1	K	371	ASN	N-CA-C	-5.10	102.03	109.63

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	853	VAL	Peptide
1	K	208	GLN	Peptide
1	K	738	TRP	Peptide
1	L	208	GLN	Peptide
1	L	853	VAL	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	7402	0	7067	351	0
1	K	7393	0	7062	356	0
1	L	7374	0	7040	364	0
2	Z	4615	0	4343	184	0
3	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Z	6	0	0	0	0
All	All	26791	0	25512	1161	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 22.

All (1161) 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:K:275:THR:HB	1:K:277:VAL:HG22	1.33	1.08
1:J:277:VAL:HB	1:J:280:MET:HG3	1.40	1.03
1:L:949:ARG:HG2	1:L:953:SER:HB2	1.52	0.90
1:J:116:TYR:HE1	1:L:858:ILE:HD11	1.36	0.89
2:Z:441:PRO:HD3	2:Z:540:TYR:HB3	1.52	0.89
1:K:378:LEU:O	1:K:381:ASP:HB3	1.73	0.88
1:K:276:SER:HB3	1:L:433:GLN:HB2	1.57	0.86
1:K:275:THR:HB	1:K:277:VAL:CG2	2.05	0.86
1:J:623:TYR:CE2	1:L:770:LYS:HE2	2.14	0.83
1:L:766:CYS:SG	1:L:767:ASN:N	2.51	0.82
1:J:843:MET:HE3	1:J:844:ARG:HH12	1.44	0.82
1:K:656:ALA:HA	1:K:929:VAL:HG22	1.61	0.82
1:K:766:CYS:SG	1:K:767:ASN:N	2.53	0.81
2:Z:53:PRO:HD2	2:Z:56:LYS:HB2	1.63	0.81
1:J:820:ASP:OD1	1:J:820:ASP:N	2.15	0.80
1:L:929:VAL:HB	1:L:950:THR:O	1.82	0.79
1:J:7:MET:SD	1:J:7:MET:N	2.55	0.79
1:J:766:CYS:SG	1:J:767:ASN:N	2.54	0.79
1:L:378:LEU:O	1:L:381:ASP:HB3	1.82	0.79
1:K:275:THR:CB	1:K:277:VAL:HG22	2.12	0.79
1:K:763:VAL:HB	1:K:770:LYS:HG2	1.65	0.79
1:L:137:GLU:O	1:L:166:LYS:HA	1.82	0.78
1:L:692:THR:O	1:L:693:LYS:C	2.24	0.78
1:J:590:TRP:HD1	1:J:591:ASN:H	1.29	0.78
2:Z:116:ASN:HB2	2:Z:124:PRO:HA	1.65	0.78
1:K:96:MET:O	1:K:97:ALA:C	2.25	0.77
1:K:874:ASP:OD1	1:K:874:ASP:N	2.18	0.76
1:J:656:ALA:HB1	1:J:927:PHE:O	1.86	0.75
1:L:757:ASP:N	1:L:757:ASP:OD1	2.19	0.75
2:Z:18:VAL:CG1	2:Z:19:CGU:OE12	2.35	0.75
1:J:335:PHE:O	1:J:553:ARG:NH1	2.20	0.75
1:L:215:GLU:HB3	1:L:220:GLU:HG2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:485:LEU:HD22	2:Z:509:GLY:HA2	1.68	0.75
1:K:495:ASN:OD1	1:K:495:ASN:N	2.20	0.74
1:L:350:ASN:HB2	1:L:591:ASN:ND2	2.02	0.74
1:K:280:MET:HE2	1:K:280:MET:H	1.51	0.74
1:K:316:ASN:N	1:K:316:ASN:OD1	2.21	0.74
1:L:336:ARG:HH12	1:L:712:ILE:H	1.35	0.74
2:Z:9:ARG:NH2	2:Z:10:LYS:HE2	2.02	0.74
1:L:680:ALA:HA	1:L:899:LEU:HD23	1.68	0.74
1:K:653:TYR:O	1:K:654:LEU:C	2.30	0.74
1:J:638:GLU:OE2	1:J:642:ARG:NE	2.20	0.74
1:J:121:TYR:HB2	1:J:242:GLY:HA2	1.71	0.73
1:J:581:LEU:HD21	1:J:586:TYR:HE1	1.54	0.73
1:K:362:ASN:ND2	1:K:364:VAL:O	2.21	0.73
1:K:844:ARG:O	1:K:844:ARG:NH1	2.22	0.73
1:J:503:ASP:OD1	1:J:503:ASP:N	2.22	0.73
1:J:371:ASN:HD21	1:J:374:LEU:CB	2.02	0.72
2:Z:229:VAL:HG23	2:Z:243:CYS:HB2	1.71	0.72
1:J:582:LEU:HB3	1:J:638:GLU:OE1	1.88	0.72
1:K:114:LYS:NZ	1:K:116:TYR:O	2.22	0.72
1:K:276:SER:CB	1:L:433:GLN:HB2	2.18	0.72
1:K:375:SER:O	1:K:376:TYR:C	2.28	0.72
1:K:276:SER:CA	1:L:433:GLN:HB2	2.19	0.72
1:J:116:TYR:CE1	1:L:858:ILE:HD11	2.22	0.72
2:Z:171:VAL:HG21	2:Z:245:LEU:HD13	1.72	0.72
1:J:284:ASN:C	1:J:286:ILE:H	1.98	0.71
1:J:831:ASN:HD21	1:K:121:TYR:HA	1.56	0.71
1:L:830:HIS:H	1:L:852:ASN:HD21	1.37	0.71
1:L:284:ASN:O	1:L:286:ILE:HD13	1.90	0.71
1:K:398:ASP:OD1	1:K:398:ASP:N	2.24	0.70
1:L:362:ASN:ND2	1:L:364:VAL:O	2.24	0.70
1:K:751:GLU:OE2	1:K:754:ARG:NE	2.25	0.70
1:L:275:THR:O	1:L:278:ASN:HB2	1.91	0.70
1:L:371:ASN:H	1:L:658:ASN:HD21	1.40	0.70
2:Z:85:GLU:OE1	2:Z:498:ARG:NH1	2.24	0.69
1:J:237:MET:HE3	1:J:316:ASN:HB2	1.74	0.69
1:J:474:ASN:OD1	1:J:474:ASN:N	2.25	0.69
1:J:472:ASN:HA	1:J:475:LEU:HD12	1.75	0.69
1:J:590:TRP:CD1	1:J:591:ASN:H	2.10	0.69
1:L:493:LYS:O	1:L:514:ARG:NH2	2.26	0.69
2:Z:347:LEU:O	2:Z:463:ASN:ND2	2.25	0.69
1:K:132:SER:HB3	1:K:230:VAL:HG23	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:79:ILE:HB	2:Z:83:GLY:HA2	1.75	0.69
1:K:930:PHE:H	1:K:950:THR:HG21	1.56	0.68
1:L:207:TYR:O	1:L:208:GLN:NE2	2.25	0.68
1:J:249:ASN:OD1	1:J:253:GLY:N	2.26	0.68
2:Z:71:THR:O	2:Z:74:ARG:NH2	2.22	0.68
1:L:277:VAL:O	1:L:278:ASN:C	2.35	0.68
2:Z:17:CYS:HA	2:Z:22:CYS:HB3	1.74	0.68
1:K:380:LEU:O	1:K:381:ASP:C	2.34	0.68
1:L:830:HIS:O	1:L:830:HIS:ND1	2.25	0.68
1:K:415:GLU:N	1:K:415:GLU:OE1	2.27	0.68
1:K:438:THR:OG1	1:K:448:ALA:N	2.27	0.68
1:L:708:TYR:CZ	1:L:710:GLY:N	2.62	0.67
1:L:348:THR:O	1:L:349:GLY:C	2.37	0.67
1:J:716:ASP:OD1	1:J:717:GLY:N	2.26	0.67
2:Z:69:LEU:O	2:Z:116:ASN:ND2	2.27	0.67
1:J:299:MET:HE1	1:L:850:PRO:HG3	1.76	0.67
1:J:246:ARG:NH1	1:L:820:ASP:OD2	2.26	0.67
1:K:276:SER:HA	1:L:433:GLN:OE1	1.95	0.67
1:L:345:TYR:O	1:L:347:SER:N	2.27	0.67
1:L:898:ASN:O	1:L:901:TYR:N	2.21	0.67
1:J:362:ASN:ND2	1:J:364:VAL:O	2.28	0.67
1:J:844:ARG:O	1:J:844:ARG:NH1	2.26	0.67
1:K:95:ASP:O	1:K:96:MET:C	2.35	0.67
1:K:429:THR:HG22	1:K:459:ILE:C	2.19	0.67
1:K:534:ASP:OD1	1:K:534:ASP:N	2.28	0.67
2:Z:18:VAL:HG13	2:Z:57:LEU:HD23	1.77	0.67
1:J:627:PHE:O	1:J:629:MET:N	2.28	0.67
1:L:694:GLU:HB3	1:L:708:TYR:CZ	2.29	0.67
1:J:90:ASP:N	1:J:90:ASP:OD1	2.25	0.67
1:K:368:GLN:O	1:K:370:ARG:N	2.28	0.67
1:K:820:ASP:OD2	1:L:246:ARG:NH1	2.28	0.66
1:K:440:GLY:H	1:K:446:THR:H	1.43	0.66
1:K:522:ASP:OD1	1:K:523:CYS:N	2.24	0.66
1:L:393:TRP:HB2	1:L:395:GLN:HG3	1.78	0.66
1:J:59:ASP:N	1:J:59:ASP:OD1	2.27	0.66
1:J:343:MET:HG2	1:J:592:PHE:CE1	2.31	0.66
1:L:811:GLN:HG3	1:L:867:THR:HG22	1.76	0.66
1:J:433:GLN:CG	1:L:276:SER:HA	2.26	0.66
1:L:303:ASP:OD1	1:L:303:ASP:N	2.27	0.66
1:J:413:GLU:O	1:J:472:ASN:ND2	2.28	0.66
1:K:62:GLN:OE1	1:K:92:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:830:HIS:H	1:L:852:ASN:ND2	1.94	0.66
1:J:178:GLY:HA3	1:J:186:LEU:HD11	1.77	0.66
1:J:595:ASP:OD2	1:J:598:MET:HG2	1.95	0.66
1:K:376:TYR:HE1	1:K:380:LEU:HG	1.61	0.66
1:L:362:ASN:OD1	1:L:363:ALA:N	2.29	0.66
1:L:382:SER:HA	1:L:797:ARG:HD3	1.77	0.65
2:Z:238:GLY:HA3	2:Z:576:GLN:HG2	1.78	0.65
1:J:450:ASP:OD1	1:J:451:ASN:N	2.28	0.65
1:K:58:THR:OG1	1:K:59:ASP:N	2.29	0.65
1:K:275:THR:C	1:K:277:VAL:N	2.47	0.65
1:K:6:MET:SD	1:K:6:MET:N	2.69	0.65
1:L:282:GLU:C	1:L:284:ASN:H	2.04	0.65
1:L:380:LEU:O	1:L:381:ASP:C	2.37	0.65
2:Z:137:GLU:HG3	2:Z:150:VAL:HG21	1.76	0.65
1:J:371:ASN:HD21	1:J:374:LEU:HB3	1.61	0.65
1:K:727:LYS:NZ	1:K:749:GLU:OE1	2.28	0.65
1:L:370:ARG:O	1:L:372:THR:N	2.27	0.65
1:J:534:ASP:N	1:J:534:ASP:OD1	2.29	0.65
1:K:403:ASP:OD1	1:K:403:ASP:N	2.28	0.65
1:J:309:LYS:NZ	1:J:314:ASP:OD2	2.29	0.64
2:Z:118:ASP:OD1	2:Z:125:TRP:NE1	2.28	0.64
1:K:219:ASN:OD1	1:K:220:GLU:N	2.26	0.64
1:L:767:ASN:N	1:L:767:ASN:OD1	2.30	0.64
1:L:298:ASN:N	1:L:298:ASN:OD1	2.26	0.64
1:J:104:ARG:NH2	1:L:759:GLU:OE1	2.31	0.64
1:K:136:ASP:N	1:K:136:ASP:OD1	2.27	0.64
1:K:332:TYR:N	1:K:603:SER:OG	2.31	0.64
1:K:374:LEU:HG	1:K:654:LEU:HD21	1.80	0.64
1:L:350:ASN:HD22	1:L:591:ASN:HD22	1.46	0.64
1:K:385:ASP:OD1	1:K:386:ARG:N	2.31	0.64
1:K:754:ARG:HD3	1:K:758:GLY:HA3	1.78	0.64
1:L:830:HIS:N	1:L:852:ASN:HD21	1.95	0.64
2:Z:114:CYS:O	2:Z:115:ARG:NH1	2.29	0.64
1:J:661:TYR:CD2	1:J:672:ILE:HG21	2.32	0.64
1:K:950:THR:OG1	1:K:951:PRO:HD2	1.98	0.64
1:K:660:LEU:HD13	1:K:922:LEU:HD13	1.80	0.63
1:L:814:ASP:OD1	1:L:815:ASP:N	2.31	0.63
1:J:642:ARG:NH1	1:J:937:GLN:O	2.31	0.63
1:K:303:ASP:N	1:K:303:ASP:OD1	2.30	0.63
1:L:316:ASN:OD1	1:L:316:ASN:N	2.20	0.63
1:L:708:TYR:CG	1:L:709:SER:N	2.66	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:292:ASP:O	2:Z:436:HIS:NE2	2.31	0.63
1:L:495:ASN:OD1	1:L:514:ARG:NH1	2.30	0.63
1:K:280:MET:H	1:K:280:MET:CE	2.11	0.63
2:Z:501:ILE:HG23	2:Z:505:MET:HE3	1.81	0.63
1:J:830:HIS:ND1	1:J:830:HIS:O	2.32	0.63
1:J:829:GLN:HA	1:J:852:ASN:HD21	1.64	0.63
1:J:369:ASP:O	1:J:370:ARG:HB2	1.98	0.63
1:J:571:GLN:OE1	1:J:572:LYS:N	2.32	0.63
1:K:278:ASN:O	1:K:279:ALA:C	2.39	0.63
1:L:6:MET:SD	1:L:6:MET:N	2.72	0.63
1:J:58:THR:OG1	1:J:59:ASP:N	2.27	0.62
1:K:208:GLN:H	1:K:229:ARG:NH1	1.97	0.62
1:J:299:MET:HE1	1:L:850:PRO:CG	2.29	0.62
1:L:237:MET:HG3	1:L:316:ASN:HD22	1.64	0.62
1:J:342:LEU:O	1:J:342:LEU:HD22	1.99	0.62
2:Z:296:ARG:O	2:Z:300:GLU:N	2.31	0.62
1:J:254:GLN:N	1:J:254:GLN:OE1	2.33	0.62
1:J:848:ALA:O	1:J:849:TYR:HB2	1.98	0.62
1:J:935:VAL:HG22	1:J:945:THR:HG22	1.82	0.62
1:K:876:THR:OG1	1:K:877:LEU:N	2.32	0.62
1:L:371:ASN:O	1:L:372:THR:C	2.42	0.62
2:Z:182:LEU:HD22	2:Z:245:LEU:HG	1.82	0.62
1:J:385:ASP:OD1	1:J:386:ARG:N	2.32	0.62
1:L:893:THR:HG23	1:L:896:GLY:H	1.65	0.62
2:Z:543:GLY:HA2	2:Z:563:VAL:HG13	1.82	0.62
1:J:370:ARG:O	1:J:372:THR:N	2.33	0.62
1:L:669:ASN:HB3	1:L:913:GLU:HG3	1.80	0.62
1:J:343:MET:O	1:J:344:TYR:C	2.40	0.62
1:K:414:ASP:OD2	1:K:470:ASN:ND2	2.29	0.62
1:L:304:THR:HG22	1:L:327:PRO:HA	1.81	0.62
1:L:347:SER:C	1:L:349:GLY:H	2.06	0.62
1:L:571:GLN:OE1	1:L:573:PHE:N	2.26	0.62
1:L:694:GLU:HB3	1:L:708:TYR:CE2	2.35	0.62
1:J:283:ALA:O	1:J:285:ALA:N	2.33	0.62
1:L:346:ASN:ND2	1:L:370:ARG:O	2.33	0.62
1:L:380:LEU:HD12	1:L:386:ARG:HD3	1.82	0.62
1:J:583:PRO:HD2	1:J:638:GLU:OE1	2.00	0.62
1:K:450:ASP:OD1	1:K:451:ASN:N	2.33	0.62
1:L:607:ASP:OD1	1:L:608:LEU:N	2.33	0.62
1:J:581:LEU:HD21	1:J:586:TYR:CE1	2.35	0.61
1:K:210:GLU:O	1:K:212:GLN:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:527:LEU:O	1:L:559:ASN:ND2	2.33	0.61
1:J:98:SER:OG	1:J:625:THR:N	2.33	0.61
1:L:949:ARG:HG2	1:L:953:SER:CB	2.28	0.61
1:K:119:THR:OG1	1:K:120:ALA:N	2.32	0.61
2:Z:219:CYS:O	2:Z:220:ARG:NH1	2.33	0.61
1:J:67:ARG:NH2	1:J:621:CYS:SG	2.72	0.61
1:K:931:ASP:OD2	1:K:949:ARG:NE	2.30	0.61
1:L:109:ARG:NH2	1:L:560:GLY:O	2.28	0.61
1:K:166:LYS:H	1:K:166:LYS:HD2	1.65	0.61
1:K:207:TYR:O	1:K:207:TYR:CG	2.54	0.61
1:L:350:ASN:O	1:L:351:MET:C	2.40	0.61
1:L:762:ASN:ND2	1:L:766:CYS:O	2.33	0.61
1:L:844:ARG:O	1:L:844:ARG:NH1	2.30	0.61
2:Z:82:SER:HB2	2:Z:155:ARG:HG3	1.83	0.61
2:Z:285:THR:O	2:Z:356:ARG:NH1	2.34	0.61
1:L:374:LEU:O	1:L:377:GLN:HB2	2.01	0.61
1:J:187:GLN:NE2	1:J:190:THR:OG1	2.34	0.60
1:J:315:ASP:OD1	1:J:315:ASP:N	2.34	0.60
1:J:527:LEU:O	1:K:559:ASN:ND2	2.34	0.60
1:J:700:SER:O	1:J:701:GLY:C	2.44	0.60
1:J:876:THR:OG1	1:J:877:LEU:N	2.34	0.60
1:L:571:GLN:OE1	1:L:572:LYS:N	2.33	0.60
1:L:691:LYS:O	1:L:692:THR:C	2.42	0.60
1:J:182:ASN:ND2	1:J:202:TYR:OH	2.34	0.60
1:K:346:ASN:ND2	1:K:370:ARG:O	2.34	0.60
1:L:371:ASN:O	1:L:373:GLU:N	2.34	0.60
1:J:284:ASN:O	1:J:286:ILE:N	2.34	0.60
1:L:695:THR:O	1:L:696:PRO:C	2.41	0.60
1:L:894:ASP:OD1	1:L:894:ASP:N	2.18	0.60
1:L:58:THR:OG1	1:L:59:ASP:N	2.34	0.60
1:J:280:MET:HB3	2:Z:52:THR:OG1	2.00	0.60
1:J:894:ASP:O	1:J:898:ASN:N	2.33	0.60
1:J:212:GLN:NE2	1:L:829:GLN:O	2.32	0.59
1:J:770:LYS:HE2	1:K:623:TYR:CE2	2.37	0.59
1:K:655:SER:O	1:K:656:ALA:HB2	2.01	0.59
1:L:948:LEU:HG	1:L:949:ARG:N	2.16	0.59
1:J:540:ASN:HD21	1:J:542:PHE:HB2	1.67	0.59
1:K:56:VAL:O	1:K:630:ALA:N	2.35	0.59
1:K:260:GLN:NE2	1:K:265:GLU:OE1	2.31	0.59
1:K:376:TYR:HD2	1:K:572:LYS:HG2	1.65	0.59
1:J:184:ASN:OD1	1:J:184:ASN:N	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:408:GLU:OE2	1:J:530:ARG:NH2	2.35	0.59
1:K:367:LEU:O	1:K:368:GLN:C	2.45	0.59
1:J:399:SER:H	1:J:547:ASN:HD21	1.49	0.59
1:J:547:ASN:OD1	1:J:550:LEU:N	2.26	0.59
1:J:845:GLU:OE2	1:K:214:GLY:N	2.36	0.59
1:L:324:GLN:N	1:L:324:GLN:OE1	2.35	0.59
1:L:607:ASP:OD1	1:L:609:ARG:N	2.33	0.59
1:J:831:ASN:OD1	1:J:832:ASN:ND2	2.36	0.59
1:K:438:THR:HG21	1:K:448:ALA:HB3	1.85	0.59
1:K:509:ASP:OD1	1:K:510:TYR:N	2.35	0.59
1:J:430:ASP:OD2	2:Z:10:LYS:CE	2.50	0.59
1:K:174:ALA:HB1	1:K:227:GLY:C	2.27	0.59
1:L:350:ASN:ND2	1:L:591:ASN:HD22	2.00	0.59
1:J:376:TYR:HE1	1:J:380:LEU:HD12	1.68	0.59
2:Z:363:HIS:ND1	2:Z:419:ASP:OD2	2.30	0.59
2:Z:392:GLU:HB3	2:Z:395:ILE:HG13	1.85	0.59
1:K:390:PHE:CE2	1:K:392:MET:HB3	2.38	0.58
1:L:341:GLY:O	1:L:593:ARG:NH1	2.36	0.58
1:J:206:THR:O	1:J:229:ARG:NH2	2.34	0.58
1:K:239:PRO:HG3	1:K:323:GLN:HG3	1.85	0.58
1:K:797:ARG:O	1:K:800:SER:OG	2.20	0.58
1:J:431:THR:HA	1:J:457:ASN:O	2.04	0.58
1:J:702:TYR:O	1:J:704:PRO:HD3	2.04	0.58
1:K:67:ARG:NH1	1:K:621:CYS:SG	2.77	0.58
1:K:830:HIS:O	1:K:830:HIS:ND1	2.35	0.58
2:Z:441:PRO:HB2	2:Z:446:ALA:HB2	1.85	0.58
1:L:874:ASP:OD1	1:L:874:ASP:N	2.20	0.58
1:J:116:TYR:CG	1:L:527:LEU:HD21	2.39	0.58
1:J:127:LYS:N	1:L:468:GLU:OE1	2.34	0.58
1:K:280:MET:HE3	2:Z:24:TYR:CE2	2.39	0.58
1:K:328:ASN:OD1	1:K:512:ASN:ND2	2.36	0.58
1:K:820:ASP:N	1:K:820:ASP:OD1	2.32	0.58
1:J:703:ASP:C	1:J:705:TYR:H	2.11	0.58
1:J:764:ALA:H	1:K:568:GLN:HE22	1.52	0.58
1:K:254:GLN:O	1:K:297:VAL:HG12	2.03	0.58
1:K:894:ASP:OD1	1:K:895:LEU:N	2.36	0.58
2:Z:18:VAL:HG11	2:Z:19:CGU:OE12	2.03	0.58
2:Z:309:GLU:HG3	2:Z:312:LEU:HD12	1.84	0.58
2:Z:327:ALA:HB2	2:Z:482:VAL:HG11	1.85	0.58
1:J:100:TYR:CE1	1:J:623:TYR:HB2	2.39	0.58
1:J:849:TYR:CD1	1:J:850:PRO:HD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:94:LEU:HB2	1:K:626:PHE:CE1	2.39	0.58
1:L:369:ASP:C	1:L:658:ASN:HD22	2.11	0.58
2:Z:176:GLN:HG2	2:Z:224:GLY:HA2	1.85	0.58
1:J:757:ASP:OD1	1:J:758:GLY:N	2.37	0.57
1:K:112:THR:O	1:K:112:THR:OG1	2.19	0.57
1:K:362:ASN:OD1	1:K:363:ALA:N	2.37	0.57
1:L:346:ASN:OD1	1:L:346:ASN:N	2.27	0.57
1:J:6:MET:N	1:J:7:MET:SD	2.77	0.57
2:Z:70:GLY:HA3	2:Z:124:PRO:HG3	1.86	0.57
2:Z:204:LYS:HE2	2:Z:205:HIS:HE1	1.69	0.57
1:J:432:TYR:HD1	1:L:275:THR:HA	1.69	0.57
1:J:623:TYR:HE2	1:L:770:LYS:HE2	1.68	0.57
1:K:131:ASN:ND2	1:K:238:LYS:O	2.38	0.57
2:Z:124:PRO:HG2	2:Z:149:THR:HG21	1.86	0.57
1:K:280:MET:HE3	2:Z:24:TYR:HE2	1.70	0.57
1:L:7:MET:HB3	1:L:8:PRO:HD3	1.86	0.57
1:J:140:THR:OG1	1:J:141:GLN:OE1	2.21	0.57
1:K:369:ASP:OD1	1:K:369:ASP:N	2.37	0.57
1:L:346:ASN:ND2	1:L:371:ASN:HA	2.19	0.57
1:L:708:TYR:CZ	1:L:710:GLY:CA	2.88	0.57
1:J:362:ASN:OD1	1:J:363:ALA:N	2.38	0.57
1:K:929:VAL:HB	1:K:950:THR:CG2	2.35	0.57
1:J:406:ILE:HG22	1:J:532:SER:HB3	1.87	0.57
1:J:581:LEU:HD11	1:J:586:TYR:CE1	2.39	0.57
1:L:815:ASP:OD1	1:L:816:THR:N	2.37	0.57
1:K:205:LYS:NZ	1:K:268:VAL:O	2.33	0.57
1:K:230:VAL:HG22	1:K:231:LEU:H	1.69	0.57
1:L:375:SER:OG	1:L:376:TYR:N	2.35	0.57
1:J:469:ILE:HB	1:L:420:CYS:HB3	1.86	0.57
1:K:230:VAL:HG22	1:K:231:LEU:N	2.20	0.57
1:K:370:ARG:HG2	1:K:371:ASN:O	2.05	0.56
1:L:768:MET:HE1	1:L:805:PHE:HE1	1.70	0.56
1:K:440:GLY:H	1:K:446:THR:N	2.02	0.56
1:L:377:GLN:O	1:L:378:LEU:C	2.46	0.56
1:L:414:ASP:OD2	1:L:470:ASN:ND2	2.39	0.56
2:Z:508:ALA:HB3	2:Z:560:TYR:HE2	1.71	0.56
1:J:371:ASN:ND2	1:J:374:LEU:HB3	2.20	0.56
1:J:414:ASP:N	1:J:415:GLU:OE2	2.37	0.56
1:K:232:LYS:HB2	1:K:295:GLU:O	2.05	0.56
2:Z:67:GLU:N	2:Z:72:ASN:OD1	2.28	0.56
1:J:647:ASP:OD2	1:J:934:ARG:NH1	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:814:ASP:CG	1:J:817:LYS:H	2.13	0.56
1:K:376:TYR:HD1	1:K:376:TYR:O	1.87	0.56
1:L:375:SER:C	1:L:377:GLN:N	2.56	0.56
1:J:345:TYR:O	1:J:347:SER:N	2.39	0.56
1:J:430:ASP:O	1:J:431:THR:C	2.48	0.56
1:L:350:ASN:HB2	1:L:591:ASN:HD21	1.69	0.56
1:L:547:ASN:OD1	1:L:550:LEU:N	2.33	0.56
1:L:582:LEU:O	1:L:586:TYR:OH	2.20	0.56
2:Z:128:THR:OG1	2:Z:133:VAL:O	2.20	0.56
1:J:284:ASN:C	1:J:286:ILE:N	2.61	0.56
2:Z:43:LYS:O	2:Z:47:CYS:N	2.28	0.56
2:Z:97:PRO:HA	2:Z:127:TYR:CZ	2.41	0.56
1:J:832:ASN:OD1	1:K:124:LEU:N	2.35	0.56
1:K:597:ASN:OD1	1:K:597:ASN:N	2.38	0.56
1:K:104:ARG:HG2	1:K:566:HIS:HB2	1.87	0.56
1:K:275:THR:HB	1:K:277:VAL:HG13	1.87	0.56
1:K:167:LYS:NZ	1:L:451:ASN:O	2.32	0.56
1:K:738:TRP:CD2	1:K:739:PRO:HD3	2.41	0.56
2:Z:242:TYR:HD1	2:Z:408:PRO:HG2	1.71	0.56
1:L:694:GLU:HB3	1:L:708:TYR:CE1	2.41	0.55
1:L:951:PRO:O	1:L:952:PHE:HB2	2.05	0.55
2:Z:94:PRO:HG2	2:Z:95:HIS:CE1	2.41	0.55
1:J:116:TYR:HE1	1:L:858:ILE:CD1	2.15	0.55
1:K:94:LEU:HB2	1:K:626:PHE:HE1	1.70	0.55
1:K:187:GLN:NE2	1:K:190:THR:OG1	2.39	0.55
1:K:607:ASP:OD1	1:K:608:LEU:N	2.39	0.55
1:L:205:LYS:H	1:L:205:LYS:HD3	1.70	0.55
1:J:894:ASP:OD1	1:J:895:LEU:N	2.37	0.55
1:K:571:GLN:OE1	1:K:572:LYS:N	2.39	0.55
1:L:794:TYR:O	1:L:797:ARG:NH1	2.39	0.55
1:L:73:ARG:NE	1:L:80:TYR:OH	2.39	0.55
2:Z:519:ASP:N	2:Z:519:ASP:OD1	2.39	0.55
1:J:899:LEU:HB3	1:J:903:ASN:ND2	2.22	0.55
1:L:403:ASP:N	1:L:403:ASP:OD1	2.39	0.55
1:J:220:GLU:OE1	1:J:221:ALA:N	2.39	0.55
2:Z:89:TRP:CZ2	2:Z:115:ARG:HB2	2.42	0.55
2:Z:385:LYS:NZ	2:Z:396:GLU:OE1	2.35	0.55
1:K:643:ASN:OD1	1:K:643:ASN:N	2.33	0.55
1:J:390:PHE:CE2	1:J:392:MET:HB3	2.42	0.55
1:K:382:SER:O	1:K:383:ILE:C	2.48	0.55
1:J:409:ASN:ND2	1:J:527:LEU:HA	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:794:TYR:CE2	1:L:795:LYS:HG3	2.42	0.55
1:K:229:ARG:HH21	1:K:295:GLU:CD	2.15	0.54
1:L:119:THR:OG1	1:L:120:ALA:N	2.37	0.54
1:J:430:ASP:OD2	2:Z:10:LYS:HE3	2.07	0.54
1:K:532:SER:OG	1:K:537:ASP:OD1	2.25	0.54
1:L:275:THR:C	1:L:278:ASN:HB2	2.33	0.54
1:L:500:GLU:OE1	1:L:501:ILE:N	2.40	0.54
1:L:899:LEU:HD22	1:L:902:ALA:HB2	1.89	0.54
1:L:899:LEU:HD13	1:L:902:ALA:HB2	1.88	0.54
2:Z:100:ASN:N	2:Z:103:THR:OG1	2.37	0.54
2:Z:206:GLN:NE2	2:Z:575:ASP:OD2	2.33	0.54
1:J:274:SER:OG	1:J:275:THR:N	2.40	0.54
1:J:592:PHE:HE2	1:J:620:ILE:HD11	1.71	0.54
2:Z:275:SER:HB3	2:Z:536:ASN:HB3	1.90	0.54
1:J:95:ASP:OD2	1:L:786:GLN:NE2	2.41	0.54
1:J:203:ALA:HB1	1:J:208:GLN:HG3	1.90	0.54
1:K:753:LYS:HD2	1:K:767:ASN:HD21	1.72	0.54
1:L:55:ASP:N	1:L:55:ASP:OD1	2.41	0.54
2:Z:229:VAL:N	2:Z:247:TYR:OH	2.39	0.54
2:Z:336:VAL:HG22	2:Z:383:ILE:HG23	1.89	0.54
1:J:369:ASP:C	1:J:658:ASN:HD21	2.16	0.54
1:L:455:GLU:HG3	1:L:456:ARG:HG3	1.88	0.54
1:L:716:ASP:OD1	1:L:717:GLY:N	2.40	0.54
1:L:737:SER:OG	1:L:738:TRP:N	2.40	0.54
1:J:249:ASN:CG	1:J:253:GLY:H	2.12	0.54
1:J:341:GLY:O	1:J:593:ARG:NH1	2.41	0.54
1:K:376:TYR:CE1	1:K:380:LEU:HG	2.43	0.54
1:L:283:ALA:O	1:L:285:ALA:N	2.41	0.54
1:L:385:ASP:OD1	1:L:386:ARG:N	2.41	0.54
2:Z:402:GLU:HG3	2:Z:426:LYS:HA	1.89	0.54
1:J:175:PRO:HG3	1:L:847:GLN:HG2	1.88	0.54
1:K:537:ASP:OD2	1:K:870:LYS:NZ	2.28	0.54
1:L:595:ASP:OD2	1:L:598:MET:N	2.35	0.54
1:L:678:ASN:OD1	1:L:679:TRP:N	2.41	0.54
1:J:632:ASN:OD1	1:J:633:THR:N	2.39	0.54
1:L:73:ARG:HH21	1:L:620:ILE:HG22	1.72	0.54
1:K:170:VAL:N	1:L:457:ASN:OD1	2.40	0.54
1:K:785:TYR:O	1:K:786:GLN:NE2	2.41	0.54
1:K:207:TYR:O	1:K:208:GLN:HB2	2.08	0.54
1:K:618:ASP:OD1	1:K:618:ASP:N	2.40	0.54
1:L:672:ILE:HG13	1:L:910:MET:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:113:PHE:CE1	1:J:115:PRO:HD3	2.43	0.53
1:J:142:VAL:HG11	1:J:164:ASN:HB3	1.90	0.53
1:J:345:TYR:O	1:J:346:ASN:C	2.48	0.53
1:K:356:GLY:HA2	1:K:586:TYR:HD1	1.73	0.53
1:L:8:PRO:O	1:L:12:TYR:HB2	2.08	0.53
1:J:342:LEU:HD23	1:J:599:VAL:HG11	1.89	0.53
1:L:219:ASN:OD1	1:L:219:ASN:N	2.39	0.53
1:K:19:ASP:N	1:K:19:ASP:OD1	2.39	0.53
1:K:68:PHE:HB2	1:K:622:LEU:HB3	1.89	0.53
1:K:753:LYS:HD2	1:K:767:ASN:ND2	2.23	0.53
1:L:678:ASN:OD1	1:L:680:ALA:N	2.41	0.53
1:K:196:GLU:HB2	1:K:199:LYS:HD3	1.89	0.53
1:K:374:LEU:O	1:K:377:GLN:HB2	2.09	0.53
2:Z:296:ARG:HB2	2:Z:299:PHE:HB2	1.91	0.53
1:J:627:PHE:CD1	1:J:627:PHE:C	2.86	0.53
1:K:209:PRO:O	1:K:229:ARG:HD2	2.09	0.53
1:K:376:TYR:CD2	1:K:572:LYS:HG2	2.43	0.53
1:L:313:SER:OG	1:L:314:ASP:N	2.40	0.53
1:K:487:TYR:OH	1:K:545:HIS:ND1	2.35	0.53
1:L:642:ARG:NH1	1:L:939:HIS:O	2.42	0.53
1:J:116:TYR:CE1	1:L:858:ILE:CD1	2.90	0.53
1:J:670:VAL:HB	1:J:912:PHE:HB2	1.90	0.53
1:L:375:SER:O	1:L:376:TYR:C	2.49	0.53
2:Z:243:CYS:O	2:Z:409:ARG:NH2	2.31	0.53
1:K:375:SER:C	1:K:377:GLN:N	2.62	0.53
1:K:607:ASP:OD1	1:K:609:ARG:N	2.32	0.53
2:Z:467:THR:HB	2:Z:468:TRP:CD1	2.44	0.53
1:J:343:MET:HG2	1:J:592:PHE:HE1	1.70	0.53
1:K:362:ASN:OD1	1:K:364:VAL:N	2.39	0.53
1:K:686:ALA:HB3	1:K:926:LEU:HB2	1.91	0.53
2:Z:185:THR:HA	2:Z:243:CYS:HA	1.90	0.53
1:J:399:SER:H	1:J:547:ASN:ND2	2.07	0.53
1:J:433:GLN:CD	1:L:276:SER:HA	2.34	0.53
1:K:347:SER:OG	1:K:699:GLY:O	2.26	0.53
1:K:632:ASN:OD1	1:K:633:THR:N	2.43	0.53
1:K:173:GLN:OE1	1:K:173:GLN:N	2.43	0.52
2:Z:204:LYS:HE2	2:Z:205:HIS:CE1	2.44	0.52
2:Z:353:ILE:HD13	2:Z:359:LEU:HB2	1.90	0.52
1:J:196:GLU:OE2	1:J:199:LYS:HB2	2.09	0.52
1:L:111:PRO:N	1:L:561:ARG:HH21	2.07	0.52
1:J:743:ARG:HB3	1:K:64:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:674:ILE:HG22	1:L:675:PRO:HD2	1.91	0.52
2:Z:401:LEU:HD23	2:Z:425:LEU:HA	1.90	0.52
1:J:651:ASN:OD1	1:J:651:ASN:N	2.42	0.52
1:K:274:SER:O	1:L:433:GLN:N	2.36	0.52
1:J:409:ASN:HD22	1:J:527:LEU:HA	1.75	0.52
1:J:413:GLU:OE2	1:K:546:ARG:NH2	2.42	0.52
1:K:950:THR:O	1:K:953:SER:OG	2.27	0.52
1:L:131:ASN:OD1	1:L:131:ASN:N	2.34	0.52
1:L:401:ASP:HB3	1:L:404:VAL:HG23	1.91	0.52
2:Z:527:GLY:N	2:Z:545:VAL:HB	2.25	0.52
1:J:112:THR:O	1:J:112:THR:OG1	2.25	0.52
1:J:558:GLY:HA3	1:L:811:GLN:HE22	1.75	0.52
1:K:640:MET:HB3	1:L:28:LEU:HD13	1.91	0.52
1:L:274:SER:HB3	1:L:278:ASN:OD1	2.10	0.52
1:J:507:THR:OG1	1:J:508:TYR:N	2.42	0.52
1:J:694:GLU:O	1:J:706:TYR:OH	2.24	0.52
2:Z:10:LYS:O	2:Z:10:LYS:HG3	2.08	0.52
2:Z:351:SER:HB3	2:Z:528:PRO:HG3	1.91	0.52
2:Z:415:ASN:ND2	2:Z:500:ARG:O	2.29	0.52
1:J:743:ARG:O	1:K:64:LEU:HB2	2.10	0.52
1:K:210:GLU:O	1:K:211:PRO:C	2.51	0.52
1:K:829:GLN:O	1:L:212:GLN:NE2	2.37	0.52
1:L:814:ASP:H	1:L:865:SER:HA	1.74	0.52
1:L:855:TYR:HD1	1:L:856:PRO:HD2	1.75	0.52
2:Z:19:CGU:N	2:Z:19:CGU:CD1	2.73	0.52
1:J:399:SER:O	1:J:547:ASN:ND2	2.43	0.52
1:J:678:ASN:OD1	1:J:680:ALA:N	2.43	0.52
1:L:63:ARG:HG3	1:L:66:LEU:HD21	1.91	0.52
1:L:398:ASP:OD1	1:L:398:ASP:N	2.43	0.52
1:J:367:LEU:O	1:J:369:ASP:N	2.38	0.51
1:J:433:GLN:HG3	1:L:276:SER:HA	1.90	0.51
1:J:723:HIS:O	1:J:753:LYS:NZ	2.28	0.51
1:K:949:ARG:HG3	1:K:950:THR:O	2.11	0.51
1:L:352:GLY:HA3	1:L:590:TRP:CE3	2.45	0.51
1:J:611:ASP:OD1	1:J:611:ASP:N	2.43	0.51
1:J:625:THR:HG22	1:J:626:PHE:H	1.74	0.51
2:Z:74:ARG:HD2	2:Z:108:ASP:HB3	1.93	0.51
1:J:232:LYS:HG3	1:J:295:GLU:O	2.11	0.51
1:K:198:ASN:OD1	1:K:198:ASN:N	2.38	0.51
1:K:313:SER:OG	1:K:314:ASP:N	2.41	0.51
2:Z:85:GLU:O	2:Z:129:THR:OG1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:137:GLU:CD	2:Z:137:GLU:H	2.19	0.51
1:J:430:ASP:OD2	2:Z:10:LYS:HE2	2.09	0.51
1:J:703:ASP:OD1	1:J:705:TYR:HB2	2.10	0.51
1:K:132:SER:CB	1:K:230:VAL:HG23	2.41	0.51
1:K:275:THR:CB	1:K:277:VAL:HG13	2.41	0.51
1:K:332:TYR:HB2	1:K:603:SER:HB3	1.93	0.51
2:Z:9:ARG:HG3	2:Z:10:LYS:N	2.25	0.51
1:J:309:LYS:HG3	1:J:310:PRO:HD2	1.92	0.51
1:J:658:ASN:N	1:J:658:ASN:ND2	2.56	0.51
1:K:94:LEU:HD12	1:K:95:ASP:H	1.76	0.51
1:K:561:ARG:HG2	1:K:562:TYR:CE2	2.46	0.51
1:L:682:PHE:CE1	1:L:927:PHE:HB3	2.45	0.51
2:Z:147:GLN:HG2	2:Z:148:VAL:H	1.75	0.51
1:J:804:ASN:OD1	1:J:804:ASN:N	2.43	0.51
1:L:382:SER:O	1:L:384:GLY:N	2.44	0.51
2:Z:48:GLU:OE1	2:Z:51:ARG:NH2	2.43	0.51
1:J:280:MET:HB3	2:Z:52:THR:HG21	1.93	0.51
1:J:904:SER:OG	1:J:905:ALA:N	2.39	0.51
1:K:759:GLU:OE2	1:L:104:ARG:NE	2.44	0.51
1:K:208:GLN:O	1:K:229:ARG:NH1	2.44	0.51
1:K:405:ARG:NH2	1:K:874:ASP:OD2	2.40	0.51
2:Z:385:LYS:NZ	2:Z:387:SER:O	2.42	0.51
2:Z:461:TRP:H	2:Z:524:ASP:CG	2.18	0.51
2:Z:552:ASP:N	2:Z:552:ASP:OD1	2.43	0.51
1:J:371:ASN:CG	1:J:371:ASN:O	2.54	0.51
1:K:138:ASP:N	1:K:138:ASP:OD1	2.41	0.51
1:K:379:LEU:O	1:K:383:ILE:HG23	2.11	0.51
1:L:379:LEU:O	1:L:383:ILE:HG23	2.11	0.51
2:Z:95:HIS:NE2	2:Z:128:THR:O	2.41	0.51
2:Z:314:GLU:HA	2:Z:455:LYS:HE3	1.92	0.51
1:J:105:GLY:HA2	1:J:618:ASP:OD1	2.11	0.50
1:J:239:PRO:O	1:J:243:SER:OG	2.28	0.50
1:J:528:GLY:O	1:K:559:ASN:ND2	2.42	0.50
1:K:794:TYR:O	1:K:797:ARG:NH1	2.43	0.50
1:L:90:ASP:OD1	1:L:90:ASP:N	2.44	0.50
1:L:261:ASN:OD1	1:L:261:ASN:N	2.44	0.50
1:L:829:GLN:HA	1:L:852:ASN:HD21	1.76	0.50
1:J:623:TYR:O	1:J:624:ALA:HB2	2.09	0.50
1:J:627:PHE:C	1:J:627:PHE:HD1	2.19	0.50
1:K:275:THR:CA	1:K:277:VAL:HG13	2.41	0.50
1:K:375:SER:OG	1:K:654:LEU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:503:ASP:OD1	1:K:503:ASP:N	2.37	0.50
1:K:924:TYR:CZ	1:K:926:LEU:HD11	2.46	0.50
1:L:347:SER:C	1:L:349:GLY:N	2.65	0.50
1:J:401:ASP:OD1	1:J:403:ASP:N	2.39	0.50
1:J:432:TYR:CD1	1:L:275:THR:HA	2.47	0.50
1:L:345:TYR:O	1:L:346:ASN:C	2.54	0.50
1:L:657:ALA:O	1:L:658:ASN:CG	2.54	0.50
2:Z:140:ILE:O	2:Z:149:THR:HG23	2.12	0.50
1:L:182:ASN:ND2	1:L:202:TYR:OH	2.37	0.50
1:L:561:ARG:NH1	1:L:562:TYR:OH	2.44	0.50
1:J:248:THR:OG1	1:J:253:GLY:O	2.25	0.50
1:J:527:LEU:HD21	1:K:116:TYR:CE2	2.47	0.50
1:K:96:MET:O	1:K:98:SER:N	2.43	0.50
1:L:286:ILE:HD13	1:L:286:ILE:H	1.77	0.50
1:J:279:ALA:O	1:J:280:MET:C	2.53	0.50
1:J:307:SER:HB3	1:J:326:MET:HB2	1.94	0.50
1:K:654:LEU:O	1:K:655:SER:HB2	2.10	0.50
1:J:94:LEU:HB2	1:J:626:PHE:HE1	1.76	0.50
1:J:579:LEU:HG	1:J:580:LEU:N	2.26	0.50
1:J:854:PRO:HG2	1:K:121:TYR:CE1	2.47	0.50
1:K:430:ASP:O	1:K:431:THR:C	2.53	0.50
1:K:510:TYR:OH	1:K:514:ARG:NH1	2.45	0.50
1:K:595:ASP:OD2	1:K:598:MET:N	2.32	0.50
1:L:204:ASP:N	1:L:208:GLN:HG3	2.26	0.50
1:L:722:ASN:HB3	1:L:878:TRP:HE1	1.77	0.50
2:Z:312:LEU:HD13	2:Z:454:TYR:HE1	1.76	0.50
1:K:276:SER:HB3	1:L:433:GLN:CB	2.36	0.50
1:L:687:PHE:CE1	1:L:878:TRP:HB2	2.46	0.50
1:J:334:ALA:HB2	1:J:554:SER:HA	1.94	0.50
1:J:495:ASN:N	1:J:495:ASN:OD1	2.44	0.50
2:Z:66:ALA:HB1	2:Z:70:GLY:HA2	1.94	0.50
1:J:316:ASN:OD1	1:J:316:ASN:N	2.45	0.49
1:J:689:ARG:NH1	1:J:724:THR:OG1	2.40	0.49
1:K:463:ASN:OD1	1:K:463:ASN:N	2.44	0.49
1:L:83:ARG:NH2	1:L:589:GLU:OE1	2.44	0.49
1:L:544:HIS:O	1:L:603:SER:HB2	2.12	0.49
2:Z:39:VAL:HG12	2:Z:43:LYS:HE3	1.93	0.49
1:J:368:GLN:C	1:J:369:ASP:CG	2.80	0.49
1:J:595:ASP:CG	1:J:597:ASN:H	2.20	0.49
1:K:223:SER:OG	1:K:224:SER:N	2.45	0.49
1:K:284:ASN:O	1:K:286:ILE:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:738:TRP:CE3	1:K:739:PRO:HD3	2.47	0.49
1:K:883:SER:OG	1:K:886:PHE:N	2.45	0.49
1:L:474:ASN:O	1:L:478:ASN:ND2	2.32	0.49
1:L:642:ARG:NH1	1:L:938:PRO:O	2.45	0.49
2:Z:306:ASP:OD1	2:Z:309:GLU:N	2.45	0.49
1:J:91:ASN:OD1	1:J:91:ASN:N	2.43	0.49
1:J:136:ASP:OD2	1:J:233:LYS:NZ	2.31	0.49
1:J:182:ASN:ND2	1:J:184:ASN:OD1	2.46	0.49
1:J:276:SER:OG	1:K:431:THR:HG22	2.12	0.49
1:J:716:ASP:OD1	1:J:718:THR:N	2.28	0.49
1:K:116:TYR:HE2	1:K:119:THR:HA	1.77	0.49
1:L:694:GLU:HB3	1:L:708:TYR:CD2	2.47	0.49
2:Z:226:GLU:OE2	2:Z:443:ARG:NH1	2.45	0.49
1:K:935:VAL:HG22	1:K:945:THR:HG22	1.93	0.49
1:L:73:ARG:HH22	1:L:619:SER:HA	1.76	0.49
1:L:112:THR:O	1:L:112:THR:OG1	2.26	0.49
1:L:507:THR:OG1	1:L:508:TYR:N	2.45	0.49
1:J:344:TYR:HE1	1:J:593:ARG:NE	2.10	0.49
1:J:371:ASN:HD21	1:J:374:LEU:HB2	1.78	0.49
1:K:275:THR:HB	1:K:277:VAL:CG1	2.42	0.49
1:K:277:VAL:HG23	2:Z:25:CGU:OE22	2.13	0.49
2:Z:248:CYS:HB2	2:Z:250:GLU:HG3	1.95	0.49
2:Z:527:GLY:H	2:Z:545:VAL:HB	1.77	0.49
1:J:218:TRP:CE2	1:J:219:ASN:HB3	2.47	0.49
1:J:540:ASN:ND2	1:J:542:PHE:H	2.11	0.49
1:J:642:ARG:NH1	1:J:939:HIS:O	2.45	0.49
1:J:109:ARG:NH2	1:J:560:GLY:O	2.23	0.49
1:J:584:GLY:HA3	1:J:586:TYR:CZ	2.46	0.49
1:K:811:GLN:NE2	1:L:560:GLY:H	2.11	0.49
2:Z:441:PRO:HG3	2:Z:542:MET:SD	2.52	0.49
1:J:42:ASN:OD1	1:J:42:ASN:N	2.46	0.49
1:L:464:ASN:N	1:L:464:ASN:OD1	2.45	0.49
1:L:692:THR:O	1:L:694:GLU:N	2.45	0.49
1:L:935:VAL:HG22	1:L:945:THR:HG22	1.95	0.49
2:Z:13:LEU:O	2:Z:17:CYS:HB2	2.12	0.49
1:J:864:ASP:OD1	1:J:864:ASP:N	2.44	0.49
1:K:657:ALA:O	1:K:658:ASN:CG	2.56	0.49
1:L:218:TRP:CZ3	1:L:424:GLY:HA3	2.47	0.49
1:J:283:ALA:C	1:J:285:ALA:N	2.70	0.49
1:J:540:ASN:OD1	1:J:543:ASN:N	2.30	0.49
1:K:362:ASN:CG	1:K:364:VAL:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:636:THR:O	1:K:640:MET:HG2	2.13	0.49
2:Z:13:LEU:HD22	2:Z:31:LEU:HD21	1.95	0.49
2:Z:93:TYR:HB2	2:Z:468:TRP:HE3	1.77	0.49
1:K:373:GLU:O	1:K:374:LEU:C	2.53	0.48
1:L:184:ASN:OD1	1:L:184:ASN:N	2.37	0.48
1:L:440:GLY:H	1:L:445:THR:HG23	1.77	0.48
1:L:544:HIS:CG	1:L:545:HIS:H	2.31	0.48
2:Z:441:PRO:CD	2:Z:540:TYR:HB3	2.32	0.48
1:J:20:ALA:HB2	1:J:47:ASN:HB3	1.95	0.48
1:J:68:PHE:CE2	1:J:86:LEU:HD12	2.47	0.48
1:J:344:TYR:CE1	1:J:593:ARG:NE	2.81	0.48
1:J:529:ALA:HB2	1:K:559:ASN:ND2	2.29	0.48
1:J:771:ASP:N	1:J:771:ASP:OD1	2.45	0.48
1:K:174:ALA:HB1	1:K:227:GLY:O	2.13	0.48
1:L:101:PHE:O	1:L:568:GLN:HA	2.13	0.48
1:L:459:ILE:HG22	1:L:460:GLY:H	1.78	0.48
1:L:708:TYR:CE1	1:L:710:GLY:HA3	2.48	0.48
1:L:830:HIS:H	1:L:852:ASN:CG	2.21	0.48
1:J:249:ASN:CG	1:J:251:ASN:H	2.22	0.48
1:J:571:GLN:OE1	1:J:573:PHE:N	2.30	0.48
1:J:737:SER:OG	1:J:739:PRO:O	2.31	0.48
1:L:760:GLY:O	1:L:770:LYS:NZ	2.46	0.48
2:Z:383:ILE:O	2:Z:396:GLU:HA	2.13	0.48
1:L:62:GLN:OE1	1:L:92:ARG:NH1	2.46	0.48
1:L:114:LYS:NZ	1:L:116:TYR:O	2.27	0.48
1:L:831:ASN:OD1	1:L:832:ASN:ND2	2.46	0.48
1:J:759:GLU:OE1	1:J:762:ASN:ND2	2.47	0.48
1:K:208:GLN:C	1:K:209:PRO:O	2.57	0.48
1:L:366:ASP:OD1	1:L:367:LEU:N	2.46	0.48
1:L:577:LYS:NZ	1:L:578:ASN:OD1	2.46	0.48
1:K:20:ALA:HA	1:K:23:TYR:CE2	2.47	0.48
1:K:275:THR:C	1:K:277:VAL:H	2.17	0.48
1:K:351:MET:HE2	1:K:366:ASP:HB3	1.96	0.48
1:K:689:ARG:O	1:K:690:LEU:HD23	2.14	0.48
2:Z:93:TYR:HB2	2:Z:468:TRP:CE3	2.47	0.48
1:J:355:ALA:O	1:J:586:TYR:HB3	2.13	0.48
1:J:704:PRO:HG2	1:J:705:TYR:CD1	2.49	0.48
1:K:276:SER:HA	1:L:433:GLN:HB2	1.95	0.48
1:K:309:LYS:HD3	1:K:498:ASN:O	2.13	0.48
1:K:590:TRP:CD1	1:K:591:ASN:H	2.32	0.48
1:L:371:ASN:H	1:L:658:ASN:ND2	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:771:ASP:N	1:L:771:ASP:OD1	2.47	0.48
2:Z:295:LEU:HA	2:Z:300:GLU:HG2	1.95	0.48
1:J:794:TYR:CE1	1:J:795:LYS:HG3	2.49	0.48
1:K:677:ARG:HG2	1:K:678:ASN:O	2.13	0.48
1:L:658:ASN:C	1:L:659:MET:SD	2.97	0.48
2:Z:404:ILE:HG23	2:Z:423:MET:HG2	1.96	0.48
1:J:204:ASP:N	1:J:208:GLN:OE1	2.40	0.48
1:J:344:TYR:HE1	1:J:593:ARG:HE	1.60	0.48
1:J:607:ASP:OD1	1:J:609:ARG:N	2.47	0.48
1:J:843:MET:HE1	1:K:218:TRP:HA	1.96	0.48
1:J:7:MET:N	1:J:8:PRO:HD2	2.29	0.48
1:J:91:ASN:HD22	1:J:631:HIS:CG	2.32	0.48
1:J:419:TYR:HD1	1:J:468:GLU:HB2	1.79	0.48
1:K:37:THR:OG1	1:K:38:TYR:N	2.45	0.48
1:L:379:LEU:O	1:L:380:LEU:C	2.53	0.48
2:Z:545:VAL:HA	2:Z:560:TYR:HD1	1.79	0.48
1:K:275:THR:HB	1:K:277:VAL:CB	2.44	0.47
1:L:176:PHE:HD2	1:L:209:PRO:HB3	1.79	0.47
1:L:205:LYS:HB2	1:L:268:VAL:HG11	1.95	0.47
1:L:381:ASP:CG	1:L:382:SER:N	2.67	0.47
1:L:948:LEU:HG	1:L:949:ARG:H	1.78	0.47
2:Z:38:ASP:HA	2:Z:41:TRP:HB3	1.96	0.47
1:J:369:ASP:CB	1:J:658:ASN:ND2	2.77	0.47
1:J:814:ASP:CG	1:J:816:THR:H	2.21	0.47
1:L:283:ALA:C	1:L:285:ALA:H	2.22	0.47
1:L:929:VAL:HG12	1:L:951:PRO:HD2	1.97	0.47
1:J:62:GLN:HG3	1:J:92:ARG:HH22	1.79	0.47
1:J:404:VAL:HG11	1:J:544:HIS:CD2	2.50	0.47
1:J:777:MET:HE3	1:J:777:MET:HB3	1.83	0.47
1:J:831:ASN:OD1	1:J:832:ASN:N	2.48	0.47
1:K:309:LYS:HB3	1:K:498:ASN:HB2	1.95	0.47
1:K:507:THR:OG1	1:K:508:TYR:N	2.47	0.47
1:K:794:TYR:CZ	1:K:795:LYS:HG3	2.49	0.47
1:L:708:TYR:CZ	1:L:710:GLY:HA3	2.49	0.47
1:L:898:ASN:O	1:L:899:LEU:HD12	2.14	0.47
1:J:357:GLN:HB2	1:J:585:SER:O	2.13	0.47
1:J:408:GLU:HB3	1:J:410:HIS:HE1	1.79	0.47
1:K:91:ASN:OD1	1:K:91:ASN:N	2.48	0.47
1:K:368:GLN:O	1:K:369:ASP:C	2.57	0.47
1:L:3:THR:HG21	1:L:7:MET:HB2	1.97	0.47
1:L:373:GLU:O	1:L:374:LEU:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:522:ASP:OD1	1:L:523:CYS:N	2.43	0.47
2:Z:14:CGU:HA	2:Z:18:VAL:HG23	1.95	0.47
1:K:829:GLN:HA	1:K:852:ASN:HD21	1.80	0.47
1:K:831:ASN:OD1	1:K:832:ASN:N	2.47	0.47
1:L:176:PHE:CD2	1:L:209:PRO:HB3	2.50	0.47
1:L:351:MET:SD	1:L:366:ASP:HB3	2.54	0.47
1:L:672:ILE:HD11	1:L:912:PHE:HE2	1.80	0.47
2:Z:225:ASP:CG	2:Z:568:LYS:HB2	2.39	0.47
1:J:49:THR:HG1	1:L:891:ALA:H	1.60	0.47
1:J:625:THR:O	1:J:626:PHE:CD1	2.67	0.47
1:K:651:ASN:OD1	1:K:932:VAL:HG13	2.15	0.47
1:K:830:HIS:HB3	1:L:212:GLN:NE2	2.30	0.47
1:L:73:ARG:NH2	1:L:618:ASP:O	2.47	0.47
1:L:187:GLN:HG3	1:L:200:GLU:HB3	1.95	0.47
1:L:275:THR:HG23	1:L:278:ASN:CG	2.40	0.47
1:L:373:GLU:C	1:L:375:SER:N	2.69	0.47
1:L:450:ASP:OD2	1:L:453:PHE:N	2.31	0.47
1:J:266:SER:OG	1:J:267:GLN:N	2.47	0.47
1:J:283:ALA:C	1:J:285:ALA:H	2.23	0.47
1:J:590:TRP:HD1	1:J:591:ASN:N	2.07	0.47
1:K:96:MET:O	1:K:99:THR:N	2.48	0.47
1:K:232:LYS:HD2	1:K:295:GLU:C	2.40	0.47
1:K:771:ASP:OD1	1:K:772:TRP:N	2.47	0.47
1:L:804:ASN:O	1:L:873:CYS:HA	2.15	0.47
2:Z:18:VAL:HG12	2:Z:19:CGU:OE12	2.12	0.47
2:Z:56:LYS:HD2	2:Z:56:LYS:HA	1.66	0.47
1:J:597:ASN:ND2	1:J:706:TYR:O	2.47	0.47
1:K:437:ALA:HA	1:K:447:TRP:HZ3	1.80	0.47
1:L:707:THR:OG1	1:L:708:TYR:N	2.45	0.47
1:K:266:SER:OG	1:K:267:GLN:N	2.46	0.47
1:K:659:MET:N	1:K:659:MET:SD	2.87	0.47
1:L:398:ASP:OD1	1:L:553:ARG:NH2	2.48	0.47
1:L:804:ASN:ND2	1:L:875:ARG:HB3	2.30	0.47
2:Z:67:GLU:HB2	2:Z:72:ASN:CG	2.40	0.47
2:Z:74:ARG:NH2	2:Z:107:ALA:HA	2.30	0.47
1:J:137:GLU:OE1	1:J:169:HIS:NE2	2.47	0.47
1:J:696:PRO:HB3	1:J:706:TYR:CE2	2.50	0.47
1:K:111:PRO:HG2	1:K:112:THR:HG22	1.97	0.47
1:K:176:PHE:CD2	1:K:209:PRO:HB3	2.50	0.47
1:K:538:ASN:HD22	1:K:917:MET:HE3	1.80	0.47
1:L:5:SER:OG	1:L:6:MET:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:56:VAL:O	1:J:630:ALA:N	2.37	0.46
1:J:230:VAL:O	1:J:294:SER:HA	2.15	0.46
1:K:527:LEU:HD21	1:L:116:TYR:CD1	2.51	0.46
1:L:687:PHE:HB3	1:L:925:VAL:HG22	1.96	0.46
2:Z:456:GLY:HA3	2:Z:529:PHE:CZ	2.50	0.46
1:J:94:LEU:HD13	1:J:626:PHE:CE1	2.49	0.46
1:K:280:MET:HG3	2:Z:24:TYR:OH	2.15	0.46
1:K:430:ASP:HB2	1:K:432:TYR:CZ	2.50	0.46
1:K:688:THR:OG1	1:K:689:ARG:N	2.48	0.46
1:L:133:CYS:SG	1:L:237:MET:HE2	2.55	0.46
1:L:347:SER:O	1:L:349:GLY:N	2.48	0.46
1:L:379:LEU:HD13	1:L:653:TYR:HB2	1.97	0.46
2:Z:118:ASP:OD2	2:Z:120:SER:HB2	2.15	0.46
2:Z:410:TYR:CE1	2:Z:412:TRP:HB3	2.50	0.46
1:L:229:ARG:NE	1:L:295:GLU:OE2	2.28	0.46
2:Z:73:TYR:O	2:Z:74:ARG:NH1	2.41	0.46
1:J:101:PHE:CD2	1:J:592:PHE:HZ	2.33	0.46
1:K:437:ALA:HB1	1:K:439:ASN:HD21	1.80	0.46
1:L:75:ASP:OD1	1:L:76:THR:N	2.49	0.46
1:L:254:GLN:HB2	1:L:297:VAL:HG12	1.98	0.46
1:L:698:LEU:HD23	1:L:698:LEU:HA	1.76	0.46
2:Z:19:CGU:OE11	2:Z:54:ARG:HB3	2.16	0.46
2:Z:457:ARG:NE	2:Z:484:ASN:OD1	2.49	0.46
1:J:138:ASP:HA	1:J:166:LYS:HG2	1.97	0.46
1:J:874:ASP:OD1	1:J:874:ASP:N	2.48	0.46
1:K:561:ARG:HG2	1:K:562:TYR:CZ	2.51	0.46
1:L:371:ASN:C	1:L:373:GLU:N	2.73	0.46
1:J:138:ASP:OD1	1:J:138:ASP:N	2.48	0.46
1:L:534:ASP:OD1	1:L:534:ASP:N	2.48	0.46
2:Z:545:VAL:HA	2:Z:560:TYR:CD1	2.50	0.46
1:J:274:SER:O	1:K:432:TYR:HB3	2.15	0.46
1:J:521:VAL:HG13	1:J:525:ILE:HG21	1.97	0.46
1:K:522:ASP:HB3	1:K:524:TYR:CE2	2.51	0.46
1:L:104:ARG:HB2	1:L:619:SER:OG	2.15	0.46
1:L:420:CYS:SG	1:L:467:MET:HB2	2.56	0.46
2:Z:95:HIS:CE1	2:Z:131:PRO:HA	2.50	0.46
1:J:559:ASN:HB3	1:L:528:GLY:O	2.15	0.46
1:K:270:MET:SD	1:K:293:TYR:HE1	2.38	0.46
1:K:282:GLU:OE1	1:K:283:ALA:N	2.49	0.46
1:L:375:SER:O	1:L:377:GLN:N	2.49	0.46
1:J:540:ASN:HB2	1:J:720:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:732:PHE:HB2	1:J:736:VAL:HG23	1.97	0.46
1:K:89:GLY:HA3	1:K:92:ARG:HE	1.81	0.46
1:K:380:LEU:HD23	1:K:380:LEU:HA	1.59	0.46
1:K:606:ASN:OD1	1:K:606:ASN:N	2.49	0.46
1:K:949:ARG:NH1	1:K:952:PHE:O	2.48	0.46
1:L:351:MET:HE2	1:L:351:MET:HB2	1.75	0.46
1:J:122:ASN:HA	1:L:832:ASN:CG	2.41	0.46
1:J:660:LEU:HD12	1:J:660:LEU:H	1.80	0.46
1:J:703:ASP:C	1:J:705:TYR:N	2.73	0.46
1:L:60:ARG:HH21	1:L:631:HIS:CE1	2.34	0.46
1:L:659:MET:SD	1:L:659:MET:N	2.89	0.46
1:L:825:GLY:O	1:L:829:GLN:HG3	2.17	0.46
2:Z:363:HIS:HB3	2:Z:416:LEU:HD22	1.98	0.46
1:J:116:TYR:HB3	1:L:527:LEU:HG	1.96	0.45
1:J:182:ASN:HD21	1:J:184:ASN:CG	2.24	0.45
1:J:313:SER:OG	1:J:315:ASP:OD1	2.34	0.45
1:K:336:ARG:HH12	1:K:712:ILE:HG13	1.81	0.45
1:K:757:ASP:OD1	1:K:757:ASP:N	2.47	0.45
1:K:889:MET:HE3	1:K:889:MET:HB2	1.85	0.45
1:L:847:GLN:HB2	1:L:848:ALA:H	1.50	0.45
1:L:876:THR:OG1	1:L:877:LEU:N	2.49	0.45
1:J:134:GLU:HB3	1:J:170:VAL:HG13	1.98	0.45
1:J:542:PHE:CE1	1:J:718:THR:HB	2.51	0.45
1:J:690:LEU:HD22	1:J:713:PRO:HB2	1.98	0.45
1:J:714:TYR:O	1:J:715:LEU:HD23	2.17	0.45
1:K:521:VAL:HG13	1:K:525:ILE:HG21	1.98	0.45
1:K:832:ASN:HD21	1:L:123:ALA:H	1.64	0.45
1:L:502:SER:OG	1:L:503:ASP:N	2.49	0.45
2:Z:19:CGU:HB2	2:Z:54:ARG:CZ	2.47	0.45
2:Z:404:ILE:HG12	2:Z:423:MET:HG2	1.98	0.45
1:J:556:LEU:HA	1:J:556:LEU:HD23	1.69	0.45
1:K:105:GLY:HA2	1:K:618:ASP:CG	2.41	0.45
1:K:215:GLU:OE1	1:K:215:GLU:N	2.26	0.45
1:K:371:ASN:HB2	1:K:658:ASN:HD21	1.80	0.45
1:K:885:ASN:N	1:K:885:ASN:OD1	2.49	0.45
1:L:811:GLN:N	1:L:811:GLN:OE1	2.49	0.45
2:Z:99:ILE:HG22	2:Z:117:PRO:HB2	1.99	0.45
1:K:819:LYS:HG3	1:K:820:ASP:OD1	2.16	0.45
1:L:346:ASN:HD21	1:L:371:ASN:HA	1.82	0.45
2:Z:77:VAL:O	2:Z:114:CYS:N	2.40	0.45
1:J:488:LEU:HD23	1:J:488:LEU:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:599:VAL:HG23	1:K:600:LEU:HG	1.99	0.45
1:K:811:GLN:HE22	1:L:558:GLY:HA3	1.81	0.45
1:L:229:ARG:HH21	1:L:295:GLU:CD	2.25	0.45
1:L:677:ARG:NE	1:L:952:PHE:CE1	2.85	0.45
1:L:722:ASN:HB3	1:L:878:TRP:NE1	2.32	0.45
2:Z:110:GLN:HG2	2:Z:115:ARG:HH21	1.81	0.45
2:Z:457:ARG:N	2:Z:530:VAL:O	2.48	0.45
1:J:421:PHE:CZ	1:K:835:PHE:HD1	2.35	0.45
1:J:557:LEU:HA	1:J:557:LEU:HD23	1.69	0.45
1:J:835:PHE:HD2	1:L:421:PHE:CZ	2.34	0.45
1:K:277:VAL:HB	2:Z:25:CGU:OE22	2.16	0.45
1:L:694:GLU:CB	1:L:708:TYR:CZ	2.98	0.45
1:L:781:TYR:OH	1:L:796:ASP:OD2	2.24	0.45
2:Z:6:CGU:C	2:Z:8:VAL:H	2.29	0.45
2:Z:508:ALA:HB3	2:Z:560:TYR:CE2	2.50	0.45
1:J:426:ILE:HD12	1:L:171:TYR:HE1	1.81	0.45
1:K:309:LYS:O	1:K:498:ASN:ND2	2.49	0.45
1:L:275:THR:HG23	1:L:278:ASN:OD1	2.17	0.45
1:L:331:ASN:OD1	1:L:603:SER:OG	2.31	0.45
1:L:456:ARG:NH1	2:Z:32:CGU:OE22	2.50	0.45
1:L:467:MET:HE3	1:L:467:MET:HB3	1.81	0.45
1:J:369:ASP:N	1:J:369:ASP:OD2	2.50	0.45
1:J:580:LEU:O	1:J:581:LEU:HB2	2.16	0.45
1:J:595:ASP:OD2	1:J:598:MET:N	2.42	0.45
1:K:280:MET:SD	1:K:280:MET:N	2.88	0.45
1:K:431:THR:CG2	1:K:456:ARG:HB3	2.47	0.45
1:K:467:MET:HG2	1:L:467:MET:HE2	1.98	0.45
1:K:811:GLN:HE22	1:L:558:GLY:C	2.25	0.45
1:J:101:PHE:O	1:J:568:GLN:HA	2.17	0.45
1:J:231:LEU:HD21	1:L:849:TYR:CE1	2.52	0.45
1:J:590:TRP:CD1	1:J:591:ASN:N	2.82	0.45
1:J:688:THR:OG1	1:J:689:ARG:N	2.45	0.45
1:K:105:GLY:HA2	1:K:618:ASP:OD1	2.17	0.45
1:K:401:ASP:OD1	1:K:403:ASP:N	2.41	0.45
2:Z:62:GLU:OE2	2:Z:64:ASN:ND2	2.50	0.45
2:Z:87:GLN:HB2	2:Z:93:TYR:O	2.16	0.45
1:J:10:TRP:N	1:J:10:TRP:CD1	2.85	0.45
1:J:342:LEU:HD23	1:J:599:VAL:CG1	2.47	0.45
1:K:369:ASP:O	1:K:658:ASN:HB2	2.17	0.45
1:L:344:TYR:O	1:L:345:TYR:CG	2.70	0.45
1:L:708:TYR:CD2	1:L:709:SER:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:829:GLN:HA	1:L:852:ASN:ND2	2.32	0.45
1:L:857:LEU:HD23	1:L:857:LEU:HA	1.77	0.45
2:Z:223:ASP:OD1	2:Z:223:ASP:N	2.40	0.45
1:J:804:ASN:HD22	1:J:875:ARG:HB3	1.82	0.44
1:K:414:ASP:N	1:K:414:ASP:OD1	2.49	0.44
1:K:622:LEU:HD12	1:K:623:TYR:H	1.82	0.44
1:L:283:ALA:C	1:L:285:ALA:N	2.73	0.44
1:L:622:LEU:HD12	1:L:623:TYR:H	1.83	0.44
1:J:713:PRO:HA	1:J:716:ASP:OD1	2.18	0.44
1:K:568:GLN:N	1:K:568:GLN:OE1	2.49	0.44
1:K:796:ASP:OD1	1:K:800:SER:OG	2.28	0.44
1:L:207:TYR:O	1:L:207:TYR:CG	2.69	0.44
1:L:345:TYR:HB3	1:L:346:ASN:OD1	2.17	0.44
1:L:918:ASP:N	1:L:918:ASP:OD1	2.48	0.44
1:J:277:VAL:CB	1:J:280:MET:HG3	2.30	0.44
1:J:527:LEU:HD21	1:K:116:TYR:CZ	2.52	0.44
1:J:657:ALA:C	1:J:658:ASN:CG	2.84	0.44
1:J:703:ASP:CG	1:J:705:TYR:H	2.26	0.44
1:K:256:VAL:HG23	1:K:296:ASP:O	2.17	0.44
1:K:778:LEU:HD23	1:K:783:ILE:O	2.17	0.44
1:L:695:THR:H	1:L:706:TYR:HE1	1.64	0.44
1:L:848:ALA:O	1:L:849:TYR:HB2	2.17	0.44
1:J:190:THR:HA	1:J:201:ILE:HG13	1.99	0.44
1:J:204:ASP:H	1:J:208:GLN:CD	2.25	0.44
1:J:607:ASP:O	1:J:608:LEU:HD23	2.17	0.44
1:K:504:ASN:HD22	1:K:507:THR:HG22	1.82	0.44
2:Z:215:VAL:HG12	2:Z:216:GLU:H	1.81	0.44
2:Z:420:ILE:HD13	2:Z:566:LEU:HD21	1.99	0.44
1:K:526:ASN:OD1	1:K:810:ARG:NH1	2.50	0.44
1:K:550:LEU:HD12	1:K:550:LEU:HA	1.71	0.44
1:L:740:GLY:O	1:L:743:ARG:HG2	2.18	0.44
2:Z:12:ASN:OD1	2:Z:13:LEU:N	2.51	0.44
1:J:582:LEU:HG	1:J:937:GLN:OE1	2.18	0.44
1:J:751:GLU:O	1:J:769:THR:OG1	2.29	0.44
1:J:770:LYS:HE2	1:K:623:TYR:HE2	1.83	0.44
1:K:678:ASN:OD1	1:K:679:TRP:N	2.50	0.44
1:K:762:ASN:ND2	1:K:767:ASN:HA	2.32	0.44
1:L:568:GLN:OE1	1:L:568:GLN:N	2.51	0.44
1:L:766:CYS:SG	1:L:768:MET:N	2.84	0.44
2:Z:433:ASP:OD1	2:Z:433:ASP:N	2.50	0.44
1:J:333:ILE:HA	1:J:601:GLN:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:411:GLY:HA3	1:K:117:SER:O	2.18	0.44
1:L:682:PHE:HE1	1:L:927:PHE:HB3	1.83	0.44
1:L:708:TYR:CD2	1:L:708:TYR:C	2.96	0.44
2:Z:127:TYR:HA	2:Z:134:ARG:O	2.18	0.44
1:J:627:PHE:CD1	1:J:628:PRO:HD2	2.53	0.44
1:K:187:GLN:NE2	1:K:190:THR:HG1	2.16	0.44
1:K:759:GLU:HG3	1:L:104:ARG:NH2	2.33	0.44
1:K:804:ASN:O	1:K:873:CYS:HA	2.18	0.44
1:L:531:TRP:CE3	1:L:810:ARG:HB3	2.53	0.44
1:L:579:LEU:HG	1:L:580:LEU:N	2.33	0.44
1:L:704:PRO:HG2	1:L:705:TYR:CD1	2.53	0.44
2:Z:173:ASP:OD1	2:Z:173:ASP:N	2.50	0.44
1:J:703:ASP:O	1:J:705:TYR:N	2.51	0.43
1:K:131:ASN:HD21	1:K:240:CYS:N	2.15	0.43
1:K:522:ASP:O	1:K:525:ILE:HG22	2.18	0.43
1:K:814:ASP:OD1	1:K:816:THR:N	2.35	0.43
1:L:680:ALA:O	1:L:951:PRO:HD3	2.18	0.43
2:Z:14:CGU:HG	2:Z:15:ARG:N	2.26	0.43
2:Z:133:VAL:HG11	2:Z:136:GLN:HB2	1.99	0.43
1:K:173:GLN:HA	1:L:459:ILE:HG22	1.99	0.43
1:K:903:ASN:OD1	1:K:903:ASN:N	2.51	0.43
1:L:279:ALA:O	1:L:280:MET:HB3	2.17	0.43
1:J:370:ARG:O	1:J:371:ASN:C	2.59	0.43
1:J:426:ILE:HD12	1:L:171:TYR:CE1	2.53	0.43
1:J:574:PHE:CG	1:J:575:ALA:N	2.86	0.43
1:K:94:LEU:HD12	1:K:95:ASP:N	2.33	0.43
1:L:290:LEU:HA	1:L:290:LEU:HD12	1.67	0.43
2:Z:86:CYS:HB2	2:Z:112:ASN:O	2.19	0.43
2:Z:93:TYR:HD1	2:Z:468:TRP:HZ3	1.66	0.43
1:J:261:ASN:OD1	1:J:261:ASN:N	2.51	0.43
1:J:763:VAL:HG12	1:J:768:MET:O	2.17	0.43
1:K:649:SER:O	1:K:650:PHE:CD1	2.71	0.43
1:L:377:GLN:O	1:L:379:LEU:N	2.52	0.43
1:L:685:TRP:HD1	1:L:927:PHE:HD1	1.66	0.43
2:Z:3:THR:O	2:Z:6:CGU:N	2.51	0.43
2:Z:382:ARG:HB3	2:Z:385:LYS:HD2	2.01	0.43
1:J:19:ASP:OD1	1:J:19:ASP:N	2.50	0.43
1:K:371:ASN:CG	1:K:372:THR:H	2.26	0.43
1:K:688:THR:HG21	1:K:719:PHE:CE2	2.54	0.43
1:L:708:TYR:CE1	1:L:710:GLY:N	2.82	0.43
1:L:780:ASN:HD22	1:L:780:ASN:C	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:87:GLN:HA	2:Z:129:THR:HG23	2.00	0.43
1:J:213:ILE:HG22	1:J:214:GLY:H	1.83	0.43
1:J:364:VAL:HG13	1:J:573:PHE:HE2	1.83	0.43
1:J:584:GLY:HA3	1:J:586:TYR:OH	2.17	0.43
1:J:655:SER:O	1:J:656:ALA:HB2	2.19	0.43
1:J:883:SER:OG	1:J:884:SER:N	2.51	0.43
1:K:88:VAL:HG12	1:K:583:PRO:HA	2.01	0.43
1:L:130:PRO:HG3	1:L:321:LEU:HB3	1.99	0.43
1:K:373:GLU:C	1:K:375:SER:N	2.72	0.43
1:K:498:ASN:N	1:K:498:ASN:OD1	2.50	0.43
1:L:437:ALA:HB2	1:L:447:TRP:CZ3	2.54	0.43
1:L:693:LYS:HB3	1:L:693:LYS:HE3	1.64	0.43
2:Z:11:GLY:HA3	2:Z:16:CGU:OE21	2.18	0.43
2:Z:337:MET:HE3	2:Z:461:TRP:CE3	2.53	0.43
1:K:131:ASN:HD21	1:K:239:PRO:C	2.26	0.43
1:K:825:GLY:O	1:K:829:GLN:NE2	2.52	0.43
1:L:204:ASP:O	1:L:208:GLN:HG2	2.19	0.43
1:L:333:ILE:HA	1:L:601:GLN:O	2.19	0.43
1:L:898:ASN:C	1:L:899:LEU:HD12	2.43	0.43
1:K:929:VAL:HB	1:K:950:THR:HG21	2.01	0.43
1:L:282:GLU:C	1:L:284:ASN:N	2.69	0.43
2:Z:458:VAL:HG23	2:Z:529:PHE:HD1	1.84	0.43
1:J:254:GLN:O	1:J:297:VAL:HG12	2.19	0.43
1:J:502:SER:HB2	1:J:509:ASP:HB2	2.01	0.43
1:K:356:GLY:HA2	1:K:586:TYR:CD1	2.52	0.43
1:K:440:GLY:HA3	1:K:446:THR:HG23	2.01	0.43
1:L:278:ASN:HD22	1:L:278:ASN:HA	1.55	0.43
1:L:597:ASN:ND2	1:L:706:TYR:O	2.52	0.43
1:L:694:GLU:CB	1:L:708:TYR:CE2	3.00	0.43
1:J:65:THR:OG1	1:J:66:LEU:N	2.52	0.42
1:J:65:THR:HG23	1:L:745:LEU:HD21	2.01	0.42
1:J:354:LEU:HA	1:J:587:THR:O	2.19	0.42
1:J:371:ASN:ND2	1:J:374:LEU:CB	2.77	0.42
1:J:790:ILE:HD12	1:J:790:ILE:H	1.85	0.42
1:K:381:ASP:CG	1:K:382:SER:N	2.74	0.42
1:K:654:LEU:HD13	1:K:654:LEU:HA	1.71	0.42
2:Z:90:ARG:HD2	2:Z:470:ALA:HB3	2.01	0.42
1:J:332:TYR:N	1:J:603:SER:OG	2.39	0.42
1:K:493:LYS:HB2	1:K:514:ARG:HH21	1.84	0.42
1:K:744:LEU:HD23	1:K:744:LEU:HA	1.82	0.42
2:Z:316:TYR:HD1	2:Z:317:ILE:HG12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:574:ILE:O	2:Z:578:GLY:N	2.52	0.42
1:J:550:LEU:HD12	1:J:550:LEU:HA	1.77	0.42
1:K:335:PHE:O	1:K:553:ARG:HD2	2.19	0.42
1:K:504:ASN:ND2	1:K:507:THR:H	2.17	0.42
1:L:276:SER:C	1:L:278:ASN:N	2.76	0.42
1:L:512:ASN:O	1:L:512:ASN:ND2	2.53	0.42
1:L:797:ARG:N	1:L:800:SER:OG	2.52	0.42
1:J:20:ALA:HA	1:J:23:TYR:HE1	1.82	0.42
1:J:68:PHE:CZ	1:J:86:LEU:HD12	2.54	0.42
1:J:782:ASN:HD21	1:J:888:SER:HB2	1.83	0.42
1:K:186:LEU:HD12	1:K:187:GLN:N	2.33	0.42
1:L:375:SER:C	1:L:377:GLN:H	2.24	0.42
1:L:393:TRP:CZ3	1:L:570:PRO:HB3	2.54	0.42
1:L:721:LEU:O	1:L:724:THR:OG1	2.32	0.42
2:Z:16:CGU:O	2:Z:22:CYS:HB3	2.18	0.42
2:Z:340:ARG:HB2	2:Z:347:LEU:HD11	2.01	0.42
1:J:98:SER:OG	1:J:624:ALA:HA	2.19	0.42
1:L:694:GLU:HB3	1:L:708:TYR:CD1	2.54	0.42
1:J:254:GLN:HB2	1:J:297:VAL:HG12	2.01	0.42
1:J:291:LEU:O	1:J:292:LEU:HD23	2.20	0.42
1:J:453:PHE:CD1	1:L:168:THR:HB	2.55	0.42
1:K:660:LEU:HD22	1:K:660:LEU:HA	1.69	0.42
1:K:769:THR:OG1	1:K:771:ASP:OD1	2.32	0.42
1:L:194:ALA:HB3	1:L:199:LYS:H	1.83	0.42
1:J:579:LEU:HD11	1:J:935:VAL:HG11	2.02	0.42
1:K:20:ALA:HA	1:K:23:TYR:CZ	2.54	0.42
1:K:470:ASN:OD1	1:K:471:LEU:N	2.53	0.42
1:L:232:LYS:HG2	1:L:294:SER:HB2	2.01	0.42
1:L:723:HIS:CE1	1:L:724:THR:HG23	2.55	0.42
2:Z:74:ARG:CZ	2:Z:107:ALA:HA	2.50	0.42
1:J:596:VAL:HB	1:J:600:LEU:HD12	2.00	0.42
1:K:10:TRP:CD1	1:K:10:TRP:N	2.87	0.42
1:K:109:ARG:HD3	1:K:333:ILE:HG22	2.01	0.42
1:K:271:GLN:O	1:K:291:LEU:HD12	2.20	0.42
1:K:657:ALA:O	1:K:658:ASN:CB	2.68	0.42
1:K:766:CYS:SG	1:K:768:MET:N	2.92	0.42
1:L:6:MET:HE2	1:L:6:MET:O	2.20	0.42
1:L:931:ASP:HA	1:L:949:ARG:HB2	2.02	0.42
2:Z:297:PRO:O	2:Z:301:LYS:HB2	2.20	0.42
2:Z:335:GLN:OE1	2:Z:459:THR:OG1	2.38	0.42
1:J:65:THR:O	1:J:66:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:14:HIS:CE1	1:K:23:TYR:CZ	3.07	0.42
1:L:292:LEU:HD23	1:L:292:LEU:HA	1.85	0.42
1:L:441:ASN:OD1	1:L:441:ASN:N	2.52	0.42
2:Z:18:VAL:HG12	2:Z:19:CGU:CD1	2.50	0.42
2:Z:240:PHE:CE1	2:Z:572:LYS:HB3	2.55	0.42
1:J:436:LYS:HZ2	1:J:450:ASP:HA	1.84	0.42
1:J:487:TYR:HE2	1:J:544:HIS:CE1	2.38	0.42
1:J:899:LEU:HD13	1:J:903:ASN:HD21	1.85	0.42
1:K:280:MET:O	1:K:281:ASN:CB	2.66	0.42
1:K:371:ASN:O	1:K:372:THR:OG1	2.27	0.42
1:K:772:TRP:HZ2	1:K:878:TRP:CE3	2.38	0.42
1:K:782:ASN:HD21	1:K:888:SER:HB2	1.84	0.42
1:L:696:PRO:HD3	1:L:706:TYR:OH	2.19	0.42
1:L:726:LYS:HE2	1:L:726:LYS:HB3	1.82	0.42
2:Z:9:ARG:CG	2:Z:10:LYS:N	2.83	0.42
1:K:376:TYR:C	1:K:376:TYR:CD1	2.97	0.41
1:K:616:LYS:HB3	1:K:616:LYS:HE2	1.86	0.41
1:K:811:GLN:N	1:K:811:GLN:OE1	2.53	0.41
1:L:409:ASN:ND2	1:L:525:ILE:O	2.53	0.41
1:L:616:LYS:HB3	1:L:616:LYS:HE2	1.85	0.41
1:L:799:TYR:N	1:L:799:TYR:CD1	2.86	0.41
1:L:944:GLU:OE1	1:L:945:THR:N	2.42	0.41
2:Z:115:ARG:O	2:Z:125:TRP:N	2.53	0.41
2:Z:277:TYR:CE1	2:Z:540:TYR:HE2	2.38	0.41
2:Z:554:ASP:N	2:Z:554:ASP:OD1	2.53	0.41
1:J:329:ARG:HG3	1:J:512:ASN:OD1	2.20	0.41
1:J:781:TYR:HB2	1:J:783:ILE:HG13	2.02	0.41
1:K:419:TYR:OH	1:L:843:MET:HA	2.20	0.41
1:K:676:SER:HA	1:K:906:HIS:O	2.20	0.41
1:K:808:MET:HE3	1:K:808:MET:HB2	1.77	0.41
1:L:256:VAL:HG23	1:L:296:ASP:O	2.20	0.41
1:K:380:LEU:O	1:K:382:SER:N	2.53	0.41
1:L:336:ARG:NH2	1:L:712:ILE:HG13	2.35	0.41
1:L:440:GLY:HA3	1:L:445:THR:HA	2.02	0.41
1:L:522:ASP:HB3	1:L:524:TYR:CE1	2.55	0.41
2:Z:48:GLU:HA	2:Z:51:ARG:CZ	2.50	0.41
2:Z:230:TRP:CZ2	2:Z:572:LYS:HD3	2.55	0.41
1:J:643:ASN:O	1:J:645:THR:N	2.53	0.41
1:J:668:THR:HG22	1:J:914:VAL:O	2.21	0.41
1:K:647:ASP:CG	1:K:936:HIS:HB2	2.45	0.41
1:K:661:TYR:CE2	1:K:672:ILE:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:847:GLN:HB3	1:L:175:PRO:HG3	2.02	0.41
2:Z:3:THR:O	2:Z:6:CGU:HB2	2.21	0.41
2:Z:506:PHE:HB3	2:Z:562:HIS:NE2	2.35	0.41
1:J:531:TRP:NE1	1:J:532:SER:O	2.53	0.41
1:J:582:LEU:O	1:J:586:TYR:OH	2.36	0.41
1:J:778:LEU:HD23	1:J:783:ILE:N	2.35	0.41
1:J:849:TYR:CD1	1:J:850:PRO:CD	3.03	0.41
1:K:207:TYR:O	1:K:208:GLN:CB	2.68	0.41
1:K:435:ILE:H	1:K:435:ILE:HG12	1.63	0.41
1:L:192:GLY:HA2	1:L:198:ASN:CG	2.46	0.41
2:Z:229:VAL:HG22	2:Z:247:TYR:OH	2.20	0.41
1:J:733:ASP:OD2	1:J:906:HIS:HB3	2.20	0.41
1:J:899:LEU:HB3	1:J:903:ASN:CG	2.46	0.41
1:J:899:LEU:HD22	1:J:903:ASN:OD1	2.20	0.41
1:K:281:ASN:HB3	1:K:282:GLU:H	1.58	0.41
1:K:469:ILE:HG12	1:K:470:ASN:N	2.36	0.41
1:K:672:ILE:CG1	1:K:910:MET:HB2	2.50	0.41
1:L:345:TYR:HB3	1:L:346:ASN:H	1.57	0.41
1:L:346:ASN:HA	1:L:366:ASP:OD2	2.21	0.41
1:L:380:LEU:HD22	1:L:380:LEU:HA	1.88	0.41
1:L:392:MET:HE2	1:L:393:TRP:CH2	2.55	0.41
2:Z:77:VAL:HG13	2:Z:79:ILE:HG12	2.02	0.41
1:J:113:PHE:CD1	1:J:113:PHE:C	2.99	0.41
1:J:134:GLU:OE1	1:J:134:GLU:N	2.53	0.41
1:J:467:MET:HG3	1:K:467:MET:HE2	2.03	0.41
1:J:501:ILE:HG13	1:J:513:LYS:HB2	2.03	0.41
1:J:855:TYR:CD2	1:J:856:PRO:HD2	2.56	0.41
1:K:76:THR:OG1	1:K:79:SER:OG	2.38	0.41
1:K:249:ASN:HD21	1:K:253:GLY:HA3	1.86	0.41
1:L:348:THR:C	1:L:350:ASN:N	2.74	0.41
1:L:522:ASP:O	1:L:525:ILE:HG22	2.21	0.41
2:Z:503:ASP:CG	2:Z:565:ARG:HH22	2.28	0.41
1:J:678:ASN:OD1	1:J:679:TRP:N	2.54	0.41
1:K:100:TYR:HD1	1:K:568:GLN:HB3	1.86	0.41
1:K:420:CYS:SG	1:K:421:PHE:N	2.93	0.41
1:K:879:ARG:NH1	1:K:928:GLU:OE2	2.54	0.41
1:L:550:LEU:HD12	1:L:550:LEU:HA	1.60	0.41
1:L:642:ARG:NH2	1:L:940:ARG:HA	2.36	0.41
2:Z:458:VAL:HA	2:Z:528:PRO:O	2.19	0.41
1:J:215:GLU:HB2	1:K:463:ASN:ND2	2.36	0.41
1:J:299:MET:HE1	1:L:850:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:689:ARG:O	1:J:690:LEU:HD23	2.20	0.41
1:J:872:LEU:HD23	1:J:872:LEU:HA	1.88	0.41
1:J:876:THR:O	1:J:877:LEU:HD23	2.21	0.41
1:K:42:ASN:OD1	1:K:42:ASN:N	2.48	0.41
1:K:368:GLN:C	1:K:370:ARG:N	2.79	0.41
1:K:504:ASN:ND2	1:K:507:THR:HG22	2.35	0.41
1:K:565:PHE:HD1	1:K:565:PHE:H	1.69	0.41
1:L:284:ASN:C	1:L:286:ILE:H	2.29	0.41
1:L:386:ARG:HD2	1:L:386:ARG:HA	1.83	0.41
1:L:644:ASP:OD1	1:L:645:THR:N	2.54	0.41
2:Z:464:LEU:HD12	2:Z:468:TRP:CD1	2.56	0.41
1:J:604:LEU:HA	1:J:604:LEU:HD23	1.81	0.41
1:J:706:TYR:HD1	1:J:706:TYR:HA	1.66	0.41
1:J:762:ASN:O	1:J:770:LYS:NZ	2.30	0.41
1:K:183:LYS:H	1:K:183:LYS:HG2	1.55	0.41
1:K:259:GLU:HA	1:K:263:LYS:O	2.21	0.41
1:K:433:GLN:NE2	1:K:449:GLN:HA	2.35	0.41
1:L:345:TYR:OH	1:L:572:LYS:HB2	2.21	0.41
1:L:953:SER:OG	1:L:954:ALA:N	2.54	0.41
2:Z:356:ARG:HB2	2:Z:424:LYS:HZ3	1.86	0.41
1:K:475:LEU:HD23	1:K:475:LEU:HA	1.92	0.40
1:L:361:LEU:HD23	1:L:361:LEU:HA	1.90	0.40
2:Z:89:TRP:HB2	2:Z:110:GLN:O	2.21	0.40
2:Z:89:TRP:NE1	2:Z:113:PHE:O	2.53	0.40
2:Z:382:ARG:HG2	2:Z:398:ILE:HG12	2.03	0.40
2:Z:460:GLY:HA3	2:Z:524:ASP:H	1.85	0.40
1:K:237:MET:HE3	1:K:316:ASN:HB3	2.02	0.40
1:K:385:ASP:OD1	1:K:387:THR:HG23	2.22	0.40
1:K:436:LYS:HE3	1:K:438:THR:HG23	2.03	0.40
1:L:277:VAL:C	1:L:279:ALA:N	2.76	0.40
2:Z:48:GLU:HA	2:Z:51:ARG:NE	2.36	0.40
2:Z:337:MET:HE3	2:Z:461:TRP:CD2	2.57	0.40
1:J:280:MET:HB3	2:Z:52:THR:CG2	2.51	0.40
1:J:591:ASN:N	1:J:591:ASN:OD1	2.54	0.40
1:J:702:TYR:CZ	1:J:704:PRO:HA	2.57	0.40
1:J:742:ASP:O	1:K:63:ARG:HD3	2.22	0.40
1:K:210:GLU:C	1:K:212:GLN:N	2.77	0.40
1:K:653:TYR:C	1:K:653:TYR:CD1	2.98	0.40
1:L:67:ARG:NH1	1:L:623:TYR:OH	2.55	0.40
1:L:204:ASP:O	1:L:206:THR:N	2.54	0.40
1:L:339:PHE:HB3	1:L:342:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:357:GLN:HB2	1:L:585:SER:O	2.21	0.40
1:L:417:PRO:HB2	1:L:419:TYR:CZ	2.56	0.40
2:Z:147:GLN:HG2	2:Z:148:VAL:N	2.35	0.40
2:Z:230:TRP:CH2	2:Z:572:LYS:HD3	2.56	0.40
1:J:566:HIS:ND1	1:J:566:HIS:O	2.53	0.40
1:J:663:ILE:HB	1:J:921:THR:OG1	2.22	0.40
1:J:778:LEU:HD23	1:J:778:LEU:HA	1.86	0.40
1:J:780:ASN:HB3	1:J:781:TYR:CE1	2.57	0.40
1:J:885:ASN:CG	1:J:887:MET:HG3	2.47	0.40
1:K:100:TYR:CE1	1:K:623:TYR:HD2	2.40	0.40
1:K:383:ILE:HG13	1:K:384:GLY:N	2.35	0.40
1:K:440:GLY:N	1:K:446:THR:H	2.15	0.40
1:K:726:LYS:HB2	1:K:913:GLU:O	2.21	0.40
1:K:826:ILE:HG23	1:K:827:ILE:HG23	2.04	0.40
1:K:934:ARG:CZ	1:L:12:TYR:HE1	2.35	0.40
2:Z:54:ARG:O	2:Z:55:ASP:C	2.64	0.40
2:Z:363:HIS:HB2	2:Z:367:TYR:CE2	2.56	0.40
1:K:292:LEU:HD23	1:K:292:LEU:HA	1.84	0.40
1:K:431:THR:HG23	1:K:456:ARG:HB3	2.02	0.40
1:K:450:ASP:CG	1:K:452:THR:H	2.30	0.40
1:L:848:ALA:O	1:L:849:TYR:CB	2.67	0.40
2:Z:566:LEU:O	2:Z:569:TRP:HB3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	927/959 (97%)	786 (85%)	124 (13%)	17 (2%)	6	34
1	K	925/959 (96%)	789 (85%)	118 (13%)	18 (2%)	6	33
1	L	923/959 (96%)	784 (85%)	119 (13%)	20 (2%)	5	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Z	567/622 (91%)	520 (92%)	44 (8%)	3 (0%)	24	62
All	All	3342/3499 (96%)	2879 (86%)	405 (12%)	58 (2%)	9	35

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	283	ALA
1	J	285	ALA
1	J	346	ASN
1	J	370	ARG
1	J	585	SER
1	K	209	PRO
1	K	281	ASN
1	K	368	GLN
1	K	369	ASP
1	K	654	LEU
1	K	658	ASN
1	K	660	LEU
1	L	280	MET
1	L	346	ASN
1	L	350	ASN
1	L	692	THR
1	L	693	LYS
1	J	284	ASN
1	J	371	ASN
1	K	372	THR
1	K	653	TYR
1	L	284	ASN
1	L	371	ASN
1	L	372	THR
1	L	383	ILE
2	Z	18	VAL
1	J	427	GLY
1	J	581	LEU
1	J	655	SER
1	K	283	ALA
1	L	345	TYR
1	L	347	SER
1	L	377	GLN
1	K	285	ALA
1	K	656	ALA
1	L	369	ASP

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Mol	Chain	Res	Type
1	L	658	ASN
1	L	708	TYR
1	L	709	SER
1	L	849	TYR
1	J	275	THR
1	J	628	PRO
1	K	655	SER
1	L	283	ALA
2	Z	54	ARG
1	J	658	ASN
1	K	97	ALA
1	K	208	GLN
1	L	351	MET
1	J	662	PRO
1	J	701	GLY
1	J	704	PRO
1	J	849	TYR
1	K	427	GLY
1	K	211	PRO
1	K	428	VAL
1	L	209	PRO
2	Z	53	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	799/824 (97%)	699 (88%)	100 (12%)	4	18
1	K	799/824 (97%)	701 (88%)	98 (12%)	4	19
1	L	797/824 (97%)	699 (88%)	98 (12%)	4	19
2	Z	486/521 (93%)	458 (94%)	28 (6%)	18	42
All	All	2881/2993 (96%)	2557 (89%)	324 (11%)	8	21

All (324) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	7	MET
1	J	42	ASN
1	J	43	ASN
1	J	47	ASN
1	J	54	HIS
1	J	55	ASP
1	J	58	THR
1	J	59	ASP
1	J	64	LEU
1	J	66	LEU
1	J	69	ILE
1	J	90	ASP
1	J	91	ASN
1	J	100	TYR
1	J	102	ASP
1	J	112	THR
1	J	114	LYS
1	J	117	SER
1	J	184	ASN
1	J	196	GLU
1	J	213	ILE
1	J	243	SER
1	J	261	ASN
1	J	266	SER
1	J	275	THR
1	J	278	ASN
1	J	284	ASN
1	J	294	SER
1	J	297	VAL
1	J	312	LYS
1	J	314	ASP
1	J	315	ASP
1	J	324	GLN
1	J	333	ILE
1	J	342	LEU
1	J	344	TYR
1	J	345	TYR
1	J	347	SER
1	J	348	THR
1	J	361	LEU
1	J	369	ASP
1	J	371	ASN
1	J	380	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	J	381	ASP
1	J	397	VAL
1	J	412	THR
1	J	413	GLU
1	J	423	LEU
1	J	428	VAL
1	J	429	THR
1	J	446	THR
1	J	467	MET
1	J	468	GLU
1	J	474	ASN
1	J	494	TYR
1	J	495	ASN
1	J	503	ASP
1	J	516	VAL
1	J	534	ASP
1	J	553	ARG
1	J	566	HIS
1	J	568	GLN
1	J	576	ILE
1	J	577	LYS
1	J	581	LEU
1	J	582	LEU
1	J	586	TYR
1	J	587	THR
1	J	593	ARG
1	J	594	LYS
1	J	595	ASP
1	J	611	ASP
1	J	615	ILE
1	J	618	ASP
1	J	622	LEU
1	J	625	THR
1	J	627	PHE
1	J	652	ASP
1	J	655	SER
1	J	658	ASN
1	J	659	MET
1	J	660	LEU
1	J	698	LEU
1	J	702	TYR
1	J	706	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	J	724	THR
1	J	736	VAL
1	J	737	SER
1	J	752	ILE
1	J	804	ASN
1	J	814	ASP
1	J	820	ASP
1	J	864	ASP
1	J	883	SER
1	J	906	HIS
1	J	914	VAL
1	J	932	VAL
1	J	933	VAL
1	J	943	ILE
1	J	950	THR
1	K	6	MET
1	K	15	ILE
1	K	19	ASP
1	K	45	PHE
1	K	49	THR
1	K	54	HIS
1	K	55	ASP
1	K	58	THR
1	K	90	ASP
1	K	91	ASN
1	K	93	VAL
1	K	112	THR
1	K	113	PHE
1	K	119	THR
1	K	136	ASP
1	K	198	ASN
1	K	208	GLN
1	K	231	LEU
1	K	250	SER
1	K	251	ASN
1	K	254	GLN
1	K	260	GLN
1	K	261	ASN
1	K	277	VAL
1	K	280	MET
1	K	282	GLU
1	K	286	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	K	295	GLU
1	K	316	ASN
1	K	317	SER
1	K	333	ILE
1	K	350	ASN
1	K	374	LEU
1	K	375	SER
1	K	381	ASP
1	K	383	ILE
1	K	397	VAL
1	K	398	ASP
1	K	403	ASP
1	K	413	GLU
1	K	420	CYS
1	K	426	ILE
1	K	428	VAL
1	K	429	THR
1	K	430	ASP
1	K	433	GLN
1	K	435	ILE
1	K	438	THR
1	K	452	THR
1	K	463	ASN
1	K	468	GLU
1	K	469	ILE
1	K	474	ASN
1	K	480	LEU
1	K	495	ASN
1	K	497	THR
1	K	498	ASN
1	K	499	VAL
1	K	501	ILE
1	K	507	THR
1	K	532	SER
1	K	534	ASP
1	K	556	LEU
1	K	565	PHE
1	K	577	LYS
1	K	595	ASP
1	K	597	ASN
1	K	618	ASP
1	K	620	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	K	631	HIS
1	K	641	LEU
1	K	643	ASN
1	K	644	ASP
1	K	652	ASP
1	K	654	LEU
1	K	659	MET
1	K	660	LEU
1	K	669	ASN
1	K	730	ILE
1	K	746	THR
1	K	752	ILE
1	K	756	VAL
1	K	766	CYS
1	K	769	THR
1	K	796	ASP
1	K	813	VAL
1	K	820	ASP
1	K	845	GLU
1	K	853	VAL
1	K	864	ASP
1	K	874	ASP
1	K	876	THR
1	K	883	SER
1	K	903	ASN
1	K	918	ASP
1	K	931	ASP
1	K	943	ILE
1	K	950	THR
1	L	6	MET
1	L	15	ILE
1	L	25	SER
1	L	37	THR
1	L	54	HIS
1	L	55	ASP
1	L	58	THR
1	L	63	ARG
1	L	78	TYR
1	L	90	ASP
1	L	91	ASN
1	L	112	THR
1	L	131	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	184	ASN
1	L	188	ILE
1	L	190	THR
1	L	243	SER
1	L	254	GLN
1	L	261	ASN
1	L	275	THR
1	L	277	VAL
1	L	278	ASN
1	L	280	MET
1	L	281	ASN
1	L	284	ASN
1	L	286	ILE
1	L	298	ASN
1	L	303	ASP
1	L	316	ASN
1	L	333	ILE
1	L	346	ASN
1	L	348	THR
1	L	350	ASN
1	L	351	MET
1	L	370	ARG
1	L	375	SER
1	L	380	LEU
1	L	381	ASP
1	L	382	SER
1	L	383	ILE
1	L	397	VAL
1	L	398	ASP
1	L	403	ASP
1	L	420	CYS
1	L	428	VAL
1	L	429	THR
1	L	445	THR
1	L	459	ILE
1	L	465	PHE
1	L	469	ILE
1	L	507	THR
1	L	516	VAL
1	L	520	LEU
1	L	550	LEU
1	L	565	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	599	VAL
1	L	614	SER
1	L	615	ILE
1	L	641	LEU
1	L	652	ASP
1	L	672	ILE
1	L	674	ILE
1	L	687	PHE
1	L	693	LYS
1	L	694	GLU
1	L	697	SER
1	L	698	LEU
1	L	708	TYR
1	L	711	SER
1	L	723	HIS
1	L	728	VAL
1	L	754	ARG
1	L	757	ASP
1	L	763	VAL
1	L	766	CYS
1	L	767	ASN
1	L	769	THR
1	L	780	ASN
1	L	790	ILE
1	L	799	TYR
1	L	813	VAL
1	L	847	GLN
1	L	849	TYR
1	L	855	TYR
1	L	858	ILE
1	L	874	ASP
1	L	876	THR
1	L	883	SER
1	L	894	ASP
1	L	899	LEU
1	L	914	VAL
1	L	926	LEU
1	L	933	VAL
1	L	943	ILE
1	L	944	GLU
1	L	948	LEU
1	L	949	ARG

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Mol	Chain	Res	Type
1	L	950	THR
2	Z	54	ARG
2	Z	55	ASP
2	Z	95	HIS
2	Z	100	ASN
2	Z	109	LEU
2	Z	112	ASN
2	Z	129	THR
2	Z	142	VAL
2	Z	152	MET
2	Z	173	ASP
2	Z	215	VAL
2	Z	223	ASP
2	Z	281	PHE
2	Z	290	GLU
2	Z	300	GLU
2	Z	316	TYR
2	Z	367	TYR
2	Z	395	ILE
2	Z	400	MET
2	Z	429	VAL
2	Z	433	ASP
2	Z	454	TYR
2	Z	479	VAL
2	Z	482	VAL
2	Z	519	ASP
2	Z	552	ASP
2	Z	554	ASP
2	Z	564	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	91	ASN
1	J	182	ASN
1	J	212	GLN
1	J	338	ASN
1	J	395	GLN
1	J	648	GLN
1	J	658	ASN
1	J	830	HIS
1	K	131	ASN

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Mol	Chain	Res	Type
1	K	261	ASN
1	K	278	ASN
1	K	298	ASN
1	K	346	ASN
1	K	377	GLN
1	K	433	GLN
1	K	439	ASN
1	K	474	ASN
1	K	646	ASN
1	L	212	GLN
1	L	328	ASN
1	L	449	GLN
1	L	474	ASN
1	L	591	ASN
1	L	658	ASN
1	L	762	ASN
1	L	780	ASN
2	Z	205	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CGU	Z	14	2,3	9,11,12	1.18	0	10,14,16	0.78	0
2	CGU	Z	29	2,3	9,11,12	1.36	0	10,14,16	0.83	0
2	CGU	Z	6	2,3	9,11,12	1.64	1 (11%)	10,14,16	0.92	0
2	CGU	Z	16	2,3	9,11,12	1.28	0	10,14,16	0.95	0
2	CGU	Z	19	2	9,11,12	1.56	1 (11%)	10,14,16	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CGU	Z	7	2,3	9,11,12	1.74	2 (22%)	10,14,16	0.89	0
2	CGU	Z	26	2,3	9,11,12	1.41	1 (11%)	10,14,16	0.81	0
2	CGU	Z	32	2	9,11,12	1.53	1 (11%)	10,14,16	0.90	0
2	CGU	Z	20	2,3	9,11,12	1.39	1 (11%)	10,14,16	0.81	0
2	CGU	Z	25	2	9,11,12	1.72	1 (11%)	10,14,16	0.90	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CGU	Z	14	2,3	-	2/13/14/16	-
2	CGU	Z	29	2,3	-	8/13/14/16	-
2	CGU	Z	6	2,3	-	3/13/14/16	-
2	CGU	Z	16	2,3	-	2/13/14/16	-
2	CGU	Z	19	2	-	3/13/14/16	-
2	CGU	Z	7	2,3	-	5/13/14/16	-
2	CGU	Z	26	2,3	-	0/13/14/16	-
2	CGU	Z	32	2	-	2/13/14/16	-
2	CGU	Z	20	2,3	-	1/13/14/16	-
2	CGU	Z	25	2	-	4/13/14/16	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	25	CGU	CG-CD2	3.54	1.56	1.52
2	Z	7	CGU	CG-CD2	3.09	1.56	1.52
2	Z	19	CGU	CG-CD1	2.97	1.55	1.52
2	Z	6	CGU	CG-CD2	2.71	1.55	1.52
2	Z	7	CGU	CG-CD1	2.12	1.54	1.52
2	Z	32	CGU	CA-N	2.07	1.53	1.48
2	Z	26	CGU	CG-CD2	2.06	1.54	1.52
2	Z	20	CGU	CG-CD2	2.04	1.54	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Z	6	CGU	C-CA-CB-CG
2	Z	6	CGU	OE21-CD2-CG-CB
2	Z	6	CGU	OE22-CD2-CG-CB
2	Z	7	CGU	N-CA-CB-CG
2	Z	14	CGU	C-CA-CB-CG
2	Z	16	CGU	CA-CB-CG-CD1
2	Z	19	CGU	N-CA-CB-CG
2	Z	19	CGU	CA-CB-CG-CD1
2	Z	20	CGU	O-C-CA-CB
2	Z	29	CGU	OE22-CD2-CG-CD1
2	Z	32	CGU	N-CA-CB-CG
2	Z	32	CGU	C-CA-CB-CG
2	Z	14	CGU	N-CA-CB-CG
2	Z	7	CGU	OE21-CD2-CG-CB
2	Z	25	CGU	OE21-CD2-CG-CB
2	Z	25	CGU	OE22-CD2-CG-CB
2	Z	29	CGU	OE21-CD2-CG-CB
2	Z	29	CGU	OE22-CD2-CG-CB
2	Z	29	CGU	OE21-CD2-CG-CD1
2	Z	7	CGU	C-CA-CB-CG
2	Z	25	CGU	N-CA-CB-CG
2	Z	29	CGU	N-CA-CB-CG
2	Z	7	CGU	OE22-CD2-CG-CB
2	Z	29	CGU	OE11-CD1-CG-CB
2	Z	29	CGU	OE12-CD1-CG-CB
2	Z	7	CGU	OE11-CD1-CG-CD2
2	Z	16	CGU	OE11-CD1-CG-CD2
2	Z	19	CGU	OE21-CD2-CG-CD1
2	Z	25	CGU	OE21-CD2-CG-CD1
2	Z	29	CGU	OE11-CD1-CG-CD2

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Z	14	CGU	2	0
2	Z	6	CGU	3	0
2	Z	16	CGU	2	0
2	Z	19	CGU	7	0
2	Z	32	CGU	1	0
2	Z	25	CGU	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

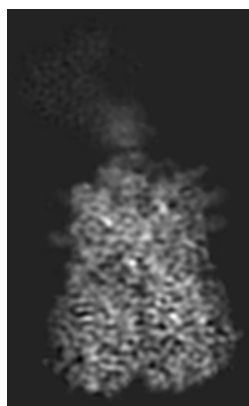
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45751. These allow visual inspection of the internal detail of the map and identification of artifacts.

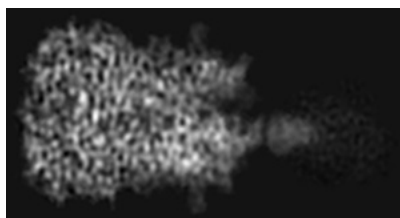
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

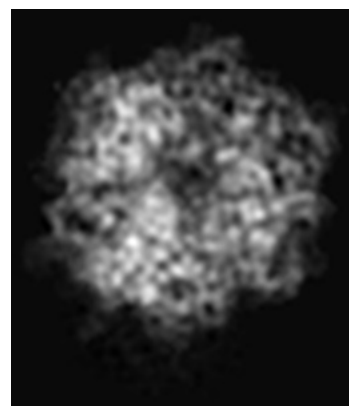
#### 6.1.1 Primary map



X

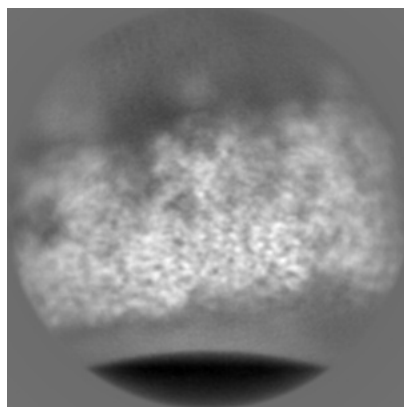


Y

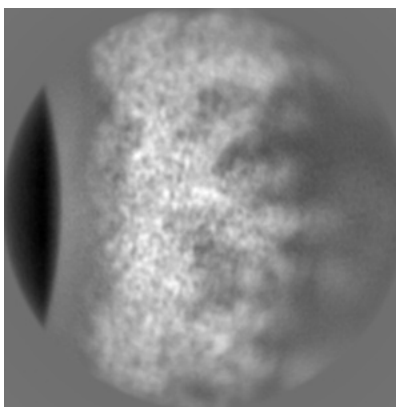


Z

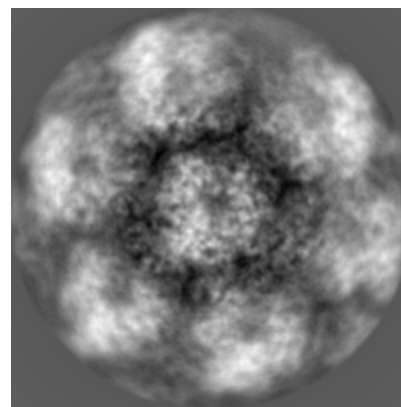
#### 6.1.2 Raw map



X



Y

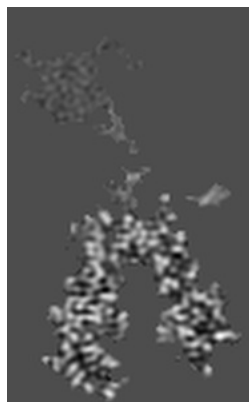


Z

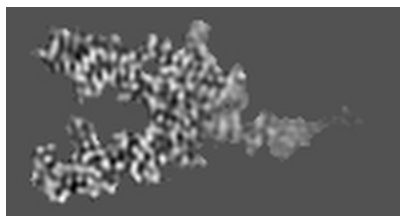
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

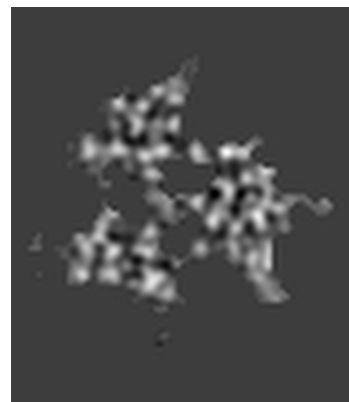
### 6.2.1 Primary map



X Index: 40

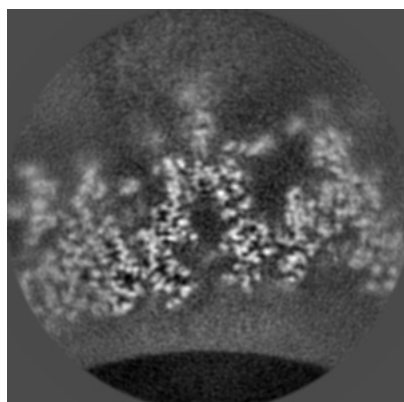


Y Index: 46

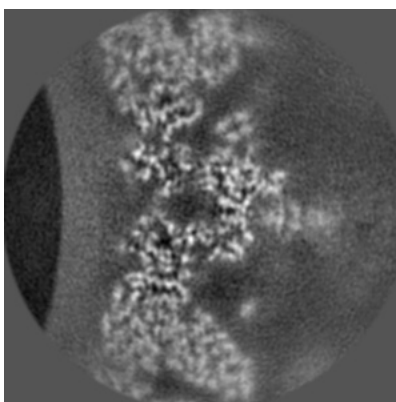


Z Index: 75

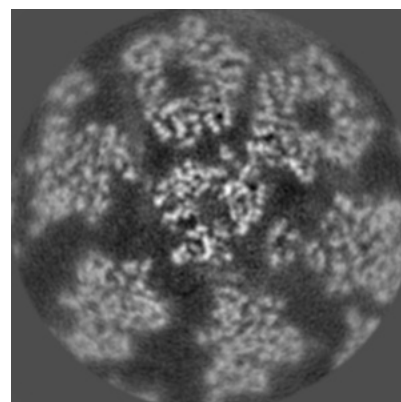
### 6.2.2 Raw map



X Index: 100



Y Index: 100

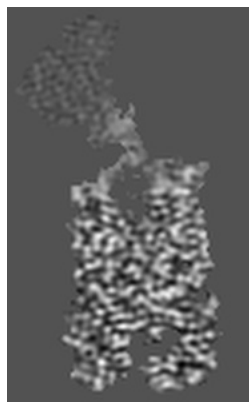


Z Index: 100

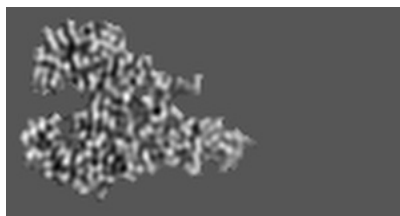
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

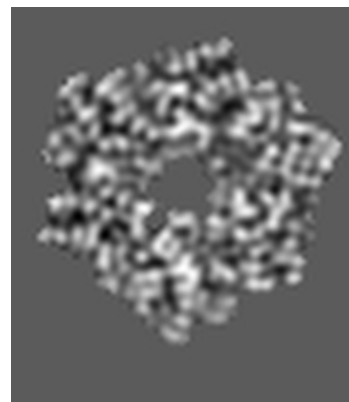
### 6.3.1 Primary map



X Index: 28

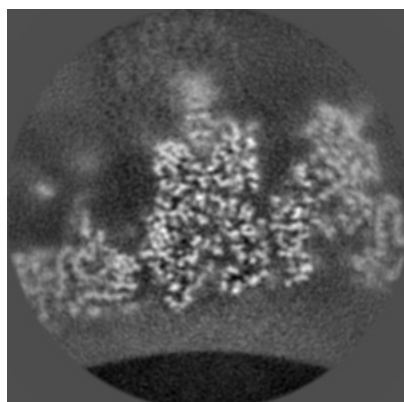


Y Index: 64

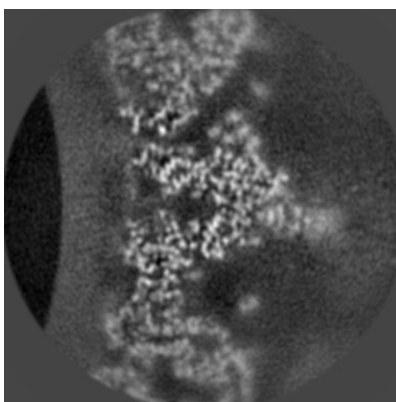


Z Index: 33

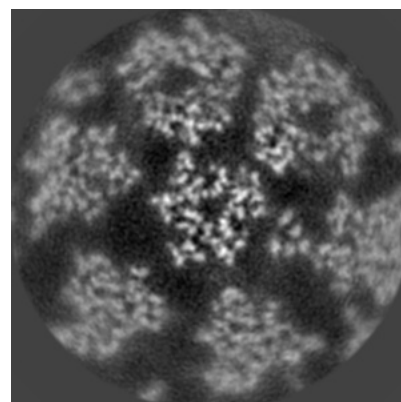
### 6.3.2 Raw map



X Index: 92



Y Index: 96

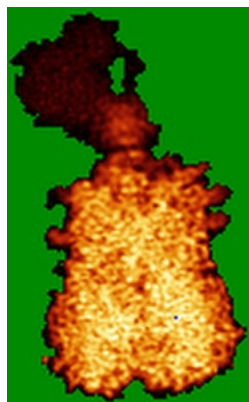


Z Index: 104

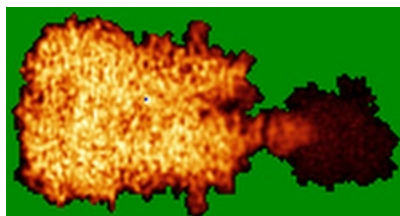
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X

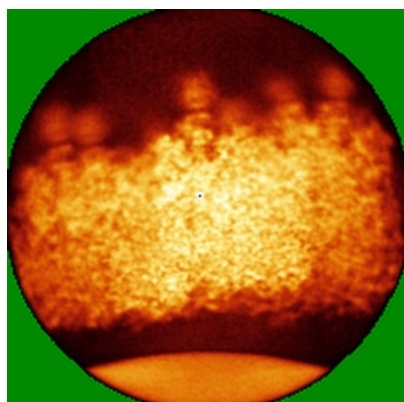


Y

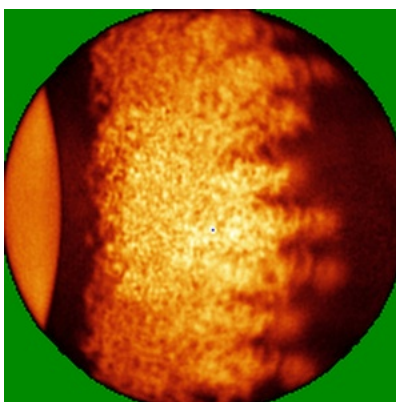


Z

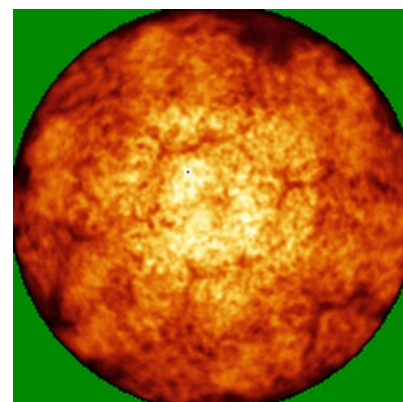
### 6.4.2 Raw map



X



Y



Z

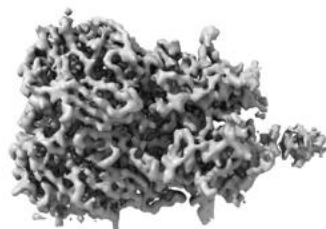
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

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

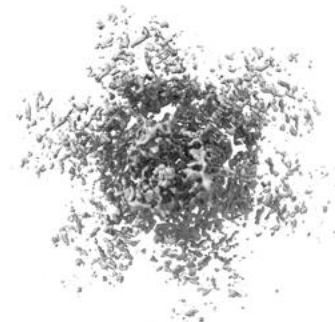
### 6.5.2 Raw map



X



Y



Z

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

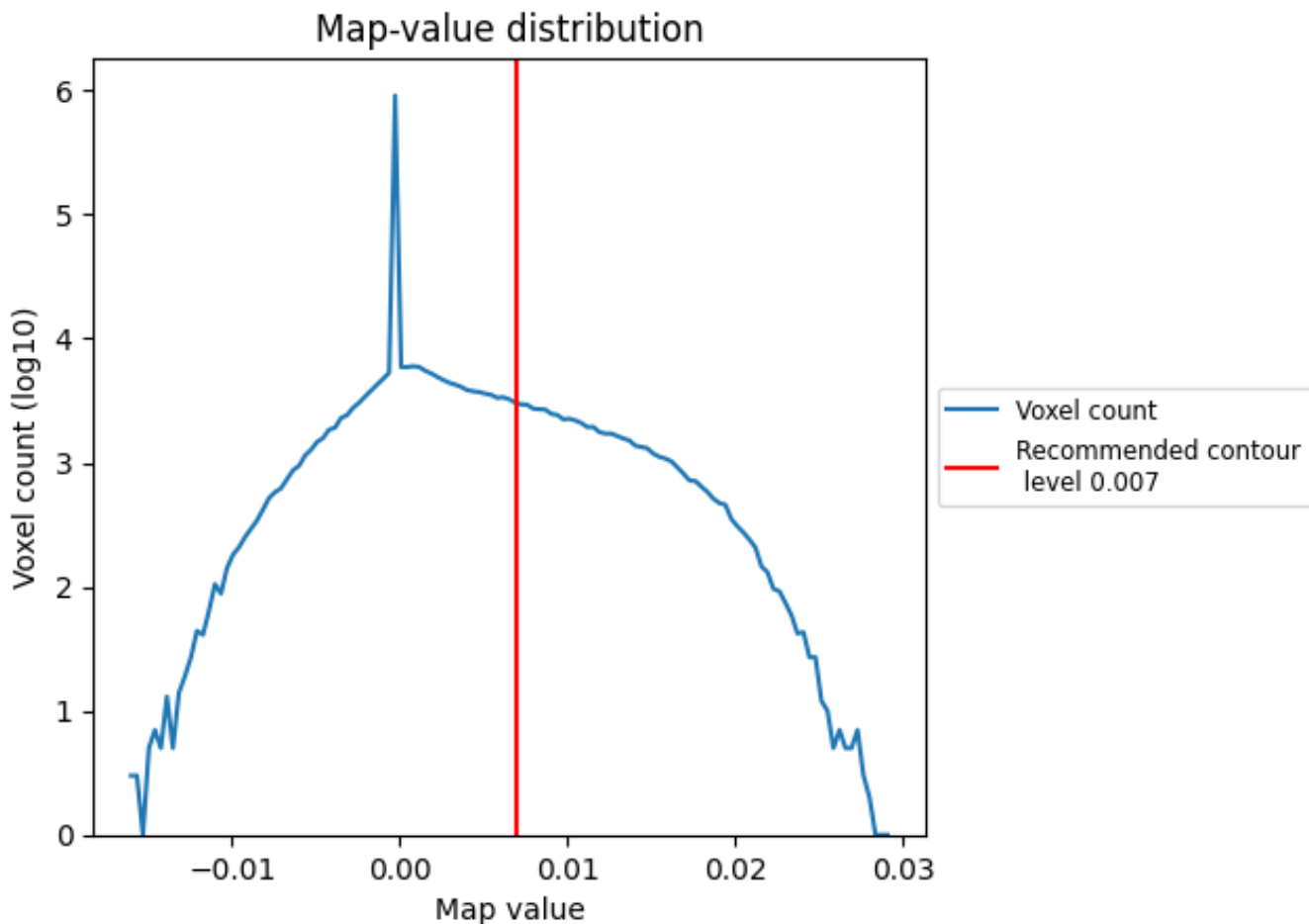
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

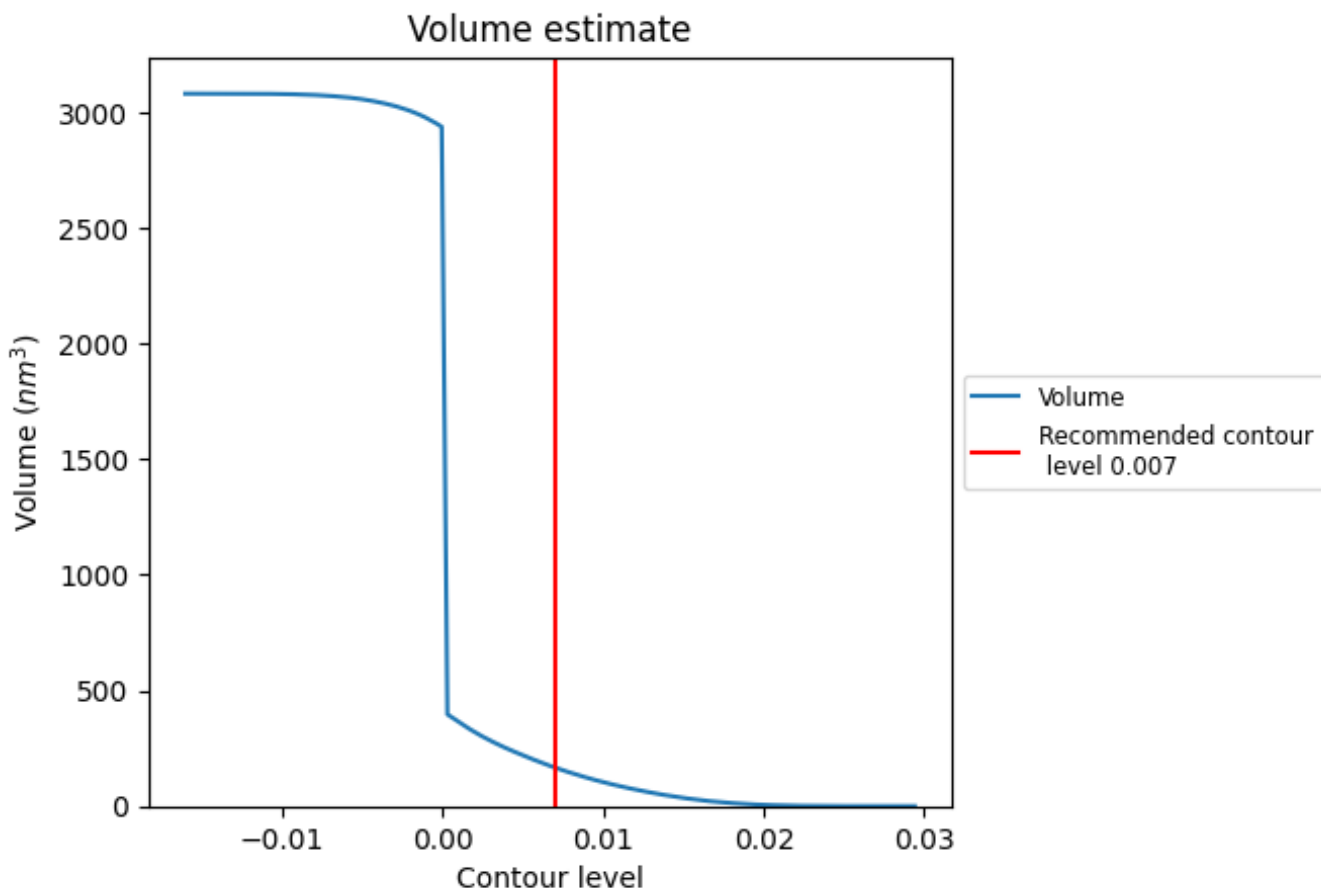
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 167 nm<sup>3</sup>; this corresponds to an approximate mass of 151 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.

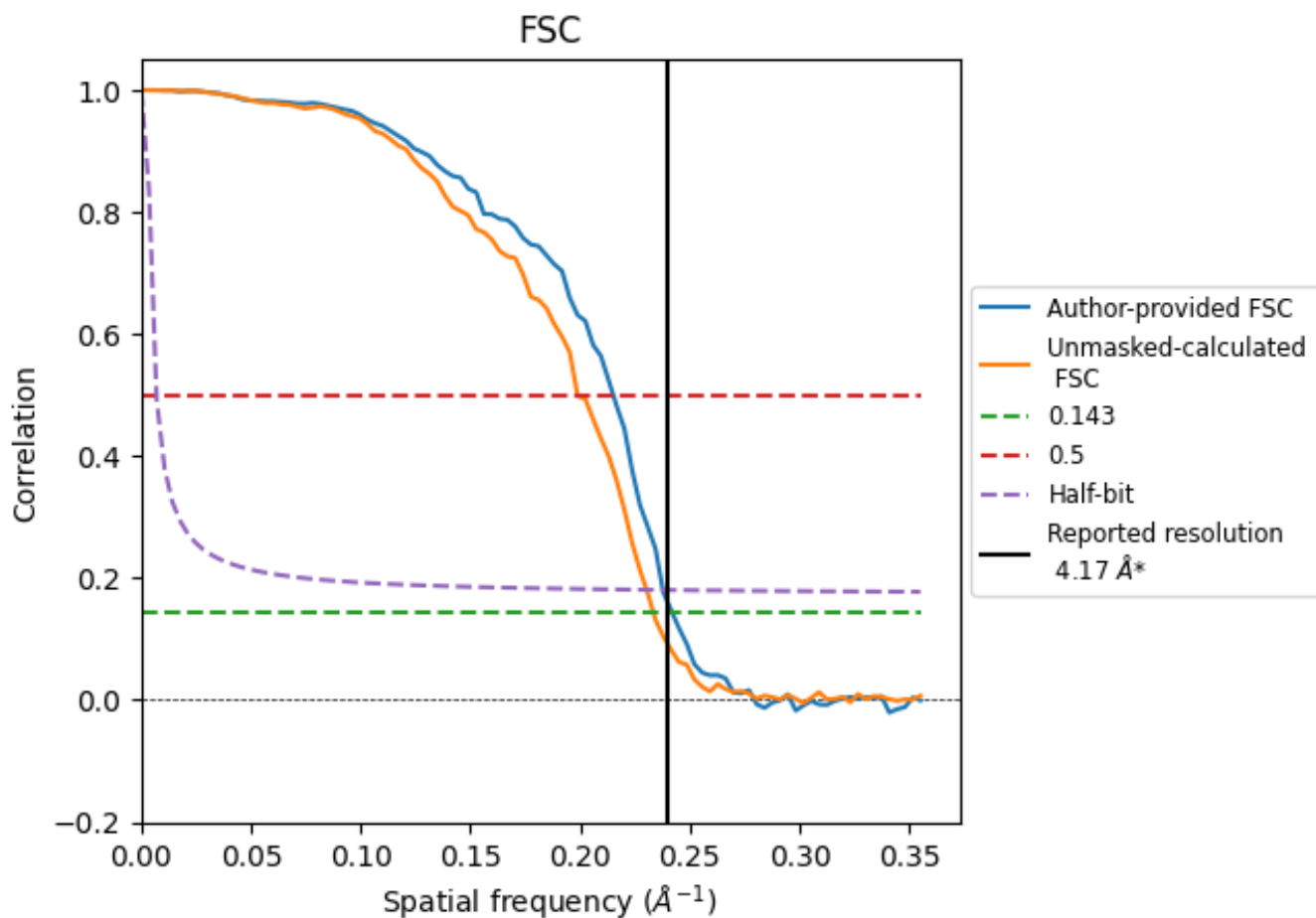
## 7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

## 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 0.240 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

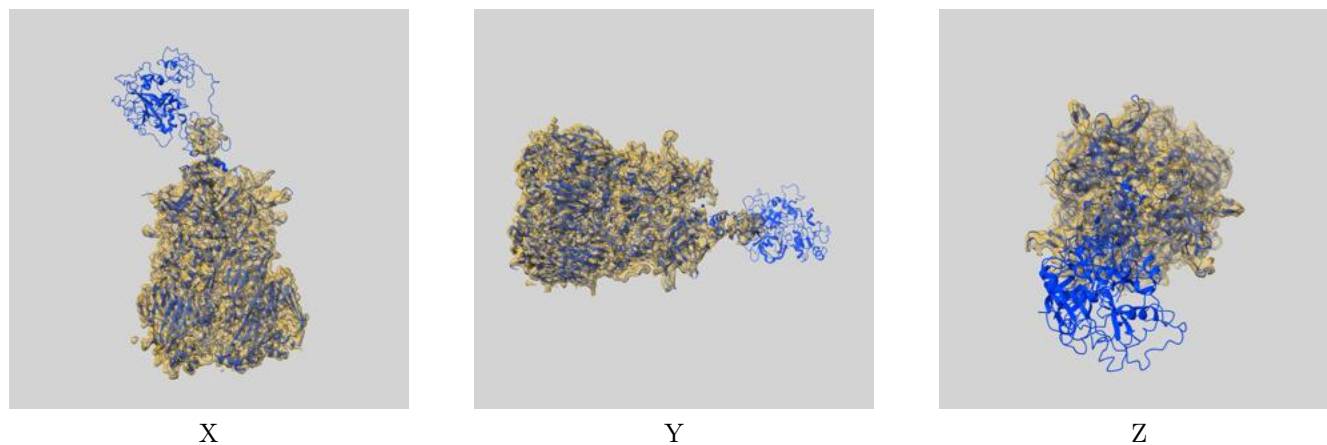
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.17	-	-
Author-provided FSC curve	4.13	4.65	4.21
Unmasked-calculated*	4.28	5.03	4.34

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

## 9 Map-model fit [i](#)

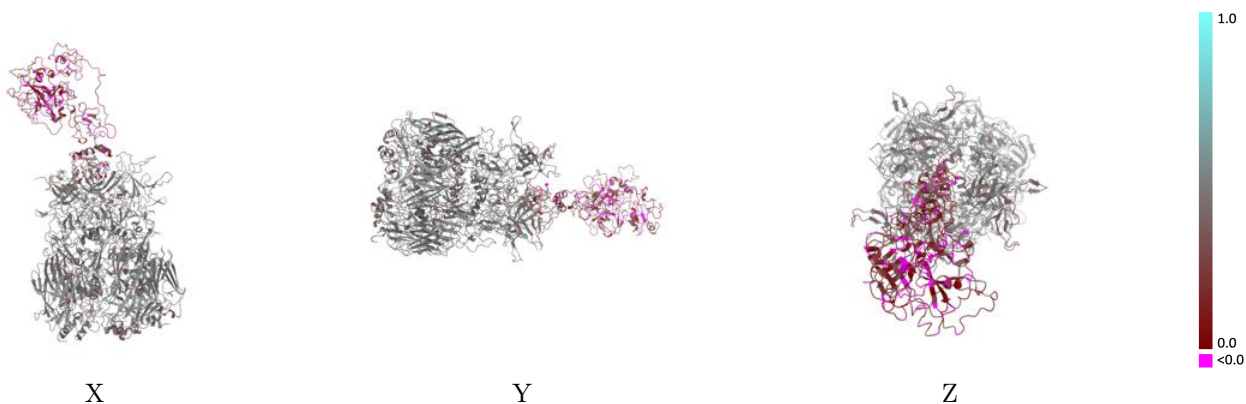
This section contains information regarding the fit between EMDB map EMD-45751 and PDB model 9CMO. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



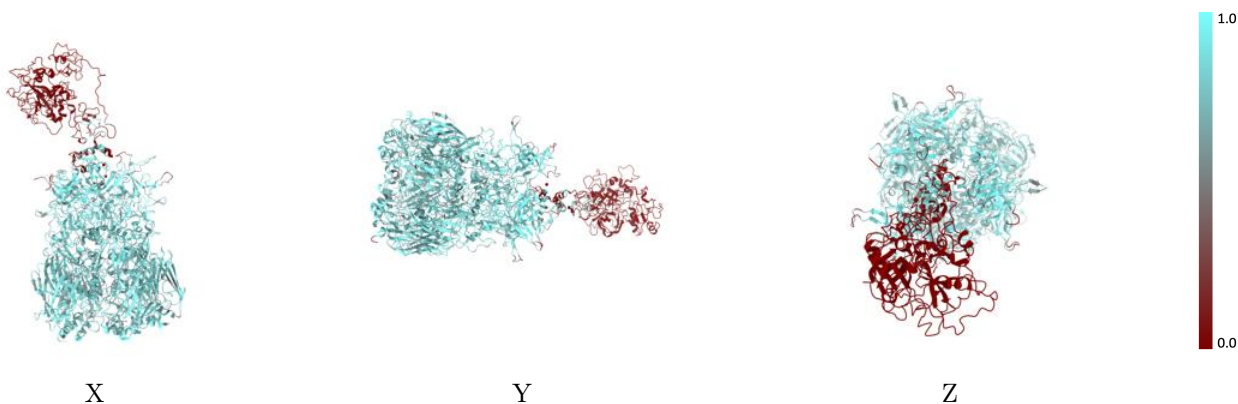
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



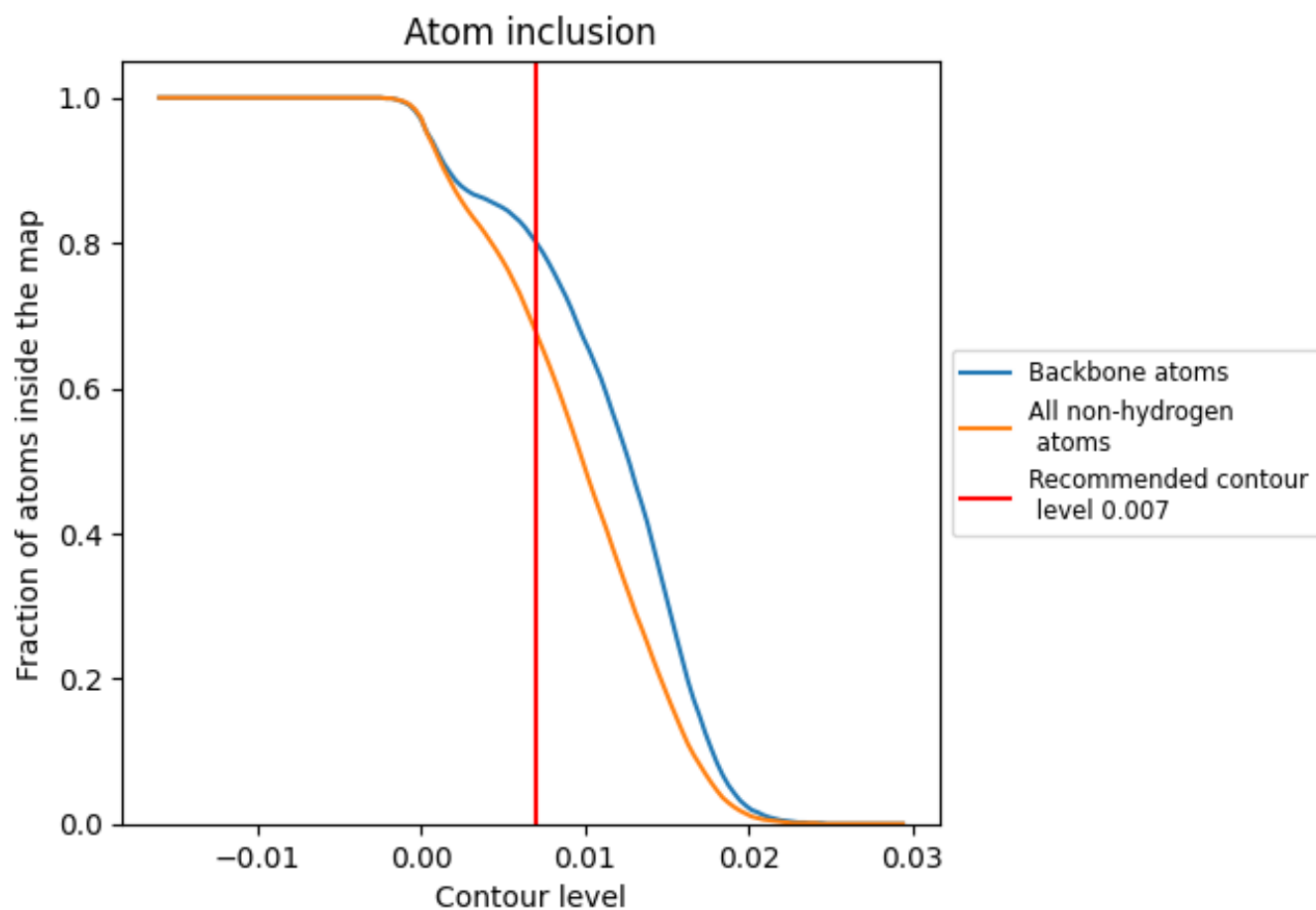
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).











## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6770	 0.4090
J	 0.7960	 0.4630
K	 0.7980	 0.4590
L	 0.8050	 0.4610
Z	 0.0860	 0.1610

