



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:54 AM UTC

PDB ID : 3JBH / pdb_00003jbh
EMDB ID : EMD-1950
Title : TWO HEAVY MEROMYOSIN INTERACTING-HEADS MOTIFS FLEXIBLE DOCKED INTO TARANTULA THICK FILAMENT 3D-MAP ALLOWS IN DEPTH STUDY OF INTRA- AND INTERMOLECULAR INTERACTIONS
Authors : Alamo, L.; Qi, D.; Wriggers, W.; Pinto, A.; Zhu, J.; Bilbao, A.; Gillilan, R.E.; Hu, S.; Padron, R.
Deposited on : 2015-09-01
Resolution : 20.00 Å(reported)
Based on initial model : 3DTP

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

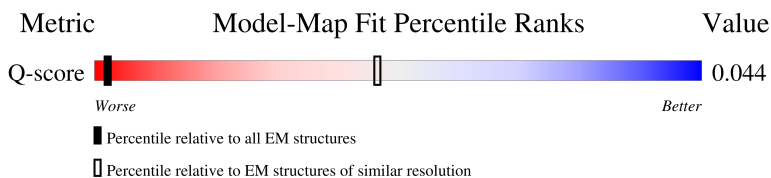
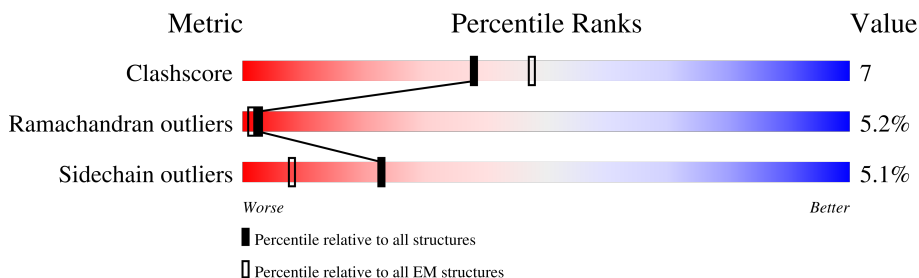
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 Å.

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



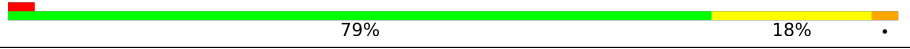
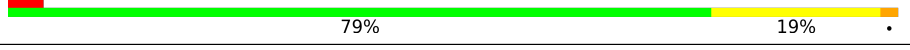
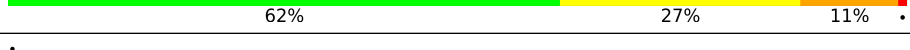
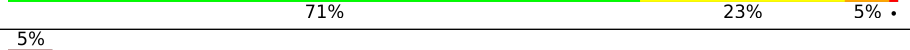
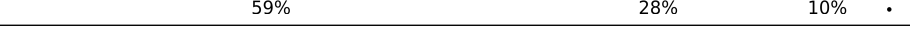
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	28 (19.50 - 20.50)

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

Mol	Chain	Length	Quality of chain
1	A	1953	
1	B	1953	
1	G	1953	

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Mol	Chain	Length	Quality of chain
1	H	1953	
2	C	156	
2	D	156	
2	I	156	
2	J	156	
3	E	196	
3	F	196	
3	K	196	
3	L	196	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 41968 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 MYOSIN 2 HEAVY CHAIN STRIATED MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	962	Total	C	N	O	S	0	0
			7721	4907	1334	1450	30		
1	B	964	Total	C	N	O	S	0	0
			7739	4918	1338	1453	30		
1	G	962	Total	C	N	O	S	0	0
			7721	4907	1334	1450	30		
1	H	964	Total	C	N	O	S	0	0
			7739	4918	1338	1453	30		

- Molecule 2 is a protein called MYOSIN 2 ESSENTIAL LIGHT CHAIN STRIATED MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	156	Total	C	N	O	S	0	0
			1233	779	199	247	8		
2	D	156	Total	C	N	O	S	0	0
			1233	779	199	247	8		
2	I	156	Total	C	N	O	S	0	0
			1233	779	199	247	8		
2	J	156	Total	C	N	O	S	0	0
			1233	779	199	247	8		

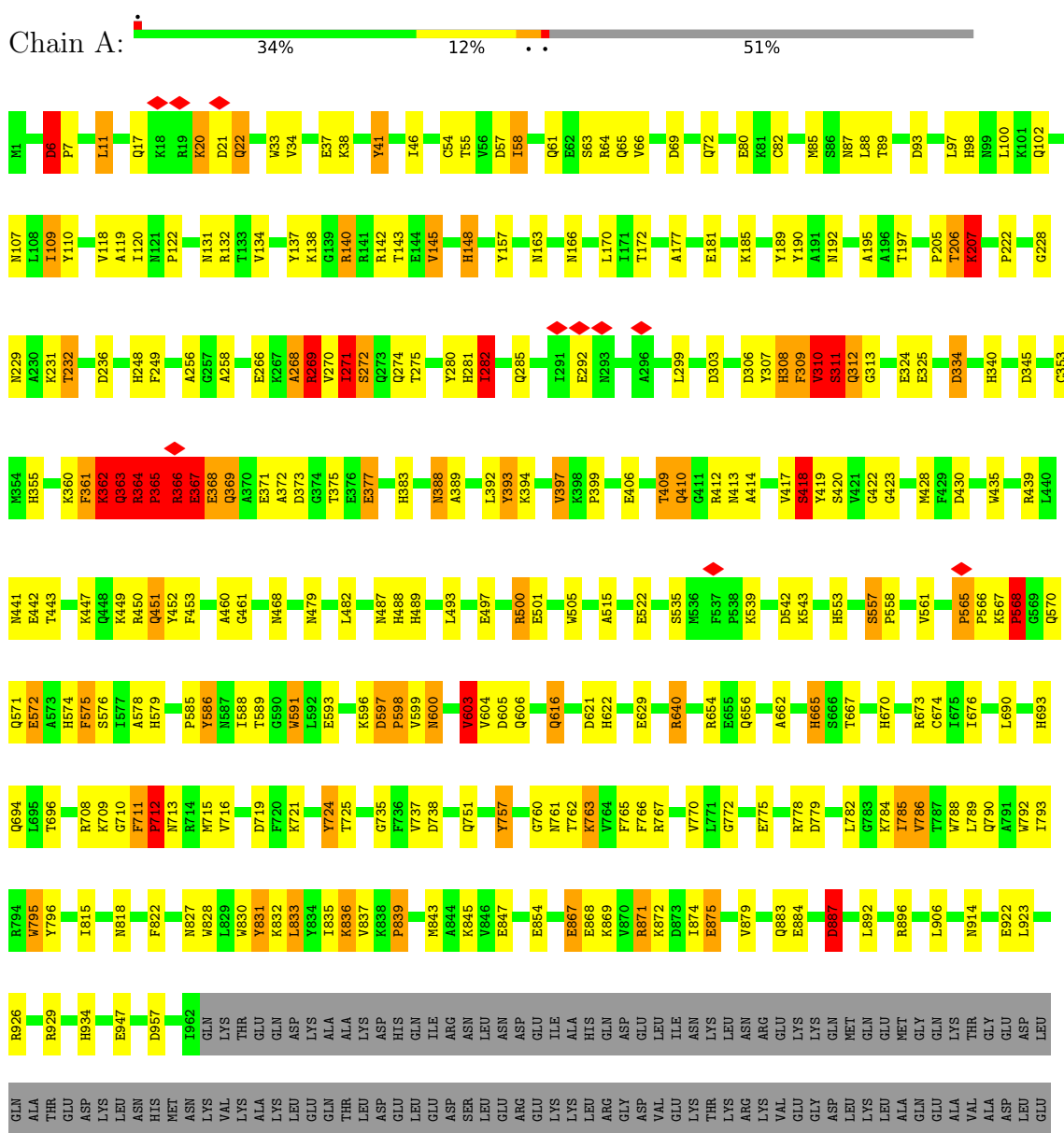
- Molecule 3 is a protein called MYOSIN 2 REGULATORY LIGHT CHAIN STRIATED MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	196	Total	C	N	O	S	0	0
			1529	952	257	314	6		
3	F	196	Total	C	N	O	S	0	0
			1529	952	257	314	6		
3	K	196	Total	C	N	O	S	0	0
			1529	952	257	314	6		
3	L	196	Total	C	N	O	S	0	0
			1529	952	257	314	6		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MYOSIN 2 HEAVY CHAIN STRIATED MUSCLE



- Molecule 1: MYOSIN 2 HEAVY CHAIN STRIATED MUSCLE



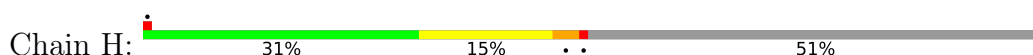
WORLDWIDE
PDB
PROTEIN DATA BANK

ASP	ARG	VAL	ILE	LEU	PHE	HIS	ALA	LYS	GLU	HIS	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889	E890	E891	E892	E893	E894	E895	E896	E897	E898	E899	E900	E901	E902	E903	E904	E905	E906	E907	E908	E909	E910	E911	E912	E913	E914	E915	E916	E917	E918	E919	E920	E921	E922	E923	E924	E925	E926	E927	E928	E929	E930	E931	E932	E933	E934	E935	E936	E937	E938	E939	E940	E941	E942	E943	E944	E945	E946	E947	E948	E949	E950	E951	E952	E953	E954	E955	E956	E957	E958	E959	E960	E961	E962	E963	E964	E965	E966	E967	E968	E969	E970	E971	E972	E973	E974	E975	E976	E977	E978	E979	E980	E981	E982	E983	E984	E985	E986	E987	E988	E989	E990	E991	E992	E993	E994	E995	E996	E997	E998	E999	D900	D901	D902	D903	D904	D905	D906	D907	D908	D909	D910	D911	D912	D913	D914	D915	D916	D917	D918	D919	D920	D921	D922	D923	D924	D925	D926	D927	D928	D929	D930	D931	D932	D933	D934	D935	D936	D937	D938	D939	D940	D941	D942	D943	D944	D945	D946	D947	D948	D949	D950	D951	D952	D953	D954	D955	D956	D957	D958	D959	D960	D961	D962	D963	D964	D965	D966	D967	D968	D969	D970	D971	D972	D973	D974	D975	D976	D977	D978	D979	D980	D981	D982	D983	D984	D985	D986	D987	D988	D989	D990	D991	D992	D993	D994	D995	D996	D997	D998	D999	C000	C001	C002	C003	C004	C005	C006	C007	C008	C009	C010	C011	C012	C013	C014	C015	C016	C017	C018	C019	C020	C021	C022	C023	C024	C025	C026	C027	C028	C029	C030	C031	C032	C033	C034	C035	C036	C037	C038	C039	C040	C041	C042	C043	C044	C045	C046	C047	C048	C049	C050	C051	C052	C053	C054	C055	C056	C057	C058	C059	C060	C061	C062	C063	C064	C065	C066	C067	C068	C069	C070	C071	C072	C073	C074	C075	C076	C077	C078	C079	C080	C081	C082	C083	C084	C085	C086	C087	C088	C089	C090	C091	C092	C093	C094	C095	C096	C097	C098	C099	C100	C101	C102	C103	C104	C105	C106	C107	C108	C109	C110	C111	C112	C113	C114	C115	C116	C117	C118	C119	C120	C121	C122	C123	C124	C125	C126	C127	C128	C129	C130	C131	C132	C133	C134	C135	C136	C137	C138	C139	C140	C141	C142	C143	C144	C145	C146	C147	C148	C149	C150	C151	C152	C153	C154	C155	C156	C157	C158	C159	C160	C161	C162	C163	C164	C165	C166	C167	C168	C169	C170	C171	C172	C173	C174	C175	C176	C177	C178	C179	C180	C181	C182	C183	C184	C185	C186	C187	C188	C189	C190	C191	C192	C193	C194	C195	C196	C197	C198	C199	B000	B001	B002	B003	B004	B005	B006	B007	B008	B009	B010	B011	B012	B013	B014	B015	B016	B017	B018	B019	B020	B021	B022	B023	B024	B025	B026	B027	B028	B029	B030	B031	B032	B033	B034	B035	B036	B037	B038	B039	B040	B041	B042	B043	B044	B045	B046	B047	B048	B049	B050	B051	B052	B053	B054	B055	B056	B057	B058	B059	B060	B061	B062	B063	B064	B065	B066	B067	B068	B069	B070	B071	B072	B073	B074	B075	B076	B077	B078	B079	B080	B081	B082	B083	B084	B085	B086	B087	B088	B089	B090	B091	B092	B093	B094	B095	B096	B097	B098	B099	A000	A001	A002	A003	A004	A005	A006	A007	A008	A009	A010	A011	A012	A013	A014	A015	A016	A017	A018	A019	A020	A021	A022	A023	A024	A025	A026	A027	A028	A029	A030	A031	A032	A033	A034	A035	A036	A037	A038	A039	A040	A041	A042	A043	A044	A045	A046	A047	A048	A049	A050	A051	A052	A053	A054	A055	A056	A057	A058	A059	A060	A061	A062	A063	A064	A065	A066	A067	A068	A069	A070	A071	A072	A073	A074	A075	A076	A077	A078	A079	A080	A081	A082	A083	A084	A085	A086	A087	A088	A089	A090	A091	A092	A093	A094	A095	A096	A097	A098	A099	Z000	Z001	Z002	Z003	Z004	Z005	Z006	Z007	Z008	Z009	Z010	Z011	Z012	Z013	Z014	Z015	Z016	Z017	Z018	Z019	Z020	Z021	Z022	Z023	Z024	Z025	Z026	Z027	Z028	Z029	Z030	Z031	Z032	Z033	Z034	Z035	Z036	Z037	Z038	Z039	Z040	Z041	Z042	Z043	Z044	Z045	Z046	Z047	Z048	Z049	Z050	Z051	Z052	Z053	Z054	Z055	Z056	Z057	Z058	Z059	Z060	Z061	Z062	Z063	Z064	Z065	Z066	Z067	Z068	Z069	Z070	Z071	Z072	Z073	Z074	Z075	Z076	Z077	Z078	Z079	Z080	Z081	Z082	Z083	Z084	Z085	Z086	Z087	Z088	Z089	Z090	Z091	Z092	Z093	Z094	Z095	Z096	Z097	Z098	Z099	R000	R001	R002	R003	R004	R005	R006	R007	R008	R009	R010	R011	R012	R013	R014	R015	R016	R017	R018	R019	R020	R021	R022	R023	R024	R025	R026	R027	R028	R029	R030	R031	R032	R033	R034	R035	R036	R037	R038	R039	R040	R041	R042	R043	R044	R045	R046	R047	R048	R049	R050	R051	R052	R053	R054	R055	R056	R057	R058	R059	R060	R061	R062	R063	R064	R065	R066	R067	R068	R069	R070	R071	R072	R073	R074	R075	R076	R077	R078	R079	R080	R081	R082	R083	R084	R085	R086	R087	R088	R089	R090	R091	R092	R093	R094	R095	R096	R097	R098	R099	Q000	Q001	Q002	Q003	Q004	Q005	Q006	Q007	Q008	Q009	Q010	Q011	Q012	Q013	Q014	Q015	Q016	Q017	Q018	Q019	Q020	Q021	Q022	Q023	Q024	Q025	Q026	Q027	Q028	Q029	Q030	Q031	Q032	Q033	Q034	Q035	Q036	Q037	Q038	Q039	Q040	Q041	Q042	Q043	Q044	Q045	Q046	Q047	Q048	Q049	Q050	Q051	Q052	Q053	Q054	Q055	Q056	Q057	Q058	Q059	Q060	Q061	Q062	Q063	Q064	Q065	Q066	Q067	Q068	Q069	Q070	Q071	Q072	Q073	Q074	Q075	Q076	Q077	Q078	Q079	Q080	Q081	Q082	Q083	Q084	Q085	Q086	Q087	Q088	Q089	Q090	Q091	Q092	Q093	Q094	Q095	Q096	Q097	Q098	Q099	P000	P001	P002	P003	P004	P005	P006	P007	P008	P009	P010	P011	P012	P013	P014	P015	P016	P017	P018	P019	P020	P021	P022	P023	P024	P025	P026	P027	P028	P029	P030	P031	P032	P033	P034	P035	P036	P037	P038	P039	P040	P041	P042	P043	P044	P045	P046	P047	P048	P049	P050	P051	P052	P053	P054	P055	P056	P057	P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- Molecule 1: MYOSIN 2 HEAVY CHAIN STRIATED MUSCLE



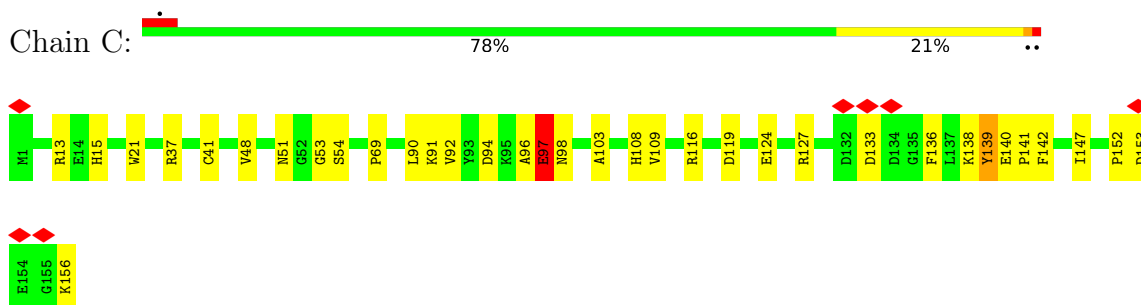
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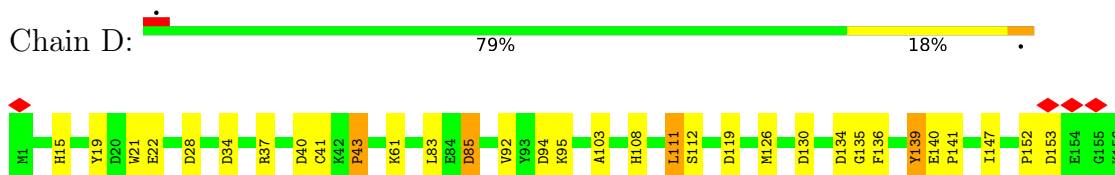


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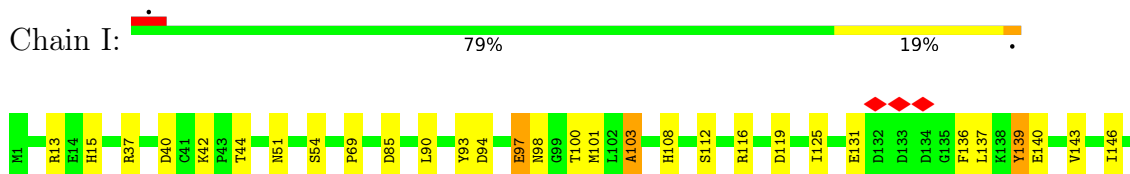
- Molecule 2: MYOSIN 2 ESSENTIAL LIGHT CHAIN STRIATED MUSCLE

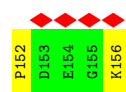


- Molecule 2: MYOSIN 2 ESSENTIAL LIGHT CHAIN STRIATED MUSCLE

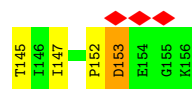
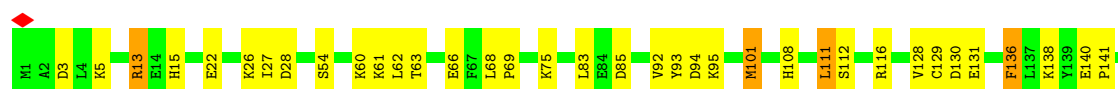


- Molecule 2: MYOSIN 2 ESSENTIAL LIGHT CHAIN STRIATED MUSCLE

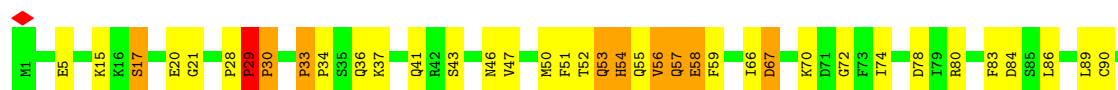




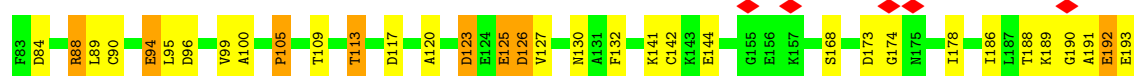
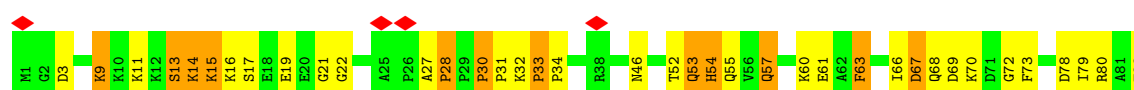
- Molecule 2: MYOSIN 2 ESSENTIAL LIGHT CHAIN STRIATED MUSCLE



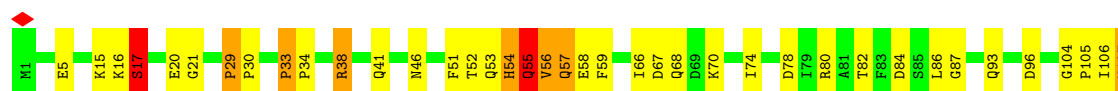
- Molecule 3: MYOSIN 2 REGULATORY LIGHT CHAIN STRIATED MUSCLE



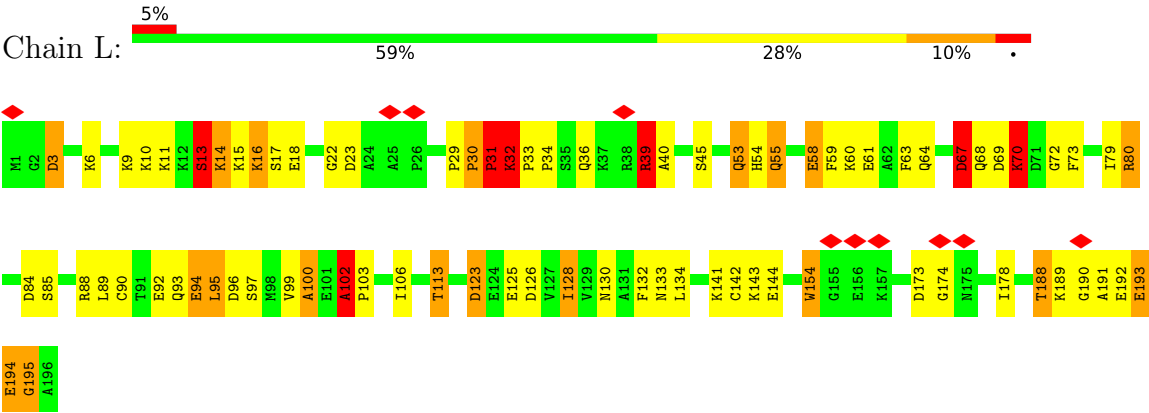
- Molecule 3: MYOSIN 2 REGULATORY LIGHT CHAIN STRIATED MUSCLE



- Molecule 3: MYOSIN 2 REGULATORY LIGHT CHAIN STRIATED MUSCLE



- Molecule 3: MYOSIN 2 REGULATORY LIGHT CHAIN STRIATED MUSCLE



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=30°, rise=100 Å, axial sym=C4	Depositor
Number of segments used	Not provided	
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI/PHILIPS CM120T	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	1950	Depositor
Maximum defocus (nm)	1950	Depositor
Magnification	35000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	247.077	Depositor
Minimum map value	-0.037	Depositor
Average map value	10.023	Depositor
Map value standard deviation	28.567	Depositor
Recommended contour level	25	Depositor
Map size (Å)	620, 620, 620.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	2.48, 2.48, 2.482	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.75	24/7867 (0.3%)	1.70	157/10591 (1.5%)
1	B	0.74	22/7885 (0.3%)	1.67	144/10614 (1.4%)
1	G	0.72	20/7867 (0.3%)	1.63	126/10591 (1.2%)
1	H	0.73	18/7885 (0.2%)	1.67	140/10614 (1.3%)
2	C	0.68	2/1251 (0.2%)	1.49	13/1674 (0.8%)
2	D	0.69	2/1251 (0.2%)	1.50	13/1674 (0.8%)
2	I	0.66	2/1251 (0.2%)	1.50	12/1674 (0.7%)
2	J	0.68	2/1251 (0.2%)	1.48	9/1674 (0.5%)
3	E	0.63	1/1554 (0.1%)	1.58	25/2081 (1.2%)
3	F	0.66	1/1554 (0.1%)	1.68	30/2081 (1.4%)
3	K	0.64	1/1554 (0.1%)	1.63	30/2081 (1.4%)
3	L	0.75	3/1554 (0.2%)	1.78	37/2081 (1.8%)
All	All	0.72	98/42724 (0.2%)	1.65	736/57430 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	32
1	B	0	20
1	G	0	25
1	H	0	19
2	D	0	1
2	I	0	1
2	J	0	4
3	E	0	1
3	F	0	3
3	K	0	2
3	L	0	8
All	All	0	116

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	364	ARG	CA-C	9.44	1.64	1.52
1	G	148	HIS	CD2-NE2	-7.44	1.29	1.37
1	A	363	GLN	CA-C	7.29	1.62	1.52
2	D	108	HIS	CD2-NE2	-7.27	1.29	1.37
1	H	489	HIS	CD2-NE2	-7.18	1.29	1.37
1	H	355	HIS	CD2-NE2	-7.12	1.30	1.37
1	A	579	HIS	CD2-NE2	-7.05	1.30	1.37
1	H	574	HIS	CD2-NE2	-7.04	1.30	1.37
3	L	31	PRO	CA-C	7.01	1.62	1.52
1	A	355	HIS	CD2-NE2	-6.99	1.30	1.37
1	B	489	HIS	CD2-NE2	-6.98	1.30	1.37
1	B	148	HIS	CD2-NE2	-6.97	1.30	1.37
1	B	383	HIS	CD2-NE2	-6.95	1.30	1.37
2	C	15	HIS	CD2-NE2	-6.93	1.30	1.37
1	H	248	HIS	CD2-NE2	-6.90	1.30	1.37
1	G	488	HIS	CD2-NE2	-6.87	1.30	1.37
1	A	488	HIS	CD2-NE2	-6.82	1.30	1.37
1	G	281	HIS	CD2-NE2	-6.76	1.30	1.37
1	G	489	HIS	CD2-NE2	-6.72	1.30	1.37
1	B	574	HIS	CD2-NE2	-6.71	1.30	1.37
1	H	553	HIS	CD2-NE2	-6.68	1.30	1.37
3	K	54	HIS	CD2-NE2	-6.67	1.30	1.37
1	A	148	HIS	CD2-NE2	-6.66	1.30	1.37
3	E	54	HIS	CD2-NE2	-6.62	1.30	1.37
1	A	281	HIS	CD2-NE2	-6.62	1.30	1.37
1	A	489	HIS	CD2-NE2	-6.61	1.30	1.37
1	B	665	HIS	CD2-NE2	-6.57	1.30	1.37
2	J	15	HIS	CD2-NE2	-6.56	1.30	1.37
1	B	340	HIS	CD2-NE2	-6.55	1.30	1.37
1	B	488	HIS	CD2-NE2	-6.55	1.30	1.37
2	D	15	HIS	CD2-NE2	-6.54	1.30	1.37
1	H	665	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	98	HIS	CD2-NE2	-6.54	1.30	1.37
1	G	622	HIS	CD2-NE2	-6.53	1.30	1.37
1	G	670	HIS	CD2-NE2	-6.52	1.30	1.37
1	G	574	HIS	CD2-NE2	-6.52	1.30	1.37
1	B	553	HIS	CD2-NE2	-6.51	1.30	1.37
3	L	54	HIS	CD2-NE2	-6.51	1.30	1.37
1	G	98	HIS	CD2-NE2	-6.51	1.30	1.37
1	A	553	HIS	CD2-NE2	-6.50	1.30	1.37
1	G	934	HIS	CD2-NE2	-6.49	1.30	1.37
1	H	693	HIS	CD2-NE2	-6.49	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	355	HIS	CD2-NE2	-6.49	1.30	1.37
1	A	670	HIS	CD2-NE2	-6.49	1.30	1.37
1	G	665	HIS	CD2-NE2	-6.47	1.30	1.37
1	H	934	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	665	HIS	CD2-NE2	-6.47	1.30	1.37
1	H	383	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	622	HIS	CD2-NE2	-6.46	1.30	1.37
1	B	248	HIS	CD2-NE2	-6.46	1.30	1.37
1	H	670	HIS	CD2-NE2	-6.46	1.30	1.37
1	G	579	HIS	CD2-NE2	-6.45	1.30	1.37
1	B	693	HIS	CD2-NE2	-6.44	1.30	1.37
1	B	355	HIS	CD2-NE2	-6.43	1.30	1.37
1	H	488	HIS	CD2-NE2	-6.43	1.30	1.37
1	G	693	HIS	CD2-NE2	-6.42	1.30	1.37
1	H	340	HIS	CD2-NE2	-6.42	1.30	1.37
1	H	308	HIS	CD2-NE2	-6.42	1.30	1.37
1	A	693	HIS	CD2-NE2	-6.42	1.30	1.37
1	B	934	HIS	CD2-NE2	-6.41	1.30	1.37
1	G	308	HIS	CD2-NE2	-6.40	1.30	1.37
1	A	340	HIS	CD2-NE2	-6.39	1.30	1.37
1	H	281	HIS	CD2-NE2	-6.38	1.30	1.37
1	G	340	HIS	CD2-NE2	-6.37	1.30	1.37
1	H	148	HIS	CD2-NE2	-6.37	1.30	1.37
1	A	248	HIS	CD2-NE2	-6.32	1.30	1.37
2	C	108	HIS	CD2-NE2	-6.29	1.30	1.37
1	A	574	HIS	CD2-NE2	-6.29	1.30	1.37
1	G	248	HIS	CD2-NE2	-6.25	1.30	1.37
3	F	54	HIS	CD2-NE2	-6.24	1.30	1.37
1	G	553	HIS	CD2-NE2	-6.24	1.30	1.37
2	I	108	HIS	CD2-NE2	-6.22	1.31	1.37
1	H	579	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	383	HIS	CD2-NE2	-6.19	1.31	1.37
1	B	308	HIS	CD2-NE2	-6.14	1.31	1.37
1	G	383	HIS	CD2-NE2	-6.08	1.31	1.37
2	I	15	HIS	CD2-NE2	-6.08	1.31	1.37
1	B	579	HIS	CD2-NE2	-6.06	1.31	1.37
1	B	281	HIS	CD2-NE2	-6.05	1.31	1.37
1	B	98	HIS	CD2-NE2	-6.04	1.31	1.37
1	A	363	GLN	N-CA	6.00	1.53	1.46
1	H	622	HIS	CD2-NE2	-5.96	1.31	1.37
1	A	934	HIS	CD2-NE2	-5.87	1.31	1.37
2	J	108	HIS	CD2-NE2	-5.84	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	622	HIS	CD2-NE2	-5.82	1.31	1.37
1	B	670	HIS	CD2-NE2	-5.82	1.31	1.37
1	A	308	HIS	CD2-NE2	-5.72	1.31	1.37
1	H	98	HIS	CD2-NE2	-5.58	1.31	1.37
1	B	670	HIS	CG-ND1	-5.38	1.32	1.38
3	L	31	PRO	N-CA	5.35	1.54	1.47
1	B	579	HIS	CG-ND1	-5.28	1.32	1.38
1	A	364	ARG	N-CA	5.26	1.53	1.46
1	G	579	HIS	CG-ND1	-5.17	1.32	1.38
1	G	665	HIS	CG-ND1	-5.13	1.32	1.38
1	B	248	HIS	CG-ND1	-5.12	1.32	1.38
1	A	665	HIS	CG-ND1	-5.11	1.32	1.38
1	B	665	HIS	CG-ND1	-5.11	1.32	1.38
1	A	148	HIS	CG-ND1	-5.10	1.32	1.38

All (736) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	565	PRO	N-CA-C	19.02	133.91	110.70
1	B	565	PRO	N-CA-C	18.55	133.34	110.70
1	A	364	ARG	CA-C-N	13.91	137.23	119.84
1	A	364	ARG	C-N-CA	13.91	137.23	119.84
1	A	365	PRO	CA-N-CD	-13.75	92.75	112.00
1	G	367	GLU	O-C-N	-12.30	106.22	122.59
1	A	365	PRO	N-CA-C	11.41	135.98	112.47
1	A	324	GLU	N-CA-C	11.36	123.22	111.07
1	A	367	GLU	O-C-N	-11.33	107.52	122.59
1	G	310	VAL	O-C-N	-11.29	108.45	122.57
1	A	206	THR	O-C-N	-11.27	110.75	121.79
1	A	362	LYS	CA-C-N	11.16	142.85	121.54
1	A	362	LYS	C-N-CA	11.16	142.85	121.54
1	A	306	ASP	N-CA-C	11.02	134.27	110.80
1	H	453	PHE	N-CA-C	10.63	124.98	109.14
3	L	3	ASP	CA-CB-CG	10.28	122.88	112.60
3	L	13	SER	O-C-N	-10.21	109.02	122.59
1	A	311	SER	N-CA-C	10.13	132.37	110.80
1	G	268	ALA	O-C-N	-10.03	111.19	122.03
3	E	192	GLU	O-C-N	-9.84	111.17	122.68
3	K	192	GLU	O-C-N	-9.83	111.27	123.17
3	K	30	PRO	N-CA-C	9.74	122.59	110.70
1	B	76	PRO	N-CA-C	9.69	119.78	110.47
1	A	313	GLY	O-C-N	-9.50	112.42	123.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	600	ASN	CA-CB-CG	9.38	121.98	112.60
1	B	597	ASP	CA-CB-CG	9.30	121.90	112.60
1	B	453	PHE	N-CA-C	9.22	123.82	109.52
1	A	603	VAL	N-CA-C	9.19	128.46	109.34
1	G	206	THR	O-C-N	-9.15	110.42	122.59
3	K	46	ASN	N-CA-C	9.11	123.97	110.30
1	B	872	LYS	CG-CD-CE	9.10	132.24	111.30
1	A	268	ALA	O-C-N	-9.04	112.63	122.03
1	H	673	ARG	N-CA-CB	-8.95	100.32	110.35
3	L	195	GLY	O-C-N	-8.85	111.20	122.70
1	H	619	PHE	N-CA-C	8.75	124.64	113.88
1	A	309	PHE	CA-CB-CG	8.72	122.52	113.80
1	H	7	PRO	N-CA-C	8.72	124.12	111.13
1	A	377	GLU	N-CA-C	8.69	120.86	108.00
2	J	28	ASP	CA-CB-CG	8.69	121.29	112.60
1	H	154	ASP	CA-CB-CG	8.68	121.28	112.60
3	F	126	ASP	CA-CB-CG	8.61	121.21	112.60
1	H	229	ASN	CA-CB-CG	8.61	121.21	112.60
1	A	451	GLN	O-C-N	-8.59	112.63	122.68
1	A	312	GLN	N-CA-C	8.58	129.08	110.80
1	A	565	PRO	N-CA-C	8.55	121.14	110.70
1	A	364	ARG	N-CA-C	8.53	128.66	109.81
1	A	306	ASP	CA-CB-CG	-8.50	104.10	112.60
1	H	76	PRO	N-CA-C	8.46	121.02	110.70
3	E	56	VAL	N-CA-C	8.43	120.19	111.00
3	E	30	PRO	N-CA-C	8.37	120.91	110.70
1	B	619	PHE	N-CA-C	8.29	123.76	112.90
3	E	41	GLN	N-CA-C	8.27	121.00	110.33
1	G	603	VAL	N-CA-C	8.27	126.54	109.34
1	B	878	ASN	CA-CB-CG	8.25	120.85	112.60
1	H	235	ASN	N-CA-C	8.22	122.40	108.02
3	E	29	PRO	N-CA-C	8.21	120.71	110.70
1	G	568	PRO	CA-N-CD	-8.19	100.54	112.00
1	G	306	ASP	N-CA-C	8.18	121.33	110.53
1	G	887	ASP	CA-CB-CG	8.06	120.66	112.60
1	G	313	GLY	O-C-N	-8.02	113.12	122.91
3	F	67	ASP	CA-CB-CG	8.00	120.60	112.60
1	A	363	GLN	N-CA-CB	-7.95	97.05	110.49
1	A	670	HIS	CB-CG-CD2	-7.92	120.90	131.20
1	A	363	GLN	N-CA-C	7.87	127.55	110.80
3	K	195	GLY	O-C-N	-7.86	112.48	122.70
1	B	868	GLU	N-CA-C	7.85	115.22	108.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	600	ASN	OD1-CG-ND2	-7.83	114.77	122.60
1	A	145	VAL	CA-C-N	7.81	125.36	119.66
1	A	145	VAL	C-N-CA	7.81	125.36	119.66
1	H	564	LYS	CA-C-N	7.71	128.32	120.38
1	H	564	LYS	C-N-CA	7.71	128.32	120.38
1	A	522	GLU	N-CA-C	7.70	119.31	111.07
1	G	712	PRO	N-CA-C	7.70	128.33	112.47
1	B	620	GLU	N-CA-C	7.64	121.93	109.94
3	K	179	ASP	CA-CB-CG	7.63	120.23	112.60
1	A	363	GLN	CA-CB-CG	7.60	129.29	114.10
3	K	29	PRO	N-CA-C	7.59	119.96	110.70
1	G	93	ASP	N-CA-C	7.57	122.18	112.34
1	B	380	ARG	NE-CZ-NH1	-7.56	113.94	121.50
1	H	322	ASP	CA-CB-CG	7.52	120.12	112.60
2	I	85	ASP	CA-CB-CG	7.50	120.09	112.60
1	A	693	HIS	CB-CG-CD2	-7.48	121.47	131.20
1	G	593	GLU	CA-CB-CG	7.48	129.06	114.10
1	A	887	ASP	CA-CB-CG	7.48	120.08	112.60
1	B	154	ASP	CA-CB-CG	7.47	120.07	112.60
1	B	75	ASN	CA-C-N	7.43	125.08	119.66
1	B	75	ASN	C-N-CA	7.43	125.08	119.66
1	H	600	ASN	CA-CB-CG	7.43	120.03	112.60
1	G	324	GLU	N-CA-C	7.41	119.00	111.07
1	B	281	HIS	CA-CB-CG	7.38	121.18	113.80
1	A	414	ALA	N-CA-C	7.33	118.97	110.97
3	L	67	ASP	N-CA-C	7.33	126.40	110.80
1	A	367	GLU	CA-C-N	7.32	134.87	121.70
1	A	367	GLU	C-N-CA	7.32	134.87	121.70
1	B	564	LYS	CA-C-N	7.29	127.89	120.38
1	B	564	LYS	C-N-CA	7.29	127.89	120.38
1	H	395	ASN	OD1-CG-ND2	-7.29	115.31	122.60
1	A	364	ARG	CD-NE-CZ	-7.28	114.21	124.40
3	K	55	GLN	OE1-CD-NE2	-7.28	115.32	122.60
1	B	7	PRO	N-CA-C	7.26	121.39	111.22
1	A	712	PRO	N-CA-C	7.23	127.36	112.47
2	C	139	TYR	N-CA-C	7.22	120.07	111.33
1	H	597	ASP	CA-CB-CG	7.18	119.78	112.60
1	A	867	GLU	N-CA-C	7.18	118.80	110.97
1	G	363	GLN	OE1-CD-NE2	-7.17	115.43	122.60
1	B	595	ASN	CA-CB-CG	7.16	119.76	112.60
1	A	579	HIS	CB-CG-CD2	-7.16	121.90	131.20
1	B	131	ASN	CA-CB-CG	7.11	119.71	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	128	ILE	N-CA-C	7.09	117.81	110.36
1	A	363	GLN	OE1-CD-NE2	-7.08	115.52	122.60
1	G	121	ASN	OD1-CG-ND2	-7.07	115.53	122.60
1	B	694	GLN	OE1-CD-NE2	-7.04	115.56	122.60
1	A	600	ASN	CA-CB-CG	7.03	119.63	112.60
1	G	355	HIS	CB-CG-CD2	-7.01	122.08	131.20
2	D	85	ASP	CA-CB-CG	7.01	119.61	112.60
1	G	522	GLU	N-CA-C	7.01	118.57	111.07
1	H	383	HIS	CB-CG-CD2	-7.01	122.09	131.20
1	B	269	ARG	N-CA-C	7.00	119.76	111.71
1	G	597	ASP	N-CA-C	7.00	125.27	109.81
3	F	195	GLY	O-C-N	-6.99	113.61	122.70
1	G	388	ASN	CA-CB-CG	6.98	119.58	112.60
1	B	75	ASN	CA-CB-CG	6.97	119.57	112.60
1	B	871	ARG	CA-C-N	6.97	129.62	120.28
1	B	871	ARG	C-N-CA	6.97	129.62	120.28
1	G	833	LEU	N-CA-C	-6.96	97.86	109.07
1	G	367	GLU	CA-C-N	6.95	134.21	121.70
1	G	367	GLU	C-N-CA	6.95	134.21	121.70
1	B	57	ASP	CA-CB-CG	6.95	119.55	112.60
3	E	195	GLY	O-C-N	-6.93	113.69	122.70
1	H	553	HIS	CB-CG-CD2	-6.91	122.22	131.20
1	B	553	HIS	CB-CG-CD2	-6.90	122.23	131.20
1	H	308	HIS	N-CA-C	6.90	120.96	112.54
1	H	281	HIS	CA-CB-CG	6.87	120.67	113.80
3	L	31	PRO	N-CA-CB	-6.87	96.04	103.25
3	L	17	SER	N-CA-C	6.87	125.43	110.80
2	D	134	ASP	N-CA-C	6.86	120.98	112.47
1	H	148	HIS	CB-CG-CD2	-6.86	122.28	131.20
1	H	598	PRO	N-CA-C	6.86	126.59	112.47
1	H	771	LEU	CA-C-N	6.84	127.72	119.99
1	H	771	LEU	C-N-CA	6.84	127.72	119.99
3	F	84	ASP	CA-CB-CG	6.84	119.44	112.60
1	H	254	LYS	N-CA-C	6.82	119.13	110.33
1	A	109	ILE	N-CA-C	6.82	118.43	111.00
1	A	818	ASN	N-CA-C	6.81	118.71	111.28
3	F	13	SER	O-C-N	-6.81	113.53	122.59
1	A	589	THR	N-CA-C	6.80	120.70	110.64
1	H	847	GLU	N-CA-C	6.80	118.34	111.07
3	F	67	ASP	N-CA-C	6.79	125.27	110.80
1	G	334	ASP	CA-CB-CG	6.79	119.39	112.60
1	A	450	ARG	N-CA-C	6.77	120.72	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	835	ILE	N-CA-C	6.75	121.86	112.35
3	E	179	ASP	CA-CB-CG	6.73	119.33	112.60
3	L	126	ASP	CA-CB-CG	6.72	119.32	112.60
1	H	601	ASP	N-CA-C	6.72	119.22	111.02
1	G	102	GLN	OE1-CD-NE2	-6.71	115.89	122.60
1	H	86	SER	N-CA-C	6.71	125.09	110.80
3	L	123	ASP	CA-CB-CG	6.70	119.30	112.60
2	C	98	ASN	OD1-CG-ND2	-6.70	115.90	122.60
1	B	210	LYS	O-C-N	-6.69	113.69	122.59
1	B	321	ASP	CA-CB-CG	6.69	119.29	112.60
1	G	761	ASN	CA-CB-CG	6.67	119.27	112.60
1	H	248	HIS	CB-CG-CD2	-6.66	122.54	131.20
1	A	606	GLN	OE1-CD-NE2	-6.64	115.96	122.60
1	H	93	ASP	N-CA-C	6.64	118.21	110.97
1	A	360	LYS	O-C-N	-6.63	114.22	123.11
1	B	254	LYS	N-CA-C	6.63	119.08	110.53
3	F	100	ALA	N-CA-C	6.63	120.24	111.75
3	L	67	ASP	CA-CB-CG	6.62	119.22	112.60
1	H	355	HIS	CB-CG-CD2	-6.62	122.59	131.20
3	L	84	ASP	CA-CB-CG	6.62	119.22	112.60
3	K	131	ALA	N-CA-C	6.61	118.48	111.28
1	B	479	ASN	OD1-CG-ND2	-6.60	116.00	122.60
1	G	140	ARG	NE-CZ-NH1	-6.59	114.91	121.50
1	H	308	HIS	CB-CG-CD2	-6.59	122.63	131.20
1	H	665	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	G	248	HIS	CA-CB-CG	6.57	120.37	113.80
1	B	818	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	A	20	LYS	N-CA-C	6.56	118.77	110.24
1	B	179	LYS	N-CA-C	6.56	119.27	111.33
1	H	600	ASN	OD1-CG-ND2	-6.54	116.06	122.60
2	I	139	TYR	N-CA-C	6.54	120.12	111.75
1	A	87	ASN	OD1-CG-ND2	-6.54	116.06	122.60
1	B	654	ARG	NE-CZ-NH1	-6.53	114.97	121.50
1	B	383	HIS	CB-CG-CD2	-6.52	122.72	131.20
1	G	488	HIS	CB-CG-CD2	-6.51	122.73	131.20
1	A	670	HIS	CB-CG-ND1	6.51	132.47	122.70
1	B	621	ASP	CA-CB-CG	6.51	119.11	112.60
2	C	54	SER	N-CA-C	6.49	119.27	109.41
1	B	149	LEU	N-CA-C	6.48	124.60	110.80
3	K	107	ASN	OD1-CG-ND2	-6.47	116.12	122.60
1	G	773	ARG	N-CA-C	-6.47	105.04	113.12
1	G	414	ALA	N-CA-C	6.46	118.02	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	658	ASN	OD1-CG-ND2	-6.46	116.14	122.60
3	E	33	PRO	CA-C-N	6.45	126.14	119.56
3	E	33	PRO	C-N-CA	6.45	126.14	119.56
1	A	785	ILE	O-C-N	-6.44	115.25	122.66
1	A	957	ASP	CA-CB-CG	6.44	119.04	112.60
2	D	28	ASP	CA-CB-CG	6.43	119.03	112.60
3	K	54	HIS	CA-CB-CG	-6.42	107.38	113.80
1	B	637	GLY	O-C-N	-6.42	114.36	122.70
1	G	605	ASP	N-CA-C	6.41	119.95	111.75
1	G	896	ARG	N-CA-C	6.40	119.07	111.71
1	B	761	ASN	OD1-CG-ND2	-6.39	116.21	122.60
3	L	31	PRO	O-C-N	-6.38	114.02	122.64
1	A	369	GLN	OE1-CD-NE2	-6.37	116.23	122.60
1	A	410	GLN	N-CA-C	6.37	119.65	108.75
1	B	872	LYS	CB-CG-CD	6.37	125.96	111.30
1	B	458	ASP	CA-CB-CG	6.36	118.96	112.60
3	K	189	LYS	N-CA-C	-6.35	99.54	109.25
1	G	83	GLU	N-CA-C	6.34	121.26	112.45
2	D	153	ASP	CA-CB-CG	6.33	118.93	112.60
1	H	57	ASP	CA-CB-CG	6.33	118.93	112.60
1	H	64	ARG	NE-CZ-NH1	-6.32	115.18	121.50
1	A	598	PRO	N-CA-C	6.31	120.41	110.50
1	H	28	GLY	O-C-N	-6.30	114.51	122.70
1	G	422	GLY	O-C-N	-6.28	114.53	122.70
1	A	6	ASP	N-CA-C	6.28	123.69	109.81
1	B	146	PRO	N-CA-CB	-6.28	96.99	103.08
2	J	111	LEU	N-CA-C	6.27	118.20	111.36
3	K	33	PRO	CA-C-N	6.27	125.84	119.19
3	K	33	PRO	C-N-CA	6.27	125.84	119.19
1	A	596	LYS	CA-CB-CG	6.27	126.63	114.10
1	H	574	HIS	CA-CB-CG	6.27	120.07	113.80
1	G	64	ARG	NE-CZ-NH1	-6.26	115.24	121.50
3	L	17	SER	O-C-N	-6.26	114.26	122.59
2	I	54	SER	N-CA-C	6.26	117.74	108.60
1	B	847	GLU	N-CA-C	6.26	118.62	111.11
1	A	268	ALA	CA-C-O	-6.26	114.43	121.00
3	L	31	PRO	N-CD-CG	-6.26	93.81	103.20
3	F	88	ARG	N-CA-C	6.25	124.11	110.80
1	H	229	ASN	OD1-CG-ND2	-6.25	116.35	122.60
1	G	451	GLN	O-C-N	-6.25	115.37	122.68
1	G	308	HIS	CB-CG-CD2	-6.24	123.09	131.20
1	A	355	HIS	CB-CG-CD2	-6.24	123.09	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	109	ILE	N-CA-C	6.23	116.86	110.82
1	B	449	LYS	O-C-N	-6.21	116.35	122.99
1	B	641	LYS	O-C-N	-6.18	113.11	123.00
3	L	102	ALA	O-C-N	-6.18	114.22	121.32
3	F	16	LYS	O-C-N	-6.18	114.38	122.59
1	A	131	ASN	CA-CB-CG	6.17	118.78	112.60
1	A	553	HIS	N-CA-C	6.17	120.76	113.23
3	E	191	ALA	N-CA-C	6.17	118.03	109.15
3	K	53	GLN	OE1-CD-NE2	-6.16	116.44	122.60
1	H	628	GLU	N-CA-C	6.16	119.83	112.93
3	F	46	ASN	OD1-CG-ND2	-6.16	116.44	122.60
3	K	66	ILE	N-CA-C	-6.15	104.85	110.82
2	D	111	LEU	N-CA-C	6.15	118.06	111.36
1	G	383	HIS	CB-CG-CD2	-6.15	123.21	131.20
1	G	786	VAL	N-CA-CB	6.15	121.95	111.50
2	D	103	ALA	N-CA-C	6.15	118.77	111.33
3	F	14	LYS	N-CA-C	6.14	128.19	111.00
1	G	778	ARG	NE-CZ-NH1	-6.14	115.36	121.50
1	A	751	GLN	N-CA-C	6.13	119.88	111.54
1	A	535	SER	N-CA-C	6.12	119.59	111.75
1	A	600	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	G	148	HIS	CB-CG-CD2	-6.12	123.24	131.20
1	A	763	LYS	N-CA-C	6.12	119.13	110.14
2	C	109	VAL	N-CA-C	6.12	116.28	110.53
1	G	601	ASP	N-CA-C	6.10	123.80	110.80
1	G	596	LYS	N-CA-CB	-6.10	101.17	110.92
3	E	53	GLN	OE1-CD-NE2	-6.09	116.51	122.60
1	G	596	LYS	CA-CB-CG	6.09	126.28	114.10
3	L	88	ARG	N-CA-C	6.09	118.41	110.43
1	A	568	PRO	CA-N-CD	-6.08	103.49	112.00
3	L	100	ALA	N-CA-C	6.08	117.58	111.07
3	L	10	LYS	N-CA-C	-6.08	105.77	113.43
3	K	93	GLN	OE1-CD-NE2	-6.07	116.53	122.60
1	A	6	ASP	CA-CB-CG	6.07	118.67	112.60
1	G	957	ASP	CA-CB-CG	6.07	118.67	112.60
2	C	153	ASP	CA-CB-CG	6.06	118.66	112.60
3	F	94	GLU	N-CA-C	6.05	119.71	112.93
1	H	902	VAL	CA-C-O	-6.05	114.76	121.05
1	H	167	GLN	OE1-CD-NE2	-6.05	116.55	122.60
1	A	596	LYS	N-CA-CB	-6.04	101.48	110.61
1	A	597	ASP	N-CA-C	6.03	123.14	109.81
1	G	282	ILE	N-CA-C	6.03	121.88	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	340	HIS	CB-CG-CD2	-6.03	123.37	131.20
3	L	39	ARG	NE-CZ-NH1	-6.01	115.49	121.50
1	A	693	HIS	CB-CG-ND1	6.00	131.70	122.70
1	B	93	ASP	N-CA-C	6.00	117.51	110.97
1	B	322	ASP	CA-CB-CG	6.00	118.60	112.60
3	L	15	LYS	N-CA-C	6.00	118.22	108.63
1	B	640	ARG	O-C-N	-5.99	116.17	123.30
1	G	420	SER	N-CA-C	5.99	120.12	112.34
1	H	340	HIS	CB-CG-CD2	-5.99	123.42	131.20
1	H	565	PRO	CA-N-CD	-5.98	103.62	112.00
1	H	929	ARG	NE-CZ-NH2	5.98	124.58	119.20
1	H	179	LYS	N-CA-C	5.98	118.29	111.11
1	H	693	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	G	489	HIS	CB-CG-CD2	-5.97	123.44	131.20
1	B	628	GLU	N-CA-C	5.97	120.18	113.02
1	A	493	LEU	N-CA-C	5.96	118.27	111.11
1	B	414	ALA	N-CA-C	5.96	121.15	111.37
2	D	108	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	B	622	HIS	N-CA-C	5.96	122.97	109.81
1	H	929	ARG	NE-CZ-NH1	-5.95	115.55	121.50
1	A	788	TRP	CG-CD2-CE3	5.94	139.84	133.90
1	B	280	TYR	N-CA-C	5.94	119.21	110.30
1	G	934	HIS	CA-CB-CG	5.93	119.73	113.80
1	B	91	LEU	N-CA-C	5.93	118.92	110.68
2	J	128	VAL	N-CA-C	5.93	117.46	111.00
1	B	102	GLN	OE1-CD-NE2	-5.92	116.68	122.60
1	H	476	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	A	515	ALA	N-CA-C	5.91	118.51	111.71
2	D	136	PHE	N-CA-C	5.91	118.15	108.52
1	A	98	HIS	CB-CG-CD2	-5.91	123.52	131.20
1	B	182	ASN	N-CA-C	5.90	117.52	111.14
3	L	16	LYS	N-CA-C	5.90	123.37	110.80
1	H	364	ARG	NE-CZ-NH1	-5.90	115.60	121.50
1	B	229	ASN	CA-CB-CG	5.90	118.50	112.60
1	B	763	LYS	N-CA-C	5.90	118.81	109.96
1	A	368	GLU	N-CA-C	5.90	127.51	111.00
1	A	622	HIS	CB-CG-CD2	-5.89	123.54	131.20
1	B	930	GLU	N-CA-C	5.89	120.31	113.18
3	E	54	HIS	CA-CB-CG	-5.89	107.91	113.80
1	G	352	SER	CA-C-O	-5.89	114.60	120.90
1	A	397	VAL	CB-CA-C	-5.87	104.24	111.92
3	E	118	ARG	NE-CZ-NH2	5.86	124.48	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	622	HIS	CB-CG-CD2	-5.86	123.58	131.20
1	B	601	ASP	CA-CB-CG	5.85	118.45	112.60
1	H	694	GLN	OE1-CD-NE2	-5.85	116.75	122.60
2	C	97	GLU	N-CA-C	5.84	123.25	110.80
2	C	136	PHE	N-CA-C	5.84	119.21	107.41
1	A	334	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	676	ILE	CB-CA-C	-5.82	104.60	110.89
1	A	310	VAL	N-CA-C	5.82	121.44	109.34
1	B	12	TYR	N-CA-CB	-5.82	102.41	110.38
1	G	535	SER	N-CA-C	5.82	119.91	112.34
1	A	441	ASN	OD1-CG-ND2	-5.82	116.78	122.60
2	I	103	ALA	N-CA-C	5.82	117.30	111.07
1	G	163	ASN	N-CA-C	5.81	120.37	113.16
1	H	142	ARG	N-CA-C	5.81	123.18	110.80
1	H	147	PRO	N-CA-C	5.80	124.42	112.47
1	B	527	ILE	N-CA-C	-5.79	106.64	113.42
1	H	416	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	B	103	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	A	57	ASP	CA-CB-CG	5.78	118.38	112.60
1	G	268	ALA	CA-C-O	-5.78	114.95	120.90
1	H	648	THR	N-CA-C	5.77	123.09	110.80
1	A	364	ARG	O-C-N	-5.77	114.69	121.32
3	L	31	PRO	N-CA-C	5.77	124.35	112.47
1	A	828	TRP	CB-CG-CD1	-5.77	118.25	126.90
1	H	500	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	A	711	PHE	CA-C-N	5.76	127.05	119.84
1	A	711	PHE	C-N-CA	5.76	127.05	119.84
2	D	134	ASP	O-C-N	-5.76	111.21	122.11
1	B	772	GLY	N-CA-C	5.76	119.18	112.50
1	B	439	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	H	145	VAL	CA-C-N	5.76	126.31	120.38
1	H	145	VAL	C-N-CA	5.76	126.31	120.38
1	B	565	PRO	CA-N-CD	-5.75	103.95	112.00
1	H	668	GLN	CA-C-N	5.75	125.51	119.76
1	H	668	GLN	C-N-CA	5.75	125.51	119.76
1	A	140	ARG	NE-CZ-NH1	-5.74	115.76	121.50
1	H	351	ALA	N-CA-C	5.74	119.54	112.54
2	I	156	LYS	CB-CG-CD	-5.74	98.11	111.30
1	B	616	GLN	OE1-CD-NE2	-5.73	116.87	122.60
1	A	340	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	G	822	PHE	CA-CB-CG	5.73	119.53	113.80
1	G	711	PHE	CA-C-N	5.72	126.99	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	711	PHE	C-N-CA	5.72	126.99	119.84
1	G	646	PHE	N-CA-C	-5.71	97.90	108.24
1	H	477	PHE	N-CA-C	5.71	119.35	112.38
1	B	801	GLU	N-CA-C	5.71	119.83	112.41
3	E	54	HIS	CB-CG-CD2	-5.71	123.78	131.20
1	B	147	PRO	N-CA-C	5.70	124.22	112.47
1	B	929	ARG	NE-CZ-NH1	-5.70	115.80	121.50
1	G	770	VAL	N-CA-C	5.69	116.34	110.36
1	A	383	HIS	CB-CG-CD2	-5.69	123.80	131.20
2	I	108	HIS	CB-CG-CD2	-5.68	123.81	131.20
1	G	716	VAL	N-CA-C	5.67	117.59	108.85
1	H	306	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	827	ASN	CA-CB-CG	5.67	118.27	112.60
1	H	64	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	H	306	ASP	N-CA-CB	-5.66	101.77	109.98
2	J	95	LYS	N-CA-C	-5.66	107.61	114.75
1	A	542	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	790	GLN	OE1-CD-NE2	-5.66	116.94	122.60
3	K	56	VAL	N-CA-C	5.66	119.02	111.44
1	B	340	HIS	CA-CB-CG	5.65	119.45	113.80
1	B	504	ASP	CA-CB-CG	5.65	118.25	112.60
1	A	303	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	306	ASP	CA-C-O	5.64	128.58	120.51
1	G	340	HIS	CB-CG-CD2	-5.64	123.86	131.20
1	A	207	LYS	N-CA-CB	5.64	120.08	110.50
3	L	70	LYS	N-CA-C	5.63	119.66	112.34
1	A	578	ALA	N-CA-C	5.63	118.40	109.50
1	B	787	THR	CA-CB-OG1	-5.63	101.16	109.60
1	H	654	ARG	NE-CZ-NH1	-5.63	115.87	121.50
1	B	33	TRP	CB-CG-CD1	-5.62	118.47	126.90
1	B	462	PHE	CA-CB-CG	-5.62	108.18	113.80
1	G	738	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	22	GLN	N-CA-C	5.60	122.73	110.80
1	A	488	HIS	CB-CG-CD2	-5.60	123.92	131.20
1	H	669	PRO	N-CA-C	5.60	119.98	111.19
1	B	737	VAL	N-CA-CB	-5.60	106.18	112.45
1	A	709	LYS	N-CA-C	5.60	118.15	111.71
1	B	448	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	B	140	ARG	NE-CZ-NH1	-5.59	115.91	121.50
2	I	97	GLU	N-CA-C	5.59	122.72	110.80
2	J	129	CYS	N-CA-C	5.59	119.09	110.42
2	D	134	ASP	CA-CB-CG	5.59	118.19	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	33	PRO	N-CA-C	5.59	117.52	110.70
1	H	146	PRO	N-CA-CB	-5.59	97.66	103.08
1	G	713	ASN	CA-CB-CG	5.58	118.18	112.60
1	H	312	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	B	93	ASP	CA-CB-CG	5.58	118.18	112.60
3	F	28	PRO	CA-C-N	5.58	123.68	119.66
3	F	28	PRO	C-N-CA	5.58	123.68	119.66
1	H	711	PHE	CA-C-N	5.58	126.44	120.47
1	H	711	PHE	C-N-CA	5.58	126.44	120.47
1	G	140	ARG	NE-CZ-NH2	5.58	124.22	119.20
1	B	479	ASN	CB-CG-ND2	5.57	124.76	116.40
1	G	450	ARG	N-CA-C	5.57	118.81	109.95
1	A	422	GLY	O-C-N	-5.57	115.46	122.70
3	E	17	SER	N-CA-C	5.57	122.67	110.80
3	L	64	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	A	822	PHE	CA-CB-CG	5.57	119.37	113.80
1	B	28	GLY	O-C-N	-5.57	115.46	122.70
1	B	647	GLN	N-CA-C	5.57	122.66	110.80
3	E	131	ALA	N-CA-C	5.57	117.35	111.28
1	B	98	HIS	CB-CG-CD2	-5.56	123.97	131.20
1	H	513	ASP	N-CA-C	5.56	117.69	108.13
1	G	199	LYS	N-CA-C	5.56	122.09	109.81
1	A	163	ASN	N-CA-C	5.55	120.04	113.16
1	B	405	ASN	OD1-CG-ND2	-5.55	117.05	122.60
1	H	790	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	B	308	HIS	CB-CG-CD2	-5.54	124.00	131.20
1	H	259	ASP	CA-CB-CG	5.54	118.14	112.60
2	C	13	ARG	NE-CZ-NH2	5.54	124.19	119.20
1	B	86	SER	N-CA-C	5.53	122.58	110.80
1	G	693	HIS	CB-CG-CD2	-5.53	124.01	131.20
3	L	154	TRP	N-CA-C	5.53	118.64	108.58
1	G	945	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	430	ASP	CA-CB-CG	5.52	118.12	112.60
1	G	751	GLN	N-CA-C	5.52	119.59	112.86
1	H	930	GLU	N-CA-C	5.52	119.86	113.18
3	K	84	ASP	CA-CB-CG	5.52	118.12	112.60
3	E	15	LYS	N-CA-C	5.51	119.31	112.59
3	L	13	SER	CA-C-N	5.51	131.61	121.70
3	L	13	SER	C-N-CA	5.51	131.61	121.70
1	G	69	ASP	CA-CB-CG	5.50	118.10	112.60
1	H	21	ASP	N-CA-C	5.50	122.52	110.80
3	E	57	GLN	CB-CG-CD	-5.50	103.25	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	68	LYS	N-CA-C	5.50	122.52	110.80
1	G	233	VAL	N-CA-C	5.50	116.56	111.45
1	H	167	GLN	CG-CD-NE2	5.50	124.64	116.40
1	H	382	ALA	N-CA-C	5.49	117.27	111.28
2	D	119	ASP	CA-CB-CG	5.49	118.09	112.60
1	B	92	ASN	OD1-CG-ND2	-5.49	117.11	122.60
3	F	126	ASP	CB-CA-C	-5.48	102.04	110.81
1	B	827	ASN	OD1-CG-ND2	-5.48	117.12	122.60
1	G	501	GLU	N-CA-C	5.48	117.96	111.33
1	G	788	TRP	CG-CD2-CE3	5.48	139.38	133.90
1	A	195	ALA	N-CA-C	5.48	117.76	110.53
1	B	794	ARG	NE-CZ-NH1	-5.48	116.02	121.50
3	F	96	ASP	CA-CB-CG	5.48	118.08	112.60
1	G	102	GLN	CG-CD-NE2	5.47	124.61	116.40
1	G	818	ASN	N-CA-C	5.47	117.25	111.28
1	G	923	LEU	N-CA-C	5.47	116.94	110.97
1	A	93	ASP	N-CA-C	5.47	119.05	112.38
1	B	345	ASP	N-CA-C	5.47	117.32	111.36
1	G	76	PRO	CA-C-N	5.47	125.14	119.56
1	G	76	PRO	C-N-CA	5.47	125.14	119.56
1	A	788	TRP	CE2-CD2-CG	-5.47	100.64	107.20
1	G	567	LYS	CA-C-N	5.46	126.67	119.84
1	G	567	LYS	C-N-CA	5.46	126.67	119.84
3	K	118	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	H	622	HIS	N-CA-C	5.46	121.87	109.81
1	G	593	GLU	CB-CA-C	-5.45	102.32	110.88
3	K	15	LYS	N-CA-C	5.45	119.92	113.16
1	A	833	LEU	N-CA-C	-5.44	100.43	109.46
1	G	355	HIS	CB-CG-ND1	5.44	130.86	122.70
1	B	73	GLN	N-CA-C	5.43	118.11	110.23
1	B	600	ASN	CB-CG-ND2	5.43	124.55	116.40
1	B	869	LYS	N-CA-C	5.43	122.37	110.80
2	I	98	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	B	6	ASP	CA-C-N	5.43	125.42	120.21
1	B	6	ASP	C-N-CA	5.43	125.42	120.21
1	B	204	ALA	N-CA-C	5.43	121.81	109.81
1	B	806	GLN	N-CA-C	5.43	117.64	111.02
1	B	693	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	G	574	HIS	CA-CB-CG	5.43	119.23	113.80
1	A	505	TRP	CE2-CD2-CG	-5.42	100.69	107.20
1	H	389	ALA	N-CA-C	5.42	117.89	111.33
2	D	95	LYS	N-CA-C	-5.42	108.44	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	54	HIS	CA-CB-CG	5.42	119.22	113.80
3	F	53	GLN	N-CA-C	5.42	122.34	110.80
3	F	63	PHE	N-CA-C	5.42	122.34	110.80
1	G	785	ILE	O-C-N	-5.42	116.43	122.66
1	B	587	ASN	CA-CB-CG	5.42	118.02	112.60
1	H	74	VAL	N-CA-C	5.42	116.07	109.30
1	H	292	GLU	N-CA-C	5.42	122.34	110.80
1	H	761	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	A	443	THR	N-CA-C	5.41	119.98	112.90
1	B	553	HIS	CB-CG-ND1	5.41	130.81	122.70
1	H	210	LYS	O-C-N	-5.40	115.40	122.59
3	K	17	SER	N-CA-C	5.40	122.31	110.80
1	G	391	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	487	ASN	OD1-CG-ND2	-5.38	117.22	122.60
3	K	118	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	B	927	LEU	N-CA-C	-5.38	104.84	111.40
1	H	92	ASN	N-CA-C	-5.38	102.50	110.46
1	B	673	ARG	N-CA-CB	-5.38	101.61	110.53
2	C	119	ASP	CA-CB-CG	5.38	117.98	112.60
3	L	95	LEU	N-CA-C	5.38	117.56	111.11
1	A	778	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	G	163	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	B	716	VAL	CA-C-N	5.37	126.80	120.09
1	B	716	VAL	C-N-CA	5.37	126.80	120.09
2	C	103	ALA	N-CA-C	5.37	117.55	111.11
1	H	595	ASN	CA-CB-CG	5.37	117.97	112.60
1	A	605	ASP	N-CA-C	5.37	117.55	111.11
1	G	670	HIS	CB-CG-CD2	-5.37	124.22	131.20
2	J	13	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	B	145	VAL	CA-C-N	5.36	125.90	120.38
1	B	145	VAL	C-N-CA	5.36	125.90	120.38
1	G	22	GLN	N-CA-C	5.36	122.21	110.80
1	G	564	LYS	N-CA-C	-5.36	98.88	108.47
1	A	268	ALA	CA-C-N	5.35	131.34	121.70
1	A	268	ALA	C-N-CA	5.35	131.34	121.70
3	F	27	ALA	CA-C-N	5.35	125.89	120.38
3	F	27	ALA	C-N-CA	5.35	125.89	120.38
1	A	365	PRO	CA-CB-CG	-5.35	94.33	104.50
2	D	139	TYR	N-CA-C	5.35	118.03	111.82
1	A	788	TRP	CB-CG-CD1	-5.35	118.87	126.90
1	A	738	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	416	GLN	OE1-CD-NE2	-5.35	117.25	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	505	TRP	CE2-CD2-CG	-5.35	100.78	107.20
1	B	303	ASP	CA-CB-CG	5.34	117.94	112.60
1	G	788	TRP	CE2-CD2-CG	-5.34	100.79	107.20
1	A	934	HIS	CA-CB-CG	5.33	119.13	113.80
1	G	210	LYS	N-CA-C	-5.33	102.02	109.69
1	B	762	THR	CA-CB-OG1	-5.33	101.61	109.60
3	E	84	ASP	CA-CB-CG	5.33	117.93	112.60
3	F	28	PRO	N-CA-C	5.33	117.20	110.70
1	A	828	TRP	CG-CD2-CE3	5.33	139.23	133.90
3	L	32	LYS	N-CA-C	5.33	121.58	109.81
1	H	75	ASN	CA-C-N	5.32	125.86	120.38
1	H	75	ASN	C-N-CA	5.32	125.86	120.38
1	A	725	THR	CA-CB-OG1	-5.32	101.62	109.60
1	H	360	LYS	N-CA-C	5.32	117.37	108.23
1	B	873	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	934	HIS	CA-CB-CG	5.31	119.11	113.80
1	A	275	THR	N-CA-C	5.31	118.20	109.76
1	A	500	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	G	360	LYS	O-C-N	-5.30	116.48	123.16
1	A	389	ALA	N-CA-C	5.30	117.97	111.82
1	H	779	ASP	CA-CB-CG	5.30	117.90	112.60
3	K	82	THR	CA-CB-OG1	-5.29	101.67	109.60
1	B	212	THR	CA-CB-OG1	-5.29	101.67	109.60
2	C	142	PHE	CA-CB-CG	5.29	119.09	113.80
3	E	154	TRP	CE2-CD2-CG	-5.29	100.86	107.20
1	G	98	HIS	CB-CG-CD2	-5.29	124.33	131.20
1	A	413	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	B	870	VAL	CA-C-O	-5.28	114.17	120.78
1	G	416	GLN	OE1-CD-NE2	-5.28	117.32	122.60
3	L	94	GLU	N-CA-C	5.28	119.41	112.92
1	A	828	TRP	CE2-CD2-CG	-5.28	100.87	107.20
1	B	725	THR	N-CA-C	5.28	122.04	110.80
2	C	156	LYS	CB-CG-CD	-5.28	99.16	111.30
3	E	93	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	A	69	ASP	CA-CB-CG	5.27	117.87	112.60
3	F	123	ASP	CA-CB-CG	5.27	117.87	112.60
1	H	697	CYS	N-CA-C	5.27	119.56	113.18
1	G	274	GLN	O-C-N	-5.27	117.49	123.13
1	H	388	ASN	CA-CB-CG	5.27	117.87	112.60
2	I	13	ARG	NE-CZ-NH2	5.27	123.94	119.20
2	I	112	SER	N-CA-C	5.26	117.82	111.40
1	H	842	THR	N-CA-C	5.26	122.01	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	836	LYS	N-CA-C	5.26	117.01	111.28
1	G	845	LYS	N-CA-C	5.26	122.00	110.80
1	A	656	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	B	292	GLU	N-CA-C	5.26	122.00	110.80
1	A	89	THR	N-CA-C	5.26	117.69	111.33
1	A	616	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	B	552	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	G	673	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	H	414	ALA	N-CA-C	5.26	122.00	110.80
3	K	158	PHE	CA-CB-CG	5.26	119.06	113.80
1	H	462	PHE	CA-CB-CG	-5.25	108.55	113.80
1	B	355	HIS	N-CA-C	5.25	118.47	111.75
1	B	658	ASN	CB-CG-ND2	5.25	124.28	116.40
1	H	148	HIS	CB-CG-ND1	5.25	130.58	122.70
3	L	40	ALA	N-CA-C	-5.25	105.23	111.69
1	H	664	LEU	N-CA-C	5.25	117.41	111.11
1	H	179	LYS	CA-C-N	5.25	127.58	120.44
1	H	179	LYS	C-N-CA	5.25	127.58	120.44
1	B	581	ALA	N-CA-C	5.25	119.40	113.15
1	H	620	GLU	N-CA-C	5.25	118.72	109.80
1	G	430	ASP	CA-CB-CG	5.25	117.85	112.60
2	C	21	TRP	CE2-CD2-CG	-5.24	100.91	107.20
3	K	54	HIS	CB-CG-CD2	-5.24	124.39	131.20
3	E	66	ILE	N-CA-C	-5.24	106.58	111.45
1	G	926	ARG	NE-CZ-NH2	5.24	123.91	119.20
1	B	405	ASN	CB-CG-ND2	5.23	124.25	116.40
3	K	96	ASP	CA-CB-CG	5.23	117.83	112.60
1	H	830	TRP	CE2-CD2-CG	-5.23	100.92	107.20
1	A	847	GLU	N-CA-C	5.23	120.00	111.37
1	A	654	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	B	33	TRP	CG-CD2-CE3	5.23	139.13	133.90
1	B	420	SER	CA-CB-OG	5.23	121.56	111.10
1	G	654	ARG	NE-CZ-NH2	5.22	123.90	119.20
3	L	102	ALA	N-CA-C	5.22	121.35	109.81
1	G	571	GLN	N-CA-C	5.22	117.02	108.52
1	H	637	GLY	O-C-N	-5.22	115.92	122.70
1	A	274	GLN	O-C-N	-5.21	117.55	123.13
1	H	705	ARG	N-CA-C	5.21	118.41	111.75
1	G	268	ALA	CA-C-N	5.20	131.06	121.70
1	G	268	ALA	C-N-CA	5.20	131.06	121.70
2	I	37	ARG	NE-CZ-NH1	-5.20	116.30	121.50
1	A	249	PHE	N-CA-C	5.20	118.16	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	476	ASN	CB-CG-ND2	5.20	124.20	116.40
1	A	258	ALA	N-CA-C	5.20	117.15	108.99
1	B	33	TRP	CE2-CD2-CG	-5.20	100.96	107.20
3	K	68	GLN	OE1-CD-NE2	-5.20	117.40	122.60
2	J	54	SER	N-CA-C	5.20	117.71	109.50
1	A	453	PHE	CA-CB-CG	5.20	119.00	113.80
1	H	553	HIS	CB-CG-ND1	5.20	130.49	122.70
1	G	132	ARG	N-CA-C	5.19	116.75	111.14
1	H	78	LYS	N-CA-C	-5.19	106.90	113.18
1	H	331	THR	CA-CB-OG1	-5.19	101.81	109.60
1	B	68	LYS	N-CA-C	5.18	121.84	110.80
1	B	355	HIS	CB-CG-CD2	-5.18	124.47	131.20
1	B	291	ILE	N-CA-C	5.17	116.68	109.80
3	K	55	GLN	CG-CD-NE2	5.17	124.16	116.40
3	K	57	GLN	CB-CG-CD	-5.17	103.81	112.60
3	L	55	GLN	OE1-CD-NE2	-5.17	117.43	122.60
3	K	151	LEU	N-CA-C	5.17	116.92	111.28
1	G	229	ASN	N-CA-C	5.17	117.18	108.96
3	L	194	GLU	N-CA-CB	-5.17	103.30	110.38
1	A	361	PHE	N-CA-CB	-5.16	101.72	110.50
1	A	82	CYS	N-CA-C	5.16	117.71	110.23
1	B	868	GLU	CA-C-O	-5.16	114.95	117.94
3	F	125	GLU	CA-C-N	5.16	127.50	120.54
3	F	125	GLU	C-N-CA	5.16	127.50	120.54
1	G	310	VAL	CA-C-O	-5.16	114.33	120.78
1	H	430	ASP	CA-CB-CG	5.16	117.76	112.60
1	G	788	TRP	CB-CG-CD1	-5.15	119.18	126.90
2	J	145	THR	CA-CB-OG1	-5.15	101.88	109.60
1	H	717	TYR	CA-C-N	5.14	124.32	118.97
1	H	717	TYR	C-N-CA	5.14	124.32	118.97
1	B	886	ASN	OD1-CG-ND2	-5.13	117.47	122.60
1	B	478	THR	CA-C-N	5.13	127.41	120.38
1	B	478	THR	C-N-CA	5.13	127.41	120.38
1	H	33	TRP	CB-CG-CD1	-5.13	119.21	126.90
1	B	872	LYS	N-CA-CB	-5.13	102.58	110.12
1	H	75	ASN	CA-CB-CG	5.13	117.73	112.60
1	H	303	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	373	ASP	N-CA-C	5.12	118.06	110.48
1	H	645	SER	CA-C-N	5.12	131.32	121.54
1	H	645	SER	C-N-CA	5.12	131.32	121.54
1	H	200	PRO	N-CA-C	5.12	123.02	112.47
1	A	505	TRP	CG-CD2-CE3	5.12	139.02	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	724	TYR	N-CA-C	5.12	119.16	113.02
1	A	148	HIS	CA-C-N	5.11	127.38	120.38
1	A	148	HIS	C-N-CA	5.11	127.38	120.38
1	H	801	GLU	N-CA-C	5.11	119.05	112.41
1	H	369	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	G	367	GLU	CA-C-O	-5.10	113.21	120.51
1	G	721	LYS	CA-CB-CG	5.10	124.31	114.10
1	H	359	MET	N-CA-C	5.10	116.79	108.63
3	F	194	GLU	CA-C-O	-5.10	115.82	121.33
1	G	921	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	A	308	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	A	605	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	535	SER	N-CA-C	5.09	121.65	110.80
1	H	808	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	B	380	ARG	NE-CZ-NH2	5.09	123.78	119.20
2	I	119	ASP	CA-CB-CG	5.09	117.69	112.60
1	H	305	TYR	CA-C-N	5.09	127.55	120.63
1	H	305	TYR	C-N-CA	5.09	127.55	120.63
3	L	54	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	H	151	ALA	CB-CA-C	-5.08	102.90	110.88
1	H	376	GLU	CA-C-N	5.08	127.34	120.38
1	H	376	GLU	C-N-CA	5.08	127.34	120.38
1	H	534	GLU	N-CA-C	5.08	121.92	113.89
1	A	575	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	489	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	G	565	PRO	N-CA-C	5.08	116.89	110.70
1	G	715	MET	N-CA-C	5.08	117.19	109.63
1	H	321	ASP	CA-CB-CG	5.08	117.67	112.60
1	G	88	LEU	N-CA-C	5.07	117.99	110.48
1	H	395	ASN	CB-CG-ND2	5.07	124.01	116.40
1	H	504	ASP	CA-CB-CG	5.07	117.67	112.60
1	G	479	ASN	CA-CB-CG	5.07	117.67	112.60
1	A	914	ASN	OD1-CG-ND2	-5.07	117.53	122.60
1	G	828	TRP	CB-CG-CD1	-5.07	119.30	126.90
1	B	220	THR	CA-CB-OG1	-5.06	102.01	109.60
1	B	375	THR	CA-CB-OG1	-5.06	102.01	109.60
2	J	153	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	325	GLU	N-CA-C	5.06	118.22	111.75
1	A	131	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	B	537	PHE	CA-C-N	5.05	124.71	119.56
1	B	537	PHE	C-N-CA	5.05	124.71	119.56
1	G	505	TRP	CG-CD2-CE3	5.05	138.95	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	345	ASP	N-CA-C	5.05	116.87	111.36
3	L	143	LYS	N-CA-C	5.05	117.77	108.58
1	G	878	ASN	N-CA-C	5.05	117.67	111.82
1	G	553	HIS	N-CA-C	5.04	119.38	113.23
1	H	580	TYR	N-CA-C	5.04	121.53	110.80
3	E	115	PHE	CA-C-N	5.04	125.67	120.03
3	E	115	PHE	C-N-CA	5.04	125.67	120.03
1	A	229	ASN	OD1-CG-ND2	-5.04	117.56	122.60
1	A	869	LYS	CB-CA-C	5.04	119.97	109.95
1	H	537	PHE	CA-C-N	5.04	124.69	119.56
1	H	537	PHE	C-N-CA	5.04	124.69	119.56
1	A	786	VAL	N-CA-CB	5.03	120.06	111.50
1	A	365	PRO	CA-C-O	5.03	129.76	120.60
1	A	292	GLU	N-CA-C	5.03	117.50	111.71
3	E	57	GLN	CB-CA-C	-5.03	102.56	110.86
3	F	32	LYS	N-CA-C	5.03	120.92	109.81
1	G	68	LYS	N-CA-C	5.03	117.41	111.33
3	F	13	SER	CA-C-N	5.03	130.74	121.70
3	F	13	SER	C-N-CA	5.03	130.74	121.70
1	B	4	ASP	CA-C-O	-5.02	115.30	120.87
1	B	830	TRP	CE2-CD2-CG	-5.02	101.18	107.20
1	G	786	VAL	CA-CB-CG2	5.02	118.93	110.40
1	H	830	TRP	CG-CD2-CE3	5.02	138.92	133.90
1	B	761	ASN	CB-CG-ND2	5.01	123.92	116.40
3	L	154	TRP	CE2-CD2-CG	-5.01	101.18	107.20
1	A	557	SER	CA-C-N	5.01	126.11	119.84
1	A	557	SER	C-N-CA	5.01	126.11	119.84
1	H	33	TRP	CG-CD2-CE3	5.01	138.91	133.90
1	A	442	GLU	CA-CB-CG	5.01	124.12	114.10
1	A	591	TRP	CE2-CD2-CG	-5.01	101.19	107.20
1	H	559	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	B	151	ALA	N-CA-C	5.01	116.43	111.07
1	H	131	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	A	388	ASN	CA-CB-CG	5.00	117.61	112.60
1	A	790	GLN	OE1-CD-NE2	-5.00	117.60	122.60
1	G	557	SER	CA-C-N	5.00	126.09	119.84
1	G	557	SER	C-N-CA	5.00	126.09	119.84
1	H	33	TRP	CE2-CD2-CG	-5.00	101.20	107.20
1	H	199	LYS	N-CA-C	5.00	120.86	109.81
1	H	591	TRP	CE2-CD2-CG	-5.00	101.20	107.20

There are no chirality outliers.

All (116) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	TYR	Sidechain
1	A	142	ARG	Sidechain
1	A	157	TYR	Sidechain
1	A	190	TYR	Sidechain
1	A	269	ARG	Sidechain
1	A	272	SER	Peptide
1	A	280	TYR	Sidechain
1	A	307	TYR	Sidechain,Peptide
1	A	310	VAL	Peptide
1	A	361	PHE	Sidechain
1	A	363	GLN	Peptide,Sidechain,Mainchain
1	A	364	ARG	Sidechain
1	A	366	ARG	Sidechain,Peptide
1	A	393	TYR	Sidechain
1	A	41	TYR	Sidechain
1	A	410	GLN	Peptide
1	A	412	ARG	Sidechain
1	A	418	SER	Peptide
1	A	567	LYS	Peptide
1	A	586	TYR	Sidechain
1	A	64	ARG	Sidechain
1	A	640	ARG	Sidechain
1	A	708	ARG	Sidechain
1	A	724	TYR	Sidechain
1	A	757	TYR	Sidechain
1	A	796	TYR	Sidechain
1	A	831	TYR	Sidechain
1	A	871	ARG	Sidechain
1	B	103	ARG	Sidechain
1	B	190	TYR	Sidechain
1	B	26	TYR	Sidechain
1	B	278	ARG	Sidechain
1	B	366	ARG	Sidechain
1	B	41	TYR	Sidechain
1	B	419	TYR	Sidechain
1	B	450	ARG	Sidechain
1	B	526	GLY	Peptide
1	B	621	ASP	Peptide
1	B	627	ALA	Peptide
1	B	639	GLY	Peptide
1	B	645	SER	Peptide
1	B	654	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	659	ARG	Sidechain
1	B	673	ARG	Sidechain
1	B	708	ARG	Sidechain
1	B	714	ARG	Sidechain
1	B	867	GLU	Peptide
1	B	941	ARG	Sidechain
2	D	111	LEU	Peptide
3	E	80	ARG	Sidechain
3	F	113	THR	Peptide
3	F	80	ARG	Sidechain
3	F	9	LYS	Peptide
1	G	10	TYR	Sidechain
1	G	123	TYR	Sidechain
1	G	157	TYR	Sidechain
1	G	164	ARG	Sidechain
1	G	190	TYR	Sidechain
1	G	272	SER	Peptide
1	G	273	GLN	Peptide
1	G	305	TYR	Sidechain,Peptide
1	G	307	TYR	Sidechain
1	G	347	TYR	Sidechain
1	G	366	ARG	Peptide
1	G	41	TYR	Sidechain
1	G	410	GLN	Peptide
1	G	418	SER	Peptide
1	G	452	TYR	Sidechain
1	G	586	TYR	Sidechain
1	G	64	ARG	Sidechain
1	G	640	ARG	Sidechain
1	G	654	ARG	Sidechain
1	G	724	TYR	Sidechain
1	G	757	TYR	Sidechain
1	G	817	ARG	Sidechain
1	G	831	TYR	Sidechain
1	G	926	ARG	Sidechain
1	H	110	TYR	Sidechain
1	H	112	TYR	Sidechain
1	H	140	ARG	Sidechain
1	H	142	ARG	Sidechain
1	H	164	ARG	Sidechain
1	H	26	TYR	Sidechain
1	H	278	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	H	347	TYR	Sidechain
1	H	419	TYR	Sidechain
1	H	462	PHE	Sidechain
1	H	571	GLN	Peptide
1	H	621	ASP	Peptide
1	H	627	ALA	Peptide
1	H	647	GLN	Peptide
1	H	654	ARG	Sidechain
1	H	673	ARG	Sidechain
1	H	767	ARG	Sidechain
1	H	79	TYR	Sidechain
1	H	941	ARG	Sidechain
2	I	93	TYR	Sidechain
2	J	111	LEU	Peptide
2	J	116	ARG	Sidechain
2	J	13	ARG	Sidechain
2	J	136	PHE	Peptide
3	K	38	ARG	Sidechain
3	K	80	ARG	Sidechain
3	L	113	THR	Peptide
3	L	29	PRO	Peptide
3	L	30	PRO	Mainchain
3	L	31	PRO	Peptide
3	L	32	LYS	Peptide,Mainchain
3	L	39	ARG	Peptide
3	L	80	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7721	0	7778	127	0
1	B	7739	0	7799	169	0
1	G	7721	0	7778	111	0
1	H	7739	0	7799	134	0
2	C	1233	0	1227	10	0
2	D	1233	0	1227	11	0
2	I	1233	0	1227	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1233	0	1227	14	0
3	E	1529	0	1491	27	0
3	F	1529	0	1491	28	0
3	K	1529	0	1491	23	0
3	L	1529	0	1491	51	0
All	All	41968	0	42026	623	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 7.

All (623) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:LYS:HE3	1:B:642:LYS:NZ	1.21	1.52
1:B:641:LYS:CE	1:B:642:LYS:NZ	2.16	1.08
1:A:364:ARG:HA	3:L:31:PRO:HG2	1.42	1.00
1:B:641:LYS:CE	1:B:642:LYS:HZ1	1.70	0.99
1:A:364:ARG:HA	3:L:31:PRO:CG	1.95	0.94
1:A:449:LYS:HD3	1:B:405:ASN:OD1	1.72	0.90
1:B:641:LYS:HE3	1:B:642:LYS:HZ2	1.07	0.90
1:B:635:LYS:HE3	1:B:904:GLU:HA	1.55	0.87
1:H:175:SER:HB2	1:H:463:GLU:HA	1.56	0.87
1:B:641:LYS:HE3	1:B:642:LYS:HZ1	1.01	0.80
1:A:369:GLN:HA	1:A:417:VAL:HG21	1.64	0.80
1:A:500:ARG:HG3	1:B:366:ARG:HB2	1.64	0.79
1:B:174:GLU:HB3	1:B:676:ILE:HD12	1.65	0.79
3:L:22:GLY:HA3	3:L:94:GLU:HG3	1.66	0.78
1:H:135:GLN:HG3	1:H:199:LYS:HE3	1.66	0.77
2:I:100:THR:HB	2:I:136:PHE:HB3	1.65	0.77
3:F:173:ASP:HB3	3:F:178:ILE:HG13	1.66	0.77
1:B:267:LYS:HD3	1:B:430:ASP:HB2	1.67	0.77
1:A:58:ILE:HB	1:A:61:GLN:HB2	1.68	0.76
1:A:833:LEU:HA	3:E:192:GLU:HG3	1.68	0.76
3:L:97:SER:HA	3:L:100:ALA:HB2	1.68	0.76
1:A:206:THR:HB	1:A:207:LYS:HB2	1.67	0.76
1:B:641:LYS:HE3	1:B:642:LYS:CE	2.17	0.75
3:E:51:PHE:HB3	3:E:56:VAL:HG21	1.67	0.75
1:G:58:ILE:HB	1:G:61:GLN:HB2	1.69	0.74
3:L:130:ASN:HA	3:L:133:ASN:HB3	1.69	0.74
3:E:192:GLU:HG2	3:E:193:GLU:HA	1.70	0.74
1:B:642:LYS:HE2	1:B:903:GLU:OE1	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:173:ASP:HB3	3:L:178:ILE:HG13	1.68	0.73
1:A:879:VAL:HG12	1:B:450:ARG:HB2	1.69	0.73
1:H:561:VAL:HB	1:H:576:SER:HB2	1.71	0.72
1:G:833:LEU:HA	3:K:192:GLU:HG3	1.73	0.70
2:I:101:MET:SD	2:I:139:TYR:HB3	2.31	0.70
1:B:902:VAL:HA	1:B:905:ARG:HB2	1.73	0.70
1:H:431:ARG:NH2	1:H:619:PHE:HA	2.07	0.70
2:J:26:LYS:HD2	2:J:61:LYS:HD3	1.73	0.69
1:A:449:LYS:HA	1:A:449:LYS:HE2	1.73	0.69
1:A:271:ILE:HD12	1:A:419:TYR:HA	1.75	0.69
1:G:716:VAL:HG12	1:G:763:LYS:HE2	1.75	0.69
1:H:597:ASP:HB3	1:H:646:PHE:HD2	1.58	0.68
1:B:7:PRO:HA	1:B:12:TYR:HE2	1.58	0.68
3:F:117:ASP:HA	3:F:120:ALA:HB3	1.76	0.67
1:B:13:ILE:HB	1:B:108:LEU:HD22	1.77	0.67
1:B:541:THR:HA	1:B:592:LEU:HD11	1.77	0.67
1:B:641:LYS:CE	1:B:642:LYS:HZ2	1.95	0.67
1:A:37:GLU:HB2	1:A:38:LYS:HD3	1.77	0.67
1:G:779:ASP:HA	1:G:782:LEU:HB2	1.77	0.67
1:A:34:VAL:HG11	1:A:58:ILE:HD12	1.75	0.67
1:G:367:GLU:HB2	1:G:369:GLN:H	1.61	0.66
1:A:309:PHE:HB2	3:L:18:GLU:HG3	1.77	0.66
1:A:772:GLY:HA2	1:A:775:GLU:HG3	1.78	0.65
1:B:175:SER:HB2	1:B:463:GLU:HA	1.76	0.65
1:A:364:ARG:HD2	1:A:371:GLU:H	1.62	0.65
3:K:51:PHE:HB2	3:L:61:GLU:HG2	1.79	0.65
1:H:244:PHE:O	1:H:260:ILE:HA	1.97	0.65
1:A:539:LYS:HD2	2:J:3:ASP:HB2	1.78	0.64
1:A:366:ARG:HA	3:L:39:ARG:HB2	1.78	0.64
1:B:716:VAL:HG13	1:B:718:PRO:HD2	1.79	0.64
1:B:431:ARG:NH2	1:B:619:PHE:HA	2.13	0.64
1:B:388:ASN:HB3	1:B:391:ASP:HB2	1.80	0.64
1:B:423:GLY:HA2	1:B:426:LYS:HE2	1.79	0.64
1:G:645:SER:HB3	1:G:647:GLN:HG3	1.80	0.64
1:A:100:LEU:HB3	1:A:120:ILE:HD11	1.78	0.63
1:B:743:THR:HA	1:B:746:VAL:HG22	1.81	0.63
1:B:635:LYS:HB3	1:B:642:LYS:CD	2.28	0.62
1:B:97:LEU:HD11	1:B:692:MET:HA	1.81	0.62
1:A:712:PRO:HD2	1:A:767:ARG:HA	1.81	0.62
1:G:500:ARG:HG3	1:H:366:ARG:HB2	1.81	0.62
1:A:364:ARG:HA	3:L:31:PRO:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:ASP:HA	2:D:37:ARG:HD2	1.81	0.62
1:G:34:VAL:HG11	1:G:58:ILE:HD12	1.82	0.62
1:A:762:THR:HG21	1:B:371:GLU:HB3	1.81	0.62
1:H:131:ASN:O	1:H:135:GLN:HB2	2.00	0.62
1:H:356:LEU:HD22	1:H:425:ALA:HB2	1.82	0.62
1:B:635:LYS:HB3	1:B:642:LYS:HD3	1.80	0.61
1:B:833:LEU:HD23	3:F:192:GLU:HG2	1.82	0.61
1:B:904:GLU:O	1:B:908:LYS:HB2	2.01	0.61
1:H:231:LYS:HB3	1:H:278:ARG:H	1.66	0.61
1:H:231:LYS:HG3	1:H:236:ASP:HA	1.83	0.61
1:A:399:PRO:O	1:A:409:THR:HA	2.01	0.61
1:G:166:ASN:ND2	1:G:667:THR:HG22	2.16	0.61
1:H:13:ILE:HB	1:H:108:LEU:HD22	1.83	0.60
1:H:171:ILE:HG12	1:H:672:VAL:HB	1.82	0.60
1:G:884:GLU:HA	1:G:887:ASP:HB2	1.82	0.60
1:G:309:PHE:HB2	1:G:362:LYS:HE3	1.84	0.60
1:H:211:ALA:HB3	1:H:214:GLU:HG2	1.82	0.60
3:E:109:THR:HG23	3:F:70:LYS:HD3	1.84	0.60
1:G:46:ILE:HG23	1:G:54:CYS:SG	2.41	0.60
1:B:431:ARG:HH22	1:B:619:PHE:HA	1.66	0.60
3:L:69:ASP:HB2	3:L:73:PHE:HB2	1.83	0.60
1:B:481:LYS:HD3	1:B:520:LEU:HA	1.84	0.60
1:G:785:ILE:HG23	1:G:786:VAL:HG23	1.83	0.60
1:G:37:GLU:HB2	1:G:38:LYS:HD3	1.82	0.59
1:H:84:ASP:HA	1:H:112:TYR:HB2	1.84	0.59
1:B:84:ASP:HA	1:B:112:TYR:HB2	1.84	0.59
1:B:142:ARG:HG2	1:B:145:VAL:HB	1.85	0.59
1:B:640:ARG:NH1	1:B:896:ARG:HG3	2.17	0.59
1:G:791:ALA:HB2	2:I:44:THR:HG22	1.85	0.59
1:H:498:TYR:HB3	1:H:503:ILE:HG12	1.83	0.59
1:H:743:THR:HA	1:H:746:VAL:HG22	1.83	0.59
1:A:256:ALA:HB1	1:A:447:LYS:HG3	1.84	0.58
1:G:287:MET:SD	1:G:360:LYS:HE2	2.43	0.58
1:H:141:ARG:NH1	1:H:776:GLU:HA	2.18	0.58
1:B:493:LEU:HA	1:B:496:GLU:HB2	1.86	0.58
1:H:114:GLY:HA2	1:H:712:PRO:HG3	1.85	0.58
1:A:109:ILE:HG21	1:A:122:PRO:HD3	1.86	0.58
1:A:884:GLU:HA	1:A:887:ASP:HB2	1.86	0.58
2:I:131:GLU:HG2	2:I:137:LEU:HD11	1.85	0.58
1:G:118:VAL:HG12	1:G:673:ARG:HB3	1.85	0.58
1:G:243:LYS:HB3	1:G:458:ASP:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:713:ASN:HB2	1:G:766:PHE:HB2	1.85	0.58
1:H:635:LYS:HB2	1:H:643:GLY:H	1.69	0.58
1:A:923:LEU:HD23	1:A:926:ARG:HH11	1.69	0.58
1:B:210:LYS:HB3	1:B:211:ALA:HA	1.86	0.58
3:K:20:GLU:HG3	3:K:109:THR:HG21	1.86	0.57
1:A:785:ILE:HG23	1:A:786:VAL:HG23	1.86	0.57
1:B:141:ARG:NH1	1:B:776:GLU:HA	2.19	0.57
1:H:546:GLN:HE22	1:H:575:PHE:HB3	1.69	0.57
3:K:109:THR:HG23	3:L:70:LYS:HD3	1.86	0.57
1:B:157:TYR:HB2	1:B:190:TYR:HE2	1.68	0.57
1:A:308:HIS:HA	3:L:13:SER:HB3	1.86	0.57
1:H:250:GLY:HA2	1:H:450:ARG:HB3	1.86	0.57
1:B:832:LYS:HD3	3:F:191:ALA:HB3	1.86	0.57
1:B:836:LYS:HB3	3:E:46:ASN:HB3	1.86	0.57
1:H:632:GLY:H	1:H:644:ALA:HB2	1.68	0.57
1:B:356:LEU:HD21	1:B:421:VAL:O	2.05	0.57
1:H:356:LEU:HD21	1:H:421:VAL:O	2.05	0.57
1:H:267:LYS:HD3	1:H:430:ASP:HB2	1.88	0.56
1:H:423:GLY:HA2	1:H:426:LYS:HE2	1.87	0.56
3:K:192:GLU:HG2	3:K:193:GLU:HA	1.87	0.56
1:B:168:SER:OG	1:B:669:PRO:HA	2.06	0.56
1:H:726:ILE:HG12	1:H:785:ILE:HB	1.86	0.56
1:B:231:LYS:HG3	1:B:236:ASP:HA	1.87	0.56
3:E:30:PRO:HB3	3:E:37:LYS:HD3	1.87	0.56
1:B:864:LEU:O	1:B:868:GLU:HG2	2.06	0.56
1:H:541:THR:HA	1:H:592:LEU:HD11	1.88	0.56
3:K:41:GLN:HG2	3:L:194:GLU:HG3	1.88	0.56
3:F:132:PHE:HB3	3:F:142:CYS:SG	2.45	0.55
1:H:457:LEU:HD23	1:H:482:LEU:HD13	1.88	0.55
1:A:906:LEU:HD13	1:B:906:LEU:HA	1.87	0.55
1:H:295:LYS:HA	1:H:300:LEU:HD12	1.87	0.55
1:H:480:GLU:HG2	1:H:518:ILE:HG12	1.87	0.55
1:H:4:ASP:HB3	1:H:15:MET:HE3	1.87	0.55
1:B:871:ARG:HB3	1:B:872:LYS:HD3	1.89	0.55
1:G:743:THR:HA	1:G:746:VAL:HG12	1.88	0.55
1:H:330:ASP:CG	1:H:343:LYS:HZ1	2.14	0.55
1:A:832:LYS:O	3:E:192:GLU:HA	2.06	0.55
1:B:642:LYS:CE	1:B:903:GLU:OE1	2.55	0.55
1:H:138:LYS:HA	1:H:193:VAL:HG13	1.89	0.55
1:B:91:LEU:HD23	1:B:705:ARG:HG2	1.89	0.55
1:G:712:PRO:HD2	1:G:767:ARG:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:GLN:HB3	1:B:332:ALA:HB1	1.89	0.54
2:D:140:GLU:HB3	2:D:141:PRO:HD3	1.87	0.54
1:A:570:GLN:HE21	2:J:26:LYS:HG3	1.71	0.54
1:B:83:GLU:HG3	1:B:84:ASP:H	1.72	0.54
1:H:542:ASP:HB3	1:H:588:ILE:HG22	1.89	0.54
1:A:874:ILE:HD12	1:B:871:ARG:HD2	1.90	0.54
1:B:740:LYS:O	1:B:743:THR:HG22	2.07	0.54
1:B:868:GLU:HG3	1:B:869:LYS:HD2	1.90	0.54
1:A:118:VAL:HA	1:A:673:ARG:O	2.07	0.54
1:A:593:GLU:HG2	1:A:598:PRO:HB3	1.89	0.54
2:J:60:LYS:HZ1	2:J:66:GLU:CD	2.15	0.54
1:H:231:LYS:HB3	1:H:278:ARG:HB2	1.89	0.54
1:G:134:VAL:HG13	1:G:189:TYR:HE1	1.73	0.54
1:B:635:LYS:CE	1:B:904:GLU:HA	2.34	0.54
1:H:732:VAL:HG11	1:H:742:VAL:HG23	1.89	0.54
1:A:33:TRP:HB2	1:A:72:GLN:HB2	1.90	0.54
1:A:711:PHE:HB3	1:A:765:PHE:HB3	1.89	0.54
1:G:451:GLN:HB3	1:G:452:TYR:HA	1.90	0.54
1:B:146:PRO:HB2	1:B:147:PRO:HD2	1.91	0.53
1:B:811:ALA:HA	3:F:127:VAL:HG13	1.91	0.53
1:A:134:VAL:HG13	1:A:189:TYR:HE1	1.73	0.53
1:B:673:ARG:HH21	1:B:673:ARG:HB3	1.72	0.53
1:G:100:LEU:HB3	1:G:120:ILE:HD11	1.90	0.53
1:H:832:LYS:HD3	3:L:191:ALA:HB3	1.90	0.53
3:E:74:ILE:HG23	3:E:78:ASP:HB2	1.91	0.53
3:K:74:ILE:HG23	3:K:78:ASP:HB2	1.91	0.53
1:A:599:VAL:HG11	1:A:604:VAL:HG23	1.91	0.53
1:B:732:VAL:HG11	1:B:742:VAL:HG23	1.89	0.53
1:G:256:ALA:HB1	1:G:447:LYS:HG3	1.91	0.53
1:G:951:LEU:HD11	1:H:952:LYS:HE3	1.90	0.53
1:H:747:LEU:HB3	1:H:752:LEU:HD23	1.90	0.53
2:I:94:ASP:HB2	2:I:139:TYR:HE2	1.73	0.53
3:L:58:GLU:HA	3:L:61:GLU:HB2	1.91	0.52
1:G:599:VAL:HG22	1:G:603:VAL:HG23	1.91	0.52
1:H:15:MET:SD	1:H:82:CYS:HA	2.50	0.52
1:H:157:TYR:HB2	1:H:190:TYR:HE2	1.74	0.52
3:K:51:PHE:HB3	3:K:56:VAL:HG21	1.91	0.52
1:G:245:ILE:HG23	1:G:260:ILE:HG12	1.90	0.52
1:G:354:MET:SD	1:G:358:GLU:HG3	2.49	0.52
1:A:721:LYS:NZ	1:B:379:GLU:OE1	2.34	0.52
1:A:837:VAL:HG21	3:E:86:LEU:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ASP:HA	1:B:189:TYR:CZ	2.45	0.52
1:B:141:ARG:HH12	1:B:779:ASP:CG	2.18	0.52
1:H:265:LEU:HD23	1:H:430:ASP:HA	1.91	0.52
1:G:422:GLY:HA2	1:G:425:ALA:H	1.75	0.52
3:L:132:PHE:HB3	3:L:142:CYS:SG	2.49	0.52
1:G:84:ASP:HB3	1:G:87:ASN:HD22	1.74	0.52
1:H:54:CYS:SG	1:H:56:VAL:HG23	2.49	0.52
1:H:356:LEU:HD11	1:H:424:LEU:HB3	1.91	0.52
1:H:677:PRO:HB2	1:H:686:ILE:HA	1.92	0.52
2:J:27:ILE:HG13	2:J:62:LEU:HB2	1.91	0.52
1:B:175:SER:HB3	1:B:234:ARG:NH2	2.24	0.51
1:B:169:MET:HB3	1:B:456:VAL:HG22	1.92	0.51
1:H:167:GLN:NE2	1:H:668:GLN:HB3	2.25	0.51
1:H:141:ARG:HH12	1:H:779:ASP:CG	2.18	0.51
1:H:166:ASN:HB3	1:H:667:THR:HG22	1.93	0.51
1:B:271:ILE:HA	1:B:309:PHE:CE1	2.46	0.51
1:H:119:ALA:O	1:H:674:CYS:HA	2.10	0.51
1:H:145:VAL:HG12	1:H:151:ALA:HB2	1.93	0.51
1:H:146:PRO:HB2	1:H:147:PRO:HD2	1.92	0.51
1:H:724:TYR:HE2	1:H:747:LEU:HD23	1.74	0.51
1:B:5:PRO:HG3	1:B:769:GLY:HA2	1.92	0.51
2:D:41:CYS:O	2:D:43:PRO:HD3	2.10	0.51
1:B:138:LYS:HA	1:B:193:VAL:HG13	1.93	0.51
1:B:930:GLU:HA	1:B:933:ALA:HB3	1.91	0.51
1:H:283:PHE:HB3	1:H:354:MET:SD	2.51	0.51
1:H:144:GLU:O	1:H:146:PRO:HD3	2.11	0.50
1:G:359:MET:HE2	1:G:418:SER:HB3	1.93	0.50
1:H:237:ASN:OD1	1:H:281:HIS:HE1	1.94	0.50
3:F:69:ASP:HB2	3:F:73:PHE:HB2	1.94	0.50
1:H:493:LEU:HA	1:H:496:GLU:HB2	1.93	0.50
1:A:55:THR:HA	1:A:65:GLN:HA	1.93	0.50
1:A:309:PHE:CE2	3:L:31:PRO:N	2.80	0.50
1:A:830:TRP:HA	3:E:195:GLY:HA3	1.94	0.50
1:B:726:ILE:HG12	1:B:785:ILE:HB	1.93	0.50
2:C:48:VAL:HG12	2:C:53:GLY:HA3	1.93	0.50
1:H:521:ILE:HB	1:H:524:PRO:HD2	1.94	0.50
2:J:140:GLU:HB3	2:J:141:PRO:HD3	1.93	0.50
3:L:6:LYS:HD3	3:L:9:LYS:O	2.11	0.50
1:G:435:TRP:O	1:G:439:ARG:HG2	2.12	0.50
1:H:240:ARG:HB3	1:H:266:GLU:HB2	1.92	0.50
1:B:278:ARG:HD2	1:B:315:ILE:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD13	1:A:482:LEU:HD11	1.94	0.50
1:G:883:GLN:OE1	1:H:450:ARG:HG3	2.12	0.50
3:L:59:PHE:O	3:L:63:PHE:HB2	2.11	0.50
1:A:364:ARG:C	3:L:31:PRO:HG2	2.37	0.49
1:A:892:LEU:HD22	1:A:896:ARG:HH22	1.76	0.49
1:H:169:MET:O	1:H:456:VAL:HA	2.11	0.49
3:L:92:GLU:HA	3:L:95:LEU:HG	1.93	0.49
1:G:795:TRP:HZ3	2:I:40:ASP:HA	1.77	0.49
1:A:875:GLU:O	1:A:879:VAL:HG23	2.13	0.49
1:B:497:GLU:HG2	1:B:668:GLN:HG3	1.94	0.49
1:B:636:GLY:H	1:B:643:GLY:HA3	1.78	0.49
1:G:310:VAL:HB	1:G:311:SER:HA	1.94	0.49
1:A:690:LEU:O	1:A:694:GLN:HG3	2.12	0.49
1:B:635:LYS:HE3	1:B:904:GLU:CA	2.34	0.49
3:F:22:GLY:HA3	3:F:94:GLU:HG2	1.94	0.49
1:H:167:GLN:HE22	1:H:668:GLN:HB3	1.78	0.49
1:H:721:LYS:HB3	2:J:92:VAL:HG12	1.95	0.49
2:J:68:LEU:HB2	2:J:69:PRO:HD3	1.95	0.49
2:I:103:ALA:HB2	2:I:137:LEU:HD13	1.95	0.49
3:E:51:PHE:HB2	3:F:61:GLU:HG2	1.95	0.49
1:A:713:ASN:HB3	1:A:715:MET:HE3	1.95	0.48
3:F:188:THR:HG22	3:F:189:LYS:H	1.78	0.48
1:G:84:ASP:HB3	1:G:87:ASN:ND2	2.27	0.48
1:A:451:GLN:HB3	1:A:452:TYR:HA	1.95	0.48
1:A:716:VAL:HG21	1:B:390:ALA:HA	1.93	0.48
1:H:97:LEU:HD12	1:H:695:LEU:HD12	1.94	0.48
3:E:67:ASP:O	3:E:70:LYS:NZ	2.47	0.48
1:G:285:GLN:NE2	1:G:326:LEU:HB2	2.27	0.48
1:H:484:GLN:HA	1:H:484:GLN:OE1	2.13	0.48
1:A:435:TRP:O	1:A:439:ARG:HG2	2.14	0.48
1:B:248:HIS:HA	1:B:452:TYR:O	2.14	0.48
1:H:930:GLU:HA	1:H:933:ALA:HB3	1.95	0.48
1:H:109:ILE:HG23	1:H:120:ILE:O	2.14	0.48
1:H:210:LYS:HB3	1:H:211:ALA:HA	1.95	0.48
1:H:714:ARG:HA	1:H:764:VAL:O	2.13	0.48
1:A:372:ALA:HB3	1:A:377:GLU:HA	1.96	0.48
1:G:221:ASN:HB3	1:G:222:PRO:HD3	1.96	0.48
1:G:863:SER:O	1:G:867:GLU:HG2	2.14	0.48
3:K:67:ASP:O	3:K:70:LYS:NZ	2.46	0.48
1:A:134:VAL:HG11	1:A:192:ASN:OD1	2.14	0.48
1:A:461:GLY:HA2	1:A:479:ASN:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:588:ILE:O	1:G:591:TRP:HB2	2.14	0.48
1:H:171:ILE:HA	1:H:672:VAL:O	2.13	0.48
1:G:109:ILE:HG21	1:G:122:PRO:HD3	1.95	0.47
1:B:419:TYR:OH	1:B:426:LYS:NZ	2.47	0.47
3:E:20:GLU:HG3	3:E:109:THR:HG21	1.95	0.47
1:B:244:PHE:O	1:B:260:ILE:HA	2.14	0.47
3:F:33:PRO:HA	3:F:34:PRO:HD3	1.83	0.47
1:G:119:ALA:O	1:G:674:CYS:HA	2.13	0.47
1:A:232:THR:O	1:A:236:ASP:HA	2.14	0.47
1:A:789:LEU:O	1:A:793:ILE:HG13	2.15	0.47
1:B:356:LEU:HD22	1:B:425:ALA:HB2	1.95	0.47
1:A:119:ALA:O	1:A:674:CYS:HA	2.14	0.47
1:B:530:ILE:HG12	1:B:548:LYS:HB2	1.95	0.47
1:G:56:VAL:HG22	1:G:64:ARG:O	2.13	0.47
1:H:169:MET:HB3	1:H:456:VAL:HG22	1.96	0.47
1:H:563:PRO:HB2	1:H:566:PRO:HD2	1.95	0.47
1:H:817:ARG:NH2	3:L:123:ASP:OD2	2.48	0.47
1:A:55:THR:HG22	1:A:65:GLN:HB3	1.96	0.47
1:B:157:TYR:HA	1:B:160:MET:HG2	1.97	0.47
1:B:711:PHE:HA	1:B:712:PRO:HD3	1.72	0.47
3:F:126:ASP:O	3:F:130:ASN:HB2	2.15	0.47
1:H:894:SER:HA	1:H:897:SER:OG	2.15	0.47
3:K:52:THR:HB	3:K:55:GLN:HE21	1.80	0.47
1:A:662:ALA:O	1:A:665:HIS:HB2	2.15	0.47
1:B:526:GLY:CA	1:B:654:ARG:HD3	2.45	0.47
1:A:353:CYS:SG	1:A:428:MET:SD	3.13	0.47
1:A:420:SER:O	1:A:423:GLY:HA3	2.14	0.47
1:A:867:GLU:OE1	1:B:872:LYS:HD2	2.15	0.47
1:H:278:ARG:HD2	1:H:315:ILE:O	2.15	0.47
1:A:272:SER:HB2	1:A:418:SER:HB2	1.97	0.47
1:B:330:ASP:CG	1:B:343:LYS:HZ1	2.22	0.47
1:G:107:ASN:O	1:G:109:ILE:HG23	2.15	0.47
1:B:242:GLY:O	1:B:262:THR:HA	2.15	0.46
1:H:33:TRP:HB2	1:H:72:GLN:HB2	1.96	0.46
1:B:142:ARG:HH11	1:B:151:ALA:HB1	1.80	0.46
1:A:6:ASP:OD1	1:A:7:PRO:HD3	2.14	0.46
1:A:362:LYS:H	3:L:32:LYS:HE3	1.80	0.46
1:B:640:ARG:HH12	1:B:896:ARG:HG3	1.79	0.46
3:F:79:ILE:HG21	3:F:99:VAL:HG22	1.97	0.46
3:F:141:LYS:NZ	3:F:173:ASP:O	2.46	0.46
1:G:80:GLU:HG3	1:G:102:GLN:HE22	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:ASP:O	1:H:219:GLN:HG2	2.14	0.46
3:L:79:ILE:HG13	3:L:99:VAL:HG13	1.96	0.46
1:A:571:GLN:HG2	1:A:572:GLU:HB2	1.95	0.46
1:A:836:LYS:HB2	3:E:192:GLU:HB3	1.98	0.46
1:B:7:PRO:HA	1:B:12:TYR:CE2	2.44	0.46
1:B:256:ALA:O	1:B:446:THR:HA	2.15	0.46
3:E:192:GLU:CG	3:E:193:GLU:HA	2.43	0.46
1:G:571:GLN:HG2	1:G:572:GLU:HB2	1.97	0.46
1:H:192:ASN:HA	1:H:197:THR:HG21	1.98	0.46
1:H:845:LYS:HE2	1:H:848:ASP:HB3	1.97	0.46
2:J:83:LEU:HD21	2:J:147:ILE:HG21	1.96	0.46
1:A:575:PHE:HD2	1:A:588:ILE:HD11	1.80	0.46
1:B:152:ILE:HG22	1:B:169:MET:HE1	1.96	0.46
3:F:30:PRO:HA	3:F:31:PRO:HD2	1.84	0.46
1:A:309:PHE:HD2	3:L:18:GLU:HG3	1.80	0.46
1:A:713:ASN:HB2	1:A:766:PHE:HB2	1.97	0.46
1:H:142:ARG:HD3	1:H:713:ASN:OD1	2.14	0.46
1:B:168:SER:O	1:B:670:HIS:HB2	2.15	0.46
2:D:22:GLU:CD	2:D:61:LYS:HZ3	2.24	0.46
3:F:54:HIS:HB2	3:F:57:GLN:OE1	2.16	0.46
1:H:248:HIS:HA	1:H:452:TYR:O	2.16	0.46
1:H:402:LYS:HE2	1:H:405:ASN:HA	1.97	0.46
2:I:90:LEU:HD22	2:I:139:TYR:HB2	1.98	0.46
1:B:252:MET:HE2	2:D:126:MET:SD	2.56	0.46
1:B:546:GLN:HE22	1:B:575:PHE:HB3	1.80	0.46
1:G:378:GLY:HA2	1:G:381:VAL:HG23	1.97	0.46
3:K:33:PRO:HA	3:K:34:PRO:HD3	1.83	0.46
1:G:164:ARG:O	1:H:400:LYS:HE3	2.16	0.46
1:H:358:GLU:HB2	1:H:377:GLU:HB3	1.97	0.46
3:L:14:LYS:HZ3	3:L:96:ASP:CG	2.23	0.46
1:A:137:TYR:O	1:A:140:ARG:HG2	2.15	0.46
1:A:629:GLU:HB2	1:A:640:ARG:HA	1.98	0.46
1:B:104:TYR:HE2	1:B:686:ILE:HB	1.80	0.46
1:B:231:LYS:HB3	1:B:278:ARG:HB2	1.98	0.46
1:H:103:ARG:HG2	1:H:111:THR:OG1	2.15	0.46
3:K:107:ASN:OD1	3:K:109:THR:HB	2.16	0.46
1:B:168:SER:HA	1:B:455:GLY:O	2.16	0.45
1:B:845:LYS:HE2	1:B:848:ASP:HB3	1.98	0.45
3:E:153:THR:O	3:E:157:LYS:NZ	2.44	0.45
1:B:9:GLU:CD	1:B:132:ARG:HH11	2.25	0.45
1:G:273:GLN:HG2	1:G:277:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:691:VAL:O	1:G:695:LEU:HG	2.16	0.45
1:H:17:GLN:NE2	1:H:81:LYS:HB2	2.31	0.45
1:H:131:ASN:ND2	1:H:207:LYS:HD3	2.31	0.45
3:L:193:GLU:HB2	3:L:194:GLU:H	1.70	0.45
1:G:174:GLU:HB2	1:G:676:ILE:HD11	1.98	0.45
1:B:142:ARG:NH1	1:B:151:ALA:HB1	2.32	0.45
1:B:423:GLY:O	1:B:426:LYS:HG2	2.16	0.45
1:B:701:LEU:HG	1:B:705:ARG:HH21	1.81	0.45
1:B:953:LYS:NZ	1:B:957:ASP:OD2	2.49	0.45
1:G:115:LEU:HD23	1:G:490:MET:SD	2.56	0.45
3:L:90:CYS:SG	3:L:95:LEU:HD23	2.57	0.45
1:B:504:ASP:HB3	1:B:758:ARG:HD2	1.99	0.45
1:B:567:LYS:HB3	1:B:568:PRO:HD3	1.99	0.45
1:G:93:ASP:HB3	1:G:701:LEU:HD22	1.98	0.45
1:H:132:ARG:HB2	1:H:204:ALA:HB1	1.98	0.45
2:C:90:LEU:HD22	2:C:139:TYR:HB2	1.98	0.45
1:G:264:LEU:HD22	1:G:474:CYS:HB2	1.98	0.45
1:G:721:LYS:HZ2	1:H:379:GLU:CD	2.25	0.45
1:A:46:ILE:HG23	1:A:54:CYS:SG	2.57	0.45
1:A:309:PHE:HE2	3:L:31:PRO:HD2	1.82	0.45
1:G:355:HIS:HB3	1:G:381:VAL:HG22	1.99	0.45
3:K:192:GLU:CG	3:K:193:GLU:HA	2.46	0.45
1:B:141:ARG:NH2	2:D:112:SER:O	2.50	0.45
1:G:891:GLN:HE21	1:G:891:GLN:HA	1.82	0.45
3:K:57:GLN:HB3	3:L:60:LYS:NZ	2.32	0.45
1:A:309:PHE:C	3:L:18:GLU:HB2	2.42	0.45
1:A:565:PRO:HA	1:A:566:PRO:HD2	1.86	0.45
1:G:137:TYR:HE2	1:G:151:ALA:HB2	1.82	0.45
1:B:868:GLU:HA	1:B:872:LYS:HG2	1.99	0.45
2:C:37:ARG:HA	2:C:41:CYS:O	2.17	0.45
1:H:953:LYS:NZ	1:H:957:ASP:OD2	2.50	0.45
1:A:375:THR:HA	1:A:377:GLU:HG3	1.99	0.44
1:A:947:GLU:HB3	1:B:948:ILE:HD11	2.00	0.44
1:B:817:ARG:NH2	3:F:123:ASP:OD2	2.50	0.44
1:G:91:LEU:HD13	1:G:705:ARG:HG2	1.98	0.44
1:G:420:SER:O	1:G:423:GLY:HA3	2.18	0.44
1:H:119:ALA:HB3	1:H:674:CYS:SG	2.57	0.44
1:H:167:GLN:O	1:H:454:ILE:HA	2.17	0.44
1:B:142:ARG:HD3	1:B:713:ASN:OD1	2.17	0.44
1:B:522:GLU:OE2	1:B:658:ASN:HB2	2.18	0.44
1:H:647:GLN:OE1	1:H:648:THR:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:702:GLU:HG3	1:H:705:ARG:NH1	2.33	0.44
1:A:561:VAL:HB	1:A:576:SER:HB2	1.99	0.44
1:A:367:GLU:HB3	1:A:368:GLU:HB2	1.99	0.44
1:G:367:GLU:HB3	1:G:368:GLU:HB2	1.98	0.44
1:G:422:GLY:O	1:G:426:LYS:HB2	2.18	0.44
1:G:832:LYS:O	3:K:192:GLU:HA	2.17	0.44
1:G:901:ASP:HB3	1:H:523:LYS:HD3	2.00	0.44
1:A:795:TRP:HA	2:C:37:ARG:HD3	1.99	0.44
1:B:790:GLN:O	1:B:794:ARG:HG2	2.18	0.44
3:F:11:LYS:HE3	3:F:11:LYS:HB2	1.81	0.44
1:G:837:VAL:HG21	3:K:86:LEU:HA	1.99	0.44
1:B:495:GLN:HA	1:B:498:TYR:CD1	2.53	0.44
1:B:926:ARG:HG2	1:B:929:ARG:HD2	1.98	0.44
3:F:66:ILE:HG23	3:F:82:THR:HG21	1.99	0.44
1:H:246:ARG:O	1:H:258:ALA:HA	2.18	0.44
1:H:601:ASP:HB3	1:H:629:GLU:HG2	2.00	0.44
1:A:468:ASN:HB2	1:A:585:PRO:O	2.18	0.44
1:B:521:ILE:HB	1:B:524:PRO:HD2	1.99	0.44
2:C:138:LYS:O	2:C:141:PRO:HD2	2.17	0.44
1:G:222:PRO:HA	1:G:225:GLU:HB2	2.00	0.44
1:G:682:GLN:HA	1:G:683:PRO:HD2	1.90	0.44
1:G:815:ILE:HD11	3:K:183:PHE:HE1	1.81	0.44
1:A:716:VAL:HG12	1:A:763:LYS:HE2	2.00	0.44
1:A:757:TYR:HB3	1:A:770:VAL:HG11	2.00	0.44
1:B:563:PRO:HB2	1:B:566:PRO:HD2	2.00	0.44
1:B:868:GLU:CA	1:B:872:LYS:HG2	2.48	0.44
1:G:232:THR:OG1	1:G:238:SER:HB3	2.17	0.44
1:A:134:VAL:HG13	1:A:189:TYR:CE1	2.51	0.44
1:A:832:LYS:HB3	3:E:191:ALA:O	2.18	0.44
1:B:714:ARG:HA	1:B:764:VAL:O	2.18	0.44
1:B:836:LYS:HD2	1:B:836:LYS:O	2.18	0.44
1:G:561:VAL:HB	1:G:576:SER:HB2	2.00	0.44
1:H:141:ARG:HH11	1:H:776:GLU:HA	1.83	0.44
3:L:11:LYS:HB2	3:L:11:LYS:HE3	1.75	0.44
1:B:488:HIS:O	1:B:492:VAL:HB	2.18	0.43
1:G:830:TRP:HA	3:K:195:GLY:HA3	1.98	0.43
1:H:159:ALA:HB2	1:H:714:ARG:O	2.18	0.43
1:H:400:LYS:HA	1:H:400:LYS:HD3	1.84	0.43
1:A:268:ALA:N	1:A:269:ARG:HB2	2.34	0.43
1:B:246:ARG:HA	1:B:454:ILE:O	2.17	0.43
1:B:723:ARG:HD2	2:D:112:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:717:TYR:CE1	1:G:764:VAL:HB	2.53	0.43
1:H:668:GLN:OE1	1:H:763:LYS:NZ	2.51	0.43
1:A:364:ARG:O	3:L:31:PRO:HG2	2.18	0.43
1:A:782:LEU:HA	1:A:785:ILE:HG13	2.01	0.43
1:B:871:ARG:HB3	1:B:872:LYS:HE2	2.00	0.43
1:H:298:LEU:HA	1:H:384:LEU:HD21	1.99	0.43
2:J:93:TYR:CZ	2:J:101:MET:HA	2.54	0.43
1:A:231:LYS:HA	1:A:236:ASP:O	2.18	0.43
1:A:835:ILE:O	1:A:839:PRO:HD2	2.17	0.43
1:G:164:ARG:HH11	1:H:606:GLN:NE2	2.17	0.43
1:A:85:MET:HA	1:A:88:LEU:HD13	2.01	0.43
1:A:166:ASN:ND2	1:A:667:THR:HG22	2.34	0.43
1:B:869:LYS:O	1:B:873:ASP:HB2	2.19	0.43
1:G:55:THR:HA	1:G:65:GLN:HA	2.01	0.43
1:G:629:GLU:HB2	1:G:640:ARG:HA	2.00	0.43
1:H:5:PRO:HG3	1:H:769:GLY:HA2	2.00	0.43
1:H:331:THR:HA	1:H:334:ASP:OD2	2.18	0.43
2:J:22:GLU:HB3	3:L:154:TRP:HZ2	1.84	0.43
2:J:136:PHE:O	2:J:138:LYS:NZ	2.43	0.43
1:A:792:TRP:CZ3	2:C:147:ILE:HA	2.54	0.43
1:A:926:ARG:O	1:A:929:ARG:HB3	2.18	0.43
1:B:523:LYS:O	1:B:527:ILE:HG13	2.18	0.43
1:H:701:LEU:O	1:H:705:ARG:HG3	2.19	0.43
1:A:17:GLN:OE1	1:A:20:LYS:NZ	2.51	0.43
1:A:107:ASN:O	1:A:109:ILE:HG23	2.19	0.43
1:B:233:VAL:HG22	1:B:275:THR:O	2.19	0.43
3:E:90:CYS:HB3	3:E:94:GLU:HB2	2.01	0.43
1:G:17:GLN:OE1	1:G:20:LYS:NZ	2.52	0.43
1:G:661:MET:O	1:G:665:HIS:HD2	2.01	0.43
1:G:843:MET:SD	3:K:57:GLN:HB2	2.59	0.43
1:H:126:PHE:HB3	1:H:128:ILE:HG13	2.00	0.43
3:L:33:PRO:HB2	3:L:34:PRO:CD	2.48	0.43
1:A:599:VAL:HG22	1:A:603:VAL:HG23	2.01	0.43
1:B:31:MET:HB2	1:B:74:VAL:HG11	2.01	0.43
1:B:155:GLY:HA2	1:B:158:SER:OG	2.18	0.43
1:B:701:LEU:HG	1:B:705:ARG:NH2	2.33	0.43
1:G:710:GLY:O	1:G:767:ARG:NH2	2.51	0.43
1:A:309:PHE:CE2	3:L:31:PRO:C	2.97	0.43
1:A:557:SER:HA	1:A:558:PRO:HD3	1.87	0.43
1:A:690:LEU:HG	1:A:694:GLN:HE21	1.84	0.43
1:B:119:ALA:O	1:B:674:CYS:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:28:PRO:HA	3:E:29:PRO:HD3	1.86	0.43
1:G:575:PHE:HD2	1:G:588:ILE:HD11	1.83	0.43
1:A:367:GLU:HB2	1:A:369:GLN:H	1.84	0.43
1:A:923:LEU:HD21	1:B:924:GLN:HG2	2.01	0.43
1:G:377:GLU:HB3	1:G:393:TYR:OH	2.19	0.43
1:H:159:ALA:HA	1:H:715:MET:HA	2.01	0.43
1:A:310:VAL:HG12	1:A:311:SER:HA	2.01	0.42
1:B:240:ARG:HB2	1:B:280:TYR:HE2	1.83	0.42
1:B:531:LEU:HG	1:B:595:ASN:ND2	2.34	0.42
1:B:534:GLU:OE1	1:B:537:PHE:CD1	2.72	0.42
1:B:109:ILE:HG21	1:B:122:PRO:HD3	1.99	0.42
1:B:875:GLU:O	1:B:878:ASN:HB3	2.20	0.42
3:E:33:PRO:HA	3:E:34:PRO:HD3	1.86	0.42
3:E:57:GLN:HB3	3:F:60:LYS:NZ	2.34	0.42
3:L:14:LYS:HD3	3:L:103:PRO:HB2	2.00	0.42
1:B:54:CYS:O	1:B:65:GLN:HA	2.20	0.42
1:B:668:GLN:OE1	1:B:763:LYS:NZ	2.51	0.42
1:H:371:GLU:HG2	1:H:397:VAL:HG21	2.01	0.42
1:B:75:ASN:HA	1:B:76:PRO:HD3	1.89	0.42
1:B:480:GLU:HG2	1:B:518:ILE:HG12	2.02	0.42
1:G:232:THR:O	1:G:236:ASP:HA	2.19	0.42
1:G:195:ALA:HB1	1:G:197:THR:HG23	2.02	0.42
1:H:342:TYR:HA	1:H:345:ASP:HB2	2.01	0.42
1:H:503:ILE:HG22	1:H:760:GLY:HA2	2.01	0.42
3:L:23:ASP:HA	3:L:93:GLN:NE2	2.34	0.42
3:L:102:ALA:HB1	3:L:106:ILE:HD11	2.00	0.42
1:A:363:GLN:C	3:L:31:PRO:HG3	2.45	0.42
1:B:654:ARG:HE	1:B:654:ARG:HA	1.84	0.42
1:B:721:LYS:HB3	2:D:92:VAL:HG12	2.02	0.42
3:E:72:GLY:O	3:E:107:ASN:HA	2.20	0.42
1:G:497:GLU:O	1:G:501:GLU:HG2	2.19	0.42
1:A:282:ILE:HA	1:A:285:GLN:OE1	2.19	0.42
1:B:702:GLU:HG3	1:B:705:ARG:NH1	2.34	0.42
1:B:743:THR:HG23	1:B:744:GLU:OE2	2.20	0.42
1:A:80:GLU:HG3	1:A:102:GLN:HE22	1.85	0.42
2:C:124:GLU:CD	2:C:127:ARG:HH11	2.28	0.42
1:G:468:ASN:HB2	1:G:585:PRO:O	2.20	0.42
3:L:188:THR:HG22	3:L:189:LYS:H	1.83	0.42
1:B:501:GLU:O	1:B:761:ASN:HB2	2.20	0.42
3:F:13:SER:HA	3:F:15:LYS:N	2.35	0.42
1:G:923:LEU:HD13	1:H:923:LEU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1:MET:HA	1:H:4:ASP:O	2.20	0.42
1:B:716:VAL:HG22	1:B:762:THR:HG22	2.02	0.42
2:D:21:TRP:H	2:D:21:TRP:CD1	2.37	0.42
2:D:83:LEU:HD21	2:D:147:ILE:HG21	2.01	0.42
1:G:906:LEU:HD13	1:H:906:LEU:HA	2.01	0.42
1:H:512:LEU:HB3	1:H:580:TYR:OH	2.20	0.42
1:H:711:PHE:HA	1:H:712:PRO:HD3	1.73	0.42
1:A:782:LEU:HD13	2:C:92:VAL:HB	2.01	0.41
1:B:157:TYR:CZ	1:B:161:LEU:HD11	2.54	0.41
1:G:134:VAL:HG13	1:G:189:TYR:CE1	2.54	0.41
1:H:142:ARG:HG2	1:H:145:VAL:HB	2.01	0.41
1:A:132:ARG:HG3	1:A:205:PRO:HB2	2.01	0.41
1:A:500:ARG:HD2	1:B:367:GLU:HB3	2.01	0.41
3:E:51:PHE:HA	3:E:56:VAL:HG11	2.01	0.41
3:E:83:PHE:HB3	3:E:89:LEU:HG	2.01	0.41
1:G:97:LEU:HD11	1:G:688:SER:HB3	2.02	0.41
1:G:282:ILE:HA	1:G:285:GLN:OE1	2.20	0.41
1:H:528:LEU:HD12	1:H:529:SER:HB3	2.01	0.41
1:H:804:LYS:HE3	3:L:134:LEU:O	2.21	0.41
1:H:894:SER:HA	1:H:897:SER:HG	1.83	0.41
1:B:727:LEU:HG	1:B:782:LEU:HD21	2.01	0.41
1:G:667:THR:O	1:G:669:PRO:HD3	2.20	0.41
1:H:654:ARG:HA	1:H:654:ARG:HE	1.85	0.41
3:K:16:LYS:NZ	3:K:17:SER:OG	2.46	0.41
3:K:104:GLY:HA3	3:K:105:PRO:HD3	1.84	0.41
1:A:364:ARG:CB	1:A:369:GLN:O	2.68	0.41
1:B:717:TYR:HE1	1:B:743:THR:HG21	1.85	0.41
3:E:5:GLU:OE2	3:F:90:CYS:HB3	2.20	0.41
1:G:889:PHE:HA	1:G:892:LEU:HD12	2.02	0.41
1:H:287:MET:HE2	1:H:354:MET:SD	2.60	0.41
1:A:181:GLU:OE2	1:A:185:LYS:NZ	2.53	0.41
1:B:402:LYS:NZ	1:B:630:LYS:O	2.46	0.41
2:D:19:TYR:O	2:D:21:TRP:HD1	2.02	0.41
3:E:43:SER:HA	3:F:193:GLU:O	2.20	0.41
1:H:541:THR:HG23	1:H:544:SER:H	1.84	0.41
1:A:406:GLU:HB3	2:J:5:LYS:HG2	2.03	0.41
1:A:501:GLU:O	1:B:364:ARG:NH2	2.54	0.41
1:G:131:ASN:ND2	1:G:204:ALA:O	2.54	0.41
1:G:217:VAL:HA	1:G:220:THR:OG1	2.20	0.41
1:G:271:ILE:HD12	1:G:419:TYR:HA	2.02	0.41
1:G:718:PRO:HG2	1:H:389:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:530:ILE:HG12	1:H:548:LYS:HB2	2.02	0.41
3:L:30:PRO:HA	3:L:31:PRO:HD3	1.84	0.41
1:A:309:PHE:CD2	3:L:18:GLU:HG3	2.55	0.41
1:A:715:MET:O	1:A:763:LYS:HD2	2.20	0.41
1:A:779:ASP:HA	1:A:782:LEU:HB2	2.02	0.41
1:B:829:LEU:O	3:F:195:GLY:HA3	2.21	0.41
1:G:715:MET:O	1:G:763:LYS:HD2	2.20	0.41
1:G:769:GLY:O	1:G:773:ARG:N	2.54	0.41
1:G:843:MET:HG2	3:L:53:GLN:O	2.20	0.41
1:A:883:GLN:NE2	1:B:451:GLN:HB3	2.35	0.41
1:B:309:PHE:HD1	1:B:309:PHE:HA	1.79	0.41
1:B:400:LYS:HD3	1:B:400:LYS:HA	1.91	0.41
1:B:894:SER:HA	1:B:897:SER:HG	1.85	0.41
2:C:94:ASP:HB2	2:C:139:TYR:HE2	1.86	0.41
1:G:33:TRP:HE1	1:G:74:VAL:HA	1.86	0.41
1:G:372:ALA:HB3	1:G:377:GLU:HG2	2.03	0.41
1:G:815:ILE:HD13	1:G:815:ILE:HA	1.95	0.41
1:H:110:TYR:OH	1:H:185:LYS:NZ	2.51	0.41
1:H:234:ARG:NH2	1:H:676:ILE:HD13	2.35	0.41
1:H:300:LEU:HA	1:H:307:TYR:OH	2.20	0.41
1:H:523:LYS:HE2	1:H:523:LYS:HB3	1.89	0.41
1:A:11:LEU:HD11	1:A:148:HIS:HB2	2.02	0.41
1:A:364:ARG:HG3	3:L:36:GLN:HG3	2.03	0.41
1:A:369:GLN:HG2	1:A:417:VAL:HG11	2.03	0.41
1:A:710:GLY:O	1:A:767:ARG:NH2	2.54	0.41
1:B:230:ALA:HB1	1:B:278:ARG:O	2.21	0.41
1:B:260:ILE:H	1:B:441:ASN:ND2	2.19	0.41
1:B:491:PHE:O	1:B:495:GLN:HG2	2.20	0.41
1:G:286:LEU:HD11	1:G:298:LEU:HD22	2.02	0.41
1:G:483:GLN:O	1:G:486:PHE:HB3	2.20	0.41
1:G:919:GLN:HA	1:G:922:GLU:HG2	2.01	0.41
3:K:5:GLU:OE2	3:L:90:CYS:HB3	2.21	0.41
1:B:612:ASN:O	1:B:614:LEU:N	2.54	0.41
3:L:141:LYS:NZ	3:L:173:ASP:O	2.47	0.41
1:A:364:ARG:HH11	3:L:33:PRO:HD3	1.85	0.40
1:B:283:PHE:HB3	1:B:354:MET:SD	2.60	0.40
3:E:33:PRO:HB2	3:E:36:GLN:NE2	2.36	0.40
1:G:892:LEU:HD22	1:G:896:ARG:HH22	1.86	0.40
1:B:163:ASN:HD21	1:B:165:GLU:HB3	1.87	0.40
1:B:169:MET:O	1:B:456:VAL:HA	2.21	0.40
3:F:9:LYS:O	3:F:13:SER:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:175:SER:HB3	1:H:234:ARG:NH2	2.36	0.40
1:H:635:LYS:HB2	1:H:643:GLY:N	2.36	0.40
1:H:723:ARG:HD2	2:J:112:SER:HB2	2.03	0.40
2:I:143:VAL:O	2:I:146:ILE:HB	2.22	0.40
2:C:91:LYS:HD3	2:C:97:GLU:HG2	2.03	0.40
1:G:527:ILE:HG23	1:G:549:LEU:HD11	2.04	0.40
1:G:793:ILE:HG23	2:I:125:ILE:HD12	2.02	0.40
3:K:41:GLN:HA	3:L:85:SER:O	2.21	0.40
1:A:41:TYR:HD1	1:A:97:LEU:HD22	1.87	0.40
1:A:922:GLU:HG3	1:A:923:LEU:N	2.36	0.40
1:B:248:HIS:ND1	1:B:453:PHE:HB3	2.37	0.40
1:B:309:PHE:CD1	1:B:357:GLY:HA3	2.57	0.40
1:B:715:MET:O	1:B:763:LYS:HA	2.21	0.40
3:F:68:GLN:OE1	3:F:78:ASP:HB2	2.21	0.40
1:H:162:ALA:O	1:H:164:ARG:NH2	2.55	0.40
1:B:41:TYR:HD1	1:B:97:LEU:HD22	1.86	0.40
1:B:359:MET:HE1	1:B:396:LEU:HD13	2.03	0.40
1:B:831:TYR:HD2	3:F:194:GLU:HB3	1.86	0.40
1:G:284:TYR:HA	1:G:287:MET:HE3	2.04	0.40
1:G:599:VAL:HG11	1:G:604:VAL:HG23	2.04	0.40
1:H:7:PRO:HA	1:H:12:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	960/1953 (49%)	772 (80%)	149 (16%)	39 (4%)	2	18
1	B	962/1953 (49%)	779 (81%)	128 (13%)	55 (6%)	1	14
1	G	960/1953 (49%)	783 (82%)	136 (14%)	41 (4%)	2	17
1	H	962/1953 (49%)	779 (81%)	125 (13%)	58 (6%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	154/156 (99%)	137 (89%)	13 (8%)	4 (3%)	4	25
2	D	154/156 (99%)	139 (90%)	11 (7%)	4 (3%)	4	25
2	I	154/156 (99%)	135 (88%)	16 (10%)	3 (2%)	6	32
2	J	154/156 (99%)	131 (85%)	19 (12%)	4 (3%)	4	25
3	E	194/196 (99%)	139 (72%)	40 (21%)	15 (8%)	1	10
3	F	194/196 (99%)	136 (70%)	41 (21%)	17 (9%)	0	8
3	K	194/196 (99%)	144 (74%)	37 (19%)	13 (7%)	1	12
3	L	194/196 (99%)	129 (66%)	46 (24%)	19 (10%)	0	7
All	All	5236/9220 (57%)	4203 (80%)	761 (14%)	272 (5%)	3	15

All (272) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	22	GLN
1	A	138	LYS
1	A	269	ARG
1	A	310	VAL
1	A	311	SER
1	A	363	GLN
1	A	365	PRO
1	A	393	TYR
1	A	394	LYS
1	A	568	PRO
1	A	603	VAL
1	A	845	LYS
1	B	68	LYS
1	B	86	SER
1	B	142	ARG
1	B	149	LEU
1	B	178	GLY
1	B	205	PRO
1	B	367	GLU
1	B	565	PRO
1	B	613	LYS
1	B	621	ASP
1	B	646	PHE
1	B	680	LEU
1	B	725	THR

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Mol	Chain	Res	Type
1	B	733	PRO
1	B	869	LYS
2	D	152	PRO
3	E	17	SER
3	E	47	VAL
3	E	50	MET
3	F	14	LYS
3	F	15	LYS
3	F	53	GLN
3	F	105	PRO
3	F	125	GLU
3	F	144	GLU
1	G	22	GLN
1	G	138	LYS
1	G	177	ALA
1	G	264	LEU
1	G	282	ILE
1	G	358	GLU
1	G	568	PRO
1	G	601	ASP
1	G	603	VAL
1	G	843	MET
1	H	21	ASP
1	H	68	LYS
1	H	86	SER
1	H	142	ARG
1	H	205	PRO
1	H	307	TYR
1	H	367	GLU
1	H	565	PRO
1	H	622	HIS
1	H	645	SER
1	H	680	LEU
1	H	725	THR
1	H	733	PRO
1	H	752	LEU
1	H	842	THR
2	I	97	GLU
3	K	17	SER
3	L	13	SER
3	L	16	LYS
3	L	31	PRO

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Mol	Chain	Res	Type
3	L	32	LYS
3	L	53	GLN
3	L	58	GLU
3	L	67	ASP
3	L	125	GLU
3	L	144	GLU
1	A	271	ILE
1	A	366	ARG
1	A	460	ALA
1	A	621	ASP
1	A	737	VAL
1	A	831	TYR
1	A	843	MET
1	B	14	SER
1	B	274	GLN
1	B	312	GLN
1	B	446	THR
1	B	447	LYS
1	B	451	GLN
1	B	517	CYS
1	B	535	SER
1	B	645	SER
1	B	752	LEU
1	B	834	TYR
1	B	842	THR
1	B	844	ALA
1	B	870	VAL
2	C	97	GLU
2	C	152	PRO
3	E	55	GLN
3	E	59	PHE
3	E	139	GLU
3	F	63	PHE
3	F	174	GLY
3	F	195	GLY
1	G	269	ARG
1	G	271	ILE
1	G	308	HIS
1	G	516	ALA
1	G	621	ASP
1	G	712	PRO
1	G	735	GLY

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Mol	Chain	Res	Type
1	G	737	VAL
1	G	831	TYR
1	H	3	GLU
1	H	11	LEU
1	H	178	GLY
1	H	356	LEU
1	H	580	TYR
1	H	613	LYS
1	H	621	ASP
1	H	646	PHE
1	H	648	THR
1	H	738	ASP
1	H	804	LYS
1	H	834	TYR
3	K	55	GLN
3	K	59	PHE
3	K	169	GLU
3	L	174	GLY
3	L	195	GLY
1	A	11	LEU
1	A	177	ALA
1	A	228	GLY
1	A	270	VAL
1	A	299	LEU
1	A	367	GLU
1	A	392	LEU
1	A	597	ASP
1	A	712	PRO
1	A	784	LYS
1	B	3	GLU
1	B	77	PRO
1	B	292	GLU
1	B	448	GLN
1	B	529	SER
1	B	567	LYS
1	B	630	LYS
1	B	751	GLN
2	C	96	ALA
2	C	116	ARG
3	E	53	GLN
3	E	58	GLU
3	E	169	GLU

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Mol	Chain	Res	Type
3	F	72	GLY
1	G	11	LEU
1	G	108	LEU
1	G	114	GLY
1	G	144	GLU
1	G	207	LYS
1	G	310	VAL
1	H	14	SER
1	H	57	ASP
1	H	109	ILE
1	H	446	THR
1	H	529	SER
1	H	567	LYS
1	H	573	ALA
1	H	751	GLN
1	H	844	ALA
2	J	152	PRO
3	K	139	GLU
3	L	72	GLY
3	L	192	GLU
1	A	207	LYS
1	A	827	ASN
1	B	20	LYS
1	B	57	ASP
1	B	601	ASP
1	B	804	LYS
1	B	871	ARG
3	E	106	ILE
3	F	28	PRO
3	F	57	GLN
3	F	95	LEU
3	F	192	GLU
1	G	9	GLU
1	G	392	LEU
1	G	460	ALA
1	G	784	LYS
1	G	827	ASN
1	H	137	TYR
1	H	200	PRO
1	H	251	PRO
1	H	375	THR
1	H	639	GLY

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Mol	Chain	Res	Type
1	H	803	LYS
2	I	116	ARG
2	J	130	ASP
3	L	70	LYS
3	L	80	ARG
3	L	188	THR
3	L	190	GLY
1	A	735	GLY
1	B	618	ILE
2	D	40	ASP
3	E	21	GLY
3	E	67	ASP
3	F	88	ARG
1	G	299	LEU
1	G	301	SER
1	G	375	THR
1	G	411	GLY
1	H	5	PRO
1	H	90	TYR
1	H	175	SER
1	H	491	PHE
1	H	597	ASP
1	H	707	CYS
2	J	75	LYS
2	J	131	GLU
3	K	138	GLY
3	L	14	LYS
1	A	719	ASP
1	B	200	PRO
1	B	251	PRO
1	B	375	THR
1	B	629	GLU
1	B	734	LYS
2	D	43	PRO
3	F	190	GLY
1	G	597	ASP
1	H	618	ILE
1	H	833	LEU
2	I	152	PRO
3	K	21	GLY
3	K	38	ARG
3	L	102	ALA

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Mol	Chain	Res	Type
1	A	66	VAL
1	A	282	ILE
1	B	846	VAL
2	D	135	GLY
3	E	29	PRO
3	E	138	GLY
1	H	58	ILE
1	H	492	VAL
3	K	106	ILE
1	G	228	GLY
1	G	839	PRO
1	H	198	PRO
1	H	599	VAL
3	K	140	GLY
1	B	404	GLY
1	G	492	VAL
1	G	760	GLY
1	H	511	GLY
3	K	29	PRO
3	K	87	GLY
3	K	190	GLY
1	A	364	ARG
1	A	760	GLY
1	A	839	PRO
1	B	58	ILE
1	B	634	GLY
1	B	639	GLY
3	F	21	GLY
1	G	66	VAL
1	H	564	LYS
1	H	631	GLY
1	B	198	PRO
1	B	750	ILE
3	E	140	GLY
1	G	786	VAL
1	H	750	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	833/1689 (49%)	792 (95%)	41 (5%)	22	43
1	B	835/1689 (49%)	778 (93%)	57 (7%)	14	36
1	G	833/1689 (49%)	795 (95%)	38 (5%)	24	45
1	H	835/1689 (49%)	788 (94%)	47 (6%)	19	40
2	C	132/132 (100%)	128 (97%)	4 (3%)	36	57
2	D	132/132 (100%)	128 (97%)	4 (3%)	36	57
2	I	132/132 (100%)	128 (97%)	4 (3%)	36	57
2	J	132/132 (100%)	127 (96%)	5 (4%)	29	50
3	E	164/164 (100%)	160 (98%)	4 (2%)	43	64
3	F	164/164 (100%)	151 (92%)	13 (8%)	11	32
3	K	164/164 (100%)	161 (98%)	3 (2%)	51	68
3	L	164/164 (100%)	155 (94%)	9 (6%)	19	41
All	All	4520/7940 (57%)	4291 (95%)	229 (5%)	23	42

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	A	58	ILE
1	A	63	SER
1	A	143	THR
1	A	145	VAL
1	A	172	THR
1	A	197	THR
1	A	222	PRO
1	A	232	THR
1	A	266	GLU
1	A	271	ILE
1	A	282	ILE
1	A	312	GLN
1	A	334	ASP
1	A	345	ASP
1	A	362	LYS
1	A	363	GLN
1	A	364	ARG
1	A	365	PRO

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Mol	Chain	Res	Type
1	A	388	ASN
1	A	397	VAL
1	A	409	THR
1	A	418	SER
1	A	497	GLU
1	A	543	LYS
1	A	568	PRO
1	A	572	GLU
1	A	586	TYR
1	A	591	TRP
1	A	600	ASN
1	A	616	GLN
1	A	696	THR
1	A	761	ASN
1	A	795	TRP
1	A	815	ILE
1	A	854	GLU
1	A	868	GLU
1	A	871	ARG
1	A	872	LYS
1	A	875	GLU
1	A	887	ASP
1	B	4	ASP
1	B	12	TYR
1	B	87	ASN
1	B	91	LEU
1	B	93	ASP
1	B	107	ASN
1	B	134	VAL
1	B	135	GLN
1	B	137	TYR
1	B	146	PRO
1	B	163	ASN
1	B	172	THR
1	B	174	GLU
1	B	180	THR
1	B	192	ASN
1	B	198	PRO
1	B	203	GLU
1	B	222	PRO
1	B	341	GLU
1	B	375	THR

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Mol	Chain	Res	Type
1	B	393	TYR
1	B	405	ASN
1	B	413	ASN
1	B	415	THR
1	B	417	VAL
1	B	448	GLN
1	B	503	ILE
1	B	524	PRO
1	B	565	PRO
1	B	584	VAL
1	B	593	GLU
1	B	608	LYS
1	B	622	HIS
1	B	647	GLN
1	B	648	THR
1	B	654	ARG
1	B	668	GLN
1	B	716	VAL
1	B	718	PRO
1	B	744	GLU
1	B	758	ARG
1	B	771	LEU
1	B	776	GLU
1	B	826	ARG
1	B	827	ASN
1	B	836	LYS
1	B	838	LYS
1	B	843	MET
1	B	862	GLU
1	B	867	GLU
1	B	870	VAL
1	B	872	LYS
1	B	873	ASP
1	B	896	ARG
1	B	911	SER
1	B	925	GLU
1	B	954	GLU
2	C	51	ASN
2	C	69	PRO
2	C	133	ASP
2	C	140	GLU
2	D	85	ASP

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Mol	Chain	Res	Type
2	D	94	ASP
2	D	130	ASP
2	D	139	TYR
3	E	52	THR
3	E	54	HIS
3	E	58	GLU
3	E	108	PHE
3	F	3	ASP
3	F	17	SER
3	F	19	GLU
3	F	30	PRO
3	F	52	THR
3	F	55	GLN
3	F	67	ASP
3	F	89	LEU
3	F	105	PRO
3	F	109	THR
3	F	113	THR
3	F	168	SER
3	F	186	ILE
1	G	4	ASP
1	G	21	ASP
1	G	165	GLU
1	G	180	THR
1	G	212	THR
1	G	215	ASP
1	G	222	PRO
1	G	243	LYS
1	G	266	GLU
1	G	271	ILE
1	G	282	ILE
1	G	306	ASP
1	G	334	ASP
1	G	345	ASP
1	G	362	LYS
1	G	381	VAL
1	G	391	ASP
1	G	470	PHE
1	G	538	PRO
1	G	543	LYS
1	G	568	PRO
1	G	576	SER

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Mol	Chain	Res	Type
1	G	586	TYR
1	G	591	TRP
1	G	600	ASN
1	G	605	ASP
1	G	616	GLN
1	G	668	GLN
1	G	713	ASN
1	G	716	VAL
1	G	721	LYS
1	G	756	ASP
1	G	761	ASN
1	G	795	TRP
1	G	815	ILE
1	G	854	GLU
1	G	865	GLU
1	G	904	GLU
1	H	4	ASP
1	H	83	GLU
1	H	91	LEU
1	H	92	ASN
1	H	93	ASP
1	H	134	VAL
1	H	145	VAL
1	H	146	PRO
1	H	180	THR
1	H	192	ASN
1	H	222	PRO
1	H	236	ASP
1	H	266	GLU
1	H	302	ASP
1	H	341	GLU
1	H	377	GLU
1	H	473	LEU
1	H	503	ILE
1	H	522	GLU
1	H	524	PRO
1	H	565	PRO
1	H	593	GLU
1	H	597	ASP
1	H	601	ASP
1	H	608	LYS
1	H	641	LYS

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Mol	Chain	Res	Type
1	H	642	LYS
1	H	645	SER
1	H	649	VAL
1	H	655	GLU
1	H	668	GLN
1	H	716	VAL
1	H	743	THR
1	H	771	LEU
1	H	776	GLU
1	H	836	LYS
1	H	838	LYS
1	H	843	MET
1	H	846	VAL
1	H	862	GLU
1	H	868	GLU
1	H	887	ASP
1	H	896	ARG
1	H	923	LEU
1	H	925	GLU
1	H	948	ILE
1	H	954	GLU
2	I	42	LYS
2	I	51	ASN
2	I	69	PRO
2	I	140	GLU
2	J	63	THR
2	J	85	ASP
2	J	94	ASP
2	J	101	MET
2	J	153	ASP
3	K	54	HIS
3	K	58	GLU
3	K	108	PHE
3	L	3	ASP
3	L	45	SER
3	L	55	GLN
3	L	67	ASP
3	L	68	GLN
3	L	89	LEU
3	L	113	THR
3	L	128	ILE
3	L	193	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	182	ASN
1	A	229	ASN
1	A	285	GLN
1	A	388	ASN
1	A	413	ASN
1	A	472	GLN
1	A	550	ASN
1	A	595	ASN
1	A	670	HIS
1	A	713	ASN
1	B	163	ASN
1	B	192	ASN
1	B	219	GLN
1	B	248	HIS
1	B	273	GLN
1	B	274	GLN
1	B	441	ASN
1	B	468	ASN
1	B	487	ASN
1	B	546	GLN
1	B	550	ASN
1	B	595	ASN
1	B	693	HIS
1	B	827	ASN
1	B	883	GLN
1	B	886	ASN
2	C	51	ASN
2	C	73	GLN
2	D	98	ASN
3	E	54	HIS
3	E	133	ASN
3	E	185	GLN
3	F	77	ASN
3	F	93	GLN
3	F	130	ASN
1	G	50	GLN
1	G	87	ASN
1	G	92	ASN
1	G	219	GLN
1	G	285	GLN

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Mol	Chain	Res	Type
1	G	293	ASN
1	G	550	ASN
1	G	595	ASN
1	G	665	HIS
1	G	670	HIS
1	G	713	ASN
1	G	878	ASN
1	G	891	GLN
1	G	919	GLN
1	H	107	ASN
1	H	192	ASN
1	H	216	GLN
1	H	219	GLN
1	H	235	ASN
1	H	281	HIS
1	H	312	GLN
1	H	546	GLN
1	H	550	ASN
1	H	595	ASN
1	H	616	GLN
1	H	670	HIS
2	I	51	ASN
2	I	73	GLN
3	K	55	GLN
3	K	133	ASN
3	L	55	GLN
3	L	77	ASN
3	L	93	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

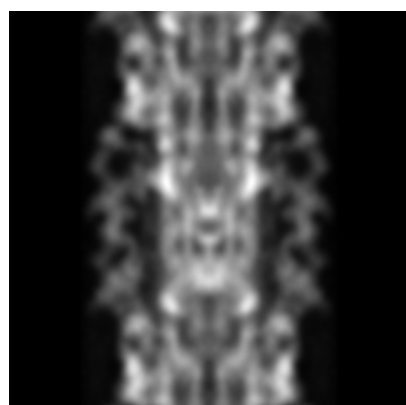
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1950. These allow visual inspection of the internal detail of the map and identification of artifacts.

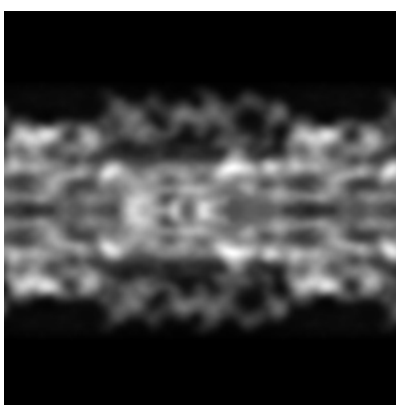
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

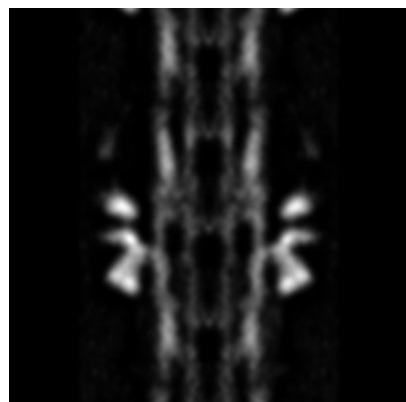


Z

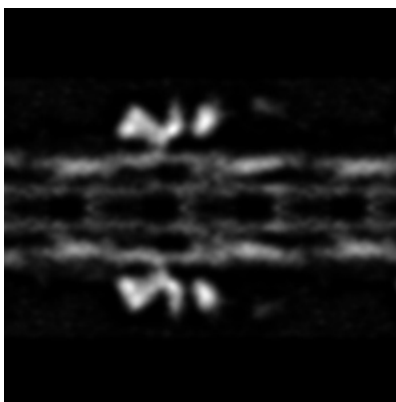
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

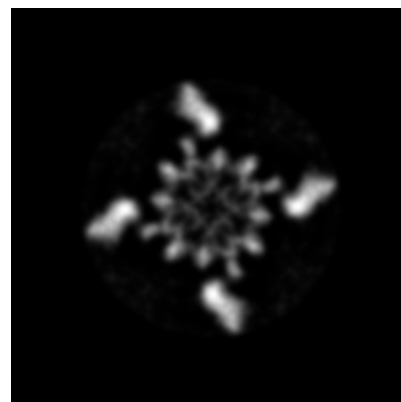
6.2.1 Primary map



X Index: 125



Y Index: 125

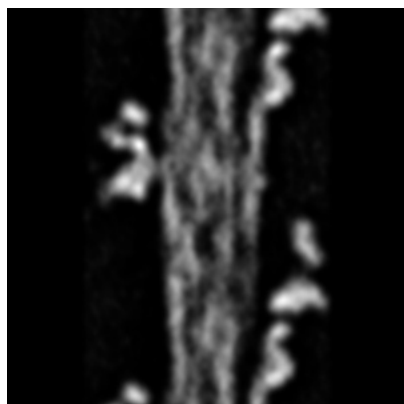


Z Index: 125

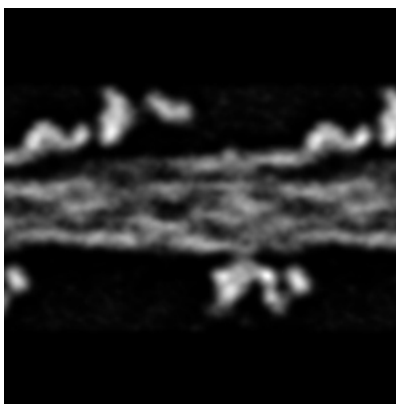
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 150



Y Index: 99

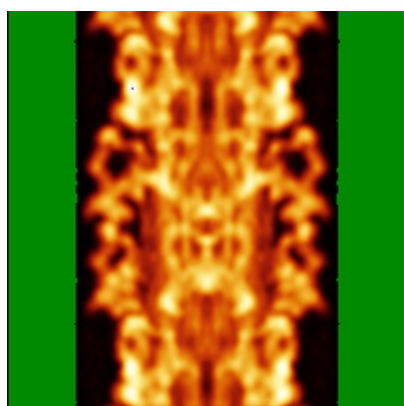


Z Index: 200

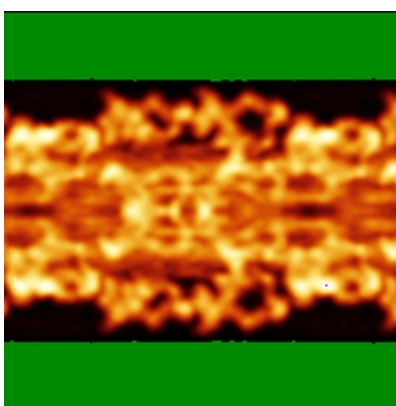
The images above show the largest variance slices of the map in three orthogonal directions.

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

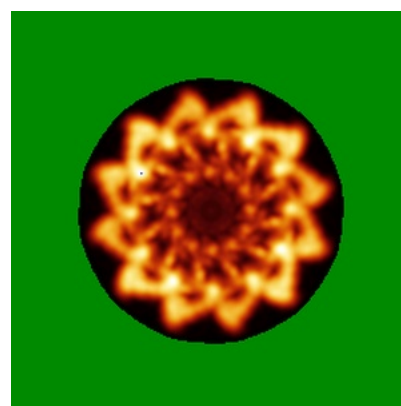
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

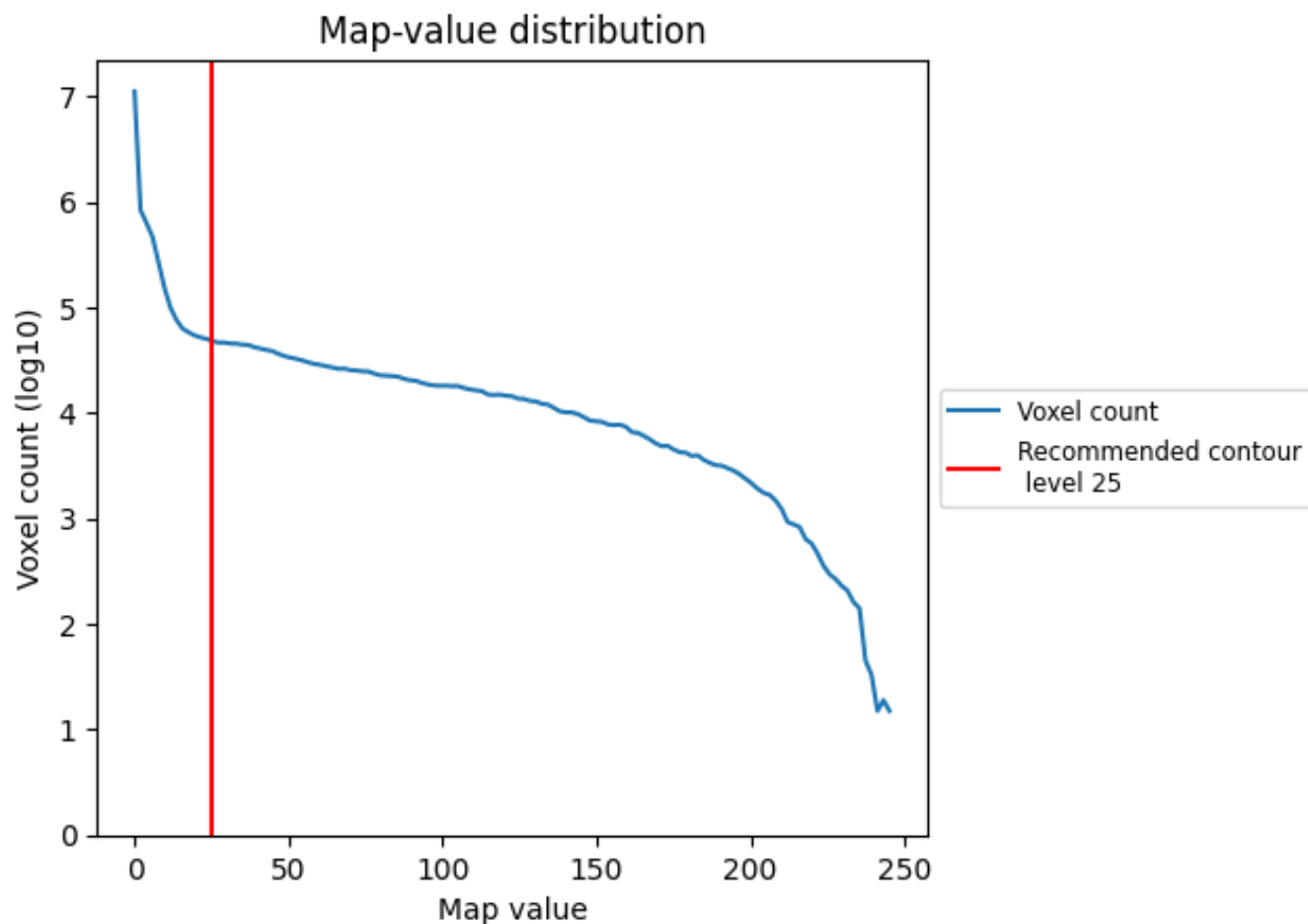
6.6 Mask visualisation

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

7 Map analysis [i](#)

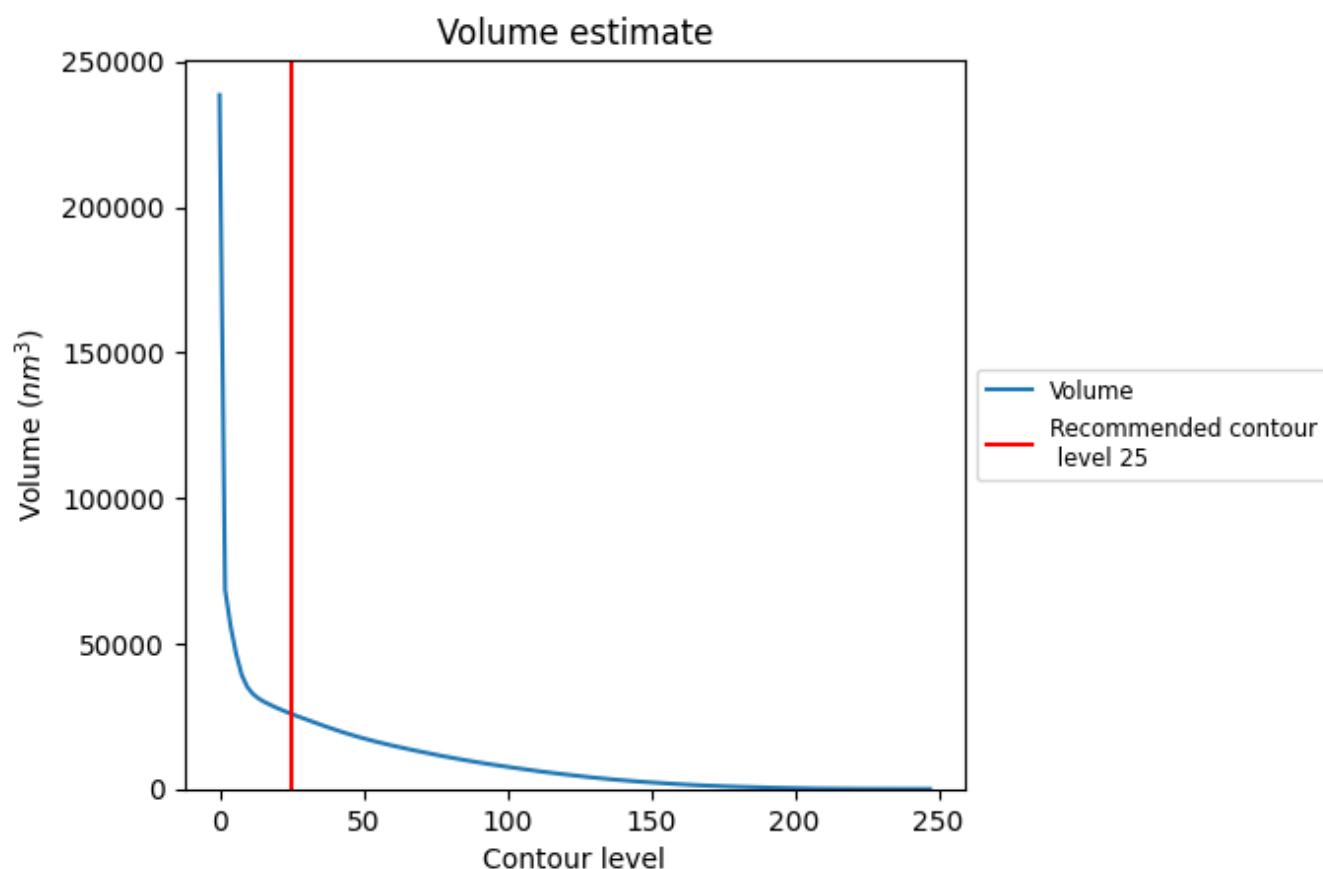
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

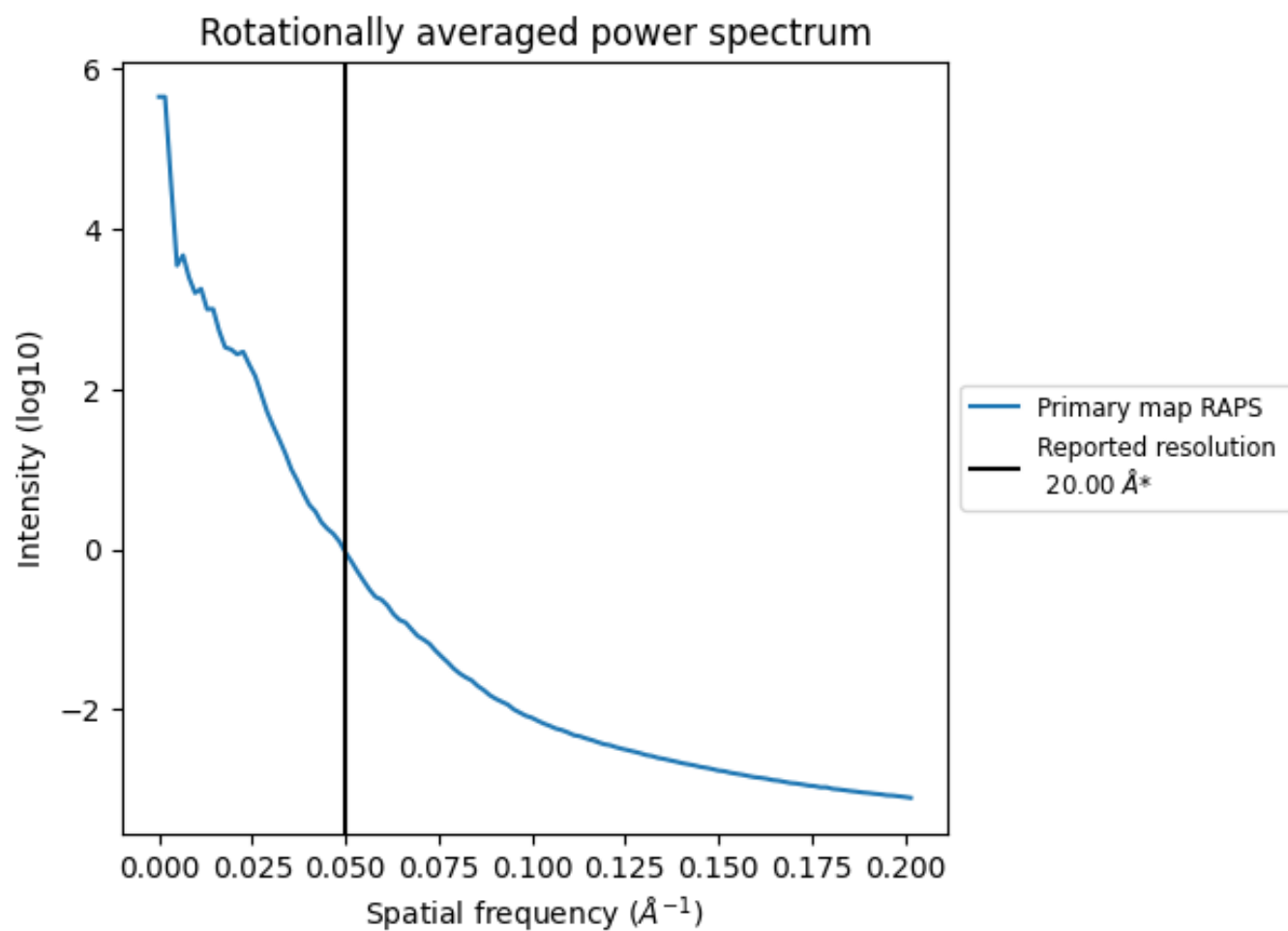
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 25767 nm³; this corresponds to an approximate mass of 23276 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.050 Å⁻¹

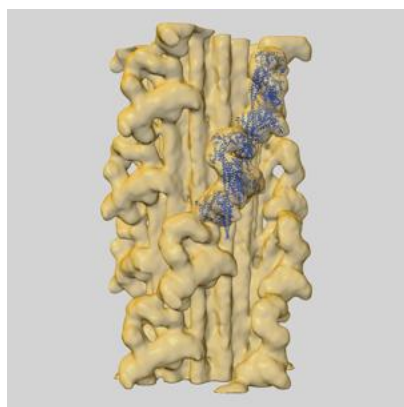
8 Fourier-Shell correlation ⓘ

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

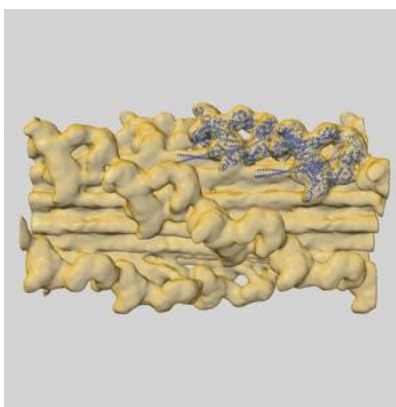
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1950 and PDB model 3JBH. Per-residue inclusion information can be found in section [3](#) on page [5](#).

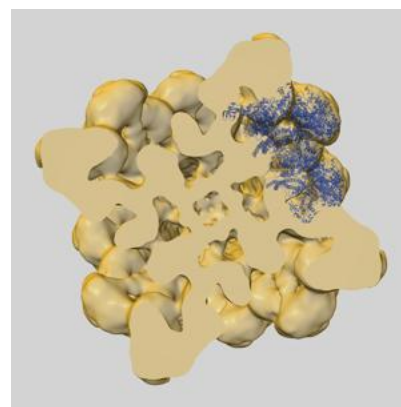
9.1 Map-model overlay [i](#)



X



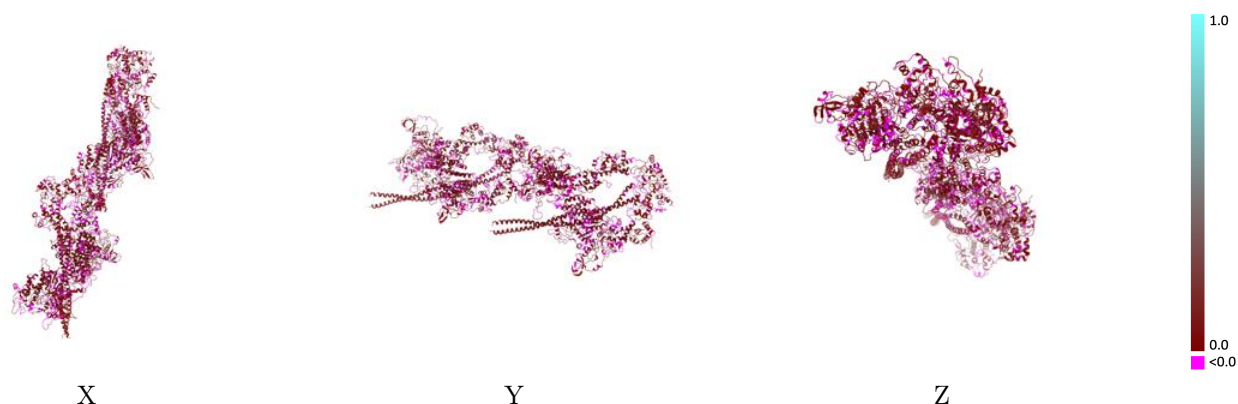
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 25.0 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](#)

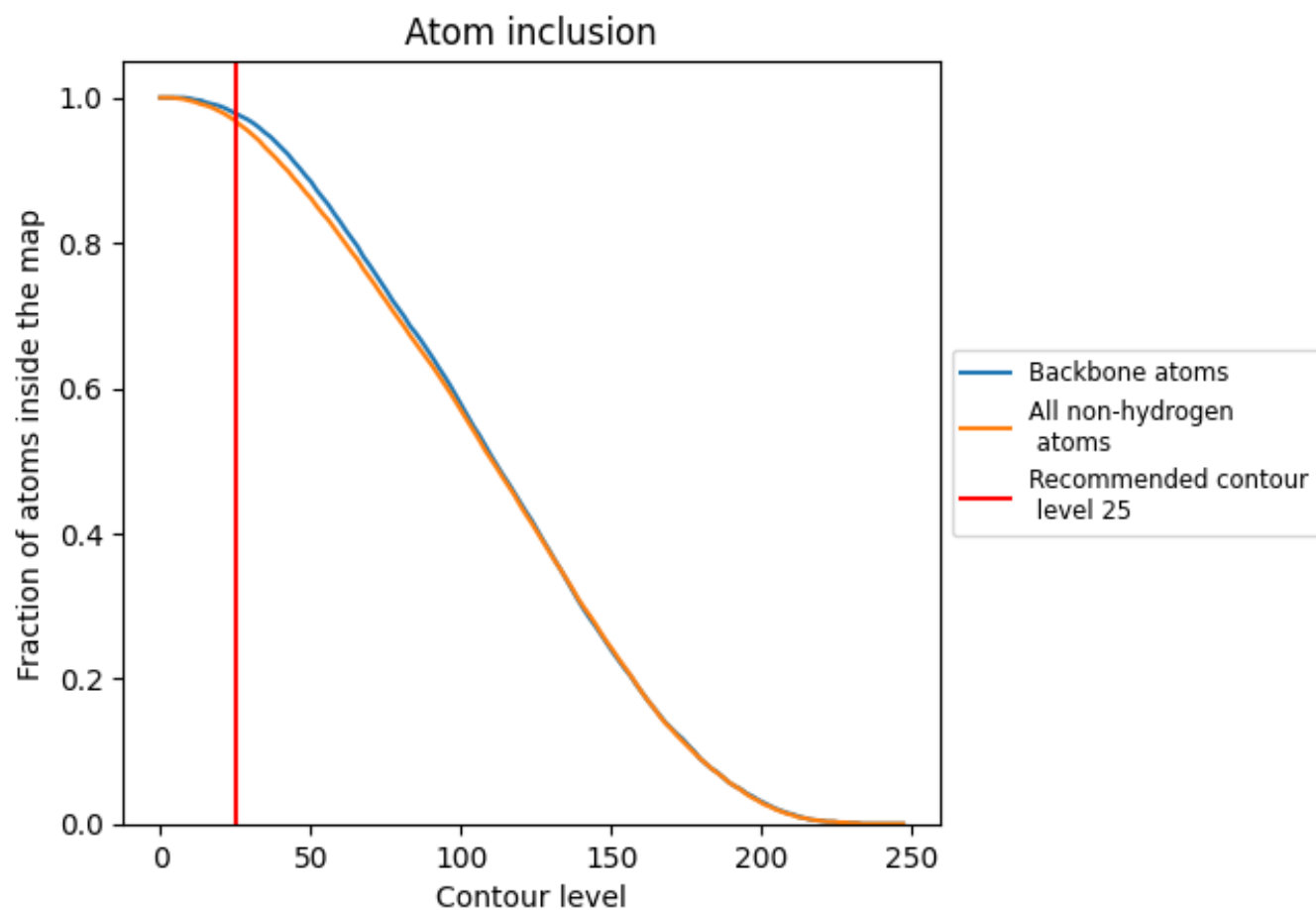


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9680	0.0440
A	0.9730	0.0440
B	0.9670	0.0430
C	0.9540	0.0530
D	0.9590	0.0410
E	0.9720	0.0430
F	0.9460	0.0440
G	0.9770	0.0460
H	0.9680	0.0430
I	0.9550	0.0520
J	0.9610	0.0380
K	0.9680	0.0440
L	0.9440	0.0440

1.0

0.0

<0.0