



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:04 PM UTC

PDB ID : 7N9C / pdb_00007n9c
EMDB ID : EMD-24256
Title : Potent neutralizing nanobodies resist convergent circulating variants of SARS-CoV-2 by targeting novel and conserved epitopes-CovS with NB95
Authors : Sun, D.; Zhang, C.; Shi, Y.
Deposited on : 2021-06-17
Resolution : 3.71 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

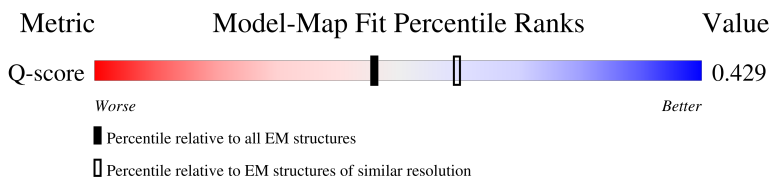
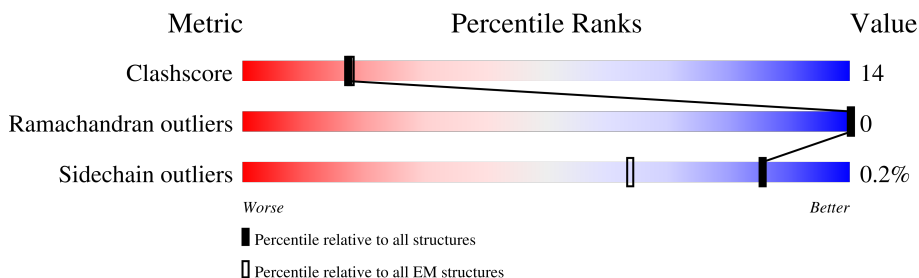
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

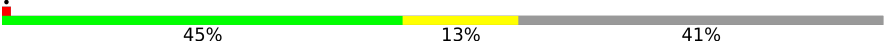
The reported resolution of this entry is 3.71 Å.

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	10534 (3.21 - 4.21)

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	1380	
1	B	1380	
1	C	1380	
2	D	155	

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Mol	Chain	Length	Quality of chain
2	E	155	63% 50% 31% 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22734 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	980	Total	C	N	O	S	0	0
			7542	4829	1259	1422	32		
1	B	812	Total	C	N	O	S	0	0
			6220	3981	1036	1177	26		
1	C	975	Total	C	N	O	S	0	0
			7018	4469	1203	1314	32		

There are 543 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0DTC2
A	2	GLY	-	expression tag	UNP P0DTC2
A	3	GLY	-	expression tag	UNP P0DTC2
A	4	GLU	-	expression tag	UNP P0DTC2
A	5	GLY	-	expression tag	UNP P0DTC2
A	6	LEU	-	expression tag	UNP P0DTC2
A	7	ARG	-	expression tag	UNP P0DTC2
A	8	ALA	-	expression tag	UNP P0DTC2
A	9	SER	-	expression tag	UNP P0DTC2
A	10	PRO	-	expression tag	UNP P0DTC2
A	11	ARG	-	expression tag	UNP P0DTC2
A	12	ARG	-	expression tag	UNP P0DTC2
A	13	ARG	-	expression tag	UNP P0DTC2
A	14	PRO	-	expression tag	UNP P0DTC2
A	15	LEU	-	expression tag	UNP P0DTC2
A	16	LEU	-	expression tag	UNP P0DTC2
A	17	PRO	-	expression tag	UNP P0DTC2
A	18	LEU	-	expression tag	UNP P0DTC2
A	19	GLN	-	expression tag	UNP P0DTC2
A	20	PRO	-	expression tag	UNP P0DTC2
A	21	ARG	-	expression tag	UNP P0DTC2
A	22	GLY	-	expression tag	UNP P0DTC2
A	23	CYS	-	expression tag	UNP P0DTC2
A	24	PRO	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ARG	-	expression tag	UNP P0DTC2
A	26	GLY	-	expression tag	UNP P0DTC2
A	27	ASP	-	expression tag	UNP P0DTC2
A	28	GLY	-	expression tag	UNP P0DTC2
A	29	CYS	-	expression tag	UNP P0DTC2
A	30	LEU	-	expression tag	UNP P0DTC2
A	31	ARG	-	expression tag	UNP P0DTC2
A	32	GLY	-	expression tag	UNP P0DTC2
A	33	GLY	-	expression tag	UNP P0DTC2
A	34	ARG	-	expression tag	UNP P0DTC2
A	35	GLY	-	expression tag	UNP P0DTC2
A	36	ARG	-	expression tag	UNP P0DTC2
A	37	ALA	-	expression tag	UNP P0DTC2
A	38	GLY	-	expression tag	UNP P0DTC2
A	39	PHE	-	expression tag	UNP P0DTC2
A	40	GLY	-	expression tag	UNP P0DTC2
A	41	PHE	-	expression tag	UNP P0DTC2
A	42	TRP	-	expression tag	UNP P0DTC2
A	43	ARG	-	expression tag	UNP P0DTC2
A	44	VAL	-	expression tag	UNP P0DTC2
A	45	THR	-	expression tag	UNP P0DTC2
A	46	GLY	-	expression tag	UNP P0DTC2
A	47	GLY	-	expression tag	UNP P0DTC2
A	48	SER	-	expression tag	UNP P0DTC2
A	49	SER	-	expression tag	UNP P0DTC2
A	50	ALA	-	expression tag	UNP P0DTC2
A	51	SER	-	expression tag	UNP P0DTC2
A	52	ALA	-	expression tag	UNP P0DTC2
A	53	ASN	-	expression tag	UNP P0DTC2
A	54	HIS	-	expression tag	UNP P0DTC2
A	55	VAL	-	expression tag	UNP P0DTC2
A	56	HIS	-	expression tag	UNP P0DTC2
A	57	ALA	-	expression tag	UNP P0DTC2
A	58	PHE	-	expression tag	UNP P0DTC2
A	59	PHE	-	expression tag	UNP P0DTC2
A	60	PHE	-	expression tag	UNP P0DTC2
A	61	PHE	-	expression tag	UNP P0DTC2
A	62	LEU	-	expression tag	UNP P0DTC2
A	63	GLN	-	expression tag	UNP P0DTC2
A	64	LEU	-	expression tag	UNP P0DTC2
A	65	LEU	-	expression tag	UNP P0DTC2
A	66	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ASN	-	expression tag	UNP P0DTC2
A	68	VAL	-	expression tag	UNP P0DTC2
A	69	LEU	-	expression tag	UNP P0DTC2
A	70	VAL	-	expression tag	UNP P0DTC2
A	71	VAL	-	expression tag	UNP P0DTC2
A	72	VAL	-	expression tag	UNP P0DTC2
A	73	LEU	-	expression tag	UNP P0DTC2
A	74	SER	-	expression tag	UNP P0DTC2
A	75	HIS	-	expression tag	UNP P0DTC2
A	76	HIS	-	expression tag	UNP P0DTC2
A	77	PHE	-	expression tag	UNP P0DTC2
A	78	GLY	-	expression tag	UNP P0DTC2
A	79	LYS	-	expression tag	UNP P0DTC2
A	80	GLU	-	expression tag	UNP P0DTC2
A	81	LEU	-	expression tag	UNP P0DTC2
A	82	ARG	-	expression tag	UNP P0DTC2
A	83	PRO	-	expression tag	UNP P0DTC2
A	84	SER	-	expression tag	UNP P0DTC2
A	85	GLN	-	expression tag	UNP P0DTC2
A	86	ALA	-	expression tag	UNP P0DTC2
A	87	GLU	-	expression tag	UNP P0DTC2
A	88	PHE	-	expression tag	UNP P0DTC2
A	89	GLY	-	expression tag	UNP P0DTC2
A	90	THR	-	expression tag	UNP P0DTC2
A	91	ALA	-	expression tag	UNP P0DTC2
A	92	THR	-	expression tag	UNP P0DTC2
A	774	GLY	ARG	engineered mutation	UNP P0DTC2
A	775	SER	ARG	engineered mutation	UNP P0DTC2
A	777	SER	ARG	engineered mutation	UNP P0DTC2
A	909	PRO	PHE	engineered mutation	UNP P0DTC2
A	984	PRO	ALA	engineered mutation	UNP P0DTC2
A	991	PRO	ALA	engineered mutation	UNP P0DTC2
A	1034	PRO	ALA	engineered mutation	UNP P0DTC2
A	1078	PRO	LYS	engineered mutation	UNP P0DTC2
A	1079	PRO	VAL	engineered mutation	UNP P0DTC2
A	1301	GLY	-	expression tag	UNP P0DTC2
A	1302	SER	-	expression tag	UNP P0DTC2
A	1303	GLY	-	expression tag	UNP P0DTC2
A	1304	TYR	-	expression tag	UNP P0DTC2
A	1305	ILE	-	expression tag	UNP P0DTC2
A	1306	PRO	-	expression tag	UNP P0DTC2
A	1307	GLU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1308	ALA	-	expression tag	UNP P0DTC2
A	1309	PRO	-	expression tag	UNP P0DTC2
A	1310	ARG	-	expression tag	UNP P0DTC2
A	1311	ASP	-	expression tag	UNP P0DTC2
A	1312	GLY	-	expression tag	UNP P0DTC2
A	1313	GLN	-	expression tag	UNP P0DTC2
A	1314	ALA	-	expression tag	UNP P0DTC2
A	1315	TYR	-	expression tag	UNP P0DTC2
A	1316	VAL	-	expression tag	UNP P0DTC2
A	1317	ARG	-	expression tag	UNP P0DTC2
A	1318	LYS	-	expression tag	UNP P0DTC2
A	1319	ASP	-	expression tag	UNP P0DTC2
A	1320	GLY	-	expression tag	UNP P0DTC2
A	1321	GLU	-	expression tag	UNP P0DTC2
A	1322	TRP	-	expression tag	UNP P0DTC2
A	1323	VAL	-	expression tag	UNP P0DTC2
A	1324	LEU	-	expression tag	UNP P0DTC2
A	1325	LEU	-	expression tag	UNP P0DTC2
A	1326	SER	-	expression tag	UNP P0DTC2
A	1327	THR	-	expression tag	UNP P0DTC2
A	1328	PHE	-	expression tag	UNP P0DTC2
A	1329	LEU	-	expression tag	UNP P0DTC2
A	1330	GLY	-	expression tag	UNP P0DTC2
A	1331	ARG	-	expression tag	UNP P0DTC2
A	1332	SER	-	expression tag	UNP P0DTC2
A	1333	LEU	-	expression tag	UNP P0DTC2
A	1334	GLU	-	expression tag	UNP P0DTC2
A	1335	VAL	-	expression tag	UNP P0DTC2
A	1336	LEU	-	expression tag	UNP P0DTC2
A	1337	PHE	-	expression tag	UNP P0DTC2
A	1338	GLN	-	expression tag	UNP P0DTC2
A	1339	GLY	-	expression tag	UNP P0DTC2
A	1340	PRO	-	expression tag	UNP P0DTC2
A	1341	GLY	-	expression tag	UNP P0DTC2
A	1342	HIS	-	expression tag	UNP P0DTC2
A	1343	HIS	-	expression tag	UNP P0DTC2
A	1344	HIS	-	expression tag	UNP P0DTC2
A	1345	HIS	-	expression tag	UNP P0DTC2
A	1346	HIS	-	expression tag	UNP P0DTC2
A	1347	HIS	-	expression tag	UNP P0DTC2
A	1348	HIS	-	expression tag	UNP P0DTC2
A	1349	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1350	SER	-	expression tag	UNP P0DTC2
A	1351	ALA	-	expression tag	UNP P0DTC2
A	1352	TRP	-	expression tag	UNP P0DTC2
A	1353	SER	-	expression tag	UNP P0DTC2
A	1354	HIS	-	expression tag	UNP P0DTC2
A	1355	PRO	-	expression tag	UNP P0DTC2
A	1356	GLN	-	expression tag	UNP P0DTC2
A	1357	PHE	-	expression tag	UNP P0DTC2
A	1358	GLU	-	expression tag	UNP P0DTC2
A	1359	LYS	-	expression tag	UNP P0DTC2
A	1360	GLY	-	expression tag	UNP P0DTC2
A	1361	GLY	-	expression tag	UNP P0DTC2
A	1362	GLY	-	expression tag	UNP P0DTC2
A	1363	SER	-	expression tag	UNP P0DTC2
A	1364	GLY	-	expression tag	UNP P0DTC2
A	1365	GLY	-	expression tag	UNP P0DTC2
A	1366	GLY	-	expression tag	UNP P0DTC2
A	1367	GLY	-	expression tag	UNP P0DTC2
A	1368	SER	-	expression tag	UNP P0DTC2
A	1369	GLY	-	expression tag	UNP P0DTC2
A	1370	GLY	-	expression tag	UNP P0DTC2
A	1371	SER	-	expression tag	UNP P0DTC2
A	1372	ALA	-	expression tag	UNP P0DTC2
A	1373	TRP	-	expression tag	UNP P0DTC2
A	1374	SER	-	expression tag	UNP P0DTC2
A	1375	HIS	-	expression tag	UNP P0DTC2
A	1376	PRO	-	expression tag	UNP P0DTC2
A	1377	GLN	-	expression tag	UNP P0DTC2
A	1378	PHE	-	expression tag	UNP P0DTC2
A	1379	GLU	-	expression tag	UNP P0DTC2
A	1380	LYS	-	expression tag	UNP P0DTC2
B	1	MET	-	initiating methionine	UNP P0DTC2
B	2	GLY	-	expression tag	UNP P0DTC2
B	3	GLY	-	expression tag	UNP P0DTC2
B	4	GLU	-	expression tag	UNP P0DTC2
B	5	GLY	-	expression tag	UNP P0DTC2
B	6	LEU	-	expression tag	UNP P0DTC2
B	7	ARG	-	expression tag	UNP P0DTC2
B	8	ALA	-	expression tag	UNP P0DTC2
B	9	SER	-	expression tag	UNP P0DTC2
B	10	PRO	-	expression tag	UNP P0DTC2
B	11	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	12	ARG	-	expression tag	UNP P0DTC2
B	13	ARG	-	expression tag	UNP P0DTC2
B	14	PRO	-	expression tag	UNP P0DTC2
B	15	LEU	-	expression tag	UNP P0DTC2
B	16	LEU	-	expression tag	UNP P0DTC2
B	17	PRO	-	expression tag	UNP P0DTC2
B	18	LEU	-	expression tag	UNP P0DTC2
B	19	GLN	-	expression tag	UNP P0DTC2
B	20	PRO	-	expression tag	UNP P0DTC2
B	21	ARG	-	expression tag	UNP P0DTC2
B	22	GLY	-	expression tag	UNP P0DTC2
B	23	CYS	-	expression tag	UNP P0DTC2
B	24	PRO	-	expression tag	UNP P0DTC2
B	25	ARG	-	expression tag	UNP P0DTC2
B	26	GLY	-	expression tag	UNP P0DTC2
B	27	ASP	-	expression tag	UNP P0DTC2
B	28	GLY	-	expression tag	UNP P0DTC2
B	29	CYS	-	expression tag	UNP P0DTC2
B	30	LEU	-	expression tag	UNP P0DTC2
B	31	ARG	-	expression tag	UNP P0DTC2
B	32	GLY	-	expression tag	UNP P0DTC2
B	33	GLY	-	expression tag	UNP P0DTC2
B	34	ARG	-	expression tag	UNP P0DTC2
B	35	GLY	-	expression tag	UNP P0DTC2
B	36	ARG	-	expression tag	UNP P0DTC2
B	37	ALA	-	expression tag	UNP P0DTC2
B	38	GLY	-	expression tag	UNP P0DTC2
B	39	PHE	-	expression tag	UNP P0DTC2
B	40	GLY	-	expression tag	UNP P0DTC2
B	41	PHE	-	expression tag	UNP P0DTC2
B	42	TRP	-	expression tag	UNP P0DTC2
B	43	ARG	-	expression tag	UNP P0DTC2
B	44	VAL	-	expression tag	UNP P0DTC2
B	45	THR	-	expression tag	UNP P0DTC2
B	46	GLY	-	expression tag	UNP P0DTC2
B	47	GLY	-	expression tag	UNP P0DTC2
B	48	SER	-	expression tag	UNP P0DTC2
B	49	SER	-	expression tag	UNP P0DTC2
B	50	ALA	-	expression tag	UNP P0DTC2
B	51	SER	-	expression tag	UNP P0DTC2
B	52	ALA	-	expression tag	UNP P0DTC2
B	53	ASN	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	54	HIS	-	expression tag	UNP P0DTC2
B	55	VAL	-	expression tag	UNP P0DTC2
B	56	HIS	-	expression tag	UNP P0DTC2
B	57	ALA	-	expression tag	UNP P0DTC2
B	58	PHE	-	expression tag	UNP P0DTC2
B	59	PHE	-	expression tag	UNP P0DTC2
B	60	PHE	-	expression tag	UNP P0DTC2
B	61	PHE	-	expression tag	UNP P0DTC2
B	62	LEU	-	expression tag	UNP P0DTC2
B	63	GLN	-	expression tag	UNP P0DTC2
B	64	LEU	-	expression tag	UNP P0DTC2
B	65	LEU	-	expression tag	UNP P0DTC2
B	66	GLY	-	expression tag	UNP P0DTC2
B	67	ASN	-	expression tag	UNP P0DTC2
B	68	VAL	-	expression tag	UNP P0DTC2
B	69	LEU	-	expression tag	UNP P0DTC2
B	70	VAL	-	expression tag	UNP P0DTC2
B	71	VAL	-	expression tag	UNP P0DTC2
B	72	VAL	-	expression tag	UNP P0DTC2
B	73	LEU	-	expression tag	UNP P0DTC2
B	74	SER	-	expression tag	UNP P0DTC2
B	75	HIS	-	expression tag	UNP P0DTC2
B	76	HIS	-	expression tag	UNP P0DTC2
B	77	PHE	-	expression tag	UNP P0DTC2
B	78	GLY	-	expression tag	UNP P0DTC2
B	79	LYS	-	expression tag	UNP P0DTC2
B	80	GLU	-	expression tag	UNP P0DTC2
B	81	LEU	-	expression tag	UNP P0DTC2
B	82	ARG	-	expression tag	UNP P0DTC2
B	83	PRO	-	expression tag	UNP P0DTC2
B	84	SER	-	expression tag	UNP P0DTC2
B	85	GLN	-	expression tag	UNP P0DTC2
B	86	ALA	-	expression tag	UNP P0DTC2
B	87	GLU	-	expression tag	UNP P0DTC2
B	88	PHE	-	expression tag	UNP P0DTC2
B	89	GLY	-	expression tag	UNP P0DTC2
B	90	THR	-	expression tag	UNP P0DTC2
B	91	ALA	-	expression tag	UNP P0DTC2
B	92	THR	-	expression tag	UNP P0DTC2
B	774	GLY	ARG	engineered mutation	UNP P0DTC2
B	775	SER	ARG	engineered mutation	UNP P0DTC2
B	777	SER	ARG	engineered mutation	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	909	PRO	PHE	engineered mutation	UNP P0DTC2
B	984	PRO	ALA	engineered mutation	UNP P0DTC2
B	991	PRO	ALA	engineered mutation	UNP P0DTC2
B	1034	PRO	ALA	engineered mutation	UNP P0DTC2
B	1078	PRO	LYS	engineered mutation	UNP P0DTC2
B	1079	PRO	VAL	engineered mutation	UNP P0DTC2
B	1301	GLY	-	expression tag	UNP P0DTC2
B	1302	SER	-	expression tag	UNP P0DTC2
B	1303	GLY	-	expression tag	UNP P0DTC2
B	1304	TYR	-	expression tag	UNP P0DTC2
B	1305	ILE	-	expression tag	UNP P0DTC2
B	1306	PRO	-	expression tag	UNP P0DTC2
B	1307	GLU	-	expression tag	UNP P0DTC2
B	1308	ALA	-	expression tag	UNP P0DTC2
B	1309	PRO	-	expression tag	UNP P0DTC2
B	1310	ARG	-	expression tag	UNP P0DTC2
B	1311	ASP	-	expression tag	UNP P0DTC2
B	1312	GLY	-	expression tag	UNP P0DTC2
B	1313	GLN	-	expression tag	UNP P0DTC2
B	1314	ALA	-	expression tag	UNP P0DTC2
B	1315	TYR	-	expression tag	UNP P0DTC2
B	1316	VAL	-	expression tag	UNP P0DTC2
B	1317	ARG	-	expression tag	UNP P0DTC2
B	1318	LYS	-	expression tag	UNP P0DTC2
B	1319	ASP	-	expression tag	UNP P0DTC2
B	1320	GLY	-	expression tag	UNP P0DTC2
B	1321	GLU	-	expression tag	UNP P0DTC2
B	1322	TRP	-	expression tag	UNP P0DTC2
B	1323	VAL	-	expression tag	UNP P0DTC2
B	1324	LEU	-	expression tag	UNP P0DTC2
B	1325	LEU	-	expression tag	UNP P0DTC2
B	1326	SER	-	expression tag	UNP P0DTC2
B	1327	THR	-	expression tag	UNP P0DTC2
B	1328	PHE	-	expression tag	UNP P0DTC2
B	1329	LEU	-	expression tag	UNP P0DTC2
B	1330	GLY	-	expression tag	UNP P0DTC2
B	1331	ARG	-	expression tag	UNP P0DTC2
B	1332	SER	-	expression tag	UNP P0DTC2
B	1333	LEU	-	expression tag	UNP P0DTC2
B	1334	GLU	-	expression tag	UNP P0DTC2
B	1335	VAL	-	expression tag	UNP P0DTC2
B	1336	LEU	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1337	PHE	-	expression tag	UNP P0DTC2
B	1338	GLN	-	expression tag	UNP P0DTC2
B	1339	GLY	-	expression tag	UNP P0DTC2
B	1340	PRO	-	expression tag	UNP P0DTC2
B	1341	GLY	-	expression tag	UNP P0DTC2
B	1342	HIS	-	expression tag	UNP P0DTC2
B	1343	HIS	-	expression tag	UNP P0DTC2
B	1344	HIS	-	expression tag	UNP P0DTC2
B	1345	HIS	-	expression tag	UNP P0DTC2
B	1346	HIS	-	expression tag	UNP P0DTC2
B	1347	HIS	-	expression tag	UNP P0DTC2
B	1348	HIS	-	expression tag	UNP P0DTC2
B	1349	HIS	-	expression tag	UNP P0DTC2
B	1350	SER	-	expression tag	UNP P0DTC2
B	1351	ALA	-	expression tag	UNP P0DTC2
B	1352	TRP	-	expression tag	UNP P0DTC2
B	1353	SER	-	expression tag	UNP P0DTC2
B	1354	HIS	-	expression tag	UNP P0DTC2
B	1355	PRO	-	expression tag	UNP P0DTC2
B	1356	GLN	-	expression tag	UNP P0DTC2
B	1357	PHE	-	expression tag	UNP P0DTC2
B	1358	GLU	-	expression tag	UNP P0DTC2
B	1359	LYS	-	expression tag	UNP P0DTC2
B	1360	GLY	-	expression tag	UNP P0DTC2
B	1361	GLY	-	expression tag	UNP P0DTC2
B	1362	GLY	-	expression tag	UNP P0DTC2
B	1363	SER	-	expression tag	UNP P0DTC2
B	1364	GLY	-	expression tag	UNP P0DTC2
B	1365	GLY	-	expression tag	UNP P0DTC2
B	1366	GLY	-	expression tag	UNP P0DTC2
B	1367	GLY	-	expression tag	UNP P0DTC2
B	1368	SER	-	expression tag	UNP P0DTC2
B	1369	GLY	-	expression tag	UNP P0DTC2
B	1370	GLY	-	expression tag	UNP P0DTC2
B	1371	SER	-	expression tag	UNP P0DTC2
B	1372	ALA	-	expression tag	UNP P0DTC2
B	1373	TRP	-	expression tag	UNP P0DTC2
B	1374	SER	-	expression tag	UNP P0DTC2
B	1375	HIS	-	expression tag	UNP P0DTC2
B	1376	PRO	-	expression tag	UNP P0DTC2
B	1377	GLN	-	expression tag	UNP P0DTC2
B	1378	PHE	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1379	GLU	-	expression tag	UNP P0DTC2
B	1380	LYS	-	expression tag	UNP P0DTC2
C	1	MET	-	initiating methionine	UNP P0DTC2
C	2	GLY	-	expression tag	UNP P0DTC2
C	3	GLY	-	expression tag	UNP P0DTC2
C	4	GLU	-	expression tag	UNP P0DTC2
C	5	GLY	-	expression tag	UNP P0DTC2
C	6	LEU	-	expression tag	UNP P0DTC2
C	7	ARG	-	expression tag	UNP P0DTC2
C	8	ALA	-	expression tag	UNP P0DTC2
C	9	SER	-	expression tag	UNP P0DTC2
C	10	PRO	-	expression tag	UNP P0DTC2
C	11	ARG	-	expression tag	UNP P0DTC2
C	12	ARG	-	expression tag	UNP P0DTC2
C	13	ARG	-	expression tag	UNP P0DTC2
C	14	PRO	-	expression tag	UNP P0DTC2
C	15	LEU	-	expression tag	UNP P0DTC2
C	16	LEU	-	expression tag	UNP P0DTC2
C	17	PRO	-	expression tag	UNP P0DTC2
C	18	LEU	-	expression tag	UNP P0DTC2
C	19	GLN	-	expression tag	UNP P0DTC2
C	20	PRO	-	expression tag	UNP P0DTC2
C	21	ARG	-	expression tag	UNP P0DTC2
C	22	GLY	-	expression tag	UNP P0DTC2
C	23	CYS	-	expression tag	UNP P0DTC2
C	24	PRO	-	expression tag	UNP P0DTC2
C	25	ARG	-	expression tag	UNP P0DTC2
C	26	GLY	-	expression tag	UNP P0DTC2
C	27	ASP	-	expression tag	UNP P0DTC2
C	28	GLY	-	expression tag	UNP P0DTC2
C	29	CYS	-	expression tag	UNP P0DTC2
C	30	LEU	-	expression tag	UNP P0DTC2
C	31	ARG	-	expression tag	UNP P0DTC2
C	32	GLY	-	expression tag	UNP P0DTC2
C	33	GLY	-	expression tag	UNP P0DTC2
C	34	ARG	-	expression tag	UNP P0DTC2
C	35	GLY	-	expression tag	UNP P0DTC2
C	36	ARG	-	expression tag	UNP P0DTC2
C	37	ALA	-	expression tag	UNP P0DTC2
C	38	GLY	-	expression tag	UNP P0DTC2
C	39	PHE	-	expression tag	UNP P0DTC2
C	40	GLY	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	41	PHE	-	expression tag	UNP P0DTC2
C	42	TRP	-	expression tag	UNP P0DTC2
C	43	ARG	-	expression tag	UNP P0DTC2
C	44	VAL	-	expression tag	UNP P0DTC2
C	45	THR	-	expression tag	UNP P0DTC2
C	46	GLY	-	expression tag	UNP P0DTC2
C	47	GLY	-	expression tag	UNP P0DTC2
C	48	SER	-	expression tag	UNP P0DTC2
C	49	SER	-	expression tag	UNP P0DTC2
C	50	ALA	-	expression tag	UNP P0DTC2
C	51	SER	-	expression tag	UNP P0DTC2
C	52	ALA	-	expression tag	UNP P0DTC2
C	53	ASN	-	expression tag	UNP P0DTC2
C	54	HIS	-	expression tag	UNP P0DTC2
C	55	VAL	-	expression tag	UNP P0DTC2
C	56	HIS	-	expression tag	UNP P0DTC2
C	57	ALA	-	expression tag	UNP P0DTC2
C	58	PHE	-	expression tag	UNP P0DTC2
C	59	PHE	-	expression tag	UNP P0DTC2
C	60	PHE	-	expression tag	UNP P0DTC2
C	61	PHE	-	expression tag	UNP P0DTC2
C	62	LEU	-	expression tag	UNP P0DTC2
C	63	GLN	-	expression tag	UNP P0DTC2
C	64	LEU	-	expression tag	UNP P0DTC2
C	65	LEU	-	expression tag	UNP P0DTC2
C	66	GLY	-	expression tag	UNP P0DTC2
C	67	ASN	-	expression tag	UNP P0DTC2
C	68	VAL	-	expression tag	UNP P0DTC2
C	69	LEU	-	expression tag	UNP P0DTC2
C	70	VAL	-	expression tag	UNP P0DTC2
C	71	VAL	-	expression tag	UNP P0DTC2
C	72	VAL	-	expression tag	UNP P0DTC2
C	73	LEU	-	expression tag	UNP P0DTC2
C	74	SER	-	expression tag	UNP P0DTC2
C	75	HIS	-	expression tag	UNP P0DTC2
C	76	HIS	-	expression tag	UNP P0DTC2
C	77	PHE	-	expression tag	UNP P0DTC2
C	78	GLY	-	expression tag	UNP P0DTC2
C	79	LYS	-	expression tag	UNP P0DTC2
C	80	GLU	-	expression tag	UNP P0DTC2
C	81	LEU	-	expression tag	UNP P0DTC2
C	82	ARG	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	83	PRO	-	expression tag	UNP P0DTC2
C	84	SER	-	expression tag	UNP P0DTC2
C	85	GLN	-	expression tag	UNP P0DTC2
C	86	ALA	-	expression tag	UNP P0DTC2
C	87	GLU	-	expression tag	UNP P0DTC2
C	88	PHE	-	expression tag	UNP P0DTC2
C	89	GLY	-	expression tag	UNP P0DTC2
C	90	THR	-	expression tag	UNP P0DTC2
C	91	ALA	-	expression tag	UNP P0DTC2
C	92	THR	-	expression tag	UNP P0DTC2
C	774	GLY	ARG	engineered mutation	UNP P0DTC2
C	775	SER	ARG	engineered mutation	UNP P0DTC2
C	777	SER	ARG	engineered mutation	UNP P0DTC2
C	909	PRO	PHE	engineered mutation	UNP P0DTC2
C	984	PRO	ALA	engineered mutation	UNP P0DTC2
C	991	PRO	ALA	engineered mutation	UNP P0DTC2
C	1034	PRO	ALA	engineered mutation	UNP P0DTC2
C	1078	PRO	LYS	engineered mutation	UNP P0DTC2
C	1079	PRO	VAL	engineered mutation	UNP P0DTC2
C	1301	GLY	-	expression tag	UNP P0DTC2
C	1302	SER	-	expression tag	UNP P0DTC2
C	1303	GLY	-	expression tag	UNP P0DTC2
C	1304	TYR	-	expression tag	UNP P0DTC2
C	1305	ILE	-	expression tag	UNP P0DTC2
C	1306	PRO	-	expression tag	UNP P0DTC2
C	1307	GLU	-	expression tag	UNP P0DTC2
C	1308	ALA	-	expression tag	UNP P0DTC2
C	1309	PRO	-	expression tag	UNP P0DTC2
C	1310	ARG	-	expression tag	UNP P0DTC2
C	1311	ASP	-	expression tag	UNP P0DTC2
C	1312	GLY	-	expression tag	UNP P0DTC2
C	1313	GLN	-	expression tag	UNP P0DTC2
C	1314	ALA	-	expression tag	UNP P0DTC2
C	1315	TYR	-	expression tag	UNP P0DTC2
C	1316	VAL	-	expression tag	UNP P0DTC2
C	1317	ARG	-	expression tag	UNP P0DTC2
C	1318	LYS	-	expression tag	UNP P0DTC2
C	1319	ASP	-	expression tag	UNP P0DTC2
C	1320	GLY	-	expression tag	UNP P0DTC2
C	1321	GLU	-	expression tag	UNP P0DTC2
C	1322	TRP	-	expression tag	UNP P0DTC2
C	1323	VAL	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1324	LEU	-	expression tag	UNP P0DTC2
C	1325	LEU	-	expression tag	UNP P0DTC2
C	1326	SER	-	expression tag	UNP P0DTC2
C	1327	THR	-	expression tag	UNP P0DTC2
C	1328	PHE	-	expression tag	UNP P0DTC2
C	1329	LEU	-	expression tag	UNP P0DTC2
C	1330	GLY	-	expression tag	UNP P0DTC2
C	1331	ARG	-	expression tag	UNP P0DTC2
C	1332	SER	-	expression tag	UNP P0DTC2
C	1333	LEU	-	expression tag	UNP P0DTC2
C	1334	GLU	-	expression tag	UNP P0DTC2
C	1335	VAL	-	expression tag	UNP P0DTC2
C	1336	LEU	-	expression tag	UNP P0DTC2
C	1337	PHE	-	expression tag	UNP P0DTC2
C	1338	GLN	-	expression tag	UNP P0DTC2
C	1339	GLY	-	expression tag	UNP P0DTC2
C	1340	PRO	-	expression tag	UNP P0DTC2
C	1341	GLY	-	expression tag	UNP P0DTC2
C	1342	HIS	-	expression tag	UNP P0DTC2
C	1343	HIS	-	expression tag	UNP P0DTC2
C	1344	HIS	-	expression tag	UNP P0DTC2
C	1345	HIS	-	expression tag	UNP P0DTC2
C	1346	HIS	-	expression tag	UNP P0DTC2
C	1347	HIS	-	expression tag	UNP P0DTC2
C	1348	HIS	-	expression tag	UNP P0DTC2
C	1349	HIS	-	expression tag	UNP P0DTC2
C	1350	SER	-	expression tag	UNP P0DTC2
C	1351	ALA	-	expression tag	UNP P0DTC2
C	1352	TRP	-	expression tag	UNP P0DTC2
C	1353	SER	-	expression tag	UNP P0DTC2
C	1354	HIS	-	expression tag	UNP P0DTC2
C	1355	PRO	-	expression tag	UNP P0DTC2
C	1356	GLN	-	expression tag	UNP P0DTC2
C	1357	PHE	-	expression tag	UNP P0DTC2
C	1358	GLU	-	expression tag	UNP P0DTC2
C	1359	LYS	-	expression tag	UNP P0DTC2
C	1360	GLY	-	expression tag	UNP P0DTC2
C	1361	GLY	-	expression tag	UNP P0DTC2
C	1362	GLY	-	expression tag	UNP P0DTC2
C	1363	SER	-	expression tag	UNP P0DTC2
C	1364	GLY	-	expression tag	UNP P0DTC2
C	1365	GLY	-	expression tag	UNP P0DTC2

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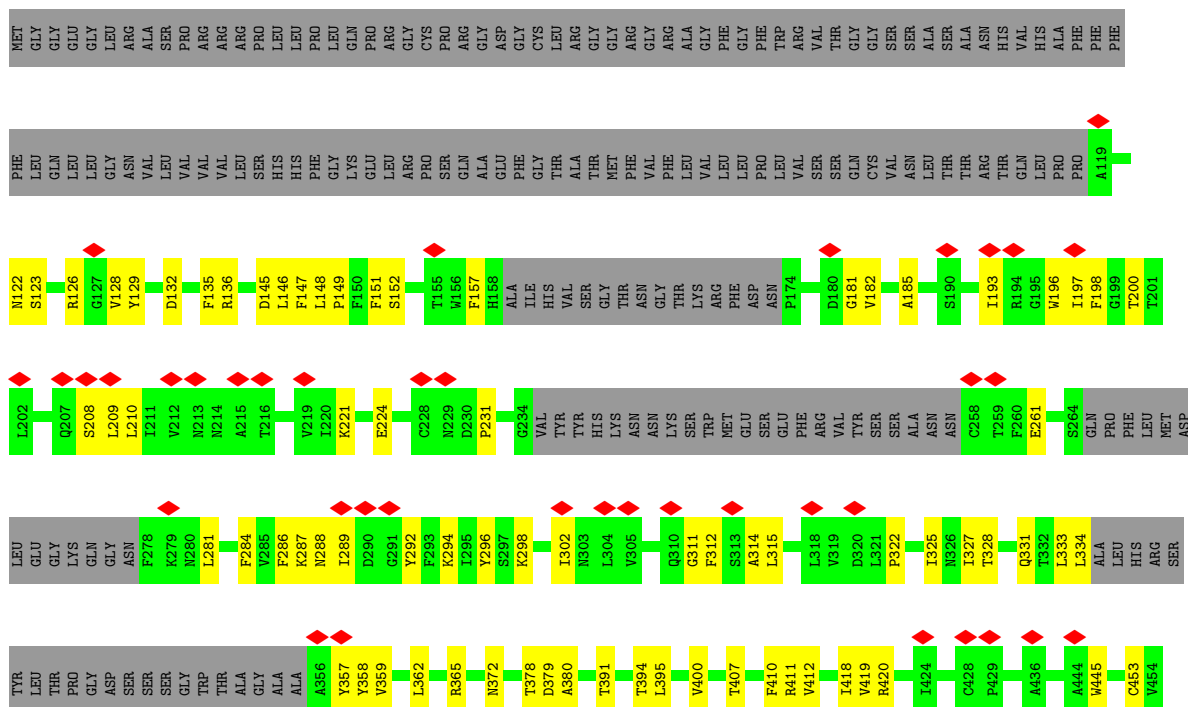
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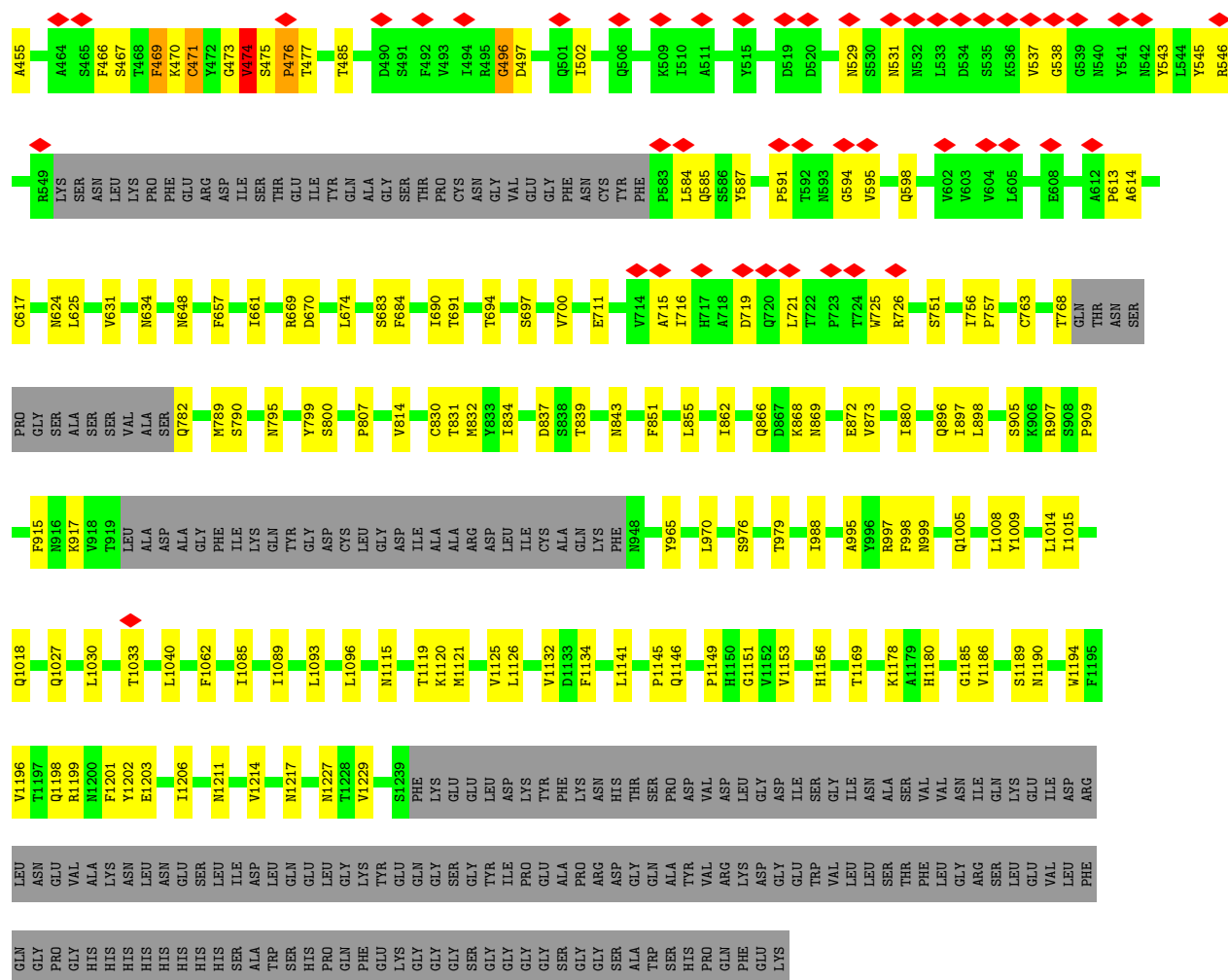
Chain	Residue	Modelled	Actual	Comment	Reference
C	1366	GLY	-	expression tag	UNP P0DTC2
C	1367	GLY	-	expression tag	UNP P0DTC2
C	1368	SER	-	expression tag	UNP P0DTC2
C	1369	GLY	-	expression tag	UNP P0DTC2
C	1370	GLY	-	expression tag	UNP P0DTC2
C	1371	SER	-	expression tag	UNP P0DTC2
C	1372	ALA	-	expression tag	UNP P0DTC2
C	1373	TRP	-	expression tag	UNP P0DTC2
C	1374	SER	-	expression tag	UNP P0DTC2
C	1375	HIS	-	expression tag	UNP P0DTC2
C	1376	PRO	-	expression tag	UNP P0DTC2
C	1377	GLN	-	expression tag	UNP P0DTC2
C	1378	PHE	-	expression tag	UNP P0DTC2
C	1379	GLU	-	expression tag	UNP P0DTC2
C	1380	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Nanobody NB95.

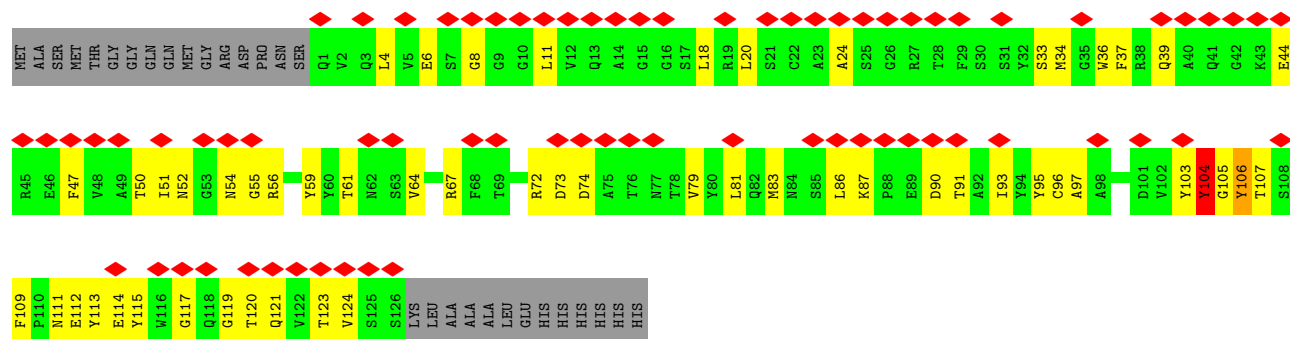
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	126	Total	C	N	O	S	0	0
			977	610	164	199	4		
2	E	126	Total	C	N	O	S	0	0
			977	610	164	199	4		

- Molecule 1: Spike glycoprotein



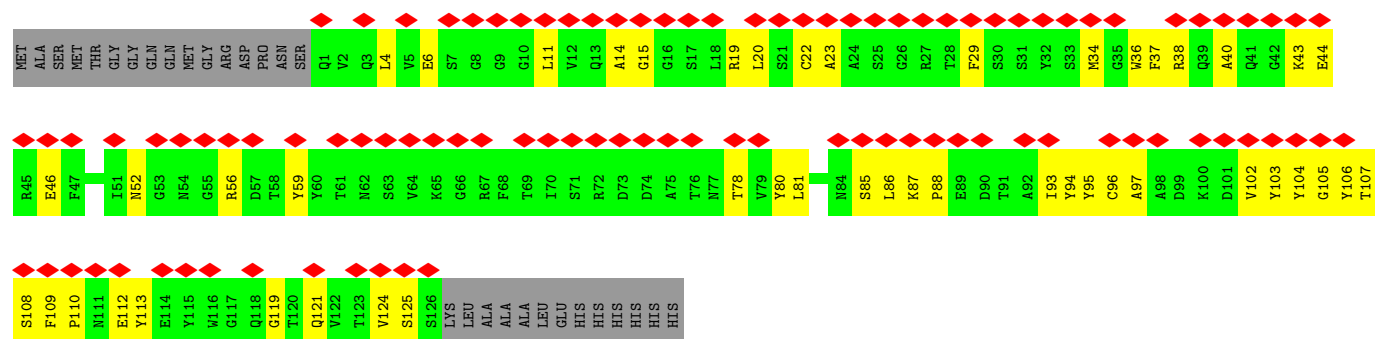


• Molecule 2: Nanobody NB95



• Molecule 2: Nanobody NB95





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68378	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.109	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	440.95996, 440.95996, 440.95996	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0.94	2/7716 (0.0%)	1.19	10/10523 (0.1%)
1	B	0.93	0/6358	1.20	8/8672 (0.1%)
1	C	0.98	5/7167 (0.1%)	1.23	13/9808 (0.1%)
2	D	1.01	1/998 (0.1%)	1.42	4/1352 (0.3%)
2	E	0.96	0/998	1.26	1/1352 (0.1%)
All	All	0.95	8/23237 (0.0%)	1.22	36/31707 (0.1%)

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	C	0	1
2	D	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	496	GLY	C-O	-11.75	1.09	1.23
2	D	106	TYR	C-O	-9.97	1.11	1.23
1	A	469	PHE	C-O	-9.39	1.12	1.23
1	C	469	PHE	C-O	-6.98	1.15	1.23
1	C	474	VAL	C-O	-5.79	1.18	1.24
1	A	1145	PRO	C-O	-5.13	1.18	1.23
1	C	1145	PRO	C-O	-5.04	1.17	1.23
1	C	800	SER	CA-CB	-5.03	1.47	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	104	TYR	OH-CZ-CE2	-11.45	85.56	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1051	LEU	N-CA-C	-9.68	101.58	113.97
1	C	476	PRO	CB-CA-C	-9.19	98.41	110.27
2	D	104	TYR	CE1-CZ-OH	9.13	147.28	119.90
1	B	1051	LEU	N-CA-C	-9.10	102.31	113.50
1	C	469	PHE	CA-C-O	7.80	129.63	120.66
1	A	692	PRO	N-CA-C	-7.30	100.47	111.41
1	C	496	GLY	CA-C-O	-7.28	113.14	121.00
1	C	474	VAL	CA-C-O	-7.17	112.62	120.43
1	C	453	CYS	CB-CA-C	-7.14	96.66	113.02
1	B	222	VAL	N-CA-C	-6.75	104.72	111.88
1	C	502	ILE	CA-C-O	-6.45	117.02	122.63
1	B	949	GLY	N-CA-C	-6.43	106.17	114.85
1	C	648	ASN	N-CA-C	-6.21	105.69	113.20
1	A	469	PHE	CA-C-O	-6.11	112.70	120.27
1	B	708	ASN	N-CA-C	-6.04	101.53	110.48
1	A	495	ARG	N-CA-C	-6.00	101.02	109.96
1	B	1077	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	949	GLY	N-CA-C	-5.87	106.88	115.63
2	D	106	TYR	CA-C-O	-5.86	114.25	121.11
1	C	898	LEU	CB-CA-C	5.82	117.59	108.63
1	C	469	PHE	O-C-N	-5.82	116.17	123.27
1	C	999	ASN	N-CA-C	-5.70	105.15	111.71
1	C	469	PHE	CB-CA-C	5.57	120.38	109.35
1	A	1049	GLN	N-CA-C	-5.45	103.34	110.53
1	C	1190	ASN	N-CA-C	-5.43	106.63	113.20
1	A	311	GLY	CA-C-O	-5.40	118.50	122.23
1	A	495	ARG	CB-CA-C	5.39	117.92	110.16
1	A	1052	ASN	N-CA-C	-5.34	105.37	111.14
2	D	55	GLY	N-CA-C	-5.29	106.11	114.10
1	B	180	ASP	N-CA-C	-5.29	108.09	114.75
2	E	29	PHE	N-CA-C	-5.18	107.34	113.97
1	B	1190	ASN	N-CA-C	-5.12	106.87	113.02
1	C	1062	PHE	N-CA-C	-5.06	105.76	112.24
1	A	1190	ASN	N-CA-C	-5.01	106.42	112.88
1	B	731	GLY	CA-C-O	-5.01	117.40	121.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	474	VAL	Mainchain
2	D	104	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7542	0	7293	241	0
1	B	6220	0	6025	139	0
1	C	7018	0	6385	183	0
2	D	977	0	907	85	0
2	E	977	0	907	64	0
All	All	22734	0	21517	600	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 14.

All (600) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:PRO:HD3	2:E:104:TYR:HB3	1.37	1.01
1:C:471:CYS:HB2	2:D:104:TYR:CE1	1.96	1.00
1:C:471:CYS:HB2	2:D:104:TYR:CZ	2.05	0.92
1:A:470:LYS:HA	2:E:105:GLY:HA3	1.52	0.90
1:A:476:PRO:HD3	2:E:104:TYR:CB	2.02	0.89
1:A:475:SER:N	2:E:103:TYR:HE2	1.70	0.87
1:C:420:ARG:HH21	1:C:670:ASP:HB2	1.40	0.85
1:A:279:LYS:N	1:A:303:ASN:HD22	1.74	0.85
1:A:468:THR:HA	2:E:107:THR:HA	1.58	0.85
1:A:804:ILE:HG23	1:A:1169:THR:HG21	1.63	0.81
1:C:476:PRO:HD3	2:D:104:TYR:CD2	2.17	0.80
1:A:198:PHE:HB2	1:A:209:LEU:HB3	1.61	0.80
1:A:476:PRO:CD	2:E:104:TYR:HB3	2.11	0.80
1:A:751:SER:HB3	1:A:790:SER:HB3	1.66	0.78
1:C:471:CYS:SG	2:D:104:TYR:OH	2.41	0.78
1:C:471:CYS:HB2	2:D:104:TYR:HE1	1.48	0.77
1:A:470:LYS:HD2	2:E:102:VAL:CG1	2.17	0.75
1:B:197:ILE:HG12	1:B:333:LEU:HD11	1.68	0.75
1:A:199:GLY:H	1:A:327:ILE:HG23	1.51	0.74
1:B:913:LEU:HD11	1:B:1031:SER:HB2	1.70	0.74
1:C:473:GLY:H	2:D:103:TYR:CB	2.01	0.73
1:A:305:VAL:HG12	1:A:306:ARG:HG2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:VAL:O	2:D:104:TYR:CE1	2.42	0.73
2:E:86:LEU:HD23	2:E:124:VAL:HG22	1.69	0.73
1:A:469:PHE:N	2:E:106:TYR:O	2.21	0.73
1:A:418:ILE:HD11	1:A:625:LEU:HA	1.71	0.72
2:E:14:ALA:HA	2:E:86:LEU:HB2	1.72	0.71
1:B:287:LYS:HD3	1:B:296:TYR:HE2	1.56	0.71
1:A:804:ILE:HG22	1:B:989:PRO:HD2	1.73	0.71
1:B:751:SER:HB3	1:B:790:SER:HB3	1.72	0.70
1:A:488:TYR:HB2	1:A:606:SER:HB3	1.72	0.70
1:B:1069:LEU:HD11	1:B:1092:ARG:HH12	1.56	0.70
1:A:600:TYR:CZ	2:E:109:PHE:CE1	2.79	0.70
1:A:659:ARG:HD3	1:A:663:ASP:HA	1.73	0.70
1:A:992:MET:HE1	1:C:1186:VAL:HG23	1.72	0.70
1:A:469:PHE:O	2:E:106:TYR:N	2.25	0.69
1:C:830:CYS:SG	1:C:831:THR:N	2.67	0.68
1:C:475:SER:HA	2:D:104:TYR:CG	2.29	0.68
1:C:476:PRO:CD	2:D:104:TYR:CD2	2.76	0.68
1:A:600:TYR:CE2	2:E:109:PHE:CE1	2.82	0.67
1:A:1070:ASN:HA	1:A:1073:LEU:HD12	1.77	0.67
1:B:768:THR:HA	1:B:782:GLN:HA	1.74	0.67
1:A:475:SER:N	2:E:103:TYR:CE2	2.59	0.66
1:A:475:SER:CB	2:E:104:TYR:CD2	2.77	0.66
2:D:51:ILE:HD13	2:D:72:ARG:HG3	1.77	0.66
2:D:114:GLU:HG3	2:D:115:TYR:HD1	1.59	0.66
1:C:897:ILE:HG13	1:C:970:LEU:HD21	1.77	0.66
1:B:1085:ILE:O	1:B:1089:ILE:HG12	1.95	0.66
1:A:395:LEU:HD12	1:A:400:VAL:HG12	1.77	0.66
1:A:495:ARG:HB2	1:A:587:TYR:HE1	1.61	0.65
1:A:595:VAL:HG21	2:E:110:PRO:CG	2.25	0.65
1:B:184:PHE:HB3	1:B:284:PHE:HB2	1.79	0.64
1:C:496:GLY:O	2:D:109:PHE:CZ	2.50	0.64
1:C:851:PHE:CD2	1:C:1093:LEU:HD21	2.33	0.64
2:D:107:THR:HB	2:D:112:GLU:HG2	1.78	0.64
1:A:412:VAL:HG22	1:A:715:ALA:HB2	1.79	0.64
1:A:475:SER:HB3	2:E:104:TYR:CD2	2.32	0.64
1:A:485:THR:HA	1:A:614:ALA:HA	1.78	0.64
1:C:469:PHE:O	2:D:106:TYR:CE2	2.51	0.63
1:C:917:LYS:NZ	1:C:1030:LEU:O	2.31	0.63
1:C:289:ILE:H	1:C:294:LYS:NZ	1.96	0.63
1:C:496:GLY:O	2:D:109:PHE:CE1	2.51	0.63
1:A:470:LYS:HD2	2:E:102:VAL:HG11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:PRO:HB3	2:D:104:TYR:CE2	2.34	0.63
1:B:136:ARG:HB2	1:B:371:TYR:CD2	2.33	0.63
1:B:791:LEU:HB2	1:C:880:ILE:HD11	1.78	0.62
2:D:83:MET:HE1	2:D:86:LEU:HG	1.81	0.62
1:A:956:LEU:HD11	1:C:757:PRO:HB2	1.82	0.61
1:A:1132:VAL:HG21	1:B:1127:GLY:HA3	1.81	0.61
2:E:19:ARG:HD2	2:E:80:TYR:HB3	1.81	0.61
1:A:422:PRO:HG3	1:A:671:PRO:HB3	1.82	0.61
1:B:1077:ASP:OD1	1:B:1078:PRO:HD2	1.99	0.61
1:A:296:TYR:HD1	1:A:317:PRO:HA	1.65	0.61
1:C:391:THR:HG22	1:C:400:VAL:HG11	1.83	0.61
1:A:464:ALA:HB1	2:E:59:TYR:HE1	1.66	0.61
1:A:612:ALA:HB1	1:A:613:PRO:HD2	1.83	0.60
1:B:421:PHE:O	1:B:672:GLN:NE2	2.34	0.60
1:C:1120:LYS:NZ	1:C:1134:PHE:O	2.33	0.60
1:A:854:GLN:OE1	1:A:857:ARG:NH1	2.34	0.60
1:C:485:THR:HA	1:C:614:ALA:HA	1.83	0.60
1:A:155:THR:HB	1:A:359:VAL:HG12	1.83	0.60
1:A:595:VAL:HG21	2:E:110:PRO:HG3	1.82	0.60
1:C:474:VAL:HA	2:D:103:TYR:CE2	2.36	0.60
1:C:851:PHE:HD2	1:C:1093:LEU:HD21	1.66	0.60
1:A:1221:VAL:HG13	1:B:1009:TYR:HB3	1.82	0.60
1:A:175:VAL:HA	1:A:331:GLN:OE1	2.01	0.60
1:C:839:THR:O	1:C:843:ASN:ND2	2.35	0.59
1:A:156:TRP:CZ3	1:A:158:HIS:HB2	2.37	0.59
1:A:474:VAL:HG13	1:A:478:LYS:HZ2	1.67	0.59
2:D:36:TRP:CD2	2:D:96:CYS:HB3	2.38	0.59
1:B:844:LEU:HD21	1:B:1086:ASP:HA	1.84	0.59
1:B:994:MET:HE1	1:B:1141:LEU:HD13	1.85	0.59
1:C:466:PHE:O	2:D:59:TYR:OH	2.18	0.59
1:A:690:ILE:HB	1:A:701:ALA:HB3	1.84	0.59
1:A:1127:GLY:HA3	1:C:1132:VAL:HG21	1.85	0.59
2:D:36:TRP:CE2	2:D:96:CYS:HB3	2.38	0.59
1:A:179:ASN:OD1	1:A:180:ASP:N	2.36	0.59
1:C:132:ASP:OD2	1:C:136:ARG:NH2	2.35	0.59
1:A:896:GLN:NE2	1:A:1027:GLN:OE1	2.35	0.58
1:A:470:LYS:HG2	2:E:105:GLY:O	2.03	0.58
1:C:1085:ILE:O	1:C:1089:ILE:HG12	2.02	0.58
2:E:87:LYS:HE2	2:E:88:PRO:HD2	1.86	0.58
2:E:52:ASN:HD21	2:E:56:ARG:HB2	1.68	0.58
1:A:467:SER:O	2:E:108:SER:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LYS:HG2	2:E:105:GLY:C	2.28	0.58
1:A:655:GLN:HG2	1:B:135:PHE:HB2	1.86	0.58
1:C:185:ALA:HB3	1:C:358:TYR:HB2	1.85	0.58
2:D:91:THR:OG1	2:D:124:VAL:N	2.34	0.58
1:B:997:ARG:NH1	1:B:1141:LEU:O	2.37	0.58
1:C:476:PRO:CB	2:D:104:TYR:CE2	2.86	0.58
1:A:119:ALA:HB3	1:A:156:TRP:HB3	1.85	0.58
1:C:909:PRO:HB2	1:C:1027:GLN:HE22	1.69	0.58
1:A:486:ASN:HB3	1:A:608:GLU:HB3	1.86	0.57
1:B:371:TYR:CE1	1:B:377:ILE:HG12	2.39	0.57
1:B:915:PHE:HD1	1:B:1149:PRO:HD3	1.70	0.57
1:C:281:LEU:HB2	1:C:302:ILE:HG12	1.85	0.57
1:B:136:ARG:HB2	1:B:371:TYR:HD2	1.70	0.57
1:C:210:LEU:HD11	1:C:221:LYS:HB2	1.87	0.57
1:C:128:VAL:HG23	1:C:314:ALA:HA	1.85	0.57
1:A:495:ARG:HG3	1:A:497:ASP:OD1	2.03	0.57
1:B:287:LYS:HE2	1:B:289:ILE:HD11	1.85	0.57
1:A:702:VAL:N	1:A:743:ILE:O	2.35	0.57
1:A:531:ASN:HB2	1:A:598:GLN:HB3	1.85	0.57
1:B:989:PRO:HG2	1:B:992:MET:SD	2.45	0.57
1:B:1069:LEU:HD11	1:B:1092:ARG:NH1	2.19	0.57
1:C:995:ALA:HB1	1:C:1005:GLN:HB2	1.87	0.56
2:E:97:ALA:HB1	2:E:113:TYR:HB3	1.87	0.56
1:A:469:PHE:HE2	1:A:476:PRO:HB3	1.70	0.56
1:B:371:TYR:HE1	1:B:377:ILE:HG12	1.69	0.56
1:B:862:ILE:O	1:B:866:GLN:HG2	2.05	0.56
1:A:474:VAL:C	2:E:103:TYR:HE2	2.12	0.56
1:C:455:ALA:N	1:C:617:CYS:O	2.37	0.56
1:C:288:ASN:HD21	1:C:327:ILE:HD12	1.71	0.56
1:C:476:PRO:CG	2:D:104:TYR:CE2	2.89	0.56
1:C:469:PHE:O	2:D:106:TYR:CZ	2.58	0.56
1:C:721:LEU:HD13	1:C:725:TRP:HB3	1.86	0.56
1:C:751:SER:HB3	1:C:790:SER:HB3	1.87	0.56
1:A:289:ILE:HG22	1:A:290:ASP:H	1.69	0.56
1:A:799:TYR:HE1	1:B:989:PRO:HA	1.71	0.56
1:C:1125:VAL:HG12	1:C:1126:LEU:HD23	1.88	0.56
1:B:363:GLN:HE21	1:B:365:ARG:HD3	1.71	0.55
2:E:36:TRP:CE2	2:E:96:CYS:HB3	2.41	0.55
1:C:470:LYS:CB	2:D:106:TYR:O	2.54	0.55
2:D:64:VAL:HA	2:D:67:ARG:HE	1.71	0.55
2:D:97:ALA:HB3	2:D:113:TYR:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:SER:O	2:E:107:THR:HA	2.06	0.55
1:C:473:GLY:H	2:D:103:TYR:HB2	1.71	0.55
1:C:473:GLY:C	2:D:103:TYR:CD2	2.85	0.55
1:C:546:ARG:HA	1:C:584:LEU:HA	1.88	0.55
1:C:1040:LEU:HD21	1:C:1151:GLY:HA3	1.88	0.55
2:D:50:THR:HG21	2:D:106:TYR:HB2	1.89	0.55
1:A:449:ARG:HH12	1:A:451:SER:HB2	1.72	0.54
1:B:408:SER:OG	1:B:409:ASN:N	2.40	0.54
1:A:304:LEU:HD11	1:A:309:PRO:HG3	1.88	0.54
1:B:285:VAL:HG13	1:B:362:LEU:HD11	1.90	0.54
1:B:652:LEU:O	1:B:669:ARG:NH2	2.40	0.54
1:B:718:ALA:O	1:B:726:ARG:NH1	2.40	0.54
1:C:412:VAL:HG21	1:C:683:SER:HB3	1.88	0.54
2:D:52:ASN:ND2	2:D:105:GLY:O	2.41	0.54
1:A:862:ILE:HD11	1:A:1104:LEU:HA	1.89	0.54
1:A:865:GLU:OE2	1:A:1111:ARG:HG3	2.07	0.54
1:B:226:GLN:O	1:B:226:GLN:HG2	2.08	0.54
1:C:690:ILE:HG23	1:C:756:ILE:HG21	1.90	0.54
1:A:814:VAL:HG22	1:A:1157:VAL:HG22	1.90	0.54
2:E:38:ARG:NH1	2:E:46:GLU:OE2	2.41	0.54
1:A:173:ASN:HB2	1:A:174:PRO:HD3	1.90	0.53
1:A:285:VAL:HB	1:A:296:TYR:HB2	1.90	0.53
1:B:915:PHE:CD1	1:B:1149:PRO:HD3	2.43	0.53
1:B:173:ASN:O	1:B:331:GLN:NE2	2.42	0.53
1:C:149:PRO:HB2	1:C:152:SER:HB3	1.89	0.53
1:B:185:ALA:O	1:B:358:TYR:N	2.41	0.53
1:B:411:ARG:NH2	1:C:832:MET:SD	2.82	0.53
1:A:184:PHE:HB3	1:A:284:PHE:HB2	1.91	0.53
1:A:212:VAL:HG23	1:A:219:VAL:HB	1.89	0.53
1:A:279:LYS:N	1:A:303:ASN:ND2	2.53	0.53
1:A:862:ILE:O	1:A:866:GLN:HG2	2.09	0.53
1:B:195:GLY:HA3	1:B:212:VAL:HA	1.91	0.53
1:B:844:LEU:HD22	1:B:1085:ILE:HG23	1.90	0.53
1:B:995:ALA:HB1	1:B:1005:GLN:HG3	1.91	0.53
1:C:200:THR:HA	1:C:328:THR:HG22	1.91	0.53
2:D:4:LEU:HB3	2:D:117:GLY:HA2	1.91	0.53
2:D:72:ARG:HG2	2:D:79:VAL:HG23	1.90	0.53
1:B:994:MET:HB3	1:B:1008:LEU:HD11	1.90	0.53
1:A:843:ASN:O	1:A:847:GLN:NE2	2.41	0.53
1:A:950:LEU:HD11	1:A:1051:LEU:HD21	1.91	0.53
1:C:471:CYS:CB	2:D:104:TYR:CZ	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:594:GLY:O	1:C:598:GLN:HG3	2.09	0.53
1:B:1069:LEU:H	1:B:1069:LEU:HD12	1.73	0.53
1:C:907:ARG:CZ	1:C:915:PHE:HD2	2.22	0.53
1:C:976:SER:O	1:C:979:THR:OG1	2.27	0.53
1:C:997:ARG:NH1	1:C:1141:LEU:O	2.42	0.53
1:A:484:PHE:HA	1:A:609:LEU:HD13	1.91	0.52
1:A:811:THR:HG23	1:A:1162:ALA:HB2	1.92	0.52
1:A:490:ASP:O	1:A:603:VAL:HA	2.10	0.52
1:C:476:PRO:HD2	1:C:477:THR:H	1.73	0.52
1:C:1198:GLN:NE2	1:C:1201:PHE:HB3	2.24	0.52
1:A:651:PHE:HB3	1:A:655:GLN:HB3	1.92	0.52
1:A:182:VAL:HB	1:A:286:PHE:HD2	1.74	0.52
2:E:40:ALA:HB3	2:E:43:LYS:HB2	1.91	0.52
1:A:497:ASP:OD1	1:A:497:ASP:N	2.42	0.52
1:A:418:ILE:HG22	1:A:632:ASN:O	2.10	0.52
1:A:460:LEU:HG	1:A:466:PHE:HE2	1.74	0.51
1:A:804:ILE:HG22	1:B:988:ILE:HA	1.91	0.51
1:A:145:ASP:OD1	1:A:146:LEU:N	2.43	0.51
1:A:445:TRP:HZ3	1:A:447:ARG:HH11	1.57	0.51
1:A:897:ILE:HD12	1:A:970:LEU:HD11	1.93	0.51
1:A:492:PHE:HE1	1:A:494:ILE:HD11	1.74	0.51
1:C:917:LYS:NZ	1:C:1033:THR:O	2.36	0.51
2:D:52:ASN:HB3	2:D:56:ARG:CZ	2.41	0.51
2:D:20:LEU:HD23	2:D:36:TRP:CZ3	2.46	0.51
1:B:946:LYS:HD2	1:B:947:PHE:H	1.76	0.51
1:C:122:ASN:HD21	1:C:151:PHE:HB3	1.75	0.51
1:A:445:TRP:CD1	1:A:445:TRP:H	2.29	0.51
1:A:998:PHE:CD2	1:A:1008:LEU:HB2	2.45	0.51
1:A:527:ALA:HB2	1:A:602:VAL:HG23	1.93	0.51
2:D:34:MET:HE2	2:D:79:VAL:HG12	1.92	0.51
1:C:473:GLY:H	2:D:103:TYR:HB3	1.76	0.50
1:C:595:VAL:HB	2:D:44:GLU:OE2	2.11	0.50
2:D:11:LEU:HA	2:D:123:THR:HB	1.93	0.50
2:D:114:GLU:HG3	2:D:115:TYR:CD1	2.45	0.50
2:E:22:CYS:H	2:E:78:THR:HG23	1.76	0.50
1:A:156:TRP:CH2	1:A:158:HIS:HB2	2.46	0.50
1:A:690:ILE:HD12	1:A:742:LEU:HD11	1.91	0.50
1:B:814:VAL:O	1:B:1026:ILE:HD11	2.11	0.50
1:C:411:ARG:HD2	1:C:684:PHE:HB2	1.91	0.50
1:C:475:SER:HA	2:D:104:TYR:CD1	2.47	0.50
1:C:998:PHE:HE1	1:C:1141:LEU:HD11	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:THR:OG1	1:A:610:LEU:O	2.29	0.50
1:C:476:PRO:CD	1:C:477:THR:N	2.74	0.50
1:C:669:ARG:HD3	1:C:674:LEU:HD22	1.94	0.50
2:E:37:PHE:N	2:E:95:TYR:O	2.41	0.50
1:B:804:ILE:HG22	1:C:988:ILE:HD12	1.93	0.50
1:B:848:TYR:OH	1:B:1086:ASP:OD1	2.28	0.50
1:C:418:ILE:HG23	1:C:631:VAL:HG21	1.94	0.50
1:C:419:VAL:HG22	1:C:634:ASN:HB3	1.94	0.50
1:A:470:LYS:HD2	2:E:102:VAL:HG13	1.91	0.50
1:C:287:LYS:HZ3	1:C:296:TYR:HE2	1.58	0.50
1:B:410:PHE:CD2	1:B:715:ALA:HB1	2.47	0.50
1:A:304:LEU:HD21	1:A:309:PRO:HB3	1.93	0.50
1:A:1140:HIS:HA	1:A:1158:THR:HG22	1.94	0.50
1:A:1076:LEU:HB3	1:A:1080:GLU:HG2	1.94	0.49
1:B:791:LEU:HB3	1:C:965:TYR:CE1	2.46	0.49
1:B:185:ALA:HB3	1:B:358:TYR:HB2	1.92	0.49
1:C:719:ASP:O	1:C:726:ARG:NH1	2.45	0.49
1:A:183:TYR:HB3	1:A:360:GLY:HA3	1.94	0.49
1:A:766:TYR:HD1	1:A:784:ILE:HD13	1.77	0.49
1:A:1220:VAL:HG23	1:A:1221:VAL:HG23	1.94	0.49
1:C:289:ILE:H	1:C:294:LYS:HZ3	1.60	0.49
1:C:412:VAL:HG22	1:C:715:ALA:HB1	1.94	0.49
1:C:470:LYS:HA	2:D:106:TYR:O	2.12	0.49
1:C:1115:ASN:O	1:C:1119:THR:HG23	2.12	0.49
1:A:534:ASP:OD1	1:A:534:ASP:N	2.45	0.49
1:A:469:PHE:O	2:E:105:GLY:CA	2.60	0.49
1:A:823:MET:HB2	1:A:1047:ASN:HD21	1.76	0.49
1:B:710:THR:OG1	1:B:711:GLU:OE1	2.30	0.49
2:D:37:PHE:HE1	2:D:47:PHE:HD1	1.59	0.49
2:E:20:LEU:HD11	2:E:94:TYR:HD2	1.77	0.49
1:A:480:ASN:OD1	1:A:619:PRO:HD2	2.13	0.49
1:B:149:PRO:HG3	1:B:363:GLN:NE2	2.28	0.49
1:B:285:VAL:HB	1:B:296:TYR:HB2	1.94	0.49
1:B:862:ILE:HD11	1:B:1104:LEU:HA	1.94	0.49
2:D:20:LEU:HB2	2:D:81:LEU:HB3	1.95	0.49
1:A:734:VAL:HG22	1:A:743:ILE:HG12	1.94	0.49
2:D:104:TYR:CD2	2:D:104:TYR:C	2.91	0.49
1:A:458:SER:O	1:A:462:ASN:ND2	2.42	0.49
1:C:476:PRO:HG3	2:D:104:TYR:CD2	2.48	0.49
2:D:6:GLU:CD	2:D:119:GLY:H	2.21	0.49
1:A:704:TYR:O	1:A:740:GLY:HA3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:15:GLY:HA2	2:E:85:SER:H	1.78	0.48
1:A:1198:GLN:HE21	1:A:1201:PHE:HB3	1.78	0.48
1:B:316:GLU:N	1:B:316:GLU:OE1	2.46	0.48
1:A:390:GLU:O	1:A:394:THR:HG23	2.13	0.48
1:C:325:ILE:HG23	1:C:327:ILE:HG13	1.95	0.48
1:A:474:VAL:C	2:E:103:TYR:CE2	2.91	0.48
1:C:1194:TRP:CD1	1:C:1227:ASN:HD22	2.31	0.48
1:A:427:LEU:HD23	1:A:454:VAL:HB	1.94	0.48
1:B:1228:THR:HB	1:B:1230:TYR:CE1	2.49	0.48
1:A:219:VAL:HA	1:A:263:VAL:HA	1.96	0.48
1:A:461:TYR:OH	1:A:479:LEU:HD12	2.14	0.48
1:A:495:ARG:NH2	1:A:598:GLN:O	2.46	0.48
1:B:746:GLU:HG3	1:B:785:ILE:HG22	1.96	0.48
1:C:469:PHE:O	2:D:106:TYR:CD2	2.67	0.48
1:A:989:PRO:HG2	1:A:992:MET:HB2	1.95	0.48
1:A:1062:PHE:O	1:A:1087:ARG:NH1	2.46	0.48
1:A:185:ALA:HB3	1:A:358:TYR:HB2	1.96	0.48
1:A:594:GLY:HA2	2:E:44:GLU:OE1	2.13	0.48
1:A:818:ILE:HD13	1:A:1037:LEU:HA	1.96	0.48
1:C:855:LEU:HD13	1:C:1096:LEU:HG	1.95	0.48
1:A:145:ASP:HB3	1:A:147:PHE:CE2	2.49	0.48
1:A:418:ILE:HD12	1:A:626:VAL:HG12	1.95	0.48
1:B:854:GLN:OE1	1:B:857:ARG:NH1	2.43	0.48
1:B:970:LEU:O	1:B:974:ILE:HG12	2.14	0.48
1:A:401:GLU:CD	1:A:401:GLU:H	2.22	0.48
1:B:296:TYR:CD1	1:B:317:PRO:HA	2.49	0.48
1:C:543:TYR:O	1:C:587:TYR:N	2.44	0.48
1:A:1080:GLU:OE1	1:A:1080:GLU:N	2.47	0.47
1:C:182:VAL:HG13	1:C:359:VAL:HG13	1.96	0.47
1:A:1234:GLN:HA	1:A:1237:LEU:HD12	1.95	0.47
1:B:379:ASP:OD1	1:B:380:ALA:N	2.46	0.47
1:C:471:CYS:O	2:D:104:TYR:CE1	2.66	0.47
1:B:200:THR:OG1	1:B:326:ASN:O	2.33	0.47
1:B:1171:PRO:HB3	1:C:1009:TYR:CE1	2.49	0.47
1:C:476:PRO:HB3	2:D:104:TYR:HE2	1.76	0.47
1:C:476:PRO:CG	2:D:104:TYR:CD2	2.97	0.47
2:E:15:GLY:H	2:E:86:LEU:H	1.61	0.47
1:A:183:TYR:O	1:A:360:GLY:N	2.46	0.47
1:A:322:PRO:HB2	1:C:613:PRO:HG3	1.96	0.47
1:A:1049:GLN:C	1:A:1051:LEU:H	2.21	0.47
1:A:688:SER:OG	1:A:705:GLN:NE2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:GLU:O	1:B:394:THR:HG23	2.13	0.47
1:C:474:VAL:CA	2:D:103:TYR:CE2	2.97	0.47
1:C:497:ASP:HA	2:D:109:PHE:CZ	2.50	0.47
1:C:538:GLY:H	1:C:591:PRO:HB3	1.80	0.47
2:E:93:ILE:HA	2:E:121:GLN:HA	1.97	0.47
1:A:823:MET:HB2	1:A:1047:ASN:ND2	2.30	0.47
1:A:1116:LEU:HD11	1:A:1120:LYS:HE2	1.96	0.47
1:B:126:ARG:HH21	1:B:309:PRO:HB2	1.80	0.47
1:B:885:PRO:O	1:B:887:LYS:HD2	2.14	0.47
1:B:894:PHE:HD1	1:B:897:ILE:HD11	1.80	0.47
1:B:1228:THR:HB	1:B:1230:TYR:HE1	1.79	0.47
1:C:469:PHE:CB	2:D:106:TYR:OH	2.63	0.47
1:C:537:VAL:HA	1:C:591:PRO:HB3	1.95	0.47
1:C:661:ILE:HD12	1:C:661:ILE:H	1.78	0.47
1:C:807:PRO:O	1:C:1202:TYR:N	2.46	0.47
2:D:4:LEU:HB3	2:D:117:GLY:CA	2.44	0.47
2:D:106:TYR:O	2:D:106:TYR:CG	2.67	0.47
1:A:536:LYS:HB3	1:A:539:GLY:O	2.14	0.47
1:B:411:ARG:O	1:B:413:GLN:NE2	2.48	0.47
1:B:957:LEU:HD23	1:B:961:MET:HE2	1.96	0.47
1:A:711:GLU:OE1	1:A:711:GLU:N	2.48	0.47
1:A:850:SER:O	1:A:854:GLN:HG2	2.15	0.47
1:B:125:THR:OG1	1:B:311:GLY:O	2.32	0.47
1:B:296:TYR:HD1	1:B:317:PRO:HA	1.80	0.47
1:C:198:PHE:HB2	1:C:209:LEU:HB3	1.97	0.47
1:C:814:VAL:HA	1:C:1156:HIS:O	2.15	0.47
1:C:298:LYS:HB3	1:C:315:LEU:HD13	1.97	0.46
1:C:1180:HIS:CD2	1:C:1214:VAL:HG22	2.49	0.46
1:C:1189:SER:HB2	1:C:1194:TRP:CD2	2.50	0.46
2:D:54:ASN:H	2:D:56:ARG:NH1	2.13	0.46
2:D:61:THR:HG22	2:D:64:VAL:HG22	1.97	0.46
1:A:412:VAL:HG23	1:A:683:SER:O	2.15	0.46
1:B:650:LYS:HE3	1:B:650:LYS:HA	1.97	0.46
1:B:657:PHE:O	1:C:135:PHE:N	2.43	0.46
1:A:387:PRO:HG3	1:A:725:TRP:CH2	2.50	0.46
1:A:469:PHE:O	2:E:105:GLY:HA3	2.15	0.46
1:A:475:SER:HB2	2:E:104:TYR:CD2	2.50	0.46
1:A:589:PHE:CE2	1:A:599:PRO:HB3	2.51	0.46
1:A:595:VAL:HG21	2:E:110:PRO:HG2	1.96	0.46
1:C:145:ASP:HB3	1:C:147:PHE:CE1	2.51	0.46
1:C:469:PHE:C	2:D:106:TYR:CZ	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:GLN:HB2	2:D:93:ILE:HG13	1.97	0.46
1:A:196:TRP:N	1:A:211:ILE:O	2.43	0.46
1:A:884:PRO:HG3	1:C:799:TYR:HD2	1.80	0.46
1:C:915:PHE:HD1	1:C:1149:PRO:HG3	1.80	0.46
2:E:37:PHE:CZ	2:E:110:PRO:HA	2.50	0.46
1:B:182:VAL:HG21	1:B:330:PHE:CE1	2.51	0.46
1:C:834:ILE:HG22	1:C:1089:ILE:HD12	1.97	0.46
1:A:474:VAL:HG13	1:A:478:LYS:NZ	2.30	0.46
1:C:869:ASN:O	1:C:873:VAL:HG23	2.16	0.46
1:A:841:CYS:HB2	1:A:1085:ILE:HD11	1.97	0.46
1:A:295:ILE:HG23	1:A:318:LEU:HB3	1.99	0.45
1:A:879:GLN:NE2	1:A:881:TYR:OH	2.49	0.45
1:C:445:TRP:H	1:C:445:TRP:CD1	2.35	0.45
1:C:1014:LEU:O	1:C:1018:GLN:HG3	2.16	0.45
2:D:20:LEU:HB3	2:D:36:TRP:CZ2	2.51	0.45
1:A:132:ASP:OD1	1:A:132:ASP:N	2.49	0.45
1:A:296:TYR:CD1	1:A:317:PRO:HA	2.48	0.45
1:B:1227:ASN:OD1	1:B:1228:THR:N	2.39	0.45
1:C:123:SER:OG	1:C:152:SER:N	2.32	0.45
1:A:501:GLN:CD	1:A:508:GLY:HA3	2.42	0.45
1:A:593:ASN:HB3	1:A:597:TYR:HB2	1.97	0.45
1:C:128:VAL:HG21	1:C:312:PHE:CE1	2.52	0.45
2:D:4:LEU:HD12	2:D:24:ALA:HB2	1.98	0.45
1:A:589:PHE:CZ	1:A:599:PRO:HB3	2.51	0.45
1:B:157:PHE:CZ	1:B:176:LEU:HD21	2.50	0.45
1:B:765:SER:OG	1:B:766:TYR:N	2.49	0.45
1:C:476:PRO:HD2	1:C:477:THR:N	2.32	0.45
1:B:994:MET:SD	1:B:1142:MET:HE3	2.56	0.45
1:C:126:ARG:NH2	1:C:311:GLY:O	2.49	0.45
1:B:136:ARG:HB2	1:B:371:TYR:CE2	2.52	0.45
1:B:736:GLN:NE2	1:B:740:GLY:O	2.49	0.45
1:C:862:ILE:O	1:C:866:GLN:HG2	2.17	0.45
1:C:998:PHE:CD2	1:C:1008:LEU:HB2	2.52	0.45
1:A:451:SER:OG	1:A:615:THR:OG1	2.35	0.45
1:A:476:PRO:HD3	2:E:104:TYR:HB2	1.94	0.45
1:B:296:TYR:HE1	1:B:317:PRO:HB3	1.82	0.45
1:A:145:ASP:HB3	1:A:147:PHE:HE2	1.81	0.45
1:A:201:THR:OG1	1:A:206:THR:OG1	2.32	0.45
1:A:466:PHE:O	2:E:59:TYR:OH	2.34	0.45
1:B:1080:GLU:OE1	1:B:1080:GLU:N	2.48	0.45
1:C:1196:VAL:HG11	1:C:1211:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:MET:HA	2:D:113:TYR:HE2	1.81	0.45
1:A:495:ARG:HH22	1:A:598:GLN:N	2.15	0.45
1:A:697:SER:OG	1:A:698:ASN:N	2.50	0.45
1:A:795:ASN:O	1:B:881:TYR:HA	2.16	0.45
1:A:1078:PRO:N	1:A:1079:PRO:HD2	2.32	0.45
1:B:670:ASP:N	1:B:675:GLU:O	2.46	0.45
1:A:998:PHE:HE2	1:A:1015:ILE:HD13	1.80	0.45
1:B:644:LEU:HD23	1:B:679:ILE:HG12	1.99	0.45
1:C:157:PHE:HB2	1:C:357:TYR:HD2	1.82	0.45
1:C:476:PRO:CD	1:C:477:THR:H	2.28	0.45
1:C:1203:GLU:O	1:C:1203:GLU:HG3	2.16	0.45
1:A:157:PHE:HE2	1:A:176:LEU:HD21	1.82	0.44
1:A:213:ASN:OD1	1:A:214:ASN:N	2.50	0.44
1:A:475:SER:HB3	2:E:104:TYR:CE2	2.52	0.44
1:A:600:TYR:CE2	2:E:109:PHE:CD1	3.05	0.44
1:C:145:ASP:OD1	1:C:146:LEU:N	2.47	0.44
1:A:199:GLY:N	1:A:327:ILE:HG23	2.27	0.44
1:B:844:LEU:HD23	1:B:1089:ILE:HG13	1.98	0.44
1:C:711:GLU:OE1	1:C:711:GLU:N	2.46	0.44
1:C:1206:ILE:O	1:C:1211:ASN:ND2	2.50	0.44
2:E:6:GLU:OE1	2:E:119:GLY:N	2.36	0.44
1:A:146:LEU:HB2	1:A:287:LYS:NZ	2.33	0.44
1:C:915:PHE:CD1	1:C:1149:PRO:HG3	2.52	0.44
1:A:437:THR:OG1	1:A:438:ARG:N	2.50	0.44
1:A:719:ASP:OD1	1:A:719:ASP:N	2.50	0.44
1:A:871:GLN:O	1:A:875:ALA:HB3	2.17	0.44
1:A:1022:ALA:O	1:A:1026:ILE:HG12	2.18	0.44
1:A:1062:PHE:HA	1:B:848:TYR:HD1	1.82	0.44
1:B:387:PRO:HG3	1:B:725:TRP:CZ3	2.52	0.44
1:C:221:LYS:HA	1:C:261:GLU:HA	2.00	0.44
2:D:52:ASN:HB2	2:D:56:ARG:HG2	1.98	0.44
1:B:1072:ILE:HG23	1:B:1076:LEU:HD12	1.99	0.44
2:D:20:LEU:HB3	2:D:36:TRP:CH2	2.52	0.44
1:A:213:ASN:HA	1:A:218:VAL:HA	2.00	0.44
1:A:799:TYR:CE1	1:B:989:PRO:HA	2.50	0.44
1:A:832:MET:SD	1:A:949:GLY:HA2	2.58	0.44
1:A:392:LYS:HE2	1:A:398:PHE:O	2.18	0.44
1:A:469:PHE:CD1	1:A:526:ILE:HG12	2.53	0.44
2:E:81:LEU:HD12	2:E:81:LEU:HA	1.91	0.44
1:B:691:THR:HB	1:B:700:VAL:HG12	2.00	0.44
1:C:670:ASP:N	1:C:670:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:SER:OG	2:D:52:ASN:ND2	2.40	0.44
2:E:34:MET:CE	2:E:96:CYS:HB2	2.47	0.44
2:E:109:PHE:HB2	2:E:112:GLU:HB2	1.99	0.44
1:A:365:ARG:HG3	1:A:366:THR:N	2.33	0.44
1:B:209:LEU:HA	1:B:222:VAL:HA	1.99	0.44
1:B:1078:PRO:N	1:B:1079:PRO:HD2	2.32	0.44
1:C:149:PRO:HG3	1:C:365:ARG:CD	2.48	0.44
1:C:905:SER:HB2	1:C:907:ARG:HG3	2.00	0.44
2:D:18:LEU:O	2:D:83:MET:HG3	2.18	0.44
2:E:11:LEU:HD11	2:E:125:SER:HB2	1.98	0.44
1:A:986:LEU:HD21	1:C:807:PRO:HG3	2.00	0.43
1:A:994:MET:HE1	1:A:1142:MET:SD	2.58	0.43
1:B:690:ILE:HG23	1:B:756:ILE:HG21	2.00	0.43
1:A:590:GLN:HB2	1:A:593:ASN:OD1	2.18	0.43
1:A:688:SER:HB2	1:A:703:LEU:HB3	2.00	0.43
1:A:1062:PHE:CD2	1:A:1091:GLY:HA3	2.54	0.43
1:B:1088:LEU:HD21	1:B:1092:ARG:CZ	2.48	0.43
1:C:1178:LYS:HE3	1:C:1178:LYS:HB2	1.62	0.43
1:A:502:ILE:O	1:A:502:ILE:HG13	2.18	0.43
1:A:530:SER:O	1:A:599:PRO:HG2	2.19	0.43
1:A:1052:ASN:O	1:A:1056:LYS:HG2	2.19	0.43
1:C:181:GLY:C	1:C:362:LEU:HD23	2.44	0.43
1:C:198:PHE:CD2	1:C:209:LEU:HD22	2.54	0.43
1:A:194:ARG:HD2	1:A:213:ASN:O	2.17	0.43
1:B:146:LEU:CD2	1:B:180:ASP:HB3	2.48	0.43
1:B:173:ASN:HB2	1:B:174:PRO:HD3	2.00	0.43
1:C:196:TRP:HB3	1:C:198:PHE:CE1	2.53	0.43
1:C:763:CYS:SG	1:C:789:MET:HE2	2.58	0.43
1:C:768:THR:HA	1:C:782:GLN:HG2	2.01	0.43
1:A:529:ASN:HA	1:A:600:TYR:CD1	2.54	0.43
1:B:697:SER:OG	1:B:698:ASN:N	2.49	0.43
1:B:795:ASN:OD1	1:B:796:SER:N	2.50	0.43
1:C:868:LYS:O	1:C:872:GLU:HG2	2.18	0.43
1:C:1146:GLN:N	1:C:1153:VAL:O	2.50	0.43
1:A:918:VAL:HG21	1:A:1149:PRO:HG2	2.01	0.43
1:A:1222:ILE:HD11	1:B:1012:GLN:NE2	2.33	0.43
1:B:703:LEU:HD11	1:B:758:ILE:HG23	2.00	0.43
1:C:476:PRO:HG3	2:D:104:TYR:CE2	2.53	0.43
1:A:494:ILE:HG22	1:A:495:ARG:N	2.33	0.43
1:A:804:ILE:CG2	1:B:989:PRO:HD2	2.47	0.43
1:B:868:LYS:O	1:B:872:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:PRO:HB2	1:C:333:LEU:HD21	2.00	0.43
1:B:209:LEU:HD12	1:B:323:ILE:HG21	2.01	0.43
1:B:811:THR:HG23	1:B:1162:ALA:HB2	2.01	0.43
1:A:1119:THR:O	1:A:1123:GLU:HG3	2.19	0.43
1:B:831:THR:O	1:B:835:CYS:HB2	2.18	0.43
1:B:998:PHE:CD2	1:B:1008:LEU:HB2	2.54	0.43
1:C:197:ILE:HB	1:C:331:GLN:HB2	2.01	0.43
2:E:4:LEU:HA	2:E:23:ALA:O	2.18	0.43
1:A:832:MET:HE3	1:A:832:MET:HB2	1.94	0.42
1:B:670:ASP:HB3	1:B:675:GLU:H	1.83	0.42
1:B:1165:LYS:HB2	1:B:1167:PHE:CE2	2.53	0.42
1:A:142:SER:HA	1:A:368:LEU:HA	2.01	0.42
1:A:464:ALA:O	2:E:59:TYR:OH	2.20	0.42
1:B:141:HIS:HD2	1:B:143:THR:HG23	1.84	0.42
1:B:1122:SER:O	1:B:1126:LEU:HB2	2.18	0.42
1:C:474:VAL:N	2:D:103:TYR:CD2	2.87	0.42
1:C:545:TYR:O	1:C:585:GLN:N	2.46	0.42
1:C:1121:MET:HE2	1:C:1121:MET:HB2	1.95	0.42
2:D:6:GLU:HB3	2:D:120:THR:HB	2.01	0.42
2:D:36:TRP:CD1	2:D:81:LEU:HD13	2.54	0.42
1:A:666:ASP:OD1	1:B:946:LYS:NZ	2.50	0.42
1:C:476:PRO:HB3	2:D:104:TYR:OH	2.19	0.42
1:A:990:PHE:HB3	1:A:991:PRO:HD3	2.02	0.42
1:A:992:MET:HG2	1:A:1009:TYR:OH	2.20	0.42
1:B:401:GLU:O	1:B:405:TYR:OH	2.36	0.42
1:B:994:MET:HB3	1:B:994:MET:HE3	1.75	0.42
1:C:694:THR:HA	1:C:697:SER:O	2.19	0.42
2:E:87:LYS:HA	2:E:87:LYS:HD2	1.89	0.42
1:A:903:LYS:HD3	1:A:912:ASP:OD2	2.20	0.42
1:A:1083:VAL:O	1:A:1087:ARG:HG3	2.19	0.42
1:B:128:VAL:O	1:B:315:LEU:N	2.52	0.42
1:B:814:VAL:HG22	1:B:1157:VAL:HG22	2.02	0.42
1:C:148:LEU:HD12	1:C:149:PRO:HD2	2.01	0.42
1:A:185:ALA:O	1:A:358:TYR:N	2.50	0.42
1:C:129:TYR:HA	1:C:315:LEU:H	1.84	0.42
1:C:624:ASN:OD1	1:C:625:LEU:N	2.52	0.42
2:D:109:PHE:CD2	2:D:111:ASN:HB3	2.55	0.42
1:A:495:ARG:HH22	1:A:598:GLN:C	2.28	0.42
1:A:665:THR:HG22	1:A:679:ILE:HD12	2.02	0.42
1:B:412:VAL:HB	1:B:682:CYS:HB3	2.01	0.42
1:C:193:ILE:HD12	1:C:334:LEU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:PHE:HB3	1:C:286:PHE:CE1	2.55	0.42
1:C:476:PRO:CD	2:D:104:TYR:CE2	3.03	0.42
1:C:1198:GLN:HE21	1:C:1201:PHE:HB3	1.85	0.42
2:D:97:ALA:CB	2:D:113:TYR:HB3	2.48	0.42
1:A:212:VAL:HG12	1:A:333:LEU:HD12	2.02	0.42
1:A:654:PHE:O	1:B:133:LYS:NZ	2.44	0.42
1:B:1182:PRO:HD3	1:B:1187:PHE:CE2	2.55	0.42
1:C:395:LEU:HD12	1:C:400:VAL:HG12	2.02	0.42
1:C:896:GLN:NE2	1:C:1027:GLN:HE21	2.18	0.42
2:D:87:LYS:HB2	2:D:90:ASP:HB2	2.02	0.42
1:A:135:PHE:CZ	1:A:137:SER:HB3	2.55	0.41
1:A:446:ASN:O	1:A:490:ASP:HA	2.20	0.41
1:A:469:PHE:O	2:E:105:GLY:C	2.63	0.41
1:A:476:PRO:CD	2:E:104:TYR:CB	2.84	0.41
1:A:860:THR:O	1:A:864:VAL:HG13	2.20	0.41
1:A:884:PRO:HG3	1:C:799:TYR:CD2	2.55	0.41
1:A:1183:ARG:NH1	1:A:1213:PHE:HB3	2.35	0.41
2:D:73:ASP:OD1	2:D:74:ASP:N	2.50	0.41
1:A:157:PHE:CE2	1:A:176:LEU:HD21	2.54	0.41
1:C:379:ASP:OD1	1:C:380:ALA:N	2.52	0.41
1:A:525:VAL:HA	1:A:604:VAL:HG23	2.02	0.41
1:A:1198:GLN:NE2	1:A:1201:PHE:HB3	2.34	0.41
1:B:198:PHE:HD2	1:B:209:LEU:HD22	1.85	0.41
1:C:467:SER:CB	1:C:529:ASN:H	2.34	0.41
1:A:366:THR:HB	1:A:383:CYS:HB3	2.03	0.41
1:A:498:GLU:O	1:A:501:GLN:HB2	2.19	0.41
1:B:411:ARG:HH12	1:C:837:ASP:HA	1.85	0.41
1:C:473:GLY:O	2:D:103:TYR:CZ	2.74	0.41
1:C:691:THR:HB	1:C:700:VAL:HG12	2.01	0.41
1:A:600:TYR:CZ	2:E:109:PHE:CD1	3.09	0.41
1:A:1121:MET:O	1:A:1125:VAL:HB	2.20	0.41
1:B:412:VAL:HG22	1:B:715:ALA:HB2	2.03	0.41
1:B:1234:GLN:CG	1:B:1235:PRO:HD3	2.51	0.41
1:A:382:ASP:O	1:A:389:SER:HB3	2.19	0.41
1:C:287:LYS:NZ	1:C:296:TYR:HE2	2.18	0.41
1:C:473:GLY:C	2:D:103:TYR:CE2	2.99	0.41
1:C:1008:LEU:HD12	1:C:1015:ILE:HD13	2.03	0.41
1:C:1217:ASN:OD1	1:C:1217:ASN:N	2.53	0.41
1:B:789:MET:H	1:B:789:MET:HG2	1.66	0.41
1:C:719:ASP:N	1:C:719:ASP:OD1	2.52	0.41
1:A:134:VAL:HG22	1:C:657:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ILE:HG22	1:A:290:ASP:OD1	2.20	0.41
1:A:1180:HIS:ND1	1:A:1214:VAL:HG22	2.36	0.41
1:C:410:PHE:HD1	1:C:716:ILE:HD13	1.85	0.41
1:A:292:TYR:CE1	1:A:322:PRO:HB3	2.56	0.41
1:A:387:PRO:O	1:A:391:THR:HG23	2.21	0.41
1:A:466:PHE:HB2	2:E:106:TYR:OH	2.21	0.41
1:A:833:TYR:CE1	1:A:1058:LEU:HD13	2.56	0.41
1:A:977:GLY:HA2	1:A:993:GLN:CD	2.46	0.41
1:A:1178:LYS:HD2	1:A:1214:VAL:HG11	2.03	0.41
1:B:896:GLN:NE2	1:B:1027:GLN:OE1	2.42	0.41
1:B:1026:ILE:HD13	1:B:1026:ILE:HA	1.90	0.41
1:C:1185:GLY:HA2	1:C:1199:ARG:HD2	2.03	0.41
2:D:93:ILE:HA	2:D:121:GLN:HG3	2.02	0.41
1:A:184:PHE:O	1:A:284:PHE:N	2.45	0.41
1:C:372:ASN:HB3	1:C:378:THR:OG1	2.21	0.41
2:D:39:GLN:HE22	2:D:95:TYR:HB2	1.86	0.41
2:D:51:ILE:HG12	2:D:52:ASN:H	1.85	0.41
1:A:289:ILE:HG22	1:A:290:ASP:N	2.35	0.40
1:A:321:LEU:HD13	1:A:321:LEU:HA	1.97	0.40
1:A:879:GLN:HE21	1:C:795:ASN:HD22	1.70	0.40
1:A:1120:LYS:NZ	1:A:1134:PHE:O	2.54	0.40
1:B:421:PHE:H	1:B:672:GLN:NE2	2.19	0.40
2:D:8:GLY:O	2:D:18:LEU:HD13	2.21	0.40
2:E:87:LYS:C	2:E:124:VAL:HG11	2.46	0.40
1:A:121:THR:O	1:A:153:ASN:HA	2.21	0.40
1:A:594:GLY:HA2	2:E:44:GLU:CD	2.46	0.40
1:B:827:SER:O	1:B:951:THR:OG1	2.33	0.40
1:B:1053:THR:O	1:B:1057:GLN:HG2	2.21	0.40
1:B:1077:ASP:OD1	1:B:1079:PRO:HD2	2.21	0.40
1:C:531:ASN:HB2	1:C:598:GLN:HG2	2.02	0.40
1:C:1178:LYS:HB3	1:C:1214:VAL:CG1	2.51	0.40
1:A:870:THR:HG23	1:A:874:PHE:HD2	1.86	0.40
1:A:989:PRO:HG3	1:C:1169:THR:HG21	2.02	0.40
1:B:1194:TRP:HB2	1:B:1227:ASN:ND2	2.36	0.40
1:C:208:SER:N	1:C:224:GLU:OE2	2.52	0.40
1:C:292:TYR:CE1	1:C:322:PRO:HB3	2.57	0.40
1:B:126:ARG:NH2	1:B:309:PRO:HB2	2.37	0.40
1:B:203:ASP:OD1	1:B:205:LYS:HG2	2.21	0.40
1:B:225:PHE:CG	1:B:226:GLN:N	2.90	0.40
1:B:1049:GLN:C	1:B:1051:LEU:H	2.30	0.40
1:A:1171:PRO:HB3	1:B:1009:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1178:LYS:HA	1:B:1217:ASN:HA	2.04	0.40
1:C:129:TYR:HB3	1:C:315:LEU:HB2	2.03	0.40
1:C:394:THR:HG21	1:C:407:THR:HB	2.03	0.40
1:C:1180:HIS:CD2	1:C:1229:VAL:HG21	2.57	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	964/1380 (70%)	938 (97%)	26 (3%)	0	100	100
1	B	796/1380 (58%)	775 (97%)	21 (3%)	0	100	100
1	C	959/1380 (70%)	938 (98%)	21 (2%)	0	100	100
2	D	124/155 (80%)	119 (96%)	5 (4%)	0	100	100
2	E	124/155 (80%)	120 (97%)	4 (3%)	0	100	100
All	All	2967/4450 (67%)	2890 (97%)	77 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	823/1185 (70%)	819 (100%)	4 (0%)	81	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	680/1185 (57%)	680 (100%)	0	100	100
1	C	677/1185 (57%)	676 (100%)	1 (0%)	88	88
2	D	102/125 (82%)	102 (100%)	0	100	100
2	E	102/125 (82%)	102 (100%)	0	100	100
All	All	2384/3805 (63%)	2379 (100%)	5 (0%)	85	86

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	636	ASN
1	A	638	LEU
1	A	645	THR
1	A	909	PRO
1	C	471	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	506	GLN
1	A	598	GLN
1	A	876	GLN
1	A	879	GLN
1	A	993	GLN
1	A	1097	GLN
1	B	141	HIS
1	B	179	ASN
1	B	717	HIS
1	B	736	GLN
1	B	876	GLN
1	B	1005	GLN
1	B	1047	ASN
1	B	1175	HIS
1	C	299	HIS
1	C	331	GLN
1	C	656	GLN
1	C	698	ASN
1	C	782	GLN
1	C	871	GLN
1	C	1027	GLN
1	C	1049	GLN

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Mol	Chain	Res	Type
1	C	1094	GLN
1	C	1180	HIS
2	D	52	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

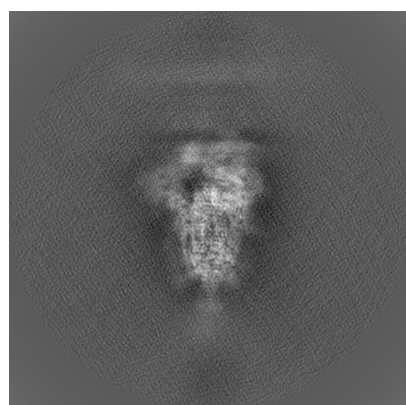
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24256. These allow visual inspection of the internal detail of the map and identification of artifacts.

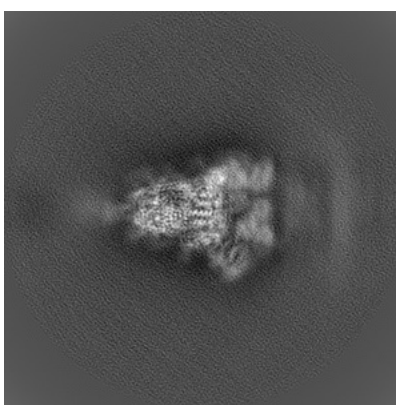
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

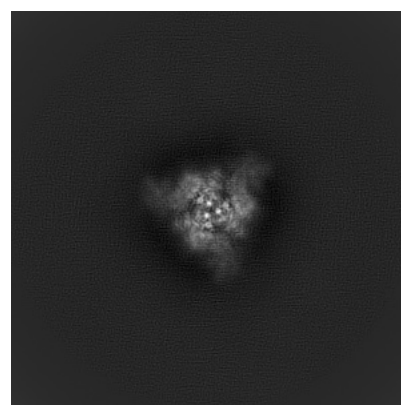
6.1.1 Primary map



X



Y

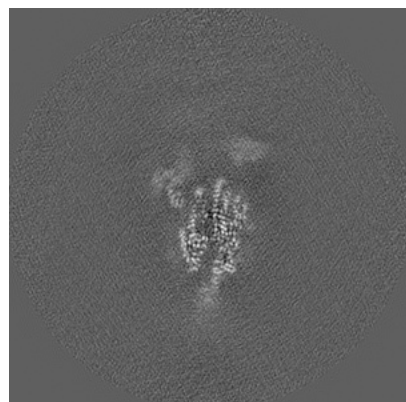


Z

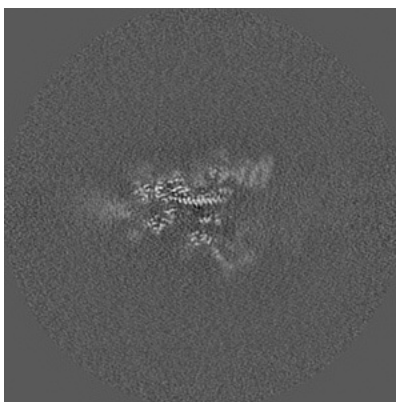
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

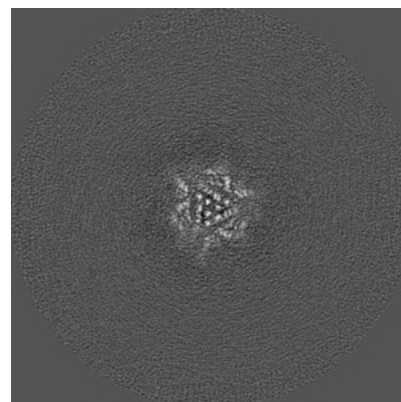
6.2.1 Primary map



X Index: 208



Y Index: 208

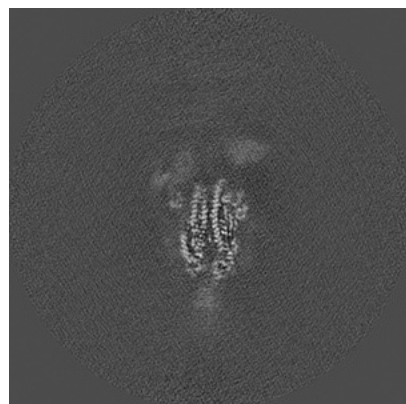


Z Index: 208

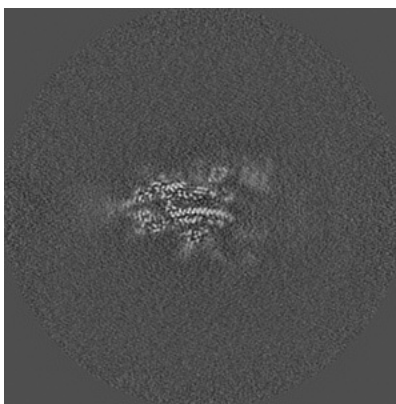
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

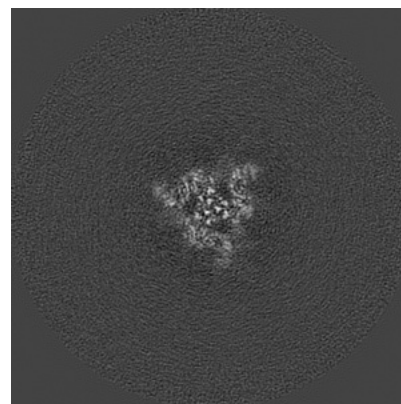
6.3.1 Primary map



X Index: 206



Y Index: 202

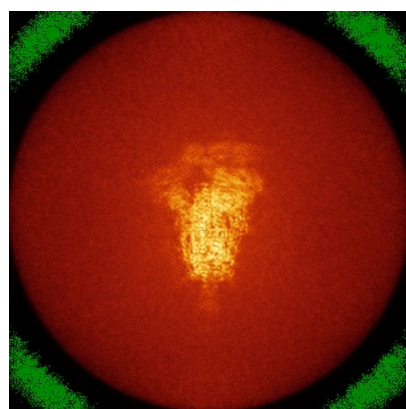


Z Index: 215

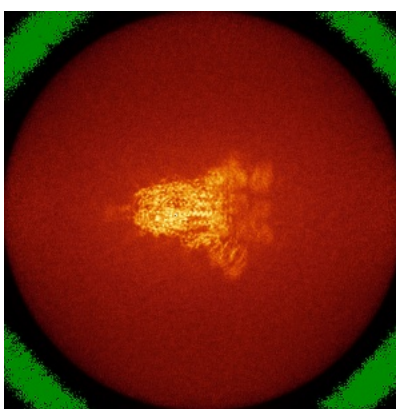
The images above show the largest variance slices of the map in three orthogonal directions.

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

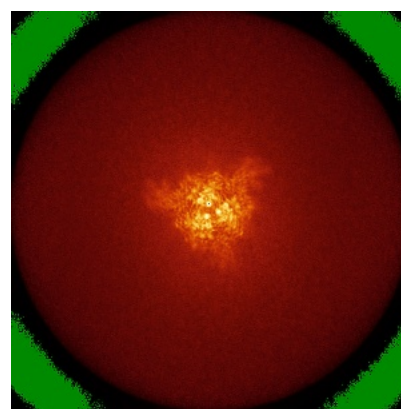
6.4.1 Primary map



X



Y

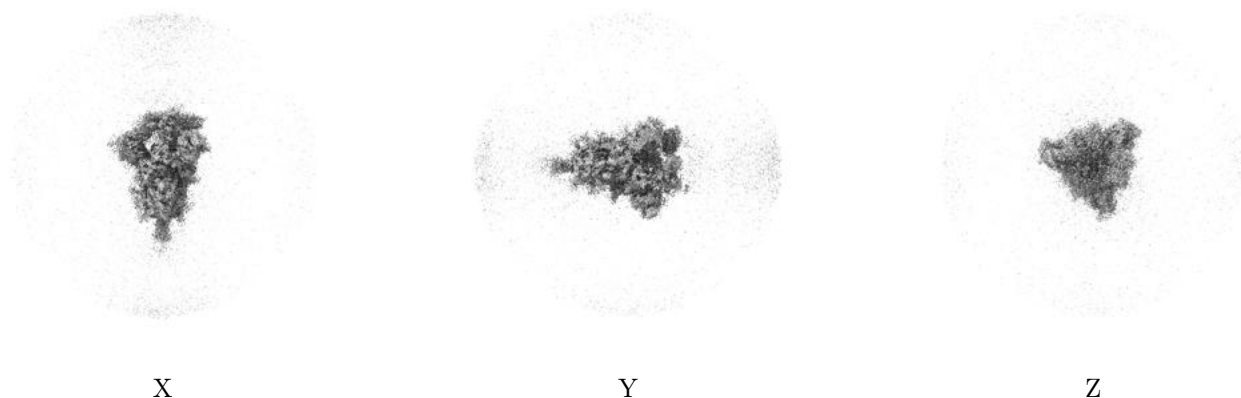


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

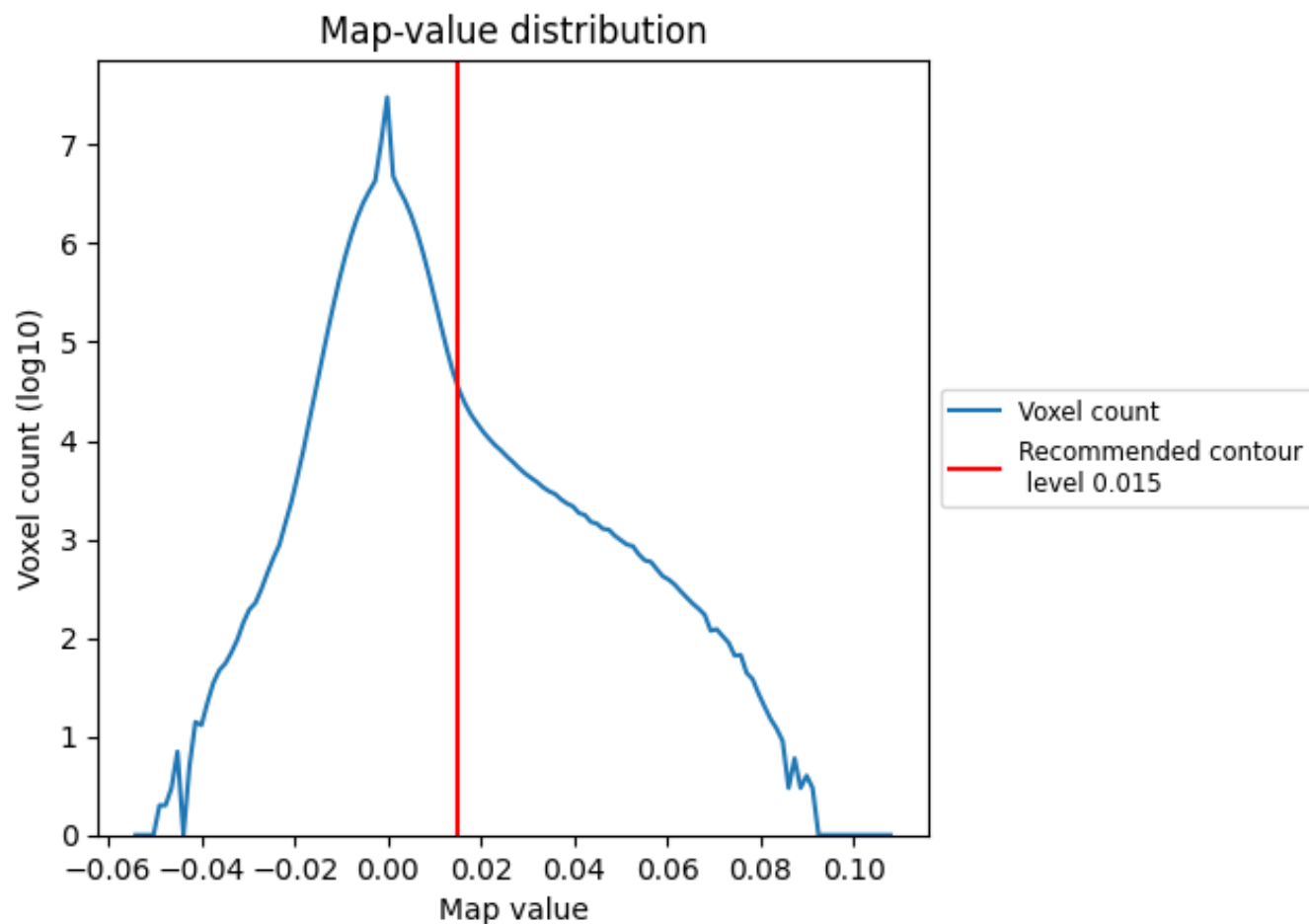
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

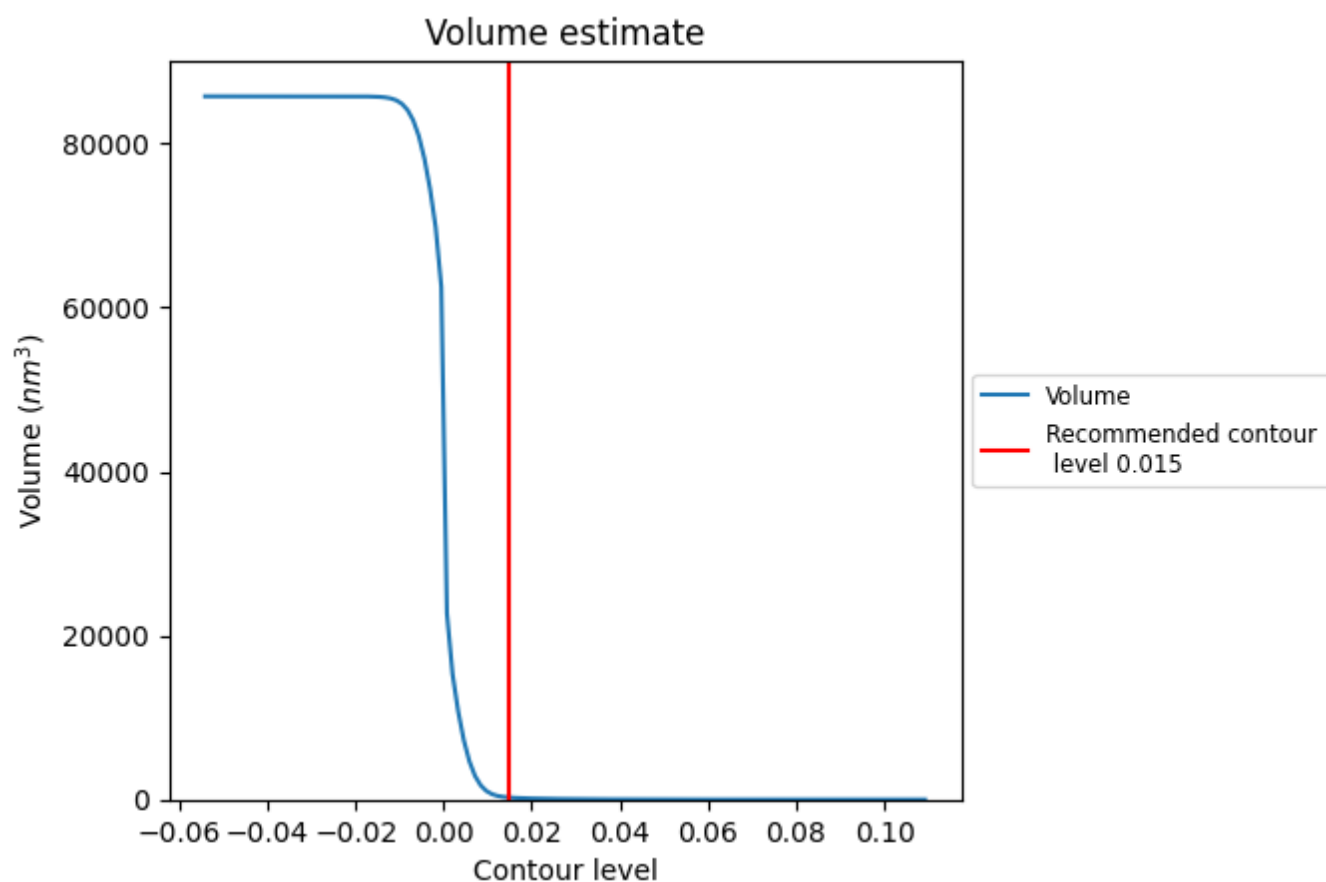
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

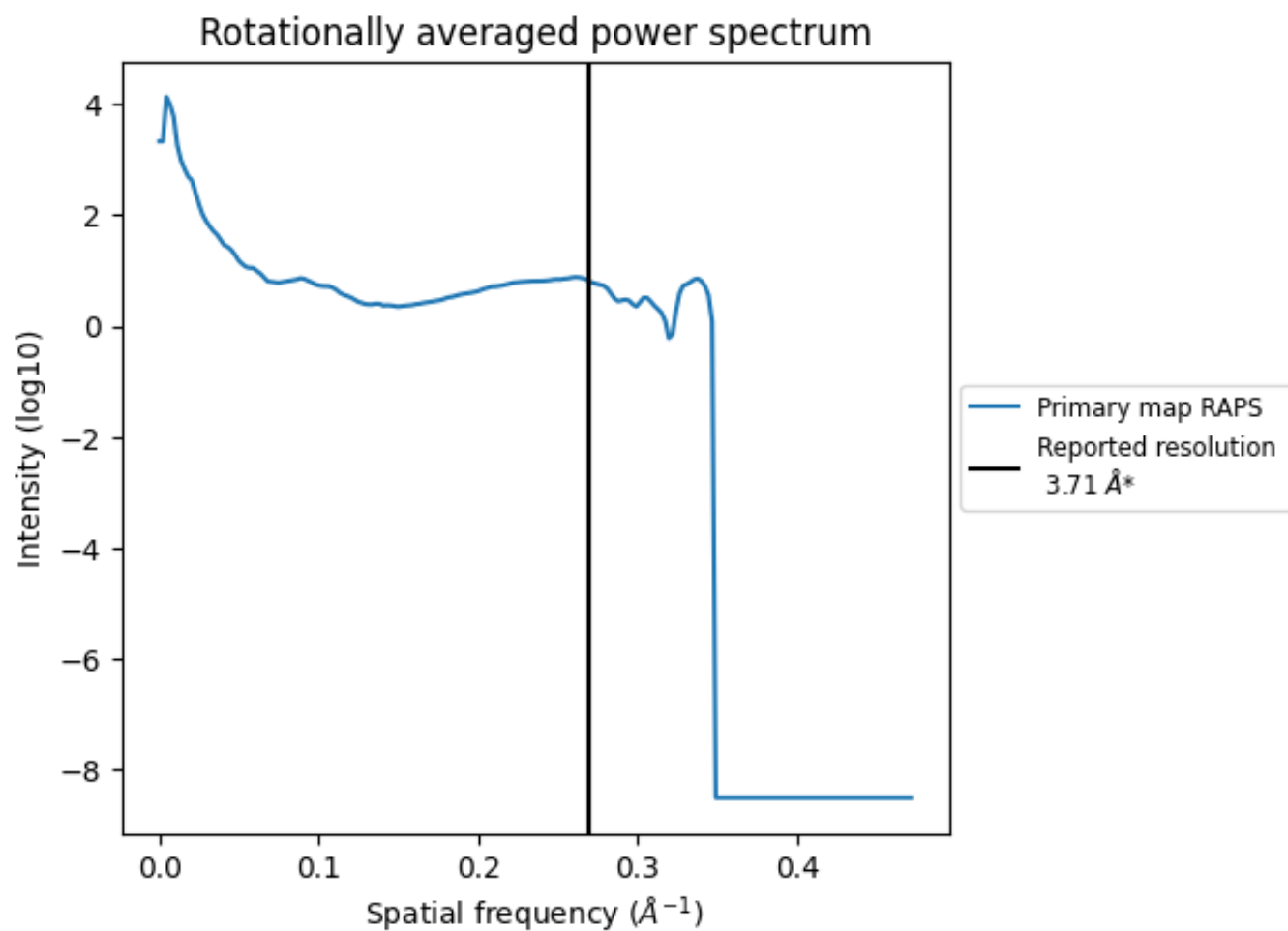
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 246 nm³; this corresponds to an approximate mass of 222 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 0.270 Å⁻¹

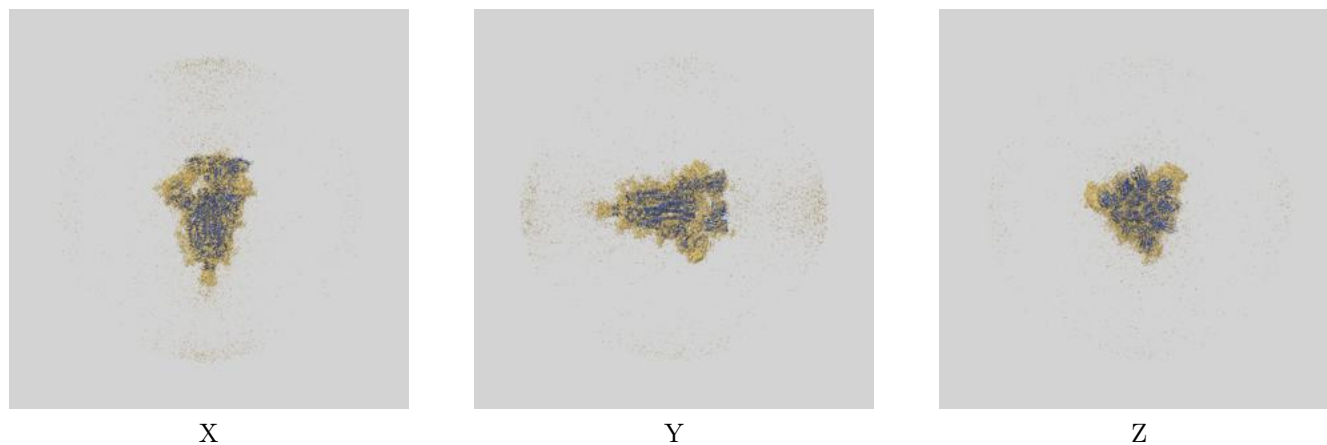
8 Fourier-Shell correlation ⓘ

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-24256 and PDB model 7N9C. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



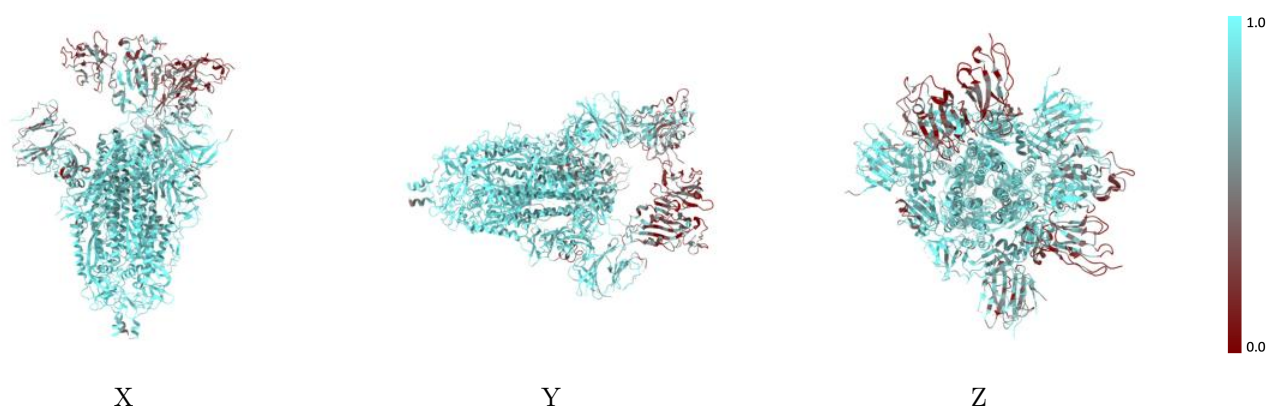
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



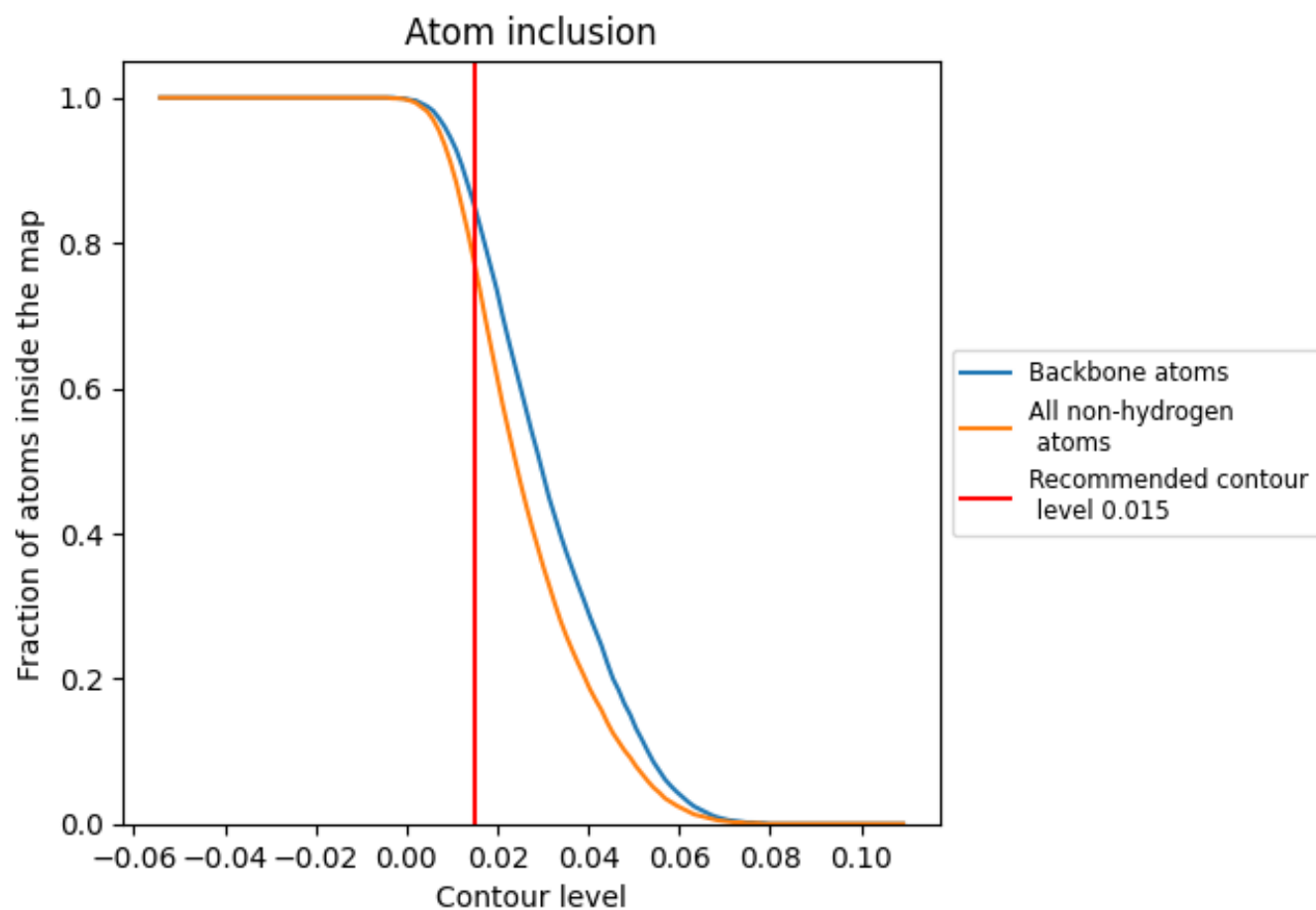
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7710	0.4290
A	0.7880	0.4340
B	0.8600	0.4700
C	0.7990	0.4380
D	0.3790	0.2510
E	0.2490	0.2430

