



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:49 PM UTC

PDB ID : 7E9N / pdb_00007e9n
EMDB ID : EMD-31033
Title : Cryo-EM structure of the SARS-CoV-2 S-6P in complex with 35B5 Fab(1 down RBD, state1)
Authors : Wang, X.F.; Zhu, Y.Q.
Deposited on : 2021-03-04
Resolution : 3.69 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
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

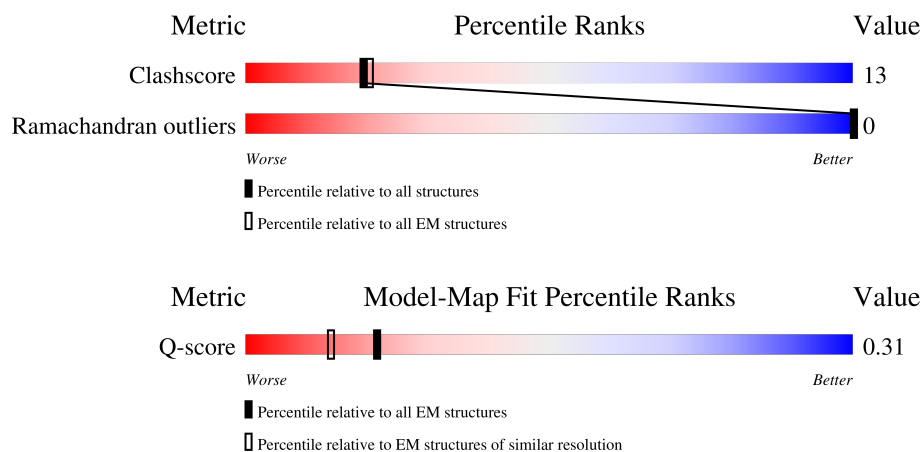
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.69 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	-
Q-score	-	25397	11284 (3.19 - 4.18)

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	1121	 67% 21% 13%
1	B	1121	 68% 22% 11%
1	C	1121	 65% 24% 11%
2	L	218	 50% 77% 23%
2	O	218	 65% 35%

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Mol	Chain	Length	Quality of chain
2	X	218	67% 33%
3	H	237	33% 73% 23% 5%
3	P	237	55% 40% 5%
3	Y	237	61% 34% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33519 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	B	1002	Total	C	N	O	S	0	0
			7805	4985	1294	1491	35		
1	A	977	Total	C	N	O	S	0	0
			7535	4817	1250	1434	34		
1	C	1002	Total	C	N	O	S	0	0
			7823	4997	1300	1491	35		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

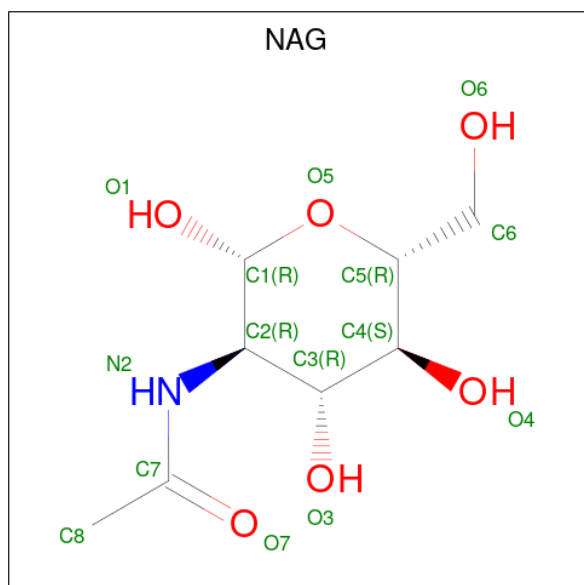
- Molecule 2 is a protein called Light chain of 35B5 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	218	Total	C	N	O	S	0	0
			1669	1048	280	335	6		
2	X	218	Total	C	N	O	S	0	0
			1655	1038	274	337	6		
2	L	218	Total	C	N	O	S	0	0
			1669	1047	279	337	6		

- Molecule 3 is a protein called Heavy chain of 35B5 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	226	Total	C	N	O	S	0	0
			1668	1048	285	327	8		
3	Y	226	Total	C	N	O	S	0	0
			1653	1038	281	327	7		
3	H	226	Total	C	N	O	S	0	0
			1664	1046	284	326	8		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

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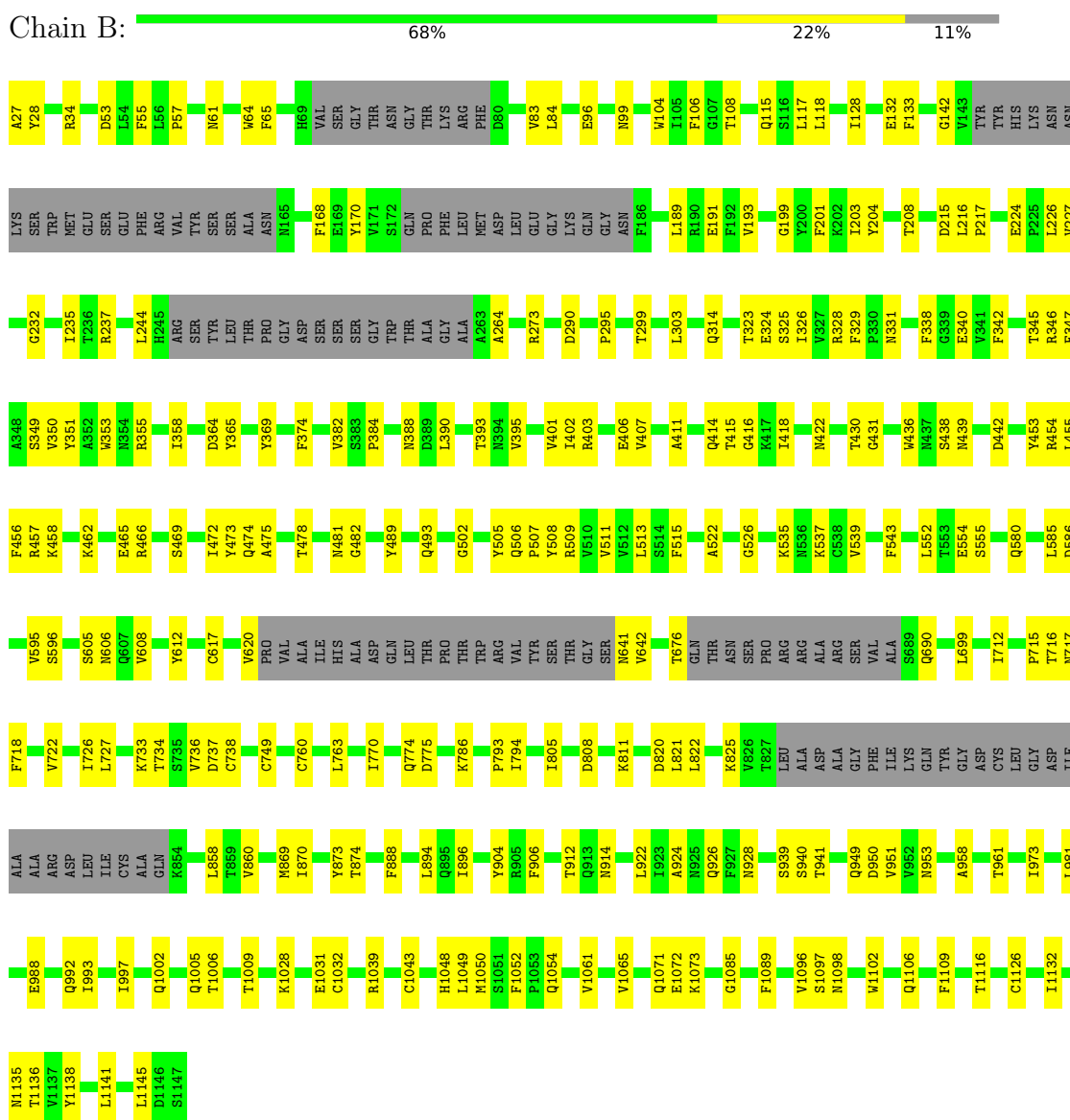
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Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots

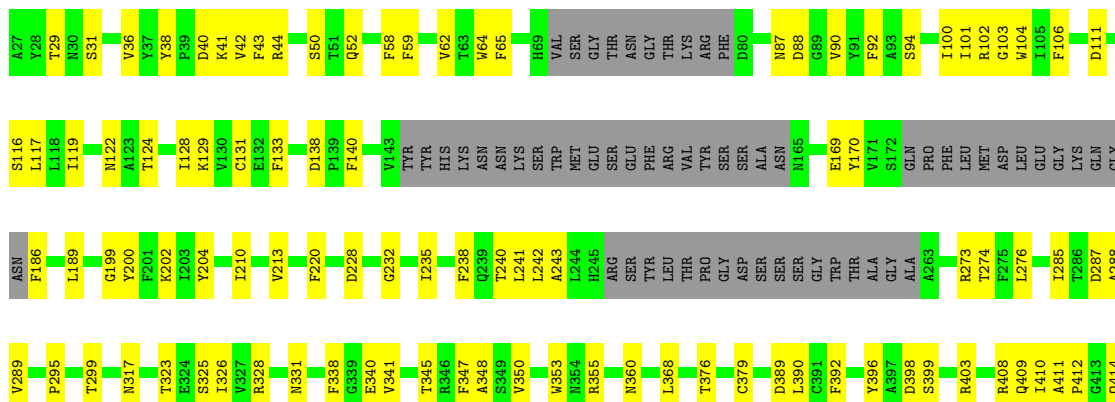
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

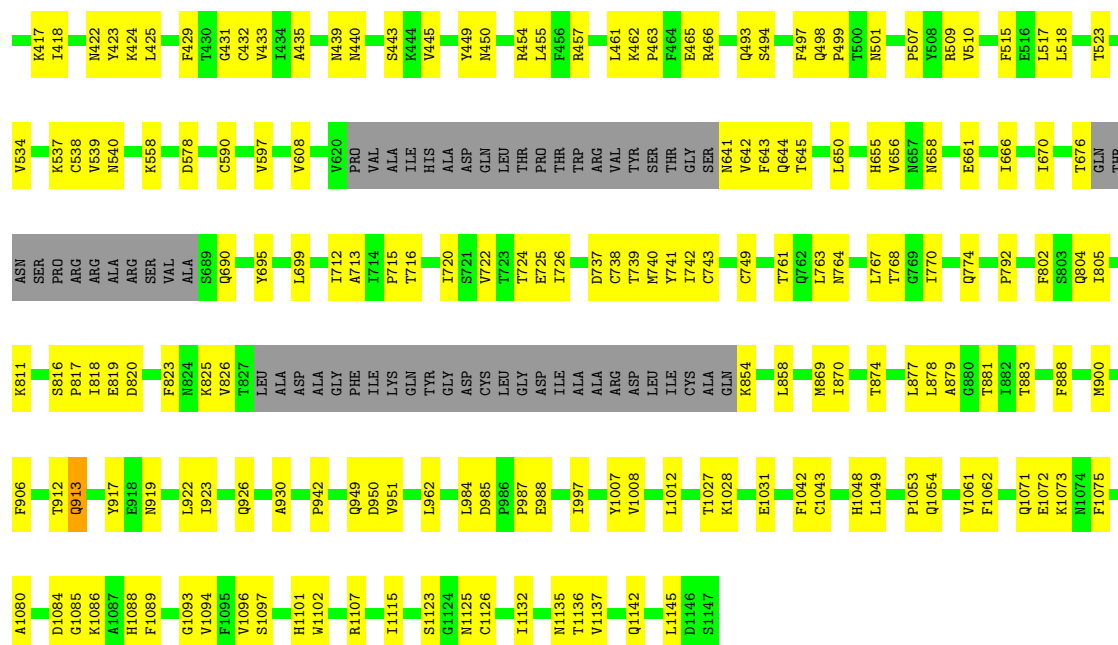
- Molecule 1: Spike glycoprotein



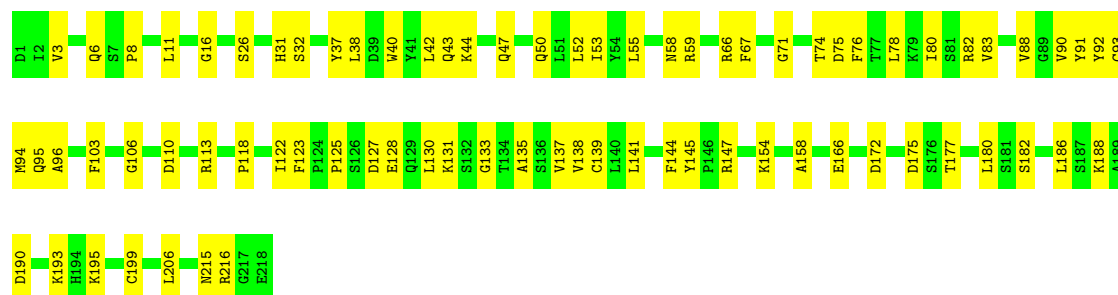
- Molecule 1: Spike glycoprotein

C1043	M902	I805	THR	V576	GLN	N360	LEU	PHE	A27
H1048	T912	K814	ASN	R577	ALA	C361	THR	ARG	Y28
	Q913		SER		GLY		THR	VAL	
V1061	N914	N914	PRO	Q580	SER	D364	GLY	TTR	R34
	N915	L822	ARG	I584	THR		ASP	SER	
H1064	N916		ALA	L585	CYS	V367	SER	SER	D53
V1065	N917	K825	ARG	L586	ASN	S371	SER	ALA	L54
	E918	T826	SER	I587	GLY		SER	ASN	F55
F1089	N919	T827	VAL	T588	VAL	F377	TRP		
		LEU	ALA		GLU		THR	N165	W64
	I923	ALA	S689	G594	GLY	T393	ALA	Y170	F65
	A930	ASP	Q630		PHE	N394	GLY	Y171	
Y1110	A930	ALA		P600		V395	ALA	S172	H89
E1111	I934	GLY	M697	T602	C488	A263	PRO	GLN	VAL
P1112		PHE	S698		Y489	A264	PHE	GLY	GLY
	L945	ILE	L699		F490	S399	LEU	LEU	THR
		LYS		V620	P491	V401	MET	ASN	THR
	L962	GLN	N703	PRO		I402	ASP	GLY	
V1129	L962	TYR	S704	VAL	T500	R403	THR	LEU	THR
K964	Q963	GLY	Y707	ALA	ASN	I410	GLY	GLY	ARG
I1132	Q965	ASP		ILE	GLY	I418		LYS	PHE
	L966	CYS	T716	HIS	V603		D287	GLN	D80
		LEU	T717	ALA		D428	GLY	GLY	
S975	S975	GLY	F718	ASP	Q506		F306	ASN	D88
V976	L977	ASP		GLN	P507		T307		
		ILE	THR	LEU	Y508	G431	V308	F186	K97
		ALA	V722	PRO	R509		E309	V193	
		ALA		THR		I434	K310		R102
L980		ARG	E725	THR	F515	A435		F201	G103
L981		ASP	I726	TRP		W436	S316		W104
		LEU		ARG	H519	N437	N317	L212	I105
L984		ILE	K733	VAL	A520			L213	F106
D985		CYS	T734	TYR	S438	P527	R328	R214	
P986		ALA	S735	SER		N439	F329	D215	Q115
		GLN	V736	THR			P330	L216	
A989		K854	GLY	GLY	L533	S443	N331	A123	
			SER	SER		LYS		T124	
I993		L858		N641	K537	VAL	N334	C219	
		T859	E748	V642		GLY			
T998				F643	F543	GLY	L223	K129	
G999		T866	L752		N544	ASN	P337	V130	
L1000				R646	V551	Y449	F338	C131	
Q1002		M869	Q755	L650		R454	G339	L229	
		L870			E554	LEU	E340	P230	F135
T1006		K871	L767	H655	S555	ARG	V341	I231	
Y1007		Q872	I770	V656	S556	PHE	F342	T235	V143
		K873		M657	K557	ARG	N343		TYR
		T874	D775	N658	K558	SER	A344		THR
L1012		L877			L560	LYS	T345	F238	HIS
T1027		T881	Q779	P665	F559	N460	R346	Q239	LYS
K1028					L560	L461	F347	T240	ASN
H1029					P661	K462	A348	L241	ASN
E1030		G889	K786	C871	F562	P463		L242	LYS
I1031		L894	Q787	A672	Q563	F464	Y351	A243	SER
			T791	V674	Q564	A465	A352	L244	THR
L1034		L895	P792	Q675	F565	R466	W353	H245	MET
				T676	D574	I472	GLU	ARG	GLU
F1042		L896	E803	C811	A576	Y472	SER	THR	CYS

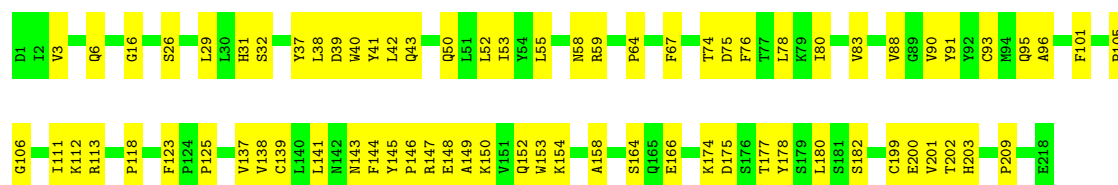




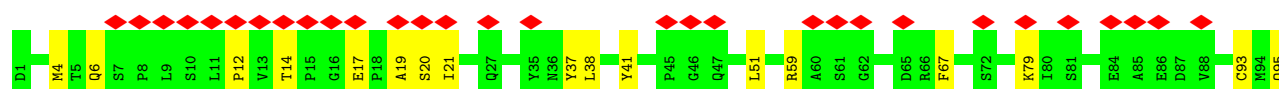
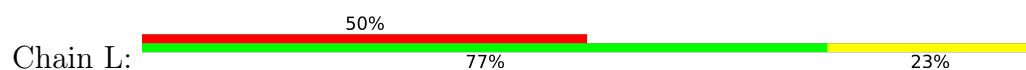
• Molecule 2: Light chain of 35B5 Fab

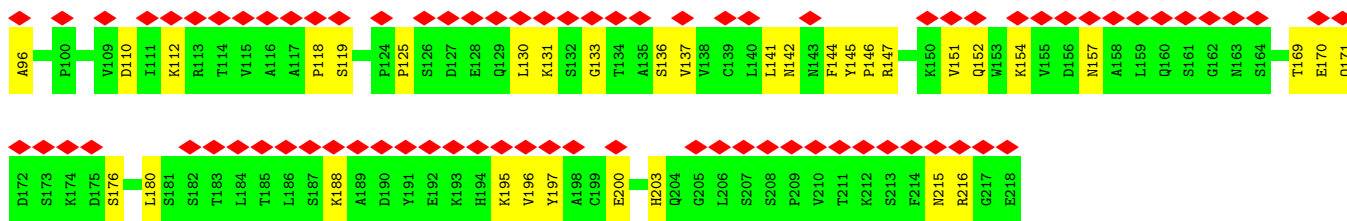


• Molecule 2: Light chain of 35B5 Fab



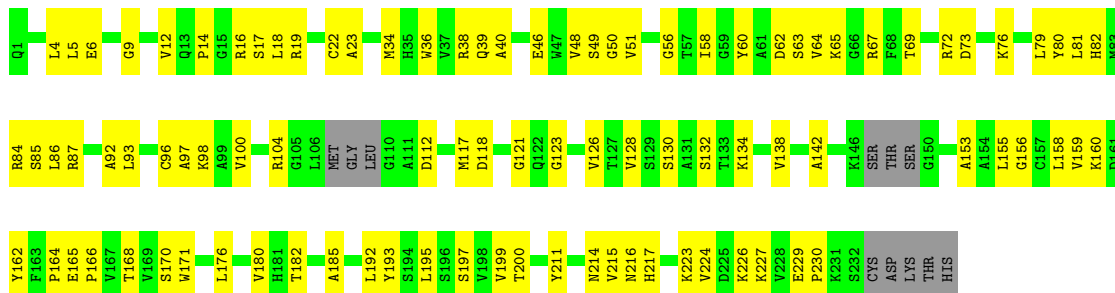
• Molecule 2: Light chain of 35B5 Fab





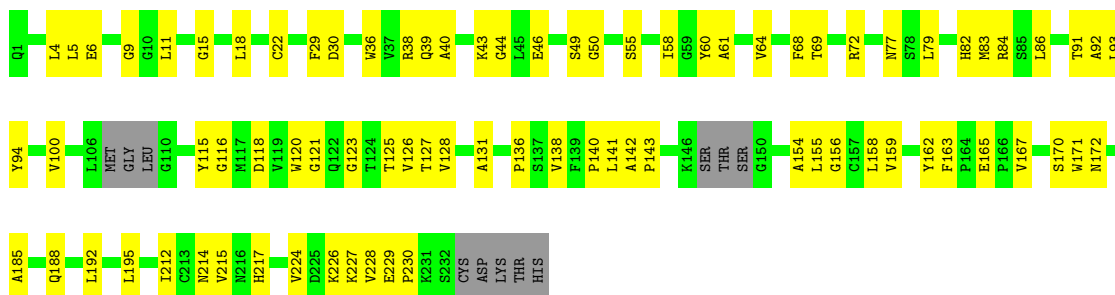
• Molecule 3: Heavy chain of 35B5 Fab

Chain P: 55% 40% 5%



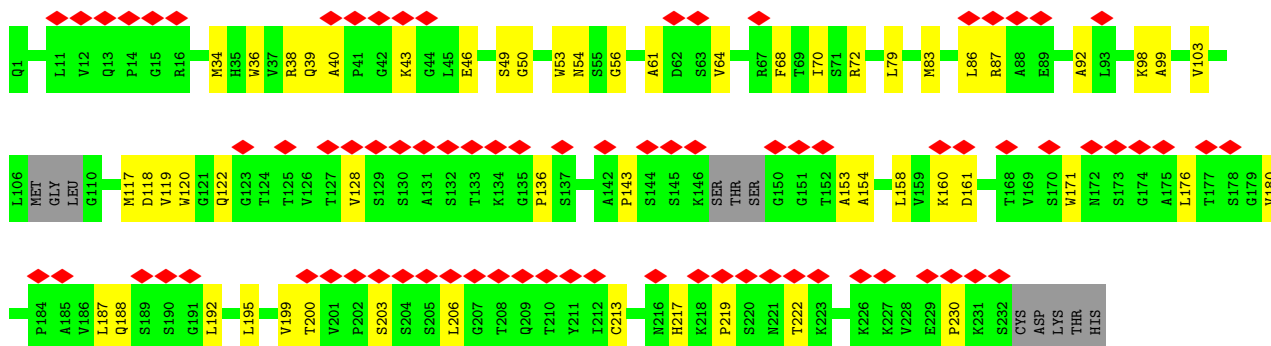
• Molecule 3: Heavy chain of 35B5 Fab

Chain Y: 61% 34% 5%



• Molecule 3: Heavy chain of 35B5 Fab

Chain H: 33% 73% 23% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	62600	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.434	Depositor
Minimum map value	-0.454	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	361.35, 361.35, 361.35	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.095, 1.095, 1.095	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.42	0/7702	0.57	1/10492 (0.0%)
1	B	0.40	0/7984	0.55	0/10874
1	C	0.39	0/8002	0.55	1/10893 (0.0%)
2	L	0.27	0/1707	0.44	0/2322
2	O	0.25	0/1707	0.48	0/2321
2	X	0.37	0/1693	0.54	0/2307
3	H	0.25	0/1702	0.44	0/2318
3	P	0.31	0/1706	0.50	0/2323
3	Y	0.22	0/1691	0.45	0/2306
All	All	0.37	0/33894	0.53	2/46156 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	913	GLN	N-CA-C	6.57	121.03	112.89
1	A	913	GLN	N-CA-C	5.31	118.92	112.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7535	0	7281	168	0
1	B	7805	0	7588	181	0
1	C	7823	0	7632	196	0
2	L	1669	0	1617	33	0
2	O	1669	0	1624	51	0
2	X	1655	0	1584	63	0
3	H	1664	0	1603	38	0
3	P	1668	0	1609	75	0
3	Y	1653	0	1573	63	0
4	A	126	0	117	3	0
4	B	126	0	117	2	0
4	C	126	0	117	2	0
All	All	33519	0	32462	828	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 13.

All (828) 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)
2:O:38:LEU:HD11	2:O:93:CYS:HB2	1.66	0.78
1:B:115:GLN:HA	1:B:132:GLU:HB3	1.65	0.76
2:O:118:PRO:HB3	2:O:144:PHE:HB3	1.67	0.75
2:O:40:TRP:HB2	2:O:53:ILE:HG22	1.70	0.73
2:X:141:LEU:HB2	2:X:180:LEU:HB3	1.70	0.73
1:A:555:SER:HB2	1:A:586:ASP:HB2	1.70	0.73
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.23	0.71
1:C:299:THR:HG21	1:C:597:VAL:HG11	1.72	0.71
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.23	0.71
1:B:676:THR:HG22	1:B:690:GLN:HG2	1.72	0.70
2:X:118:PRO:HB3	2:X:144:PHE:HB3	1.73	0.70
2:X:3:VAL:HB	2:X:26:SER:HB3	1.74	0.70
1:B:474:GLN:NE2	1:B:478:THR:O	2.25	0.69
1:B:502:GLY:H	1:B:505:TYR:HB2	1.56	0.69
2:X:123:PHE:HB2	2:X:138:VAL:HB	1.73	0.69
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.25	0.69
1:B:431:GLY:HA3	1:B:513:LEU:O	1.93	0.69
1:C:355:ARG:HD2	1:C:396:TYR:HD1	1.57	0.69
2:O:38:LEU:HA	2:O:94:MET:O	1.93	0.69
3:Y:156:GLY:HA2	3:Y:171:TRP:HH2	1.58	0.68
1:B:1028:LYS:O	1:B:1032:CYS:HB2	1.93	0.68
1:C:1135:ASN:OD1	1:C:1136:THR:N	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:34:MET:SD	3:P:79:LEU:HD22	2.34	0.68
2:X:50:GLN:HA	3:Y:120:TRP:CZ3	2.29	0.68
2:X:59:ARG:NH2	2:X:64:PRO:O	2.27	0.67
1:A:986:PRO:O	1:A:989:ALA:N	2.27	0.67
3:Y:227:LYS:NZ	3:Y:229:GLU:OE1	2.26	0.67
1:B:422:ASN:O	1:B:454:ARG:NH2	2.22	0.67
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.75	0.67
1:B:737:ASP:OD2	1:C:317:ASN:ND2	2.28	0.67
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.76	0.67
3:P:63:SER:O	3:P:67:ARG:NH2	2.28	0.67
1:B:418:ILE:HA	1:B:422:ASN:HB2	1.75	0.67
1:A:115:GLN:NE2	1:A:130:VAL:O	2.27	0.67
2:O:195:LYS:NZ	2:O:216:ARG:O	2.28	0.67
1:B:340:GLU:OE1	3:P:104:ARG:NH1	2.27	0.67
1:B:108:THR:O	1:B:237:ARG:NH2	2.28	0.66
1:A:671:CYS:SG	1:A:697:MET:HB3	2.35	0.66
2:O:172:ASP:HB3	2:O:177:THR:HB	1.76	0.66
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.28	0.66
3:P:138:VAL:HG21	3:P:215:VAL:HG11	1.77	0.66
3:P:12:VAL:HG21	3:P:18:LEU:HD11	1.78	0.66
2:O:166:GLU:HB3	2:O:180:LEU:HD21	1.78	0.66
1:B:793:PRO:HG2	1:B:794:ILE:HD12	1.77	0.66
1:C:412:PRO:HG3	1:C:429:PHE:HD2	1.60	0.65
3:Y:100:VAL:HG23	3:Y:118:ASP:HB3	1.77	0.65
1:A:328:ARG:HE	1:A:533:LEU:HD23	1.60	0.65
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.27	0.65
3:Y:15:GLY:H	3:Y:86:LEU:HB2	1.62	0.65
1:C:348:ALA:HB2	3:Y:55:SER:O	1.96	0.65
2:O:3:VAL:HB	2:O:26:SER:HB3	1.79	0.65
3:P:180:VAL:HA	3:P:199:VAL:HG22	1.79	0.65
1:C:1085:GLY:O	1:C:1126:CYS:N	2.22	0.65
2:L:38:LEU:HD11	2:L:93:CYS:HB2	1.78	0.65
2:L:133:GLY:HA2	2:L:188:LYS:HB2	1.79	0.64
2:L:171:GLN:HE21	2:L:176:SER:HB3	1.62	0.64
1:C:443:SER:HB3	1:C:499:PRO:HD3	1.79	0.64
1:B:106:PHE:HB3	1:B:235:ILE:HD11	1.79	0.64
1:B:822:LEU:HD21	1:B:1061:VAL:HG11	1.78	0.64
1:B:388:ASN:HB2	1:B:526:GLY:HA3	1.78	0.64
2:L:147:ARG:O	2:L:147:ARG:NH1	2.31	0.64
2:O:123:PHE:HB2	2:O:138:VAL:HB	1.79	0.64
3:Y:39:GLN:O	3:Y:93:LEU:N	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:142:ALA:HB1	3:Y:230:PRO:HA	1.79	0.64
1:B:351:TYR:HB3	1:B:454:ARG:HB2	1.80	0.64
2:O:133:GLY:HA2	2:O:188:LYS:HD2	1.80	0.64
1:C:676:THR:HA	1:C:690:GLN:HA	1.78	0.64
1:A:104:TRP:HB3	1:A:106:PHE:CE1	2.33	0.64
1:B:369:TYR:HE1	1:B:384:PRO:HB2	1.62	0.63
1:C:103:GLY:HA3	1:C:119:ILE:O	1.98	0.63
3:P:39:GLN:HB3	3:P:93:LEU:HB3	1.80	0.63
1:B:353:TRP:HE1	1:B:466:ARG:HA	1.62	0.63
1:C:328:ARG:NH1	1:C:578:ASP:OD1	2.32	0.63
1:C:1043:CYS:HB3	1:C:1048:HIS:CD2	2.33	0.63
2:X:145:TYR:HA	2:X:147:ARG:H	1.62	0.63
1:B:458:LYS:HD3	1:B:475:ALA:HA	1.78	0.63
3:P:69:THR:HG23	3:P:84:ARG:HH12	1.62	0.63
1:A:317:ASN:HA	1:A:594:GLY:HA2	1.80	0.63
1:A:393:THR:HG21	1:A:519:HIS:H	1.64	0.63
1:B:482:GLY:HA3	3:P:17:SER:H	1.64	0.63
1:C:1126:CYS:HB2	1:C:1132:ILE:HD13	1.81	0.62
1:A:64:TRP:HD1	1:A:65:PHE:N	1.96	0.62
3:P:39:GLN:H	3:P:92:ALA:HB1	1.64	0.62
2:X:40:TRP:HB2	2:X:53:ILE:HG22	1.80	0.62
1:A:562:PHE:HD2	1:C:41:LYS:HZ2	1.45	0.62
1:A:557:LYS:NZ	1:A:574:ASP:O	2.32	0.62
1:A:403:ARG:HA	1:A:507:PRO:HA	1.80	0.62
1:A:977:LEU:HA	1:A:980:ILE:HD13	1.81	0.62
3:P:38:ARG:HB2	3:P:48:VAL:HB	1.82	0.62
2:X:145:TYR:CG	2:X:146:PRO:HA	2.35	0.62
1:B:555:SER:OG	1:B:586:ASP:N	2.33	0.61
3:P:168:THR:OG1	3:P:216:ASN:HB2	2.00	0.61
1:B:808:ASP:HB2	1:B:811:LYS:HG2	1.82	0.61
1:B:726:ILE:HG12	1:B:1061:VAL:HG23	1.81	0.61
1:A:170:TYR:HE2	1:A:172:SER:HB3	1.65	0.61
3:P:62:ASP:HA	3:P:65:LYS:HE3	1.82	0.61
2:O:91:TYR:O	2:O:106:GLY:HA2	2.00	0.61
2:O:128:GLU:HA	2:O:131:LYS:HG3	1.82	0.61
1:A:562:PHE:HZ	1:C:38:TYR:HD2	1.48	0.61
1:A:707:TYR:HD2	1:C:792:PRO:HG3	1.65	0.61
3:H:98:LYS:NZ	3:H:99:ALA:O	2.34	0.61
1:A:431:GLY:HA2	1:A:515:PHE:HD1	1.66	0.61
2:L:136:SER:OG	3:H:160:LYS:NZ	2.33	0.60
1:B:118:LEU:HD22	1:B:133:PHE:HZ	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:12:VAL:HG11	3:P:18:LEU:HD21	1.83	0.60
1:A:402:ILE:HD11	1:A:418:ILE:HG13	1.82	0.60
1:A:277:LEU:HD23	1:A:285:ILE:HD13	1.83	0.60
3:Y:83:MET:HE2	3:Y:86:LEU:HD21	1.83	0.60
2:L:6:GLN:NE2	2:L:93:CYS:SG	2.74	0.60
1:A:646:ARG:O	1:A:646:ARG:NH1	2.35	0.60
1:A:703:ASN:OD1	1:A:704:SER:N	2.33	0.60
1:A:228:ASP:OD1	1:A:229:LEU:N	2.35	0.60
1:C:379:CYS:HA	1:C:432:CYS:HA	1.83	0.60
1:B:716:THR:HG21	1:B:1073:LYS:HE3	1.84	0.60
3:P:165:GLU:N	3:P:166:PRO:HD2	2.17	0.60
2:X:153:TRP:NE1	2:X:182:SER:OG	2.35	0.60
1:C:1089:PHE:CE1	1:C:1123:SER:HB3	2.37	0.59
1:C:950:ASP:OD1	1:C:951:VAL:N	2.35	0.59
1:A:825:LYS:HD2	1:A:945:LEU:HD23	1.83	0.59
3:Y:18:LEU:HB2	3:Y:83:MET:HB2	1.84	0.59
1:A:1106:GLN:NE2	1:A:1111:GLU:OE1	2.36	0.59
3:P:134:LYS:HE2	3:P:192:LEU:HD21	1.83	0.59
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.85	0.59
1:B:64:TRP:HD1	1:B:65:PHE:N	2.01	0.59
3:P:5:LEU:O	3:P:22:CYS:HA	2.03	0.59
2:L:118:PRO:HB3	2:L:144:PHE:HB3	1.85	0.59
1:B:346:ARG:HA	1:B:509:ARG:NH2	2.18	0.59
1:C:323:THR:HG21	1:C:537:LYS:HD2	1.85	0.58
3:P:142:ALA:HB1	3:P:230:PRO:HA	1.85	0.58
1:C:722:VAL:HG12	1:C:930:ALA:HB1	1.85	0.58
2:X:29:LEU:HD11	2:X:95:GLN:HB2	1.84	0.58
2:X:37:TYR:HA	2:X:55:LEU:HD22	1.84	0.58
3:Y:138:VAL:HG11	3:Y:215:VAL:HG21	1.85	0.58
3:Y:156:GLY:HA2	3:Y:171:TRP:CH2	2.38	0.58
1:B:353:TRP:O	1:B:466:ARG:NH1	2.36	0.58
1:A:34:ARG:HD2	1:A:216:LEU:HD13	1.84	0.58
1:C:345:THR:O	1:C:509:ARG:NH1	2.29	0.58
1:A:439:ASN:ND2	1:A:506:GLN:OE1	2.36	0.58
1:A:912:THR:O	1:A:915:VAL:HG12	2.01	0.58
1:B:439:ASN:HB2	1:B:506:GLN:HG2	1.85	0.58
3:P:104:ARG:HA	3:P:104:ARG:NE	2.19	0.58
2:X:42:LEU:HB2	2:X:52:LEU:HD11	1.85	0.58
3:Y:30:ASP:HA	3:Y:72:ARG:HH22	1.67	0.58
3:H:83:MET:SD	3:H:86:LEU:HD21	2.44	0.58
3:Y:9:GLY:HA2	3:Y:126:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:143:PRO:HB3	3:Y:155:LEU:HB3	1.86	0.58
3:H:217:HIS:CD2	3:H:219:PRO:HD2	2.39	0.58
1:C:40:ASP:OD2	1:C:44:ARG:NH1	2.37	0.58
1:B:418:ILE:HD13	1:B:422:ASN:ND2	2.19	0.57
1:C:742:ILE:HD11	1:C:997:ILE:HG23	1.85	0.57
1:C:1093:GLY:H	1:C:1107:ARG:HH12	1.51	0.57
1:A:722:VAL:HG22	1:A:930:ALA:HB1	1.86	0.57
3:P:97:ALA:HB3	3:P:117:MET:HE3	1.85	0.57
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.86	0.57
1:B:1098:ASN:HD22	4:B:1308:NAG:H61	1.69	0.57
1:C:138:ASP:HB3	1:C:140:PHE:CE1	2.39	0.57
1:A:770:ILE:HD11	1:A:1012:LEU:HD12	1.85	0.57
2:X:144:PHE:CE2	2:X:180:LEU:HB2	2.39	0.57
1:B:382:VAL:HG21	1:B:390:LEU:HD21	1.85	0.57
1:A:656:VAL:HG12	1:A:658:ASN:H	1.69	0.57
1:C:392:PHE:HD2	1:C:515:PHE:HB3	1.70	0.57
3:P:100:VAL:HG23	3:P:118:ASP:HB3	1.85	0.57
2:X:91:TYR:O	2:X:106:GLY:HA2	2.04	0.57
1:B:1116:THR:HG22	1:B:1138:TYR:HB3	1.87	0.57
1:C:411:ALA:HB3	1:C:414:GLN:HB2	1.86	0.57
3:Y:50:GLY:HA3	3:Y:58:ILE:HD12	1.87	0.57
1:A:736:VAL:HG22	1:A:858:LEU:HD23	1.86	0.57
3:P:227:LYS:NZ	3:P:229:GLU:OE1	2.33	0.57
2:X:143:ASN:HA	2:X:177:THR:HB	1.87	0.56
3:H:161:ASP:HA	3:H:192:LEU:HB3	1.87	0.56
3:Y:39:GLN:H	3:Y:92:ALA:HB1	1.71	0.56
3:H:68:PHE:CE1	3:H:83:MET:HG3	2.40	0.56
1:B:924:ALA:O	1:B:928:ASN:ND2	2.39	0.56
1:C:1043:CYS:HB3	1:C:1048:HIS:HD2	1.70	0.56
1:A:733:LYS:NZ	1:A:775:ASP:OD2	2.37	0.56
1:B:894:LEU:HD21	1:C:715:PRO:HD3	1.87	0.56
1:C:295:PRO:HB2	1:C:608:VAL:HG21	1.88	0.56
3:P:17:SER:HB2	3:P:82:HIS:NE2	2.20	0.56
3:H:203:SER:HA	3:H:206:LEU:HG	1.88	0.56
1:B:617:CYS:HA	1:B:620:VAL:HG23	1.86	0.56
2:X:39:ASP:OD1	2:X:55:LEU:HD23	2.05	0.56
1:B:466:ARG:HH21	3:P:72:ARG:H	1.54	0.56
1:A:115:GLN:HE22	1:A:131:CYS:HA	1.72	0.55
2:O:53:ILE:HD11	2:O:59:ARG:NE	2.20	0.55
2:O:190:ASP:HA	2:O:193:LYS:HG2	1.88	0.55
3:P:138:VAL:HG22	3:P:159:VAL:HG22	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:PHE:HB2	1:B:401:VAL:HG23	1.88	0.55
2:O:141:LEU:HB2	2:O:180:LEU:HB3	1.87	0.55
3:P:6:GLU:HG3	3:P:22:CYS:SG	2.46	0.55
1:A:889:GLY:HA3	1:A:1034:LEU:HD12	1.89	0.55
1:C:742:ILE:HD11	1:C:997:ILE:HA	1.88	0.55
1:B:473:TYR:HD2	1:B:489:TYR:HB2	1.71	0.55
1:A:676:THR:HG22	1:A:690:GLN:HG2	1.88	0.55
1:C:299:THR:CG2	1:C:597:VAL:HG11	2.37	0.55
3:Y:40:ALA:HA	3:Y:92:ALA:HA	1.89	0.55
3:P:9:GLY:HA2	3:P:126:VAL:HG22	1.87	0.55
3:H:176:LEU:HD21	3:H:199:VAL:HG11	1.88	0.55
1:C:716:THR:HG22	1:C:1071:GLN:O	2.07	0.55
1:B:329:PHE:O	1:B:580:GLN:NE2	2.37	0.55
1:A:1043:CYS:HB3	1:A:1048:HIS:CD2	2.41	0.55
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.40	0.55
1:C:64:TRP:HD1	1:C:65:PHE:N	2.05	0.55
1:B:716:THR:N	1:B:1071:GLN:O	2.29	0.55
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.89	0.55
1:A:802:PHE:HD2	1:A:805:ILE:HD11	1.72	0.55
1:A:980:ILE:HG23	1:A:984:LEU:HD12	1.89	0.55
2:X:67:PHE:HB3	2:X:78:LEU:HD11	1.89	0.55
1:A:229:LEU:HD23	1:A:231:ILE:HD11	1.89	0.54
1:A:328:ARG:NE	1:A:533:LEU:HD23	2.21	0.54
2:O:113:ARG:H	2:O:145:TYR:HE2	1.54	0.54
3:H:153:ALA:HB3	3:H:206:LEU:HD11	1.88	0.54
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.41	0.54
1:B:993:ILE:O	1:B:997:ILE:HG12	2.07	0.54
1:C:1084:ASP:HB2	1:C:1086:LYS:NZ	2.23	0.54
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.89	0.54
1:B:712:ILE:HD13	1:A:896:ILE:HD12	1.88	0.54
1:C:422:ASN:HD21	1:C:454:ARG:HD2	1.72	0.54
3:Y:38:ARG:N	3:Y:46:GLU:O	2.41	0.54
1:C:410:ILE:HG12	1:C:433:VAL:HG11	1.89	0.54
1:C:418:ILE:HA	1:C:422:ASN:HD22	1.73	0.54
2:O:38:LEU:HD13	2:O:95:GLN:NE2	2.22	0.54
3:Y:138:VAL:HA	3:Y:158:LEU:O	2.08	0.54
1:B:734:THR:HG22	1:B:860:VAL:HG12	1.89	0.54
1:A:348:ALA:O	1:A:401:VAL:N	2.40	0.54
1:A:487:ASN:N	1:A:489:TYR:HH	2.06	0.54
1:C:92:PHE:HE2	1:C:94:SER:HB2	1.73	0.54
2:O:71:GLY:HA3	2:O:76:PHE:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ILE:HD11	1:A:418:ILE:HG22	1.90	0.53
1:A:1089:PHE:HE1	1:C:917:TYR:HD1	1.56	0.53
1:A:1105:THR:HG22	1:A:1112:PRO:HA	1.89	0.53
2:L:141:LEU:HD12	2:L:180:LEU:HD22	1.88	0.53
2:X:74:THR:OG1	2:X:75:ASP:OD2	2.24	0.53
2:X:139:CYS:HB3	2:X:182:SER:HB3	1.89	0.53
1:A:353:TRP:HA	1:A:399:SER:O	2.08	0.53
1:C:879:ALA:O	1:C:883:THR:HG22	2.08	0.53
2:O:6:GLN:HE22	2:O:92:TYR:HA	1.73	0.53
2:O:195:LYS:HE3	2:O:215:ASN:HB3	1.90	0.53
1:A:316:SER:OG	1:A:317:ASN:N	2.38	0.53
1:A:337:PRO:HB2	1:A:340:GLU:HB2	1.89	0.53
1:C:87:ASN:OD1	1:C:88:ASP:N	2.41	0.53
3:P:6:GLU:HG2	3:P:123:GLY:HA2	1.90	0.53
1:C:104:TRP:HB3	1:C:106:PHE:CE1	2.42	0.53
1:B:462:LYS:N	1:B:465:GLU:OE1	2.38	0.53
1:B:749:CYS:SG	1:B:997:ILE:HD11	2.49	0.53
1:A:722:VAL:HG12	1:A:1065:VAL:HG22	1.90	0.53
1:C:338:PHE:O	1:C:341:VAL:HG12	2.09	0.53
1:C:737:ASP:HB3	1:C:740:MET:HB2	1.90	0.53
2:X:144:PHE:CE1	2:X:147:ARG:HA	2.44	0.53
1:C:106:PHE:CD1	1:C:238:PHE:HB2	2.44	0.53
2:L:19:ALA:O	2:L:79:LYS:HA	2.08	0.53
1:B:106:PHE:HB3	1:B:235:ILE:CD1	2.38	0.53
1:A:346:ARG:HE	3:H:56:GLY:HA3	1.74	0.53
2:O:74:THR:OG1	2:O:75:ASP:OD2	2.25	0.53
1:B:395:VAL:HG23	1:B:515:PHE:HD1	1.74	0.52
1:A:102:ARG:HE	1:A:243:ALA:HB2	1.74	0.52
1:C:725:GLU:HG2	1:C:1062:PHE:HB2	1.92	0.52
1:C:1027:THR:O	1:C:1031:GLU:HG3	2.09	0.52
2:X:153:TRP:CD1	2:X:164:SER:HB2	2.45	0.52
3:H:118:ASP:OD1	3:H:119:VAL:N	2.42	0.52
1:C:186:PHE:HB3	1:C:213:VAL:HA	1.90	0.52
2:O:42:LEU:O	2:O:50:GLN:N	2.31	0.52
1:A:339:GLY:O	1:A:343:ASN:HB2	2.09	0.52
1:A:334:ASN:ND2	1:A:360:ASN:O	2.40	0.52
3:P:73:ASP:HB2	3:P:80:TYR:HE1	1.73	0.52
3:Y:131:ALA:HB3	3:Y:163:PHE:CE1	2.44	0.52
1:B:106:PHE:CD1	1:B:235:ILE:HD11	2.44	0.52
1:B:595:VAL:HG12	1:B:612:TYR:CD2	2.44	0.52
1:B:736:VAL:HG22	1:B:858:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:PHE:HD1	1:A:342:PHE:HE2	1.56	0.52
1:C:38:TYR:CE1	1:C:285:ILE:HG12	2.45	0.52
1:C:410:ILE:HD12	1:C:425:LEU:HD11	1.92	0.52
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.75	0.52
3:H:180:VAL:HA	3:H:199:VAL:HG22	1.92	0.52
1:B:1102:TRP:CD1	1:B:1135:ASN:HD22	2.28	0.52
1:B:1089:PHE:HE1	1:A:917:TYR:HD1	1.57	0.52
1:C:725:GLU:OE2	1:C:1028:LYS:HE2	2.10	0.52
3:Y:4:LEU:HB2	3:Y:121:GLY:HA3	1.92	0.52
1:C:537:LYS:O	1:C:539:VAL:HG13	2.10	0.52
1:C:656:VAL:HG12	1:C:658:ASN:H	1.75	0.52
2:X:6:GLN:HG3	2:X:105:PRO:HD2	1.92	0.52
2:X:37:TYR:HB3	2:X:96:ALA:HB3	1.91	0.52
2:X:152:GLN:HB2	2:X:200:GLU:HB3	1.91	0.52
2:L:4:MET:HE3	2:L:95:GLN:HB3	1.90	0.52
2:L:145:TYR:O	2:L:203:HIS:NE2	2.37	0.52
3:P:156:GLY:HA2	3:P:171:TRP:HH2	1.75	0.51
3:Y:188:GLN:HB2	3:Y:192:LEU:HB2	1.92	0.51
2:L:119:SER:HB2	2:L:142:ASN:OD1	2.09	0.51
1:B:193:VAL:HG22	1:B:204:TYR:HB2	1.92	0.51
1:C:100:ILE:HG22	1:C:242:LEU:HG	1.92	0.51
1:C:985:ASP:OD2	1:C:987:PRO:HD2	2.10	0.51
3:P:164:PRO:HD2	3:P:217:HIS:HE1	1.74	0.51
1:B:346:ARG:HA	1:B:509:ARG:CZ	2.38	0.51
1:A:962:LEU:HD11	1:A:1007:TYR:CD2	2.45	0.51
2:L:154:LYS:HE2	2:L:157:ASN:HA	1.91	0.51
1:A:97:LYS:HB3	1:A:186:PHE:HA	1.91	0.51
1:A:462:LYS:NZ	1:A:464:PHE:O	2.35	0.51
1:B:369:TYR:OH	1:B:384:PRO:O	2.26	0.51
1:B:455:LEU:HD22	1:B:493:GLN:HB2	1.91	0.51
1:A:282:ASN:OD1	4:A:1301:NAG:N2	2.44	0.51
1:B:353:TRP:NE1	1:B:465:GLU:O	2.44	0.51
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.75	0.51
1:A:64:TRP:CD1	1:A:65:PHE:N	2.78	0.51
1:A:643:PHE:HB3	1:A:650:LEU:HG	1.92	0.51
1:C:200:TYR:HB3	1:C:228:ASP:OD1	2.10	0.51
1:C:331:ASN:OD1	4:C:1302:NAG:N2	2.43	0.51
3:Y:69:THR:HG23	3:Y:84:ARG:HH12	1.75	0.51
1:B:403:ARG:HB2	1:B:406:GLU:HG2	1.92	0.51
1:A:329:PHE:CE2	1:A:544:ASN:HA	2.46	0.51
1:A:786:LYS:HG3	1:A:787:GLN:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:LEU:O	1:A:881:THR:HG23	2.11	0.51
3:Y:30:ASP:OD1	3:Y:72:ARG:NH2	2.44	0.51
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.76	0.50
1:A:393:THR:HB	1:A:520:ALA:HB3	1.93	0.50
1:C:661:GLU:O	1:C:695:TYR:OH	2.25	0.50
3:Y:138:VAL:HG22	3:Y:159:VAL:HG22	1.93	0.50
2:L:37:TYR:HB3	2:L:96:ALA:HB3	1.92	0.50
2:X:40:TRP:CE2	2:X:78:LEU:HB2	2.47	0.50
2:X:166:GLU:HB2	2:X:180:LEU:HD21	1.93	0.50
1:B:472:ILE:HD11	3:P:84:ARG:HG2	1.94	0.50
1:A:329:PHE:O	1:A:580:GLN:NE2	2.44	0.50
1:B:457:ARG:NH2	1:B:469:SER:OG	2.40	0.50
1:B:458:LYS:HG3	1:B:473:TYR:HE1	1.76	0.50
3:Y:185:ALA:HB2	3:Y:195:LEU:HB3	1.93	0.50
1:A:27:ALA:C	1:A:28:TYR:HD2	2.20	0.50
1:A:351:TYR:O	1:A:466:ARG:NH2	2.45	0.50
1:A:775:ASP:O	1:A:779:GLN:HG2	2.12	0.50
1:A:998:THR:O	1:A:1002:GLN:HG2	2.12	0.50
2:X:41:TYR:OH	3:Y:116:GLY:HA2	2.12	0.50
1:A:986:PRO:HA	1:A:989:ALA:HB3	1.93	0.50
1:C:1115:ILE:HG22	1:C:1137:VAL:HG13	1.93	0.50
1:A:53:ASP:HB3	1:A:55:PHE:HE2	1.77	0.49
2:O:37:TYR:HB3	2:O:96:ALA:HB3	1.93	0.49
2:X:40:TRP:CD2	2:X:78:LEU:HB2	2.47	0.49
1:B:438:SER:OG	1:B:507:PRO:O	2.28	0.49
1:B:770:ILE:O	1:B:774:GLN:HG2	2.13	0.49
3:P:85:SER:O	3:P:87:ARG:NH1	2.44	0.49
1:B:314:GLN:HA	1:B:596:SER:HA	1.94	0.49
1:A:1002:GLN:O	1:A:1006:THR:HG23	2.11	0.49
3:P:185:ALA:HB2	3:P:195:LEU:HB3	1.95	0.49
1:B:1043:CYS:HB3	1:B:1048:HIS:HD1	1.78	0.49
1:C:643:PHE:HD2	1:C:650:LEU:HD21	1.77	0.49
2:X:146:PRO:HD2	2:X:203:HIS:NE2	2.27	0.49
1:B:328:ARG:HG3	1:B:543:PHE:CE2	2.46	0.49
1:A:912:THR:HG23	1:A:1106:GLN:OE1	2.12	0.49
1:C:129:LYS:HE2	1:C:169:GLU:HB2	1.94	0.49
1:C:742:ILE:HG23	1:C:743:CYS:N	2.27	0.49
1:C:922:LEU:O	1:C:926:GLN:HG3	2.12	0.49
3:Y:83:MET:HB3	3:Y:86:LEU:HD21	1.94	0.49
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.94	0.49
3:P:132:SER:HB2	3:P:134:LYS:NZ	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:133:GLY:HA2	2:L:188:LYS:HE3	1.92	0.49
3:H:203:SER:O	3:H:206:LEU:HB2	2.13	0.49
1:B:83:VAL:HG11	1:B:237:ARG:HH11	1.76	0.49
1:B:712:ILE:HG21	1:B:1096:VAL:HG12	1.94	0.49
1:C:189:LEU:HB2	1:C:210:ILE:HD13	1.95	0.49
1:C:287:ASP:OD1	1:C:288:ALA:N	2.44	0.49
3:P:138:VAL:HA	3:P:158:LEU:O	2.13	0.49
1:B:117:LEU:HD23	1:B:118:LEU:N	2.27	0.49
1:A:377:PHE:CD1	1:A:434:ILE:HG12	2.48	0.49
1:C:350:VAL:HG21	1:C:418:ILE:HG23	1.95	0.49
2:O:53:ILE:HD11	2:O:59:ARG:HE	1.78	0.49
3:P:50:GLY:HA3	3:P:58:ILE:HD12	1.94	0.49
3:H:61:ALA:HB3	3:H:64:VAL:HG12	1.94	0.49
1:B:1141:LEU:HD22	1:B:1145:LEU:HD23	1.94	0.49
1:A:985:ASP:OD1	1:A:986:PRO:HD2	2.13	0.49
1:C:713:ALA:HA	1:C:1073:LYS:O	2.13	0.49
1:B:27:ALA:HB3	1:B:64:TRP:HB3	1.95	0.49
1:A:551:VAL:HG13	1:A:588:THR:HB	1.94	0.49
2:O:118:PRO:HD2	2:O:206:LEU:HG	1.95	0.48
2:O:122:ILE:HD12	2:O:199:CYS:HB3	1.95	0.48
3:P:97:ALA:HB3	3:P:117:MET:CE	2.43	0.48
3:Y:29:PHE:CD2	3:Y:77:ASN:HA	2.48	0.48
1:B:96:GLU:OE2	1:B:99:ASN:N	2.46	0.48
1:B:481:ASN:O	3:P:16:ARG:HD3	2.14	0.48
1:B:896:ILE:HD12	1:C:712:ILE:HG12	1.95	0.48
1:A:170:TYR:CE2	1:A:172:SER:HB3	2.46	0.48
1:C:338:PHE:HE2	1:C:368:LEU:HD11	1.78	0.48
1:C:725:GLU:CG	1:C:1062:PHE:HB2	2.44	0.48
1:C:854:LYS:HA	1:C:858:LEU:HD11	1.94	0.48
1:C:1102:TRP:HB2	1:C:1135:ASN:ND2	2.28	0.48
1:B:201:PHE:HE2	1:B:203:ILE:HD11	1.78	0.48
1:B:552:LEU:HD13	1:B:585:LEU:HD13	1.94	0.48
1:A:436:TRP:HE1	1:A:509:ARG:HD2	1.78	0.48
1:A:438:SER:HB2	1:A:509:ARG:HG3	1.95	0.48
1:A:870:ILE:O	1:A:874:THR:HG23	2.13	0.48
1:C:106:PHE:CD2	1:C:117:LEU:HD22	2.49	0.48
1:B:350:VAL:HG11	1:B:422:ASN:HB3	1.95	0.48
1:C:455:LEU:HD22	1:C:493:GLN:HB2	1.95	0.48
2:O:113:ARG:NH2	2:O:175:ASP:HA	2.28	0.48
1:B:502:GLY:N	1:B:505:TYR:HB2	2.27	0.48
1:B:949:GLN:HG3	1:B:953:ASN:HD21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:HE3	1:A:131:CYS:HB2	1.94	0.48
1:A:364:ASP:HA	1:A:527:PRO:HD3	1.95	0.48
1:C:804:GLN:O	1:C:818:ILE:HG13	2.14	0.48
2:X:6:GLN:NE2	2:X:93:CYS:SG	2.86	0.48
2:X:67:PHE:CE1	2:X:80:ILE:HG12	2.48	0.48
1:B:1005:GLN:O	1:B:1009:THR:HG23	2.14	0.48
1:A:34:ARG:NH1	1:A:219:GLY:O	2.47	0.48
1:C:64:TRP:CD1	1:C:65:PHE:N	2.82	0.48
1:C:726:ILE:HG23	1:C:1061:VAL:HG12	1.96	0.48
1:C:988:GLU:OE1	1:C:988:GLU:N	2.47	0.48
2:X:38:LEU:HD13	2:X:76:PHE:HB2	1.95	0.48
3:Y:224:VAL:HG12	3:Y:226:LYS:HG3	1.96	0.48
2:L:59:ARG:NH1	2:L:67:PHE:O	2.45	0.48
3:H:203:SER:HA	3:H:206:LEU:CG	2.44	0.48
1:B:65:PHE:CZ	1:B:84:LEU:HD11	2.49	0.48
1:B:338:PHE:HB3	1:B:342:PHE:HE2	1.77	0.48
1:B:738:CYS:HB3	1:B:760:CYS:HB2	1.73	0.48
2:X:52:LEU:HD22	2:X:67:PHE:CE2	2.48	0.48
3:Y:143:PRO:HD3	3:Y:228:VAL:HG12	1.96	0.48
1:A:989:ALA:O	1:A:993:ILE:HG12	2.14	0.48
1:C:1097:SER:OG	1:C:1101:HIS:O	2.27	0.48
1:A:554:GLU:CD	1:A:554:GLU:H	2.20	0.48
1:C:38:TYR:HE1	1:C:285:ILE:HG12	1.78	0.48
3:H:203:SER:HA	3:H:206:LEU:HD12	1.95	0.48
1:B:727:LEU:HD11	1:B:1028:LYS:HD2	1.96	0.48
1:B:950:ASP:OD1	1:B:951:VAL:N	2.46	0.48
1:C:819:GLU:O	1:C:823:PHE:HD2	1.96	0.48
1:A:358:ILE:HB	1:A:395:VAL:HG13	1.96	0.47
1:A:1089:PHE:CE1	1:C:917:TYR:HD1	2.30	0.47
1:C:31:SER:HB3	1:C:62:VAL:HG13	1.96	0.47
1:C:1075:PHE:HB3	1:C:1096:VAL:HG13	1.95	0.47
2:X:148:GLU:HB3	2:X:203:HIS:CD2	2.49	0.47
3:H:217:HIS:HB3	3:H:222:THR:HG22	1.96	0.47
3:Y:141:LEU:HD12	3:Y:158:LEU:HD11	1.95	0.47
2:L:146:PRO:HD2	2:L:203:HIS:CE1	2.49	0.47
1:B:786:LYS:NZ	1:B:888:PHE:O	2.47	0.47
1:C:439:ASN:OD1	1:C:440:ASN:N	2.47	0.47
1:C:641:ASN:OD1	1:C:642:VAL:N	2.46	0.47
2:X:31:HIS:CG	2:X:32:SER:H	2.32	0.47
3:H:203:SER:HA	3:H:206:LEU:CD1	2.44	0.47
1:C:106:PHE:O	1:C:116:SER:OG	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LEU:HD21	1:C:119:ILE:HD11	1.96	0.47
1:B:226:LEU:HB3	1:B:227:VAL:HG23	1.96	0.47
1:A:472:ILE:HA	1:A:491:PRO:HG3	1.96	0.47
1:A:866:THR:O	1:A:869:MET:N	2.44	0.47
1:C:403:ARG:HE	1:C:497:PHE:HE1	1.61	0.47
2:X:144:PHE:HB2	2:X:149:ALA:HB3	1.97	0.47
3:H:49:SER:OG	3:H:50:GLY:N	2.47	0.47
1:B:295:PRO:HB2	1:B:608:VAL:HG21	1.96	0.47
1:C:408:ARG:CZ	1:C:409:GLN:HG2	2.45	0.47
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.97	0.47
2:X:153:TRP:CH2	2:X:199:CYS:HB2	2.50	0.47
3:Y:11:LEU:HA	3:Y:127:THR:HB	1.97	0.47
2:L:195:LYS:HD3	2:L:216:ARG:HB2	1.97	0.47
3:H:34:MET:HG2	3:H:72:ARG:CZ	2.45	0.47
1:B:28:TYR:HD2	1:B:61:ASN:HB3	1.80	0.47
1:B:430:THR:OG1	1:B:515:PHE:O	2.33	0.47
1:B:904:TYR:OH	1:C:1094:VAL:HG22	2.15	0.47
1:B:1085:GLY:O	1:B:1126:CYS:N	2.41	0.47
1:A:308:VAL:HG22	1:A:602:THR:HG23	1.96	0.47
1:A:334:ASN:HB2	1:A:361:CYS:HA	1.96	0.47
1:A:537:LYS:HE2	1:A:537:LYS:HB3	1.65	0.47
1:C:870:ILE:O	1:C:874:THR:HG23	2.15	0.47
1:C:877:LEU:O	1:C:881:THR:HG23	2.15	0.47
1:C:922:LEU:HG	1:C:926:GLN:HE21	1.78	0.47
1:C:962:LEU:HD11	1:C:1007:TYR:CD2	2.50	0.47
3:P:38:ARG:HG3	3:P:92:ALA:CB	2.44	0.47
3:P:224:VAL:HG12	3:P:226:LYS:HG3	1.96	0.47
3:Y:155:LEU:HD12	3:Y:171:TRP:HZ3	1.80	0.47
1:B:353:TRP:CZ3	1:B:355:ARG:HB2	2.50	0.47
1:B:364:ASP:OD1	1:B:365:TYR:N	2.48	0.47
1:A:201:PHE:HB3	1:A:229:LEU:HB2	1.97	0.47
1:C:131:CYS:HB2	1:C:133:PHE:CE1	2.49	0.47
2:O:154:LYS:HG2	2:O:158:ALA:O	2.14	0.47
1:C:743:CYS:SG	1:C:749:CYS:C	2.98	0.47
3:Y:82:HIS:CD2	3:Y:84:ARG:HH21	2.33	0.47
1:B:1039:ARG:NH2	1:A:1031:GLU:OE2	2.48	0.47
3:Y:22:CYS:HB2	3:Y:79:LEU:HG	1.97	0.47
2:L:130:LEU:O	2:L:131:LYS:HE2	2.14	0.47
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.96	0.46
1:B:506:GLN:HB2	1:B:508:TYR:HE1	1.80	0.46
1:B:988:GLU:N	1:B:988:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ASP:OD2	1:A:88:ASP:N	2.48	0.46
1:C:129:LYS:HG3	1:C:131:CYS:H	1.80	0.46
2:X:175:ASP:OD1	2:X:177:THR:OG1	2.27	0.46
1:C:199:GLY:HA2	1:C:232:GLY:HA2	1.97	0.46
2:L:41:TYR:OH	3:H:117:MET:N	2.34	0.46
3:P:4:LEU:HB2	3:P:121:GLY:HA3	1.97	0.46
1:B:342:PHE:HE1	1:B:511:VAL:HG11	1.80	0.46
1:A:367:VAL:O	1:A:371:SER:N	2.48	0.46
3:P:19:ARG:NE	3:P:82:HIS:HD1	2.14	0.46
3:Y:140:PRO:HB3	3:Y:228:VAL:HA	1.98	0.46
2:L:110:ASP:OD1	2:L:110:ASP:N	2.48	0.46
1:B:53:ASP:HB3	1:B:55:PHE:CE1	2.51	0.46
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.41	0.46
1:C:738:CYS:O	1:C:742:ILE:HG22	2.15	0.46
3:P:36:TRP:CD1	3:P:81:LEU:HD12	2.50	0.46
2:L:20:SER:C	2:L:21:ILE:HG13	2.40	0.46
1:C:90:VAL:HG21	1:C:238:PHE:CE1	2.51	0.46
2:O:103:PHE:CD2	3:P:46:GLU:HA	2.51	0.46
3:P:162:TYR:HE2	3:P:165:GLU:O	1.99	0.46
1:B:869:MET:HG2	1:C:699:LEU:HD11	1.97	0.46
1:B:912:THR:HG22	1:B:914:ASN:H	1.81	0.46
1:C:326:ILE:HD11	1:C:534:VAL:HG22	1.97	0.46
1:C:390:LEU:HB3	1:C:392:PHE:CE1	2.51	0.46
1:C:431:GLY:HA2	1:C:515:PHE:CE2	2.51	0.46
1:C:645:THR:OG1	1:C:670:ILE:HD12	2.16	0.46
1:B:65:PHE:O	1:B:264:ALA:HB1	2.16	0.46
1:B:104:TRP:HB3	1:B:106:PHE:CE2	2.51	0.46
1:A:331:ASN:OD1	4:A:1303:NAG:N2	2.48	0.46
1:A:902:MET:HE2	1:A:902:MET:HA	1.98	0.46
1:C:737:ASP:OD2	1:C:740:MET:HG3	2.16	0.46
3:P:22:CYS:HB2	3:P:79:LEU:CG	2.46	0.46
3:P:73:ASP:OD2	3:P:76:LYS:HG2	2.15	0.46
1:B:64:TRP:CD1	1:B:65:PHE:N	2.82	0.46
3:H:122:GLN:H	3:H:122:GLN:CD	2.24	0.46
1:A:229:LEU:HB3	1:A:231:ILE:HG12	1.98	0.45
1:A:287:ASP:HB3	1:A:306:PHE:HE2	1.81	0.45
1:B:106:PHE:HD1	1:B:235:ILE:HD11	1.81	0.45
1:A:106:PHE:HB3	1:A:235:ILE:HG21	1.98	0.45
1:A:106:PHE:CD1	1:A:238:PHE:HB2	2.51	0.45
1:C:424:LYS:NZ	1:C:463:PRO:HA	2.31	0.45
2:O:67:PHE:CE1	2:O:80:ILE:HG12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:40:TRP:HB2	2:X:53:ILE:CG2	2.44	0.45
1:B:388:ASN:O	1:B:526:GLY:N	2.49	0.45
1:B:763:LEU:HD21	1:B:1005:GLN:OE1	2.17	0.45
1:A:586:ASP:OD2	1:A:587:ILE:N	2.49	0.45
2:O:135:ALA:HB3	2:O:186:LEU:HB2	1.97	0.45
1:C:666:ILE:HB	1:C:670:ILE:O	2.17	0.45
3:P:215:VAL:O	3:P:223:LYS:HA	2.16	0.45
2:X:201:VAL:O	2:X:209:PRO:HA	2.16	0.45
1:B:1089:PHE:CE1	1:A:917:TYR:HD1	2.33	0.45
1:A:212:LEU:HD21	1:A:214:ARG:NH2	2.32	0.45
2:O:40:TRP:CE2	2:O:78:LEU:HB2	2.51	0.45
1:B:403:ARG:O	1:B:407:VAL:HG23	2.17	0.45
1:C:43:PHE:C	1:C:44:ARG:HD2	2.41	0.45
1:C:52:GLN:HA	1:C:274:THR:HA	1.99	0.45
1:C:111:ASP:N	1:C:111:ASP:OD1	2.47	0.45
1:C:128:ILE:HD12	1:C:170:TYR:HD2	1.81	0.45
3:P:170:SER:OG	3:P:214:ASN:HB2	2.17	0.45
3:Y:15:GLY:H	3:Y:86:LEU:CB	2.27	0.45
1:B:1002:GLN:O	1:B:1006:THR:HG23	2.17	0.45
1:A:103:GLY:HA3	1:A:241:LEU:HB2	1.98	0.45
1:A:345:THR:C	1:A:346:ARG:HG3	2.41	0.45
1:A:557:LYS:NZ	1:A:575:ALA:HB2	2.32	0.45
1:C:878:LEU:HD11	1:C:1054:GLN:HE22	1.81	0.45
1:C:29:THR:HB	1:C:62:VAL:HG23	1.99	0.45
1:C:102:ARG:HB2	1:C:241:LEU:HD12	1.99	0.45
1:C:353:TRP:CE2	1:C:466:ARG:HD3	2.51	0.45
2:O:8:PRO:HG2	2:O:11:LEU:HB3	1.99	0.45
2:X:55:LEU:HD12	2:X:58:ASN:HB2	1.98	0.45
2:X:101:PHE:CE2	3:Y:115:TYR:HB3	2.51	0.45
1:B:821:LEU:HD21	1:B:939:SER:HB3	1.98	0.45
1:A:565:PHE:O	1:C:42:VAL:HA	2.17	0.45
1:A:665:PRO:HA	1:A:671:CYS:HB3	1.99	0.45
1:C:360:ASN:H	1:C:523:THR:HG23	1.80	0.45
1:C:498:GLN:HB3	1:C:501:ASN:OD1	2.17	0.45
3:P:159:VAL:HG12	3:P:162:TYR:CD1	2.52	0.45
2:X:43:GLN:HB3	2:X:90:VAL:CG1	2.47	0.45
2:X:125:PRO:HD3	2:X:137:VAL:HA	1.98	0.45
1:A:748:GLU:H	1:A:748:GLU:CD	2.23	0.44
1:C:742:ILE:HG23	1:C:743:CYS:H	1.81	0.44
2:O:42:LEU:HD22	2:O:52:LEU:HD21	1.99	0.44
3:Y:93:LEU:HD11	3:Y:125:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1106:GLN:HE21	1:B:1109:PHE:HB3	1.82	0.44
1:C:58:PHE:HB3	1:C:59:PHE:CD1	2.53	0.44
1:B:1031:GLU:OE2	1:C:1042:PHE:HB2	2.16	0.44
1:A:673:SER:OG	1:A:674:TYR:N	2.51	0.44
3:P:34:MET:HG3	3:P:97:ALA:O	2.16	0.44
3:P:155:LEU:HD21	3:P:211:TYR:CE1	2.52	0.44
3:Y:43:LYS:HE3	3:Y:44:GLY:H	1.81	0.44
1:B:870:ILE:O	1:B:874:THR:HG23	2.16	0.44
1:B:940:SER:OG	1:B:941:THR:N	2.50	0.44
1:C:462:LYS:HB3	1:C:463:PRO:HD2	1.99	0.44
3:Y:30:ASP:HA	3:Y:72:ARG:NH2	2.32	0.44
1:B:349:SER:OG	1:B:350:VAL:N	2.51	0.44
1:A:1030:SER:O	1:A:1034:LEU:HB2	2.18	0.44
1:C:826:VAL:HG23	1:C:949:GLN:OE1	2.18	0.44
3:H:136:PRO:HD3	3:H:217:HIS:ND1	2.31	0.44
1:A:105:ILE:HG21	1:A:135:PHE:CZ	2.52	0.44
1:C:517:LEU:C	1:C:518:LEU:HD12	2.43	0.44
2:O:66:ARG:HB2	2:O:82:ARG:HB2	1.99	0.44
2:O:125:PRO:HD3	2:O:137:VAL:HA	1.99	0.44
3:P:79:LEU:HD11	3:P:96:CYS:SG	2.58	0.44
2:X:42:LEU:HD23	2:X:43:GLN:N	2.32	0.44
1:B:142:GLY:HA2	1:B:244:LEU:H	1.82	0.44
1:B:323:THR:OG1	1:B:324:GLU:HG2	2.18	0.44
1:C:1093:GLY:N	1:C:1107:ARG:HH12	2.14	0.44
1:A:822:LEU:HD23	1:A:945:LEU:HD21	1.99	0.44
1:C:1080:ALA:HB3	1:C:1132:ILE:HG13	2.00	0.44
2:X:145:TYR:HA	2:X:147:ARG:N	2.29	0.44
3:Y:92:ALA:HB3	3:Y:94:TYR:CZ	2.52	0.44
1:B:402:ILE:O	1:B:508:TYR:HB2	2.18	0.44
1:C:558:LYS:HD2	1:C:558:LYS:HA	1.86	0.44
2:O:16:GLY:H	2:O:83:VAL:HG21	1.82	0.44
2:O:37:TYR:HA	2:O:55:LEU:HD22	2.00	0.44
2:X:141:LEU:HD13	2:X:180:LEU:HD22	1.99	0.44
3:H:188:GLN:HB2	3:H:192:LEU:O	2.17	0.44
1:B:411:ALA:HB3	1:B:414:GLN:HB2	2.00	0.43
1:B:442:ASP:OD2	1:B:509:ARG:NE	2.47	0.43
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.51	0.43
1:C:106:PHE:HB3	1:C:235:ILE:HG21	2.00	0.43
1:B:331:ASN:OD1	4:B:1309:NAG:N2	2.51	0.43
1:B:537:LYS:O	1:B:539:VAL:HG13	2.18	0.43
1:B:894:LEU:CD2	1:C:715:PRO:HD3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:LEU:CD1	1:C:38:TYR:HE2	2.30	0.43
1:A:966:LEU:O	1:A:975:SER:OG	2.36	0.43
1:C:431:GLY:HA2	1:C:515:PHE:HE2	1.83	0.43
1:C:919:ASN:O	1:C:923:ILE:HG13	2.18	0.43
2:O:44:LYS:HB2	2:O:47:GLN:HB2	2.00	0.43
3:Y:6:GLU:HG2	3:Y:123:GLY:HA2	1.99	0.43
2:L:152:GLN:HB2	2:L:200:GLU:HB2	2.00	0.43
1:B:199:GLY:HA2	1:B:232:GLY:HA2	2.00	0.43
1:C:340:GLU:N	1:C:340:GLU:OE1	2.52	0.43
1:C:1072:GLU:N	1:C:1072:GLU:OE1	2.51	0.43
2:O:127:ASP:HA	2:O:130:LEU:HD12	2.00	0.43
3:P:227:LYS:NZ	3:P:229:GLU:HB2	2.33	0.43
3:Y:40:ALA:HB3	3:Y:43:LYS:HB2	1.99	0.43
3:H:38:ARG:HG2	3:H:46:GLU:HB3	2.00	0.43
1:B:717:ASN:OD1	1:B:718:PHE:N	2.51	0.43
1:B:825:LYS:HZ1	1:B:939:SER:HA	1.83	0.43
1:B:958:ALA:O	1:B:961:THR:OG1	2.30	0.43
1:A:543:PHE:HE2	1:A:576:VAL:HG11	1.84	0.43
1:A:802:PHE:CD2	1:A:805:ILE:HD11	2.54	0.43
1:A:1123:SER:O	1:A:1123:SER:OG	2.35	0.43
2:X:123:PHE:CD2	3:Y:141:LEU:HD21	2.53	0.43
3:H:39:GLN:O	3:H:92:ALA:HB1	2.19	0.43
1:B:555:SER:HG	1:B:586:ASP:H	1.65	0.43
1:B:699:LEU:HD12	1:A:872:GLN:NE2	2.33	0.43
1:C:273:ARG:HD3	1:C:273:ARG:HA	1.71	0.43
2:L:151:VAL:HA	2:L:200:GLU:O	2.18	0.43
3:H:87:ARG:O	3:H:128:VAL:HG21	2.18	0.43
3:H:171:TRP:CZ3	3:H:213:CYS:HB3	2.54	0.43
1:A:557:LYS:HB2	1:A:584:ILE:HG21	1.99	0.43
1:A:643:PHE:CE1	1:A:655:HIS:HB2	2.54	0.43
1:A:699:LEU:HD11	1:C:869:MET:HG2	2.00	0.43
1:C:417:LYS:HA	1:C:417:LYS:HD3	1.72	0.43
1:C:770:ILE:O	1:C:774:GLN:HG2	2.19	0.43
3:P:14:PRO:O	3:P:16:ARG:NH1	2.52	0.43
3:P:22:CYS:HB2	3:P:79:LEU:HG	2.01	0.43
1:B:456:PHE:HB3	1:B:473:TYR:CD2	2.53	0.43
1:B:873:TYR:CZ	1:C:699:LEU:HD22	2.54	0.43
1:C:435:ALA:HB2	1:C:510:VAL:HG22	2.01	0.43
1:C:816:SER:OG	1:C:819:GLU:HG3	2.19	0.43
1:B:393:THR:HA	1:B:522:ALA:HA	1.99	0.43
1:B:554:GLU:OE1	1:B:555:SER:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	2.00	0.43
1:C:825:LYS:HB3	1:C:825:LYS:HE3	1.73	0.43
1:C:1086:LYS:HA	1:C:1125:ASN:HA	2.00	0.43
2:O:55:LEU:HB2	2:O:58:ASN:HB2	2.00	0.43
2:O:144:PHE:HE1	2:O:147:ARG:HA	1.83	0.43
3:H:158:LEU:HD12	3:H:195:LEU:O	2.19	0.43
1:B:1043:CYS:HB3	1:B:1048:HIS:ND1	2.32	0.43
1:A:348:ALA:HB3	1:A:352:ALA:O	2.19	0.43
1:A:722:VAL:HG23	1:A:722:VAL:O	2.19	0.43
1:A:934:ILE:HD13	1:A:934:ILE:HA	1.87	0.43
1:A:1129:VAL:HG13	1:A:1132:ILE:HB	2.01	0.43
1:C:454:ARG:HH21	1:C:457:ARG:N	2.17	0.43
3:H:53:TRP:CG	3:H:103:VAL:HG21	2.54	0.43
1:B:458:LYS:HG3	1:B:473:TYR:CE1	2.54	0.43
1:B:981:LEU:HD21	1:B:993:ILE:HD11	2.00	0.43
1:A:345:THR:HG23	1:A:346:ARG:N	2.34	0.43
1:A:555:SER:HB3	1:A:584:ILE:HG22	2.01	0.43
1:C:325:SER:HA	1:C:540:ASN:O	2.19	0.43
1:C:538:CYS:HB2	1:C:590:CYS:HB3	1.74	0.43
1:C:739:THR:C	1:C:741:TYR:N	2.77	0.43
1:C:767:LEU:HD23	1:C:767:LEU:HA	1.91	0.43
1:C:1142:GLN:HA	1:C:1145:LEU:HG	1.99	0.43
2:X:113:ARG:H	2:X:145:TYR:HE2	1.65	0.43
2:X:118:PRO:HB3	2:X:144:PHE:CB	2.44	0.43
3:Y:136:PRO:HA	3:Y:162:TYR:HB3	2.01	0.43
1:B:922:LEU:O	1:B:926:GLN:HG3	2.19	0.42
1:B:1050:MET:HE2	1:B:1052:PHE:CZ	2.54	0.42
1:C:643:PHE:CZ	1:C:655:HIS:ND1	2.87	0.42
1:A:543:PHE:CE2	1:A:576:VAL:HG11	2.54	0.42
2:O:88:VAL:HG12	2:O:110:ASP:HA	2.01	0.42
2:X:149:ALA:HA	2:X:202:THR:O	2.19	0.42
2:L:41:TYR:CD1	2:L:51:LEU:HA	2.55	0.42
1:B:326:ILE:HD13	1:B:326:ILE:HA	1.86	0.42
1:B:402:ILE:HG13	1:B:407:VAL:HG22	2.01	0.42
1:B:825:LYS:HE2	1:B:825:LYS:HB2	1.65	0.42
4:A:1307:NAG:O6	4:A:1307:NAG:O4	2.30	0.42
1:C:119:ILE:HD12	1:C:128:ILE:HG12	2.01	0.42
1:C:497:PHE:CE2	1:C:507:PRO:HB3	2.55	0.42
1:C:825:LYS:NZ	1:C:942:PRO:HA	2.34	0.42
1:C:1086:LYS:HE2	1:C:1088:HIS:NE2	2.34	0.42
3:H:53:TRP:CE2	3:H:54:ASN:OD1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:36:TRP:HB2	3:P:49:SER:OG	2.20	0.42
2:X:112:LYS:HA	2:X:145:TYR:OH	2.19	0.42
2:X:144:PHE:CD1	2:X:147:ARG:HA	2.54	0.42
1:A:240:THR:OG1	1:A:241:LEU:N	2.52	0.42
1:C:742:ILE:CD1	1:C:997:ILE:HG23	2.49	0.42
2:O:43:GLN:HB3	2:O:90:VAL:CG1	2.48	0.42
3:H:154:ALA:HA	3:H:200:THR:HA	2.01	0.42
1:A:506:GLN:NE2	1:A:508:TYR:OH	2.52	0.42
1:C:101:ILE:HD11	1:C:240:THR:OG1	2.19	0.42
1:C:347:PHE:CZ	1:C:399:SER:HB2	2.54	0.42
1:C:715:PRO:HA	1:C:1072:GLU:HA	2.00	0.42
3:Y:91:THR:HG23	3:Y:128:VAL:HB	2.01	0.42
3:H:70:ILE:HD11	3:H:79:LEU:HD11	2.01	0.42
1:B:57:PRO:HB3	1:B:273:ARG:NH2	2.34	0.42
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.45	0.42
1:A:436:TRP:NE1	1:A:509:ARG:HD2	2.34	0.42
1:C:202:LYS:HB3	1:C:204:TYR:CE1	2.54	0.42
3:P:86:LEU:HD12	3:P:128:VAL:HG11	2.01	0.42
3:P:182:THR:HA	3:P:197:SER:HA	2.01	0.42
1:C:276:LEU:HB3	1:C:289:VAL:CG2	2.49	0.42
1:C:720:ILE:HG13	1:C:923:ILE:HG23	2.02	0.42
3:P:14:PRO:HD2	3:P:130:SER:HB2	2.01	0.42
3:P:51:VAL:HG23	3:P:56:GLY:C	2.44	0.42
3:P:60:TYR:HB3	3:P:64:VAL:HG13	2.00	0.42
2:L:4:MET:CE	2:L:95:GLN:HB3	2.50	0.42
1:B:906:PHE:CD1	1:B:1049:LEU:HD11	2.54	0.42
1:A:317:ASN:N	1:A:317:ASN:OD1	2.52	0.42
1:A:919:ASN:O	1:A:923:ILE:HG13	2.19	0.42
1:C:58:PHE:HB3	1:C:59:PHE:HD1	1.85	0.42
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	2.02	0.42
1:C:984:LEU:HD23	1:C:984:LEU:HA	1.90	0.42
3:P:4:LEU:HA	3:P:23:ALA:O	2.20	0.42
3:P:69:THR:OG1	3:P:82:HIS:HB3	2.20	0.42
3:Y:36:TRP:HB2	3:Y:49:SER:OG	2.20	0.42
3:H:117:MET:O	3:H:120:TRP:NE1	2.41	0.42
1:B:358:ILE:HB	1:B:395:VAL:CG1	2.49	0.42
1:A:791:THR:OG1	1:A:792:PRO:HD2	2.20	0.42
1:C:449:TYR:O	1:C:494:SER:HB2	2.19	0.42
2:X:123:PHE:HZ	3:Y:154:ALA:HB3	1.85	0.42
2:X:154:LYS:HA	2:X:158:ALA:O	2.20	0.42
3:Y:5:LEU:O	3:Y:22:CYS:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:143:PRO:HG2	3:H:230:PRO:HB3	2.01	0.42
1:B:224:GLU:N	1:B:224:GLU:OE1	2.53	0.41
1:A:551:VAL:CG1	1:A:588:THR:HB	2.50	0.41
1:C:445:VAL:O	1:C:498:GLN:NE2	2.53	0.41
1:C:724:THR:HA	1:C:1062:PHE:O	2.19	0.41
1:C:900:MET:HA	1:C:917:TYR:OH	2.20	0.41
2:O:38:LEU:HD12	2:O:94:MET:O	2.20	0.41
2:L:41:TYR:HD1	2:L:51:LEU:HA	1.85	0.41
1:B:430:THR:OG1	1:B:430:THR:O	2.36	0.41
1:A:64:TRP:HD1	1:A:65:PHE:H	1.64	0.41
2:O:67:PHE:HE1	2:O:80:ILE:HG12	1.84	0.41
2:L:169:THR:OG1	2:L:170:GLU:N	2.53	0.41
1:B:395:VAL:HG23	1:B:515:PHE:CD1	2.55	0.41
1:A:123:ALA:O	1:A:124:THR:HG22	2.21	0.41
1:A:473:TYR:O	1:A:489:TYR:N	2.52	0.41
1:A:722:VAL:HA	1:A:1064:HIS:O	2.20	0.41
1:C:50:SER:HB2	1:C:276:LEU:HD13	2.01	0.41
1:C:376:THR:HG22	1:C:435:ALA:HB3	2.01	0.41
1:C:912:THR:HG22	1:C:913:GLN:H	1.86	0.41
3:P:176:LEU:HD21	3:P:199:VAL:HG11	2.02	0.41
3:Y:6:GLU:HG3	3:Y:22:CYS:SG	2.60	0.41
1:B:453:TYR:CE1	1:B:493:GLN:HB3	2.55	0.41
1:B:535:LYS:O	1:B:537:LYS:HG3	2.21	0.41
1:A:431:GLY:HA2	1:A:515:PHE:CD1	2.51	0.41
1:C:122:ASN:O	1:C:124:THR:N	2.53	0.41
1:C:389:ASP:OD1	1:C:390:LEU:N	2.53	0.41
2:X:88:VAL:HG11	2:X:111:ILE:HG12	2.01	0.41
1:B:973:ILE:HG13	1:B:992:GLN:OE1	2.21	0.41
1:A:716:THR:HG22	1:A:1110:TYR:HB2	2.01	0.41
1:A:717:ASN:OD1	1:A:718:PHE:N	2.54	0.41
1:A:767:LEU:HD23	1:A:767:LEU:HA	1.87	0.41
1:A:976:VAL:HG23	1:A:976:VAL:O	2.21	0.41
1:C:450:ASN:HD21	3:Y:60:TYR:HD2	1.67	0.41
1:C:644:GLN:HG3	1:C:645:THR:N	2.36	0.41
2:L:14:THR:HG23	2:L:17:GLU:OE1	2.20	0.41
2:L:215:ASN:OD1	2:L:215:ASN:N	2.51	0.41
3:H:40:ALA:HB3	3:H:43:LYS:HB2	2.02	0.41
1:B:189:LEU:HB3	1:B:208:THR:HG23	2.03	0.41
1:B:215:ASP:CG	1:B:216:LEU:H	2.29	0.41
1:A:393:THR:HG21	1:A:520:ALA:H	1.86	0.41
1:A:814:LYS:HA	1:A:814:LYS:HD3	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:16:GLY:H	2:X:83:VAL:HG21	1.85	0.41
1:B:345:THR:CG2	3:P:112:ASP:HB2	2.51	0.41
1:B:605:SER:OG	1:B:606:ASN:N	2.53	0.41
1:A:193:VAL:HG23	1:A:223:LEU:HD21	2.03	0.41
1:A:964:LYS:HE2	1:A:964:LYS:HB2	1.81	0.41
1:A:1027:THR:O	1:A:1031:GLU:HG3	2.20	0.41
1:C:881:THR:HG22	1:C:888:PHE:HE2	1.85	0.41
2:O:43:GLN:HB3	2:O:90:VAL:HG12	2.03	0.41
1:B:168:PHE:CE2	1:B:170:TYR:HB2	2.56	0.41
1:B:299:THR:O	1:B:303:LEU:HG	2.20	0.41
1:B:415:THR:OG1	1:B:416:GLY:N	2.53	0.41
1:B:715:PRO:HD3	1:A:894:LEU:HD13	2.03	0.41
1:B:1097:SER:HB3	1:B:1102:TRP:CE3	2.55	0.41
1:A:752:LEU:O	1:A:755:GLN:HG2	2.20	0.41
1:C:36:VAL:HG11	1:C:220:PHE:CZ	2.56	0.41
1:C:242:LEU:HG	1:C:243:ALA:H	1.85	0.41
1:C:398:ASP:OD2	1:C:423:TYR:OH	2.24	0.41
3:Y:167:VAL:HG12	3:Y:217:HIS:HA	2.02	0.41
3:Y:170:SER:OG	3:Y:214:ASN:HB2	2.21	0.41
3:H:36:TRP:HE1	3:H:79:LEU:HG	1.85	0.41
1:B:325:SER:O	1:B:326:ILE:HD13	2.21	0.41
1:A:428:ASP:OD1	1:A:428:ASP:N	2.53	0.41
1:C:138:ASP:HB3	1:C:140:PHE:HE1	1.84	0.41
1:C:761:THR:C	1:C:763:LEU:H	2.29	0.41
1:C:816:SER:HB2	1:C:817:PRO:HD2	2.01	0.41
1:C:1101:HIS:HD2	4:C:1308:NAG:H5	1.85	0.41
3:P:34:MET:HE1	3:P:72:ARG:HG2	2.03	0.41
1:B:436:TRP:CE2	1:B:509:ARG:HB2	2.57	0.40
1:A:977:LEU:O	1:A:981:LEU:HG	2.21	0.40
2:O:31:HIS:CG	2:O:32:SER:H	2.40	0.40
2:O:139:CYS:HB3	2:O:182:SER:HB3	2.03	0.40
2:X:145:TYR:CD1	2:X:178:TYR:HE1	2.40	0.40
2:X:150:LYS:O	2:X:201:VAL:HA	2.21	0.40
3:Y:138:VAL:HB	3:Y:226:LYS:HD2	2.03	0.40
3:Y:172:ASN:HA	3:Y:212:ILE:HG13	2.02	0.40
2:L:196:VAL:C	2:L:197:TYR:HD1	2.28	0.40
1:B:345:THR:HG23	3:P:112:ASP:H	1.85	0.40
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.37	0.40
1:A:564:GLN:O	1:A:577:ARG:HB3	2.21	0.40
1:C:643:PHE:CD2	1:C:650:LEU:HD21	2.55	0.40
2:O:141:LEU:HB3	2:O:144:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:38:ARG:N	3:P:46:GLU:O	2.54	0.40
3:Y:61:ALA:HB3	3:Y:64:VAL:HG12	2.04	0.40
1:B:189:LEU:HD22	1:B:217:PRO:HG2	2.02	0.40
1:A:559:PHE:HE2	1:A:565:PHE:HA	1.85	0.40
2:X:101:PHE:HE2	3:Y:115:TYR:HB3	1.86	0.40
2:X:144:PHE:HB2	2:X:149:ALA:CB	2.51	0.40
2:X:174:LYS:HG3	2:X:175:ASP:OD1	2.22	0.40
3:Y:162:TYR:OH	3:Y:165:GLU:OE2	2.35	0.40
2:L:12:PRO:HB2	2:L:112:LYS:HB2	2.03	0.40
3:H:187:LEU:HD23	3:H:188:GLN:O	2.21	0.40
1:B:805:ILE:HB	1:B:1054:GLN:HE22	1.86	0.40
1:A:353:TRP:CD1	1:A:353:TRP:H	2.40	0.40
1:C:461:LEU:HB3	1:C:465:GLU:HB3	2.03	0.40
1:C:906:PHE:CD1	1:C:1049:LEU:HD11	2.56	0.40
1:C:962:LEU:HA	1:C:962:LEU:HD23	1.91	0.40
3:P:18:LEU:O	3:P:82:HIS:HA	2.22	0.40
3:P:38:ARG:NH1	3:P:40:ALA:HB2	2.37	0.40
3:P:98:LYS:HG3	3:P:118:ASP:OD1	2.20	0.40
3:P:160:LYS:HA	3:P:193:TYR:O	2.21	0.40
3:Y:64:VAL:HG21	3:Y:68:PHE:CE2	2.56	0.40
2:L:125:PRO:HD3	2:L:137:VAL:HG22	2.02	0.40
1:B:641:ASN:OD1	1:B:642:VAL:N	2.55	0.40
1:A:735:SER:OG	1:A:859:THR:OG1	2.30	0.40
1:C:764:ASN:O	1:C:768:THR:HG23	2.22	0.40
2:O:113:ARG:HB2	2:O:145:TYR:CE2	2.56	0.40
3:P:153:ALA:O	3:P:200:THR:HA	2.22	0.40
3:Y:39:GLN:HB3	3:Y:93:LEU:HB3	2.04	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	953/1121 (85%)	871 (91%)	82 (9%)	0	100	100
1	B	986/1121 (88%)	896 (91%)	90 (9%)	0	100	100
1	C	986/1121 (88%)	891 (90%)	95 (10%)	0	100	100
2	L	216/218 (99%)	201 (93%)	15 (7%)	0	100	100
2	O	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
2	X	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
3	H	220/237 (93%)	207 (94%)	13 (6%)	0	100	100
3	P	220/237 (93%)	204 (93%)	16 (7%)	0	100	100
3	Y	220/237 (93%)	209 (95%)	11 (5%)	0	100	100
All	All	4233/4728 (90%)	3892 (92%)	341 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

27 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1304	1	14,14,15	1.94	4 (28%)	17,19,21	1.35	3 (17%)
4	NAG	B	1303	1	14,14,15	1.82	3 (21%)	17,19,21	1.30	2 (11%)
4	NAG	A	1308	1	14,14,15	1.85	4 (28%)	17,19,21	1.25	2 (11%)
4	NAG	C	1303	1	14,14,15	1.93	5 (35%)	17,19,21	1.06	1 (5%)
4	NAG	A	1301	1	14,14,15	2.04	4 (28%)	17,19,21	1.22	2 (11%)
4	NAG	B	1306	1	14,14,15	1.82	4 (28%)	17,19,21	1.23	1 (5%)
4	NAG	B	1308	1	14,14,15	1.99	4 (28%)	17,19,21	1.05	0
4	NAG	A	1305	1	14,14,15	1.96	5 (35%)	17,19,21	2.10	5 (29%)
4	NAG	A	1307	1	14,14,15	1.93	4 (28%)	17,19,21	1.29	3 (17%)
4	NAG	A	1303	1	14,14,15	1.86	4 (28%)	17,19,21	1.30	3 (17%)
4	NAG	A	1309	1	14,14,15	1.92	4 (28%)	17,19,21	1.09	0
4	NAG	C	1306	1	14,14,15	1.84	4 (28%)	17,19,21	1.48	2 (11%)
4	NAG	A	1306	1	14,14,15	1.99	4 (28%)	17,19,21	1.09	2 (11%)
4	NAG	C	1307	1	14,14,15	1.86	3 (21%)	17,19,21	0.87	1 (5%)
4	NAG	C	1302	1	14,14,15	1.80	3 (21%)	17,19,21	1.38	3 (17%)
4	NAG	B	1304	1	14,14,15	1.98	5 (35%)	17,19,21	1.43	3 (17%)
4	NAG	B	1302	1	14,14,15	1.98	4 (28%)	17,19,21	1.35	3 (17%)
4	NAG	A	1302	1	14,14,15	1.90	4 (28%)	17,19,21	1.25	2 (11%)
4	NAG	B	1307	1	14,14,15	1.86	4 (28%)	17,19,21	1.32	4 (23%)
4	NAG	C	1305	1	14,14,15	1.92	5 (35%)	17,19,21	1.27	3 (17%)
4	NAG	C	1301	1	14,14,15	1.89	5 (35%)	17,19,21	1.11	1 (5%)
4	NAG	C	1309	1	14,14,15	1.73	3 (21%)	17,19,21	1.91	3 (17%)
4	NAG	C	1308	1	14,14,15	1.87	4 (28%)	17,19,21	1.27	3 (17%)
4	NAG	B	1305	1	14,14,15	1.88	3 (21%)	17,19,21	1.37	4 (23%)
4	NAG	B	1301	1	14,14,15	1.90	4 (28%)	17,19,21	0.83	0
4	NAG	B	1309	1	14,14,15	1.95	4 (28%)	17,19,21	1.32	3 (17%)
4	NAG	C	1304	1	14,14,15	1.81	4 (28%)	17,19,21	1.17	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1308	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	0/6/23/26	0/1/1/1

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1301	NAG	O5-C1	4.53	1.51	1.43
4	B	1302	NAG	O5-C1	4.49	1.51	1.43
4	B	1309	NAG	O5-C1	4.44	1.51	1.43
4	A	1304	NAG	O5-C1	4.42	1.51	1.43
4	B	1305	NAG	O5-C1	4.41	1.51	1.43
4	B	1308	NAG	O5-C1	4.38	1.51	1.43
4	B	1304	NAG	O5-C1	4.30	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1307	NAG	O5-C1	4.28	1.50	1.43
4	C	1301	NAG	O5-C1	4.24	1.50	1.43
4	A	1302	NAG	O5-C1	4.20	1.50	1.43
4	A	1307	NAG	O5-C1	4.18	1.50	1.43
4	C	1305	NAG	O5-C1	4.18	1.50	1.43
4	A	1308	NAG	O5-C1	4.15	1.50	1.43
4	A	1306	NAG	O5-C1	4.13	1.50	1.43
4	A	1305	NAG	O5-C1	4.12	1.50	1.43
4	B	1301	NAG	O5-C1	4.11	1.50	1.43
4	C	1306	NAG	O5-C1	4.07	1.50	1.43
4	C	1303	NAG	O5-C1	4.02	1.50	1.43
4	C	1308	NAG	O5-C1	4.01	1.50	1.43
4	A	1303	NAG	O5-C1	4.00	1.50	1.43
4	B	1303	NAG	O5-C1	4.00	1.50	1.43
4	A	1309	NAG	O5-C1	4.00	1.50	1.43
4	B	1307	NAG	O5-C1	3.91	1.50	1.43
4	B	1306	NAG	O5-C1	3.90	1.50	1.43
4	C	1304	NAG	O5-C1	3.88	1.50	1.43
4	A	1305	NAG	C7-N2	3.81	1.46	1.34
4	A	1306	NAG	C7-N2	3.76	1.46	1.34
4	C	1302	NAG	O5-C1	3.74	1.50	1.43
4	A	1309	NAG	C7-N2	3.66	1.46	1.34
4	A	1301	NAG	C7-N2	3.65	1.46	1.34
4	C	1309	NAG	O5-C1	3.62	1.49	1.43
4	C	1303	NAG	C7-N2	3.60	1.46	1.34
4	B	1308	NAG	C7-N2	3.58	1.45	1.34
4	B	1301	NAG	C7-N2	3.55	1.45	1.34
4	A	1302	NAG	C7-N2	3.54	1.45	1.34
4	B	1302	NAG	C7-N2	3.51	1.45	1.34
4	A	1307	NAG	C7-N2	3.51	1.45	1.34
4	C	1309	NAG	C7-N2	3.50	1.45	1.34
4	C	1302	NAG	C7-N2	3.49	1.45	1.34
4	B	1307	NAG	C7-N2	3.48	1.45	1.34
4	B	1306	NAG	C7-N2	3.47	1.45	1.34
4	C	1301	NAG	C7-N2	3.46	1.45	1.34
4	C	1308	NAG	C7-N2	3.43	1.45	1.34
4	A	1303	NAG	C7-N2	3.42	1.45	1.34
4	C	1305	NAG	C7-N2	3.41	1.45	1.34
4	B	1309	NAG	C7-N2	3.41	1.45	1.34
4	A	1304	NAG	C7-N2	3.40	1.45	1.34
4	A	1308	NAG	C7-N2	3.38	1.45	1.34
4	B	1304	NAG	C7-N2	3.37	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1307	NAG	C7-N2	3.34	1.45	1.34
4	C	1304	NAG	C7-N2	3.32	1.45	1.34
4	B	1303	NAG	C7-N2	3.24	1.44	1.34
4	C	1306	NAG	C7-N2	3.23	1.44	1.34
4	B	1305	NAG	C7-N2	3.22	1.44	1.34
4	A	1306	NAG	C2-N2	2.74	1.50	1.46
4	A	1305	NAG	C2-N2	2.70	1.50	1.46
4	B	1304	NAG	O5-C5	2.61	1.48	1.43
4	A	1301	NAG	C2-N2	2.61	1.50	1.46
4	B	1308	NAG	O5-C5	2.56	1.48	1.43
4	C	1303	NAG	C2-N2	2.51	1.50	1.46
4	A	1309	NAG	C2-N2	2.48	1.50	1.46
4	B	1302	NAG	O5-C5	2.48	1.48	1.43
4	B	1301	NAG	C2-N2	2.44	1.50	1.46
4	B	1304	NAG	C3-C2	-2.42	1.47	1.52
4	A	1304	NAG	O5-C5	2.38	1.48	1.43
4	B	1308	NAG	C2-N2	2.33	1.50	1.46
4	A	1307	NAG	C3-C2	-2.28	1.47	1.52
4	C	1303	NAG	O5-C5	2.26	1.47	1.43
4	C	1306	NAG	O5-C5	2.26	1.47	1.43
4	C	1305	NAG	C3-C2	-2.24	1.47	1.52
4	A	1309	NAG	O5-C5	2.21	1.47	1.43
4	A	1303	NAG	O5-C5	2.21	1.47	1.43
4	B	1309	NAG	O5-C5	2.20	1.47	1.43
4	A	1301	NAG	O5-C5	2.20	1.47	1.43
4	C	1309	NAG	C2-N2	2.19	1.49	1.46
4	C	1308	NAG	O5-C5	2.19	1.47	1.43
4	A	1307	NAG	C2-N2	2.19	1.49	1.46
4	C	1301	NAG	C2-N2	2.19	1.49	1.46
4	A	1308	NAG	C2-N2	2.18	1.49	1.46
4	B	1307	NAG	O5-C5	2.16	1.47	1.43
4	A	1302	NAG	C2-N2	2.15	1.49	1.46
4	A	1304	NAG	C2-N2	2.13	1.49	1.46
4	B	1302	NAG	C2-N2	2.13	1.49	1.46
4	C	1304	NAG	O5-C5	2.11	1.47	1.43
4	C	1302	NAG	C2-N2	2.10	1.49	1.46
4	A	1306	NAG	O5-C5	2.09	1.47	1.43
4	A	1305	NAG	O7-C7	-2.08	1.18	1.23
4	B	1309	NAG	C2-N2	2.08	1.49	1.46
4	A	1303	NAG	C2-N2	2.07	1.49	1.46
4	B	1307	NAG	C3-C2	-2.07	1.48	1.52
4	A	1308	NAG	O7-C7	-2.06	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1306	NAG	O7-C7	-2.06	1.18	1.23
4	A	1302	NAG	O5-C5	2.06	1.47	1.43
4	B	1303	NAG	O7-C7	-2.05	1.18	1.23
4	C	1307	NAG	C2-N2	2.04	1.49	1.46
4	B	1301	NAG	O5-C5	2.04	1.47	1.43
4	B	1306	NAG	C2-N2	2.04	1.49	1.46
4	C	1304	NAG	C3-C2	-2.03	1.48	1.52
4	B	1306	NAG	O5-C5	2.03	1.47	1.43
4	C	1301	NAG	O7-C7	-2.03	1.18	1.23
4	B	1304	NAG	O7-C7	-2.02	1.18	1.23
4	C	1303	NAG	O7-C7	-2.02	1.18	1.23
4	C	1305	NAG	C2-N2	2.02	1.49	1.46
4	C	1301	NAG	O5-C5	2.02	1.47	1.43
4	B	1305	NAG	O5-C5	2.01	1.47	1.43
4	C	1305	NAG	O5-C5	2.01	1.47	1.43
4	C	1308	NAG	C3-C2	-2.01	1.48	1.52
4	A	1305	NAG	O5-C5	2.00	1.47	1.43

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1309	NAG	C4-C3-C2	5.63	119.27	111.02
4	A	1305	NAG	C8-C7-N2	5.43	125.12	116.12
4	C	1306	NAG	C2-N2-C7	-4.30	117.14	122.90
4	A	1305	NAG	C2-N2-C7	3.78	127.96	122.90
4	B	1304	NAG	C2-N2-C7	-3.37	118.38	122.90
4	C	1302	NAG	C1-O5-C5	-3.08	108.06	112.19
4	B	1303	NAG	C2-N2-C7	-3.07	118.79	122.90
4	B	1305	NAG	C2-N2-C7	-2.99	118.89	122.90
4	B	1302	NAG	C2-N2-C7	-2.97	118.93	122.90
4	C	1305	NAG	C2-N2-C7	-2.96	118.93	122.90
4	C	1308	NAG	C2-N2-C7	-2.80	119.15	122.90
4	B	1307	NAG	C2-N2-C7	-2.78	119.17	122.90
4	C	1309	NAG	C3-C4-C5	2.71	115.14	110.23
4	A	1305	NAG	O7-C7-N2	-2.70	117.22	121.98
4	B	1309	NAG	C8-C7-N2	2.65	120.51	116.12
4	C	1301	NAG	C8-C7-N2	2.65	120.51	116.12
4	B	1304	NAG	C8-C7-N2	2.61	120.45	116.12
4	C	1308	NAG	C8-C7-N2	2.60	120.42	116.12
4	A	1307	NAG	C8-C7-N2	2.58	120.40	116.12
4	B	1302	NAG	C8-C7-N2	2.57	120.38	116.12
4	A	1308	NAG	C4-C3-C2	2.57	114.78	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1309	NAG	C1-O5-C5	2.55	115.60	112.19
4	A	1302	NAG	C2-N2-C7	-2.53	119.51	122.90
4	A	1301	NAG	O5-C1-C2	2.47	115.11	111.29
4	A	1305	NAG	O7-C7-C8	-2.46	117.67	122.05
4	A	1302	NAG	C8-C7-N2	2.44	120.17	116.12
4	C	1306	NAG	C8-C7-N2	2.44	120.17	116.12
4	C	1305	NAG	C8-C7-N2	2.40	120.10	116.12
4	C	1304	NAG	C2-N2-C7	-2.40	119.68	122.90
4	B	1303	NAG	C8-C7-N2	2.40	120.09	116.12
4	A	1301	NAG	C1-O5-C5	2.38	115.37	112.19
4	A	1307	NAG	C2-N2-C7	-2.36	119.73	122.90
4	B	1307	NAG	C8-C7-N2	2.33	119.98	116.12
4	A	1308	NAG	C8-C7-N2	2.31	119.96	116.12
4	B	1306	NAG	C1-C2-N2	-2.31	106.80	110.43
4	B	1304	NAG	C4-C3-C2	-2.30	107.64	111.02
4	B	1309	NAG	C2-N2-C7	-2.29	119.83	122.90
4	C	1302	NAG	C8-C7-N2	2.27	119.89	116.12
4	B	1307	NAG	C6-C5-C4	-2.27	107.45	113.02
4	A	1304	NAG	C8-C7-N2	2.24	119.83	116.12
4	C	1302	NAG	C3-C4-C5	2.22	114.26	110.23
4	C	1304	NAG	C1-C2-N2	-2.22	106.94	110.43
4	B	1305	NAG	C1-O5-C5	2.19	115.12	112.19
4	A	1303	NAG	C8-C7-N2	2.19	119.74	116.12
4	C	1308	NAG	C6-C5-C4	-2.17	107.69	113.02
4	A	1306	NAG	C2-N2-C7	2.17	125.81	122.90
4	A	1304	NAG	C1-O5-C5	2.14	115.05	112.19
4	B	1305	NAG	C6-C5-C4	-2.13	107.79	113.02
4	A	1306	NAG	O7-C7-C8	-2.11	118.29	122.05
4	C	1309	NAG	C8-C7-N2	2.11	119.61	116.12
4	B	1305	NAG	C8-C7-N2	2.11	119.61	116.12
4	A	1303	NAG	C2-N2-C7	-2.11	120.08	122.90
4	C	1303	NAG	C3-C4-C5	2.10	114.04	110.23
4	A	1307	NAG	C6-C5-C4	-2.08	107.90	113.02
4	B	1307	NAG	C1-O5-C5	2.08	114.97	112.19
4	A	1304	NAG	C2-N2-C7	-2.07	120.13	122.90
4	A	1303	NAG	C3-C4-C5	2.06	113.97	110.23
4	B	1302	NAG	C1-O5-C5	2.06	114.94	112.19
4	A	1305	NAG	O5-C1-C2	2.04	114.44	111.29
4	C	1307	NAG	C8-C7-N2	2.01	119.45	116.12
4	C	1305	NAG	C6-C5-C4	-2.01	108.10	113.02

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1306	NAG	C1-C2-N2-C7
4	C	1305	NAG	C4-C5-C6-O6
4	A	1308	NAG	O5-C5-C6-O6
4	C	1309	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	A	1308	NAG	C4-C5-C6-O6
4	C	1309	NAG	C4-C5-C6-O6
4	C	1301	NAG	C4-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	A	1307	NAG	C4-C5-C6-O6
4	B	1301	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	A	1305	NAG	C8-C7-N2-C2
4	A	1305	NAG	O7-C7-N2-C2
4	C	1301	NAG	C8-C7-N2-C2
4	C	1301	NAG	O7-C7-N2-C2
4	B	1309	NAG	C4-C5-C6-O6
4	A	1304	NAG	O5-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	A	1306	NAG	C4-C5-C6-O6
4	C	1302	NAG	C4-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	C	1308	NAG	C4-C5-C6-O6
4	B	1301	NAG	C1-C2-N2-C7
4	C	1303	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	B	1306	NAG	O5-C5-C6-O6
4	A	1304	NAG	C4-C5-C6-O6
4	B	1308	NAG	C3-C2-N2-C7
4	A	1305	NAG	C3-C2-N2-C7
4	A	1309	NAG	C3-C2-N2-C7
4	B	1308	NAG	O5-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	B	1303	NAG	C4-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	B	1308	NAG	C1-C2-N2-C7
4	A	1301	NAG	C1-C2-N2-C7
4	A	1309	NAG	C1-C2-N2-C7
4	B	1301	NAG	C3-C2-N2-C7
4	A	1301	NAG	C3-C2-N2-C7
4	C	1302	NAG	C3-C2-N2-C7
4	C	1303	NAG	C3-C2-N2-C7
4	A	1303	NAG	C4-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1301	NAG	1	0
4	B	1308	NAG	1	0
4	A	1307	NAG	1	0
4	A	1303	NAG	1	0
4	C	1302	NAG	1	0
4	C	1308	NAG	1	0
4	B	1309	NAG	1	0

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.

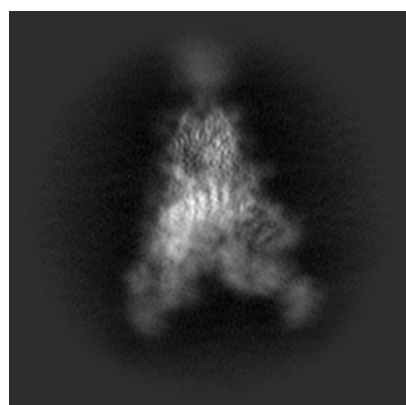
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31033. These allow visual inspection of the internal detail of the map and identification of artifacts.

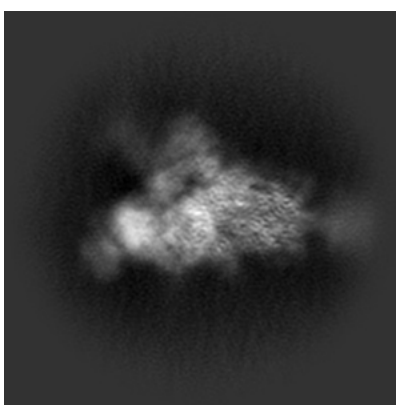
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

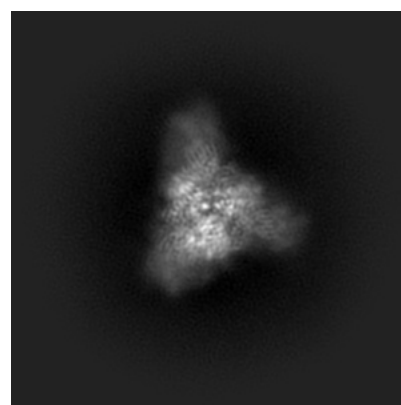
6.1.1 Primary map



X



Y

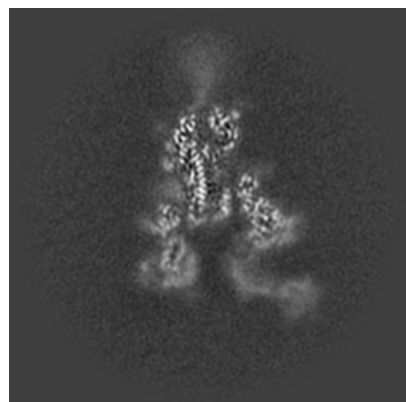


Z

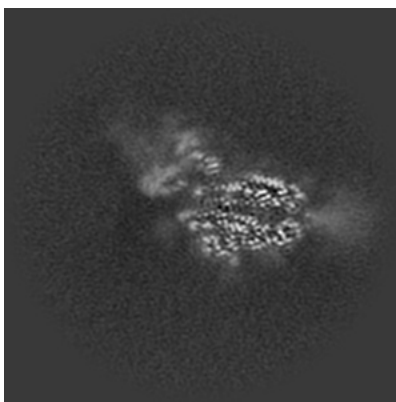
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

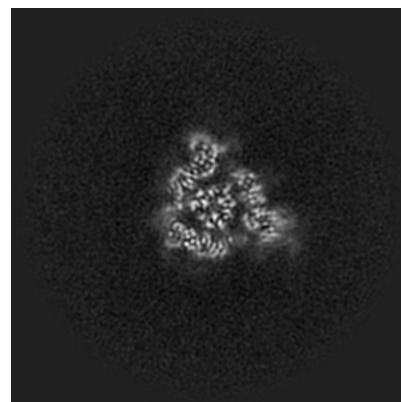
6.2.1 Primary map



X Index: 165



Y Index: 165

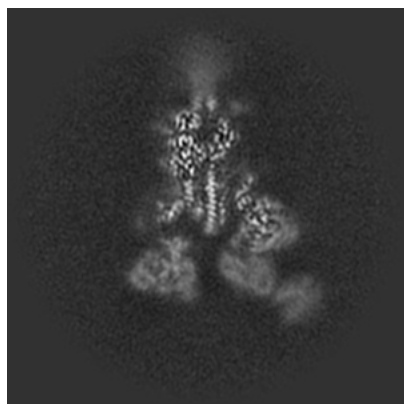


Z Index: 165

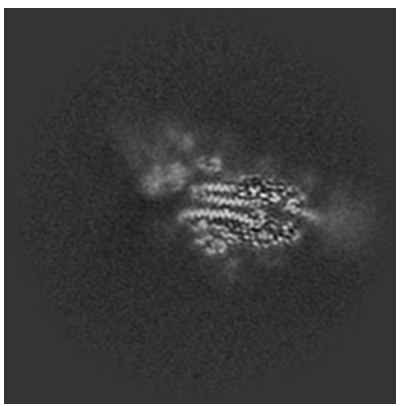
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

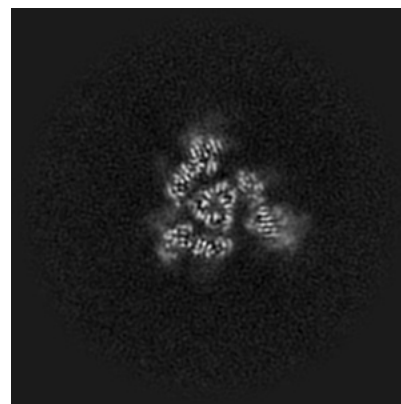
6.3.1 Primary map



X Index: 159



Y Index: 168

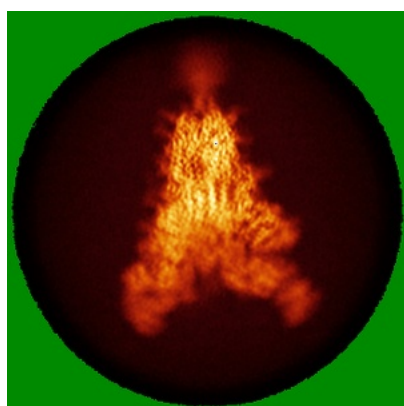


Z Index: 160

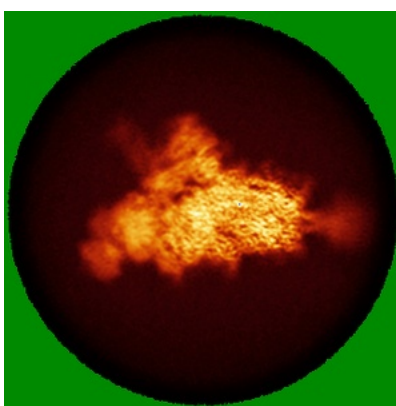
The images above show the largest variance slices of the map in three orthogonal directions.

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

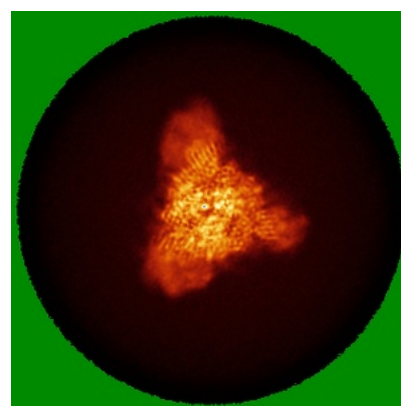
6.4.1 Primary map



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.

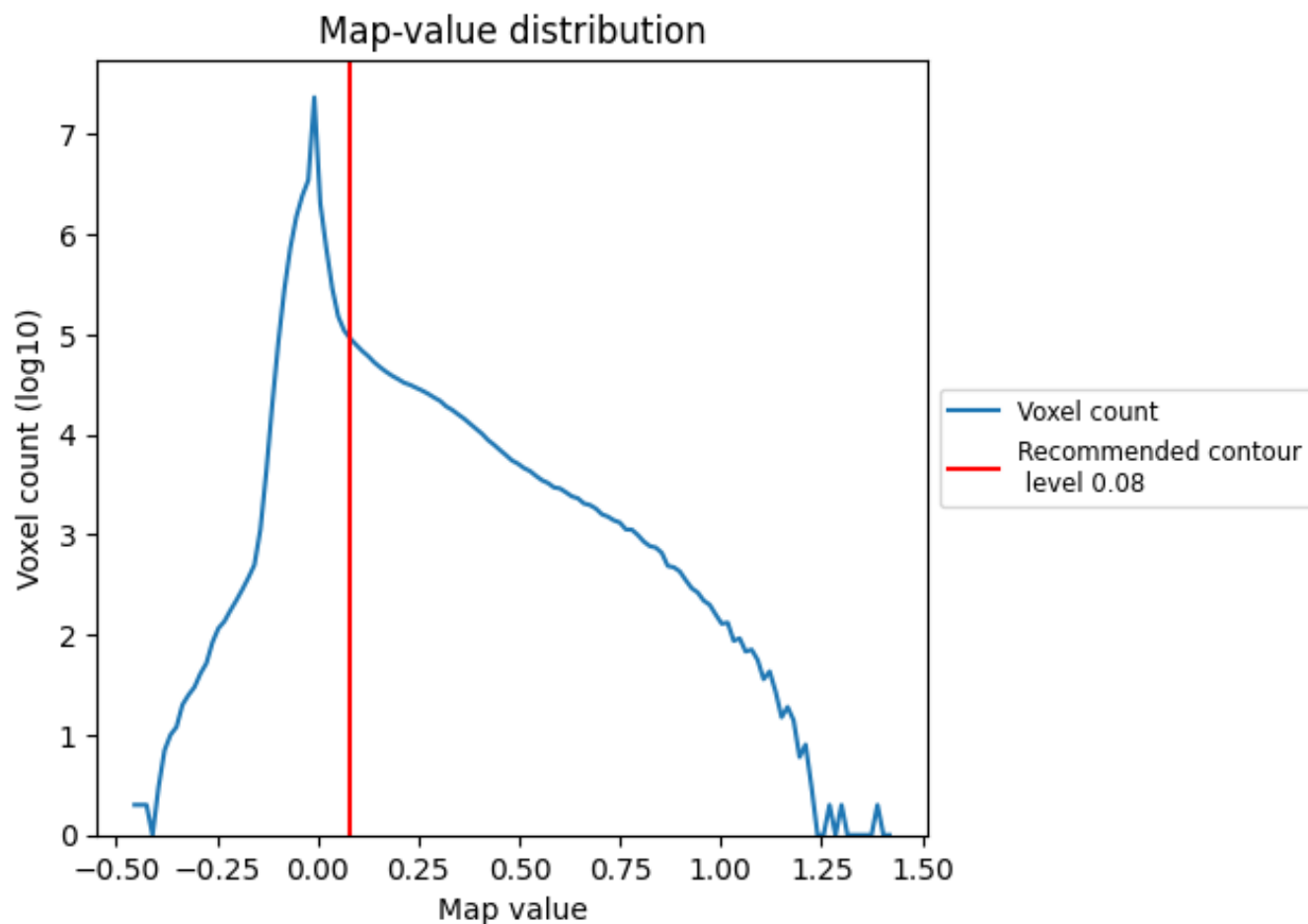
6.6 Mask visualisation

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

7 Map analysis [i](#)

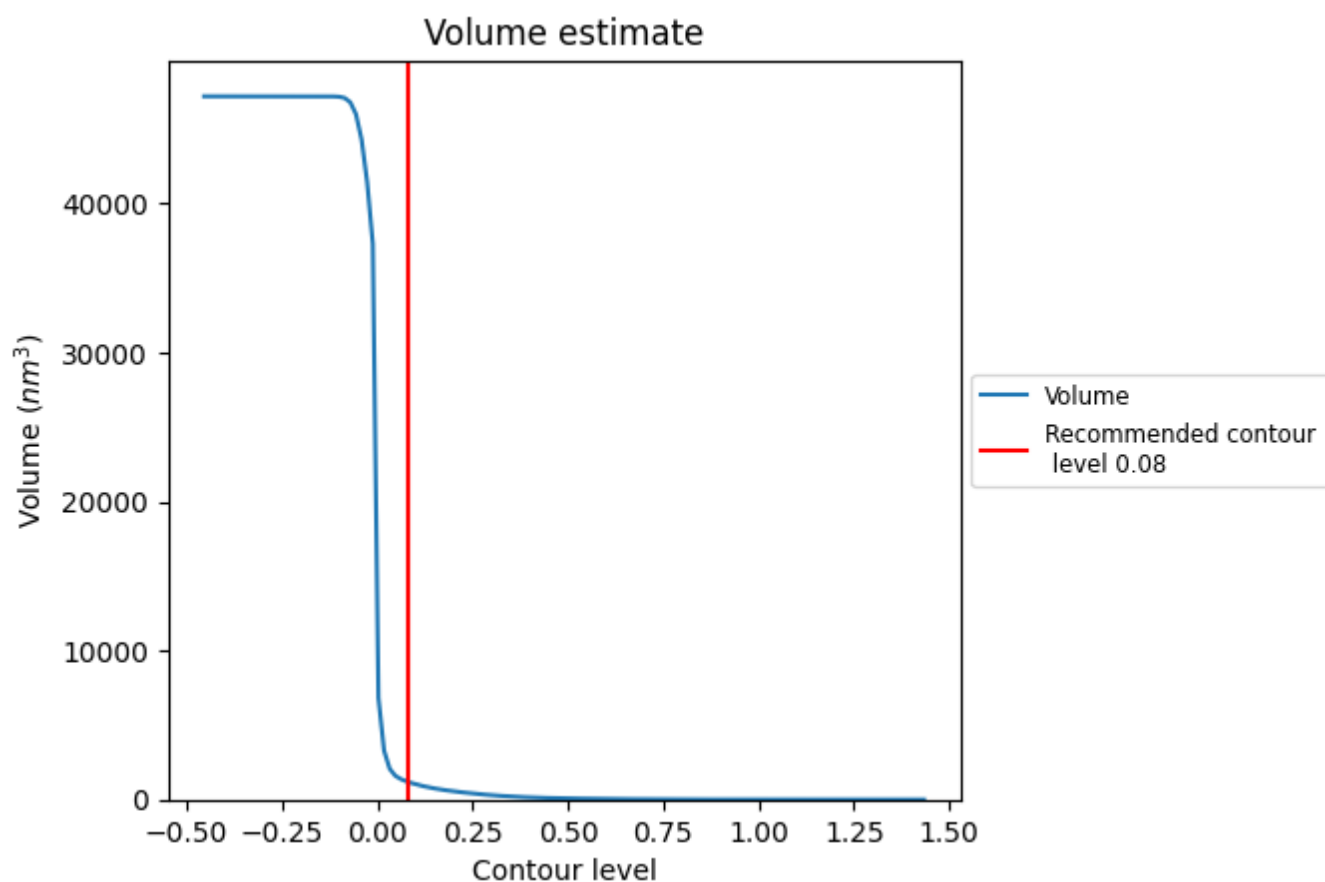
This section contains the results of statistical analysis of the map.

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.

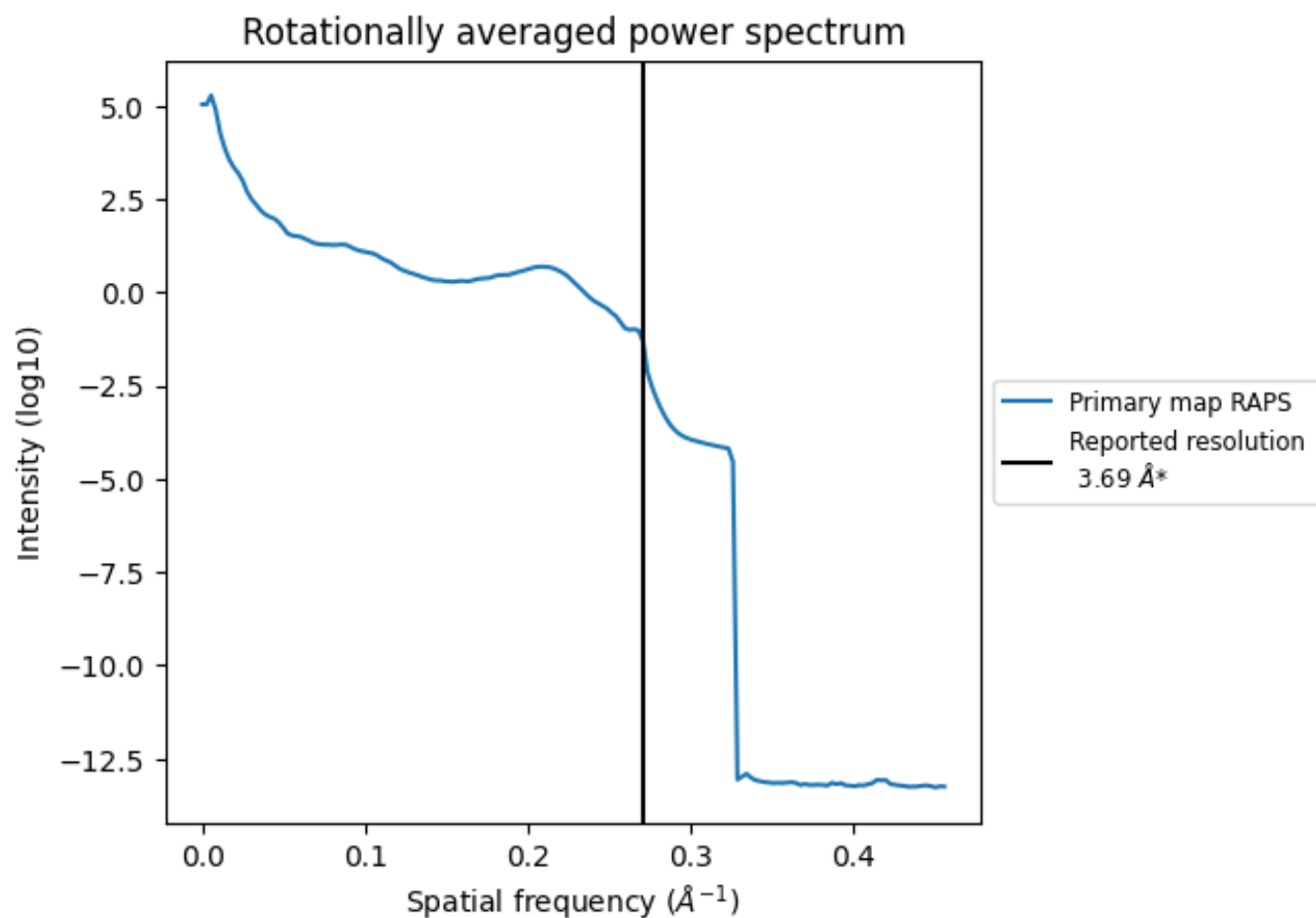
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1192 nm³; this corresponds to an approximate mass of 1077 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 0.271 Å⁻¹

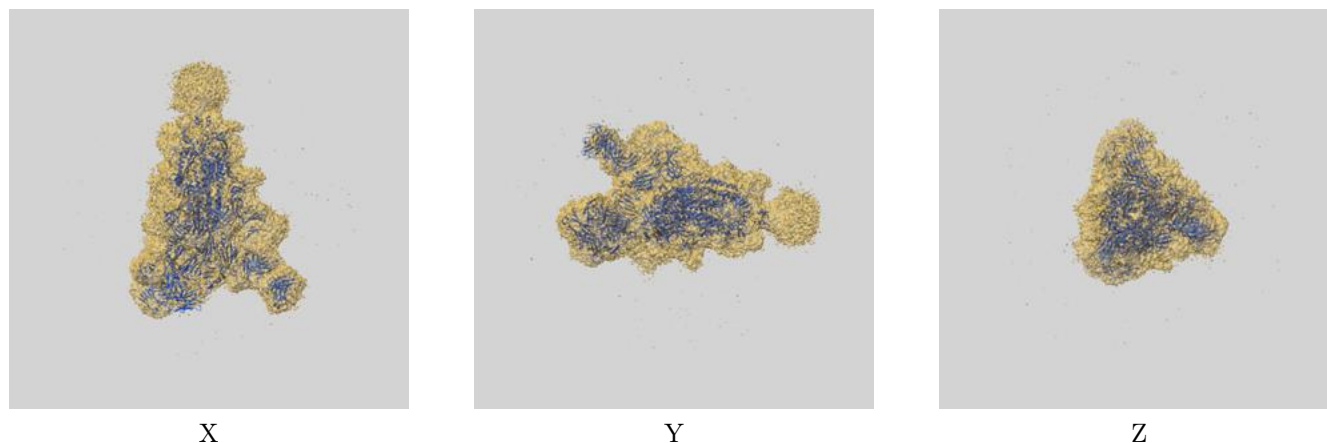
8 Fourier-Shell correlation

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-31033 and PDB model 7E9N. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



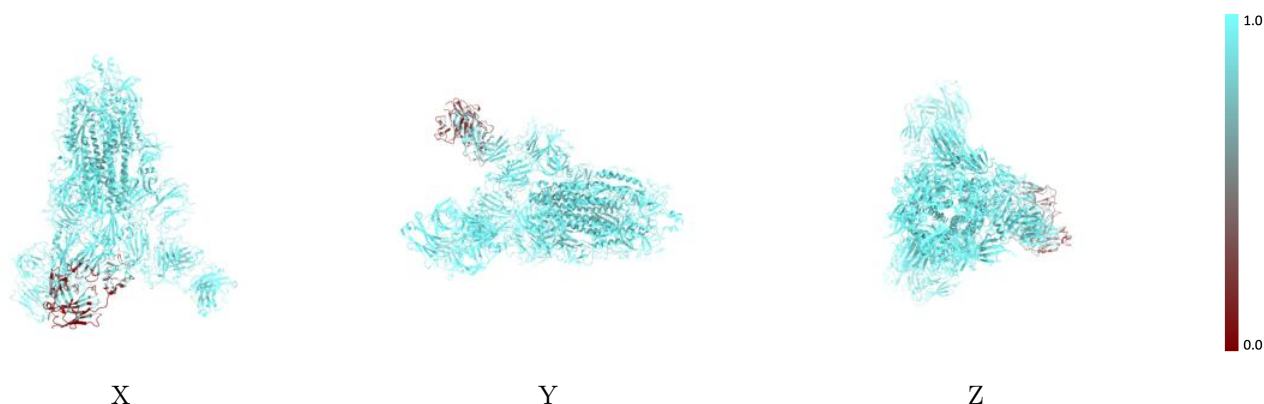
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



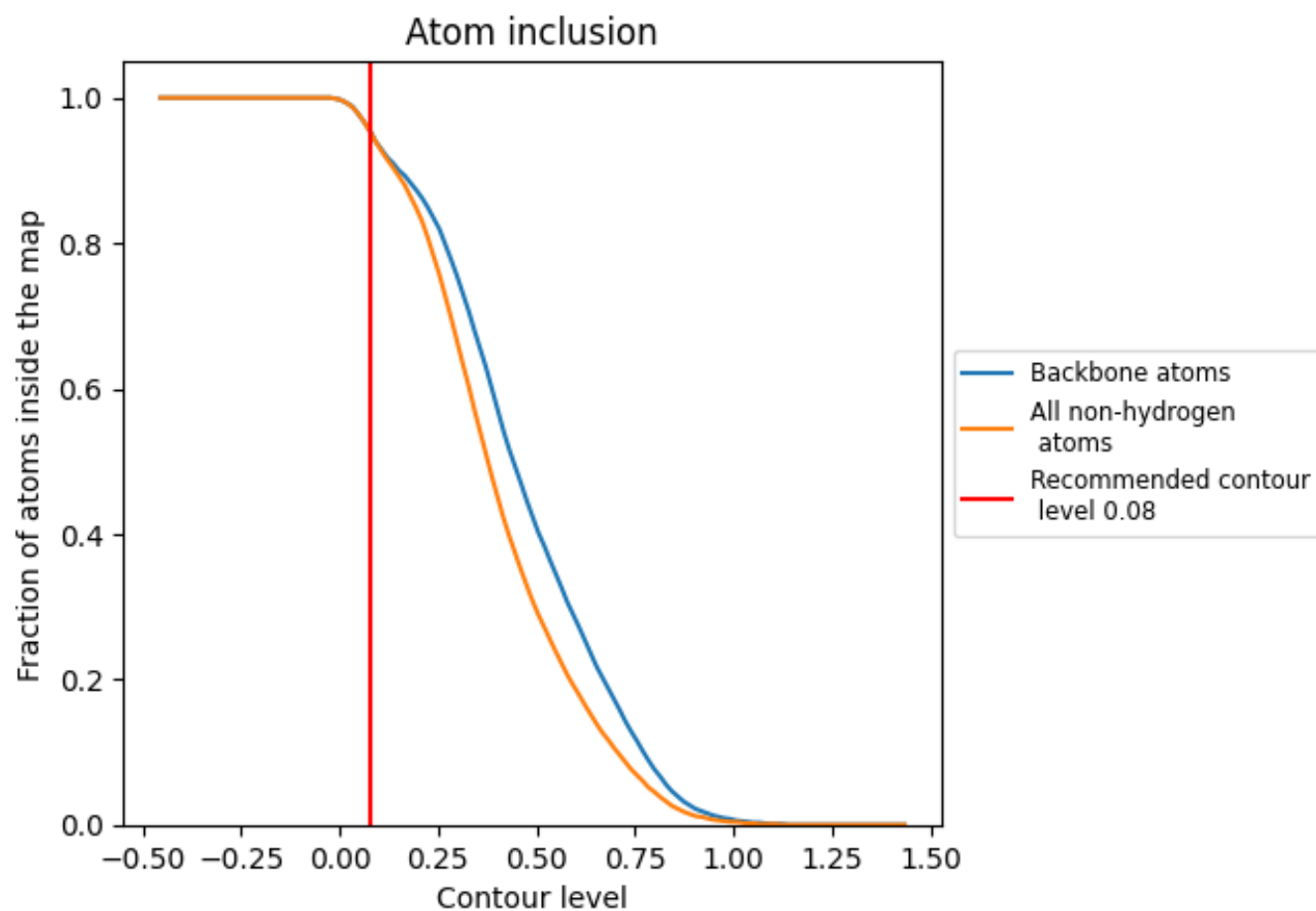
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9510	0.3100
A	0.9990	0.4020
B	0.9990	0.3900
C	0.9990	0.3830
H	0.6140	0.0190
L	0.4410	0.0440
O	0.9930	0.1240
P	0.9930	0.1540
X	0.9950	0.1650
Y	0.9980	0.2000

1.0

0.0

<0.0