



## Full wwPDB EM Validation Report ⓘ

Jun 15, 2025 – 12:49 AM JST

PDB ID : 9JQR / pdb\_00009jqr  
EMDB ID : EMD-61740  
Title : Cryo-EM structure of the Vgamma9Vdelta2 TCR-engaged BTN3A1-BTN3A2-BTN2A1 complex  
Authors : Zhang, M.; Wang, Y.Q.; Xiao, J.Y.  
Deposited on : 2024-09-28  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

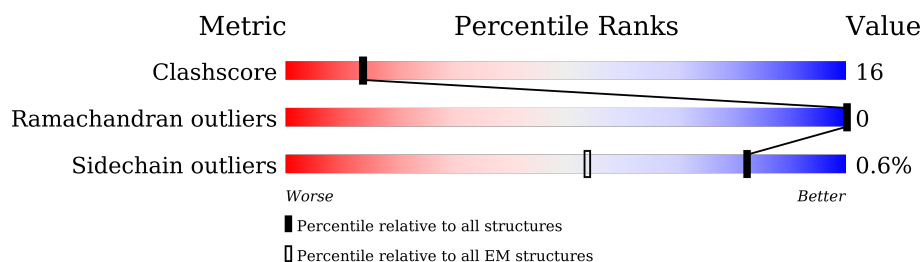
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	527	 55%      33%      • 10%
2	B	318	 59%      32%      • 8%
3	D	274	 62%      12%      26%
4	E	532	 61%      28%      11%
4	F	532	 61%      29%      11%
5	G	295	 62%      16%      23%
6	C	3	 33%      33%      33%
6	H	3	 67%      33%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17295 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 Butyrophilin subfamily 3 member A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	475	Total	C	N	O	S	0	0
			3767	2403	650	698	16		

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	485	GLY	-	expression tag	UNP O00481
A	486	GLY	-	expression tag	UNP O00481
A	487	GLY	-	expression tag	UNP O00481
A	488	GLY	-	expression tag	UNP O00481
A	489	SER	-	expression tag	UNP O00481
A	490	GLY	-	expression tag	UNP O00481
A	491	GLY	-	expression tag	UNP O00481
A	492	GLY	-	expression tag	UNP O00481
A	493	GLY	-	expression tag	UNP O00481
A	494	SER	-	expression tag	UNP O00481
A	495	GLY	-	expression tag	UNP O00481
A	496	GLY	-	expression tag	UNP O00481
A	497	GLY	-	expression tag	UNP O00481
A	498	GLY	-	expression tag	UNP O00481
A	499	SER	-	expression tag	UNP O00481
A	500	TRP	-	expression tag	UNP O00481
A	501	SER	-	expression tag	UNP O00481
A	502	HIS	-	expression tag	UNP O00481
A	503	PRO	-	expression tag	UNP O00481
A	504	GLN	-	expression tag	UNP O00481
A	505	PHE	-	expression tag	UNP O00481
A	506	GLU	-	expression tag	UNP O00481
A	507	LYS	-	expression tag	UNP O00481
A	508	GLY	-	expression tag	UNP O00481
A	509	GLY	-	expression tag	UNP O00481
A	510	GLY	-	expression tag	UNP O00481
A	511	SER	-	expression tag	UNP O00481
A	512	GLY	-	expression tag	UNP O00481

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Chain	Residue	Modelled	Actual	Comment	Reference
A	513	GLY	-	expression tag	UNP O00481
A	514	GLY	-	expression tag	UNP O00481
A	515	SER	-	expression tag	UNP O00481
A	516	GLY	-	expression tag	UNP O00481
A	517	GLY	-	expression tag	UNP O00481
A	518	SER	-	expression tag	UNP O00481
A	519	ALA	-	expression tag	UNP O00481
A	520	TRP	-	expression tag	UNP O00481
A	521	SER	-	expression tag	UNP O00481
A	522	HIS	-	expression tag	UNP O00481
A	523	PRO	-	expression tag	UNP O00481
A	524	GLN	-	expression tag	UNP O00481
A	525	PHE	-	expression tag	UNP O00481
A	526	GLU	-	expression tag	UNP O00481
A	527	LYS	-	expression tag	UNP O00481

- Molecule 2 is a protein called Butyrophilin subfamily 3 member A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	294	Total	C	N	O	S	0	0
			2260	1430	385	435	10		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	306	GLY	-	expression tag	UNP P78410
B	307	GLY	-	expression tag	UNP P78410
B	308	GLY	-	expression tag	UNP P78410
B	309	GLY	-	expression tag	UNP P78410
B	310	SER	-	expression tag	UNP P78410
B	311	ASP	-	expression tag	UNP P78410
B	312	TYR	-	expression tag	UNP P78410
B	313	LYS	-	expression tag	UNP P78410
B	314	ASP	-	expression tag	UNP P78410
B	315	ASP	-	expression tag	UNP P78410
B	316	ASP	-	expression tag	UNP P78410
B	317	ASP	-	expression tag	UNP P78410
B	318	LYS	-	expression tag	UNP P78410

- Molecule 3 is a protein called Vdelta2 T cell receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	203	Total	C	N	O	S	0	0
			1598	1015	267	307	9		

- Molecule 4 is a protein called Butyrophilin subfamily 2 member A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	475	Total	C	N	O	S	0	0
			3821	2426	669	704	22		
4	F	475	Total	C	N	O	S	0	0
			3815	2418	668	706	23		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	500	GLY	-	expression tag	UNP Q7KYR7
E	501	GLY	-	expression tag	UNP Q7KYR7
E	502	GLY	-	expression tag	UNP Q7KYR7
E	503	GLY	-	expression tag	UNP Q7KYR7
E	504	SER	-	expression tag	UNP Q7KYR7
E	505	TRP	-	expression tag	UNP Q7KYR7
E	506	SER	-	expression tag	UNP Q7KYR7
E	507	HIS	-	expression tag	UNP Q7KYR7
E	508	PRO	-	expression tag	UNP Q7KYR7
E	509	GLN	-	expression tag	UNP Q7KYR7
E	510	PHE	-	expression tag	UNP Q7KYR7
E	511	GLU	-	expression tag	UNP Q7KYR7
E	512	LYS	-	expression tag	UNP Q7KYR7
E	513	GLY	-	expression tag	UNP Q7KYR7
E	514	GLY	-	expression tag	UNP Q7KYR7
E	515	GLY	-	expression tag	UNP Q7KYR7
E	516	SER	-	expression tag	UNP Q7KYR7
E	517	GLY	-	expression tag	UNP Q7KYR7
E	518	GLY	-	expression tag	UNP Q7KYR7
E	519	GLY	-	expression tag	UNP Q7KYR7
E	520	SER	-	expression tag	UNP Q7KYR7
E	521	GLY	-	expression tag	UNP Q7KYR7
E	522	GLY	-	expression tag	UNP Q7KYR7
E	523	SER	-	expression tag	UNP Q7KYR7
E	524	ALA	-	expression tag	UNP Q7KYR7
E	525	TRP	-	expression tag	UNP Q7KYR7
E	526	SER	-	expression tag	UNP Q7KYR7
E	527	HIS	-	expression tag	UNP Q7KYR7
E	528	PRO	-	expression tag	UNP Q7KYR7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	529	GLN	-	expression tag	UNP Q7KYR7
E	530	PHE	-	expression tag	UNP Q7KYR7
E	531	GLU	-	expression tag	UNP Q7KYR7
E	532	LYS	-	expression tag	UNP Q7KYR7
F	500	GLY	-	expression tag	UNP Q7KYR7
F	501	GLY	-	expression tag	UNP Q7KYR7
F	502	GLY	-	expression tag	UNP Q7KYR7
F	503	GLY	-	expression tag	UNP Q7KYR7
F	504	SER	-	expression tag	UNP Q7KYR7
F	505	TRP	-	expression tag	UNP Q7KYR7
F	506	SER	-	expression tag	UNP Q7KYR7
F	507	HIS	-	expression tag	UNP Q7KYR7
F	508	PRO	-	expression tag	UNP Q7KYR7
F	509	GLN	-	expression tag	UNP Q7KYR7
F	510	PHE	-	expression tag	UNP Q7KYR7
F	511	GLU	-	expression tag	UNP Q7KYR7
F	512	LYS	-	expression tag	UNP Q7KYR7
F	513	GLY	-	expression tag	UNP Q7KYR7
F	514	GLY	-	expression tag	UNP Q7KYR7
F	515	GLY	-	expression tag	UNP Q7KYR7
F	516	SER	-	expression tag	UNP Q7KYR7
F	517	GLY	-	expression tag	UNP Q7KYR7
F	518	GLY	-	expression tag	UNP Q7KYR7
F	519	GLY	-	expression tag	UNP Q7KYR7
F	520	SER	-	expression tag	UNP Q7KYR7
F	521	GLY	-	expression tag	UNP Q7KYR7
F	522	GLY	-	expression tag	UNP Q7KYR7
F	523	SER	-	expression tag	UNP Q7KYR7
F	524	ALA	-	expression tag	UNP Q7KYR7
F	525	TRP	-	expression tag	UNP Q7KYR7
F	526	SER	-	expression tag	UNP Q7KYR7
F	527	HIS	-	expression tag	UNP Q7KYR7
F	528	PRO	-	expression tag	UNP Q7KYR7
F	529	GLN	-	expression tag	UNP Q7KYR7
F	530	PHE	-	expression tag	UNP Q7KYR7
F	531	GLU	-	expression tag	UNP Q7KYR7
F	532	LYS	-	expression tag	UNP Q7KYR7

- Molecule 5 is a protein called Vgamma9 T cell receptor.

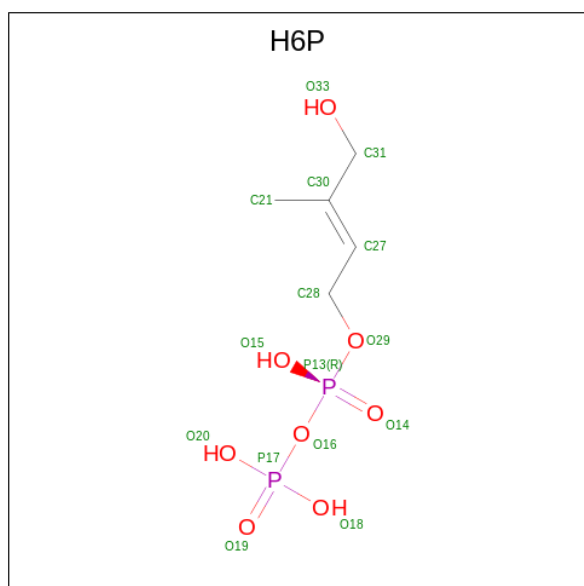
Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	228	Total	C	N	O	S	0	0
			1815	1158	302	349	6		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
6	C	3	Total	C	N	O	0	0
			39	22	2	15		
6	H	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is (2E)-4-hydroxy-3-methylbut-2-en-1-yl trihydrogen diphosphate (CCD ID: H6P) (formula:  $C_5H_{12}O_8P_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	O	P	0
			15	5	8	2	

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



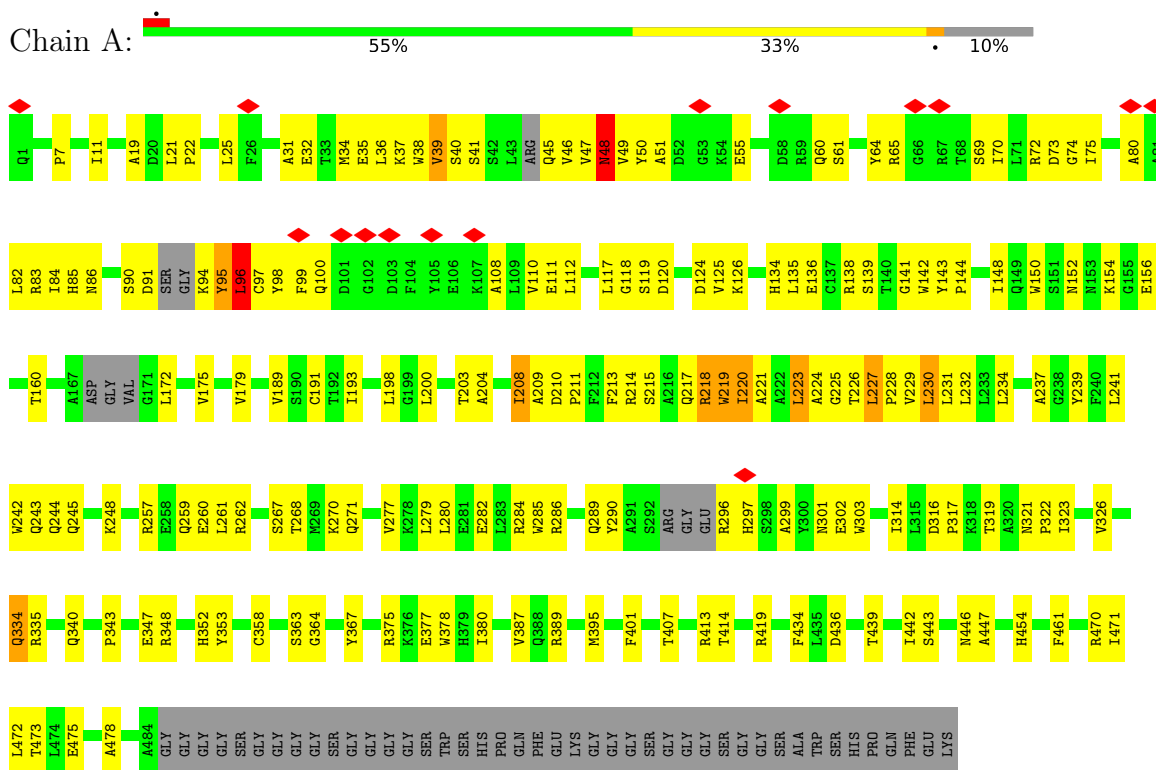
Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	F	1	Total	C	N	O	0
			14	8	1	5	
8	F	1	Total	C	N	O	0
			14	8	1	5	
8	F	1	Total	C	N	O	0
			14	8	1	5	
8	F	1	Total	C	N	O	0
			14	8	1	5	



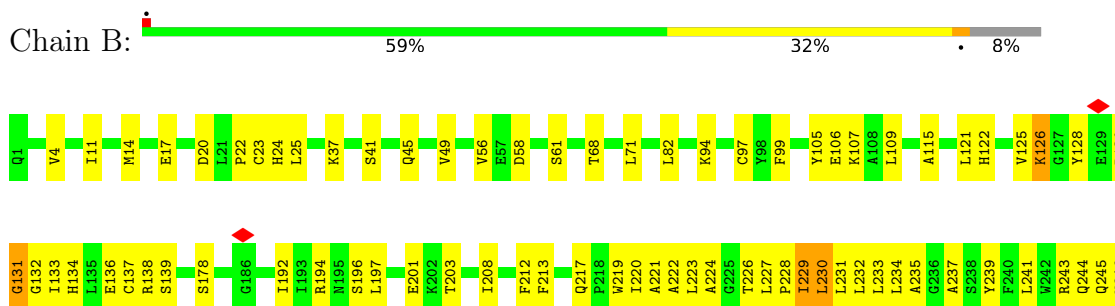
### 3 Residue-property plots

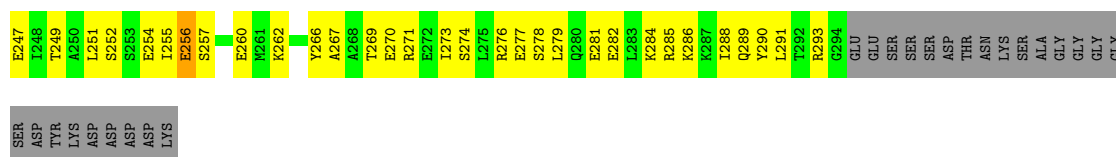
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Butyrophilin subfamily 3 member A1

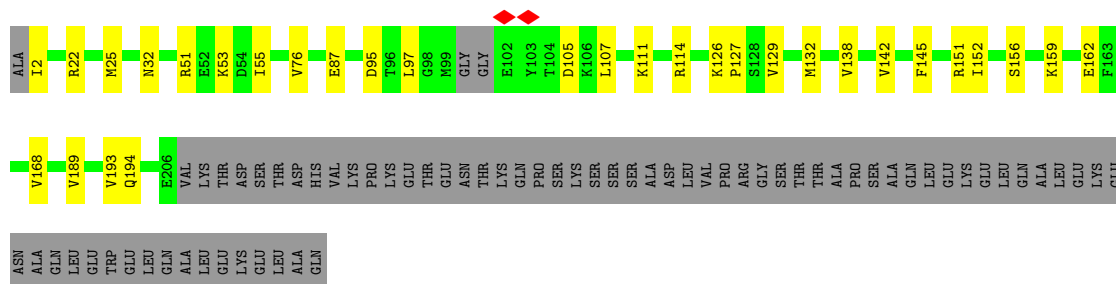


#### • Molecule 2: Butyrophilin subfamily 3 member A2

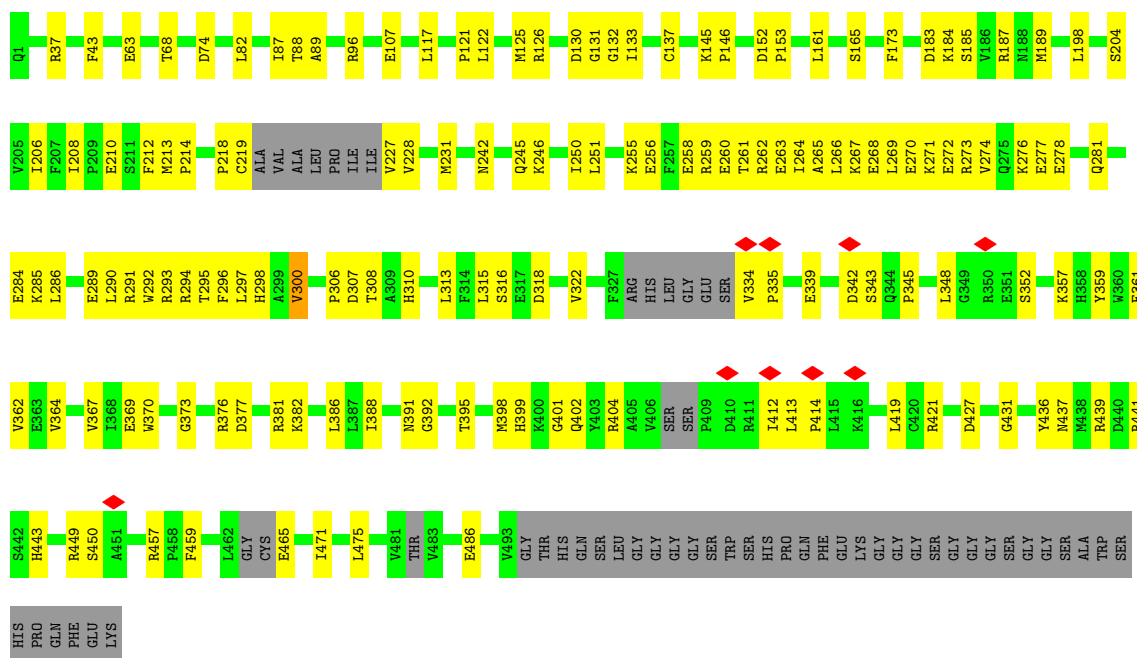




• Molecule 3: Vdelta2 T cell receptor

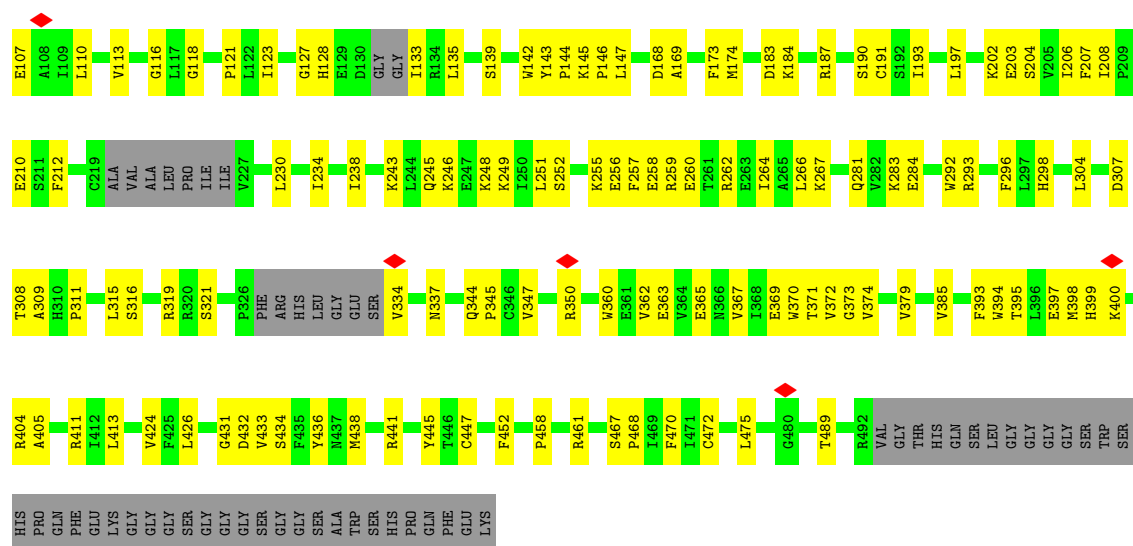


• Molecule 4: Butyrophilin subfamily 2 member A1

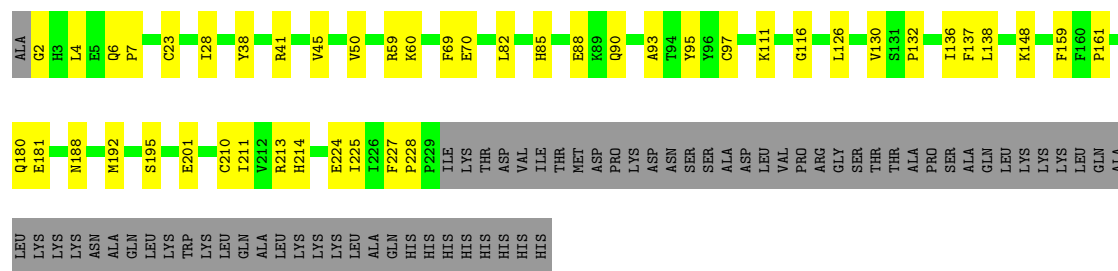


• Molecule 4: Butyrophilin subfamily 2 member A1





• Molecule 5: Vgamma9 T cell receptor



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	282479	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60.0	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	19.269	Depositor
Minimum map value	-0.100	Depositor
Average map value	-0.021	Depositor
Map value standard deviation	0.336	Depositor
Recommended contour level	2	Depositor
Map size (Å)	399.0, 399.0, 399.0	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, H6P

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.28	0/3857	0.55	6/5224 (0.1%)
2	B	0.37	0/2303	0.64	4/3117 (0.1%)
3	D	0.18	0/1632	0.36	0/2208
4	E	0.20	0/3905	0.42	0/5279
4	F	0.14	0/3900	0.36	0/5277
5	G	0.21	0/1854	0.39	1/2511 (0.0%)
All	All	0.24	0/17451	0.46	11/23616 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	131	GLY	N-CA-C	-7.89	104.99	115.40
1	A	227	LEU	CA-C-N	-7.18	111.13	119.32
1	A	227	LEU	C-N-CA	-7.18	111.13	119.32
1	A	96	LEU	CB-CA-C	-6.36	101.37	111.17
1	A	48	ASN	N-CA-C	6.08	118.09	108.79
1	A	95	TYR	N-CA-C	5.61	116.67	108.14
2	B	24	HIS	N-CA-C	5.60	117.49	109.14
1	A	39	VAL	N-CA-C	5.54	116.46	108.48
5	G	188	ASN	CB-CA-C	-5.20	110.59	116.63
2	B	256	GLU	N-CA-CB	5.13	117.66	110.12
2	B	126	LYS	N-CA-C	5.11	116.93	111.36

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	3767	0	3730	173	0
2	B	2260	0	2252	112	0
3	D	1598	0	1581	23	0
4	E	3821	0	3791	118	0
4	F	3815	0	3781	126	0
5	G	1815	0	1829	30	0
6	C	39	0	34	4	0
6	H	39	0	34	0	0
7	A	15	0	9	2	0
8	B	14	0	13	0	0
8	E	42	0	39	0	0
8	F	70	0	65	1	0
All	All	17295	0	17158	538	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 16.

All (538) 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:39:VAL:HG12	1:A:41:SER:H	1.23	1.00
1:A:35:GLU:HB3	1:A:100:GLN:O	1.71	0.88
1:A:224:ALA:O	1:A:228:PRO:HD2	1.77	0.84
1:A:241:LEU:O	1:A:244:GLN:HG3	1.79	0.82
1:A:39:VAL:HG13	1:A:46:VAL:HG22	1.64	0.79
1:A:39:VAL:HB	1:A:96:LEU:HB2	1.65	0.79
1:A:37:LYS:HG3	1:A:49:VAL:HG22	1.65	0.78
1:A:234:LEU:HB3	2:B:234:LEU:HD11	1.65	0.78
4:E:298:HIS:CE1	4:E:300:VAL:HG13	2.19	0.77
1:A:118:GLY:HA3	1:A:142:TRP:CE2	2.20	0.76
1:A:83:ARG:HG2	1:A:85:HIS:CE1	2.22	0.74
2:B:224:ALA:O	2:B:228:PRO:HD2	1.88	0.73
4:F:371:THR:HB	4:F:461:ARG:HB3	1.69	0.73
4:E:286:LEU:HA	4:E:289:GLU:HG2	1.69	0.73
1:A:237:ALA:HB1	2:B:241:LEU:HD11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:LYS:HB2	2:B:134:HIS:CD2	2.25	0.72
4:F:118:GLY:HA3	4:F:142:TRP:CE2	2.24	0.72
3:D:22:ARG:HG2	3:D:76:VAL:HG22	1.72	0.71
4:E:298:HIS:CE1	4:F:296:PHE:HB3	2.25	0.71
1:A:242:TRP:O	1:A:245:GLN:HG2	1.90	0.71
1:A:261:LEU:HD11	2:B:262:LYS:HE3	1.73	0.70
1:A:223:LEU:CD1	2:B:223:LEU:HD23	2.21	0.70
2:B:134:HIS:HE1	2:B:178:SER:HB3	1.57	0.70
1:A:90:SER:O	1:A:91:ASP:C	2.33	0.70
2:B:11:ILE:HD11	2:B:22:PRO:HD2	1.73	0.70
2:B:128:TYR:CD2	2:B:131:GLY:HA2	2.26	0.69
2:B:126:LYS:HB2	2:B:134:HIS:HD2	1.57	0.69
2:B:136:GLU:OE1	2:B:138:ARG:NH2	2.25	0.69
5:G:38:TYR:OH	5:G:111:LYS:NZ	2.25	0.69
1:A:148:ILE:HG12	1:A:193:ILE:HG22	1.73	0.69
1:A:213:PHE:C	1:A:215:SER:H	2.00	0.69
4:E:270:GLU:HA	4:E:273:ARG:HG2	1.73	0.69
1:A:375:ARG:HH21	1:A:471:ILE:HB	1.57	0.68
2:B:227:LEU:O	2:B:230:LEU:HG	1.93	0.68
1:A:35:GLU:HA	1:A:51:ALA:HB2	1.76	0.68
2:B:251:LEU:O	2:B:254:GLU:HG3	1.94	0.68
1:A:39:VAL:HG12	1:A:41:SER:N	2.05	0.67
1:A:124:ASP:OD2	1:A:138:ARG:NH1	2.30	0.65
2:B:192:ILE:HG12	2:B:203:THR:HG22	1.78	0.65
1:A:286:ARG:HH11	1:A:290:TYR:HE1	1.42	0.65
1:A:227:LEU:HB3	1:A:228:PRO:HD2	1.78	0.65
4:F:399:HIS:HE2	4:F:404:ARG:HE	1.44	0.65
4:F:190:SER:HA	4:F:204:SER:O	1.96	0.65
4:E:449:ARG:NH1	4:E:450:SER:O	2.30	0.64
4:F:264:ILE:HA	4:F:267:LYS:HE2	1.78	0.64
1:A:31:ALA:HA	1:A:34:MET:HE2	1.79	0.64
4:F:98:TYR:HD1	4:F:107:GLU:HG3	1.63	0.64
2:B:133:ILE:HG21	2:B:208:ILE:CD1	2.28	0.64
2:B:243:ARG:HH11	2:B:246:LYS:NZ	1.97	0.63
4:E:292:TRP:HB2	4:E:296:PHE:CZ	2.34	0.63
1:A:208:ILE:HA	2:B:125:VAL:CG2	2.29	0.63
1:A:210:ASP:N	1:A:211:PRO:HD2	2.13	0.63
1:A:198:LEU:HG	1:A:200:LEU:HD13	1.81	0.62
4:E:125:MET:HE2	4:E:208:ILE:HG12	1.81	0.62
1:A:37:LYS:HB3	1:A:98:TYR:HB2	1.81	0.62
1:A:223:LEU:HD13	2:B:223:LEU:HD23	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:441:ARG:NH1	4:F:472:CYS:SG	2.73	0.62
1:A:7:PRO:HB3	1:A:22:PRO:HG2	1.82	0.62
2:B:229:ILE:HG12	2:B:230:LEU:HD23	1.81	0.62
1:A:239:TYR:O	1:A:243:GLN:HG2	2.00	0.61
1:A:290:TYR:HB3	1:A:303:TRP:HE1	1.66	0.61
4:F:257:PHE:O	4:F:260:GLU:HG2	2.01	0.61
4:F:38:TRP:CZ3	4:F:82:LEU:HB2	2.35	0.61
1:A:223:LEU:HD22	2:B:223:LEU:HB3	1.81	0.61
1:A:220:ILE:O	1:A:223:LEU:HG	2.01	0.60
2:B:257:SER:O	2:B:260:GLU:HG3	2.01	0.60
4:E:227:VAL:HG23	4:F:230:LEU:HD21	1.82	0.60
4:F:127:GLY:O	4:F:133:ILE:N	2.35	0.60
4:F:373:GLY:HA3	4:F:395:THR:HG22	1.82	0.60
1:A:39:VAL:CB	1:A:96:LEU:HB2	2.30	0.60
1:A:214:ARG:HA	1:A:214:ARG:HH21	1.66	0.60
2:B:217:GLN:O	2:B:220:ILE:HG12	2.02	0.60
4:E:412:ILE:HG13	4:E:414:PRO:HD3	1.84	0.60
4:E:436:TYR:HD2	4:F:475:LEU:HD13	1.67	0.60
1:A:83:ARG:CG	1:A:85:HIS:CE1	2.85	0.60
4:F:48:PHE:CE2	4:F:50:TYR:HB2	2.37	0.60
4:F:135:LEU:HD11	4:F:208:ILE:HD11	1.83	0.60
2:B:134:HIS:CE1	2:B:178:SER:HB3	2.37	0.59
2:B:262:LYS:HG2	2:B:266:TYR:CE2	2.37	0.59
1:A:414:THR:HG21	1:A:454:HIS:CD2	2.37	0.59
4:F:394:TRP:HB3	4:F:433:VAL:HG11	1.83	0.59
1:A:227:LEU:HB3	1:A:228:PRO:CD	2.32	0.59
1:A:227:LEU:O	1:A:231:LEU:HG	2.02	0.59
4:F:38:TRP:HZ2	4:F:80:VAL:HB	1.67	0.59
1:A:95:TYR:C	1:A:96:LEU:HD12	2.27	0.59
2:B:267:ALA:O	2:B:270:GLU:HG2	2.02	0.59
2:B:278:SER:O	2:B:281:GLU:HG3	2.01	0.59
4:F:363:GLU:HB3	4:F:470:PHE:HB2	1.85	0.59
2:B:244:GLN:NE2	2:B:245:GLN:HG3	2.18	0.58
2:B:243:ARG:HH11	2:B:246:LYS:HZ1	1.51	0.58
2:B:107:LYS:HE3	3:D:97:LEU:HD22	1.84	0.58
4:E:145:LYS:HE3	4:E:165:SER:HB2	1.86	0.58
4:E:369:GLU:OE1	4:E:465:GLU:N	2.36	0.58
1:A:213:PHE:CG	1:A:214:ARG:N	2.70	0.58
4:E:37:ARG:NH1	4:E:43:PHE:O	2.36	0.58
1:A:39:VAL:O	1:A:95:TYR:HA	2.03	0.58
4:E:291:ARG:O	4:E:295:THR:HG23	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:213:MET:SD	4:E:214:PRO:HD2	2.43	0.58
4:F:365:GLU:O	4:F:467:SER:OG	2.22	0.58
4:F:37:ARG:NH1	4:F:48:PHE:O	2.36	0.58
2:B:279:LEU:O	2:B:282:GLU:HG3	2.04	0.57
2:B:126:LYS:HD3	2:B:134:HIS:CD2	2.39	0.57
4:E:398:MET:HE2	4:E:401:GLY:H	1.69	0.57
4:E:306:PRO:HB3	4:E:315:LEU:HD22	1.85	0.57
1:A:220:ILE:HB	2:B:219:TRP:CH2	2.38	0.57
1:A:231:LEU:O	1:A:234:LEU:HG	2.04	0.57
4:E:218:PRO:O	4:E:219:CYS:C	2.48	0.57
4:E:315:LEU:HG	4:E:322:VAL:HG12	1.85	0.57
2:B:126:LYS:CB	2:B:134:HIS:HD2	2.18	0.57
2:B:130:ASP:C	2:B:132:GLY:H	2.12	0.57
2:B:133:ILE:HG21	2:B:208:ILE:HD13	1.86	0.57
1:A:38:TRP:CB	1:A:82:LEU:HD22	2.35	0.57
4:E:130:ASP:OD1	4:E:131:GLY:N	2.36	0.57
4:F:370:TRP:HZ3	4:F:372:VAL:HG22	1.69	0.57
1:A:35:GLU:HA	1:A:51:ALA:CB	2.35	0.57
1:A:280:LEU:O	1:A:284:ARG:HG3	2.04	0.57
4:F:345:PRO:HD2	4:F:461:ARG:HG2	1.87	0.57
1:A:94:LYS:O	1:A:95:TYR:CG	2.59	0.56
1:A:213:PHE:HE2	2:B:128:TYR:CD1	2.24	0.56
4:F:245:GLN:O	4:F:248:LYS:HG3	2.05	0.56
1:A:32:GLU:O	1:A:72:ARG:NH2	2.38	0.56
1:A:224:ALA:O	1:A:228:PRO:CD	2.50	0.56
2:B:288:ILE:HD13	2:B:291:LEU:HD21	1.88	0.56
1:A:48:ASN:OD1	1:A:82:LEU:HD11	2.06	0.56
2:B:239:TYR:OH	2:B:243:ARG:NH2	2.32	0.56
3:D:87:GLU:OE2	3:D:114:ARG:NH2	2.39	0.56
4:F:24:HIS:CD2	4:F:25:LEU:HD23	2.41	0.56
5:G:60:LYS:NZ	5:G:69:PHE:O	2.36	0.56
2:B:4:VAL:HG22	2:B:25:LEU:CD2	2.36	0.56
4:E:291:ARG:HA	4:E:294:ARG:NH1	2.21	0.55
2:B:68:THR:HB	2:B:82:LEU:HD11	1.88	0.55
3:D:156:SER:HB3	3:D:189:VAL:HG12	1.88	0.55
4:E:291:ARG:HA	4:E:294:ARG:CZ	2.36	0.55
4:F:144:PRO:CG	4:F:197:LEU:CD1	2.85	0.55
4:F:311:PRO:HB3	4:F:334:VAL:HG11	1.87	0.55
1:A:296:ARG:HB2	1:A:299:ALA:HB3	1.87	0.55
2:B:97:CYS:O	2:B:107:LYS:HA	2.06	0.55
4:E:255:LYS:HG3	4:F:251:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:2:GLY:HA2	5:G:28:ILE:HB	1.89	0.55
3:D:105:ASP:OD1	5:G:59:ARG:NH1	2.39	0.55
4:F:145:LYS:HA	4:F:173:PHE:CD2	2.42	0.55
5:G:70:GLU:OE2	5:G:85:HIS:NE2	2.26	0.55
1:A:82:LEU:O	1:A:82:LEU:HG	2.06	0.55
4:E:291:ARG:NH1	4:E:295:THR:HG21	2.22	0.55
4:E:273:ARG:O	4:E:276:LYS:HG3	2.06	0.54
1:A:290:TYR:HB3	1:A:303:TRP:NE1	2.22	0.54
1:A:316:ASP:OD2	1:A:319:THR:N	2.40	0.54
4:F:22:ARG:NH2	4:F:79:SER:OG	2.41	0.54
1:A:285:TRP:O	1:A:289:GLN:HG3	2.08	0.54
4:F:144:PRO:HG2	4:F:197:LEU:CD1	2.38	0.54
1:A:39:VAL:CG2	1:A:96:LEU:HB2	2.37	0.54
3:D:95:ASP:HB2	3:D:107:LEU:HD23	1.90	0.54
4:F:252:SER:O	4:F:255:LYS:HG3	2.07	0.54
2:B:244:GLN:O	2:B:247:GLU:HG2	2.08	0.54
4:F:434:SER:HA	4:F:445:TYR:O	2.07	0.54
5:G:138:LEU:HD21	5:G:228:PRO:HD2	1.90	0.54
1:A:119:SER:O	1:A:139:SER:OG	2.22	0.54
4:F:144:PRO:HD3	4:F:197:LEU:HD12	1.90	0.54
4:E:250:ILE:HG13	4:E:251:LEU:HD12	1.90	0.54
1:A:152:ASN:HA	1:A:189:VAL:HG12	1.90	0.53
1:A:38:TRP:HB3	1:A:82:LEU:HD22	1.90	0.53
1:A:50:TYR:HB3	1:A:70:ILE:HD12	1.90	0.53
4:F:144:PRO:CD	4:F:197:LEU:HD12	2.38	0.53
4:E:292:TRP:HB2	4:E:296:PHE:CE2	2.44	0.53
1:A:120:ASP:OD2	2:B:203:THR:OG1	2.25	0.53
2:B:230:LEU:O	2:B:233:LEU:HB3	2.08	0.53
4:F:142:TRP:HH2	4:F:202:LYS:HE2	1.73	0.53
1:A:436:ASP:OD2	1:A:439:THR:OG1	2.25	0.53
1:A:69:SER:O	1:A:82:LEU:HD12	2.09	0.53
2:B:192:ILE:HG23	2:B:201:GLU:HG3	1.91	0.53
1:A:61:SER:HB3	1:A:64:TYR:HB2	1.91	0.53
1:A:118:GLY:HA3	1:A:142:TRP:NE1	2.23	0.53
4:F:168:ASP:OD1	4:F:169:ALA:N	2.40	0.53
1:A:73:ASP:OD1	1:A:74:GLY:N	2.41	0.53
1:A:150:TRP:CD2	1:A:191:CYS:HB3	2.43	0.53
1:A:321:ASN:ND2	1:A:352:HIS:O	2.42	0.53
2:B:4:VAL:HG23	2:B:106:GLU:HB3	1.91	0.52
4:F:255:LYS:HA	4:F:258:GLU:HG3	1.90	0.52
4:F:316:SER:OG	4:F:321:SER:OG	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:VAL:HA	1:A:46:VAL:HG13	1.90	0.52
3:D:142:VAL:HG11	3:D:193:VAL:HG11	1.91	0.52
1:A:214:ARG:HH22	2:B:212:PHE:HD2	1.58	0.52
1:A:223:LEU:HD12	1:A:224:ALA:N	2.24	0.52
4:E:291:ARG:CZ	4:E:295:THR:HG21	2.38	0.52
1:A:38:TRP:HH2	1:A:80:ALA:HB3	1.74	0.52
1:A:85:HIS:O	1:A:86:ASN:C	2.52	0.52
2:B:122:HIS:HB3	2:B:138:ARG:HG2	1.90	0.52
4:E:183:ASP:OD1	4:E:185:SER:N	2.37	0.52
4:F:344:GLN:HE22	4:F:385:VAL:H	1.55	0.52
4:F:405:ALA:HB2	4:F:413:LEU:HD21	1.91	0.52
2:B:246:LYS:O	2:B:249:THR:HG22	2.09	0.52
2:B:262:LYS:HG2	2:B:266:TYR:HE2	1.74	0.52
4:F:38:TRP:CZ2	4:F:80:VAL:HB	2.45	0.52
1:A:118:GLY:HA2	1:A:141:GLY:O	2.10	0.52
4:F:39:PHE:CE2	4:F:96:ARG:HD2	2.45	0.52
1:A:124:ASP:OD1	1:A:136:GLU:HB2	2.09	0.51
1:A:442:ILE:HD11	1:A:461:PHE:HZ	1.75	0.51
2:B:219:TRP:CE3	2:B:223:LEU:HD22	2.46	0.51
4:F:69:THR:HB	4:F:83:VAL:HB	1.92	0.51
1:A:11:ILE:HB	1:A:112:LEU:HD12	1.91	0.51
1:A:227:LEU:HD12	1:A:230:LEU:HD11	1.91	0.51
1:A:317:PRO:HG3	1:A:326:VAL:HG11	1.92	0.51
3:D:111:LYS:HG2	5:G:45:VAL:HG12	1.92	0.51
1:A:419:ARG:NH1	7:A:601:H6P:O18	2.44	0.51
2:B:226:THR:O	2:B:229:ILE:HG12	2.10	0.51
2:B:252:SER:O	2:B:256:GLU:OE1	2.28	0.51
3:D:138:VAL:HG11	3:D:189:VAL:HG21	1.91	0.51
4:E:298:HIS:ND1	4:E:300:VAL:HG22	2.25	0.51
4:F:370:TRP:NE1	4:F:398:MET:HE2	2.25	0.51
1:A:375:ARG:NH2	1:A:473:THR:O	2.43	0.51
4:F:370:TRP:HE1	4:F:398:MET:HE2	1.75	0.51
1:A:209:ALA:HB3	1:A:214:ARG:HG3	1.92	0.51
4:E:242:ASN:O	4:E:245:GLN:HG2	2.10	0.51
1:A:154:LYS:HG3	1:A:156:GLU:HG3	1.92	0.51
3:D:132:MET:HE2	5:G:137:PHE:HB3	1.93	0.51
4:E:264:ILE:HA	4:E:267:LYS:HD3	1.93	0.51
1:A:213:PHE:C	1:A:215:SER:N	2.62	0.51
1:A:323:ILE:HG13	1:A:353:TYR:CE1	2.45	0.50
4:E:370:TRP:NE1	4:E:398:MET:HB2	2.26	0.50
3:D:127:PRO:HB3	3:D:145:PHE:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:304:LEU:HD22	4:F:347:VAL:HB	1.92	0.50
1:A:220:ILE:HG12	1:A:221:ALA:N	2.25	0.50
4:F:48:PHE:HE2	4:F:50:TYR:HB2	1.77	0.50
2:B:128:TYR:CG	2:B:131:GLY:HA2	2.46	0.50
2:B:230:LEU:HA	2:B:233:LEU:HB3	1.93	0.50
3:D:51:ARG:HB3	3:D:55:ILE:HB	1.93	0.50
2:B:4:VAL:HG22	2:B:25:LEU:HD23	1.93	0.50
4:E:334:VAL:N	4:E:335:PRO:HD2	2.27	0.50
1:A:143:TYR:CD1	1:A:144:PRO:HA	2.47	0.50
2:B:219:TRP:CZ3	2:B:223:LEU:HD22	2.46	0.50
1:A:50:TYR:CD1	1:A:50:TYR:C	2.90	0.50
1:A:94:LYS:HZ3	1:A:111:GLU:HB3	1.77	0.50
4:E:132:GLY:HA2	4:E:213:MET:HE1	1.94	0.50
4:E:256:GLU:O	4:E:259:ARG:HG3	2.11	0.50
4:E:258:GLU:O	4:E:262:ARG:HG2	2.12	0.50
4:E:261:THR:O	4:E:264:ILE:HG12	2.11	0.50
4:E:475:LEU:HD21	4:F:441:ARG:HE	1.76	0.50
5:G:136:ILE:HG23	6:C:1:NAG:H2	1.92	0.50
1:A:223:LEU:CD2	2:B:223:LEU:HD23	2.41	0.50
1:A:39:VAL:HB	1:A:96:LEU:CB	2.40	0.49
1:A:267:SER:HA	1:A:270:LYS:HG2	1.94	0.49
1:A:472:LEU:HD22	7:A:601:H6P:H31	1.93	0.49
5:G:7:PRO:O	5:G:213:ARG:NH2	2.42	0.49
1:A:227:LEU:O	1:A:228:PRO:C	2.52	0.49
4:E:152:ASP:HB2	4:E:153:PRO:HD2	1.94	0.49
4:E:297:LEU:HD13	4:E:357:LYS:HG3	1.93	0.49
4:E:352:SER:OG	4:E:457:ARG:NH2	2.41	0.49
4:E:63:GLU:OE1	4:E:63:GLU:N	2.43	0.49
2:B:290:TYR:O	2:B:293:ARG:HG2	2.12	0.49
5:G:88:GLU:OE1	5:G:90:GLN:NE2	2.30	0.49
4:F:307:ASP:OD1	4:F:337:ASN:ND2	2.46	0.49
5:G:136:ILE:HG22	6:C:1:NAG:H4	1.95	0.49
1:A:319:THR:HG22	1:A:347:GLU:HB3	1.94	0.49
4:E:298:HIS:CE1	4:F:296:PHE:CD1	3.00	0.49
4:F:438:MET:N	4:F:438:MET:HE2	2.27	0.49
4:F:371:THR:HG23	4:F:397:GLU:HG3	1.95	0.48
1:A:83:ARG:HG2	1:A:85:HIS:NE2	2.28	0.48
1:A:94:LYS:HZ2	1:A:110:VAL:C	2.21	0.48
4:E:290:LEU:HD23	4:E:290:LEU:O	2.12	0.48
4:F:321:SER:HB2	4:F:468:PRO:HB2	1.95	0.48
4:E:298:HIS:NE2	4:F:296:PHE:CD1	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:144:PRO:CG	4:F:197:LEU:HD12	2.44	0.48
1:A:217:GLN:HG3	1:A:218:ARG:CZ	2.44	0.48
1:A:367:TYR:HB2	1:A:434:PHE:CD1	2.49	0.48
4:E:278:GLU:HA	4:E:281:GLN:NE2	2.29	0.48
4:E:292:TRP:HZ3	4:F:298:HIS:NE2	2.11	0.48
1:A:220:ILE:CG1	2:B:219:TRP:HH2	2.26	0.48
1:A:228:PRO:HA	1:A:231:LEU:HD12	1.94	0.48
1:A:378:TRP:HZ3	1:A:380:ILE:HG12	1.78	0.48
2:B:228:PRO:O	2:B:232:LEU:HG	2.14	0.48
1:A:234:LEU:HB3	2:B:234:LEU:CD1	2.39	0.48
2:B:234:LEU:O	2:B:237:ALA:N	2.47	0.48
4:F:19:THR:HB	4:F:87:ILE:HD11	1.95	0.48
2:B:221:ALA:O	2:B:224:ALA:HB3	2.13	0.48
2:B:234:LEU:O	2:B:235:ALA:C	2.57	0.48
4:E:300:VAL:HG13	4:F:296:PHE:CD1	2.48	0.48
1:A:413:ARG:HD2	1:A:419:ARG:HB3	1.96	0.48
4:E:298:HIS:NE2	4:F:296:PHE:CG	2.82	0.48
1:A:210:ASP:N	1:A:211:PRO:CD	2.77	0.48
2:B:14:MET:HB2	2:B:17:GLU:CD	2.39	0.48
4:E:419:LEU:HA	4:E:439:ARG:HH12	1.79	0.48
4:F:37:ARG:HH12	4:F:49:VAL:HA	1.78	0.48
4:E:264:ILE:O	4:E:267:LYS:HG2	2.14	0.47
4:F:424:VAL:HG12	4:F:424:VAL:O	2.14	0.47
4:E:266:LEU:HA	4:E:269:LEU:HD12	1.95	0.47
4:E:362:VAL:HG22	4:E:471:ILE:HG12	1.96	0.47
2:B:252:SER:HA	2:B:255:ILE:HG12	1.95	0.47
4:F:245:GLN:O	4:F:249:LYS:HG2	2.14	0.47
4:F:374:VAL:HG21	4:F:426:LEU:HD12	1.95	0.47
5:G:70:GLU:O	5:G:82:LEU:HD12	2.14	0.47
2:B:115:ALA:HB2	2:B:197:LEU:HD23	1.97	0.47
2:B:276:ARG:O	2:B:279:LEU:HG	2.13	0.47
4:E:339:GLU:HA	4:E:381:ARG:HH11	1.79	0.47
4:F:116:GLY:N	4:F:143:TYR:O	2.47	0.47
1:A:40:SER:HB2	1:A:45:GLN:O	2.14	0.47
1:A:94:LYS:C	1:A:95:TYR:CG	2.92	0.47
4:E:343:SER:OG	4:E:382:LYS:O	2.32	0.47
5:G:41:ARG:HG2	5:G:93:ALA:HB2	1.96	0.47
1:A:387:VAL:HG21	1:A:401:PHE:CE2	2.50	0.47
1:A:395:MET:HG3	1:A:470:ARG:HH12	1.80	0.47
4:E:161:LEU:H	4:E:161:LEU:HD23	1.79	0.47
4:F:144:PRO:HG2	4:F:197:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:413:LEU:HD11	4:F:489:THR:HB	1.97	0.47
4:F:243:LYS:O	4:F:246:LYS:HG2	2.15	0.47
1:A:50:TYR:HD2	1:A:55:GLU:CA	2.28	0.47
1:A:125:VAL:HG12	1:A:135:LEU:HD23	1.96	0.47
2:B:229:ILE:CG1	2:B:230:LEU:N	2.77	0.47
4:F:433:VAL:HG12	4:F:447:CYS:SG	2.54	0.47
4:E:187:ARG:NH1	4:E:210:GLU:HB3	2.29	0.46
1:A:148:ILE:HD11	1:A:175:VAL:HB	1.97	0.46
4:E:268:GLU:O	4:E:272:GLU:OE1	2.33	0.46
1:A:375:ARG:NH1	1:A:475:GLU:HB3	2.31	0.46
3:D:129:VAL:HG22	3:D:142:VAL:HG12	1.96	0.46
4:E:96:ARG:NH1	4:E:107:GLU:OE2	2.49	0.46
4:E:121:PRO:O	4:E:204:SER:OG	2.24	0.46
4:F:183:ASP:OD1	4:F:184:LYS:N	2.49	0.46
4:E:293:ARG:O	4:E:293:ARG:HD3	2.14	0.46
4:E:285:LYS:O	4:E:289:GLU:HG2	2.15	0.46
4:E:437:ASN:O	4:E:441:ARG:N	2.47	0.46
1:A:434:PHE:HB2	1:A:443:SER:OG	2.15	0.46
2:B:126:LYS:CB	2:B:134:HIS:CD2	2.96	0.46
4:E:437:ASN:HD21	4:E:439:ARG:NH1	2.14	0.46
4:F:123:ILE:HD11	4:F:191:CYS:HB2	1.97	0.46
4:F:315:LEU:HD23	4:F:319:ARG:HG3	1.98	0.46
2:B:269:THR:O	2:B:273:ILE:HG23	2.15	0.46
2:B:281:GLU:HA	2:B:284:LYS:HG2	1.97	0.46
4:E:307:ASP:OD1	4:E:308:THR:N	2.49	0.46
4:F:283:LYS:O	4:F:283:LYS:HD3	2.16	0.46
4:F:399:HIS:ND1	4:F:400:LYS:HE2	2.31	0.46
4:E:68:THR:HB	4:E:82:LEU:HD11	1.97	0.46
4:E:293:ARG:HD3	4:E:293:ARG:C	2.41	0.46
1:A:150:TRP:CE2	1:A:191:CYS:HB3	2.50	0.45
1:A:241:LEU:C	1:A:241:LEU:HD23	2.41	0.45
4:E:475:LEU:HB3	4:F:436:TYR:HE2	1.81	0.45
5:G:132:PRO:HD3	5:G:214:HIS:ND1	2.30	0.45
1:A:36:LEU:O	1:A:49:VAL:HG13	2.17	0.45
1:A:277:VAL:O	1:A:280:LEU:HG	2.16	0.45
4:F:113:VAL:HG22	8:F:603:NAG:H62	1.99	0.45
4:F:292:TRP:CD1	4:F:293:ARG:HH21	2.34	0.45
1:A:241:LEU:O	1:A:242:TRP:C	2.59	0.45
4:E:263:GLU:O	4:E:266:LEU:HG	2.17	0.45
4:F:24:HIS:HD2	4:F:25:LEU:HD23	1.82	0.45
4:F:256:GLU:O	4:F:259:ARG:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:4:LEU:HD12	5:G:23:CYS:SG	2.56	0.45
5:G:50:VAL:HG12	5:G:60:LYS:HG2	1.98	0.45
1:A:223:LEU:O	1:A:226:THR:HG22	2.16	0.45
2:B:270:GLU:HG2	2:B:271:ARG:N	2.31	0.45
4:F:304:LEU:O	4:F:350:ARG:NH1	2.50	0.45
1:A:268:THR:O	1:A:271:GLN:HG3	2.16	0.45
4:F:4:VAL:HG21	4:F:99:PHE:CD1	2.51	0.45
2:B:231:LEU:C	2:B:231:LEU:HD23	2.42	0.45
3:D:152:ILE:HG12	3:D:193:VAL:HG12	1.99	0.45
4:E:427:ASP:O	4:E:431:GLY:N	2.49	0.45
5:G:136:ILE:HG13	5:G:227:PHE:CE2	2.52	0.45
1:A:96:LEU:HB3	1:A:98:TYR:CE1	2.52	0.45
1:A:228:PRO:O	1:A:232:LEU:HD23	2.17	0.45
4:E:133:ILE:HG23	4:F:212:PHE:HZ	1.82	0.45
4:E:260:GLU:O	4:E:264:ILE:HG23	2.16	0.45
4:F:38:TRP:HZ3	4:F:82:LEU:HB2	1.80	0.45
4:F:187:ARG:HA	4:F:187:ARG:HD3	1.76	0.45
4:F:262:ARG:HG2	4:F:266:LEU:HD23	1.98	0.45
2:B:37:LYS:HG3	2:B:49:VAL:HG22	1.99	0.45
4:E:265:ALA:HA	4:E:268:GLU:CD	2.41	0.45
4:F:24:HIS:CD2	4:F:25:LEU:H	2.35	0.45
1:A:343:PRO:O	1:A:348:ARG:NH2	2.50	0.45
2:B:222:ALA:O	2:B:226:THR:HG23	2.17	0.45
2:B:270:GLU:O	2:B:273:ILE:HG12	2.17	0.45
4:F:61:MET:HG2	4:F:63:GLU:OE1	2.17	0.45
1:A:225:GLY:O	1:A:229:VAL:HG23	2.17	0.44
2:B:121:LEU:HD12	2:B:137:CYS:SG	2.57	0.44
4:E:313:LEU:HD21	4:E:345:PRO:HB3	1.98	0.44
4:F:281:GLN:HA	4:F:284:GLU:OE1	2.17	0.44
1:A:82:LEU:O	1:A:83:ARG:C	2.59	0.44
4:E:286:LEU:HA	4:E:289:GLU:CG	2.42	0.44
4:E:370:TRP:HE1	4:E:398:MET:HB2	1.81	0.44
1:A:220:ILE:HB	2:B:219:TRP:HH2	1.81	0.44
1:A:334:GLN:HG2	1:A:478:ALA:HB2	1.98	0.44
2:B:285:ARG:O	2:B:289:GLN:OE1	2.35	0.44
4:E:145:LYS:HA	4:E:146:PRO:HD3	1.83	0.44
1:A:223:LEU:HD12	1:A:224:ALA:H	1.83	0.44
4:E:145:LYS:HA	4:E:173:PHE:HD2	1.82	0.44
2:B:41:SER:OG	3:D:32:ASN:OD1	2.36	0.44
4:E:388:ILE:HG13	4:E:391:ASN:H	1.81	0.44
1:A:299:ALA:O	1:A:302:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:53:LYS:HA	3:D:53:LYS:HD2	1.61	0.44
4:E:486:GLU:O	4:F:411:ARG:NH1	2.44	0.44
4:F:121:PRO:HB3	4:F:193:ILE:HD11	1.99	0.44
4:E:274:VAL:O	4:E:277:GLU:HB3	2.17	0.44
4:E:290:LEU:O	4:E:291:ARG:C	2.60	0.44
4:F:146:PRO:C	4:F:147:LEU:HD22	2.42	0.44
2:B:270:GLU:HA	2:B:273:ILE:HG12	1.99	0.44
4:E:361:GLU:OE2	4:E:421:ARG:HB2	2.17	0.44
1:A:334:GLN:OE1	1:A:335:ARG:N	2.38	0.44
1:A:257:ARG:HA	1:A:260:GLU:HG2	2.00	0.43
1:A:279:LEU:O	1:A:282:GLU:HG3	2.18	0.43
2:B:241:LEU:O	2:B:244:GLN:HG3	2.18	0.43
4:F:36:VAL:HA	4:F:98:TYR:O	2.18	0.43
4:F:37:ARG:O	4:F:97:CYS:HA	2.17	0.43
4:E:125:MET:O	4:E:126:ARG:HD2	2.18	0.43
4:E:268:GLU:O	4:E:271:LYS:HB3	2.19	0.43
4:F:206:ILE:HG13	4:F:207:PHE:H	1.83	0.43
1:A:117:LEU:HG	1:A:118:GLY:H	1.82	0.43
1:A:219:TRP:CE2	2:B:220:ILE:HD12	2.53	0.43
1:A:446:ASN:OD1	1:A:447:ALA:N	2.51	0.43
2:B:194:ARG:HH12	2:B:196:SER:HB3	1.84	0.43
2:B:274:SER:HA	2:B:277:GLU:HG2	1.99	0.43
2:B:58:ASP:N	2:B:58:ASP:OD1	2.50	0.43
4:E:228:VAL:HA	4:E:231:MET:HB3	2.00	0.43
4:E:297:LEU:HG	4:E:359:TYR:HE1	1.83	0.43
4:F:362:VAL:HG11	4:F:372:VAL:HG11	2.01	0.43
5:G:136:ILE:CG2	6:C:1:NAG:H2	2.48	0.43
4:E:342:ASP:OD1	4:E:342:ASP:N	2.52	0.43
1:A:25:LEU:HD21	1:A:99:PHE:CG	2.54	0.43
2:B:262:LYS:HE2	2:B:266:TYR:OH	2.17	0.43
4:E:316:SER:OG	4:E:318:ASP:OD1	2.30	0.43
4:F:292:TRP:NE1	4:F:293:ARG:HH21	2.16	0.43
1:A:19:ALA:N	1:A:84:ILE:O	2.49	0.43
1:A:21:LEU:HD21	1:A:110:VAL:HG21	2.00	0.43
4:E:373:GLY:HA3	4:E:395:THR:HG22	2.00	0.43
4:F:187:ARG:NH2	4:F:210:GLU:HB2	2.33	0.43
1:A:39:VAL:HG22	1:A:46:VAL:HG13	2.01	0.43
1:A:227:LEU:CB	1:A:228:PRO:CD	2.97	0.43
3:D:164:ASP:OD1	3:D:164:ASP:N	2.52	0.43
4:F:367:VAL:HG12	4:F:369:GLU:H	1.84	0.43
1:A:261:LEU:HD11	2:B:262:LYS:CE	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:187:ARG:HH22	4:F:210:GLU:HB2	1.82	0.43
4:F:432:ASP:OD1	4:F:434:SER:N	2.51	0.43
1:A:126:LYS:HE3	1:A:134:HIS:CE1	2.53	0.43
1:A:317:PRO:HA	1:A:326:VAL:HG21	2.00	0.43
2:B:122:HIS:HB3	2:B:138:ARG:CG	2.49	0.43
5:G:95:TYR:O	5:G:116:GLY:HA2	2.19	0.43
5:G:159:PHE:HB2	5:G:214:HIS:CE1	2.54	0.43
6:C:1:NAG:O3	6:C:1:NAG:C7	2.67	0.43
2:B:286:LYS:HD2	2:B:286:LYS:HA	1.90	0.42
4:E:267:LYS:O	4:E:270:GLU:HG3	2.18	0.42
4:E:74:ASP:N	4:E:74:ASP:OD1	2.49	0.42
4:E:88:THR:HG22	4:E:89:ALA:N	2.34	0.42
5:G:211:ILE:CD1	5:G:224:GLU:HG2	2.48	0.42
2:B:45:GLN:HB3	2:B:61:SER:OG	2.19	0.42
2:B:232:LEU:O	2:B:233:LEU:C	2.61	0.42
1:A:47:VAL:HG23	1:A:64:TYR:HB3	2.00	0.42
1:A:363:SER:OG	1:A:364:GLY:N	2.52	0.42
4:E:189:MET:HB2	4:E:206:ILE:HG22	2.01	0.42
4:E:364:VAL:HG13	4:E:367:VAL:HB	2.02	0.42
4:F:38:TRP:HH2	4:F:70:PHE:HE1	1.66	0.42
4:F:144:PRO:CG	4:F:197:LEU:HD11	2.49	0.42
2:B:227:LEU:O	2:B:228:PRO:C	2.61	0.42
4:F:49:VAL:HG11	4:F:56:ARG:HB2	2.02	0.42
4:F:88:THR:OG1	4:F:91:GLU:OE1	2.35	0.42
1:A:314:ILE:HG23	1:A:358:CYS:HB2	2.02	0.42
3:D:159:LYS:HD3	3:D:162:GLU:HG3	2.00	0.42
4:F:281:GLN:O	4:F:284:GLU:HG2	2.20	0.42
1:A:245:GLN:O	1:A:248:LYS:HG2	2.20	0.42
4:E:386:LEU:HG	4:E:388:ILE:HG23	2.01	0.42
4:F:432:ASP:OD1	4:F:433:VAL:N	2.53	0.42
1:A:270:LYS:HG3	1:A:271:GLN:N	2.33	0.42
1:A:377:GLU:HG3	1:A:407:THR:HA	2.01	0.42
4:F:369:GLU:OE2	4:F:461:ARG:NH1	2.36	0.42
1:A:297:HIS:O	1:A:301:ASN:ND2	2.53	0.42
4:F:49:VAL:HG12	4:F:49:VAL:O	2.20	0.42
4:F:139:SER:O	4:F:174:MET:HB2	2.20	0.42
4:F:292:TRP:HE1	4:F:293:ARG:HH21	1.67	0.42
1:A:40:SER:O	1:A:41:SER:HB3	2.20	0.41
1:A:50:TYR:O	1:A:51:ALA:HB2	2.20	0.41
4:E:117:LEU:HG	4:E:198:LEU:HD12	2.02	0.41
1:A:94:LYS:C	1:A:95:TYR:CD2	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:CYS:SG	2:B:99:PHE:HE1	2.43	0.41
4:E:122:LEU:O	4:E:137:CYS:HA	2.20	0.41
4:E:242:ASN:O	4:E:246:LYS:HG2	2.20	0.41
4:E:386:LEU:HD23	4:E:386:LEU:H	1.84	0.41
4:F:11:ILE:HD12	4:F:110:LEU:HD21	2.01	0.41
4:F:431:GLY:HA2	4:F:452:PHE:CE1	2.55	0.41
5:G:161:PRO:HD2	5:G:214:HIS:CE1	2.55	0.41
5:G:210:CYS:HB3	5:G:225:ILE:HB	2.02	0.41
1:A:39:VAL:CG1	1:A:96:LEU:HD13	2.50	0.41
1:A:72:ARG:HB3	1:A:75:ILE:HB	2.02	0.41
1:A:347:GLU:O	1:A:389:ARG:NH1	2.53	0.41
4:F:191:CYS:O	4:F:203:GLU:HA	2.20	0.41
4:F:379:VAL:HG11	4:F:393:PHE:HE1	1.86	0.41
1:A:97:CYS:SG	1:A:108:ALA:HB3	2.60	0.41
1:A:203:THR:HG22	1:A:204:ALA:N	2.35	0.41
2:B:14:MET:HE3	2:B:14:MET:HB3	1.89	0.41
2:B:281:GLU:O	2:B:284:LYS:HG2	2.21	0.41
3:D:168:VAL:HG11	5:G:180:GLN:HB3	2.02	0.41
4:E:183:ASP:OD1	4:E:184:LYS:N	2.54	0.41
1:A:208:ILE:HG22	2:B:125:VAL:HG21	2.02	0.41
4:E:348:LEU:HD21	4:E:459:PHE:HD1	1.85	0.41
4:E:399:HIS:O	4:E:402:GLN:NE2	2.54	0.41
4:F:25:LEU:HD23	4:F:25:LEU:H	1.85	0.41
1:A:213:PHE:CE2	2:B:128:TYR:CD1	3.08	0.41
2:B:105:TYR:CE2	3:D:53:LYS:HD3	2.55	0.41
1:A:279:LEU:HD11	2:B:279:LEU:HD13	2.01	0.41
2:B:219:TRP:O	2:B:223:LEU:HD13	2.21	0.41
2:B:252:SER:O	2:B:255:ILE:HG12	2.20	0.41
4:F:283:LYS:HD3	4:F:283:LYS:C	2.46	0.41
4:F:309:ALA:HA	4:F:347:VAL:HG22	2.03	0.41
1:A:160:THR:HA	1:A:179:VAL:HG22	2.03	0.41
4:F:94:THR:OG1	4:F:110:LEU:O	2.27	0.41
4:F:360:TRP:CH2	4:F:458:PRO:HG3	2.55	0.41
1:A:172:LEU:HD23	1:A:172:LEU:HA	1.96	0.41
1:A:321:ASN:OD1	1:A:322:PRO:HD2	2.20	0.41
2:B:94:LYS:HB3	2:B:109:LEU:HD11	2.02	0.41
2:B:226:THR:O	2:B:229:ILE:HG23	2.20	0.41
4:E:310:HIS:HB3	4:E:313:LEU:HG	2.03	0.41
4:E:376:ARG:HG3	4:E:392:GLY:HA3	2.03	0.41
4:F:91:GLU:OE1	4:F:91:GLU:N	2.54	0.41
4:F:234:ILE:O	4:F:238:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:6:GLN:NE2	5:G:97:CYS:SG	2.94	0.41
1:A:60:GLN:O	1:A:65:ARG:NH2	2.54	0.41
2:B:56:VAL:O	2:B:56:VAL:HG23	2.21	0.41
2:B:130:ASP:C	2:B:132:GLY:N	2.72	0.41
1:A:259:GLN:O	1:A:262:ARG:HB3	2.21	0.40
2:B:133:ILE:HG12	2:B:213:PHE:CE1	2.57	0.40
2:B:230:LEU:O	2:B:231:LEU:C	2.64	0.40
4:E:212:PHE:HA	4:F:128:HIS:HD2	1.86	0.40
2:B:121:LEU:HD13	2:B:139:SER:HB2	2.03	0.40
3:D:2:ILE:N	3:D:25:MET:HE3	2.36	0.40
4:E:87:ILE:HD13	4:E:87:ILE:HA	1.97	0.40
4:E:436:TYR:HE1	4:E:443:HIS:ND1	2.19	0.40
4:F:308:THR:HG23	4:F:347:VAL:HG13	2.04	0.40
5:G:181:GLU:HG2	5:G:195:SER:HB2	2.02	0.40
4:E:298:HIS:CG	4:E:300:VAL:HG22	2.56	0.40
4:E:399:HIS:CG	4:E:404:ARG:HE	2.40	0.40
1:A:118:GLY:HA3	1:A:142:TRP:CZ2	2.55	0.40
2:B:20:ASP:OD2	2:B:71:LEU:HD21	2.22	0.40
4:E:281:GLN:O	4:E:284:GLU:HG2	2.21	0.40
5:G:192:MET:HE3	5:G:192:MET:HB3	1.85	0.40
1:A:223:LEU:HA	1:A:226:THR:HG22	2.03	0.40
1:A:322:PRO:HB3	1:A:340:GLN:O	2.22	0.40
3:D:126:LYS:HG3	3:D:127:PRO:HD2	2.04	0.40
3:D:151:ARG:HB2	3:D:194:GLN:HB2	2.04	0.40
4:E:145:LYS:HA	4:E:173:PHE:CD2	2.56	0.40
4:E:377:ASP:N	4:E:377:ASP:OD1	2.51	0.40
4:E:421:ARG:HH22	4:F:441:ARG:HD2	1.87	0.40
4:E:475:LEU:HD12	4:F:436:TYR:CE2	2.56	0.40
4:F:206:ILE:HD12	4:F:206:ILE:HA	1.97	0.40
5:G:126:LEU:HD23	5:G:130:VAL:HG11	2.03	0.40
5:G:148:LYS:HG3	5:G:201:GLU:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	465/527 (88%)	439 (94%)	26 (6%)	0	100	100
2	B	292/318 (92%)	283 (97%)	9 (3%)	0	100	100
3	D	199/274 (73%)	188 (94%)	11 (6%)	0	100	100
4	E	463/532 (87%)	443 (96%)	20 (4%)	0	100	100
4	F	467/532 (88%)	444 (95%)	23 (5%)	0	100	100
5	G	226/295 (77%)	212 (94%)	14 (6%)	0	100	100
All	All	2112/2478 (85%)	2009 (95%)	103 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/434 (94%)	397 (98%)	9 (2%)	47	76
2	B	239/258 (93%)	237 (99%)	2 (1%)	79	90
3	D	180/240 (75%)	180 (100%)	0	100	100
4	E	424/463 (92%)	423 (100%)	1 (0%)	92	97
4	F	425/463 (92%)	425 (100%)	0	100	100
5	G	207/265 (78%)	207 (100%)	0	100	100
All	All	1881/2123 (89%)	1869 (99%)	12 (1%)	82	93

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	96	LEU
1	A	208	ILE
1	A	218	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	219	TRP
1	A	220	ILE
1	A	223	LEU
1	A	230	LEU
1	A	334	GLN
2	B	229	ILE
2	B	230	LEU
4	E	300	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	GLN
1	A	366	HIS
1	A	421	ASN
1	A	454	HIS
2	B	120	ASN
2	B	134	HIS
3	D	124	HIS
4	E	358	HIS
4	E	437	ASN
4	F	24	HIS
4	F	90	GLN
4	F	491	HIS
5	G	103	GLN
5	G	147	GLN
5	G	188	ASN
5	G	214	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

6 monosaccharides 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	$\# Z  > 2$
6	NAG	C	1	3,6	14,14,15	0.43	0	17,19,21	1.11	2 (11%)
6	NAG	C	2	6	14,14,15	0.55	0	17,19,21	1.29	2 (11%)
6	BMA	C	3	6	11,11,12	0.30	0	15,15,17	0.88	0
6	NAG	H	1	6,4	14,14,15	0.47	0	17,19,21	1.20	1 (5%)
6	NAG	H	2	6	14,14,15	0.41	0	17,19,21	0.77	0
6	BMA	H	3	6	11,11,12	0.24	0	15,15,17	0.70	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1	3,6	-	4/6/23/26	0/1/1/1
6	NAG	C	2	6	-	0/6/23/26	0/1/1/1
6	BMA	C	3	6	-	0/2/19/22	0/1/1/1
6	NAG	H	1	6,4	-	4/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
6	BMA	H	3	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1	NAG	C1-O5-C5	3.71	117.22	112.19
6	C	2	NAG	O5-C1-C2	-2.87	106.76	111.29
6	C	1	NAG	C1-O5-C5	2.38	115.41	112.19
6	C	2	NAG	C2-N2-C7	-2.34	119.56	122.90
6	C	1	NAG	O5-C1-C2	-2.22	107.78	111.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

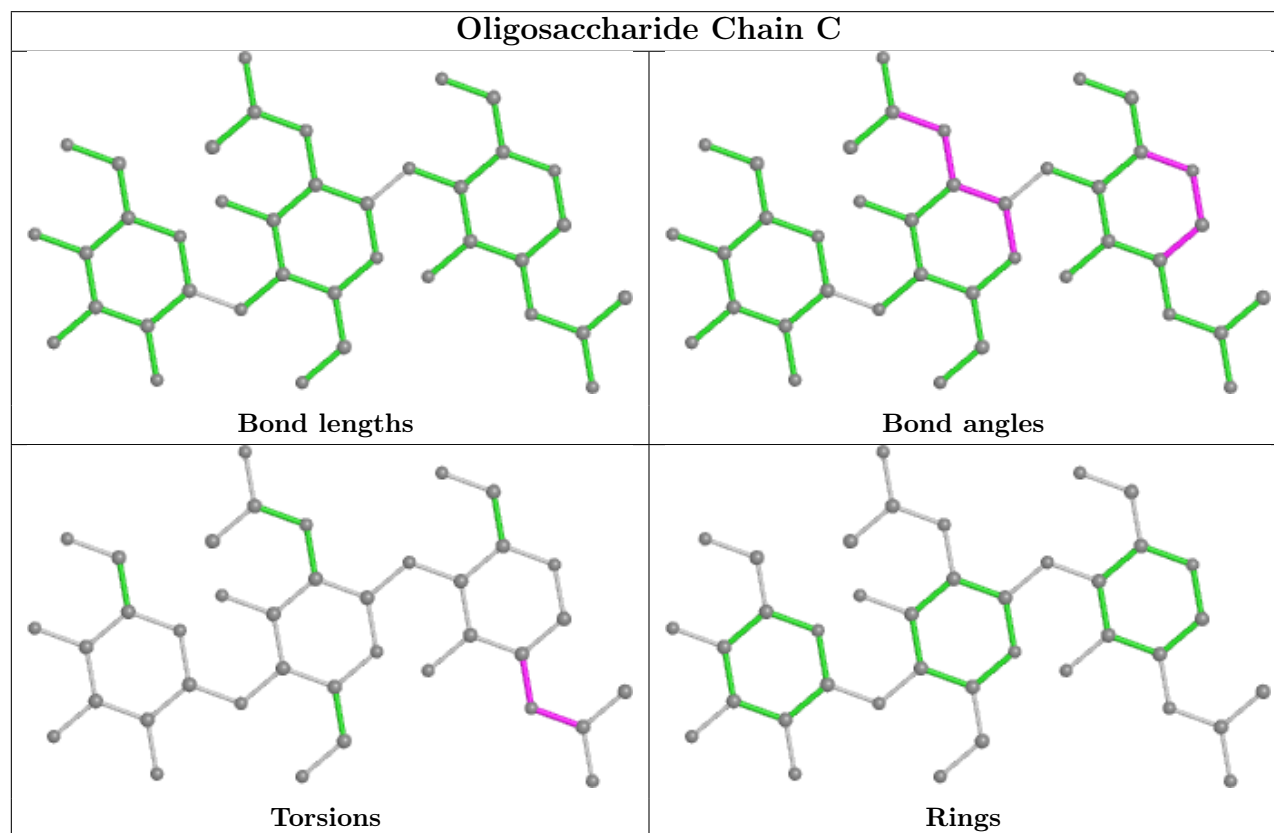
Mol	Chain	Res	Type	Atoms
6	C	1	NAG	C3-C2-N2-C7
6	C	1	NAG	C8-C7-N2-C2
6	C	1	NAG	O7-C7-N2-C2
6	H	1	NAG	C8-C7-N2-C2
6	H	1	NAG	O7-C7-N2-C2
6	H	1	NAG	C1-C2-N2-C7
6	C	1	NAG	C1-C2-N2-C7
6	H	1	NAG	O5-C5-C6-O6

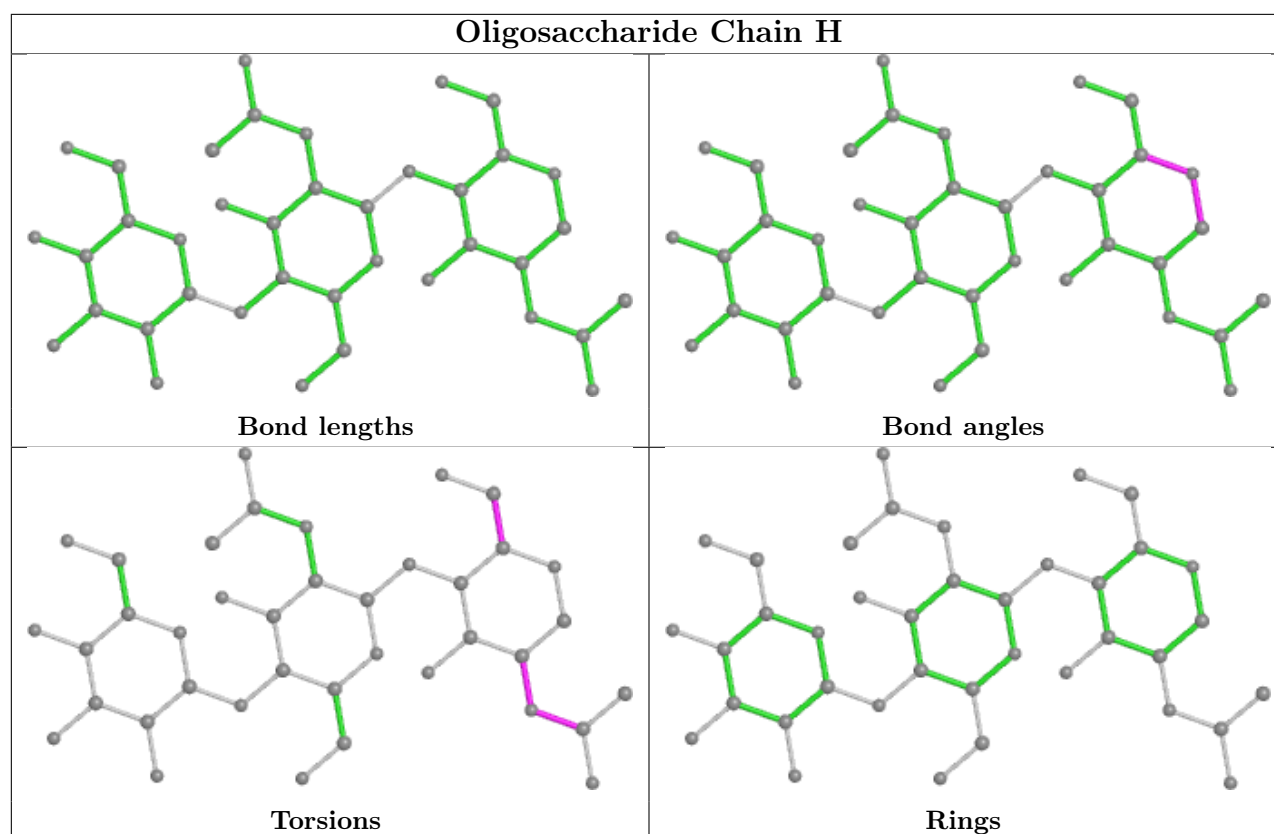
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





## 5.6 Ligand geometry [i](#)

10 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	$\# Z  > 2$
8	NAG	F	602	4	14,14,15	0.21	0	17,19,21	0.44	0
8	NAG	F	605	4	14,14,15	0.29	0	17,19,21	0.35	0
8	NAG	F	603	4	14,14,15	0.26	0	17,19,21	0.55	0
8	NAG	F	601	4	14,14,15	0.23	0	17,19,21	0.44	0
8	NAG	E	601	4	14,14,15	0.33	0	17,19,21	0.73	0
8	NAG	B	401	2	14,14,15	0.23	0	17,19,21	0.42	0
8	NAG	E	602	4	14,14,15	0.34	0	17,19,21	0.77	0
8	NAG	E	603	4	14,14,15	0.38	0	17,19,21	0.79	0
8	NAG	F	604	4	14,14,15	0.27	0	17,19,21	0.58	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	H6P	A	601	-	11,14,14	0.81	0	13,20,20	1.28	1 (7%)

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
8	NAG	F	602	4	-	2/6/23/26	0/1/1/1
8	NAG	F	605	4	-	3/6/23/26	0/1/1/1
8	NAG	F	603	4	-	4/6/23/26	0/1/1/1
8	NAG	F	601	4	-	0/6/23/26	0/1/1/1
8	NAG	E	601	4	-	2/6/23/26	0/1/1/1
8	NAG	B	401	2	-	0/6/23/26	0/1/1/1
8	NAG	E	602	4	-	2/6/23/26	0/1/1/1
8	NAG	E	603	4	-	4/6/23/26	0/1/1/1
8	NAG	F	604	4	-	3/6/23/26	0/1/1/1
7	H6P	A	601	-	-	4/15/15/15	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	601	H6P	O20-P17-O18	2.25	116.22	107.64

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	601	H6P	P13-O16-P17-O20
8	E	601	NAG	O7-C7-N2-C2
8	E	601	NAG	C8-C7-N2-C2
8	F	602	NAG	O5-C5-C6-O6
8	F	602	NAG	C4-C5-C6-O6
8	F	605	NAG	O5-C5-C6-O6
8	F	603	NAG	O5-C5-C6-O6
8	E	602	NAG	C8-C7-N2-C2
8	E	602	NAG	O7-C7-N2-C2
8	E	603	NAG	C8-C7-N2-C2

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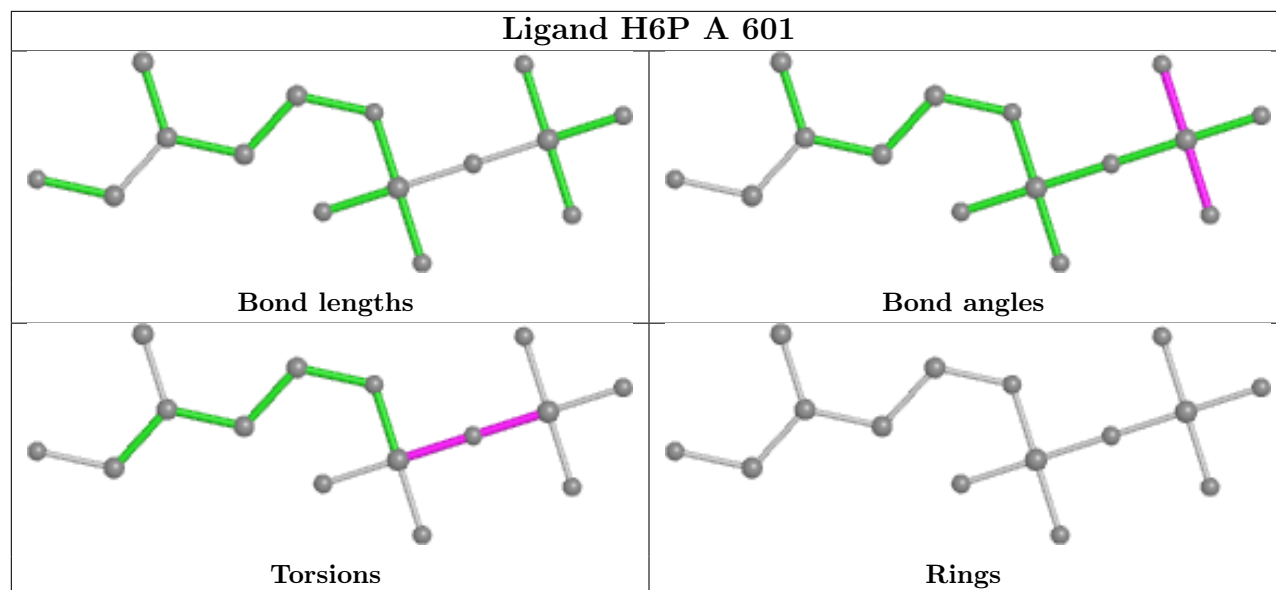
Mol	Chain	Res	Type	Atoms
8	F	603	NAG	C8-C7-N2-C2
8	F	603	NAG	O7-C7-N2-C2
8	F	603	NAG	C4-C5-C6-O6
8	F	605	NAG	C4-C5-C6-O6
8	E	603	NAG	O7-C7-N2-C2
8	E	603	NAG	C1-C2-N2-C7
8	F	604	NAG	C4-C5-C6-O6
7	A	601	H6P	P17-O16-P13-O29
8	F	604	NAG	O5-C5-C6-O6
8	F	604	NAG	C3-C2-N2-C7
8	F	605	NAG	C1-C2-N2-C7
7	A	601	H6P	P13-O16-P17-O18
8	E	603	NAG	C3-C2-N2-C7
7	A	601	H6P	P13-O16-P17-O19

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	603	NAG	1	0
7	A	601	H6P	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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.

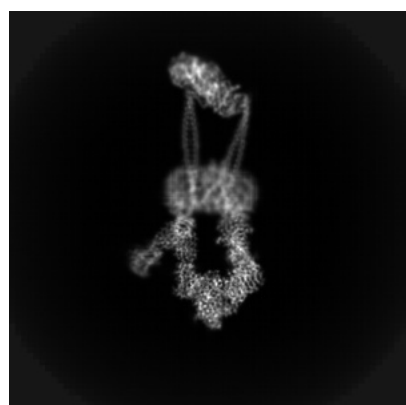
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61740. These allow visual inspection of the internal detail of the map and identification of artifacts.

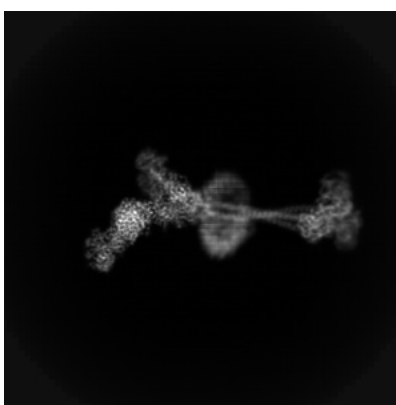
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

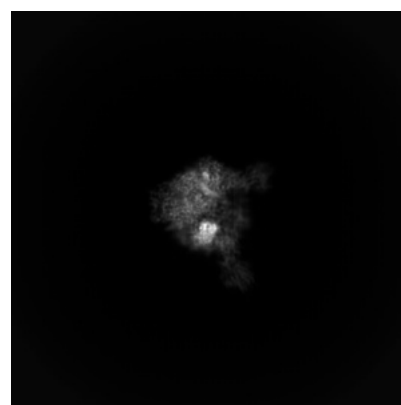
#### 6.1.1 Primary map



X



Y

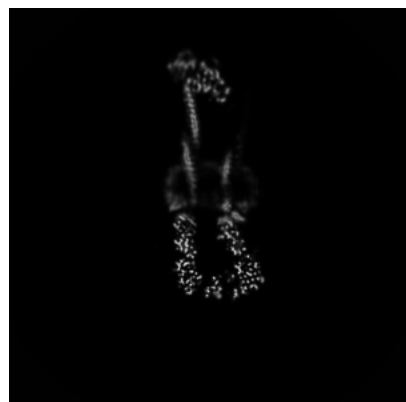


Z

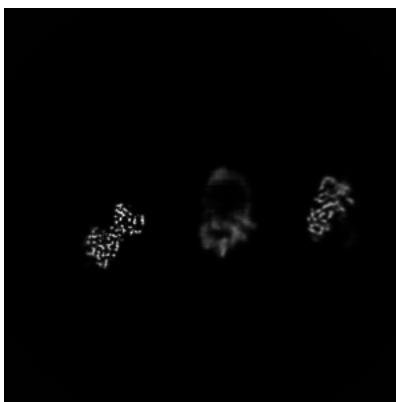
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

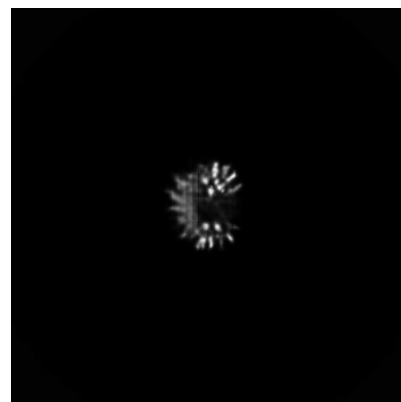
#### 6.2.1 Primary map



X Index: 210



Y Index: 210

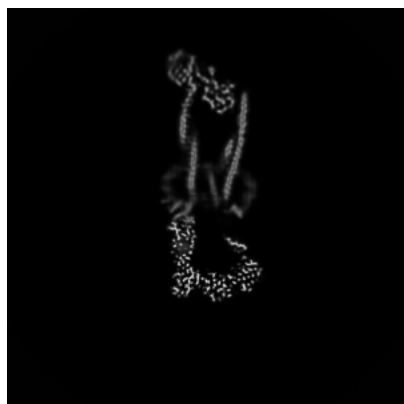


Z Index: 210

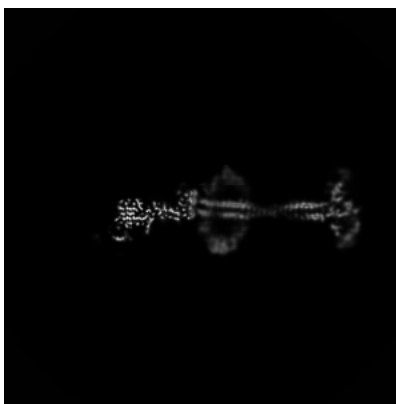
The images above show central slices of the map in three orthogonal directions.

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

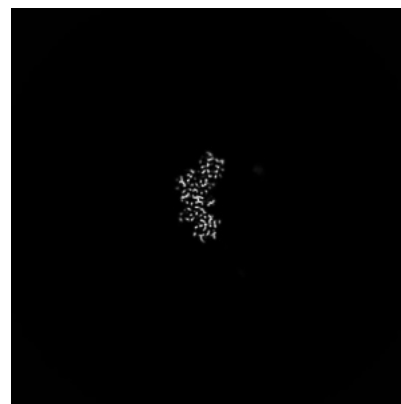
### 6.3.1 Primary map



X Index: 203



Y Index: 191



Z Index: 136

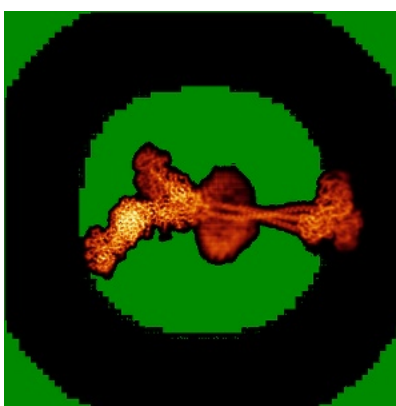
The images above show the largest variance slices of the map in three orthogonal directions.

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

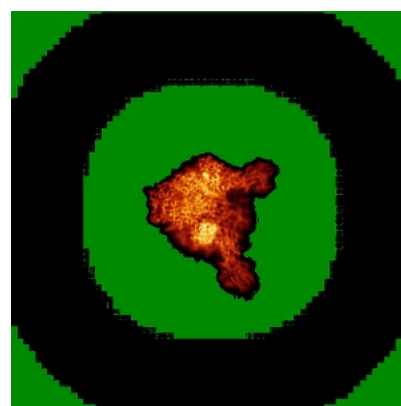
### 6.4.1 Primary map



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](#)

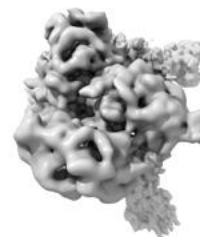
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

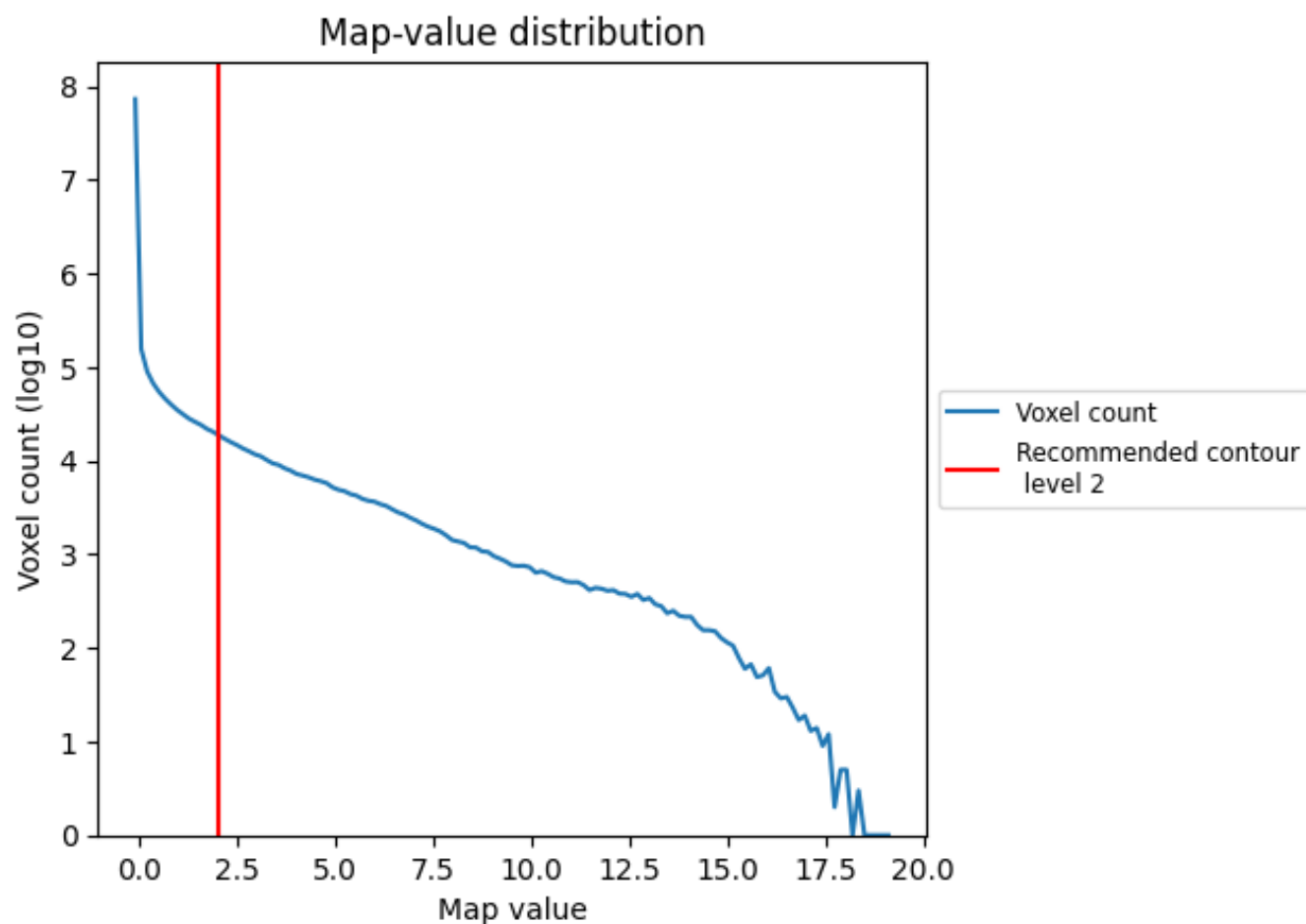
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

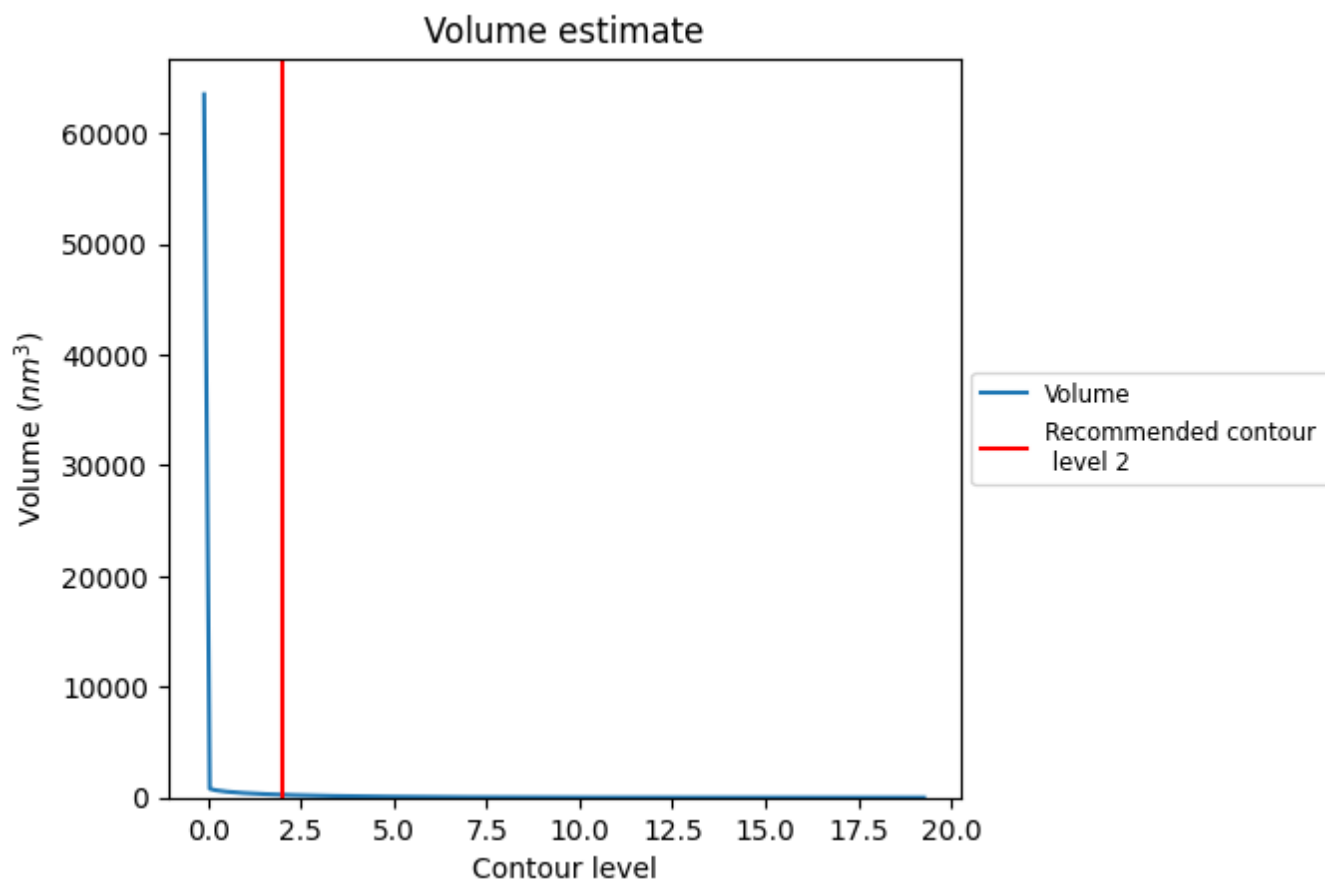
This section contains the results of statistical analysis of the map.

### 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](#)

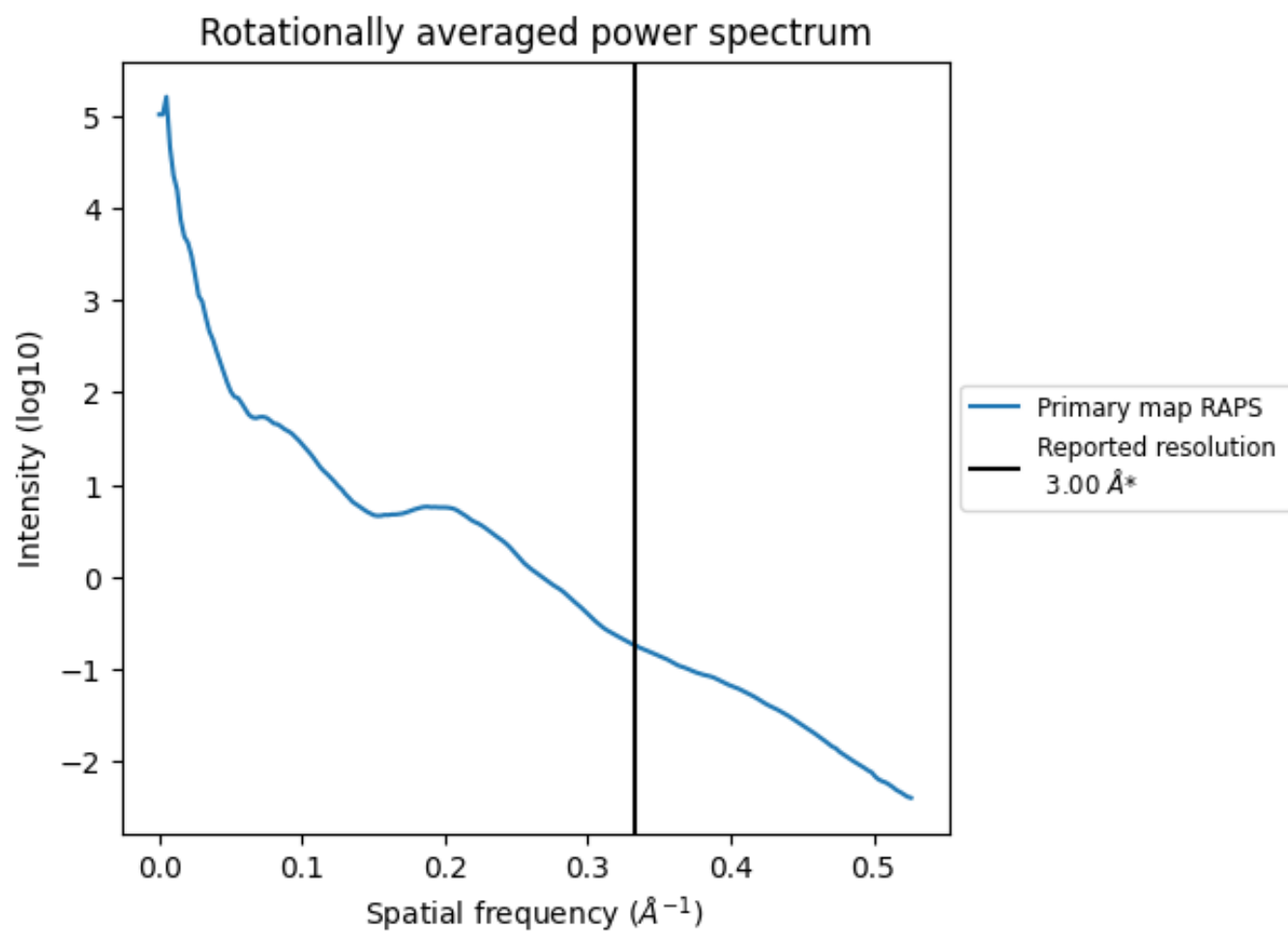


The volume at the recommended contour level is 253 nm<sup>3</sup>; this corresponds to an approximate mass of 229 kDa.

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 0.333 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

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

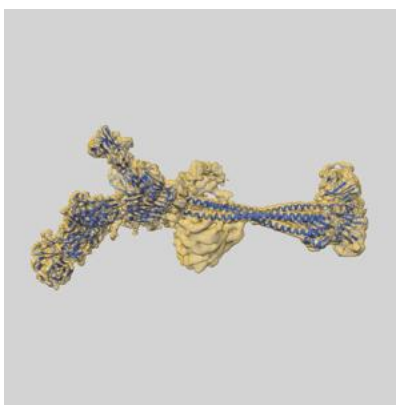
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61740 and PDB model 9JQR. Per-residue inclusion information can be found in section [3](#) on page [9](#).

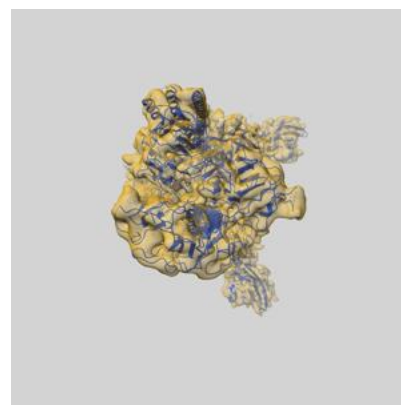
### 9.1 Map-model overlay [i](#)



X



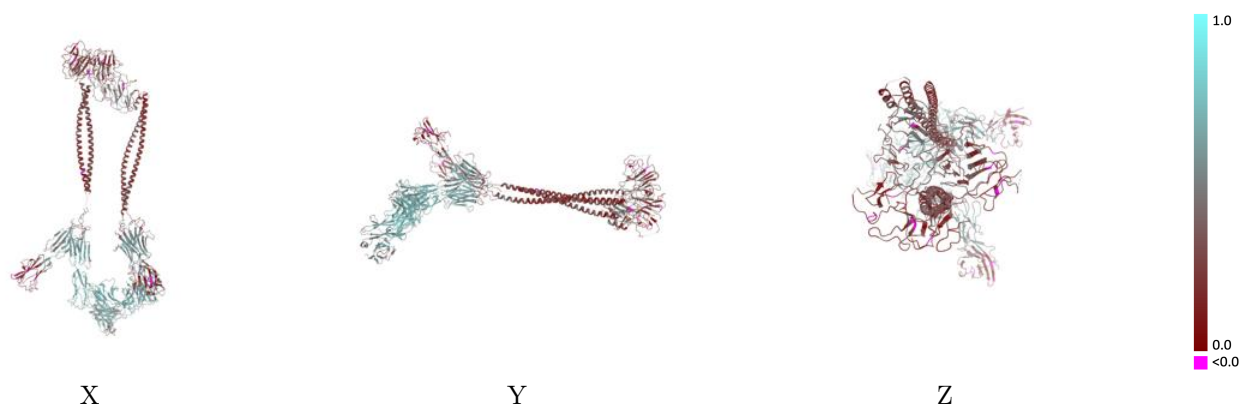
Y



Z

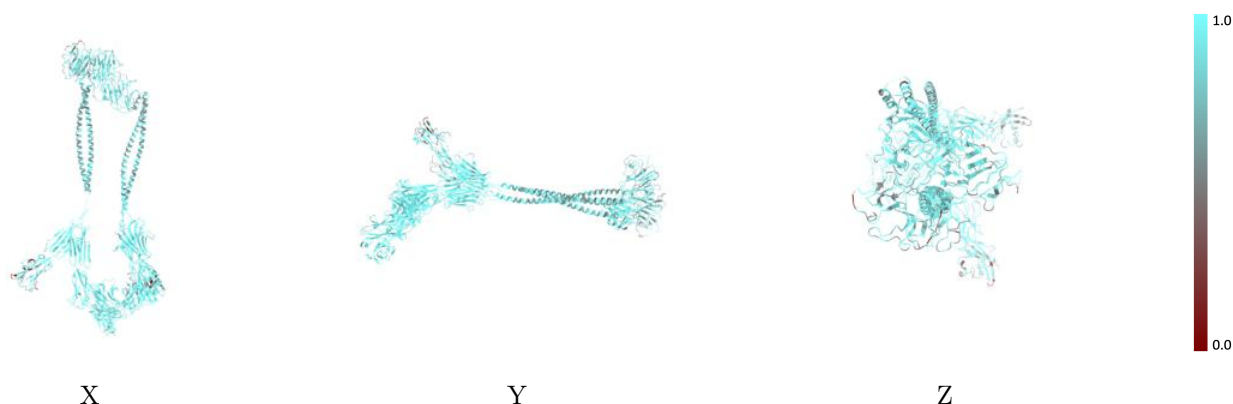
The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



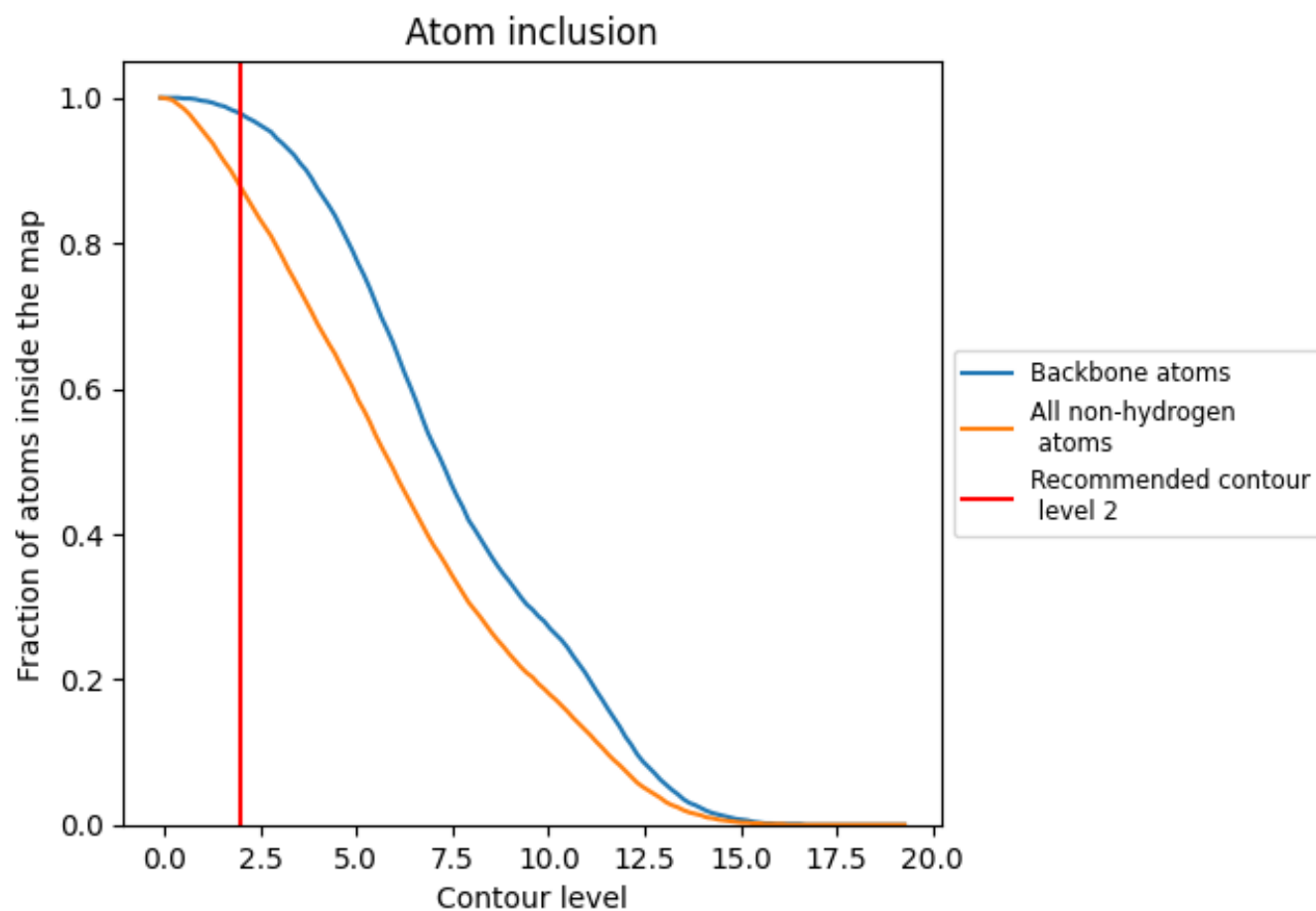
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 88% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8760</div>	<div><div></div>0.4180</div>
A	<div><div></div>0.8470</div>	<div><div></div>0.3420</div>
B	<div><div></div>0.9030</div>	<div><div></div>0.4710</div>
C	<div><div></div>0.8970</div>	<div><div></div>0.5040</div>
D	<div><div></div>0.9580</div>	<div><div></div>0.5880</div>
E	<div><div></div>0.8770</div>	<div><div></div>0.4060</div>
F	<div><div></div>0.8170</div>	<div><div></div>0.3160</div>
G	<div><div></div>0.9500</div>	<div><div></div>0.5990</div>
H	<div><div></div>0.9490</div>	<div><div></div>0.5260</div>

1.0

0.0

<0.0