



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 01:56 AM UTC

PDB ID : 7O7N / pdb_00007o7n
EMDB ID : EMD-12750
Title : (h-alpha2M)4 semiactivated I state
Authors : Luque, D.; Goulas, T.; Mata, C.P.; Mendes, S.R.; Gomis-Ruth, F.X.; Caston, J.R.
Deposited on : 2021-04-13
Resolution : 7.30 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:

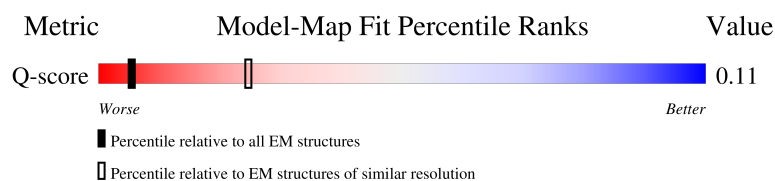
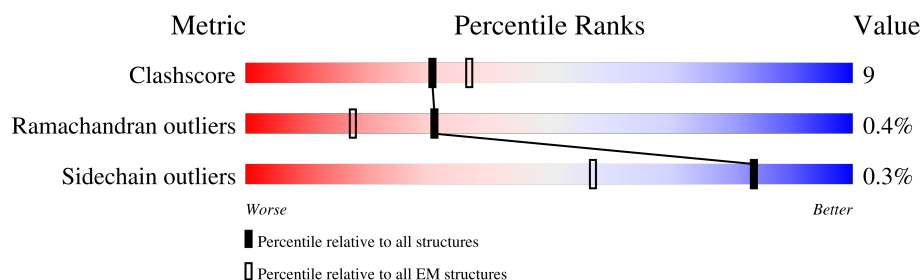
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 7.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	436 (6.80 - 7.80)

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	1474	<div> <div>30%</div> <div>68%</div> <div>19%</div> <div>14%</div> </div>
1	B	1474	<div> <div>57%</div> <div>76%</div> <div>19%</div> <div>• •</div> </div>
1	C	1474	<div> <div>30%</div> <div>68%</div> <div>19%</div> <div>14%</div> </div>
1	D	1474	<div> <div>58%</div> <div>76%</div> <div>19%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	2	<div> <div>100%</div> <div>100%</div> </div>
2	F	2	<div> <div>50%</div> <div>50%</div> <div>50%</div> </div>
2	G	2	<div> <div>100%</div> <div>100%</div> </div>
2	H	2	<div> <div>50%</div> <div>50%</div> <div>50%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	2005	X	-	-	-
3	NAG	D	2005	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 42372 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 Alpha-2-macroglobulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1275	Total	C	N	O	S	0	0
			9944	6322	1670	1909	43		
1	B	1410	Total	C	N	O	S	0	0
			11004	6999	1840	2117	48		
1	C	1275	Total	C	N	O	S	0	0
			9944	6322	1670	1909	43		
1	D	1410	Total	C	N	O	S	0	0
			11004	6999	1840	2117	48		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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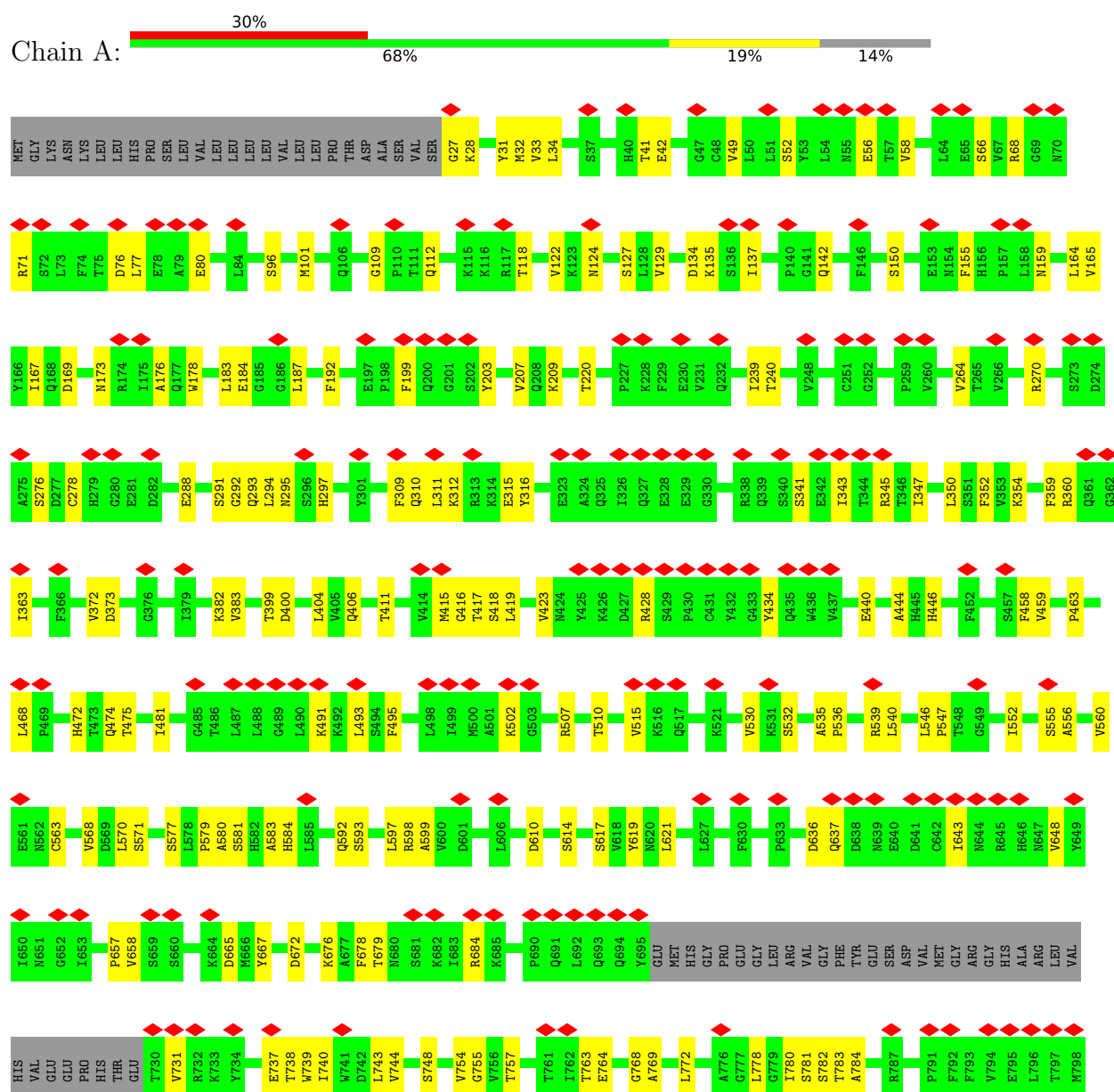
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Mol	Chain	Residues	Atoms				AltConf
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	C	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C	N	O	0
			14	8	1	5	
3	D	1	Total	C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

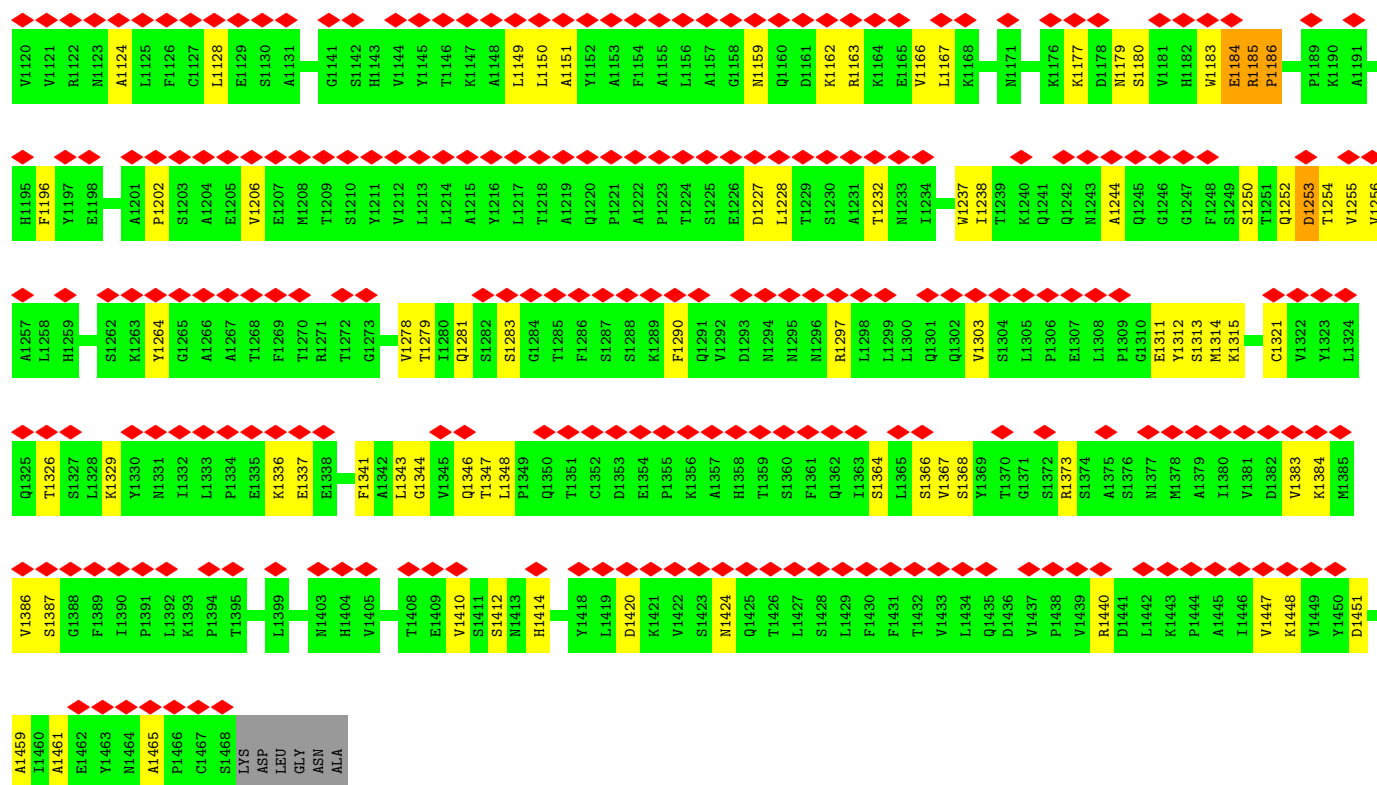
3 Residue-property plots

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.

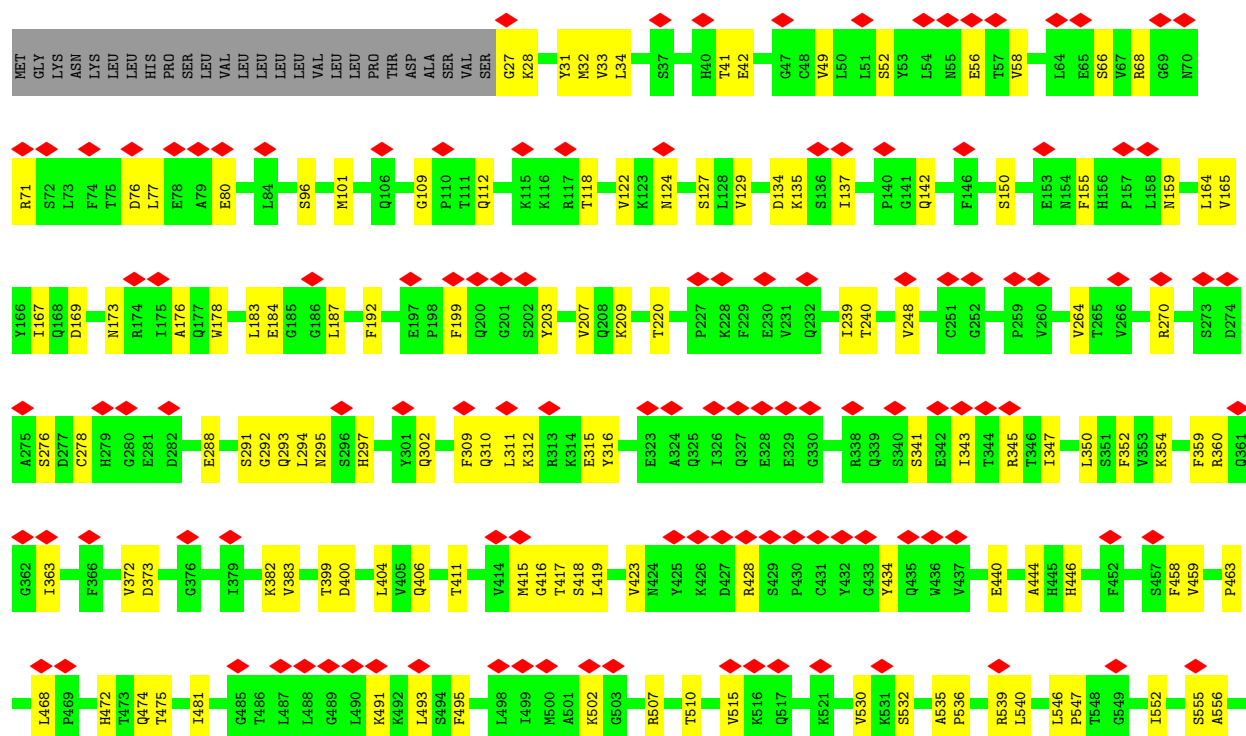
• Molecule 1: Alpha-2-macroglobulin



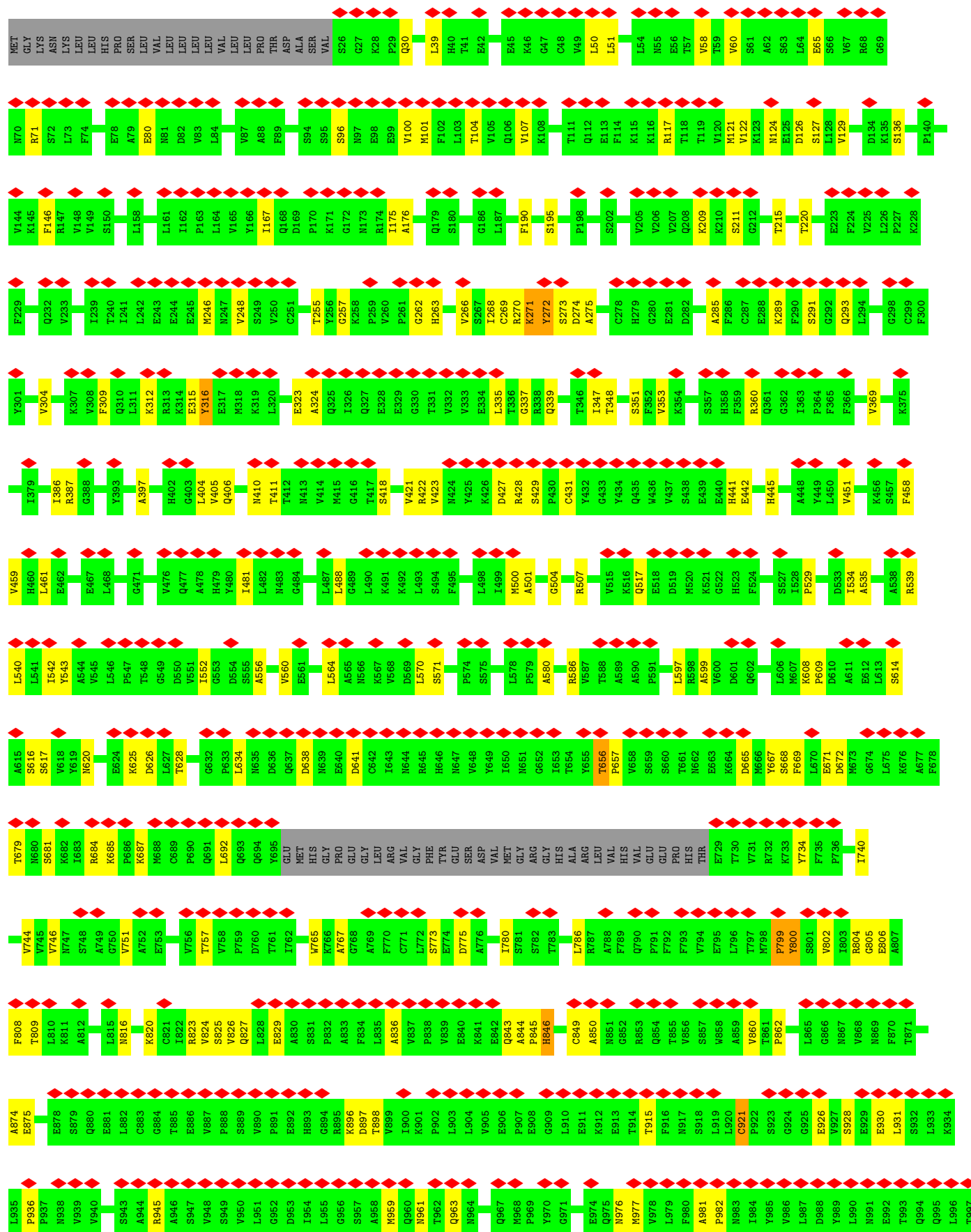


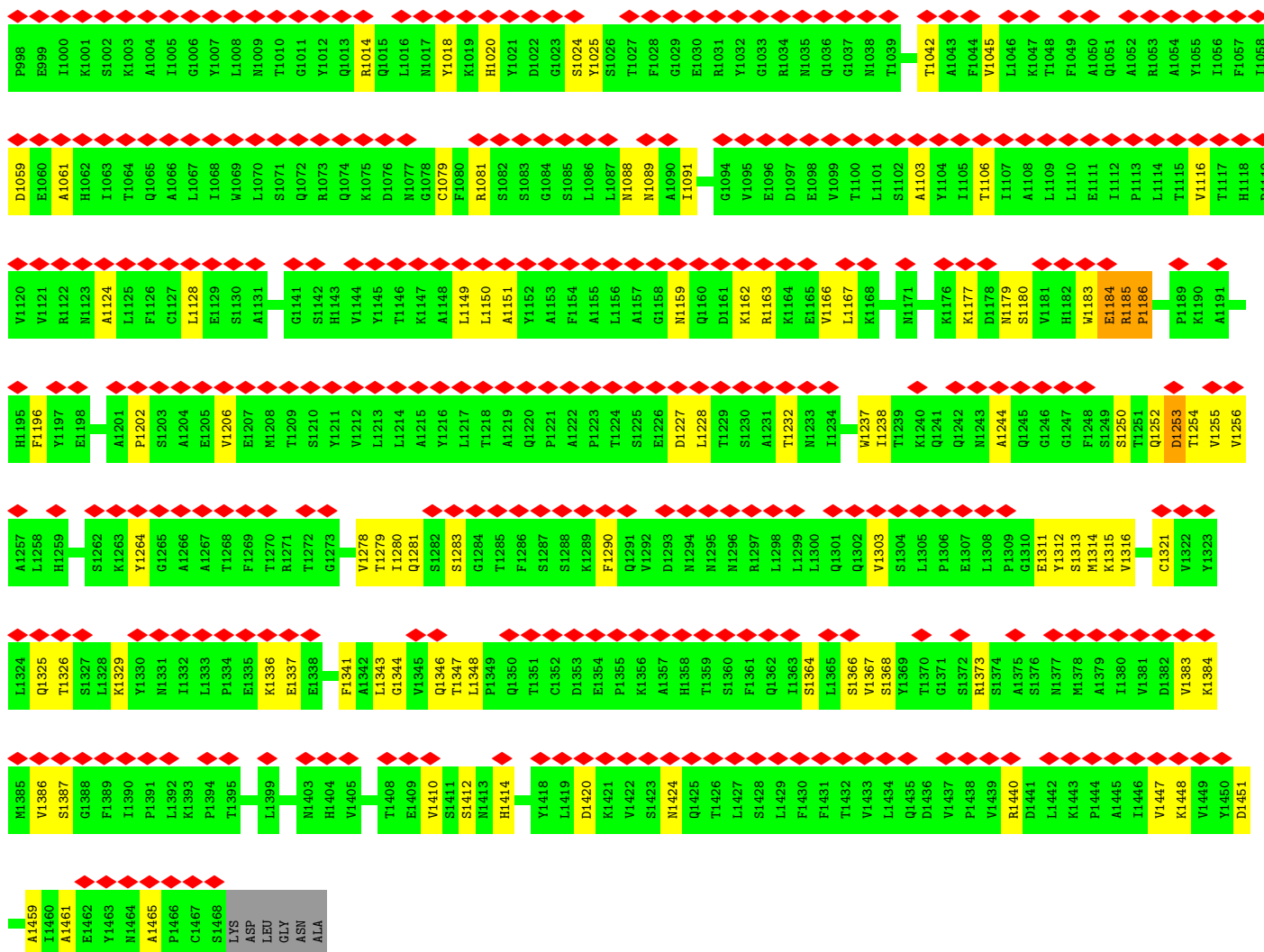


• Molecule 1: Alpha-2-macroglobulin









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



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



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



- Molecule 2: 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, C2	Depositor
Number of particles used	35993	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	47775	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.056	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0135	Depositor
Map size (\AA)	335.04, 335.04, 335.04	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.047, 1.047, 1.047	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.25	0/10165	0.54	9/13811 (0.1%)
1	B	0.33	4/11249 (0.0%)	0.58	6/15286 (0.0%)
1	C	0.25	0/10165	0.54	9/13811 (0.1%)
1	D	0.33	4/11249 (0.0%)	0.58	6/15286 (0.0%)
All	All	0.30	8/42828 (0.0%)	0.56	30/58194 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	845	PRO	CA-CB	-10.44	1.39	1.53
1	D	845	PRO	CA-CB	-10.44	1.39	1.53
1	B	845	PRO	N-CA	9.11	1.58	1.47
1	D	845	PRO	N-CA	9.11	1.58	1.47
1	B	846	HIS	CA-C	-6.84	1.46	1.53
1	D	846	HIS	CA-C	-6.84	1.46	1.53
1	B	846	HIS	N-CA	6.17	1.54	1.46
1	D	846	HIS	N-CA	6.17	1.54	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	821	CYS	CA-C-N	10.48	139.51	122.64
1	A	821	CYS	C-N-CA	10.48	139.51	122.64
1	C	821	CYS	CA-C-N	10.48	139.51	122.64
1	C	821	CYS	C-N-CA	10.48	139.51	122.64
1	A	821	CYS	O-C-N	-9.63	110.99	123.13
1	C	821	CYS	O-C-N	-9.63	110.99	123.13
1	A	849	CYS	CA-CB-SG	7.47	131.58	114.40
1	C	849	CYS	CA-CB-SG	7.47	131.58	114.40
1	B	845	PRO	N-CA-C	-7.23	97.58	112.47
1	D	845	PRO	N-CA-C	-7.23	97.58	112.47
1	B	845	PRO	CB-CA-C	6.40	122.12	111.56
1	D	845	PRO	CB-CA-C	6.40	122.12	111.56
1	A	822	ILE	CA-C-N	6.02	129.26	120.71
1	A	822	ILE	C-N-CA	6.02	129.26	120.71
1	C	822	ILE	CA-C-N	6.02	129.26	120.71
1	C	822	ILE	C-N-CA	6.02	129.26	120.71
1	B	1116	VAL	N-CA-C	-5.76	107.20	112.96
1	D	1116	VAL	N-CA-C	-5.76	107.20	112.96
1	A	52	SER	CA-C-N	5.27	131.61	121.54
1	A	52	SER	C-N-CA	5.27	131.61	121.54
1	C	52	SER	CA-C-N	5.27	131.61	121.54
1	C	52	SER	C-N-CA	5.27	131.61	121.54
1	B	316	TYR	CA-C-N	5.24	128.78	121.02
1	B	316	TYR	C-N-CA	5.24	128.78	121.02
1	D	316	TYR	CA-C-N	5.24	128.78	121.02
1	D	316	TYR	C-N-CA	5.24	128.78	121.02
1	A	822	ILE	N-CA-CB	-5.13	100.50	111.37
1	C	822	ILE	N-CA-CB	-5.13	100.50	111.37
1	B	921	CYS	CA-CB-SG	5.10	126.13	114.40
1	D	921	CYS	CA-CB-SG	5.10	126.13	114.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	821	CYS	Mainchain
1	C	821	CYS	Mainchain

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	9944	0	9843	175	0
1	B	11004	0	10889	194	0
1	C	9944	0	9843	175	0
1	D	11004	0	10889	195	0
2	E	28	0	25	1	0
2	F	28	0	25	5	0
2	G	28	0	25	0	0
2	H	28	0	25	5	0
3	A	70	0	65	1	0
3	B	112	0	104	1	0
3	C	70	0	65	1	0
3	D	112	0	104	1	0
All	All	42372	0	41902	746	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 9.

All (746) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1185:ARG:HB3	1:B:1186:PRO:CD	1.98	0.93
1:B:656:THR:HB	1:B:657:PRO:CD	1.99	0.92
1:D:1185:ARG:HB3	1:D:1186:PRO:CD	1.98	0.92
1:D:656:THR:HB	1:D:657:PRO:CD	1.99	0.91
1:D:597:LEU:HD11	1:D:744:VAL:HG22	1.62	0.80
2:F:2:NAG:H3	2:F:2:NAG:C8	2.12	0.80
1:B:597:LEU:HD11	1:B:744:VAL:HG22	1.62	0.79
2:H:2:NAG:C8	2:H:2:NAG:H3	2.12	0.79
1:B:539:ARG:NH1	1:B:672:ASP:O	2.17	0.78
1:A:946:ALA:HB2	1:A:1328:LEU:HD13	1.66	0.78
1:D:539:ARG:NH1	1:D:672:ASP:O	2.17	0.77
1:C:822:ILE:HA	1:C:887:VAL:HG23	1.66	0.77
1:C:946:ALA:HB2	1:C:1328:LEU:HD13	1.66	0.76
1:B:1185:ARG:HB3	1:B:1186:PRO:HD3	1.67	0.76
1:A:822:ILE:HA	1:A:887:VAL:HG23	1.66	0.75
1:B:269:CYS:SG	1:B:289:LYS:NZ	2.59	0.75
1:B:805:GLY:O	1:B:1440:ARG:NH2	2.20	0.75
1:D:805:GLY:O	1:D:1440:ARG:NH2	2.20	0.75
1:A:127:SER:O	1:A:209:LYS:NZ	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:CYS:SG	1:D:289:LYS:NZ	2.59	0.75
1:D:1185:ARG:HB3	1:D:1186:PRO:HD3	1.67	0.74
1:B:843:GLN:NE2	1:B:844:ALA:O	2.20	0.74
1:B:1079:CYS:O	1:B:1081:ARG:NH1	2.21	0.74
1:D:843:GLN:NE2	1:D:844:ALA:O	2.20	0.74
1:B:656:THR:HB	1:B:657:PRO:HD3	1.70	0.73
1:B:360:ARG:NH1	1:B:459:VAL:O	2.21	0.73
1:C:127:SER:O	1:C:209:LYS:NZ	2.20	0.73
1:D:656:THR:HB	1:D:657:PRO:HD2	1.70	0.73
1:B:656:THR:CB	1:B:657:PRO:CD	2.67	0.73
1:C:849:CYS:O	1:C:852:GLY:N	2.22	0.73
1:A:849:CYS:O	1:A:852:GLY:N	2.22	0.73
1:A:295:ASN:ND2	1:A:297:HIS:O	2.22	0.72
1:B:656:THR:HB	1:B:657:PRO:HD2	1.70	0.72
1:D:360:ARG:NH1	1:D:459:VAL:O	2.21	0.72
1:D:656:THR:CB	1:D:657:PRO:CD	2.67	0.72
1:C:295:ASN:ND2	1:C:297:HIS:O	2.22	0.72
1:D:656:THR:HB	1:D:657:PRO:HD3	1.70	0.72
1:D:270:ARG:NE	1:D:316:TYR:O	2.23	0.72
1:C:1180:SER:OG	1:C:1233:ASN:O	2.08	0.72
1:D:1184:GLU:OE1	1:D:1184:GLU:HA	1.89	0.71
1:D:1079:CYS:O	1:D:1081:ARG:NH1	2.21	0.71
1:A:964:ASN:ND2	1:A:1245:GLN:O	2.24	0.71
1:A:1180:SER:OG	1:A:1233:ASN:O	2.08	0.71
1:B:1184:GLU:OE1	1:B:1184:GLU:HA	1.89	0.71
1:B:571:SER:O	1:B:586:ARG:N	2.24	0.71
1:B:860:VAL:HG22	1:B:862:PRO:HD3	1.72	0.71
1:C:964:ASN:ND2	1:C:1245:GLN:O	2.24	0.71
1:C:434:TYR:OH	1:D:274:ASP:OD1	2.09	0.70
1:A:434:TYR:OH	1:B:274:ASP:OD1	2.09	0.70
1:C:823:ARG:NH1	1:C:824:VAL:O	2.24	0.70
1:B:270:ARG:NE	1:B:316:TYR:O	2.23	0.70
1:C:96:SER:O	1:C:124:ASN:ND2	2.24	0.70
1:D:571:SER:O	1:D:586:ARG:N	2.24	0.70
1:D:860:VAL:HG22	1:D:862:PRO:HD3	1.72	0.70
1:D:353:VAL:HG21	1:D:404:LEU:HD13	1.73	0.69
1:B:608:LYS:NZ	1:B:609:PRO:O	2.25	0.69
1:C:1185:ARG:O	1:C:1187:GLN:NE2	2.25	0.69
1:C:1250:SER:O	1:C:1254:THR:OG1	2.09	0.69
1:C:536:PRO:O	1:C:560:VAL:N	2.26	0.69
1:A:96:SER:O	1:A:124:ASN:ND2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:LEU:O	1:B:517:GLN:NE2	2.26	0.69
1:B:1250:SER:HB3	1:B:1253:ASP:HB2	1.74	0.69
1:D:418:SER:OG	1:D:445:HIS:NE2	2.25	0.69
1:A:507:ARG:NH2	1:A:532:SER:O	2.26	0.69
1:A:536:PRO:O	1:A:560:VAL:N	2.26	0.69
1:A:1185:ARG:O	1:A:1187:GLN:NE2	2.25	0.69
1:B:418:SER:OG	1:B:445:HIS:NE2	2.25	0.69
1:C:270:ARG:NH1	1:C:309:PHE:O	2.26	0.69
1:C:495:PHE:O	1:C:510:THR:OG1	2.11	0.69
1:D:488:LEU:O	1:D:517:GLN:NE2	2.26	0.69
1:A:270:ARG:NH1	1:A:309:PHE:O	2.26	0.69
1:C:614:SER:O	1:C:617:SER:OG	2.09	0.69
1:A:637:GLN:O	1:A:684:ARG:NH1	2.26	0.68
1:C:637:GLN:O	1:C:684:ARG:NH1	2.26	0.68
1:A:823:ARG:NH1	1:A:824:VAL:O	2.24	0.68
1:B:1106:THR:HG21	1:B:1124:ALA:HB3	1.75	0.68
1:C:507:ARG:NH2	1:C:532:SER:O	2.26	0.68
1:D:608:LYS:NZ	1:D:609:PRO:O	2.25	0.68
1:B:353:VAL:HG21	1:B:404:LEU:HD13	1.73	0.68
1:D:1250:SER:HB3	1:D:1253:ASP:HB2	1.74	0.68
1:B:507:ARG:NH1	1:B:529:PRO:O	2.26	0.68
1:C:288:GLU:N	1:C:288:GLU:OE1	2.27	0.68
1:D:507:ARG:NH1	1:D:529:PRO:O	2.26	0.68
1:A:288:GLU:OE1	1:A:288:GLU:N	2.27	0.67
1:B:626:ASP:OD2	1:B:628:THR:OG1	2.12	0.67
1:C:33:VAL:HG12	1:C:49:VAL:HG23	1.77	0.67
1:B:255:THR:HG1	1:B:734:TYR:HH	1.42	0.67
1:C:415:MET:SD	1:C:416:GLY:N	2.68	0.67
1:D:1232:THR:HG22	1:D:1264:TYR:OH	1.95	0.67
1:D:626:ASP:OD2	1:D:628:THR:OG1	2.12	0.67
1:D:825:SER:N	1:D:875:GLU:O	2.28	0.67
1:D:773:SER:OG	1:D:775:ASP:OD1	2.10	0.66
1:A:415:MET:SD	1:A:416:GLY:N	2.68	0.66
1:D:255:THR:HG1	1:D:734:TYR:HH	1.44	0.66
1:B:1177:LYS:N	1:B:1180:SER:O	2.29	0.66
1:C:270:ARG:NH2	1:C:315:GLU:O	2.29	0.66
1:A:614:SER:O	1:A:617:SER:OG	2.09	0.66
1:B:1185:ARG:HD3	1:B:1196:PHE:HB2	1.76	0.66
1:D:1106:THR:HG21	1:D:1124:ALA:HB3	1.75	0.66
1:A:400:ASP:OD1	1:A:404:LEU:N	2.28	0.66
1:A:33:VAL:HG12	1:A:49:VAL:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:825:SER:N	1:B:875:GLU:O	2.28	0.66
1:D:1177:LYS:N	1:D:1180:SER:O	2.29	0.66
1:C:400:ASP:OD1	1:C:404:LEU:N	2.28	0.66
1:B:271:LYS:O	1:B:272:TYR:HB2	1.95	0.66
1:D:823:ARG:NH1	1:D:846:HIS:O	2.29	0.66
1:D:1185:ARG:HB3	1:D:1186:PRO:HD2	1.78	0.66
1:C:363:ILE:O	1:C:411:THR:OG1	2.15	0.65
1:B:823:ARG:NH1	1:B:846:HIS:O	2.29	0.65
1:D:800:TYR:O	1:D:802:VAL:HG13	1.96	0.65
1:B:1185:ARG:CB	1:B:1186:PRO:CD	2.75	0.65
1:B:1232:THR:HG22	1:B:1264:TYR:OH	1.95	0.65
1:B:800:TYR:O	1:B:802:VAL:HG13	1.96	0.65
1:B:1185:ARG:HB3	1:B:1186:PRO:HD2	1.78	0.65
1:D:1185:ARG:HD3	1:D:1196:PHE:HB2	1.76	0.65
1:A:363:ILE:O	1:A:411:THR:OG1	2.15	0.65
1:A:270:ARG:NH2	1:A:315:GLU:O	2.29	0.64
1:A:495:PHE:O	1:A:510:THR:OG1	2.11	0.64
1:A:1250:SER:O	1:A:1254:THR:OG1	2.09	0.64
1:D:638:ASP:OD2	1:D:641:ASP:N	2.31	0.64
1:D:271:LYS:O	1:D:272:TYR:HB2	1.95	0.64
1:B:1373:ARG:HD2	1:B:1373:ARG:O	1.98	0.64
1:D:1228:LEU:O	1:D:1232:THR:HG23	1.98	0.63
1:B:976:ASN:OD1	1:B:1014:ARG:NH1	2.31	0.63
1:C:458:PHE:CZ	1:C:481:ILE:HD11	2.33	0.63
1:C:360:ARG:O	1:C:411:THR:OG1	2.12	0.63
1:D:976:ASN:OD1	1:D:1014:ARG:NH1	2.31	0.63
1:A:458:PHE:CZ	1:A:481:ILE:HD11	2.33	0.63
1:B:1228:LEU:O	1:B:1232:THR:HG23	1.98	0.63
1:C:1129:GLU:OE1	1:C:1162:LYS:NZ	2.31	0.63
2:F:2:NAG:H3	2:F:2:NAG:H82	1.81	0.63
1:B:616:SER:O	1:B:620:ASN:ND2	2.32	0.63
1:D:616:SER:O	1:D:620:ASN:ND2	2.32	0.63
1:D:915:THR:OG1	1:D:1326:THR:O	2.05	0.63
1:A:1117:THR:O	1:A:1122:ARG:NH1	2.32	0.63
1:D:1373:ARG:HD2	1:D:1373:ARG:O	1.98	0.63
1:A:1129:GLU:OE1	1:A:1162:LYS:NZ	2.31	0.62
1:B:638:ASP:OD2	1:B:641:ASP:N	2.31	0.62
1:C:769:ALA:HB3	1:C:781:SER:HB3	1.81	0.62
1:A:769:ALA:HB3	1:A:781:SER:HB3	1.81	0.62
1:C:1019:LYS:NZ	1:C:1020:HIS:O	2.20	0.62
1:C:293:GLN:NE2	1:C:294:LEU:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:928:SER:OG	1:C:1314:MET:O	2.11	0.62
1:D:270:ARG:O	1:D:285:ALA:N	2.32	0.62
1:B:270:ARG:O	1:B:285:ALA:N	2.32	0.62
1:B:195:SER:N	1:B:963:GLN:OE1	2.33	0.62
1:B:404:LEU:O	1:B:406:GLN:NE2	2.33	0.62
1:D:195:SER:N	1:D:963:GLN:OE1	2.33	0.62
1:D:620:ASN:O	1:D:625:LYS:NZ	2.26	0.62
1:A:293:GLN:NE2	1:A:294:LEU:O	2.33	0.62
1:B:620:ASN:O	1:B:625:LYS:NZ	2.26	0.61
1:C:580:ALA:O	1:C:757:THR:OG1	2.14	0.61
1:D:404:LEU:O	1:D:406:GLN:NE2	2.33	0.61
2:F:2:NAG:H3	2:F:2:NAG:H83	1.82	0.61
2:H:2:NAG:H3	2:H:2:NAG:H82	1.81	0.61
1:B:915:THR:OG1	1:B:1326:THR:O	2.05	0.61
1:C:383:VAL:O	1:C:423:VAL:HG23	2.00	0.61
1:C:1117:THR:O	1:C:1122:ARG:NH1	2.32	0.61
1:D:816:ASN:ND2	1:D:820:LYS:O	2.34	0.61
1:A:383:VAL:O	1:A:423:VAL:HG23	2.00	0.61
1:B:540:LEU:O	1:B:556:ALA:N	2.33	0.61
2:H:2:NAG:H3	2:H:2:NAG:H83	1.82	0.61
1:A:360:ARG:O	1:A:411:THR:OG1	2.12	0.61
1:D:1103:ALA:HB1	1:D:1149:LEU:HD13	1.83	0.61
1:B:1103:ALA:HB1	1:B:1149:LEU:HD13	1.83	0.60
1:B:1089:ASN:ND2	1:B:1420:ASP:O	2.35	0.60
1:C:1005:ILE:O	1:C:1009:ASN:ND2	2.34	0.60
1:D:540:LEU:O	1:D:556:ALA:N	2.33	0.60
1:D:614:SER:O	1:D:617:SER:OG	2.15	0.60
1:B:428:ARG:NH2	1:B:441:HIS:O	2.34	0.60
1:B:816:ASN:ND2	1:B:820:LYS:O	2.34	0.60
1:D:428:ARG:NH2	1:D:441:HIS:O	2.34	0.60
1:B:1185:ARG:NE	1:B:1185:ARG:HA	2.16	0.60
1:A:1005:ILE:O	1:A:1009:ASN:ND2	2.34	0.60
1:D:981:ALA:HB3	1:D:982:PRO:HD3	1.84	0.60
1:D:1089:ASN:ND2	1:D:1420:ASP:O	2.35	0.60
1:D:1185:ARG:HA	1:D:1185:ARG:NE	2.16	0.60
1:C:955:LEU:HD23	1:C:958:ALA:HB3	1.84	0.59
1:D:1185:ARG:HA	1:D:1185:ARG:HE	1.67	0.59
1:D:1278:VAL:N	1:D:1290:PHE:O	2.36	0.59
1:B:1185:ARG:HA	1:B:1185:ARG:HE	1.67	0.59
1:A:955:LEU:HD23	1:A:958:ALA:HB3	1.84	0.59
1:B:799:PRO:O	1:B:800:TYR:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ARG:NH1	1:D:315:GLU:HB2	2.18	0.59
1:B:981:ALA:HB3	1:B:982:PRO:HD3	1.84	0.59
1:B:1278:VAL:N	1:B:1290:PHE:O	2.36	0.59
1:C:169:ASP:N	1:C:173:ASN:O	2.36	0.58
1:A:68:ARG:NH2	1:C:1060:GLU:OE1	2.36	0.58
1:A:169:ASP:N	1:A:173:ASN:O	2.36	0.58
1:B:270:ARG:NH1	1:B:315:GLU:HB2	2.18	0.58
1:A:636:ASP:O	1:C:1072:GLN:NE2	2.36	0.58
1:B:60:VAL:HG12	1:B:107:VAL:HA	1.86	0.58
1:D:799:PRO:O	1:D:800:TYR:HB2	2.02	0.58
1:A:491:LYS:O	1:A:515:VAL:HG22	2.04	0.58
1:A:1072:GLN:NE2	1:C:636:ASP:O	2.36	0.58
1:B:312:LYS:HB2	1:B:315:GLU:HG2	1.86	0.58
1:D:60:VAL:HG12	1:D:107:VAL:HA	1.86	0.58
1:B:773:SER:OG	1:B:775:ASP:OD1	2.10	0.57
1:D:312:LYS:HB2	1:D:315:GLU:HG2	1.86	0.57
1:A:1060:GLU:OE1	1:C:68:ARG:NH2	2.36	0.57
1:B:273:SER:N	1:B:316:TYR:HB3	2.19	0.57
1:A:580:ALA:O	1:A:757:THR:OG1	2.14	0.57
1:A:979:LEU:O	1:A:983:ASN:ND2	2.38	0.57
1:A:540:LEU:O	1:A:556:ALA:N	2.37	0.57
1:A:928:SER:OG	1:A:1314:MET:O	2.11	0.57
1:B:614:SER:O	1:B:617:SER:OG	2.15	0.57
1:C:459:VAL:HG23	1:C:552:ILE:HD12	1.86	0.57
1:D:959:MET:SD	1:D:959:MET:N	2.77	0.57
1:B:959:MET:SD	1:B:959:MET:N	2.77	0.56
1:D:1250:SER:CB	1:D:1253:ASP:HB2	2.35	0.56
1:A:782:SER:OG	1:A:783:THR:N	2.38	0.56
1:A:1027:THR:HG21	1:A:1087:LEU:HD11	1.88	0.56
1:C:979:LEU:O	1:C:983:ASN:ND2	2.38	0.56
1:A:459:VAL:HG23	1:A:552:ILE:HD12	1.86	0.56
1:B:1283:SER:OG	1:B:1311:GLU:OE2	2.20	0.56
1:C:491:LYS:O	1:C:515:VAL:HG22	2.04	0.56
1:C:540:LEU:O	1:C:556:ALA:N	2.37	0.56
1:D:273:SER:N	1:D:316:TYR:HB3	2.19	0.56
1:A:165:VAL:HG22	1:A:207:VAL:HG22	1.87	0.56
1:C:493:LEU:HD21	1:C:546:LEU:CD2	2.36	0.56
1:D:921:CYS:HB2	1:D:1321:CYS:HA	1.88	0.56
1:D:126:ASP:OD2	1:D:211:SER:OG	2.22	0.56
1:D:1020:HIS:N	1:D:1024:SER:O	2.39	0.56
1:D:1283:SER:OG	1:D:1311:GLU:OE2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:LYS:NZ	1:A:1020:HIS:O	2.20	0.56
1:B:1020:HIS:N	1:B:1024:SER:O	2.39	0.56
1:B:1250:SER:CB	1:B:1253:ASP:HB2	2.35	0.56
1:C:592:GLN:OE1	1:C:748:SER:OG	2.23	0.56
1:A:493:LEU:HD21	1:A:546:LEU:CD2	2.36	0.56
1:B:1341:PHE:O	1:B:1461:ALA:HB2	2.06	0.56
1:C:56:GLU:O	1:C:58:VAL:HG12	2.06	0.56
1:C:1027:THR:HG21	1:C:1087:LEU:HD11	1.88	0.56
1:B:634:LEU:O	1:B:687:LYS:NZ	2.30	0.55
1:B:1106:THR:HG21	1:B:1124:ALA:CB	2.36	0.55
1:C:782:SER:OG	1:C:783:THR:N	2.38	0.55
1:C:165:VAL:HG22	1:C:207:VAL:HG22	1.87	0.55
1:C:354:LYS:NZ	1:C:463:PRO:O	2.32	0.55
1:C:583:ALA:O	1:C:755:GLY:N	2.39	0.55
1:C:579:PRO:HB3	1:C:731:VAL:HG12	1.88	0.55
2:F:1:NAG:H83	2:F:1:NAG:C1	2.37	0.55
1:C:929:GLU:O	1:C:1314:MET:N	2.39	0.55
1:A:583:ALA:O	1:A:755:GLY:N	2.39	0.55
1:A:592:GLN:OE1	1:A:748:SER:OG	2.23	0.55
1:C:472:HIS:O	1:C:530:VAL:N	2.39	0.55
1:C:822:ILE:HG21	1:C:876:ALA:HB1	1.89	0.55
1:D:1341:PHE:O	1:D:1461:ALA:HB2	2.06	0.55
1:B:921:CYS:HB2	1:B:1321:CYS:HA	1.88	0.55
1:C:345:ARG:O	1:C:440:GLU:N	2.39	0.54
1:D:827:GLN:NE2	1:D:829:GLU:OE2	2.40	0.54
1:A:56:GLU:O	1:A:58:VAL:HG12	2.06	0.54
1:A:345:ARG:O	1:A:440:GLU:N	2.39	0.54
1:D:127:SER:O	1:D:209:LYS:NZ	2.35	0.54
2:H:1:NAG:C1	2:H:1:NAG:H83	2.37	0.54
1:B:96:SER:O	1:B:124:ASN:ND2	2.41	0.54
1:D:30:GLN:O	1:D:51:LEU:HD12	2.08	0.54
1:A:382:LYS:N	1:A:399:THR:OG1	2.40	0.54
1:A:948:VAL:HG12	1:A:1305:LEU:HD11	1.90	0.54
1:D:96:SER:O	1:D:124:ASN:ND2	2.41	0.54
1:A:109:GLY:N	1:A:112:GLN:O	2.41	0.54
1:A:579:PRO:HB3	1:A:731:VAL:HG12	1.88	0.54
1:B:827:GLN:NE2	1:B:829:GLU:OE2	2.40	0.54
1:C:31:TYR:O	1:C:679:THR:HG23	2.08	0.54
1:D:351:SER:O	1:D:369:VAL:HG13	2.08	0.54
1:D:1185:ARG:CB	1:D:1186:PRO:CD	2.75	0.54
1:A:382:LYS:HE2	1:A:423:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:SER:O	1:B:369:VAL:HG13	2.08	0.54
1:C:382:LYS:N	1:C:399:THR:OG1	2.40	0.54
1:C:885:THR:OG1	1:C:886:GLU:OE1	2.11	0.54
1:C:955:LEU:HD21	1:C:995:GLN:OE1	2.08	0.54
1:D:656:THR:CB	1:D:657:PRO:HD2	2.36	0.54
1:A:31:TYR:O	1:A:679:THR:HG23	2.08	0.54
1:A:1027:THR:HG21	1:A:1087:LEU:CD1	2.38	0.54
1:C:539:ARG:NH1	1:C:672:ASP:O	2.41	0.54
1:C:822:ILE:HD11	1:C:889:SER:H	1.73	0.54
1:C:1027:THR:HG21	1:C:1087:LEU:CD1	2.38	0.54
1:D:1106:THR:HG21	1:D:1124:ALA:CB	2.36	0.54
1:A:929:GLU:O	1:A:1314:MET:N	2.39	0.54
1:C:1100:THR:CG2	1:C:1146:THR:HG22	2.38	0.54
1:C:109:GLY:N	1:C:112:GLN:O	2.41	0.54
1:A:539:ARG:NH1	1:A:672:ASP:O	2.41	0.54
1:B:262:GLY:O	1:B:293:GLN:NE2	2.40	0.53
1:D:271:LYS:O	1:D:271:LYS:NZ	2.26	0.53
1:A:822:ILE:HD11	1:A:889:SER:H	1.73	0.53
1:C:892:GLU:N	1:C:892:GLU:OE1	2.41	0.53
1:A:1100:THR:CG2	1:A:1146:THR:HG22	2.38	0.53
1:C:382:LYS:HE2	1:C:423:VAL:HG21	1.89	0.53
1:D:262:GLY:O	1:D:293:GLN:NE2	2.40	0.53
1:A:892:GLU:N	1:A:892:GLU:OE1	2.41	0.53
1:B:126:ASP:OD2	1:B:211:SER:OG	2.22	0.53
1:C:948:VAL:HG12	1:C:1305:LEU:HD11	1.90	0.53
1:D:129:VAL:HG23	1:D:215:THR:HG21	1.90	0.53
1:D:580:ALA:O	1:D:757:THR:OG1	2.20	0.53
1:A:946:ALA:HB3	1:A:1305:LEU:HB2	1.90	0.53
3:C:2004:NAG:O7	3:C:2004:NAG:O3	2.24	0.53
1:A:955:LEU:HD21	1:A:995:GLN:OE1	2.08	0.53
1:B:30:GLN:O	1:B:51:LEU:HD12	2.08	0.53
1:D:599:ALA:HB3	1:D:740:ILE:HG13	1.91	0.53
1:D:836:ALA:HA	1:D:860:VAL:HG23	1.90	0.53
1:A:822:ILE:HG21	1:A:876:ALA:HB1	1.89	0.53
1:B:136:SER:O	1:B:220:THR:N	2.42	0.53
1:B:1346:GLN:NE2	1:B:1348:LEU:O	2.42	0.53
1:A:584:HIS:NE2	1:A:754:VAL:HG22	2.24	0.53
1:A:472:HIS:O	1:A:530:VAL:N	2.39	0.52
1:B:129:VAL:HG23	1:B:215:THR:HG21	1.90	0.52
1:B:599:ALA:HB3	1:B:740:ILE:HG13	1.91	0.52
1:D:1346:GLN:NE2	1:D:1348:LEU:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:665:ASP:O	1:B:668:SER:OG	2.27	0.52
1:B:127:SER:O	1:B:209:LYS:NZ	2.35	0.52
1:B:836:ALA:HA	1:B:860:VAL:HG23	1.90	0.52
1:C:276:SER:OG	1:C:278:CYS:O	2.27	0.52
1:C:584:HIS:NE2	1:C:754:VAL:HG22	2.24	0.52
1:B:1014:ARG:O	1:B:1018:TYR:N	2.43	0.52
1:B:1451:ASP:OD1	1:B:1451:ASP:N	2.43	0.52
1:C:974:GLU:O	1:C:978:VAL:HG23	2.10	0.52
1:A:974:GLU:O	1:A:978:VAL:HG23	2.10	0.52
3:A:2004:NAG:O7	3:A:2004:NAG:O3	2.24	0.52
1:C:946:ALA:HB3	1:C:1305:LEU:HB2	1.90	0.52
1:D:136:SER:O	1:D:220:THR:N	2.42	0.52
1:A:239:ILE:HG22	1:A:341:SER:HB3	1.92	0.52
1:A:918:SER:O	1:A:1324:LEU:N	2.42	0.52
1:A:1242:GLN:NE2	1:A:1243:ASN:O	2.43	0.52
1:D:1336:LYS:NZ	1:D:1337:GLU:OE1	2.36	0.51
1:D:1014:ARG:O	1:D:1018:TYR:N	2.43	0.51
1:A:936:PRO:O	1:A:939:VAL:HG12	2.11	0.51
1:B:50:LEU:HD11	1:B:543:TYR:CE1	2.45	0.51
1:B:1252:GLN:O	1:B:1253:ASP:C	2.54	0.51
1:A:276:SER:OG	1:A:278:CYS:O	2.27	0.51
1:B:1344:GLY:O	1:B:1366:SER:N	2.41	0.51
1:C:936:PRO:O	1:C:939:VAL:HG12	2.11	0.51
1:D:50:LEU:HD11	1:D:543:TYR:CE1	2.45	0.51
1:B:167:ILE:HD12	1:B:176:ALA:HB3	1.93	0.51
1:B:1336:LYS:NZ	1:B:1337:GLU:OE1	2.36	0.51
1:C:239:ILE:HG22	1:C:341:SER:HB3	1.92	0.51
1:D:167:ILE:HD12	1:D:176:ALA:HB3	1.93	0.51
1:D:945:ARG:O	1:D:1329:LYS:N	2.44	0.51
1:D:1252:GLN:O	1:D:1253:ASP:C	2.54	0.51
1:C:135:LYS:NZ	1:C:142:GLN:OE1	2.44	0.51
1:A:579:PRO:O	1:A:581:SER:N	2.44	0.51
1:B:599:ALA:HB3	1:B:740:ILE:CG1	2.40	0.51
1:C:1242:GLN:NE2	1:C:1243:ASN:O	2.43	0.51
1:D:665:ASP:O	1:D:668:SER:OG	2.27	0.51
1:A:350:LEU:HD11	1:A:444:ALA:HB2	1.93	0.51
1:A:648:VAL:HG22	1:A:658:VAL:HG13	1.93	0.51
1:B:945:ARG:O	1:B:1329:LYS:N	2.44	0.51
1:D:928:SER:OG	1:D:1314:MET:O	2.10	0.51
1:D:1344:GLY:O	1:D:1366:SER:N	2.41	0.51
1:C:33:VAL:C	1:C:34:LEU:HD12	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:874:ALA:N	1:D:897:ASP:O	2.44	0.50
1:D:667:TYR:OH	1:D:684:ARG:NH1	2.45	0.50
1:A:1180:SER:OG	1:A:1181:VAL:N	2.44	0.50
1:C:563:CYS:O	1:C:619:TYR:OH	2.29	0.50
1:A:598:ARG:O	1:A:768:GLY:N	2.43	0.50
1:B:874:ALA:N	1:B:897:ASP:O	2.44	0.50
1:B:1151:ALA:HB2	1:B:1167:LEU:HD11	1.93	0.50
1:C:579:PRO:O	1:C:581:SER:N	2.44	0.50
1:D:599:ALA:HB3	1:D:740:ILE:CG1	2.40	0.50
1:D:1024:SER:OG	1:D:1025:TYR:N	2.45	0.50
1:A:33:VAL:C	1:A:34:LEU:HD12	2.35	0.50
1:A:563:CYS:O	1:A:619:TYR:OH	2.29	0.50
1:D:1151:ALA:HB2	1:D:1167:LEU:HD11	1.93	0.50
1:B:667:TYR:OH	1:B:684:ARG:NH1	2.45	0.50
1:B:1024:SER:OG	1:B:1025:TYR:N	2.45	0.50
1:C:41:THR:OG1	1:C:42:GLU:OE1	2.26	0.50
1:C:350:LEU:HD11	1:C:444:ALA:HB2	1.93	0.50
1:D:1150:LEU:HD13	1:D:1166:VAL:HG21	1.94	0.50
1:A:135:LYS:NZ	1:A:142:GLN:OE1	2.44	0.50
1:B:849:CYS:SG	1:B:850:ALA:N	2.85	0.49
1:C:66:SER:OG	1:C:71:ARG:N	2.45	0.49
1:C:875:GLU:OE1	1:C:875:GLU:N	2.45	0.49
1:C:648:VAL:HG21	1:C:657:PRO:HA	1.94	0.49
1:C:648:VAL:HG22	1:C:658:VAL:HG13	1.93	0.49
2:F:2:NAG:C8	2:F:2:NAG:C3	2.84	0.49
1:A:875:GLU:N	1:A:875:GLU:OE1	2.45	0.49
1:B:580:ALA:O	1:B:757:THR:OG1	2.20	0.49
1:D:167:ILE:HD12	1:D:176:ALA:CB	2.43	0.49
1:C:1180:SER:OG	1:C:1181:VAL:N	2.44	0.49
1:A:474:GLN:NE2	1:A:475:THR:O	2.43	0.49
1:A:648:VAL:HG21	1:A:657:PRO:HA	1.94	0.49
1:C:167:ILE:HD12	1:C:176:ALA:HB3	1.94	0.49
1:C:183:LEU:HD22	1:C:187:LEU:C	2.38	0.49
1:C:598:ARG:O	1:C:768:GLY:N	2.43	0.49
1:B:167:ILE:HD12	1:B:176:ALA:CB	2.43	0.49
1:C:593:SER:OG	1:C:772:LEU:O	2.13	0.49
1:D:634:LEU:O	1:D:687:LYS:NZ	2.30	0.49
1:D:1451:ASP:N	1:D:1451:ASP:OD1	2.43	0.49
1:A:41:THR:OG1	1:A:42:GLU:OE1	2.26	0.49
1:B:1150:LEU:HD13	1:B:1166:VAL:HG21	1.94	0.49
1:B:1163:ARG:O	1:B:1167:LEU:HD13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:GLN:NE2	1:C:475:THR:O	2.43	0.49
1:C:555:SER:OG	1:C:556:ALA:N	2.46	0.49
1:D:146:PHE:O	1:D:190:PHE:N	2.46	0.49
1:A:66:SER:OG	1:A:71:ARG:N	2.45	0.48
1:B:255:THR:HG23	1:B:257:GLY:H	1.78	0.48
1:B:1253:ASP:O	1:B:1256:VAL:N	2.42	0.48
1:D:411:THR:O	3:D:2005:NAG:N2	2.45	0.48
1:A:129:VAL:HG12	1:A:150:SER:CB	2.44	0.48
1:A:183:LEU:HD22	1:A:187:LEU:C	2.38	0.48
1:C:176:ALA:HB2	1:C:192:PHE:CE1	2.48	0.48
1:C:810:LEU:O	1:C:858:TRP:N	2.47	0.48
1:D:255:THR:HG23	1:D:257:GLY:H	1.78	0.48
1:D:1042:THR:HA	1:D:1045:VAL:HG12	1.96	0.48
1:A:167:ILE:HD12	1:A:176:ALA:HB3	1.94	0.48
1:B:146:PHE:O	1:B:190:PHE:N	2.46	0.48
1:C:27:GLY:HA3	1:C:547:PRO:HB2	1.96	0.48
1:C:32:MET:HE2	1:C:34:LEU:HD11	1.95	0.48
1:A:555:SER:OG	1:A:556:ALA:N	2.46	0.48
1:C:918:SER:O	1:C:1324:LEU:N	2.42	0.48
1:D:339:GLN:OE1	1:D:339:GLN:N	2.44	0.48
1:D:534:ILE:HG23	1:D:560:VAL:HG11	1.96	0.48
1:D:1183:TRP:CE3	1:D:1184:GLU:HB2	2.48	0.48
1:A:27:GLY:HA3	1:A:547:PRO:HB2	1.96	0.48
1:B:411:THR:O	3:B:2005:NAG:N2	2.45	0.48
1:A:32:MET:HE2	1:A:34:LEU:HD11	1.95	0.48
1:C:665:ASP:OD1	1:C:667:TYR:N	2.44	0.48
1:D:387:ARG:HB2	1:D:423:VAL:HG11	1.95	0.48
1:A:570:LEU:HD22	1:A:784:ALA:CB	2.44	0.48
1:D:1163:ARG:O	1:D:1167:LEU:HD13	2.13	0.48
1:B:339:GLN:OE1	1:B:339:GLN:N	2.44	0.47
1:B:1183:TRP:CE3	1:B:1184:GLU:HB2	2.48	0.47
1:B:387:ARG:HB2	1:B:423:VAL:HG11	1.95	0.47
1:B:1383:VAL:HG23	1:B:1414:HIS:HA	1.96	0.47
1:C:270:ARG:NE	1:C:316:TYR:O	2.45	0.47
1:D:1383:VAL:HG23	1:D:1414:HIS:HA	1.96	0.47
1:A:810:LEU:O	1:A:858:TRP:N	2.47	0.47
1:C:129:VAL:HG12	1:C:150:SER:CB	2.44	0.47
1:A:176:ALA:HB2	1:A:192:PHE:CE1	2.48	0.47
1:A:1118:HIS:HB3	1:A:1121:VAL:HG12	1.96	0.47
1:B:58:VAL:HG12	1:B:60:VAL:HG13	1.97	0.47
1:B:656:THR:CB	1:B:657:PRO:HD2	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:ILE:HG22	1:D:348:THR:HG23	1.96	0.47
1:B:534:ILE:HG23	1:B:560:VAL:HG11	1.96	0.47
1:B:268:ILE:HD11	1:B:309:PHE:CE1	2.50	0.47
1:C:418:SER:C	1:C:419:LEU:HD12	2.39	0.47
1:D:58:VAL:HG12	1:D:60:VAL:HG13	1.97	0.47
1:A:291:SER:OG	1:A:292:GLY:N	2.47	0.47
1:A:885:THR:OG1	1:A:886:GLU:OE1	2.11	0.47
1:A:910:LEU:HD22	1:A:1332:ILE:HD11	1.96	0.47
1:B:1042:THR:HA	1:B:1045:VAL:HG12	1.96	0.47
1:B:347:ILE:HG22	1:B:348:THR:HG23	1.96	0.47
1:C:419:LEU:N	1:C:446:HIS:O	2.45	0.47
1:C:570:LEU:HD22	1:C:784:ALA:CB	2.44	0.47
1:C:1323:TYR:C	1:C:1324:LEU:HD12	2.40	0.47
1:D:323:GLU:OE1	1:D:324:ALA:N	2.48	0.47
1:D:387:ARG:HG3	1:D:423:VAL:HG11	1.97	0.47
1:D:1279:THR:N	1:D:1315:LYS:O	2.45	0.47
1:B:458:PHE:CE1	1:B:481:ILE:HD11	2.50	0.47
1:A:418:SER:C	1:A:419:LEU:HD12	2.39	0.46
1:C:1118:HIS:HB3	1:C:1121:VAL:HG12	1.96	0.46
1:C:910:LEU:HD22	1:C:1332:ILE:HD11	1.96	0.46
1:B:1279:THR:N	1:B:1315:LYS:O	2.45	0.46
1:D:312:LYS:HB2	1:D:315:GLU:CG	2.45	0.46
1:D:427:ASP:OD1	1:D:428:ARG:N	2.48	0.46
1:A:270:ARG:NE	1:A:316:TYR:O	2.45	0.46
1:C:291:SER:OG	1:C:292:GLY:N	2.47	0.46
1:D:458:PHE:CE1	1:D:481:ILE:HD11	2.50	0.46
1:A:593:SER:OG	1:A:772:LEU:O	2.13	0.46
1:B:1384:LYS:H	1:B:1447:VAL:HG11	1.81	0.46
1:D:369:VAL:O	1:D:405:VAL:HG12	2.16	0.46
1:B:312:LYS:HB2	1:B:315:GLU:CG	2.45	0.46
1:B:369:VAL:O	1:B:405:VAL:HG12	2.16	0.46
1:B:564:LEU:CD1	1:B:780:ILE:HG22	2.46	0.46
1:D:1343:LEU:H	1:D:1461:ALA:HB3	1.81	0.46
1:B:427:ASP:OD1	1:B:428:ARG:N	2.48	0.46
1:B:1343:LEU:H	1:B:1461:ALA:HB3	1.81	0.46
1:C:883:CYS:SG	1:C:884:GLY:N	2.89	0.46
1:D:263:HIS:NE2	1:D:291:SER:OG	2.48	0.46
1:D:268:ILE:HD11	1:D:309:PHE:CE1	2.50	0.46
1:A:76:ASP:OD1	1:A:77:LEU:N	2.49	0.46
1:A:1322:VAL:HG23	1:A:1324:LEU:HD11	1.98	0.46
1:B:323:GLU:OE1	1:B:324:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:GLU:OE1	1:B:685:LYS:NZ	2.49	0.46
1:C:76:ASP:OD1	1:C:77:LEU:N	2.49	0.46
1:D:671:GLU:OE1	1:D:685:LYS:NZ	2.49	0.46
1:A:350:LEU:CD1	1:A:444:ALA:HB2	2.46	0.46
1:B:387:ARG:HG3	1:B:423:VAL:HG11	1.97	0.46
1:C:1322:VAL:HG23	1:C:1324:LEU:HD11	1.98	0.46
1:D:1184:GLU:HG3	1:D:1185:ARG:O	2.16	0.46
1:D:1384:LYS:H	1:D:1447:VAL:HG11	1.81	0.46
1:A:665:ASP:OD1	1:A:667:TYR:N	2.44	0.46
1:A:1323:TYR:C	1:A:1324:LEU:HD12	2.40	0.46
1:C:763:THR:HG23	1:C:764:GLU:O	2.16	0.46
1:D:804:ARG:NH2	1:D:806:GLU:OE2	2.49	0.46
1:A:187:LEU:HD11	1:A:743:LEU:HD21	1.99	0.45
1:A:883:CYS:SG	1:A:884:GLY:N	2.89	0.45
1:B:1184:GLU:HG3	1:B:1185:ARG:O	2.16	0.45
1:C:953:ASP:OD1	1:C:953:ASP:N	2.50	0.45
1:C:966:LEU:HD22	1:C:1000:ILE:HD11	1.97	0.45
1:D:246:MET:N	1:D:304:VAL:O	2.49	0.45
1:A:804:ARG:NH2	1:A:863:LYS:O	2.50	0.45
1:D:931:LEU:HD23	1:D:1314:MET:CE	2.47	0.45
1:A:570:LEU:HD23	1:A:571:SER:N	2.32	0.45
1:B:570:LEU:HD22	1:B:767:ALA:HB3	1.99	0.45
1:A:345:ARG:NE	1:A:440:GLU:OE1	2.50	0.45
1:A:598:ARG:NH2	1:A:610:ASP:OD2	2.49	0.45
1:C:80:GLU:N	1:C:80:GLU:OE1	2.50	0.45
1:C:570:LEU:HD23	1:C:571:SER:N	2.32	0.45
1:B:271:LYS:O	1:B:271:LYS:NZ	2.26	0.45
1:B:657:PRO:CG	1:B:692:LEU:HD23	2.46	0.45
1:C:598:ARG:NH2	1:C:610:ASP:OD2	2.49	0.45
1:B:246:MET:N	1:B:304:VAL:O	2.49	0.45
1:C:310:GLN:O	1:C:312:LYS:N	2.50	0.45
1:C:954:ILE:HG22	1:C:1297:ARG:NH2	2.32	0.45
1:D:657:PRO:CG	1:D:692:LEU:HD23	2.46	0.45
1:C:599:ALA:HB3	1:C:740:ILE:HB	1.99	0.45
1:D:564:LEU:CD1	1:D:780:ILE:HG22	2.46	0.45
1:C:137:ILE:HG22	1:C:220:THR:HB	1.99	0.45
1:D:599:ALA:HB3	1:D:740:ILE:HB	1.99	0.45
1:D:1346:GLN:O	1:D:1364:SER:N	2.50	0.45
1:A:137:ILE:HG22	1:A:220:THR:HB	1.99	0.45
1:A:599:ALA:HB3	1:A:740:ILE:HB	1.99	0.45
1:A:966:LEU:HD22	1:A:1000:ILE:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:ALA:O	1:B:560:VAL:HG21	2.16	0.45
1:C:345:ARG:NE	1:C:440:GLU:OE1	2.50	0.45
1:A:763:THR:HG23	1:A:764:GLU:O	2.16	0.44
1:B:80:GLU:OE1	1:B:80:GLU:N	2.47	0.44
1:B:931:LEU:HD23	1:B:1314:MET:CE	2.47	0.44
1:A:80:GLU:N	1:A:80:GLU:OE1	2.50	0.44
1:B:1346:GLN:O	1:B:1364:SER:N	2.50	0.44
1:D:1255:VAL:HG23	1:D:1256:VAL:HG23	2.00	0.44
1:B:71:ARG:HG2	1:B:101:MET:HE3	1.99	0.44
1:B:1059:ASP:OD1	1:B:1061:ALA:HB3	2.17	0.44
1:D:1206:VAL:HB	1:D:1253:ASP:OD2	2.17	0.44
1:A:372:VAL:HG12	1:A:373:ASP:N	2.32	0.44
1:B:422:ARG:NH1	1:B:442:GLU:O	2.51	0.44
1:D:535:ALA:O	1:D:560:VAL:HG21	2.16	0.44
1:B:451:VAL:HG23	1:B:669:PHE:HZ	1.83	0.44
1:C:350:LEU:CD1	1:C:444:ALA:HB2	2.46	0.44
1:C:352:PHE:CZ	1:C:444:ALA:HB1	2.53	0.44
1:A:502:LYS:H	1:A:535:ALA:HB2	1.82	0.44
1:A:952:GLY:O	1:A:1297:ARG:NH1	2.49	0.44
1:B:1255:VAL:HG23	1:B:1256:VAL:HG23	2.00	0.44
1:C:187:LEU:HD11	1:C:743:LEU:HD21	1.99	0.44
1:A:428:ARG:NH2	1:A:440:GLU:OE2	2.49	0.44
1:C:134:ASP:OD1	1:C:738:THR:OG1	2.28	0.44
1:A:310:GLN:O	1:A:312:LYS:N	2.50	0.44
1:A:881:GLU:HG3	1:A:887:VAL:HG12	1.99	0.44
1:B:804:ARG:NH2	1:B:806:GLU:OE2	2.49	0.44
1:B:926:GLU:OE2	1:B:1315:LYS:NZ	2.42	0.44
1:B:1206:VAL:HB	1:B:1253:ASP:OD2	2.17	0.44
1:C:264:VAL:O	1:C:292:GLY:N	2.51	0.44
1:C:372:VAL:HG12	1:C:373:ASP:N	2.32	0.44
1:C:804:ARG:NH2	1:C:863:LYS:O	2.50	0.44
1:B:39:LEU:HD12	1:B:122:VAL:HG12	2.00	0.44
1:D:71:ARG:HG2	1:D:101:MET:HE3	1.99	0.44
1:D:570:LEU:HD22	1:D:767:ALA:HB3	1.99	0.44
1:A:1039:THR:O	1:A:1042:THR:OG1	2.29	0.43
1:B:599:ALA:HB3	1:B:740:ILE:HB	1.99	0.43
1:C:341:SER:O	1:C:343:ILE:HD12	2.18	0.43
1:C:428:ARG:NH2	1:C:440:GLU:OE2	2.49	0.43
1:C:502:LYS:H	1:C:535:ALA:HB2	1.82	0.43
1:C:822:ILE:CD1	1:C:889:SER:H	2.29	0.43
1:C:881:GLU:HG3	1:C:887:VAL:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1059:ASP:OD1	1:D:1061:ALA:HB3	2.17	0.43
1:A:822:ILE:CD1	1:A:889:SER:H	2.29	0.43
1:A:954:ILE:HG22	1:A:1297:ARG:NH2	2.32	0.43
1:B:1347:THR:HG21	1:B:1465:ALA:HA	2.00	0.43
1:C:199:PHE:O	1:C:203:TYR:OH	2.30	0.43
1:D:1341:PHE:HB2	1:D:1459:ALA:HB1	1.99	0.43
1:D:1347:THR:HG21	1:D:1465:ALA:HA	2.00	0.43
1:C:164:LEU:HD12	1:C:178:TRP:O	2.18	0.43
1:D:80:GLU:OE1	1:D:80:GLU:N	2.47	0.43
1:D:422:ARG:NH1	1:D:442:GLU:O	2.51	0.43
1:D:429:SER:O	1:D:431:CYS:N	2.48	0.43
1:D:849:CYS:SG	1:D:850:ALA:N	2.85	0.43
1:A:164:LEU:HD12	1:A:178:TRP:O	2.18	0.43
1:A:173:ASN:OD1	1:A:173:ASN:N	2.51	0.43
1:A:264:VAL:O	1:A:292:GLY:N	2.51	0.43
1:A:352:PHE:CZ	1:A:444:ALA:HB1	2.53	0.43
2:H:2:NAG:C8	2:H:2:NAG:C3	2.84	0.43
1:B:1341:PHE:HB2	1:B:1459:ALA:HB1	1.99	0.43
1:C:964:ASN:O	1:C:966:LEU:N	2.51	0.43
1:D:1253:ASP:O	1:D:1256:VAL:N	2.42	0.43
1:B:104:THR:HG22	1:B:117:ARG:HA	2.00	0.43
1:C:359:PHE:CE1	1:C:417:THR:HG22	2.54	0.43
1:D:679:THR:HG22	1:D:681:SER:H	1.84	0.43
1:A:1052:ALA:O	1:A:1056:ILE:N	2.50	0.43
1:B:931:LEU:O	1:B:1312:TYR:N	2.48	0.43
1:B:1227:ASP:N	1:B:1227:ASP:OD1	2.51	0.43
1:C:33:VAL:HG12	1:C:49:VAL:CG2	2.47	0.43
1:C:1039:THR:O	1:C:1042:THR:OG1	2.29	0.43
1:A:311:LEU:C	1:A:312:LYS:HG2	2.44	0.43
1:A:739:TRP:O	1:A:740:ILE:HD13	2.19	0.43
1:C:118:THR:HG22	1:C:678:PHE:HZ	1.84	0.43
1:D:1163:ARG:HA	1:D:1166:VAL:HG22	2.01	0.43
1:D:1410:VAL:HG22	1:D:1412:SER:H	1.84	0.43
1:A:134:ASP:OD1	1:A:738:THR:OG1	2.28	0.43
1:B:679:THR:HG22	1:B:681:SER:H	1.84	0.43
1:C:173:ASN:OD1	1:C:173:ASN:N	2.51	0.43
1:C:887:VAL:O	1:C:887:VAL:HG13	2.19	0.43
1:D:104:THR:HG22	1:D:117:ARG:HA	2.00	0.43
1:D:335:LEU:HD23	1:D:337:GLY:N	2.34	0.43
1:D:1386:VAL:HG12	1:D:1387:SER:H	1.84	0.43
1:A:359:PHE:CE1	1:A:417:THR:HG22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:964:ASN:O	1:A:966:LEU:N	2.51	0.43
1:B:896:LYS:O	1:B:898:THR:HG23	2.19	0.43
1:A:406:GLN:OE1	1:A:406:GLN:N	2.52	0.42
1:A:802:VAL:HG23	1:A:905:VAL:HG23	2.00	0.42
1:A:941:GLU:OE1	1:A:942:GLU:N	2.52	0.42
1:A:1105:ILE:O	1:A:1109:LEU:HD23	2.19	0.42
1:B:501:ALA:N	1:B:504:GLY:O	2.49	0.42
1:C:802:VAL:HG23	1:C:905:VAL:HG23	2.00	0.42
1:C:961:ASN:OD1	1:C:1247:GLY:N	2.50	0.42
1:D:39:LEU:HD12	1:D:122:VAL:HG12	2.00	0.42
1:D:926:GLU:OE2	1:D:1315:LYS:NZ	2.42	0.42
1:B:571:SER:N	1:B:586:ARG:O	2.52	0.42
1:C:248:VAL:N	1:C:302:GLN:O	2.51	0.42
1:A:419:LEU:N	1:A:446:HIS:O	2.45	0.42
1:A:953:ASP:OD1	1:A:953:ASP:N	2.50	0.42
1:C:1151:ALA:HA	1:C:1166:VAL:HG11	2.01	0.42
1:D:571:SER:N	1:D:586:ARG:O	2.52	0.42
1:D:657:PRO:HG3	1:D:692:LEU:HD23	2.02	0.42
1:D:826:VAL:HG12	1:D:874:ALA:HB1	2.01	0.42
1:D:1227:ASP:N	1:D:1227:ASP:OD1	2.51	0.42
1:B:1163:ARG:HA	1:B:1166:VAL:HG22	2.01	0.42
1:B:1410:VAL:HG22	1:B:1412:SER:H	1.84	0.42
1:C:159:ASN:ND2	1:C:184:GLU:O	2.53	0.42
1:C:406:GLN:OE1	1:C:406:GLN:N	2.52	0.42
1:C:822:ILE:HG12	1:C:889:SER:OG	2.20	0.42
1:C:880:GLN:H	1:C:887:VAL:HG11	1.84	0.42
1:D:896:LYS:O	1:D:898:THR:HG23	2.19	0.42
1:D:977:MET:SD	1:D:1091:ILE:HD12	2.60	0.42
1:B:1386:VAL:HG12	1:B:1387:SER:H	1.84	0.42
1:C:737:GLU:O	1:C:738:THR:OG1	2.38	0.42
1:C:1052:ALA:O	1:C:1056:ILE:N	2.50	0.42
1:D:451:VAL:HG23	1:D:669:PHE:HZ	1.83	0.42
1:A:880:GLN:H	1:A:887:VAL:HG11	1.84	0.42
1:B:335:LEU:HD23	1:B:337:GLY:N	2.34	0.42
1:C:739:TRP:O	1:C:740:ILE:HD13	2.19	0.42
1:A:155:PHE:HB3	1:A:778:LEU:HD22	2.00	0.42
1:A:822:ILE:HG12	1:A:889:SER:OG	2.20	0.42
1:A:1236:LYS:NZ	1:A:1325:GLN:OE1	2.53	0.42
1:B:458:PHE:HB3	1:B:552:ILE:HG21	2.02	0.42
1:C:155:PHE:HB3	1:C:778:LEU:HD22	2.00	0.42
1:C:311:LEU:C	1:C:312:LYS:HG2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1144:VAL:HG23	1:C:1145:TYR:N	2.35	0.42
1:D:248:VAL:HG21	1:D:266:VAL:HG11	2.02	0.42
1:D:746:VAL:HG23	1:D:751:VAL:H	1.84	0.42
1:D:1088:ASN:HB3	1:D:1091:ILE:HG22	2.01	0.42
1:D:1367:VAL:O	1:D:1368:SER:OG	2.29	0.42
1:B:1179:ASN:HB2	1:B:1237:TRP:HB2	2.02	0.42
1:D:1447:VAL:O	1:D:1447:VAL:HG13	2.19	0.42
1:A:341:SER:O	1:A:343:ILE:HD12	2.18	0.42
1:A:887:VAL:O	1:A:887:VAL:HG13	2.19	0.42
1:B:421:VAL:HG12	1:B:422:ARG:H	1.85	0.42
1:A:159:ASN:ND2	1:A:184:GLU:O	2.53	0.42
1:D:765:TRP:HB2	1:D:786:LEU:HD22	2.02	0.42
1:D:1128:LEU:HD21	1:D:1150:LEU:HD21	2.02	0.42
1:D:1281:GLN:NE2	1:D:1313:SER:OG	2.53	0.42
1:A:118:THR:HG22	1:A:678:PHE:HZ	1.84	0.41
1:A:1051:GLN:O	1:A:1054:ALA:HB3	2.20	0.41
1:A:1144:VAL:HG23	1:A:1145:TYR:N	2.35	0.41
1:B:167:ILE:O	1:B:175:ILE:N	2.53	0.41
1:B:764:GLU:OE1	1:B:764:GLU:N	2.51	0.41
1:B:977:MET:SD	1:B:1091:ILE:HD12	2.60	0.41
1:B:1343:LEU:HD13	1:B:1448:LYS:HG3	2.02	0.41
1:B:1447:VAL:O	1:B:1447:VAL:HG13	2.19	0.41
1:C:1236:LYS:NZ	1:C:1325:GLN:OE1	2.53	0.41
1:B:657:PRO:HG3	1:B:692:LEU:HD23	2.02	0.41
1:B:663:GLU:OE1	1:B:663:GLU:N	2.52	0.41
1:C:577:SER:OG	1:C:580:ALA:HB2	2.21	0.41
1:D:458:PHE:HB3	1:D:552:ILE:HG21	2.02	0.41
1:A:1151:ALA:HA	1:A:1166:VAL:HG11	2.01	0.41
1:B:930:GLU:C	1:B:931:LEU:HD22	2.46	0.41
1:C:617:SER:O	1:C:621:LEU:HD13	2.20	0.41
1:C:643:ILE:O	1:C:643:ILE:HG22	2.20	0.41
1:D:461:LEU:HD11	1:D:542:ILE:CG2	2.51	0.41
1:D:824:VAL:HG13	1:D:824:VAL:O	2.20	0.41
1:D:1343:LEU:HD13	1:D:1448:LYS:HG3	2.02	0.41
1:A:737:GLU:O	1:A:738:THR:OG1	2.38	0.41
1:B:461:LEU:HD11	1:B:542:ILE:CG2	2.51	0.41
1:C:952:GLY:O	1:C:1297:ARG:NH1	2.49	0.41
1:D:1202:PRO:HB2	1:D:1253:ASP:CG	2.46	0.41
1:A:468:LEU:HD23	1:A:560:VAL:HG22	2.02	0.41
1:A:643:ILE:HG22	1:A:643:ILE:O	2.20	0.41
1:B:961:ASN:ND2	1:B:1238:ILE:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1105:ILE:O	1:C:1109:LEU:HD23	2.19	0.41
1:D:1159:ASN:O	1:D:1162:LYS:NZ	2.53	0.41
1:D:1278:VAL:HG22	1:D:1316:VAL:HG12	2.03	0.41
1:A:617:SER:O	1:A:621:LEU:HD13	2.20	0.41
1:B:826:VAL:HG12	1:B:874:ALA:HB1	2.01	0.41
1:B:1281:GLN:NE2	1:B:1313:SER:OG	2.53	0.41
1:D:386:ILE:HD11	1:D:397:ALA:HB3	2.03	0.41
1:D:421:VAL:HG12	1:D:422:ARG:H	1.85	0.41
1:A:240:THR:OG1	1:A:347:ILE:HD12	2.21	0.41
1:B:765:TRP:HB2	1:B:786:LEU:HD22	2.02	0.41
1:B:1159:ASN:O	1:B:1162:LYS:NZ	2.53	0.41
1:B:1202:PRO:HB2	1:B:1253:ASP:CG	2.46	0.41
1:C:28:LYS:N	1:C:547:PRO:O	2.53	0.41
1:D:100:VAL:HG12	1:D:121:MET:HE1	2.03	0.41
1:D:167:ILE:O	1:D:175:ILE:N	2.53	0.41
1:D:272:TYR:CB	1:D:275:ALA:HB2	2.51	0.41
1:D:961:ASN:ND2	1:D:1238:ILE:O	2.51	0.41
1:A:577:SER:OG	1:A:580:ALA:HB2	2.21	0.41
1:B:386:ILE:HD11	1:B:397:ALA:HB3	2.03	0.41
1:B:952:GLY:N	1:B:1297:ARG:O	2.54	0.41
1:B:1128:LEU:HD21	1:B:1150:LEU:HD21	2.02	0.41
1:C:101:MET:SD	1:C:122:VAL:HG11	2.61	0.41
1:A:28:LYS:N	1:A:547:PRO:O	2.53	0.41
1:A:101:MET:SD	1:A:122:VAL:HG11	2.61	0.41
1:B:248:VAL:HG21	1:B:266:VAL:HG11	2.02	0.41
1:B:746:VAL:HG23	1:B:751:VAL:H	1.84	0.41
1:B:824:VAL:HG13	1:B:824:VAL:O	2.20	0.41
1:B:1088:ASN:HB3	1:B:1091:ILE:HG22	2.01	0.41
1:C:468:LEU:HD23	1:C:560:VAL:HG22	2.02	0.41
1:C:775:ASP:OD1	1:C:776:ALA:N	2.54	0.41
1:C:864:SER:OG	1:C:865:LEU:N	2.54	0.41
1:D:1177:LYS:O	1:D:1325:GLN:NE2	2.54	0.41
1:A:354:LYS:NZ	1:A:463:PRO:O	2.32	0.41
1:B:1367:VAL:O	1:B:1368:SER:OG	2.29	0.41
1:B:1373:ARG:O	1:B:1373:ARG:CD	2.69	0.41
1:C:1051:GLN:O	1:C:1054:ALA:HB3	2.20	0.41
1:D:65:GLU:OE2	1:D:104:THR:OG1	2.39	0.41
1:D:501:ALA:N	1:D:504:GLY:O	2.49	0.41
1:D:1179:ASN:HB2	1:D:1237:TRP:HB2	2.02	0.41
1:D:1252:GLN:O	1:D:1254:THR:N	2.54	0.41
1:A:864:SER:OG	1:A:865:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:HD11	1:B:543:TYR:CZ	2.56	0.40
1:B:500:MET:SD	1:B:504:GLY:N	2.94	0.40
1:C:493:LEU:HD21	1:C:546:LEU:HD23	2.02	0.40
1:C:568:VAL:HG11	1:C:780:ILE:N	2.36	0.40
1:C:778:LEU:H	1:C:778:LEU:HD23	1.85	0.40
1:A:118:THR:HG21	1:A:676:LYS:HD2	2.03	0.40
1:A:568:VAL:HG11	1:A:780:ILE:N	2.36	0.40
1:A:778:LEU:H	1:A:778:LEU:HD23	1.85	0.40
1:A:822:ILE:CA	1:A:887:VAL:HG23	2.44	0.40
1:B:1252:GLN:O	1:B:1254:THR:N	2.54	0.40
2:E:1:NAG:H61	2:E:2:NAG:HN2	1.87	0.40
1:A:1181:VAL:HG22	1:A:1233:ASN:CB	2.51	0.40
1:B:272:TYR:CB	1:B:275:ALA:HB2	2.51	0.40
1:B:282:ASP:OD1	1:B:282:ASP:N	2.55	0.40
1:B:963:GLN:O	1:B:1244:ALA:HB1	2.21	0.40
1:C:240:THR:OG1	1:C:347:ILE:HD12	2.21	0.40
1:C:821:CYS:HB3	1:C:849:CYS:HB3	1.88	0.40
1:D:50:LEU:HD11	1:D:543:TYR:CZ	2.56	0.40
1:D:270:ARG:HD3	1:D:315:GLU:HB3	2.03	0.40
1:D:930:GLU:C	1:D:931:LEU:HD22	2.46	0.40
1:D:931:LEU:O	1:D:1312:TYR:N	2.48	0.40
1:D:1280:ILE:HD13	1:D:1314:MET:HG3	2.03	0.40
1:A:33:VAL:HG12	1:A:49:VAL:CG2	2.47	0.40
1:A:199:PHE:O	1:A:203:TYR:OH	2.30	0.40
1:B:263:HIS:NE2	1:B:291:SER:OG	2.48	0.40
1:B:270:ARG:HD3	1:B:315:GLU:HB3	2.03	0.40
1:B:363:ILE:HG22	1:B:460:HIS:HB3	2.02	0.40
1:D:195:SER:OG	1:D:1244:ALA:O	2.39	0.40
1:D:500:MET:SD	1:D:504:GLY:N	2.94	0.40
1:A:597:LEU:HD13	1:A:744:VAL:HG22	2.04	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	1271/1474 (86%)	1138 (90%)	133 (10%)	0	100	100
1	B	1406/1474 (95%)	1198 (85%)	197 (14%)	11 (1%)	16	54
1	C	1271/1474 (86%)	1138 (90%)	133 (10%)	0	100	100
1	D	1406/1474 (95%)	1198 (85%)	197 (14%)	11 (1%)	16	54
All	All	5354/5896 (91%)	4672 (87%)	660 (12%)	22 (0%)	31	67

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	272	TYR
1	B	800	TYR
1	B	1253	ASP
1	D	272	TYR
1	D	800	TYR
1	D	1253	ASP
1	B	1186	PRO
1	D	1186	PRO
1	B	799	PRO
1	B	809	THR
1	B	1184	GLU
1	D	799	PRO
1	D	809	THR
1	D	1184	GLU
1	B	808	PHE
1	D	808	PHE
1	B	1185	ARG
1	D	1185	ARG
1	B	656	THR
1	B	936	PRO
1	D	656	THR
1	D	936	PRO

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	1112/1290 (86%)	1109 (100%)	3 (0%)	86	86
1	B	1236/1290 (96%)	1232 (100%)	4 (0%)	86	86
1	C	1112/1290 (86%)	1109 (100%)	3 (0%)	86	86
1	D	1236/1290 (96%)	1232 (100%)	4 (0%)	86	86
All	All	4696/5160 (91%)	4682 (100%)	14 (0%)	84	86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	822	ILE
1	A	849	CYS
1	A	991	ASN
1	B	271	LYS
1	B	410	ASN
1	B	1303	VAL
1	B	1424	ASN
1	C	822	ILE
1	C	849	CYS
1	C	991	ASN
1	D	271	LYS
1	D	410	ASN
1	D	1303	VAL
1	D	1424	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	389	ASN
1	A	413	ASN
1	A	994	GLN
1	A	1072	GLN
1	B	474	GLN
1	B	479	HIS
1	B	620	ASN
1	B	827	GLN
1	B	843	GLN
1	B	1013	GLN
1	B	1015	GLN

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Mol	Chain	Res	Type
1	B	1143	HIS
1	B	1259	HIS
1	B	1281	GLN
1	B	1295	ASN
1	B	1377	ASN
1	B	1413	ASN
1	C	40	HIS
1	C	389	ASN
1	C	413	ASN
1	C	1072	GLN
1	D	479	HIS
1	D	620	ASN
1	D	639	ASN
1	D	827	GLN
1	D	843	GLN
1	D	1013	GLN
1	D	1015	GLN
1	D	1143	HIS
1	D	1259	HIS
1	D	1281	GLN
1	D	1295	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

8 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
2	NAG	E	1	1,2	14,14,15	0.25	0	17,19,21	0.57	0
2	NAG	E	2	2	14,14,15	0.31	0	17,19,21	0.48	0
2	NAG	F	1	2	14,14,15	0.41	0	17,19,21	1.18	2 (11%)
2	NAG	F	2	2	14,14,15	0.30	0	17,19,21	0.51	0
2	NAG	G	1	1,2	14,14,15	0.25	0	17,19,21	0.57	0
2	NAG	G	2	2	14,14,15	0.31	0	17,19,21	0.48	0
2	NAG	H	1	2	14,14,15	0.41	0	17,19,21	1.18	2 (11%)
2	NAG	H	2	2	14,14,15	0.30	0	17,19,21	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	5/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	2	-	4/6/23/26	0/1/1/1
2	NAG	H	2	2	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C4-C3-C2	3.16	115.65	111.02
2	H	1	NAG	C4-C3-C2	3.16	115.65	111.02
2	F	1	NAG	C2-N2-C7	-2.33	119.78	122.90
2	H	1	NAG	C2-N2-C7	-2.33	119.78	122.90

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2

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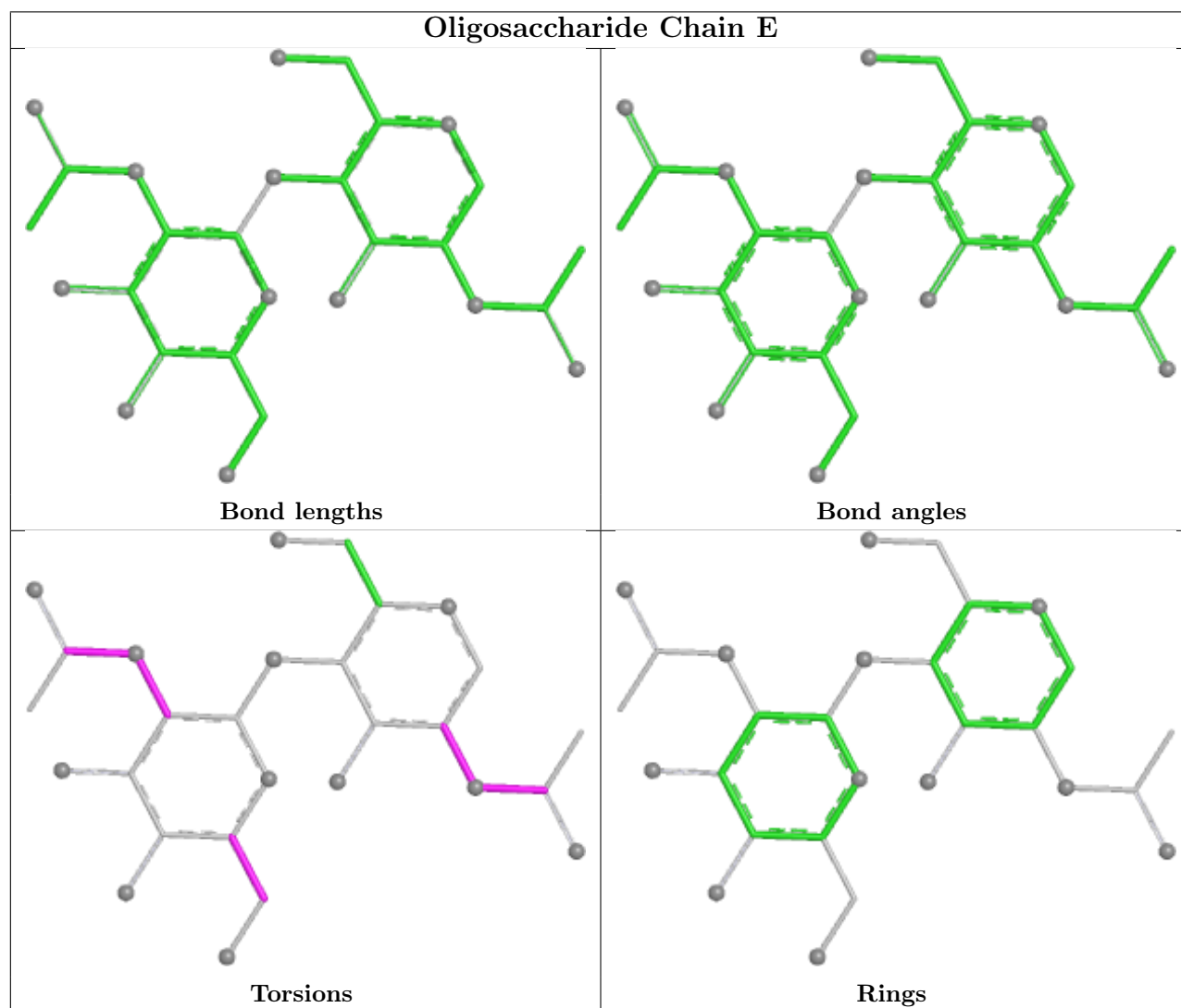
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C3-C2-N2-C7
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C1-C2-N2-C7
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C3-C2-N2-C7
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	F	1	NAG	C3-C2-N2-C7
2	H	1	NAG	C3-C2-N2-C7
2	E	1	NAG	C3-C2-N2-C7
2	F	2	NAG	C3-C2-N2-C7
2	G	1	NAG	C3-C2-N2-C7
2	H	2	NAG	C3-C2-N2-C7

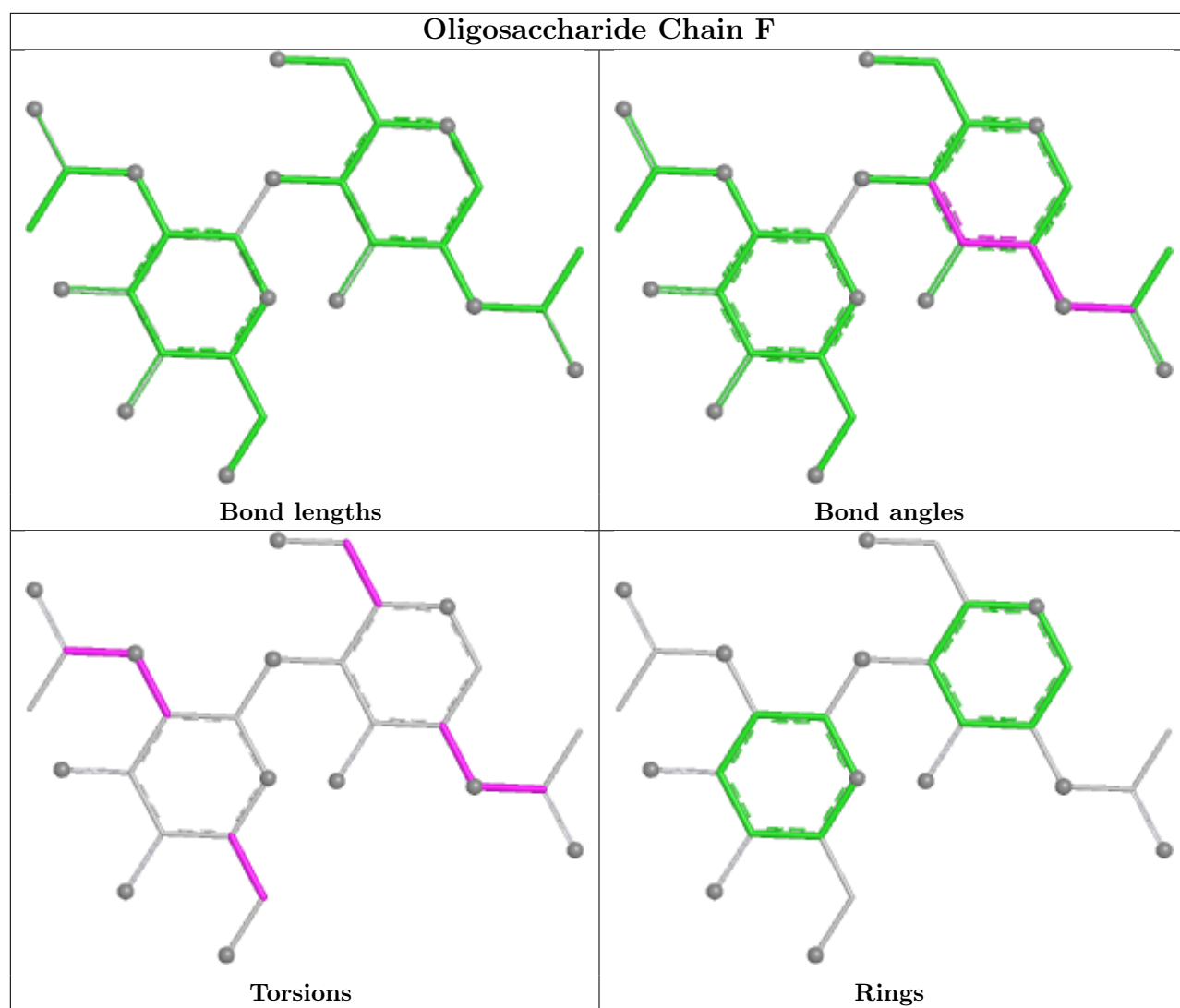
There are no ring outliers.

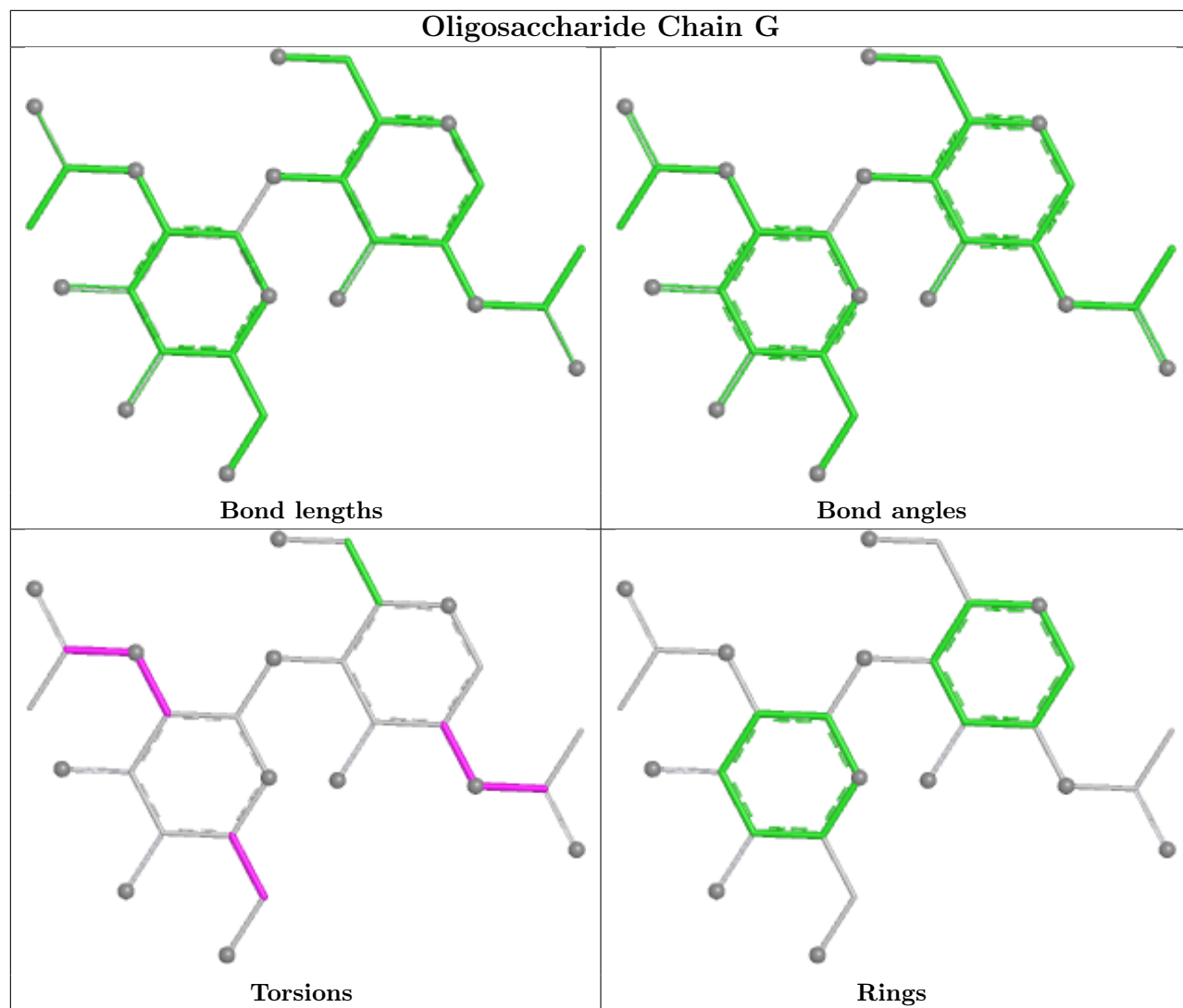
6 monomers are involved in 11 short contacts:

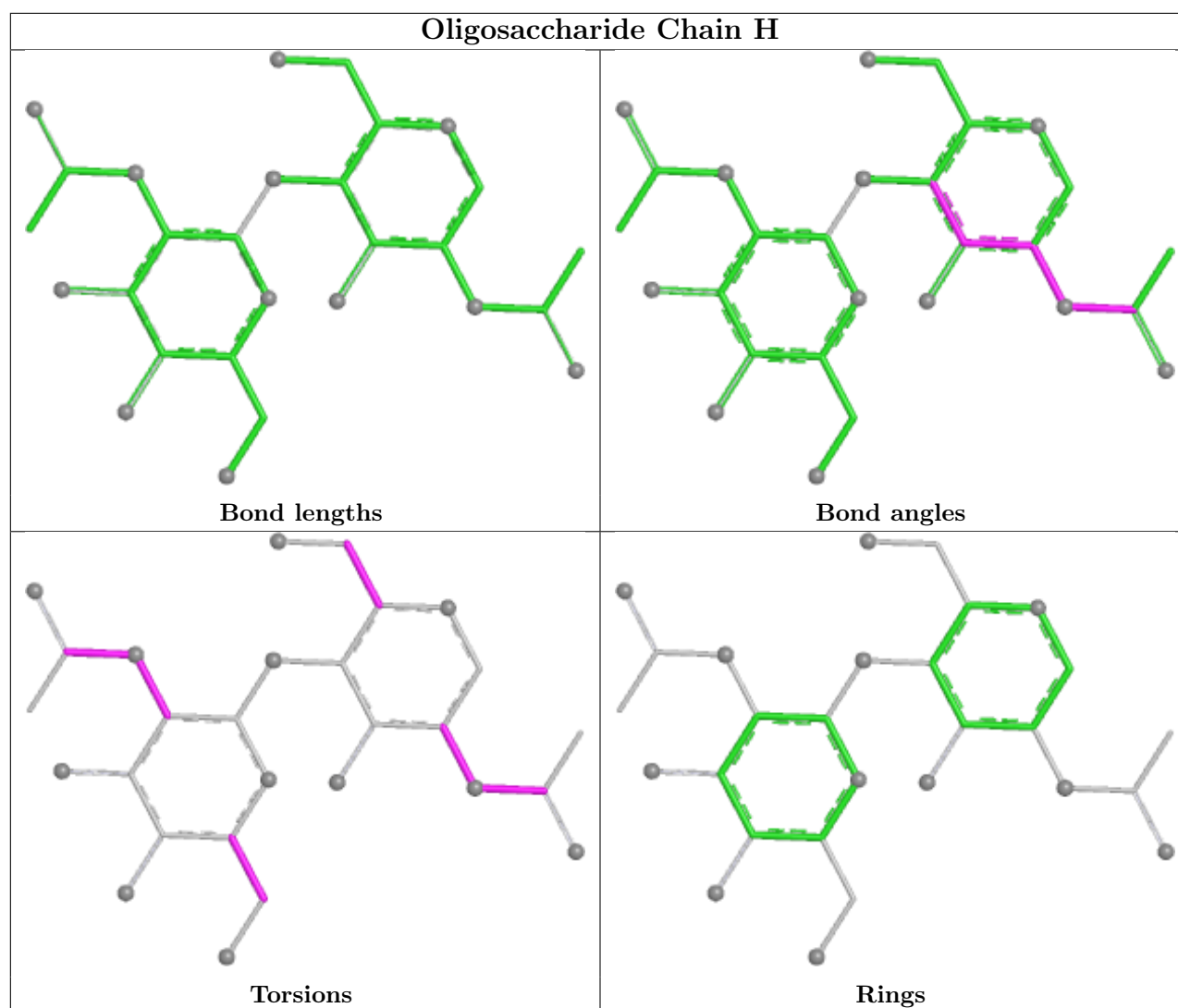
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2	NAG	4	0
2	E	1	NAG	1	0
2	F	1	NAG	1	0
2	E	2	NAG	1	0
2	H	2	NAG	4	0
2	H	1	NAG	1	0

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](#)

26 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	$\# Z > 2$
3	NAG	C	2003	1	14,14,15	1.84	6 (42%)	17,19,21	1.10	1 (5%)
3	NAG	D	2002	1	14,14,15	0.31	0	17,19,21	0.48	0
3	NAG	D	2004	1	14,14,15	0.33	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	2007	1	14,14,15	0.29	0	17,19,21	0.66	0
3	NAG	D	2005	1	14,14,15	0.35	0	17,19,21	0.70	1 (5%)
3	NAG	A	2001	1	14,14,15	2.12	4 (28%)	17,19,21	2.08	5 (29%)
3	NAG	C	2001	1	14,14,15	2.12	4 (28%)	17,19,21	2.08	5 (29%)
3	NAG	D	2003	1	14,14,15	0.28	0	17,19,21	0.91	0
3	NAG	D	2008	1	14,14,15	0.32	0	17,19,21	0.44	0
3	NAG	C	2005	1	14,14,15	1.93	5 (35%)	17,19,21	1.47	2 (11%)
3	NAG	B	2003	1	14,14,15	0.28	0	17,19,21	0.91	0
3	NAG	B	2004	1	14,14,15	0.33	0	17,19,21	0.58	0
3	NAG	A	2005	1	14,14,15	1.93	5 (35%)	17,19,21	1.47	2 (11%)
3	NAG	D	2001	1	14,14,15	0.27	0	17,19,21	1.28	2 (11%)
3	NAG	B	2005	1	14,14,15	0.35	0	17,19,21	0.70	1 (5%)
3	NAG	B	2001	1	14,14,15	0.27	0	17,19,21	1.28	2 (11%)
3	NAG	C	2004	1	14,14,15	1.80	3 (21%)	17,19,21	1.35	2 (11%)
3	NAG	D	2006	1	14,14,15	0.31	0	17,19,21	0.81	0
3	NAG	B	2002	1	14,14,15	0.31	0	17,19,21	0.48	0
3	NAG	B	2007	1	14,14,15	0.29	0	17,19,21	0.66	0
3	NAG	A	2003	1	14,14,15	1.84	6 (42%)	17,19,21	1.10	1 (5%)
3	NAG	B	2006	1	14,14,15	0.31	0	17,19,21	0.81	0
3	NAG	A	2004	1	14,14,15	1.80	3 (21%)	17,19,21	1.35	2 (11%)
3	NAG	A	2002	-	14,14,15	1.94	3 (21%)	17,19,21	1.07	1 (5%)
3	NAG	B	2008	1	14,14,15	0.32	0	17,19,21	0.44	0
3	NAG	C	2002	-	14,14,15	1.94	3 (21%)	17,19,21	1.07	1 (5%)

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
3	NAG	C	2003	1	-	2/6/23/26	0/1/1/1
3	NAG	D	2002	1	-	3/6/23/26	0/1/1/1
3	NAG	D	2004	1	-	4/6/23/26	0/1/1/1
3	NAG	D	2007	1	-	3/6/23/26	0/1/1/1
3	NAG	D	2005	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	A	2001	1	-	4/6/23/26	0/1/1/1
3	NAG	C	2001	1	-	4/6/23/26	0/1/1/1
3	NAG	D	2003	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	2008	1	-	4/6/23/26	0/1/1/1
3	NAG	C	2005	1	-	3/6/23/26	0/1/1/1
3	NAG	B	2003	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2004	1	-	4/6/23/26	0/1/1/1
3	NAG	A	2005	1	-	3/6/23/26	0/1/1/1
3	NAG	D	2001	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2005	1	1/1/5/7	3/6/23/26	0/1/1/1
3	NAG	B	2001	1	-	2/6/23/26	0/1/1/1
3	NAG	C	2004	1	-	1/6/23/26	0/1/1/1
3	NAG	D	2006	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2002	1	-	3/6/23/26	0/1/1/1
3	NAG	B	2007	1	-	3/6/23/26	0/1/1/1
3	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
3	NAG	B	2006	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2004	1	-	1/6/23/26	0/1/1/1
3	NAG	A	2002	-	-	3/6/23/26	0/1/1/1
3	NAG	B	2008	1	-	4/6/23/26	0/1/1/1
3	NAG	C	2002	-	-	3/6/23/26	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	NAG	O5-C1	4.38	1.51	1.43
3	C	2001	NAG	O5-C1	4.38	1.51	1.43
3	A	2002	NAG	O5-C1	4.18	1.50	1.43
3	C	2002	NAG	O5-C1	4.18	1.50	1.43
3	A	2005	NAG	O5-C1	3.98	1.50	1.43
3	C	2005	NAG	O5-C1	3.98	1.50	1.43
3	A	2001	NAG	C7-N2	3.89	1.46	1.34
3	C	2001	NAG	C7-N2	3.89	1.46	1.34
3	A	2003	NAG	O5-C1	3.77	1.50	1.43
3	C	2003	NAG	O5-C1	3.77	1.50	1.43
3	A	2004	NAG	O5-C1	3.74	1.50	1.43
3	C	2004	NAG	O5-C1	3.74	1.50	1.43
3	A	2002	NAG	C7-N2	3.65	1.46	1.34
3	C	2002	NAG	C7-N2	3.65	1.46	1.34
3	A	2005	NAG	C7-N2	3.57	1.45	1.34
3	C	2005	NAG	C7-N2	3.57	1.45	1.34
3	A	2004	NAG	C7-N2	3.50	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2004	NAG	C7-N2	3.50	1.45	1.34
3	A	2003	NAG	C7-N2	3.47	1.45	1.34
3	C	2003	NAG	C7-N2	3.47	1.45	1.34
3	A	2001	NAG	C2-N2	3.08	1.51	1.46
3	C	2001	NAG	C2-N2	3.08	1.51	1.46
3	A	2002	NAG	C2-N2	2.61	1.50	1.46
3	C	2002	NAG	C2-N2	2.61	1.50	1.46
3	A	2005	NAG	O5-C5	2.33	1.48	1.43
3	C	2005	NAG	O5-C5	2.33	1.48	1.43
3	A	2004	NAG	C2-N2	2.30	1.50	1.46
3	C	2004	NAG	C2-N2	2.30	1.50	1.46
3	A	2005	NAG	C2-N2	2.23	1.49	1.46
3	C	2005	NAG	C2-N2	2.23	1.49	1.46
3	A	2005	NAG	C3-C2	-2.19	1.47	1.52
3	C	2005	NAG	C3-C2	-2.19	1.47	1.52
3	A	2003	NAG	O5-C5	2.08	1.47	1.43
3	C	2003	NAG	O5-C5	2.08	1.47	1.43
3	A	2003	NAG	C2-N2	2.06	1.49	1.46
3	C	2003	NAG	C2-N2	2.06	1.49	1.46
3	A	2003	NAG	C3-C2	-2.03	1.48	1.52
3	C	2003	NAG	C3-C2	-2.03	1.48	1.52
3	A	2001	NAG	O7-C7	-2.03	1.18	1.23
3	C	2001	NAG	O7-C7	-2.03	1.18	1.23
3	A	2003	NAG	O7-C7	-2.01	1.18	1.23
3	C	2003	NAG	O7-C7	-2.01	1.18	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	NAG	C8-C7-N2	5.70	125.58	116.12
3	C	2001	NAG	C8-C7-N2	5.70	125.58	116.12
3	B	2001	NAG	C1-O5-C5	3.92	117.44	112.19
3	D	2001	NAG	C1-O5-C5	3.92	117.44	112.19
3	A	2005	NAG	C8-C7-N2	3.82	122.45	116.12
3	C	2005	NAG	C8-C7-N2	3.82	122.45	116.12
3	A	2001	NAG	C1-C2-N2	3.24	115.54	110.43
3	C	2001	NAG	C1-C2-N2	3.24	115.54	110.43
3	A	2001	NAG	C2-N2-C7	3.05	126.98	122.90
3	C	2001	NAG	C2-N2-C7	3.05	126.98	122.90
3	A	2001	NAG	O7-C7-C8	-3.04	116.64	122.05
3	C	2001	NAG	O7-C7-C8	-3.04	116.64	122.05
3	A	2003	NAG	C1-O5-C5	-3.03	108.13	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2003	NAG	C1-O5-C5	-3.03	108.13	112.19
3	A	2004	NAG	C8-C7-N2	2.52	120.29	116.12
3	C	2004	NAG	C8-C7-N2	2.52	120.29	116.12
3	A	2001	NAG	O7-C7-N2	-2.38	117.78	121.98
3	C	2001	NAG	O7-C7-N2	-2.38	117.78	121.98
3	A	2005	NAG	C6-C5-C4	-2.37	107.21	113.02
3	C	2005	NAG	C6-C5-C4	-2.37	107.21	113.02
3	A	2002	NAG	C1-O5-C5	2.30	115.28	112.19
3	C	2002	NAG	C1-O5-C5	2.30	115.28	112.19
3	B	2001	NAG	C4-C3-C2	-2.17	107.84	111.02
3	D	2001	NAG	C4-C3-C2	-2.17	107.84	111.02
3	A	2004	NAG	C1-C2-N2	-2.10	107.12	110.43
3	C	2004	NAG	C1-C2-N2	-2.10	107.12	110.43
3	B	2005	NAG	C1-O5-C5	-2.04	109.45	112.19
3	D	2005	NAG	C1-O5-C5	-2.04	109.45	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	2005	NAG	C1
3	D	2005	NAG	C1

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2002	NAG	C3-C2-N2-C7
3	B	2002	NAG	C8-C7-N2-C2
3	B	2002	NAG	O7-C7-N2-C2
3	B	2004	NAG	C8-C7-N2-C2
3	B	2004	NAG	O7-C7-N2-C2
3	B	2005	NAG	C3-C2-N2-C7
3	B	2005	NAG	C8-C7-N2-C2
3	B	2005	NAG	O7-C7-N2-C2
3	B	2006	NAG	C8-C7-N2-C2
3	B	2006	NAG	O7-C7-N2-C2
3	B	2007	NAG	C3-C2-N2-C7
3	B	2007	NAG	C8-C7-N2-C2
3	B	2007	NAG	O7-C7-N2-C2
3	B	2008	NAG	C8-C7-N2-C2
3	B	2008	NAG	O7-C7-N2-C2
3	D	2002	NAG	C3-C2-N2-C7
3	D	2002	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	D	2002	NAG	O7-C7-N2-C2
3	D	2004	NAG	C8-C7-N2-C2
3	D	2004	NAG	O7-C7-N2-C2
3	D	2005	NAG	C3-C2-N2-C7
3	D	2005	NAG	C8-C7-N2-C2
3	D	2005	NAG	O7-C7-N2-C2
3	D	2006	NAG	C8-C7-N2-C2
3	D	2006	NAG	O7-C7-N2-C2
3	D	2007	NAG	C3-C2-N2-C7
3	D	2007	NAG	C8-C7-N2-C2
3	D	2007	NAG	O7-C7-N2-C2
3	D	2008	NAG	C8-C7-N2-C2
3	D	2008	NAG	O7-C7-N2-C2
3	A	2001	NAG	C8-C7-N2-C2
3	A	2001	NAG	O7-C7-N2-C2
3	A	2005	NAG	C8-C7-N2-C2
3	A	2005	NAG	O7-C7-N2-C2
3	C	2001	NAG	C8-C7-N2-C2
3	C	2001	NAG	O7-C7-N2-C2
3	C	2005	NAG	C8-C7-N2-C2
3	C	2005	NAG	O7-C7-N2-C2
3	B	2008	NAG	O5-C5-C6-O6
3	D	2008	NAG	O5-C5-C6-O6
3	A	2005	NAG	O5-C5-C6-O6
3	C	2005	NAG	O5-C5-C6-O6
3	A	2002	NAG	O5-C5-C6-O6
3	C	2002	NAG	O5-C5-C6-O6
3	B	2004	NAG	C4-C5-C6-O6
3	D	2004	NAG	C4-C5-C6-O6
3	A	2003	NAG	C1-C2-N2-C7
3	B	2001	NAG	C1-C2-N2-C7
3	C	2003	NAG	C1-C2-N2-C7
3	D	2001	NAG	C1-C2-N2-C7
3	A	2002	NAG	C3-C2-N2-C7
3	A	2004	NAG	C3-C2-N2-C7
3	B	2008	NAG	C3-C2-N2-C7
3	C	2002	NAG	C3-C2-N2-C7
3	C	2004	NAG	C3-C2-N2-C7
3	D	2008	NAG	C3-C2-N2-C7
3	A	2001	NAG	C1-C2-N2-C7
3	A	2002	NAG	C1-C2-N2-C7
3	C	2001	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	C	2002	NAG	C1-C2-N2-C7
3	B	2004	NAG	O5-C5-C6-O6
3	D	2004	NAG	O5-C5-C6-O6
3	A	2001	NAG	C3-C2-N2-C7
3	A	2003	NAG	C3-C2-N2-C7
3	B	2001	NAG	C3-C2-N2-C7
3	C	2001	NAG	C3-C2-N2-C7
3	C	2003	NAG	C3-C2-N2-C7
3	D	2001	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2005	NAG	1	0
3	B	2005	NAG	1	0
3	C	2004	NAG	1	0
3	A	2004	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.

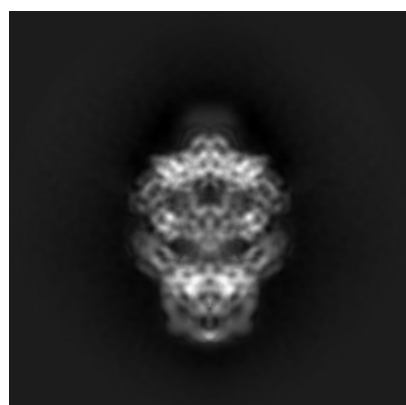
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12750. These allow visual inspection of the internal detail of the map and identification of artifacts.

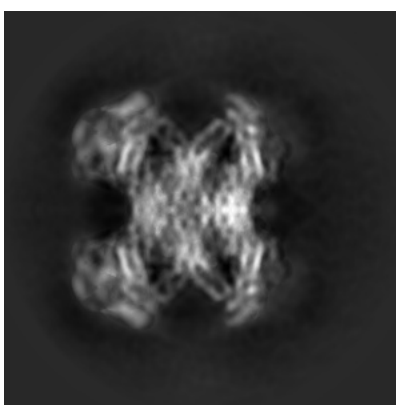
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

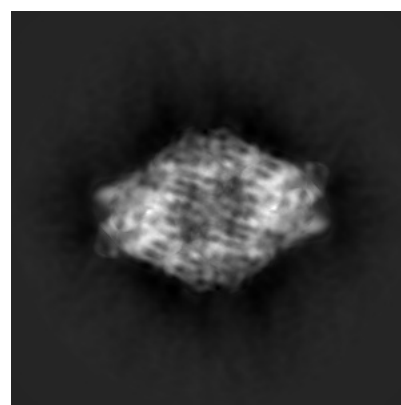
6.1.1 Primary map



X



Y



Z

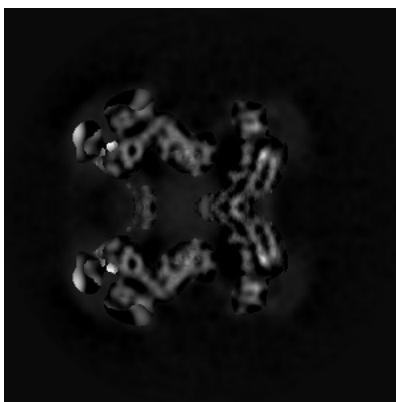
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

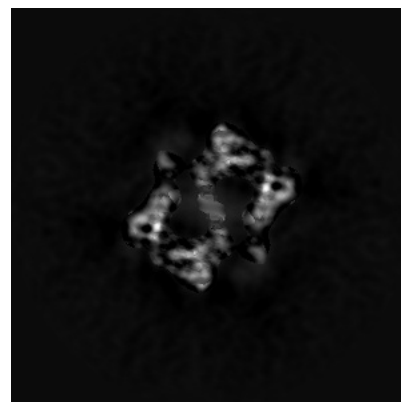
6.2.1 Primary map



X Index: 160



Y Index: 160

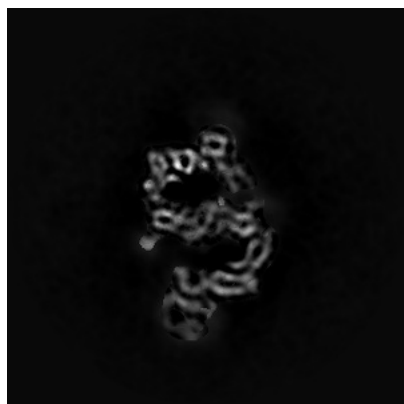


Z Index: 160

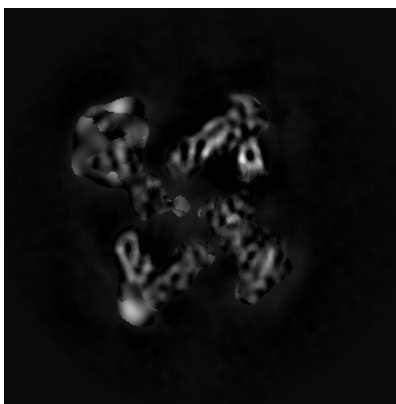
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

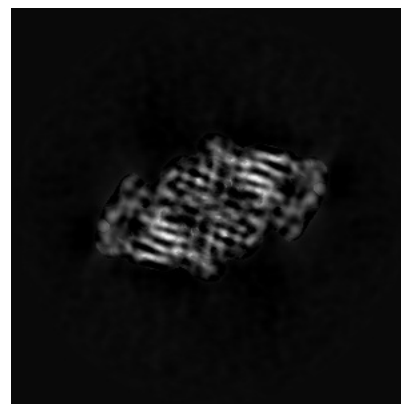
6.3.1 Primary map



X Index: 124



Y Index: 174

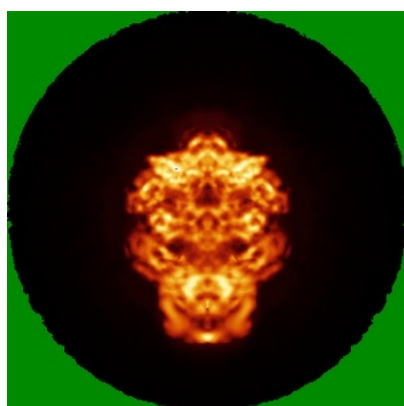


Z Index: 192

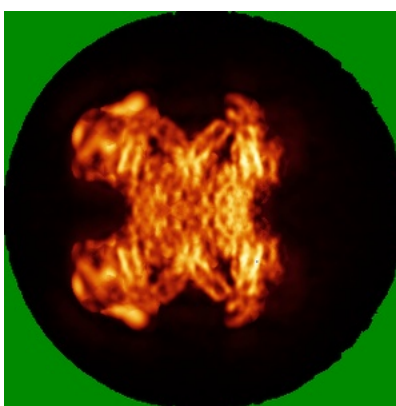
The images above show the largest variance slices of the map in three orthogonal directions.

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

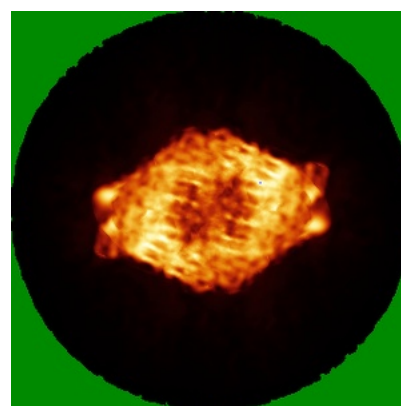
6.4.1 Primary map



X



Y

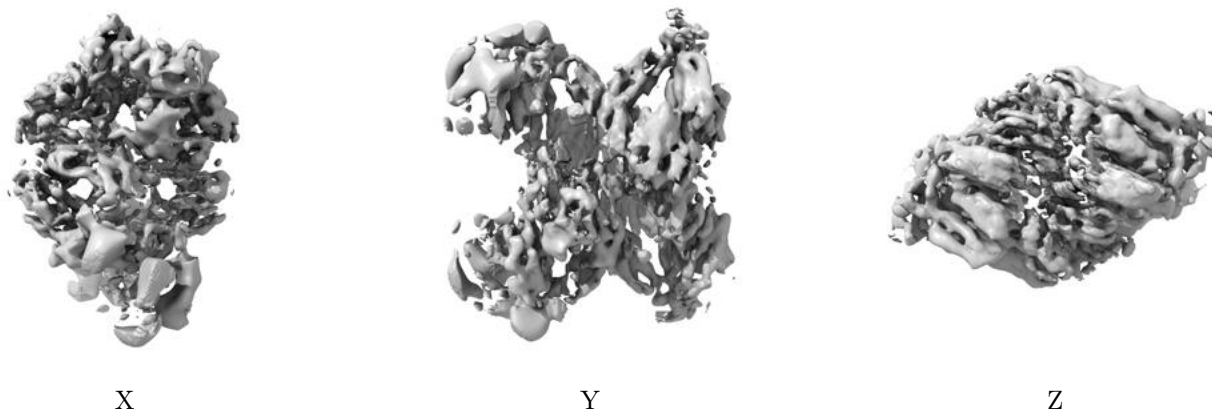


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

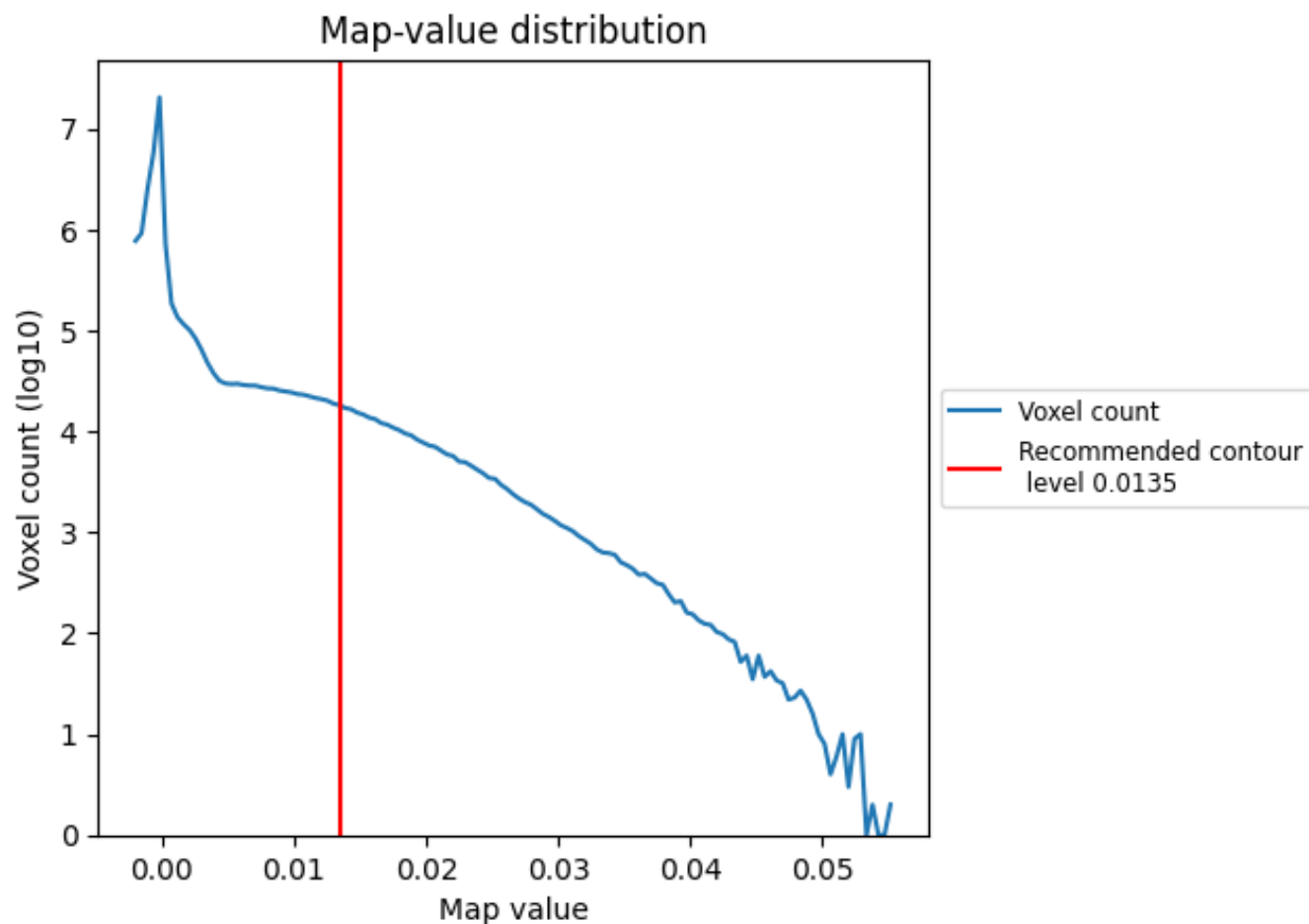
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

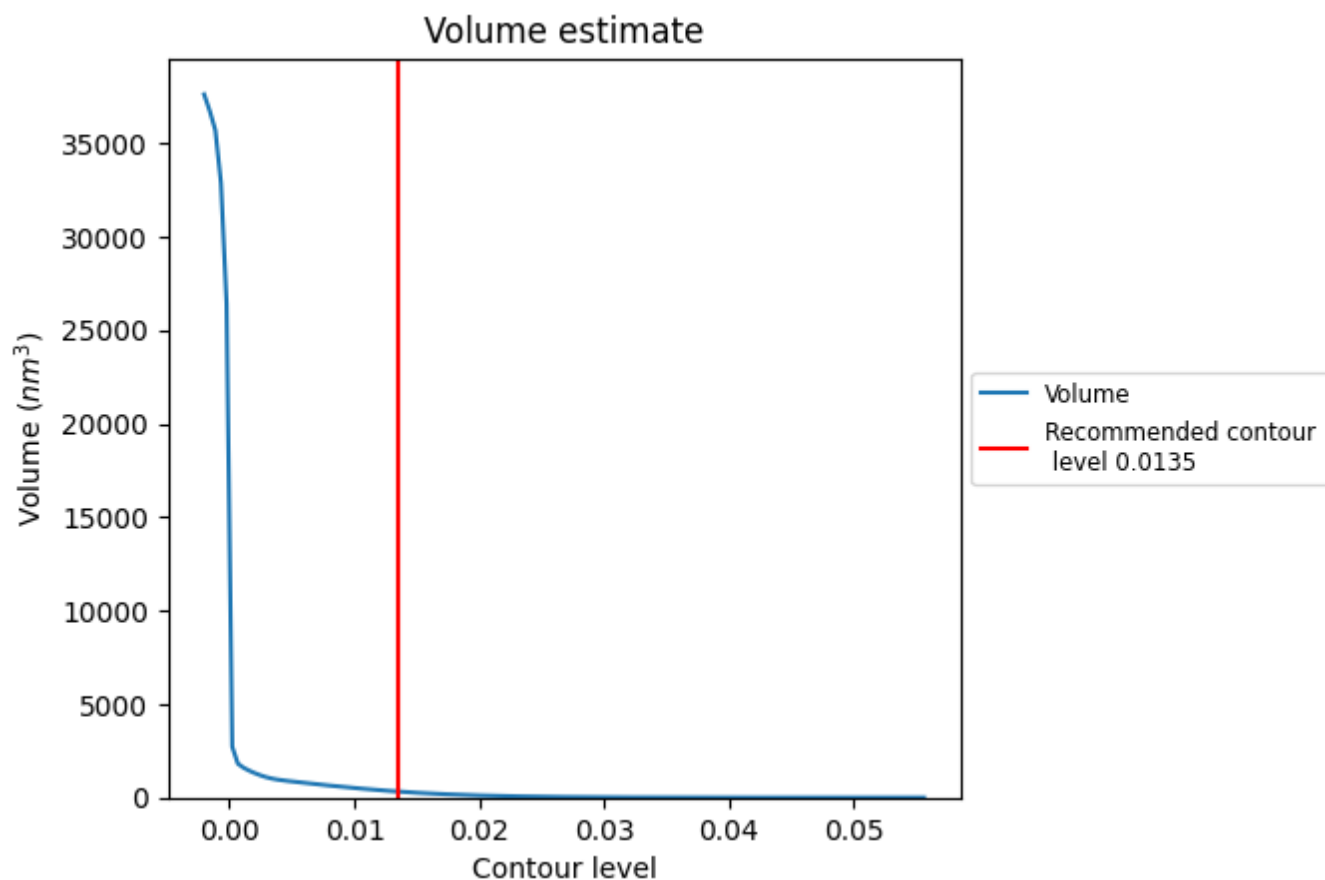
This section contains the results of statistical analysis of the map.

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.

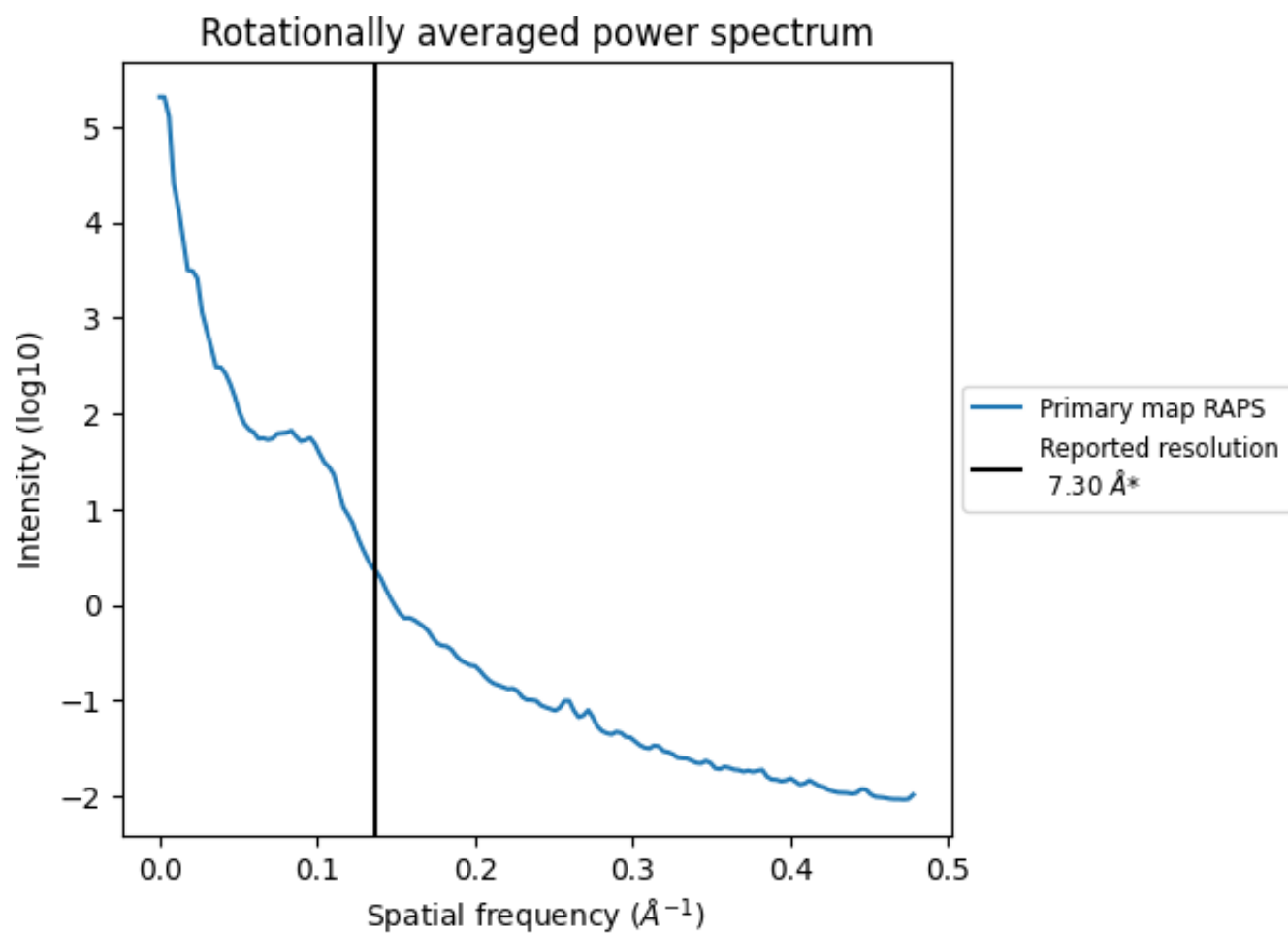
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 322 nm³; this corresponds to an approximate mass of 291 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 0.137 Å⁻¹

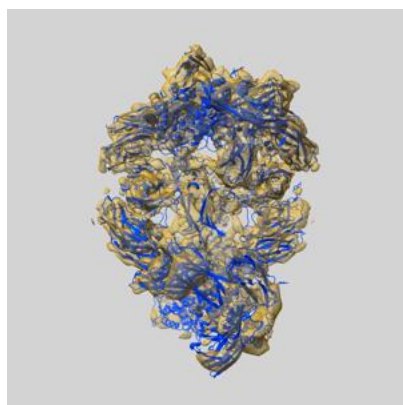
8 Fourier-Shell correlation ⓘ

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

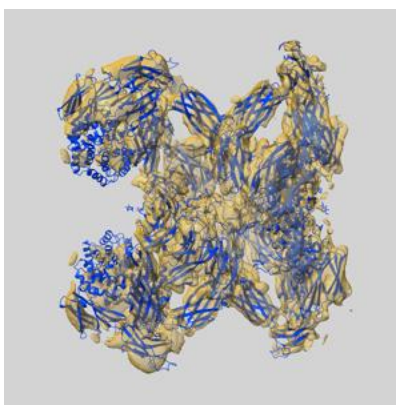
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12750 and PDB model 7O7N. Per-residue inclusion information can be found in section [3](#) on page [7](#).

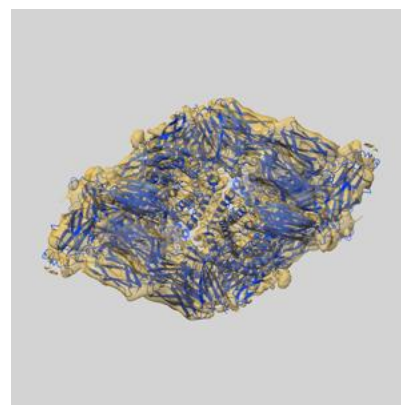
9.1 Map-model overlay [i](#)



X



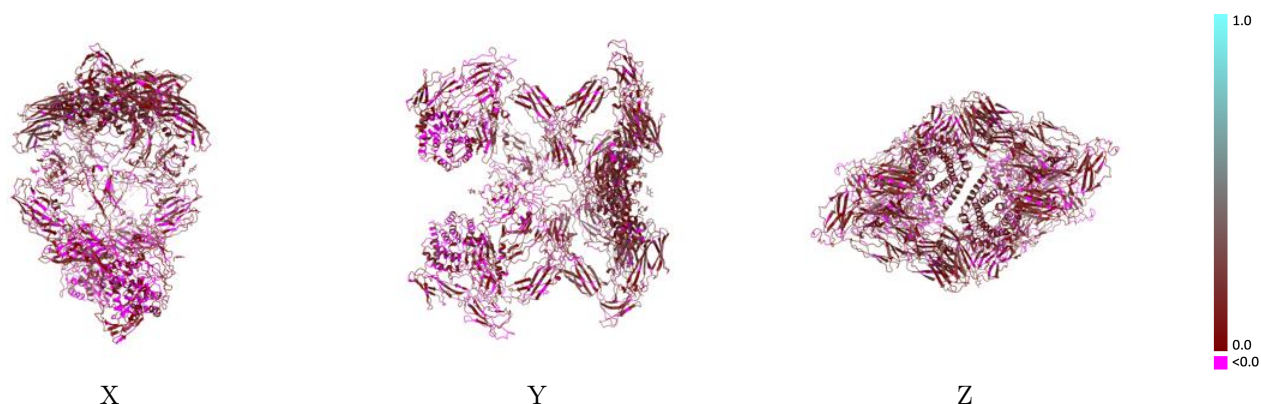
Y



Z

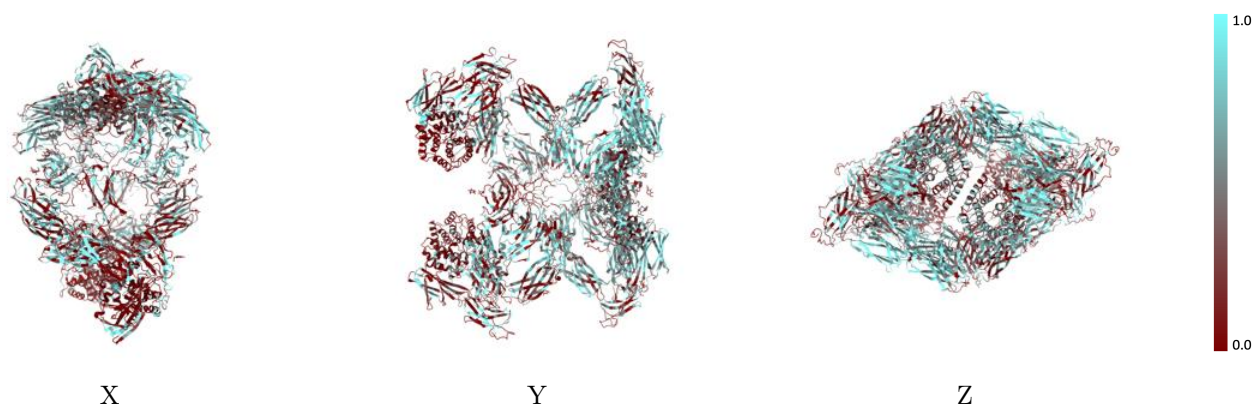
The images above show the 3D surface view of the map at the recommended contour level 0.0135 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



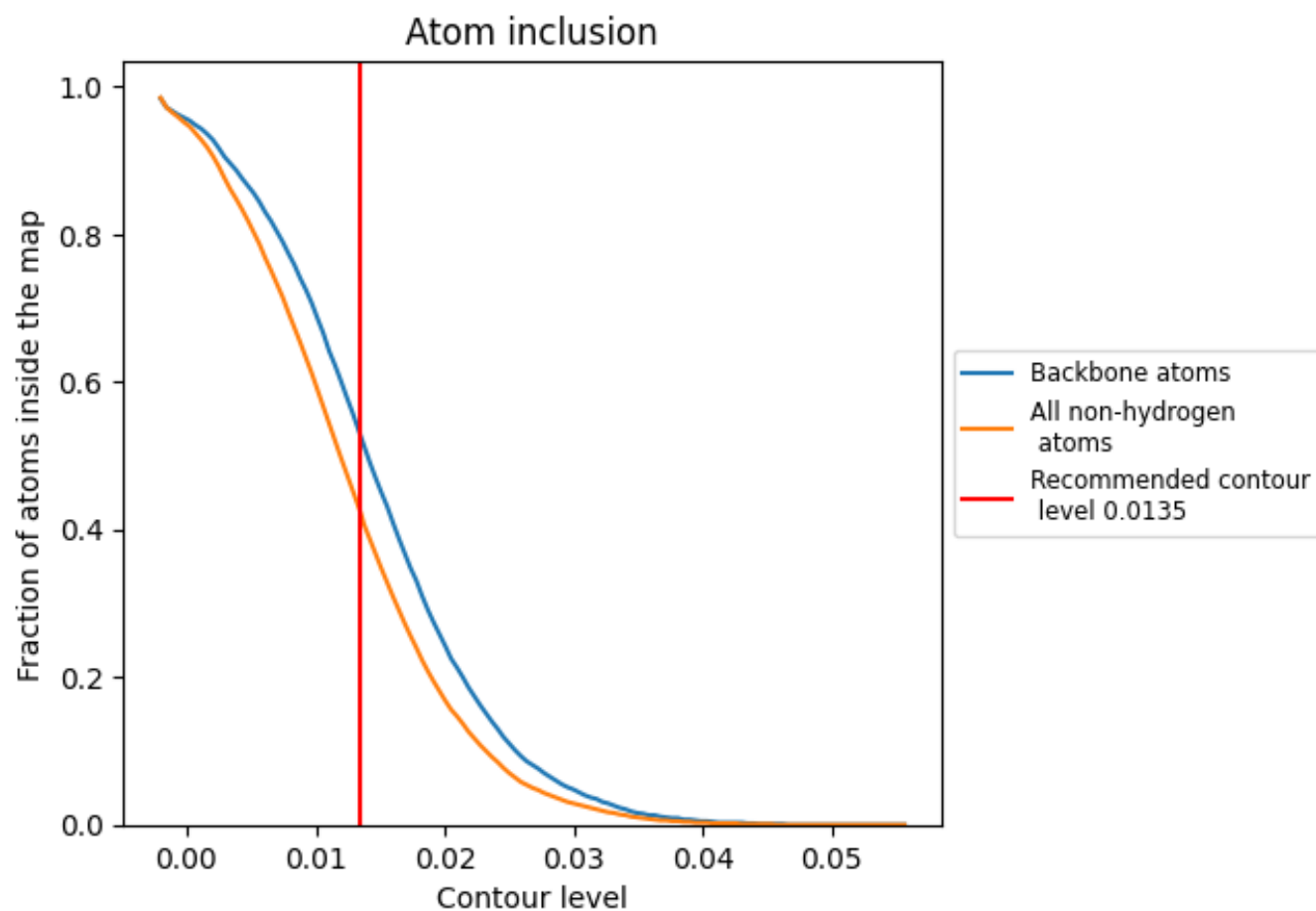
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0135).

9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 42% 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 (0.0135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4220	<div></div> 0.1100
A	<div></div> 0.5150	<div></div> 0.1550
B	<div></div> 0.3380	<div></div> 0.0690
C	<div></div> 0.5160	<div></div> 0.1550
D	<div></div> 0.3380	<div></div> 0.0690
E	<div></div> 0.0360	<div></div> 0.0970
F	<div></div> 0.2860	<div></div> 0.2640
G	<div></div> 0.0360	<div></div> 0.0790
H	<div></div> 0.2860	<div></div> 0.2510

