



## Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 07:37 AM EST

PDB ID : 8CS9  
EMDB ID : EMD-26960  
Title : Composite reconstruction of Class 1 of the erythrocyte ankyrin-1 complex  
Authors : Vallese, F.; Kim, K.; Yen, L.Y.; Johnston, J.D.; Noble, A.J.; Cali, T.; Clarke, O.B.  
Deposited on : 2022-05-12  
Resolution : 2.74 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.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

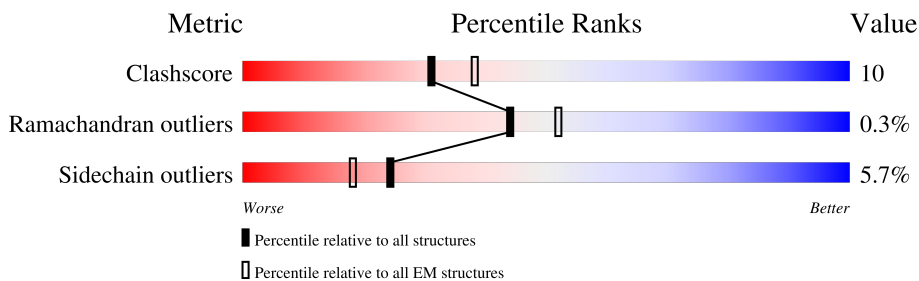
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.74 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1881	
2	K	417	
3	L	409	
3	Q	409	
4	X	691	
5	P	91	
6	R	150	
6	S	150	

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Mol	Chain	Length	Quality of chain
6	T	150	 5% 15% 9% 75%
6	a	150	 23% 75%
6	b	150	 5% 24% 75%
6	c	150	 21% 78%
7	V	911	 68% 19% 11%
7	Y	911	 60% 24% 14%
7	Z	911	 68% 17% 14%
7	e	911	 82% 6% 12%
7	f	911	 83% 5% 12%
7	g	911	 85% 6% 9%
8	B	2	 50% 100%
8	C	2	 100%
8	D	2	 100%

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 60944 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 Ankyrin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	796	6017	3768	1116	1113	20	0	0

- Molecule 2 is a protein called Blood group Rh(CE) polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	K	380	2943	1959	476	490	18	2	0

- Molecule 3 is a protein called Ammonium transporter Rh type A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	388	2938	1928	473	513	24	0	0
3	Q	390	2954	1940	475	515	24	0	0

- Molecule 4 is a protein called Protein 4.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	X	656	5162	3276	914	949	23	0	0

- Molecule 5 is a protein called Glycophorin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	P	33	248	168	40	38	2	0	0

- Molecule 6 is a protein called Glycophorin-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	36	Total	C	N	O	S	0	0
			277	183	47	46	1		
6	a	37	Total	C	N	O	S	0	0
			284	188	48	47	1		
6	S	33	Total	C	N	O	S	0	0
			255	169	43	42	1		
6	b	38	Total	C	N	O	S	0	0
			289	191	49	48	1		
6	T	37	Total	C	N	O	S	0	0
			284	188	48	47	1		
6	c	33	Total	C	N	O	S	0	0
			255	169	43	42	1		

- Molecule 7 is a protein called Band 3 anion transport protein.

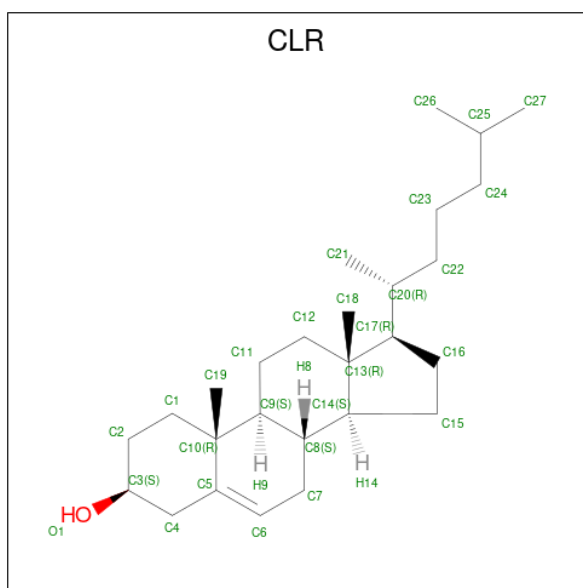
Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	810	Total	C	N	O	S	0	0
			6386	4195	1056	1111	24		
7	e	804	Total	C	N	O	S	0	0
			6339	4170	1047	1098	24		
7	Y	786	Total	C	N	O	S	0	0
			6226	4099	1028	1075	24		
7	f	802	Total	C	N	O	S	0	0
			6331	4164	1047	1096	24		
7	Z	786	Total	C	N	O	S	0	0
			6226	4099	1028	1075	24		
7	g	832	Total	C	N	O	S	0	0
			6556	4301	1079	1149	27		

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



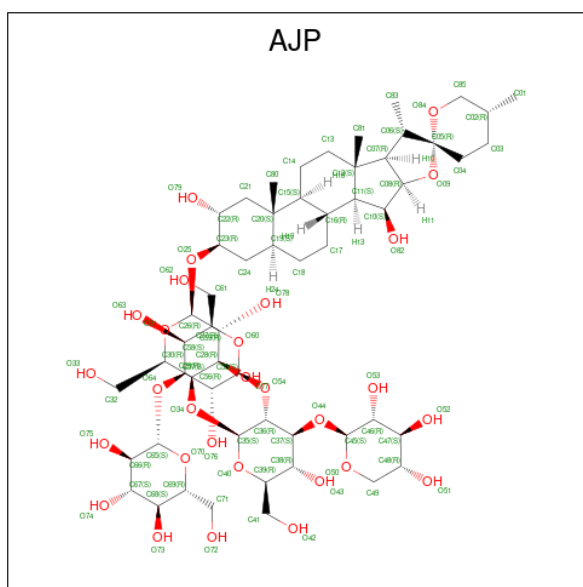
Mol	Chain	Residues	Atoms				AltConf	Trace
8	B	2	Total	C	N	O	0	0
			28	16	2	10		
8	C	2	Total	C	N	O	0	0
			28	16	2	10		
8	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 9 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



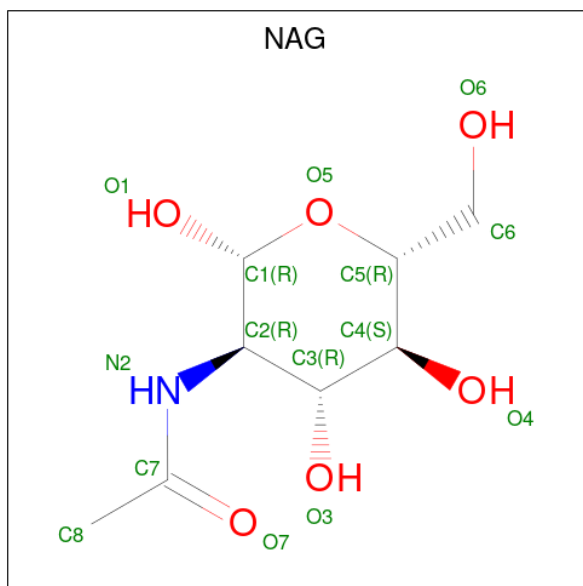
Mol	Chain	Residues	Atoms			AltConf
9	L	1	Total	C	O	0
			56	54	2	
9	L	1	Total	C	O	0
			56	54	2	
9	V	1	Total	C	O	0
			28	27	1	
9	e	1	Total	C	O	0
			28	27	1	
9	Y	1	Total	C	O	0
			28	27	1	
9	f	1	Total	C	O	0
			28	27	1	
9	c	1	Total	C	O	0
			28	27	1	
9	Z	1	Total	C	O	0
			28	27	1	

- Molecule 10 is Digitonin (three-letter code: AJP) (formula:  $C_{56}H_{92}O_{29}$ ).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	Q	1	32	27	5	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



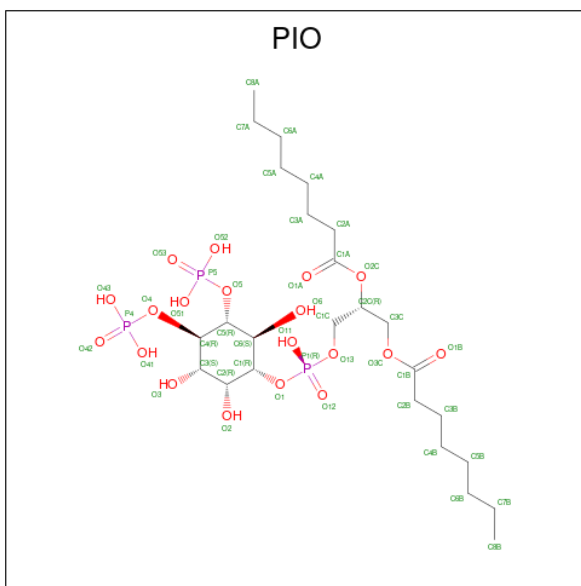
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	V	1	28	16	2	10	0
11	V	1	28	16	2	10	0

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Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
11	Y	1	Total	C	N	O	0
			28	16	2	10	
11	Y	1	Total	C	N	O	0
			28	16	2	10	
11	Z	1	Total	C	N	O	0
			28	16	2	10	
11	Z	1	Total	C	N	O	0
			28	16	2	10	

- Molecule 12 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonoxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (three-letter code: PIO) (formula: C<sub>25</sub>H<sub>49</sub>O<sub>19</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
12	V	1	Total	C	O	P	0
			47	25	19	3	
12	e	1	Total	C	O	P	0
			47	25	19	3	
12	Y	1	Total	C	O	P	0
			47	25	19	3	
12	f	1	Total	C	O	P	0
			47	25	19	3	
12	g	1	Total	C	O	P	0
			94	50	38	6	
12	g	1	Total	C	O	P	0
			94	50	38	6	



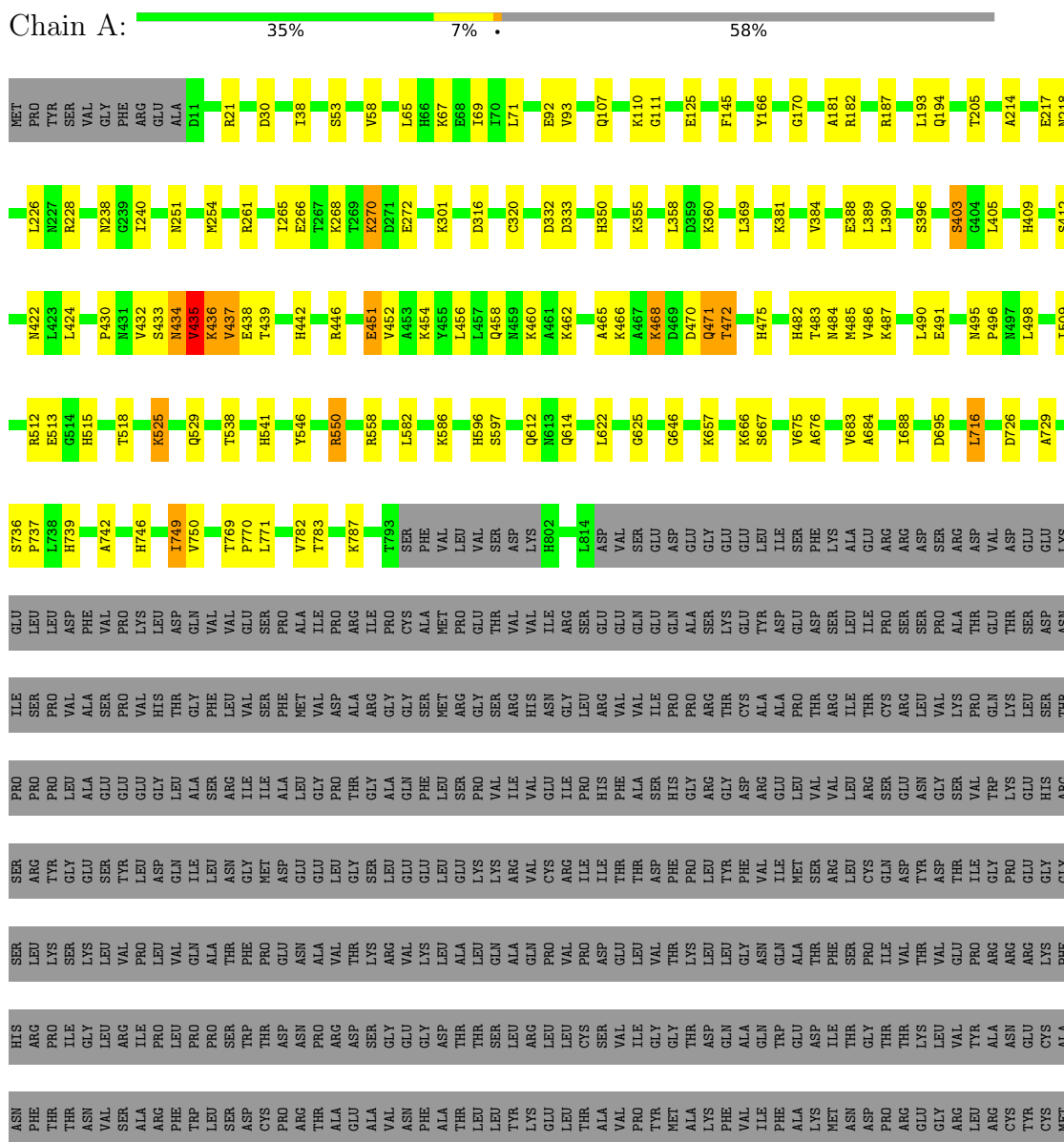
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	32	Total 32	O 32	0
13	K	18	Total 18	O 18	0
13	L	46	Total 46	O 46	0
13	Q	34	Total 34	O 34	0
13	X	112	Total 112	O 112	0
13	V	17	Total 17	O 17	0
13	e	4	Total 4	O 4	0
13	f	2	Total 2	O 2	0
13	g	3	Total 3	O 3	0

### 3 Residue-property plots [i](#)

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.

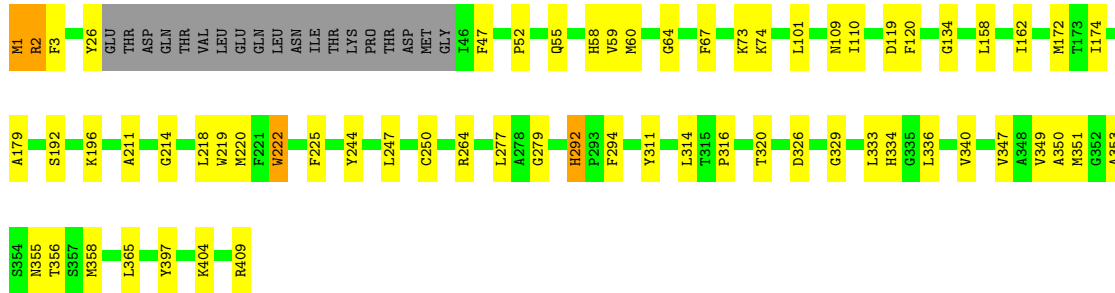
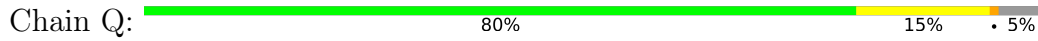
#### • Molecule 1: Ankyrin-1



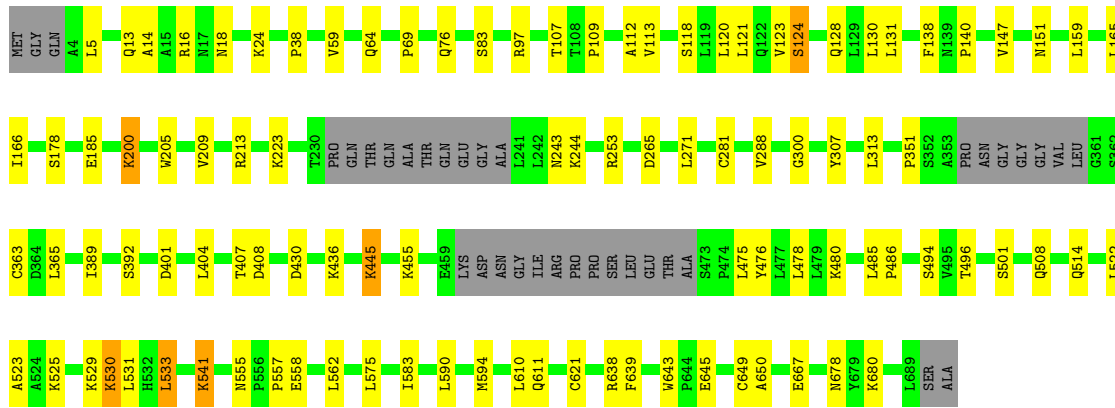
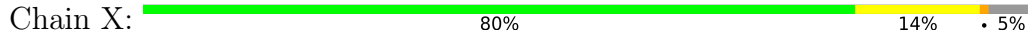




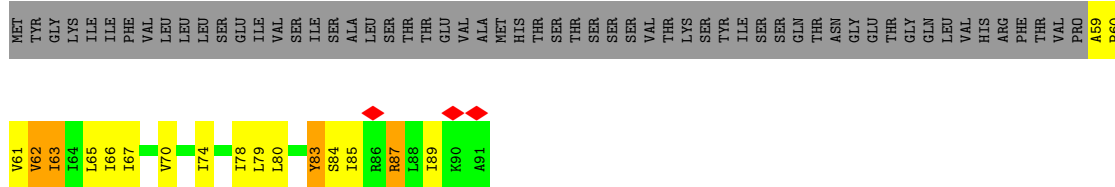
• Molecule 3: Ammonium transporter Rh type A



• Molecule 4: Protein 4.2



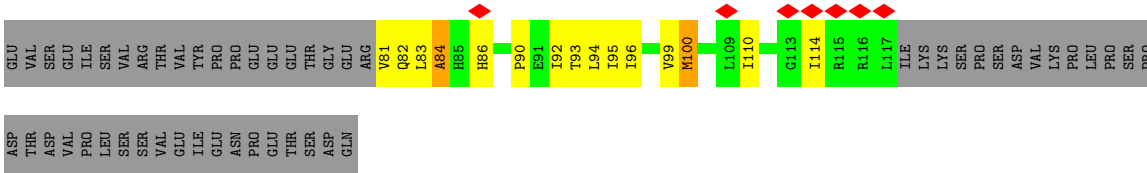
• Molecule 5: Glycophorin-B



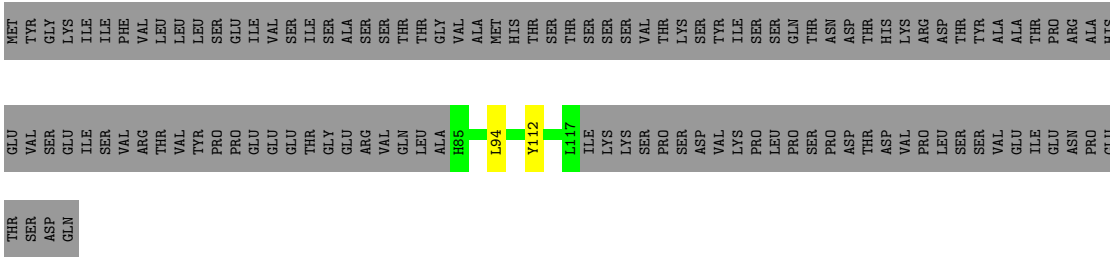
• Molecule 6: Glycophorin-A



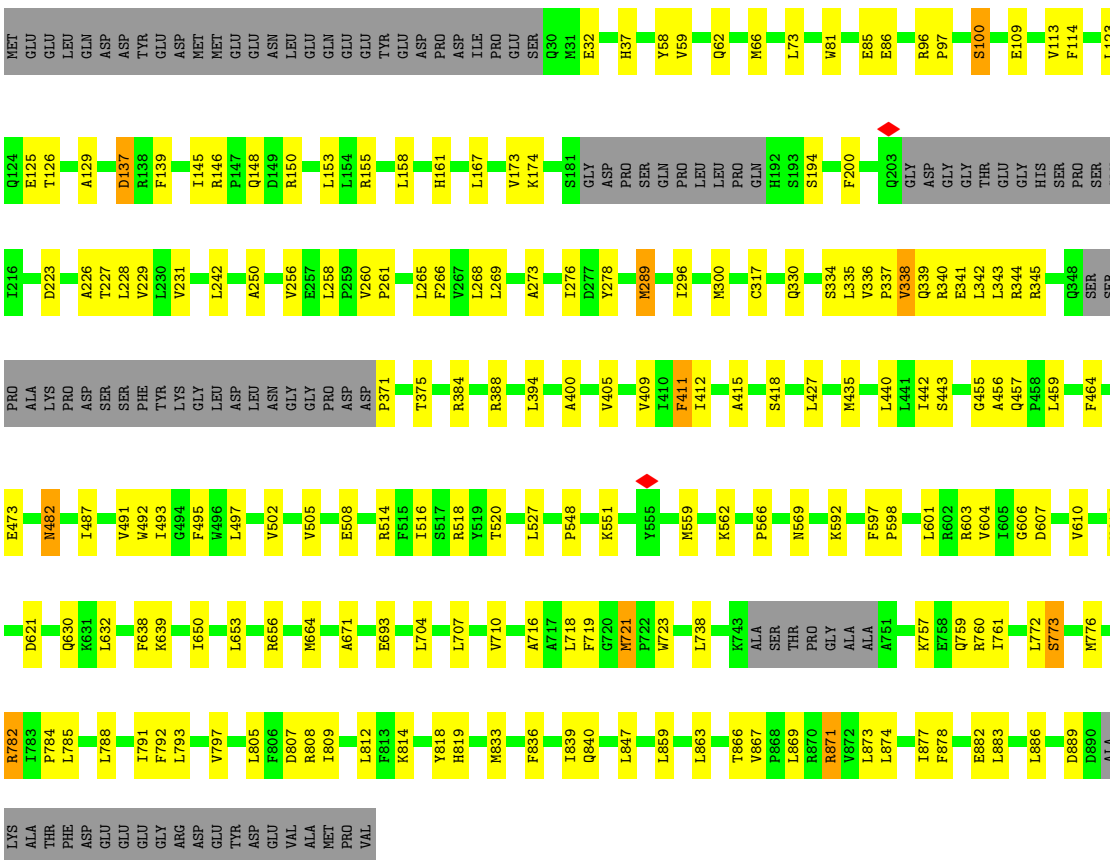




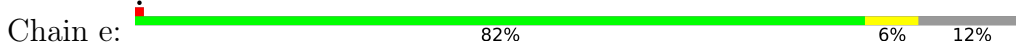
### Molecule 6: Glycophorin-A

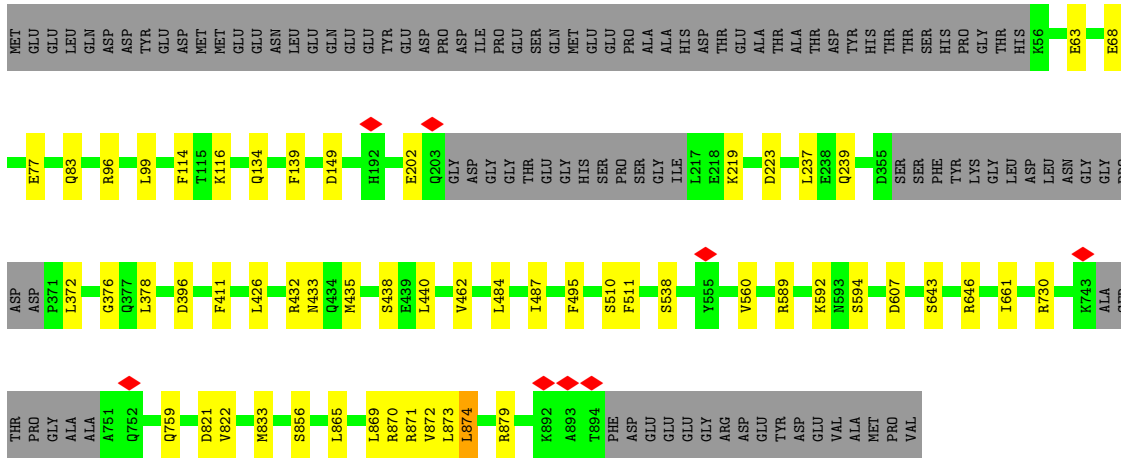


### Molecule 7: Band 3 anion transport protein

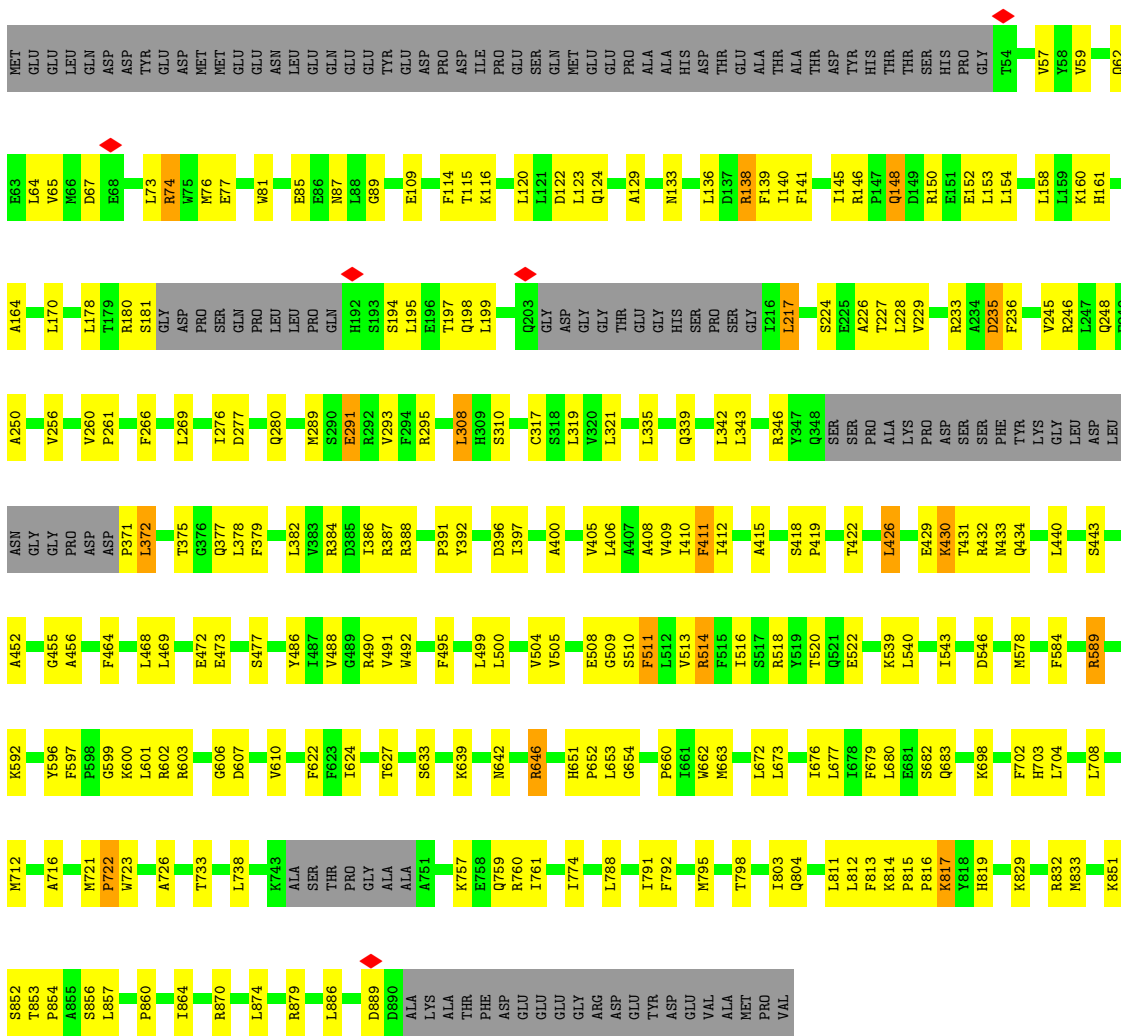


### Molecule 7: Band 3 anion transport protein

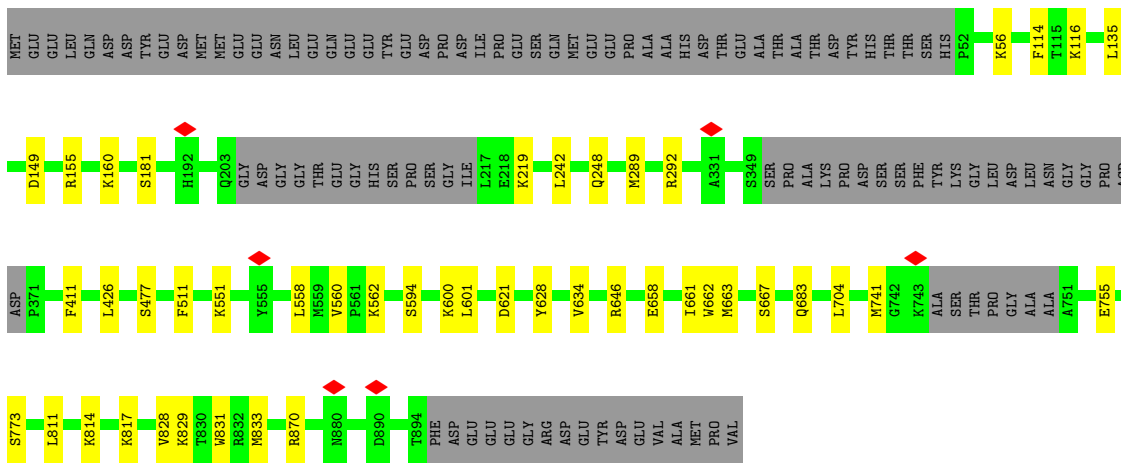
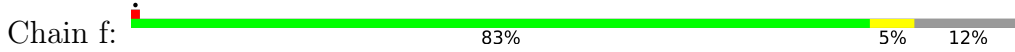




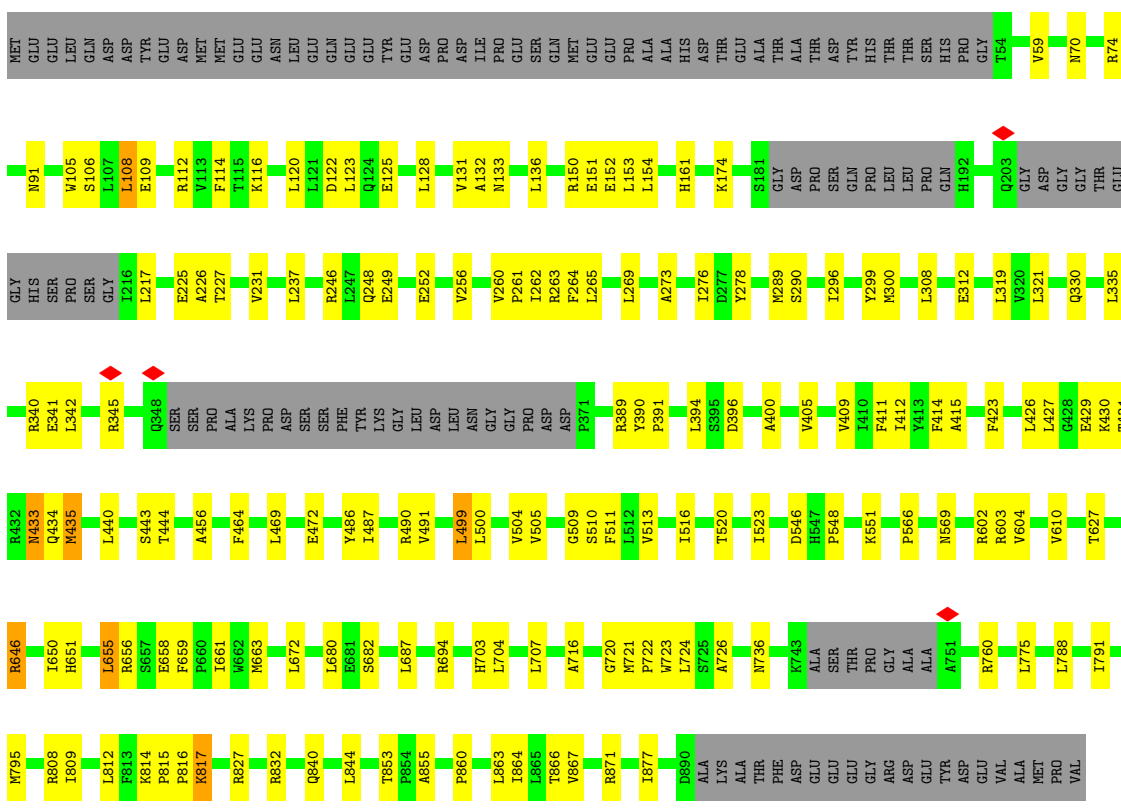
- Molecule 7: Band 3 anion transport protein



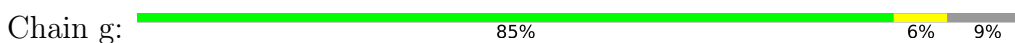
- Molecule 7: Band 3 anion transport protein



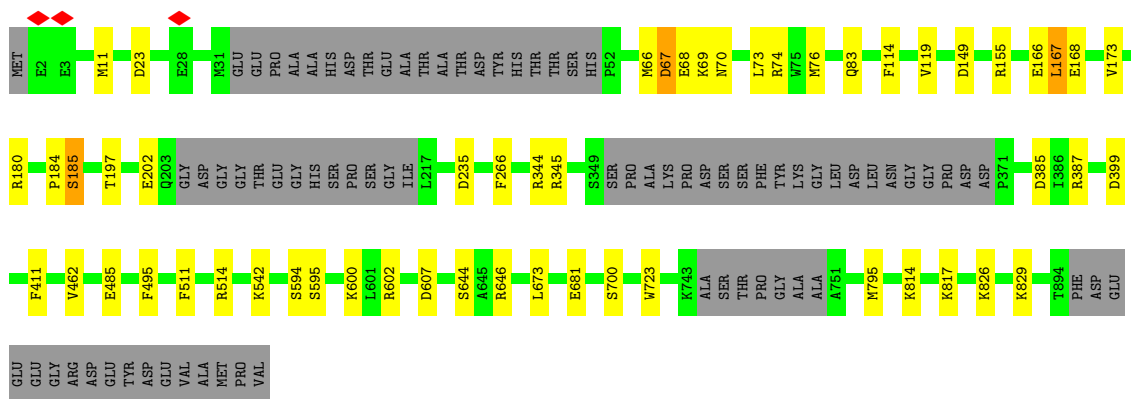
• Molecule 7: Band 3 anion transport protein



• Molecule 7: Band 3 anion transport protein







- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: 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, C1	Depositor
Number of particles used	126197	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Patch CTF (cryoSPARC v3) followed by per particle defocus refinement and refinement of higher order aberrations (cryoSPARC v3)	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.911	Depositor
Minimum map value	0.000	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.101	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	373.5, 373.5, 373.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.31	0/6127	0.49	0/8331
2	K	0.31	0/3016	0.51	0/4105
3	L	0.29	0/3008	0.46	0/4075
3	Q	0.31	0/3025	0.50	0/4098
4	X	0.27	0/5269	0.51	0/7149
5	P	0.52	0/249	0.64	0/336
6	R	0.38	0/282	0.56	0/381
6	S	0.25	0/260	0.55	0/351
6	T	0.41	0/289	0.58	0/391
6	a	0.24	0/289	0.54	0/391
6	b	0.25	0/294	0.52	0/398
6	c	0.40	0/260	0.55	0/351
7	V	0.29	0/6536	0.52	0/8885
7	Y	0.33	0/6371	0.54	0/8655
7	Z	0.30	0/6371	0.51	0/8655
7	e	0.35	0/6489	0.54	0/8822
7	f	0.36	0/6481	0.56	0/8808
7	g	0.35	0/6709	0.55	0/9118
All	All	0.32	0/61325	0.52	0/83300

There are no bond length outliers.

There are no bond angle outliers.

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	6017	0	6114	87	0
2	K	2943	0	3056	43	0
3	L	2938	0	2978	40	0
3	Q	2954	0	2989	40	0
4	X	5162	0	5173	52	0
5	P	248	0	298	18	0
6	R	277	0	289	15	0
6	S	255	0	265	5	0
6	T	284	0	298	9	0
6	a	284	0	298	0	0
6	b	289	0	300	0	0
6	c	255	0	265	0	0
7	V	6386	0	6558	107	0
7	Y	6226	0	6437	145	0
7	Z	6226	0	6437	102	0
7	e	6339	0	6541	0	0
7	f	6331	0	6536	0	0
7	g	6556	0	6703	0	0
8	B	28	0	25	0	0
8	C	28	0	25	0	0
8	D	28	0	25	0	0
9	L	56	0	92	4	0
9	V	28	0	46	9	0
9	Y	28	0	46	1	0
9	Z	28	0	46	4	0
9	c	28	0	46	0	0
9	e	28	0	46	0	0
9	f	28	0	46	0	0
10	Q	32	0	0	1	0
11	V	28	0	25	0	0
11	Y	28	0	25	0	0
11	Z	28	0	25	0	0
12	V	47	0	44	3	0
12	Y	47	0	44	3	0
12	e	47	0	44	0	0
12	f	47	0	44	0	0
12	g	94	0	88	0	0
13	A	32	0	0	0	0
13	K	18	0	0	0	0
13	L	46	0	0	0	0
13	Q	34	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	V	17	0	0	0	0
13	X	112	0	0	1	0
13	e	4	0	0	0	0
13	f	2	0	0	0	0
13	g	3	0	0	0	0
All	All	60944	0	62317	641	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 10.

All (641) 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)
7:Y:57:VAL:HB	7:Y:295:ARG:HD3	1.62	0.82
7:V:495:PHE:HB3	9:V:1001:CLR:H261	1.62	0.79
3:Q:350:ALA:HB2	3:Q:358:MET:SD	2.23	0.79
4:X:59:VAL:HG22	4:X:123:VAL:HG22	1.65	0.78
7:Z:136:LEU:HD12	7:Z:154:LEU:HB2	1.64	0.77
6:R:87:PHE:HB3	6:R:91:GLU:HB3	1.66	0.77
1:A:454:LYS:HD2	1:A:458:GLN:HE22	1.50	0.76
7:Y:708:LEU:O	7:Y:712:MET:HG3	1.87	0.75
4:X:121:LEU:CD2	4:X:123:VAL:HG23	2.16	0.75
7:Y:456:ALA:HB2	7:Y:704:LEU:HD23	1.69	0.75
7:V:58:TYR:HE2	7:V:258:LEU:HD12	1.52	0.74
7:Z:650:ILE:HG23	7:Z:655:LEU:HD21	1.67	0.74
5:P:62:VAL:O	5:P:66:ILE:HG23	1.87	0.74
7:Y:392:TYR:CD2	7:Y:698:LYS:HG3	2.23	0.73
3:L:1:MET:HG2	3:L:3:PHE:H	1.52	0.72
7:Z:131:VAL:HG11	7:Z:265:LEU:HD13	1.71	0.72
7:Z:414:PHE:HB3	7:Z:788:LEU:HD11	1.71	0.72
7:V:598:PRO:HD3	12:V:1004:PIO:H5A	1.69	0.72
7:Z:431:THR:HG21	7:Z:435:MET:H	1.55	0.71
7:V:618:VAL:HG11	7:V:782:ARG:NH1	2.06	0.70
7:Y:293:VAL:HG21	7:Y:346:ARG:HG3	1.73	0.70
7:Z:426:LEU:HB3	7:Z:430:LYS:HE3	1.73	0.70
1:A:490:LEU:HB3	1:A:525:LYS:HG2	1.75	0.69
7:Z:226:ALA:HB2	7:Z:260:VAL:HG23	1.74	0.69
1:A:436:LYS:HD3	1:A:468:LYS:HB2	1.72	0.69
7:Y:124:GLN:HG3	7:Y:248:GLN:HG3	1.75	0.69
1:A:238:ASN:O	1:A:270:LYS:HD2	1.93	0.68
7:V:341:GLU:OE2	7:V:344:ARG:HD3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:867:VAL:O	7:Z:871:ARG:HG3	1.94	0.68
7:Y:250:ALA:HB1	7:Y:261:PRO:HB2	1.76	0.67
1:A:436:LYS:HD2	1:A:438:GLU:HG3	1.74	0.67
7:Y:680:LEU:HD11	7:Y:864:ILE:HD11	1.76	0.67
7:Y:738:LEU:HB3	7:Y:757:LYS:HB2	1.75	0.67
1:A:491:GLU:OE1	1:A:525:LYS:NZ	2.28	0.67
6:T:95:ILE:O	6:T:99:VAL:HG23	1.95	0.66
7:Z:809:ILE:HA	7:Z:812:LEU:HD12	1.76	0.66
5:P:60:PRO:HA	5:P:63:ILE:HG13	1.77	0.66
7:V:772:LEU:O	7:V:776:MET:HG2	1.96	0.66
1:A:454:LYS:CD	1:A:458:GLN:HE22	2.08	0.66
5:P:79:LEU:O	5:P:83:TYR:HB2	1.96	0.66
7:Y:226:ALA:HB2	7:Y:260:VAL:HG23	1.78	0.66
7:Z:427:LEU:HD13	7:Z:469:LEU:HD12	1.77	0.66
7:Z:853:THR:HG22	7:Z:855:ALA:H	1.59	0.66
7:Y:396:ASP:OD2	7:Y:760:ARG:NH1	2.30	0.65
7:Y:434:GLN:O	7:Y:646:ARG:NH1	2.29	0.65
6:S:87:PHE:HB2	6:S:92:ILE:HG13	1.78	0.65
7:Y:592:LYS:HB2	7:Y:606:GLY:HA3	1.79	0.65
3:L:377:LEU:HD11	9:L:502:CLR:H213	1.78	0.64
7:Y:488:VAL:HG11	7:Y:654:GLY:HA2	1.79	0.64
5:P:63:ILE:HG22	5:P:67:ILE:HD11	1.80	0.64
7:Y:500:LEU:HD21	7:Y:672:LEU:HD22	1.78	0.64
7:Z:340:ARG:HH22	7:Z:341:GLU:HB2	1.61	0.64
2:K:70:ARG:HG2	2:K:202:ALA:HB2	1.79	0.64
7:Y:510:SER:HB2	7:Y:703:HIS:CE1	2.33	0.63
6:T:100:MET:HG3	7:Z:499:LEU:HD12	1.80	0.63
7:V:371:PRO:HA	7:V:384:ARG:HH21	1.63	0.63
1:A:436:LYS:O	1:A:438:GLU:N	2.30	0.63
6:R:90:PRO:O	6:R:94:LEU:HG	1.99	0.63
2:K:123:VAL:HG11	2:K:143:VAL:HA	1.81	0.63
7:Z:227:THR:HG21	7:Z:289:MET:HG2	1.81	0.62
12:Y:1004:PIO:H8BA	12:Y:1004:PIO:H7A	1.80	0.62
3:Q:347:VAL:HG12	3:Q:351:MET:HE2	1.81	0.62
2:K:34[B]:TYR:HH	3:L:237:CYS:HG	1.48	0.62
4:X:590:LEU:HD13	4:X:610:LEU:HD12	1.80	0.62
7:Y:443:SER:HB2	7:Y:721:MET:HB3	1.81	0.62
7:Z:431:THR:CG2	7:Z:435:MET:H	2.13	0.62
7:Z:340:ARG:NH2	7:Z:341:GLU:HB2	2.14	0.62
3:Q:2:ARG:HG2	3:Q:3:PHE:CE1	2.35	0.62
7:Z:109:GLU:HG2	7:Z:276:ILE:HG12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:120:LEU:HD22	7:Z:123:LEU:HD13	1.82	0.62
7:V:518:ARG:NH2	7:V:693:GLU:OE1	2.28	0.61
7:Y:464:PHE:HE2	7:Y:469:LEU:HB2	1.65	0.61
1:A:726:ASP:HB3	1:A:729:ALA:HB2	1.82	0.61
1:A:783:THR:O	1:A:787:LYS:HB2	2.01	0.61
4:X:140:PRO:HG2	4:X:159:LEU:HD22	1.83	0.61
3:L:286:CYS:HB3	3:L:291:ILE:HG21	1.82	0.61
7:Z:694:ARG:NH2	7:Z:736:ASN:OD1	2.34	0.61
7:Y:468:LEU:O	7:Y:472:GLU:HG2	2.00	0.61
1:A:435:VAL:HG23	1:A:436:LYS:H	1.65	0.60
7:V:384:ARG:NH2	7:V:388:ARG:HH22	1.98	0.60
3:Q:73:LYS:HG3	3:Q:74:LYS:HG3	1.83	0.60
7:Y:64:LEU:HD22	7:Y:73:LEU:HD22	1.83	0.60
7:Y:115:THR:HA	7:Y:308:LEU:HD11	1.82	0.60
3:L:314:LEU:HD12	3:L:317:LEU:HD23	1.82	0.60
7:V:336:VAL:N	7:V:337:PRO:HD2	2.17	0.60
4:X:121:LEU:HD21	4:X:123:VAL:HG23	1.84	0.59
4:X:64:GLN:NE2	4:X:76:GLN:OE1	2.35	0.59
4:X:244:LYS:NZ	4:X:667:GLU:OE1	2.35	0.59
2:K:153:LEU:HD23	2:K:376:ILE:HD12	1.84	0.59
7:V:491:VAL:HG22	7:V:718:LEU:HA	1.83	0.59
1:A:482:HIS:HD2	1:A:485:MET:CB	2.16	0.59
7:Y:853:THR:HB	7:Y:854:PRO:HD2	1.85	0.59
1:A:472:THR:OG1	1:A:475:HIS:ND1	2.35	0.59
7:Y:738:LEU:HD11	7:Y:759:GLN:HE22	1.68	0.59
7:V:400:ALA:HA	7:V:405:VAL:HG21	1.84	0.59
4:X:590:LEU:O	4:X:678:ASN:ND2	2.35	0.59
5:P:66:ILE:HG13	5:P:67:ILE:N	2.17	0.59
2:K:235:LYS:HE3	3:Q:47:PHE:CG	2.38	0.58
7:V:58:TYR:CE2	7:V:258:LEU:HD12	2.36	0.58
7:Y:870:ARG:HA	7:Y:874:LEU:HD23	1.86	0.58
1:A:193:LEU:HD13	1:A:228:ARG:HG3	1.84	0.58
1:A:226:LEU:HD13	1:A:261:ARG:HG3	1.85	0.58
1:A:612:GLN:OE1	1:A:614:GLN:NE2	2.36	0.58
7:Y:504:VAL:HG13	7:Y:509:GLY:HA3	1.85	0.58
5:P:61:VAL:O	5:P:65:LEU:HG	2.03	0.58
5:P:63:ILE:HG22	5:P:67:ILE:CD1	2.34	0.58
7:V:527:LEU:HD22	7:V:847:LEU:HD23	1.86	0.58
5:P:84:SER:O	5:P:87:ARG:HG2	2.04	0.57
7:V:226:ALA:HB2	7:V:260:VAL:HG23	1.86	0.57
7:V:440:LEU:HD11	7:V:464:PHE:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:122:ASP:OD2	7:Y:246:ARG:NH2	2.37	0.57
7:Y:759:GLN:N	7:Y:759:GLN:OE1	2.37	0.57
7:V:882:GLU:O	7:V:886:LEU:HB2	2.03	0.57
7:Y:235:ASP:OD1	7:Y:236:PHE:N	2.37	0.57
4:X:209:VAL:HG13	4:X:365:LEU:HD12	1.85	0.57
7:Z:659:PHE:CZ	7:Z:663:MET:HG2	2.39	0.57
7:Y:400:ALA:HA	7:Y:405:VAL:HG21	1.86	0.57
7:Y:610:VAL:HG13	7:Y:791:ILE:HD12	1.87	0.57
7:Z:153:LEU:HD22	7:Z:269:LEU:HD13	1.85	0.57
7:Y:148:GLN:HA	7:Y:829:LYS:HE2	1.86	0.57
7:Y:488:VAL:HA	7:Y:491:VAL:HG12	1.86	0.57
7:Z:456:ALA:HB2	7:Z:704:LEU:HD23	1.85	0.56
7:Z:400:ALA:HA	7:Z:405:VAL:HG21	1.87	0.56
1:A:58:VAL:HG11	1:A:92:GLU:HG3	1.87	0.56
1:A:214:ALA:O	1:A:251:ASN:ND2	2.37	0.56
7:Z:472:GLU:OE2	7:Z:486:TYR:OH	2.22	0.56
7:Z:863:LEU:O	7:Z:866:THR:OG1	2.22	0.56
6:R:100:MET:HG3	9:V:1001:CLR:H25	1.88	0.56
7:Y:733:THR:HG21	7:Y:795:MET:HE2	1.87	0.56
1:A:646:GLY:HA2	1:A:683:VAL:HG21	1.87	0.56
7:Y:522:GLU:HB3	7:Y:803:ILE:HG23	1.87	0.56
7:Y:522:GLU:OE2	7:Y:804:GLN:N	2.39	0.56
7:Y:422:THR:O	7:Y:426:LEU:HG	2.06	0.56
7:V:412:ILE:HA	7:V:415:ALA:HB3	1.88	0.56
7:V:738:LEU:HB3	7:V:757:LYS:HB2	1.88	0.56
7:Y:680:LEU:HD21	7:Y:864:ILE:HD11	1.89	0.55
2:K:189:LYS:HD2	2:K:189:LYS:N	2.22	0.55
7:V:610:VAL:HG13	7:V:791:ILE:HD12	1.89	0.55
7:Y:382:LEU:O	7:Y:386:ILE:HG13	2.07	0.55
7:Y:511:PHE:O	7:Y:514:ARG:HG2	2.07	0.55
1:A:622:LEU:HD13	1:A:657:LYS:HG3	1.87	0.55
6:R:114:ILE:HG22	6:R:115:ARG:HG3	1.89	0.55
7:Y:386:ILE:HG12	7:Y:704:LEU:HD22	1.89	0.55
12:V:1004:PIO:H7AA	12:V:1004:PIO:H5B	1.88	0.55
3:L:147:LEU:HD12	3:L:379:THR:HG23	1.89	0.54
5:P:63:ILE:HA	5:P:66:ILE:HG12	1.89	0.54
7:V:456:ALA:HB2	7:V:704:LEU:HD23	1.89	0.54
7:V:497:LEU:HD22	7:V:710:VAL:HG13	1.90	0.54
2:K:34[B]:TYR:OH	3:L:237:CYS:SG	2.61	0.54
2:K:88:VAL:HG11	3:L:244:TYR:HE2	1.72	0.54
7:V:516:ILE:HG23	7:V:520:THR:HB	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:HD21	1:A:71:LEU:HD13	1.90	0.54
1:A:484:ASN:OD1	1:A:484:ASN:N	2.39	0.54
4:X:113:VAL:HG13	4:X:205:TRP:HB2	1.90	0.54
6:T:83:LEU:O	6:T:84:ALA:C	2.46	0.54
7:V:296:ILE:HG23	7:V:300:MET:HE3	1.89	0.54
7:Y:396:ASP:CG	7:Y:760:ARG:HG3	2.28	0.54
7:Z:426:LEU:HA	7:Z:429:GLU:HG2	1.89	0.54
1:A:30:ASP:OD1	4:X:97:ARG:NH2	2.30	0.54
7:V:139:PHE:HB3	7:V:145:ILE:HG12	1.89	0.54
7:Y:540:LEU:HD13	7:Y:578:MET:HE3	1.90	0.54
7:Z:427:LEU:HD11	7:Z:472:GLU:HG3	1.90	0.54
3:L:69:MET:HE3	3:L:130:GLY:HA2	1.90	0.53
7:Z:815:PRO:O	7:Z:817:LYS:N	2.41	0.53
3:Q:316:PRO:O	3:Q:320:THR:OG1	2.24	0.53
7:Y:129:ALA:O	7:Y:133:ASN:ND2	2.30	0.53
7:Y:146:ARG:HG3	7:Y:146:ARG:HH11	1.73	0.53
1:A:466:LYS:HE3	1:A:498:LEU:HD23	1.89	0.53
2:K:123:VAL:HG22	2:K:146:GLU:HG2	1.91	0.53
7:V:296:ILE:HG23	7:V:300:MET:CE	2.38	0.53
7:V:867:VAL:O	7:V:871:ARG:HG2	2.09	0.53
1:A:107:GLN:NE2	1:A:111:GLY:HA2	2.23	0.53
7:V:229:VAL:HG22	7:V:266:PHE:HB2	1.91	0.53
7:Y:198:GLN:O	7:Y:199:LEU:HD12	2.08	0.53
7:Y:412:ILE:HA	7:Y:415:ALA:HB3	1.91	0.53
1:A:240:ILE:HD11	1:A:270:LYS:NZ	2.24	0.53
3:Q:336:LEU:O	3:Q:340:VAL:HG23	2.09	0.53
7:V:664:MET:SD	9:V:1001:CLR:H182	2.49	0.53
7:Y:89:GLY:HA2	7:Y:197:THR:CG2	2.39	0.53
7:Y:378:LEU:O	7:Y:379:PHE:HB2	2.08	0.53
3:Q:1:MET:HG2	3:Q:2:ARG:H	1.74	0.53
4:X:38:PRO:HB3	4:X:107:THR:HG22	1.91	0.53
7:V:296:ILE:O	7:V:300:MET:HE3	2.09	0.53
7:Y:153:LEU:HD22	7:Y:269:LEU:HD13	1.91	0.53
7:Z:659:PHE:CE2	7:Z:663:MET:HG2	2.44	0.53
7:V:400:ALA:HB2	7:V:759:GLN:HG3	1.91	0.52
7:Y:85:GLU:OE2	7:Y:87:ASN:ND2	2.40	0.52
6:T:82:GLN:OE1	7:Z:655:LEU:HD12	2.09	0.52
1:A:439:THR:OG1	1:A:442:HIS:HD2	1.92	0.52
2:K:217:TRP:NE1	2:K:245:LEU:HB3	2.24	0.52
2:K:396:PRO:HB3	2:K:406:VAL:HG11	1.91	0.52
7:Y:455:GLY:O	7:Y:760:ARG:NH2	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:92:ILE:O	6:T:96:ILE:HD12	2.09	0.52
1:A:437:VAL:HG23	1:A:468:LYS:HE3	1.91	0.52
3:L:59:VAL:HA	3:Q:220:MET:SD	2.50	0.52
4:X:307:TYR:HE2	4:X:404:LEU:HD21	1.75	0.52
7:Y:321:LEU:HD13	7:Y:335:LEU:HD11	1.91	0.52
7:Y:440:LEU:HD21	7:Y:464:PHE:HB2	1.92	0.52
4:X:650:ALA:HA	7:V:32:GLU:HB3	1.91	0.52
7:Y:511:PHE:CE1	7:Y:514:ARG:HD3	2.45	0.52
7:Z:680:LEU:HD11	7:Z:864:ILE:HG13	1.92	0.52
1:A:355:LYS:HA	1:A:389:LEU:HD11	1.91	0.52
1:A:486:VAL:HG21	1:A:518:THR:HG23	1.92	0.52
4:X:313:LEU:HD13	4:X:525:LYS:HD3	1.92	0.52
7:Y:860:PRO:O	7:Y:864:ILE:HG12	2.10	0.52
1:A:596:HIS:NE2	1:A:625:GLY:O	2.40	0.52
4:X:485:LEU:HD12	4:X:486:PRO:HD2	1.91	0.52
7:V:317:CYS:HA	7:V:342:LEU:HD11	1.92	0.52
7:Y:738:LEU:CD1	7:Y:759:GLN:HE22	2.22	0.52
1:A:268:LYS:HB3	1:A:272:GLU:HA	1.92	0.51
7:V:371:PRO:HA	7:V:384:ARG:NH2	2.24	0.51
1:A:38:ILE:HG12	1:A:69:ILE:HD12	1.93	0.51
3:Q:277:LEU:HB2	3:Q:333:LEU:HD11	1.91	0.51
7:Z:231:VAL:HG13	7:Z:278:TYR:HB3	1.91	0.51
1:A:482:HIS:HD2	1:A:485:MET:HB3	1.74	0.51
7:V:859:LEU:O	7:V:859:LEU:HD23	2.11	0.51
7:Y:811:LEU:HD23	7:Y:814:LYS:HD3	1.93	0.51
7:Z:431:THR:HG23	7:Z:434:GLN:N	2.25	0.51
7:Z:440:LEU:HD11	7:Z:464:PHE:HB2	1.92	0.51
7:Y:683:GLN:NE2	7:Y:702:PHE:HB3	2.26	0.51
7:Y:813:PHE:HD1	12:Y:1004:PIO:H7AA	1.76	0.51
3:L:187:GLY:HA3	9:L:502:CLR:H161	1.92	0.51
7:V:418:SER:HB2	7:V:792:PHE:HZ	1.76	0.51
7:Z:321:LEU:HD13	7:Z:335:LEU:HD11	1.93	0.51
7:Z:133:ASN:OD1	7:Z:150:ARG:NH2	2.44	0.51
5:P:85:ILE:HG21	7:Z:390:TYR:HD1	1.76	0.51
7:Y:452:ALA:O	7:Y:760:ARG:HD3	2.10	0.51
1:A:125:GLU:CD	1:A:125:GLU:H	2.14	0.51
3:Q:314:LEU:HD23	3:Q:336:LEU:HD11	1.93	0.51
7:Y:89:GLY:HA2	7:Y:197:THR:HG23	1.92	0.51
7:Y:227:THR:HG21	7:Y:289:MET:HG2	1.93	0.50
7:Y:371:PRO:HG2	7:Y:372:LEU:HG	1.91	0.50
7:Z:500:LEU:HD11	7:Z:672:LEU:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LYS:HB2	1:A:465:ALA:HB2	1.94	0.50
2:K:312:LEU:HD13	2:K:330:SER:HB2	1.94	0.50
3:Q:347:VAL:HG12	3:Q:351:MET:CE	2.41	0.50
7:Y:540:LEU:HD13	7:Y:578:MET:CE	2.41	0.50
7:Z:161:HIS:CG	7:Z:256:VAL:HG22	2.46	0.50
7:V:805:LEU:O	7:V:809:ILE:HG13	2.12	0.50
6:S:89:GLU:HG3	7:Y:651:HIS:CD2	2.47	0.50
7:Z:319:LEU:HD13	7:Z:342:LEU:HD22	1.92	0.50
7:V:242:LEU:HD12	7:V:268:LEU:HD21	1.91	0.50
7:Z:153:LEU:HD11	7:Z:237:LEU:HD21	1.92	0.50
4:X:69:PRO:HB2	4:X:76:GLN:HB2	1.93	0.50
7:Y:57:VAL:HB	7:Y:295:ARG:CD	2.36	0.50
7:Y:624:ILE:HD13	7:Y:627:THR:HB	1.94	0.50
7:Z:431:THR:HG23	7:Z:434:GLN:H	1.77	0.50
3:L:222:TRP:HB3	3:L:247:LEU:HD11	1.94	0.49
7:Y:65:VAL:HG21	7:Y:76:MET:HB2	1.94	0.49
1:A:166:TYR:OH	1:A:170:GLY:O	2.25	0.49
7:Y:592:LYS:NZ	7:Y:607:ASP:OD1	2.33	0.49
2:K:218:MET:HG2	3:Q:58:HIS:CD2	2.48	0.49
3:L:340:VAL:HG13	9:L:501:CLR:H273	1.95	0.49
7:Z:505:VAL:HG21	7:Z:707:LEU:HB2	1.95	0.49
1:A:53:SER:HA	1:A:93:VAL:HG11	1.94	0.49
4:X:594:MET:O	4:X:680:LYS:NZ	2.46	0.49
6:R:96:ILE:HG21	7:V:495:PHE:CZ	2.48	0.49
7:Y:375:THR:OG1	7:Y:508:GLU:OE2	2.28	0.49
7:V:62:GLN:OE1	7:V:161:HIS:ND1	2.39	0.49
7:V:632:LEU:HD11	7:V:788:LEU:HD11	1.94	0.49
7:Y:815:PRO:O	7:Y:817:LYS:N	2.40	0.49
1:A:384:VAL:O	1:A:388:GLU:HG3	2.12	0.49
1:A:729:ALA:O	1:A:737:PRO:HD3	2.13	0.49
7:V:493:ILE:HG23	7:V:671:ALA:HA	1.94	0.49
7:Y:140:ILE:HD11	7:Y:150:ARG:HB2	1.94	0.49
7:Z:443:SER:HB2	7:Z:721:MET:HB3	1.93	0.49
7:Z:548:PRO:HD2	7:Z:566:PRO:HB3	1.95	0.49
3:Q:2:ARG:HG2	3:Q:3:PHE:CD1	2.48	0.49
7:Y:396:ASP:OD1	7:Y:760:ARG:N	2.46	0.49
7:Y:433:ASN:O	7:Y:642:ASN:HB2	2.13	0.49
1:A:529:GLN:NE2	1:A:558:ARG:O	2.46	0.48
1:A:676:ALA:HA	1:A:716:LEU:HD22	1.95	0.48
4:X:13:GLN:OE1	4:X:16:ARG:NH1	2.46	0.48
7:Y:120:LEU:HD23	7:Y:123:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:716:ALA:HB1	7:Y:721:MET:HB2	1.95	0.48
7:Z:486:TYR:CZ	7:Z:490:ARG:HD2	2.47	0.48
7:V:231:VAL:HG13	7:V:278:TYR:HB3	1.96	0.48
7:Z:308:LEU:O	7:Z:312:GLU:HG2	2.13	0.48
1:A:538:THR:OG1	1:A:541:HIS:ND1	2.43	0.48
2:K:217:TRP:CD1	2:K:245:LEU:HD22	2.49	0.48
6:R:92:ILE:CD1	9:V:1001:CLR:H6	2.43	0.48
7:Z:791:ILE:O	7:Z:795:MET:HG3	2.13	0.48
2:K:382:LEU:O	2:K:386:LEU:HD22	2.14	0.48
3:L:69:MET:CE	3:L:130:GLY:HA2	2.42	0.48
4:X:138:PHE:HB3	4:X:147:VAL:HG21	1.95	0.48
4:X:223:LYS:HD3	4:X:271:LEU:HD22	1.94	0.48
7:V:785:LEU:HD23	7:V:788:LEU:HD12	1.96	0.48
7:Y:178:LEU:HD23	7:Y:236:PHE:CZ	2.48	0.48
7:V:487:ILE:HG21	7:V:650:ILE:HG12	1.95	0.48
1:A:771:LEU:HD11	1:A:783:THR:HG23	1.95	0.48
2:K:20:LEU:HD11	2:K:144:LEU:HD11	1.96	0.48
3:Q:120:PHE:HB3	3:Q:174:ILE:HD11	1.95	0.48
7:V:716:ALA:HB1	7:V:721:MET:HB2	1.94	0.48
7:Y:62:GLN:HG3	7:Y:228:LEU:HD11	1.96	0.48
2:K:249:VAL:HG22	2:K:274:VAL:HG12	1.95	0.48
6:R:96:ILE:HD11	7:V:492:TRP:CH2	2.48	0.48
1:A:301:LYS:NZ	1:A:333:ASP:OD2	2.47	0.48
1:A:424:LEU:HD11	1:A:456:LEU:HD23	1.96	0.48
4:X:166:ILE:HD12	4:X:288:VAL:HG11	1.96	0.48
7:Y:408:ALA:O	7:Y:412:ILE:HG12	2.14	0.48
7:Z:122:ASP:OD1	7:Z:246:ARG:NH2	2.41	0.48
7:Z:431:THR:HG21	7:Z:435:MET:N	2.27	0.48
3:Q:179:ALA:HB2	3:Q:334:HIS:HB2	1.95	0.47
5:P:59:ALA:N	5:P:60:PRO:HD2	2.30	0.47
7:Y:889:ASP:OD1	7:Y:889:ASP:N	2.47	0.47
2:K:108:ILE:HD12	3:L:293:PRO:HG2	1.95	0.47
2:K:267:MET:HG3	2:K:271:HIS:CE1	2.49	0.47
4:X:300:GLY:O	4:X:455:LYS:NZ	2.43	0.47
4:X:480:LYS:HB3	4:X:494:SER:HB2	1.97	0.47
4:X:120:LEU:HD13	4:X:128:GLN:OE1	2.15	0.47
1:A:451:GLU:CD	1:A:451:GLU:H	2.18	0.47
1:A:746:HIS:HB3	1:A:749:ILE:HG13	1.96	0.47
3:L:24:VAL:O	3:Q:292:HIS:NE2	2.47	0.47
6:R:96:ILE:HG13	9:V:1001:CLR:H151	1.97	0.47
7:V:137:ASP:OD2	7:V:150:ARG:NH2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:443:SER:HB2	7:V:721:MET:HB3	1.96	0.47
7:Y:418:SER:HB2	7:Y:788:LEU:HD13	1.95	0.47
7:Y:490:ARG:NH2	7:Y:722:PRO:HA	2.29	0.47
7:Y:539:LYS:O	7:Y:543:ILE:HG22	2.15	0.47
7:Z:832:ARG:NH2	7:Z:877:ILE:O	2.47	0.47
1:A:582:LEU:HG	1:A:586:LYS:HD2	1.96	0.47
1:A:769:THR:HG23	1:A:771:LEU:H	1.80	0.47
7:Z:273:ALA:HB3	7:Z:276:ILE:HD12	1.97	0.47
7:Z:427:LEU:HD21	7:Z:435:MET:HE3	1.97	0.47
3:L:130:GLY:HA3	3:L:330:VAL:HG11	1.96	0.47
3:L:348:ALA:HB1	3:L:353:ALA:HB3	1.97	0.47
7:V:621:ASP:OD2	7:V:784:PRO:HG3	2.14	0.47
7:Y:59:VAL:HB	7:Y:81:TRP:HB2	1.96	0.47
7:Y:136:LEU:O	7:Y:140:ILE:HG13	2.14	0.47
7:Y:178:LEU:HD23	7:Y:236:PHE:HZ	1.80	0.47
7:Y:660:PRO:HB2	7:Y:662:TRP:CD1	2.50	0.47
3:L:350:ALA:HA	3:L:358:MET:HE1	1.97	0.47
7:Y:589:ARG:NH1	7:Y:798:THR:HG22	2.30	0.47
3:L:50:LEU:HB2	3:L:112:ILE:HG21	1.97	0.47
4:X:185:GLU:OE1	4:X:253:ARG:NH2	2.48	0.47
4:X:523:ALA:HB1	4:X:557:PRO:HG2	1.96	0.47
7:Y:516:ILE:HG23	7:Y:520:THR:HB	1.97	0.47
3:L:387:LEU:HD22	5:P:83:TYR:HE1	1.79	0.47
7:V:719:PHE:HB2	7:V:721:MET:HG3	1.97	0.47
7:Y:397:ILE:HG23	7:Y:761:ILE:HD11	1.96	0.47
7:Y:472:GLU:OE2	7:Y:472:GLU:HA	2.15	0.47
1:A:217:GLU:HA	1:A:254:MET:HE3	1.97	0.46
7:V:228:LEU:HD22	7:V:256:VAL:HG11	1.95	0.46
7:V:342:LEU:O	7:V:342:LEU:HG	2.15	0.46
7:Y:74:ARG:NH2	7:Y:160:LYS:HD2	2.31	0.46
7:Z:248:GLN:O	7:Z:248:GLN:NE2	2.47	0.46
2:K:218:MET:SD	3:Q:59:VAL:HA	2.55	0.46
3:L:67:PHE:O	3:L:211:ALA:HA	2.15	0.46
4:X:445:LYS:HB3	4:X:445:LYS:HE3	1.58	0.46
7:Z:411:PHE:CD1	7:Z:610:VAL:HG11	2.50	0.46
1:A:217:GLU:HG3	1:A:251:ASN:HB3	1.97	0.46
7:V:551:LYS:HB2	7:V:551:LYS:HE3	1.74	0.46
3:L:64:GLY:HA2	3:L:214:GLY:HA2	1.97	0.46
7:Y:596:TYR:O	7:Y:597:PHE:HB2	2.14	0.46
7:Z:132:ALA:O	7:Z:136:LEU:HG	2.15	0.46
1:A:107:GLN:HE21	1:A:107:GLN:HB3	1.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:LEU:HD21	1:A:430:PRO:HB3	1.97	0.46
1:A:550:ARG:HA	1:A:550:ARG:NE	2.31	0.46
7:V:96:ARG:HH21	7:V:200:PHE:HA	1.80	0.46
1:A:433:SER:HA	1:A:438:GLU:O	2.15	0.46
2:K:343:TYR:HE2	2:K:347:LEU:HD13	1.81	0.46
3:L:261:VAL:HB	3:L:312:LYS:HG2	1.97	0.46
3:Q:172:MET:HG2	3:Q:365:LEU:HD13	1.97	0.46
12:V:1004:PIO:P5	12:V:1004:PIO:HO6	2.39	0.46
7:Y:67:ASP:HB3	7:Y:170:LEU:HD13	1.97	0.46
7:Y:440:LEU:HG	7:Y:722:PRO:HG2	1.97	0.46
4:X:109:PRO:HG2	4:X:112:ALA:HB2	1.97	0.46
6:R:87:PHE:HB3	6:R:91:GLU:CB	2.42	0.46
7:Z:680:LEU:HD23	7:Z:680:LEU:HA	1.81	0.46
4:X:478:LEU:HB3	4:X:496:THR:HB	1.98	0.46
7:Y:77:GLU:OE1	7:Y:164:ALA:N	2.49	0.46
7:Z:225:GLU:OE1	7:Z:263:ARG:NH1	2.49	0.46
1:A:550:ARG:HB3	1:A:550:ARG:CZ	2.45	0.46
5:P:59:ALA:HA	5:P:62:VAL:HG13	1.96	0.46
7:V:59:VAL:HB	7:V:81:TRP:HB2	1.98	0.46
7:V:273:ALA:HB3	7:V:276:ILE:HD12	1.98	0.46
7:Z:396:ASP:HB3	7:Z:760:ARG:HG3	1.98	0.46
7:Z:516:ILE:HG23	7:Z:520:THR:HB	1.97	0.46
3:L:120:PHE:HB3	3:L:174:ILE:HD11	1.97	0.46
4:X:408:ASP:HB2	4:X:575:LEU:HD21	1.98	0.46
7:V:818:TYR:O	7:V:819:HIS:C	2.54	0.46
1:A:405:LEU:HD22	1:A:409:HIS:HB3	1.97	0.45
7:V:863:LEU:O	7:V:866:THR:HG22	2.15	0.45
6:S:108:LEU:HG	7:Y:378:LEU:HD13	1.98	0.45
7:Y:430:LYS:HB3	7:Y:473:GLU:OE2	2.16	0.45
7:Z:610:VAL:HG13	7:Z:791:ILE:HD12	1.98	0.45
1:A:442:HIS:HE1	1:A:471:GLN:O	1.98	0.45
6:R:92:ILE:CD1	7:V:653:LEU:HD21	2.46	0.45
7:V:227:THR:HG21	7:V:289:MET:HG3	1.97	0.45
4:X:120:LEU:HD23	4:X:130:LEU:HA	1.98	0.45
12:Y:1004:PIO:H3B	12:Y:1004:PIO:H5A	1.97	0.45
2:K:308:GLY:HA3	2:K:331:ILE:HD13	1.97	0.45
7:Y:510:SER:HB2	7:Y:703:HIS:ND1	2.31	0.45
9:Y:1001:CLR:H221	9:Y:1001:CLR:H162	1.48	0.45
4:X:621:CYS:HB3	4:X:639:PHE:CZ	2.52	0.45
5:P:84:SER:O	5:P:87:ARG:N	2.49	0.45
7:Y:317:CYS:HA	7:Y:342:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Z:319:LEU:HD13	7:Z:342:LEU:CD2	2.47	0.45
1:A:358:LEU:HD11	1:A:390:LEU:HD23	1.98	0.45
9:V:1001:CLR:H221	9:V:1001:CLR:H162	1.27	0.45
2:K:68:ASN:ND2	2:K:206:SER:OG	2.48	0.45
4:X:165:LEU:HD23	4:X:178:SER:HA	1.98	0.45
7:V:342:LEU:O	7:V:343:LEU:HD23	2.16	0.45
7:Z:227:THR:HG23	7:Z:264:PHE:HB2	1.98	0.45
1:A:214:ALA:HA	1:A:254:MET:HG2	1.98	0.45
4:X:529:LYS:HZ3	4:X:531:LEU:HD21	1.82	0.45
5:P:66:ILE:O	5:P:70:VAL:HG23	2.17	0.45
7:V:497:LEU:HD22	7:V:710:VAL:CG1	2.46	0.45
7:Z:59:VAL:HG13	7:Z:227:THR:HB	1.99	0.45
7:Z:423:PHE:HA	7:Z:426:LEU:HD12	1.99	0.45
7:Z:444:THR:HA	7:Z:724:LEU:HD11	1.99	0.45
7:Z:504:VAL:HG13	7:Z:509:GLY:HA3	1.99	0.45
4:X:562:LEU:HB2	4:X:583:ILE:HB	1.99	0.45
5:P:74:ILE:O	5:P:78:ILE:HG13	2.17	0.45
7:Z:394:LEU:HD12	7:Z:394:LEU:HA	1.80	0.45
9:Z:1001:CLR:H213	9:Z:1001:CLR:H232	1.84	0.45
1:A:468:LYS:HD3	1:A:468:LYS:HA	1.59	0.44
1:A:750:VAL:HG21	1:A:782:VAL:HG13	1.99	0.44
7:Y:405:VAL:HA	7:Y:738:LEU:HD21	1.99	0.44
7:Z:513:VAL:HG12	7:Z:687:LEU:HD11	1.98	0.44
2:K:218:MET:HG2	3:Q:58:HIS:HD2	1.82	0.44
2:K:370:LEU:O	2:K:374:ILE:HG12	2.17	0.44
3:Q:311:TYR:CE1	3:Q:329:GLY:HA3	2.52	0.44
7:V:250:ALA:HB1	7:V:261:PRO:HB2	1.99	0.44
7:V:384:ARG:NH2	7:V:388:ARG:NH2	2.64	0.44
7:Z:487:ILE:O	7:Z:491:VAL:HG23	2.17	0.44
3:Q:347:VAL:HB	10:Q:501:AJP:O82	2.17	0.44
1:A:265:ILE:HD12	1:A:265:ILE:HA	1.84	0.44
4:X:5:LEU:HD12	4:X:5:LEU:HA	1.88	0.44
6:R:92:ILE:HD11	9:V:1001:CLR:H6	2.00	0.44
7:V:874:LEU:HB3	7:V:883:LEU:HD21	1.99	0.44
7:Y:392:TYR:HD2	7:Y:698:LYS:HG3	1.77	0.44
7:Y:673:LEU:O	7:Y:676:ILE:HG13	2.17	0.44
7:Z:523:ILE:HG23	7:Z:844:LEU:HD22	1.98	0.44
6:R:96:ILE:HG21	7:V:495:PHE:CE2	2.52	0.44
7:V:394:LEU:HD23	7:V:394:LEU:HA	1.81	0.44
7:V:442:ILE:HD11	7:V:638:PHE:HD1	1.82	0.44
7:Y:277:ASP:HB3	7:Y:280:GLN:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ASN:ND2	1:A:436:LYS:O	2.50	0.44
7:V:411:PHE:CD1	7:V:610:VAL:HG11	2.52	0.44
7:V:759:GLN:HG2	7:V:761:ILE:H	1.82	0.44
7:V:877:ILE:HG23	7:V:878:PHE:HD1	1.83	0.44
1:A:181:ALA:O	1:A:218:ASN:ND2	2.45	0.44
2:K:49:GLN:NE2	3:Q:52:PRO:HG3	2.32	0.44
7:V:427:LEU:HD21	7:V:435:MET:HE3	2.00	0.44
7:Y:406:LEU:O	7:Y:410:ILE:HG12	2.18	0.44
7:Z:551:LYS:HB2	7:Z:551:LYS:HE2	1.75	0.44
5:P:89:ILE:HG13	7:Z:391:PRO:HD3	1.98	0.44
7:V:375:THR:OG1	7:V:508:GLU:OE2	2.34	0.44
7:V:869:LEU:HD12	7:V:873:LEU:HB2	1.99	0.44
7:Y:431:THR:O	7:Y:432:ARG:C	2.56	0.44
1:A:238:ASN:HB2	1:A:270:LYS:CE	2.48	0.44
4:X:389:ILE:O	4:X:436:LYS:NZ	2.44	0.44
4:X:638:ARG:NH2	7:V:37:HIS:NE2	2.65	0.44
7:Z:716:ALA:HB1	7:Z:721:MET:HB2	1.99	0.44
1:A:742:ALA:HA	1:A:782:VAL:HG11	2.00	0.43
7:V:109:GLU:O	7:V:113:VAL:HG22	2.18	0.43
7:Y:217:LEU:HD23	7:Y:217:LEU:HA	1.83	0.43
2:K:42:LYS:H	2:K:42:LYS:HG2	1.43	0.43
6:R:96:ILE:HG21	7:V:495:PHE:CE1	2.54	0.43
7:Y:833:MET:HG3	7:Y:886:LEU:HD21	1.99	0.43
7:Y:152:GLU:OE2	7:Y:181:SER:N	2.49	0.43
7:Y:599:GLY:HA2	7:Y:602:ARG:CZ	2.49	0.43
1:A:270:LYS:CD	1:A:270:LYS:H	2.31	0.43
2:K:288:ILE:HG23	2:K:293:LEU:HB3	2.01	0.43
3:Q:67:PHE:O	3:Q:211:ALA:HA	2.18	0.43
4:X:123:VAL:O	4:X:124:SER:C	2.57	0.43
7:V:603:ARG:O	7:V:606:GLY:N	2.51	0.43
7:Z:440:LEU:HD13	7:Z:722:PRO:HG2	2.00	0.43
3:L:190:TYR:CZ	3:L:323:ARG:HG2	2.54	0.43
7:V:223:ASP:OD1	7:V:223:ASP:N	2.44	0.43
7:Y:513:VAL:HG23	7:Y:516:ILE:HD12	2.01	0.43
7:Y:518:ARG:HG2	7:Y:522:GLU:HG3	2.00	0.43
7:Z:296:ILE:O	7:Z:300:MET:HG2	2.19	0.43
7:Z:433:ASN:HD22	7:Z:433:ASN:HA	1.65	0.43
1:A:110:LYS:HB3	1:A:110:LYS:HE2	1.91	0.43
7:V:597:PHE:CD2	7:V:601:LEU:HD12	2.53	0.43
7:Y:64:LEU:HD23	7:Y:64:LEU:HA	1.91	0.43
7:Y:229:VAL:HG22	7:Y:266:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:HIS:CE1	1:A:770:PRO:HG3	2.53	0.43
3:Q:64:GLY:HA3	3:Q:218:LEU:HG	2.00	0.43
7:Y:74:ARG:CZ	7:Y:160:LYS:HD2	2.47	0.43
7:Y:679:PHE:O	7:Y:683:GLN:HG2	2.19	0.43
7:Y:682:SER:HA	7:Y:726:ALA:HB3	2.00	0.43
9:Z:1001:CLR:H221	9:Z:1001:CLR:H162	1.51	0.43
1:A:666:LYS:HA	1:A:666:LYS:HD3	1.87	0.43
7:V:129:ALA:HA	7:V:158:LEU:HD21	2.01	0.43
3:Q:158:LEU:HD12	3:Q:162:ILE:HB	2.00	0.43
6:S:92:ILE:HD13	7:Y:653:LEU:CD2	2.49	0.43
7:Y:138:ARG:NH1	7:Y:141:PHE:CD1	2.87	0.43
7:Y:195:LEU:HD12	7:Y:199:LEU:HD13	2.01	0.43
7:Z:248:GLN:HG3	7:Z:249:GLU:OE1	2.19	0.43
7:Z:252:GLU:HG2	7:Z:261:PRO:HB3	2.01	0.43
3:L:57:VAL:O	3:L:61:ILE:HG12	2.19	0.43
9:L:502:CLR:H222	9:L:502:CLR:H162	1.69	0.43
6:R:104:ILE:HD13	7:V:502:VAL:HG11	2.00	0.43
7:Z:646:ARG:HH12	7:Z:720:GLY:HA3	1.84	0.43
1:A:482:HIS:CD2	1:A:485:MET:H	2.37	0.42
2:K:200:GLN:HE21	2:K:200:GLN:HA	1.84	0.42
3:L:326:ASP:OD2	3:L:330:VAL:N	2.52	0.42
7:Y:161:HIS:CG	7:Y:256:VAL:HG22	2.53	0.42
7:Y:680:LEU:HD12	7:Y:680:LEU:HA	1.80	0.42
3:L:144:MET:HG3	3:L:379:THR:HG21	2.00	0.42
3:Q:222:TRP:HB3	3:Q:247:LEU:HD11	2.01	0.42
7:Z:136:LEU:CD1	7:Z:154:LEU:HB2	2.41	0.42
3:Q:349:VAL:HG11	3:Q:356:THR:O	2.19	0.42
7:V:455:GLY:O	7:V:760:ARG:NH1	2.44	0.42
7:Z:651:HIS:H	7:Z:655:LEU:HD11	1.85	0.42
4:X:514:GLN:HE21	4:X:522:LEU:HB3	1.83	0.42
7:V:405:VAL:O	7:V:409:VAL:HG23	2.19	0.42
7:V:457:GLN:HE21	7:V:459:LEU:H	1.67	0.42
7:Y:339:GLN:O	7:Y:343:LEU:HG	2.20	0.42
1:A:513:GLU:HB2	1:A:515:HIS:CD2	2.54	0.42
4:X:121:LEU:HD12	4:X:131:LEU:HD11	2.00	0.42
4:X:365:LEU:HD23	4:X:365:LEU:HA	1.80	0.42
7:V:505:VAL:HG21	7:V:707:LEU:HB2	2.02	0.42
7:Z:226:ALA:HB3	7:Z:262:ILE:HD13	2.00	0.42
7:Z:248:GLN:O	7:Z:263:ARG:NH2	2.53	0.42
7:Z:682:SER:HA	7:Z:726:ALA:HB3	2.01	0.42
9:Z:1001:CLR:H272	9:Z:1001:CLR:H231	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ARG:HD2	1:A:546:TYR:CE2	2.53	0.42
2:K:34[B]:TYR:CE2	3:L:238:ARG:HG2	2.55	0.42
2:K:57:MET:HG2	2:K:216:LEU:HA	2.00	0.42
3:L:243:THR:HA	3:L:283:VAL:HG11	2.02	0.42
3:L:349:VAL:HG12	3:L:358:MET:SD	2.59	0.42
7:V:335:LEU:HA	7:V:338:VAL:HG23	2.01	0.42
6:S:104:ILE:O	6:S:108:LEU:HD13	2.19	0.42
7:Y:387:ARG:O	7:Y:391:PRO:HD2	2.19	0.42
7:Z:108:LEU:HD23	7:Z:108:LEU:HA	1.84	0.42
1:A:490:LEU:HD21	1:A:496:PRO:HG3	2.01	0.42
4:X:530:LYS:C	4:X:531:LEU:HD23	2.39	0.42
7:Y:677:LEU:HD11	7:Y:857:LEU:HD22	2.02	0.42
4:X:243:ASN:ND2	4:X:558:GLU:OE1	2.53	0.42
7:V:153:LEU:HD22	7:V:269:LEU:HD13	2.01	0.42
3:L:64:GLY:O	3:L:68:LEU:HB2	2.19	0.42
5:P:85:ILE:HG23	5:P:89:ILE:HD13	2.01	0.42
7:V:86:GLU:OE2	7:V:97:PRO:HG3	2.20	0.42
7:V:836:PHE:O	7:V:839:ILE:HG22	2.19	0.42
3:Q:60:MET:SD	3:Q:225:PHE:HB2	2.60	0.42
3:Q:219:TRP:CD1	3:Q:247:LEU:HD22	2.55	0.42
7:V:73:LEU:HD12	7:V:73:LEU:HA	1.81	0.42
7:Y:291:GLU:O	7:Y:295:ARG:HB2	2.20	0.42
7:Z:815:PRO:C	7:Z:817:LYS:H	2.22	0.42
1:A:369:LEU:HD23	1:A:369:LEU:HA	1.86	0.41
1:A:436:LYS:HD2	1:A:438:GLU:CG	2.46	0.41
2:K:344:ILE:HD12	2:K:366:SER:OG	2.19	0.41
4:X:14:ALA:O	4:X:18:ASN:HB2	2.20	0.41
4:X:200:LYS:HA	4:X:200:LYS:HD3	1.89	0.41
4:X:475:LEU:HD12	4:X:476:TYR:H	1.85	0.41
7:V:603:ARG:O	7:V:604:VAL:C	2.58	0.41
7:Y:418:SER:HG	7:Y:792:PHE:HZ	1.68	0.41
7:Z:109:GLU:OE2	7:Z:112:ARG:NH1	2.53	0.41
1:A:107:GLN:HE21	1:A:111:GLY:HA2	1.85	0.41
1:A:495:ASN:HB3	1:A:498:LEU:HD13	2.02	0.41
2:K:61:GLY:HA3	2:K:216:LEU:HG	2.02	0.41
6:T:90:PRO:HA	6:T:93:THR:HG22	2.02	0.41
2:K:75:SER:O	2:K:79:PHE:HB2	2.20	0.41
3:L:60:MET:SD	3:L:225:PHE:HB2	2.60	0.41
3:Q:55:GLN:O	3:Q:59:VAL:HG23	2.20	0.41
3:Q:134:GLY:HA3	3:Q:397:TYR:CD1	2.56	0.41
4:X:533:LEU:HD22	4:X:541:LYS:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:664:MET:CE	9:V:1001:CLR:H191	2.50	0.41
7:Z:105:TRP:CE3	7:Z:108:LEU:HD12	2.56	0.41
7:Z:510:SER:HB2	7:Z:703:HIS:CD2	2.55	0.41
7:Z:661:ILE:HD12	9:Z:1001:CLR:H193	2.02	0.41
7:Y:109:GLU:HG2	7:Y:276:ILE:HG13	2.02	0.41
7:Y:405:VAL:O	7:Y:409:VAL:HG23	2.21	0.41
7:Y:426:LEU:HG	7:Y:426:LEU:H	1.41	0.41
7:Z:412:ILE:HA	7:Z:415:ALA:HB3	2.03	0.41
2:K:204:ILE:N	2:K:205:PRO:CD	2.83	0.41
7:V:123:LEU:HG	7:V:125:GLU:HB2	2.02	0.41
7:V:630:GLN:HE21	7:V:630:GLN:HB3	1.59	0.41
7:Y:411:PHE:CD1	7:Y:610:VAL:HG11	2.56	0.41
7:Z:123:LEU:HG	7:Z:125:GLU:HG2	2.02	0.41
7:Z:431:THR:O	7:Z:434:GLN:HG3	2.21	0.41
2:K:207:LEU:HD23	2:K:207:LEU:HA	1.82	0.41
3:L:93:TRP:CD1	3:L:146:ILE:HA	2.56	0.41
7:V:146:ARG:HB3	7:V:148:GLN:HE22	1.85	0.41
7:Y:387:ARG:O	7:Y:391:PRO:CD	2.68	0.41
7:Y:492:TRP:NE1	7:Y:652:PRO:O	2.48	0.41
7:Y:540:LEU:HD12	7:Y:540:LEU:HA	1.95	0.41
1:A:316:ASP:HB2	1:A:350:HIS:CE1	2.56	0.41
1:A:412:SER:HA	1:A:452:VAL:HG11	2.03	0.41
1:A:483:THR:O	1:A:487:LYS:HG3	2.21	0.41
2:K:20:LEU:HD12	2:K:86:LEU:HD11	2.03	0.41
3:Q:2:ARG:HG3	3:Q:2:ARG:HH11	1.85	0.41
3:Q:250:CYS:SG	3:Q:279:GLY:N	2.92	0.41
7:V:482:ASN:OD1	7:V:482:ASN:N	2.54	0.41
7:V:559:MET:CE	7:V:559:MET:HA	2.50	0.41
7:Z:569:ASN:HB2	7:Z:627:THR:HG23	2.01	0.41
7:Z:680:LEU:HD12	7:Z:860:PRO:HB3	2.02	0.41
1:A:403:SER:O	1:A:435:VAL:HG22	2.21	0.41
3:Q:26:TYR:HE1	3:Q:110:ILE:HD11	1.85	0.41
3:Q:64:GLY:HA2	3:Q:214:GLY:HA2	2.02	0.41
7:Z:405:VAL:O	7:Z:409:VAL:HG23	2.21	0.41
1:A:675:VAL:HG11	1:A:684:ALA:HB2	2.03	0.41
2:K:88:VAL:HG11	3:L:244:TYR:CE2	2.54	0.41
2:K:242[A]:TYR:HE1	3:Q:58:HIS:CE1	2.39	0.41
3:Q:101:LEU:HA	3:Q:101:LEU:HD23	1.84	0.41
4:X:638:ARG:NE	7:V:37:HIS:CD2	2.88	0.41
7:V:548:PRO:HD2	7:V:566:PRO:HB3	2.02	0.41
7:V:773:SER:HA	7:V:776:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:145:ILE:HD13	7:Y:153:LEU:HD12	2.02	0.41
7:Y:386:ILE:HD11	7:Y:704:LEU:HD13	2.03	0.41
6:T:90:PRO:O	6:T:94:LEU:HD23	2.21	0.41
1:A:512:ARG:HD2	1:A:546:TYR:CZ	2.56	0.41
2:K:57:MET:HG2	2:K:216:LEU:HD23	2.03	0.41
3:L:259:SER:O	3:L:265:GLY:HA2	2.21	0.41
7:Y:384:ARG:HH21	7:Y:387:ARG:NH1	2.19	0.41
7:Y:832:ARG:H	7:Y:832:ARG:HG2	1.69	0.41
6:T:100:MET:HE2	6:T:100:MET:HB2	1.89	0.41
6:T:110:ILE:O	6:T:114:ILE:HG12	2.21	0.41
2:K:117:THR:O	2:K:121:MET:HG3	2.21	0.40
4:X:213:ARG:NH2	13:X:716:HOH:O	2.53	0.40
7:V:85:GLU:OE1	7:V:100:SER:OG	2.33	0.40
7:V:562:LYS:HB2	7:V:562:LYS:HE2	1.86	0.40
7:Y:152:GLU:CD	7:Y:180:ARG:HA	2.41	0.40
7:Y:319:LEU:HD21	7:Y:335:LEU:HD13	2.01	0.40
7:Y:426:LEU:HA	7:Y:429:GLU:OE1	2.21	0.40
7:Z:808:ARG:NH1	7:Z:840:GLN:OE1	2.43	0.40
3:Q:355:ASN:OD1	3:Q:355:ASN:N	2.54	0.40
7:V:167:LEU:HD11	7:V:173:VAL:HB	2.04	0.40
7:Y:136:LEU:HD23	7:Y:136:LEU:HA	1.90	0.40
7:Y:680:LEU:HD21	7:Y:864:ILE:CD1	2.50	0.40
1:A:403:SER:O	1:A:403:SER:OG	2.39	0.40
2:K:136:LEU:HD12	2:K:136:LEU:HA	1.93	0.40
3:L:135:LYS:HE3	3:L:135:LYS:HB2	1.82	0.40
3:L:140:GLN:HG2	3:L:383:LEU:HD22	2.03	0.40
6:R:95:ILE:H	6:R:95:ILE:HG13	1.75	0.40
7:V:793:LEU:O	7:V:797:VAL:HG22	2.21	0.40
7:Y:154:LEU:O	7:Y:158:LEU:HG	2.21	0.40
7:Z:487:ILE:HG23	7:Z:650:ILE:HG21	2.03	0.40
2:K:274:VAL:HG23	2:K:275:LEU:HD23	2.02	0.40
9:V:1001:CLR:H242	9:V:1001:CLR:C16	2.52	0.40
7:Y:120:LEU:HB2	7:Y:245:VAL:HG22	2.04	0.40
3:L:115:MET:HG2	3:Q:244:TYR:CE2	2.57	0.40
4:X:351:PRO:HA	4:X:363:CYS:HA	2.02	0.40
7:V:808:ARG:NH1	7:V:840:GLN:OE1	2.44	0.40
7:Z:128:LEU:C	7:Z:128:LEU:HD23	2.42	0.40
7:Z:151:GLU:O	7:Z:152:GLU:C	2.59	0.40
7:Z:389:ARG:HA	7:Z:389:ARG:HD2	1.88	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	792/1881 (42%)	772 (98%)	18 (2%)	2 (0%)	41	61
2	K	370/417 (89%)	362 (98%)	8 (2%)	0	100	100
3	L	384/409 (94%)	380 (99%)	4 (1%)	0	100	100
3	Q	386/409 (94%)	380 (98%)	4 (1%)	2 (0%)	29	48
4	X	648/691 (94%)	639 (99%)	8 (1%)	1 (0%)	47	69
5	P	31/91 (34%)	31 (100%)	0	0	100	100
6	R	34/150 (23%)	31 (91%)	2 (6%)	1 (3%)	4	7
6	S	31/150 (21%)	31 (100%)	0	0	100	100
6	T	35/150 (23%)	32 (91%)	1 (3%)	2 (6%)	1	2
6	a	35/150 (23%)	35 (100%)	0	0	100	100
6	b	36/150 (24%)	36 (100%)	0	0	100	100
6	c	31/150 (21%)	31 (100%)	0	0	100	100
7	V	800/911 (88%)	789 (99%)	11 (1%)	0	100	100
7	Y	776/911 (85%)	754 (97%)	20 (3%)	2 (0%)	41	61
7	Z	776/911 (85%)	761 (98%)	14 (2%)	1 (0%)	51	75
7	e	796/911 (87%)	765 (96%)	25 (3%)	6 (1%)	19	36
7	f	794/911 (87%)	766 (96%)	27 (3%)	1 (0%)	51	75
7	g	822/911 (90%)	792 (96%)	26 (3%)	4 (0%)	29	48
All	All	7577/10264 (74%)	7387 (98%)	168 (2%)	22 (0%)	44	61

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	e	873	LEU
7	e	874	LEU
7	f	181	SER
1	A	437	VAL

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Mol	Chain	Res	Type
7	e	376	GLY
7	Y	194	SER
7	g	185	SER
4	X	124	SER
7	e	83	GLN
7	e	433	ASN
6	T	84	ALA
6	T	86	HIS
7	Z	816	PRO
7	g	67	ASP
1	A	435	VAL
3	Q	353	ALA
6	R	100	MET
7	e	872	VAL
7	Y	816	PRO
7	g	167	LEU
7	g	184	PRO
3	Q	292	HIS

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	643/1594 (40%)	606 (94%)	37 (6%)	20	35
2	K	317/348 (91%)	299 (94%)	18 (6%)	20	36
3	L	307/328 (94%)	302 (98%)	5 (2%)	62	78
3	Q	308/328 (94%)	296 (96%)	12 (4%)	32	53
4	X	558/588 (95%)	536 (96%)	22 (4%)	32	53
5	P	28/81 (35%)	23 (82%)	5 (18%)	2	2
6	R	29/136 (21%)	27 (93%)	2 (7%)	15	27
6	S	27/136 (20%)	26 (96%)	1 (4%)	34	54
6	T	30/136 (22%)	28 (93%)	2 (7%)	16	29
6	a	30/136 (22%)	28 (93%)	2 (7%)	16	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	b	30/136 (22%)	28 (93%)	2 (7%)	16	29
6	c	27/136 (20%)	25 (93%)	2 (7%)	13	24
7	V	692/786 (88%)	657 (95%)	35 (5%)	24	41
7	Y	679/786 (86%)	631 (93%)	48 (7%)	14	26
7	Z	679/786 (86%)	649 (96%)	30 (4%)	28	47
7	e	689/786 (88%)	638 (93%)	51 (7%)	13	24
7	f	689/786 (88%)	644 (94%)	45 (6%)	17	30
7	g	710/786 (90%)	657 (92%)	53 (8%)	13	24
All	All	6472/8799 (74%)	6100 (94%)	372 (6%)	24	36

All (372) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ARG
1	A	67	LYS
1	A	145	PHE
1	A	182	ARG
1	A	187	ARG
1	A	194	GLN
1	A	205	THR
1	A	266	GLU
1	A	270	LYS
1	A	320	CYS
1	A	332	ASP
1	A	360	LYS
1	A	381	LYS
1	A	396	SER
1	A	403	SER
1	A	422	ASN
1	A	432	VAL
1	A	434	ASN
1	A	435	VAL
1	A	436	LYS
1	A	446	ARG
1	A	451	GLU
1	A	460	LYS
1	A	468	LYS
1	A	470	ASP
1	A	471	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	472	THR
1	A	509	ILE
1	A	525	LYS
1	A	550	ARG
1	A	597	SER
1	A	667	SER
1	A	688	ILE
1	A	695	ASP
1	A	716	LEU
1	A	736	SER
1	A	749	ILE
2	K	2	SER
2	K	7	ARG
2	K	20	LEU
2	K	26	LEU
2	K	33	HIS
2	K	42	LYS
2	K	68	ASN
2	K	153	LEU
2	K	200	GLN
2	K	230	SER
2	K	235	LYS
2	K	248	SER
2	K	262	GLN
2	K	267	MET
2	K	311	CYS
2	K	330	SER
2	K	343	TYR
2	K	391	LYS
3	L	69	MET
3	L	222	TRP
3	L	269	MET
3	L	323	ARG
3	L	407	LYS
3	Q	1	MET
3	Q	2	ARG
3	Q	109	ASN
3	Q	119	ASP
3	Q	192	SER
3	Q	196	LYS
3	Q	222	TRP
3	Q	264	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	Q	294	PHE
3	Q	326	ASP
3	Q	404	LYS
3	Q	409	ARG
4	X	24	LYS
4	X	83	SER
4	X	118	SER
4	X	151	ASN
4	X	200	LYS
4	X	265	ASP
4	X	281	CYS
4	X	392	SER
4	X	401	ASP
4	X	407	THR
4	X	430	ASP
4	X	445	LYS
4	X	501	SER
4	X	508	GLN
4	X	530	LYS
4	X	533	LEU
4	X	541	LYS
4	X	555	ASN
4	X	611	GLN
4	X	643	TRP
4	X	645	GLU
4	X	649	CYS
5	P	62	VAL
5	P	63	ILE
5	P	80	LEU
5	P	83	TYR
5	P	87	ARG
6	R	91	GLU
6	R	96	ILE
6	a	86	HIS
6	a	87	PHE
7	V	66	MET
7	V	100	SER
7	V	114	PHE
7	V	126	THR
7	V	137	ASP
7	V	155	ARG
7	V	174	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	V	194	SER
7	V	265	LEU
7	V	289	MET
7	V	330	GLN
7	V	334	SER
7	V	338	VAL
7	V	339	GLN
7	V	340	ARG
7	V	345	ARG
7	V	411	PHE
7	V	473	GLU
7	V	482	ASN
7	V	514	ARG
7	V	569	ASN
7	V	592	LYS
7	V	607	ASP
7	V	639	LYS
7	V	656	ARG
7	V	721	MET
7	V	723	TRP
7	V	773	SER
7	V	782	ARG
7	V	807	ASP
7	V	812	LEU
7	V	814	LYS
7	V	833	MET
7	V	871	ARG
7	V	889	ASP
7	e	63	GLU
7	e	68	GLU
7	e	77	GLU
7	e	96	ARG
7	e	99	LEU
7	e	114	PHE
7	e	116	LYS
7	e	134	GLN
7	e	139	PHE
7	e	149	ASP
7	e	202	GLU
7	e	219	LYS
7	e	223	ASP
7	e	237	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	e	239	GLN
7	e	372	LEU
7	e	378	LEU
7	e	396	ASP
7	e	411	PHE
7	e	426	LEU
7	e	432	ARG
7	e	435	MET
7	e	438	SER
7	e	440	LEU
7	e	462	VAL
7	e	484	LEU
7	e	487	ILE
7	e	495	PHE
7	e	510	SER
7	e	511	PHE
7	e	538	SER
7	e	560	VAL
7	e	589	ARG
7	e	592	LYS
7	e	594	SER
7	e	607	ASP
7	e	643	SER
7	e	646	ARG
7	e	661	ILE
7	e	730	ARG
7	e	759	GLN
7	e	821	ASP
7	e	822	VAL
7	e	833	MET
7	e	856	SER
7	e	865	LEU
7	e	869	LEU
7	e	870	ARG
7	e	871	ARG
7	e	874	LEU
7	e	879	ARG
6	S	100	MET
6	b	82	GLN
6	b	112	TYR
7	Y	74	ARG
7	Y	114	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	Y	116	LYS
7	Y	138	ARG
7	Y	139	PHE
7	Y	148	GLN
7	Y	217	LEU
7	Y	224	SER
7	Y	233	ARG
7	Y	235	ASP
7	Y	291	GLU
7	Y	308	LEU
7	Y	310	SER
7	Y	372	LEU
7	Y	377	GLN
7	Y	388	ARG
7	Y	411	PHE
7	Y	419	PRO
7	Y	426	LEU
7	Y	430	LYS
7	Y	477	SER
7	Y	486	TYR
7	Y	495	PHE
7	Y	499	LEU
7	Y	505	VAL
7	Y	511	PHE
7	Y	514	ARG
7	Y	546	ASP
7	Y	584	PHE
7	Y	589	ARG
7	Y	600	LYS
7	Y	601	LEU
7	Y	603	ARG
7	Y	622	PHE
7	Y	633	SER
7	Y	639	LYS
7	Y	646	ARG
7	Y	663	MET
7	Y	722	PRO
7	Y	723	TRP
7	Y	774	ILE
7	Y	812	LEU
7	Y	817	LYS
7	Y	819	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	Y	851	LYS
7	Y	852	SER
7	Y	856	SER
7	Y	879	ARG
7	f	56	LYS
7	f	114	PHE
7	f	116	LYS
7	f	135	LEU
7	f	149	ASP
7	f	155	ARG
7	f	160	LYS
7	f	219	LYS
7	f	242	LEU
7	f	248	GLN
7	f	289	MET
7	f	292	ARG
7	f	411	PHE
7	f	426	LEU
7	f	477	SER
7	f	511	PHE
7	f	551	LYS
7	f	558	LEU
7	f	560	VAL
7	f	562	LYS
7	f	594	SER
7	f	600	LYS
7	f	601	LEU
7	f	621	ASP
7	f	628	TYR
7	f	634	VAL
7	f	646	ARG
7	f	658	GLU
7	f	661	ILE
7	f	662	TRP
7	f	663	MET
7	f	667	SER
7	f	683	GLN
7	f	704	LEU
7	f	741	MET
7	f	755	GLU
7	f	773	SER
7	f	811	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	f	814	LYS
7	f	817	LYS
7	f	828	VAL
7	f	829	LYS
7	f	831	TRP
7	f	833	MET
7	f	870	ARG
6	T	81	VAL
6	T	100	MET
6	c	94	LEU
6	c	112	TYR
7	Z	70	ASN
7	Z	74	ARG
7	Z	91	ASN
7	Z	106	SER
7	Z	108	LEU
7	Z	114	PHE
7	Z	116	LYS
7	Z	174	LYS
7	Z	217	LEU
7	Z	290	SER
7	Z	299	TYR
7	Z	330	GLN
7	Z	345	ARG
7	Z	433	ASN
7	Z	435	MET
7	Z	499	LEU
7	Z	511	PHE
7	Z	546	ASP
7	Z	602	ARG
7	Z	603	ARG
7	Z	604	VAL
7	Z	646	ARG
7	Z	655	LEU
7	Z	656	ARG
7	Z	658	GLU
7	Z	723	TRP
7	Z	775	LEU
7	Z	814	LYS
7	Z	817	LYS
7	Z	827	ARG
7	g	11	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	g	23	ASP
7	g	66	MET
7	g	67	ASP
7	g	68	GLU
7	g	69	LYS
7	g	70	ASN
7	g	73	LEU
7	g	74	ARG
7	g	76	MET
7	g	83	GLN
7	g	114	PHE
7	g	119	VAL
7	g	149	ASP
7	g	155	ARG
7	g	166	GLU
7	g	167	LEU
7	g	168	GLU
7	g	173	VAL
7	g	180	ARG
7	g	185	SER
7	g	197	THR
7	g	202	GLU
7	g	235	ASP
7	g	266	PHE
7	g	344	ARG
7	g	345	ARG
7	g	385	ASP
7	g	387	ARG
7	g	399	ASP
7	g	411	PHE
7	g	462	VAL
7	g	485	GLU
7	g	495	PHE
7	g	511	PHE
7	g	514	ARG
7	g	542	LYS
7	g	594	SER
7	g	595	SER
7	g	600	LYS
7	g	602	ARG
7	g	607	ASP
7	g	644	SER

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Mol	Chain	Res	Type
7	g	646	ARG
7	g	673	LEU
7	g	681	GLU
7	g	700	SER
7	g	723	TRP
7	g	795	MET
7	g	814	LYS
7	g	817	LYS
7	g	826	LYS
7	g	829	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	A	442	HIS
1	A	458	GLN
1	A	459	ASN
2	K	200	GLN
2	K	405	GLN
3	L	102	GLN
7	V	148	GLN
7	V	630	GLN
7	Y	683	GLN
7	f	547	HIS
7	f	564	GLN
7	f	819	HIS
7	f	834	HIS
7	f	884	GLN
6	T	86	HIS
7	Z	433	ASN
7	g	62	GLN
7	g	457	GLN

### 5.3.3 RNA

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](#)

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
8	NAG	B	1	8,7	14,14,15	0.22	0	17,19,21	0.38	0
8	NAG	B	2	8	14,14,15	0.40	0	17,19,21	0.40	0
8	NAG	C	1	8,7	14,14,15	0.24	0	17,19,21	0.45	0
8	NAG	C	2	8	14,14,15	0.37	0	17,19,21	0.39	0
8	NAG	D	1	8,7	14,14,15	0.22	0	17,19,21	0.42	0
8	NAG	D	2	8	14,14,15	0.39	0	17,19,21	0.42	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
8	NAG	B	1	8,7	-	2/6/23/26	0/1/1/1
8	NAG	B	2	8	-	2/6/23/26	0/1/1/1
8	NAG	C	1	8,7	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	2/6/23/26	0/1/1/1
8	NAG	D	1	8,7	-	1/6/23/26	0/1/1/1
8	NAG	D	2	8	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

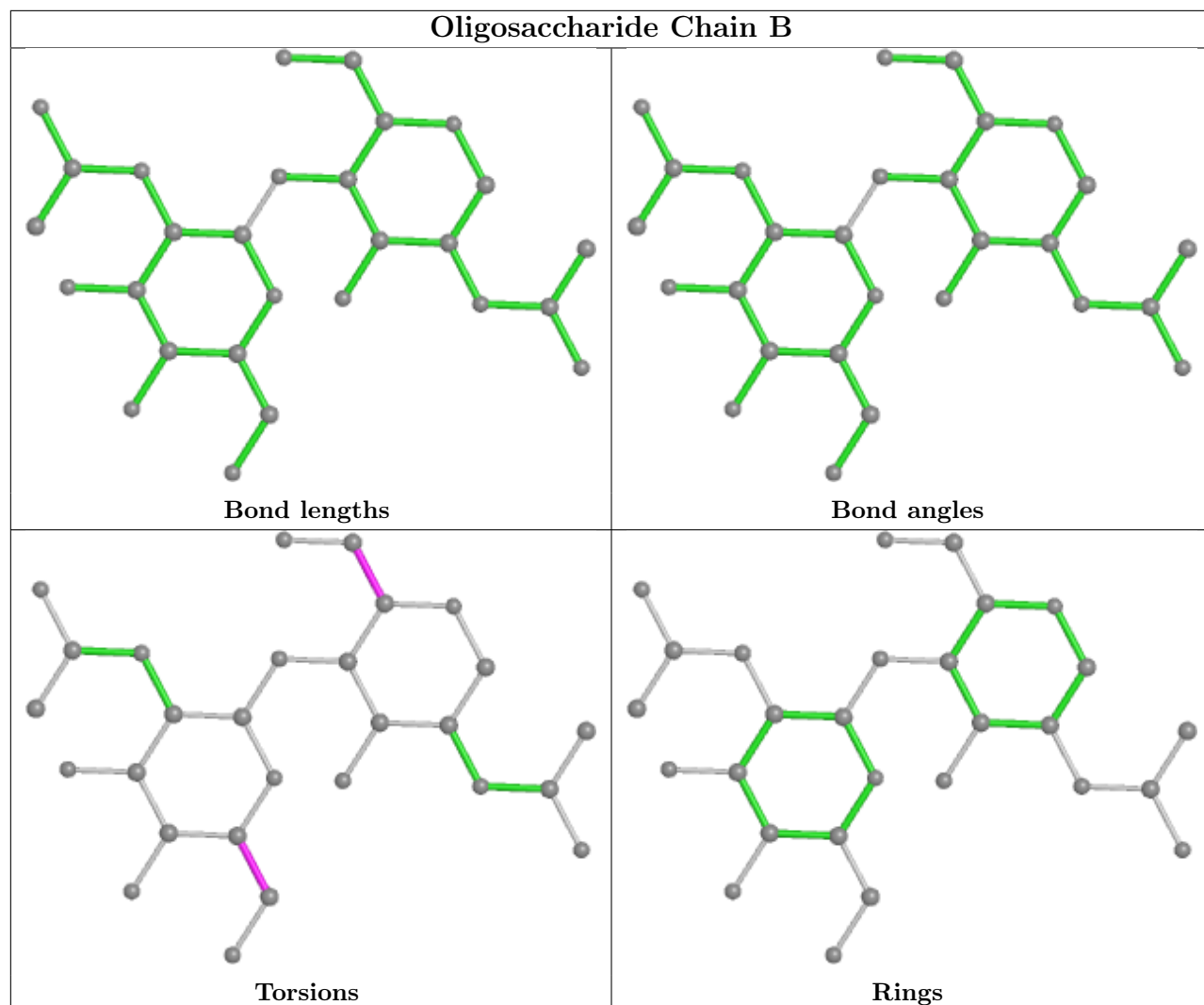
All (11) torsion outliers are listed below:

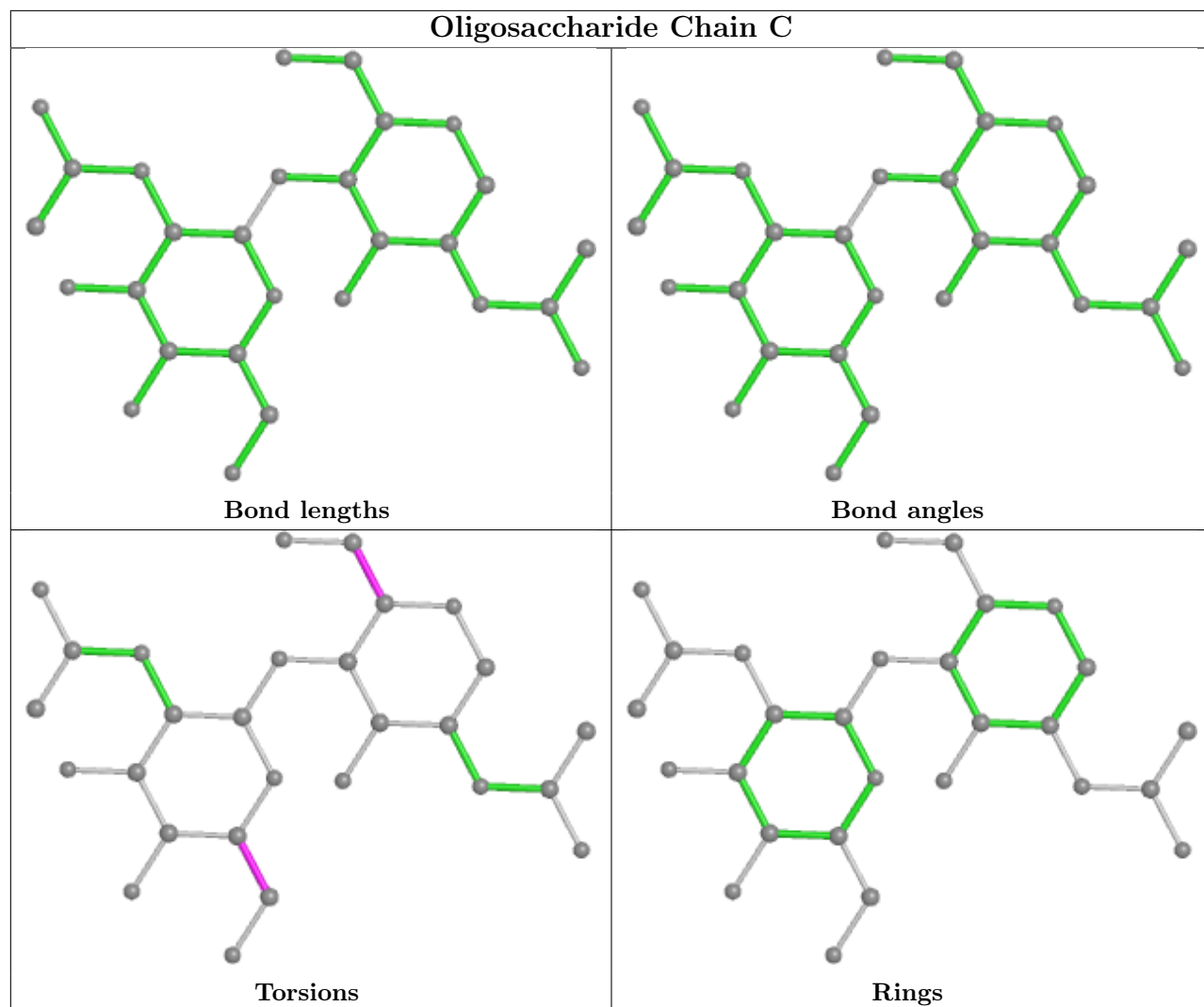
Mol	Chain	Res	Type	Atoms
8	B	1	NAG	O5-C5-C6-O6
8	B	1	NAG	C4-C5-C6-O6
8	D	2	NAG	C4-C5-C6-O6
8	C	1	NAG	O5-C5-C6-O6
8	C	1	NAG	C4-C5-C6-O6
8	B	2	NAG	C4-C5-C6-O6
8	C	2	NAG	C4-C5-C6-O6
8	D	2	NAG	O5-C5-C6-O6
8	B	2	NAG	O5-C5-C6-O6
8	C	2	NAG	O5-C5-C6-O6
8	D	1	NAG	O5-C5-C6-O6

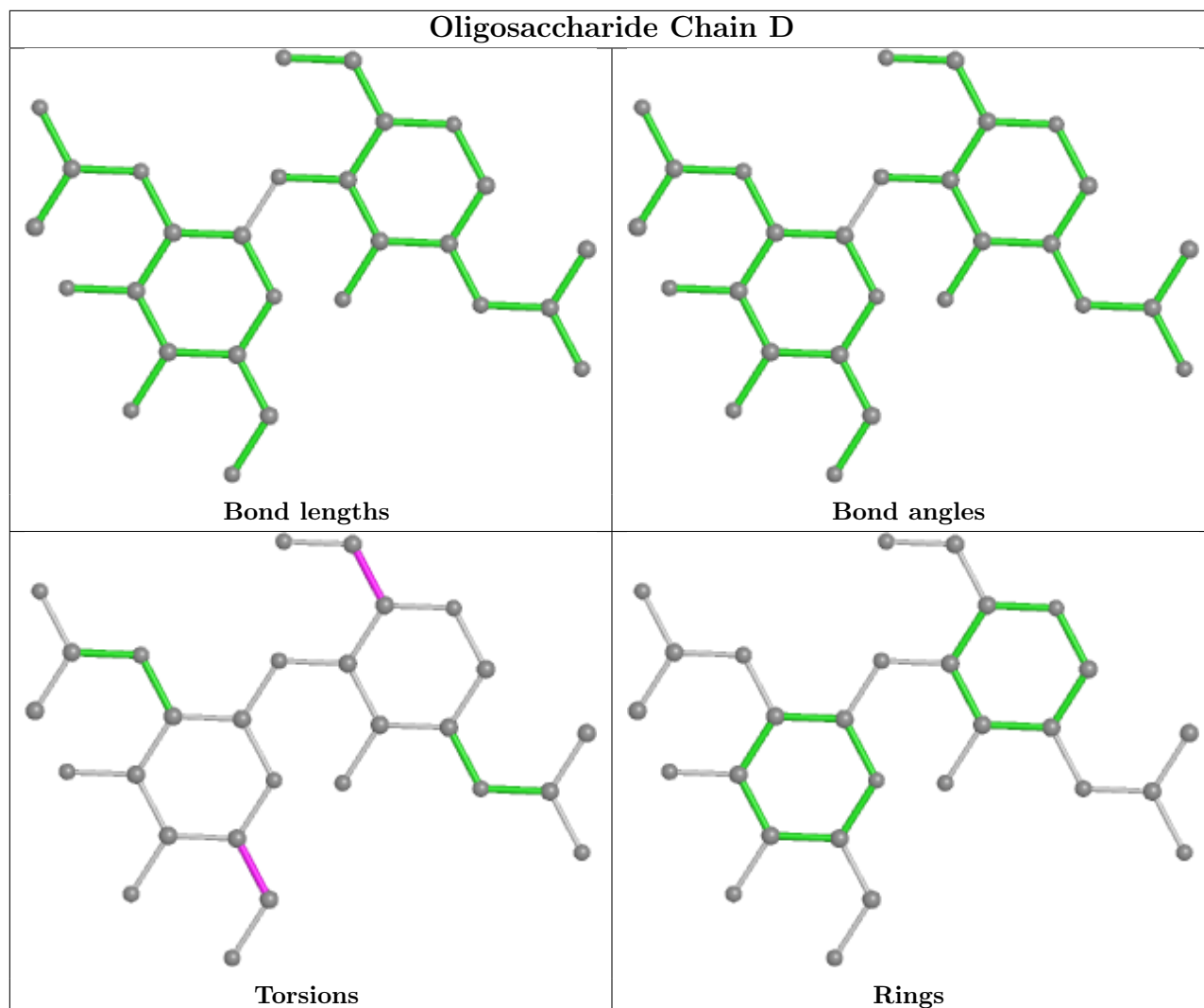
There are no ring outliers.

No monomer is involved in short contacts.

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](#)

21 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	$\# Z  > 2$
11	NAG	V	1003	11	14,14,15	0.38	0	17,19,21	0.37	0
9	CLR	Z	1001	-	31,31,31	0.28	0	48,48,48	0.37	0
11	NAG	Z	1003	11	14,14,15	0.43	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	AJP	Q	501	-	37,37,95	0.47	0	58,62,149	0.65	1 (1%)
9	CLR	V	1001	-	31,31,31	0.32	0	48,48,48	0.53	0
9	CLR	Y	1001	-	31,31,31	0.36	0	48,48,48	0.59	0
9	CLR	c	201	-	31,31,31	0.35	0	48,48,48	0.79	0
9	CLR	f	1001	-	31,31,31	0.28	0	48,48,48	0.49	0
11	NAG	Z	1002	11,7	14,14,15	0.21	0	17,19,21	0.43	0
9	CLR	e	1001	-	31,31,31	0.36	0	48,48,48	0.60	0
11	NAG	V	1002	11,7	14,14,15	0.24	0	17,19,21	0.41	0
12	PIO	Y	1004	-	47,47,47	0.50	0	61,65,65	0.43	0
11	NAG	Y	1003	11	14,14,15	0.37	0	17,19,21	0.38	0
12	PIO	g	1001	-	47,47,47	0.46	0	61,65,65	0.42	0
9	CLR	L	501	-	31,31,31	0.40	0	48,48,48	0.82	0
12	PIO	g	1002	-	47,47,47	0.43	0	61,65,65	0.48	0
12	PIO	e	1002	-	47,47,47	0.47	0	61,65,65	0.41	0
12	PIO	f	1002	-	47,47,47	0.48	0	61,65,65	0.41	0
12	PIO	V	1004	-	47,47,47	0.48	0	61,65,65	0.50	0
11	NAG	Y	1002	11,7	14,14,15	0.21	0	17,19,21	0.42	0
9	CLR	L	502	-	31,31,31	0.43	0	48,48,48	0.92	2 (4%)

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
11	NAG	V	1003	11	-	0/6/23/26	0/1/1/1
9	CLR	Z	1001	-	-	10/10/68/68	0/4/4/4
11	NAG	Z	1003	11	-	2/6/23/26	0/1/1/1
10	AJP	Q	501	-	-	-	0/6/6/11
9	CLR	V	1001	-	-	10/10/68/68	0/4/4/4
9	CLR	Y	1001	-	-	8/10/68/68	0/4/4/4
9	CLR	c	201	-	-	8/10/68/68	0/4/4/4
9	CLR	f	1001	-	-	8/10/68/68	0/4/4/4
11	NAG	Z	1002	11,7	-	2/6/23/26	0/1/1/1
9	CLR	e	1001	-	-	8/10/68/68	0/4/4/4
11	NAG	V	1002	11,7	-	0/6/23/26	0/1/1/1
12	PIO	Y	1004	-	-	14/44/68/68	0/1/1/1
11	NAG	Y	1003	11	-	2/6/23/26	0/1/1/1
12	PIO	g	1001	-	-	11/44/68/68	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CLR	L	501	-	-	5/10/68/68	0/4/4/4
12	PIO	g	1002	-	-	26/44/68/68	0/1/1/1
12	PIO	e	1002	-	-	27/44/68/68	0/1/1/1
12	PIO	f	1002	-	-	23/44/68/68	0/1/1/1
12	PIO	V	1004	-	-	19/44/68/68	0/1/1/1
11	NAG	Y	1002	11,7	-	2/6/23/26	0/1/1/1
9	CLR	L	502	-	-	7/10/68/68	0/4/4/4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	502	CLR	C16-C15-C14	-3.83	97.53	105.13
10	Q	501	AJP	C19-C24-C23	-2.90	111.26	114.46
9	L	502	CLR	C7-C8-C9	2.13	112.29	109.71

There are no chirality outliers.

All (192) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	V	1004	PIO	C1-O1-P1-O11
12	V	1004	PIO	C1-O1-P1-O12
12	V	1004	PIO	C4-C5-O5-P5
12	V	1004	PIO	C6-C5-O5-P5
12	V	1004	PIO	C2A-C1A-O2C-C2C
12	e	1002	PIO	C1C-O13-P1-O1
12	e	1002	PIO	C1C-O13-P1-O11
12	e	1002	PIO	C5-O5-P5-O53
12	e	1002	PIO	C2A-C1A-O2C-C2C
12	Y	1004	PIO	C1-O1-P1-O11
12	Y	1004	PIO	C5-O5-P5-O53
12	f	1002	PIO	C1-O1-P1-O11
12	f	1002	PIO	C1C-O13-P1-O11
12	f	1002	PIO	C1C-O13-P1-O12
12	f	1002	PIO	C4-C5-O5-P5
12	f	1002	PIO	C6-C5-O5-P5
12	g	1002	PIO	O1A-C1A-O2C-C2C
12	g	1002	PIO	C2A-C1A-O2C-C2C
12	g	1002	PIO	O2C-C2C-C3C-O3C

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Mol	Chain	Res	Type	Atoms
9	V	1001	CLR	C21-C20-C22-C23
9	V	1001	CLR	C16-C17-C20-C21
9	e	1001	CLR	C16-C17-C20-C21
9	V	1001	CLR	C13-C17-C20-C21
9	e	1001	CLR	C13-C17-C20-C21
9	V	1001	CLR	C13-C17-C20-C22
12	V	1004	PIO	O1A-C1A-O2C-C2C
12	e	1002	PIO	O1A-C1A-O2C-C2C
12	e	1002	PIO	C2B-C1B-O3C-C3C
9	e	1001	CLR	C21-C20-C22-C23
9	Y	1001	CLR	C21-C20-C22-C23
9	f	1001	CLR	C21-C20-C22-C23
9	c	201	CLR	C21-C20-C22-C23
9	Y	1001	CLR	C16-C17-C20-C21
9	c	201	CLR	C16-C17-C20-C21
9	V	1001	CLR	C16-C17-C20-C22
9	e	1001	CLR	C13-C17-C20-C22
11	Y	1003	NAG	C4-C5-C6-O6
12	e	1002	PIO	O1B-C1B-O3C-C3C
9	Z	1001	CLR	C16-C17-C20-C21
9	e	1001	CLR	C16-C17-C20-C22
9	L	501	CLR	C17-C20-C22-C23
9	Z	1001	CLR	C21-C20-C22-C23
9	Y	1001	CLR	C17-C20-C22-C23
9	L	501	CLR	C21-C20-C22-C23
9	Y	1001	CLR	C13-C17-C20-C21
9	c	201	CLR	C13-C17-C20-C21
12	Y	1004	PIO	C1A-C2A-C3A-C4A
9	e	1001	CLR	C17-C20-C22-C23
9	f	1001	CLR	C17-C20-C22-C23
9	c	201	CLR	C17-C20-C22-C23
12	g	1002	PIO	C2B-C1B-O3C-C3C
12	e	1002	PIO	C1-O1-P1-O13
12	g	1002	PIO	C1-O1-P1-O13
9	Y	1001	CLR	C13-C17-C20-C22
9	c	201	CLR	C13-C17-C20-C22
9	Z	1001	CLR	C13-C17-C20-C22
11	Y	1003	NAG	O5-C5-C6-O6
9	Z	1001	CLR	C13-C17-C20-C21
9	Z	1001	CLR	C16-C17-C20-C22
9	f	1001	CLR	C13-C17-C20-C22
9	f	1001	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
9	c	201	CLR	C22-C23-C24-C25
9	V	1001	CLR	C17-C20-C22-C23
9	e	1001	CLR	C22-C23-C24-C25
9	f	1001	CLR	C16-C17-C20-C21
9	Y	1001	CLR	C16-C17-C20-C22
9	c	201	CLR	C16-C17-C20-C22
9	Z	1001	CLR	C17-C20-C22-C23
12	Y	1004	PIO	C1B-C2B-C3B-C4B
12	f	1002	PIO	C2A-C1A-O2C-C2C
12	g	1002	PIO	O1B-C1B-O3C-C3C
9	Y	1001	CLR	C20-C22-C23-C24
9	Y	1001	CLR	C22-C23-C24-C25
11	Z	1002	NAG	O5-C5-C6-O6
9	f	1001	CLR	C13-C17-C20-C21
12	e	1002	PIO	C1B-C2B-C3B-C4B
9	V	1001	CLR	C20-C22-C23-C24
9	f	1001	CLR	C22-C23-C24-C25
9	Z	1001	CLR	C22-C23-C24-C25
9	L	501	CLR	C22-C23-C24-C25
12	f	1002	PIO	C1C-O13-P1-O1
12	f	1002	PIO	C2B-C1B-O3C-C3C
9	c	201	CLR	C20-C22-C23-C24
12	f	1002	PIO	O1A-C1A-O2C-C2C
12	V	1004	PIO	C1-O1-P1-O13
12	Y	1004	PIO	C1-O1-P1-O13
12	f	1002	PIO	C1-O1-P1-O13
11	Z	1002	NAG	C4-C5-C6-O6
12	g	1001	PIO	C1A-C2A-C3A-C4A
12	f	1002	PIO	C3A-C4A-C5A-C6A
12	g	1001	PIO	C3A-C4A-C5A-C6A
12	g	1002	PIO	C1C-C2C-O2C-C1A
11	Y	1002	NAG	O5-C5-C6-O6
12	f	1002	PIO	C1B-C2B-C3B-C4B
12	Y	1004	PIO	C2B-C3B-C4B-C5B
9	e	1001	CLR	C20-C22-C23-C24
12	e	1002	PIO	C2B-C3B-C4B-C5B
12	e	1002	PIO	C3A-C4A-C5A-C6A
12	g	1001	PIO	C3B-C4B-C5B-C6B
12	g	1002	PIO	C4B-C5B-C6B-C7B
12	f	1002	PIO	C3B-C4B-C5B-C6B
12	f	1002	PIO	C2A-C3A-C4A-C5A
12	f	1002	PIO	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
12	f	1002	PIO	O1B-C1B-O3C-C3C
12	g	1002	PIO	C1A-C2A-C3A-C4A
12	g	1001	PIO	C5B-C6B-C7B-C8B
12	Y	1004	PIO	C5B-C6B-C7B-C8B
12	e	1002	PIO	C5B-C6B-C7B-C8B
12	f	1002	PIO	C2B-C3B-C4B-C5B
12	g	1002	PIO	C3A-C4A-C5A-C6A
12	Y	1004	PIO	O1A-C1A-O2C-C2C
12	Y	1004	PIO	C2A-C1A-O2C-C2C
12	Y	1004	PIO	O2C-C2C-C3C-O3C
12	g	1001	PIO	C2B-C3B-C4B-C5B
12	e	1002	PIO	O13-C1C-C2C-C3C
12	g	1001	PIO	C4A-C5A-C6A-C7A
12	g	1002	PIO	C1B-C2B-C3B-C4B
12	V	1004	PIO	C1A-C2A-C3A-C4A
12	g	1002	PIO	C1C-C2C-C3C-O3C
11	Z	1003	NAG	C4-C5-C6-O6
12	g	1002	PIO	C5B-C6B-C7B-C8B
12	V	1004	PIO	C5A-C6A-C7A-C8A
12	V	1004	PIO	C4A-C5A-C6A-C7A
12	e	1002	PIO	C2C-C1C-O13-P1
12	Y	1004	PIO	C1C-C2C-C3C-O3C
12	e	1002	PIO	C1-O1-P1-O12
12	Y	1004	PIO	C1-O1-P1-O12
12	f	1002	PIO	C1-O1-P1-O12
12	g	1002	PIO	C1-O1-P1-O12
12	g	1002	PIO	C5A-C6A-C7A-C8A
9	L	502	CLR	C20-C22-C23-C24
12	g	1002	PIO	O13-C1C-C2C-C3C
12	e	1002	PIO	C2A-C3A-C4A-C5A
9	Z	1001	CLR	C20-C22-C23-C24
12	f	1002	PIO	C5-O5-P5-O53
12	e	1002	PIO	C3C-C2C-O2C-C1A
12	f	1002	PIO	C2C-C1C-O13-P1
12	g	1001	PIO	C2C-C1C-O13-P1
12	e	1002	PIO	O13-C1C-C2C-O2C
12	g	1002	PIO	O13-C1C-C2C-O2C
11	Z	1003	NAG	O5-C5-C6-O6
12	Y	1004	PIO	C5-O5-P5-O51
12	e	1002	PIO	C1A-C2A-C3A-C4A
12	V	1004	PIO	C1C-O13-P1-O1
12	e	1002	PIO	C1C-O13-P1-O12

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Mol	Chain	Res	Type	Atoms
9	V	1001	CLR	C23-C24-C25-C27
9	L	502	CLR	C16-C17-C20-C22
9	f	1001	CLR	C16-C17-C20-C22
9	V	1001	CLR	C22-C23-C24-C25
12	g	1002	PIO	C2B-C3B-C4B-C5B
12	V	1004	PIO	C1C-C2C-O2C-C1A
12	g	1001	PIO	O2C-C2C-C3C-O3C
9	Z	1001	CLR	C23-C24-C25-C27
9	V	1001	CLR	C23-C24-C25-C26
12	g	1001	PIO	C5A-C6A-C7A-C8A
9	L	502	CLR	C16-C17-C20-C21
12	e	1002	PIO	C4A-C5A-C6A-C7A
9	L	501	CLR	C16-C17-C20-C22
11	Y	1002	NAG	C4-C5-C6-O6
12	e	1002	PIO	C5A-C6A-C7A-C8A
9	L	502	CLR	C13-C17-C20-C21
12	g	1002	PIO	C4A-C5A-C6A-C7A
12	V	1004	PIO	C2C-C3C-O3C-C1B
12	e	1002	PIO	C3-C4-O4-P4
12	g	1002	PIO	C3-C4-O4-P4
9	L	502	CLR	C13-C17-C20-C22
12	V	1004	PIO	O2C-C2C-C3C-O3C
12	V	1004	PIO	C5-O5-P5-O53
9	L	501	CLR	C13-C17-C20-C21
12	f	1002	PIO	C5B-C6B-C7B-C8B
12	e	1002	PIO	O3C-C1B-C2B-C3B
12	e	1002	PIO	O2C-C2C-C3C-O3C
12	g	1002	PIO	O3C-C1B-C2B-C3B
12	V	1004	PIO	C5-O5-P5-O51
12	e	1002	PIO	C4-O4-P4-O43
12	Y	1004	PIO	C3-C4-O4-P4
12	g	1002	PIO	C4-O4-P4-O43
12	g	1002	PIO	C5-O5-P5-O51
9	Z	1001	CLR	C23-C24-C25-C26
12	V	1004	PIO	O2C-C1A-C2A-C3A
12	f	1002	PIO	O2C-C1A-C2A-C3A
12	g	1002	PIO	O2C-C1A-C2A-C3A
9	L	502	CLR	C22-C23-C24-C25
12	g	1001	PIO	C1C-C2C-C3C-O3C
12	f	1002	PIO	O1A-C1A-C2A-C3A
9	L	502	CLR	C21-C20-C22-C23
12	e	1002	PIO	O1B-C1B-C2B-C3B

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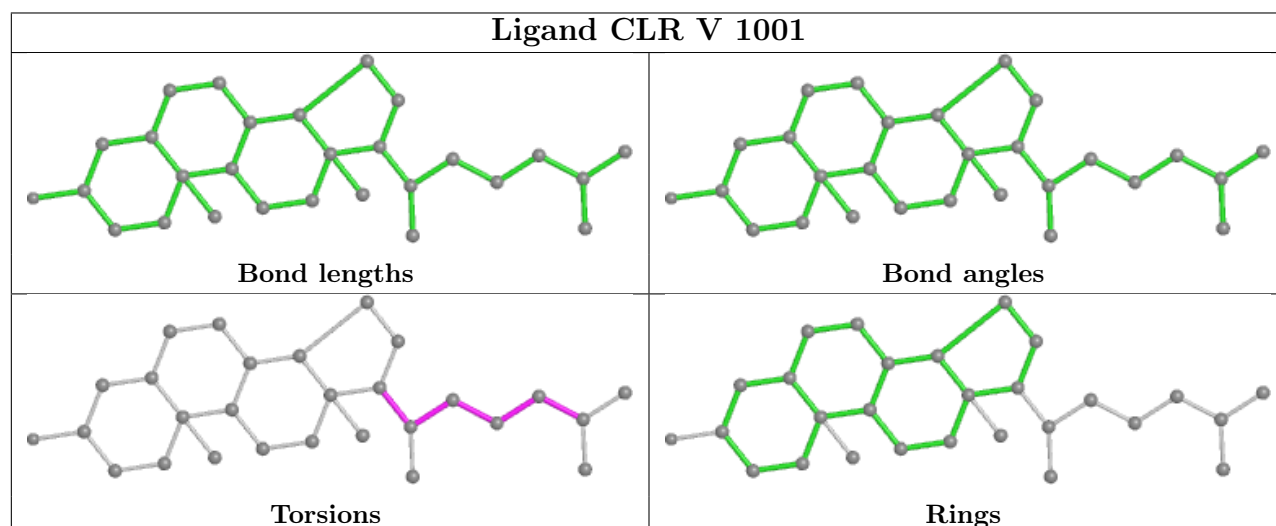
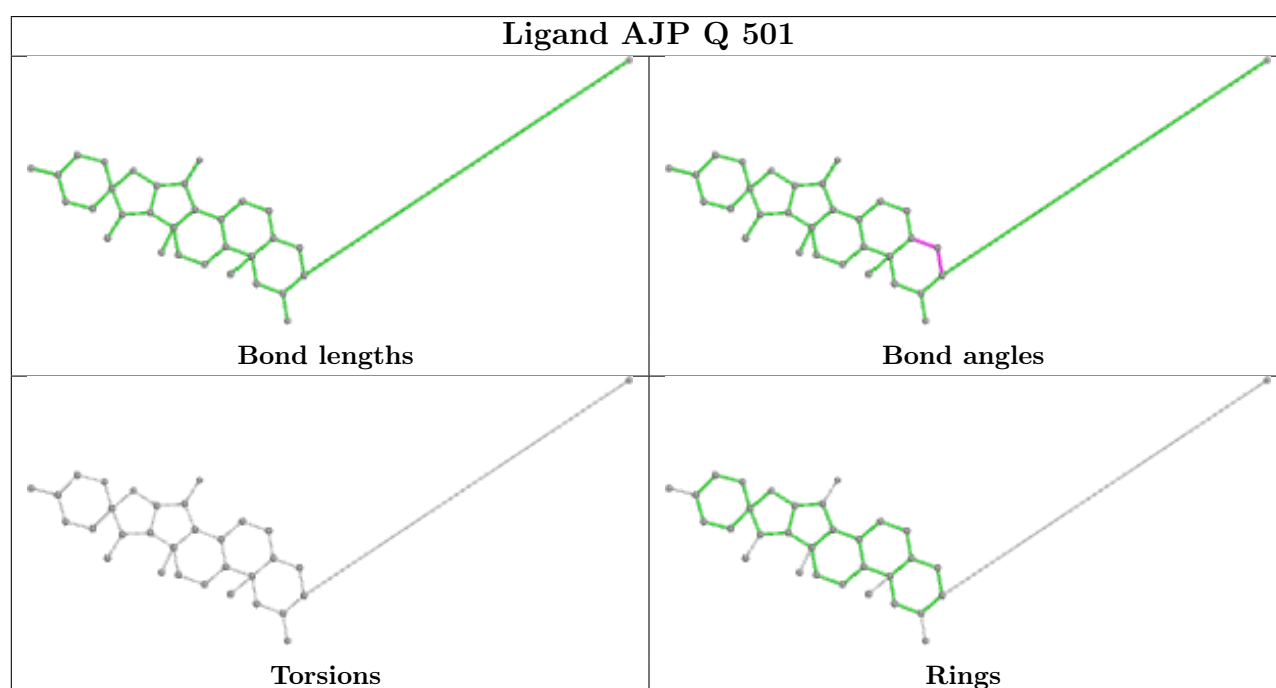
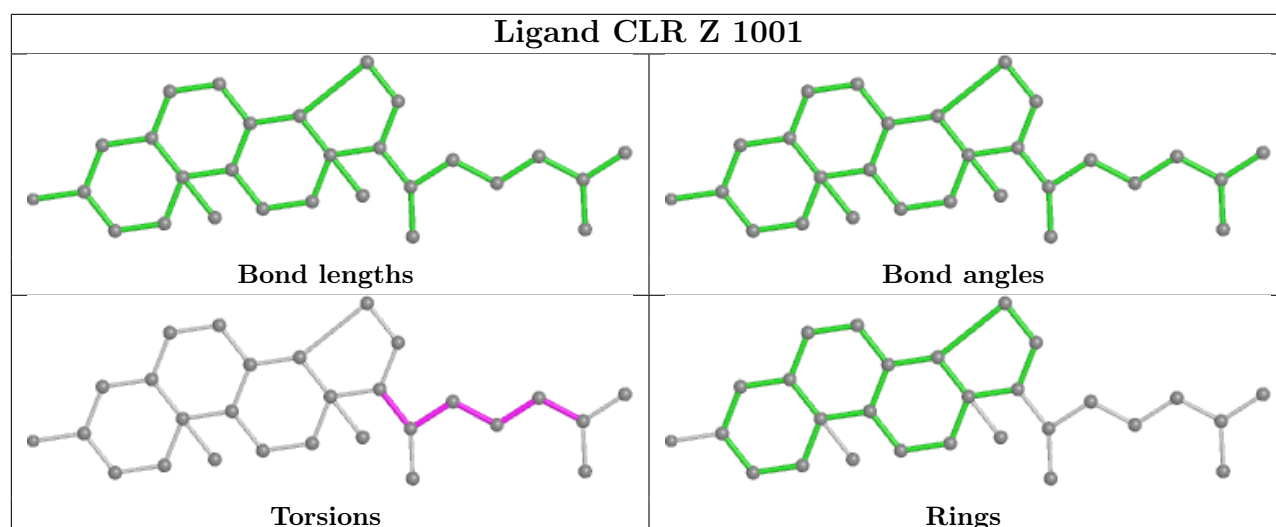
Mol	Chain	Res	Type	Atoms
12	V	1004	PIO	O1A-C1A-C2A-C3A
12	g	1002	PIO	O1A-C1A-C2A-C3A
12	g	1001	PIO	O2C-C1A-C2A-C3A
12	g	1002	PIO	O1B-C1B-C2B-C3B
12	V	1004	PIO	O3C-C1B-C2B-C3B

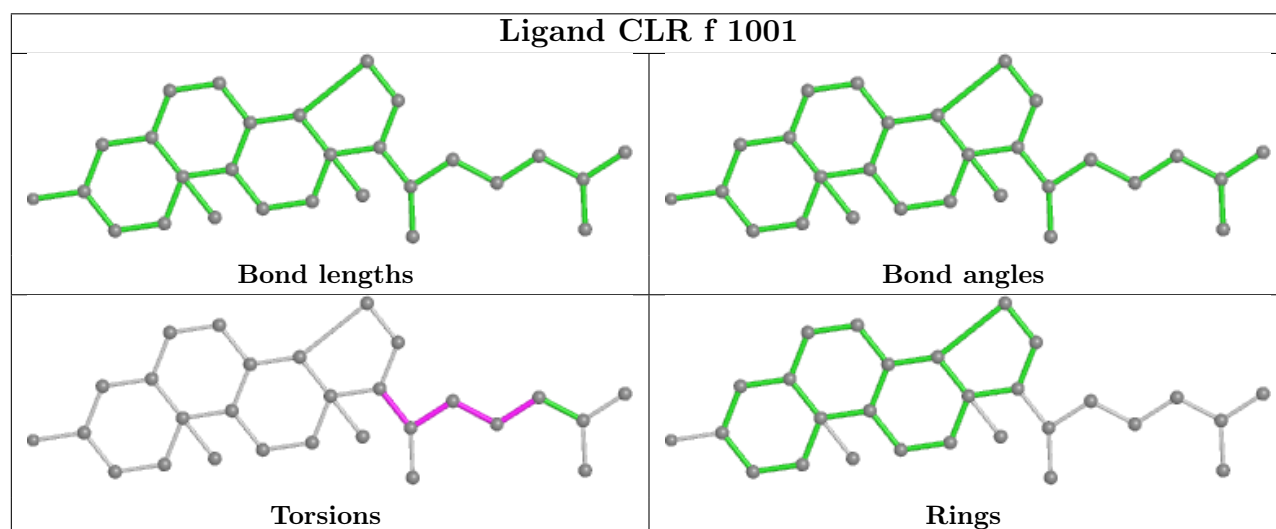
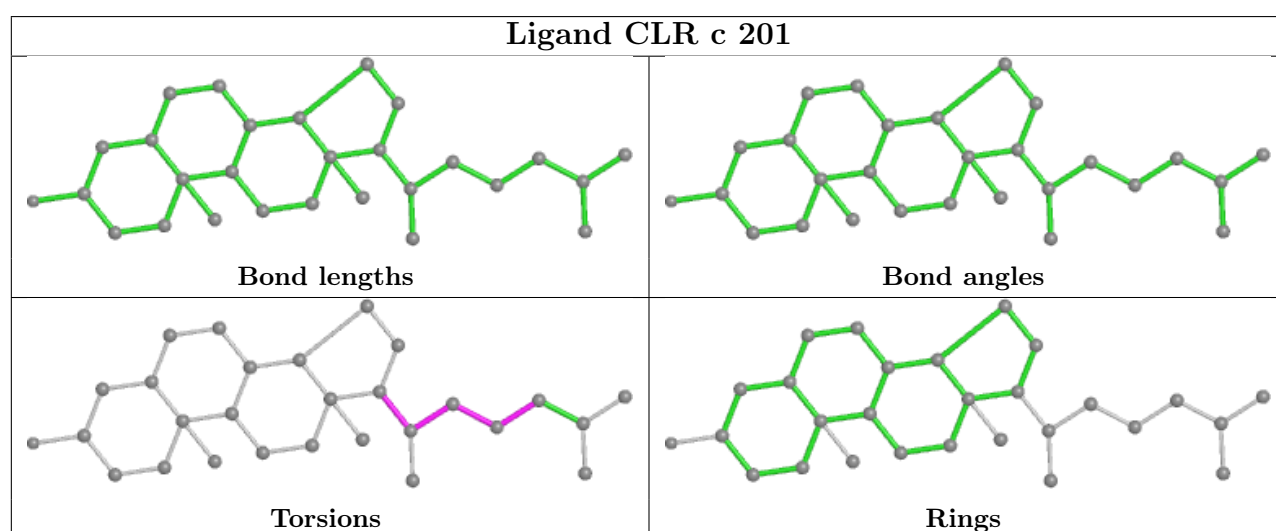
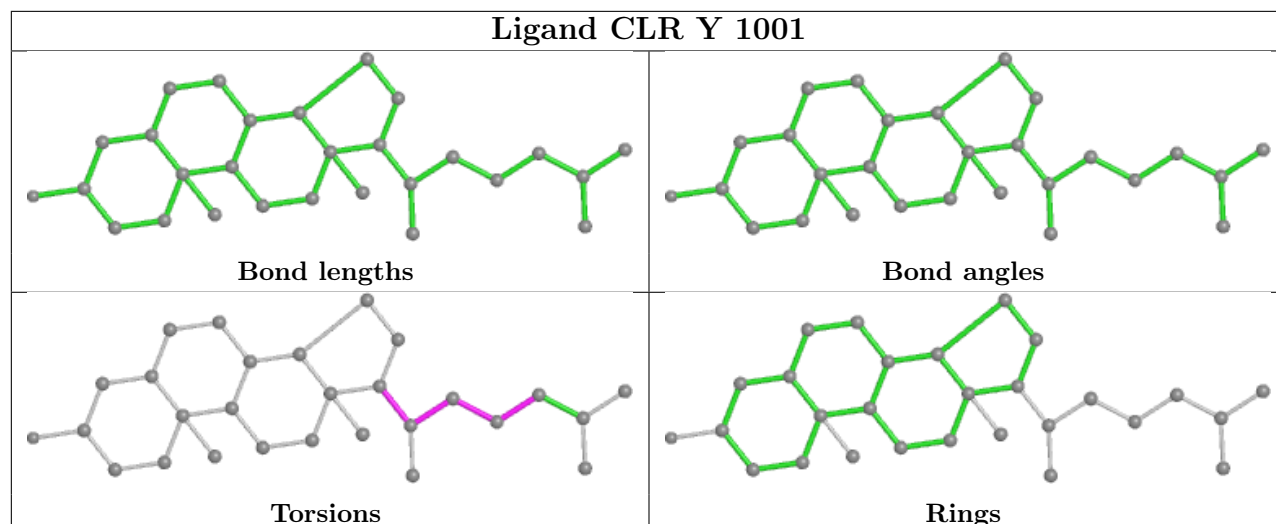
There are no ring outliers.

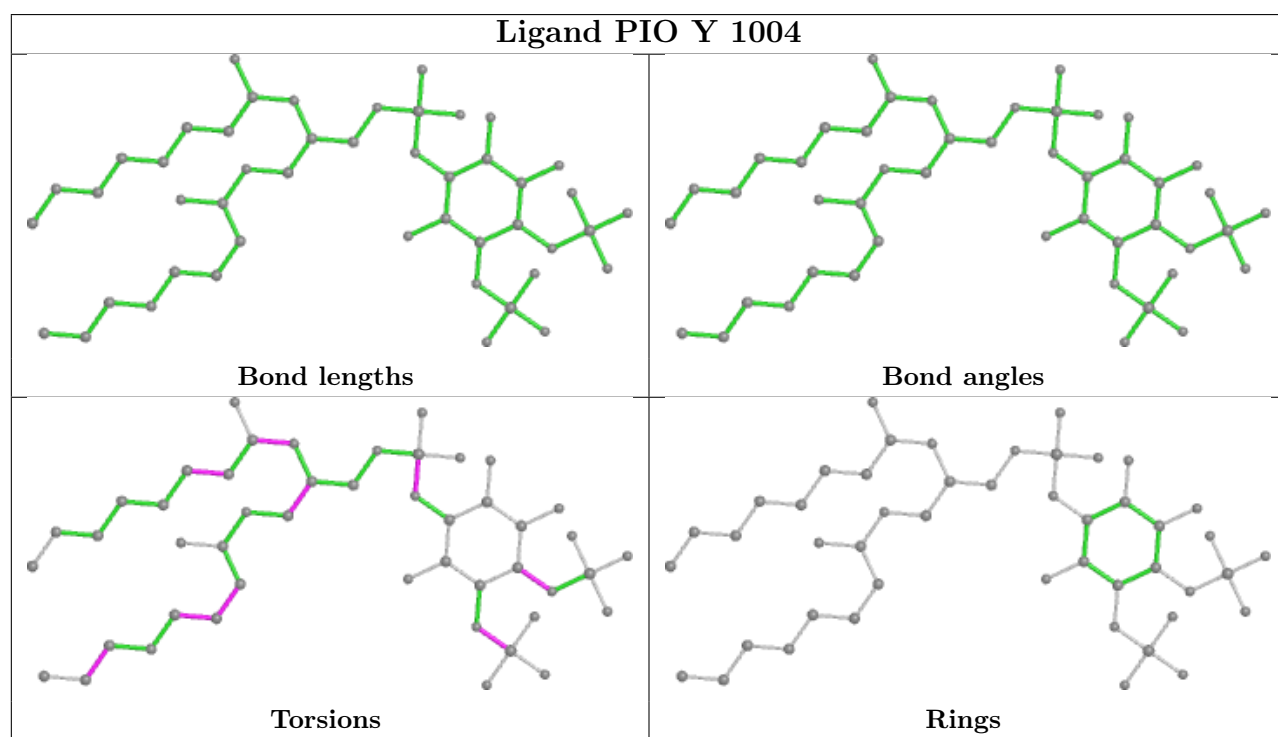
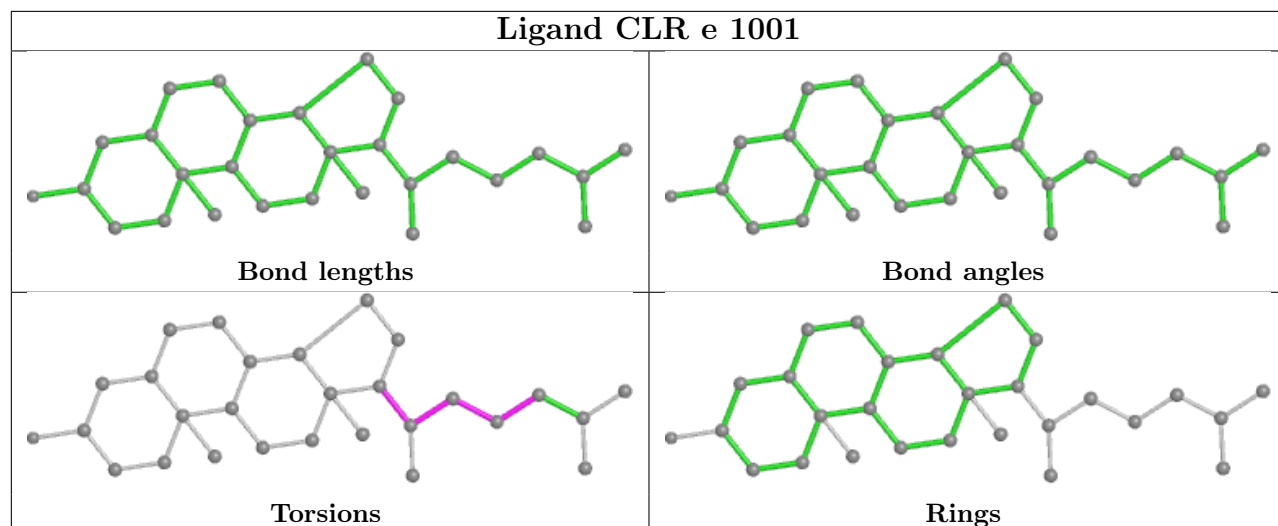
8 monomers are involved in 25 short contacts:

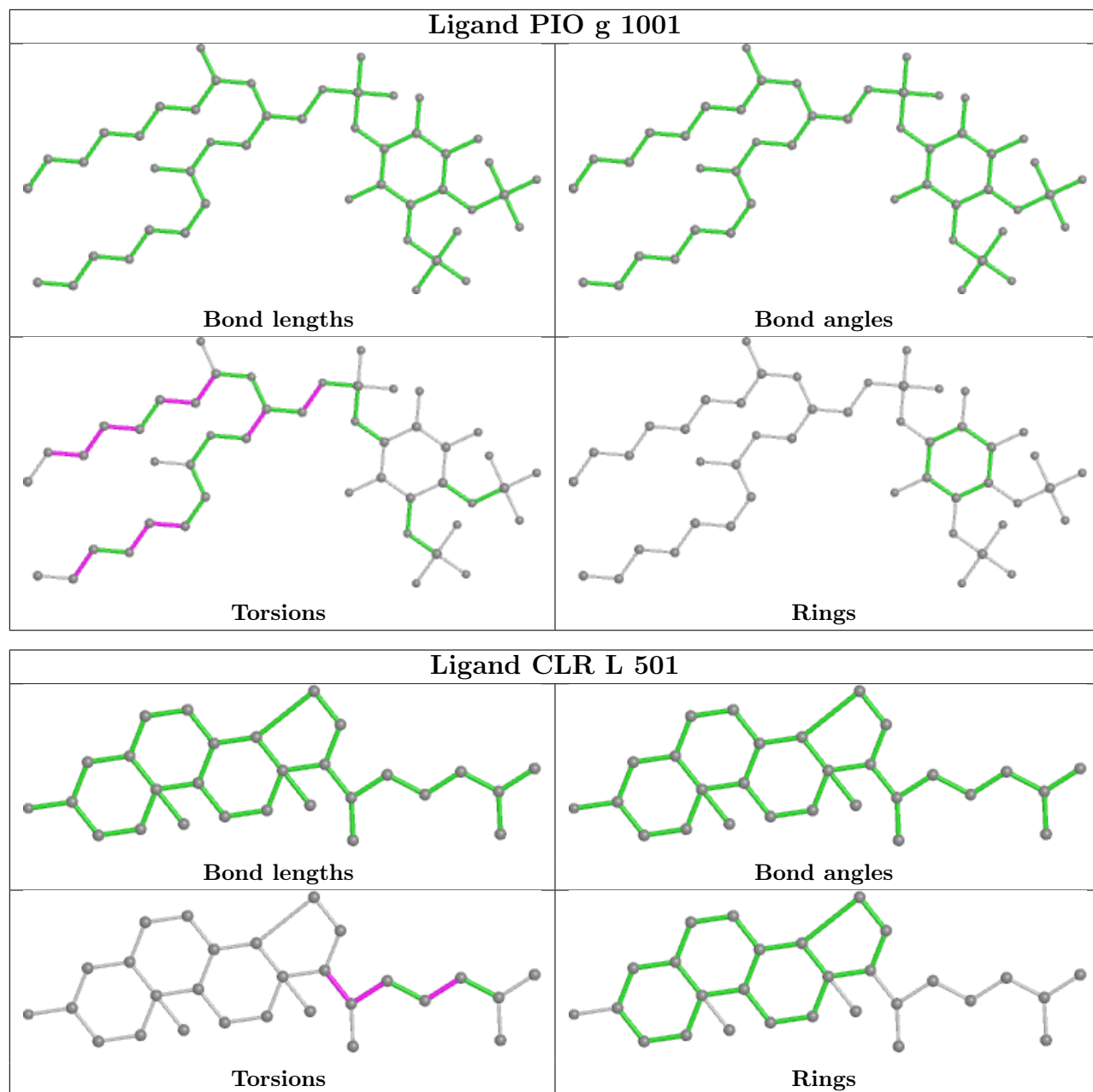
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Z	1001	CLR	4	0
10	Q	501	AJP	1	0
9	V	1001	CLR	9	0
9	Y	1001	CLR	1	0
12	Y	1004	PIO	3	0
9	L	501	CLR	1	0
12	V	1004	PIO	3	0
9	L	502	CLR	3	0

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.

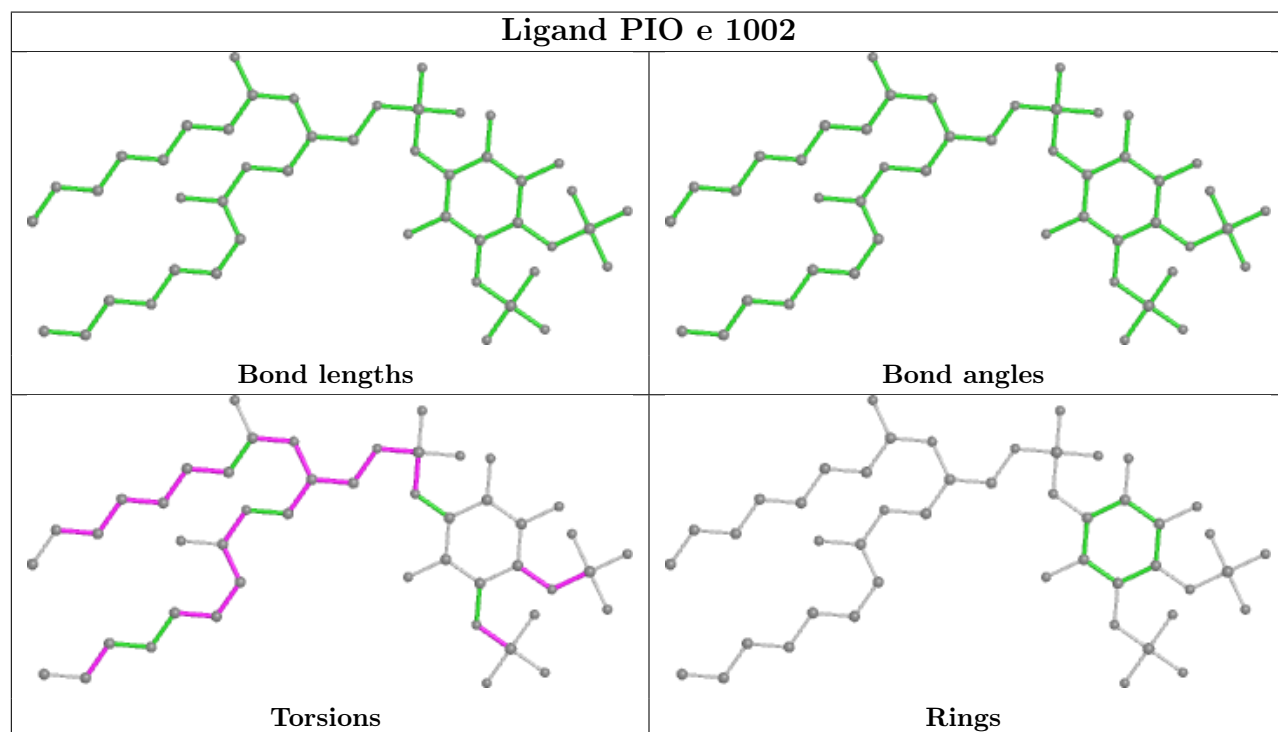
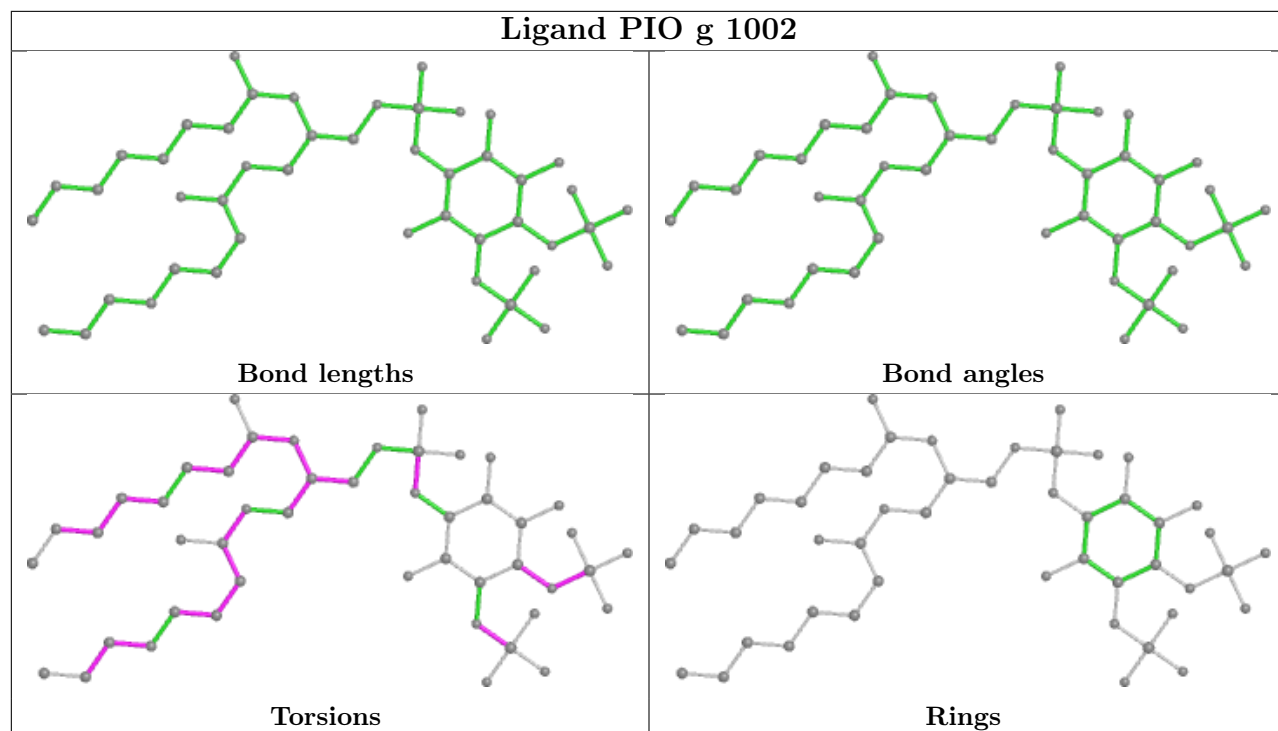


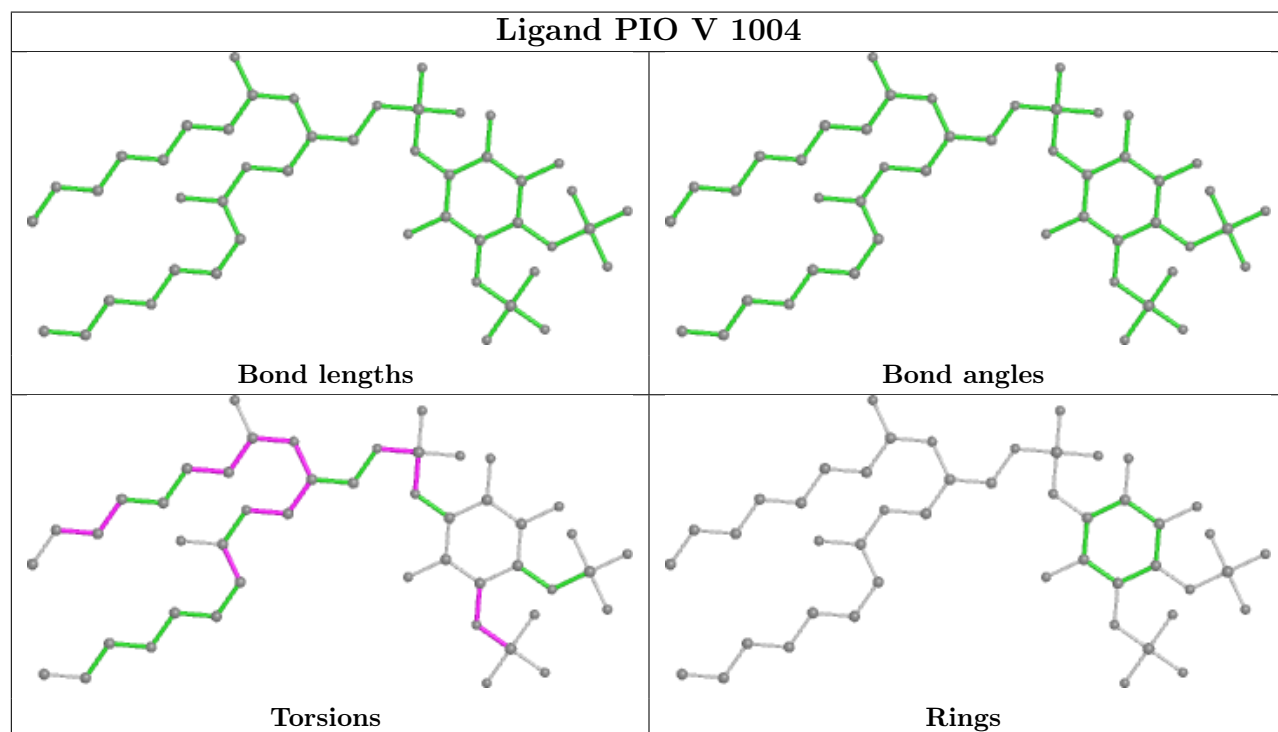
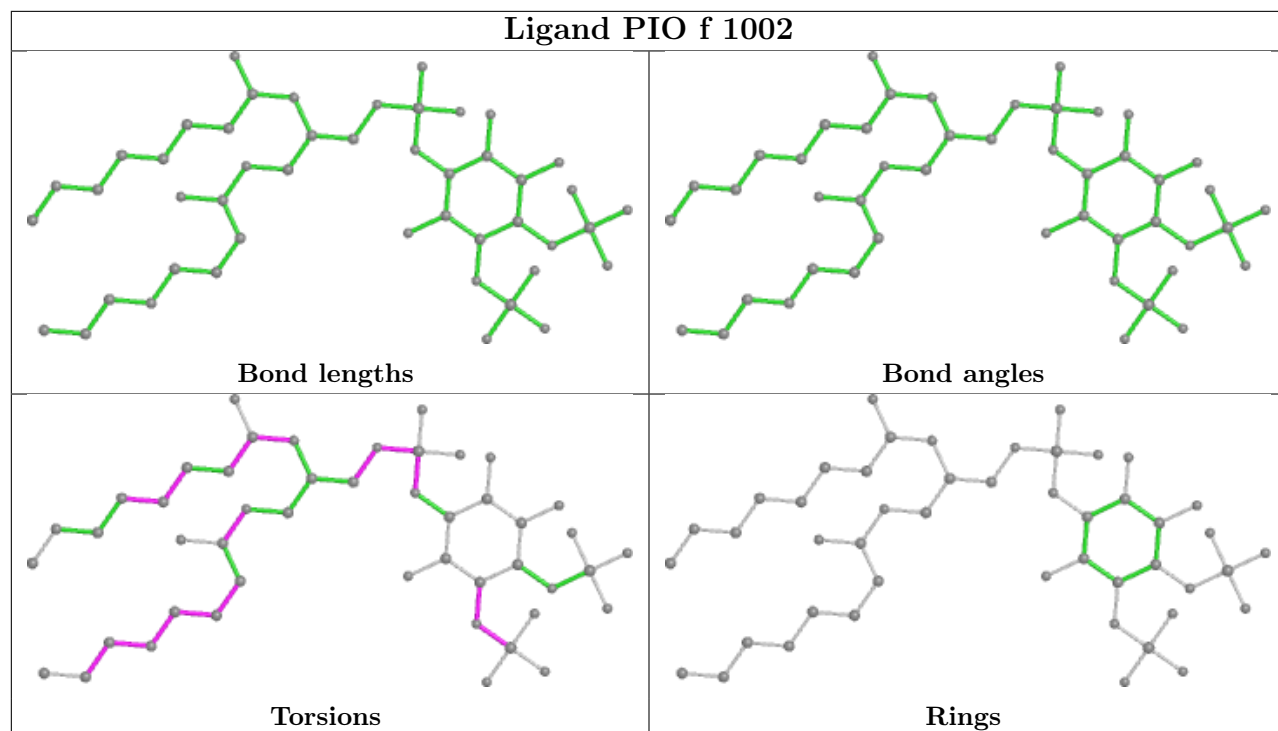


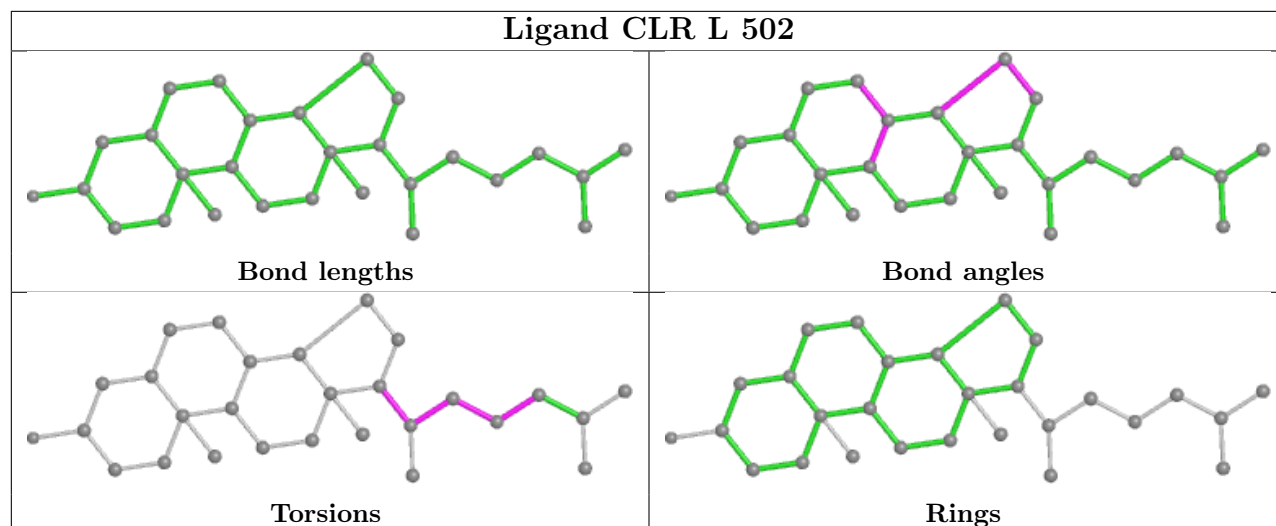












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

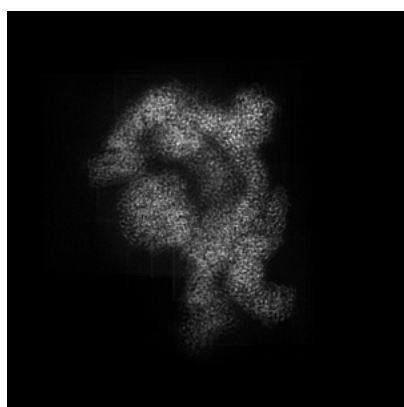
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26960. These allow visual inspection of the internal detail of the map and identification of artifacts.

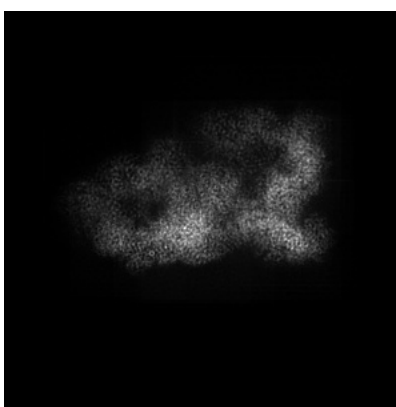
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

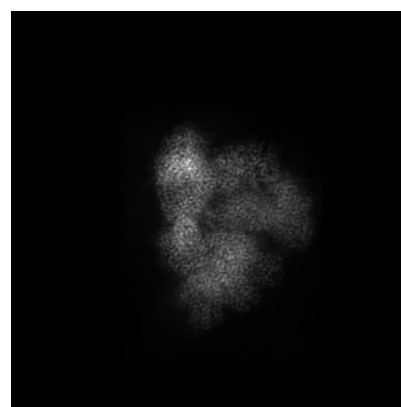
#### 6.1.1 Primary map



X



Y

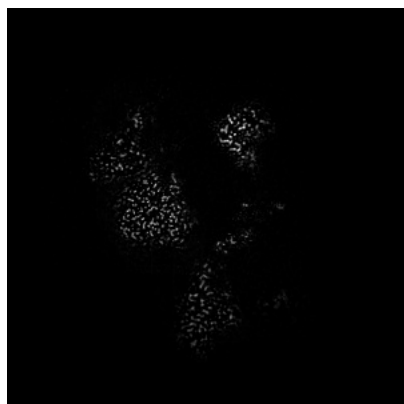


Z

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

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

#### 6.2.1 Primary map



X Index: 225



Y Index: 225

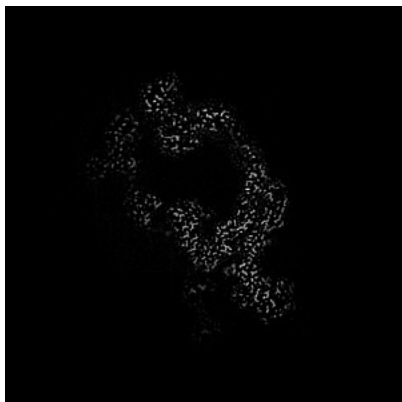


Z Index: 225

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: 199



Y Index: 272



Z Index: 324

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

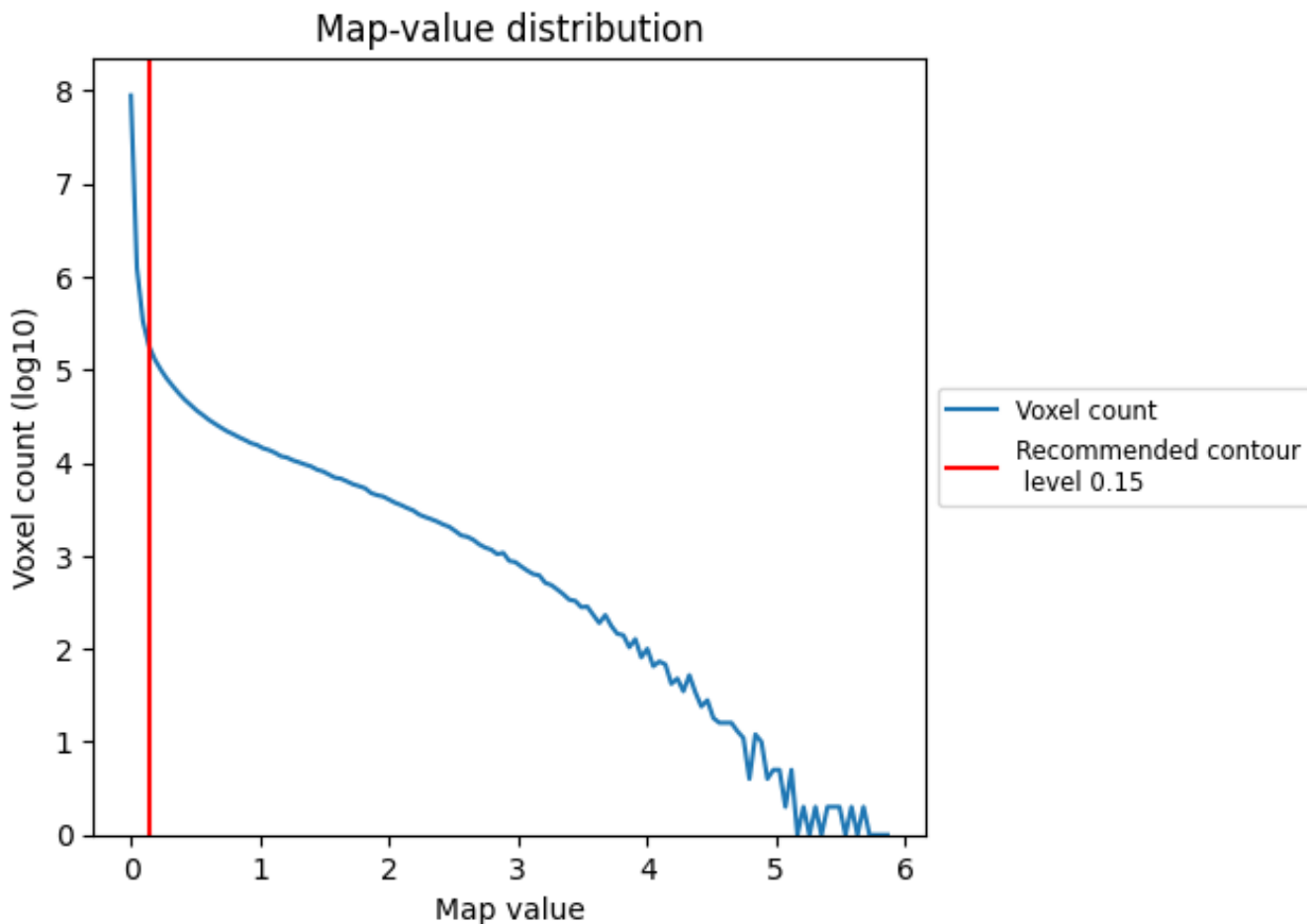
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

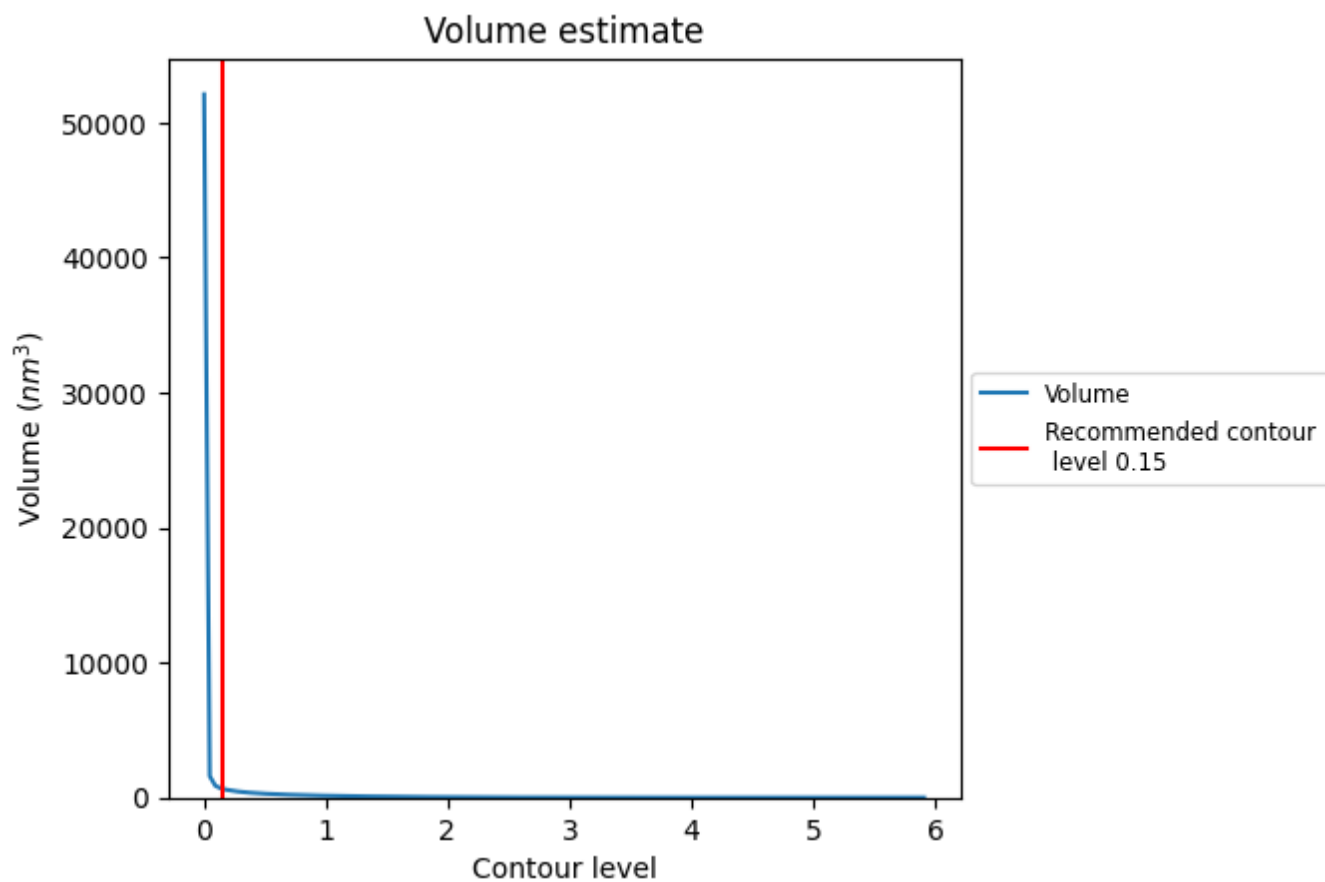
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

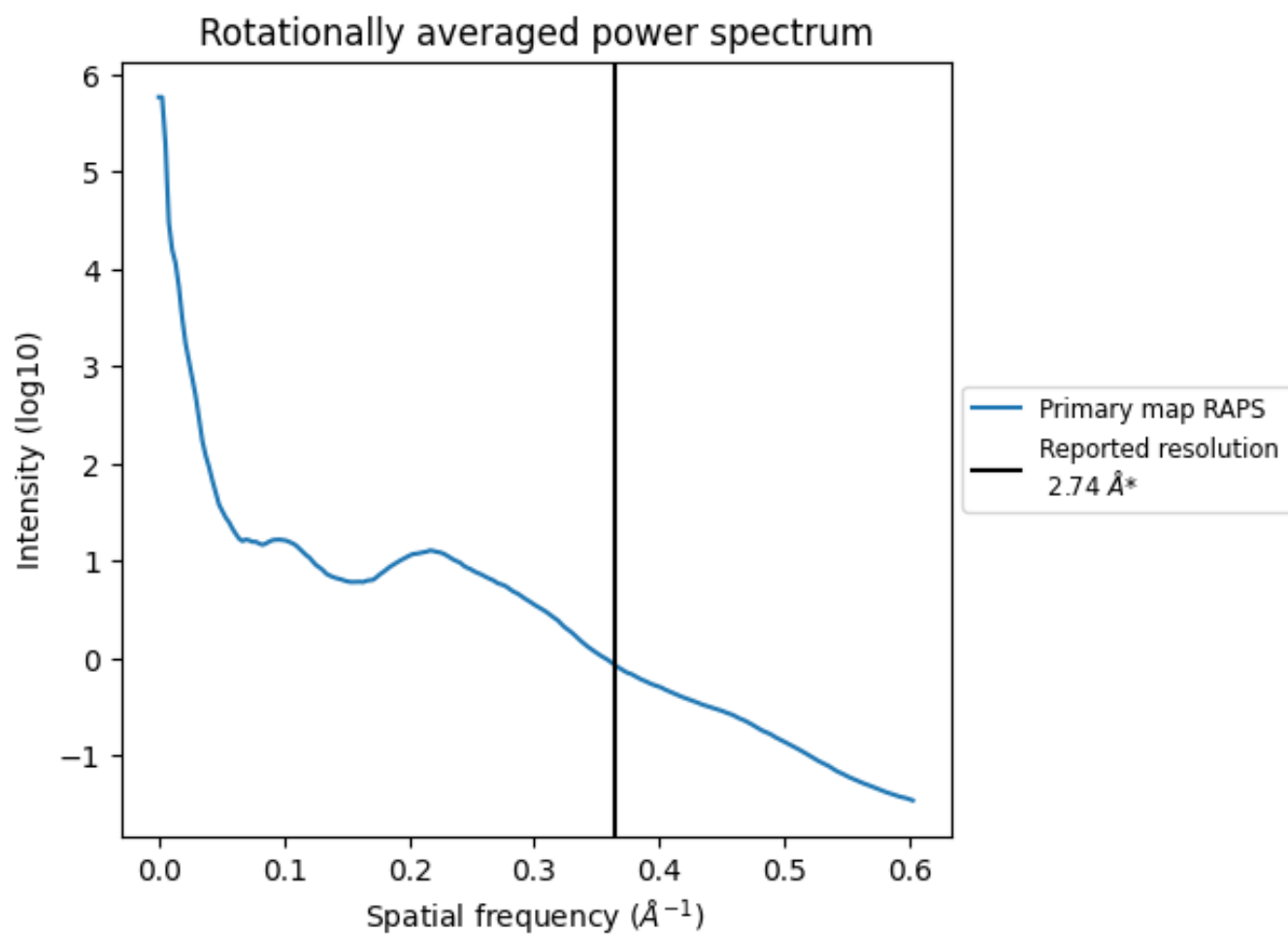


The volume at the recommended contour level is 656  $\text{nm}^3$ ; this corresponds to an approximate mass of 592 kDa.

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 [i](#)

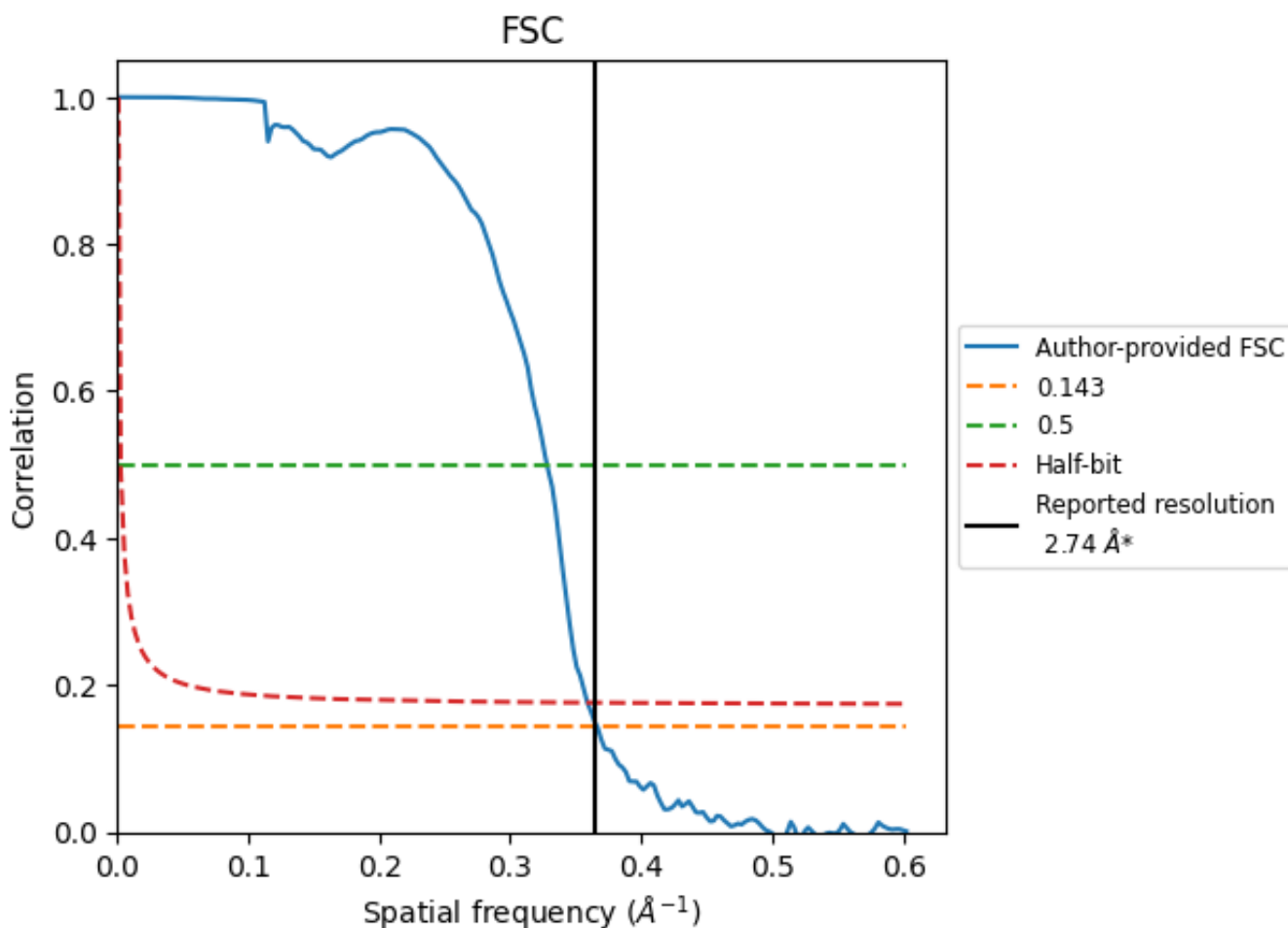


\*Reported resolution corresponds to spatial frequency of 0.365 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.365 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

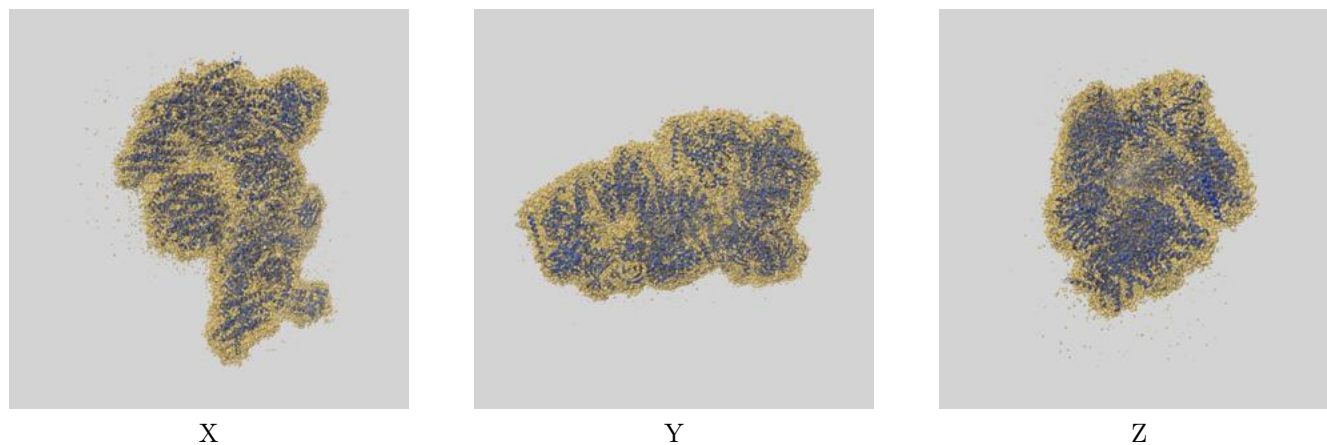
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.73	3.05	2.79
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

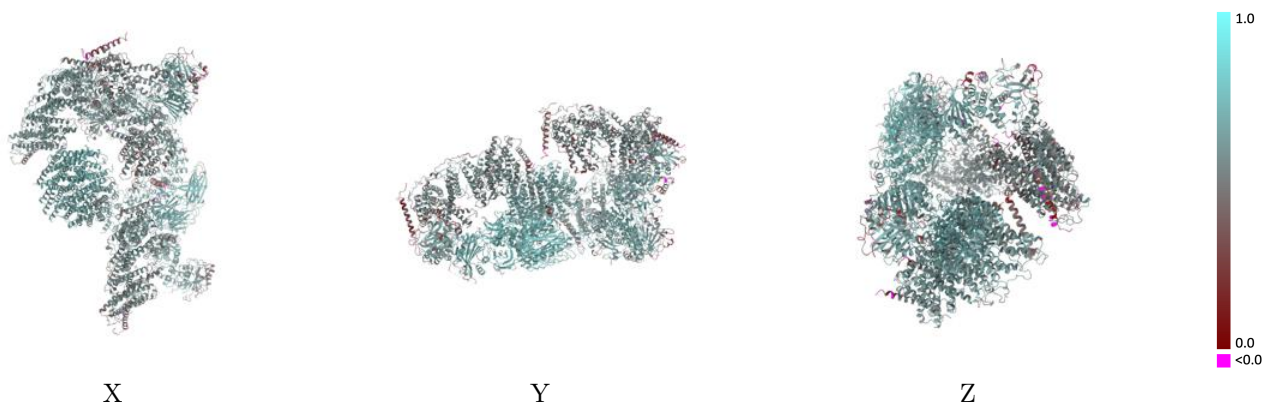
This section contains information regarding the fit between EMDB map EMD-26960 and PDB model 8CS9. Per-residue inclusion information can be found in section [3](#) on page [10](#).

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



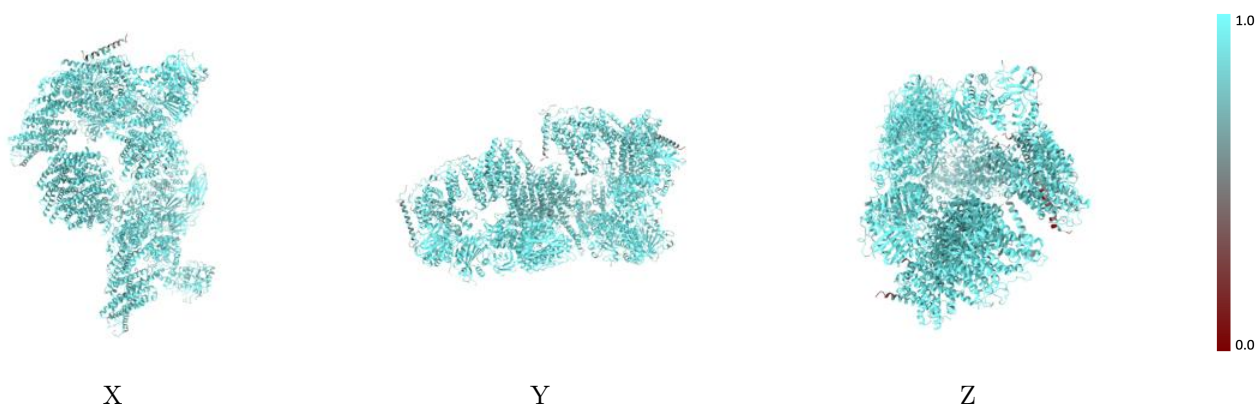
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



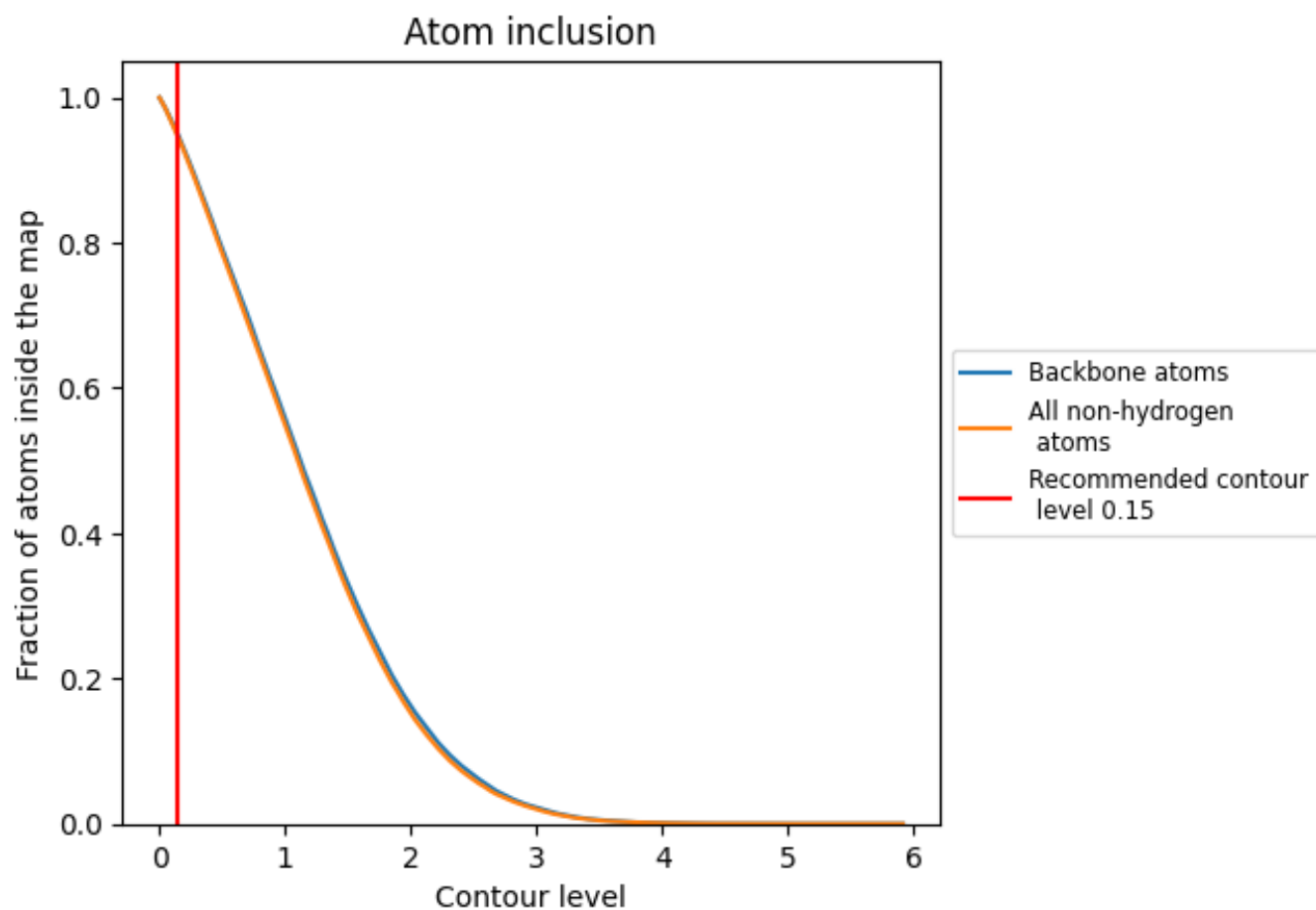
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).













































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9453	 0.5880
A	 0.9933	 0.6630
B	 0.5357	 0.3070
C	 0.6786	 0.3330
D	 0.6786	 0.2980
K	 0.9823	 0.6590
L	 0.9960	 0.7190
P	 0.7654	 0.4020
Q	 0.9949	 0.7160
R	 0.7831	 0.3860
S	 0.4640	 0.2070
T	 0.6810	 0.3260
V	 0.9482	 0.5680
X	 0.9826	 0.7050
Y	 0.9234	 0.5200
Z	 0.9572	 0.5640
a	 0.6416	 0.2870
b	 0.6479	 0.2950
c	 0.8201	 0.4250
e	 0.9087	 0.5260
f	 0.9210	 0.5290
g	 0.9625	 0.5830

