



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:54 PM UTC

PDB ID : 7U06 / pdb_00007u06
EMDB ID : EMD-26255
Title : Structure of the yeast TRAPP2-Rab11/Ypt32 complex in the closed/open state (composite structure)
Authors : Bagde, S.R.; Fromme, J.C.
Deposited on : 2022-02-17
Resolution : 4.20 Å (reported)
Based on initial models : 3RWO, 3CUE, 3PR6

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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

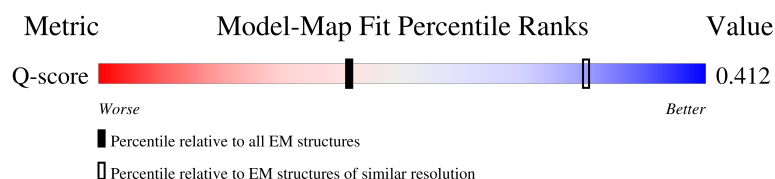
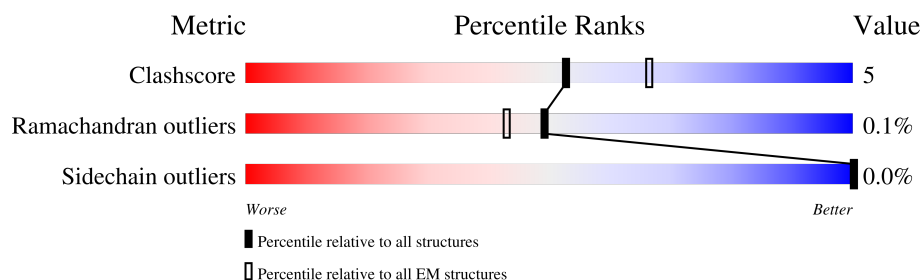
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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.



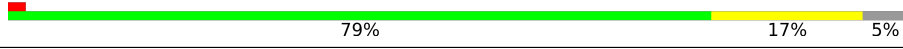
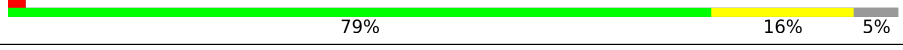
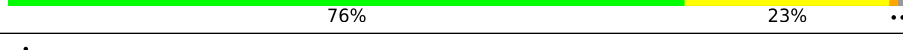
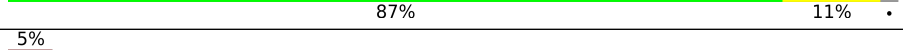
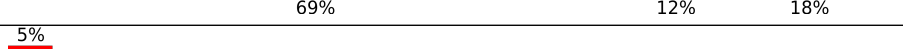
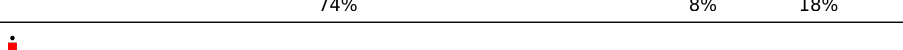
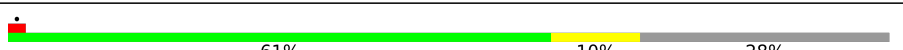
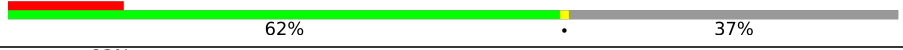
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	C	560	
1	c	560	
2	D	152	
2	d	152	

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Mol	Chain	Length	Quality of chain
3	E	268	
3	e	268	
4	F	193	
4	I	193	
4	f	193	
4	i	193	
5	G	159	
5	g	159	
6	H	219	
6	h	219	
7	J	283	
7	j	283	
8	K	175	
8	k	175	
9	l	227	
10	B	1104	
10	b	1104	
11	A	1289	
11	a	1289	
12	M	293	
12	m	293	
13	N	210	
13	n	210	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 127470 atoms, of which 63610 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 Trafficking protein particle complex II-specific subunit 65.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	C	286	Total	C	H	N	O	S	0	0
			4650	1488	2351	372	434	5		
1	c	286	Total	C	H	N	O	S	0	0
			4652	1488	2353	372	434	5		

- Molecule 2 is a protein called TRAPP-associated protein TCA17.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	146	Total	C	H	N	O	S	0	0
			2344	754	1183	181	222	4		
2	d	140	Total	C	H	N	O	S	1	0
			2270	731	1150	175	210	4		

- Molecule 3 is a protein called Trafficking protein particle complex subunit 33.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	212	Total	C	H	N	O	S	0	0
			3495	1117	1766	288	315	9		
3	e	207	Total	C	H	N	O	S	0	0
			3430	1092	1736	286	308	8		

- Molecule 4 is a protein called Trafficking protein particle complex subunit BET3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	F	184	Total	C	H	N	O	S	0	0
			2975	948	1491	244	281	11		
4	I	183	Total	C	H	N	O	S	0	0
			2964	945	1486	243	279	11		
4	f	186	Total	C	H	N	O	S	0	0
			2996	955	1499	246	285	11		
4	i	184	Total	C	H	N	O	S	0	0
			2971	947	1489	244	280	11		

- Molecule 5 is a protein called Trafficking protein particle complex subunit BET5.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	158	Total	C	H	N	O	S	0	0
			2544	821	1257	220	240	6		
5	g	156	Total	C	H	N	O	S	0	0
			2518	813	1245	216	238	6		

- Molecule 6 is a protein called Trafficking protein particle complex subunit 23.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	H	179	Total	C	H	N	O	S	0	0
			2862	921	1431	230	272	8		
6	h	179	Total	C	H	N	O	S	0	0
			2863	921	1432	230	272	8		

- Molecule 7 is a protein called Trafficking protein particle complex subunit 31.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	J	210	Total	C	H	N	O	S	0	0
			3350	1079	1656	288	318	9		
7	j	210	Total	C	H	N	O	S	0	0
			3350	1079	1656	288	318	9		

- Molecule 8 is a protein called Trafficking protein particle complex subunit 20.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	K	146	Total	C	H	N	O	S	0	0
			2342	766	1152	197	222	5		
8	k	146	Total	C	H	N	O	S	0	0
			2342	766	1152	197	222	5		

- Molecule 9 is a protein called GTP-binding protein YPT32/YPT11.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	l	191	Total	C	H	N	O	S	0	0
			2958	943	1464	252	295	4		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	221	HIS	-	expression tag	UNP P51996
1	222	HIS	-	expression tag	UNP P51996
1	223	HIS	-	expression tag	UNP P51996

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Chain	Residue	Modelled	Actual	Comment	Reference
1	224	HIS	-	expression tag	UNP P51996
1	225	HIS	-	expression tag	UNP P51996
1	226	HIS	-	expression tag	UNP P51996
1	227	HIS	-	expression tag	UNP P51996

- Molecule 10 is a protein called Trafficking protein particle complex II-specific subunit 130.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	B	791	Total	C	H	N	O	S	0	0
			12974	4183	6512	1042	1209	28		
10	b	791	Total	C	H	N	O	S	0	0
			12979	4188	6513	1042	1208	28		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1103	ALA	-	expression tag	UNP Q03660
B	1104	ALA	-	expression tag	UNP Q03660
b	1103	ALA	-	expression tag	UNP Q03660
b	1104	ALA	-	expression tag	UNP Q03660

- Molecule 11 is a protein called Trafficking protein particle complex II-specific subunit 120.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	A	1106	Total	C	H	N	O	S	0	0
			18239	5857	9206	1466	1668	42		
11	a	1114	Total	C	H	N	O	S	0	0
			18374	5905	9270	1477	1680	42		

- Molecule 12 is a protein called Trafficking protein particle complex II-specific subunit 130.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	247	Total	C	H	N	O	0	0
			2221	741	986	247	247		
12	m	249	Total	C	H	N	O	0	0
			2239	747	994	249	249		

- Molecule 13 is a protein called Trafficking protein particle complex II-specific subunit 65.

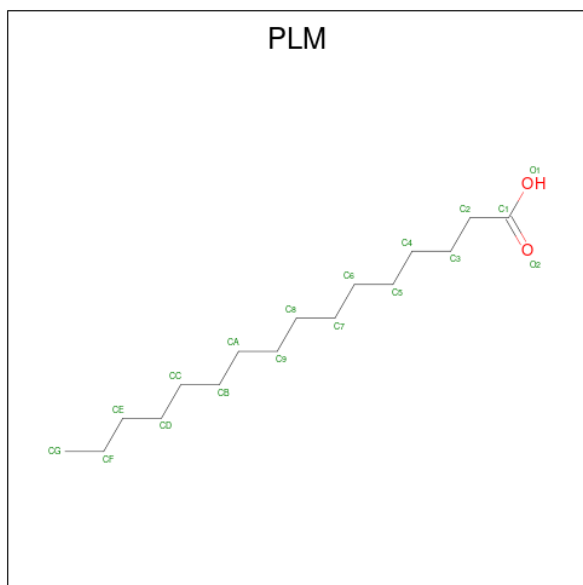
Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	132	Total	C	H	N	O	0	0
			1188	396	528	132	132		

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Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	132	Total	C	H	N	O	0	0
			1188	396	528	132	132		

- Molecule 14 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).

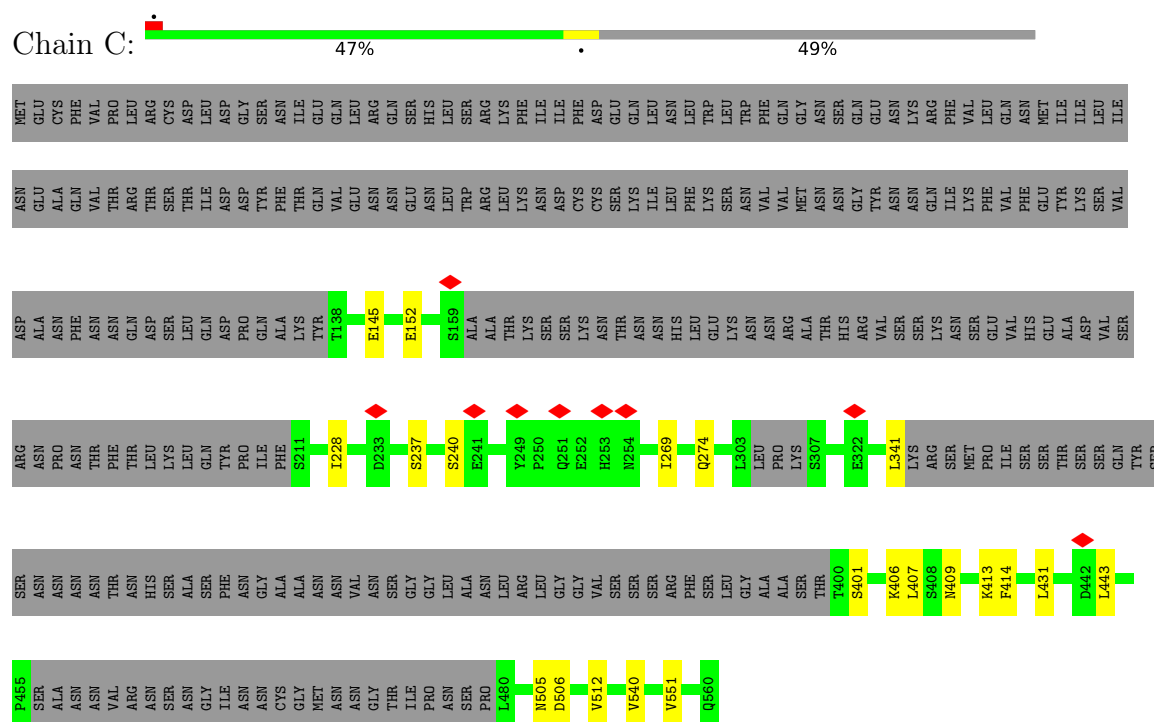


Mol	Chain	Residues	Atoms				AltConf
14	F	1	Total	C	H	O	0
			48	16	31	1	
14	I	1	Total	C	H	O	0
			48	16	31	1	
14	f	1	Total	C	H	O	0
			48	16	31	1	
14	i	1	Total	C	H	O	0
			48	16	31	1	

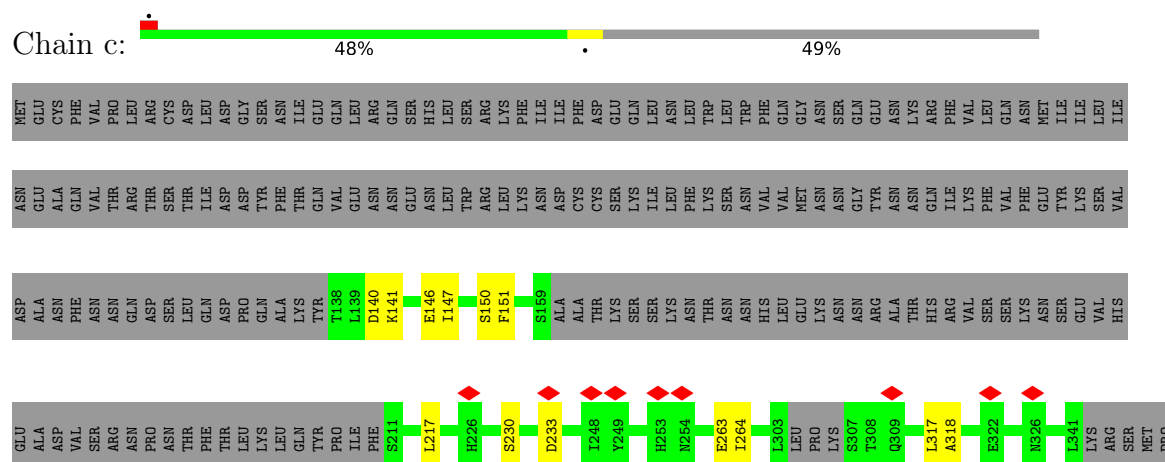
3 Residue-property plots

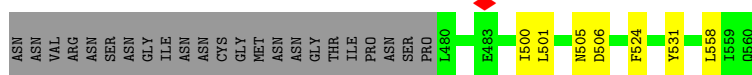
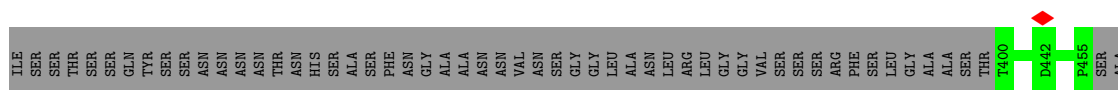
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Trafficking protein particle complex II-specific subunit 65

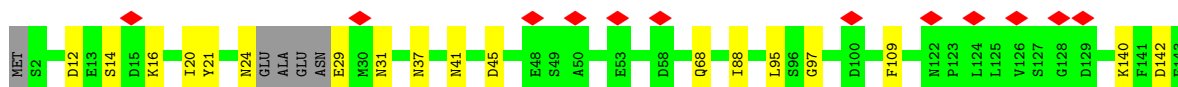
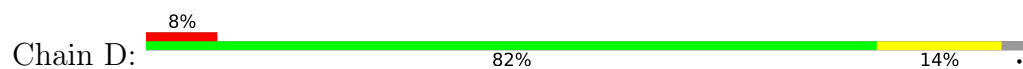


- Molecule 1: Trafficking protein particle complex II-specific subunit 65

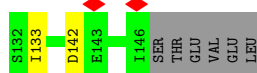
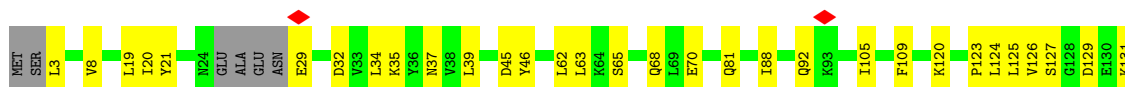




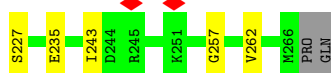
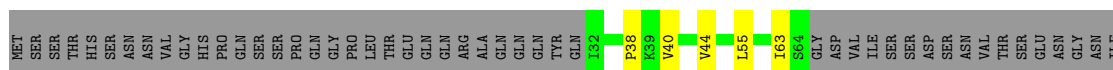
• Molecule 2: TRAPP-associated protein TCA17



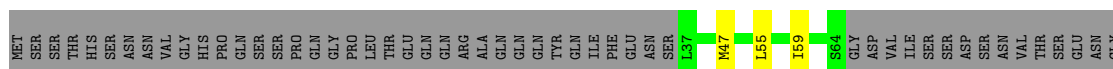
• Molecule 2: TRAPP-associated protein TCA17

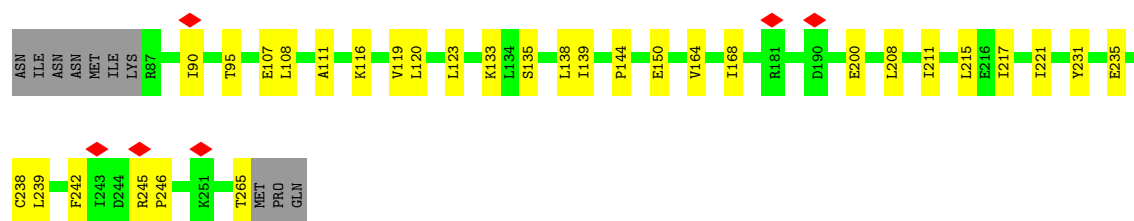


• Molecule 3: Trafficking protein particle complex subunit 33



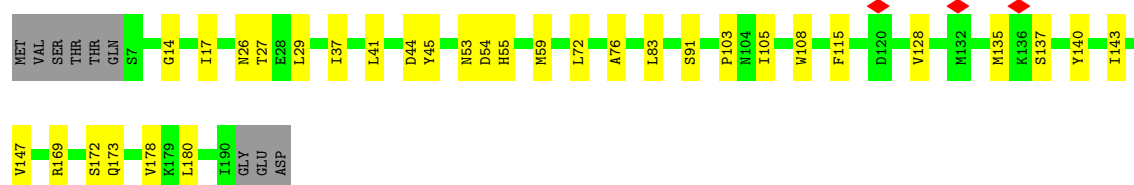
• Molecule 3: Trafficking protein particle complex subunit 33





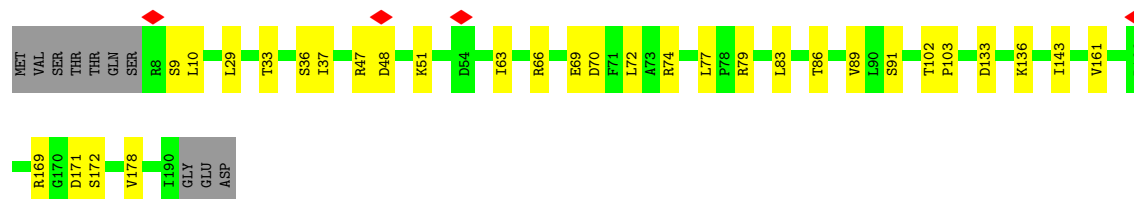
- Molecule 4: Trafficking protein particle complex subunit BET3

Chain F: 79% 17% 5%



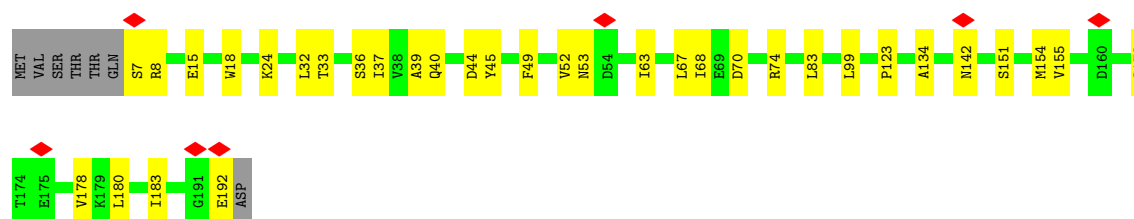
- Molecule 4: Trafficking protein particle complex subunit BET3

Chain I: 79% 16% 5%



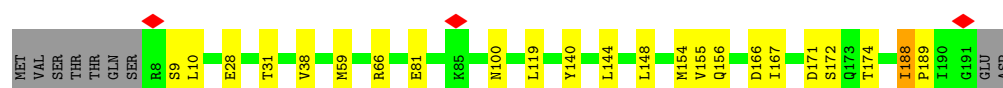
- Molecule 4: Trafficking protein particle complex subunit BET3

Chain f: 79% 18% 5%

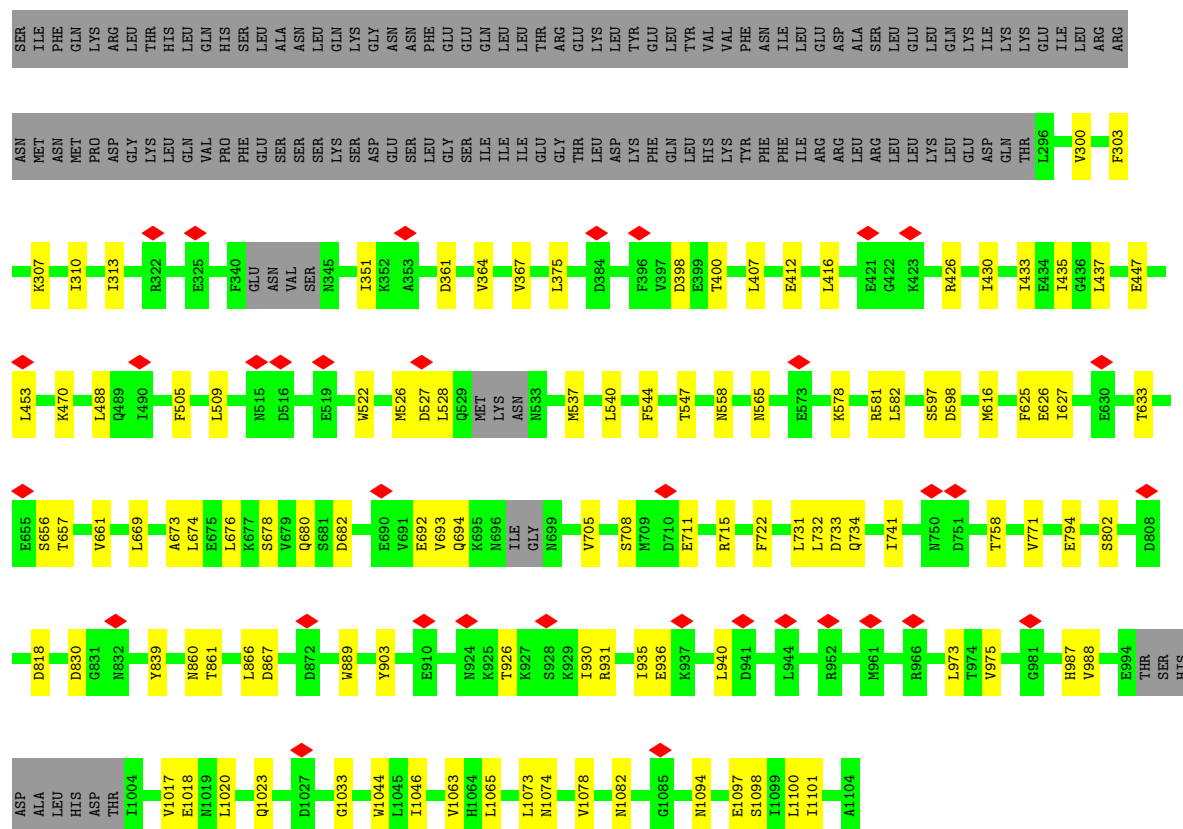


- Molecule 4: Trafficking protein particle complex subunit BET3

Chain i: 83% 11% 5%

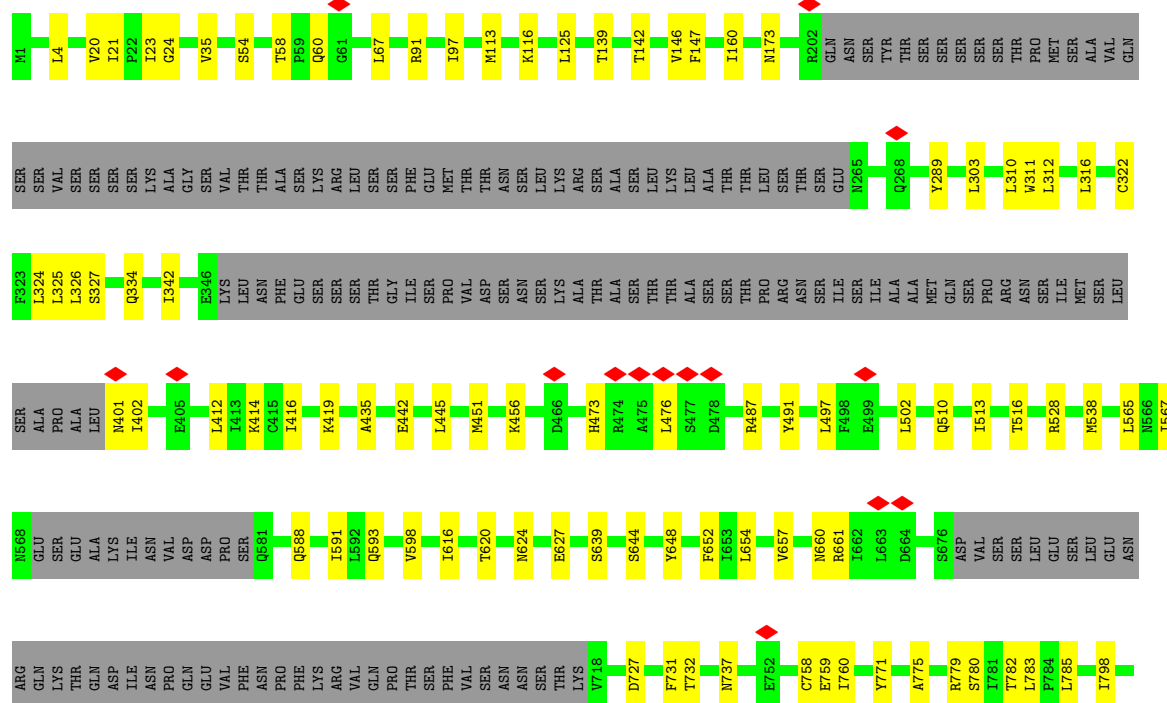


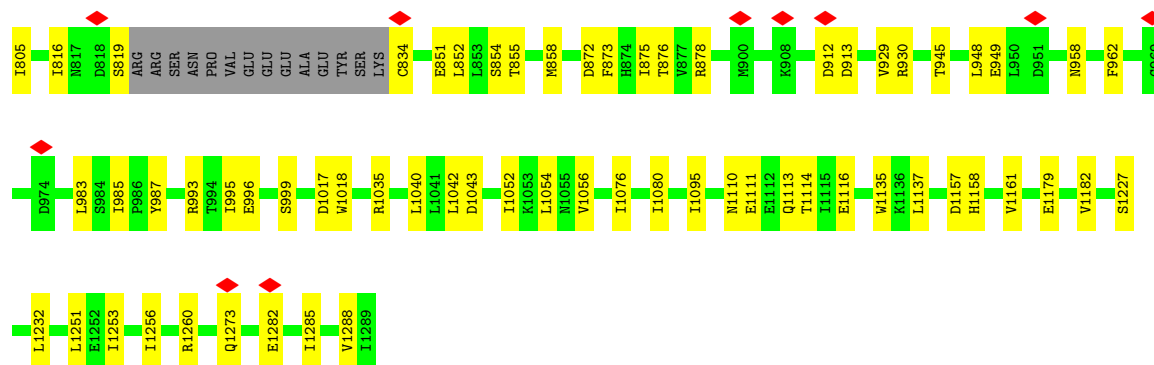
- Molecule 5: Trafficking protein particle complex subunit BET5



• Molecule 11: Trafficking protein particle complex II-specific subunit 120

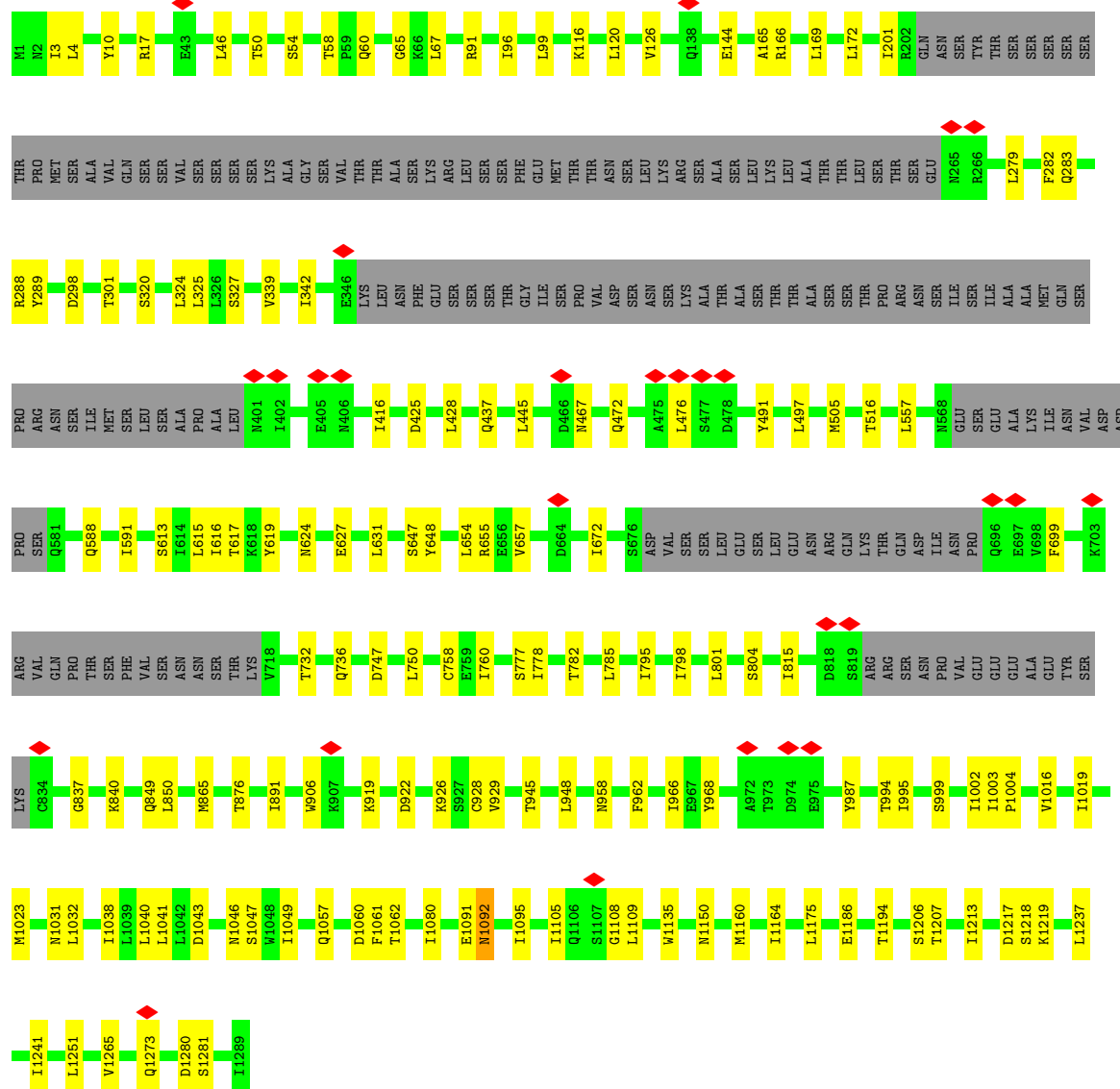
Chain A: 74% 12% 14%



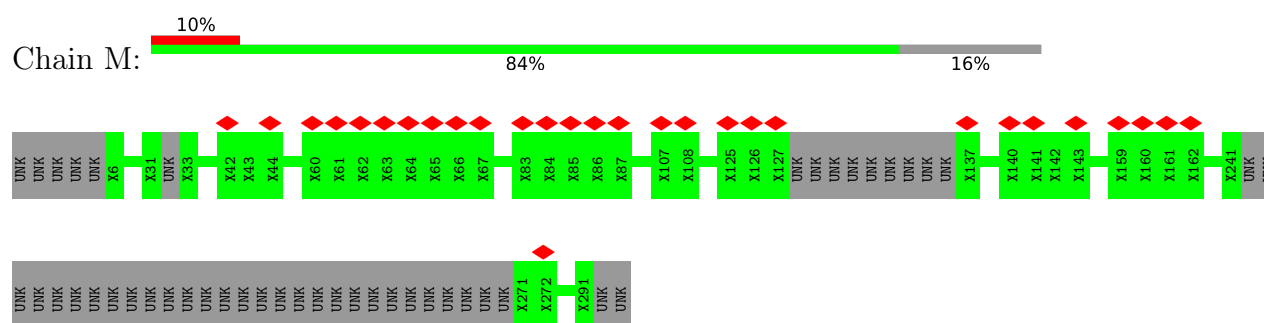


• Molecule 11: Trafficking protein particle complex II-specific subunit 120

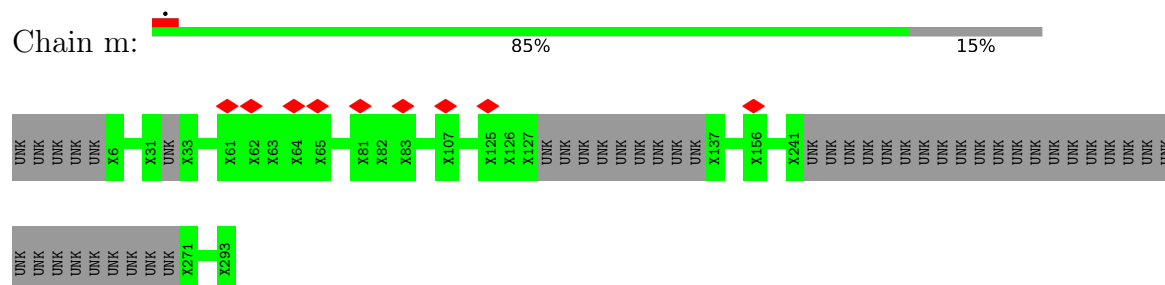
Chain a: 75% 12% 14%



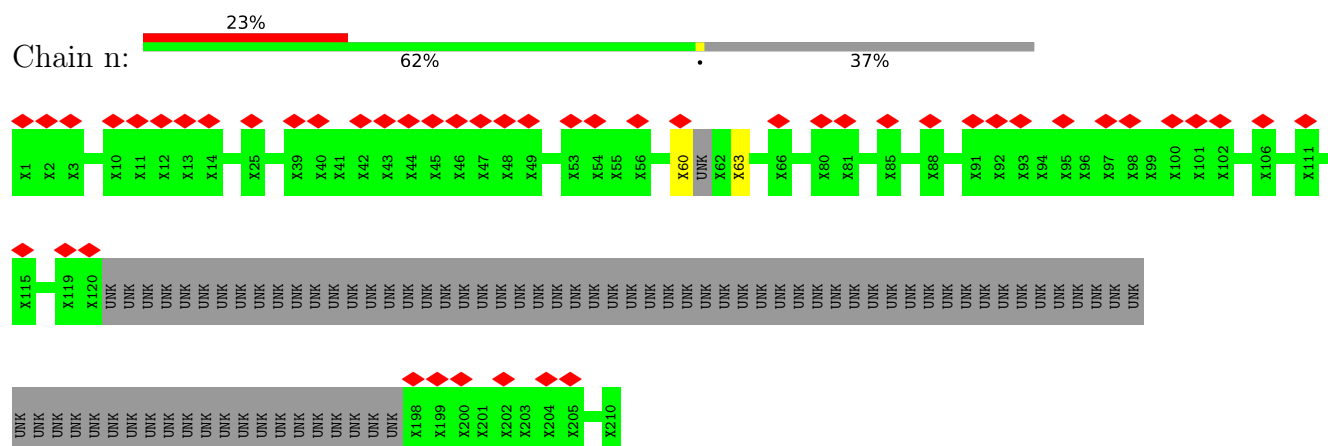
• Molecule 12: Trafficking protein particle complex II-specific subunit 130



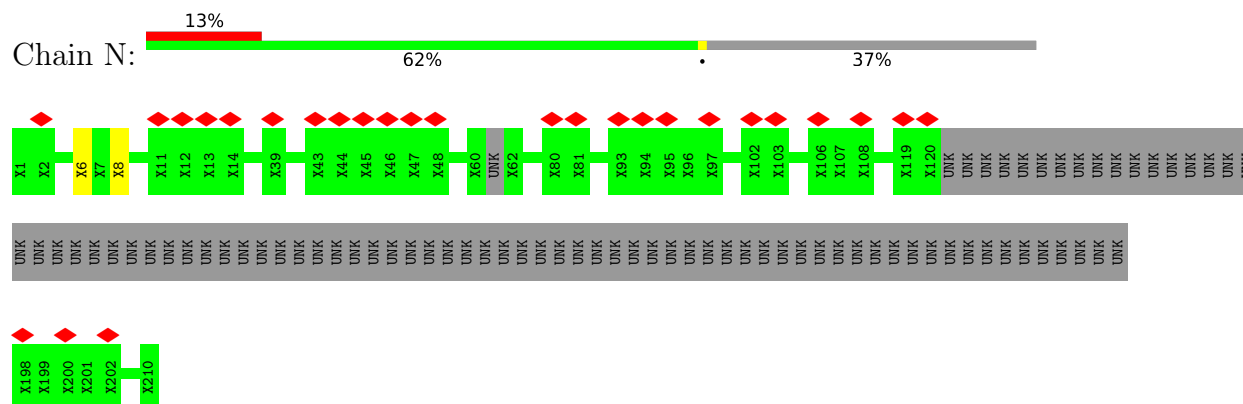
- Molecule 12: Trafficking protein particle complex II-specific subunit 130



- Molecule 13: Trafficking protein particle complex II-specific subunit 65



- Molecule 13: Trafficking protein particle complex II-specific subunit 65



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	149906	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	63000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	55.359	Depositor
Minimum map value	-39.084	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.716	Depositor
Recommended contour level	3	Depositor
Map size (Å)	572.8, 572.8, 572.8	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4319999, 1.4319999, 1.4319999	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: PLM

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	C	0.19	0/2344	0.44	0/3176
1	c	0.18	0/2344	0.43	0/3176
2	D	0.20	0/1179	0.48	0/1590
2	d	0.24	0/1141	0.53	0/1538
3	E	0.23	0/1762	0.55	0/2372
3	e	0.22	0/1726	0.50	0/2323
4	F	0.22	0/1511	0.48	0/2043
4	I	0.19	0/1505	0.43	0/2035
4	f	0.21	0/1524	0.46	0/2060
4	i	0.20	0/1509	0.48	0/2040
5	G	0.22	0/1316	0.49	0/1777
5	g	0.20	0/1302	0.50	0/1758
6	H	0.21	0/1457	0.48	0/1968
6	h	0.19	0/1457	0.45	0/1968
7	J	0.20	0/1730	0.46	0/2333
7	j	0.22	0/1730	0.48	0/2333
8	K	0.20	0/1221	0.43	0/1655
8	k	0.21	0/1221	0.47	0/1655
9	l	0.19	0/1519	0.47	0/2055
10	B	0.20	0/6585	0.44	0/8883
10	b	0.19	0/6590	0.44	0/8889
11	A	0.20	0/9230	0.45	0/12505
11	a	0.20	0/9303	0.46	0/12602
All	All	0.20	0/61206	0.46	0/82734

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
11	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	A	1135	TRP	Peptide

5.2 Too-close contacts [i](#)

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	C	2299	2351	2353	14	0
1	c	2299	2353	2353	14	0
2	D	1161	1183	1179	19	0
2	d	1120	1150	1146	28	0
3	E	1729	1766	1762	29	0
3	e	1694	1736	1736	25	0
4	F	1484	1491	1491	26	0
4	I	1478	1486	1486	26	0
4	f	1497	1499	1500	26	0
4	i	1482	1489	1489	18	0
5	G	1287	1257	1257	27	0
5	g	1273	1245	1245	14	0
6	H	1431	1431	1430	22	0
6	h	1431	1432	1430	14	0
7	J	1694	1656	1656	16	0
7	j	1694	1656	1656	21	0
8	K	1190	1152	1152	14	0
8	k	1190	1152	1152	16	0
9	l	1494	1464	1465	19	0
10	B	6462	6512	6512	72	0
10	b	6466	6513	6514	72	0
11	A	9033	9206	9206	106	0
11	a	9104	9270	9272	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	M	1235	986	267	0	0
12	m	1245	994	268	0	0
13	N	660	528	148	1	0
13	n	660	528	149	1	0
14	F	17	31	31	1	0
14	I	17	31	31	0	0
14	f	17	31	31	0	0
14	i	17	31	31	0	0
All	All	63860	63610	61398	665	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 5.

All (665) 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)
11:A:876:THR:HG22	11:A:945:THR:HG22	1.38	1.06
3:e:47:MET:HE1	4:f:67:LEU:HD13	1.55	0.88
10:B:661:VAL:HG21	10:B:742:ILE:HG21	1.56	0.87
11:A:54:SER:OG	11:A:173:ASN:ND2	2.13	0.81
11:A:593:GLN:NE2	11:A:627:GLU:OE2	2.14	0.79
4:i:28:GLU:OE1	7:j:190:TYR:OH	2.00	0.79
5:G:114:TYR:O	5:G:142:ASN:ND2	2.17	0.78
4:F:83:LEU:HD21	4:F:180:LEU:HD13	1.65	0.78
4:I:37:ILE:HD11	7:J:69:MET:HE2	1.65	0.78
2:D:24:ASN:OD1	3:E:181:ARG:NH2	2.18	0.77
10:B:989:GLN:NE2	10:B:991:GLU:OE2	2.17	0.76
2:D:21:TYR:OH	2:D:142:ASP:OD1	2.04	0.75
2:d:120:LYS:O	3:e:133:LYS:NZ	2.20	0.75
4:F:172:SER:OG	4:F:173:GLN:OE1	2.03	0.73
11:a:1213:ILE:HD13	11:a:1251:LEU:HD22	1.70	0.73
10:B:802:SER:O	10:B:839:TYR:OH	2.06	0.73
9:l:128:SER:HG	9:l:156:SER:HG	1.33	0.73
3:e:47:MET:HE3	4:f:63:ILE:HG23	1.70	0.73
11:a:876:THR:HG22	11:a:945:THR:HG22	1.70	0.73
11:a:747:ASP:OD1	11:a:804:SER:OG	2.04	0.72
6:H:183:TYR:OH	4:I:69:GLU:OE2	2.06	0.72
10:B:440:TYR:OH	10:B:477:ASP:OD2	2.07	0.72
5:G:38:GLU:OE1	5:G:42:LYS:NZ	2.23	0.72
11:A:54:SER:O	11:A:58:THR:OG1	2.07	0.72
8:k:126:ASP:OD2	8:k:129:ASN:ND2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:135:LEU:HD23	4:I:72:LEU:HD11	1.71	0.71
11:a:54:SER:O	11:a:58:THR:OG1	2.07	0.71
11:a:467:ASN:ND2	11:a:472:GLN:O	2.24	0.71
10:B:529:GLN:NE2	10:B:533:ASN:OD1	2.24	0.71
5:g:112:VAL:O	5:g:116:SER:OG	2.08	0.71
3:E:161:CYS:SG	3:E:173:ILE:HG21	2.31	0.70
10:B:690:GLU:OE2	10:B:715:ARG:NH1	2.24	0.70
11:A:538:MET:CE	11:A:598:VAL:HG11	2.21	0.70
3:E:196:SER:O	5:G:118:ASN:ND2	2.25	0.70
9:l:128:SER:OG	9:l:156:SER:OG	2.07	0.70
11:A:661:ARG:NH1	11:A:727:ASP:OD2	2.25	0.70
7:J:51:LEU:O	7:J:105:ARG:NE	2.25	0.70
10:b:1073:LEU:HD12	10:b:1101:ILE:HD13	1.73	0.69
7:j:172:ARG:NH2	8:k:86:ASN:O	2.26	0.69
11:A:993:ARG:NH2	11:A:996:GLU:OE1	2.25	0.69
2:d:125:LEU:HD21	2:d:133:ILE:HD11	1.75	0.69
3:e:235:GLU:OE2	3:e:265:THR:N	2.26	0.69
11:a:732:THR:HG22	11:a:782:THR:HG22	1.73	0.69
10:b:1094:ASN:ND2	10:b:1097:GLU:OE1	2.27	0.68
4:F:91:SER:OG	4:F:103:PRO:O	2.11	0.68
11:A:779:ARG:NH1	11:A:780:SER:O	2.26	0.68
5:G:2:GLY:O	5:G:92:SER:OG	2.09	0.68
1:C:401:SER:OG	1:C:413:LYS:NZ	2.27	0.67
11:a:324:LEU:O	11:a:327:SER:OG	2.12	0.67
8:k:93:ASP:OD1	11:a:491:TYR:OH	2.11	0.67
11:a:922:ASP:OD2	11:a:926:LYS:NZ	2.28	0.67
2:D:37:ASN:ND2	10:B:466:SER:OG	2.28	0.67
3:E:122:ARG:NH1	4:F:44:ASP:OD1	2.28	0.67
11:A:930:ARG:NH2	11:A:949:GLU:OE1	2.27	0.66
11:a:750:LEU:HD21	11:a:760:ILE:HD12	1.77	0.66
5:g:77:VAL:HG22	5:g:91:LEU:HD22	1.75	0.66
5:g:69:SER:OG	6:h:123:CYS:SG	2.49	0.66
10:b:692:GLU:OE1	10:b:715:ARG:NH2	2.29	0.66
4:i:28:GLU:OE1	7:j:105:ARG:NH2	2.29	0.66
11:A:342:ILE:O	11:A:419:LYS:NZ	2.29	0.65
10:b:537:MET:SD	10:b:633:THR:OG1	2.53	0.65
10:b:802:SER:O	10:b:839:TYR:OH	2.13	0.65
2:d:20:ILE:HG21	2:d:37:ASN:OD1	1.96	0.65
11:A:1110:ASN:OD1	11:A:1113:GLN:NE2	2.29	0.65
11:A:616:ILE:O	11:A:620:THR:OG1	2.15	0.65
8:K:100:ILE:HG12	8:K:114:ILE:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:11:ARG:NH1	5:G:124:ASP:OD2	2.30	0.65
11:A:334:GLN:OE1	11:A:402:ILE:N	2.30	0.65
2:D:95:LEU:HD22	10:B:315:ILE:HD11	1.79	0.64
11:A:1040:LEU:HD13	11:A:1080:ILE:HD12	1.79	0.64
11:A:819:SER:O	11:A:834:CYS:N	2.30	0.64
7:J:62:MET:HE3	7:J:218:LEU:HD21	1.80	0.64
2:d:68:GLN:NE2	2:d:92:GLN:OE1	2.31	0.63
3:E:183:THR:OG1	3:E:262:VAL:O	2.07	0.63
5:G:144:ASN:O	5:G:148:VAL:HG12	1.98	0.63
11:a:445:LEU:HD22	11:a:516:THR:CG2	2.29	0.63
11:A:639:SER:OG	11:A:644:SER:OG	2.12	0.63
4:f:70:ASP:OD2	4:f:74:ARG:NH1	2.32	0.63
3:e:215:LEU:HD11	3:e:242:PHE:CE2	2.34	0.63
7:J:197:ASP:OD2	7:J:214:ASN:ND2	2.31	0.63
2:d:8:VAL:HA	2:d:88:ILE:HG22	1.81	0.63
11:a:279:LEU:HD23	11:a:283:GLN:OE1	1.98	0.62
11:A:758:CYS:HB2	11:A:785:LEU:HD21	1.81	0.62
3:E:115:GLU:O	3:E:119:VAL:HG23	1.99	0.62
5:g:51:LEU:HD12	5:g:70:ILE:HD13	1.81	0.62
11:a:891:ILE:HD12	11:a:966:ILE:HG22	1.81	0.62
11:a:994:THR:HG22	11:a:995:ILE:H	1.65	0.62
5:G:5:SER:O	5:G:90:LEU:HD12	2.00	0.62
10:b:794:GLU:N	10:b:794:GLU:OE1	2.33	0.62
4:f:68:ILE:HD13	4:f:151:SER:OG	2.00	0.62
3:E:198:SER:OG	5:G:142:ASN:OD1	2.18	0.61
10:B:321:VAL:O	10:B:388:LYS:N	2.32	0.61
11:A:732:THR:HG22	11:A:782:THR:HG22	1.81	0.61
4:I:29:LEU:HD13	7:J:191:LEU:HD22	1.81	0.61
6:h:196:TYR:O	4:i:66:ARG:NH2	2.33	0.61
3:E:224:GLY:O	3:E:227:SER:N	2.34	0.61
4:I:91:SER:OG	4:I:103:PRO:O	2.16	0.61
10:B:788:LEU:HD13	10:B:799:LEU:HD21	1.82	0.61
5:g:19:ARG:NH2	5:g:150:GLU:OE1	2.33	0.61
4:I:70:ASP:OD1	4:I:74:ARG:NH1	2.33	0.60
10:B:493:GLU:N	10:B:493:GLU:OE1	2.33	0.60
10:B:457:GLU:OE2	10:B:461:GLN:NE2	2.35	0.60
7:j:100:GLU:OE2	8:k:107:SER:N	2.33	0.60
10:B:426:ARG:O	10:B:430:ILE:HD12	2.01	0.60
10:B:693:VAL:HG21	10:B:705:VAL:CG1	2.31	0.60
11:A:771:TYR:HE2	11:A:783:LEU:HD21	1.66	0.60
3:e:47:MET:CE	4:f:67:LEU:HD13	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:946:CYS:O	10:B:950:VAL:HG23	2.01	0.60
10:b:581:ARG:NH1	10:b:626:GLU:OE1	2.34	0.60
4:i:59:MET:HE2	7:j:72:GLN:HG3	1.84	0.60
7:J:161:SER:OG	7:J:164:ASN:OD1	2.18	0.60
2:d:29:GLU:N	2:d:32:ASP:OD2	2.35	0.60
9:l:130:LEU:O	9:l:134:ARG:NH1	2.35	0.59
1:C:152:GLU:OE2	11:a:116:LYS:NZ	2.35	0.59
9:l:49:GLU:N	9:l:68:ASP:OD1	2.33	0.59
11:a:1003:ILE:HD11	11:a:1041:LEU:HD11	1.84	0.59
3:E:160:ILE:HD12	3:E:225:VAL:CG1	2.33	0.59
11:a:1213:ILE:HG23	11:a:1237:LEU:HD22	1.84	0.59
8:K:85:ASP:OD2	8:K:131:ARG:NH1	2.36	0.59
9:l:72:GLN:OE1	4:f:192:GLU:N	2.35	0.59
11:A:1251:LEU:HD23	11:A:1253:ILE:HD11	1.84	0.59
4:f:68:ILE:HG21	4:f:154:MET:HB2	1.84	0.59
11:A:502:LEU:O	11:A:510:GLN:NE2	2.36	0.59
11:A:20:VAL:HG22	11:A:97:ILE:CG2	2.33	0.59
10:b:398:ASP:OD2	10:b:400:THR:OG1	2.20	0.58
11:a:50:THR:OG1	11:a:166:ARG:NE	2.36	0.58
9:l:16:ILE:HG22	9:l:88:GLY:HA3	1.86	0.58
7:j:231:TYR:OH	7:j:251:THR:OG1	2.13	0.58
2:d:65:SER:O	10:b:307:LYS:NZ	2.36	0.58
11:a:445:LEU:HD22	11:a:516:THR:HG21	1.83	0.58
10:b:656:SER:N	10:b:680:GLN:OE1	2.36	0.58
6:h:15:LEU:HD21	6:h:18:GLN:HB2	1.85	0.57
11:A:456:LYS:NZ	11:A:473:HIS:O	2.37	0.57
8:k:100:ILE:HG12	8:k:114:ILE:HG22	1.86	0.57
10:b:693:VAL:HG11	10:b:705:VAL:CG1	2.34	0.57
2:D:148:THR:HG21	3:E:180:HIS:NE2	2.19	0.57
5:G:68:ARG:NH1	6:H:125:ASP:OD1	2.37	0.57
5:G:77:VAL:HG22	5:G:91:LEU:CD2	2.34	0.57
11:A:334:GLN:OE1	11:A:401:ASN:N	2.36	0.57
11:A:414:LYS:NZ	11:A:451:MET:SD	2.75	0.57
11:a:758:CYS:HB2	11:a:785:LEU:HD21	1.85	0.57
11:a:17:ARG:NH1	11:a:91:ARG:O	2.37	0.57
11:A:316:LEU:HD21	11:A:342:ILE:HD11	1.87	0.57
11:A:125:LEU:HD21	11:A:146:VAL:HG12	1.87	0.57
1:c:140:ASP:OD1	1:c:141:LYS:N	2.37	0.57
2:d:3:LEU:HD23	2:d:105:ILE:HD11	1.87	0.56
11:A:983:LEU:HD21	11:A:985:ILE:HG23	1.87	0.56
10:b:987:HIS:NE2	10:b:1018:GLU:OE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:866:LEU:HD23	10:b:903:TYR:CD2	2.40	0.56
10:B:547:THR:OG1	10:B:565:ASN:OD1	2.19	0.56
3:e:133:LYS:HG3	4:f:32:LEU:HD22	1.87	0.56
10:b:303:PHE:CG	10:b:351:ILE:HD12	2.41	0.56
10:b:731:LEU:HD23	10:b:732:LEU:N	2.21	0.56
10:b:771:VAL:HG11	10:b:975:VAL:HG21	1.87	0.56
11:a:1175:LEU:HD21	11:a:1265:VAL:HG21	1.86	0.56
3:E:40:VAL:HG23	4:F:27:THR:HG22	1.87	0.56
11:a:865:MET:HA	11:a:865:MET:HE2	1.86	0.56
5:G:22:THR:OG1	5:G:23:LEU:N	2.39	0.56
1:c:146:GLU:OE1	1:c:147:ILE:N	2.38	0.55
6:h:191:MET:O	4:i:66:ARG:NH1	2.38	0.55
2:d:81:GLN:NE2	3:e:144:PRO:O	2.39	0.55
2:d:126:VAL:HG23	2:d:127:SER:H	1.71	0.55
7:J:212:VAL:HG12	7:J:265:VAL:HG23	1.88	0.55
8:K:50:ASP:OD1	11:A:487:ARG:NH1	2.39	0.55
6:H:200:MET:HE3	6:H:201:PRO:HD3	1.87	0.55
11:A:852:LEU:HD22	11:A:985:ILE:HG21	1.87	0.55
11:a:58:THR:O	11:a:288:ARG:NH2	2.40	0.55
10:B:317:TYR:O	10:B:320:SER:OG	2.23	0.55
2:d:70:GLU:N	10:b:361:ASP:OD2	2.38	0.55
10:b:578:LYS:O	10:b:597:SER:OG	2.11	0.55
10:B:644:GLU:N	10:B:644:GLU:OE1	2.40	0.55
6:h:205:ASN:OD1	6:h:206:LEU:HD22	2.07	0.55
11:A:565:LEU:HD12	11:A:591:ILE:HD11	1.89	0.54
11:A:929:VAL:HG21	11:A:962:PHE:CZ	2.42	0.54
10:B:693:VAL:HG21	10:B:705:VAL:HG11	1.89	0.54
7:j:252:ALA:O	7:j:253:HIS:ND1	2.40	0.54
9:l:137:PRO:HB3	11:a:1105:ILE:HD11	1.90	0.54
2:d:123:PRO:O	2:d:124:LEU:HD22	2.07	0.54
3:E:243:ILE:O	3:E:257:GLY:N	2.40	0.54
11:A:445:LEU:HD21	11:A:513:ILE:HG13	1.90	0.54
2:d:34:LEU:HD21	10:b:470:LYS:HE2	1.88	0.54
11:A:648:TYR:CE1	11:A:805:ILE:HG21	2.43	0.54
11:A:1040:LEU:HD13	11:A:1080:ILE:CD1	2.36	0.54
5:g:22:THR:HG22	5:g:28:ALA:HB1	1.89	0.54
10:b:931:ARG:NH1	10:b:940:LEU:HD21	2.23	0.54
6:H:120:ARG:NH2	6:H:176:ASP:OD2	2.41	0.54
10:B:536:LEU:HD23	10:B:537:MET:O	2.07	0.54
10:B:785:LYS:HE2	10:B:836:ILE:HD12	1.88	0.54
10:b:547:THR:OG1	10:b:565:ASN:OD1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:314:SER:O	10:B:318:ARG:NH1	2.41	0.54
11:A:116:LYS:NZ	1:c:151:PHE:O	2.28	0.54
2:d:34:LEU:HD21	10:b:470:LYS:CE	2.38	0.54
10:B:384:ASP:OD1	10:B:385:VAL:N	2.41	0.54
11:A:412:LEU:O	11:A:416:ILE:HD12	2.07	0.54
6:H:208:ASP:OD1	6:H:209:GLU:N	2.41	0.53
3:E:157:MET:HA	3:E:160:ILE:HG22	1.91	0.53
5:G:55:THR:HG21	5:G:67:ILE:HG23	1.91	0.53
6:H:173:GLN:OE1	6:H:173:GLN:N	2.42	0.53
10:B:1069:LYS:HB3	10:B:1073:LEU:HD11	1.88	0.53
11:A:445:LEU:HD22	11:A:516:THR:CG2	2.39	0.53
3:e:138:LEU:CD1	3:e:164:VAL:HG22	2.38	0.53
1:C:409:ASN:O	1:C:409:ASN:ND2	2.40	0.53
8:K:161:PHE:O	8:K:165:VAL:HG23	2.08	0.53
10:B:489:GLN:OE1	10:B:489:GLN:N	2.42	0.53
11:A:782:THR:O	11:A:783:LEU:HD23	2.09	0.53
3:e:150:GLU:O	3:e:231:TYR:OH	2.27	0.53
5:g:77:VAL:HG22	5:g:91:LEU:CD2	2.37	0.53
1:c:217:LEU:HD11	1:c:230:SER:OG	2.09	0.53
7:j:161:SER:OG	8:k:136:GLU:OE1	2.27	0.53
4:I:66:ARG:NH1	7:J:67:GLN:OE1	2.42	0.53
4:I:161:VAL:HG22	4:I:178:VAL:HG22	1.91	0.53
10:B:913:ILE:HG23	10:B:955:ALA:HB2	1.91	0.53
4:f:99:LEU:HD12	4:f:123:PRO:HG2	1.90	0.53
4:F:14:GLY:HA2	4:F:17:ILE:HG22	1.91	0.53
5:G:6:PHE:HD2	5:G:90:LEU:HD13	1.74	0.53
11:A:1035:ARG:NH1	11:A:1282:GLU:OE1	2.41	0.53
9:l:89:ALA:CB	9:l:111:LEU:HD21	2.39	0.53
10:B:425:GLN:N	10:B:425:GLN:OE1	2.42	0.53
6:h:208:ASP:OD1	6:h:209:GLU:N	2.42	0.53
2:D:16:LYS:NZ	10:B:463:ASN:OD1	2.22	0.52
10:B:912:ARG:NH1	10:B:957:CYS:O	2.41	0.52
7:J:271:ASP:OD1	7:J:272:ARG:N	2.42	0.52
6:h:15:LEU:HD22	6:h:33:TYR:HB3	1.89	0.52
11:a:1016:VAL:HG23	11:a:1019:ILE:HG22	1.92	0.52
11:A:58:THR:HG22	11:A:60:GLN:H	1.74	0.52
11:A:1017:ASP:OD1	11:A:1018:TRP:N	2.42	0.52
4:f:18:TRP:O	4:f:24:LYS:NZ	2.38	0.52
7:j:180:LEU:HD21	7:j:199:LEU:HD11	1.91	0.52
11:a:624:ASN:N	11:a:627:GLU:OE2	2.42	0.52
11:a:778:ILE:O	11:a:778:ILE:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:h:43:VAL:HA	6:h:46:ILE:HG22	1.90	0.52
6:h:29:ASN:OD1	6:h:30:SER:N	2.42	0.52
10:B:683:ALA:O	10:B:684:LEU:HD12	2.10	0.52
5:g:22:THR:CG2	5:g:28:ALA:HB1	2.40	0.52
4:I:63:ILE:HD12	4:I:143:ILE:HD11	1.92	0.52
10:B:1073:LEU:HD12	10:B:1101:ILE:HD13	1.90	0.52
2:d:34:LEU:HD21	10:b:470:LYS:NZ	2.25	0.52
2:d:88:ILE:HD11	2:d:109:PHE:CE1	2.45	0.52
8:k:39:PHE:HE1	11:a:591:ILE:HD11	1.75	0.52
4:I:63:ILE:CD1	4:I:143:ILE:HD11	2.41	0.52
3:E:149:LYS:H	3:E:151:MET:HE1	1.74	0.51
10:B:917:LEU:O	10:B:920:SER:OG	2.28	0.51
11:A:147:PHE:HD2	11:A:160:ILE:HG23	1.75	0.51
11:A:873:PHE:CE1	11:A:948:LEU:HD22	2.45	0.51
4:i:119:LEU:HB2	4:i:174:THR:HG23	1.92	0.51
10:b:426:ARG:O	10:b:430:ILE:HD12	2.09	0.51
11:a:172:LEU:O	11:a:172:LEU:HD23	2.10	0.51
11:a:616:ILE:HG22	11:a:616:ILE:O	2.11	0.51
5:G:110:ILE:HD11	5:G:148:VAL:HG13	1.93	0.51
11:a:1206:SER:OG	11:a:1207:THR:N	2.42	0.51
1:C:145:GLU:N	1:C:145:GLU:OE1	2.44	0.51
3:E:149:LYS:N	3:E:151:MET:HE1	2.25	0.51
6:H:196:TYR:O	4:I:66:ARG:NH2	2.44	0.51
8:K:32:ASP:OD1	8:K:33:LEU:N	2.43	0.51
9:l:46:ILE:HG13	9:l:47:GLY:H	1.74	0.51
2:d:62:LEU:HD23	2:d:63:LEU:N	2.26	0.51
3:e:116:LYS:O	3:e:120:LEU:HD23	2.11	0.51
10:b:669:LEU:HD12	10:b:975:VAL:HG22	1.92	0.51
3:E:160:ILE:HD12	3:E:225:VAL:HG11	1.92	0.51
4:F:128:VAL:HG11	4:F:140:TYR:CE2	2.46	0.51
11:A:855:THR:HG21	11:A:858:MET:HG3	1.93	0.51
5:G:142:ASN:O	5:G:146:ILE:HD12	2.10	0.51
4:i:171:ASP:OD1	4:i:172:SER:N	2.44	0.51
10:b:300:VAL:O	10:b:303:PHE:N	2.44	0.51
10:b:733:ASP:OD1	10:b:734:GLN:N	2.44	0.51
11:a:1160:MET:O	11:a:1164:ILE:HG22	2.11	0.51
11:a:1108:GLY:C	11:a:1109:LEU:HD12	2.36	0.51
2:d:34:LEU:HD11	10:b:470:LYS:HE2	1.91	0.51
10:b:582:LEU:HD13	10:b:625:PHE:HD1	1.76	0.51
11:a:798:ILE:HG23	11:a:798:ILE:O	2.11	0.51
11:A:91:ARG:NH1	11:A:442:GLU:OE1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:l:167:PHE:CE1	9:l:171:ILE:HD11	2.46	0.51
10:B:733:ASP:OD1	10:B:734:GLN:N	2.44	0.51
10:B:845:ASN:OD1	10:B:846:ASN:N	2.43	0.51
11:A:67:LEU:HD23	11:A:67:LEU:O	2.11	0.51
10:b:407:LEU:CD1	10:b:435:ILE:HG23	2.41	0.51
4:I:47:ARG:NH2	4:I:133:ASP:OD1	2.44	0.50
1:c:501:LEU:HD13	1:c:524:PHE:CE1	2.47	0.50
7:J:96:ILE:HD13	7:J:243:ASN:CG	2.36	0.50
11:A:798:ILE:HG23	11:A:798:ILE:O	2.11	0.50
10:b:889:TRP:HZ3	10:b:935:ILE:HD12	1.76	0.50
1:C:505:ASN:OD1	1:C:506:ASP:N	2.45	0.50
11:A:657:VAL:O	11:A:657:VAL:HG22	2.12	0.50
3:E:112:ASP:OD1	3:E:113:GLU:N	2.41	0.50
4:I:9:SER:C	4:I:10:LEU:HD12	2.37	0.50
10:B:330:PHE:CE1	10:B:334:MET:HE1	2.46	0.50
4:f:40:GLN:NE2	4:f:44:ASP:OD2	2.43	0.50
6:h:142:ALA:HB2	6:h:179:LEU:HD21	1.92	0.50
10:B:661:VAL:HG22	10:B:676:LEU:CD2	2.42	0.50
11:A:983:LEU:CD2	11:A:985:ILE:HG23	2.42	0.50
11:a:201:ILE:HG22	11:a:201:ILE:O	2.11	0.50
4:f:99:LEU:HD12	4:f:123:PRO:CG	2.42	0.50
10:b:447:GLU:N	10:b:447:GLU:OE1	2.43	0.50
11:a:1046:ASN:OD1	11:a:1047:SER:N	2.45	0.50
11:A:737:ASN:ND2	11:A:775:ALA:O	2.45	0.50
11:A:759:GLU:N	11:A:759:GLU:OE1	2.43	0.50
7:j:172:ARG:NH1	8:k:52:GLN:O	2.45	0.50
11:a:654:LEU:HD13	11:a:801:LEU:HD21	1.93	0.50
3:E:235:GLU:N	3:E:235:GLU:OE1	2.45	0.49
1:c:233:ASP:OD1	1:c:233:ASP:N	2.45	0.49
10:b:1033:GLY:O	10:b:1082:ASN:OD1	2.30	0.49
11:a:99:LEU:HD23	11:a:126:VAL:HG23	1.94	0.49
3:E:63:ILE:HD11	4:F:45:TYR:CB	2.42	0.49
4:I:77:LEU:HD22	4:I:89:VAL:HG21	1.94	0.49
10:B:331:ILE:HD12	10:B:355:LEU:HD11	1.94	0.49
11:A:21:ILE:HD11	11:A:113:MET:SD	2.53	0.49
1:c:558:LEU:HD21	10:b:1100:LEU:HD21	1.93	0.49
3:e:135:SER:O	3:e:139:ILE:HD12	2.12	0.49
4:i:154:MET:O	4:i:156:GLN:NE2	2.45	0.49
11:a:1040:LEU:HD13	11:a:1080:ILE:CD1	2.42	0.49
5:G:118:ASN:O	5:G:121:SER:N	2.45	0.49
10:B:870:ILE:HD12	10:B:903:TYR:OH	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:90:ILE:HG13	3:e:95:THR:HG22	1.93	0.49
2:d:20:ILE:O	2:d:20:ILE:HG22	2.13	0.49
2:D:95:LEU:HD22	10:B:315:ILE:CD1	2.41	0.49
2:D:146:ILE:HG22	2:D:146:ILE:O	2.13	0.49
11:A:1260:ARG:HH22	11:A:1285:ILE:HD12	1.77	0.49
10:b:1044:TRP:NE1	10:b:1074:ASN:O	2.44	0.49
10:B:693:VAL:HG23	10:B:703:LEU:HD11	1.94	0.49
11:a:1280:ASP:OD1	11:a:1281:SER:N	2.46	0.49
10:B:776:ILE:HB	10:B:783:PHE:HB2	1.95	0.49
11:A:1260:ARG:NH2	11:A:1285:ILE:HD12	2.28	0.49
2:D:88:ILE:HD13	2:D:109:PHE:CE2	2.48	0.48
4:I:171:ASP:OD1	4:I:172:SER:N	2.46	0.48
10:b:540:LEU:HD21	10:b:544:PHE:HB2	1.94	0.48
11:a:1049:ILE:O	11:a:1049:ILE:HG22	2.13	0.48
4:I:37:ILE:HD12	7:J:65:LEU:HD11	1.93	0.48
11:a:655:ARG:NE	11:a:736:GLN:OE1	2.46	0.48
1:C:269:ILE:HD11	1:C:274:GLN:NE2	2.28	0.48
4:F:115:PHE:CE1	4:F:178:VAL:HG11	2.48	0.48
11:A:324:LEU:O	11:A:327:SER:OG	2.25	0.48
11:a:999:SER:OG	11:a:1043:ASP:OD2	2.30	0.48
11:a:1186:GLU:N	11:a:1186:GLU:OE1	2.46	0.48
9:l:167:PHE:HE1	9:l:171:ILE:HD11	1.77	0.48
10:b:673:ALA:C	10:b:674:LEU:HD12	2.38	0.48
11:A:660:ASN:OD1	11:A:661:ARG:N	2.46	0.48
6:h:29:ASN:N	6:h:32:GLU:OE2	2.43	0.48
11:a:96:ILE:HD11	11:a:120:LEU:CD2	2.44	0.48
3:E:153:LEU:O	3:E:155:LEU:N	2.46	0.48
10:B:536:LEU:HD23	10:B:537:MET:N	2.28	0.48
7:j:72:GLN:OE1	7:j:75:ARG:NH2	2.44	0.48
5:G:58:LEU:HD12	5:G:58:LEU:O	2.13	0.48
10:B:505:PHE:O	10:B:509:LEU:HD23	2.14	0.48
4:f:15:GLU:OE2	4:f:15:GLU:N	2.47	0.48
7:j:233:VAL:O	7:j:237:ILE:HD12	2.14	0.48
10:b:1098:SER:O	11:a:1219:LYS:NZ	2.46	0.48
1:C:237:SER:O	1:C:240:SER:OG	2.27	0.48
4:F:135:MET:O	4:F:169:ARG:NH2	2.46	0.48
8:K:12:ASP:OD2	11:A:528:ARG:NE	2.47	0.48
10:b:830:ASP:OD2	10:b:830:ASP:N	2.47	0.48
8:K:169:ALA:HB1	8:K:173:LEU:HD12	1.95	0.48
10:b:860:ASN:OD1	10:b:861:THR:N	2.45	0.48
11:a:10:TYR:CD2	11:a:324:LEU:HD22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:849:GLN:C	11:a:850:LEU:HD12	2.39	0.48
9:l:55:ILE:HD11	9:l:171:ILE:HG21	1.96	0.47
11:A:322:CYS:O	11:A:326:LEU:HD23	2.14	0.47
7:j:199:LEU:HD12	7:j:210:MET:O	2.14	0.47
11:a:1213:ILE:CG2	11:a:1237:LEU:HD22	2.44	0.47
2:D:45:ASP:O	10:B:424:ARG:NH1	2.47	0.47
11:A:654:LEU:O	11:A:654:LEU:HD23	2.14	0.47
11:A:1043:ASP:N	11:A:1043:ASP:OD1	2.47	0.47
4:I:29:LEU:HD13	7:J:191:LEU:CD2	2.43	0.47
8:K:93:ASP:OD1	8:K:94:HIS:N	2.45	0.47
9:l:126:ASN:OD1	9:l:127:LYS:N	2.47	0.47
3:e:59:ILE:HD11	4:f:45:TYR:HD1	1.79	0.47
10:b:936:GLU:OE1	10:b:936:GLU:N	2.47	0.47
11:a:654:LEU:O	11:a:654:LEU:HD23	2.13	0.47
10:b:988:VAL:HG21	10:b:1078:VAL:HG21	1.95	0.47
11:a:96:ILE:HD11	11:a:120:LEU:HD22	1.97	0.47
8:K:85:ASP:OD1	8:K:86:ASN:N	2.47	0.47
11:A:854:SER:OG	11:A:876:THR:OG1	2.09	0.47
4:f:49:PHE:CE2	4:f:134:ALA:HB2	2.50	0.47
11:a:99:LEU:HD23	11:a:126:VAL:CG2	2.45	0.47
11:a:144:GLU:N	11:a:144:GLU:OE1	2.47	0.47
9:l:80:SER:O	9:l:114:ASN:ND2	2.47	0.47
10:B:712:ILE:O	10:B:712:ILE:HG23	2.15	0.47
11:A:24:GLY:O	1:c:150:SER:OG	2.32	0.47
5:g:142:ASN:O	5:g:146:ILE:HD12	2.15	0.47
4:F:115:PHE:CZ	4:F:178:VAL:HG11	2.50	0.47
5:G:54:ILE:HD12	6:H:36:LEU:HG	1.97	0.47
6:H:113:ASN:OD1	6:H:114:TRP:N	2.48	0.47
10:B:363:TRP:HE1	10:B:395:THR:HG21	1.79	0.47
4:i:166:ASP:OD1	4:i:167:ILE:N	2.48	0.47
10:b:694:GLN:CD	10:b:741:ILE:HD12	2.40	0.47
11:a:777:SER:OG	11:a:778:ILE:N	2.48	0.47
10:B:540:LEU:HD21	10:B:544:PHE:HB2	1.97	0.47
10:b:505:PHE:O	10:b:509:LEU:HD23	2.15	0.47
11:a:445:LEU:HD23	11:a:497:LEU:HD11	1.96	0.47
11:a:750:LEU:HD21	11:a:760:ILE:CD1	2.45	0.47
4:F:173:GLN:OE1	4:F:173:GLN:N	2.48	0.46
10:B:572:PRO:O	10:B:603:LYS:NZ	2.35	0.46
11:A:624:ASN:O	11:A:627:GLU:N	2.46	0.46
11:A:771:TYR:CE2	11:A:783:LEU:HD21	2.47	0.46
5:G:110:ILE:CD1	5:G:148:VAL:HG13	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:173:GLN:OE1	4:f:173:GLN:N	2.49	0.46
11:a:320:SER:HB2	11:a:416:ILE:HG21	1.97	0.46
11:a:1040:LEU:HD13	11:a:1080:ILE:HD11	1.98	0.46
1:C:414:PHE:CZ	1:C:431:LEU:HD13	2.51	0.46
4:I:102:THR:HG23	4:I:102:THR:O	2.16	0.46
10:B:766:TYR:HH	10:B:791:SER:HG	1.61	0.46
2:d:123:PRO:O	4:f:39:ALA:HB2	2.15	0.46
2:d:129:ASP:OD1	2:d:131:LYS:NZ	2.25	0.46
4:f:83:LEU:HD21	4:f:180:LEU:HD13	1.98	0.46
8:k:126:ASP:OD1	8:k:127:ASP:N	2.47	0.46
11:a:425:ASP:O	11:a:428:LEU:HD12	2.15	0.46
11:a:1043:ASP:N	11:a:1043:ASP:OD1	2.46	0.46
6:H:8:VAL:HG23	6:H:16:ILE:CG1	2.45	0.46
7:J:97:ARG:NH1	8:K:145:LEU:O	2.49	0.46
7:j:212:VAL:HG12	7:j:265:VAL:HG23	1.97	0.46
8:k:128:ASN:OD1	8:k:129:ASN:N	2.48	0.46
10:b:926:THR:O	10:b:930:ILE:HD12	2.16	0.46
11:a:588:GLN:OE1	11:a:619:TYR:OH	2.14	0.46
4:F:83:LEU:CD2	4:F:180:LEU:HD13	2.42	0.46
3:e:200:GLU:OE1	5:g:141:THR:OG1	2.30	0.46
11:a:298:ASP:HA	11:a:301:THR:HG22	1.97	0.46
3:E:137:LEU:HD22	3:E:139:ILE:HG22	1.95	0.46
4:F:128:VAL:O	4:F:128:VAL:HG12	2.15	0.46
11:A:567:ILE:HD13	11:A:588:GLN:HE21	1.81	0.46
11:a:339:VAL:HA	11:a:342:ILE:HG22	1.96	0.46
5:G:111:TYR:O	5:G:115:VAL:N	2.44	0.46
10:b:582:LEU:HD13	10:b:625:PHE:CD1	2.51	0.46
5:G:82:THR:HG21	5:G:107:TYR:CE1	2.50	0.46
11:A:445:LEU:HD23	11:A:497:LEU:HD11	1.98	0.46
11:A:652:PHE:HD1	11:A:816:ILE:HD13	1.81	0.46
10:b:678:SER:OG	10:b:722:PHE:O	2.31	0.46
11:a:657:VAL:HG22	11:a:657:VAL:O	2.15	0.46
10:B:1038:ILE:HG12	10:B:1078:VAL:HG12	1.99	0.46
11:A:999:SER:OG	11:A:1043:ASP:OD2	2.34	0.46
4:f:53:ASN:O	4:f:142:ASN:ND2	2.49	0.46
2:D:20:ILE:HG21	2:D:37:ASN:OD1	2.15	0.45
11:A:4:LEU:O	11:A:4:LEU:HD12	2.17	0.45
2:d:81:GLN:N	2:d:81:GLN:OE1	2.49	0.45
8:k:39:PHE:CE1	11:a:591:ILE:HD11	2.50	0.45
11:a:165:ALA:O	11:a:169:LEU:HD23	2.17	0.45
11:a:891:ILE:HD12	11:a:966:ILE:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:1057:GLN:HG2	11:a:1062:THR:HG22	1.97	0.45
11:a:1194:THR:HG21	11:a:1241:ILE:HD12	1.99	0.45
4:F:91:SER:CB	4:F:105:ILE:HD11	2.46	0.45
11:A:289:TYR:CE1	11:A:325:LEU:HD23	2.51	0.45
4:f:7:SER:OG	4:f:8:ARG:N	2.49	0.45
11:a:1023:MET:HE3	11:a:1023:MET:HA	1.98	0.45
4:F:26:ASN:OD1	4:F:29:LEU:N	2.49	0.45
10:B:306:ILE:HD11	10:B:334:MET:SD	2.56	0.45
8:k:136:GLU:HB3	8:k:168:LEU:HD21	1.98	0.45
6:H:186:TYR:OH	6:H:191:MET:HE3	2.17	0.45
10:B:827:ILE:HD12	10:B:835:PHE:HB3	1.98	0.45
11:A:639:SER:HG	11:A:644:SER:HG	1.57	0.45
11:A:731:PHE:CE1	11:A:760:ILE:HD12	2.51	0.45
4:i:155:VAL:HG12	4:i:155:VAL:O	2.15	0.45
11:a:1194:THR:HG21	11:a:1241:ILE:CD1	2.46	0.45
4:I:136:LYS:O	4:I:169:ARG:NH2	2.49	0.45
7:j:227:VAL:HG13	7:j:227:VAL:O	2.17	0.45
7:j:234:CYS:SG	7:j:252:ALA:HB2	2.56	0.45
11:a:613:SER:O	11:a:617:THR:HG22	2.17	0.45
11:a:1091:GLU:OE1	11:a:1091:GLU:N	2.48	0.45
6:H:50:LEU:HD23	6:H:50:LEU:O	2.17	0.45
11:a:795:ILE:HD12	11:a:840:LYS:HE3	1.98	0.45
11:A:1056:VAL:HG11	11:A:1076:ILE:HG21	1.98	0.45
2:d:88:ILE:HD11	2:d:109:PHE:HE1	1.80	0.45
5:g:65:ASN:ND2	6:h:126:GLN:OE1	2.49	0.45
4:i:81:GLU:OE2	4:i:81:GLU:N	2.49	0.45
10:b:412:GLU:O	10:b:416:LEU:HD23	2.17	0.45
13:n:60:UNK:O	13:n:63:UNK:N	2.50	0.45
2:D:29:GLU:OE1	2:D:31:ASN:N	2.49	0.45
3:e:107:GLU:O	3:e:111:ALA:HB2	2.17	0.45
7:J:45:ILE:HG23	7:J:46:TYR:CD1	2.52	0.45
9:l:146:MET:HE1	11:a:699:PHE:CE2	2.52	0.45
11:A:20:VAL:HG11	11:A:35:VAL:HG22	1.98	0.45
1:c:500:ILE:HG21	11:a:1003:ILE:CD1	2.46	0.45
4:i:100:ASN:OD1	7:j:56:GLU:O	2.35	0.45
10:b:597:SER:OG	10:b:598:ASP:N	2.50	0.45
10:b:889:TRP:CZ3	10:b:935:ILE:HD12	2.51	0.45
13:N:6:UNK:O	13:N:8:UNK:N	2.49	0.45
10:B:661:VAL:HG22	10:B:676:LEU:HD22	1.99	0.44
9:l:169:GLU:HA	9:l:172:VAL:HG12	1.99	0.44
8:k:95:PHE:O	8:k:97:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:708:SER:OG	10:b:711:GLU:O	2.35	0.44
3:E:63:ILE:HD11	4:F:45:TYR:HB3	2.00	0.44
11:a:906:TRP:CZ3	11:a:1105:ILE:HD12	2.51	0.44
4:F:53:ASN:ND2	4:F:137:SER:O	2.51	0.44
6:H:43:VAL:HA	6:H:46:ILE:HG22	2.00	0.44
11:A:872:ASP:OD1	11:A:872:ASP:N	2.51	0.44
1:C:512:VAL:O	1:C:512:VAL:HG23	2.18	0.44
4:F:105:ILE:HG21	4:F:108:TRP:HE1	1.83	0.44
11:A:1035:ARG:NH2	11:A:1282:GLU:OE2	2.51	0.44
2:d:45:ASP:OD1	2:d:46:TYR:N	2.51	0.44
10:b:1046:ILE:HD12	10:b:1065:LEU:HD23	1.99	0.44
1:c:264:ILE:HD12	1:c:317:LEU:HD22	2.00	0.44
2:d:21:TYR:OH	2:d:142:ASP:OD1	2.15	0.44
4:i:9:SER:C	4:i:10:LEU:HD22	2.43	0.44
10:b:558:ASN:ND2	10:b:657:THR:O	2.51	0.44
11:a:1004:PRO:HB3	11:a:1038:ILE:HG22	1.98	0.44
4:I:48:ASP:OD2	4:I:51:LYS:NZ	2.30	0.44
8:K:47:ILE:HD11	11:A:491:TYR:CZ	2.52	0.44
11:A:958:ASN:OD1	11:A:958:ASN:N	2.51	0.44
4:i:38:VAL:HG11	4:i:140:TYR:CE1	2.52	0.44
3:E:217:ILE:O	3:E:221:ILE:HD12	2.17	0.44
10:B:479:LEU:HD13	10:B:485:LEU:HD13	2.00	0.44
11:a:1060:ASP:OD1	11:a:1061:PHE:N	2.51	0.44
2:D:68:GLN:OE1	2:D:68:GLN:N	2.51	0.43
3:E:44:VAL:HG21	14:F:201:PLM:HG3	1.99	0.43
4:F:37:ILE:O	4:F:41:LEU:HD23	2.18	0.43
4:i:9:SER:O	4:i:10:LEU:HD22	2.18	0.43
10:b:1020:LEU:HD23	10:b:1020:LEU:O	2.18	0.43
10:b:1046:ILE:HD11	10:b:1063:VAL:HG21	2.00	0.43
11:a:437:GLN:OE1	11:a:505:MET:HE2	2.18	0.43
8:K:47:ILE:HD11	11:A:491:TYR:CE2	2.53	0.43
9:l:153:THR:OG1	9:l:162:ASN:OD1	2.34	0.43
10:B:586:ASN:OD1	10:B:587:MET:N	2.51	0.43
11:A:139:THR:O	11:A:142:THR:OG1	2.36	0.43
11:a:58:THR:HG22	11:a:60:GLN:H	1.83	0.43
10:B:785:LYS:NZ	11:A:1227:SER:OG	2.31	0.43
11:a:750:LEU:HD12	11:a:798:ILE:HD11	1.99	0.43
11:a:1002:ILE:HD13	11:a:1040:LEU:HD12	2.00	0.43
2:D:12:ASP:OD2	2:D:14:SER:OG	2.36	0.43
2:D:41:ASN:OD1	10:B:430:ILE:HD11	2.18	0.43
11:A:851:GLU:OE1	11:A:878:ARG:NH2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:20:ILE:HD13	2:d:37:ASN:OD1	2.19	0.43
5:g:51:LEU:HD21	6:h:43:VAL:HG11	2.00	0.43
10:b:364:VAL:HA	10:b:367:VAL:HG22	1.99	0.43
11:a:4:LEU:HD11	11:a:557:LEU:HD13	1.99	0.43
11:a:928:CYS:SG	11:a:929:VAL:N	2.83	0.43
1:c:531:TYR:HD1	1:c:558:LEU:HD13	1.82	0.43
11:A:727:ASP:OD1	11:A:727:ASP:N	2.51	0.43
8:k:105:SER:OG	8:k:106:TYR:N	2.50	0.43
5:G:51:LEU:HD21	6:H:122:LEU:HD12	2.00	0.43
6:H:53:LYS:HE3	6:H:53:LYS:HA	2.01	0.43
11:A:310:LEU:HD11	11:A:435:ALA:HA	2.00	0.43
11:A:538:MET:HE1	11:A:598:VAL:HG11	2.01	0.43
11:A:995:ILE:HD12	11:A:1054:LEU:HD11	2.01	0.43
4:f:49:PHE:HA	4:f:52:VAL:HG12	2.00	0.43
10:b:661:VAL:HG23	10:b:676:LEU:CD2	2.49	0.43
10:b:988:VAL:HG12	10:b:1017:VAL:HG22	2.01	0.43
11:a:850:LEU:HD13	11:a:968:TYR:CD1	2.54	0.43
1:C:431:LEU:HD11	1:C:551:VAL:HG21	2.00	0.43
3:e:245:ARG:NH1	3:e:246:PRO:O	2.52	0.43
10:b:433:ILE:O	10:b:437:LEU:HD23	2.19	0.43
11:a:929:VAL:CG2	11:a:948:LEU:HD21	2.49	0.43
1:C:431:LEU:HD11	1:C:551:VAL:CG2	2.48	0.43
11:A:962:PHE:O	11:A:987:TYR:N	2.50	0.43
11:a:647:SER:OG	11:a:648:TYR:N	2.50	0.43
1:c:263:GLU:HG3	1:c:318:ALA:HB3	2.00	0.42
10:b:973:LEU:CD2	10:b:975:VAL:HG23	2.49	0.42
11:a:906:TRP:HZ3	11:a:1105:ILE:HD12	1.84	0.42
6:H:135:LEU:HD11	4:I:79:ARG:NH1	2.34	0.42
7:J:96:ILE:HD13	7:J:243:ASN:CB	2.49	0.42
11:A:316:LEU:HD22	11:A:416:ILE:HG23	2.01	0.42
11:a:1092:ASN:O	11:a:1092:ASN:ND2	2.48	0.42
1:C:406:LYS:C	1:C:407:LEU:HD23	2.44	0.42
2:D:95:LEU:HD23	2:D:97:GLY:N	2.33	0.42
3:e:108:LEU:HD12	3:e:119:VAL:HG11	2.01	0.42
10:b:625:PHE:CE2	10:b:627:ILE:HD11	2.53	0.42
3:E:38:PRO:HB2	4:F:27:THR:HG21	2.01	0.42
4:I:37:ILE:CD1	7:J:65:LEU:HD11	2.49	0.42
10:B:584:LEU:HD12	10:B:594:PHE:HE2	1.85	0.42
10:b:867:ASP:OD1	10:b:903:TYR:OH	2.25	0.42
1:C:443:LEU:HD12	1:C:540:VAL:HG21	2.00	0.42
8:K:90:GLY:O	8:K:92:VAL:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:l:19:ILE:HD11	9:l:107:TRP:CZ3	2.55	0.42
10:b:818:ASP:OD1	10:b:818:ASP:N	2.52	0.42
7:j:49:SER:OG	7:j:50:LEU:N	2.51	0.42
11:a:1108:GLY:O	11:a:1109:LEU:HD12	2.19	0.42
9:l:32:ARG:NH2	9:l:160:SER:OG	2.53	0.42
3:e:138:LEU:HD12	3:e:164:VAL:HG22	2.02	0.42
8:k:85:ASP:OD1	8:k:86:ASN:N	2.53	0.42
10:b:616:MET:HE2	10:b:758:THR:HG21	2.01	0.42
4:F:72:LEU:O	4:F:76:ALA:N	2.53	0.42
8:K:136:GLU:HB3	8:K:168:LEU:HD21	2.01	0.42
1:c:505:ASN:OD1	1:c:506:ASP:N	2.51	0.42
3:e:238:CYS:C	3:e:239:LEU:HD22	2.45	0.42
6:H:191:MET:HE1	4:I:69:GLU:HG3	2.00	0.42
6:H:200:MET:HE3	6:H:200:MET:HA	2.02	0.42
10:B:407:LEU:HD12	10:B:438:LEU:HD22	2.02	0.42
10:B:1033:GLY:O	10:B:1082:ASN:ND2	2.52	0.42
2:d:35:LYS:O	2:d:39:LEU:HD23	2.20	0.42
10:b:527:ASP:OD1	10:b:528:LEU:N	2.53	0.42
11:a:3:ILE:HG23	11:a:4:LEU:N	2.35	0.42
11:a:172:LEU:HD21	11:a:282:PHE:CD1	2.54	0.42
5:G:54:ILE:HD11	6:H:39:THR:OG1	2.20	0.42
10:B:612:CYS:SG	10:B:613:ARG:N	2.93	0.42
10:B:699:ASN:C	10:B:700:MET:HE2	2.44	0.42
4:f:183:ILE:HG23	4:f:183:ILE:O	2.20	0.42
7:j:73:LEU:HD22	7:j:86:LYS:HB3	2.02	0.42
10:b:453:LEU:HD11	10:b:488:LEU:HB3	2.01	0.42
11:a:67:LEU:HD21	11:a:165:ALA:HB1	2.02	0.42
11:a:962:PHE:O	11:a:987:TYR:N	2.53	0.42
11:a:994:THR:HG21	11:a:1135:TRP:CZ2	2.54	0.42
4:I:83:LEU:HA	4:I:86:THR:HG22	2.02	0.41
4:f:178:VAL:O	4:f:178:VAL:HG13	2.20	0.41
11:A:912:ASP:OD1	11:A:913:ASP:N	2.53	0.41
3:e:55:LEU:HD21	4:f:37:ILE:HG23	2.01	0.41
3:e:238:CYS:O	3:e:239:LEU:HD22	2.20	0.41
7:j:100:GLU:OE1	8:k:105:SER:OG	2.37	0.41
10:b:310:ILE:HA	10:b:313:ILE:HG22	2.02	0.41
11:a:672:ILE:HD12	11:a:672:ILE:H	1.84	0.41
10:B:528:LEU:HD23	10:B:529:GLN:N	2.35	0.41
11:A:303:LEU:HD21	11:A:311:TRP:HB2	2.01	0.41
2:d:19:LEU:HD21	2:d:21:TYR:HB2	2.01	0.41
10:b:407:LEU:HD13	10:b:435:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:a:289:TYR:CE1	11:a:325:LEU:HD23	2.54	0.41
11:a:958:ASN:OD1	11:a:958:ASN:N	2.52	0.41
11:a:1031:ASN:OD1	11:a:1032:LEU:N	2.53	0.41
10:B:582:LEU:HD13	10:B:625:PHE:HD1	1.86	0.41
11:A:538:MET:HE3	11:A:598:VAL:HG11	1.98	0.41
3:e:208:LEU:HA	3:e:211:ILE:HG22	2.02	0.41
4:f:155:VAL:HG12	4:f:155:VAL:O	2.20	0.41
10:b:522:TRP:CH2	10:b:526:MET:HE3	2.56	0.41
11:a:1217:ASP:O	11:a:1218:SER:OG	2.33	0.41
2:D:140:LYS:O	2:D:144:LEU:HD23	2.20	0.41
11:A:125:LEU:CD2	11:A:146:VAL:HG12	2.49	0.41
11:A:1179:GLU:OE1	11:A:1179:GLU:N	2.54	0.41
3:e:123:LEU:HD11	3:e:217:ILE:CG2	2.50	0.41
5:G:28:ALA:O	5:G:30:GLY:N	2.53	0.41
4:I:33:THR:O	4:I:36:SER:OG	2.25	0.41
10:B:331:ILE:HG23	10:B:355:LEU:HD11	2.02	0.41
10:B:666:ASN:O	10:B:726:ARG:NH1	2.53	0.41
10:b:364:VAL:HG21	10:b:375:LEU:HD23	2.02	0.41
11:A:648:TYR:HE1	11:A:805:ILE:HG21	1.86	0.41
5:G:32:ILE:HG22	5:G:33:ASN:OD1	2.21	0.41
11:A:1182:VAL:HG23	11:A:1288:VAL:HG23	2.02	0.41
4:i:188:ILE:HB	4:i:189:PRO:HD2	2.02	0.41
11:a:919:LYS:NZ	11:a:1150:ASN:OD1	2.54	0.41
1:C:228:ILE:HD12	1:C:341:LEU:HD11	2.03	0.41
2:D:148:THR:OG1	3:E:178:THR:O	2.22	0.41
3:E:55:LEU:HD22	4:F:59:MET:CE	2.51	0.41
4:F:54:ASP:OD1	4:F:55:HIS:N	2.54	0.41
5:G:6:PHE:CD2	5:G:90:LEU:HD13	2.54	0.41
6:H:140:PHE:HB3	6:H:179:LEU:HD22	2.02	0.41
6:H:192:LYS:NZ	4:I:70:ASP:OD2	2.54	0.41
10:B:394:GLU:OE1	10:B:394:GLU:N	2.54	0.41
10:B:546:VAL:HG11	10:B:625:PHE:CE2	2.55	0.41
11:A:312:LEU:O	11:A:312:LEU:HD23	2.21	0.41
4:f:33:THR:O	4:f:36:SER:OG	2.31	0.41
5:g:5:SER:O	5:g:90:LEU:HD12	2.20	0.41
5:g:43:LEU:HB2	6:h:46:ILE:HD11	2.02	0.41
4:i:28:GLU:HA	4:i:31:THR:HG22	2.03	0.41
10:b:1020:LEU:HD21	10:b:1023:GLN:CD	2.46	0.41
11:a:1003:ILE:HD11	11:a:1041:LEU:CD1	2.50	0.41
11:a:1095:ILE:HD12	11:a:1095:ILE:H	1.86	0.41
4:F:143:ILE:O	4:F:147:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:691:VAL:HG22	10:B:742:ILE:HG22	2.03	0.41
11:A:1095:ILE:HD12	11:A:1095:ILE:H	1.85	0.41
4:i:144:LEU:O	4:i:148:LEU:HD23	2.21	0.41
7:j:73:LEU:HD21	7:j:90:TYR:CE2	2.56	0.41
11:a:815:ILE:HG21	11:a:837:GLY:O	2.21	0.41
3:E:55:LEU:HD13	4:F:59:MET:CE	2.51	0.40
11:A:1052:ILE:HG12	11:A:1137:LEU:HD23	2.04	0.40
3:e:168:ILE:HD13	3:e:221:ILE:HD13	2.02	0.40
10:b:1046:ILE:HD11	10:b:1063:VAL:CG2	2.51	0.40
11:a:46:LEU:HD12	11:a:65:GLY:HA3	2.02	0.40
11:A:23:ILE:HD12	1:c:151:PHE:CE2	2.56	0.40
11:A:1040:LEU:HD23	11:A:1042:LEU:HD21	2.03	0.40
11:A:1111:GLU:HA	11:A:1114:THR:HG22	2.03	0.40
11:A:1232:LEU:HD13	11:A:1256:ILE:HG13	2.03	0.40
2:D:20:ILE:HG22	2:D:20:ILE:O	2.21	0.40
10:B:769:LEU:HD23	10:B:770:SER:N	2.36	0.40
11:a:1175:LEU:HD21	11:a:1265:VAL:CG2	2.50	0.40
3:E:194:ILE:O	3:E:194:ILE:HG23	2.21	0.40
5:G:72:THR:OG1	5:G:73:GLY:N	2.55	0.40
10:B:860:ASN:OD1	10:B:861:THR:N	2.53	0.40
11:A:1116:GLU:OE2	11:A:1158:HIS:NE2	2.55	0.40
11:a:615:LEU:HD23	11:a:631:LEU:HD11	2.02	0.40
10:B:868:CYS:HA	10:B:871:THR:HG22	2.04	0.40
11:A:855:THR:HG23	11:A:875:ILE:HD13	2.03	0.40
11:A:1157:ASP:O	11:A:1161:VAL:HG23	2.22	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	C	276/560 (49%)	244 (88%)	32 (12%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	c	276/560 (49%)	252 (91%)	24 (9%)	0	100	100
2	D	142/152 (93%)	131 (92%)	11 (8%)	0	100	100
2	d	137/152 (90%)	119 (87%)	18 (13%)	0	100	100
3	E	208/268 (78%)	169 (81%)	39 (19%)	0	100	100
3	e	203/268 (76%)	177 (87%)	26 (13%)	0	100	100
4	F	182/193 (94%)	159 (87%)	23 (13%)	0	100	100
4	I	181/193 (94%)	167 (92%)	14 (8%)	0	100	100
4	f	184/193 (95%)	174 (95%)	10 (5%)	0	100	100
4	i	182/193 (94%)	160 (88%)	21 (12%)	1 (0%)	24	62
5	G	156/159 (98%)	130 (83%)	25 (16%)	1 (1%)	21	58
5	g	154/159 (97%)	128 (83%)	26 (17%)	0	100	100
6	H	173/219 (79%)	152 (88%)	21 (12%)	0	100	100
6	h	173/219 (79%)	151 (87%)	22 (13%)	0	100	100
7	J	204/283 (72%)	179 (88%)	25 (12%)	0	100	100
7	j	204/283 (72%)	181 (89%)	22 (11%)	1 (0%)	24	62
8	K	142/175 (81%)	128 (90%)	13 (9%)	1 (1%)	18	54
8	k	142/175 (81%)	129 (91%)	12 (8%)	1 (1%)	18	54
9	l	187/227 (82%)	161 (86%)	26 (14%)	0	100	100
10	B	781/1104 (71%)	696 (89%)	85 (11%)	0	100	100
10	b	781/1104 (71%)	706 (90%)	74 (10%)	1 (0%)	48	82
11	A	1094/1289 (85%)	973 (89%)	119 (11%)	2 (0%)	43	77
11	a	1100/1289 (85%)	981 (89%)	117 (11%)	2 (0%)	43	77
All	All	7262/9417 (77%)	6447 (89%)	805 (11%)	10 (0%)	49	82

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	b	682	ASP
4	i	188	ILE
11	A	476	LEU
11	a	476	LEU
5	G	22	THR
8	k	30	PRO
11	A	1273	GLN

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Mol	Chain	Res	Type
7	j	171	ARG
11	a	1273	GLN
8	K	30	PRO

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	C	270/518 (52%)	270 (100%)	0	100	100
1	c	270/518 (52%)	270 (100%)	0	100	100
2	D	133/142 (94%)	133 (100%)	0	100	100
2	d	128/142 (90%)	128 (100%)	0	100	100
3	E	195/248 (79%)	195 (100%)	0	100	100
3	e	192/248 (77%)	192 (100%)	0	100	100
4	F	170/178 (96%)	170 (100%)	0	100	100
4	I	169/178 (95%)	169 (100%)	0	100	100
4	f	171/178 (96%)	171 (100%)	0	100	100
4	i	169/178 (95%)	169 (100%)	0	100	100
5	G	143/145 (99%)	143 (100%)	0	100	100
5	g	142/145 (98%)	142 (100%)	0	100	100
6	H	162/199 (81%)	162 (100%)	0	100	100
6	h	162/199 (81%)	162 (100%)	0	100	100
7	J	188/249 (76%)	188 (100%)	0	100	100
7	j	188/249 (76%)	188 (100%)	0	100	100
8	K	132/152 (87%)	132 (100%)	0	100	100
8	k	132/152 (87%)	132 (100%)	0	100	100
9	l	161/194 (83%)	161 (100%)	0	100	100
10	B	729/1023 (71%)	729 (100%)	0	100	100
10	b	729/1023 (71%)	729 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	A	1046/1213 (86%)	1046 (100%)	0	100	100
11	a	1054/1213 (87%)	1053 (100%)	1 (0%)	88	88
All	All	6835/8684 (79%)	6834 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	a	1092	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	262	GLN
1	C	311	HIS
1	C	489	HIS
2	D	37	ASN
3	E	103	ASN
6	H	219	GLN
7	J	92	HIS
7	J	184	HIS
7	J	193	ASN
8	K	42	HIS
8	K	129	ASN
9	l	182	GLN
10	B	529	GLN
10	B	666	ASN
10	B	1019	ASN
11	A	173	ASN
11	A	847	GLN
11	A	1209	ASN
1	c	449	ASN
2	d	122	ASN
4	f	20	ASN
4	f	55	HIS
6	h	60	GLN
8	k	120	ASN
10	b	507	ASN
10	b	1082	ASN
11	a	6	HIS
11	a	430	HIS

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Mol	Chain	Res	Type
11	a	473	HIS
11	a	510	GLN
11	a	1006	ASN
11	a	1055	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
14	PLM	I	201	4	15,16,17	0.51	0	14,15,17	0.39	0
14	PLM	f	201	4	15,16,17	0.54	0	14,15,17	0.41	0
14	PLM	i	201	4	15,16,17	0.50	0	14,15,17	0.39	0
14	PLM	F	201	4	15,16,17	0.52	0	14,15,17	0.39	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
14	PLM	I	201	4	-	3/14/14/15	-
14	PLM	f	201	4	-	6/14/14/15	-
14	PLM	i	201	4	-	4/14/14/15	-
14	PLM	F	201	4	-	6/14/14/15	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	F	201	PLM	O2-C1-C2-C3
14	I	201	PLM	O2-C1-C2-C3
14	i	201	PLM	O2-C1-C2-C3
14	f	201	PLM	C2-C3-C4-C5
14	F	201	PLM	C2-C3-C4-C5
14	i	201	PLM	CB-CC-CD-CE
14	F	201	PLM	C4-C5-C6-C7
14	f	201	PLM	C4-C5-C6-C7
14	f	201	PLM	C3-C4-C5-C6
14	I	201	PLM	C7-C8-C9-CA
14	F	201	PLM	C3-C4-C5-C6
14	I	201	PLM	CB-CC-CD-CE
14	f	201	PLM	CD-CE-CF-CG
14	F	201	PLM	C7-C8-C9-CA
14	f	201	PLM	CB-CC-CD-CE
14	i	201	PLM	C7-C8-C9-CA
14	f	201	PLM	C7-C8-C9-CA
14	i	201	PLM	C8-C9-CA-CB
14	F	201	PLM	CD-CE-CF-CG

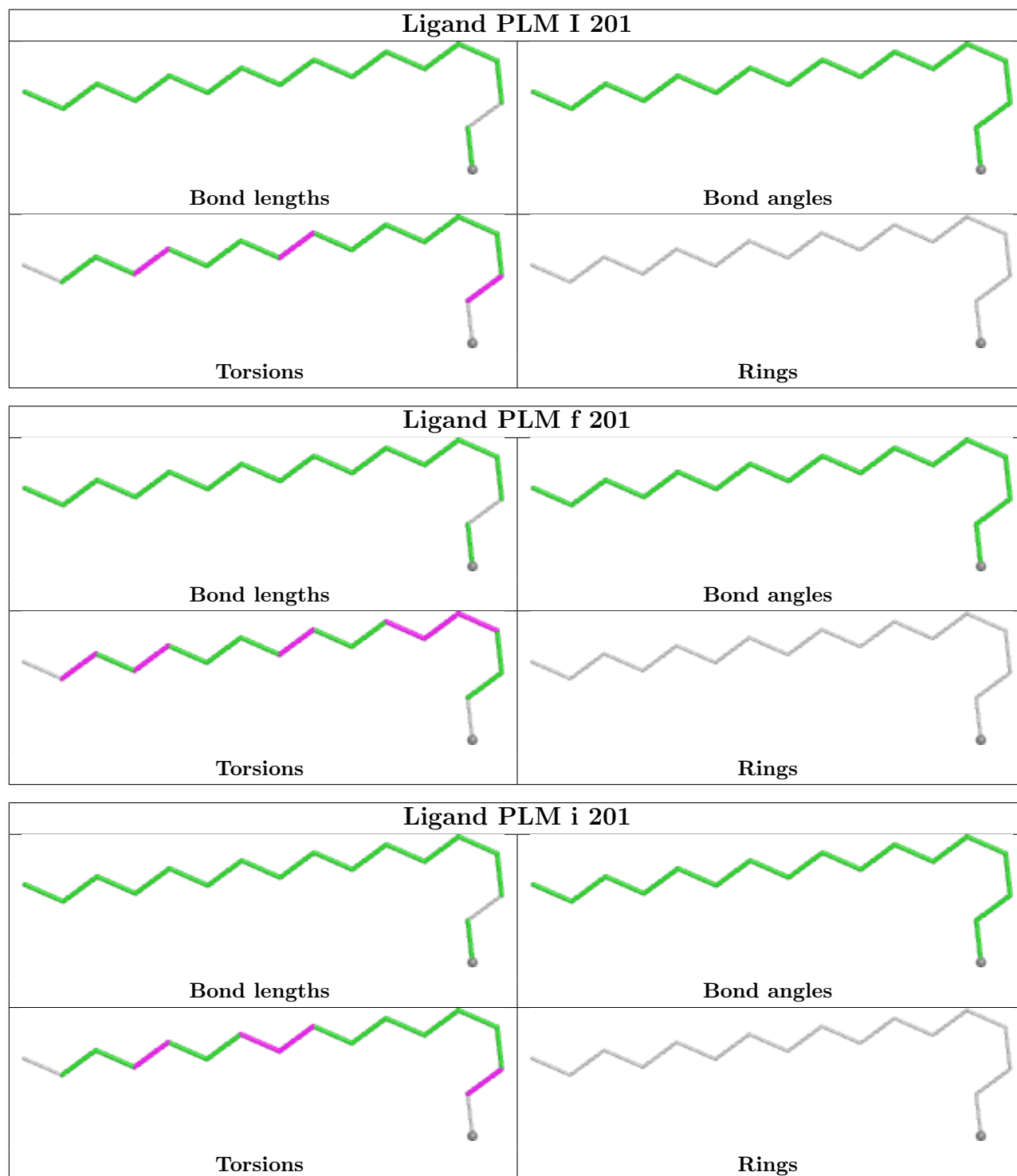
There are no ring outliers.

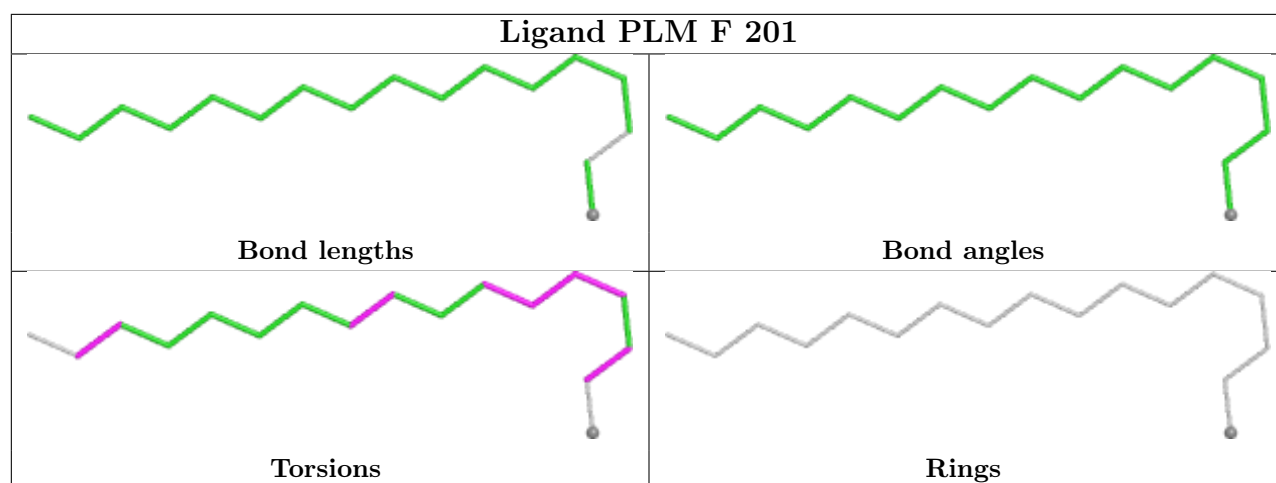
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	F	201	PLM	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 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-26255. These allow visual inspection of the internal detail of the map and identification of artifacts.

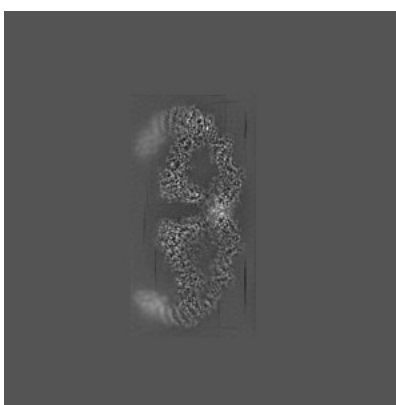
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

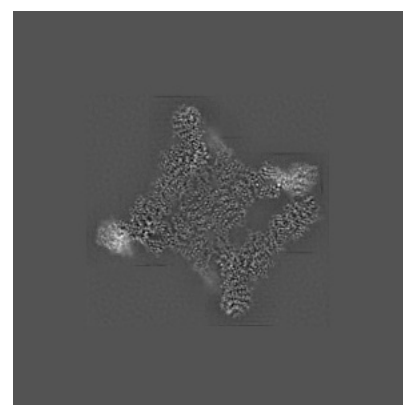
6.1.1 Primary map



X



Y



Z

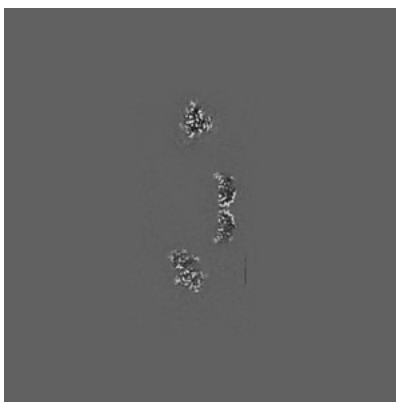
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

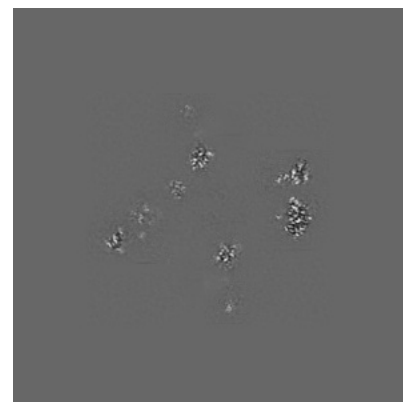
6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

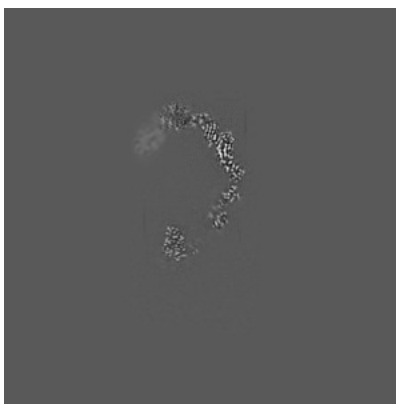
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

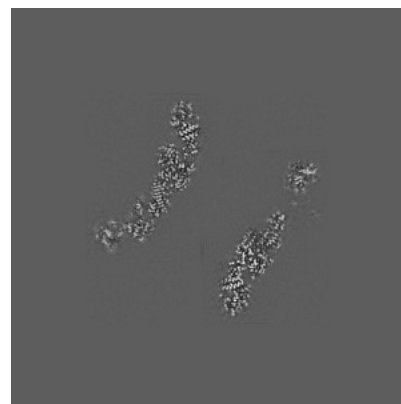
6.3.1 Primary map



X Index: 182



Y Index: 233

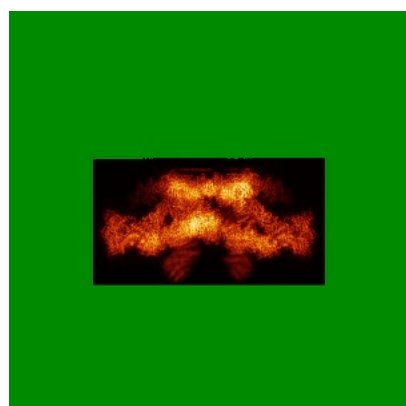


Z Index: 174

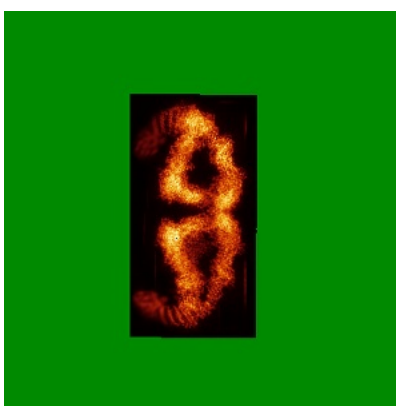
The images above show the largest variance slices of the map in three orthogonal directions.

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

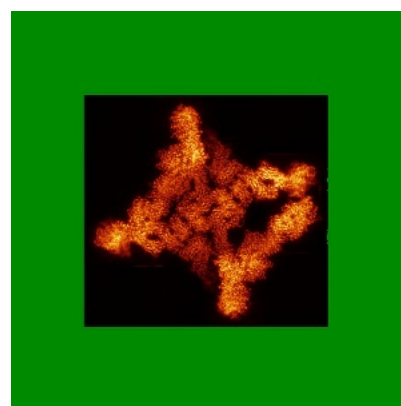
6.4.1 Primary map



X



Y

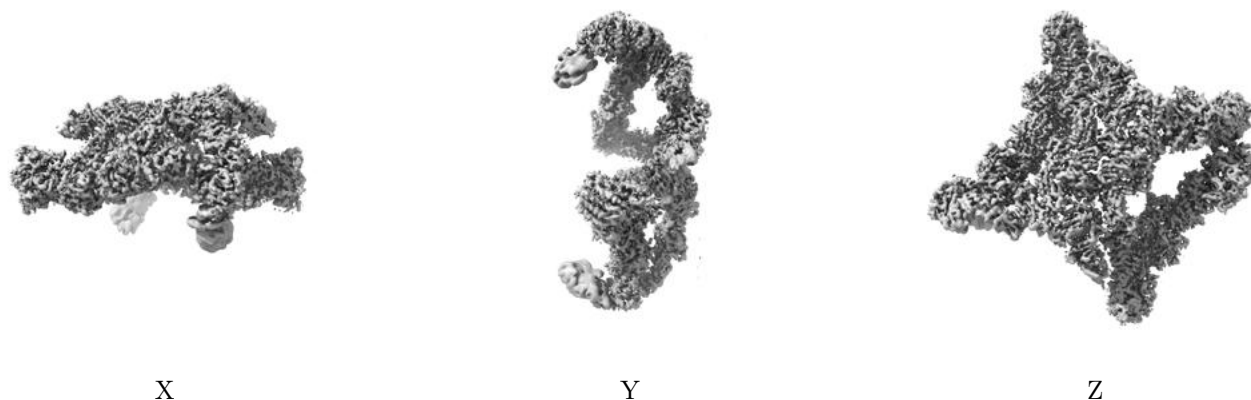


Z

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 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

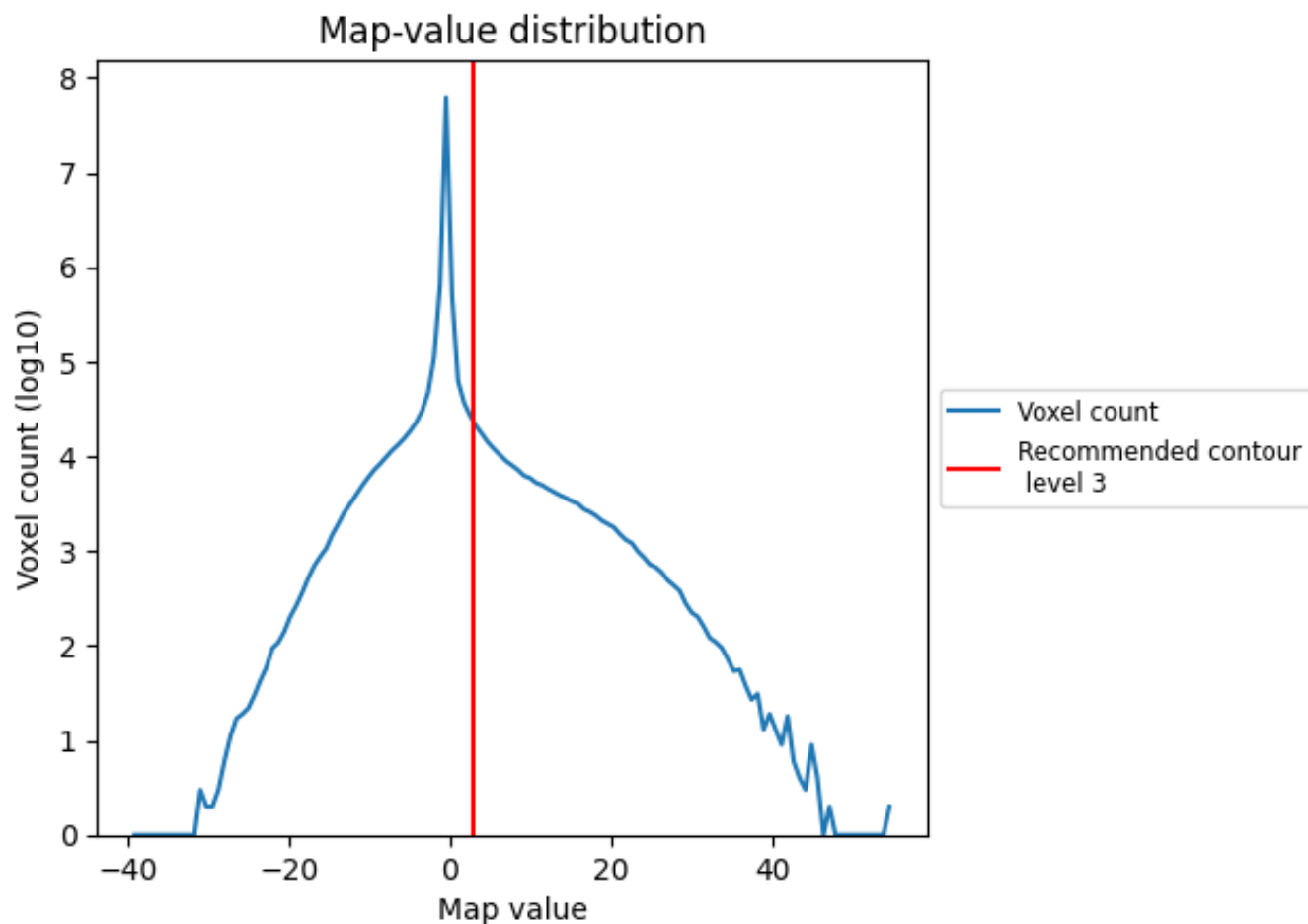
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

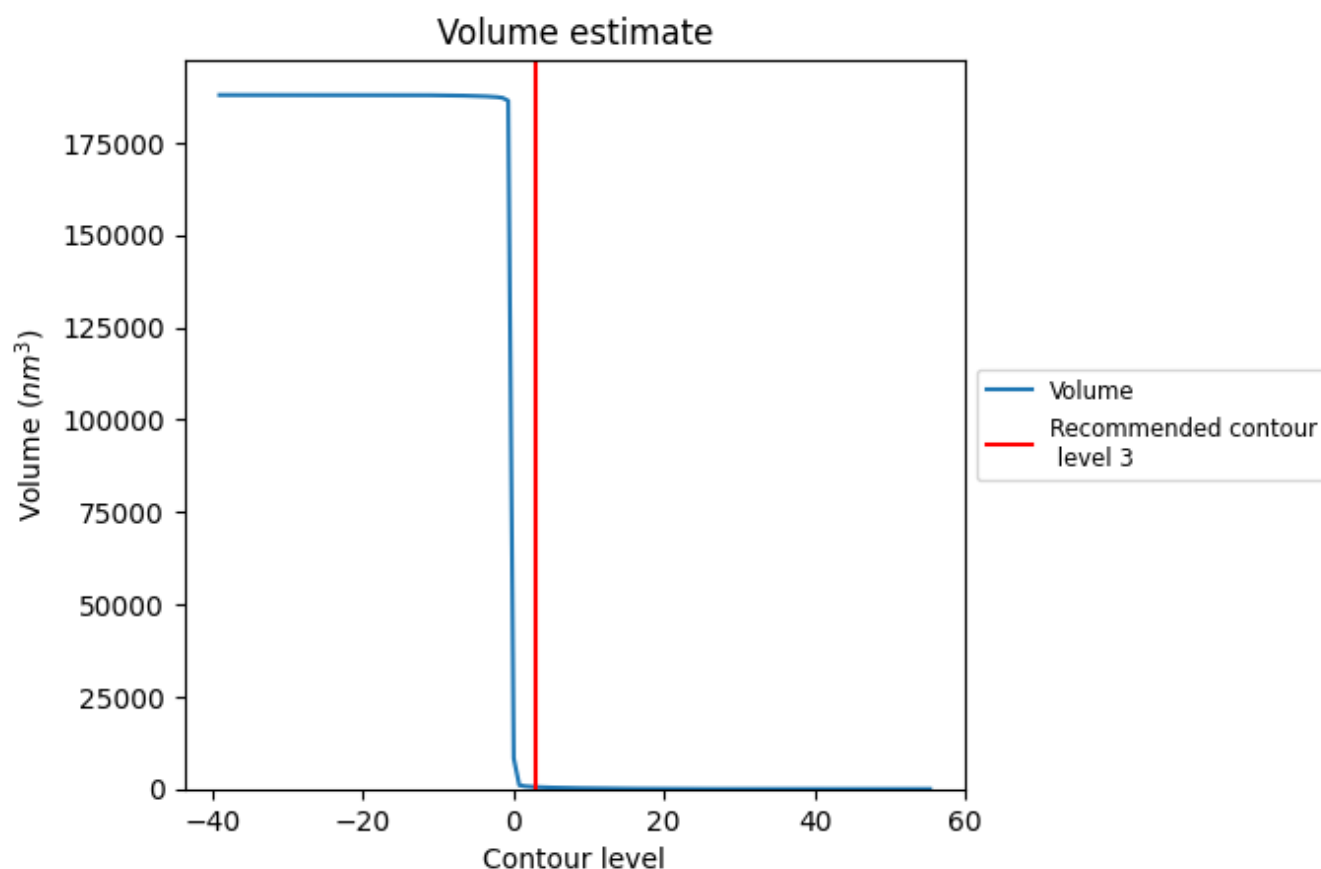
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

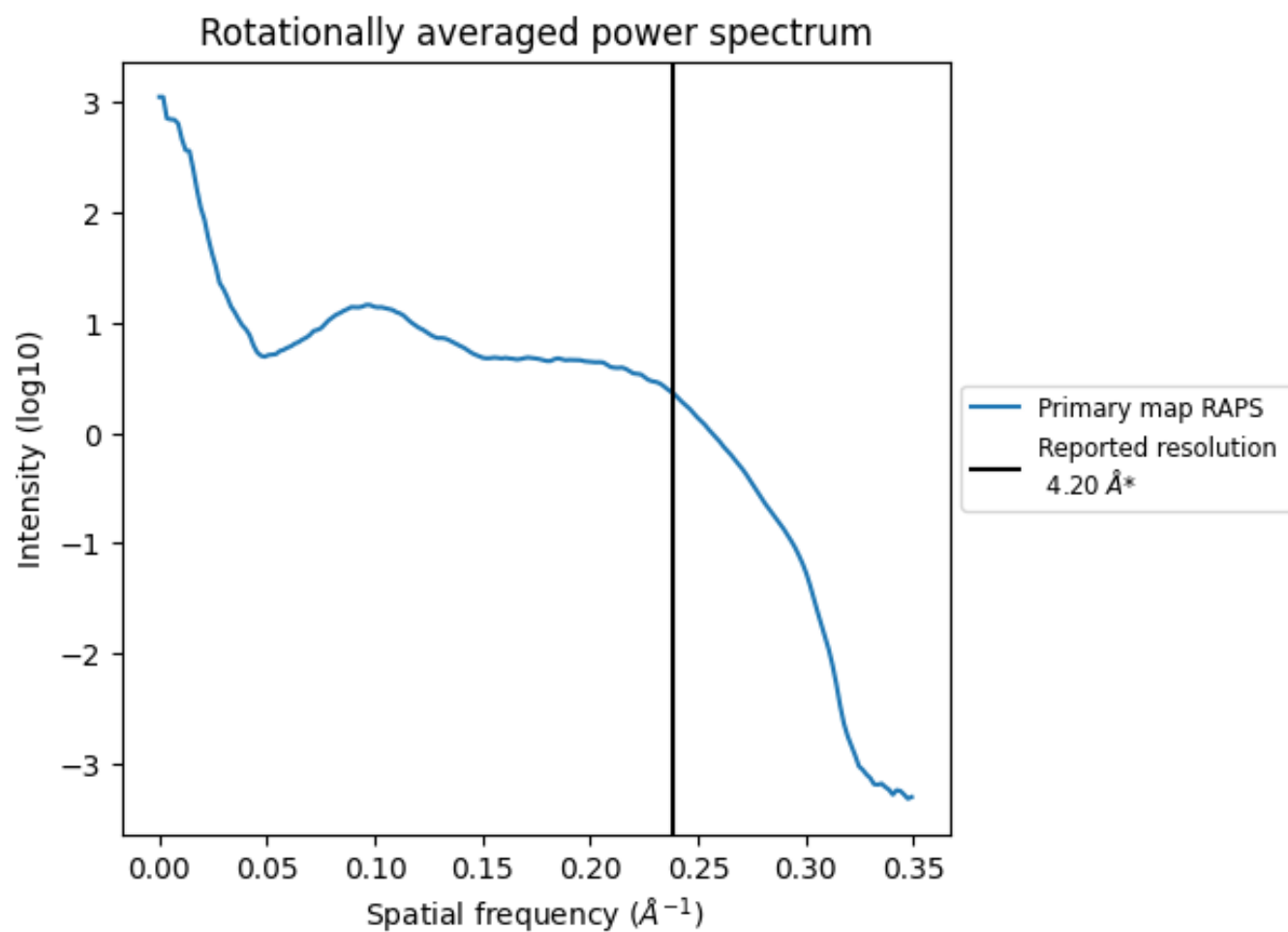
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 524 nm^3 ; this corresponds to an approximate mass of 474 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 0.238 Å⁻¹

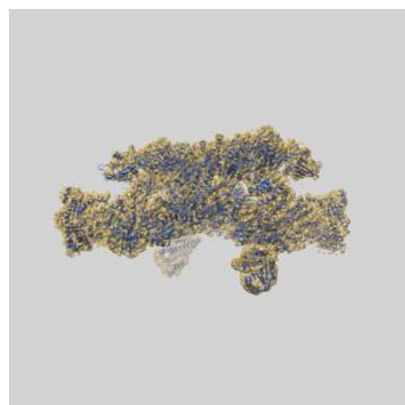
8 Fourier-Shell correlation

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

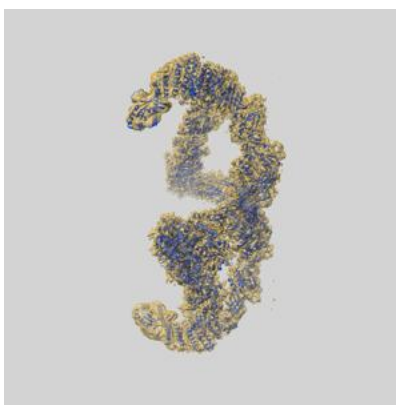
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26255 and PDB model 7U06. Per-residue inclusion information can be found in section [3](#) on page [8](#).

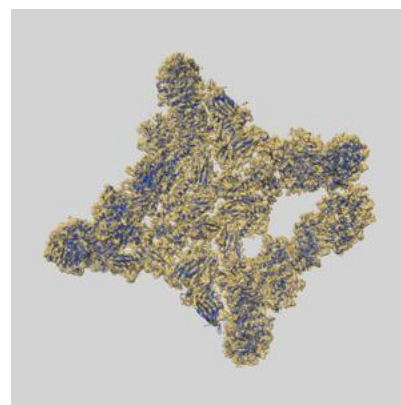
9.1 Map-model overlay [i](#)



X



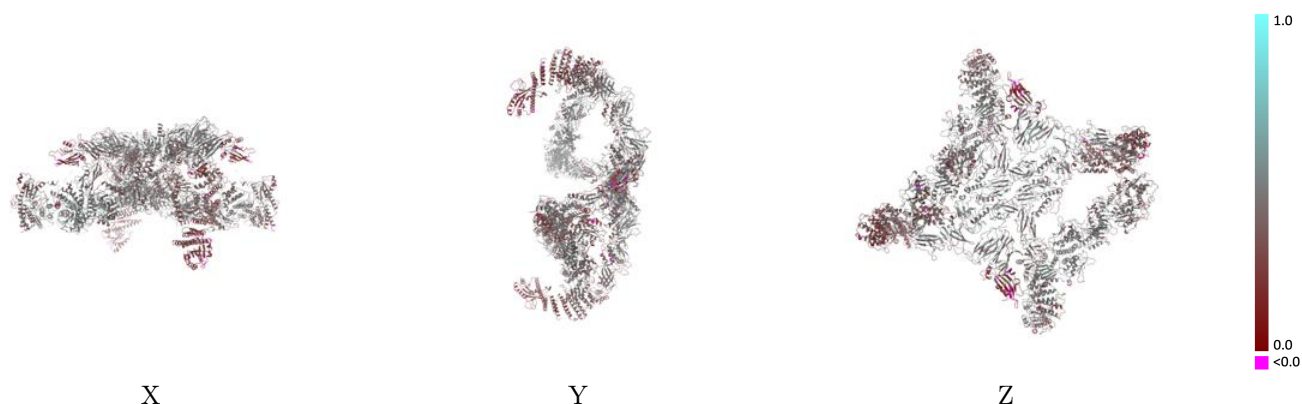
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

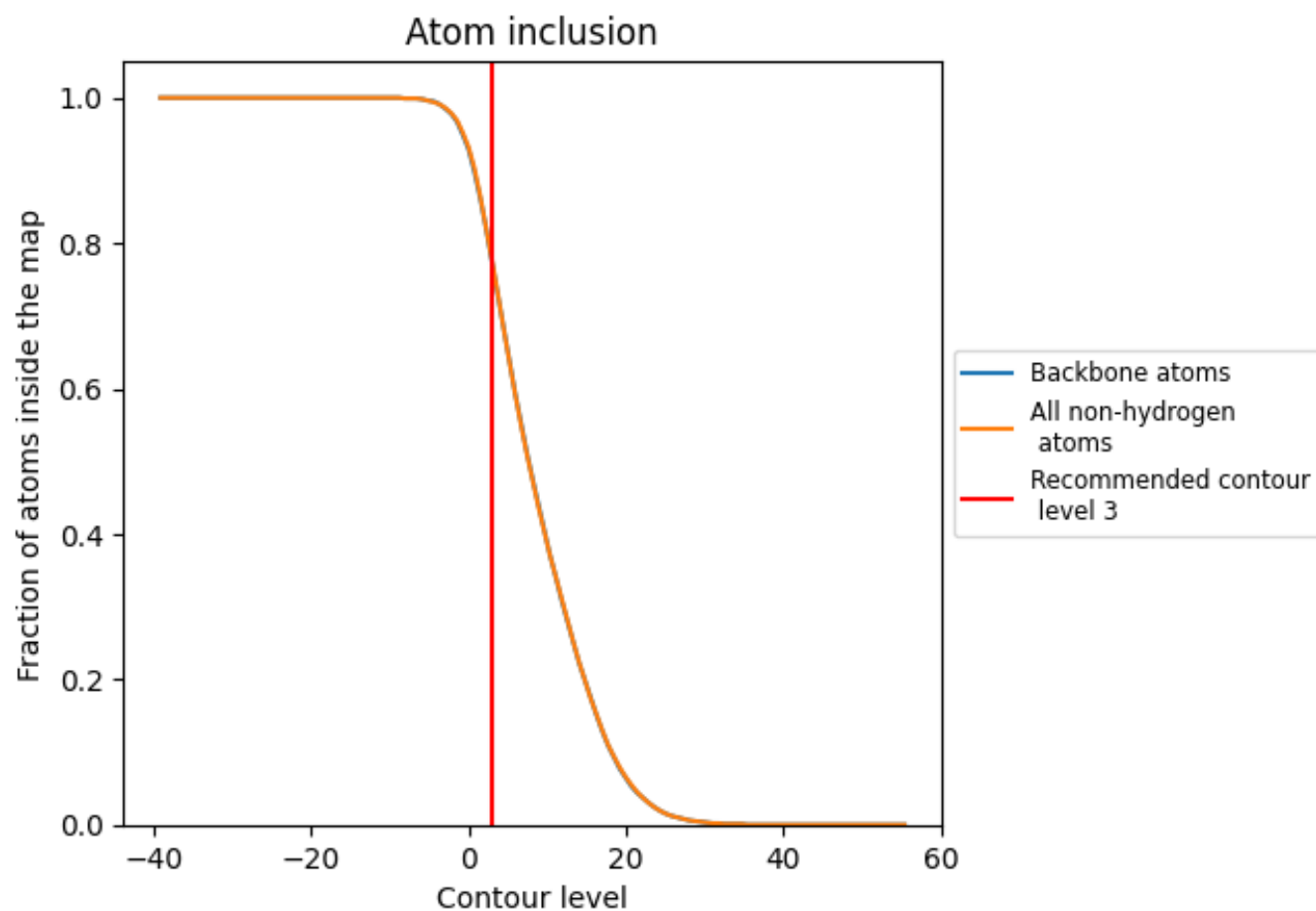


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 77% of all backbone atoms, 78% 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 (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7760	 0.4120
A	 0.7990	 0.4410
B	 0.7860	 0.3980
C	 0.7580	 0.4410
D	 0.7270	 0.3550
E	 0.8020	 0.4140
F	 0.8160	 0.4280
G	 0.8420	 0.4610
H	 0.7540	 0.4360
I	 0.7890	 0.4620
J	 0.8320	 0.4650
K	 0.8430	 0.4800
M	 0.8660	 0.2150
N	 0.7420	 0.2460
a	 0.7790	 0.4270
b	 0.7350	 0.3790
c	 0.7400	 0.4340
d	 0.7770	 0.4020
e	 0.7600	 0.4060
f	 0.7930	 0.4410
g	 0.7890	 0.4360
h	 0.7400	 0.4360
i	 0.7780	 0.4520
j	 0.8060	 0.4440
k	 0.8300	 0.4570
l	 0.5250	 0.3730
m	 0.9520	 0.2310
n	 0.5830	 0.2120

