



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 01:01 AM UTC

PDB ID : 6GCS / pdb_00006gcs
EMDB ID : EMD-4384
Title : Cryo-EM structure of respiratory complex I from *Yarrowia lipolytica*
Authors : Parey, K.; Vonck, J.
Deposited on : 2018-04-19
Resolution : 4.32 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

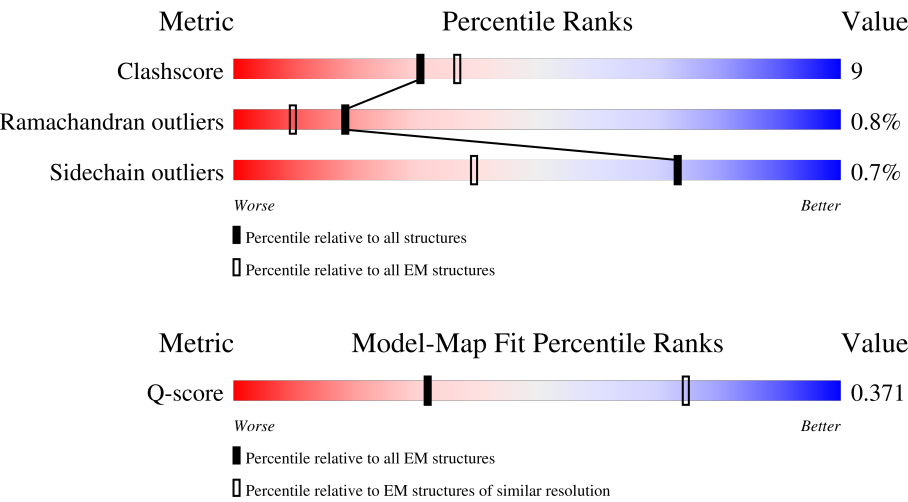
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.32 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.



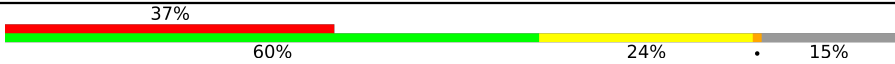
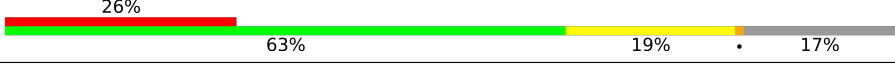
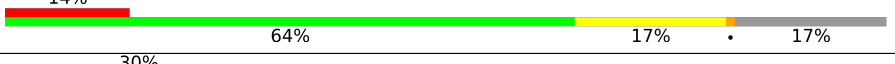
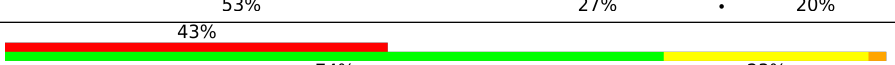
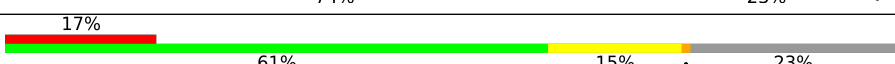
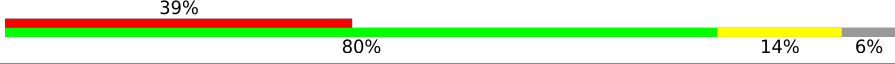
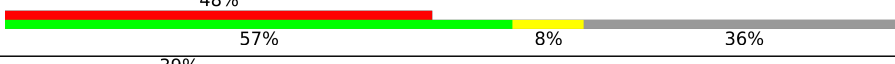
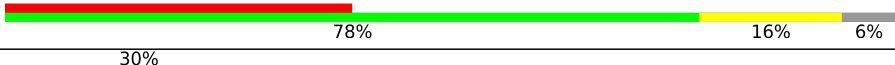
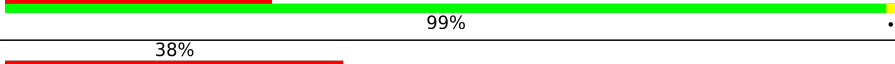
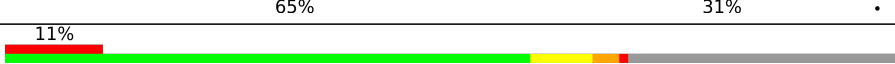
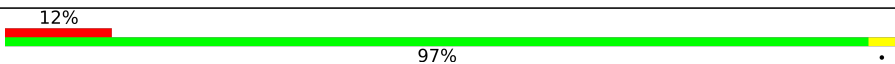
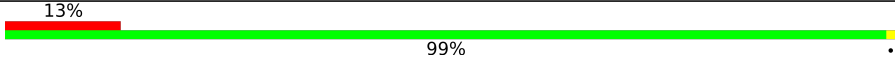
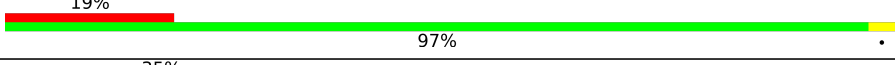
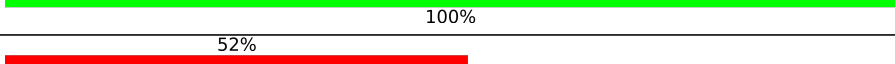
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3853 (3.83 - 4.82)

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

Mol	Chain	Length	Quality of chain
1	A	728	34% 75% 20% 5%
2	B	488	39% 70% 20% 9%
3	C	466	33% 63% 25% • 11%
4	D	87	39% 72% 18% • 8%

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Mol	Chain	Length	Quality of chain
5	E	375	
6	F	144	
7	G	281	
8	H	243	
9	I	229	
10	J	198	
11	K	210	
12	L	86	
13	M	136	
14	O	109	
15	P	124	
16	Q	132	
17	R	109	
18	S	159	
19	U	172	
20	W	123	
21	X	169	
22	Y	161	
23	Z	137	
24	a	100	
25	b	64	
26	c	60	
27	d	92	
28	e	45	
29	f	87	

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Mol	Chain	Length	Quality of chain
30	g	63	
31	h	138	
32	i	53	
33	j	93	
34	n	93	
35	1	341	
36	2	469	
37	3	128	
38	4	486	
39	5	655	
40	6	185	
41	8	99	
42	9	89	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
43	SF4	A	802	-	-	X	-
43	SF4	B	501	-	-	X	-
43	SF4	I	302	-	-	X	-

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 55137 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 75-KDA PROTEIN (NUAM).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	689	Total	C	N	O	S	0	0
			5236	3251	921	1035	29		

- Molecule 2 is a protein called 51-KDA PROTEIN (NUBM).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	443	Total	C	N	O	S	0	0
			3380	2132	595	630	23		

- Molecule 3 is a protein called 49-KDA PROTEIN (NUCM).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	416	Total	C	N	O	S	0	0
			3190	2032	548	589	21		

- Molecule 4 is a protein called NIMM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	80	Total	C	N	O	S	0	0
			559	352	103	101	3		

- Molecule 5 is a protein called NUEM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	318	Total	C	N	O	S	0	0
			2546	1621	445	471	9		

- Molecule 6 is a protein called NUFM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	119	Total	C	N	O	S	0	0
			915	578	155	181	1		

- Molecule 7 is a protein called 30-KDA PROTEIN (NUGM).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	232	Total	C	N	O	S	0	0
			1680	1069	294	313	4		

- Molecule 8 is a protein called 24-KDA SUBUNIT (NUHM).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	185	Total	C	N	O	S	0	0
			1385	870	232	266	17		

- Molecule 9 is a protein called TYKY SUBUNIT (NUIM).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	180	Total	C	N	O	S	0	0
			1441	915	240	276	10		

- Molecule 10 is a protein called NUJM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	140	Total	C	N	O	S	0	0
			961	612	174	170	5		

- Molecule 11 is a protein called PSST SUBUNIT (NUKM).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	169	Total	C	N	O	S	0	0
			1339	852	235	238	14		

- Molecule 12 is a protein called ND4L SUBUNIT (NULM).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	86	Total	C	N	O	S	0	0
			668	447	106	112	3		

- Molecule 13 is a protein called NUMM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	105	Total	C	N	O	S	0	0
			726	449	136	136	5		

- Molecule 14 is a protein called ACPM1 SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	77	Total	C	N	O	0	0
			591	373	93	125		

- Molecule 15 is a protein called NB4M SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	116	Total	C	N	O	S	0	0
			982	633	170	177	2		

- Molecule 16 is a protein called ACPM2 SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	85	Total	C	N	O	S	0	0
			648	405	103	138	2		

- Molecule 17 is a protein called NI2M SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	102	Total	C	N	O	S	0	0
			820	517	159	142	2		

- Molecule 18 is a protein called NESM SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S	159	Total	C	N	O	0	0
			796	477	159	160		

- Molecule 19 is a protein called NUPM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	158	Total	C	N	O	S	0	0
			1141	707	205	219	10		

- Molecule 20 is a protein called NB6M SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	118	Total	C	N	O	S	0	0
			929	590	174	160	5		

- Molecule 21 is a protein called NUXM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	117	Total	C	N	O	S	0	0
			638	392	124	121	1		

- Molecule 22 is a protein called NUYM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	115	Total	C	N	O	S	0	0
			957	610	173	172	2		

- Molecule 23 is a protein called NUZM SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	Z	137	Total	C	N	O	0	0
			686	411	137	138		

- Molecule 24 is a protein called NIAM SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	a	100	Total	C	N	O	0	0
			501	300	100	101		

- Molecule 25 is a protein called NEBM SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	b	64	Total	C	N	O	0	0
			321	192	64	65		

- Molecule 26 is a protein called NB2M SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	c	42	Total	C	N	O	0	0
			251	163	43	45		

- Molecule 27 is a protein called NIDM SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	89	Total	C	N	O	S	0	0
			752	467	136	146	3		

- Molecule 28 is a protein called NUUM SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	e	45	Total	C	N	O	0	0
			226	135	45	46		

- Molecule 29 is a protein called NI8M SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	80	Total	C	N	O	S	0
			629	394	119	115	1	0

- Molecule 30 is a protein called NI9M SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	g	60	Total	C	N	O		0
			492	328	88	76		0

- Molecule 31 is a protein called N7BM SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	h	130	Total	C	N	O	S	0
			1081	697	184	198	2	0

- Molecule 32 is a protein called UNKNOWN SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	i	53	Total	C	N	O		0
			266	159	53	54		0

- Molecule 33 is a protein called NB5M SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	j	73	Total	C	N	O		0
			436	266	87	83		0

- Molecule 34 is a protein called NUNM SUBUNIT.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	n	93	Total	C	N	O		0
			466	279	93	94		0

- Molecule 35 is a protein called ND1 SUBUNIT (NU1M).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1	340	Total	C	N	O	S	0	0
			2608	1766	390	445	7		

- Molecule 36 is a protein called ND2 SUBUNIT (NU2M).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	2	452	Total	C	N	O	S	0	0
			3376	2263	511	590	12		

- Molecule 37 is a protein called ND3 SUBUNIT (NU3M).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3	110	Total	C	N	O	S	0	0
			871	600	129	140	2		

- Molecule 38 is a protein called ND4 SUBUNIT (NU4M).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	4	475	Total	C	N	O	S	0	0
			3312	2188	533	581	10		

- Molecule 39 is a protein called ND5 SUBUNIT (NU5M).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	5	639	Total	C	N	O	S	0	0
			4599	3032	723	817	27		

- Molecule 40 is a protein called ND6 SUBUNIT (NU6M).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	6	183	Total	C	N	O	S	0	0
			1211	812	189	203	7		

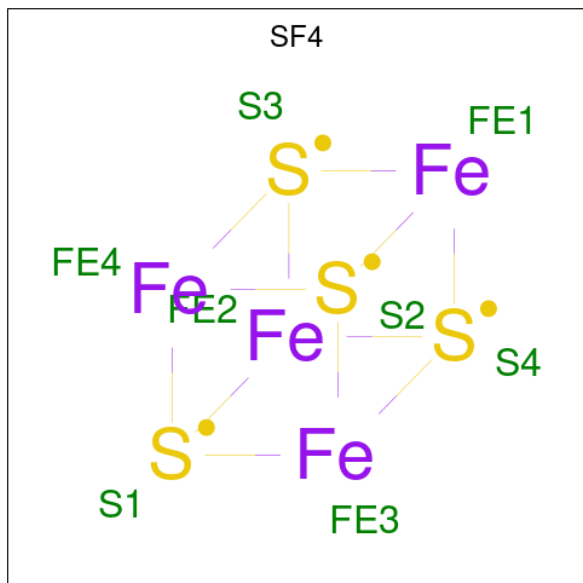
- Molecule 41 is a protein called NB8M SUBUNIT.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	8	82	Total	C	N	O	S	0	0
			672	426	122	116	8		

- Molecule 42 is a protein called NIPM SUBUNIT.

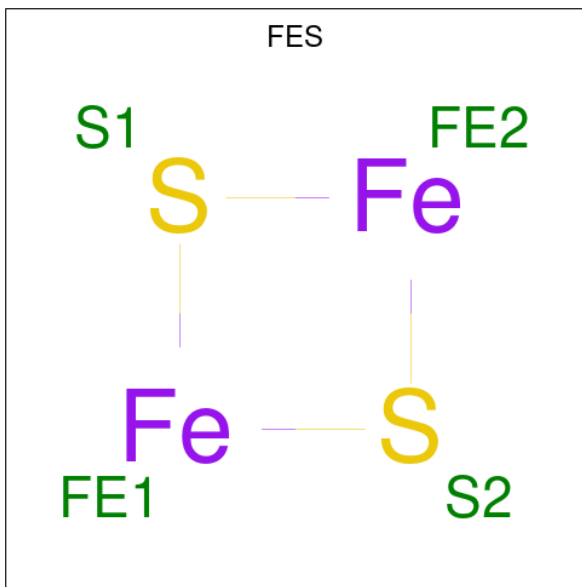
Mol	Chain	Residues	Atoms					AltConf	Trace
42	9	59	Total	C	N	O	S	0	0
			468	290	85	87	6		

- Molecule 43 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



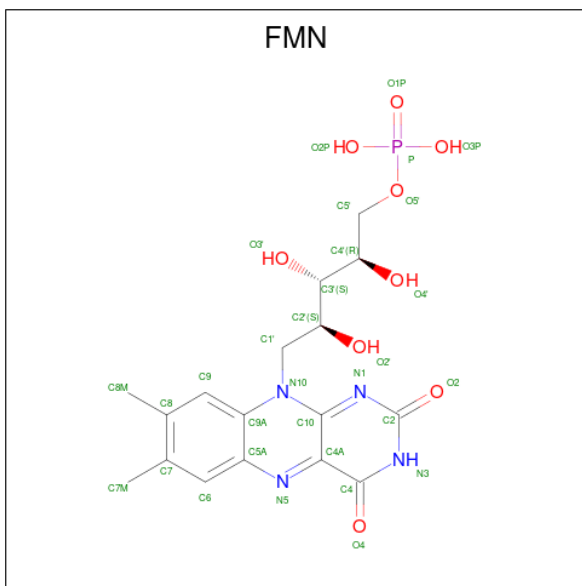
Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total	Fe	S	0
			8	4	4	
43	A	1	Total	Fe	S	0
			8	4	4	
43	B	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	K	1	Total	Fe	S	0
			8	4	4	

- Molecule 44 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
44	A	1	Total 4	Fe 2	S 2	0
44	H	1	Total 4	Fe 2	S 2	0

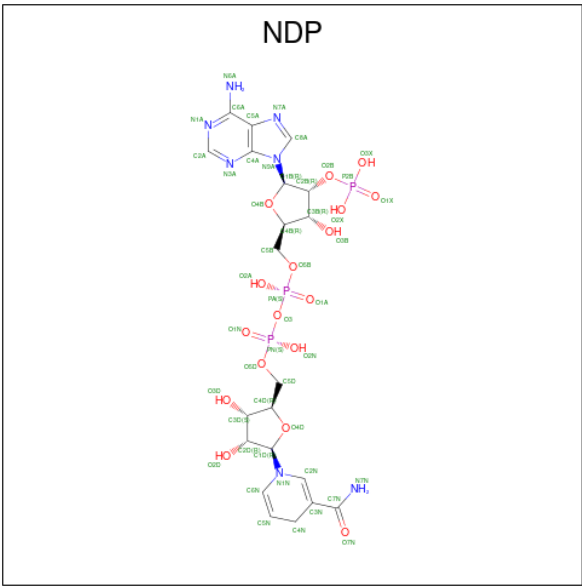
- Molecule 45 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
45	B	1	Total 31	C 17	N 4	O 9	P 1	0

- Molecule 46 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

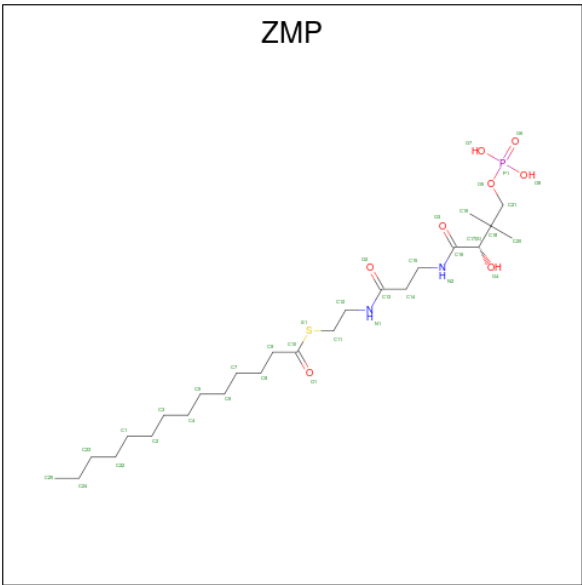


Mol	Chain	Residues	Atoms					AltConf
46	E	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 47 is ZINC ION (CCD ID: ZN) (formula: Zn).

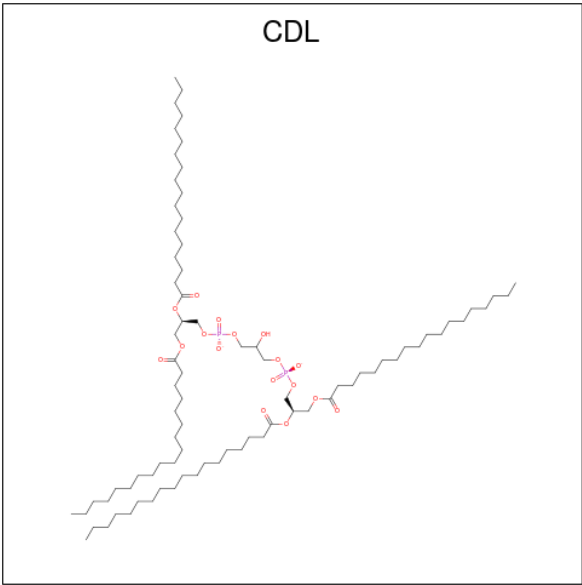
Mol	Chain	Residues	Atoms		AltConf
47	M	1	Total	Zn	0
			1	1	

- Molecule 48 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



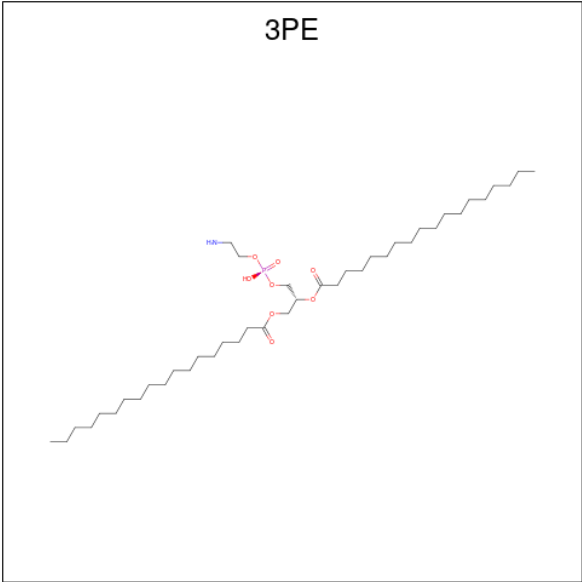
Mol	Chain	Residues	Atoms					AltConf	
48	O	1	Total	C	N	O	P	S	0
			29	18	2	7	1	1	

- Molecule 49 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
49	g	1	Total	C	O	P	0
			83	64	17	2	

- Molecule 50 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).

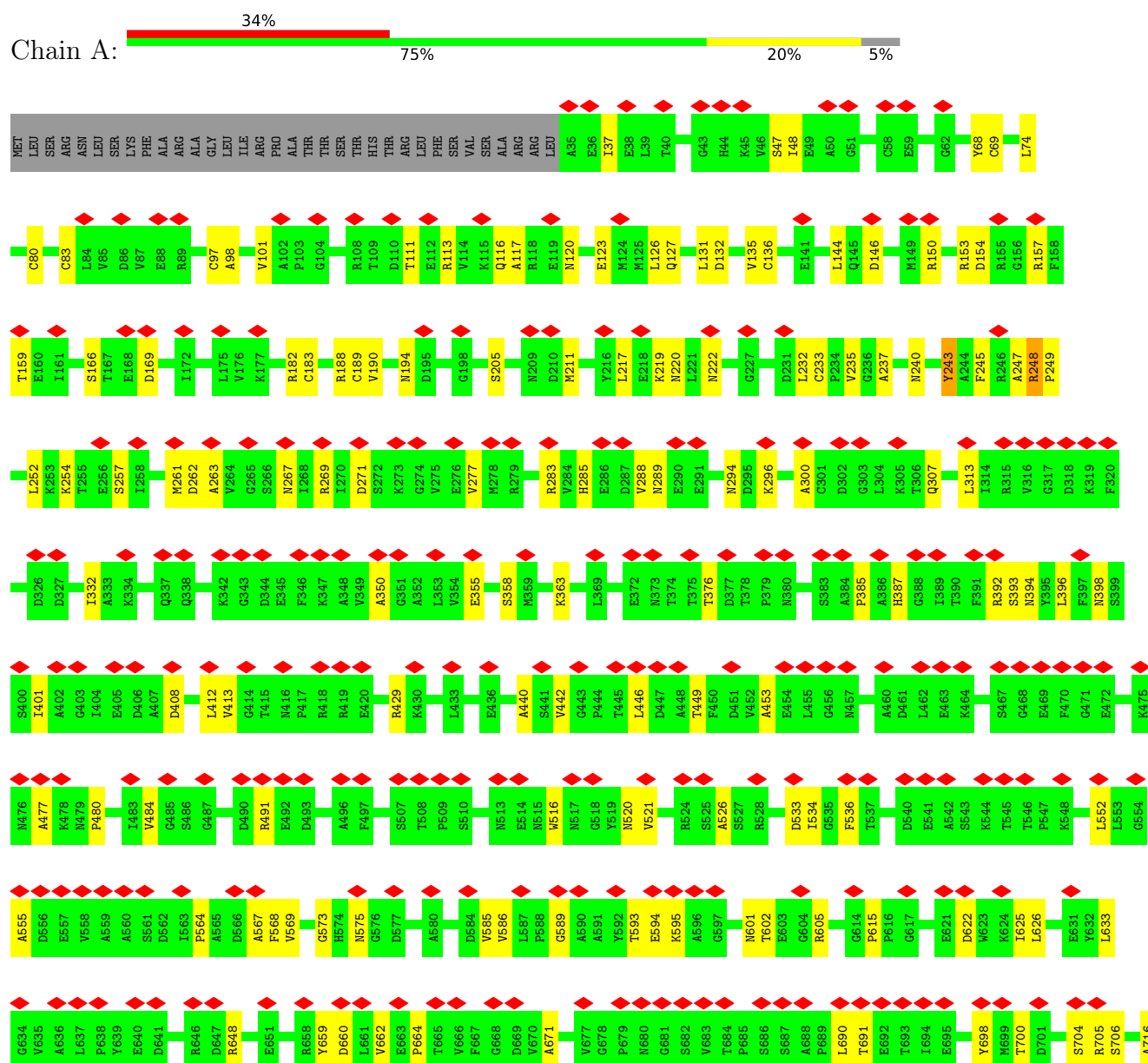


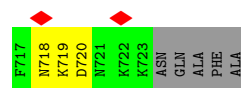
Mol	Chain	Residues	Atoms					AltConf
50	g	1	Total	C	N	O	P	0
			43	33	1	8	1	
50	1	1	Total	C	N	O	P	0
			51	41	1	8	1	
50	4	1	Total	C	N	O	P	0
			43	33	1	8	1	

3 Residue-property plots [i](#)

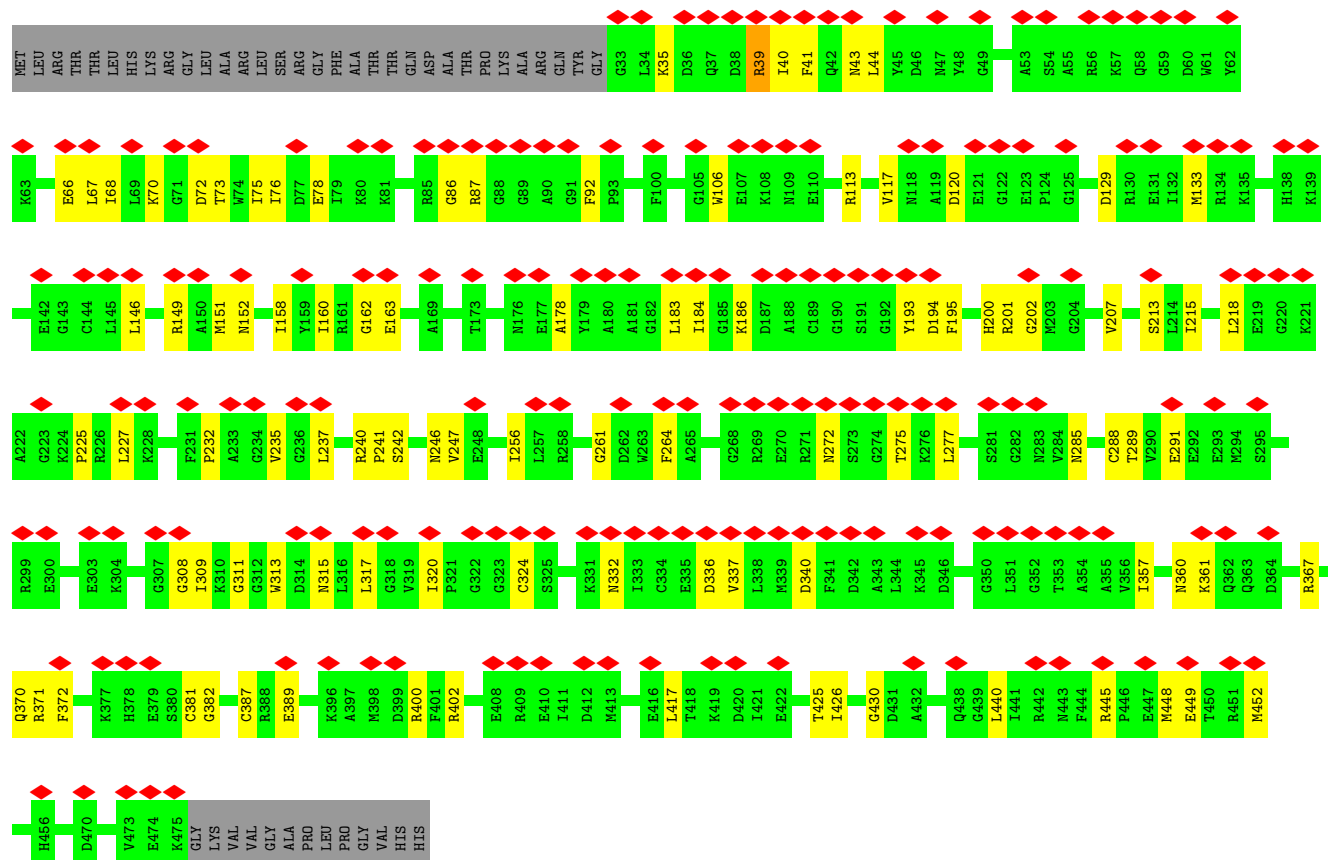
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 75-KDA PROTEIN (NUAM)

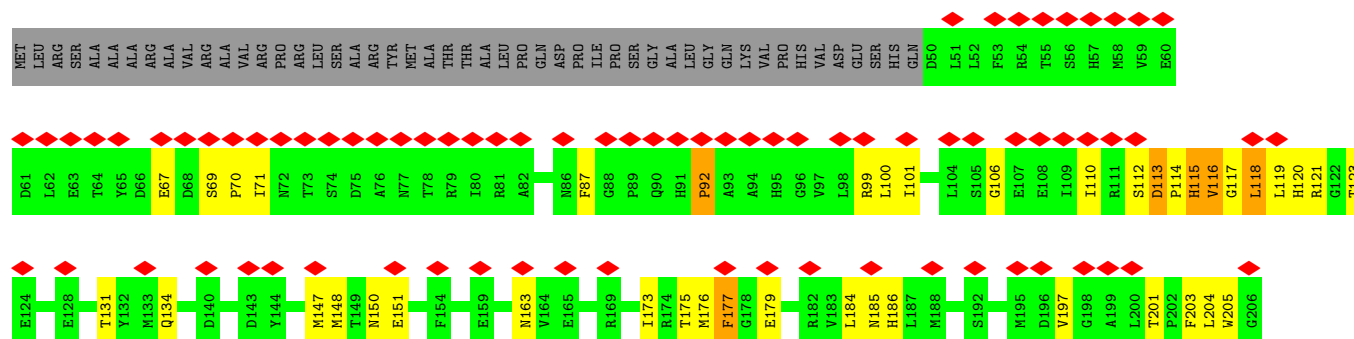


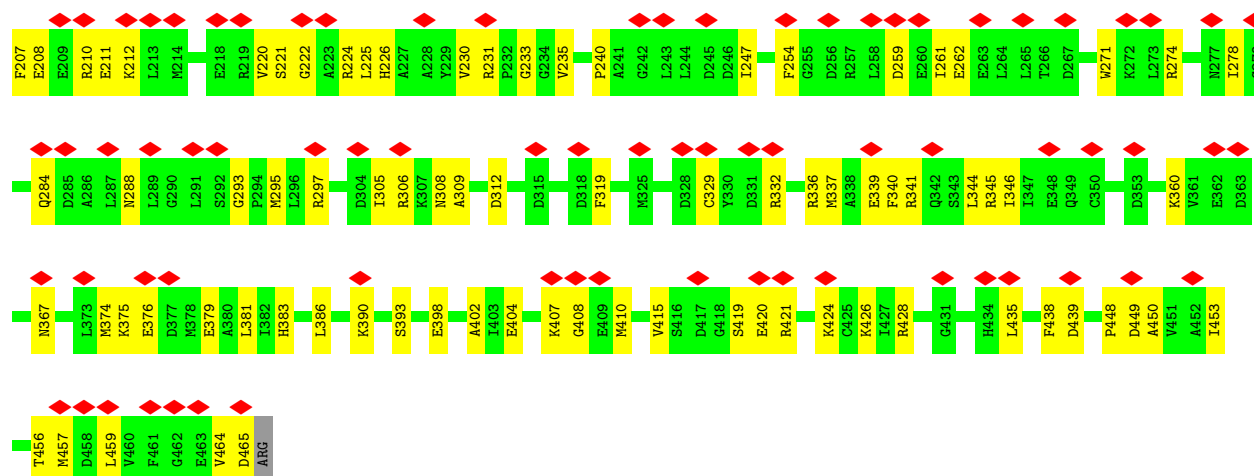


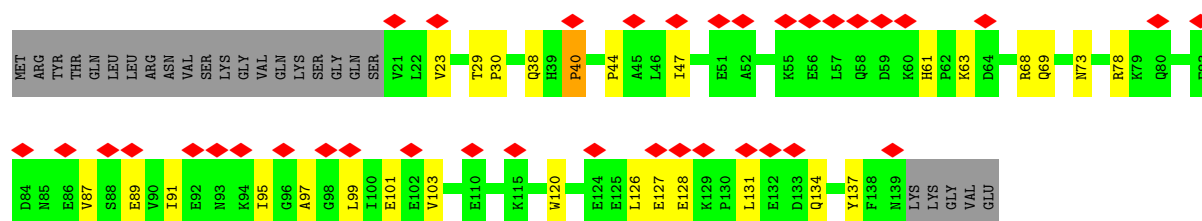
• Molecule 2: 51-KDA PROTEIN (NUBM)



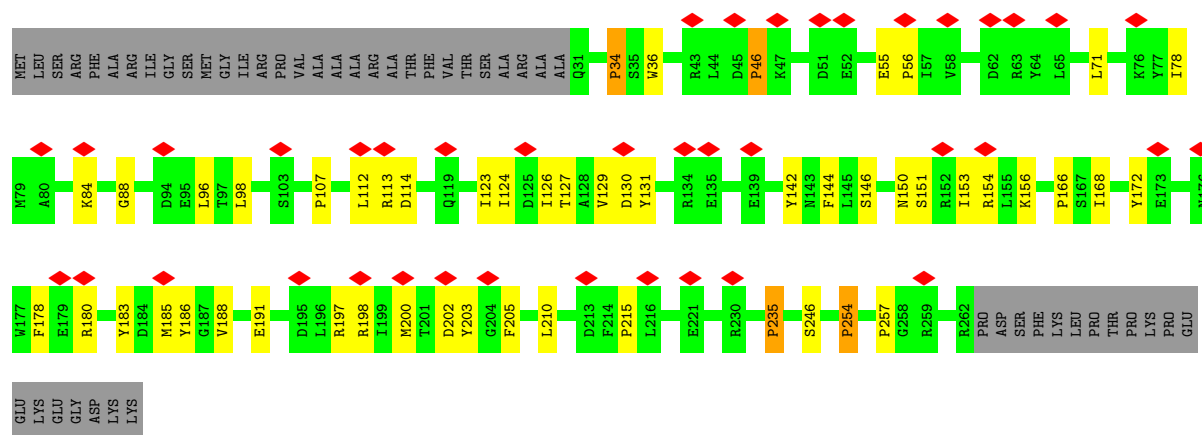
• Molecule 3: 49-KDA PROTEIN (NUCM)



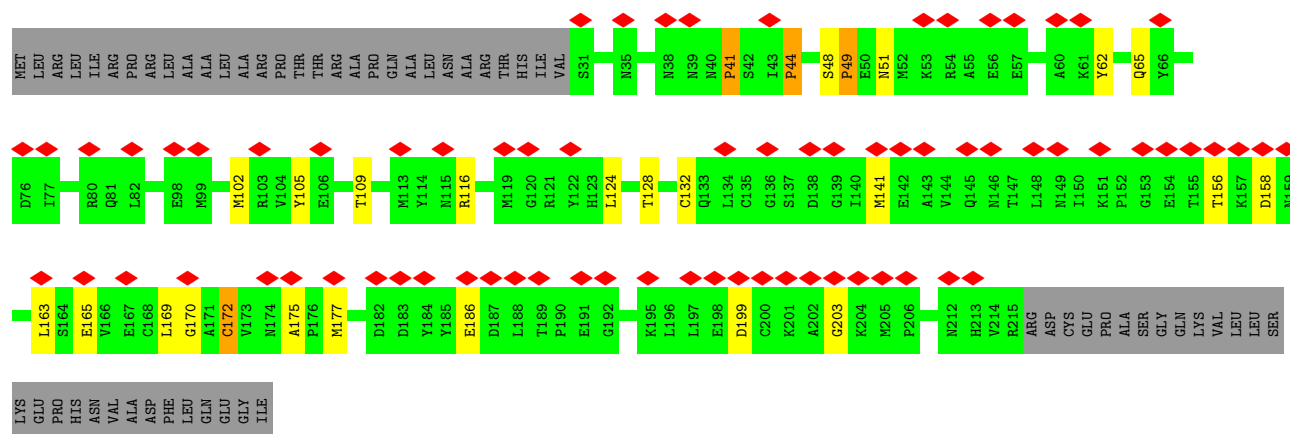




• Molecule 7: 30-KDA PROTEIN (NUGM)

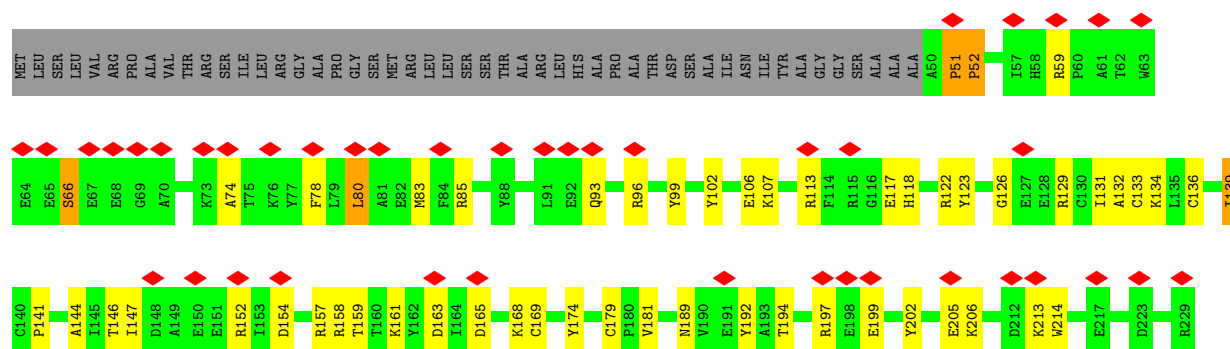


• Molecule 8: 24-KDA SUBUNIT (NUHM)

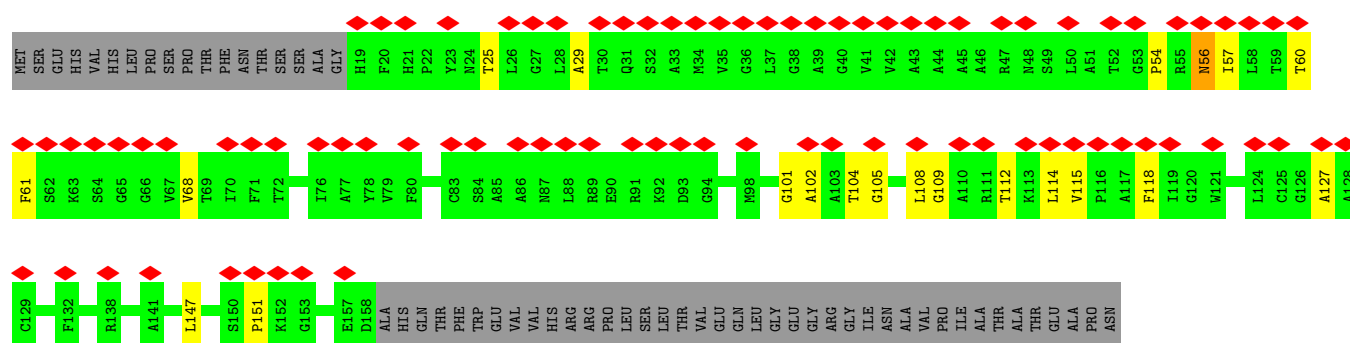


• Molecule 9: TYKY SUBUNIT (NUIM)

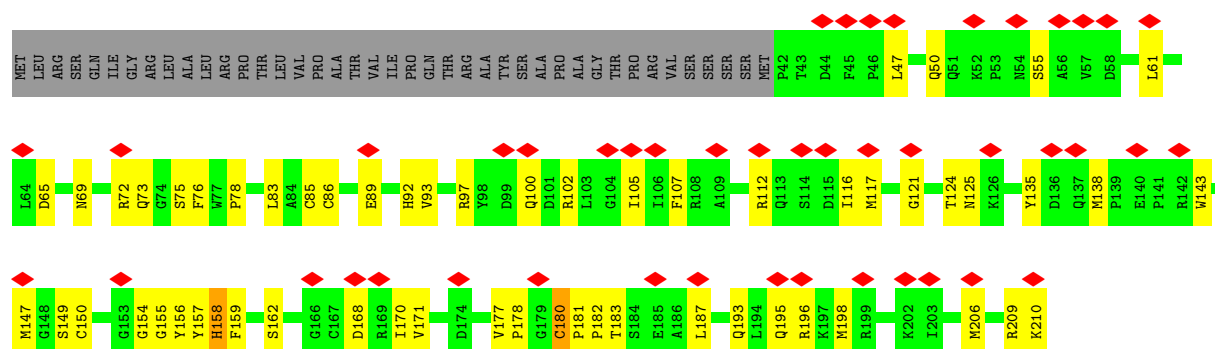




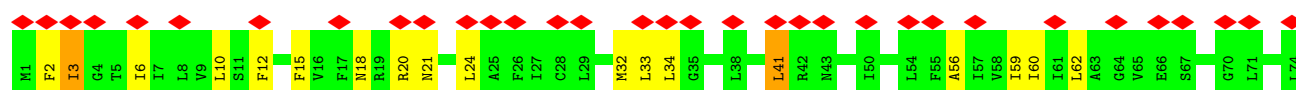
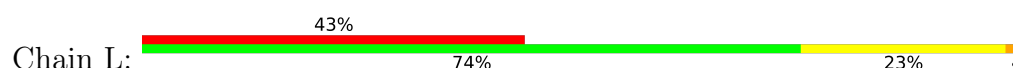
- Molecule 10: NUJM SUBUNIT

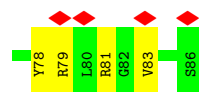


- Molecule 11: PSST SUBUNIT (NUKM)

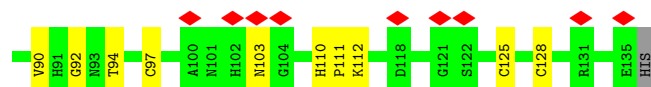
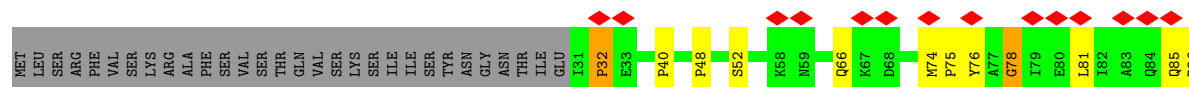


- Molecule 12: ND4L SUBUNIT (NULM)

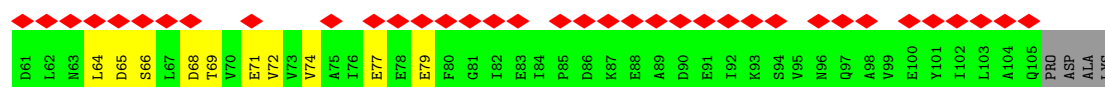
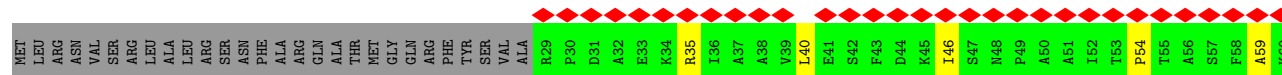




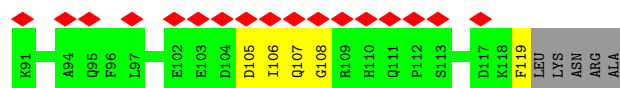
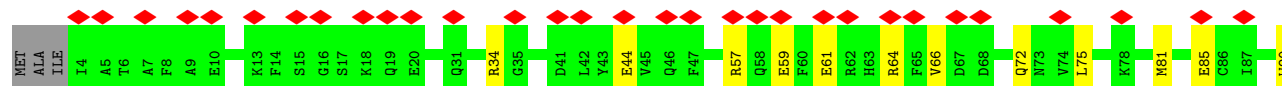
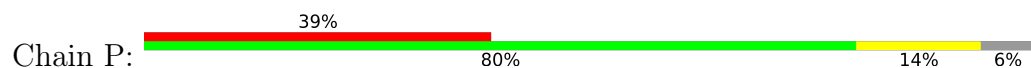
• Molecule 13: NUMM SUBUNIT



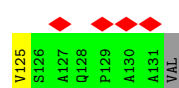
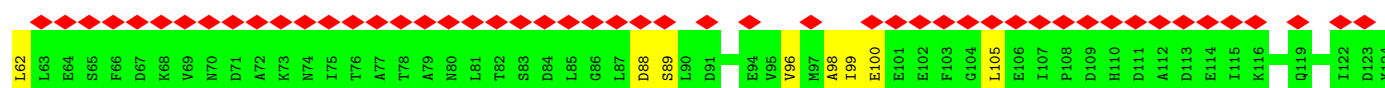
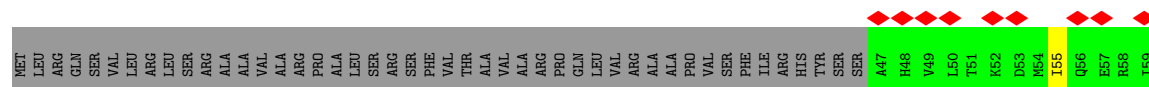
• Molecule 14: ACPM1 SUBUNIT



• Molecule 15: NB4M SUBUNIT

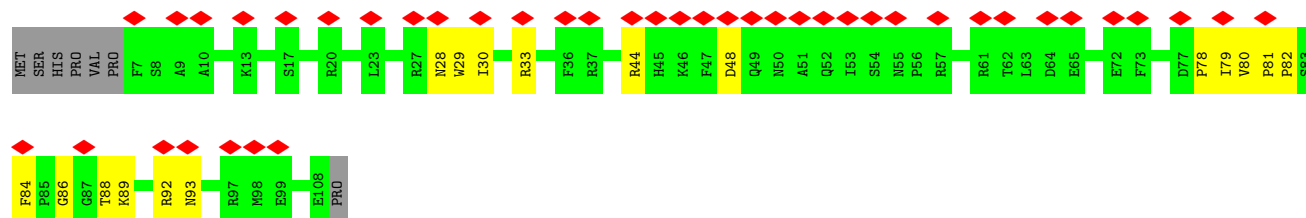


• Molecule 16: ACPM2 SUBUNIT



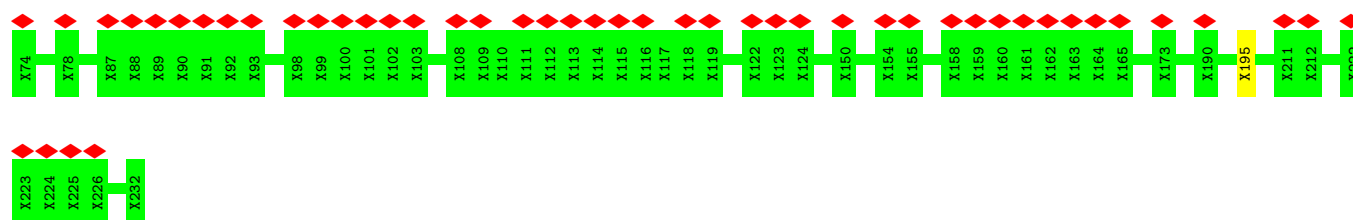
- Molecule 17: NI2M SUBUNIT

Chain R:



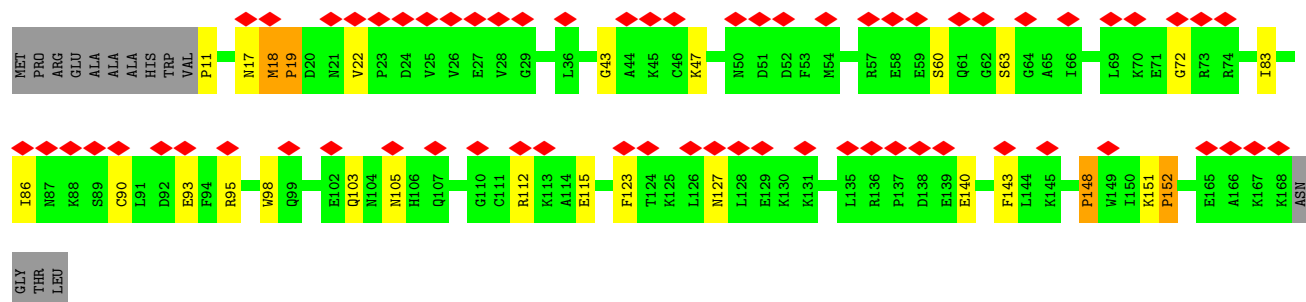
- Molecule 18: NESM SUBUNIT

Chain S:



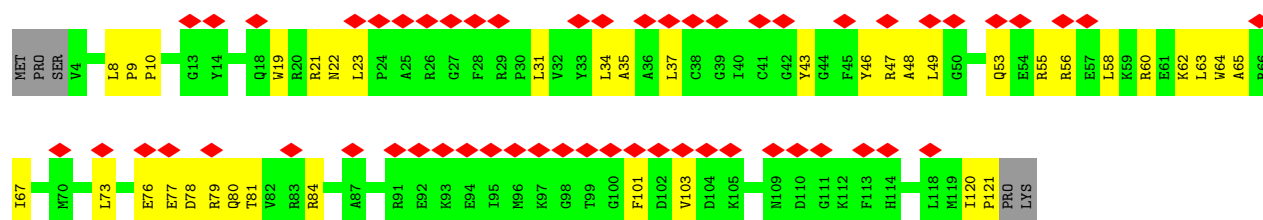
- Molecule 19: NUPM SUBUNIT

Chain U:



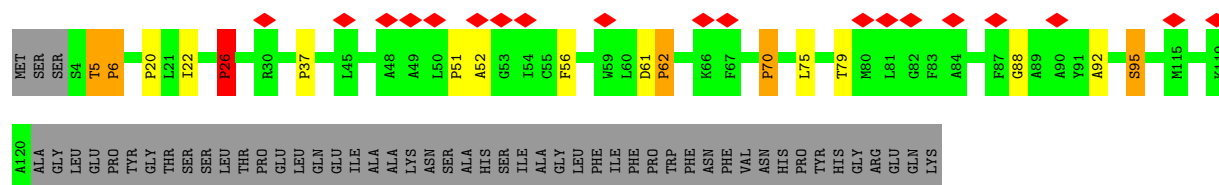
- Molecule 20: NB6M SUBUNIT

Chain W:

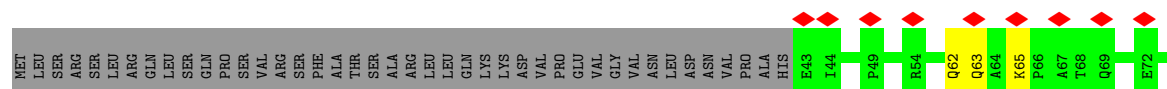


- Molecule 21: NUXM SUBUNIT

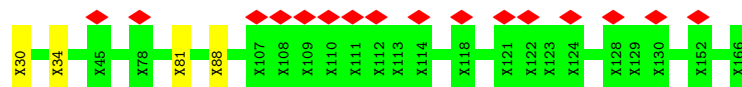
Chain X:



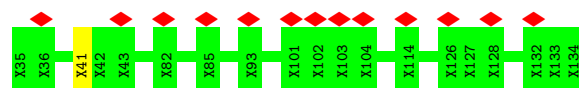
• Molecule 22: NUYM SUBUNIT



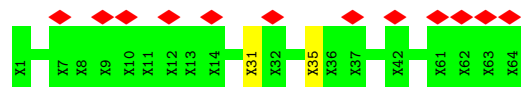
• Molecule 23: NUZM SUBUNIT



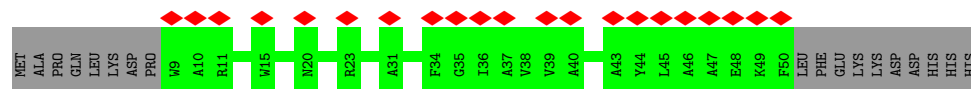
• Molecule 24: NIAM SUBUNIT



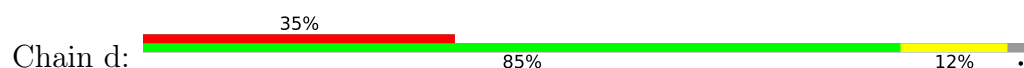
• Molecule 25: NEBM SUBUNIT

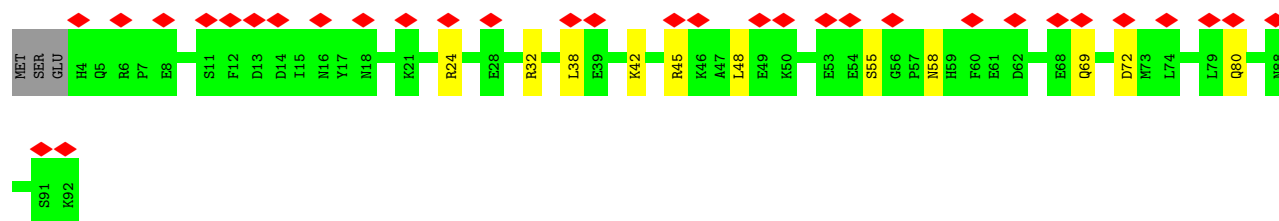


• Molecule 26: NB2M SUBUNIT

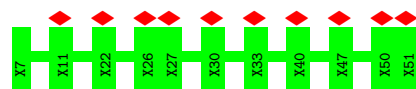


• Molecule 27: NIDM SUBUNIT

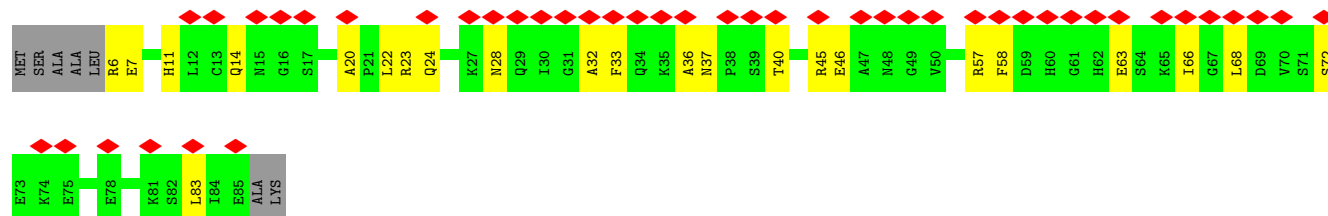




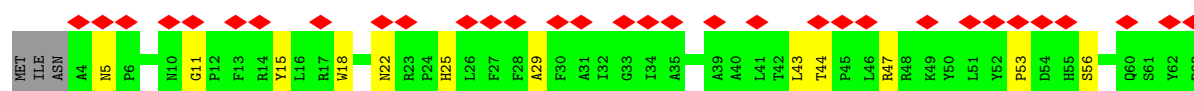
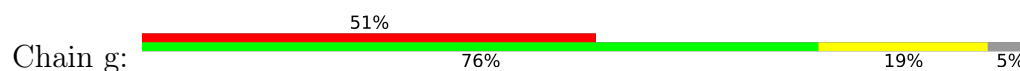
• Molecule 28: NUUM SUBUNIT



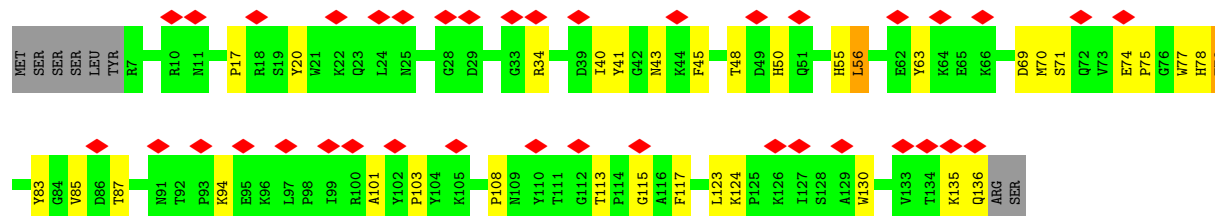
• Molecule 29: NI8M SUBUNIT



• Molecule 30: NI9M SUBUNIT

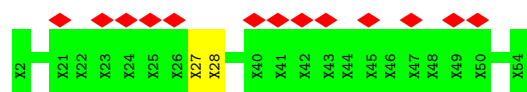


• Molecule 31: N7BM SUBUNIT

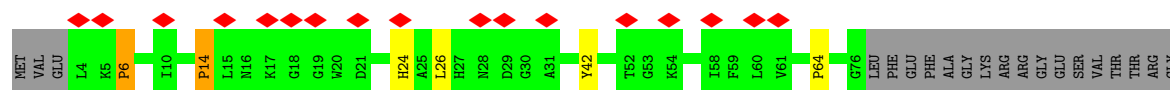
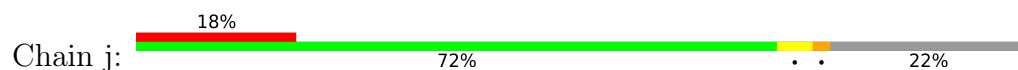


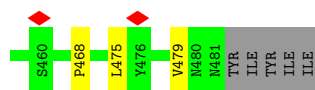
• Molecule 32: UNKNOWN SUBUNIT





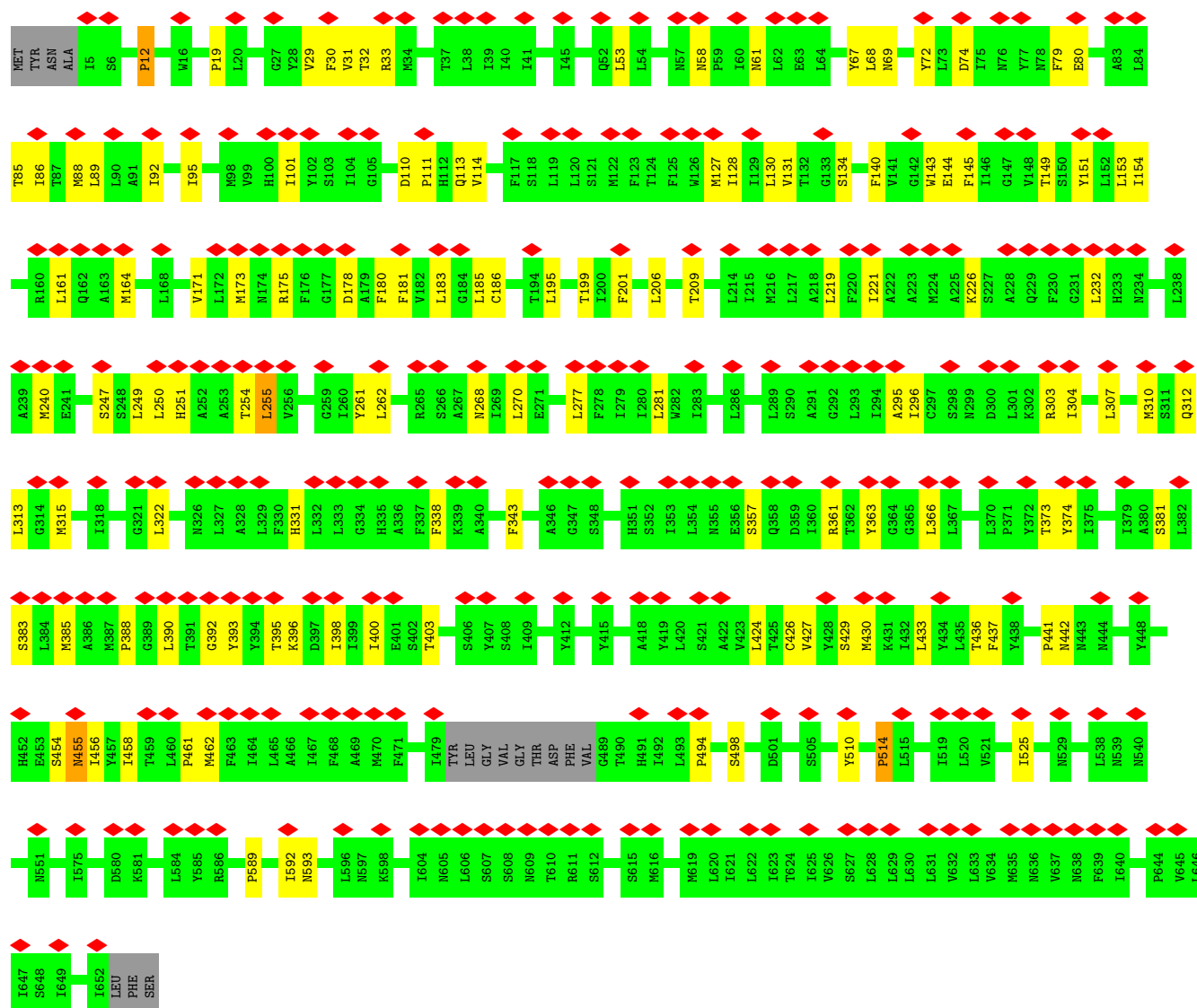
- Molecule 33: NB5M SUBUNIT





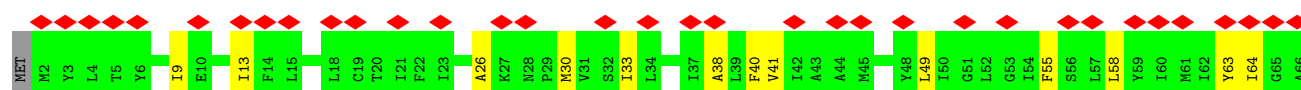
• Molecule 39: ND5 SUBUNIT (NU5M)

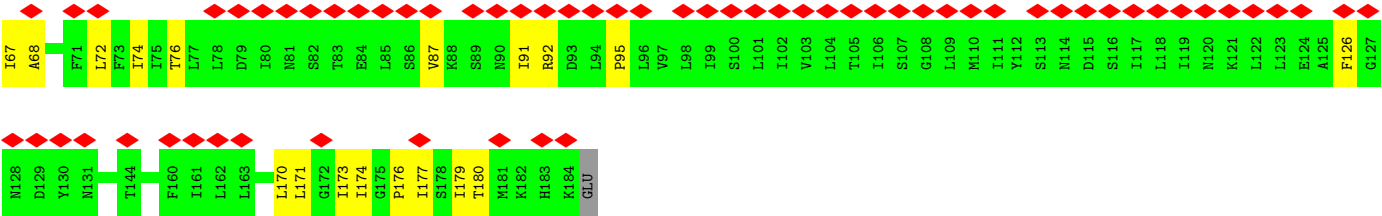
Chain 5: 41% 78% 19% ..



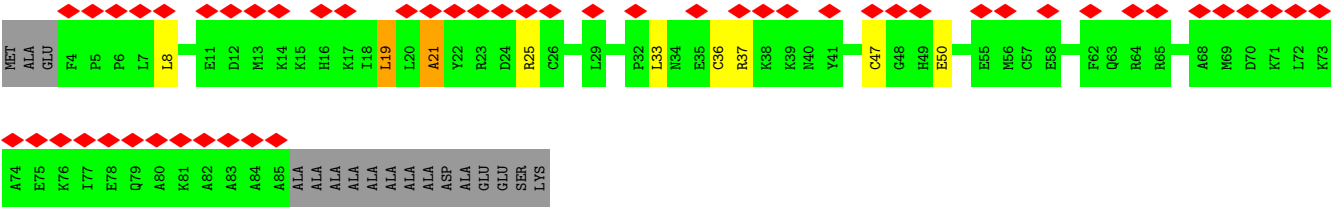
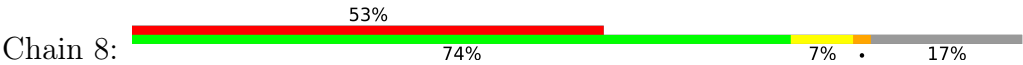
• Molecule 40: ND6 SUBUNIT (NU6M)

Chain 6: 52% 82% 17% .

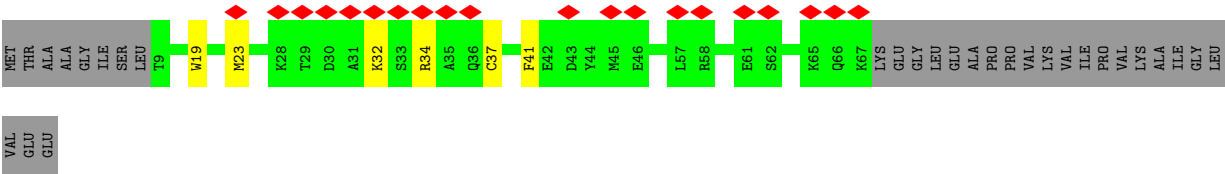




• Molecule 41: NB8M SUBUNIT



• Molecule 42: NIPM SUBUNIT



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124626	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.5	Depositor
Minimum defocus (nm)	-1.5	Depositor
Maximum defocus (nm)	-3.0	Depositor
Magnification	45872	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.256	Depositor
Minimum map value	-0.057	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.045	Depositor
Map size ($\text{\AA}$)	497.04, 497.04, 497.04	wwPDB
Map dimensions	456, 456, 456	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.09, 1.09, 1.09	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FES, NDP, CDL, FMN, SF4, ZMP, 3PE

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	0.40	0/5329	0.68	4/7232 (0.1%)
2	B	0.36	0/3451	0.70	4/4660 (0.1%)
3	C	0.48	0/3260	0.80	6/4421 (0.1%)
4	D	0.40	0/568	0.80	1/770 (0.1%)
5	E	0.39	0/2604	0.72	0/3529
6	F	0.36	0/932	0.75	4/1265 (0.3%)
7	G	0.51	0/1721	0.88	6/2356 (0.3%)
8	H	0.37	0/1411	0.74	3/1919 (0.2%)
9	I	0.51	0/1475	0.85	4/1998 (0.2%)
10	J	0.30	0/983	0.79	4/1343 (0.3%)
11	K	0.49	0/1377	0.79	0/1872
12	L	0.49	0/676	0.82	0/913
13	M	0.38	0/741	0.83	4/1009 (0.4%)
14	O	0.29	0/598	0.57	0/813
15	P	0.40	0/1007	0.65	0/1355
16	Q	0.25	0/654	0.66	0/890
17	R	0.28	0/840	0.61	0/1136
19	U	0.35	0/1157	0.90	6/1568 (0.4%)
20	W	0.36	0/948	0.79	2/1275 (0.2%)
21	X	0.35	0/641	1.05	9/881 (1.0%)
22	Y	0.46	0/985	0.66	0/1330
26	c	0.22	0/255	0.57	0/349
27	d	0.35	0/768	0.72	0/1031
29	f	0.36	0/639	0.76	0/856
30	g	0.38	0/516	0.73	0/707
31	h	0.39	0/1118	0.75	1/1522 (0.1%)
33	j	0.35	0/444	0.79	3/611 (0.5%)
35	1	0.44	0/2674	0.89	6/3656 (0.2%)
36	2	0.50	0/3440	0.82	0/4696
37	3	0.42	0/890	0.90	2/1213 (0.2%)
38	4	0.45	0/3373	0.80	4/4630 (0.1%)
39	5	0.39	0/4692	0.77	7/6430 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
40	6	0.38	0/1229	0.74	1/1686 (0.1%)
41	8	0.31	0/686	0.64	0/918
42	9	0.33	0/477	0.66	0/637
All	All	0.41	0/52559	0.77	81/71477 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	2
5	E	0	5
7	G	0	2
9	I	0	1
10	J	0	1
11	K	0	1
12	L	0	1
19	U	0	2
20	W	0	1
21	X	0	2
24	a	0	1
29	f	0	1
30	g	0	1
31	h	0	1
33	j	0	1
34	n	0	1
35	1	0	9
36	2	0	2
38	4	0	3
39	5	0	1
41	8	0	1
All	All	0	43

There are no bond length outliers.

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	115	HIS	N-CA-C	12.05	128.07	112.41
3	C	113	ASP	CA-C-N	-9.41	110.30	119.89
3	C	113	ASP	C-N-CA	-9.41	110.30	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	5	398	ILE	N-CA-C	-9.27	104.90	113.71
19	U	19	PRO	N-CA-CB	8.86	112.55	103.25
8	H	41	PRO	N-CA-CB	8.31	111.98	103.25
37	3	119	PRO	N-CA-CB	8.26	111.93	103.25
7	G	46	PRO	N-CA-CB	8.14	111.80	103.25
10	J	56	ASN	N-CA-C	8.14	119.84	110.97
4	D	71	PRO	N-CA-CB	8.10	111.75	103.25
7	G	254	PRO	N-CA-CB	8.08	111.73	103.25
21	X	26	PRO	N-CA-CB	7.85	111.50	103.25
21	X	70	PRO	N-CA-CB	7.72	111.36	103.25
33	j	14	PRO	N-CA-CB	7.52	111.14	103.25
9	I	51	PRO	N-CA-CB	7.51	110.37	103.08
19	U	152	PRO	N-CA-CB	7.51	111.14	103.25
21	X	62	PRO	N-CA-CB	7.49	111.12	103.25
20	W	9	PRO	N-CA-CB	7.48	110.34	103.08
7	G	257	PRO	N-CA-CB	7.45	111.07	103.25
21	X	51	PRO	N-CA-CB	7.42	110.64	103.51
9	I	52	PRO	N-CA-CB	7.37	110.99	103.25
13	M	32	PRO	N-CA-CB	7.35	110.97	103.25
38	4	65	PRO	N-CA-CB	7.34	110.96	103.25
35	1	217	THR	CA-C-N	7.25	133.07	122.63
35	1	217	THR	C-N-CA	7.25	133.07	122.63
33	j	6	PRO	N-CA-CB	7.14	110.75	103.25
8	H	44	PRO	N-CA-CB	7.14	110.75	103.25
21	X	20	PRO	N-CA-CB	7.11	109.62	103.36
7	G	56	PRO	N-CA-CB	7.08	110.68	103.25
38	4	468	PRO	N-CA-CB	7.05	110.65	103.25
7	G	235	PRO	N-CA-CB	7.00	110.60	103.25
3	C	70	PRO	N-CA-CB	6.97	110.57	103.25
21	X	6	PRO	N-CA-CB	6.94	110.54	103.25
39	5	494	PRO	N-CA-CB	6.91	110.51	103.25
35	1	181	PRO	N-CA-CB	6.91	110.14	103.51
39	5	441	PRO	N-CA-CB	6.83	110.42	103.25
19	U	11	PRO	N-CA-CB	6.78	110.45	103.00
13	M	40	PRO	N-CA-CB	6.59	110.17	103.25
10	J	151	PRO	N-CA-CB	6.57	110.15	103.25
39	5	514	PRO	N-CA-CB	6.57	110.48	103.52
13	M	48	PRO	N-CA-CB	6.49	110.07	103.25
6	F	40	PRO	N-CA-CB	6.48	110.05	103.25
19	U	148	PRO	N-CA-CB	6.42	109.99	103.25
3	C	92	PRO	N-CA-CB	6.41	109.98	103.25
21	X	37	PRO	N-CA-CB	6.35	110.25	103.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	W	10	PRO	N-CA-CB	6.35	109.92	103.25
33	j	64	PRO	N-CA-CB	6.31	110.50	103.44
39	5	19	PRO	N-CA-CB	6.29	110.49	103.44
39	5	12	PRO	N-CA-CB	6.20	109.76	103.25
6	F	30	PRO	N-CA-CB	6.10	111.02	103.15
8	H	49	PRO	N-CA-CB	6.07	109.62	103.25
6	F	131	LEU	CA-C-N	6.00	133.00	121.54
6	F	131	LEU	C-N-CA	6.00	133.00	121.54
37	3	68	LEU	CA-CB-CG	5.98	137.24	116.30
3	C	118	LEU	N-CA-C	-5.94	104.81	111.28
40	6	95	PRO	N-CA-CB	5.84	109.75	103.33
10	J	68	VAL	CA-C-N	5.51	132.07	121.54
10	J	68	VAL	C-N-CA	5.51	132.07	121.54
19	U	18	MET	CA-C-N	5.43	126.62	119.84
19	U	18	MET	C-N-CA	5.43	126.62	119.84
1	A	289	ASN	CA-C-N	5.39	128.25	120.38
1	A	289	ASN	C-N-CA	5.39	128.25	120.38
13	M	74	MET	N-CA-C	5.29	121.50	109.81
35	1	58	LEU	CA-C-N	5.28	131.62	121.54
35	1	58	LEU	C-N-CA	5.28	131.62	121.54
9	I	66	SER	CA-C-N	5.27	131.60	121.54
9	I	66	SER	C-N-CA	5.27	131.60	121.54
7	G	34	PRO	N-CA-CB	5.25	108.77	103.25
21	X	95	SER	CA-C-N	5.21	131.48	121.54
21	X	95	SER	C-N-CA	5.21	131.48	121.54
39	5	455	ASN	N-CA-CB	-5.14	101.81	110.49
2	B	337	VAL	CA-C-N	5.08	131.25	121.54
2	B	337	VAL	C-N-CA	5.08	131.25	121.54
31	h	56	LEU	CA-CB-CG	5.07	134.04	116.30
35	1	218	GLU	CA-CB-CG	5.07	124.24	114.10
1	A	659	TYR	CA-C-N	5.04	131.16	121.54
1	A	659	TYR	C-N-CA	5.04	131.16	121.54
38	4	240	LEU	CA-C-N	5.01	131.11	121.54
38	4	240	LEU	C-N-CA	5.01	131.11	121.54
2	B	39	ARG	CA-C-N	5.01	130.98	121.97
2	B	39	ARG	C-N-CA	5.01	130.98	121.97

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	1	149	ILE	Peptide

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Mol	Chain	Res	Type	Group
35	1	176	VAL	Peptide
35	1	199	ARG	Peptide
35	1	203	ASP	Peptide
35	1	303	PHE	Peptide
35	1	324	PHE	Peptide
35	1	57	LEU	Peptide
35	1	93	LEU	Peptide
35	1	94	GLY	Peptide
36	2	258	LEU	Peptide
36	2	84	GLY	Peptide
38	4	226	PRO	Peptide
38	4	389	THR	Peptide
38	4	391	ASN	Peptide
39	5	454	SER	Peptide
41	8	21	ALA	Peptide
1	A	243	TYR	Peptide
1	A	248	ARG	Peptide
1	A	633	LEU	Peptide
2	B	151	MET	Peptide
2	B	445	ARG	Peptide
5	E	175	SER	Peptide
5	E	265	GLN	Peptide
5	E	349	ARG	Peptide
5	E	40	LEU	Peptide
5	E	63	GLY	Peptide
7	G	130	ASP	Peptide
7	G	36	TRP	Peptide
9	I	117	GLU	Peptide
10	J	54	PRO	Peptide
11	K	180	CYS	Peptide
12	L	78	TYR	Peptide
19	U	143	PHE	Peptide
19	U	22	VAL	Peptide
20	W	22	ASN	Peptide
21	X	26	PRO	Peptide
21	X	95	SER	Peptide
24	a	41	UNK	Peptide
29	f	72	SER	Peptide
30	g	56	SER	Peptide
31	h	101	ALA	Peptide
33	j	42	TYR	Peptide
34	n	117	UNK	Peptide

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	5236	0	5140	99	0
2	B	3380	0	3293	69	0
3	C	3190	0	3049	114	0
4	D	559	0	496	12	0
5	E	2546	0	2538	64	0
6	F	915	0	842	18	0
7	G	1680	0	1433	43	0
8	H	1385	0	1317	17	0
9	I	1441	0	1373	60	0
10	J	961	0	895	12	0
11	K	1339	0	1317	48	0
12	L	668	0	731	21	0
13	M	726	0	615	13	0
14	O	591	0	585	9	0
15	P	982	0	954	21	0
16	Q	648	0	637	6	0
17	R	820	0	800	13	0
18	S	796	0	168	1	0
19	U	1141	0	1041	15	0
20	W	929	0	917	27	0
21	X	638	0	414	4	0
22	Y	957	0	912	21	0
23	Z	686	0	159	3	0
24	a	501	0	112	0	0
25	b	321	0	67	1	0
26	c	251	0	197	0	0
27	d	752	0	715	9	0
28	e	226	0	51	0	0
29	f	629	0	640	15	0
30	g	492	0	476	8	0
31	h	1081	0	1036	23	0
32	i	266	0	58	2	0
33	j	436	0	280	2	0
34	n	466	0	101	0	0
35	1	2608	0	2641	74	0
36	2	3376	0	3352	71	0
37	3	871	0	923	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	4	3312	0	3110	67	0
39	5	4599	0	4314	76	0
40	6	1211	0	1074	24	0
41	8	672	0	677	6	0
42	9	468	0	437	3	0
43	A	16	0	0	2	0
43	B	8	0	0	3	0
43	I	16	0	0	7	0
43	K	8	0	0	0	0
44	A	4	0	0	0	0
44	H	4	0	0	0	0
45	B	31	0	19	2	0
46	E	48	0	23	5	0
47	M	1	0	0	0	0
48	O	29	0	30	3	0
49	g	83	0	116	2	0
50	1	51	0	82	2	0
50	4	43	0	63	2	0
50	g	43	0	63	3	0
All	All	55137	0	50283	939	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (939) 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)
3:C:116:VAL:HG22	3:C:117:GLY:H	1.06	1.13
3:C:116:VAL:HG22	3:C:117:GLY:N	1.79	0.97
3:C:116:VAL:HG21	3:C:464:VAL:HG21	1.50	0.93
7:G:197:ARG:HD3	15:P:90:TRP:CH2	2.04	0.93
3:C:119:LEU:HD13	3:C:121:ARG:HH11	1.34	0.90
15:P:85:GLU:HG2	15:P:90:TRP:HE3	1.34	0.90
35:1:200:PRO:HG2	35:1:203:ASP:H	1.39	0.87
3:C:116:VAL:CG2	3:C:117:GLY:H	1.88	0.87
15:P:85:GLU:HG2	15:P:90:TRP:CE3	2.11	0.84
3:C:118:LEU:O	11:K:124:THR:HG21	1.79	0.83
3:C:116:VAL:HB	3:C:435:LEU:HD21	1.61	0.81
3:C:197:VAL:HG13	3:C:274:ARG:HE	1.48	0.78
1:A:37:ILE:O	1:A:47:SER:HA	1.84	0.77
10:J:56:ASN:HB3	40:6:92:ARG:HA	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:5:61:ASN:HB3	39:5:79:PHE:HB2	1.68	0.76
36:2:211:LYS:HG2	36:2:240:PRO:HB2	1.68	0.75
3:C:119:LEU:HD13	3:C:121:ARG:NH1	2.03	0.73
1:A:233:CYS:HA	43:A:802:SF4:S2	2.28	0.72
41:8:33:LEU:O	41:8:36:CYS:HB3	1.90	0.72
9:I:133:CYS:HB3	43:I:302:SF4:S2	2.31	0.71
3:C:115:HIS:O	3:C:115:HIS:ND1	2.23	0.70
3:C:112:SER:HB3	3:C:439:ASP:HA	1.74	0.69
7:G:197:ARG:HD3	15:P:90:TRP:HH2	1.58	0.69
3:C:116:VAL:CG2	3:C:464:VAL:HG21	2.21	0.69
9:I:189:ASN:HD21	31:h:75:PRO:HB3	1.58	0.69
3:C:150:ASN:ND2	3:C:410:MET:SD	2.67	0.68
3:C:116:VAL:HG21	3:C:464:VAL:CG2	2.24	0.68
10:J:57:ILE:O	10:J:60:THR:HG22	1.92	0.68
31:h:17:PRO:HA	31:h:20:TYR:HB3	1.76	0.68
2:B:317:LEU:HB2	2:B:361:LYS:HA	1.77	0.67
2:B:381:CYS:SG	2:B:382:GLY:N	2.68	0.67
7:G:71:LEU:HD21	7:G:96:LEU:HB2	1.76	0.66
2:B:387:CYS:HB3	43:B:501:SF4:S4	2.36	0.66
11:K:193:GLN:HE22	11:K:196:ARG:HH11	1.44	0.66
27:d:38:LEU:HD11	39:5:72:TYR:H	1.60	0.65
50:g:202:3PE:H341	37:3:103:VAL:HG12	1.78	0.65
39:5:498:SER:HA	41:8:21:ALA:HB2	1.79	0.65
9:I:93:GLN:HG2	35:1:35:ARG:HH21	1.62	0.65
9:I:152:ARG:HD2	9:I:154:ASP:H	1.62	0.65
30:g:29:ALA:HB2	35:1:319:LEU:HD22	1.79	0.65
3:C:224:ARG:HD2	11:K:183:THR:HG23	1.79	0.65
3:C:147:MET:SD	3:C:147:MET:N	2.70	0.64
20:W:53:GLN:O	20:W:56:ARG:HB3	1.97	0.64
3:C:134:GLN:HE21	9:I:139:ILE:HA	1.63	0.64
7:G:197:ARG:HD3	15:P:90:TRP:CZ3	2.33	0.64
5:E:126:VAL:HG12	5:E:164:ILE:HB	1.80	0.64
19:U:43:GLY:O	19:U:47:LYS:HB2	1.97	0.64
35:1:161:VAL:HG11	35:1:169:ILE:HG13	1.78	0.64
39:5:589:PRO:HA	39:5:592:ILE:HB	1.80	0.64
5:E:227:ASN:ND2	5:E:289:LEU:O	2.31	0.64
1:A:189:CYS:SG	1:A:190:VAL:N	2.71	0.64
36:2:315:GLN:HG3	36:2:378:LEU:HG	1.80	0.64
9:I:133:CYS:CB	43:I:302:SF4:S2	2.86	0.63
1:A:261:MET:HB3	1:A:296:LYS:HE3	1.78	0.63
17:R:28:ASN:HB3	17:R:79:ILE:HG13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:424:LYS:HG2	7:G:129:VAL:HG22	1.81	0.63
2:B:186:LYS:HA	2:B:194:ASP:HA	1.81	0.63
35:1:243:GLY:HA2	35:1:247:LEU:HB3	1.79	0.63
3:C:329:CYS:SG	3:C:332:ARG:NH2	2.71	0.63
1:A:205:SER:O	1:A:211:MET:HA	1.99	0.62
5:E:61:ALA:HA	5:E:66:GLY:HA3	1.81	0.62
9:I:133:CYS:N	43:I:302:SF4:S2	2.69	0.62
12:L:62:LEU:HD21	36:2:131:GLU:HG2	1.81	0.62
2:B:288:CYS:SG	2:B:289:THR:N	2.72	0.62
37:3:64:LEU:HD11	40:6:67:ILE:HG22	1.82	0.62
39:5:151:TYR:HB2	39:5:171:VAL:HG21	1.81	0.62
1:A:394:ASN:HB3	1:A:671:ALA:HB1	1.81	0.62
35:1:161:VAL:HG12	35:1:163:SER:H	1.64	0.62
3:C:457:MET:HG3	3:C:459:LEU:HD13	1.82	0.62
6:F:69:GLN:O	6:F:73:ASN:ND2	2.32	0.62
13:M:125:CYS:HB3	13:M:128:CYS:SG	2.40	0.62
1:A:69:CYS:SG	1:A:80:CYS:N	2.68	0.62
9:I:132:ALA:HB2	9:I:159:THR:HG22	1.81	0.62
38:4:417:VAL:HG12	39:5:175:ARG:HD2	1.82	0.61
1:A:262:ASP:OD2	1:A:294:ASN:ND2	2.33	0.61
9:I:179:CYS:HB2	43:I:302:SF4:S3	2.41	0.61
5:E:109:LEU:HD12	46:E:401:NDP:H61A	1.66	0.61
39:5:80:GLU:H	39:5:134:SER:HB2	1.64	0.61
35:1:110:LEU:HB2	35:1:154:PHE:HZ	1.66	0.61
35:1:130:LYS:HZ2	37:3:49:ARG:HD2	1.66	0.61
1:A:116:GLN:O	1:A:120:ASN:ND2	2.33	0.61
3:C:119:LEU:HA	11:K:124:THR:HG21	1.82	0.61
3:C:116:VAL:HG11	3:C:435:LEU:HD23	1.83	0.60
42:9:32:LYS:O	42:9:34:ARG:NH2	2.34	0.60
11:K:100:GLN:HB3	11:K:105:ILE:HB	1.83	0.60
20:W:37:LEU:HD11	35:1:184:PRO:HG3	1.83	0.60
20:W:34:LEU:O	20:W:37:LEU:HB3	2.00	0.60
9:I:132:ALA:O	9:I:157:ARG:NH2	2.35	0.60
3:C:211:GLU:OE2	11:K:92:HIS:ND1	2.35	0.60
11:K:150:CYS:HA	11:K:155:GLY:HA3	1.83	0.60
5:E:150:ARG:NH1	11:K:47:LEU:O	2.34	0.60
20:W:73:LEU:O	20:W:76:GLU:HB3	2.02	0.60
1:A:363:LYS:HB2	1:A:536:PHE:HE1	1.67	0.59
4:D:36:VAL:HA	19:U:103:GLN:HE21	1.67	0.59
6:F:95:ILE:HG23	6:F:97:ALA:H	1.68	0.59
20:W:60:ARG:NH1	30:g:53:PRO:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1:117:VAL:HG21	35:1:144:ILE:HG23	1.84	0.59
7:G:198:ARG:NH2	7:G:203:TYR:O	2.35	0.59
13:M:90:VAL:HG12	13:M:92:GLY:H	1.67	0.59
1:A:355:GLU:HG3	1:A:358:SER:H	1.68	0.59
1:A:648:ARG:NH1	29:f:63:GLU:OE2	2.35	0.59
14:O:71:GLU:OE1	15:P:57:ARG:NH2	2.35	0.59
20:W:62:LYS:O	20:W:65:ALA:HB3	2.02	0.59
29:f:6:ARG:HG2	29:f:58:PHE:HA	1.84	0.59
11:K:116:ILE:HG22	11:K:143:TRP:HB2	1.84	0.59
9:I:96:ARG:HD2	35:1:35:ARG:HH22	1.68	0.59
2:B:240:ARG:HH12	22:Y:150:HIS:HA	1.68	0.59
2:B:371:ARG:NH2	8:H:128:THR:OG1	2.36	0.59
12:L:12:PHE:HA	12:L:32:MET:HE2	1.85	0.59
36:2:255:ILE:HG23	36:2:303:ASN:HB2	1.83	0.59
39:5:312:GLN:HE22	39:5:396:LYS:HD2	1.68	0.59
2:B:237:LEU:HB2	2:B:242:SER:HB2	1.85	0.58
3:C:114:PRO:HG3	3:C:438:PHE:HD2	1.66	0.58
6:F:127:GLU:HG3	6:F:128:GLU:HG3	1.85	0.58
35:1:203:ASP:HB2	35:1:302:ARG:HG2	1.85	0.58
1:A:413:VAL:HG12	1:A:442:VAL:HB	1.84	0.58
2:B:367:ARG:HG2	2:B:402:ARG:HE	1.69	0.58
3:C:116:VAL:CB	3:C:435:LEU:HD21	2.31	0.58
39:5:373:THR:HG23	39:5:462:MET:HE1	1.84	0.58
35:1:93:LEU:HG	35:1:95:PRO:HA	1.86	0.58
39:5:331:HIS:ND1	39:5:395:THR:O	2.36	0.58
1:A:205:SER:HA	8:H:109:THR:HG21	1.86	0.58
9:I:93:GLN:NE2	35:1:33:MET:O	2.34	0.58
2:B:66:GLU:HG2	2:B:70:LYS:HE2	1.84	0.58
3:C:295:MET:HE1	3:C:457:MET:HE2	1.85	0.58
36:2:252:ASN:ND2	36:2:303:ASN:OD1	2.37	0.58
1:A:393:SER:O	1:A:398:ASN:ND2	2.37	0.58
1:A:601:ASN:OD1	1:A:605:ARG:N	2.37	0.58
5:E:99:LEU:HB3	22:Y:95:LEU:HD13	1.86	0.58
5:E:275:MET:HB3	5:E:344:MET:HE1	1.86	0.58
12:L:79:ARG:HE	12:L:83:VAL:HG21	1.68	0.58
14:O:35:ARG:NH2	14:O:79:GLU:OE2	2.37	0.58
3:C:113:ASP:O	3:C:114:PRO:C	2.44	0.58
9:I:165:ASP:HB3	9:I:168:LYS:HG2	1.85	0.58
2:B:240:ARG:NH2	22:Y:149:VAL:O	2.37	0.58
19:U:17:ASN:HD21	20:W:84:ARG:HG3	1.69	0.58
35:1:251:LEU:HD13	35:1:253:PHE:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:106:GLY:O	37:3:53:ASN:ND2	2.32	0.57
9:I:136:CYS:HB3	43:I:302:SF4:S3	2.43	0.57
39:5:366:LEU:HG	39:5:374:TYR:HB2	1.86	0.57
40:6:9:ILE:HG23	40:6:49:LEU:HD11	1.86	0.57
3:C:297:ARG:NH2	3:C:404:GLU:OE2	2.37	0.57
5:E:110:ARG:NH2	11:K:50:GLN:OE1	2.37	0.57
5:E:146:GLU:OE1	5:E:150:ARG:NH2	2.37	0.57
1:A:220:ASN:ND2	1:A:720:ASP:OD2	2.37	0.57
31:h:34:ARG:HG3	31:h:48:THR:HG23	1.87	0.57
36:2:24:ILE:HG22	36:2:104:ILE:HG21	1.87	0.57
39:5:281:LEU:HD21	39:5:322:LEU:HG	1.85	0.57
48:O:201:ZMP:H11A	15:P:75:LEU:HB3	1.87	0.57
35:1:206:GLU:O	35:1:302:ARG:NH2	2.38	0.57
39:5:110:ASP:HB2	39:5:113:GLN:HB3	1.87	0.57
4:D:46:ASP:O	4:D:50:MET:N	2.38	0.57
11:K:86:CYS:HB2	11:K:121:GLY:H	1.70	0.57
20:W:43:TYR:O	20:W:46:TYR:HB3	2.05	0.57
36:2:299:LEU:HA	36:2:302:LEU:HD23	1.86	0.57
37:3:58:LEU:HD11	40:6:177:ILE:HD13	1.87	0.57
36:2:374:ILE:HD12	36:2:376:PRO:HD2	1.87	0.56
7:G:197:ARG:CD	15:P:90:TRP:HH2	2.18	0.56
38:4:384:ILE:HD11	38:4:421:ALA:HA	1.86	0.56
3:C:420:GLU:HG3	3:C:421:ARG:HG3	1.87	0.56
5:E:247:ARG:NH1	5:E:334:ASP:O	2.39	0.56
12:L:6:ILE:HD12	40:6:13:ILE:HD11	1.87	0.56
38:4:103:ASN:HD21	38:4:240:LEU:HB3	1.69	0.56
7:G:185:MET:HE3	7:G:210:LEU:HB2	1.88	0.56
11:K:78:PRO:HG2	11:K:107:PHE:HB3	1.87	0.56
36:2:257:SER:HB2	36:2:301:LEU:HD22	1.86	0.56
39:5:385:MET:HG2	39:5:426:CYS:HA	1.88	0.56
1:A:222:ASN:ND2	1:A:716:ALA:O	2.38	0.56
1:A:240:ASN:HB3	1:A:243:TYR:HB3	1.87	0.56
4:D:55:ARG:NH1	4:D:70:ALA:O	2.39	0.56
21:X:5:THR:O	37:3:85:ASN:ND2	2.39	0.56
22:Y:86:ASP:O	22:Y:89:ASN:ND2	2.38	0.56
9:I:118:HIS:NE2	9:I:169:CYS:SG	2.76	0.56
3:C:426:LYS:HG2	7:G:127:THR:HG21	1.87	0.56
6:F:63:LYS:O	6:F:69:GLN:NE2	2.38	0.56
25:b:31:UNK:O	25:b:35:UNK:N	2.38	0.56
36:2:164:LEU:HD13	36:2:210:PHE:HB2	1.86	0.56
38:4:293:LEU:O	38:4:426:LYS:NZ	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:161:LYS:NZ	22:Y:97:GLY:O	2.38	0.56
35:1:57:LEU:HD11	35:1:225:VAL:HB	1.88	0.56
36:2:209:LEU:HB3	36:2:214:ILE:HD13	1.87	0.56
36:2:214:ILE:HA	36:2:268:LEU:HD13	1.88	0.56
1:A:533:ASP:OD1	29:f:45:ARG:NH2	2.39	0.56
35:1:67:GLU:HG2	35:1:126:SER:HB2	1.88	0.56
39:5:366:LEU:N	39:5:436:THR:O	2.39	0.56
38:4:245:ILE:O	38:4:249:LEU:N	2.38	0.56
39:5:85:THR:HG23	39:5:131:VAL:HG12	1.88	0.55
4:D:55:ARG:NH2	20:W:76:GLU:OE2	2.40	0.55
5:E:217:MET:HB3	5:E:276:VAL:HG11	1.89	0.55
7:G:198:ARG:NH1	7:G:205:PHE:O	2.39	0.55
29:f:24:GLN:O	29:f:28:ASN:ND2	2.39	0.55
3:C:308:ASN:O	7:G:150:ASN:ND2	2.37	0.55
1:A:247:ALA:HB1	1:A:252:LEU:HD11	1.87	0.55
8:H:156:THR:HG22	8:H:158:ASP:H	1.70	0.55
13:M:97:CYS:SG	13:M:110:HIS:HE1	2.19	0.55
13:M:103:ASN:ND2	31:h:94:LYS:O	2.40	0.55
22:Y:86:ASP:HB2	22:Y:89:ASN:HB3	1.87	0.55
9:I:157:ARG:O	9:I:158:ARG:NH1	2.39	0.55
36:2:108:LEU:HA	36:2:111:ILE:HD12	1.88	0.55
30:g:25:HIS:HB2	35:1:315:ILE:HD13	1.89	0.55
39:5:67:TYR:HD2	39:5:68:LEU:HD22	1.70	0.55
9:I:179:CYS:HA	43:I:302:SF4:S3	2.47	0.55
11:K:170:ILE:HG22	11:K:171:VAL:HG13	1.88	0.55
36:2:78:VAL:HG11	36:2:321:LEU:HD21	1.88	0.55
3:C:259:ASP:OD1	3:C:341:ARG:NH1	2.39	0.55
11:K:72:ARG:HD3	11:K:143:TRP:HH2	1.72	0.55
22:Y:63:GLN:OE1	22:Y:79:ARG:NH1	2.39	0.55
1:A:132:ASP:O	1:A:136:CYS:N	2.35	0.55
1:A:491:ARG:HH22	1:A:691:THR:H	1.53	0.55
3:C:185:ASN:HD21	3:C:407:LYS:HG3	1.71	0.55
9:I:179:CYS:CB	43:I:302:SF4:S3	2.95	0.55
3:C:336:ARG:NH2	3:C:456:THR:O	2.38	0.55
18:S:195:UNK:O	27:d:32:ARG:NH2	2.40	0.55
36:2:346:TYR:HB2	36:2:349:GLN:HG2	1.89	0.55
1:A:98:ALA:HB3	2:B:227:LEU:HD23	1.89	0.54
3:C:163:ASN:ND2	23:Z:81:UNK:O	2.39	0.54
1:A:552:LEU:HD22	1:A:555:ALA:HB3	1.89	0.54
3:C:379:GLU:OE2	3:C:383:HIS:NE2	2.39	0.54
3:C:398:GLU:HG2	3:C:415:VAL:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:4:152:ILE:HA	38:4:239:PRO:HG2	1.90	0.54
9:I:192:TYR:CG	11:K:178:PRO:HG3	2.43	0.54
35:1:240:ALA:O	35:1:244:TYR:N	2.40	0.54
12:L:20:ARG:NH2	40:6:26:ALA:O	2.40	0.54
22:Y:62:GLN:NE2	22:Y:75:THR:O	2.41	0.54
36:2:233:THR:HG21	36:2:282:LYS:HD2	1.89	0.54
39:5:32:THR:OG1	39:5:33:ARG:N	2.40	0.54
17:R:44:ARG:O	17:R:48:ASP:HB2	2.07	0.54
1:A:288:VAL:HG22	1:A:401:ILE:HD13	1.90	0.54
2:B:162:GLY:O	2:B:201:ARG:NH1	2.40	0.54
36:2:226:GLU:HA	36:2:282:LYS:HG2	1.89	0.54
1:A:307:GLN:HB3	31:h:130:TRP:HD1	1.71	0.54
21:X:88:GLY:O	21:X:92:ALA:N	2.40	0.54
36:2:369:PHE:HB3	36:2:374:ILE:HG12	1.89	0.54
38:4:382:ALA:O	38:4:391:ASN:ND2	2.41	0.54
2:B:207:VAL:HG21	2:B:381:CYS:HB3	1.90	0.54
17:R:29:TRP:HD1	17:R:30:ILE:HG23	1.72	0.54
36:2:83:TYR:HE1	36:2:231:LEU:HB3	1.73	0.54
3:C:116:VAL:HG11	3:C:435:LEU:CD2	2.38	0.53
5:E:129:ILE:HG22	46:E:401:NDP:H8A	1.89	0.53
5:E:162:ARG:NH1	5:E:251:ASP:O	2.41	0.53
5:E:132:GLU:OE2	5:E:316:ARG:NH2	2.41	0.53
6:F:137:TYR:OH	7:G:156:LYS:NZ	2.38	0.53
38:4:91:LEU:HD23	38:4:333:VAL:HG23	1.90	0.53
39:5:201:PHE:HA	39:5:268:ASN:HD22	1.74	0.53
39:5:295:ALA:HB2	39:5:307:LEU:HB2	1.90	0.53
1:A:68:TYR:O	1:A:188:ARG:NH2	2.41	0.53
5:E:266:LYS:HB3	5:E:268:THR:HG23	1.90	0.53
15:P:66:VAL:O	15:P:72:GLN:NE2	2.42	0.53
20:W:47:ARG:NH2	35:1:175:VAL:O	2.38	0.53
38:4:211:TRP:HZ2	38:4:277:ILE:HD11	1.74	0.53
39:5:31:VAL:HG11	39:5:114:VAL:HG13	1.90	0.53
2:B:184:ILE:HD11	2:B:195:PHE:HD2	1.73	0.53
17:R:33:ARG:NH1	39:5:442:ASN:O	2.42	0.53
1:A:217:LEU:HD22	1:A:219:LYS:HD2	1.91	0.53
2:B:272:ASN:HD22	2:B:340:ASP:HB2	1.74	0.53
3:C:208:GLU:OE2	3:C:212:LYS:NZ	2.42	0.53
3:C:271:TRP:H	3:C:274:ARG:HB3	1.73	0.53
6:F:61:HIS:O	6:F:68:ARG:NH1	2.41	0.53
38:4:85:SER:HB3	38:4:260:ARG:HH21	1.73	0.53
1:A:573:GLY:O	1:A:589:GLY:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:221:SER:OG	3:C:222:GLY:N	2.41	0.52
17:R:28:ASN:HD22	17:R:78:PRO:HA	1.74	0.52
36:2:292:ASN:HA	36:2:295:TYR:HD2	1.74	0.52
3:C:226:HIS:HD2	11:K:181:PRO:HD3	1.75	0.52
3:C:262:GLU:OE2	20:W:21:ARG:NH2	2.39	0.52
3:C:428:ARG:HE	7:G:124:ILE:HG13	1.74	0.52
10:J:105:GLY:O	10:J:109:GLY:N	2.40	0.52
40:6:179:ILE:HG23	40:6:180:THR:HG23	1.92	0.52
3:C:424:LYS:HE3	7:G:210:LEU:HD21	1.91	0.52
7:G:144:PHE:HB2	7:G:153:ILE:HG22	1.89	0.52
7:G:166:PRO:HA	7:G:191:GLU:HB3	1.91	0.52
15:P:61:GLU:OE2	15:P:64:ARG:NH2	2.43	0.52
1:A:194:ASN:ND2	22:Y:157:HIS:H	2.07	0.52
1:A:252:LEU:HD23	1:A:271:ASP:HB3	1.92	0.52
19:U:72:GLY:O	20:W:79:ARG:NH1	2.43	0.52
35:1:117:VAL:HG23	35:1:143:LEU:HD23	1.92	0.52
36:2:59:LEU:HB2	36:2:121:ASN:HB2	1.90	0.52
39:5:400:ILE:O	39:5:403:THR:OG1	2.28	0.52
1:A:363:LYS:NZ	1:A:534:ILE:O	2.42	0.52
1:A:698:TYR:O	1:A:704:SER:OG	2.27	0.52
35:1:72:ILE:HA	35:1:75:ILE:HG22	1.91	0.52
1:A:123:GLU:OE2	1:A:157:ARG:NH1	2.42	0.52
5:E:164:ILE:HG12	5:E:198:THR:HB	1.92	0.52
7:G:126:ILE:HG13	7:G:178:PHE:HB3	1.90	0.52
8:H:102:MET:HA	8:H:105:TYR:HD2	1.74	0.52
29:f:14:GLN:O	29:f:23:ARG:NH1	2.40	0.52
1:A:480:PRO:O	1:A:516:TRP:NE1	2.38	0.52
10:J:25:THR:O	10:J:29:ALA:HB2	2.10	0.52
1:A:131:LEU:HD22	3:C:381:LEU:HD12	1.91	0.52
3:C:87:PHE:HB3	3:C:100:LEU:HB3	1.92	0.52
36:2:387:LEU:HD21	36:2:402:LEU:HD22	1.91	0.52
1:A:429:ARG:NH1	1:A:449:THR:O	2.42	0.52
2:B:309:ILE:HD12	2:B:313:TRP:HA	1.91	0.52
5:E:81:VAL:HG13	5:E:105:LEU:HD23	1.91	0.52
35:1:153:ILE:HD11	35:1:189:PHE:HD1	1.75	0.52
5:E:129:ILE:O	46:E:401:NDP:O3D	2.27	0.51
39:5:589:PRO:O	39:5:593:ASN:N	2.40	0.51
1:A:69:CYS:HB3	1:A:80:CYS:HB3	1.93	0.51
3:C:240:PRO:HD3	9:I:113:ARG:HH22	1.74	0.51
1:A:267:ASN:HD22	1:A:285:HIS:HB3	1.73	0.51
1:A:398:ASN:N	1:A:520:ASN:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:LEU:HB3	2:B:146:LEU:HD11	1.92	0.51
9:I:122:ARG:HB2	9:I:126:GLY:HA3	1.92	0.51
17:R:89:LYS:HA	17:R:92:ARG:HD2	1.93	0.51
36:2:333:TYR:OH	36:2:357:ASN:ND2	2.43	0.51
3:C:220:VAL:HA	9:I:113:ARG:HH21	1.76	0.51
9:I:99:TYR:HE2	35:1:35:ARG:HD3	1.76	0.51
9:I:194:THR:HB	9:I:199:GLU:HB3	1.92	0.51
17:R:80:VAL:HG13	17:R:86:GLY:HA3	1.91	0.51
17:R:88:THR:O	17:R:92:ARG:NH1	2.44	0.51
37:3:99:ILE:HA	37:3:102:PHE:HD2	1.74	0.51
5:E:115:ILE:HG21	5:E:151:ILE:HG22	1.92	0.51
7:G:123:ILE:HG21	7:G:172:TYR:CZ	2.45	0.51
10:J:105:GLY:HA2	10:J:108:LEU:HB2	1.92	0.51
14:O:68:ASP:HB2	15:P:57:ARG:HH12	1.76	0.51
22:Y:65:LYS:HG2	22:Y:75:THR:HG22	1.93	0.51
1:A:484:VAL:HB	1:A:521:VAL:HG12	1.92	0.51
29:f:33:PHE:O	29:f:37:ASN:N	2.44	0.51
35:1:30:LEU:O	35:1:34:GLN:N	2.43	0.51
1:A:150:ARG:HH11	3:C:393:SER:HB3	1.76	0.51
9:I:80:LEU:HB2	9:I:83:MET:HB3	1.92	0.51
9:I:168:LYS:HA	11:K:155:GLY:HA2	1.93	0.51
6:F:91:ILE:O	6:F:95:ILE:HB	2.11	0.51
30:g:5:ASN:O	30:g:22:ASN:ND2	2.41	0.51
36:2:268:LEU:HD11	36:2:290:LEU:HD21	1.93	0.51
6:F:99:LEU:O	6:F:103:VAL:N	2.44	0.51
7:G:78:ILE:HG21	7:G:98:LEU:HD21	1.93	0.51
31:h:48:THR:HG22	31:h:50:HIS:H	1.74	0.51
35:1:175:VAL:HG13	35:1:176:VAL:HG23	1.93	0.51
38:4:137:PHE:O	38:4:141:PHE:HB2	2.11	0.51
38:4:400:GLN:NE2	39:5:186:CYS:SG	2.84	0.51
39:5:383:SER:HA	39:5:390:LEU:HD11	1.93	0.51
3:C:211:GLU:HB3	11:K:97:ARG:HE	1.76	0.51
5:E:207:GLY:H	5:E:210:ASP:CG	2.19	0.51
11:K:55:SER:HB2	11:K:210:LYS:HE2	1.92	0.51
17:R:93:ASN:HD22	39:5:111:PRO:HD3	1.75	0.51
21:X:52:ALA:O	21:X:56:PHE:N	2.43	0.51
36:2:72:ILE:HD11	36:2:242:ILE:HD11	1.91	0.51
5:E:39:THR:OG1	5:E:40:LEU:N	2.44	0.50
21:X:75:LEU:O	21:X:79:THR:N	2.40	0.50
39:5:366:LEU:H	39:5:437:PHE:HA	1.76	0.50
1:A:183:CYS:HA	43:A:802:SF4:S3	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:199:ASP:O	8:H:203:GLY:N	2.44	0.50
37:3:65:PRO:HA	37:3:68:LEU:HD23	1.94	0.50
2:B:320:ILE:HB	2:B:357:ILE:HB	1.93	0.50
3:C:201:THR:HG23	35:1:298:ALA:HB1	1.92	0.50
3:C:293:GLY:HA3	3:C:408:GLY:HA2	1.93	0.50
9:I:152:ARG:HE	9:I:154:ASP:HB2	1.76	0.50
11:K:93:VAL:HG21	11:K:187:LEU:HD23	1.93	0.50
19:U:60:SER:HB2	19:U:63:SER:HB3	1.92	0.50
35:1:157:ILE:O	35:1:178:TYR:OH	2.29	0.50
36:2:215:ALA:HB3	36:2:267:THR:HG23	1.93	0.50
36:2:259:VAL:HG12	36:2:262:ILE:HD11	1.93	0.50
39:5:92:ILE:HD11	39:5:128:ILE:HD13	1.92	0.50
2:B:213:SER:HB2	2:B:225:PRO:HG3	1.93	0.50
14:O:74:VAL:HA	14:O:77:GLU:HG2	1.92	0.50
35:1:287:VAL:HA	35:1:290:MET:HE3	1.93	0.50
2:B:120:ASP:O	45:B:502:FMN:N3	2.44	0.50
6:F:126:LEU:HA	7:G:84:LYS:HA	1.93	0.50
38:4:429:ASN:HB2	39:5:164:MET:HG3	1.94	0.50
2:B:232:PRO:HB2	2:B:237:LEU:HD11	1.94	0.50
3:C:306:ARG:NH2	3:C:404:GLU:OE1	2.44	0.50
27:d:80:GLN:NE2	38:4:475:LEU:O	2.45	0.50
38:4:171:THR:O	38:4:175:SER:OG	2.28	0.50
38:4:309:HIS:NE2	38:4:383:ASN:OD1	2.43	0.50
5:E:202:PRO:HA	5:E:261:LEU:HB2	1.92	0.50
11:K:147:MET:HA	11:K:177:VAL:HB	1.93	0.50
14:O:40:LEU:HD13	14:O:72:VAL:HG21	1.94	0.50
3:C:284:GLN:O	3:C:288:ASN:ND2	2.45	0.50
5:E:169:PHE:HB2	5:E:321:GLN:HE22	1.77	0.50
6:F:127:GLU:HB3	7:G:84:LYS:HE3	1.93	0.50
39:5:388:PRO:HA	39:5:393:TYR:HB2	1.94	0.50
3:C:306:ARG:HH11	3:C:319:PHE:HZ	1.60	0.50
7:G:88:GLY:HA3	23:Z:88:UNK:HA	1.94	0.50
13:M:76:TYR:CZ	31:h:103:PRO:HD2	2.47	0.50
49:g:201:CDL:HB22	36:2:15:MET:HG2	1.94	0.50
35:1:146:TYR:HD1	35:1:149:ILE:HD11	1.77	0.50
2:B:160:ILE:O	2:B:202:GLY:N	2.42	0.49
12:L:60:ILE:HD12	40:6:63:TYR:HE2	1.76	0.49
36:2:212:ILE:HD12	36:2:293:ALA:HB1	1.94	0.49
39:5:251:HIS:HB2	39:5:343:PHE:HE2	1.77	0.49
1:A:263:ALA:HA	1:A:526:ALA:HA	1.94	0.49
5:E:277:SER:HB2	5:E:282:LYS:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:126:ILE:HG21	7:G:168:ILE:HD11	1.94	0.49
8:H:132:CYS:HA	8:H:175:ALA:HB1	1.94	0.49
9:I:144:ALA:HB2	9:I:168:LYS:HG3	1.93	0.49
20:W:49:LEU:O	20:W:53:GLN:N	2.39	0.49
39:5:510:TYR:O	39:5:514:PRO:N	2.45	0.49
2:B:163:GLU:HG2	8:H:169:LEU:HD22	1.94	0.49
31:h:79:PHE:O	31:h:83:TYR:N	2.45	0.49
36:2:230:ILE:HA	36:2:233:THR:HG22	1.94	0.49
5:E:99:LEU:HD21	9:I:197:ARG:HD2	1.94	0.49
1:A:392:ARG:HB2	29:f:45:ARG:HG3	1.94	0.49
9:I:74:ALA:O	9:I:78:PHE:HB2	2.13	0.49
27:d:48:LEU:HD23	39:5:199:THR:HG23	1.93	0.49
4:D:37:ARG:H	19:U:103:GLN:HG3	1.77	0.49
5:E:67:SER:HA	5:E:93:LEU:HD11	1.95	0.49
22:Y:91:TRP:NE1	22:Y:100:SER:OG	2.45	0.49
36:2:276:LEU:HD22	36:2:412:TYR:HB3	1.95	0.49
38:4:86:LEU:HA	38:4:89:ILE:HD12	1.94	0.49
39:5:86:ILE:HA	39:5:89:LEU:HG	1.94	0.49
3:C:439:ASP:OD1	3:C:439:ASP:N	2.43	0.49
5:E:295:GLN:O	5:E:298:THR:OG1	2.27	0.49
11:K:75:SER:OG	11:K:76:PHE:N	2.45	0.49
29:f:37:ASN:HB3	29:f:40:THR:HB	1.94	0.49
31:h:43:ASN:ND2	31:h:63:TYR:O	2.45	0.49
38:4:158:SER:OG	38:4:159:ASP:N	2.41	0.49
2:B:425:THR:HG21	2:B:430:GLY:HA3	1.95	0.49
7:G:180:ARG:HH22	7:G:197:ARG:CZ	2.25	0.49
1:A:700:THR:HA	1:A:705:ARG:HH21	1.76	0.49
2:B:129:ASP:O	2:B:133:MET:N	2.44	0.49
3:C:101:ILE:HG22	3:C:115:HIS:HB2	1.95	0.48
3:C:184:LEU:HD21	3:C:210:ARG:HH21	1.77	0.48
31:h:45:PHE:HE2	31:h:77:TRP:HB3	1.78	0.48
3:C:116:VAL:CG1	3:C:435:LEU:HD21	2.43	0.48
5:E:69:LEU:HD22	5:E:245:LEU:HD22	1.95	0.48
5:E:155:VAL:HA	5:E:160:ILE:HD12	1.93	0.48
7:G:113:ARG:NH1	7:G:114:ASP:OD2	2.46	0.48
36:2:6:ILE:HD13	36:2:109:ILE:HG22	1.95	0.48
36:2:326:ILE:HG21	36:2:364:MET:HB2	1.95	0.48
1:A:154:ASP:HA	3:C:379:GLU:HG2	1.95	0.48
6:F:38:GLN:HA	6:F:101:GLU:HG2	1.95	0.48
12:L:81:ARG:HB3	37:3:52:PHE:CG	2.48	0.48
27:d:24:ARG:NH1	38:4:195:ILE:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:3:1:MET:HA	37:3:5:ILE:HD12	1.95	0.48
1:A:48:ILE:HD11	1:A:101:VAL:HG21	1.95	0.48
6:F:23:VAL:HA	37:3:122:ASP:HA	1.94	0.48
38:4:350:LEU:O	38:4:362:TYR:OH	2.31	0.48
40:6:55:PHE:HA	40:6:58:LEU:HB2	1.96	0.48
1:A:194:ASN:HD21	22:Y:157:HIS:H	1.62	0.48
2:B:285:ASN:HB3	2:B:308:GLY:H	1.78	0.48
6:F:99:LEU:HD23	9:I:59:ARG:HD3	1.95	0.48
16:Q:62:LEU:HD11	16:Q:98:ALA:HB1	1.96	0.48
20:W:101:PHE:HD2	20:W:103:VAL:HG23	1.78	0.48
35:1:289:LEU:O	35:1:292:SER:OG	2.27	0.48
39:5:357:SER:O	39:5:363:TYR:OH	2.28	0.48
2:B:160:ILE:HD11	2:B:201:ARG:HG2	1.96	0.48
9:I:123:TYR:HA	9:I:129:ARG:HH21	1.79	0.48
2:B:194:ASP:OD1	2:B:194:ASP:N	2.47	0.48
7:G:112:LEU:HD21	7:G:153:ILE:HD13	1.95	0.48
36:2:214:ILE:O	36:2:217:LEU:N	2.43	0.48
22:Y:95:LEU:HD23	22:Y:96:ILE:HG12	1.96	0.48
31:h:113:THR:HG22	31:h:115:GLY:H	1.79	0.48
39:5:180:PHE:HD2	39:5:221:ILE:HG21	1.78	0.48
1:A:117:ALA:HA	1:A:120:ASN:HD22	1.79	0.48
2:B:215:ILE:HG13	2:B:237:LEU:HD22	1.94	0.48
3:C:278:ILE:HD11	3:C:449:ASP:HB3	1.95	0.48
12:L:3:ILE:H	12:L:3:ILE:HG13	1.50	0.48
23:Z:30:UNK:O	23:Z:34:UNK:N	2.47	0.48
29:f:66:ILE:HG22	29:f:83:LEU:HD11	1.96	0.48
41:8:47:CYS:HB3	41:8:50:GLU:HB2	1.94	0.48
7:G:197:ARG:CD	15:P:90:TRP:CH2	2.86	0.47
1:A:166:SER:HB3	13:M:94:THR:HG23	1.95	0.47
3:C:197:VAL:HG12	35:1:301:PRO:HB2	1.95	0.47
3:C:254:PHE:HD2	3:C:344:LEU:HD12	1.79	0.47
9:I:123:TYR:HB2	9:I:126:GLY:HA2	1.95	0.47
11:K:154:GLY:HA3	11:K:158:HIS:HD2	1.79	0.47
30:g:11:GLY:O	30:g:15:TYR:N	2.41	0.47
32:i:28:UNK:N	39:5:58:ASN:O	2.47	0.47
36:2:202:ILE:HD13	36:2:260:ILE:HG21	1.95	0.47
36:2:214:ILE:HG22	36:2:216:PRO:HD2	1.96	0.47
38:4:241:ALA:HA	38:4:244:MET:HG2	1.94	0.47
38:4:244:MET:HG3	38:4:245:ILE:HG12	1.95	0.47
38:4:386:THR:O	38:4:392:PHE:HB2	2.14	0.47
39:5:219:LEU:HD23	39:5:262:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:8:33:LEU:HD21	41:8:37:ARG:HH11	1.77	0.47
5:E:146:GLU:HG2	5:E:149:ARG:HE	1.79	0.47
20:W:48:ALA:HA	35:1:176:VAL:HG21	1.96	0.47
35:1:323:ILE:HD11	50:1:401:3PE:H3E1	1.96	0.47
38:4:387:PRO:HB3	39:5:144:GLU:HB3	1.96	0.47
1:A:248:ARG:HD2	9:I:134:LYS:HB2	1.97	0.47
3:C:204:LEU:HD22	35:1:34:GLN:HB3	1.96	0.47
3:C:421:ARG:NH1	7:G:246:SER:O	2.47	0.47
5:E:131:ARG:NH1	46:E:401:NDP:O2B	2.47	0.47
8:H:141:MET:HE1	8:H:165:GLU:HB3	1.96	0.47
27:d:42:LYS:HG2	27:d:45:ARG:HH12	1.80	0.47
36:2:12:PHE:O	36:2:16:SER:OG	2.31	0.47
37:3:24:LEU:HD12	37:3:25:LEU:HB3	1.97	0.47
38:4:381:PHE:HA	38:4:384:ILE:HB	1.96	0.47
2:B:332:ASN:OD1	2:B:332:ASN:N	2.45	0.47
5:E:245:LEU:HA	5:E:248:ILE:HG22	1.97	0.47
10:J:60:THR:HG23	10:J:61:PHE:CD2	2.50	0.47
14:O:46:ILE:HD11	14:O:64:LEU:HD21	1.96	0.47
22:Y:103:ASP:HB3	22:Y:106:GLN:HB2	1.95	0.47
36:2:380:PHE:HE2	38:4:135:ILE:HG23	1.79	0.47
39:5:250:LEU:HA	39:5:255:LEU:HD23	1.97	0.47
1:A:169:ASP:OD1	1:A:169:ASP:N	2.46	0.47
5:E:170:ASN:ND2	5:E:320:SER:O	2.47	0.47
30:g:43:LEU:HG	35:1:333:ILE:HA	1.96	0.47
37:3:8:ILE:HD12	37:3:9:ILE:HG13	1.97	0.47
38:4:106:ASN:ND2	38:4:352:ASP:OD1	2.48	0.47
40:6:64:ILE:HA	40:6:68:ALA:HB3	1.97	0.47
1:A:111:THR:HG22	1:A:113:ARG:H	1.80	0.47
2:B:449:GLU:HA	2:B:452:MET:HE2	1.97	0.47
3:C:99:ARG:O	3:C:115:HIS:HB3	2.15	0.47
3:C:116:VAL:CG1	3:C:435:LEU:CD2	2.92	0.47
3:C:184:LEU:HG	3:C:210:ARG:HE	1.79	0.47
3:C:186:HIS:NE2	3:C:339:GLU:OE1	2.48	0.47
5:E:107:MET:HA	5:E:114:SER:HB2	1.97	0.47
7:G:180:ARG:NH2	7:G:197:ARG:CZ	2.78	0.47
9:I:131:ILE:HG22	9:I:157:ARG:HG3	1.95	0.47
19:U:18:MET:SD	19:U:18:MET:N	2.88	0.47
30:g:44:THR:HG22	30:g:47:ARG:HH12	1.80	0.47
31:h:40:ILE:HG22	31:h:41:TYR:H	1.79	0.47
35:1:220:SER:HA	35:1:224:PHE:HB2	1.96	0.47
39:5:270:LEU:HB3	39:5:277:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ILE:HD11	1:A:585:VAL:HG11	1.97	0.47
1:A:595:LYS:NZ	1:A:622:ASP:OD2	2.47	0.47
2:B:78:GLU:OE2	2:B:261:GLY:N	2.48	0.47
2:B:232:PRO:HA	2:B:235:VAL:HG12	1.97	0.47
2:B:311:GLY:O	2:B:315:ASN:ND2	2.42	0.47
17:R:81:PRO:HB2	17:R:84:PHE:HD2	1.80	0.47
38:4:250:ILE:HA	38:4:253:LEU:HD23	1.97	0.47
5:E:72:LYS:HE2	5:E:243:ALA:HA	1.97	0.47
14:O:59:ALA:HA	14:O:64:LEU:H	1.79	0.47
19:U:90:CYS:HB3	19:U:93:GLU:HB2	1.96	0.47
38:4:330:VAL:HA	38:4:333:VAL:HG12	1.96	0.47
3:C:177:PHE:HZ	3:C:220:VAL:HG21	1.80	0.47
7:G:202:ASP:HB2	7:G:205:PHE:HB2	1.97	0.47
9:I:192:TYR:CD1	11:K:178:PRO:HG3	2.50	0.47
12:L:33:LEU:HD23	12:L:59:ILE:HD11	1.97	0.47
39:5:143:TRP:HE1	39:5:226:LYS:HG3	1.80	0.47
2:B:200:HIS:ND1	8:H:62:TYR:OH	2.47	0.46
3:C:176:MET:HE1	3:C:247:ILE:HD13	1.97	0.46
3:C:207:PHE:HA	3:C:210:ARG:HB2	1.96	0.46
9:I:66:SER:HB3	30:g:18:TRP:HZ2	1.80	0.46
9:I:163:ASP:OD2	22:Y:98:TRP:NE1	2.47	0.46
19:U:83:ILE:HA	19:U:86:ILE:HG22	1.98	0.46
39:5:390:LEU:HD12	39:5:392:GLY:H	1.80	0.46
2:B:117:VAL:HB	2:B:158:ILE:HA	1.97	0.46
20:W:56:ARG:HH22	35:1:336:SER:HB3	1.79	0.46
36:2:257:SER:HG	36:2:261:SER:H	1.61	0.46
37:3:74:LEU:HA	37:3:77:VAL:HG12	1.98	0.46
2:B:370:GLN:OE1	2:B:402:ARG:NH1	2.42	0.46
9:I:102:TYR:O	9:I:106:GLU:N	2.49	0.46
39:5:206:LEU:HB2	39:5:209:THR:HA	1.98	0.46
1:A:408:ASP:HB3	1:A:477:ALA:HB1	1.96	0.46
3:C:115:HIS:HD1	3:C:115:HIS:C	2.23	0.46
5:E:207:GLY:N	5:E:210:ASP:OD1	2.48	0.46
5:E:270:LYS:O	5:E:273:ILE:HB	2.16	0.46
36:2:309:TYR:CZ	36:2:313:ILE:HD11	2.51	0.46
4:D:55:ARG:HD2	4:D:73:ALA:HA	1.97	0.46
5:E:260:GLU:OE2	5:E:321:GLN:NE2	2.48	0.46
14:O:65:ASP:O	14:O:69:THR:N	2.48	0.46
3:C:450:ALA:HA	3:C:453:ILE:HG22	1.98	0.46
12:L:62:LEU:HD11	36:2:131:GLU:HB3	1.98	0.46
36:2:103:LEU:HD13	36:2:107:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:231:GLU:H	5:E:269:GLN:HB3	1.81	0.46
38:4:238:SER:HB2	38:4:244:MET:HB2	1.98	0.46
35:1:8:ILE:HD11	37:3:7:PHE:HB2	1.98	0.46
38:4:207:GLN:HE21	38:4:266:LEU:HA	1.80	0.46
6:F:78:ARG:HG2	6:F:95:ILE:HD11	1.98	0.46
8:H:48:SER:H	8:H:51:ASN:HD22	1.64	0.46
11:K:117:MET:HE1	11:K:135:TYR:HB2	1.98	0.46
31:h:135:LYS:HG3	31:h:136:GLN:H	1.81	0.46
38:4:252:LYS:HE3	38:4:306:SER:HB3	1.97	0.46
38:4:265:LEU:HD12	38:4:266:LEU:HD22	1.98	0.46
42:9:19:TRP:O	42:9:23:MET:N	2.42	0.46
2:B:381:CYS:HB3	43:B:501:SF4:S1	2.55	0.46
12:L:2:PHE:HZ	40:6:126:PHE:HA	1.81	0.46
12:L:15:PHE:O	12:L:18:ASN:ND2	2.49	0.46
14:O:77:GLU:OE2	15:P:34:ARG:NE	2.49	0.46
48:O:201:ZMP:H5A	15:P:59:GLU:HG3	1.97	0.46
20:W:78:ASP:HA	20:W:81:THR:HG22	1.97	0.46
36:2:398:ILE:HA	36:2:401:VAL:HG12	1.97	0.46
3:C:360:LYS:HB3	3:C:367:ASN:HD21	1.81	0.45
5:E:270:LYS:HB3	5:E:273:ILE:HD12	1.98	0.45
7:G:146:SER:HG	7:G:151:SER:H	1.62	0.45
8:H:109:THR:HA	8:H:116:ARG:NH1	2.31	0.45
12:L:3:ILE:HG22	40:6:13:ILE:HB	1.98	0.45
31:h:69:ASP:N	31:h:69:ASP:OD1	2.48	0.45
40:6:87:VAL:O	40:6:91:ILE:N	2.47	0.45
6:F:120:TRP:CD2	7:G:107:PRO:HB3	2.51	0.45
7:G:142:TYR:O	7:G:154:ARG:HA	2.17	0.45
11:K:112:ARG:HH11	35:1:218:GLU:HG3	1.81	0.45
16:Q:96:VAL:HA	16:Q:99:ILE:HD12	1.98	0.45
35:1:188:ILE:HA	35:1:191:ILE:HG22	1.97	0.45
39:5:53:LEU:HD11	39:5:86:ILE:HG21	1.98	0.45
39:5:173:MET:HB3	39:5:232:LEU:HD13	1.97	0.45
9:I:107:LYS:HE2	31:h:78:HIS:CE1	2.51	0.45
10:J:102:ALA:HB2	10:J:127:ALA:HB2	1.98	0.45
22:Y:116:GLU:HA	22:Y:119:ILE:HG22	1.98	0.45
29:f:20:ALA:HA	29:f:23:ARG:HB2	1.98	0.45
39:5:392:GLY:HA2	39:5:395:THR:HG22	1.97	0.45
39:5:430:MET:HG3	39:5:525:ILE:HA	1.97	0.45
1:A:261:MET:HE1	1:A:300:ALA:HB2	1.98	0.45
1:A:263:ALA:O	1:A:602:THR:N	2.50	0.45
5:E:237:HIS:CG	5:E:343:LEU:HD21	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:115:VAL:HG12	10:J:118:PHE:H	1.80	0.45
11:K:73:GLN:HE21	11:K:195:GLN:HB3	1.81	0.45
11:K:89:GLU:HG2	11:K:182:PRO:O	2.16	0.45
39:5:381:SER:HB2	39:5:429:SER:HB2	1.98	0.45
3:C:402:ALA:HA	3:C:410:MET:O	2.17	0.45
3:C:121:ARG:HG3	3:C:123:THR:HG23	1.98	0.45
5:E:228:LYS:HE3	5:E:318:PHE:HD1	1.82	0.45
35:1:13:VAL:O	35:1:17:PHE:HB2	2.16	0.45
35:1:179:CYS:SG	35:1:180:ILE:N	2.90	0.45
39:5:250:LEU:HA	39:5:255:LEU:HB2	1.99	0.45
40:6:170:LEU:O	40:6:174:ILE:HG12	2.16	0.45
41:8:19:LEU:H	41:8:19:LEU:HG	1.72	0.45
1:A:491:ARG:HH22	1:A:690:LEU:HA	1.82	0.45
2:B:73:THR:HA	2:B:76:ILE:HD12	1.98	0.45
3:C:114:PRO:HG3	3:C:438:PHE:CD2	2.49	0.45
9:I:141:PRO:HB2	11:K:156:TYR:HE1	1.81	0.45
35:1:185:LEU:O	35:1:188:ILE:HG13	2.17	0.45
39:5:310:MET:HA	39:5:313:LEU:HG	1.99	0.45
2:B:215:ILE:HD12	2:B:237:LEU:HB3	1.98	0.45
13:M:52:SER:HA	31:h:123:LEU:HA	1.98	0.45
38:4:125:ILE:HA	38:4:128:ASN:HB2	1.99	0.45
2:B:68:ILE:HG23	2:B:149:ARG:HD3	1.99	0.45
2:B:106:TRP:HZ2	2:B:152:ASN:HD22	1.64	0.45
2:B:162:GLY:N	2:B:202:GLY:O	2.46	0.45
9:I:131:ILE:HD11	9:I:181:VAL:HG11	1.99	0.44
17:R:79:ILE:HA	39:5:361:ARG:HH21	1.83	0.44
33:j:26:LEU:HD11	38:4:354:TYR:HA	1.98	0.44
38:4:114:TYR:HB2	38:4:155:TYR:CE2	2.52	0.44
38:4:245:ILE:HG21	38:4:343:PHE:CG	2.52	0.44
1:A:132:ASP:HB2	1:A:182:ARG:HD3	1.99	0.44
3:C:179:GLU:HG3	3:C:346:ILE:HG21	2.00	0.44
3:C:375:LYS:HA	13:M:111:PRO:HB3	1.97	0.44
10:J:101:GLY:O	10:J:104:THR:HB	2.17	0.44
35:1:91:ILE:HG13	35:1:100:GLY:H	1.82	0.44
36:2:403:ILE:HG23	38:4:176:LEU:HG	1.99	0.44
3:C:119:LEU:HD11	11:K:83:LEU:O	2.17	0.44
9:I:102:TYR:HD1	11:K:102:ARG:HH21	1.65	0.44
31:h:123:LEU:HG	31:h:124:LYS:H	1.83	0.44
36:2:115:LEU:HA	36:2:118:VAL:HG22	1.98	0.44
39:5:424:LEU:HA	39:5:427:VAL:HG22	2.00	0.44
40:6:176:PRO:HA	40:6:179:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:ILE:HD11	2:B:264:PHE:HB2	1.99	0.44
3:C:203:PHE:HD2	3:C:204:LEU:HD12	1.82	0.44
5:E:135:THR:OG1	5:E:138:PHE:N	2.50	0.44
6:F:87:VAL:HG23	6:F:89:GLU:H	1.81	0.44
15:P:106:ILE:HG23	15:P:107:GLN:HG3	2.00	0.44
37:3:101:GLY:HA3	40:6:173:ILE:HD11	1.98	0.44
39:5:29:VAL:HG12	39:5:30:PHE:H	1.82	0.44
1:A:194:ASN:HD21	22:Y:156:LYS:HB2	1.83	0.44
1:A:254:LYS:HB2	1:A:269:ARG:HD3	1.99	0.44
1:A:332:ILE:HA	1:A:568:PHE:HZ	1.83	0.44
6:F:134:GLN:O	7:G:131:TYR:OH	2.34	0.44
7:G:197:ARG:NE	15:P:90:TRP:HH2	2.16	0.44
38:4:262:LEU:HA	38:4:266:LEU:HD23	1.99	0.44
1:A:146:ASP:OD1	3:C:390:LYS:NZ	2.51	0.44
3:C:114:PRO:HD3	3:C:439:ASP:HB3	1.99	0.44
5:E:51:ARG:HA	5:E:77:GLY:HA3	1.99	0.44
5:E:155:VAL:HG13	5:E:160:ILE:HB	1.98	0.44
11:K:149:SER:OG	11:K:180:CYS:SG	2.75	0.44
12:L:20:ARG:HG3	12:L:24:LEU:HD21	1.99	0.44
39:5:175:ARG:HD3	39:5:178:ASP:HB2	1.99	0.44
1:A:69:CYS:CB	1:A:80:CYS:HB3	2.48	0.44
3:C:131:THR:HA	3:C:421:ARG:HG2	1.99	0.44
9:I:202:TYR:CD1	9:I:206:LYS:HG2	2.53	0.44
11:K:112:ARG:HH12	35:1:64:LEU:HD21	1.82	0.44
17:R:81:PRO:HA	17:R:82:PRO:HD3	1.82	0.44
32:i:27:UNK:HA	39:5:58:ASN:HB2	2.00	0.44
35:1:236:ILE:H	35:1:236:ILE:HG13	1.73	0.44
38:4:147:LEU:HD21	50:4:501:3PE:H272	2.00	0.44
38:4:415:ILE:HG23	38:4:418:LEU:HD12	1.99	0.44
2:B:86:GLY:N	2:B:92:PHE:O	2.42	0.44
3:C:175:THR:OG1	3:C:312:ASP:O	2.34	0.44
5:E:170:ASN:HD21	5:E:319:LEU:HD12	1.83	0.44
10:J:112:THR:HG23	10:J:114:LEU:HD13	1.98	0.44
29:f:7:GLU:HG2	29:f:57:ARG:HH21	1.82	0.44
35:1:317:LEU:HD21	37:3:102:PHE:CE1	2.52	0.44
38:4:158:SER:HB3	38:4:237:GLU:HB2	1.98	0.44
2:B:178:ALA:HB1	2:B:183:LEU:HB2	1.99	0.44
5:E:349:ARG:HH22	15:P:44:GLU:HG2	1.83	0.44
48:O:201:ZMP:O2	48:O:201:ZMP:N2	2.47	0.44
39:5:88:MET:HE3	39:5:88:MET:HB2	1.77	0.44
39:5:315:MET:HE3	39:5:315:MET:HB3	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:VAL:HG21	1:A:593:THR:HG21	2.00	0.43
1:A:605:ARG:HB3	1:A:660:ASP:HA	1.99	0.43
3:C:116:VAL:CG2	3:C:117:GLY:N	2.53	0.43
36:2:385:ASN:HA	36:2:388:MET:HG2	1.98	0.43
3:C:205:TRP:HE3	3:C:261:ILE:HG22	1.82	0.43
5:E:146:GLU:OE2	5:E:149:ARG:NH1	2.51	0.43
11:K:61:LEU:O	11:K:65:ASP:HB2	2.19	0.43
35:1:191:ILE:HD12	35:1:191:ILE:HA	1.81	0.43
39:5:69:ASN:OD1	39:5:69:ASN:N	2.50	0.43
39:5:247:SER:HA	39:5:250:LEU:HB3	2.00	0.43
2:B:87:ARG:NH2	2:B:275:THR:O	2.51	0.43
3:C:376:GLU:HG2	13:M:112:LYS:HE3	2.00	0.43
5:E:210:ASP:HB2	5:E:214:LEU:HB2	1.99	0.43
11:K:117:MET:HB2	11:K:138:MET:HE1	2.00	0.43
35:1:257:TYR:O	35:1:261:ILE:N	2.39	0.43
38:4:381:PHE:HE1	38:4:425:LEU:HD21	1.83	0.43
7:G:215:PRO:HG3	22:Y:105:MET:HA	2.01	0.43
11:K:69:ASN:ND2	11:K:198:MET:O	2.35	0.43
11:K:100:GLN:HE22	11:K:107:PHE:HE1	1.67	0.43
12:L:41:LEU:HD13	12:L:41:LEU:HA	1.78	0.43
38:4:414:CYS:HB2	39:5:183:LEU:HD12	2.00	0.43
50:4:501:3PE:H2A2	50:4:501:3PE:H2D2	1.78	0.43
1:A:127:GLN:N	2:B:389:GLU:OE2	2.52	0.43
2:B:149:ARG:HA	2:B:193:TYR:HE2	1.84	0.43
2:B:440:LEU:HD11	2:B:448:MET:HE3	2.00	0.43
4:D:38:ASP:O	19:U:105:ASN:ND2	2.52	0.43
5:E:232:THR:HG21	5:E:270:LYS:HE3	2.01	0.43
46:E:401:NDP:O1X	11:K:209:ARG:NH2	2.50	0.43
20:W:55:ARG:HA	20:W:58:LEU:HB2	1.99	0.43
29:f:11:HIS:HB2	29:f:46:GLU:HB2	2.00	0.43
35:1:217:THR:HB	35:1:219:TYR:HD1	1.83	0.43
1:A:662:VAL:HG12	1:A:664:PRO:HD3	2.01	0.43
19:U:112:ARG:NH1	19:U:140:GLU:O	2.44	0.43
38:4:388:LEU:HG	39:5:145:PHE:HE2	1.82	0.43
40:6:176:PRO:O	40:6:180:THR:OG1	2.36	0.43
4:D:34:GLY:O	4:D:36:VAL:N	2.49	0.43
39:5:127:MET:HE3	39:5:254:THR:HB	2.00	0.43
39:5:140:PHE:HB2	39:5:181:PHE:HE2	1.84	0.43
1:A:267:ASN:O	1:A:283:ARG:N	2.52	0.43
1:A:567:ALA:HB1	1:A:569:VAL:HG23	2.00	0.43
2:B:381:CYS:N	43:B:501:SF4:S1	2.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:MET:HE3	3:C:225:LEU:HB2	2.00	0.43
9:I:93:GLN:OE1	35:1:35:ARG:NE	2.52	0.43
35:1:91:ILE:HG21	35:1:100:GLY:H	1.83	0.43
38:4:283:LEU:O	38:4:287:LEU:HB2	2.19	0.43
5:E:87:GLU:HG3	11:K:206:MET:HE1	2.01	0.43
5:E:98:ASP:OD1	9:I:197:ARG:NH2	2.52	0.43
5:E:188:GLN:NE2	5:E:192:ASP:OD1	2.50	0.43
33:j:24:HIS:O	33:j:26:LEU:N	2.51	0.43
35:1:188:ILE:O	35:1:192:ALA:N	2.50	0.43
38:4:88:PHE:O	38:4:91:LEU:HB3	2.19	0.43
1:A:625:ILE:HA	15:P:119:PHE:HE2	1.84	0.43
6:F:44:PRO:HA	6:F:47:ILE:HG22	1.99	0.43
16:Q:100:GLU:HA	16:Q:105:LEU:HA	2.01	0.43
35:1:133:LEU:HD12	40:6:76:THR:HB	2.01	0.43
36:2:160:MET:HE2	36:2:160:MET:HB3	1.93	0.43
36:2:222:ILE:HG22	36:2:283:ARG:HD2	2.01	0.43
36:2:288:SER:OG	36:2:289:GLY:N	2.52	0.43
38:4:91:LEU:HD11	38:4:250:ILE:HD12	2.01	0.43
5:E:117:GLU:OE1	13:M:66:GLN:NE2	2.48	0.42
13:M:78:GLY:HA2	13:M:81:LEU:HB2	2.01	0.42
38:4:409:ILE:H	38:4:409:ILE:HG13	1.65	0.42
5:E:247:ARG:HE	15:P:108:GLY:HA2	1.84	0.42
9:I:134:LYS:HD3	9:I:147:ILE:HD12	2.01	0.42
50:g:202:3PE:H332	50:g:202:3PE:H361	1.76	0.42
35:1:85:LEU:HB3	37:3:11:ILE:HD13	2.00	0.42
35:1:91:ILE:O	35:1:93:LEU:N	2.52	0.42
38:4:121:ILE:H	38:4:121:ILE:HG13	1.70	0.42
38:4:241:ALA:HA	38:4:244:MET:HE3	2.01	0.42
38:4:258:ILE:HG23	38:4:317:VAL:HG11	2.01	0.42
42:9:37:CYS:O	42:9:41:PHE:N	2.45	0.42
7:G:183:TYR:HE2	15:P:81:MET:HE1	1.85	0.42
9:I:213:LYS:HD2	9:I:214:TRP:CZ3	2.54	0.42
22:Y:78:TRP:CZ2	22:Y:115:LYS:HB2	2.54	0.42
35:1:22:LEU:HD12	35:1:22:LEU:HA	1.91	0.42
36:2:139:LEU:HD23	36:2:139:LEU:HA	1.86	0.42
38:4:245:ILE:HG13	38:4:343:PHE:CD1	2.54	0.42
1:A:440:ALA:HA	1:A:453:ALA:H	1.85	0.42
27:d:42:LYS:HG2	27:d:45:ARG:NH1	2.34	0.42
31:h:85:VAL:HG22	31:h:87:THR:H	1.84	0.42
2:B:218:LEU:HD23	2:B:218:LEU:HA	1.91	0.42
3:C:233:GLY:HA3	3:C:367:ASN:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:86:ILE:HD12	19:U:86:ILE:HA	1.87	0.42
35:1:195:ALA:HB2	35:1:202:PHE:HE2	1.84	0.42
36:2:9:LEU:HA	36:2:12:PHE:HB3	2.01	0.42
36:2:282:LYS:HA	36:2:282:LYS:HD3	1.88	0.42
38:4:87:THR:O	38:4:91:LEU:N	2.52	0.42
39:5:185:LEU:HD11	39:5:195:LEU:HD21	2.01	0.42
39:5:338:PHE:CE1	39:5:383:SER:HB3	2.55	0.42
39:5:433:LEU:HA	39:5:436:THR:HG22	2.01	0.42
2:B:256:ILE:HD12	2:B:256:ILE:HA	1.82	0.42
2:B:371:ARG:NE	8:H:128:THR:O	2.53	0.42
3:C:465:ASP:HA	7:G:200:MET:HE1	2.02	0.42
5:E:237:HIS:HD2	5:E:239:ILE:HG22	1.85	0.42
7:G:146:SER:OG	7:G:151:SER:N	2.38	0.42
12:L:56:ALA:O	12:L:60:ILE:HG12	2.19	0.42
35:1:323:ILE:HD12	35:1:323:ILE:HA	1.90	0.42
39:5:240:MET:HE2	39:5:303:ARG:HG3	2.01	0.42
1:A:235:VAL:HG23	1:A:237:ALA:H	1.85	0.42
4:D:11:TYR:HA	4:D:14:ILE:HG22	2.01	0.42
5:E:275:MET:O	5:E:278:GLU:HB3	2.19	0.42
7:G:202:ASP:OD2	11:K:125:ASN:ND2	2.53	0.42
10:J:147:LEU:H	38:4:206:LEU:HD12	1.85	0.42
20:W:77:GLU:O	20:W:80:GLN:HB2	2.19	0.42
3:C:345:ARG:HH21	20:W:19:TRP:HE1	1.67	0.42
22:Y:79:ARG:NH2	22:Y:109:GLN:OE1	2.53	0.42
29:f:68:LEU:HD12	29:f:68:LEU:HA	1.80	0.42
31:h:74:GLU:HA	31:h:75:PRO:HD3	1.82	0.42
38:4:246:LEU:HG	38:4:340:PRO:HB3	2.02	0.42
39:5:458:ILE:HA	39:5:461:PRO:HD2	2.01	0.42
1:A:127:GLN:HE22	2:B:417:LEU:HD11	1.85	0.42
5:E:281:ARG:HG3	5:E:283:GLU:HB3	2.00	0.42
12:L:20:ARG:HH12	40:6:26:ALA:H	1.65	0.42
29:f:22:LEU:HG	29:f:68:LEU:HD23	2.01	0.42
38:4:343:PHE:HA	38:4:346:VAL:HG12	2.01	0.42
39:5:143:TRP:NE1	39:5:226:LYS:HG3	2.34	0.42
40:6:38:ALA:HA	40:6:41:VAL:HG12	2.02	0.42
1:A:83:CYS:SG	1:A:97:CYS:N	2.93	0.42
1:A:257:SER:O	1:A:283:ARG:NH1	2.53	0.42
1:A:412:LEU:HD11	1:A:446:LEU:HD21	2.02	0.42
1:A:594:GLU:HG2	1:A:615:PRO:HA	2.02	0.42
2:B:39:ARG:O	2:B:41:PHE:N	2.53	0.42
2:B:72:ASP:HA	2:B:75:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:197:ARG:NE	11:K:168:ASP:OD2	2.53	0.42
29:f:32:ALA:O	29:f:36:ALA:CB	2.68	0.42
38:4:306:SER:HA	38:4:335:HIS:CE1	2.55	0.42
1:A:245:PHE:CD1	9:I:157:ARG:HD2	2.55	0.41
2:B:324:CYS:HB2	2:B:372:PHE:CE1	2.54	0.41
5:E:73:LEU:O	5:E:78:THR:OG1	2.30	0.41
16:Q:105:LEU:HD13	17:R:81:PRO:HB3	2.02	0.41
35:1:143:LEU:HD12	35:1:143:LEU:HA	1.86	0.41
36:2:243:SER:OG	36:2:244:ILE:N	2.53	0.41
36:2:313:ILE:HG21	36:2:313:ILE:HD13	1.83	0.41
38:4:177:PHE:CG	38:4:216:ILE:HD11	2.55	0.41
2:B:360:ASN:OD1	2:B:361:LYS:N	2.53	0.41
3:C:274:ARG:NH2	3:C:448:PRO:O	2.53	0.41
3:C:337:MET:HA	3:C:340:PHE:HD2	1.84	0.41
4:D:42:ILE:HG22	4:D:45:TRP:HB3	2.03	0.41
5:E:234:ASN:HA	5:E:267:PHE:HA	2.02	0.41
5:E:237:HIS:CD2	5:E:239:ILE:HG22	2.55	0.41
20:W:120:ILE:HD12	20:W:121:PRO:HD2	2.02	0.41
36:2:215:ALA:HB2	36:2:268:LEU:HA	2.02	0.41
38:4:281:SER:O	38:4:284:THR:OG1	2.27	0.41
45:B:502:FMN:H9	45:B:502:FMN:H1'1	1.85	0.41
3:C:305:ILE:O	3:C:309:ALA:N	2.36	0.41
5:E:212:TRP:CD1	5:E:313:GLN:HE22	2.38	0.41
9:I:80:LEU:H	9:I:80:LEU:HG	1.63	0.41
35:1:153:ILE:HD11	35:1:189:PHE:CD1	2.56	0.41
1:A:74:LEU:HD23	1:A:74:LEU:HA	1.86	0.41
3:C:151:GLU:HB3	3:C:230:VAL:HB	2.02	0.41
3:C:386:LEU:HA	3:C:386:LEU:HD23	1.86	0.41
3:C:398:GLU:OE2	7:G:156:LYS:NZ	2.51	0.41
4:D:21:GLY:O	4:D:25:MET:HG2	2.21	0.41
20:W:60:ARG:HA	20:W:63:LEU:HG	2.02	0.41
35:1:156:ILE:HB	35:1:327:ILE:HD11	2.01	0.41
35:1:159:MET:HE1	35:1:328:PRO:HB3	2.02	0.41
35:1:324:PHE:HA	35:1:327:ILE:HG13	2.02	0.41
36:2:137:ILE:O	36:2:141:THR:OG1	2.35	0.41
38:4:301:ILE:H	38:4:301:ILE:HG13	1.66	0.41
41:8:8:LEU:HD21	41:8:25:ARG:HG2	2.01	0.41
1:A:564:PRO:HG2	1:A:567:ALA:HA	2.03	0.41
1:A:575:ASN:HD21	1:A:706:SER:HB3	1.85	0.41
8:H:163:LEU:HD23	8:H:163:LEU:HA	1.92	0.41
11:K:209:ARG:HD3	11:K:209:ARG:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:10:LEU:HD23	12:L:10:LEU:HA	1.94	0.41
12:L:21:ASN:HB2	12:L:24:LEU:HD23	2.02	0.41
35:1:191:ILE:HD13	50:1:401:3PE:H292	2.03	0.41
2:B:113:ARG:HG2	2:B:241:PRO:HG2	2.02	0.41
2:B:246:ASN:OD1	2:B:247:VAL:N	2.53	0.41
8:H:170:GLY:O	8:H:172:CYS:SG	2.79	0.41
9:I:158:ARG:HA	9:I:158:ARG:HD3	1.91	0.41
12:L:34:LEU:HD12	40:6:40:PHE:CE1	2.55	0.41
31:h:55:HIS:CD2	31:h:56:LEU:HD23	2.55	0.41
35:1:81:LEU:HD21	37:3:15:GLY:HA3	2.03	0.41
35:1:321:PHE:HE2	37:3:98:LEU:HD23	1.86	0.41
36:2:109:ILE:HD11	40:6:171:LEU:HD22	2.01	0.41
39:5:149:THR:O	39:5:153:LEU:HB2	2.20	0.41
2:B:336:ASP:OD1	2:B:336:ASP:N	2.54	0.41
3:C:345:ARG:HE	20:W:19:TRP:CD1	2.38	0.41
9:I:205:GLU:HG3	13:M:75:PRO:HG3	2.03	0.41
27:d:55:SER:HB2	27:d:58:ASN:HB2	2.02	0.41
27:d:69:GLN:HA	27:d:72:ASP:HB2	2.01	0.41
35:1:144:ILE:HD13	37:3:63:PHE:CG	2.56	0.41
35:1:321:PHE:HB3	37:3:99:ILE:HD11	2.03	0.41
36:2:110:ASN:HD22	36:2:235:TYR:HE2	1.69	0.41
36:2:257:SER:OG	36:2:261:SER:N	2.51	0.41
1:A:718:ASN:HB3	1:A:719:LYS:H	1.76	0.41
2:B:43:ASN:HB3	2:B:44:LEU:HD12	2.02	0.41
3:C:148:MET:HE3	3:C:148:MET:HB2	1.84	0.41
20:W:64:TRP:O	20:W:67:ILE:HG13	2.20	0.41
36:2:297:MET:HB3	36:2:297:MET:HE2	1.86	0.41
38:4:345:ILE:HG21	38:4:376:ILE:HD11	2.02	0.41
40:6:30:MET:HB2	40:6:33:ILE:HD11	2.03	0.41
1:A:135:VAL:HB	9:I:157:ARG:HD3	2.03	0.41
1:A:153:ARG:HH22	1:A:157:ARG:HH22	1.68	0.41
1:A:313:LEU:H	1:A:586:VAL:HB	1.86	0.41
1:A:385:PRO:HB2	1:A:387:HIS:CE1	2.56	0.41
2:B:227:LEU:HA	2:B:426:ILE:HG23	2.02	0.41
3:C:120:HIS:O	11:K:162:SER:OG	2.25	0.41
3:C:374:MET:HG3	3:C:375:LYS:HG3	2.03	0.41
8:H:124:LEU:HA	8:H:124:LEU:HD12	1.89	0.41
9:I:85:ARG:NH2	20:W:23:LEU:O	2.54	0.41
15:P:105:ASP:OD1	15:P:105:ASP:N	2.54	0.41
20:W:31:LEU:O	20:W:35:ALA:N	2.49	0.41
49:g:201:CDL:H1	36:2:15:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:40:ILE:HG12	31:h:77:TRP:CD1	2.56	0.41
31:h:70:MET:HG2	31:h:71:SER:H	1.86	0.41
35:1:121:LEU:HD12	40:6:72:LEU:HB3	2.03	0.41
35:1:290:MET:HB3	35:1:290:MET:HE2	1.78	0.41
36:2:1:MET:SD	36:2:1:MET:N	2.79	0.41
36:2:181:SER:OG	36:2:182:TYR:N	2.54	0.41
39:5:249:LEU:O	39:5:254:THR:OG1	2.35	0.41
1:A:159:THR:HB	2:B:400:ARG:HH12	1.86	0.41
1:A:232:LEU:HD12	1:A:232:LEU:HA	1.90	0.41
3:C:419:SER:OG	3:C:420:GLU:N	2.48	0.41
4:D:13:ILE:HD13	35:1:21:TYR:HD2	1.85	0.41
5:E:228:LYS:HD2	5:E:318:PHE:HA	2.02	0.41
8:H:65:GLN:HG3	22:Y:151:SER:HB2	2.03	0.41
11:K:72:ARG:HD3	11:K:143:TRP:CH2	2.53	0.41
19:U:123:PHE:HA	19:U:127:ASN:HA	2.02	0.41
36:2:54:VAL:HB	36:2:58:LEU:HB3	2.03	0.41
39:5:296:ILE:HD11	39:5:424:LEU:HG	2.02	0.41
1:A:126:LEU:HD21	1:A:144:LEU:HD21	2.03	0.40
2:B:72:ASP:OD1	2:B:72:ASP:N	2.52	0.40
13:M:85:GLN:HA	13:M:86:PRO:HD3	1.93	0.40
36:2:214:ILE:HG21	36:2:264:ALA:HB1	2.03	0.40
38:4:225:PHE:CE1	38:4:280:ILE:HG13	2.56	0.40
2:B:35:LYS:HD3	2:B:35:LYS:HA	1.88	0.40
2:B:277:LEU:HA	2:B:291:GLU:HA	2.03	0.40
3:C:67:GLU:O	36:2:280:LYS:NZ	2.42	0.40
9:I:141:PRO:HB2	11:K:156:TYR:CE1	2.55	0.40
9:I:146:THR:HB	9:I:163:ASP:HB3	2.04	0.40
11:K:157:TYR:C	11:K:159:PHE:H	2.30	0.40
19:U:95:ARG:HA	19:U:98:TRP:NE1	2.36	0.40
19:U:112:ARG:HD2	19:U:115:GLU:HG3	2.02	0.40
50:g:202:3PE:H281	50:g:202:3PE:H252	1.88	0.40
36:2:3:ILE:O	36:2:7:ILE:HG12	2.20	0.40
36:2:133:GLN:O	36:2:137:ILE:HG12	2.21	0.40
38:4:232:PRO:HA	38:4:235:HIS:HB2	2.03	0.40
39:5:74:ASP:OD1	39:5:74:ASP:N	2.54	0.40
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.83	0.40
1:A:132:ASP:OD2	1:A:182:ARG:NH1	2.48	0.40
1:A:350:ALA:HB3	1:A:376:THR:HG22	2.03	0.40
3:C:231:ARG:NH2	9:I:174:TYR:OH	2.53	0.40
5:E:134:GLU:OE2	5:E:140:TYR:N	2.49	0.40
16:Q:55:ILE:HD11	16:Q:125:VAL:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:4:207:GLN:HE22	38:4:268:GLU:H	1.68	0.40
1:A:396:LEU:H	1:A:396:LEU:HG	1.70	0.40
1:A:626:LEU:HD23	1:A:626:LEU:HA	1.90	0.40
7:G:186:TYR:HB3	7:G:188:VAL:HG23	2.03	0.40
8:H:177:MET:HB3	8:H:186:GLU:HA	2.04	0.40
9:I:206:LYS:HB2	31:h:117:PHE:CZ	2.56	0.40
12:L:15:PHE:CE2	36:2:163:ILE:HD11	2.57	0.40
36:2:369:PHE:HA	36:2:372:ILE:HG12	2.04	0.40
38:4:274:THR:HA	38:4:278:TYR:HD2	1.86	0.40
1:A:249:PRO:HA	1:A:252:LEU:HD13	2.04	0.40
3:C:115:HIS:O	3:C:115:HIS:CG	2.73	0.40
3:C:119:LEU:HA	11:K:124:THR:CG2	2.50	0.40
3:C:120:HIS:CD2	7:G:200:MET:HB3	2.56	0.40
3:C:173:ILE:HD11	3:C:235:VAL:HG21	2.03	0.40
3:C:305:ILE:HG23	3:C:309:ALA:HB3	2.04	0.40
3:C:381:LEU:HA	3:C:381:LEU:HD23	1.79	0.40
10:J:60:THR:HG23	10:J:61:PHE:N	2.37	0.40
11:K:73:GLN:NE2	11:K:195:GLN:OE1	2.55	0.40
16:Q:88:ASP:OD1	16:Q:89:SER:N	2.55	0.40
20:W:58:LEU:HD23	20:W:58:LEU:HA	1.94	0.40
36:2:164:LEU:HD23	36:2:164:LEU:HA	1.88	0.40
38:4:376:ILE:HD13	38:4:376:ILE:HA	1.92	0.40
39:5:88:MET:HE1	39:5:261:TYR:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	687/728 (94%)	604 (88%)	83 (12%)	0	100	100
2	B	441/488 (90%)	391 (89%)	49 (11%)	1 (0%)	43	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	414/466 (89%)	371 (90%)	39 (9%)	4 (1%)	12	47
4	D	78/87 (90%)	66 (85%)	11 (14%)	1 (1%)	9	41
5	E	316/375 (84%)	261 (83%)	55 (17%)	0	100	100
6	F	117/144 (81%)	101 (86%)	14 (12%)	2 (2%)	7	35
7	G	230/281 (82%)	180 (78%)	45 (20%)	5 (2%)	5	29
8	H	183/243 (75%)	151 (82%)	29 (16%)	3 (2%)	7	36
9	I	178/229 (78%)	148 (83%)	28 (16%)	2 (1%)	11	45
10	J	138/198 (70%)	123 (89%)	15 (11%)	0	100	100
11	K	167/210 (80%)	143 (86%)	23 (14%)	1 (1%)	21	58
12	L	84/86 (98%)	69 (82%)	15 (18%)	0	100	100
13	M	103/136 (76%)	84 (82%)	17 (16%)	2 (2%)	6	32
14	O	75/109 (69%)	68 (91%)	6 (8%)	1 (1%)	9	41
15	P	114/124 (92%)	103 (90%)	11 (10%)	0	100	100
16	Q	83/132 (63%)	70 (84%)	13 (16%)	0	100	100
17	R	100/109 (92%)	90 (90%)	10 (10%)	0	100	100
19	U	156/172 (91%)	128 (82%)	24 (15%)	4 (3%)	4	25
20	W	116/123 (94%)	104 (90%)	11 (10%)	1 (1%)	14	49
21	X	115/169 (68%)	81 (70%)	27 (24%)	7 (6%)	1	13
22	Y	113/161 (70%)	95 (84%)	18 (16%)	0	100	100
26	c	40/60 (67%)	35 (88%)	5 (12%)	0	100	100
27	d	87/92 (95%)	78 (90%)	9 (10%)	0	100	100
29	f	78/87 (90%)	66 (85%)	12 (15%)	0	100	100
30	g	58/63 (92%)	42 (72%)	16 (28%)	0	100	100
31	h	128/138 (93%)	103 (80%)	24 (19%)	1 (1%)	16	52
33	j	71/93 (76%)	62 (87%)	7 (10%)	2 (3%)	4	24
35	1	338/341 (99%)	291 (86%)	46 (14%)	1 (0%)	36	71
36	2	448/469 (96%)	400 (89%)	46 (10%)	2 (0%)	30	66
37	3	106/128 (83%)	87 (82%)	18 (17%)	1 (1%)	14	49
38	4	473/486 (97%)	394 (83%)	72 (15%)	7 (2%)	8	38
39	5	635/655 (97%)	554 (87%)	78 (12%)	3 (0%)	24	62
40	6	181/185 (98%)	162 (90%)	19 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	8	80/99 (81%)	71 (89%)	9 (11%)	0	100	100
42	9	57/89 (64%)	52 (91%)	5 (9%)	0	100	100
All	All	6788/7755 (88%)	5828 (86%)	909 (13%)	51 (1%)	18	52

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	116	VAL
4	D	71	PRO
6	F	29	THR
7	G	34	PRO
7	G	46	PRO
7	G	55	GLU
7	G	235	PRO
7	G	254	PRO
8	H	41	PRO
8	H	44	PRO
9	I	52	PRO
13	M	32	PRO
19	U	19	PRO
19	U	148	PRO
21	X	5	THR
21	X	6	PRO
21	X	26	PRO
21	X	70	PRO
33	j	6	PRO
36	2	259	VAL
37	3	119	PRO
38	4	448	ILE
39	5	12	PRO
2	B	40	ILE
20	W	8	LEU
38	4	65	PRO
38	4	241	ALA
39	5	455	ASN
39	5	456	ILE
21	X	61	ASP
38	4	386	THR
11	K	158	HIS
33	j	14	PRO
3	C	92	PRO

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Mol	Chain	Res	Type
9	I	51	PRO
19	U	151	LYS
21	X	22	ILE
21	X	62	PRO
36	2	429	ILE
3	C	69	SER
13	M	78	GLY
38	4	109	PHE
19	U	152	PRO
6	F	40	PRO
8	H	49	PRO
14	O	54	PRO
31	h	108	PRO
38	4	227	ILE
38	4	479	VAL
3	C	71	ILE
35	1	200	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	563/595 (95%)	563 (100%)	0	100	100
2	B	340/389 (87%)	340 (100%)	0	100	100
3	C	320/394 (81%)	318 (99%)	2 (1%)	78	80
4	D	44/69 (64%)	44 (100%)	0	100	100
5	E	275/329 (84%)	272 (99%)	3 (1%)	65	73
6	F	89/129 (69%)	89 (100%)	0	100	100
7	G	143/245 (58%)	143 (100%)	0	100	100
8	H	144/212 (68%)	143 (99%)	1 (1%)	76	79
9	I	148/187 (79%)	146 (99%)	2 (1%)	59	71
10	J	80/147 (54%)	80 (100%)	0	100	100
11	K	146/180 (81%)	145 (99%)	1 (1%)	76	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	75/75 (100%)	73 (97%)	2 (3%)	39	60
13	M	60/115 (52%)	60 (100%)	0	100	100
14	O	65/91 (71%)	64 (98%)	1 (2%)	57	70
15	P	104/110 (94%)	104 (100%)	0	100	100
16	Q	72/111 (65%)	72 (100%)	0	100	100
17	R	84/100 (84%)	84 (100%)	0	100	100
19	U	110/148 (74%)	110 (100%)	0	100	100
20	W	89/102 (87%)	89 (100%)	0	100	100
21	X	17/133 (13%)	17 (100%)	0	100	100
22	Y	98/140 (70%)	98 (100%)	0	100	100
26	c	11/45 (24%)	11 (100%)	0	100	100
27	d	82/85 (96%)	82 (100%)	0	100	100
29	f	69/73 (94%)	69 (100%)	0	100	100
30	g	49/52 (94%)	49 (100%)	0	100	100
31	h	115/123 (94%)	114 (99%)	1 (1%)	70	76
33	j	17/73 (23%)	17 (100%)	0	100	100
35	1	272/302 (90%)	267 (98%)	5 (2%)	51	66
36	2	340/433 (78%)	333 (98%)	7 (2%)	47	65
37	3	93/114 (82%)	93 (100%)	0	100	100
38	4	295/434 (68%)	292 (99%)	3 (1%)	68	75
39	5	426/580 (73%)	419 (98%)	7 (2%)	55	69
40	6	88/167 (53%)	87 (99%)	1 (1%)	65	73
41	8	69/76 (91%)	68 (99%)	1 (1%)	59	71
42	9	49/76 (64%)	49 (100%)	0	100	100
All	All	5041/6634 (76%)	5004 (99%)	37 (1%)	73	79

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	110	ILE
3	C	177	PHE
5	E	82	VAL
5	E	115	ILE
5	E	129	ILE

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Mol	Chain	Res	Type
8	H	172	CYS
9	I	80	LEU
9	I	139	ILE
11	K	85	CYS
12	L	3	ILE
12	L	41	LEU
14	O	66	SER
31	h	79	PHE
35	1	79	ILE
35	1	175	VAL
35	1	236	ILE
35	1	247	LEU
35	1	286	LEU
36	2	105	ILE
36	2	106	LEU
36	2	208	LEU
36	2	214	ILE
36	2	236	ILE
36	2	344	ILE
36	2	377	LEU
38	4	121	ILE
38	4	227	ILE
38	4	349	ILE
39	5	95	ILE
39	5	101	ILE
39	5	130	LEU
39	5	154	ILE
39	5	161	LEU
39	5	255	LEU
39	5	304	ILE
40	6	74	ILE
41	8	19	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	127	GLN
1	A	147	GLN
1	A	185	HIS
1	A	194	ASN
1	A	459	HIS

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Mol	Chain	Res	Type
1	A	499	ASN
1	A	575	ASN
2	B	102	ASN
2	B	152	ASN
3	C	120	HIS
3	C	185	ASN
3	C	193	HIS
3	C	268	ASN
3	C	308	ASN
5	E	76	HIS
5	E	170	ASN
5	E	237	HIS
6	F	85	ASN
6	F	106	GLN
7	G	149	HIS
7	G	208	HIS
8	H	115	ASN
8	H	125	GLN
9	I	58	HIS
9	I	189	ASN
11	K	73	GLN
11	K	100	GLN
11	K	193	GLN
13	M	85	GLN
13	M	103	ASN
15	P	63	HIS
15	P	84	GLN
15	P	95	GLN
19	U	17	ASN
19	U	50	ASN
20	W	53	GLN
22	Y	62	GLN
22	Y	132	GLN
22	Y	146	ASN
27	d	20	HIS
29	f	28	ASN
30	g	21	HIS
31	h	78	HIS
35	1	173	GLN
36	2	193	ASN
36	2	339	ASN
36	2	357	ASN

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Mol	Chain	Res	Type
38	4	103	ASN
38	4	207	GLN
38	4	335	HIS
38	4	400	GLN
39	5	112	HIS
39	5	229	GLN
39	5	312	GLN
40	6	28	ASN
42	9	50	HIS

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](#)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 for Mogul analysis.

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	$\# Z > 2$
43	SF4	I	302	9	0,12,12	-	-	-		
43	SF4	A	802	1	0,12,12	-	-	-		
48	ZMP	O	201	14	23,28,36	1.89	6 (26%)	27,35,45	2.13	9 (33%)
44	FES	A	803	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	3PE	4	501	-	42,42,50	0.96	4 (9%)	45,47,55	1.15	3 (6%)
43	SF4	K	301	11	0,12,12	-	-	-	-	-
50	3PE	g	202	-	42,42,50	0.94	4 (9%)	45,47,55	1.12	2 (4%)
43	SF4	I	301	9	0,12,12	-	-	-	-	-
43	SF4	A	801	1	0,12,12	-	-	-	-	-
44	FES	H	301	8	0,4,4	-	-	-	-	-
45	FMN	B	502	-	33,33,33	2.57	10 (30%)	48,50,50	1.58	11 (22%)
49	CDL	g	201	-	82,82,99	0.96	7 (8%)	88,94,111	1.17	5 (5%)
50	3PE	1	401	-	50,50,50	0.86	4 (8%)	53,55,55	1.15	2 (3%)
43	SF4	B	501	2	0,12,12	-	-	-	-	-
46	NDP	E	401	-	51,52,52	3.60	24 (47%)	71,80,80	2.14	19 (26%)

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
48	ZMP	O	201	14	-	6/33/35/43	-
43	SF4	A	802	1	-	-	0/6/5/5
43	SF4	I	302	9	-	-	0/6/5/5
50	3PE	4	501	-	-	18/46/46/54	-
44	FES	A	803	1	-	-	0/1/1/1
43	SF4	K	301	11	-	-	0/6/5/5
43	SF4	B	501	2	-	-	0/6/5/5
43	SF4	I	301	9	-	-	0/6/5/5
49	CDL	g	201	-	-	43/93/93/110	-
45	FMN	B	502	-	-	13/18/18/18	0/3/3/3
50	3PE	1	401	-	-	27/54/54/54	-
43	SF4	A	801	1	-	-	0/6/5/5
44	FES	H	301	8	-	-	0/1/1/1
50	3PE	g	202	-	-	21/46/46/54	-
46	NDP	E	401	-	-	7/34/77/77	0/5/5/5

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	E	401	NDP	C2B-C1B	-9.34	1.30	1.53
46	E	401	NDP	O4B-C1B	8.54	1.61	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	E	401	NDP	O4D-C1D	8.22	1.61	1.42
46	E	401	NDP	C2D-C1D	-7.50	1.29	1.53
46	E	401	NDP	C6N-C5N	7.13	1.55	1.33
46	E	401	NDP	O4D-C4D	-6.99	1.29	1.45
46	E	401	NDP	O4B-C4B	-6.23	1.31	1.45
45	B	502	FMN	C10-N1	6.06	1.45	1.33
45	B	502	FMN	C4A-N5	6.02	1.43	1.30
46	E	401	NDP	C2N-C3N	5.43	1.50	1.35
46	E	401	NDP	PA-O3	5.34	1.65	1.59
48	O	201	ZMP	C13-N1	5.21	1.45	1.33
46	E	401	NDP	C6A-N6A	5.17	1.47	1.34
45	B	502	FMN	C2-N1	5.06	1.48	1.36
48	O	201	ZMP	C16-N2	4.81	1.44	1.33
45	B	502	FMN	C5A-N5	4.62	1.47	1.39
46	E	401	NDP	PN-O3	4.58	1.64	1.59
45	B	502	FMN	C2-N3	4.49	1.48	1.39
46	E	401	NDP	C7N-N7N	4.37	1.46	1.33
45	B	502	FMN	C9A-N10	3.76	1.47	1.41
45	B	502	FMN	C4-N3	3.36	1.45	1.38
46	E	401	NDP	C4N-C5N	3.30	1.57	1.49
45	B	502	FMN	O2-C2	-3.29	1.17	1.24
46	E	401	NDP	C5A-N7A	-3.15	1.33	1.39
45	B	502	FMN	C10-N10	3.11	1.44	1.37
46	E	401	NDP	O3D-C3D	-2.88	1.35	1.43
49	g	201	CDL	OB6-CB4	-2.85	1.39	1.46
49	g	201	CDL	OA6-CA4	-2.85	1.39	1.46
46	E	401	NDP	C7N-C3N	2.84	1.54	1.48
46	E	401	NDP	C5A-C4A	-2.80	1.34	1.39
46	E	401	NDP	O2D-C2D	2.79	1.49	1.43
45	B	502	FMN	O4-C4	-2.76	1.18	1.23
46	E	401	NDP	O3B-C3B	-2.75	1.36	1.43
50	g	202	3PE	O21-C2	-2.62	1.40	1.46
48	O	201	ZMP	O3-C16	-2.60	1.18	1.23
48	O	201	ZMP	C10-S1	2.51	1.82	1.76
46	E	401	NDP	P2B-O2B	2.50	1.63	1.59
46	E	401	NDP	C6N-N1N	2.46	1.43	1.37
50	1	401	3PE	O31-C31	2.44	1.40	1.33
46	E	401	NDP	O7N-C7N	-2.43	1.18	1.24
50	4	501	3PE	O21-C2	-2.41	1.40	1.46
50	4	501	3PE	O31-C31	2.41	1.40	1.33
46	E	401	NDP	C8A-N9A	-2.39	1.33	1.37
49	g	201	CDL	OA8-CA7	2.36	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	g	202	3PE	O31-C31	2.36	1.40	1.33
46	E	401	NDP	C4N-C3N	2.35	1.54	1.50
48	O	201	ZMP	O2-C13	-2.34	1.18	1.23
50	4	501	3PE	O21-C21	2.34	1.40	1.34
50	1	401	3PE	O21-C21	2.30	1.40	1.34
50	1	401	3PE	O31-C3	-2.29	1.40	1.45
48	O	201	ZMP	C9-C10	2.28	1.53	1.50
50	g	202	3PE	O31-C3	-2.28	1.40	1.45
49	g	201	CDL	OB8-CB7	2.27	1.40	1.33
50	4	501	3PE	O31-C3	-2.25	1.40	1.45
49	g	201	CDL	OB8-CB6	-2.23	1.40	1.45
50	g	202	3PE	O21-C21	2.21	1.40	1.34
49	g	201	CDL	OA8-CA6	-2.18	1.40	1.45
50	1	401	3PE	O21-C2	-2.11	1.41	1.46
49	g	201	CDL	OA6-CA5	2.06	1.40	1.34

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	E	401	NDP	C5A-C4A-N3A	-7.28	116.70	126.72
46	E	401	NDP	N6A-C6A-N1A	-6.75	103.35	118.38
48	O	201	ZMP	C9-C10-S1	6.57	121.24	113.40
46	E	401	NDP	N3A-C2A-N1A	-6.32	119.01	128.58
46	E	401	NDP	N3A-C4A-N9A	5.34	136.25	127.17
46	E	401	NDP	C5A-C6A-N6A	4.80	135.16	123.29
50	1	401	3PE	O21-C21-C22	4.66	121.56	111.48
46	E	401	NDP	C2A-N3A-C4A	4.63	123.14	111.83
50	4	501	3PE	O21-C21-C22	4.24	120.66	111.48
49	g	201	CDL	OB6-CB5-C51	4.14	120.44	111.48
48	O	201	ZMP	O1-C10-C9	-4.10	119.25	123.98
50	g	202	3PE	O21-C21-C22	4.04	120.21	111.48
49	g	201	CDL	OA6-CA5-C11	3.98	120.08	111.48
45	B	502	FMN	C4-N3-C2	-3.93	118.66	125.64
45	B	502	FMN	C7M-C7-C6	-3.60	113.23	119.57
46	E	401	NDP	C2B-C1B-N9A	3.50	119.52	113.75
45	B	502	FMN	O4-C4-C4A	-2.93	118.80	126.53
48	O	201	ZMP	C11-S1-C10	2.92	110.48	101.84
50	g	202	3PE	O31-C31-C32	2.90	120.68	111.83
48	O	201	ZMP	C20-C18-C17	2.87	113.66	108.77
48	O	201	ZMP	C14-C15-N2	-2.86	105.91	112.00
46	E	401	NDP	N9A-C8A-N7A	-2.84	109.91	113.94
50	4	501	3PE	O31-C31-C32	2.77	120.29	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	g	201	CDL	OA8-CA7-C31	2.73	120.14	111.83
49	g	201	CDL	OB8-CB7-C71	2.64	119.87	111.83
45	B	502	FMN	C4'-C3'-C2'	-2.59	109.26	113.57
45	B	502	FMN	C4-C4A-C10	2.58	121.36	116.93
46	E	401	NDP	C3D-C2D-C1D	2.58	106.34	101.46
50	1	401	3PE	O31-C31-C32	2.53	119.56	111.83
49	g	201	CDL	CB4-OB6-CB5	-2.51	111.79	117.80
48	O	201	ZMP	O1-C10-S1	-2.49	119.51	122.68
46	E	401	NDP	C6A-C5A-C4A	2.45	120.52	117.18
45	B	502	FMN	C4A-C4-N3	2.45	119.48	113.25
45	B	502	FMN	C5A-C9A-N10	2.44	120.18	117.97
45	B	502	FMN	C7M-C7-C8	2.37	125.60	120.76
46	E	401	NDP	C5B-C4B-C3B	-2.32	106.85	115.21
46	E	401	NDP	C3N-C7N-N7N	2.32	121.79	117.67
46	E	401	NDP	C5A-N7A-C8A	2.30	107.06	103.45
46	E	401	NDP	O4B-C1B-C2B	-2.29	102.65	106.59
48	O	201	ZMP	O3-C16-N2	-2.27	118.18	122.98
48	O	201	ZMP	C14-C13-N1	2.26	120.46	116.34
46	E	401	NDP	C3N-C2N-N1N	-2.22	119.95	123.20
48	O	201	ZMP	C15-C14-C13	-2.14	108.82	112.39
45	B	502	FMN	C4A-C10-N10	2.11	119.50	116.48
46	E	401	NDP	C4A-N9A-C1B	-2.09	121.74	126.63
50	4	501	3PE	C3-C2-C1	-2.09	106.92	111.78
46	E	401	NDP	C1B-N9A-C8A	2.05	131.65	127.09
46	E	401	NDP	O4B-C1B-N9A	-2.04	104.17	108.09
45	B	502	FMN	C5'-C4'-C3'	-2.03	108.39	112.22
46	E	401	NDP	C4D-O4D-C1D	-2.01	105.03	109.47
45	B	502	FMN	O5'-P-O1P	2.00	111.85	106.44

There are no chirality outliers.

All (135) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	B	502	FMN	N10-C1'-C2'-O2'
45	B	502	FMN	N10-C1'-C2'-C3'
45	B	502	FMN	C1'-C2'-C3'-O3'
45	B	502	FMN	C1'-C2'-C3'-C4'
45	B	502	FMN	O2'-C2'-C3'-C4'
45	B	502	FMN	C3'-C4'-C5'-O5'
45	B	502	FMN	O4'-C4'-C5'-O5'
45	B	502	FMN	C5'-O5'-P-O2P
45	B	502	FMN	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
46	E	401	NDP	C1B-C2B-O2B-P2B
48	O	201	ZMP	S1-C11-C12-N1
48	O	201	ZMP	C12-C11-S1-C10
48	O	201	ZMP	C7-C8-C9-C10
49	g	201	CDL	CA2-OA2-PA1-OA3
49	g	201	CDL	CA2-OA2-PA1-OA5
49	g	201	CDL	CB2-OB2-PB2-OB3
49	g	201	CDL	CB2-OB2-PB2-OB4
49	g	201	CDL	CB2-OB2-PB2-OB5
49	g	201	CDL	CB3-OB5-PB2-OB2
49	g	201	CDL	CB3-OB5-PB2-OB4
50	g	202	3PE	C11-O13-P-O11
50	g	202	3PE	O22-C21-O21-C2
50	g	202	3PE	C22-C21-O21-C2
50	1	401	3PE	C22-C21-O21-C2
50	4	501	3PE	C1-O11-P-O12
50	4	501	3PE	C1-O11-P-O13
50	4	501	3PE	C1-O11-P-O14
50	4	501	3PE	O13-C11-C12-N
49	g	201	CDL	OB9-CB7-OB8-CB6
50	1	401	3PE	O22-C21-O21-C2
49	g	201	CDL	C71-CB7-OB8-CB6
50	g	202	3PE	C36-C37-C38-C39
45	B	502	FMN	O2'-C2'-C3'-O3'
46	E	401	NDP	O4B-C4B-C5B-O5B
50	4	501	3PE	C31-C32-C33-C34
49	g	201	CDL	CA5-C11-C12-C13
49	g	201	CDL	CA7-C31-C32-C33
49	g	201	CDL	CB7-C71-C72-C73
50	1	401	3PE	C2B-C2C-C2D-C2E
50	g	202	3PE	C23-C24-C25-C26
50	1	401	3PE	C29-C2A-C2B-C2C
50	1	401	3PE	C37-C38-C39-C3A
49	g	201	CDL	C13-C14-C15-C16
49	g	201	CDL	C40-C41-C42-C43
50	g	202	3PE	C2E-C2F-C2G-C2H
49	g	201	CDL	C11-CA5-OA6-CA4
49	g	201	CDL	C51-CB5-OB6-CB4
49	g	201	CDL	C15-C16-C17-C18
50	1	401	3PE	C21-C22-C23-C24
50	1	401	3PE	C2A-C2B-C2C-C2D
50	g	202	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
50	g	202	3PE	C31-C32-C33-C34
49	g	201	CDL	C36-C37-C38-C39
50	4	501	3PE	C33-C34-C35-C36
50	g	202	3PE	C27-C28-C29-C2A
50	1	401	3PE	C36-C37-C38-C39
50	1	401	3PE	C39-C3A-C3B-C3C
49	g	201	CDL	OA7-CA5-OA6-CA4
49	g	201	CDL	OB7-CB5-OB6-CB4
48	O	201	ZMP	C6-C7-C8-C9
50	g	202	3PE	C34-C35-C36-C37
50	1	401	3PE	C28-C29-C2A-C2B
49	g	201	CDL	C76-C77-C78-C79
50	g	202	3PE	C2B-C2C-C2D-C2E
50	1	401	3PE	C32-C33-C34-C35
50	1	401	3PE	C2E-C2F-C2G-C2H
49	g	201	CDL	C73-C74-C75-C76
50	4	501	3PE	C21-C22-C23-C24
50	4	501	3PE	C2D-C2E-C2F-C2G
50	4	501	3PE	O21-C2-C3-O31
50	g	202	3PE	C28-C29-C2A-C2B
49	g	201	CDL	C33-C34-C35-C36
49	g	201	CDL	C75-C76-C77-C78
46	E	401	NDP	C3B-C4B-C5B-O5B
48	O	201	ZMP	C5-C6-C7-C8
50	g	202	3PE	C33-C34-C35-C36
49	g	201	CDL	C12-C13-C14-C15
45	B	502	FMN	C5'-O5'-P-O1P
50	g	202	3PE	C29-C2A-C2B-C2C
50	4	501	3PE	C24-C25-C26-C27
50	1	401	3PE	C1-C2-O21-C21
49	g	201	CDL	C11-C12-C13-C14
49	g	201	CDL	C39-C40-C41-C42
50	g	202	3PE	C37-C38-C39-C3A
49	g	201	CDL	C35-C36-C37-C38
50	4	501	3PE	C2B-C2C-C2D-C2E
50	4	501	3PE	C28-C29-C2A-C2B
50	4	501	3PE	C22-C23-C24-C25
49	g	201	CDL	C37-C38-C39-C40
50	g	202	3PE	C1-C2-C3-O31
50	4	501	3PE	C1-C2-C3-O31
49	g	201	CDL	CB5-C51-C52-C53
50	g	202	3PE	O21-C2-C3-O31

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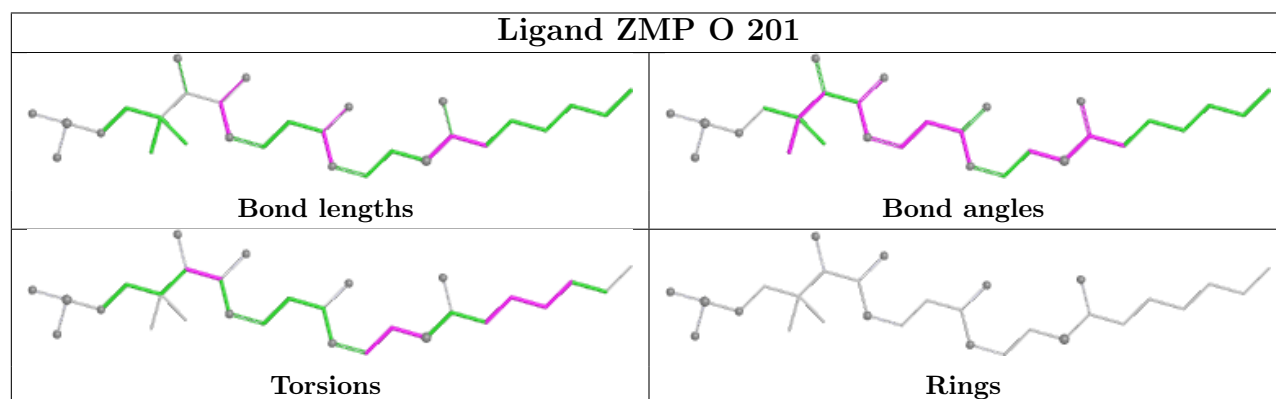
Mol	Chain	Res	Type	Atoms
50	4	501	3PE	C34-C35-C36-C37
50	1	401	3PE	C26-C27-C28-C29
46	E	401	NDP	O4D-C1D-N1N-C6N
49	g	201	CDL	C38-C39-C40-C41
49	g	201	CDL	OB6-CB4-CB6-OB8
50	1	401	3PE	C1-C2-C3-O31
49	g	201	CDL	C31-CA7-OA8-CA6
46	E	401	NDP	C2B-C1B-N9A-C4A
46	E	401	NDP	C5D-O5D-PN-O1N
49	g	201	CDL	CA2-OA2-PA1-OA4
50	g	202	3PE	C11-O13-P-O14
50	g	202	3PE	O13-C11-C12-N
50	1	401	3PE	C1-O11-P-O12
50	1	401	3PE	C1-O11-P-O13
50	1	401	3PE	C1-O11-P-O14
49	g	201	CDL	OA9-CA7-OA8-CA6
46	E	401	NDP	C2B-C1B-N9A-C8A
50	1	401	3PE	C3B-C3C-C3D-C3E
49	g	201	CDL	CB3-CB4-CB6-OB8
45	B	502	FMN	C2'-C3'-C4'-O4'
50	4	501	3PE	C23-C24-C25-C26
49	g	201	CDL	C16-C17-C18-C19
50	1	401	3PE	C3C-C3D-C3E-C3F
50	g	202	3PE	C32-C33-C34-C35
50	1	401	3PE	C2-C1-O11-P
49	g	201	CDL	C31-C32-C33-C34
49	g	201	CDL	C52-C53-C54-C55
50	1	401	3PE	C2C-C2D-C2E-C2F
49	g	201	CDL	CA4-CA3-OA5-PA1
50	4	501	3PE	C2A-C2B-C2C-C2D
49	g	201	CDL	C19-C20-C21-C22
50	1	401	3PE	C33-C34-C35-C36
50	1	401	3PE	C3D-C3E-C3F-C3G
45	B	502	FMN	O3'-C3'-C4'-O4'
49	g	201	CDL	CB4-CB3-OB5-PB2
50	4	501	3PE	C25-C26-C27-C28
50	1	401	3PE	C22-C23-C24-C25
50	1	401	3PE	C24-C25-C26-C27
50	g	202	3PE	O21-C21-C22-C23
48	O	201	ZMP	N2-C16-C17-O4
49	g	201	CDL	C17-C18-C19-C20
50	1	401	3PE	O21-C21-C22-C23

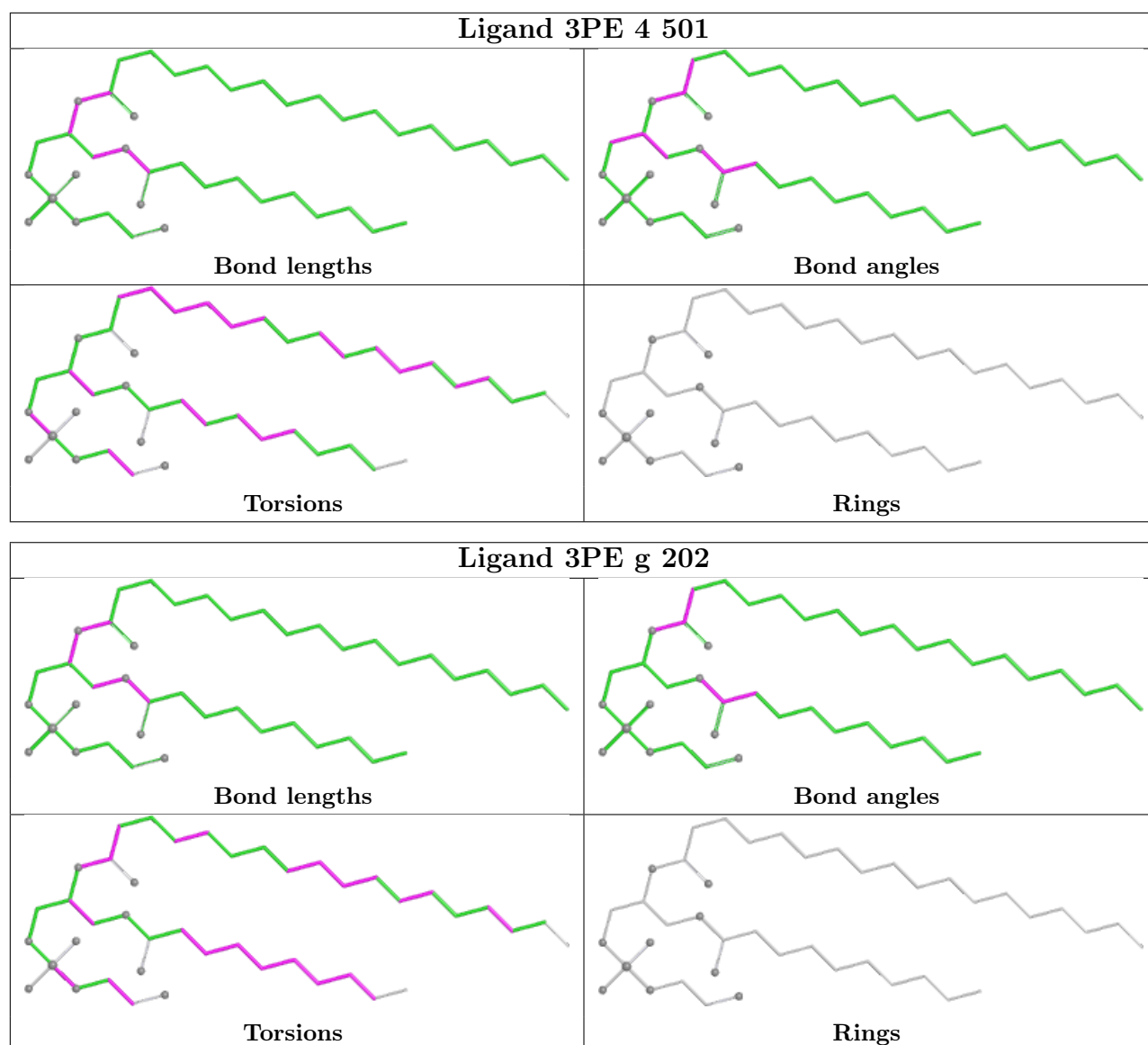
There are no ring outliers.

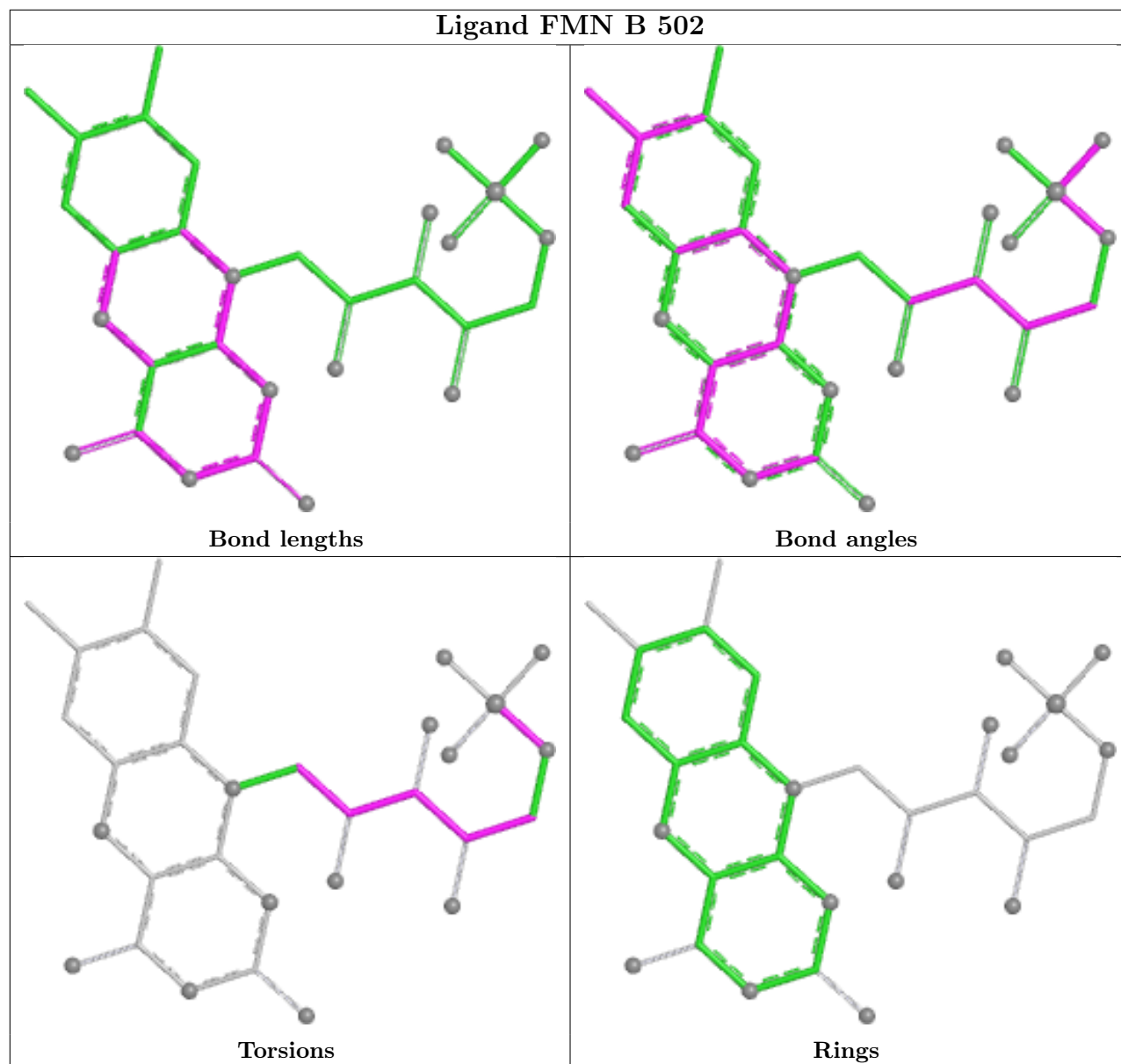
10 monomers are involved in 31 short contacts:

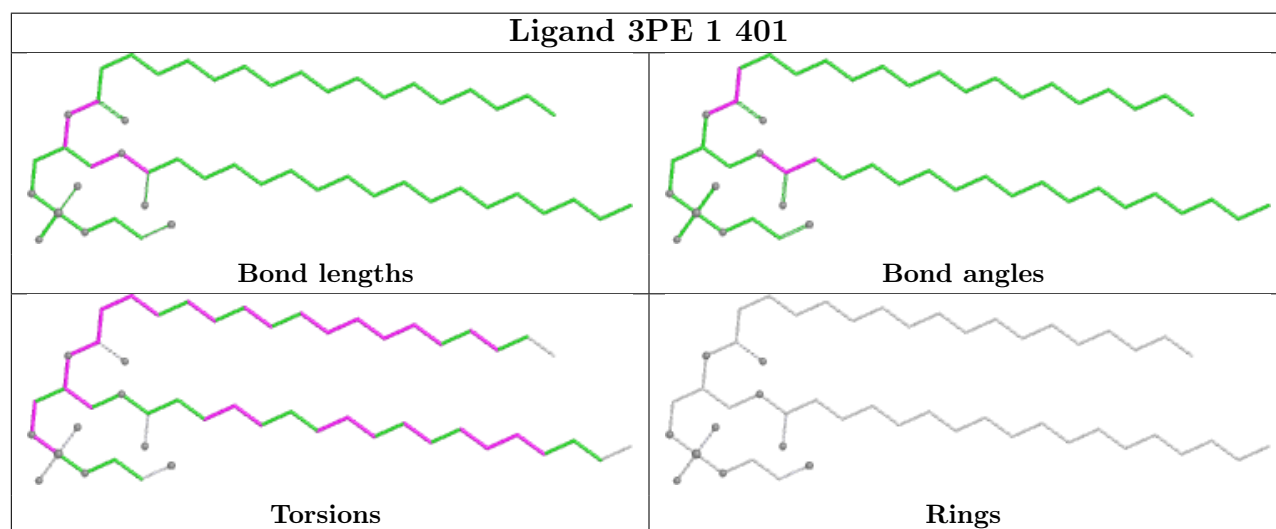
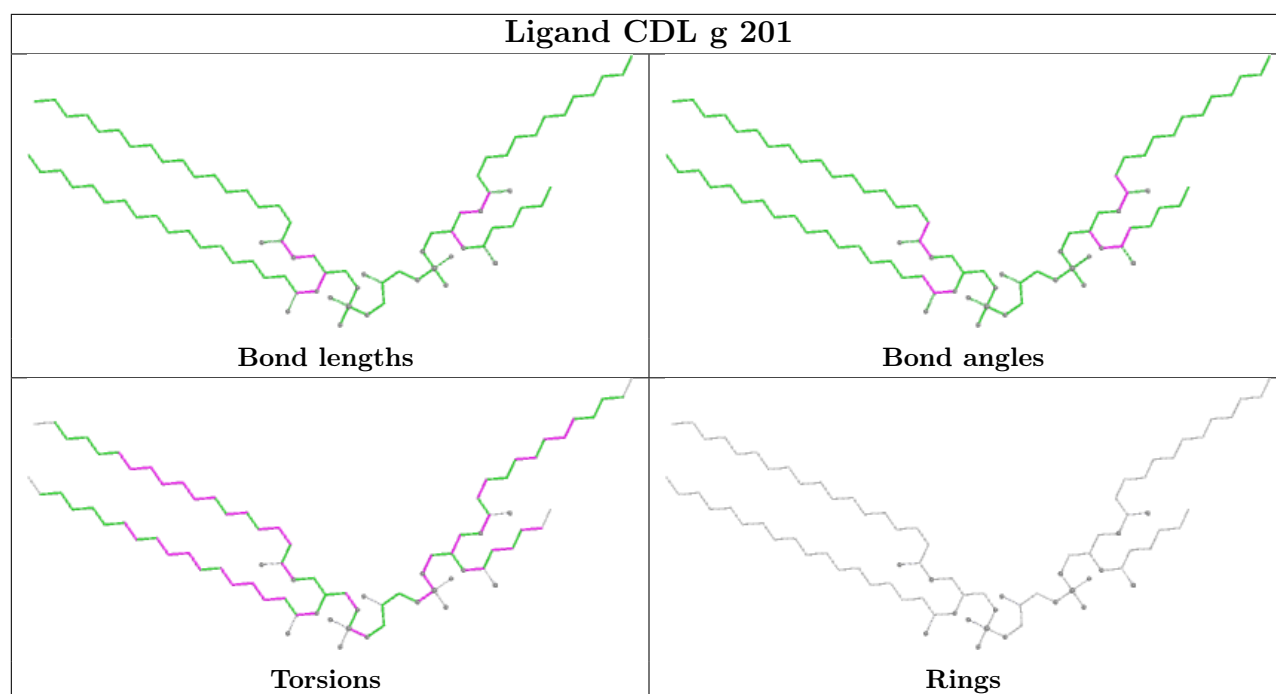
Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	I	302	SF4	7	0
43	A	802	SF4	2	0
48	O	201	ZMP	3	0
50	4	501	3PE	2	0
50	g	202	3PE	3	0
45	B	502	FMN	2	0
49	g	201	CDL	2	0
50	1	401	3PE	2	0
43	B	501	SF4	3	0
46	E	401	NDP	5	0

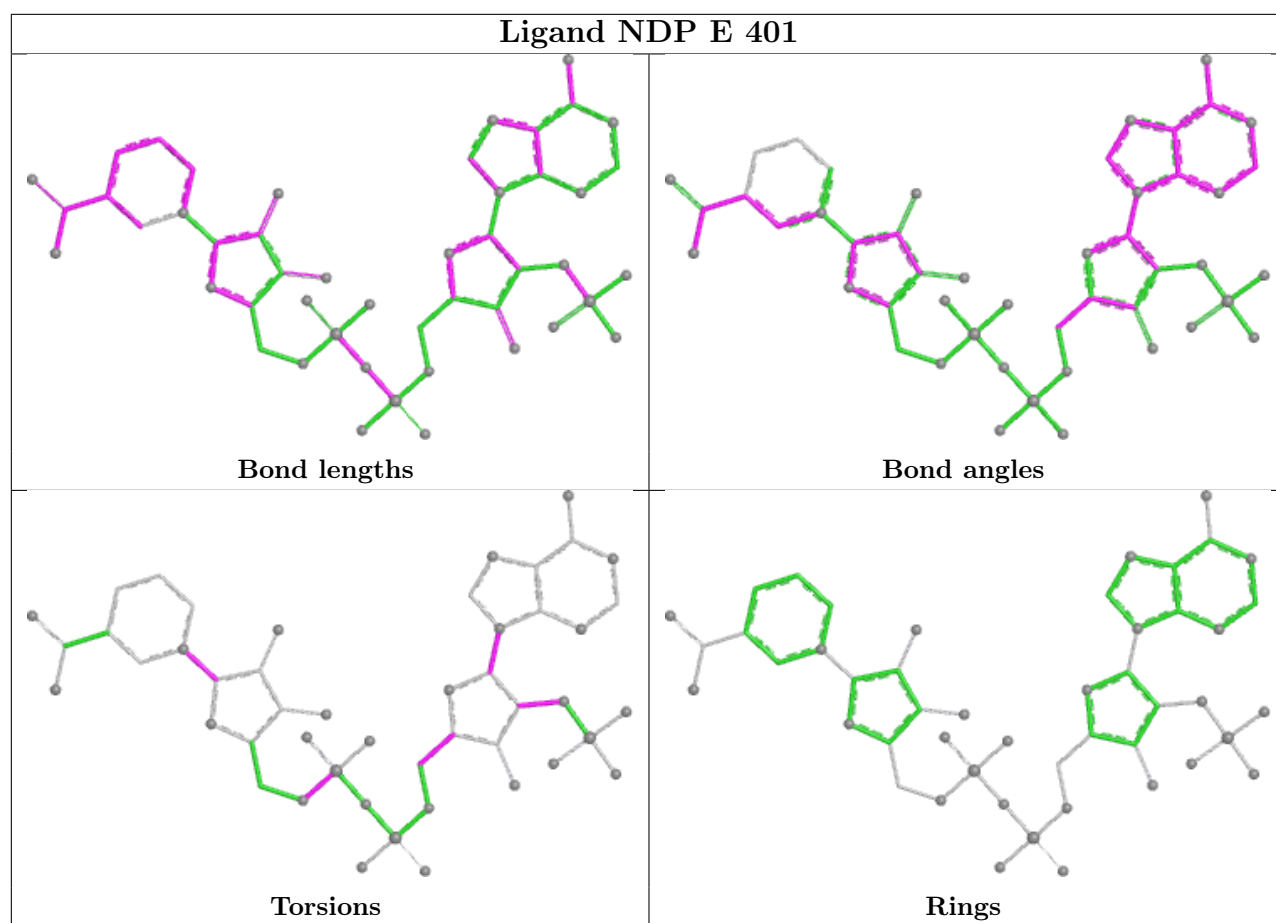
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

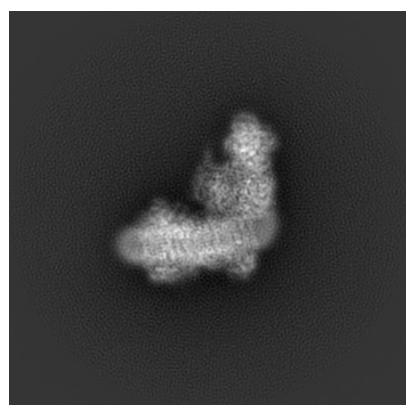
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4384. These allow visual inspection of the internal detail of the map and identification of artifacts.

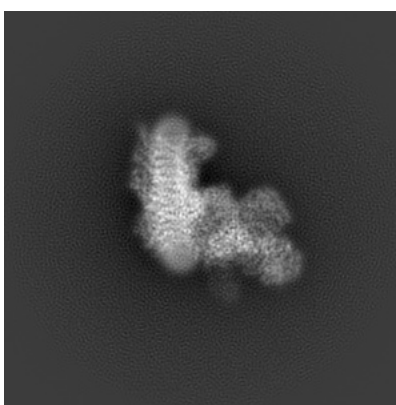
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

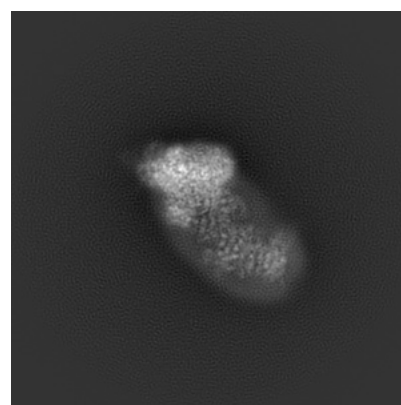
6.1.1 Primary map



X



Y

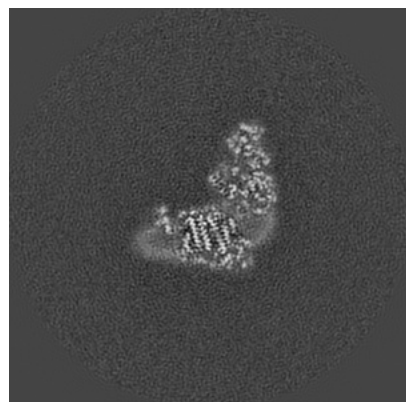


Z

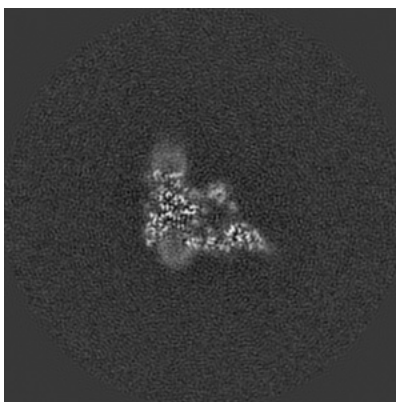
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

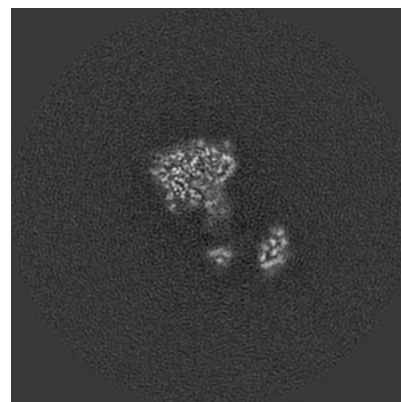
6.2.1 Primary map



X Index: 228



Y Index: 228

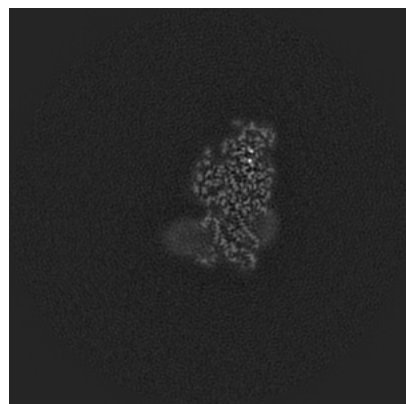


Z Index: 228

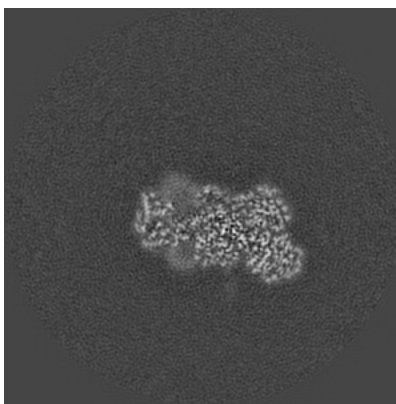
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

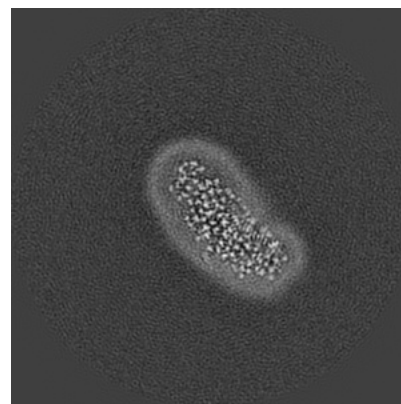
6.3.1 Primary map



X Index: 192



Y Index: 268

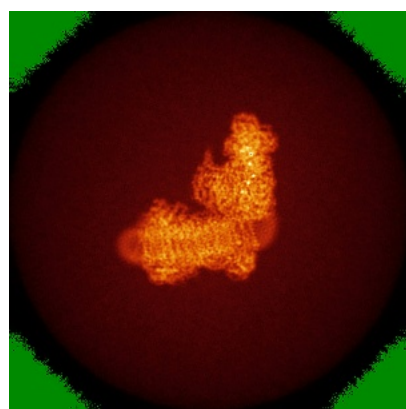


Z Index: 201

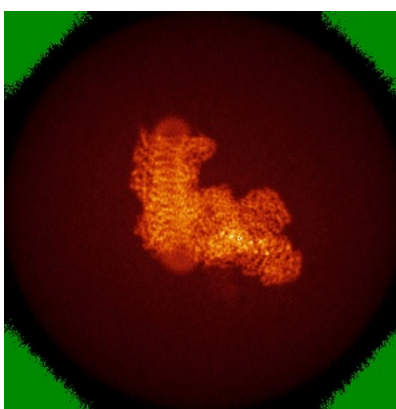
The images above show the largest variance slices of the map in three orthogonal directions.

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

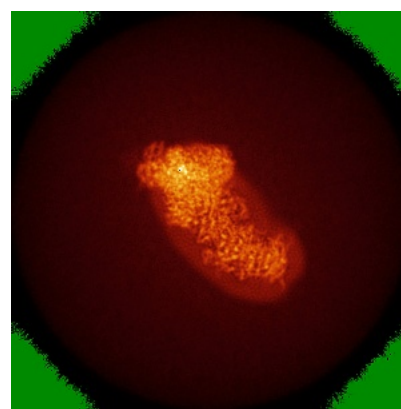
6.4.1 Primary map



X



Y

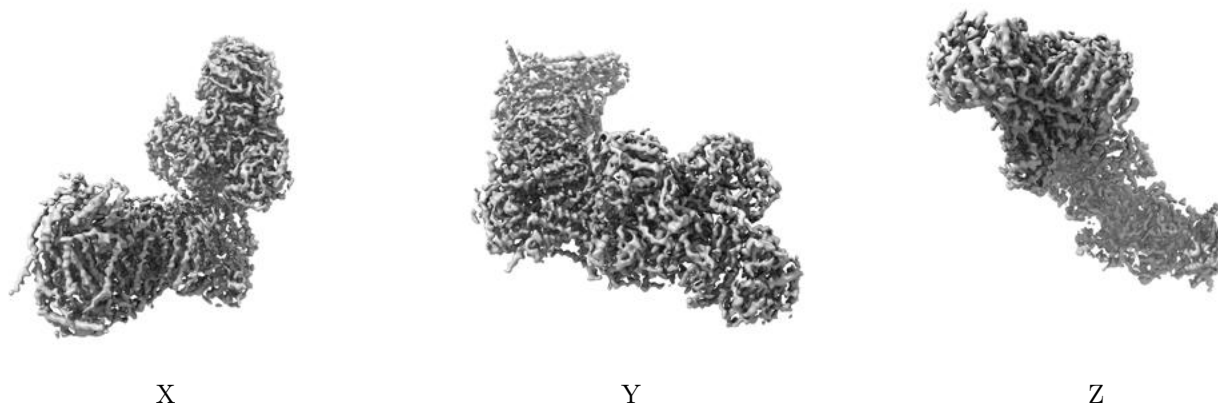


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

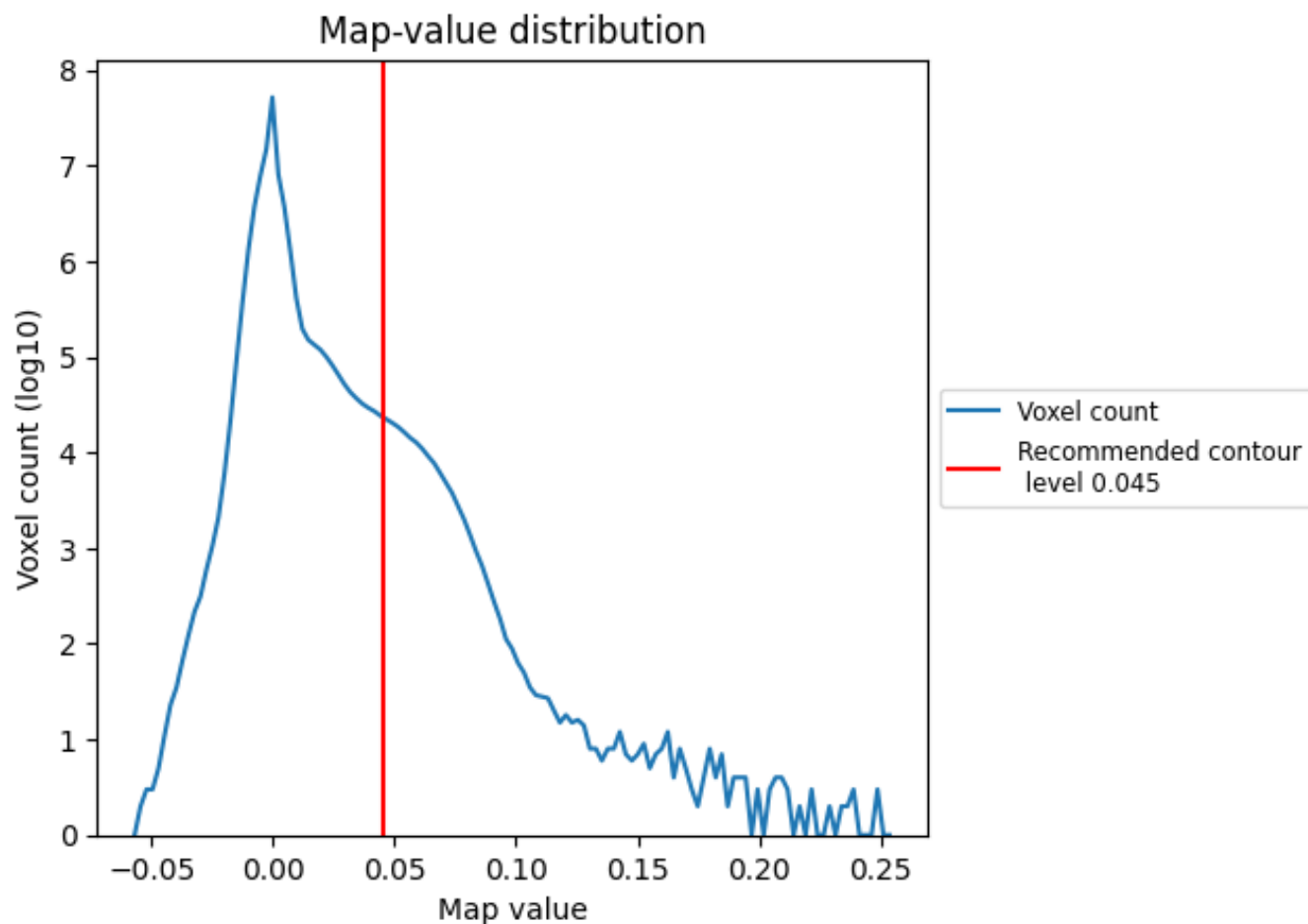
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

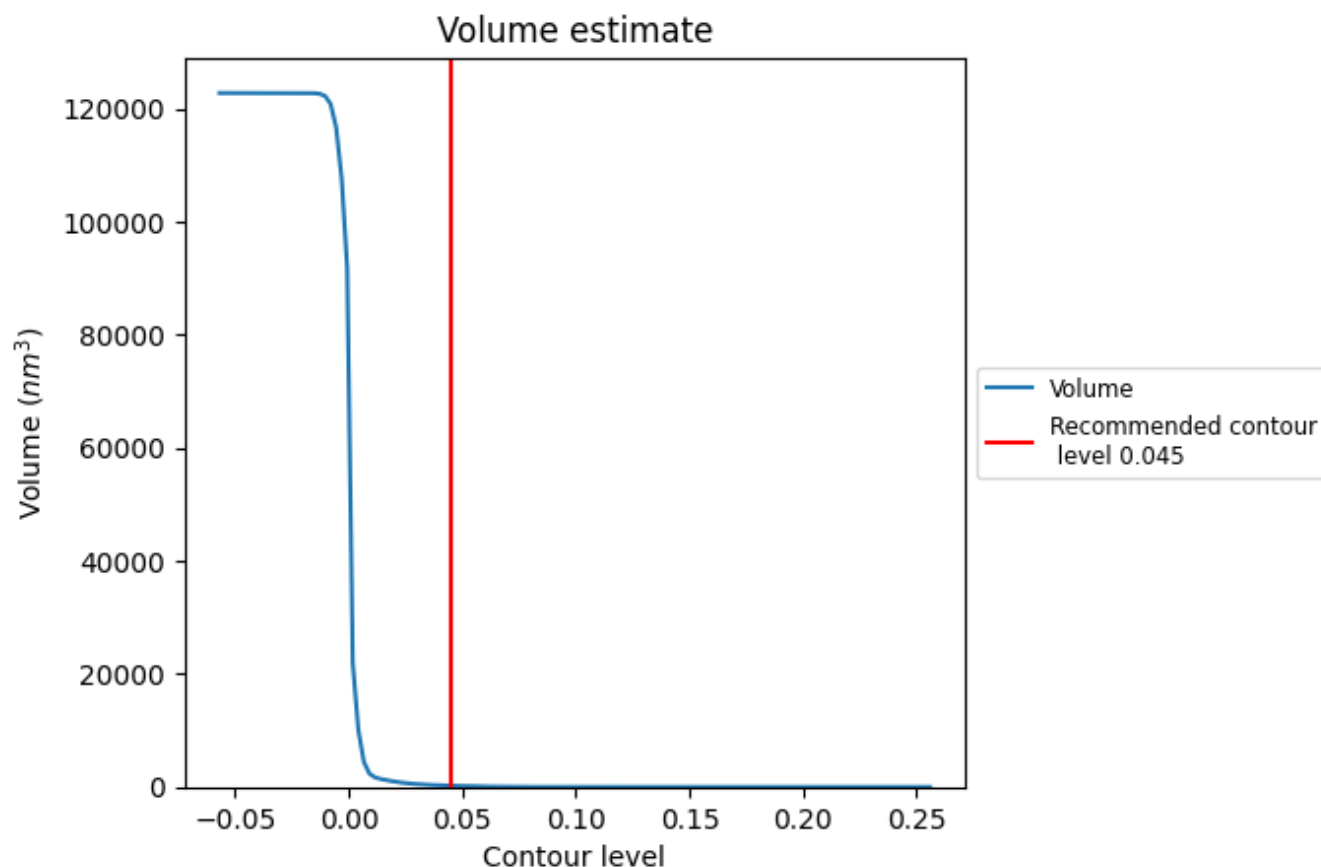
This section contains the results of statistical analysis of the map.

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.

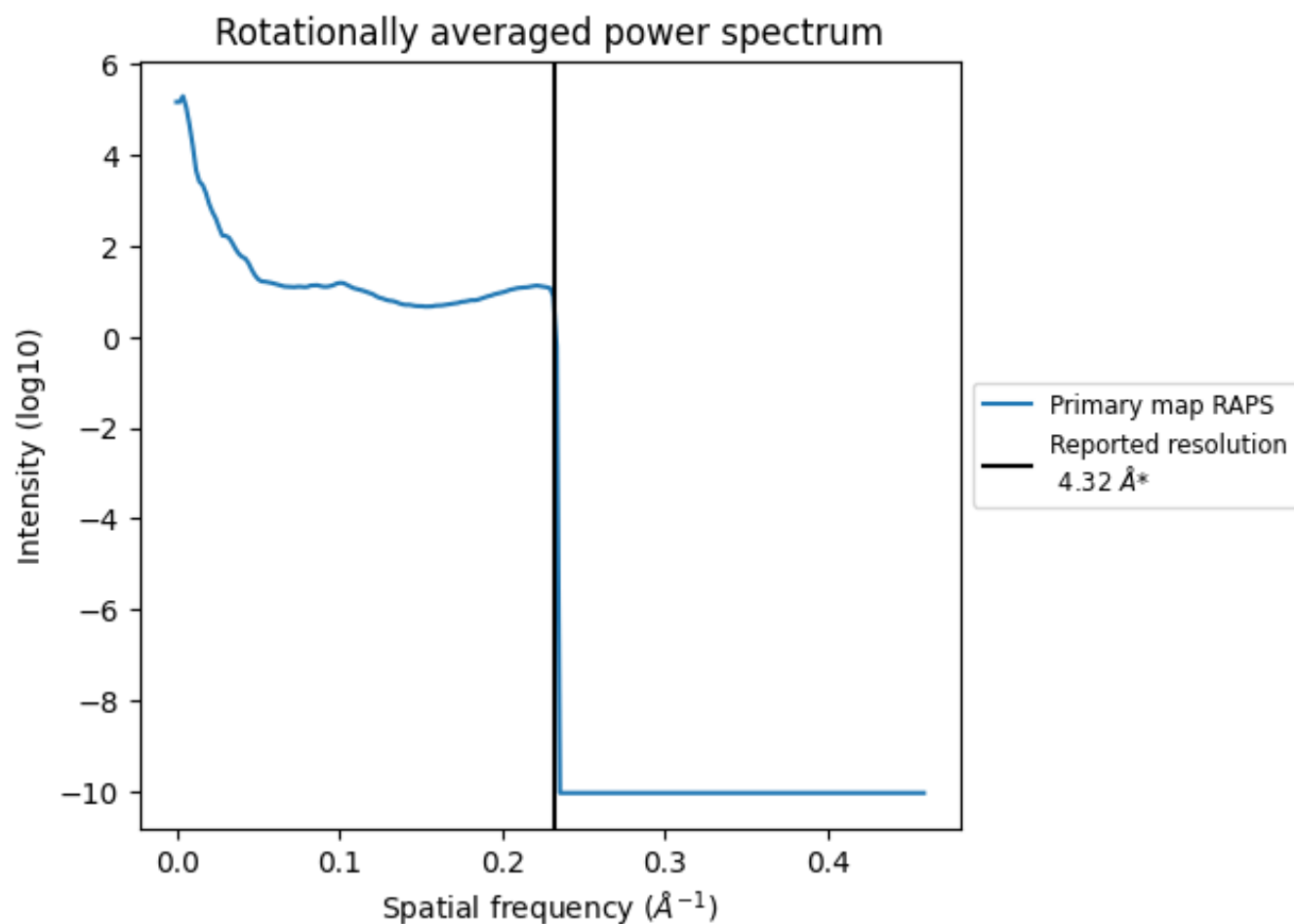
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 223 nm^3 ; this corresponds to an approximate mass of 202 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 ⓘ

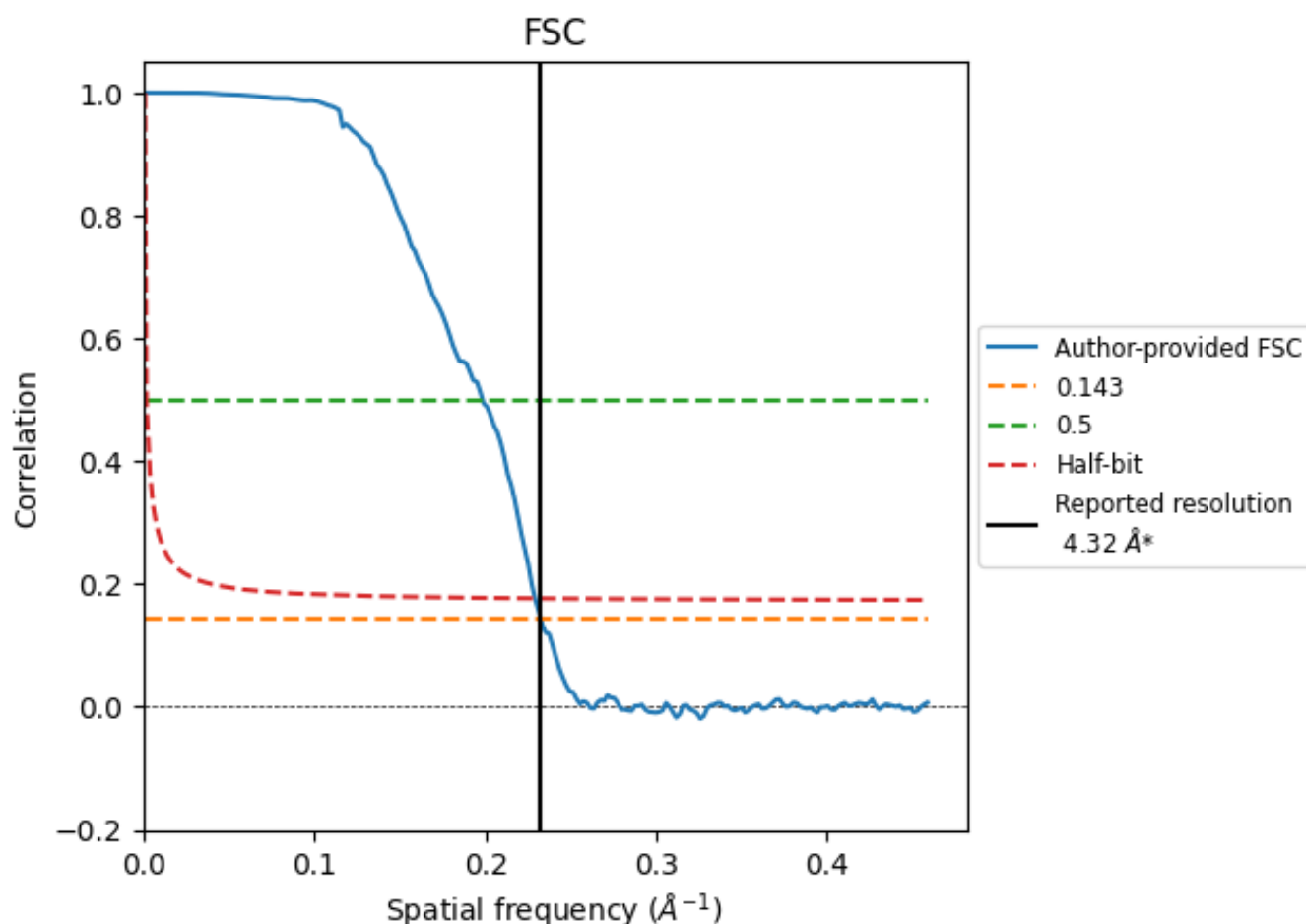


*Reported resolution corresponds to spatial frequency of 0.231 Å⁻¹

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 0.231 Å⁻¹

8.2 Resolution estimates [i](#)

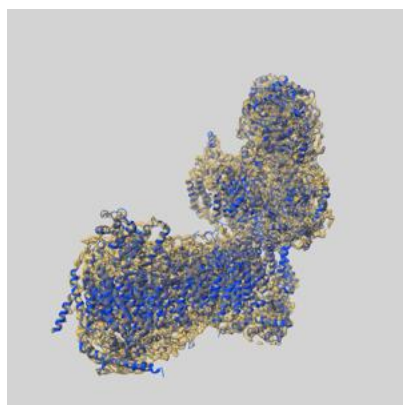
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.32	-	-
Author-provided FSC curve	4.30	5.04	4.36
Unmasked-calculated*	-	-	-

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

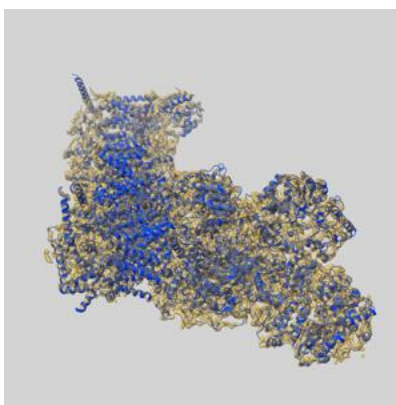
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4384 and PDB model 6GCS. Per-residue inclusion information can be found in section 3 on page 16.

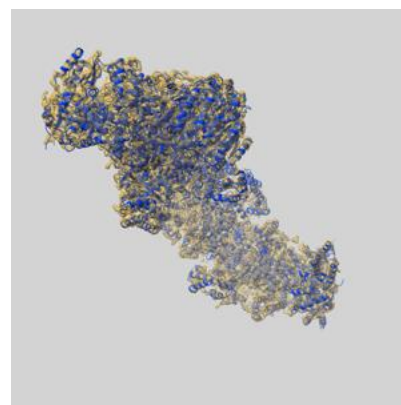
9.1 Map-model overlay [i](#)



X



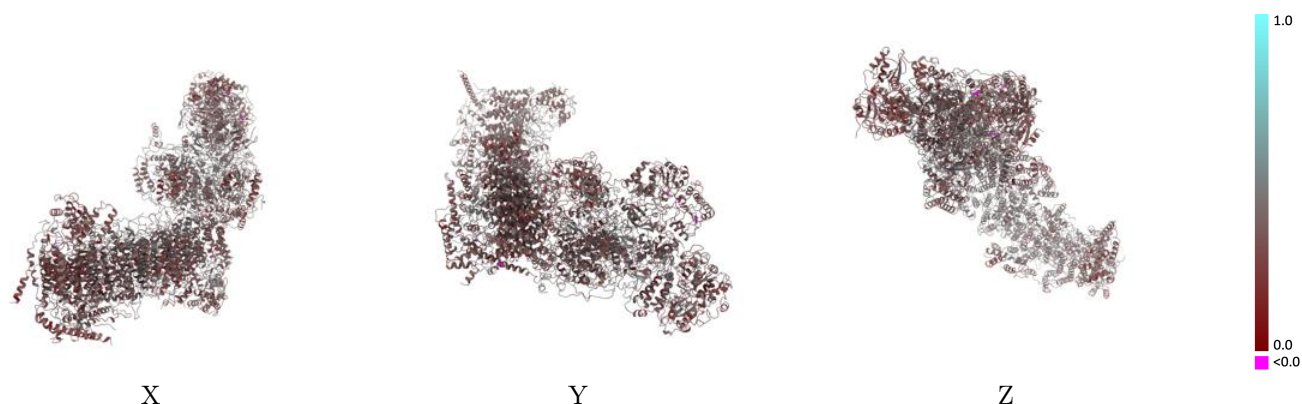
Y



Z

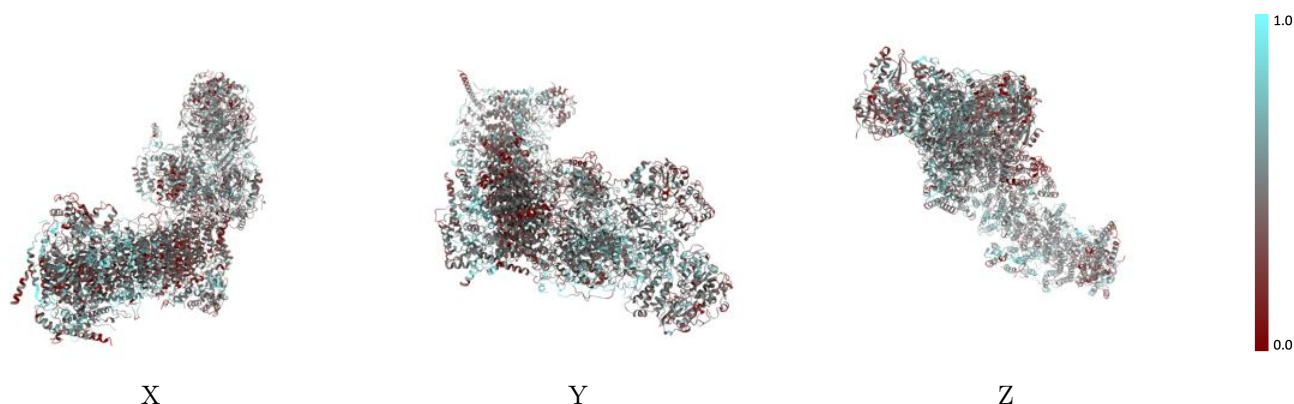
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



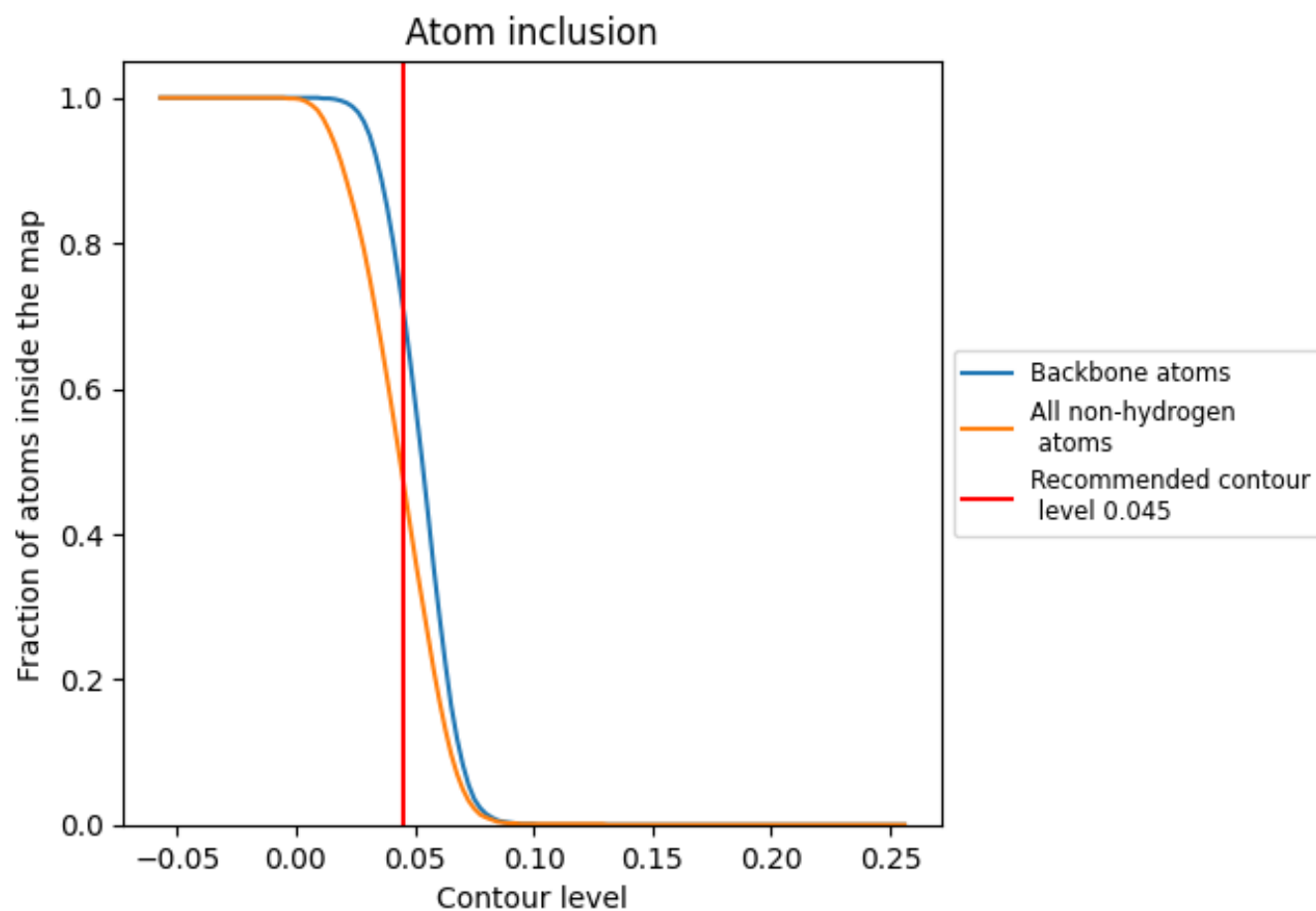
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 48% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4760	 0.3710
1	 0.4040	 0.3510
2	 0.5170	 0.3900
3	 0.3210	 0.3650
4	 0.4920	 0.3770
5	 0.4510	 0.3460
6	 0.3990	 0.3890
8	 0.3540	 0.3110
9	 0.4630	 0.3350
A	 0.4730	 0.3650
B	 0.4500	 0.3440
C	 0.4780	 0.3900
D	 0.4820	 0.3780
E	 0.4480	 0.3640
F	 0.4970	 0.3730
G	 0.5750	 0.4070
H	 0.4820	 0.3450
I	 0.5320	 0.3770
J	 0.3470	 0.3500
K	 0.5320	 0.3860
L	 0.4240	 0.3750
M	 0.5720	 0.4050
O	 0.2150	 0.3280
P	 0.4490	 0.3790
Q	 0.2880	 0.3160
R	 0.4530	 0.3550
S	 0.6020	 0.3880
U	 0.4660	 0.3660
W	 0.4460	 0.3610
X	 0.6380	 0.4220
Y	 0.4960	 0.3990
Z	 0.7390	 0.4500
a	 0.6890	 0.4510
b	 0.6510	 0.3740
c	 0.4160	 0.3580



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Chain	Atom inclusion	Q-score
d	 0.4810	 0.3480
e	 0.6280	 0.4130
f	 0.3840	 0.3520
g	 0.3760	 0.3870
h	 0.5030	 0.3900
i	 0.6350	 0.3870
j	 0.5920	 0.4240
n	 0.7100	 0.4180