



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:59 PM UTC

PDB ID : 6F3A / pdb_00006f3a
EMDB ID : EMD-2860
Title : Cryo-EM structure of a single dynein tail domain bound to dynactin and BICD2N
Authors : Urnavicius, L.; Lau, C.K.; Elshenawy, M.M.; Morales-Rios, E.; Motz, C.; Yildiz, A.; Carter, A.P.
Deposited on : 2017-11-28
Resolution : 8.20 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

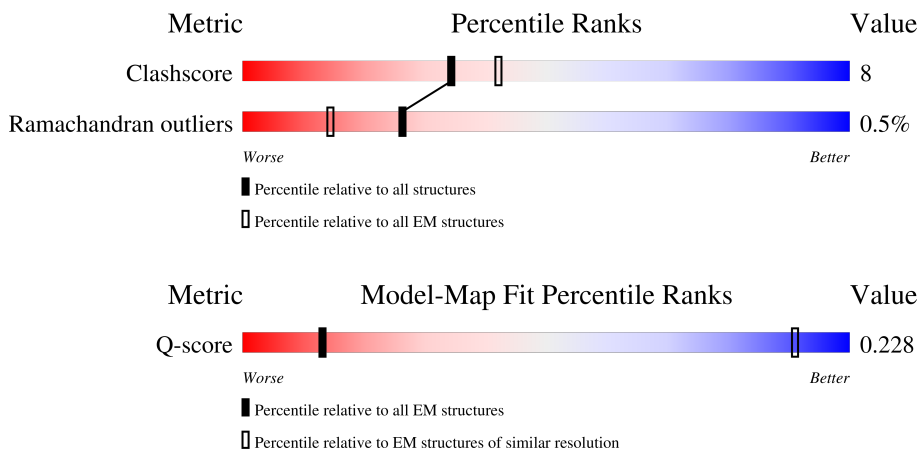
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

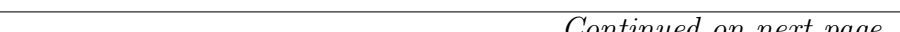
The reported resolution of this entry is 8.20 Å.

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



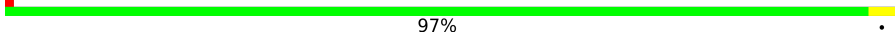
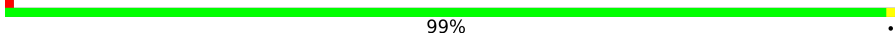
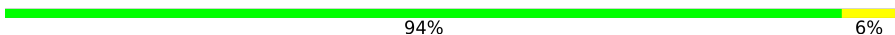
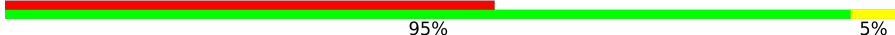
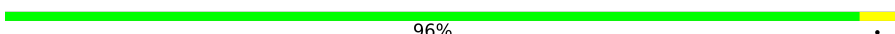
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	337 (7.70 - 8.70)

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

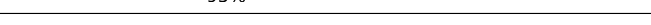
Mol	Chain	Length	Quality of chain
1	A	376	 85% 13% .
1	B	376	 80% 19% .
1	C	376	 84% 14% ..
1	D	376	 82% 17% .
1	E	376	 80% 18% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	376	
1	G	376	
1	I	376	
2	H	375	
3	J	390	
4	K	286	
5	L	272	
6	M	587	
7	N	616	
8	O	65	
8	P	65	
9	Q	87	
9	R	87	
10	U	190	
11	V	182	
12	Y	264	
13	Z	52	
14	a	68	
15	b	89	
15	c	89	
15	d	89	
16	e	1455	
16	f	1455	
17	g	612	
17	h	612	

Continued on next page...

Mol	Chain	Length	Quality of chain
18	j	492	 97%
19	k	96	 85% 95%
19	l	96	 39% 93%
20	z	53	 8% 100%
21	5	275	 18% 81% 19%
21	6	275	 16% 81% 19%

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 48864 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 ARP1 actin related protein 1 homolog A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	B	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	C	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	D	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	E	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	F	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	G	370	Total	C	N	O	0	0
			1822	1082	370	370		
1	I	370	Total	C	N	O	0	0
			1822	1082	370	370		

- Molecule 2 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	370	Total	C	N	O	0	0
			1822	1082	370	370		

- Molecule 3 is a protein called Actin related protein 10 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	369	Total	C	N	O	0	0
			1819	1081	369	369		

- Molecule 4 is a protein called Capping protein (Actin filament) muscle Z-line, alpha 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	278	Total	C	N	O	0	0
			1378	822	278	278		

- Molecule 5 is a protein called F-actin capping protein beta subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	L	269	Total	C	N	O	0	0
			1327	789	269	269		

- Molecule 6 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	M	587	Total	C	N	O	0	0
			2935	1761	587	587		

- Molecule 7 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	N	616	Total	C	N	O	0	0
			3080	1848	616	616		

- Molecule 8 is a protein called Dynactin Subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	O	65	Total	C	N	O	0	0
			323	193	65	65		
8	P	65	Total	C	N	O	0	0
			323	193	65	65		

- Molecule 9 is a protein called Dynactin Subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	Q	87	Total	C	N	O	0	0
			435	261	87	87		
9	R	87	Total	C	N	O	0	0
			435	261	87	87		

- Molecule 10 is a protein called Dynactin 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	U	172	Total	C	N	O	0	1
			843	500	171	172		

- Molecule 11 is a protein called Dynactin subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	V	165	Total	C	N	O	0	0
			812	482	165	165		

- Molecule 12 is a protein called Dynactin Subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Y	264	Total	C	N	O	0	0
			1320	792	264	264		

- Molecule 13 is a protein called Dynactin Subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Z	52	Total	C	N	O	0	0
			260	156	52	52		

- Molecule 14 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	a	52	Total	C	N	O	0	0
			259	155	52	52		

- Molecule 15 is a protein called Dynactin subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	b	75	Total	C	N	O	0	0
			369	219	75	75		
15	c	35	Total	C	N	O	0	0
			174	104	35	35		
15	d	24	Total	C	N	O	0	0
			119	71	24	24		

- Molecule 16 is a protein called Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	e	785	Total	C	N	O	0	0
			3898	2328	785	785		
16	f	832	Total	C	N	O	0	0
			4128	2470	832	826		

- Molecule 17 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	g	397	Total	C	N	O	0	0
			1961	1167	397	397		
17	h	401	Total	C	N	O	0	0
			1980	1178	401	401		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	484	SER	THR	conflict	UNP Q13409
g	499	GLY	ASP	conflict	UNP Q13409
h	484	SER	THR	conflict	UNP Q13409
h	499	GLY	ASP	conflict	UNP Q13409

- Molecule 18 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	j	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 19 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	k	93	Total	C	N	O	0	0
			462	276	93	93		
19	l	93	Total	C	N	O	0	0
			462	276	93	93		

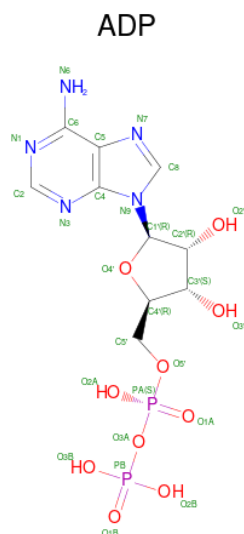
- Molecule 20 is a protein called Dynactin Subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	z	53	Total	C	N	O	0	0
			265	159	53	53		

- Molecule 21 is a protein called BICD2N.

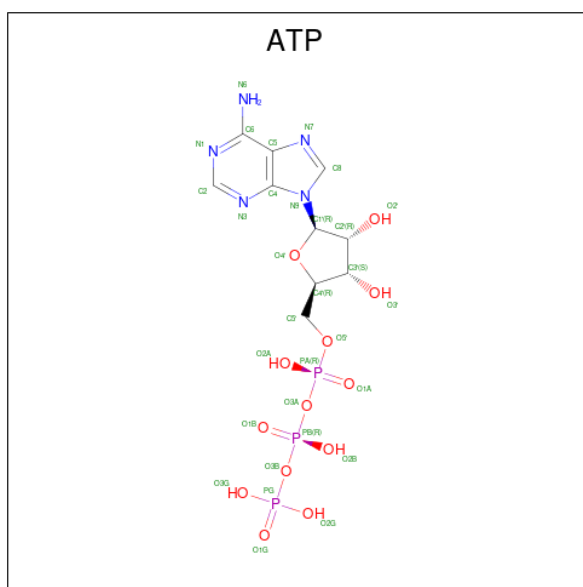
Mol	Chain	Residues	Atoms				AltConf	Trace
21	5	275	Total	C	N	O	0	0
			1375	825	275	275		
21	6	275	Total	C	N	O	0	0
			1375	825	275	275		

- Molecule 22 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 27	C 10	N 5	O 10	P 2	0
22	B	1	Total 27	C 10	N 5	O 10	P 2	0
22	C	1	Total 27	C 10	N 5	O 10	P 2	0
22	D	1	Total 27	C 10	N 5	O 10	P 2	0
22	E	1	Total 27	C 10	N 5	O 10	P 2	0
22	F	1	Total 27	C 10	N 5	O 10	P 2	0
22	G	1	Total 27	C 10	N 5	O 10	P 2	0
22	I	1	Total 27	C 10	N 5	O 10	P 2	0
22	J	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 23 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

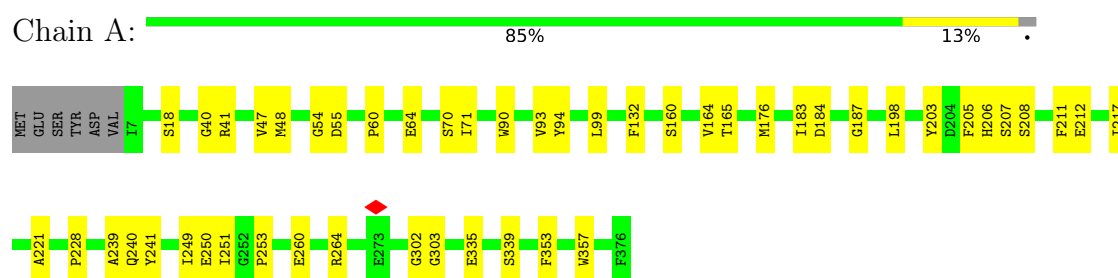


Mol	Chain	Residues	Atoms					AltConf
23	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

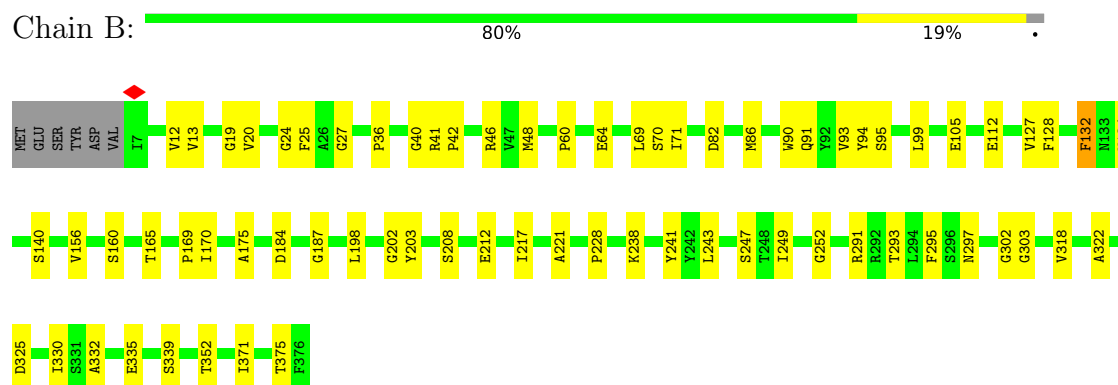
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

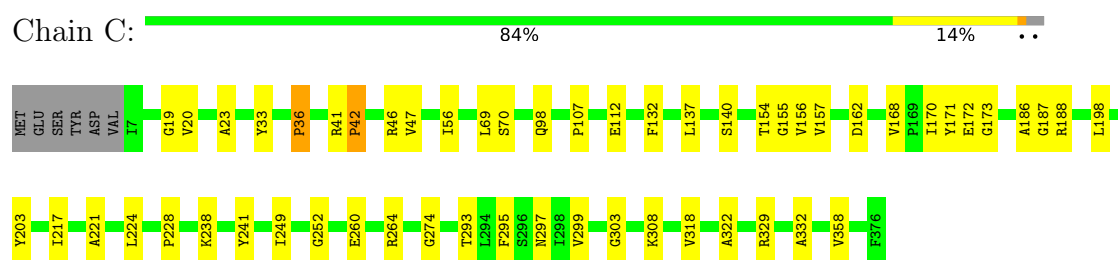
- Molecule 1: ARP1 actin related protein 1 homolog A



- Molecule 1: ARP1 actin related protein 1 homolog A



- Molecule 1: ARP1 actin related protein 1 homolog A



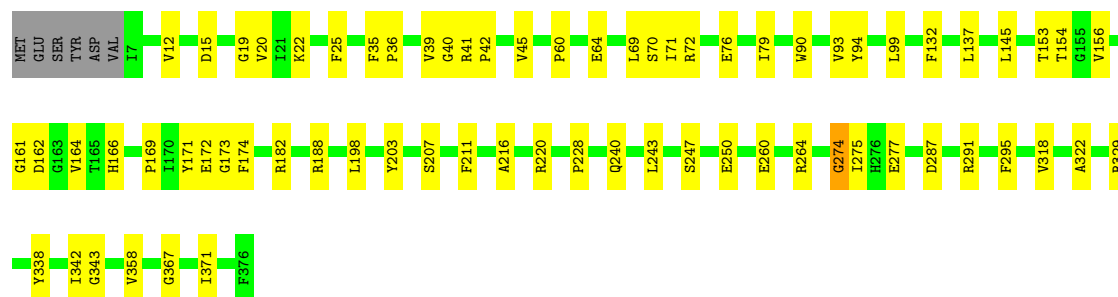
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain D:  82% 17% .



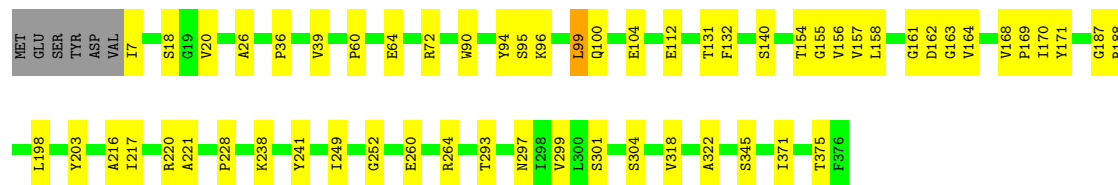
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain E:  80% 18% .



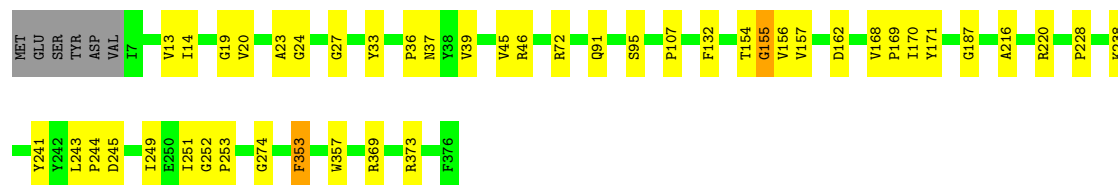
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain F:  83% 15% .



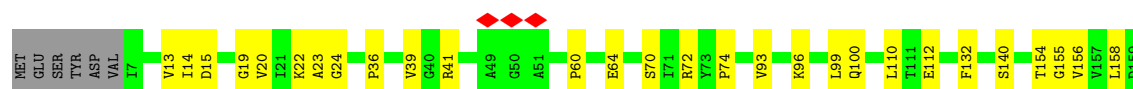
- Molecule 1: ARP1 actin related protein 1 homolog A

Chain G:  86% 11% ..



- Molecule 1: ARP1 actin related protein 1 homolog A

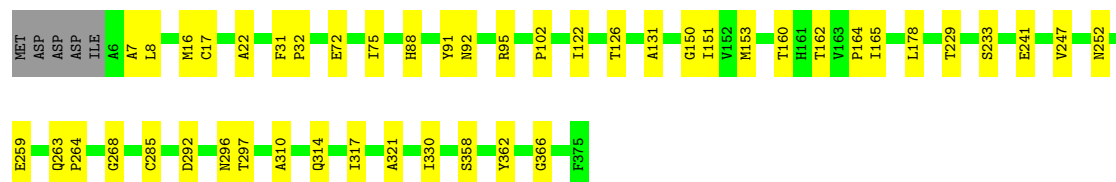
Chain I:  84% 15% .





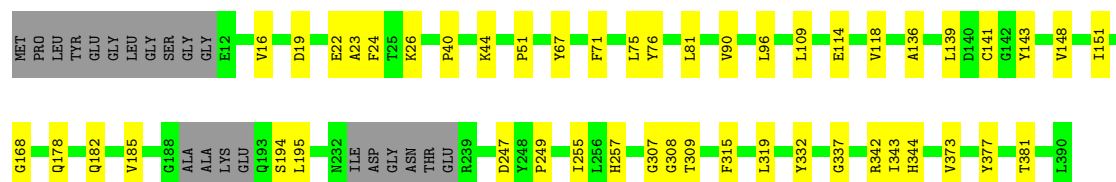
- Molecule 2: Actin, cytoplasmic 1

Chain H: 86% 12% .



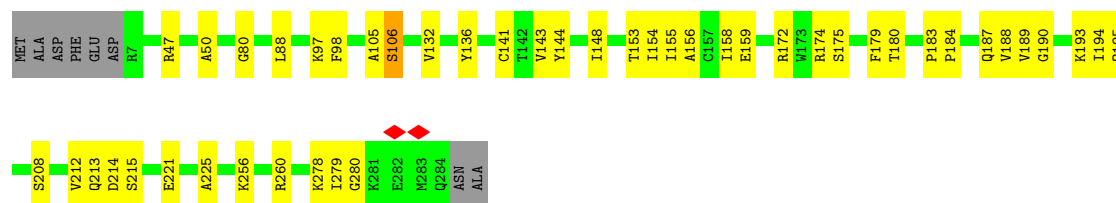
- Molecule 3: Actin related protein 10 homolog

Chain J: 82% 12% 5%



- Molecule 4: Capping protein (Actin filament) muscle Z-line, alpha 1

Chain K: 81% 16% .



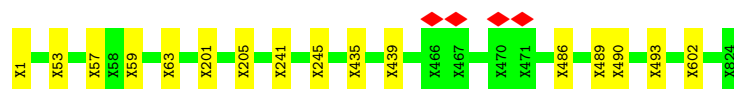
- Molecule 5: F-actin capping protein beta subunit

Chain L: 89% 10% .

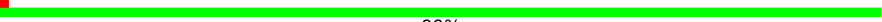


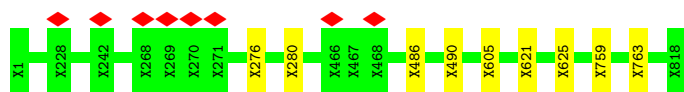
- Molecule 6: Dynactin Subunit 2

Chain M: 97% .



- Molecule 7: Dynactin Subunit 2

Chain N:  99% .



- Molecule 8: Dynactin Subunit 3

Chain O:  89% 11%



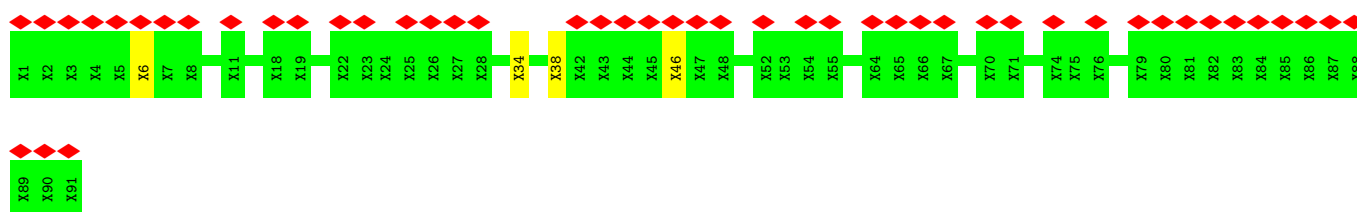
- Molecule 8: Dynactin Subunit 3

Chain P:  94% 6%

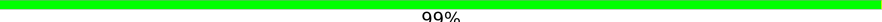


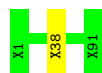
- Molecule 9: Dynactin Subunit 2

Chain Q:  55% 95% 5%



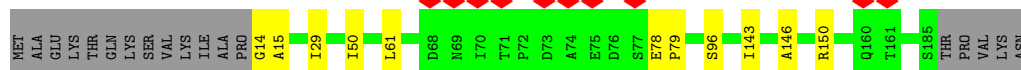
- Molecule 9: Dynactin Subunit 2

Chain R:  99% .



- Molecule 10: Dynactin 6

Chain U:  5% 85% 6% 9%

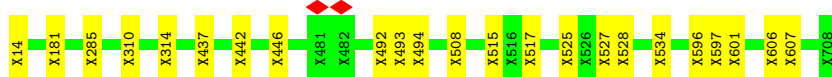


- Molecule 11: Dynactin subunit 5

Chain V:  77% 14% 9%



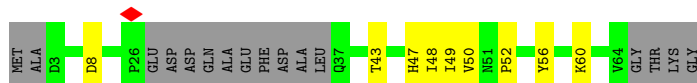
• Molecule 12: Dynactin Subunit 4



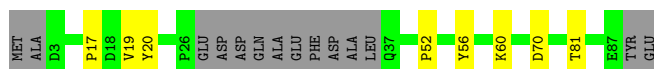
• Molecule 13: Dynactin Subunit 1



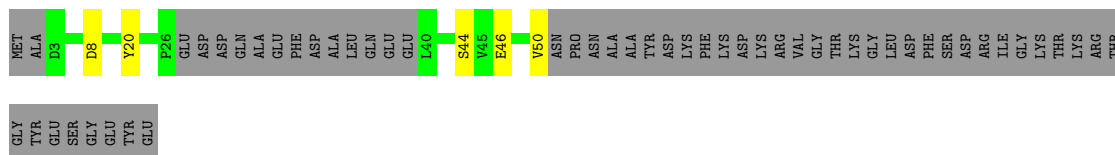
• Molecule 14: Dynactin subunit 2



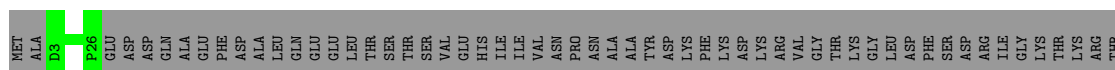
• Molecule 15: Dynactin subunit 2



• Molecule 15: Dynactin subunit 2



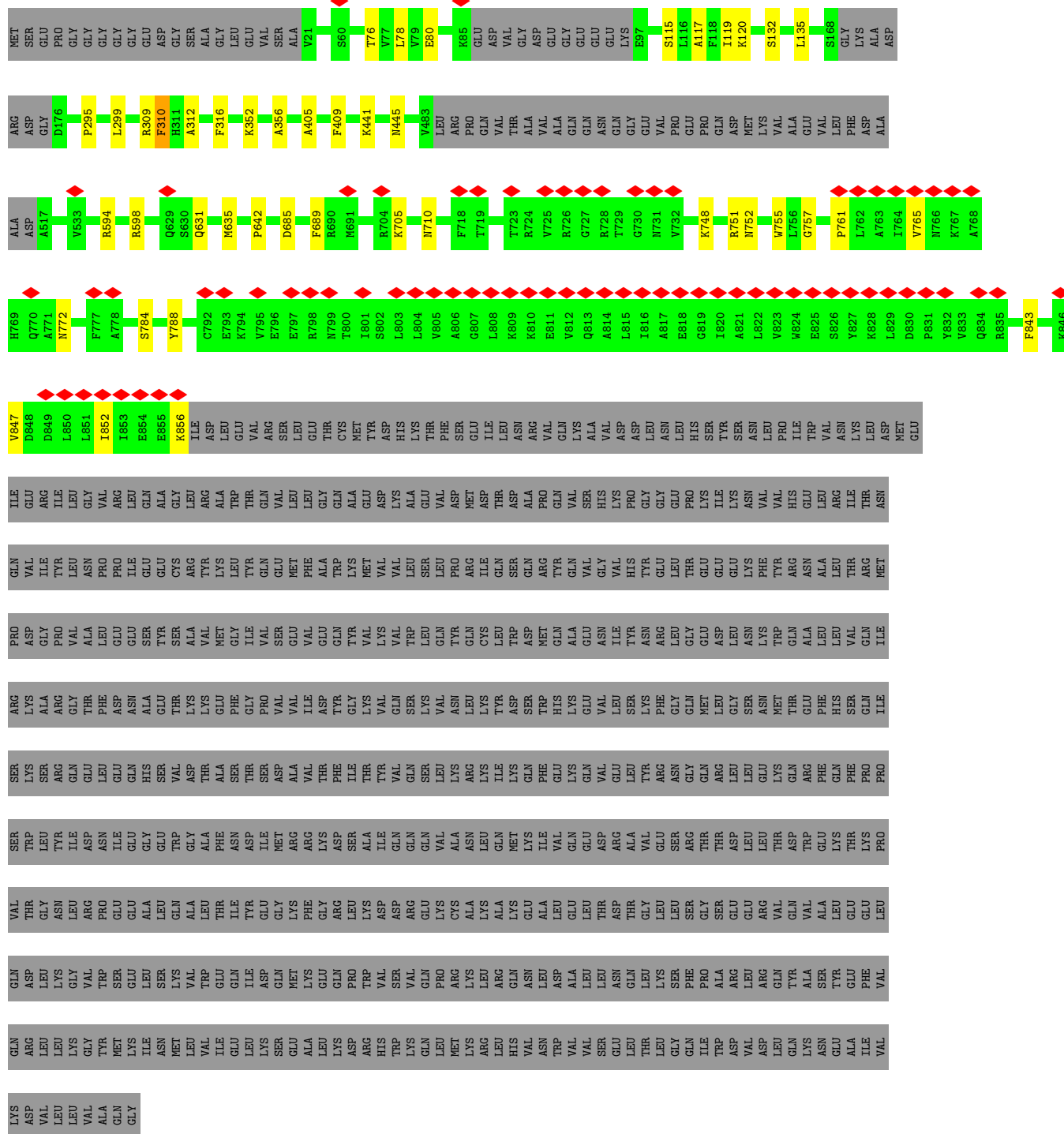
• Molecule 15: Dynactin subunit 2



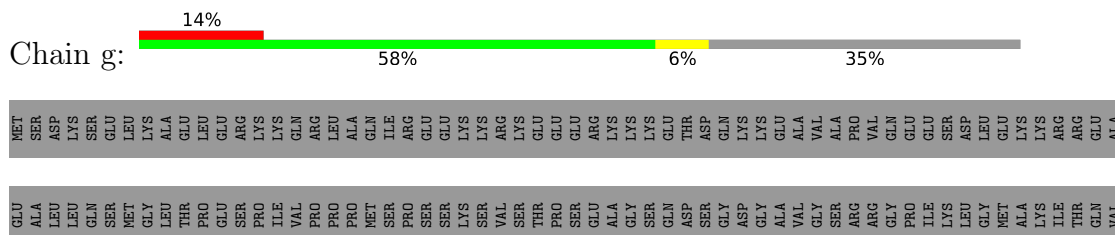
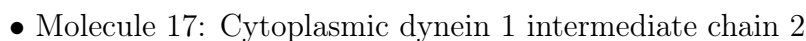
GLY
TYR
GLU
SER
PRO
GLY
GLY
TYR
GLU

• Molecule 16: Cytoplasmic dynein 1 heavy chain 1

Chain e: 



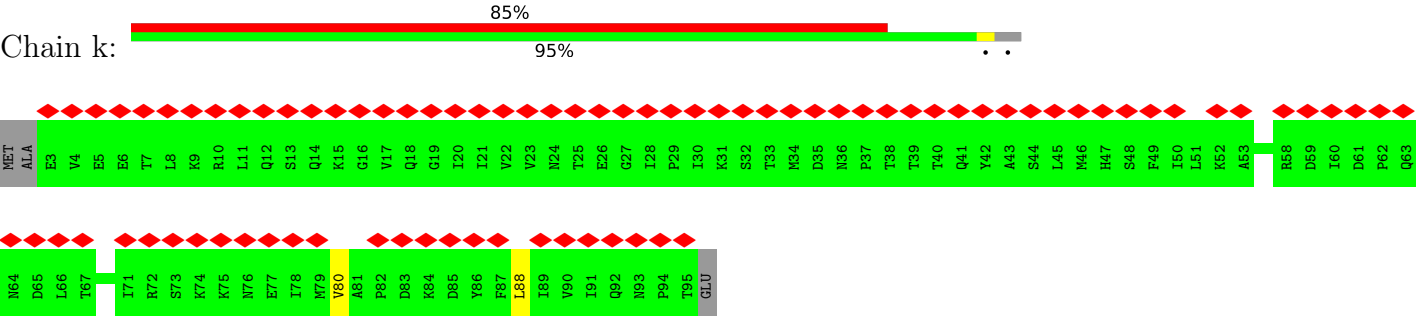
• Molecule 16: Cytoplasmic dynein 1 heavy chain 1



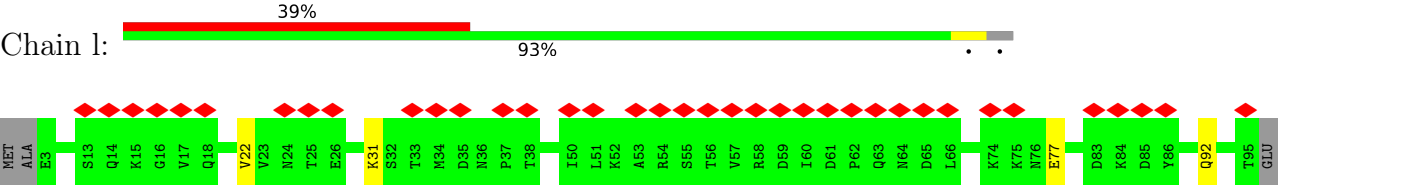




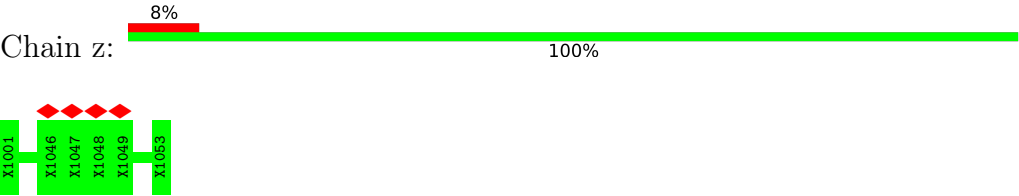
● Molecule 19: Dynein light chain roadblock-type 1



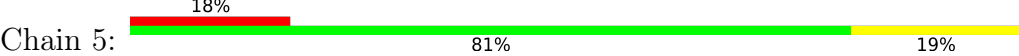
● Molecule 19: Dynein light chain roadblock-type 1

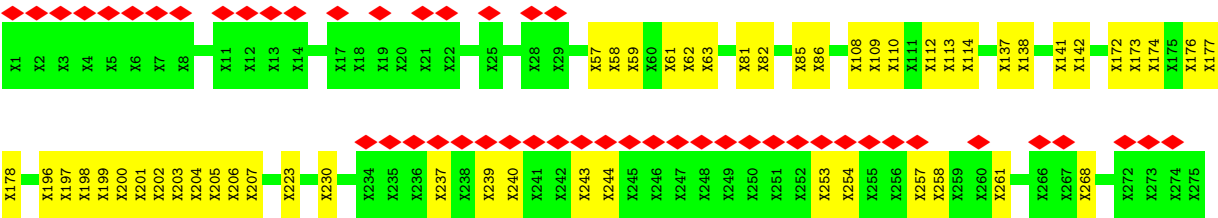


● Molecule 20: Dynactin Subunit 1

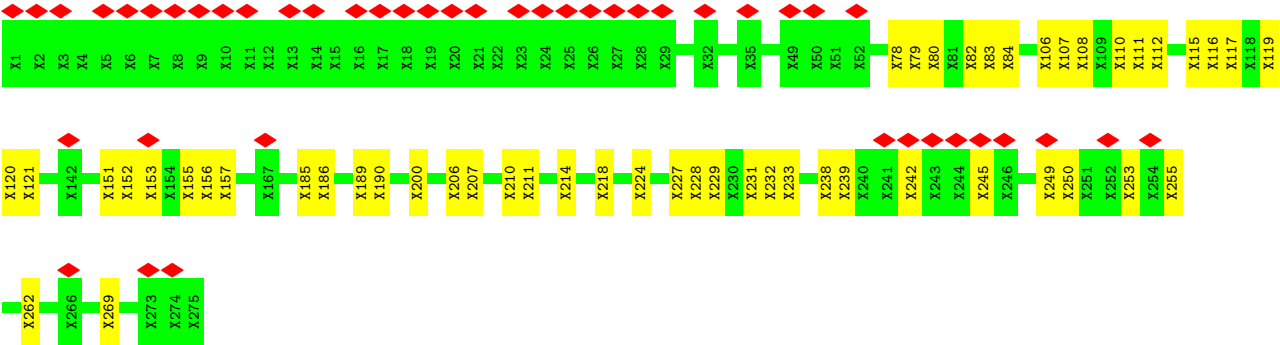
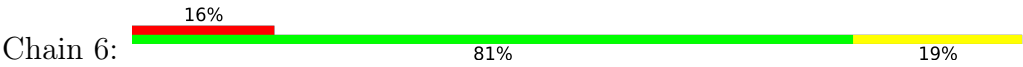


● Molecule 21: BICD2N





• Molecule 21: BICD2N



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	85744	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.371	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	578.88, 578.88, 578.88	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP

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	0.44	0/1821	1.05	8/2531 (0.3%)
1	B	0.49	0/1821	1.07	5/2531 (0.2%)
1	C	0.53	0/1821	1.18	8/2531 (0.3%)
1	D	0.56	0/1821	1.11	3/2531 (0.1%)
1	E	0.56	0/1821	1.14	3/2531 (0.1%)
1	F	0.58	0/1821	1.13	4/2531 (0.2%)
1	G	0.56	0/1821	1.21	10/2531 (0.4%)
1	I	0.49	0/1821	1.05	3/2531 (0.1%)
2	H	0.51	0/1821	1.10	3/2531 (0.1%)
3	J	0.51	1/1816 (0.1%)	1.05	0/2522
4	K	0.41	0/1377	1.07	6/1919 (0.3%)
5	L	0.47	0/1326	1.00	3/1844 (0.2%)
10	U	0.43	0/841	0.92	0/1168
11	V	0.26	0/811	0.74	0/1126
14	a	0.43	0/257	1.36	5/356 (1.4%)
15	b	0.47	0/367	1.22	2/507 (0.4%)
15	c	0.41	0/172	1.13	1/237 (0.4%)
15	d	0.40	0/118	0.87	0/163
16	e	0.30	1/3894 (0.0%)	0.75	3/5429 (0.1%)
16	f	0.38	0/4123	0.91	2/5745 (0.0%)
17	g	0.36	0/1959	0.97	0/2725
17	h	0.39	0/1978	1.09	6/2751 (0.2%)
18	j	0.26	0/74	0.72	0/102
19	k	0.30	0/461	0.82	0/642
19	l	0.30	0/461	0.71	0/642
All	All	0.45	2/36424 (0.0%)	1.02	75/50657 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	195	LEU	C-O	-8.90	1.19	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	e	310	PHE	CA-C	-5.16	1.45	1.52

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	274	GLY	N-CA-C	-11.27	86.47	113.18
1	I	274	GLY	N-CA-C	-9.68	90.23	113.18
16	e	309	ARG	CA-C-N	9.16	139.04	121.54
16	e	309	ARG	C-N-CA	9.16	139.04	121.54
1	A	205	PHE	CA-C-N	8.88	133.35	120.38
1	A	205	PHE	C-N-CA	8.88	133.35	120.38
1	C	274	GLY	N-CA-C	-8.87	92.16	113.18
1	A	206	HIS	N-CA-C	8.73	122.92	111.75
14	a	50	VAL	N-CA-C	8.62	118.43	111.62
1	G	274	GLY	N-CA-C	-7.99	94.24	113.18
1	E	274	GLY	N-CA-C	-7.61	95.16	113.18
1	G	155	GLY	N-CA-C	7.28	119.63	110.96
5	L	127	GLY	N-CA-C	-7.26	100.66	110.97
16	f	221	TYR	N-CA-C	-6.83	106.15	114.75
1	C	56	ILE	N-CA-C	-6.81	95.17	109.34
1	A	176	MET	N-CA-C	-6.79	99.37	109.42
15	c	8	ASP	N-CA-C	6.65	118.22	110.97
17	h	331	ILE	N-CA-C	-6.64	99.22	108.12
17	h	491	LEU	CA-C-N	6.58	131.11	121.31
17	h	491	LEU	C-N-CA	6.58	131.11	121.31
2	H	252	ASN	CA-C-N	6.45	133.85	121.54
2	H	252	ASN	C-N-CA	6.45	133.85	121.54
4	K	278	LYS	CA-C-N	6.39	133.47	121.97
4	K	278	LYS	C-N-CA	6.39	133.47	121.97
1	A	132	PHE	N-CA-C	-6.30	101.16	110.48
16	e	757	GLY	N-CA-C	-6.29	103.07	114.46
1	C	36	PRO	CA-C-N	6.14	133.26	121.54
1	C	36	PRO	C-N-CA	6.14	133.26	121.54
1	F	131	THR	N-CA-C	-6.11	103.36	111.24
1	B	105	GLU	N-CA-C	6.02	117.93	111.36
1	I	269	GLY	N-CA-C	-5.99	98.98	113.18
17	h	418	VAL	CA-C-N	5.98	132.96	121.54
17	h	418	VAL	C-N-CA	5.98	132.96	121.54
1	G	244	PRO	CA-C-N	5.98	131.13	121.98
1	G	244	PRO	C-N-CA	5.98	131.13	121.98
1	D	253	PRO	CA-C-N	5.95	128.53	120.38
1	D	253	PRO	C-N-CA	5.95	128.53	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	132	PHE	N-CA-C	-5.95	101.72	110.52
1	G	253	PRO	CA-C-N	5.90	129.67	120.82
1	G	253	PRO	C-N-CA	5.90	129.67	120.82
1	I	132	PHE	N-CA-C	-5.88	102.62	110.55
1	F	163	GLY	N-CA-C	-5.87	99.28	113.18
16	f	669	LEU	N-CA-C	-5.81	98.93	108.41
17	h	492	TYR	N-CA-C	5.76	118.42	110.35
2	H	285	CYS	N-CA-C	5.68	115.78	108.34
5	L	68	GLY	N-CA-C	-5.62	99.86	113.18
1	C	132	PHE	N-CA-C	-5.61	102.98	110.55
1	A	253	PRO	CA-C-N	5.59	128.04	120.38
1	A	253	PRO	C-N-CA	5.59	128.04	120.38
15	b	17	PRO	CA-C-N	5.53	129.11	120.82
15	b	17	PRO	C-N-CA	5.53	129.11	120.82
1	E	132	PHE	N-CA-C	-5.50	103.12	110.55
5	L	127	GLY	CA-C-O	-5.48	116.99	121.76
14	a	8	ASP	N-CA-C	5.45	116.91	110.97
1	B	132	PHE	N-CA-C	-5.44	102.47	110.52
1	A	54	GLY	N-CA-C	-5.41	100.35	113.18
4	K	106	SER	CA-C-N	5.37	134.90	121.80
4	K	106	SER	C-N-CA	5.37	134.90	121.80
1	E	35	PHE	N-CA-C	-5.34	103.32	108.13
1	G	107	PRO	N-CA-C	-5.32	102.80	111.68
1	C	98	GLN	N-CA-C	5.31	122.11	110.80
1	F	99	LEU	CB-CA-C	-5.29	102.47	111.26
14	a	49	ILE	CA-C-N	-5.25	117.59	123.16
14	a	49	ILE	C-N-CA	-5.25	117.59	123.16
1	C	107	PRO	N-CA-C	-5.20	102.43	111.32
1	F	132	PHE	N-CA-C	-5.18	102.86	110.52
4	K	148	ILE	CA-C-N	5.15	131.38	121.54
4	K	148	ILE	C-N-CA	5.15	131.38	121.54
1	B	352	THR	CA-C-N	5.12	131.32	121.54
1	B	352	THR	C-N-CA	5.12	131.32	121.54
14	a	43	THR	N-CA-C	5.12	117.52	111.33
1	G	251	ILE	N-CA-C	5.11	115.66	111.62
1	G	27	GLY	N-CA-C	-5.10	101.10	113.18
1	B	27	GLY	N-CA-C	-5.08	107.64	114.25
1	C	42	PRO	N-CA-C	5.01	119.07	111.15

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1822	0	820	22	0
1	B	1822	0	820	38	0
1	C	1822	0	820	30	0
1	D	1822	0	820	31	0
1	E	1822	0	820	35	0
1	F	1822	0	820	30	0
1	G	1822	0	820	23	0
1	I	1822	0	820	30	0
2	H	1822	0	835	22	0
3	J	1819	0	794	28	0
4	K	1378	0	611	22	0
5	L	1327	0	585	13	0
6	M	2935	0	601	9	0
7	N	3080	0	632	5	0
8	O	323	0	73	4	0
8	P	323	0	74	2	0
9	Q	435	0	93	3	0
9	R	435	0	93	1	0
10	U	843	0	376	5	0
11	V	812	0	344	14	0
12	Y	1320	0	339	14	0
13	Z	260	0	57	1	0
14	a	259	0	110	4	0
15	b	369	0	161	6	0
15	c	174	0	71	4	0
15	d	119	0	50	0	0
16	e	3898	0	1725	22	0
16	f	4128	0	1822	21	0
17	g	1961	0	883	21	0
17	h	1980	0	889	26	0
18	j	75	0	32	0	0
19	k	462	0	192	1	0
19	l	462	0	192	2	0
20	z	265	0	57	0	0
21	5	1375	0	277	53	0
21	6	1375	0	277	43	0
22	A	27	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B	27	0	12	1	0
22	C	27	0	12	2	0
22	D	27	0	12	0	0
22	E	27	0	12	1	0
22	F	27	0	12	2	0
22	G	27	0	12	2	0
22	I	27	0	12	1	0
22	J	27	0	12	4	0
23	H	31	0	12	0	0
All	All	48864	0	18925	548	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 8.

All (548) 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)
21:5:268:UNK:CB	21:6:269:UNK:CB	1.95	1.44
21:5:137:UNK:O	21:5:141:UNK:N	1.68	1.25
21:6:238:UNK:O	21:6:242:UNK:N	1.70	1.24
21:5:138:UNK:O	21:5:142:UNK:N	1.90	1.05
21:6:117:UNK:O	21:6:121:UNK:N	1.92	1.02
21:5:82:UNK:O	21:5:86:UNK:N	1.95	1.00
17:g:245:PHE:O	17:g:567:GLN:HA	1.61	0.99
21:5:109:UNK:O	21:5:113:UNK:N	1.94	0.99
21:5:174:UNK:O	21:5:178:UNK:N	1.98	0.95
21:5:240:UNK:O	21:5:244:UNK:N	2.01	0.94
21:6:151:UNK:O	21:6:155:UNK:N	2.02	0.92
21:5:110:UNK:O	21:5:114:UNK:N	2.03	0.91
17:g:420:ASN:HA	17:g:433:ALA:O	1.70	0.90
21:5:174:UNK:O	21:5:178:UNK:CB	2.20	0.90
21:5:230:UNK:CB	21:6:231:UNK:CB	2.51	0.88
21:5:109:UNK:O	21:5:113:UNK:CB	2.20	0.88
21:5:202:UNK:O	21:5:206:UNK:N	2.07	0.87
21:5:201:UNK:O	21:5:205:UNK:N	2.09	0.85
21:5:199:UNK:O	21:5:203:UNK:N	2.10	0.84
21:5:223:UNK:CB	21:6:224:UNK:CB	2.58	0.81
21:6:239:UNK:HA	21:6:242:UNK:CB	2.10	0.81
17:g:431:TYR:HA	17:g:444:GLU:O	1.80	0.81
21:6:228:UNK:O	21:6:232:UNK:N	2.15	0.80
17:h:420:ASN:HA	17:h:433:ALA:O	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:g:423:VAL:O	17:g:430:VAL:HA	1.84	0.78
21:5:81:UNK:O	21:5:85:UNK:N	2.17	0.78
21:5:58:UNK:O	21:5:62:UNK:N	2.18	0.77
10:U:146:ALA:HB2	11:V:149:CYS:CB	2.15	0.76
17:h:513:LEU:HA	17:h:526:TRP:O	1.86	0.75
21:5:201:UNK:O	21:5:205:UNK:CB	2.34	0.75
21:6:106:UNK:O	21:6:110:UNK:N	2.19	0.75
21:5:244:UNK:CB	21:6:245:UNK:CB	2.65	0.74
21:5:138:UNK:O	21:5:142:UNK:CB	2.35	0.74
21:6:116:UNK:O	21:6:120:UNK:N	2.20	0.74
21:5:173:UNK:O	21:5:177:UNK:N	2.20	0.73
21:6:238:UNK:O	21:6:242:UNK:CB	2.35	0.73
1:G:238:LYS:HA	1:G:252:GLY:H	1.53	0.73
21:5:203:UNK:O	21:5:207:UNK:N	2.21	0.73
17:h:422:VAL:HA	17:h:431:TYR:O	1.89	0.71
21:5:108:UNK:O	21:5:112:UNK:N	2.23	0.71
21:5:237:UNK:CB	21:6:238:UNK:CB	2.69	0.71
17:h:514:PHE:O	17:h:525:LEU:HA	1.91	0.71
21:6:107:UNK:O	21:6:111:UNK:N	2.24	0.71
21:5:57:UNK:O	21:5:61:UNK:N	2.24	0.70
1:B:160:SER:H	1:B:302:GLY:HA3	1.55	0.70
21:6:186:UNK:O	21:6:190:UNK:N	2.25	0.70
21:6:116:UNK:O	21:6:120:UNK:CB	2.40	0.69
21:5:202:UNK:O	21:5:206:UNK:CB	2.41	0.69
21:6:79:UNK:O	21:6:83:UNK:N	2.25	0.68
4:K:221:GLU:O	4:K:225:ALA:HB2	1.93	0.68
17:h:561:VAL:O	17:h:568:ILE:HA	1.94	0.68
1:I:200:LYS:HA	3:J:96:LEU:HA	1.75	0.68
21:6:227:UNK:O	21:6:231:UNK:N	2.27	0.67
21:6:238:UNK:O	21:6:242:UNK:CA	2.43	0.67
17:g:514:PHE:O	17:g:525:LEU:HA	1.95	0.66
1:A:40:GLY:HA2	1:A:71:ILE:HA	1.77	0.66
17:h:505:MET:O	17:h:514:PHE:HA	1.94	0.66
1:E:41:ARG:O	1:E:70:SER:N	2.28	0.66
2:H:151:ILE:HA	2:H:164:PRO:HA	1.78	0.66
17:g:260:ASP:O	17:g:269:LEU:HA	1.96	0.66
21:6:207:UNK:O	21:6:211:UNK:N	2.29	0.66
17:h:428:GLY:H	17:h:452:PRO:HA	1.61	0.66
3:J:139:LEU:HA	3:J:148:VAL:HA	1.79	0.65
1:G:20:VAL:HA	1:G:36:PRO:HA	1.78	0.65
1:A:48:MET:H	1:C:173:GLY:HA3	1.62	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:6:249:UNK:O	21:6:253:UNK:N	2.29	0.65
1:B:165:THR:H	1:B:184:ASP:HA	1.62	0.65
1:C:46:ARG:HA	1:E:174:PHE:HA	1.78	0.65
16:f:523:VAL:O	16:f:527:TYR:CB	2.46	0.64
1:B:42:PRO:HA	1:B:69:LEU:HA	1.81	0.63
8:P:25:UNK:HA	8:P:36:UNK:HA	1.80	0.63
4:K:47:ARG:HA	4:K:50:ALA:HB3	1.82	0.62
21:5:59:UNK:O	21:5:63:UNK:N	2.32	0.62
1:D:20:VAL:HA	1:D:36:PRO:HA	1.80	0.62
11:V:146:PHE:HA	11:V:153:PHE:HA	1.81	0.62
21:5:172:UNK:O	21:5:176:UNK:N	2.33	0.62
1:F:7:ILE:N	1:F:104:GLU:O	2.33	0.62
2:H:88:HIS:O	2:H:92:ASN:CB	2.48	0.62
2:H:153:MET:HA	2:H:162:THR:HA	1.82	0.62
5:L:164:THR:HA	5:L:202:THR:HA	1.81	0.61
1:G:369:ARG:O	1:G:373:ARG:CB	2.48	0.61
1:E:20:VAL:HA	1:E:36:PRO:HA	1.82	0.61
11:V:51:ASP:CB	21:6:250:UNK:CB	2.78	0.61
21:5:198:UNK:O	21:5:202:UNK:N	2.33	0.61
21:6:80:UNK:O	21:6:84:UNK:CB	2.49	0.61
1:D:60:PRO:O	1:D:64:GLU:CB	2.48	0.60
21:6:214:UNK:O	21:6:218:UNK:N	2.34	0.60
4:K:187:GLN:HA	4:K:215:SER:HA	1.83	0.60
12:Y:527:UNK:HA	12:Y:607:UNK:HA	1.83	0.60
17:h:549:ARG:O	17:h:561:VAL:HA	2.02	0.60
21:5:137:UNK:O	21:5:141:UNK:CB	2.50	0.60
1:G:156:VAL:HA	1:G:169:PRO:HA	1.83	0.60
5:L:20:GLN:O	5:L:24:ASN:N	2.29	0.60
12:Y:14:UNK:N	12:Y:437:UNK:O	2.35	0.60
1:B:325:ASP:HA	15:c:50:VAL:HA	1.84	0.60
1:E:19:GLY:N	22:E:800:ADP:O3B	2.32	0.60
21:6:152:UNK:O	21:6:156:UNK:N	2.34	0.60
7:N:486:UNK:O	7:N:490:UNK:N	2.34	0.60
4:K:80:GLY:O	4:K:88:LEU:N	2.31	0.60
17:h:480:VAL:O	17:h:494:PHE:N	2.34	0.59
1:B:40:GLY:HA2	1:B:71:ILE:HA	1.85	0.59
1:F:112:GLU:N	1:F:140:SER:O	2.34	0.59
1:I:217:ILE:O	1:I:221:ALA:N	2.34	0.59
16:f:423:TRP:O	16:f:427:TYR:CB	2.51	0.59
1:A:60:PRO:O	1:A:64:GLU:CB	2.51	0.59
1:A:217:ILE:O	1:A:221:ALA:N	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:e:132:SER:H	16:f:44:ASP:HA	1.67	0.59
1:B:93:VAL:O	1:B:99:LEU:N	2.33	0.59
6:M:486:UNK:O	6:M:490:UNK:N	2.36	0.59
16:e:352:LYS:O	16:e:356:ALA:HB2	2.03	0.59
1:C:318:VAL:O	1:C:322:ALA:N	2.36	0.59
1:B:238:LYS:HA	1:B:252:GLY:H	1.67	0.58
4:K:189:VAL:HA	4:K:213:GLN:HA	1.85	0.58
16:e:78:LEU:HA	16:e:117:ALA:HA	1.85	0.58
21:5:110:UNK:O	21:5:114:UNK:CB	2.52	0.58
1:E:39:VAL:O	1:E:72:ARG:N	2.36	0.58
21:5:109:UNK:O	21:5:113:UNK:CA	2.51	0.58
1:I:154:THR:HA	1:I:171:TYR:HA	1.85	0.58
1:C:241:TYR:N	1:C:249:ILE:O	2.35	0.58
17:g:504:VAL:HA	17:g:515:ALA:O	2.04	0.58
21:6:78:UNK:O	21:6:82:UNK:N	2.37	0.58
1:B:217:ILE:O	1:B:221:ALA:N	2.35	0.57
5:L:52:ASP:O	5:L:56:GLY:N	2.35	0.57
17:h:453:ILE:HA	17:h:474:SER:O	2.03	0.57
1:A:160:SER:O	1:A:303:GLY:N	2.34	0.57
5:L:12:LEU:O	5:L:16:LEU:N	2.36	0.57
11:V:31:SER:HA	11:V:50:GLY:H	1.70	0.57
21:5:240:UNK:HA	21:5:243:UNK:CB	2.34	0.57
1:G:353:PHE:O	1:G:357:TRP:N	2.37	0.57
1:I:156:VAL:HA	1:I:169:PRO:HA	1.84	0.57
2:H:264:PRO:O	2:H:268:GLY:N	2.38	0.57
4:K:144:TYR:N	4:K:155:ILE:O	2.37	0.57
5:L:90:SER:O	5:L:94:ARG:N	2.36	0.57
1:C:20:VAL:HA	1:C:36:PRO:HA	1.87	0.57
1:E:166:HIS:HA	1:E:182:ARG:HA	1.87	0.57
4:K:132:VAL:O	4:K:136:TYR:N	2.36	0.56
16:e:312:ALA:O	16:e:316:PHE:CB	2.53	0.56
1:B:20:VAL:HA	1:B:36:PRO:HA	1.86	0.56
1:B:198:LEU:O	1:B:203:TYR:N	2.35	0.56
1:D:239:ALA:O	1:D:251:ILE:N	2.36	0.56
3:J:143:TYR:O	3:J:168:GLY:N	2.37	0.56
1:D:217:ILE:O	1:D:221:ALA:N	2.38	0.56
7:N:276:UNK:O	7:N:280:UNK:CB	2.54	0.56
16:f:431:GLN:O	16:f:435:ARG:CB	2.53	0.56
3:J:141:CYS:H	3:J:307:GLY:HA3	1.71	0.56
21:5:137:UNK:O	21:5:141:UNK:CA	2.53	0.56
1:C:224:LEU:N	1:C:308:LYS:O	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:217:ILE:O	1:F:221:ALA:N	2.38	0.56
1:B:41:ARG:O	1:B:70:SER:N	2.38	0.56
1:F:20:VAL:HA	1:F:36:PRO:HA	1.87	0.56
1:F:155:GLY:N	1:F:170:ILE:O	2.31	0.56
21:5:174:UNK:O	21:5:178:UNK:CA	2.53	0.56
1:B:156:VAL:HA	1:B:169:PRO:HA	1.87	0.56
5:L:181:LYS:O	5:L:185:GLY:N	2.39	0.56
11:V:33:ASN:H	11:V:50:GLY:HA3	1.71	0.56
21:5:254:UNK:HA	21:5:257:UNK:CB	2.36	0.55
1:C:41:ARG:O	1:C:70:SER:N	2.32	0.55
1:E:216:ALA:O	1:E:220:ARG:CB	2.54	0.55
1:E:156:VAL:HA	1:E:169:PRO:HA	1.87	0.55
10:U:14:GLY:O	10:U:15:ALA:N	2.39	0.55
17:h:309:VAL:HA	17:h:326:THR:HA	1.87	0.55
21:5:58:UNK:O	21:5:62:UNK:CB	2.54	0.55
1:C:217:ILE:O	1:C:221:ALA:N	2.31	0.55
11:V:103:GLN:O	11:V:122:LEU:N	2.32	0.55
1:A:260:GLU:O	1:A:264:ARG:N	2.39	0.55
1:C:241:TYR:O	1:C:249:ILE:N	2.39	0.55
1:C:303:GLY:N	22:C:800:ADP:O1A	2.37	0.55
1:D:154:THR:HA	1:D:171:TYR:HA	1.89	0.54
1:E:162:ASP:O	1:E:188:ARG:N	2.37	0.54
1:G:39:VAL:O	1:G:72:ARG:N	2.38	0.54
1:C:42:PRO:HA	1:C:69:LEU:HA	1.89	0.54
1:G:154:THR:HA	1:G:171:TYR:HA	1.90	0.54
16:e:751:ARG:O	16:e:755:TRP:CB	2.55	0.54
21:6:108:UNK:O	21:6:112:UNK:N	2.39	0.54
1:G:216:ALA:O	1:G:220:ARG:CB	2.55	0.54
2:H:150:GLY:N	2:H:165:ILE:O	2.37	0.54
3:J:19:ASP:N	3:J:26:LYS:O	2.40	0.54
3:J:343:ILE:O	12:Y:493:UNK:N	2.40	0.54
1:A:41:ARG:O	1:A:70:SER:N	2.39	0.54
1:F:293:THR:O	1:F:297:ASN:N	2.40	0.54
16:e:594:ARG:O	16:e:598:ARG:N	2.41	0.54
17:h:548:ASN:N	17:h:562:GLY:O	2.40	0.54
4:K:172:ARG:O	4:K:195:GLN:N	2.38	0.54
1:F:60:PRO:O	1:F:64:GLU:CB	2.56	0.54
12:Y:515:UNK:O	12:Y:527:UNK:N	2.40	0.54
1:E:243:LEU:N	1:E:247:SER:O	2.39	0.54
17:g:470:LEU:HA	17:g:484:SER:HA	1.90	0.54
2:H:241:GLU:HA	2:H:247:VAL:HA	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:g:325:GLY:HA2	17:g:331:ILE:HA	1.90	0.53
1:D:157:VAL:O	1:D:168:VAL:N	2.36	0.53
1:G:241:TYR:N	1:G:249:ILE:O	2.35	0.53
19:l:77:GLU:CB	19:l:92:GLN:O	2.56	0.53
1:A:353:PHE:O	1:A:357:TRP:N	2.42	0.53
1:B:60:PRO:O	1:B:64:GLU:CB	2.57	0.53
1:F:198:LEU:O	1:F:203:TYR:N	2.39	0.53
3:J:315:PHE:O	3:J:319:LEU:CB	2.57	0.53
16:e:76:THR:HA	16:e:119:ILE:HA	1.91	0.53
1:F:216:ALA:O	1:F:220:ARG:CB	2.57	0.53
1:I:263:PHE:HA	1:I:274:GLY:HA3	1.91	0.53
17:h:559:ILE:O	17:h:570:ILE:HA	2.08	0.53
1:C:155:GLY:O	1:C:170:ILE:N	2.38	0.53
21:5:81:UNK:O	21:5:85:UNK:CB	2.57	0.53
1:F:95:SER:O	1:F:99:LEU:N	2.43	0.52
2:H:362:TYR:O	2:H:366:GLY:N	2.40	0.52
3:J:24:PHE:HA	3:J:40:PRO:HA	1.91	0.52
21:5:138:UNK:O	21:5:142:UNK:CA	2.57	0.52
21:6:80:UNK:O	21:6:84:UNK:N	2.42	0.52
1:C:154:THR:HA	1:C:171:TYR:HA	1.90	0.52
21:5:239:UNK:O	21:5:243:UNK:N	2.42	0.52
1:C:156:VAL:O	1:C:299:VAL:N	2.40	0.52
1:F:158:LEU:O	1:F:301:SER:N	2.39	0.52
17:h:455:GLY:HA3	17:h:503:ASP:HA	1.90	0.52
1:C:137:LEU:O	1:C:358:VAL:N	2.43	0.52
1:F:158:LEU:N	1:F:299:VAL:O	2.39	0.52
16:e:120:LYS:HA	16:e:135:LEU:HA	1.92	0.52
16:f:20:ALA:N	16:f:124:VAL:O	2.42	0.52
1:C:238:LYS:HA	1:C:252:GLY:H	1.73	0.52
1:E:153:THR:O	1:E:172:GLU:N	2.43	0.52
1:F:241:TYR:O	1:F:249:ILE:N	2.43	0.52
17:h:289:VAL:O	17:h:300:GLU:N	2.42	0.52
1:G:23:ALA:N	1:G:33:TYR:O	2.41	0.52
1:I:112:GLU:N	1:I:140:SER:O	2.42	0.52
1:B:82:ASP:O	1:B:86:MET:N	2.41	0.52
16:e:748:LYS:O	16:e:752:ASN:CB	2.58	0.52
21:6:229:UNK:O	21:6:233:UNK:N	2.43	0.52
3:J:249:PRO:HA	3:J:255:ILE:HA	1.92	0.52
16:f:723:THR:N	16:f:822:LEU:O	2.43	0.52
1:F:161:GLY:N	1:F:164:VAL:O	2.43	0.51
16:f:79:VAL:HA	16:f:103:ILE:HA	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:f:217:ALA:O	16:f:221:TYR:CB	2.58	0.51
1:C:19:GLY:N	22:C:800:ADP:O1B	2.37	0.51
6:M:241:UNK:O	6:M:245:UNK:CB	2.58	0.51
15:b:52:PRO:O	15:b:56:TYR:CB	2.59	0.51
5:L:157:GLN:O	5:L:166:HIS:N	2.40	0.51
1:D:112:GLU:N	1:D:140:SER:O	2.44	0.51
2:H:8:LEU:N	2:H:102:PRO:O	2.42	0.51
1:I:371:ILE:O	1:I:375:THR:CB	2.59	0.51
1:A:164:VAL:HA	1:A:184:ASP:HA	1.93	0.51
1:B:371:ILE:O	1:B:375:THR:N	2.39	0.51
11:V:144:THR:HA	11:V:156:GLU:HA	1.93	0.51
1:C:157:VAL:O	1:C:168:VAL:N	2.43	0.51
16:e:441:LYS:O	16:e:445:ASN:N	2.43	0.51
1:A:160:SER:H	1:A:302:GLY:HA3	1.76	0.51
1:B:335:GLU:O	1:B:339:SER:N	2.44	0.51
1:D:17:GLY:H	1:D:21:ILE:HA	1.76	0.51
2:H:229:THR:O	2:H:233:SER:N	2.41	0.51
2:H:297:THR:O	2:H:330:ILE:N	2.37	0.51
1:D:95:SER:O	1:D:99:LEU:N	2.43	0.51
4:K:158:ILE:O	4:K:175:SER:N	2.34	0.51
1:E:42:PRO:HA	1:E:69:LEU:HA	1.92	0.50
3:J:16:VAL:O	3:J:90:VAL:N	2.41	0.50
3:J:332:TYR:O	3:J:337:GLY:N	2.41	0.50
1:B:208:SER:O	1:B:212:GLU:N	2.44	0.50
2:H:310:ALA:O	2:H:314:GLN:CB	2.60	0.50
16:f:409:PHE:O	16:f:413:MET:CB	2.59	0.50
1:D:39:VAL:O	1:D:72:ARG:N	2.45	0.50
1:G:45:VAL:O	1:I:175:ALA:N	2.45	0.50
2:H:16:MET:HA	2:H:32:PRO:HA	1.92	0.50
3:J:178:GLN:O	3:J:182:GLN:N	2.44	0.50
3:J:247:ASP:HA	3:J:257:HIS:HA	1.92	0.50
4:K:190:GLY:N	4:K:212:VAL:O	2.44	0.50
1:F:260:GLU:O	1:F:264:ARG:N	2.44	0.50
16:f:66:ARG:O	16:f:70:SER:CB	2.60	0.50
1:A:241:TYR:N	1:A:249:ILE:O	2.42	0.50
1:B:46:ARG:HA	1:D:174:PHE:HA	1.94	0.50
1:C:23:ALA:N	1:C:33:TYR:O	2.44	0.50
7:N:759:UNK:O	7:N:763:UNK:N	2.45	0.50
16:e:784:SER:O	16:e:788:TYR:CB	2.60	0.50
1:B:330:ILE:H	15:c:46:GLU:HA	1.77	0.50
1:F:162:ASP:O	1:F:188:ARG:N	2.37	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:154:ILE:N	4:K:179:PHE:O	2.44	0.50
1:F:39:VAL:O	1:F:72:ARG:N	2.38	0.50
4:K:188:VAL:N	4:K:214:ASP:O	2.45	0.50
1:D:318:VAL:O	1:D:322:ALA:N	2.34	0.49
1:F:154:THR:HA	1:F:171:TYR:HA	1.93	0.49
1:I:110:LEU:O	1:I:140:SER:N	2.43	0.49
3:J:136:ALA:O	3:J:151:ILE:N	2.39	0.49
21:6:79:UNK:O	21:6:83:UNK:CB	2.60	0.49
21:6:206:UNK:O	21:6:210:UNK:N	2.45	0.49
1:A:165:THR:N	1:A:183:ILE:O	2.41	0.49
1:B:90:TRP:O	1:B:94:TYR:N	2.37	0.49
1:E:287:ASP:O	1:E:291:ARG:N	2.44	0.49
6:M:602:UNK:HA	9:Q:38:UNK:HA	1.93	0.49
1:A:93:VAL:O	1:A:99:LEU:N	2.35	0.49
1:I:41:ARG:O	1:I:70:SER:N	2.44	0.49
4:K:256:LYS:HA	4:K:260:ARG:HA	1.94	0.49
16:f:77:VAL:H	16:f:119:ILE:HA	1.78	0.49
21:6:107:UNK:O	21:6:111:UNK:CB	2.60	0.49
1:B:243:LEU:N	1:B:247:SER:O	2.33	0.49
6:M:53:UNK:O	6:M:57:UNK:N	2.45	0.49
7:N:621:UNK:O	7:N:625:UNK:CB	2.60	0.49
1:I:155:GLY:N	1:I:170:ILE:O	2.42	0.49
21:5:261:UNK:CB	21:6:262:UNK:CB	2.91	0.49
1:A:208:SER:O	1:A:212:GLU:N	2.46	0.49
1:B:112:GLU:N	1:B:140:SER:O	2.44	0.49
2:H:259:GLU:O	2:H:263:GLN:N	2.46	0.49
17:g:380:LYS:HA	17:g:396:MET:O	2.13	0.49
17:h:561:VAL:CB	17:h:569:VAL:O	2.61	0.49
21:5:59:UNK:O	21:5:63:UNK:CB	2.60	0.49
21:5:254:UNK:O	21:5:258:UNK:N	2.46	0.49
1:E:76:GLU:N	1:E:79:ILE:O	2.43	0.49
1:G:157:VAL:O	1:G:168:VAL:N	2.40	0.49
1:A:47:VAL:N	1:C:173:GLY:O	2.46	0.48
1:A:335:GLU:O	1:A:339:SER:N	2.47	0.48
1:E:161:GLY:N	1:E:164:VAL:O	2.41	0.48
16:f:38:VAL:O	16:f:42:LEU:CB	2.61	0.48
1:I:208:SER:O	1:I:212:GLU:N	2.46	0.48
11:V:19:GLY:HA3	11:V:39:LYS:H	1.78	0.48
21:5:199:UNK:CB	21:6:200:UNK:CB	2.91	0.48
1:E:93:VAL:O	1:E:99:LEU:N	2.36	0.48
1:E:318:VAL:O	1:E:322:ALA:N	2.39	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:VAL:HA	1:F:169:PRO:HA	1.95	0.48
3:J:76:TYR:O	3:J:81:LEU:N	2.45	0.48
8:P:89:UNK:O	8:P:93:UNK:CB	2.60	0.48
1:A:198:LEU:O	1:A:203:TYR:N	2.46	0.48
1:B:198:LEU:O	1:B:202:GLY:N	2.46	0.48
19:l:22:VAL:N	19:l:31:LYS:O	2.46	0.48
1:B:291:ARG:O	1:B:295:PHE:N	2.46	0.48
17:h:308:ALA:O	17:h:327:TYR:N	2.47	0.48
1:D:110:LEU:O	1:D:140:SER:N	2.42	0.48
5:L:138:GLY:HA3	5:L:146:GLY:H	1.78	0.48
16:e:295:PRO:O	16:e:299:LEU:CB	2.62	0.48
1:C:47:VAL:N	1:E:173:GLY:O	2.36	0.48
1:D:160:SER:H	1:D:302:GLY:HA3	1.78	0.48
1:E:45:VAL:HA	15:b:81:THR:HA	1.95	0.48
1:D:362:GLU:O	1:D:366:ASP:N	2.46	0.48
1:E:90:TRP:O	1:E:94:TYR:N	2.34	0.48
19:k:80:VAL:HA	19:k:88:LEU:O	2.13	0.48
21:6:117:UNK:O	21:6:121:UNK:CB	2.62	0.48
1:C:260:GLU:O	1:C:264:ARG:N	2.46	0.47
1:I:96:LYS:HA	1:I:100:GLN:HA	1.95	0.47
21:5:253:UNK:O	21:5:257:UNK:N	2.47	0.47
2:H:122:ILE:O	2:H:126:THR:CB	2.62	0.47
4:K:153:THR:HA	4:K:180:THR:HA	1.96	0.47
6:M:489:UNK:O	6:M:493:UNK:N	2.47	0.47
16:e:705:LYS:O	16:e:710:ASN:N	2.47	0.47
21:5:173:UNK:O	21:5:177:UNK:CB	2.63	0.47
1:B:332:ALA:H	15:c:44:SER:HA	1.79	0.47
2:H:17:CYS:N	2:H:31:PHE:O	2.46	0.47
15:b:56:TYR:O	15:b:60:LYS:CB	2.62	0.47
11:V:19:GLY:H	11:V:38:GLY:HA2	1.78	0.47
14:a:52:PRO:O	14:a:56:TYR:CB	2.62	0.47
16:e:80:GLU:HA	16:e:115:SER:HA	1.96	0.47
1:C:293:THR:O	1:C:297:ASN:N	2.46	0.47
1:G:243:LEU:C	1:G:245:ASP:H	2.23	0.47
1:I:298:ILE:O	1:I:331:SER:N	2.45	0.47
3:J:44:LYS:HA	3:J:51:PRO:HA	1.97	0.47
5:L:50:ALA:O	5:L:59:TYR:N	2.37	0.47
6:M:59:UNK:O	6:M:63:UNK:CB	2.62	0.47
12:Y:528:UNK:N	12:Y:606:UNK:O	2.48	0.47
16:e:631:GLN:O	16:e:635:MET:CB	2.63	0.47
1:E:198:LEU:O	1:E:203:TYR:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:308:GLY:H	22:J:800:ADP:H5'1	1.80	0.47
5:L:132:ILE:N	5:L:152:HIS:O	2.31	0.47
16:f:145:PRO:O	16:f:149:LEU:CB	2.63	0.47
21:5:254:UNK:CB	21:6:255:UNK:CB	2.92	0.47
21:6:185:UNK:O	21:6:189:UNK:N	2.48	0.47
1:E:240:GLN:HA	1:E:250:GLU:HA	1.95	0.47
2:H:72:GLU:N	2:H:75:ILE:O	2.48	0.47
1:D:156:VAL:HA	1:D:169:PRO:HA	1.97	0.47
1:G:39:VAL:N	1:G:72:ARG:O	2.46	0.47
1:G:373:ARG:O	15:b:70:ASP:HA	2.15	0.47
1:I:331:SER:HA	15:b:19:VAL:HA	1.96	0.47
1:F:238:LYS:HA	1:F:252:GLY:H	1.80	0.46
2:H:7:ALA:HB3	2:H:22:ALA:HB2	1.96	0.46
3:J:377:TYR:O	3:J:381:THR:CB	2.63	0.46
13:Z:1028:UNK:O	13:Z:1032:UNK:CB	2.63	0.46
16:f:118:PHE:HA	16:f:137:VAL:HA	1.97	0.46
1:B:12:VAL:HA	1:B:25:PHE:HA	1.97	0.46
1:B:241:TYR:N	1:B:249:ILE:O	2.36	0.46
1:F:96:LYS:HA	1:F:100:GLN:H	1.79	0.46
1:B:318:VAL:O	1:B:322:ALA:N	2.37	0.46
3:J:67:TYR:O	3:J:71:PHE:CB	2.63	0.46
1:C:332:ALA:O	14:a:48:ILE:N	2.36	0.46
1:E:367:GLY:O	1:E:371:ILE:N	2.44	0.46
1:I:160:SER:O	1:I:303:GLY:N	2.48	0.46
1:E:40:GLY:HA2	1:E:71:ILE:HA	1.98	0.46
5:L:165:ALA:N	5:L:201:GLU:O	2.47	0.46
1:B:91:GLN:O	1:B:95:SER:N	2.49	0.46
1:G:19:GLY:O	1:G:37:ASN:N	2.41	0.46
4:K:194:ILE:N	4:K:208:SER:O	2.47	0.46
8:O:27:UNK:HA	8:O:34:UNK:HA	1.98	0.46
14:a:56:TYR:O	14:a:60:LYS:CB	2.64	0.46
1:C:295:PHE:O	1:C:329:ARG:N	2.44	0.46
1:I:20:VAL:HA	1:I:36:PRO:HA	1.96	0.46
4:K:159:GLU:HA	4:K:174:ARG:HA	1.98	0.46
17:g:548:ASN:N	17:g:562:GLY:O	2.49	0.46
21:6:106:UNK:O	21:6:110:UNK:CB	2.64	0.46
1:C:162:ASP:O	1:C:188:ARG:N	2.44	0.46
1:E:60:PRO:O	1:E:64:GLU:CB	2.64	0.46
3:J:109:LEU:O	3:J:114:GLU:N	2.48	0.46
1:D:127:VAL:O	1:D:132:PHE:N	2.43	0.46
1:D:158:LEU:HA	1:D:167:ALA:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:VAL:O	1:G:24:GLY:N	2.49	0.46
1:I:330:ILE:N	15:b:20:TYR:O	2.37	0.45
3:J:344:HIS:HA	12:Y:492:UNK:HA	1.99	0.45
21:6:115:UNK:O	21:6:119:UNK:N	2.49	0.45
1:B:48:MET:H	1:D:173:GLY:HA3	1.81	0.45
1:F:96:LYS:O	1:F:100:GLN:N	2.50	0.45
1:I:160:SER:O	1:I:304:SER:N	2.38	0.45
11:V:143:PHE:O	11:V:157:LEU:N	2.43	0.45
12:Y:442:UNK:O	12:Y:446:UNK:N	2.49	0.45
16:e:761:PRO:O	16:e:765:VAL:N	2.49	0.45
12:Y:596:UNK:O	12:Y:601:UNK:N	2.49	0.45
17:g:478:TRP:O	17:g:497:ASN:N	2.47	0.45
1:B:170:ILE:HA	1:B:175:ALA:HA	1.97	0.45
17:h:409:THR:N	17:h:424:GLY:O	2.48	0.45
1:E:15:ASP:O	1:E:22:LYS:N	2.38	0.45
1:I:39:VAL:O	1:I:72:ARG:N	2.35	0.45
16:e:405:ALA:O	16:e:409:PHE:N	2.45	0.45
16:e:685:ASP:O	16:e:689:PHE:CB	2.64	0.45
1:F:238:LYS:HA	1:F:252:GLY:N	2.32	0.45
1:E:12:VAL:HA	1:E:25:PHE:HA	1.97	0.45
3:J:342:ARG:HA	12:Y:494:UNK:HA	1.98	0.45
10:U:61:LEU:O	10:U:96:SER:N	2.46	0.45
1:A:239:ALA:O	1:A:251:ILE:N	2.50	0.45
1:E:145:LEU:O	1:E:343:GLY:HA3	2.17	0.45
1:I:158:LEU:N	1:I:299:VAL:O	2.47	0.45
3:J:118:VAL:O	3:J:373:VAL:N	2.50	0.45
11:V:121:VAL:O	11:V:140:VAL:N	2.49	0.45
21:6:152:UNK:O	21:6:156:UNK:CB	2.64	0.45
1:G:14:ILE:HA	1:G:23:ALA:HA	1.99	0.45
12:Y:181:UNK:H2	12:Y:285:UNK:HA	1.81	0.45
1:G:155:GLY:N	1:G:170:ILE:O	2.51	0.44
5:L:166:HIS:HA	5:L:200:ASP:HA	1.99	0.44
4:K:97:LYS:N	4:K:106:SER:O	2.50	0.44
10:U:29:ILE:HA	10:U:50:ILE:H	1.82	0.44
16:f:193:LEU:O	16:f:197:GLN:CB	2.66	0.44
16:f:376:ARG:O	16:f:380:LEU:CB	2.65	0.44
1:D:287:ASP:O	1:D:291:ARG:N	2.48	0.44
4:K:174:ARG:N	4:K:193:LYS:O	2.41	0.44
1:A:240:GLN:HA	1:A:250:GLU:HA	2.00	0.44
1:G:46:ARG:HA	1:I:175:ALA:H	1.83	0.44
17:h:430:VAL:O	17:h:445:MET:HA	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:THR:O	1:D:172:GLU:N	2.51	0.44
1:D:330:ILE:N	15:c:20:TYR:O	2.43	0.44
1:F:318:VAL:O	1:F:322:ALA:N	2.36	0.44
1:G:162:ASP:H	22:G:800:ADP:PB	2.41	0.44
2:H:292:ASP:O	2:H:296:ASN:N	2.47	0.44
8:O:26:UNK:O	8:O:35:UNK:N	2.50	0.44
5:L:149:ASP:N	5:L:174:MET:O	2.43	0.44
1:D:145:LEU:O	1:D:343:GLY:HA3	2.18	0.44
17:g:428:GLY:N	17:g:451:GLY:O	2.51	0.44
21:6:153:UNK:O	21:6:157:UNK:CB	2.66	0.44
1:A:207:SER:O	1:A:211:PHE:N	2.51	0.43
1:C:198:LEU:O	1:C:203:TYR:N	2.42	0.43
17:g:513:LEU:HA	17:g:526:TRP:O	2.18	0.43
21:5:197:UNK:O	21:5:201:UNK:N	2.51	0.43
6:M:201:UNK:O	6:M:205:UNK:N	2.51	0.43
17:h:553:THR:N	17:h:558:GLU:O	2.51	0.43
1:F:18:SER:N	22:F:800:ADP:O2B	2.48	0.43
3:J:22:GLU:N	22:J:800:ADP:O1B	2.51	0.43
12:Y:517:UNK:N	12:Y:525:UNK:O	2.51	0.43
1:B:160:SER:O	1:B:303:GLY:N	2.51	0.43
1:D:12:VAL:N	1:D:107:PRO:O	2.38	0.43
1:D:41:ARG:O	1:D:70:SER:N	2.28	0.43
1:D:216:ALA:O	1:D:220:ARG:CB	2.67	0.43
1:F:371:ILE:O	1:F:375:THR:N	2.52	0.43
2:H:160:THR:O	2:H:178:LEU:N	2.52	0.43
16:e:352:LYS:O	16:e:356:ALA:CB	2.66	0.43
4:K:143:VAL:HA	4:K:156:ALA:HA	2.00	0.43
11:V:86:HIS:O	11:V:104:ILE:N	2.41	0.43
12:Y:597:UNK:O	12:Y:601:UNK:N	2.44	0.43
17:h:526:TRP:CB	17:h:536:THR:H	2.30	0.43
6:M:1:UNK:N	8:O:41:UNK:O	2.52	0.43
7:N:605:UNK:N	9:R:38:UNK:O	2.52	0.43
3:J:185:VAL:N	3:J:194:SER:O	2.51	0.43
1:F:157:VAL:O	1:F:168:VAL:N	2.38	0.43
16:e:843:PHE:O	16:e:847:VAL:CB	2.67	0.43
16:e:852:ILE:O	16:e:856:LYS:C	2.62	0.43
2:H:317:ILE:O	2:H:321:ALA:N	2.51	0.43
17:g:464:ALA:HB1	17:g:580:PRO:HA	2.00	0.43
17:h:558:GLU:HA	17:h:571:TYR:O	2.18	0.43
1:G:162:ASP:N	22:G:800:ADP:O3A	2.52	0.42
17:g:455:GLY:HA3	17:g:503:ASP:HA	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:ILE:HA	1:I:23:ALA:HA	2.01	0.42
11:V:145:VAL:O	11:V:154:SER:N	2.52	0.42
1:A:18:SER:H	22:A:800:ADP:PB	2.42	0.42
1:B:293:THR:O	1:B:297:ASN:N	2.53	0.42
1:E:260:GLU:O	1:E:264:ARG:N	2.52	0.42
8:O:28:UNK:N	8:O:33:UNK:O	2.52	0.42
1:E:338:TYR:O	1:E:342:ILE:N	2.37	0.42
1:I:15:ASP:N	1:I:22:LYS:O	2.49	0.42
1:I:19:GLY:H	22:I:800:ADP:PB	2.42	0.42
21:5:196:UNK:O	21:5:200:UNK:N	2.52	0.42
21:5:200:UNK:O	21:5:204:UNK:CB	2.68	0.42
21:5:200:UNK:O	21:5:204:UNK:N	2.53	0.42
1:B:13:VAL:N	1:B:24:GLY:O	2.50	0.42
1:F:90:TRP:O	1:F:94:TYR:N	2.36	0.42
4:K:98:PHE:HA	4:K:105:ALA:HA	2.02	0.42
16:e:772:ASN:HA	17:g:405:ALA:HB3	2.01	0.42
16:f:81:ARG:HA	16:f:101:TYR:HA	2.00	0.42
3:J:23:ALA:N	22:J:800:ADP:O1B	2.31	0.42
16:f:527:TYR:O	16:f:531:LYS:CB	2.67	0.42
1:E:295:PHE:O	1:E:329:ARG:N	2.49	0.42
21:6:228:UNK:O	21:6:232:UNK:CB	2.68	0.42
1:B:160:SER:N	1:B:302:GLY:HA3	2.29	0.41
3:J:71:PHE:O	3:J:75:LEU:CB	2.68	0.41
1:D:76:GLU:N	1:D:79:ILE:O	2.49	0.41
2:H:91:TYR:HA	2:H:95:ARG:HA	2.00	0.41
9:Q:34:UNK:O	9:Q:38:UNK:N	2.54	0.41
17:g:308:ALA:O	17:g:327:TYR:N	2.53	0.41
17:g:380:LYS:HA	17:g:397:GLU:HA	2.01	0.41
2:H:131:ALA:HA	2:H:358:SER:HA	2.02	0.41
1:I:166:HIS:HA	1:I:182:ARG:HA	2.02	0.41
1:D:162:ASP:C	1:D:186:ALA:HB3	2.46	0.41
1:I:13:VAL:O	1:I:24:GLY:N	2.42	0.41
4:K:183:PRO:HA	4:K:184:PRO:HA	1.74	0.41
10:U:143:ILE:HA	10:U:150:ARG:O	2.21	0.41
1:B:127:VAL:O	1:B:132:PHE:N	2.50	0.41
1:E:207:SER:O	1:E:211:PHE:N	2.49	0.41
1:I:93:VAL:O	1:I:99:LEU:N	2.50	0.41
16:f:81:ARG:N	16:f:115:SER:HA	2.36	0.41
1:G:91:GLN:O	1:G:95:SER:N	2.54	0.41
1:A:90:TRP:O	1:A:94:TYR:N	2.48	0.41
1:C:332:ALA:HB3	14:a:47:HIS:HA	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:MET:HA	1:D:80:VAL:HA	2.03	0.41
1:E:137:LEU:O	1:E:358:VAL:N	2.54	0.41
1:E:154:THR:HA	1:E:171:TYR:HA	2.02	0.41
1:F:304:SER:HA	22:F:800:ADP:N3	2.36	0.41
12:Y:310:UNK:N	12:Y:314:UNK:O	2.54	0.41
16:f:373:PRO:O	16:f:377:ALA:N	2.46	0.41
17:h:479:THR:HA	17:h:495:GLU:HA	2.02	0.41
1:B:128:PHE:O	1:B:134:VAL:N	2.54	0.41
6:M:435:UNK:O	6:M:439:UNK:CB	2.69	0.41
16:f:81:ARG:H	16:f:115:SER:HA	1.86	0.41
17:g:379:GLY:O	17:g:398:LEU:N	2.47	0.41
17:h:240:SER:N	17:h:572:ASP:O	2.54	0.41
1:B:19:GLY:N	22:B:800:ADP:O1A	2.35	0.40
1:C:112:GLU:N	1:C:140:SER:O	2.54	0.40
1:C:162:ASP:C	1:C:186:ALA:HB3	2.46	0.40
1:I:60:PRO:O	1:I:64:GLU:CB	2.70	0.40
3:J:309:THR:N	22:J:800:ADP:O4'	2.54	0.40
21:6:239:UNK:CA	21:6:242:UNK:CB	2.93	0.40
1:D:298:ILE:O	1:D:331:SER:N	2.54	0.40
1:E:274:GLY:O	1:E:277:GLU:N	2.48	0.40
4:K:141:CYS:HA	4:K:158:ILE:HA	2.02	0.40
11:V:173:TYR:O	11:V:177:LEU:CB	2.69	0.40
17:h:257:SER:N	17:h:272:SER:O	2.44	0.40
21:5:108:UNK:O	21:5:112:UNK:CB	2.69	0.40
1:D:42:PRO:HA	1:D:69:LEU:HA	2.03	0.40
1:F:26:ALA:HA	1:F:345:SER:HA	2.03	0.40
1:I:160:SER:N	1:I:301:SER:O	2.52	0.40
17:g:468:SER:O	17:g:470:LEU:N	2.54	0.40
17:h:382:CYS:HA	17:h:395:SER:HA	2.03	0.40
21:5:201:UNK:O	21:5:205:UNK:CA	2.69	0.40
9:Q:6:UNK:HA	9:Q:46:UNK:HA	2.03	0.40
12:Y:508:UNK:N	12:Y:534:UNK:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/376 (98%)	319 (87%)	46 (12%)	3 (1%)	16	54
1	B	368/376 (98%)	321 (87%)	45 (12%)	2 (0%)	24	63
1	C	368/376 (98%)	325 (88%)	40 (11%)	3 (1%)	16	54
1	D	368/376 (98%)	316 (86%)	49 (13%)	3 (1%)	16	54
1	E	368/376 (98%)	321 (87%)	45 (12%)	2 (0%)	24	63
1	F	368/376 (98%)	316 (86%)	50 (14%)	2 (0%)	24	63
1	G	368/376 (98%)	325 (88%)	40 (11%)	3 (1%)	16	54
1	I	368/376 (98%)	333 (90%)	30 (8%)	5 (1%)	9	40
2	H	368/375 (98%)	326 (89%)	42 (11%)	0	100	100
3	J	363/390 (93%)	310 (85%)	53 (15%)	0	100	100
4	K	276/286 (96%)	236 (86%)	38 (14%)	2 (1%)	18	56
5	L	267/272 (98%)	237 (89%)	30 (11%)	0	100	100
10	U	169/190 (89%)	126 (75%)	41 (24%)	2 (1%)	10	44
11	V	163/182 (90%)	126 (77%)	36 (22%)	1 (1%)	21	59
14	a	48/68 (71%)	39 (81%)	9 (19%)	0	100	100
15	b	71/89 (80%)	55 (78%)	16 (22%)	0	100	100
15	c	31/89 (35%)	22 (71%)	9 (29%)	0	100	100
15	d	22/89 (25%)	18 (82%)	4 (18%)	0	100	100
16	e	777/1455 (53%)	694 (89%)	81 (10%)	2 (0%)	36	72
16	f	822/1455 (56%)	750 (91%)	71 (9%)	1 (0%)	48	83
17	g	393/612 (64%)	341 (87%)	52 (13%)	0	100	100
17	h	397/612 (65%)	328 (83%)	67 (17%)	2 (0%)	24	63
18	j	13/492 (3%)	11 (85%)	2 (15%)	0	100	100
19	k	91/96 (95%)	75 (82%)	16 (18%)	0	100	100
19	l	91/96 (95%)	85 (93%)	6 (7%)	0	100	100
All	All	7306/9856 (74%)	6355 (87%)	918 (13%)	33 (0%)	26	63

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	K	279	ILE
10	U	79	PRO
17	h	491	LEU
1	A	187	GLY
1	B	187	GLY
1	F	187	GLY
1	I	275	ILE
16	f	225	GLU
1	A	55	ASP
1	B	228	PRO
1	C	228	PRO
1	E	228	PRO
1	F	228	PRO
1	G	228	PRO
1	I	333	PRO
1	A	228	PRO
1	C	172	GLU
1	D	228	PRO
1	D	275	ILE
1	G	353	PHE
1	I	172	GLU
1	I	187	GLY
16	e	310	PHE
16	e	642	PRO
17	h	490	PRO
4	K	280	GLY
1	C	187	GLY
1	D	187	GLY
1	E	275	ILE
1	G	187	GLY
11	V	84	PRO
1	I	74	PRO
10	U	78	GLU

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	ADP	F	800	-	28,29,29	1.40	5 (17%)	43,45,45	1.95	12 (27%)
22	ADP	G	800	-	28,29,29	1.39	5 (17%)	43,45,45	1.87	11 (25%)
23	ATP	H	401	-	32,33,33	1.35	6 (18%)	48,52,52	1.82	10 (20%)
22	ADP	A	800	-	28,29,29	1.37	4 (14%)	43,45,45	1.89	11 (25%)
22	ADP	B	800	-	28,29,29	1.43	5 (17%)	43,45,45	2.01	15 (34%)
22	ADP	C	800	-	28,29,29	1.39	5 (17%)	43,45,45	2.14	14 (32%)
22	ADP	I	800	-	28,29,29	1.40	5 (17%)	43,45,45	1.73	10 (23%)
22	ADP	D	800	-	28,29,29	1.36	5 (17%)	43,45,45	1.99	14 (32%)
22	ADP	J	800	-	28,29,29	1.45	4 (14%)	43,45,45	1.94	14 (32%)
22	ADP	E	800	-	28,29,29	1.46	5 (17%)	43,45,45	2.02	15 (34%)

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
22	ADP	F	800	-	-	2/16/32/32	0/3/3/3
22	ADP	G	800	-	-	1/16/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	ATP	H	401	-	-	1/22/38/38	0/3/3/3
22	ADP	A	800	-	-	3/16/32/32	0/3/3/3
22	ADP	B	800	-	-	1/16/32/32	0/3/3/3
22	ADP	C	800	-	-	6/16/32/32	0/3/3/3
22	ADP	I	800	-	-	1/16/32/32	0/3/3/3
22	ADP	D	800	-	-	3/16/32/32	0/3/3/3
22	ADP	J	800	-	-	5/16/32/32	0/3/3/3
22	ADP	E	800	-	-	6/16/32/32	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	800	ADP	C5-C4	4.52	1.47	1.39
22	F	800	ADP	C5-C4	4.37	1.46	1.39
23	H	401	ATP	C5-C4	4.35	1.46	1.39
22	E	800	ADP	C5-C4	4.29	1.46	1.39
22	G	800	ADP	C5-C4	4.27	1.46	1.39
22	I	800	ADP	C5-C4	4.22	1.46	1.39
22	B	800	ADP	C5-C4	4.17	1.46	1.39
22	J	800	ADP	C5-C4	4.15	1.46	1.39
22	C	800	ADP	C5-C4	4.08	1.46	1.39
22	D	800	ADP	C5-C4	3.85	1.46	1.39
22	B	800	ADP	C4-N9	-3.13	1.31	1.37
22	J	800	ADP	C4-N9	-3.00	1.31	1.37
22	E	800	ADP	C4-N9	-2.91	1.31	1.37
22	I	800	ADP	C4-N9	-2.86	1.31	1.37
22	D	800	ADP	C4-N9	-2.81	1.31	1.37
22	E	800	ADP	C5-C6	2.66	1.48	1.41
22	G	800	ADP	C5-C6	2.66	1.48	1.41
23	H	401	ATP	C5-C6	2.66	1.48	1.41
22	A	800	ADP	C5-C6	2.63	1.48	1.41
22	I	800	ADP	C5-C6	2.63	1.48	1.41
22	B	800	ADP	C5-C6	2.63	1.48	1.41
22	F	800	ADP	C5-C6	2.58	1.48	1.41
23	H	401	ATP	C5-N7	-2.57	1.34	1.39
22	C	800	ADP	C4-N9	-2.57	1.32	1.37
22	B	800	ADP	C8-N7	2.56	1.36	1.31
22	G	800	ADP	C4-N9	-2.56	1.32	1.37
22	E	800	ADP	C5-N7	-2.52	1.34	1.39
22	I	800	ADP	C5-N7	-2.51	1.34	1.39
22	E	800	ADP	C8-N7	2.49	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	J	800	ADP	C5-N7	-2.49	1.34	1.39
22	F	800	ADP	C5-N7	-2.48	1.34	1.39
22	C	800	ADP	C5-N7	-2.46	1.34	1.39
22	D	800	ADP	C5-C6	2.43	1.47	1.41
22	A	800	ADP	C5-N7	-2.42	1.34	1.39
22	C	800	ADP	C5-C6	2.41	1.47	1.41
22	G	800	ADP	C5-N7	-2.38	1.34	1.39
22	G	800	ADP	C8-N7	2.35	1.36	1.31
22	D	800	ADP	C8-N7	2.30	1.36	1.31
22	F	800	ADP	C8-N7	2.28	1.36	1.31
22	I	800	ADP	C8-N7	2.28	1.36	1.31
23	H	401	ATP	C4-N9	-2.27	1.33	1.37
22	J	800	ADP	C5-C6	2.25	1.47	1.41
22	A	800	ADP	C8-N7	2.23	1.36	1.31
22	D	800	ADP	C5-N7	-2.23	1.35	1.39
22	C	800	ADP	C8-N7	2.22	1.35	1.31
22	B	800	ADP	C5-N7	-2.19	1.35	1.39
22	F	800	ADP	C4-N9	-2.15	1.33	1.37
23	H	401	ATP	C8-N9	-2.14	1.33	1.37
23	H	401	ATP	C8-N7	2.04	1.35	1.31

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	800	ADP	C5-C4-N3	-6.05	118.39	126.72
23	H	401	ATP	C5-C4-N3	-6.00	118.45	126.72
22	A	800	ADP	C5-C4-N3	-6.00	118.46	126.72
22	G	800	ADP	C5-C4-N3	-5.30	119.41	126.72
22	E	800	ADP	C5-C4-N3	-5.21	119.54	126.72
22	A	800	ADP	N3-C4-N9	4.94	135.57	127.17
23	H	401	ATP	N3-C4-N9	4.93	135.55	127.17
22	C	800	ADP	C5-C4-N3	-4.90	119.97	126.72
22	D	800	ADP	C5-C4-N3	-4.84	120.06	126.72
22	C	800	ADP	C4'-O4'-C1'	-4.77	98.94	109.47
22	I	800	ADP	C5-C4-N3	-4.74	120.19	126.72
22	C	800	ADP	C2'-C1'-N9	4.72	125.03	113.30
22	B	800	ADP	C4-C5-N7	-4.55	105.38	110.58
22	B	800	ADP	C2'-C1'-N9	-4.55	102.01	113.30
22	J	800	ADP	C5-C4-N3	-4.46	120.57	126.72
22	B	800	ADP	C5-C4-N3	-4.35	120.73	126.72
22	F	800	ADP	N3-C4-N9	4.25	134.40	127.17
22	F	800	ADP	C4-C5-N7	-4.18	105.81	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	E	800	ADP	C4-C5-N7	-4.16	105.82	110.58
22	I	800	ADP	C4-C5-N7	-4.07	105.92	110.58
22	C	800	ADP	N3-C4-N9	4.06	134.07	127.17
22	J	800	ADP	C4-N9-C8	3.98	109.92	105.74
22	G	800	ADP	C4-C5-N7	-3.97	106.05	110.58
22	J	800	ADP	N3-C4-N9	3.94	133.87	127.17
22	D	800	ADP	C4-N9-C8	3.90	109.84	105.74
22	D	800	ADP	N3-C4-N9	3.81	133.65	127.17
22	G	800	ADP	N3-C4-N9	3.76	133.56	127.17
23	H	401	ATP	C2-N3-C4	3.73	120.93	111.83
22	J	800	ADP	N3-C2-N1	-3.69	123.00	128.58
22	F	800	ADP	C2-N3-C4	3.67	120.79	111.83
22	A	800	ADP	C2-N3-C4	3.67	120.78	111.83
22	C	800	ADP	N3-C2-N1	-3.64	123.07	128.58
22	C	800	ADP	C4-N9-C8	3.61	109.53	105.74
22	D	800	ADP	C4-C5-N7	-3.61	106.45	110.58
22	C	800	ADP	C2-N3-C4	3.56	120.52	111.83
22	E	800	ADP	C2-N3-C4	3.50	120.39	111.83
22	F	800	ADP	C5'-C4'-C3'	-3.50	102.61	115.21
22	D	800	ADP	C2-N3-C4	3.42	120.17	111.83
23	H	401	ATP	C4-C5-N7	-3.41	106.68	110.58
22	A	800	ADP	C4-C5-N7	-3.38	106.72	110.58
22	E	800	ADP	N3-C4-N9	3.38	132.91	127.17
22	G	800	ADP	C2-N3-C4	3.33	119.95	111.83
22	C	800	ADP	C4-C5-N7	-3.28	106.83	110.58
22	J	800	ADP	C2-N3-C4	3.28	119.83	111.83
22	E	800	ADP	C5'-C4'-C3'	-3.27	103.44	115.21
22	B	800	ADP	O4'-C1'-N9	3.17	114.17	108.09
22	B	800	ADP	C6-C5-N7	3.15	138.16	132.09
22	I	800	ADP	N3-C4-N9	3.14	132.50	127.17
22	D	800	ADP	O4'-C1'-N9	3.13	114.10	108.09
23	H	401	ATP	C4-N9-C8	3.10	108.99	105.74
22	A	800	ADP	C4-N9-C8	3.10	108.99	105.74
22	D	800	ADP	N3-C2-N1	-3.03	124.00	128.58
22	J	800	ADP	C2'-C1'-N9	-2.99	105.87	113.30
22	I	800	ADP	C2-N3-C4	2.98	119.10	111.83
23	H	401	ATP	N3-C2-N1	-2.96	124.09	128.58
22	J	800	ADP	O3A-PB-O1B	-2.96	95.48	111.04
22	G	800	ADP	C2'-C1'-N9	-2.91	106.08	113.30
22	J	800	ADP	O3'-C3'-C2'	-2.90	102.52	111.82
22	B	800	ADP	C2-N3-C4	2.90	118.92	111.83
22	D	800	ADP	N9-C8-N7	-2.89	109.84	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	800	ADP	C4-N9-C1'	-2.86	119.94	126.63
22	J	800	ADP	C4-C5-N7	-2.86	107.31	110.58
22	E	800	ADP	C6-C5-N7	2.85	137.59	132.09
22	B	800	ADP	C4-N9-C8	2.85	108.73	105.74
22	F	800	ADP	C5-N7-C8	2.81	107.86	103.45
22	D	800	ADP	C6-C5-N7	2.78	137.45	132.09
22	B	800	ADP	C5-N7-C8	2.77	107.80	103.45
22	I	800	ADP	C6-C5-N7	2.75	137.39	132.09
22	G	800	ADP	C4-N9-C8	2.74	108.62	105.74
22	A	800	ADP	C2'-C1'-N9	-2.74	106.50	113.30
22	A	800	ADP	N3-C2-N1	-2.68	124.52	128.58
22	D	800	ADP	O3'-C3'-C2'	-2.68	103.23	111.82
22	G	800	ADP	C5-N7-C8	2.66	107.64	103.45
22	I	800	ADP	C5-N7-C8	2.66	107.63	103.45
22	E	800	ADP	N3-C2-N1	-2.66	124.56	128.58
22	B	800	ADP	O3B-PB-O2B	2.63	117.65	107.80
22	D	800	ADP	C5-N7-C8	2.63	107.58	103.45
22	C	800	ADP	N9-C8-N7	-2.62	110.22	113.94
22	J	800	ADP	C2-N1-C6	2.59	122.99	118.73
22	B	800	ADP	N9-C8-N7	-2.59	110.26	113.94
22	I	800	ADP	C4-N9-C8	2.58	108.45	105.74
22	A	800	ADP	C5-N7-C8	2.57	107.50	103.45
22	E	800	ADP	C5-N7-C8	2.57	107.48	103.45
22	G	800	ADP	C6-C5-N7	2.54	136.99	132.09
22	B	800	ADP	N3-C4-N9	2.54	131.48	127.17
22	D	800	ADP	C4-N9-C1'	-2.53	120.71	126.63
22	F	800	ADP	N3-C2-N1	-2.50	124.79	128.58
22	G	800	ADP	N3-C2-N1	-2.50	124.80	128.58
22	C	800	ADP	C5-N7-C8	2.49	107.37	103.45
22	E	800	ADP	O3B-PB-O3A	-2.48	96.31	104.64
22	C	800	ADP	C6-C5-N7	2.48	136.87	132.09
23	H	401	ATP	C5-N7-C8	2.47	107.33	103.45
22	E	800	ADP	O3A-PA-O1A	-2.46	103.30	110.70
22	F	800	ADP	C6-C5-N7	2.46	136.83	132.09
22	E	800	ADP	C4-N9-C8	2.45	108.31	105.74
22	J	800	ADP	N9-C8-N7	-2.42	110.50	113.94
22	E	800	ADP	O5'-C5'-C4'	2.38	117.11	108.99
22	I	800	ADP	O3B-PB-O2B	2.34	116.56	107.80
22	G	800	ADP	N9-C8-N7	-2.31	110.67	113.94
22	I	800	ADP	N9-C8-N7	-2.30	110.67	113.94
23	H	401	ATP	C3'-C2'-C1'	2.30	105.82	101.46
22	J	800	ADP	C6-C5-N7	2.25	136.42	132.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	F	800	ADP	C4-N9-C8	2.23	108.08	105.74
22	D	800	ADP	C3'-C2'-C1'	-2.22	97.27	101.46
22	A	800	ADP	C6-C5-N7	2.20	136.32	132.09
22	B	800	ADP	O2A-PA-O1A	2.19	122.66	112.44
22	A	800	ADP	N9-C8-N7	-2.19	110.82	113.94
22	E	800	ADP	N9-C8-N7	-2.18	110.84	113.94
22	B	800	ADP	O5'-C5'-C4'	-2.18	101.56	108.99
22	A	800	ADP	O3B-PB-O2B	2.17	115.93	107.80
22	C	800	ADP	O3'-C3'-C4'	-2.16	104.87	111.08
22	C	800	ADP	C2-N1-C6	2.16	122.28	118.73
22	J	800	ADP	C5-N7-C8	2.15	106.83	103.45
22	E	800	ADP	O2A-PA-O1A	2.15	122.43	112.44
22	J	800	ADP	O3B-PB-O2B	2.13	115.80	107.80
22	D	800	ADP	C4'-O4'-C1'	-2.13	104.77	109.47
22	C	800	ADP	O3B-PB-O2B	2.11	115.71	107.80
22	B	800	ADP	N3-C2-N1	-2.10	125.40	128.58
23	H	401	ATP	N9-C8-N7	-2.07	111.00	113.94
22	F	800	ADP	O2B-PB-O1B	2.07	118.91	110.83
23	H	401	ATP	C6-C5-N7	2.07	136.08	132.09
22	E	800	ADP	O3B-PB-O2B	2.05	115.50	107.80
22	F	800	ADP	N9-C8-N7	-2.04	111.04	113.94
22	I	800	ADP	N3-C2-N1	-2.03	125.51	128.58
22	G	800	ADP	C3'-C2'-C1'	2.01	105.27	101.46
22	F	800	ADP	C3'-C2'-C1'	2.00	105.25	101.46

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	800	ADP	O4'-C4'-C5'-O5'
22	A	800	ADP	C3'-C4'-C5'-O5'
22	C	800	ADP	C5'-O5'-PA-O3A
22	C	800	ADP	C3'-C4'-C5'-O5'
22	D	800	ADP	O4'-C4'-C5'-O5'
22	D	800	ADP	C3'-C4'-C5'-O5'
22	J	800	ADP	C5'-O5'-PA-O3A
22	E	800	ADP	C3'-C4'-C5'-O5'
22	J	800	ADP	O4'-C4'-C5'-O5'
22	J	800	ADP	C3'-C4'-C5'-O5'
22	C	800	ADP	O4'-C4'-C5'-O5'
22	E	800	ADP	O4'-C4'-C5'-O5'
22	E	800	ADP	C2'-C1'-N9-C8

Continued on next page...

Continued from previous page...

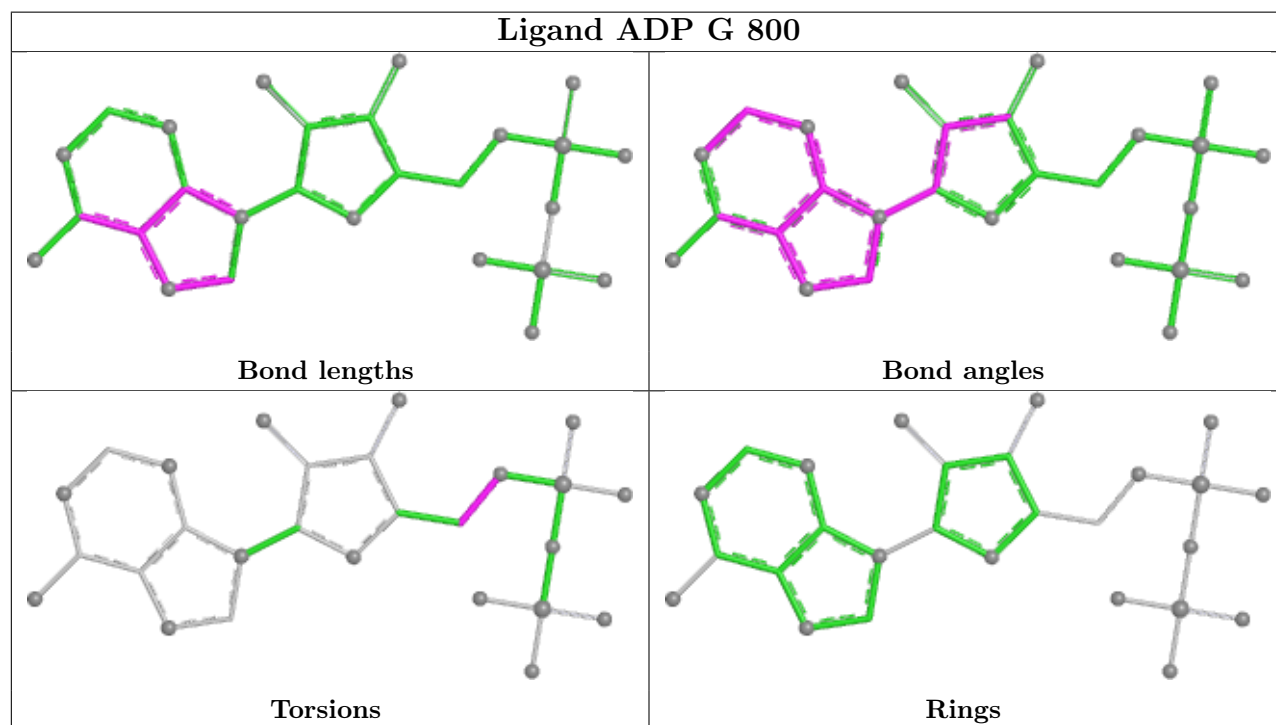
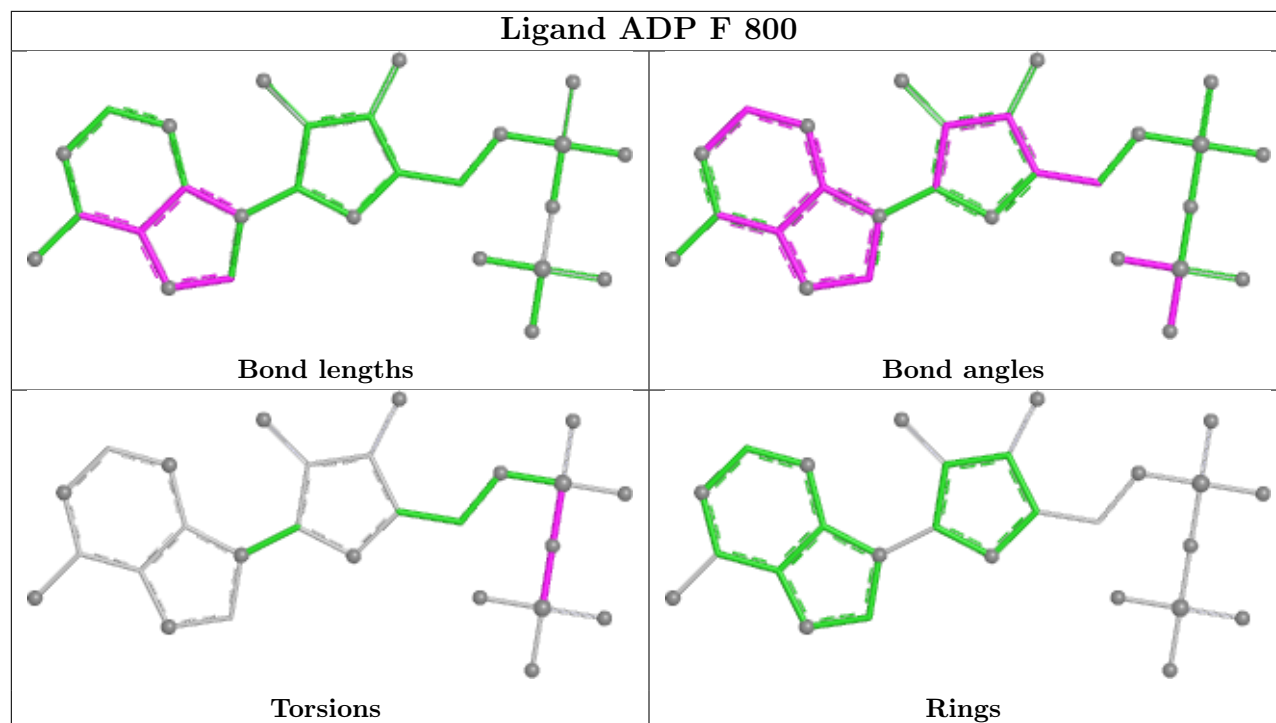
Mol	Chain	Res	Type	Atoms
22	C	800	ADP	PB-O3A-PA-O2A
22	A	800	ADP	C5'-O5'-PA-O1A
22	C	800	ADP	C5'-O5'-PA-O1A
23	H	401	ATP	C5'-O5'-PA-O3A
22	D	800	ADP	C4'-C5'-O5'-PA
22	E	800	ADP	C4'-C5'-O5'-PA
22	J	800	ADP	C4'-C5'-O5'-PA
22	F	800	ADP	PA-O3A-PB-O3B
22	G	800	ADP	C4'-C5'-O5'-PA
22	I	800	ADP	C4'-C5'-O5'-PA
22	E	800	ADP	O4'-C1'-N9-C8
22	J	800	ADP	C2'-C1'-N9-C8
22	E	800	ADP	C2'-C1'-N9-C4
22	B	800	ADP	C3'-C4'-C5'-O5'
22	C	800	ADP	PB-O3A-PA-O1A
22	F	800	ADP	PB-O3A-PA-O2A

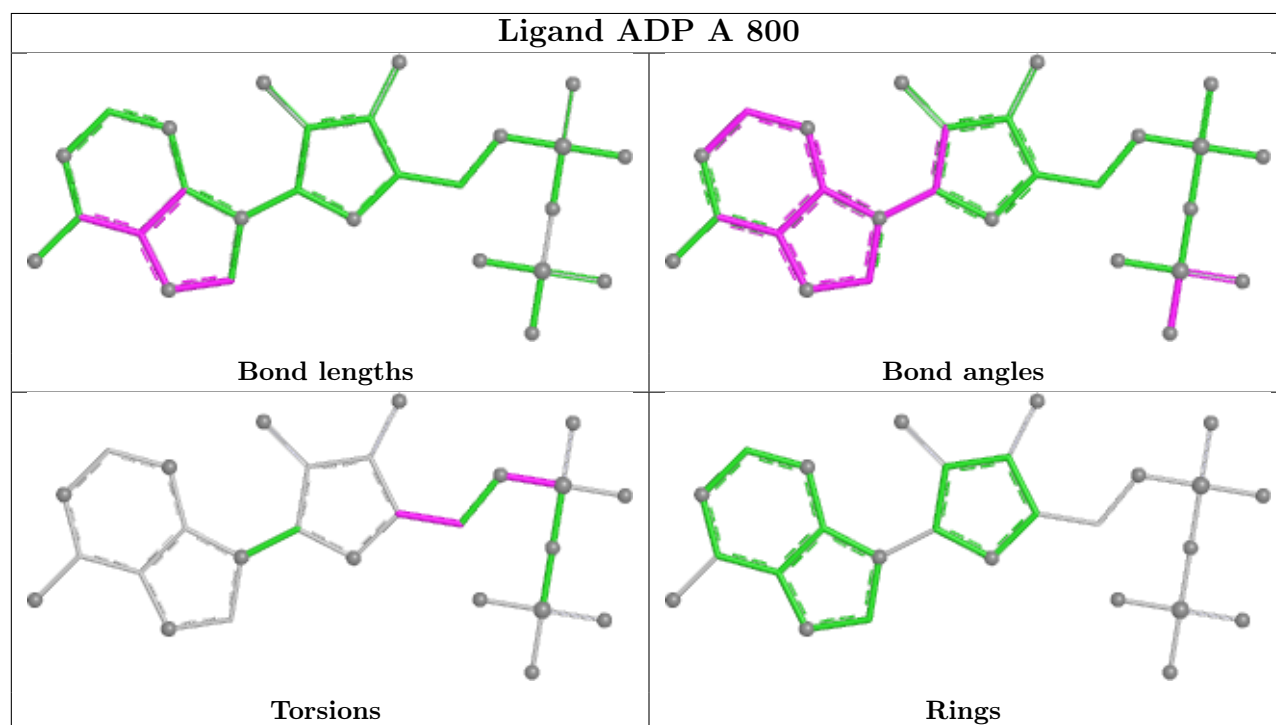
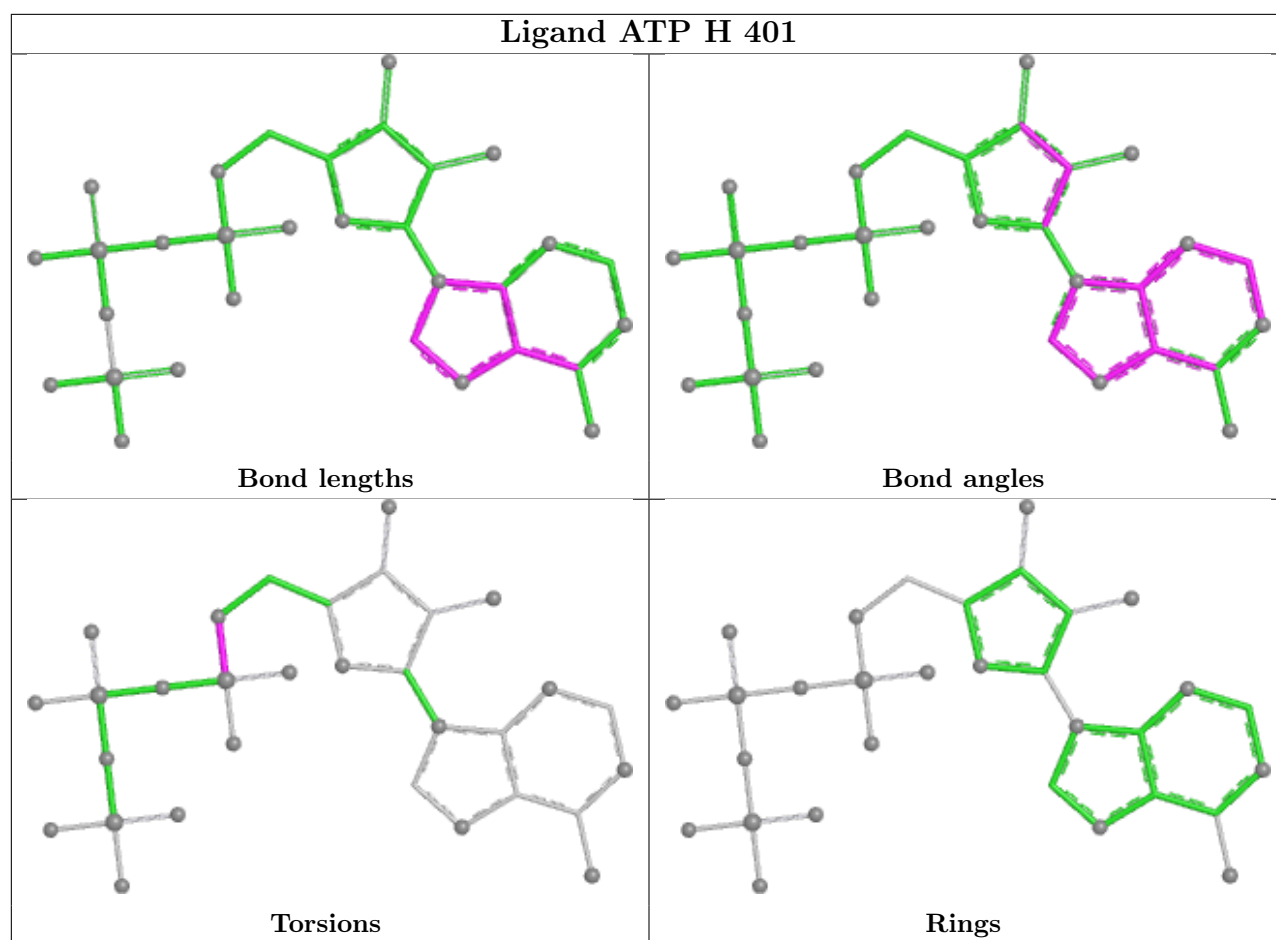
There are no ring outliers.

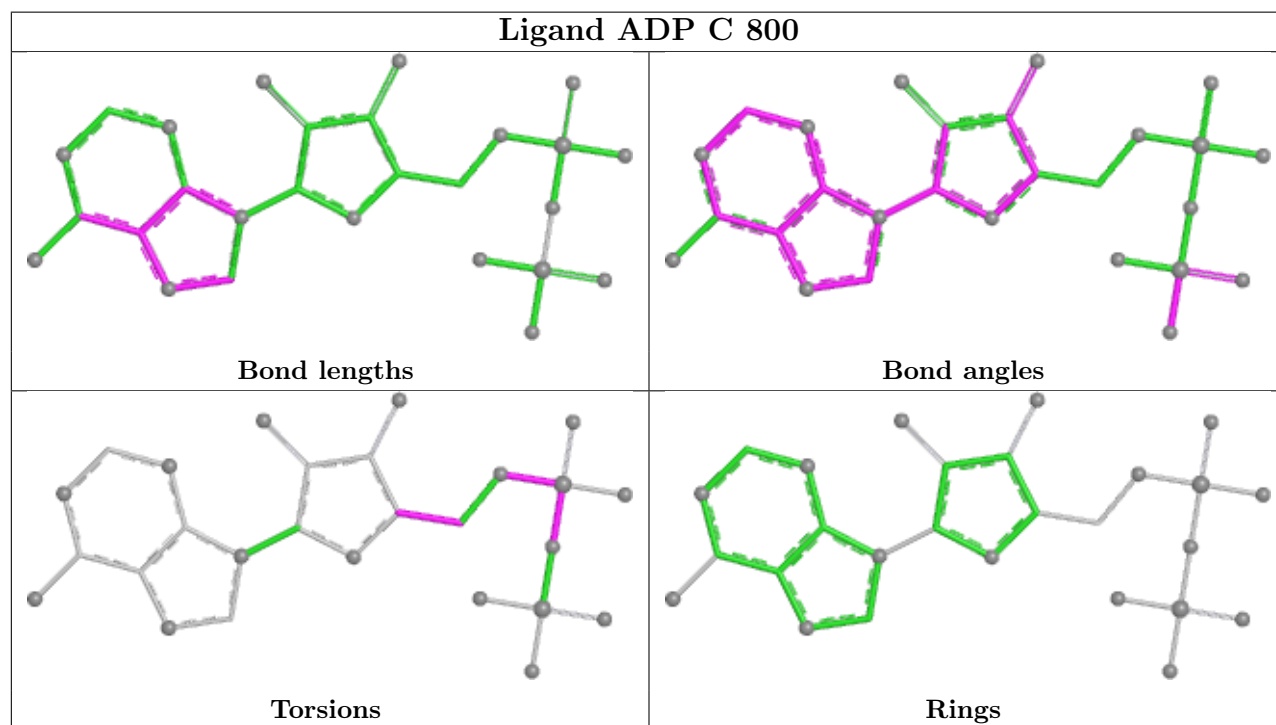
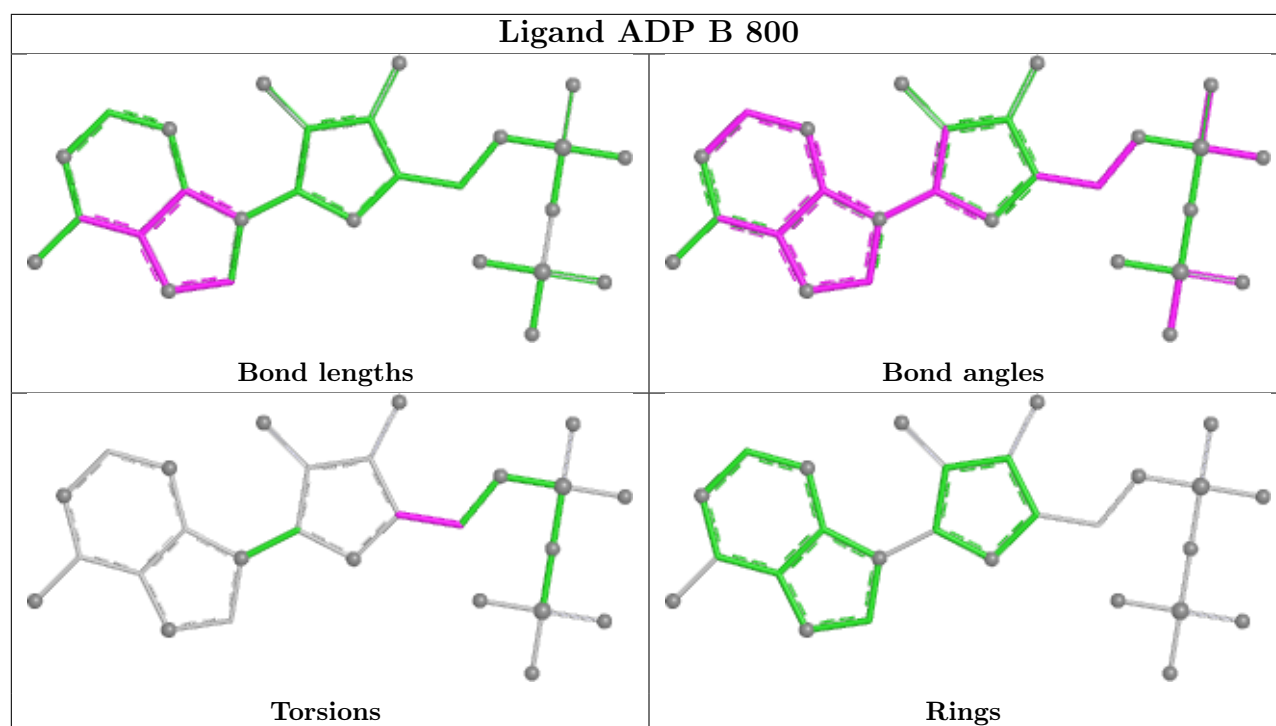
8 monomers are involved in 14 short contacts:

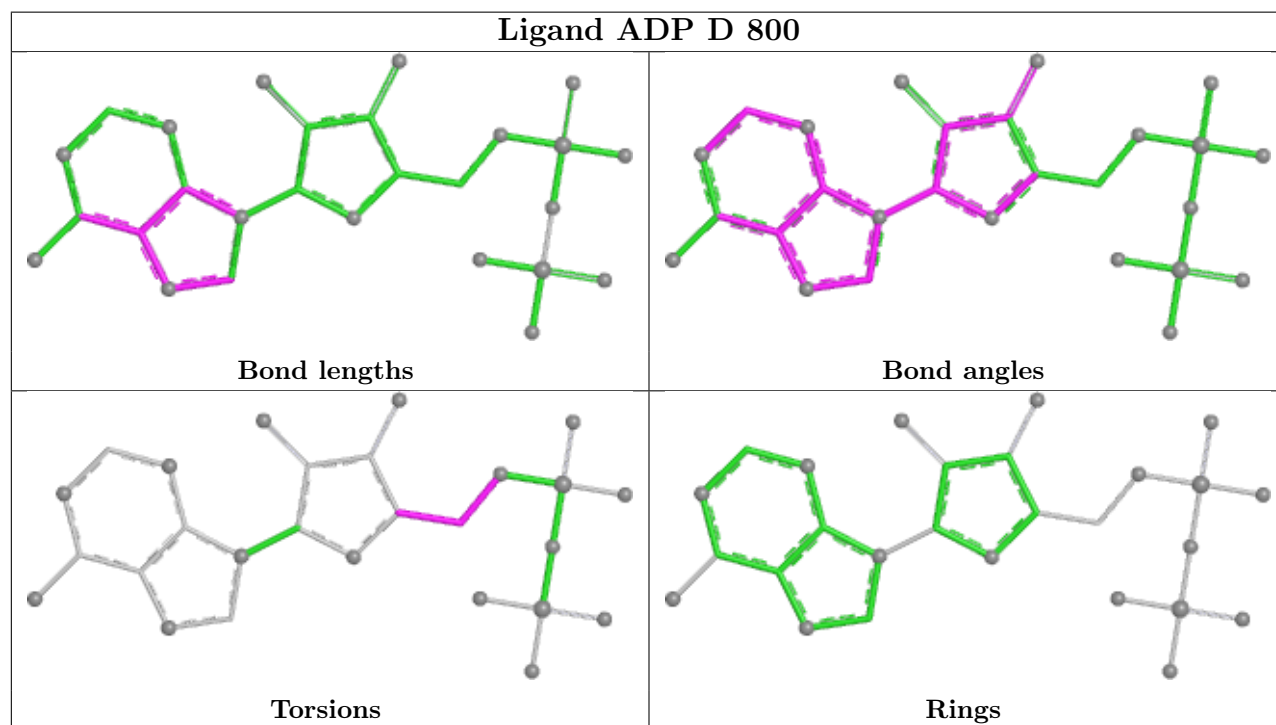
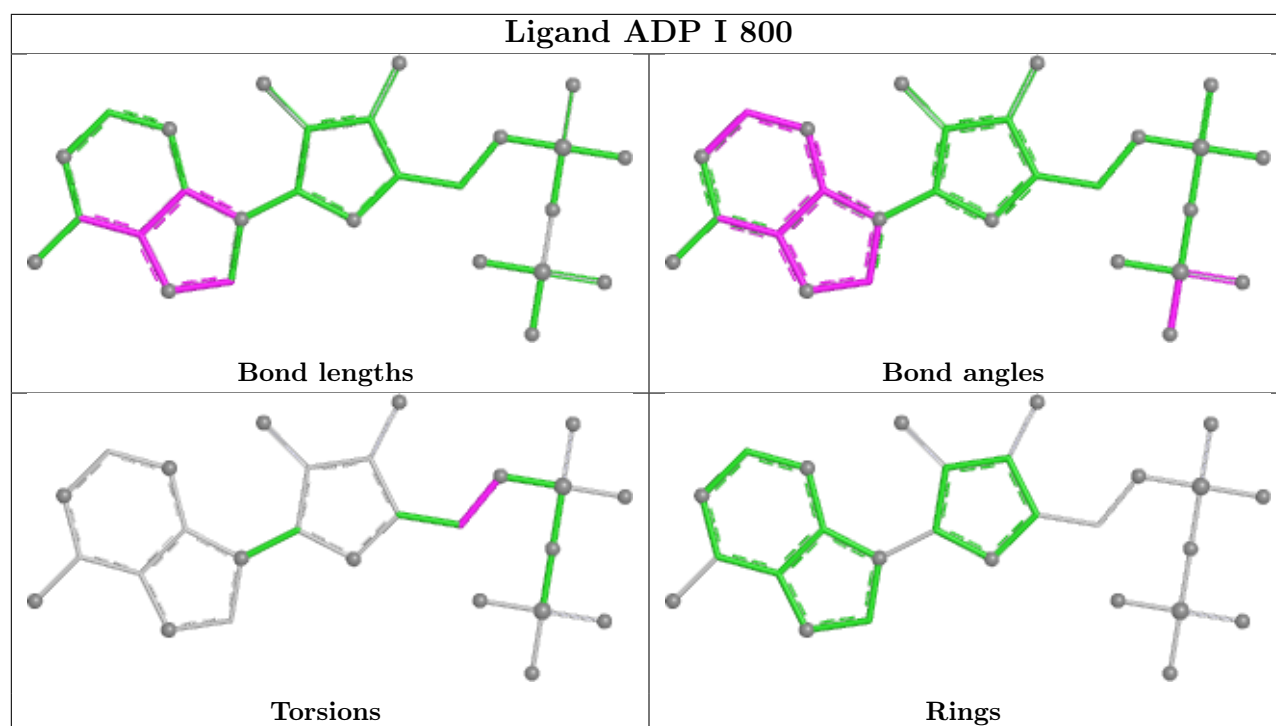
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	F	800	ADP	2	0
22	G	800	ADP	2	0
22	A	800	ADP	1	0
22	B	800	ADP	1	0
22	C	800	ADP	2	0
22	I	800	ADP	1	0
22	J	800	ADP	4	0
22	E	800	ADP	1	0

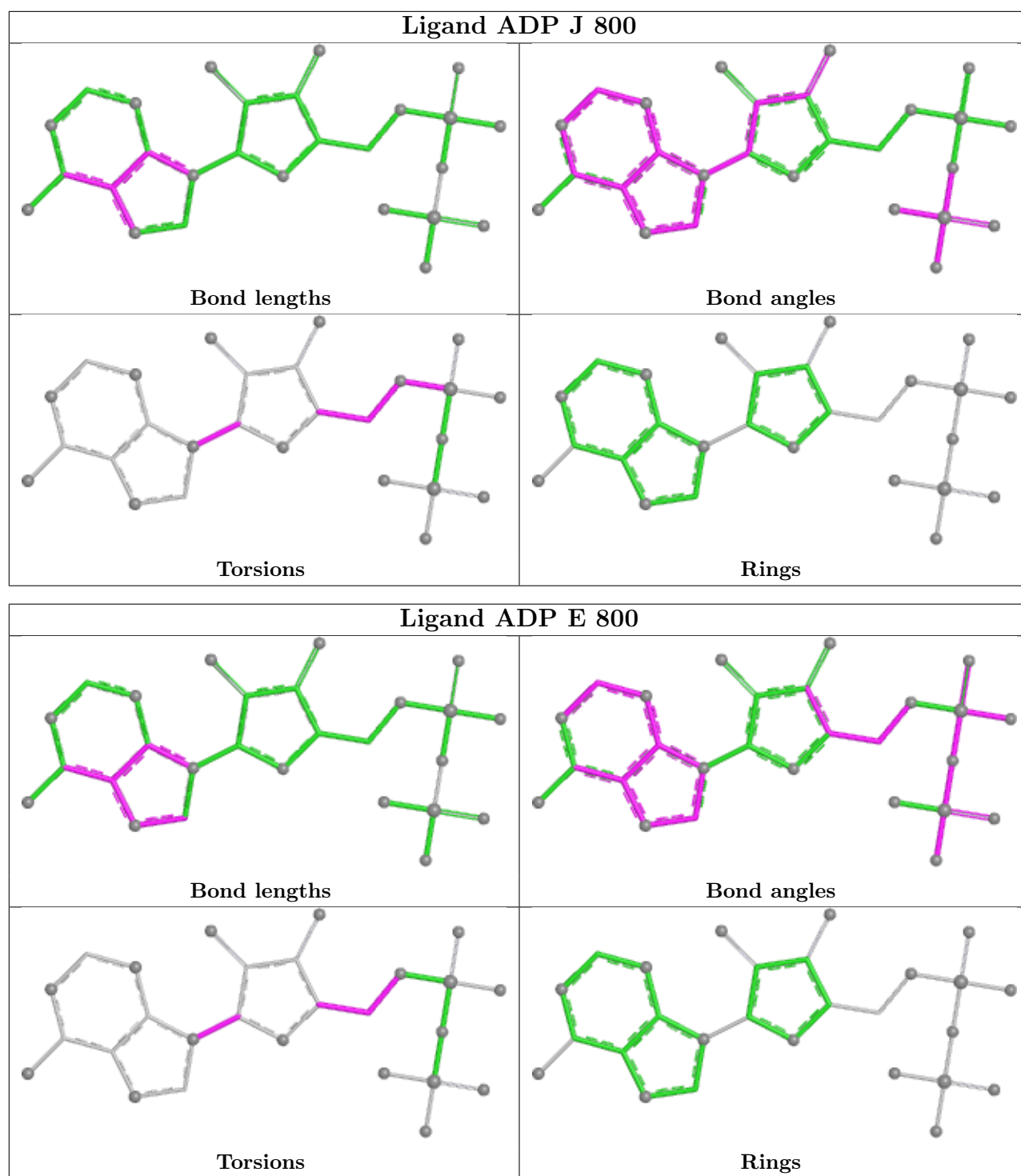
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
12	Y	12
7	N	5
6	M	5
8	O	3
8	P	3
9	R	2
9	Q	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	171:UNK	C	201:UNK	N	103.17
1	N	367:UNK	C	401:UNK	N	94.98
1	M	171:UNK	C	201:UNK	N	93.67
1	M	367:UNK	C	401:UNK	N	83.48
1	N	634:UNK	C	701:UNK	N	69.69
1	Y	26:UNK	C	155:UNK	N	62.83
1	Y	502:UNK	C	508:UNK	N	62.38
1	M	625:UNK	C	701:UNK	N	61.53
1	R	38:UNK	C	42:UNK	N	55.45
1	Q	38:UNK	C	42:UNK	N	50.32
1	Y	359:UNK	C	415:UNK	N	43.28
1	M	741:UNK	C	801:UNK	N	38.54
1	N	768:UNK	C	801:UNK	N	33.82
1	N	559:UNK	C	602:UNK	N	28.02
1	O	41:UNK	C	64:UNK	N	27.62
1	Y	193:UNK	C	282:UNK	N	25.54
1	Y	160:UNK	C	181:UNK	N	23.35
1	P	41:UNK	C	64:UNK	N	22.66
1	M	559:UNK	C	601:UNK	N	20.21
1	Y	620:UNK	C	703:UNK	N	16.86
1	Y	535:UNK	C	580:UNK	N	16.10
1	R	62:UNK	C	64:UNK	N	14.28
1	O	94:UNK	C	96:UNK	N	14.16
1	Q	62:UNK	C	64:UNK	N	13.53
1	Y	611:UNK	C	615:UNK	N	13.46
1	P	78:UNK	C	80:UNK	N	12.72
1	P	94:UNK	C	96:UNK	N	11.57
1	O	78:UNK	C	80:UNK	N	11.54
1	Y	421:UNK	C	423:UNK	N	7.76

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Y	586:UNK	C	588:UNK	N	5.98
1	Y	298:UNK	C	300:UNK	N	4.47
1	Y	597:UNK	C	601:UNK	N	3.21

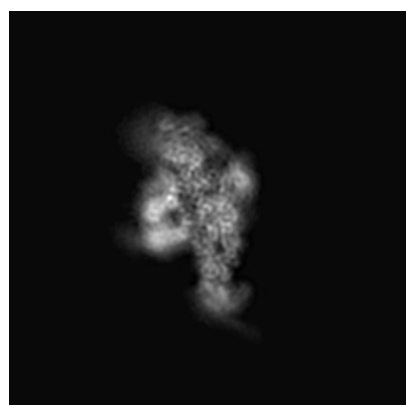
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2860. These allow visual inspection of the internal detail of the map and identification of artifacts.

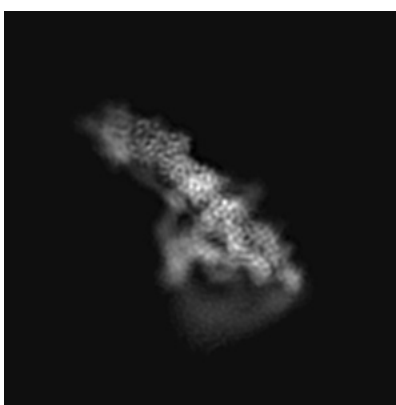
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

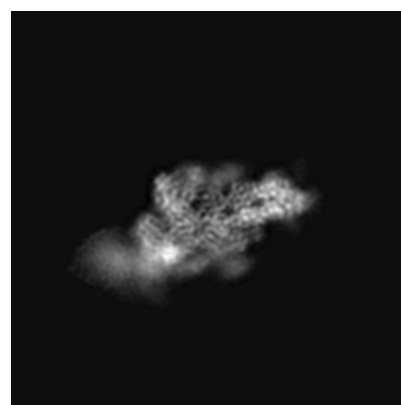
6.1.1 Primary map



X



Y

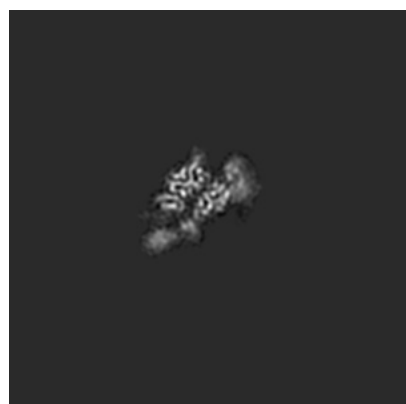


Z

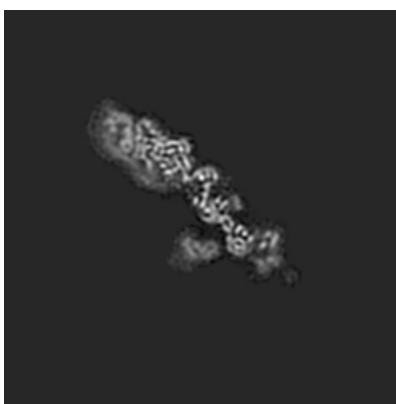
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

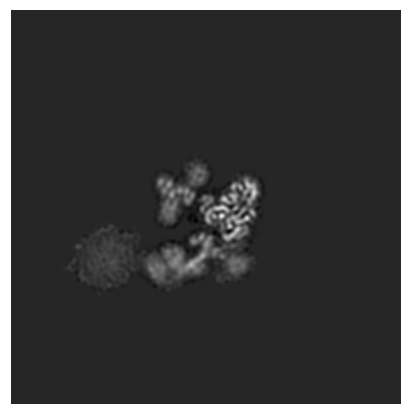
6.2.1 Primary map



X Index: 216



Y Index: 216

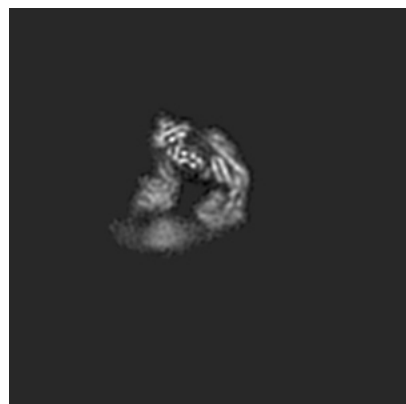


Z Index: 216

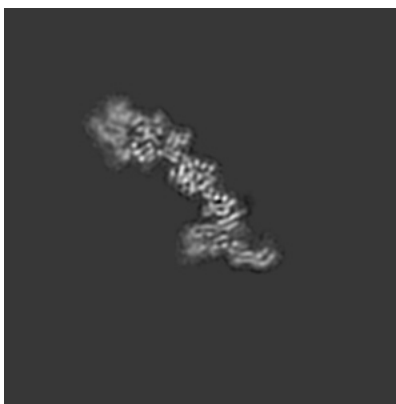
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

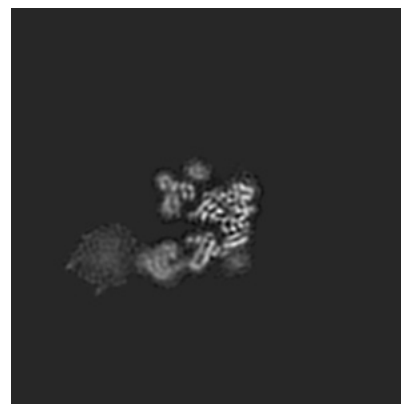
6.3.1 Primary map



X Index: 166



Y Index: 230

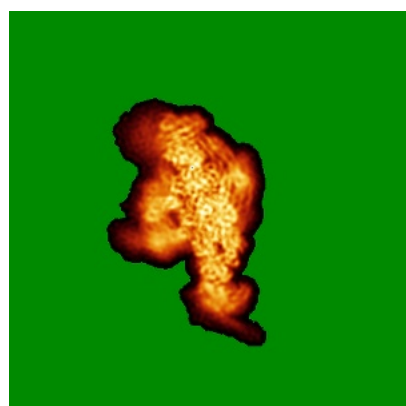


Z Index: 221

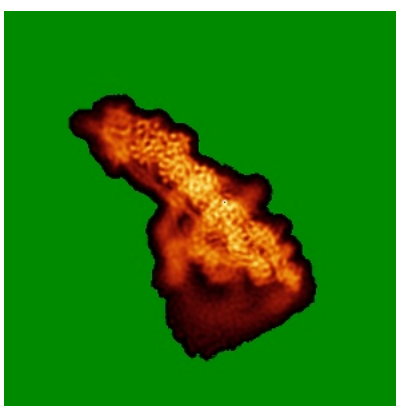
The images above show the largest variance slices of the map in three orthogonal directions.

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

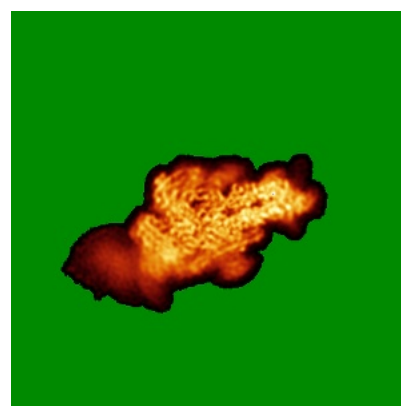
6.4.1 Primary map



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

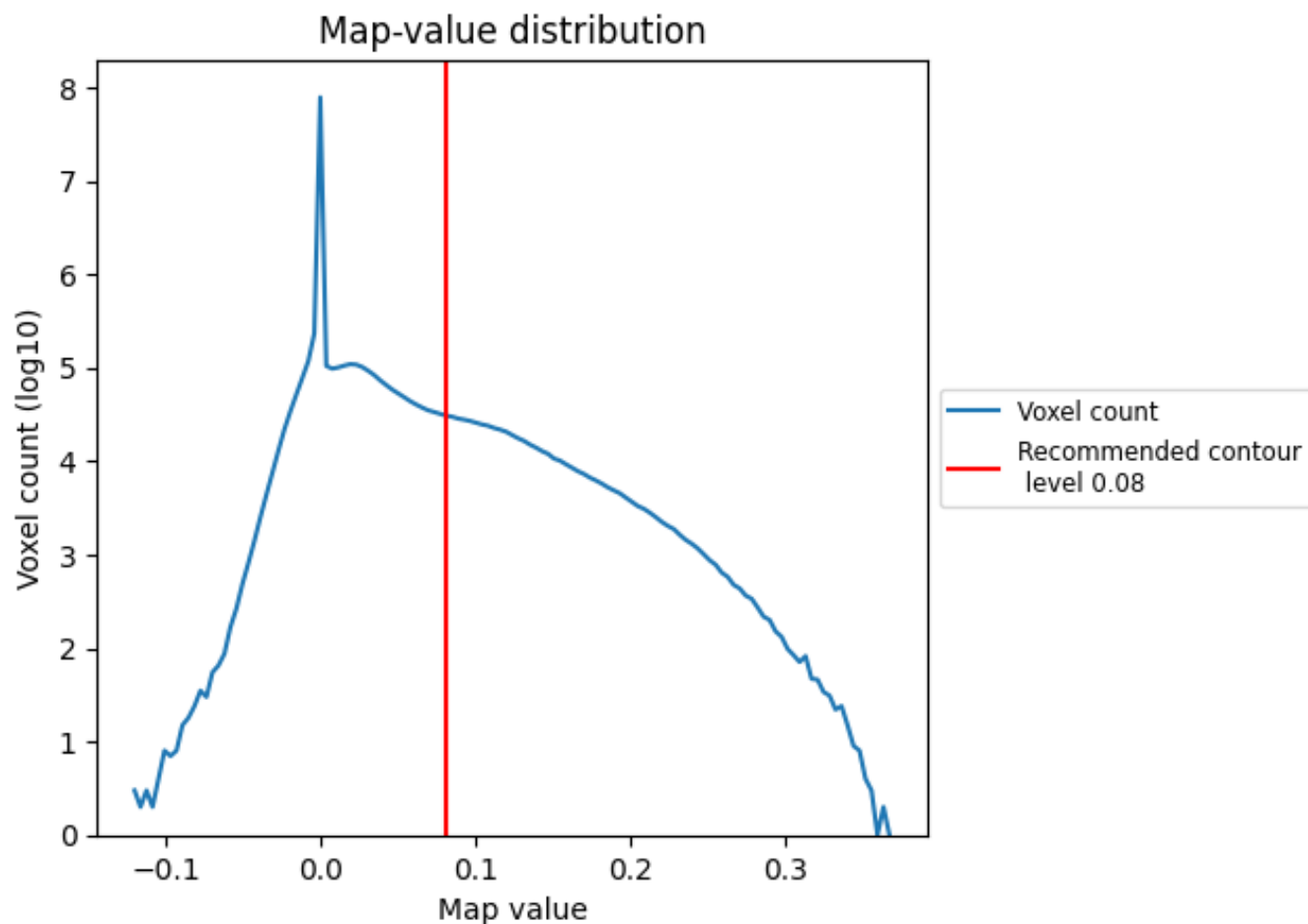
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

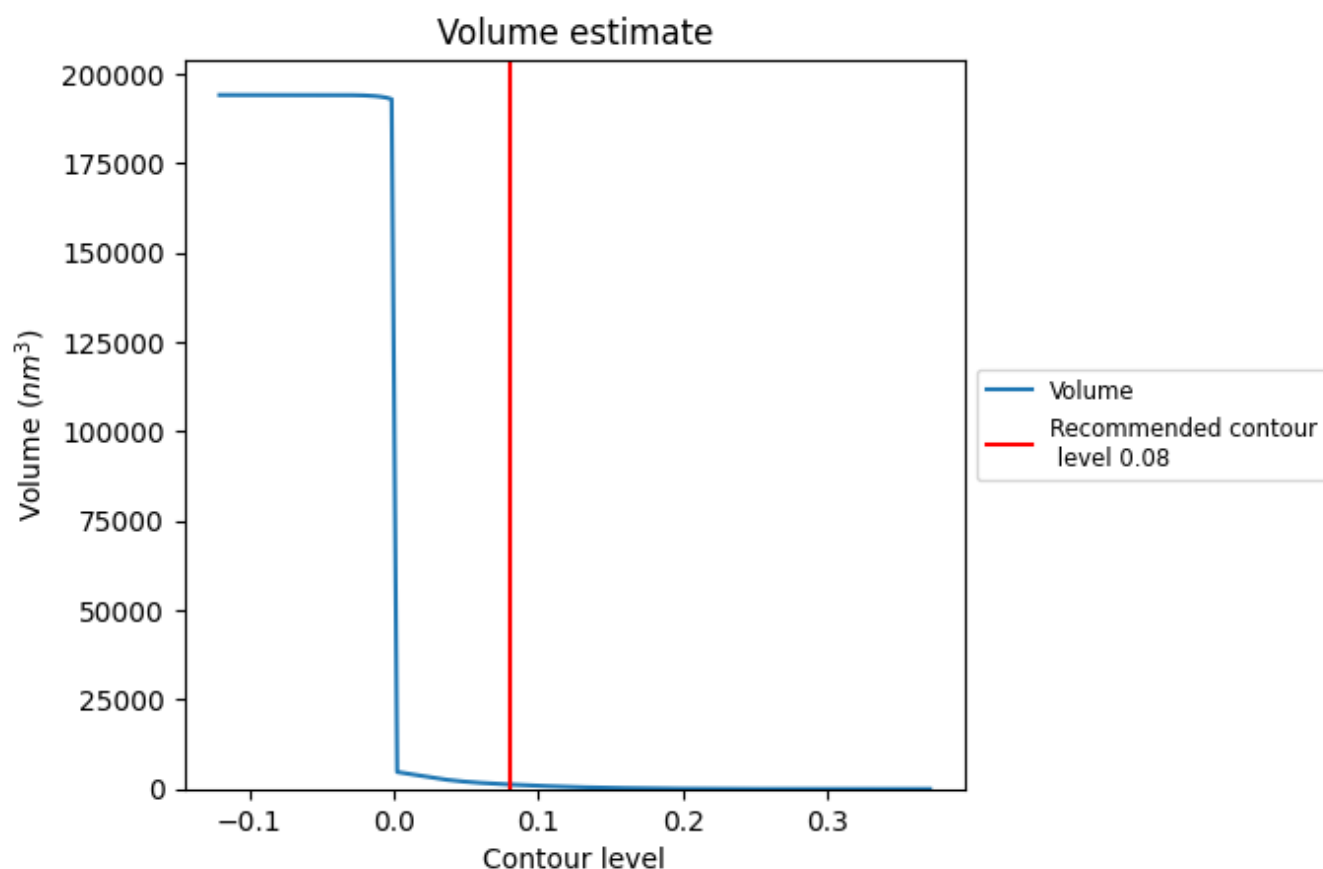
This section contains the results of statistical analysis of the map.

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.

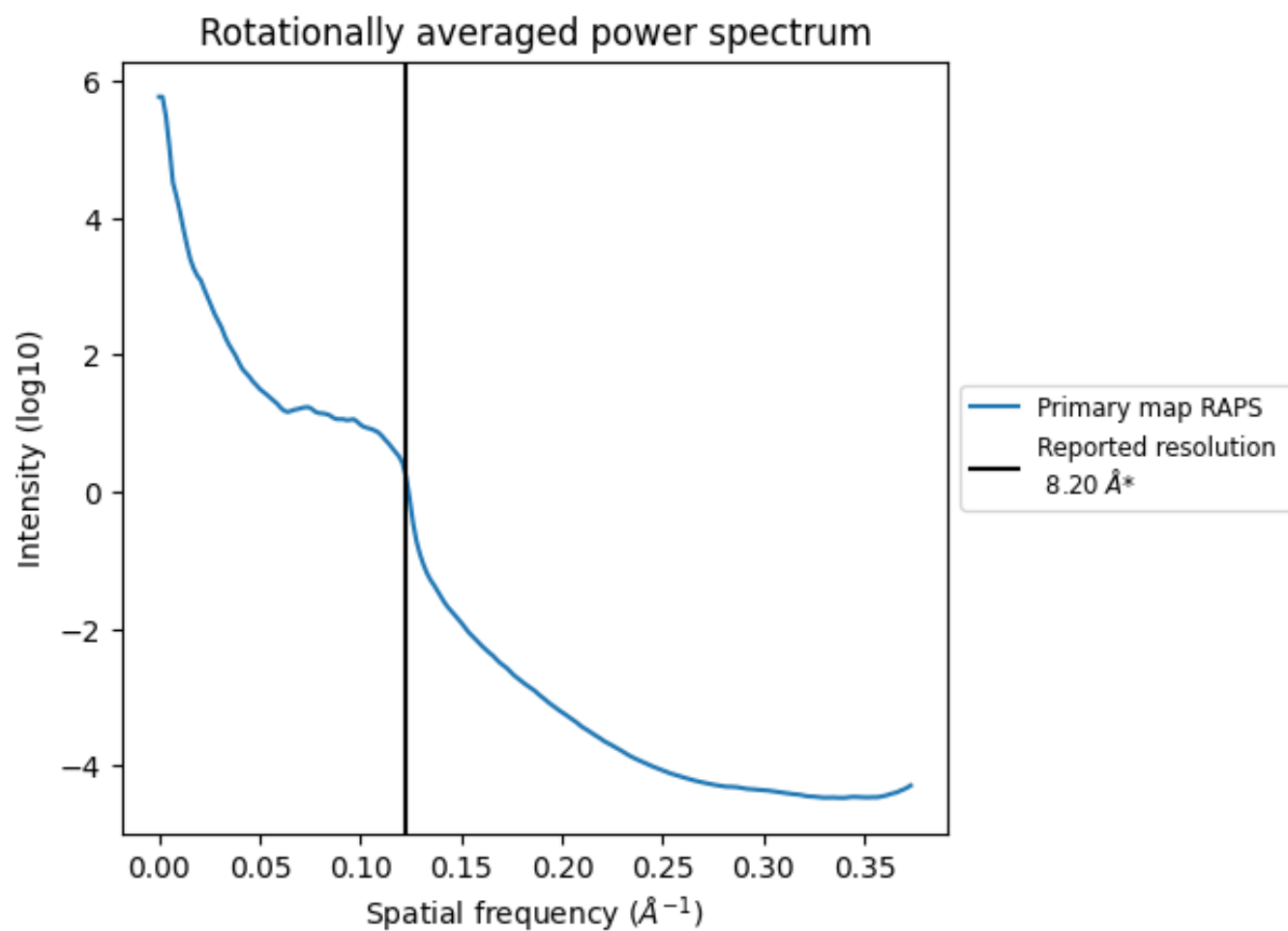
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1254 nm^3 ; this corresponds to an approximate mass of 1133 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 0.122 Å⁻¹

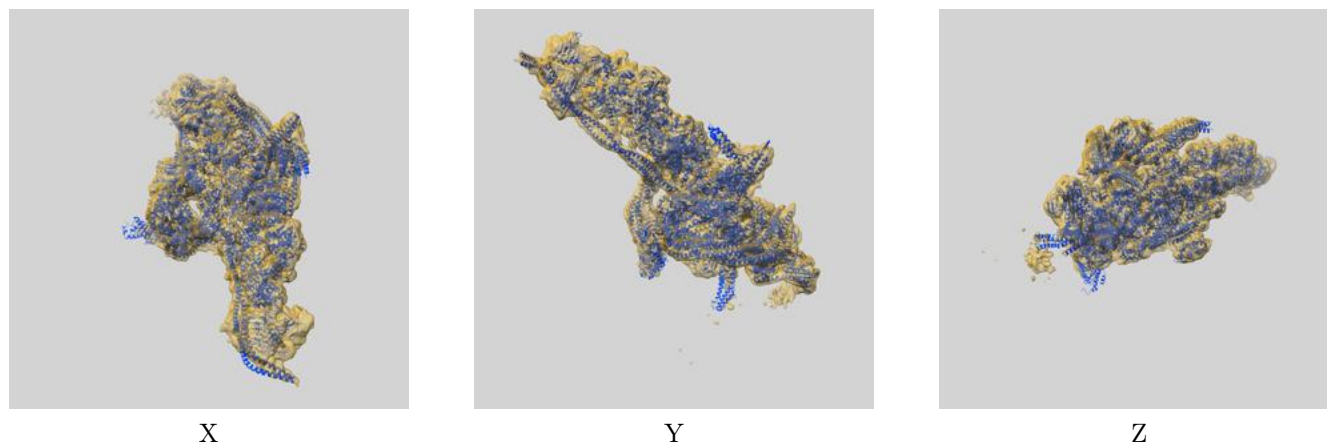
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2860 and PDB model 6F3A. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



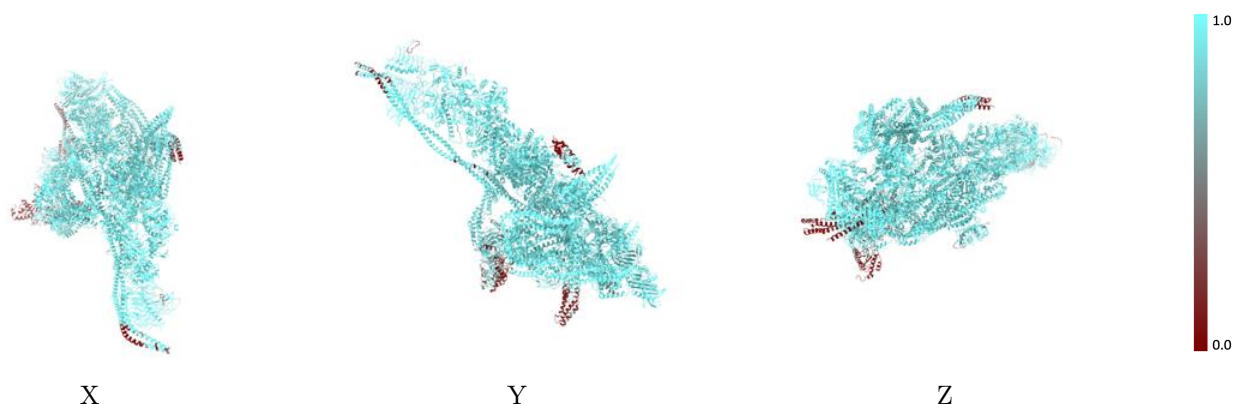
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



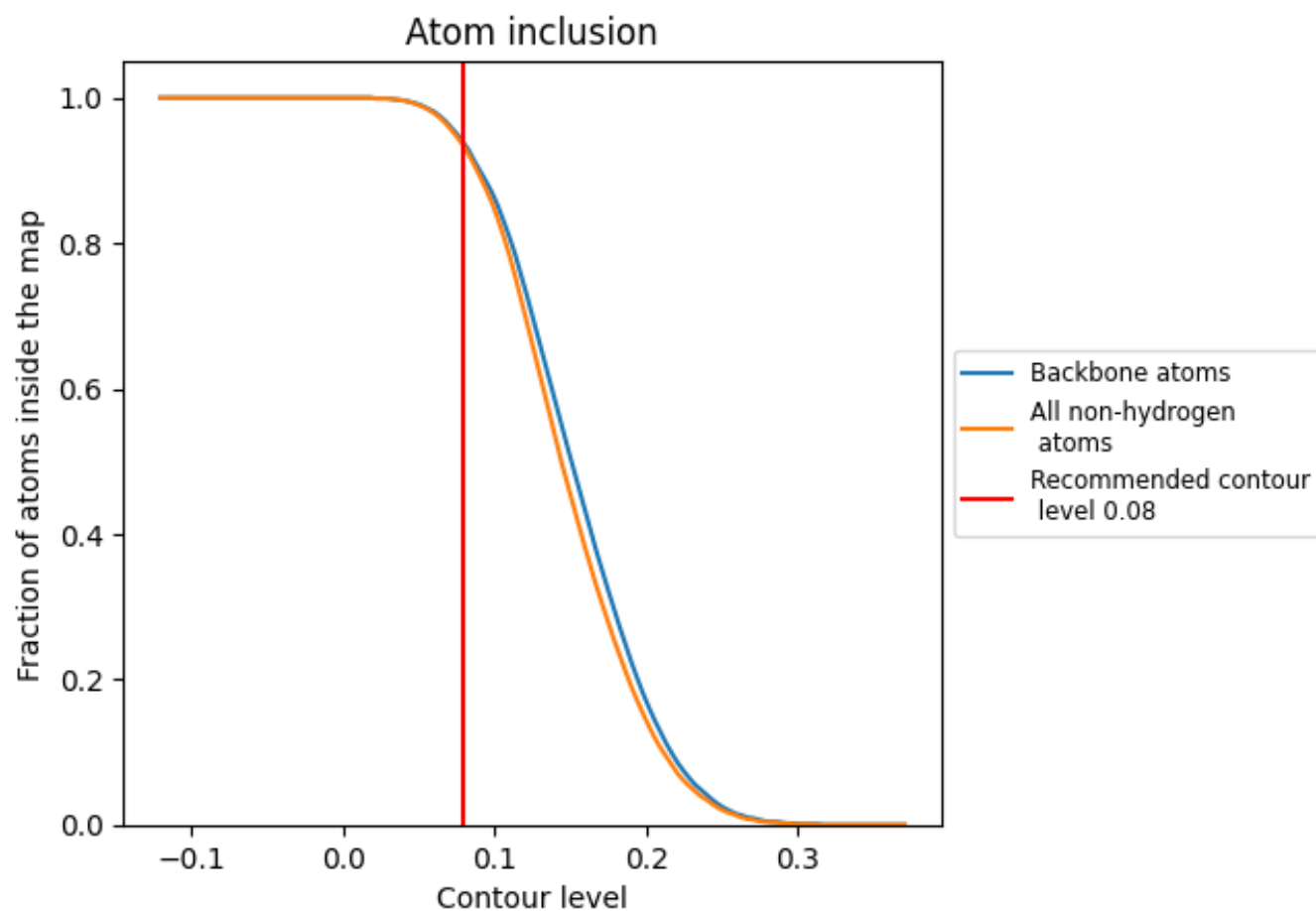
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9330	 0.2280
5	 0.8180	 0.2340
6	 0.8180	 0.2130
A	 0.9970	 0.2510
B	 0.9970	 0.2640
C	 0.9940	 0.2690
D	 0.9970	 0.2650
E	 0.9960	 0.2720
F	 0.9940	 0.2680
G	 0.9980	 0.2650
H	 0.9960	 0.2690
I	 0.9890	 0.2510
J	 0.9980	 0.2680
K	 0.9910	 0.2460
L	 0.9990	 0.2550
M	 0.9880	 0.2430
N	 0.9820	 0.2570
O	 1.0000	 0.2620
P	 1.0000	 0.2870
Q	 0.4410	 0.1280
R	 1.0000	 0.2840
U	 0.9370	 0.1700
V	 1.0000	 0.2350
Y	 0.9910	 0.2810
Z	 1.0000	 0.2800
a	 0.9770	 0.3170
b	 0.9970	 0.3000
c	 0.9830	 0.2780
d	 0.9830	 0.2960
e	 0.8970	 0.1650
f	 0.8740	 0.2210
g	 0.7790	 0.0560
h	 0.8560	 0.1380
j	 0.5330	 0.1620
k	 0.1390	 0.0480



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
l	 0.5890	 0.0700
z	 0.9210	 0.2330