Full wwPDB EM Validation Report

Apr 23, 2024 – 06:54 am BST

PDB ID	:	6ZYW
EMDB ID	:	EMD-11576
Title	:	Outer Dynein Arm-Shulin complex - overall structure (Tetrahymena thermophila)
Authors	:	Mali, G.R.; Abid Ali, F.; Lau, C.K.; Carter, A.P.
Deposited on	:	2020-08-03
Resolution	:	8.78 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:

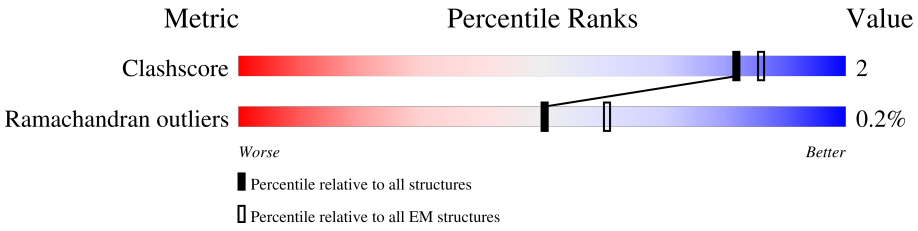
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 8.78 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	4168	85% 6% 9%
2	B	4595	91% · 5%
3	C	4620	94% · ·
4	D	667	47% · 52%
4	d	667	19% 81%
5	E	670	51% 49%
5	e	670	15% 85%
6	F	133	74% 26%
7	G	103	90% · 8%
8	H	92	90% · 8%

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Mol	Chain	Length	Quality of chain
9	I	110	81% 19%
10	J	93	90% 10%
11	K	111	86% 14%
12	L	111	87% 13%
13	M	87	99%
14	N	132	83% 17%
15	O	117	93% 5%
16	P	110	90% 6%
17	Y	1200	94% 6%

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 73897 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 Dynein-1-alpha heavy chain, flagellar inner arm I1 complex protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	3795	Total 18787	C 11198	N 3795	O 3794	0	0

- Molecule 2 is a protein called Outer arm dynein beta heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	4370	Total 20008	C 12102	N 3953	O 3953	0	417

- Molecule 3 is a protein called Dynein heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	4433	Total 19737	C 11997	N 3870	O 3870	0	563

- Molecule 4 is a protein called Dynein intermediate chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	321	Total 1588	C 946	N 321	O 321	0	0
4	d	128	Total 637	C 381	N 128	O 128	0	0

- Molecule 5 is a protein called Flagellar outer dynein arm intermediate protein, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	341	Total 1678	C 996	N 341	O 341	0	0
5	e	102	Total 501	C 297	N 102	O 102	0	0

- Molecule 6 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	98	Total 486	C 290	N 98	O 98	0	0

- Molecule 7 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	95	Total 470	C 280	N 95	O 95	0	0

- Molecule 8 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	85	Total 420	C 250	N 85	O 85	0	0

- Molecule 9 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	89	Total 439	C 261	N 89	O 89	0	0

- Molecule 10 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	84	Total 416	C 248	N 84	O 84	0	0

- Molecule 11 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	95	Total 470	C 280	N 95	O 95	0	0

- Molecule 12 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	97	Total 479	C 285	N 97	O 97	0	0

- Molecule 13 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	86	Total 426	C 254	N 86	O 86	0	0

- Molecule 14 is a protein called Dynein light chain 2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	109	Total 537	C 319	N 109	O 109	0	0

- Molecule 15 is a protein called Dynein light chain tctex-type 1 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	111	Total 550	C 328	N 111	O 111	0	0

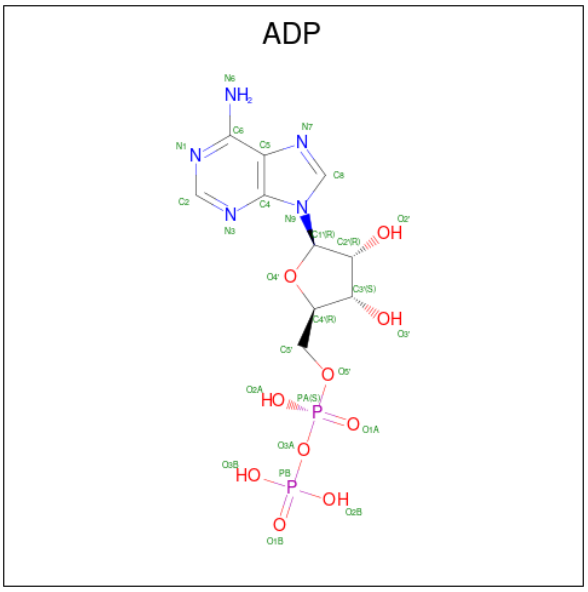
- Molecule 16 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	103	Total 513	C 307	N 103	O 103	0	0

- Molecule 17 is a protein called Shulin.

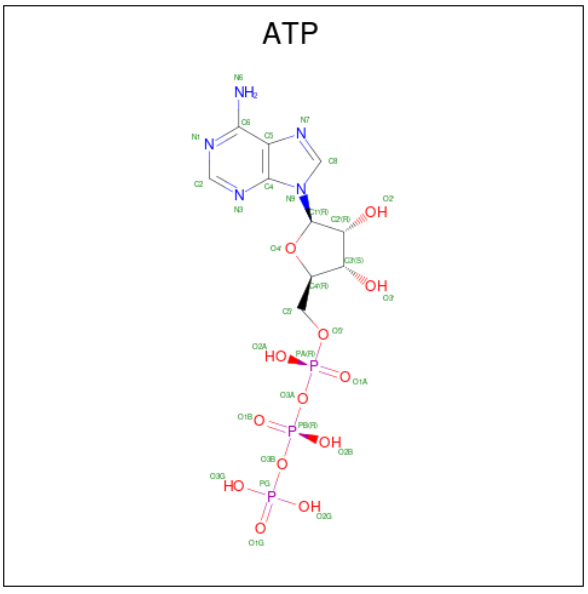
Mol	Chain	Residues	Atoms				AltConf	Trace
17	Y	1133	Total 5611	C 3345	N 1133	O 1133	0	0

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



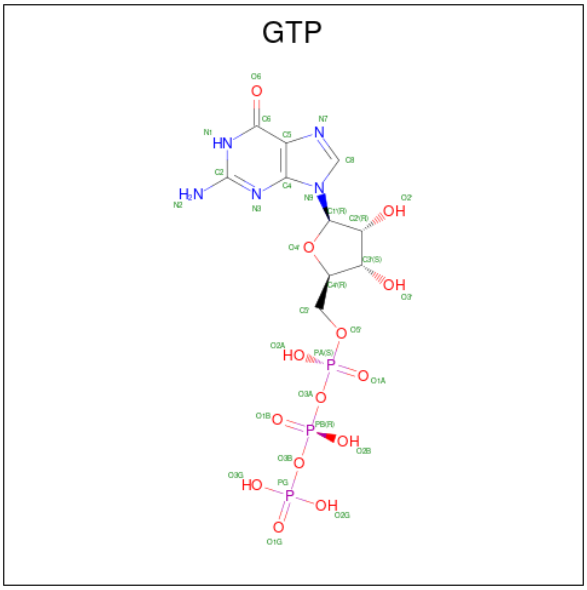
Mol	Chain	Residues	Atoms					AltConf
18	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
18	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
18	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 20 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



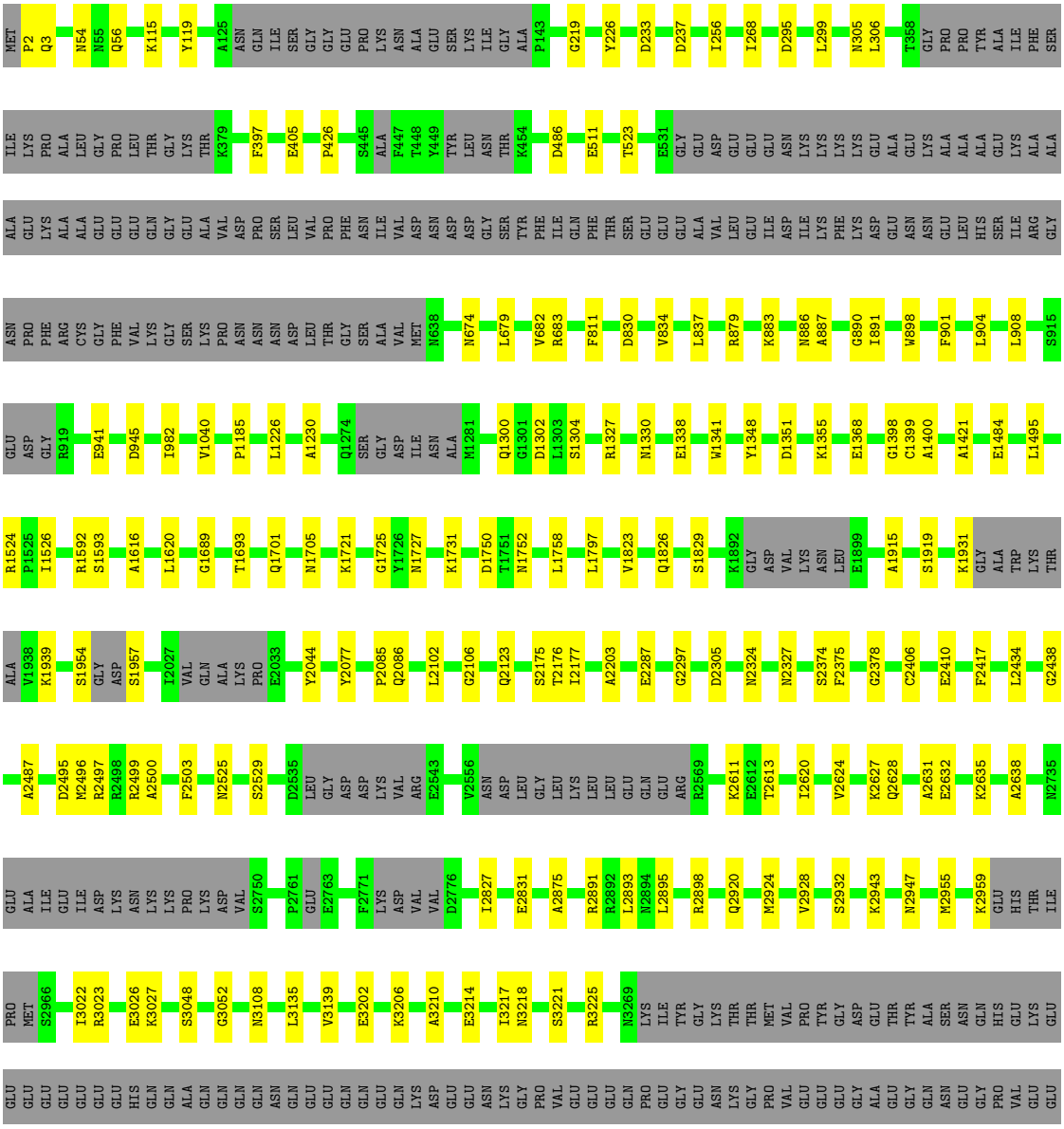
Mol	Chain	Residues	Atoms					AltConf
20	Y	1	Total	C	N	O	P	0
			32	10	5	14	3	

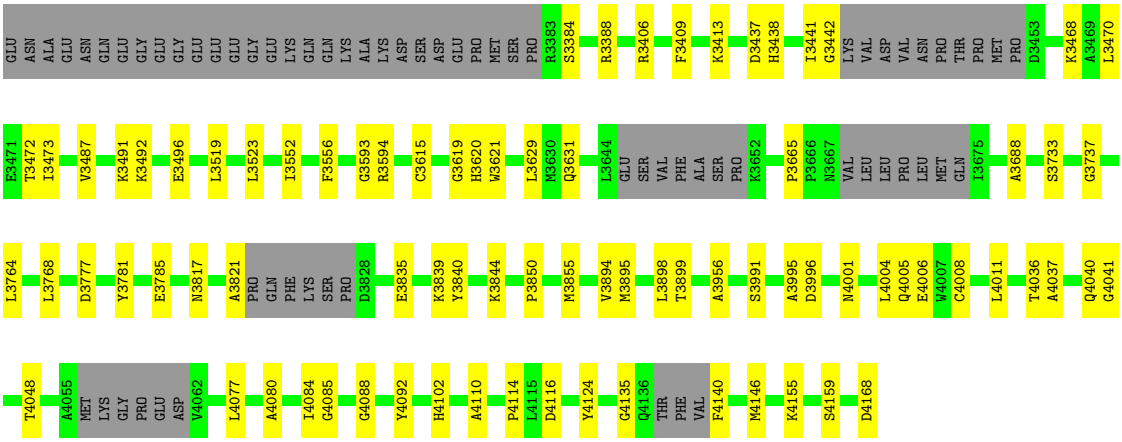
3 Residue-property plots (i)

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. 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. 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: Dynein-1-alpha heavy chain, flagellar inner arm I1 complex protein, putative

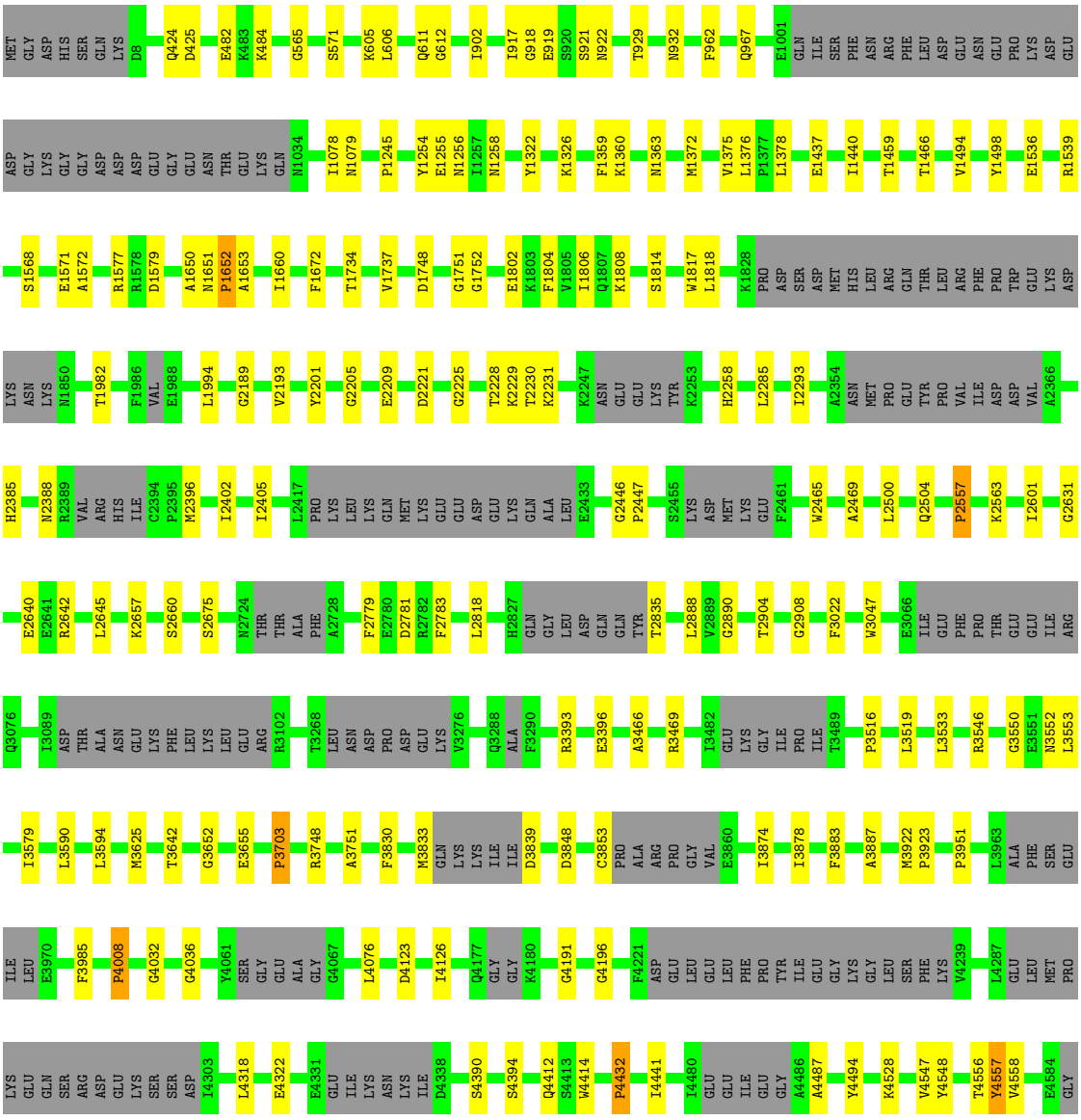
Chain A:





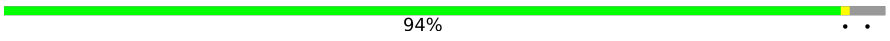
• Molecule 2: Outer arm dynein beta heavy chain

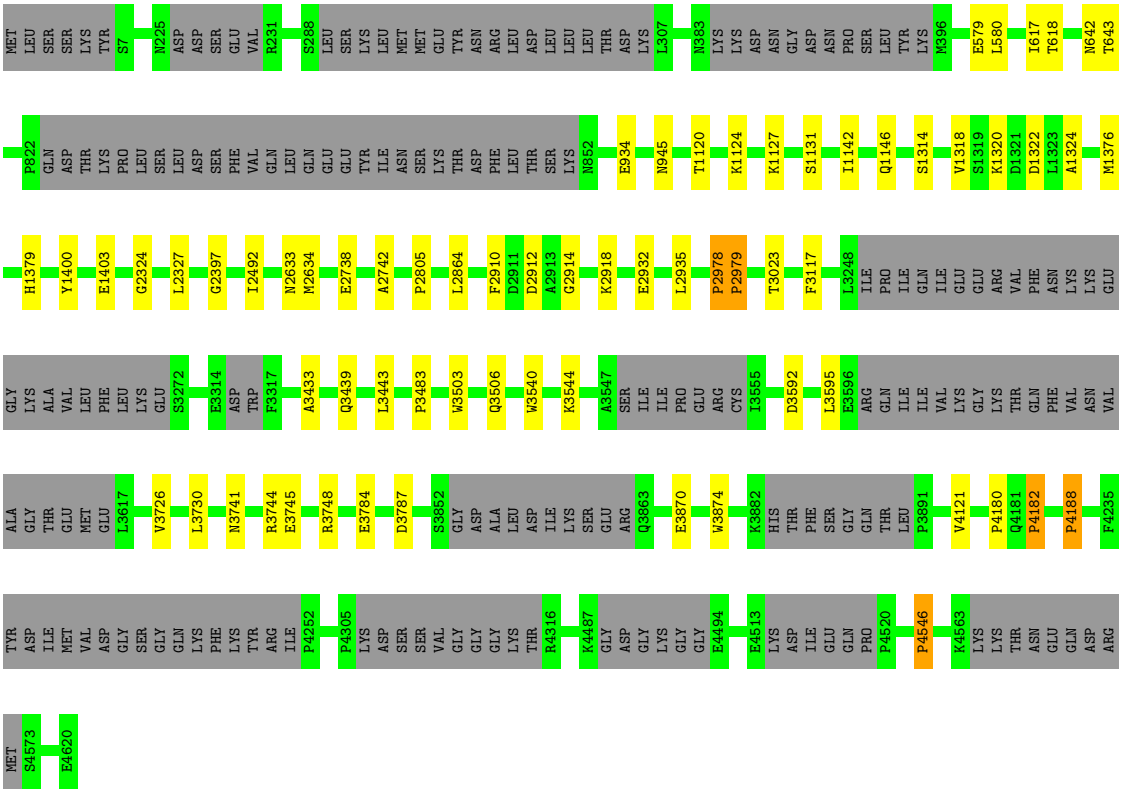
Chain B:



• Molecule 3: Dynein heavy chain, outer arm protein

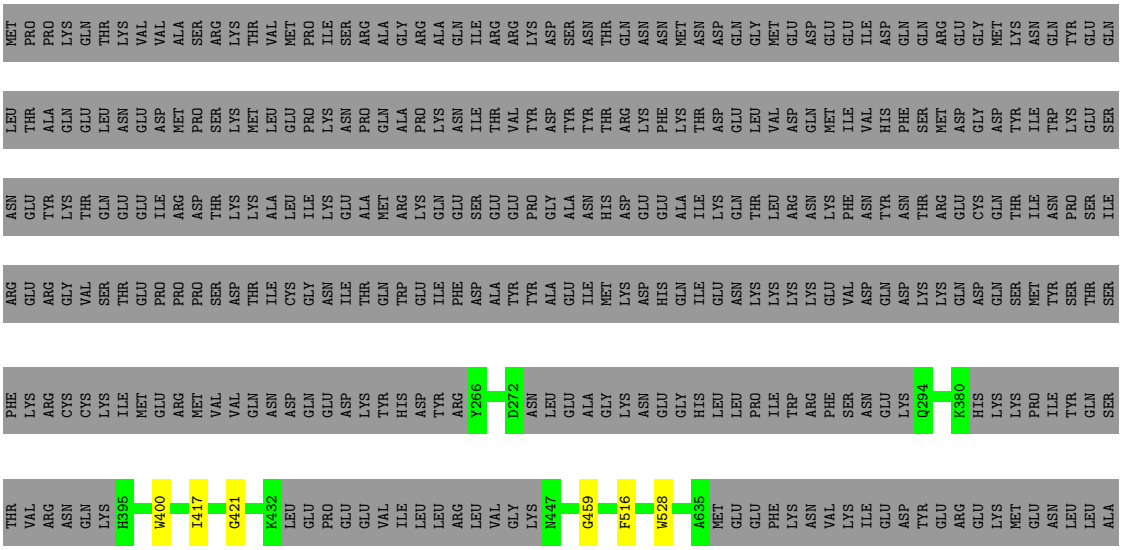
Chain C:





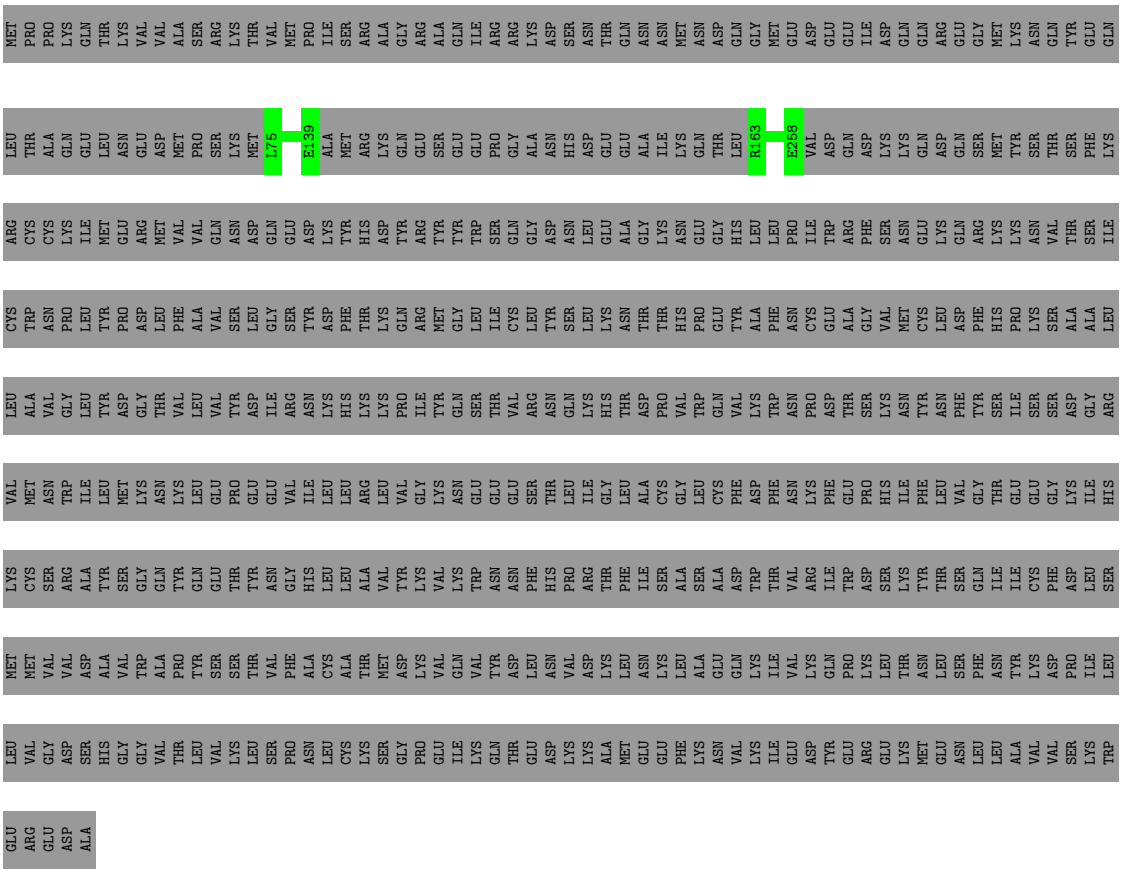
• Molecule 4: Dynein intermediate chain 2

Chain D:



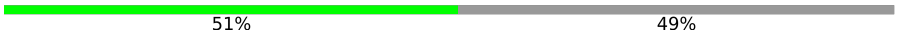
• Molecule 4: Dynein intermediate chain 2

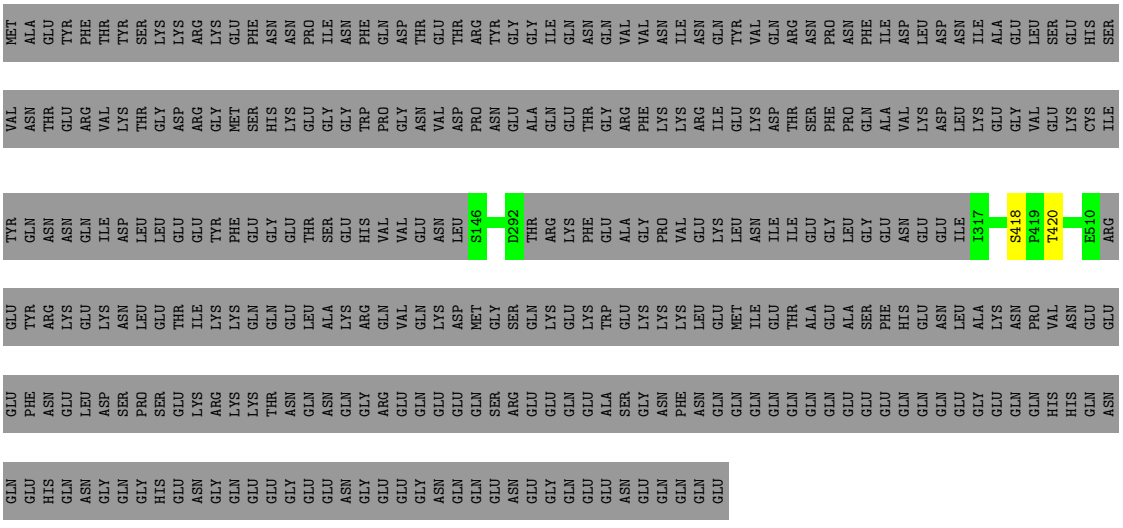
Chain d:



• Molecule 5: Flagellar outer dynein arm intermediate protein, putative

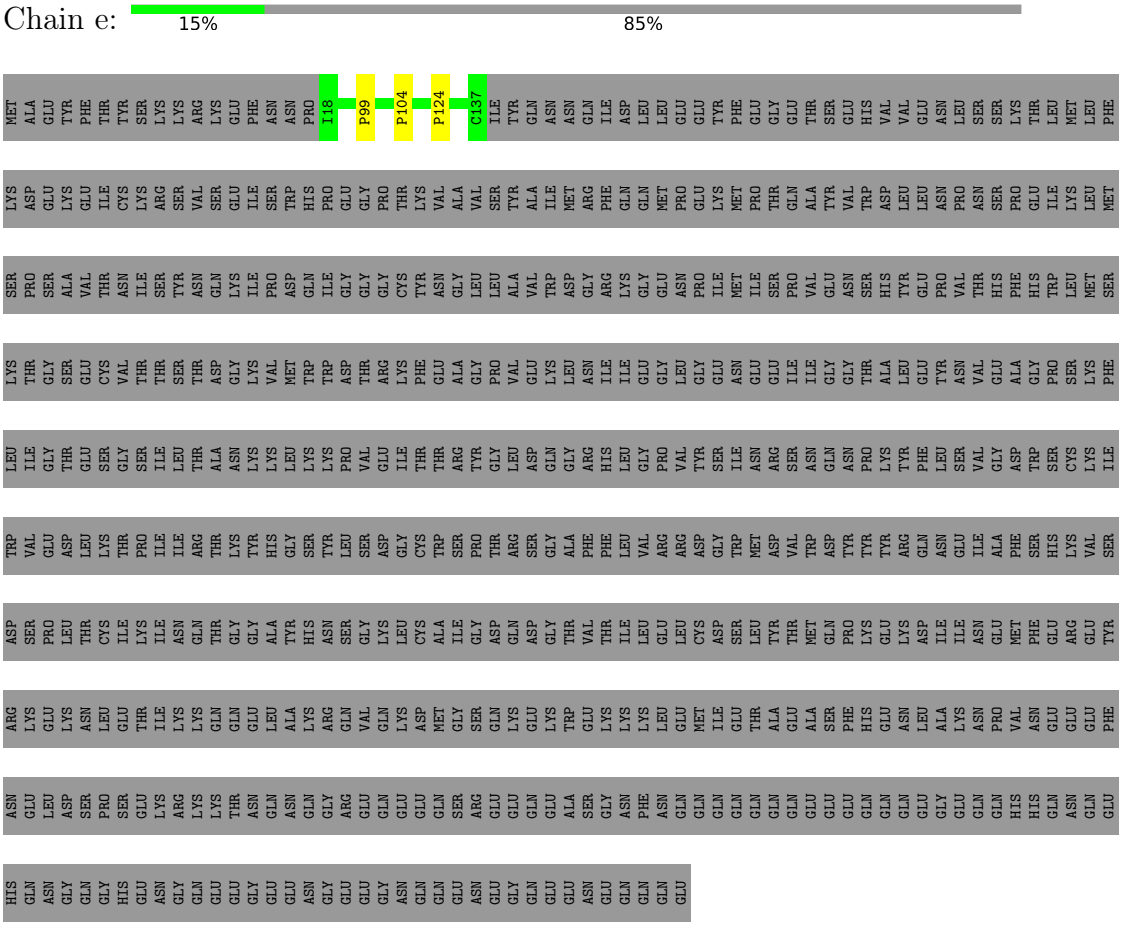
Chain E:





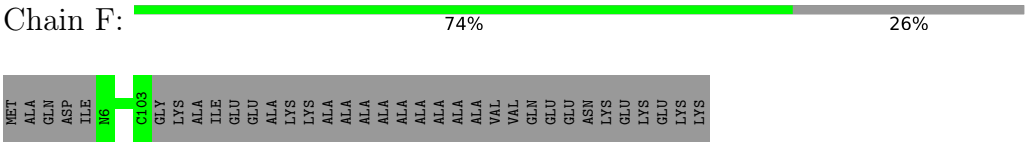
• Molecule 5: Flagellar outer dynein arm intermediate protein, putative

Chain e:



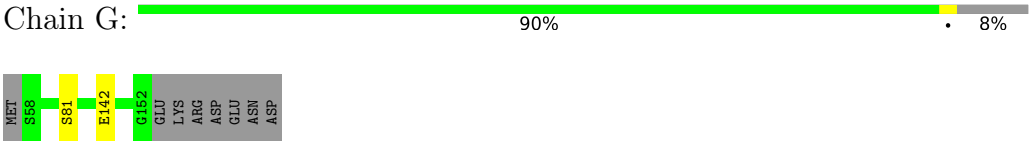
• Molecule 6: Dynein light chain roadblock-type 2 protein

Chain F:



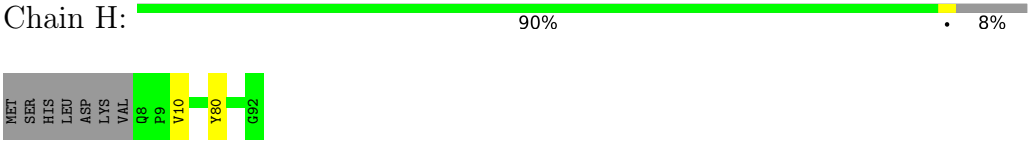
• Molecule 7: Dynein light chain roadblock-type 2 protein

Chain G:



• Molecule 8: Dynein light chain

Chain H:



• Molecule 9: Dynein light chain

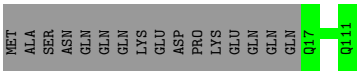
Chain I:

• Molecule 10: Dynein light chain

Chain J:

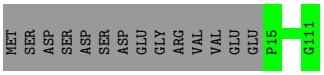
• Molecule 11: Dynein light chain

Chain K:



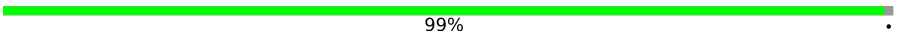
• Molecule 12: Dynein light chain

Chain L:



• Molecule 13: Dynein light chain

Chain M:

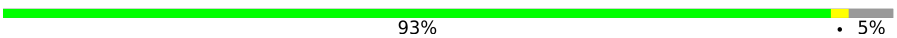


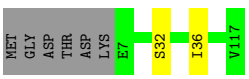
• Molecule 14: Dynein light chain 2A

Chain N:

• Molecule 15: Dynein light chain tctex-type 1 protein

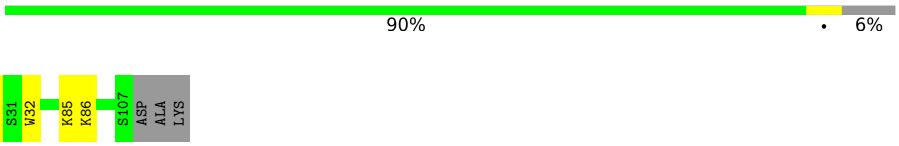
Chain O:





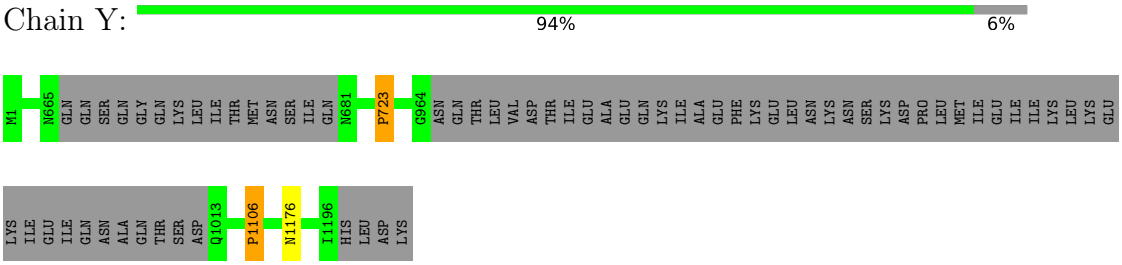
• Molecule 16: Thioredoxin

Chain P:



• Molecule 17: Shulin

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131142	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.34	0/18743	0.69	1/26057 (0.0%)
2	B	0.39	0/19561	0.65	6/27233 (0.0%)
3	C	0.31	0/19162	0.56	8/26702 (0.0%)
4	D	0.36	0/1584	0.84	0/2201
4	d	0.31	0/634	0.61	0/881
5	E	0.36	0/1676	0.78	0/2327
5	e	0.44	0/498	0.76	3/687 (0.4%)
6	F	0.46	0/485	0.86	0/675
7	G	0.37	0/469	0.73	0/652
8	H	0.42	0/419	0.84	0/582
9	I	0.40	0/438	0.86	0/608
10	J	0.31	0/415	0.57	0/577
11	K	0.28	0/469	0.56	0/652
12	L	0.28	0/478	0.57	0/664
13	M	0.29	0/425	0.55	0/591
14	N	0.28	0/536	0.57	0/744
15	O	0.24	0/549	0.50	0/764
16	P	0.78	0/512	0.92	0/714
17	Y	0.29	1/5608 (0.0%)	0.55	2/7814 (0.0%)
All	All	0.35	1/72661 (0.0%)	0.64	20/101125 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	1176	ASN	C-N	6.01	1.47	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	4432	PRO	N-CA-CB	8.75	113.80	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	4182	PRO	N-CA-CB	6.65	111.28	103.30
3	C	4188	PRO	N-CA-CB	6.65	111.28	103.30
17	Y	1106	PRO	N-CA-CB	6.55	111.16	103.30
3	C	2978	PRO	N-CA-CB	6.33	110.89	103.30
3	C	4180	PRO	N-CA-CB	6.29	110.85	103.30
17	Y	723	PRO	N-CA-CB	6.25	110.81	103.30
2	B	4008	PRO	N-CA-CB	6.21	110.76	103.30
5	e	99	PRO	N-CA-CB	6.21	110.76	103.30
3	C	4546	PRO	N-CA-CB	6.21	110.75	103.30
2	B	3703	PRO	N-CA-CB	6.20	110.74	103.30
3	C	2979	PRO	N-CA-CB	6.20	110.73	103.30
2	B	1652	PRO	N-CA-CB	5.83	110.29	103.30
5	e	124	PRO	N-CA-CB	5.76	110.21	103.30
1	A	1185	PRO	N-CA-CB	5.71	110.16	103.30
3	C	2805	PRO	N-CA-CB	5.63	110.06	103.30
3	C	3483	PRO	N-CA-CB	5.61	110.03	103.30
5	e	104	PRO	N-CA-CB	5.38	109.75	103.30
2	B	3951	PRO	N-CA-CB	5.29	109.65	103.30
2	B	2557	PRO	N-CA-CB	5.08	109.40	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18787	0	8282	131	0
2	B	20008	0	8566	89	0
3	C	19737	0	8300	29	0
4	D	1588	0	693	3	0
4	d	637	0	261	0	0
5	E	1678	0	724	1	0
5	e	501	0	215	0	0
6	F	486	0	218	0	0
7	G	470	0	203	1	0
8	H	420	0	185	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	439	0	202	0	0
10	J	416	0	184	0	0
11	K	470	0	215	0	0
12	L	479	0	209	0	0
13	M	426	0	189	0	0
14	N	537	0	231	0	0
15	O	550	0	247	1	0
16	P	513	0	213	2	0
17	Y	5611	0	2410	0	0
18	C	81	0	36	0	0
19	C	31	0	12	0	0
20	Y	32	0	12	0	0
All	All	73897	0	31807	258	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 2.

All (258) 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)
2:B:917:ILE:O	2:B:921:SER:CB	2.17	0.92
3:C:617:ILE:C	3:C:618:THR:CA	2.46	0.84
2:B:4318:LEU:O	2:B:4322:GLU:N	2.12	0.83
3:C:642:ASN:CA	3:C:643:THR:N	2.43	0.81
2:B:2229:LYS:O	2:B:2230:THR:N	2.13	0.81
2:B:4032:GLY:O	2:B:4036:GLY:N	2.15	0.80
2:B:424:GLN:CA	2:B:425:ASP:N	2.45	0.80
1:A:4124:TYR:N	1:A:4146:MET:O	2.15	0.79
3:C:1314:SER:O	3:C:1318:VAL:N	2.14	0.79
1:A:2611:LYS:O	1:A:2613:THR:N	2.15	0.78
2:B:3830:PHE:O	2:B:3839:ASP:N	2.16	0.78
1:A:4048:THR:O	1:A:4110:ALA:N	2.16	0.78
1:A:2631:ALA:O	1:A:2635:LYS:N	2.16	0.77
2:B:3552:ASN:O	2:B:3553:LEU:N	2.18	0.76
2:B:3546:ARG:O	2:B:3550:GLY:N	2.19	0.76
3:C:579:GLU:CA	3:C:580:LEU:N	2.49	0.75
2:B:2201:TYR:O	2:B:2205:GLY:N	2.19	0.75
2:B:2228:THR:O	2:B:2231:LYS:N	2.21	0.74
1:A:2496:MET:O	1:A:2500:ALA:N	2.20	0.74
1:A:2297:GLY:N	1:A:2375:PHE:O	2.21	0.73
1:A:4004:LEU:O	1:A:4008:CYS:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1954:SER:O	1:A:1957:SER:N	2.21	0.73
2:B:1568:SER:O	2:B:1572:ALA:N	2.21	0.73
2:B:2396:MET:N	2:B:2447:PRO:O	2.22	0.72
1:A:3:GLN:N	1:A:305:ASN:O	2.23	0.72
2:B:1650:ALA:N	2:B:1653:ALA:O	2.22	0.72
1:A:2627:LYS:O	1:A:2631:ALA:N	2.23	0.71
1:A:3895:MET:O	1:A:3899:THR:N	2.24	0.71
1:A:1400:ALA:N	1:A:1524:ARG:O	2.23	0.71
1:A:426:PRO:O	1:A:486:ASP:N	2.24	0.70
2:B:2209:GLU:N	2:B:2258:HIS:O	2.25	0.70
2:B:2221:ASP:O	2:B:2225:GLY:N	2.23	0.69
1:A:3221:SER:O	1:A:3225:ARG:N	2.25	0.69
2:B:3848:ASP:O	2:B:3853:CYS:N	2.24	0.69
1:A:2044:TYR:O	1:A:2086:GLN:N	2.26	0.68
1:A:2893:LEU:O	1:A:2898:ARG:N	2.26	0.68
2:B:3833:MET:O	2:B:3839:ASP:N	2.25	0.68
1:A:886:ASN:O	1:A:890:GLY:N	2.27	0.68
1:A:1484:GLU:O	1:A:1495:LEU:N	2.27	0.68
1:A:3519:LEU:O	1:A:3523:LEU:N	2.26	0.68
1:A:3384:SER:O	1:A:3388:ARG:N	2.26	0.68
1:A:898:TRP:O	1:A:901:PHE:N	2.27	0.67
1:A:3781:TYR:O	1:A:3785:GLU:N	2.26	0.67
2:B:4441:ILE:N	2:B:4494:TYR:O	2.27	0.67
1:A:1931:LYS:O	1:A:1939:LYS:N	2.28	0.67
1:A:3470:LEU:O	1:A:3473:ILE:N	2.28	0.67
2:B:606:LEU:HA	2:B:612:GLY:HA2	1.77	0.67
2:B:4123:ASP:O	2:B:4126:ILE:N	2.26	0.67
1:A:3835:GLU:O	1:A:3839:LYS:N	2.27	0.67
3:C:3741:ASN:O	3:C:3745:GLU:N	2.27	0.67
1:A:3594:ARG:O	1:A:3621:TRP:N	2.26	0.67
2:B:918:GLY:O	2:B:921:SER:C	2.34	0.67
1:A:679:LEU:O	1:A:683:ARG:N	2.26	0.66
1:A:2495:ASP:O	1:A:2496:MET:N	2.29	0.65
3:C:1127:LYS:O	3:C:1131:SER:N	2.29	0.65
1:A:2374:SER:O	1:A:2378:GLY:N	2.29	0.65
2:B:2285:LEU:N	2:B:2293:ILE:O	2.30	0.65
2:B:1804:PHE:O	2:B:1808:LYS:N	2.28	0.65
2:B:2465:TRP:O	2:B:2469:ALA:N	2.30	0.65
1:A:1592:ARG:O	1:A:1593:SER:N	2.29	0.65
3:C:2492:ILE:O	3:C:2634:MET:N	2.29	0.65
2:B:2890:GLY:N	2:B:3022:PHE:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1398:GLY:O	1:A:1524:ARG:N	2.32	0.63
2:B:2189:GLY:O	2:B:2193:VAL:N	2.31	0.63
1:A:2928:VAL:O	1:A:2932:SER:N	2.29	0.63
1:A:1616:ALA:O	1:A:1620:LEU:N	2.32	0.62
3:C:3870:GLU:O	3:C:3874:TRP:N	2.31	0.62
3:C:2910:PHE:O	3:C:2914:GLY:N	2.31	0.62
2:B:1748:ASP:O	2:B:1752:GLY:N	2.31	0.62
1:A:3406:ARG:O	1:A:3688:ALA:N	2.33	0.62
1:A:2175:SER:O	1:A:2177:ILE:N	2.32	0.62
2:B:605:LYS:CB	2:B:611:GLN:CB	2.79	0.61
2:B:3393:ARG:O	2:B:3396:GLU:N	2.34	0.61
2:B:3516:PRO:O	2:B:3519:LEU:N	2.32	0.61
1:A:834:VAL:O	1:A:837:LEU:N	2.34	0.61
1:A:3487:VAL:O	1:A:3491:LYS:N	2.33	0.61
1:A:1915:ALA:O	1:A:1919:SER:N	2.33	0.61
2:B:918:GLY:O	2:B:922:ASN:N	2.34	0.60
7:G:81:SER:N	7:G:142:GLU:O	2.34	0.60
2:B:2904:THR:O	2:B:2908:GLY:N	2.34	0.60
2:B:3590:LEU:O	2:B:3594:LEU:N	2.31	0.60
1:A:1348:TYR:O	1:A:1355:LYS:N	2.34	0.60
1:A:3206:LYS:O	1:A:3210:ALA:N	2.32	0.60
2:B:1802:GLU:O	2:B:1806:ILE:N	2.30	0.60
1:A:3135:LEU:O	1:A:3139:VAL:N	2.35	0.59
2:B:1660:ILE:O	2:B:1672:PHE:N	2.35	0.59
1:A:1701:GLN:O	1:A:1705:ASN:N	2.35	0.59
2:B:902:ILE:O	2:B:1079:ASN:N	2.36	0.59
1:A:3214:GLU:O	1:A:3218:ASN:N	2.35	0.59
1:A:2628:GLN:O	1:A:2632:GLU:N	2.34	0.58
2:B:2657:LYS:O	2:B:2660:SER:N	2.36	0.58
1:A:3023:ARG:O	1:A:3027:LYS:N	2.37	0.58
2:B:1734:THR:O	2:B:1737:VAL:N	2.37	0.58
3:C:2912:ASP:O	3:C:2918:LYS:N	2.37	0.58
5:E:418:SER:O	5:E:420:THR:N	2.37	0.58
2:B:2781:ASP:O	2:B:3047:TRP:N	2.37	0.57
1:A:3615:CYS:O	1:A:3619:GLY:N	2.37	0.57
2:B:606:LEU:HA	2:B:612:GLY:CA	2.34	0.57
2:B:4547:VAL:O	2:B:4558:VAL:N	2.36	0.57
1:A:1400:ALA:O	1:A:1526:ILE:N	2.38	0.57
2:B:4191:GLY:O	2:B:4196:GLY:N	2.38	0.57
1:A:4135:GLY:O	1:A:4140:PHE:N	2.38	0.57
4:D:400:TRP:N	4:D:417:ILE:O	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:ASP:O	1:A:834:VAL:N	2.38	0.56
2:B:2818:LEU:N	2:B:2835:THR:O	2.38	0.56
1:A:674:ASN:HA	1:A:811:PHE:HA	1.87	0.56
1:A:1689:GLY:O	1:A:1693:THR:N	2.38	0.56
3:C:3117:PHE:CB	3:C:3433:ALA:HB2	2.36	0.56
1:A:2417:PHE:N	1:A:2487:ALA:O	2.38	0.56
2:B:1255:GLU:O	2:B:1256:ASN:C	2.43	0.55
3:C:1120:THR:O	3:C:1124:LYS:N	2.40	0.55
2:B:3579:ILE:O	2:B:3625:MET:N	2.39	0.55
1:A:3492:LYS:O	1:A:3496:GLU:N	2.39	0.55
1:A:1727:ASN:O	1:A:1731:LYS:N	2.39	0.55
1:A:4080:ALA:HB1	1:A:4092:TYR:O	2.07	0.55
3:C:1376:MET:O	3:C:1379:HIS:N	2.40	0.54
1:A:2102:LEU:O	1:A:2106:GLY:N	2.40	0.54
1:A:2499:ARG:O	1:A:2503:PHE:N	2.40	0.54
2:B:1437:GLU:O	2:B:1440:ILE:N	2.41	0.54
2:B:1254:TYR:O	2:B:1258:ASN:CB	2.55	0.54
1:A:3733:SER:O	1:A:3737:GLY:N	2.41	0.54
1:A:3438:HIS:O	1:A:3442:GLY:N	2.41	0.53
1:A:2176:THR:O	1:A:2177:ILE:N	2.40	0.53
1:A:3048:SER:O	1:A:3052:GLY:N	2.41	0.53
1:A:4006:GLU:O	1:A:4011:LEU:N	2.41	0.53
1:A:3894:VAL:O	1:A:3898:LEU:N	2.39	0.53
1:A:219:GLY:O	1:A:226:TYR:N	2.41	0.53
2:B:3874:ILE:O	2:B:3878:ILE:N	2.40	0.53
3:C:2324:GLY:O	3:C:2327:LEU:N	2.41	0.53
1:A:3817:ASN:O	1:A:3821:ALA:N	2.41	0.52
2:B:1982:THR:O	2:B:1994:LEU:N	2.42	0.52
1:A:1327:ARG:O	1:A:1330:ASN:N	2.42	0.52
2:B:4390:SER:O	2:B:4394:SER:N	2.43	0.51
1:A:2287:GLU:N	1:A:2305:ASP:O	2.43	0.51
15:O:32:SER:O	15:O:36:ILE:N	2.43	0.51
1:A:3850:PRO:O	1:A:3855:MET:N	2.43	0.51
1:A:3991:SER:O	1:A:3995:ALA:HB3	2.10	0.51
1:A:2920:GLN:O	1:A:2924:MET:N	2.41	0.51
2:B:3533:LEU:N	2:B:3642:THR:O	2.43	0.51
1:A:3409:PHE:O	1:A:3413:LYS:N	2.43	0.51
2:B:902:ILE:O	2:B:1078:ILE:HA	2.11	0.51
1:A:1302:ASP:O	1:A:1304:SER:N	2.44	0.51
1:A:3552:ILE:O	1:A:3556:PHE:N	2.43	0.51
1:A:679:LEU:O	1:A:682:VAL:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:565:GLY:HA2	2:B:571:SER:H	1.75	0.50
3:C:2397:GLY:O	3:C:2633:ASN:N	2.43	0.50
1:A:2077:TYR:N	1:A:2123:GLN:O	2.42	0.50
2:B:3985:PHE:N	2:B:4076:LEU:O	2.42	0.50
1:A:3615:CYS:O	1:A:3620:HIS:N	2.43	0.50
4:D:516:PHE:O	4:D:528:TRP:N	2.45	0.50
1:A:4036:THR:O	1:A:4040:GLN:N	2.45	0.49
2:B:605:LYS:O	2:B:612:GLY:HA3	2.12	0.49
1:A:4155:LYS:O	1:A:4159:SER:N	2.45	0.49
1:A:4037:ALA:O	1:A:4041:GLY:N	2.41	0.49
1:A:115:LYS:O	1:A:119:TYR:N	2.46	0.49
1:A:2324:ASN:HA	1:A:2327:ASN:O	2.13	0.49
1:A:4085:GLY:O	1:A:4088:GLY:N	2.46	0.49
2:B:1577:ARG:O	2:B:1579:ASP:N	2.45	0.49
1:A:3764:LEU:O	1:A:3768:LEU:N	2.38	0.49
3:C:2932:GLU:O	3:C:2935:LEU:N	2.42	0.49
1:A:3217:ILE:O	1:A:3221:SER:N	2.40	0.48
2:B:2446:GLY:O	2:B:2675:SER:N	2.43	0.48
1:A:3840:TYR:O	1:A:3844:LYS:N	2.44	0.48
1:A:2891:ARG:O	1:A:2895:LEU:N	2.44	0.48
1:A:3468:LYS:O	1:A:3472:THR:N	2.44	0.48
1:A:4077:LEU:O	1:A:4102:HIS:N	2.47	0.48
1:A:3996:ASP:HA	1:A:4168:ASP:HA	1.96	0.48
3:C:2864:LEU:N	3:C:3023:THR:O	2.45	0.48
1:A:1721:LYS:O	1:A:1725:GLY:N	2.45	0.48
2:B:2888:LEU:O	2:B:3022:PHE:N	2.46	0.48
3:C:3592:ASP:O	3:C:3595:LEU:N	2.47	0.48
1:A:4124:TYR:O	1:A:4146:MET:N	2.46	0.47
1:A:2827:ILE:O	1:A:2831:GLU:N	2.44	0.47
2:B:1814:SER:O	2:B:1818:LEU:N	2.39	0.47
3:C:1142:ILE:O	3:C:1146:GLN:N	2.47	0.47
2:B:919:GLU:O	2:B:921:SER:O	2.33	0.47
1:A:4001:ASN:O	1:A:4005:GLN:N	2.39	0.47
2:B:1322:TYR:O	2:B:1326:LYS:N	2.47	0.47
2:B:1459:THR:N	2:B:1466:THR:O	2.43	0.47
2:B:4548:TYR:HA	2:B:4557:TYR:HA	1.97	0.47
1:A:2955:MET:O	1:A:2959:LYS:N	2.47	0.47
1:A:2406:CYS:O	1:A:2410:GLU:N	2.38	0.47
2:B:1372:MET:O	2:B:1376:LEU:N	2.48	0.46
2:B:4412:GLN:O	2:B:4414:TRP:N	2.48	0.46
3:C:3744:ARG:O	3:C:3748:ARG:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1372:MET:O	2:B:1375:VAL:N	2.48	0.46
2:B:962:PHE:O	2:B:967:GLN:N	2.37	0.46
1:A:1300:GLN:O	1:A:1302:ASP:N	2.44	0.46
1:A:2638:ALA:HB2	1:A:2875:ALA:HB1	1.97	0.46
2:B:1568:SER:O	2:B:1571:GLU:N	2.44	0.46
2:B:2631:GLY:O	2:B:2645:LEU:N	2.42	0.46
1:A:233:ASP:O	1:A:237:ASP:N	2.48	0.45
1:A:1826:GLN:O	1:A:1829:SER:N	2.50	0.45
3:C:2738:GLU:O	3:C:2742:ALA:N	2.49	0.45
1:A:1338:GLU:O	1:A:1341:TRP:N	2.50	0.45
2:B:2500:LEU:O	2:B:2504:GLN:N	2.50	0.45
3:C:1320:LYS:HA	3:C:1324:ALA:HB1	1.99	0.45
1:A:887:ALA:O	1:A:891:ILE:N	2.32	0.44
2:B:1359:PHE:O	2:B:1363:ASN:N	2.41	0.44
2:B:1814:SER:O	2:B:1817:TRP:N	2.50	0.44
2:B:2779:PHE:O	2:B:2783:PHE:N	2.50	0.44
1:A:3777:ASP:O	1:A:3781:TYR:N	2.46	0.44
1:A:2525:ASN:O	1:A:2529:SER:CB	2.66	0.44
2:B:929:THR:O	2:B:932:ASN:N	2.50	0.44
16:P:85:LYS:O	16:P:86:LYS:CB	2.65	0.44
1:A:54:ASN:C	1:A:56:GLN:H	2.21	0.44
1:A:879:ARG:O	1:A:883:LYS:N	2.45	0.44
1:A:1399:CYS:HA	1:A:1524:ARG:C	2.38	0.44
1:A:3996:ASP:HA	1:A:4168:ASP:O	2.17	0.44
3:C:3439:GLN:O	3:C:3443:LEU:N	2.42	0.44
1:A:2:PRO:HA	1:A:306:LEU:HA	2.00	0.43
1:A:256:ILE:O	1:A:268:ILE:HA	2.18	0.43
1:A:4114:PRO:O	1:A:4116:ASP:N	2.51	0.43
2:B:1375:VAL:O	2:B:1378:LEU:N	2.51	0.43
16:P:30:ALA:C	16:P:32:TRP:H	2.21	0.43
1:A:1399:CYS:HA	1:A:1524:ARG:O	2.18	0.43
2:B:3748:ARG:O	2:B:3751:ALA:HB3	2.18	0.43
1:A:397:PHE:O	1:A:405:GLU:HA	2.19	0.43
1:A:2044:TYR:HA	1:A:2085:PRO:HA	2.00	0.43
2:B:482:GLU:O	2:B:484:LYS:N	2.52	0.43
3:C:1400:TYR:O	3:C:1403:GLU:N	2.47	0.43
3:C:3503:TRP:O	3:C:3506:GLN:N	2.52	0.43
1:A:1758:LEU:N	1:A:1797:LEU:O	2.47	0.43
1:A:3437:ASP:O	1:A:3441:ILE:N	2.44	0.42
1:A:2943:LYS:O	1:A:2947:ASN:N	2.44	0.42
2:B:3466:ALA:O	2:B:3469:ARG:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3726:VAL:O	3:C:3730:LEU:N	2.44	0.42
8:H:10:VAL:N	8:H:80:TYR:O	2.50	0.42
3:C:3540:TRP:O	3:C:3544:LYS:N	2.50	0.42
1:A:904:LEU:O	1:A:908:LEU:N	2.51	0.42
1:A:4077:LEU:N	1:A:4102:HIS:O	2.51	0.42
2:B:1494:VAL:O	2:B:1498:TYR:N	2.52	0.42
1:A:295:ASP:O	1:A:299:LEU:N	2.53	0.42
1:A:2203:ALA:HB2	1:A:3956:ALA:HA	2.02	0.42
2:B:3883:PHE:O	2:B:3887:ALA:N	2.44	0.42
3:C:3784:GLU:O	3:C:3787:ASP:N	2.53	0.42
1:A:2620:ILE:O	1:A:2624:VAL:N	2.48	0.41
2:B:2402:ILE:O	2:B:2405:ILE:N	2.52	0.41
2:B:3652:GLY:O	2:B:3655:GLU:N	2.53	0.41
2:B:2563:LYS:N	2:B:2601:ILE:O	2.52	0.41
2:B:1748:ASP:O	2:B:1751:GLY:N	2.46	0.41
2:B:1360:LYS:HA	2:B:1363:ASN:CB	2.50	0.41
4:D:421:GLY:HA2	4:D:459:GLY:O	2.20	0.41
1:A:3202:GLU:O	1:A:3206:LYS:N	2.52	0.41
1:A:2434:LEU:O	1:A:2438:GLY:N	2.48	0.41
2:B:1536:GLU:O	2:B:1539:ARG:N	2.53	0.41
1:A:3629:LEU:O	1:A:3631:GLN:N	2.54	0.41
3:C:934:GLU:O	3:C:945:ASN:N	2.41	0.41
1:A:1226:LEU:O	1:A:1230:ALA:HB2	2.20	0.41
1:A:1368:GLU:O	1:A:1421:ALA:HB1	2.21	0.41
1:A:3022:ILE:O	1:A:3026:GLU:N	2.51	0.41
2:B:2640:GLU:O	2:B:2642:ARG:N	2.54	0.41
2:B:4487:ALA:HB2	2:B:4528:LYS:H	1.86	0.41
1:A:2495:ASP:O	1:A:2497:ARG:N	2.54	0.40
2:B:2385:HIS:O	2:B:2388:ASN:N	2.54	0.40
1:A:941:GLU:O	1:A:945:ASP:CB	2.69	0.40
1:A:511:GLU:HA	1:A:523:THR:HA	2.02	0.40
1:A:1750:ASP:O	1:A:1752:ASN:N	2.55	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	3707/4168 (89%)	3206 (86%)	493 (13%)	8 (0%)	47	81
2	B	3893/4595 (85%)	3484 (90%)	398 (10%)	11 (0%)	41	77
3	C	3846/4620 (83%)	3509 (91%)	330 (9%)	7 (0%)	47	81
4	D	313/667 (47%)	268 (86%)	45 (14%)	0	100	100
4	d	122/667 (18%)	112 (92%)	10 (8%)	0	100	100
5	E	337/670 (50%)	287 (85%)	50 (15%)	0	100	100
5	e	96/670 (14%)	86 (90%)	10 (10%)	0	100	100
6	F	96/133 (72%)	79 (82%)	17 (18%)	0	100	100
7	G	93/103 (90%)	81 (87%)	12 (13%)	0	100	100
8	H	83/92 (90%)	76 (92%)	7 (8%)	0	100	100
9	I	87/110 (79%)	79 (91%)	8 (9%)	0	100	100
10	J	82/93 (88%)	77 (94%)	5 (6%)	0	100	100
11	K	93/111 (84%)	83 (89%)	10 (11%)	0	100	100
12	L	95/111 (86%)	90 (95%)	5 (5%)	0	100	100
13	M	84/87 (97%)	77 (92%)	7 (8%)	0	100	100
14	N	107/132 (81%)	100 (94%)	7 (6%)	0	100	100
15	O	109/117 (93%)	99 (91%)	10 (9%)	0	100	100
16	P	101/110 (92%)	97 (96%)	4 (4%)	0	100	100
17	Y	1127/1200 (94%)	1071 (95%)	54 (5%)	2 (0%)	47	81
All	All	14471/18456 (78%)	12961 (90%)	1482 (10%)	28 (0%)	50	81

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1823	VAL
2	B	1651	ASN
2	B	1652	PRO
2	B	2557	PRO
2	B	3703	PRO
2	B	4008	PRO
2	B	4432	PRO
3	C	2978	PRO

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Mol	Chain	Res	Type
3	C	2979	PRO
3	C	4182	PRO
3	C	4188	PRO
3	C	4546	PRO
17	Y	723	PRO
17	Y	1106	PRO
1	A	1351	ASP
1	A	4084	ILE
2	B	4556	THR
3	C	1322	ASP
2	B	1245	PRO
2	B	3923	PRO
1	A	982	ILE
1	A	3108	ASN
2	B	4557	TYR
1	A	1040	VAL
1	A	3665	PRO
2	B	3922	MET
3	C	4121	VAL
1	A	3593	GLY

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

5 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	$\#\|Z\| > 2$
20	GTP	Y	1301	-	26,34,34	1.21	2 (7%)	32,54,54	1.65	6 (18%)
18	ADP	C	4704	-	24,29,29	0.92	1 (4%)	29,45,45	1.49	4 (13%)
18	ADP	C	4701	-	24,29,29	0.96	1 (4%)	29,45,45	1.49	3 (10%)
19	ATP	C	4702	-	26,33,33	0.87	1 (3%)	31,52,52	1.68	5 (16%)
18	ADP	C	4703	-	24,29,29	0.93	1 (4%)	29,45,45	1.54	4 (13%)

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
20	GTP	Y	1301	-	-	6/18/38/38	0/3/3/3
18	ADP	C	4704	-	-	3/12/32/32	0/3/3/3
18	ADP	C	4701	-	-	1/12/32/32	0/3/3/3
19	ATP	C	4702	-	-	4/18/38/38	0/3/3/3
18	ADP	C	4703	-	-	4/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Y	1301	GTP	C5-C6	-4.38	1.38	1.47
18	C	4704	ADP	C5-C4	2.25	1.46	1.40
18	C	4701	ADP	C5-C4	2.18	1.46	1.40
20	Y	1301	GTP	C2-N3	2.17	1.38	1.33
18	C	4703	ADP	C5-C4	2.13	1.46	1.40
19	C	4702	ATP	C5-C4	2.03	1.46	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	C	4702	ATP	PA-O3A-PB	-5.12	115.25	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	C	4701	ADP	PA-O3A-PB	-4.56	117.17	132.83
18	C	4704	ADP	PA-O3A-PB	-4.21	118.36	132.83
19	C	4702	ATP	PB-O3B-PG	-4.13	118.64	132.83
18	C	4703	ADP	PA-O3A-PB	-4.13	118.66	132.83
20	Y	1301	GTP	PA-O3A-PB	-4.09	118.78	132.83
20	Y	1301	GTP	PB-O3B-PG	-3.93	119.33	132.83
18	C	4703	ADP	N3-C2-N1	-3.65	122.97	128.68
19	C	4702	ATP	N3-C2-N1	-3.65	122.97	128.68
18	C	4704	ADP	N3-C2-N1	-3.52	123.17	128.68
20	Y	1301	GTP	C5-C6-N1	3.39	119.94	113.95
18	C	4703	ADP	C3'-C2'-C1'	3.17	105.76	100.98
20	Y	1301	GTP	C2-N1-C6	-3.14	119.31	125.10
18	C	4701	ADP	N3-C2-N1	-3.13	123.78	128.68
18	C	4701	ADP	C4-C5-N7	-2.94	106.34	109.40
20	Y	1301	GTP	C8-N7-C5	2.85	108.42	102.99
18	C	4704	ADP	C3'-C2'-C1'	2.79	105.18	100.98
18	C	4704	ADP	C4-C5-N7	-2.54	106.75	109.40
20	Y	1301	GTP	O6-C6-C5	-2.24	120.00	124.37
19	C	4702	ATP	C4-C5-N7	-2.15	107.16	109.40
19	C	4702	ATP	N6-C6-N1	2.15	123.03	118.57
18	C	4703	ADP	C4-C5-N7	-2.09	107.22	109.40

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	C	4703	ADP	C5'-O5'-PA-O1A
18	C	4703	ADP	C5'-O5'-PA-O2A
18	C	4704	ADP	C5'-O5'-PA-O2A
19	C	4702	ATP	C5'-O5'-PA-O1A
19	C	4702	ATP	C5'-O5'-PA-O3A
19	C	4702	ATP	C3'-C4'-C5'-O5'
20	Y	1301	GTP	C5'-O5'-PA-O3A
20	Y	1301	GTP	O4'-C4'-C5'-O5'
20	Y	1301	GTP	C3'-C4'-C5'-O5'
19	C	4702	ATP	O4'-C4'-C5'-O5'
18	C	4704	ADP	C5'-O5'-PA-O3A
18	C	4704	ADP	C5'-O5'-PA-O1A
20	Y	1301	GTP	C5'-O5'-PA-O1A
20	Y	1301	GTP	PB-O3A-PA-O5'
18	C	4703	ADP	C5'-O5'-PA-O3A
20	Y	1301	GTP	PG-O3B-PB-O2B

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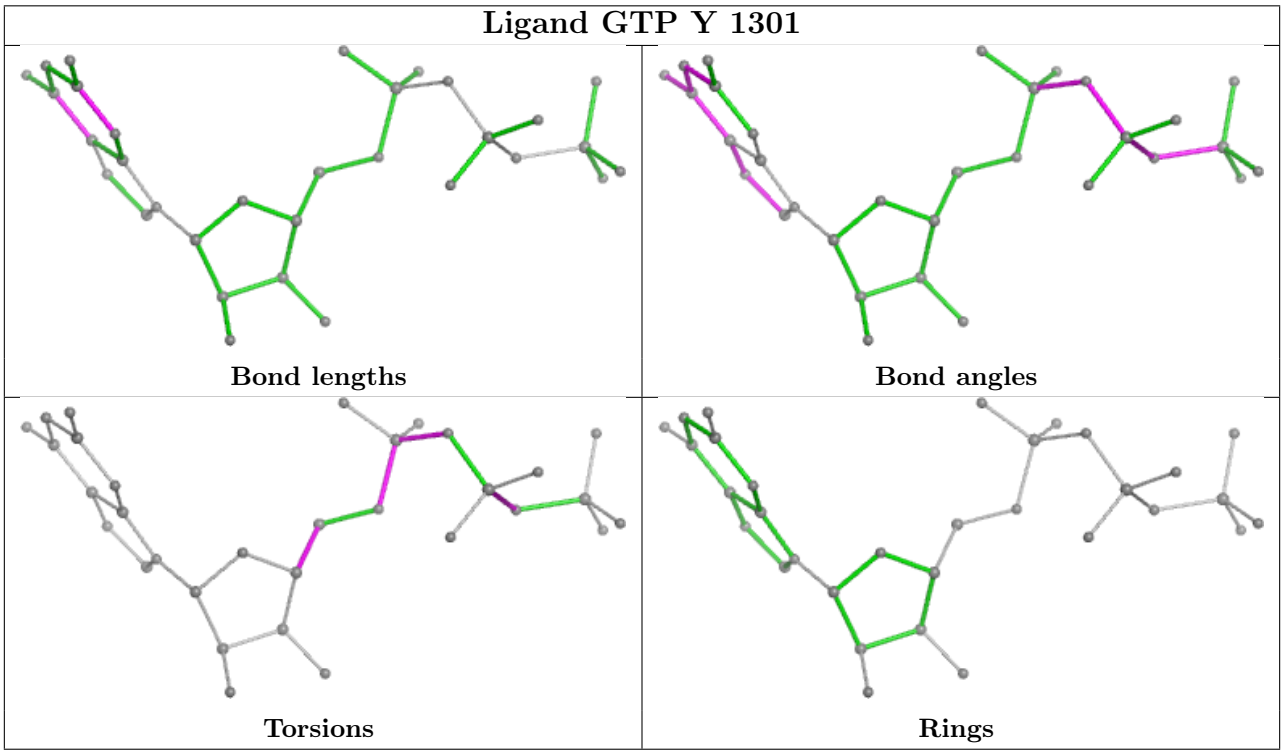
Mol	Chain	Res	Type	Atoms
18	C	4701	ADP	C5'-O5'-PA-O1A
18	C	4703	ADP	O4'-C4'-C5'-O5'

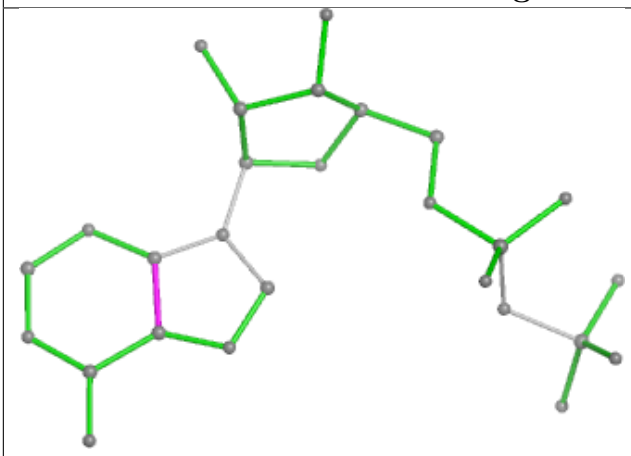
There are no ring outliers.

No monomer is involved in short contacts.

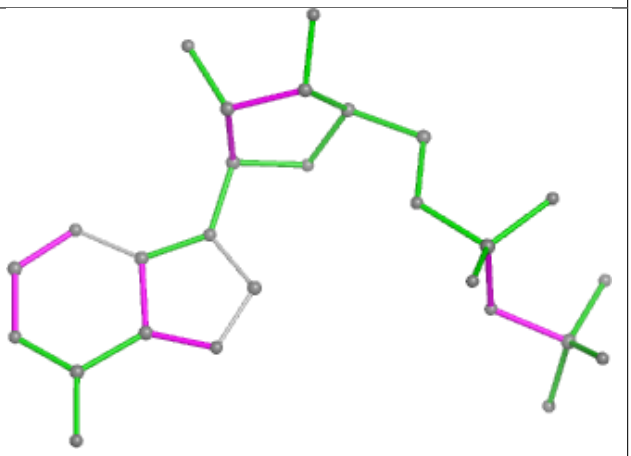
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



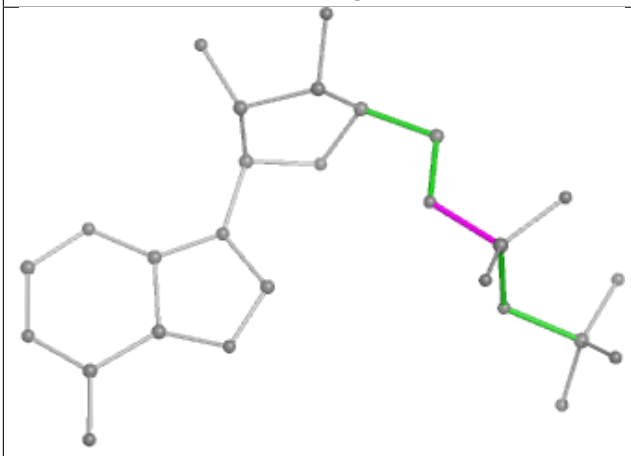
Ligand ADP C 4704



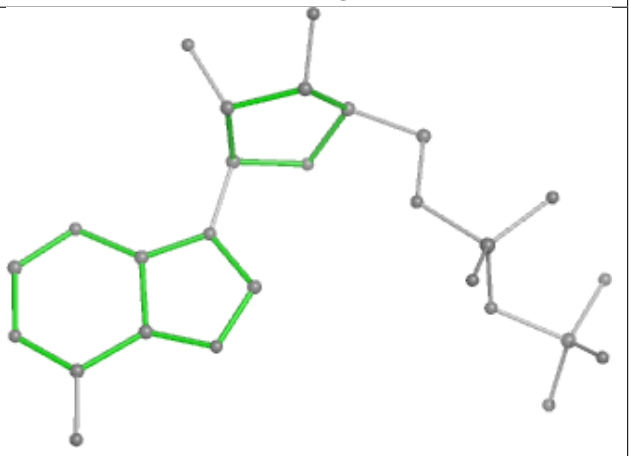
Bond lengths



Bond angles

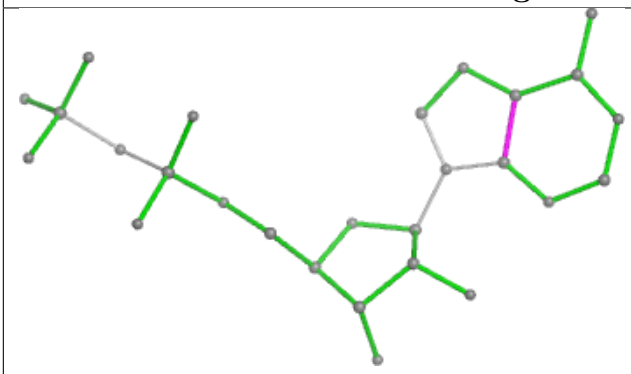


Torsions

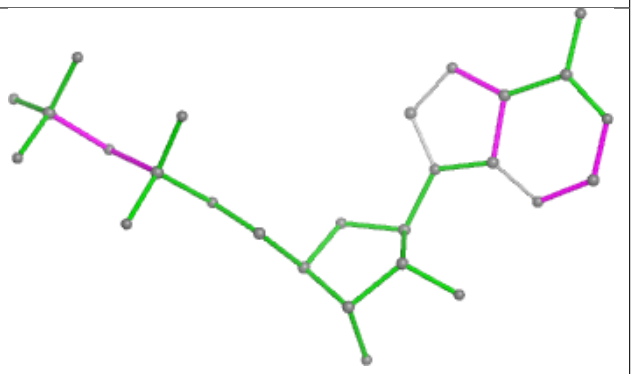


Rings

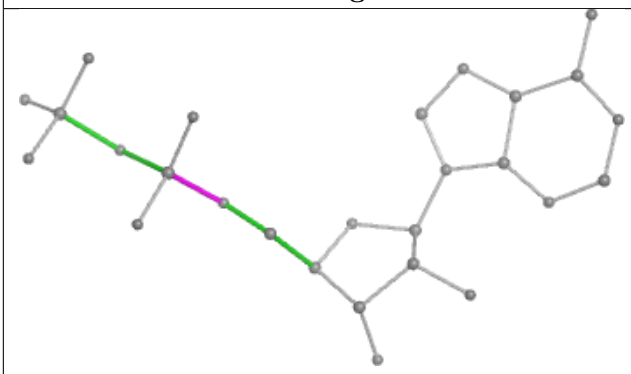
Ligand ADP C 4701



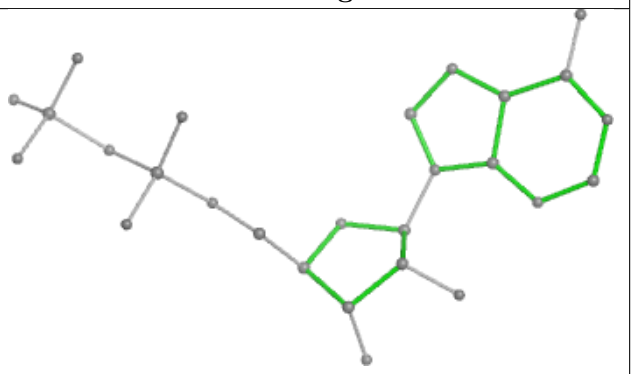
Bond lengths



Bond angles

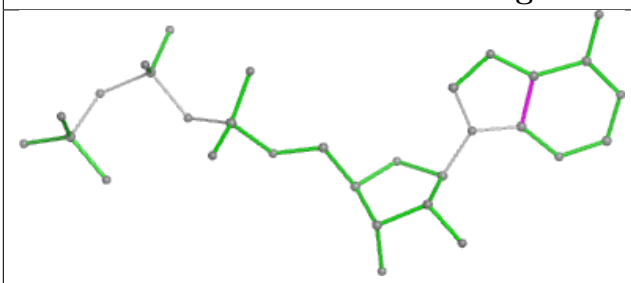


Torsions

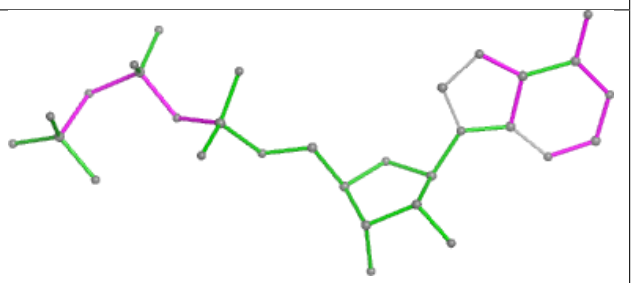


Rings

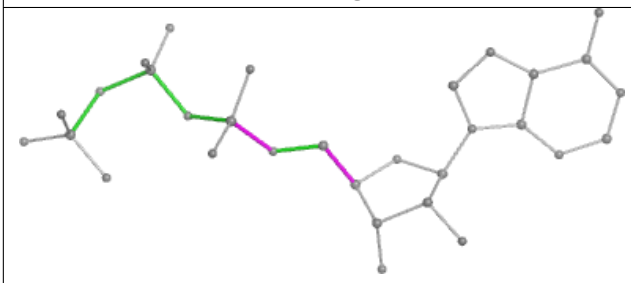
Ligand ATP C 4702



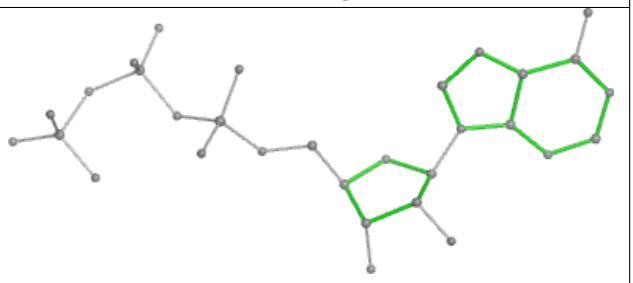
Bond lengths



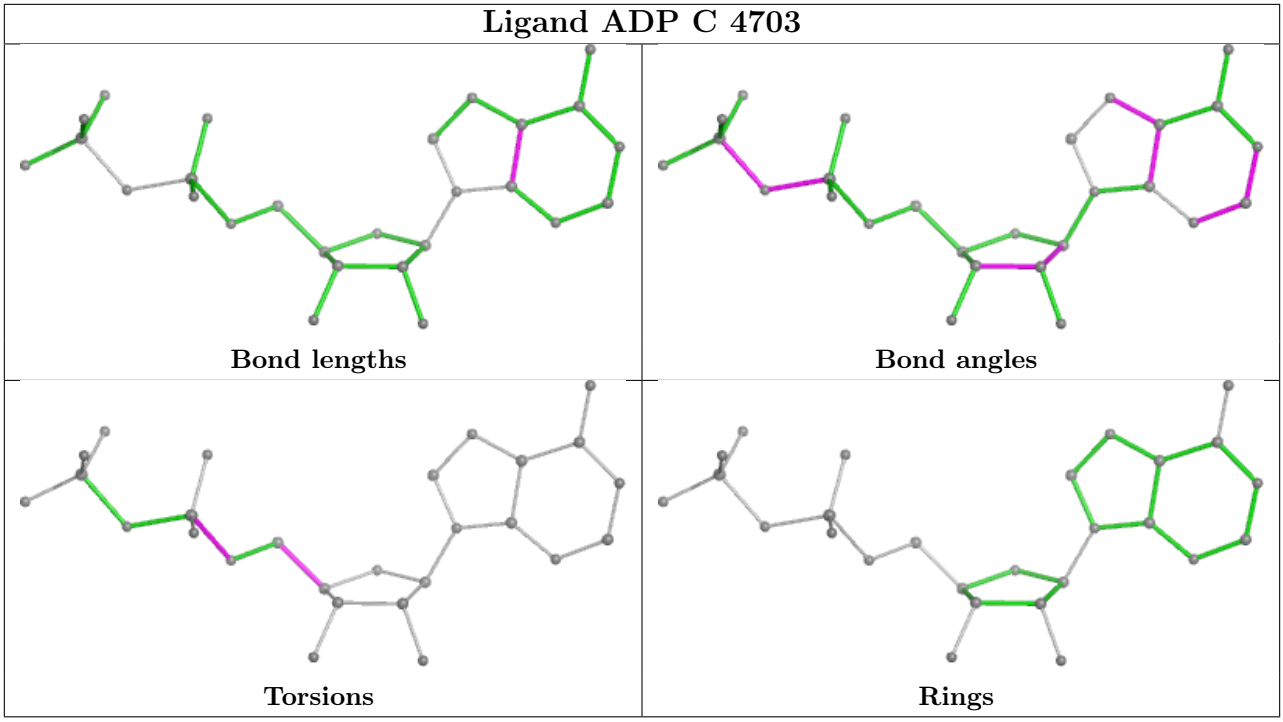
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	23
2	B	12
5	e	2
4	d	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	d	201:GLN	C	235:TRP	N	31.73
1	A	389:ASP	C	390:THR	N	29.62
1	A	486:ASP	C	487:GLN	N	21.39
1	A	1299:VAL	C	1300:GLN	N	17.01
1	A	2300:SER	C	2301:ASP	N	13.90
1	A	2232:GLU	C	2233:PRO	N	13.48
1	B	4440:MET	C	4441:ILE	N	12.83

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1507:PRO	C	1508:GLY	N	12.62
1	B	2495:LYS	C	2496:VAL	N	12.29
1	A	2533:PRO	C	2534:VAL	N	10.43
1	A	4018:CYS	C	4019:ILE	N	10.38
1	B	2583:MET	C	2584:VAL	N	9.43
1	A	2296:ALA	C	2297:GLY	N	9.01
1	A	4109:ASN	C	4110:ALA	N	8.24
1	A	2058:THR	C	2059:LEU	N	8.10
1	A	2897:GLN	C	2898:ARG	N	6.96
1	A	1972:PHE	C	1973:ASP	N	6.76
1	B	1775:VAL	C	1776:ARG	N	6.38
1	e	66:VAL	C	72:LYS	N	6.29
1	e	81:LYS	C	95:GLU	N	6.23
1	A	2132:ALA	C	2133:GLY	N	5.82
1	A	3472:THR	C	3473:ILE	N	5.79
1	A	3921:LYS	C	3922:THR	N	5.38
1	B	2658:SER	C	2659:GLY	N	5.09
1	A	2630:GLU	C	2631:ALA	N	4.86
1	B	2091:ARG	C	2092:GLY	N	4.86
1	B	3793:ASP	C	3794:GLU	N	4.35
1	A	1725:GLY	C	1726:TYR	N	4.16
1	A	2000:LEU	C	2001:MET	N	3.91
1	A	2612:GLU	C	2613:THR	N	3.44
1	B	4123:ASP	C	4124:PRO	N	3.30
1	B	2229:LYS	C	2230:THR	N	3.20
1	B	3552:ASN	C	3553:LEU	N	3.19
1	A	2495:ASP	C	2496:MET	N	3.16
1	B	2702:LYS	C	2703:ALA	N	3.15
1	B	2006:PRO	C	2007:GLY	N	3.09
1	A	1592:ARG	C	1593:SER	N	3.08
1	A	2176:THR	C	2177:ILE	N	3.05