Full wwPDB EM Validation Report (i)

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PDB ID	:	5T0H
EMDB ID	:	EMD-8335
Title	:	Structural basis for dynamic regulation of the human 26S proteasome
Authors	:	Chen, S.; Wu, J.; Lu, Y.; Ma, Y.B.; Lee, B.H.; Yu, Z.; Ouyang, Q.; Finley, D.; Kirschner, M.W.; Mao, Y.
Deposited on	:	2016-08-16
Resolution	:	6.80 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 (i) 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 (1)) were used in the production of this report:

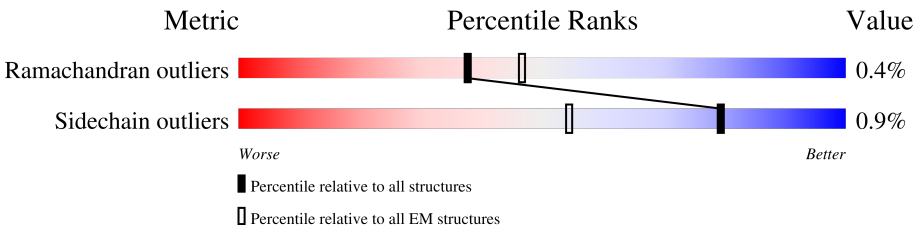
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.80 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	433	82% • 17%
2	B	440	75% • 22%
3	C	398	93% • •
4	D	418	90% • 9%
5	E	403	87% • 12%
6	F	439	81% • 17%
7	G	245	98% •
8	H	233	98% •
9	I	260	96% •
10	J	247	96% • •

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Mol	Chain	Length	Quality of chain
11	K	240	94% • 5%
12	L	268	88% 11%
13	M	254	94% 6%
14	N	238	80% 20%
15	O	276	80% 20%
16	P	204	100%
17	Q	201	99% •
18	R	262	77% 23%
19	S	240	89% 11%
20	T	263	81% 18%
21	U	953	84% • 15%
22	V	533	88% • 10%
23	W	456	51% • 48%
24	X	422	19% 81%
25	Y	389	95% • •
26	Z	324	87% • 12%
27	a	376	98% • •
28	b	377	50% 49%
29	c	309	90% • 7%
30	d	349	72% • 26%
31	e	70	34% 66%
32	f	749	90% • 7%

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 73509 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 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	361	2835	1788	501	528	18	0	0

- Molecule 2 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	341	2662	1671	453	526	12	0	0

- Molecule 3 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	384	3015	1894	540	564	17	0	0

- Molecule 4 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	380	3040	1923	524	580	13	0	0

- Molecule 5 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	353	2790	1755	494	525	16	0	0

- Molecule 6 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	366	2863	1802	496	549	16	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	240	1826	1160	305	348	13	0	0

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	232	1708	1081	289	333	5	0	0

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	250	1912	1204	329	371	8	0	0

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	239	1704	1056	308	335	5	0	0

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	228	1722	1080	284	348	10	0	0

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	238	1850	1159	334	346	11	0	0

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	240	1856	1178	314	353	11	0	0

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	191	1430	893	245	280	12	0	0

- Molecule 15 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	220	1643	1033	280	318	12	0	0

- Molecule 16 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	204	1585	1010	262	294	19	0	0

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	199	1570	1006	265	290	9	0	0

- Molecule 18 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	201	1548	974	273	292	9	0	0

- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	213	1641	1036	282	313	10	0	0

- Molecule 20 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	215	1667	1052	285	318	12	0	0

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	U	806	6287	3990	1075	1178	44	0	0

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	V	480	3852	2444	684	710	14	0	0

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	W	236	1940	1237	331	361	11	0	0

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	X	81	647	414	107	124	2	0	0

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Y	378	3115	1987	533	578	17	0	0

- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Z	286	2281	1457	392	427	5	0	0

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	a	373	2995	1911	510	559	15	0	0

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	b	191	1458	910	261	279	8	0	0

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	c	287	2260	1430	389	422	19	0	0

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	d	257	2116	1371	346	390	9	0	0

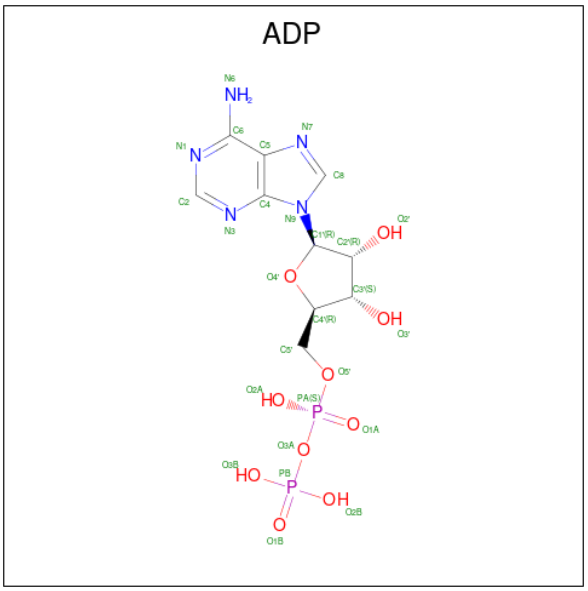
- Molecule 31 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	e	24	197	121	34	40	2	0	0

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	f	694	5331	3364	899	1027	41	0	0

- Molecule 33 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

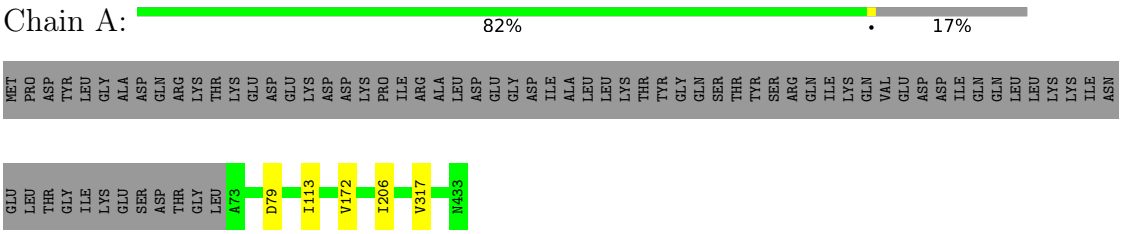
Mol	Chain	Residues	Atoms		AltConf
34	c	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

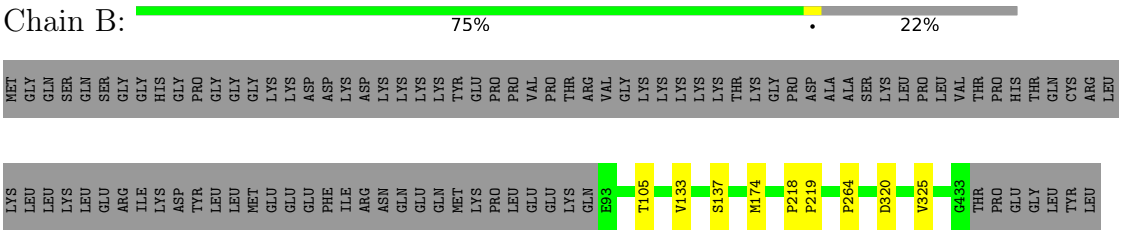
- Molecule 1: 26S protease regulatory subunit 7

Chain A:



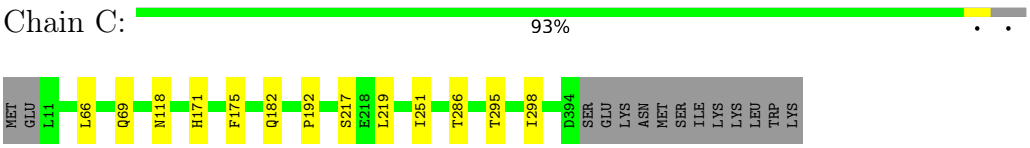
- Molecule 2: 26S protease regulatory subunit 4

Chain B:



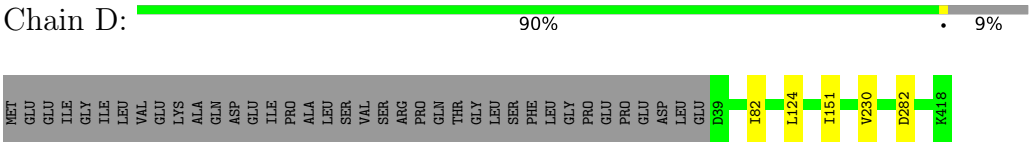
- Molecule 3: 26S protease regulatory subunit 8

Chain C:



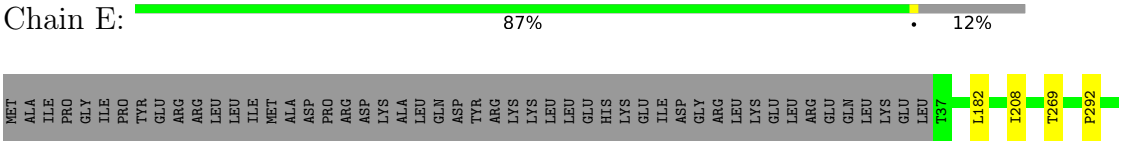
- Molecule 4: 26S protease regulatory subunit 6B

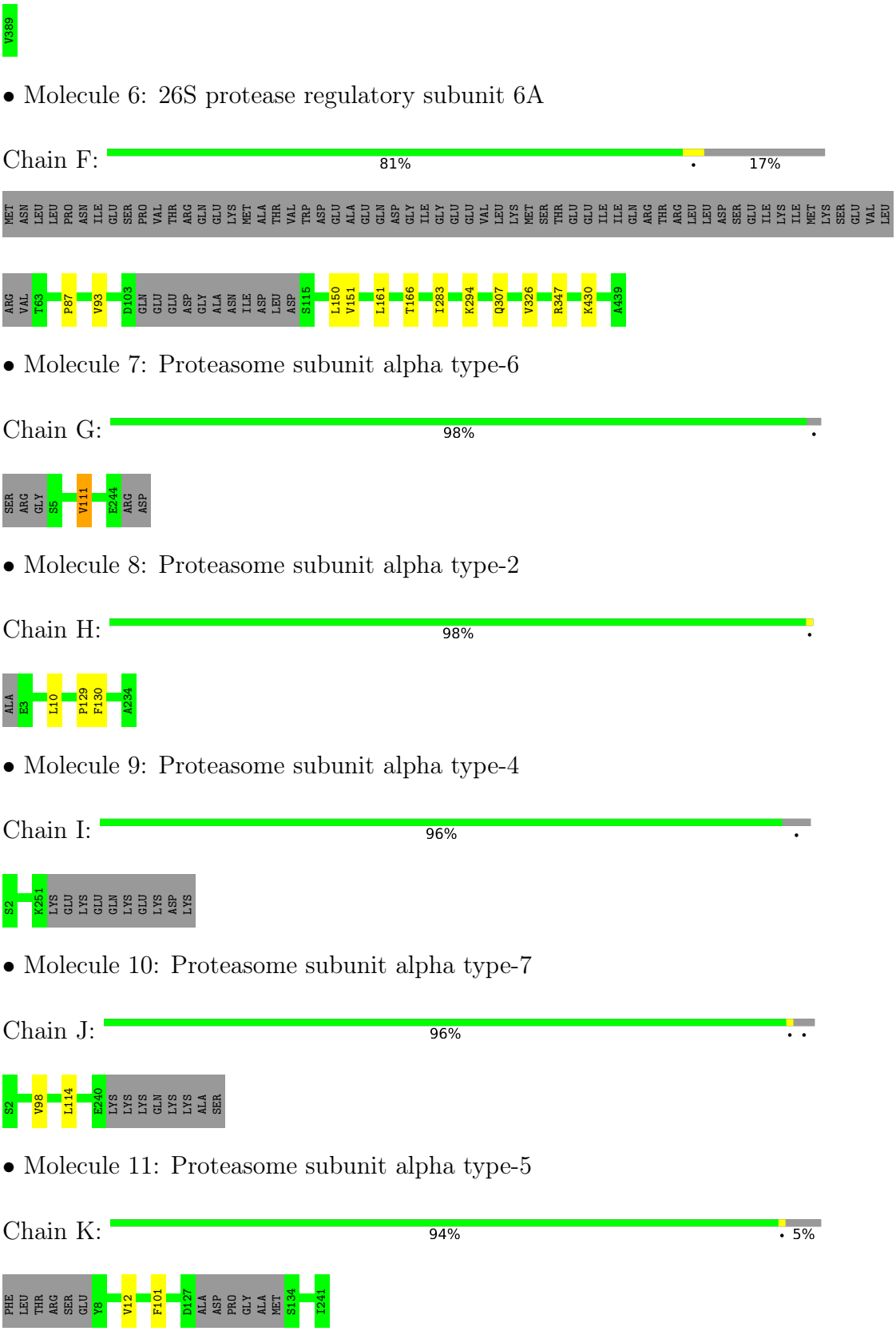
Chain D:



- Molecule 5: 26S protease regulatory subunit 10B

Chain E:




V389
• Molecule 6: 26S protease regulatory subunit 6A
Chain F:
81%
17%
MET ASN LEU LEU PRO ASN ILE GLU SER PRO VAL THR ARG GLN GLU LYS MET ALA THR VAL TRP ASP GLU ALA GLU GLN ASP GLY ILE GLY GLU GLU VAL LEU LYS MET SER THR GLU GLU ILE ILE GLN ARG THR ARG LEU LEU ASP SER GLU ILE LYS ILE MET LYS SER GLU VAL LEU
ARG VAL T63 P87 V93 D103 GLN GLU GLU ASP GLY ALA ASN ILE ASP LEU ASP S115 L150 V151 L161 T166 I283 K294 Q307 V326 R347 K430 A439
• Molecule 7: Proteasome subunit alpha type-6
Chain G:
98%
SER ARG GLY S5 V111 E244 ARG ASP
• Molecule 8: Proteasome subunit alpha type-2
Chain H:
98%
ALA E3 L10 P129 F130 A234
• Molecule 9: Proteasome subunit alpha type-4
Chain I:
96%
S2 K251 LYS GLU LYS GLU GLN LYS GLU LYS ASP LYS
• Molecule 10: Proteasome subunit alpha type-7
Chain J:
96%
S2 V98 L114 E240 LYS LYS LYS GLN LYS LYS ALA SER
• Molecule 11: Proteasome subunit alpha type-5
Chain K:
94%
5%
PHE LEU THR ARG SER GLU Y8 V12 F101 D127 ALA ASP PRO GLY ALA MET S134 I241
• Molecule 12: Proteasome subunit alpha type-1

Chain L: 88% 11%

GLN LEU SER LYS VAL LYS PHE ARG N4 L46 Q241 ARG LYS ALA GLN PRO ALA GLN PRO ALA ASP GLU PRO ALA GLU LYS ALA ASP GLU PRO MET GLU HIS

• Molecule 13: Proteasome subunit alpha type-3

Chain M: 94% 6%

SER SER ILE GLY T5 V227 K244 GLU GLU ASP GLU SER ASP ASP ASP ASN MET

• Molecule 14: Proteasome subunit beta type-6

Chain N: 80% 20%

ALA ALA THR LEU LEU ALA ALA ARG GLY ALA GLY PRO ALA PRO ALA TRP GLY PRO GLU ALA PHE THR PRO ASP TRP GLU SER ARG GLU VAL SER THR GLY T1 G191 ASP GLN ILE PRO LYS PHE ALA VAL ALA THR LEU PRO PRO ALA

• Molecule 15: Proteasome subunit beta type-7

Chain O: 80% 20%

ALA ALA VAL SER VAL TYR ALA PRO PRO VAL GLY GLY PHE SER PHE ASP ASN CYS ARG ARG ASN ALA VAL LEU GLU ALA ASP PHE ALA LYS ARG GLY TYR LYS LEU PRO LYS VAL ARG LYS THR GLY T1 E220 ILE GLU VAL LEU GLU GLU THR VAL GLN THR MET ASP THR SER

• Molecule 16: Proteasome subunit beta type-3

Chain P: 100%

There are no outlier residues recorded for this chain.

• Molecule 17: Proteasome subunit beta type-2

Chain Q: 99%

M1 Q199 GLY SER

• Molecule 18: Proteasome subunit beta type-5

Chain R: 77% 23%

ALA LEU ALA SER VAL LEU GLU ARG PRO LEU PRO VAL ASN GLN ARG GLY PHE PHE GLY LEU GLY GLY ARG ALA ASP LEU LEU ASP LEU GLY PRO GLY SER LEU SER ASP GLY LEU SER LEU ALA ALA PRO GLY TRP GLY VAL PRO GLU GLU PRO GLY ILE GLU MET LEU HIS GLY T1

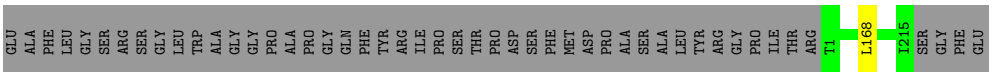
G201 SER THR PRO

• Molecule 19: Proteasome subunit beta type-1

Chain S: 89% 11%

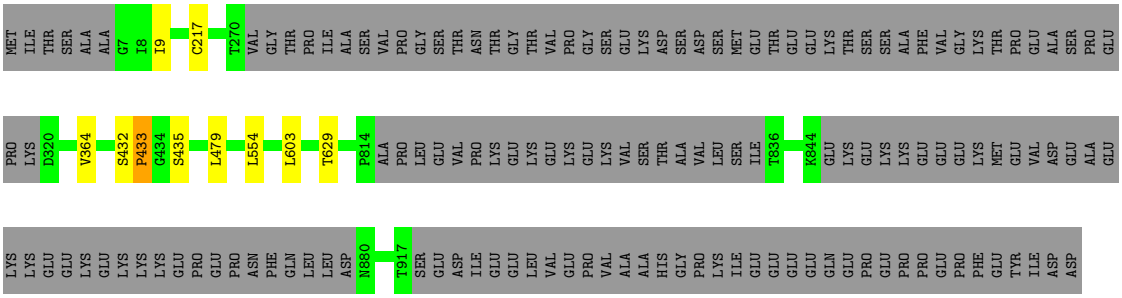
• Molecule 20: Proteasome subunit beta type-4

Chain T: 81% 18%



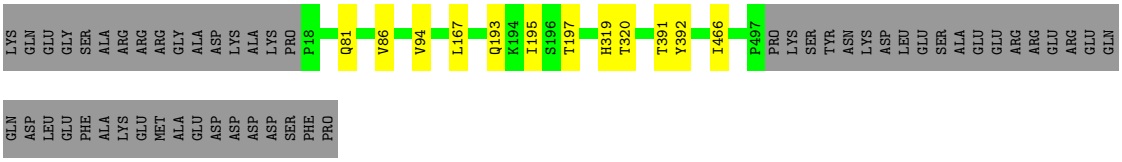
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

Chain U: 84% • 15%



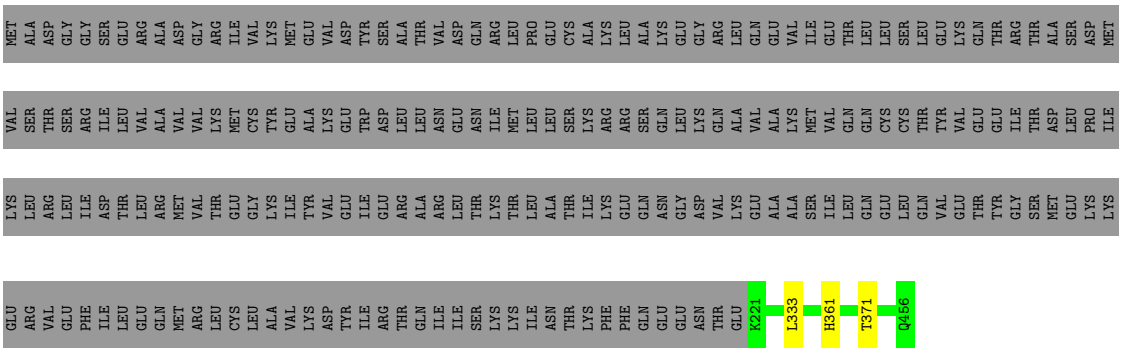
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

Chain V: 88% • 10%



• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

Chain W: 51% • 48%



• Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 19% 81%

MET ALA ALA ALA ALA VAL VAL GLU PHE GLN ARG ALA GLN SER LEU LEU SER THR ASP ARG GLU ALA SER ILE ASP ILE LEU HIS SER ILE VAL LYS ARG ASP ILE GLN GLU ASN ASP GLU GLU ALA VAL GLN VAL LYS GLU GLN SER ILE LEU GLU LEU GLY SER LEU LEU ALA LYS THR

GLY GLN ALA ALA GLU LEU GLY GLY LEU LEU LYS TYR VAL ARG PRO PHE LEU ASN SER ILE SER LYS ALA LYS ALA ALA ARG LEU VAL ARG SER LEU LEU ASP LEU PHE LEU ASP MET GLU ALA ALA THR GLY GLN GLU VAL GLU LEU CYS LEU GLU CYS ILE GLU TRP ALA LYS SER GLU

LYS ARG THR PHE LEU ARG GLN ALA LEU GLU GLU ALA ARG LEU VAL SER LEU TYR PHE ASP THR LYS ARG TYR GLN GLU ALA LEU HIS LEU GLY SER GLN LEU LEU ARG GLU LEU LYS LYS MET ASP ASP LYS ALA LEU LEU VAL GLU VAL GLN LEU LEU GLU SER LYS THR TYR HIS ALA LEU

SER ASN LEU PRO LYS ALA ARG ALA ALA LEU THR SER ALA ARG THR THR ALA ASN ALA ILE TYR CYS PRO PRO LYS LEU GLN ALA THR LEU ASP MET GLN SER GLN ILE ILE HIS ALA ALA GLU GLU LYS ASP TRP LYS THR ALA TYR SER TYR PHE TYR GLU ALA PHE GLU GLY TYR ASP

SER ILE ASP SER PRO LYS ALA ILE THR SER LEU LYS TYR MET LEU LEU CYS LYS ILE MET LEU ASN THR PRO GLU ASP VAL GLN ALA LEU VAL SER GLY LYS LEU ALA LEU ARG TYR ALA GLY ARG GLN THR GLU ALA LEU LYS CYS VAL ALA GLN ALA SER LYS ASN ARG SER LEU ALA

ASP PHE GLU LYS ALA LEU THR ASP TYR ARG ALA GLU LEU ARG ASP ASP PRO ILE ILE SER THR HIS LEU ALA LYS LEU TYR ASP ASN LEU LEU GLU GLN ASN LEU ILE ARG VAL ILE GLU PRO F342 T422

• Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 95%

MET PRO LEU GLU ASN LEU GLU GLU GLU GLY LEU P12 W63 V67 L287 T315 F323 L343 V350 T356 N357 M389

• Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 87% 12%

MET PRO GLU LEU A5 L133 V144 T186 I191 Y228 G290 GLN GLU LYS GLU GLU SER LYS LYS ASP ARG LYS GLU ASP LYS GLU LYS ASP LYS ASP LYS GLU LYS SER ASP VAL LYS LYS GLU GLU LYS LYS GLU LYS

• Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 98%

MET LYS ASP V4 E215 V336 V340 T376

• Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

Chain b: 50% 49%

M1 T53 G191 GLU GLY GLY ALA MET LEU GLY LEU GLY ALA SER ASP PHE GLU PHE GLY VAL ASP PRO SER ALA ASP PRO GLU LEU ALA LEU ALA LEU ARG VAL SER MET GLU GLU GLN ARG GLN ARG GLN GLU GLU GLU ALA ARG ARG ALA ALA ALA ALA ALA SER ALA ALA GLU ALA

GLY ILE ALA THR THR GLY THR GLU ASP SER ASP ASP ALA LEU LEU LYS LYS MET THR ILE SER GLN GLN GLU PHE GLY ARG THR GLY LEU PRO ASP LEU SER SER MET THR GLU GLU GLU GLN ILE ALA TYR ALA MET GLN MET SER LEU GLN GLY ALA GLU PHE GLY GLN ALA GLU SER ALA

ASP ILE ASP ALA SER SER ALA MET ASP THR SER GLU PRO ALA LYS GLU GLU ASP ASP TYR ASP VAL MET GLN ASP PRO GLU PHE LEU GLN SER VAL LEU GLU ASN LEU PRO GLY VAL ASP PRO ASN ASN GLU ALA ILE ARG ASN ALA MET GLY SER LEU ALA SER GLN ALA THR LYS ASP

GLY LYS LYS ASP LYS LYS GLU GLU ASP LYS LYS

- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

Chain c: 90% • 7%

ASP ARG LEU LEU ARG LEU GLY GLY GLY MET PRO GLY LEU GLY GLN GLY PRO PRO THR ASP ALA PRO A24 V156 I157 I189 H194 E227 G228 L229 S243 V244 K310

- Molecule 30: 26S proteasome non-ATPase regulatory subunit 8

Chain d: 72% • 26%

PHE ILE LYS GLY ARG ALA PRO ARG ALA PRO PRO ARG GLU ARG ARG ARG ALA THR ARG GLY GLY LEU ARG GLN VAL VAL ALA PRO PRO ARG ALA LEU GLY SER THR SER ARG PRO HIS PHE ARG ARG ALA SER VAL CYS ARG ARG ARG CYS ARG LYS SER GLY GLY LEU LEU ALA ALA SER

ARG LYS MET ALA ALA ALA VAL ASN GLY ALA ALA GLY PHE SER SER SER GLY PRO ALA ALA THR SER GLY ALA VAL LEU GLN ALA ALA THR GLY M1 Y2 E3 L107 H116 R121 R213 V257

- Molecule 31: 26S proteasome complex subunit DSS1

Chain e: 34% 66%

M1 D9 LEU GLY LEU LEU GLU GLU ASP ASP GLU PHE GLU GLU PHE PRO ALA GLU ASP TRP ALA GLY LEU ASP GLU ASP GLU ASP ALA HIS VAL TRP GLU ASP ASN TRP ASP ASP ASP ASN VAL GLU ASP ASP PHE SER ASN GLN L56 S70

- Molecule 32: 26S proteasome non-ATPase regulatory subunit 2

Chain f: 90% • 7%

M1 I62 L107 V131 I281 T317 C371 L391 V447 E459 T526 L600 G636 G661 Q667 L681 R686 Q689 V694 GLY GLN ALA GLY LYS PRO LYS THR ILE THR GLY PHE GLN THR HIS THR THR PRO VAL LEU LEU ALA HIS

GLY GLU ARG ALA GLU LEU ALA THR GLU GLU PHE LEU PRO VAL THR PRO ILE LEU GLU GLY PHE VAL ILE LEU ARG LYS ASN PRO ASN TYR ASP LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.27	0/2886	0.54	0/3899
2	B	0.27	0/2700	0.55	0/3645
3	C	0.25	0/3054	0.52	1/4107 (0.0%)
4	D	0.26	0/3090	0.53	0/4168
5	E	0.25	0/2835	0.48	0/3821
6	F	0.26	0/2903	0.54	0/3912
7	G	0.23	0/1859	0.45	0/2523
8	H	0.25	0/1743	0.46	0/2372
9	I	0.23	0/1942	0.45	0/2628
10	J	0.23	0/1728	0.44	0/2358
11	K	0.24	0/1747	0.44	0/2364
12	L	0.24	0/1885	0.44	0/2552
13	M	0.23	0/1891	0.42	0/2552
14	N	0.24	0/1454	0.42	0/1967
15	O	0.23	0/1670	0.43	0/2265
16	P	0.24	0/1614	0.41	0/2177
17	Q	0.23	0/1603	0.41	0/2174
18	R	0.23	0/1579	0.39	0/2134
19	S	0.24	0/1671	0.41	0/2253
20	T	0.25	0/1700	0.41	0/2305
21	U	0.23	0/6396	0.42	0/8646
22	V	0.25	0/3929	0.52	2/5309 (0.0%)
23	W	0.24	0/1975	0.46	0/2659
24	X	0.22	0/655	0.40	0/877
25	Y	0.24	0/3173	0.47	2/4273 (0.0%)
26	Z	1.86	6/2324 (0.3%)	0.53	0/3150
27	a	1.52	2/3052 (0.1%)	0.55	4/4130 (0.1%)
28	b	0.25	0/1478	0.43	0/2001
29	c	0.25	0/2302	0.53	2/3110 (0.1%)
30	d	0.25	0/2162	0.51	0/2919
31	e	0.24	0/198	0.53	0/258
32	f	0.27	1/5413 (0.0%)	0.53	3/7317 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.51	9/74611 (0.0%)	0.48	14/100825 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
3	C	0	1
5	E	0	1
6	F	0	2
21	U	0	3
22	V	0	2
25	Y	0	1
30	d	0	1
32	f	0	2
All	All	0	15

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	215	GLU	CG-CD	82.57	2.75	1.51
26	Z	228	TYR	CD2-CE2	46.09	2.08	1.39
26	Z	228	TYR	CD1-CE1	45.24	2.07	1.39
26	Z	228	TYR	CE1-CZ	34.72	1.83	1.38
26	Z	228	TYR	CE2-CZ	33.47	1.82	1.38
26	Z	228	TYR	CG-CD1	26.67	1.73	1.39
26	Z	228	TYR	CG-CD2	26.35	1.73	1.39
27	a	215	GLU	CB-CG	6.88	1.65	1.52
32	f	681	LEU	C-N	6.33	1.46	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	215	GLU	OE1-CD-OE2	-19.13	100.35	123.30
27	a	215	GLU	CG-CD-OE1	6.35	131.00	118.30
29	c	243	SER	C-N-CA	6.19	137.17	121.70
27	a	215	GLU	CB-CG-CD	6.17	130.86	114.20
32	f	459	GLU	N-CA-C	6.13	127.56	111.00
3	C	217	SER	C-N-CA	5.99	136.67	121.70
25	Y	63	TRP	C-N-CA	5.79	136.19	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	f	661	GLY	N-CA-C	5.68	127.29	113.10
25	Y	287	LEU	CA-CB-CG	5.54	128.04	115.30
22	V	195	ILE	C-N-CA	5.32	135.00	121.70
32	f	636	GLY	N-CA-C	5.27	126.28	113.10
27	a	215	GLU	CG-CD-OE2	5.17	128.65	118.30
29	c	243	SER	CA-C-N	5.09	128.40	117.20
22	V	81	GLN	C-N-CA	5.07	134.37	121.70

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	133	VAL	Peptide
2	B	264	PRO	Peptide
3	C	171	HIS	Peptide
5	E	292	PRO	Peptide
6	F	294	LYS	Peptide
6	F	87	PRO	Peptide
21	U	432	SER	Peptide
21	U	433	PRO	Peptide
21	U	435	SER	Peptide
22	V	193	GLN	Peptide
22	V	319	HIS	Peptide
25	Y	357	ASN	Peptide
30	d	3	GLU	Peptide
32	f	667	GLN	Peptide
32	f	681	LEU	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	359/433 (83%)	304 (85%)	53 (15%)	2 (1%)	25	66
2	B	339/440 (77%)	298 (88%)	38 (11%)	3 (1%)	17	57
3	C	382/398 (96%)	317 (83%)	62 (16%)	3 (1%)	19	60
4	D	378/418 (90%)	328 (87%)	49 (13%)	1 (0%)	41	77
5	E	351/403 (87%)	299 (85%)	51 (14%)	1 (0%)	41	77
6	F	362/439 (82%)	316 (87%)	45 (12%)	1 (0%)	41	77
7	G	238/245 (97%)	221 (93%)	16 (7%)	1 (0%)	34	72
8	H	230/233 (99%)	210 (91%)	19 (8%)	1 (0%)	34	72
9	I	248/260 (95%)	230 (93%)	18 (7%)	0	100	100
10	J	237/247 (96%)	221 (93%)	15 (6%)	1 (0%)	34	72
11	K	224/240 (93%)	203 (91%)	20 (9%)	1 (0%)	34	72
12	L	236/268 (88%)	222 (94%)	14 (6%)	0	100	100
13	M	238/254 (94%)	218 (92%)	20 (8%)	0	100	100
14	N	189/238 (79%)	175 (93%)	14 (7%)	0	100	100
15	O	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
16	P	202/204 (99%)	188 (93%)	14 (7%)	0	100	100
17	Q	197/201 (98%)	183 (93%)	14 (7%)	0	100	100
18	R	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
19	S	211/240 (88%)	199 (94%)	12 (6%)	0	100	100
20	T	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
21	U	798/953 (84%)	729 (91%)	67 (8%)	2 (0%)	41	77
22	V	478/533 (90%)	416 (87%)	60 (13%)	2 (0%)	34	72
23	W	234/456 (51%)	213 (91%)	21 (9%)	0	100	100
24	X	79/422 (19%)	75 (95%)	4 (5%)	0	100	100
25	Y	376/389 (97%)	336 (89%)	38 (10%)	2 (0%)	29	69
26	Z	284/324 (88%)	251 (88%)	32 (11%)	1 (0%)	34	72
27	a	369/376 (98%)	340 (92%)	27 (7%)	2 (0%)	29	69
28	b	189/377 (50%)	178 (94%)	11 (6%)	0	100	100
29	c	285/309 (92%)	242 (85%)	39 (14%)	4 (1%)	11	46
30	d	255/349 (73%)	219 (86%)	34 (13%)	2 (1%)	19	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	e	20/70 (29%)	16 (80%)	4 (20%)	0	100	100
32	f	686/749 (92%)	574 (84%)	108 (16%)	4 (1%)	25	66
All	All	9304/11269 (83%)	8324 (90%)	946 (10%)	34 (0%)	38	72

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	111	VAL
11	K	12	VAL
21	U	364	VAL
25	Y	350	VAL
29	c	244	VAL
32	f	62	ILE
32	f	447	VAL
1	A	206	ILE
32	f	131	VAL
3	C	298	ILE
29	c	157	ILE
4	D	151	ILE
8	H	10	LEU
25	Y	67	VAL
26	Z	144	VAL
27	a	336	VAL
27	a	340	VAL
29	c	156	VAL
32	f	281	ILE
30	d	121	ARG
22	V	466	ILE
30	d	213	ARG
21	U	433	PRO
2	B	218	PRO
2	B	219	PRO
2	B	325	VAL
5	E	208	ILE
22	V	86	VAL
3	C	192	PRO
3	C	251	ILE
10	J	98	VAL
29	c	189	ILE
1	A	172	VAL
6	F	326	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/372 (83%)	305 (99%)	3 (1%)	76	86
2	B	298/385 (77%)	294 (99%)	4 (1%)	69	82
3	C	332/346 (96%)	324 (98%)	8 (2%)	49	69
4	D	333/366 (91%)	329 (99%)	4 (1%)	71	83
5	E	308/353 (87%)	306 (99%)	2 (1%)	86	92
6	F	312/379 (82%)	303 (97%)	9 (3%)	42	64
7	G	193/209 (92%)	192 (100%)	1 (0%)	88	93
8	H	164/190 (86%)	162 (99%)	2 (1%)	71	83
9	I	193/220 (88%)	193 (100%)	0	100	100
10	J	152/210 (72%)	151 (99%)	1 (1%)	84	90
11	K	186/202 (92%)	185 (100%)	1 (0%)	88	93
12	L	198/229 (86%)	197 (100%)	1 (0%)	88	93
13	M	192/211 (91%)	191 (100%)	1 (0%)	88	93
14	N	148/180 (82%)	148 (100%)	0	100	100
15	O	177/227 (78%)	177 (100%)	0	100	100
16	P	172/173 (99%)	172 (100%)	0	100	100
17	Q	164/171 (96%)	164 (100%)	0	100	100
18	R	153/201 (76%)	153 (100%)	0	100	100
19	S	174/198 (88%)	174 (100%)	0	100	100
20	T	175/214 (82%)	174 (99%)	1 (1%)	86	92
21	U	685/816 (84%)	679 (99%)	6 (1%)	78	87
22	V	414/459 (90%)	408 (99%)	6 (1%)	67	80
23	W	218/416 (52%)	215 (99%)	3 (1%)	67	80
24	X	74/362 (20%)	74 (100%)	0	100	100
25	Y	334/344 (97%)	330 (99%)	4 (1%)	71	83
26	Z	257/295 (87%)	254 (99%)	3 (1%)	71	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	a	333/336 (99%)	333 (100%)	0	100	100
28	b	167/312 (54%)	166 (99%)	1 (1%)	86	92
29	c	252/267 (94%)	249 (99%)	3 (1%)	71	83
30	d	231/293 (79%)	229 (99%)	2 (1%)	78	87
31	e	22/63 (35%)	22 (100%)	0	100	100
32	f	582/628 (93%)	574 (99%)	8 (1%)	67	80
All	All	7901/9627 (82%)	7827 (99%)	74 (1%)	79	87

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ASP
1	A	113	ILE
1	A	317	VAL
2	B	105	THR
2	B	137	SER
2	B	174	MET
2	B	320	ASP
3	C	66	LEU
3	C	69	GLN
3	C	118	ASN
3	C	175	PHE
3	C	182	GLN
3	C	219	LEU
3	C	286	THR
3	C	295	THR
4	D	82	ILE
4	D	124	LEU
4	D	230	VAL
4	D	282	ASP
5	E	182	LEU
5	E	269	THR
6	F	93	VAL
6	F	150	LEU
6	F	151	VAL
6	F	161	LEU
6	F	166	THR
6	F	283	ILE
6	F	307	GLN
6	F	347	ARG

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Mol	Chain	Res	Type
6	F	430	LYS
7	G	111	VAL
8	H	129	PRO
8	H	130	PHE
10	J	114	LEU
11	K	101	PHE
12	L	46	LEU
13	M	227	VAL
20	T	168	LEU
21	U	9	ILE
21	U	217	CYS
21	U	479	LEU
21	U	554	LEU
21	U	603	LEU
21	U	629	THR
22	V	94	VAL
22	V	167	LEU
22	V	197	THR
22	V	320	THR
22	V	391	THR
22	V	392	TYR
23	W	333	LEU
23	W	361	HIS
23	W	371	THR
25	Y	315	THR
25	Y	323	PHE
25	Y	343	LEU
25	Y	356	THR
26	Z	133	LEU
26	Z	186	THR
26	Z	191	ILE
28	b	53	THR
29	c	194	HIS
29	c	227	GLU
29	c	229	LEU
30	d	107	LEU
30	d	116	HIS
32	f	107	LEU
32	f	317	THR
32	f	371	CYS
32	f	391	LEU
32	f	526	THR

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Mol	Chain	Res	Type
32	f	600	LEU
32	f	686	ARG
32	f	689	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	304	ASN
1	A	305	GLN
1	A	358	HIS
1	A	414	ASN
2	B	119	ASN
2	B	154	HIS
2	B	193	GLN
2	B	314	ASN
3	C	32	GLN
3	C	40	GLN
3	C	182	GLN
3	C	279	GLN
3	C	296	ASN
4	D	65	GLN
4	D	91	GLN
4	D	99	ASN
4	D	193	GLN
4	D	222	HIS
4	D	304	ASN
4	D	376	ASN
5	E	55	GLN
5	E	141	GLN
6	F	83	ASN
6	F	207	ASN
6	F	258	GLN
6	F	323	ASN
6	F	392	ASN
7	G	123	GLN
7	G	127	GLN
11	K	23	GLN
19	S	108	ASN
21	U	107	HIS
21	U	115	ASN
21	U	421	GLN

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Mol	Chain	Res	Type
21	U	685	GLN
21	U	734	GLN
22	V	177	ASN
22	V	242	HIS
22	V	329	HIS
22	V	400	HIS
23	W	264	GLN
23	W	444	HIS
24	X	406	ASN
25	Y	77	ASN
25	Y	351	ASN
26	Z	235	ASN
27	a	86	GLN
27	a	193	GLN
28	b	76	HIS
29	c	44	HIS
29	c	101	GLN
29	c	172	HIS
29	c	190	GLN
29	c	241	ASN
29	c	287	HIS
30	d	245	GLN
32	f	86	ASN
32	f	246	HIS
32	f	269	GLN
32	f	372	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
33	ADP	E	401	-	24,29,29	1.00	2 (8%)	29,45,45	1.47	4 (13%)
33	ADP	A	501	-	24,29,29	0.99	1 (4%)	29,45,45	1.42	4 (13%)
33	ADP	C	501	-	24,29,29	0.98	1 (4%)	29,45,45	1.44	4 (13%)
33	ADP	B	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.35	4 (13%)
33	ADP	D	501	-	24,29,29	0.93	1 (4%)	29,45,45	1.41	4 (13%)
33	ADP	F	501	-	24,29,29	1.01	2 (8%)	29,45,45	1.34	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
33	ADP	E	401	-	-	6/12/32/32	0/3/3/3
33	ADP	A	501	-	-	3/12/32/32	0/3/3/3
33	ADP	C	501	-	-	4/12/32/32	0/3/3/3
33	ADP	B	501	-	-	5/12/32/32	0/3/3/3
33	ADP	D	501	-	-	2/12/32/32	0/3/3/3
33	ADP	F	501	-	-	7/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	501	ADP	C5-C4	2.63	1.47	1.40
33	C	501	ADP	C5-C4	2.56	1.47	1.40
33	F	501	ADP	C5-C4	2.55	1.47	1.40
33	E	401	ADP	C5-C4	2.48	1.47	1.40
33	B	501	ADP	C5-C4	2.44	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	501	ADP	C5-C4	2.43	1.47	1.40
33	E	401	ADP	O4'-C1'	2.14	1.44	1.41
33	F	501	ADP	O4'-C1'	2.10	1.44	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	C	501	ADP	PA-O3A-PB	-3.48	120.87	132.83
33	A	501	ADP	PA-O3A-PB	-3.28	121.56	132.83
33	C	501	ADP	C3'-C2'-C1'	3.28	105.91	100.98
33	E	401	ADP	PA-O3A-PB	-3.26	121.63	132.83
33	E	401	ADP	N3-C2-N1	-3.26	123.59	128.68
33	B	501	ADP	N3-C2-N1	-3.24	123.61	128.68
33	A	501	ADP	C3'-C2'-C1'	3.18	105.77	100.98
33	D	501	ADP	N3-C2-N1	-3.18	123.71	128.68
33	F	501	ADP	N3-C2-N1	-3.17	123.72	128.68
33	D	501	ADP	C3'-C2'-C1'	3.15	105.72	100.98
33	D	501	ADP	PA-O3A-PB	-3.08	122.26	132.83
33	E	401	ADP	C3'-C2'-C1'	3.06	105.58	100.98
33	A	501	ADP	N3-C2-N1	-3.05	123.92	128.68
33	C	501	ADP	N3-C2-N1	-3.02	123.96	128.68
33	B	501	ADP	C4-C5-N7	-2.89	106.39	109.40
33	F	501	ADP	C3'-C2'-C1'	2.82	105.22	100.98
33	E	401	ADP	C4-C5-N7	-2.82	106.46	109.40
33	B	501	ADP	C3'-C2'-C1'	2.82	105.22	100.98
33	C	501	ADP	C4-C5-N7	-2.75	106.54	109.40
33	F	501	ADP	C4-C5-N7	-2.66	106.62	109.40
33	D	501	ADP	C4-C5-N7	-2.57	106.72	109.40
33	B	501	ADP	PA-O3A-PB	-2.34	124.79	132.83
33	A	501	ADP	C4-C5-N7	-2.28	107.02	109.40
33	F	501	ADP	PA-O3A-PB	-2.26	125.08	132.83

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	A	501	ADP	O4'-C4'-C5'-O5'
33	B	501	ADP	PA-O3A-PB-O3B
33	B	501	ADP	C5'-O5'-PA-O3A
33	C	501	ADP	C5'-O5'-PA-O1A
33	E	401	ADP	C5'-O5'-PA-O1A
33	F	501	ADP	C5'-O5'-PA-O1A

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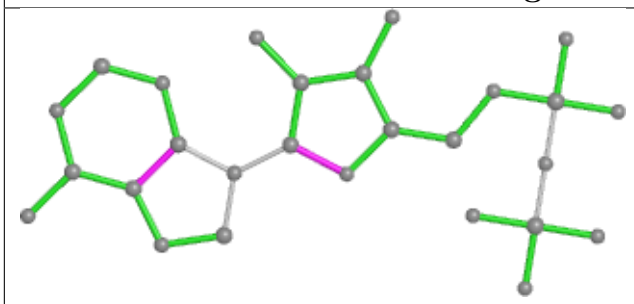
Mol	Chain	Res	Type	Atoms
33	F	501	ADP	C5'-O5'-PA-O2A
33	F	501	ADP	C5'-O5'-PA-O3A
33	F	501	ADP	O4'-C4'-C5'-O5'
33	F	501	ADP	C3'-C4'-C5'-O5'
33	A	501	ADP	C3'-C4'-C5'-O5'
33	B	501	ADP	O4'-C4'-C5'-O5'
33	F	501	ADP	PA-O3A-PB-O2B
33	F	501	ADP	PA-O3A-PB-O3B
33	C	501	ADP	C5'-O5'-PA-O3A
33	B	501	ADP	C5'-O5'-PA-O1A
33	C	501	ADP	C5'-O5'-PA-O2A
33	E	401	ADP	C5'-O5'-PA-O2A
33	E	401	ADP	C4'-C5'-O5'-PA
33	D	501	ADP	C3'-C4'-C5'-O5'
33	D	501	ADP	O4'-C4'-C5'-O5'
33	B	501	ADP	PA-O3A-PB-O1B
33	C	501	ADP	O4'-C4'-C5'-O5'
33	E	401	ADP	C5'-O5'-PA-O3A
33	E	401	ADP	PB-O3A-PA-O1A
33	E	401	ADP	PB-O3A-PA-O2A
33	A	501	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

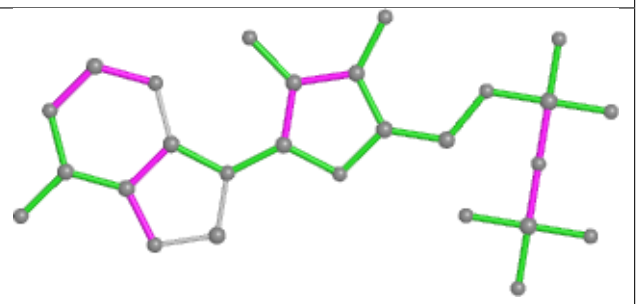
No monomer is involved in short contacts.

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.

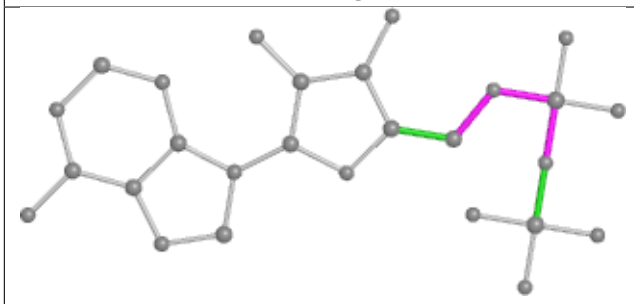
Ligand ADP E 401



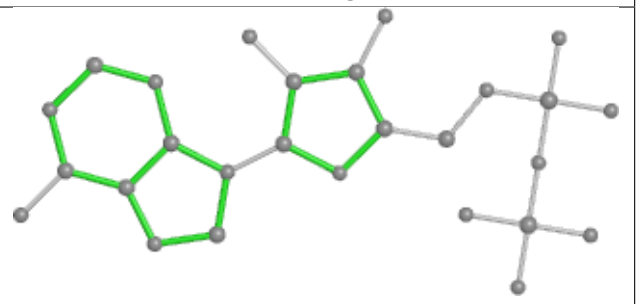
Bond lengths



Bond angles

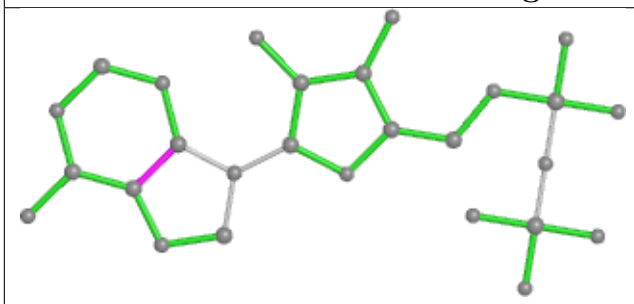


Torsions

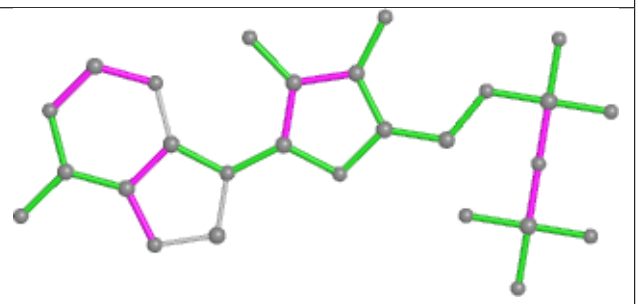


Rings

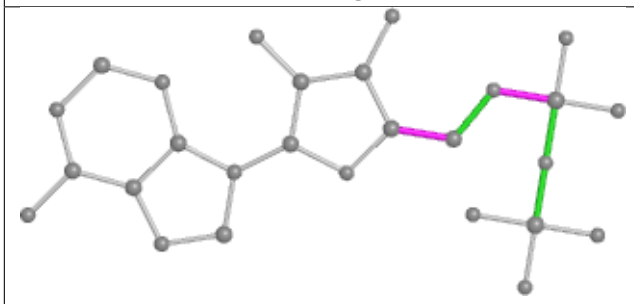
Ligand ADP A 501



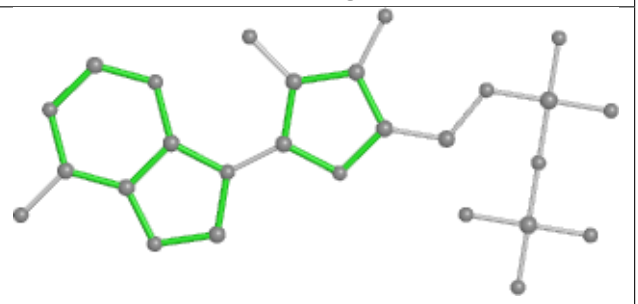
Bond lengths



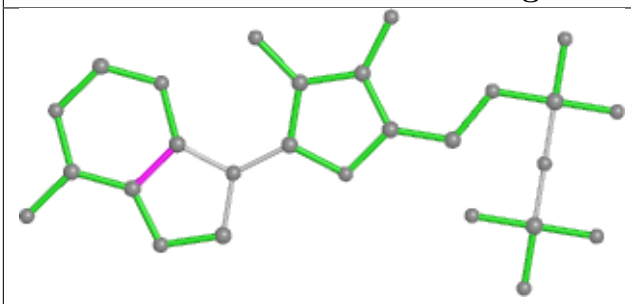
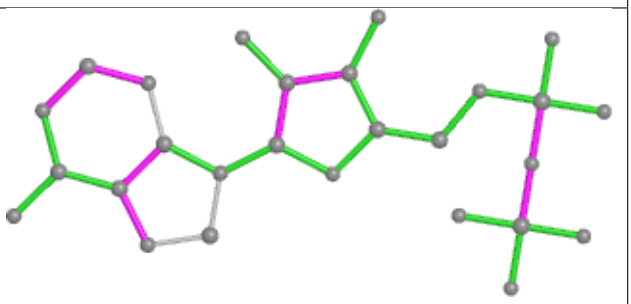
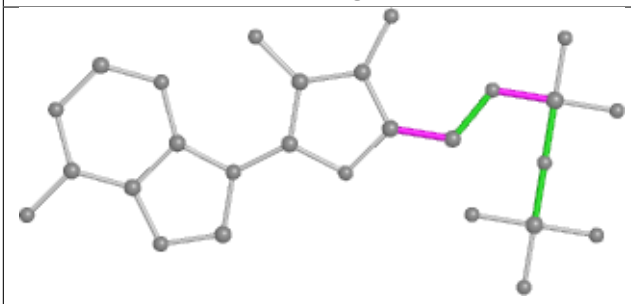
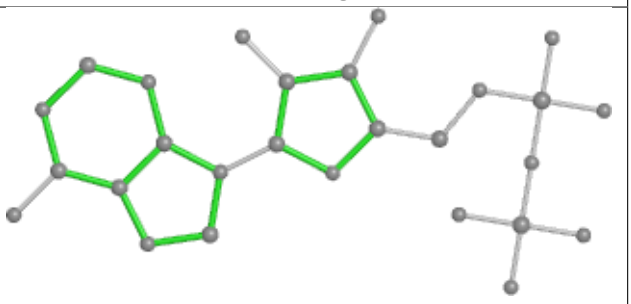
Bond angles

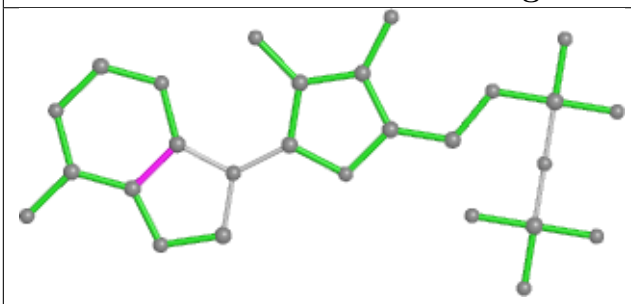
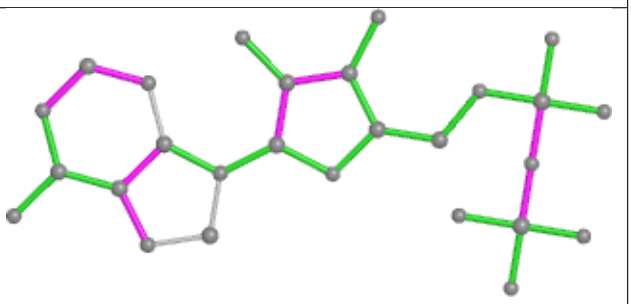
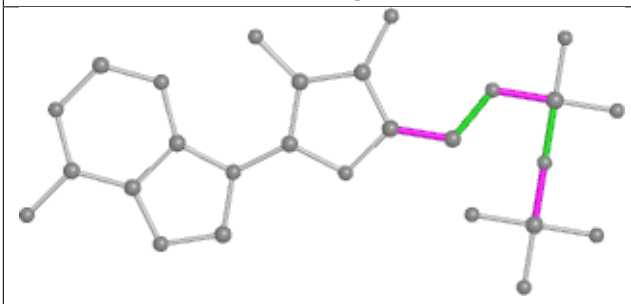
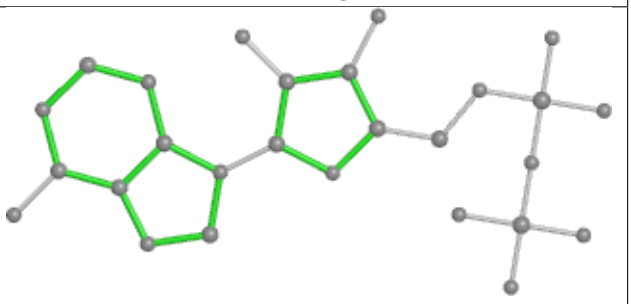


Torsions

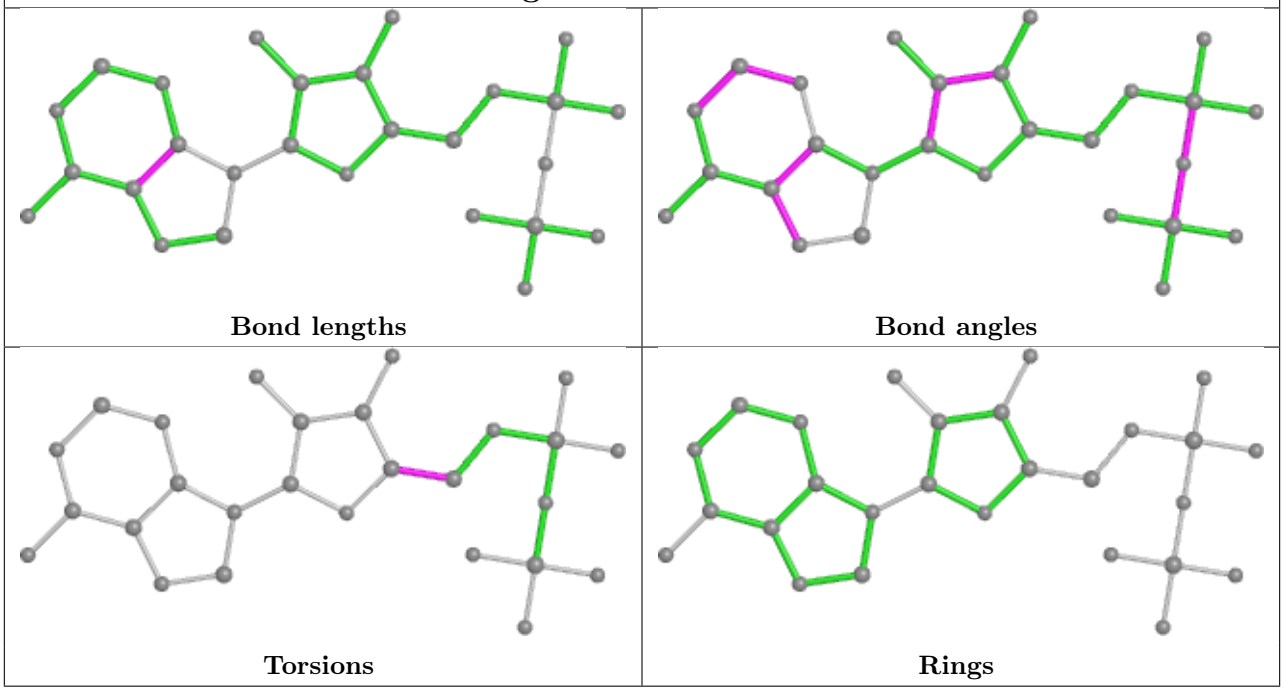


Rings

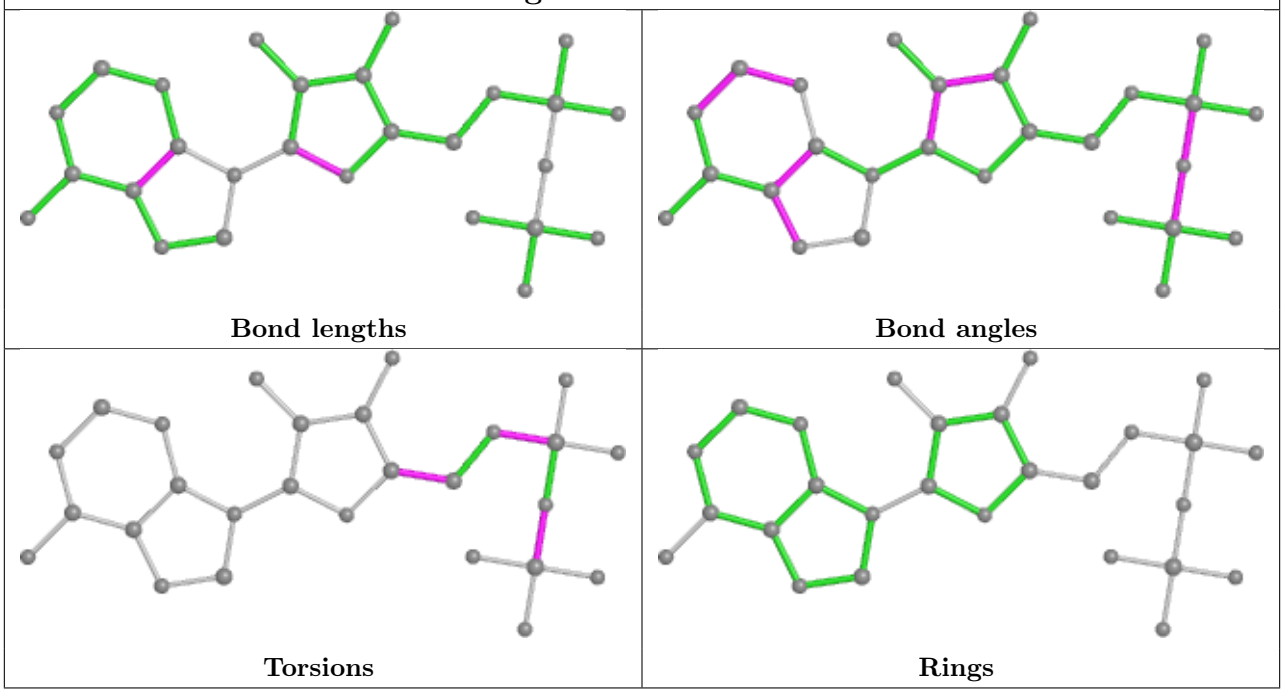
Ligand ADP C 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP B 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D 501



Ligand ADP F 501



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
32	f	3
27	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	f	110:ALA	C	111:LEU	N	8.67
1	f	79:ASN	C	80:TYR	N	7.26
1	f	348:ASP	C	349:SER	N	6.44
1	a	341:LEU	C	342:ASP	N	5.77

6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-8335. 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)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal surface views (i)

This section was not generated.

6.5 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)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

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

9 Map-model fit (i)

This section was not generated.