wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Jun 11, 2019 – 01:46 PM EDT

PDB ID	:	6I3M
EMDB ID:	:	EMD-4404
Title	:	eIF2B:eIF2 complex, phosphorylated on eIF2 alpha serine 52.
Authors	:	Adomavicius, T.; Roseman, A.M.; Pavitt, G.D.
Deposited on	:	2018-11-06
Resolution	:	3.93 Å(reported)
Based on PDB ID	:	3JAP, 5B04

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB 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.

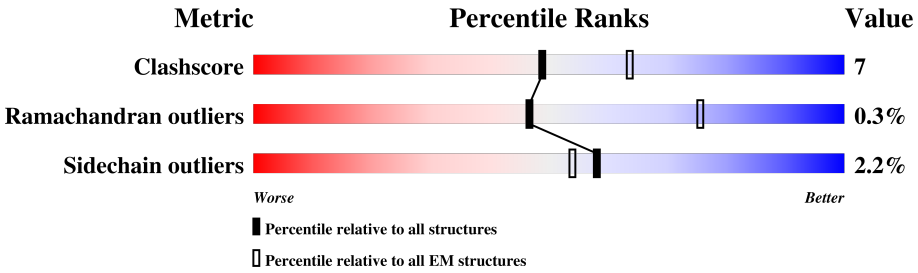
MolProbity	:	4.02b-467
Mogul	:	1.8.0 (224370), CSD as540be (2019)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.3.2

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 3.93 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	305	82% 18%
1	B	305	82% 18%
2	C	651	44% 9% 47%
2	D	651	44% 8% 47%
3	E	381	73% 20% 7%
3	F	381	74% 19% 7%
4	G	712	47% 11% 42%
4	H	712	46% 11% 42%
5	I	578	38% 8% 54%

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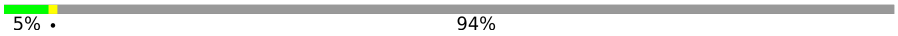
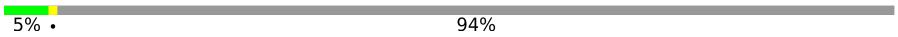
Mol	Chain	Length	Quality of chain
5	J	578	
6	K	304	
6	L	304	
7	M	285	
7	N	285	
8	O	527	
8	P	527	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 37012 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 Translation initiation factor eIF-2B subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	305	Total	C	N	O	S	0	0
			2393	1526	400	456	11		
1	B	305	Total	C	N	O	S	0	0
			2393	1526	400	456	11		

- Molecule 2 is a protein called Translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	342	Total	C	N	O	S	0	0
			2677	1715	446	505	11		
2	D	342	Total	C	N	O	S	0	0
			2677	1715	446	505	11		

- Molecule 3 is a protein called Translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	354	Total	C	N	O	S	0	0
			2797	1774	484	530	9		
3	F	354	Total	C	N	O	S	0	0
			2797	1774	484	530	9		

- Molecule 4 is a protein called Translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	410	Total	C	N	O	S	0	0
			3265	2061	549	635	20		
4	H	410	Total	C	N	O	S	0	0
			3265	2061	549	635	20		

- Molecule 5 is a protein called Translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	268	Total	C	N	O	S	0	0
			2187	1398	372	408	9		
5	J	268	Total	C	N	O	S	0	0
			2187	1398	372	408	9		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	K	249	Total	C	N	O	P	S	0	0
			2010	1283	333	385	1	8		
6	L	249	Total	C	N	O	P	S	0	0
			2010	1283	333	385	1	8		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	M	17	Total	C	N	O	0	0
			143	96	24	23		
7	N	17	Total	C	N	O	0	0
			143	96	24	23		

- Molecule 8 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

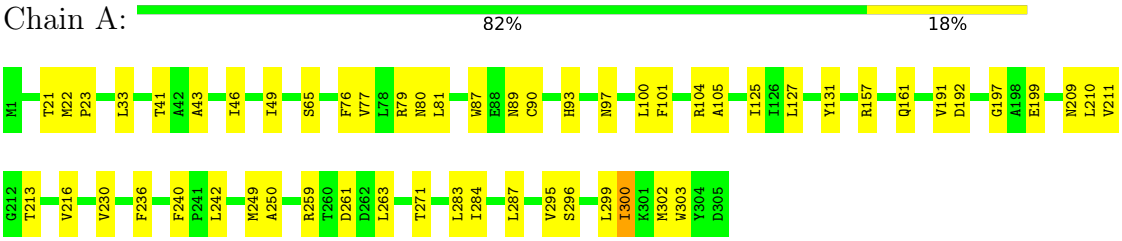
Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	396	Total	C	N	O	S	0	0
			3034	1932	542	544	16		
8	P	396	Total	C	N	O	S	0	0
			3034	1932	542	544	16		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

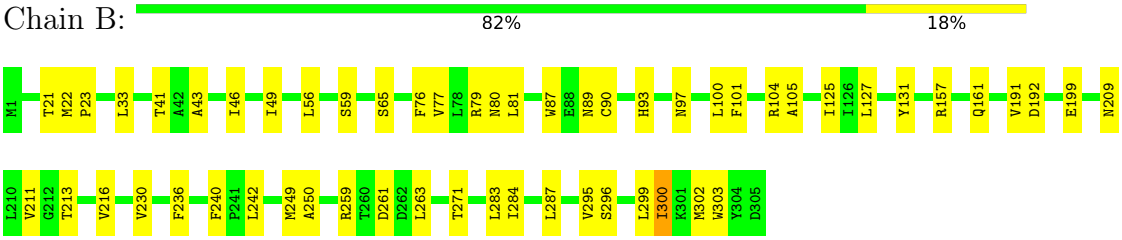
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain A:



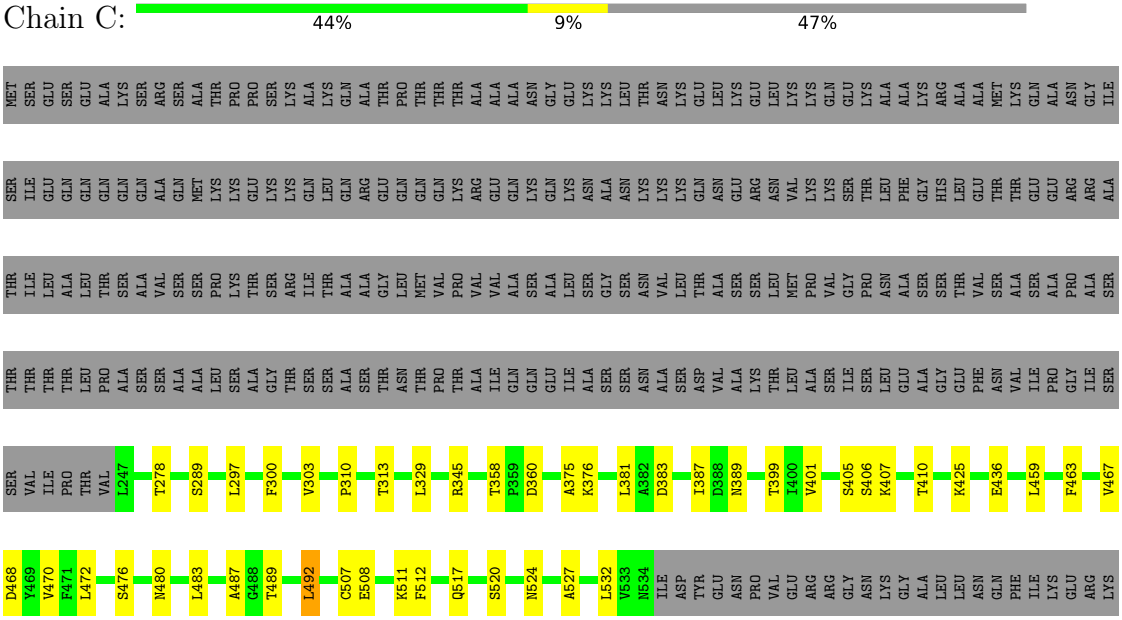
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

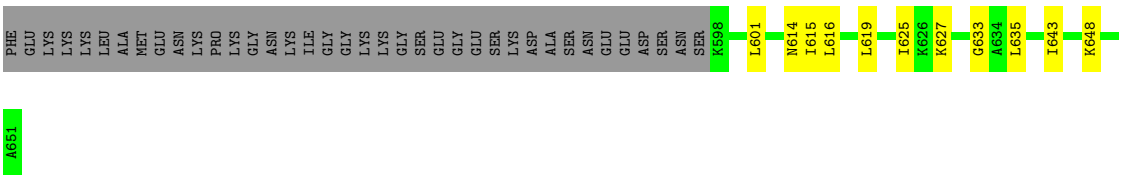
Chain B:



• Molecule 2: Translation initiation factor eIF-2B subunit delta

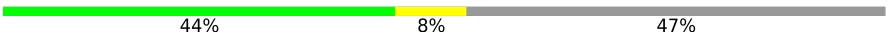
Chain C:

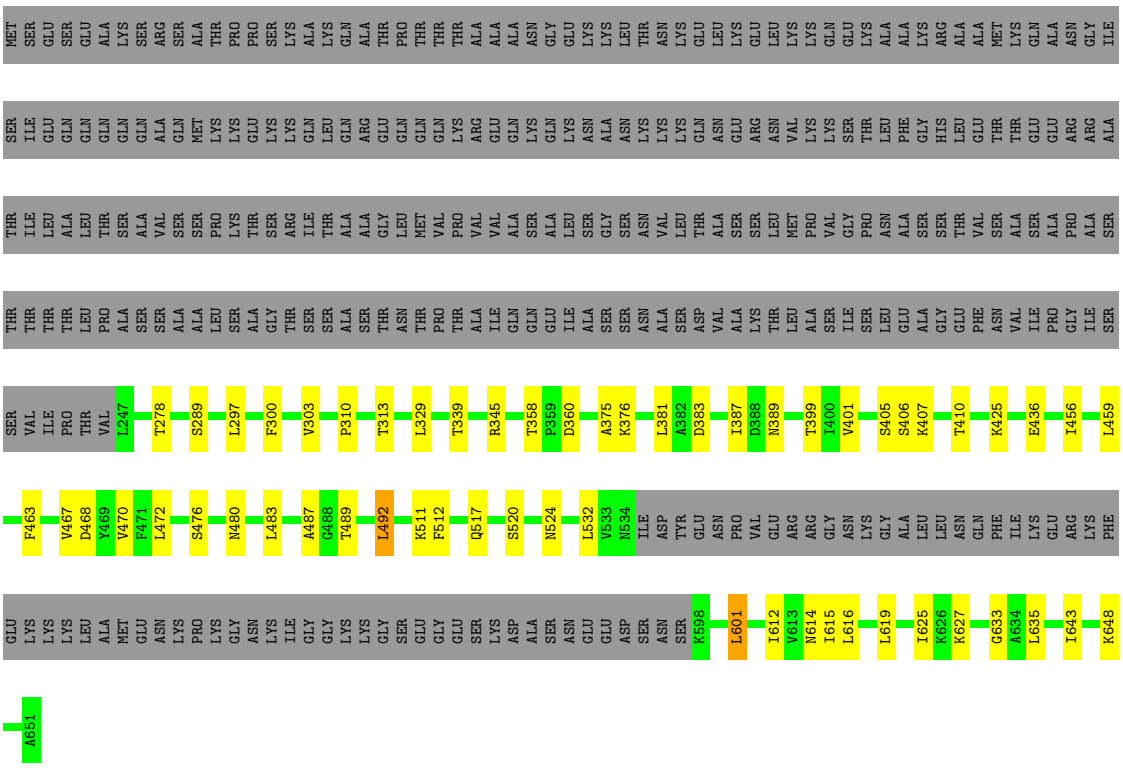




• Molecule 2: Translation initiation factor eIF-2B subunit delta

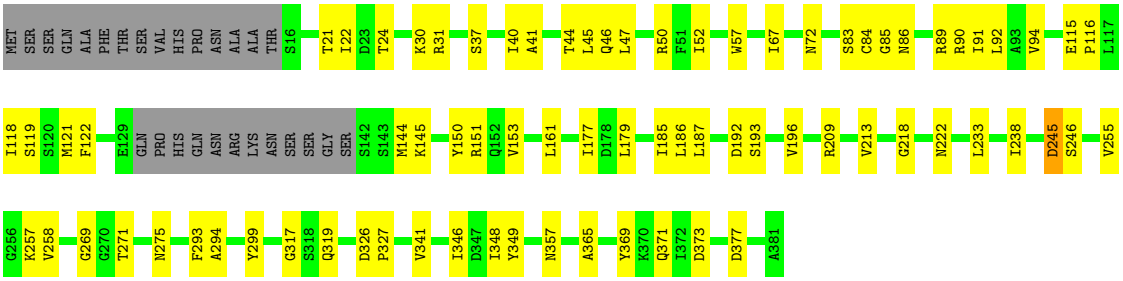
Chain D:





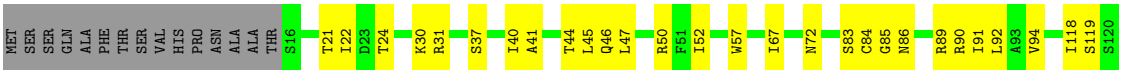
• Molecule 3: Translation initiation factor eIF-2B subunit beta

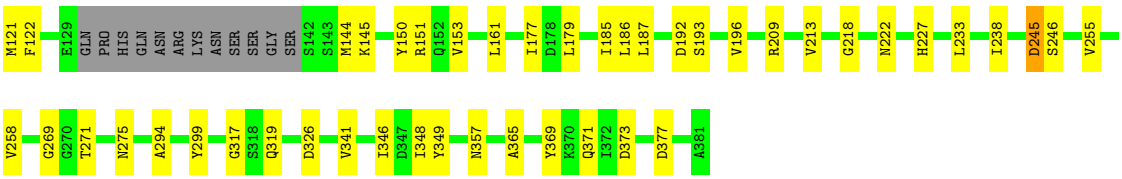
Chain E:



• Molecule 3: Translation initiation factor eIF-2B subunit beta

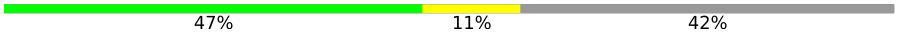
Chain F:

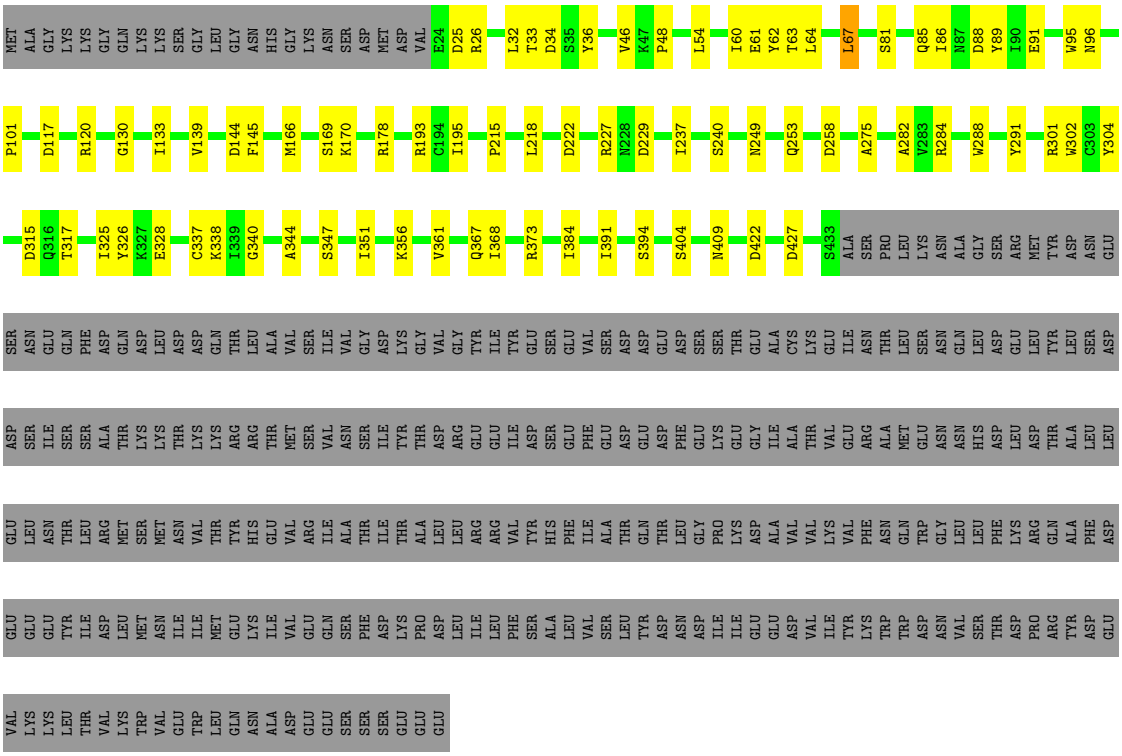




• Molecule 4: Translation initiation factor eIF-2B subunit epsilon

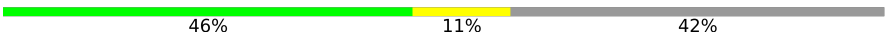
Chain G:

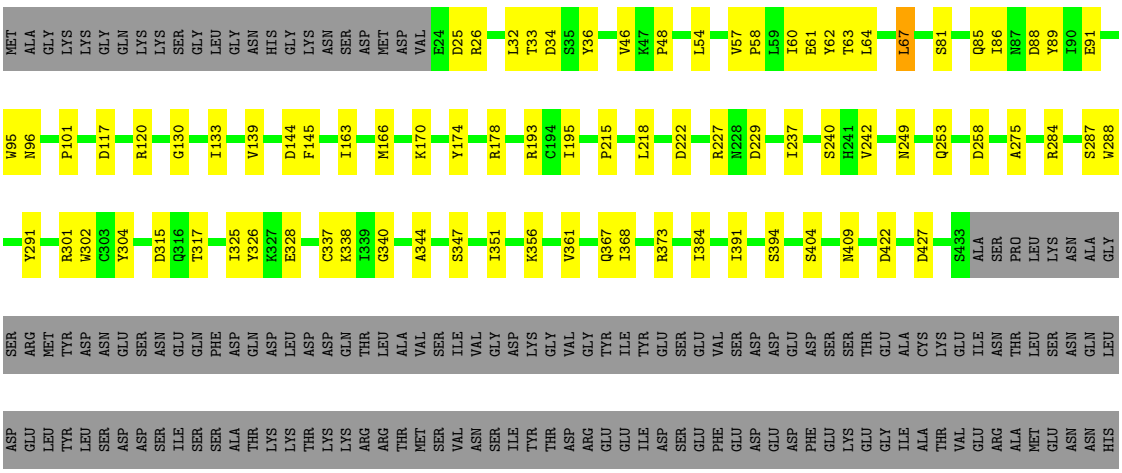




• Molecule 4: Translation initiation factor eIF-2B subunit epsilon

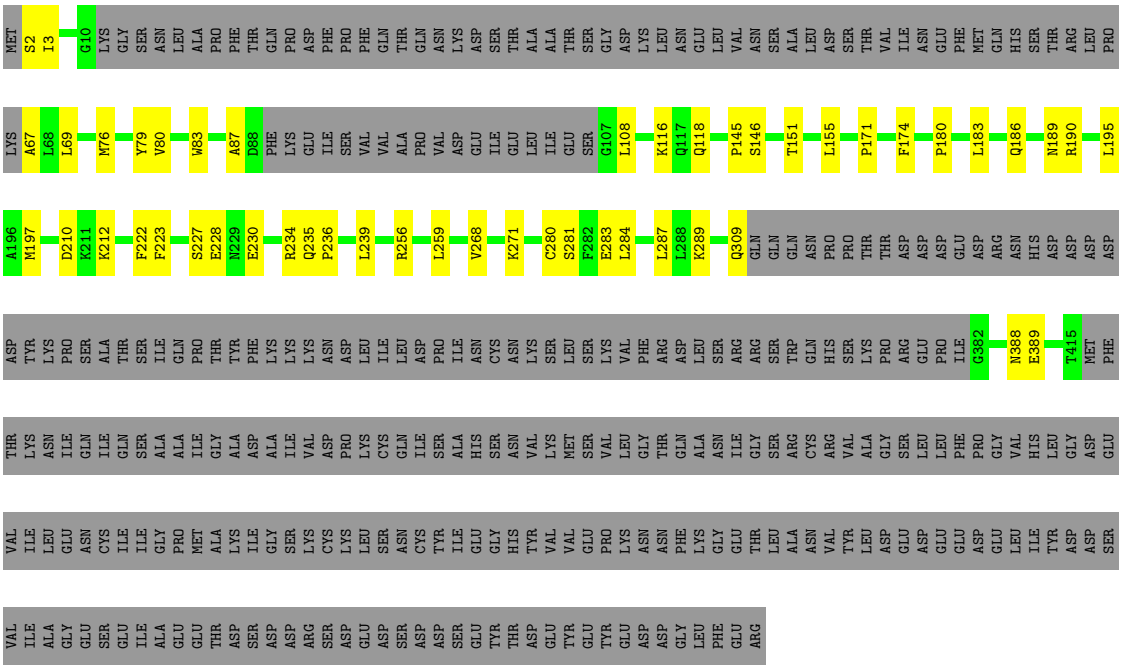
Chain H:





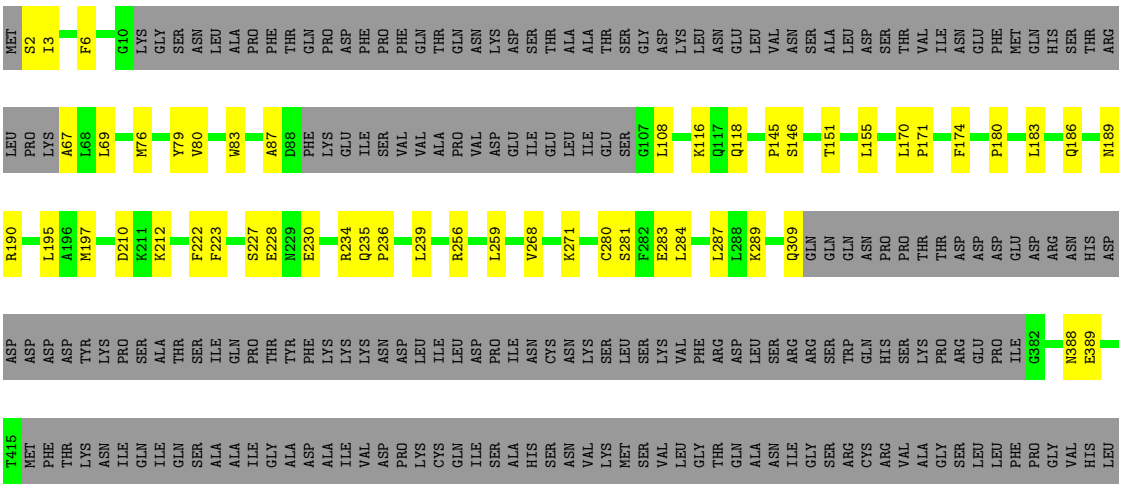
• Molecule 5: Translation initiation factor eIF-2B subunit gamma

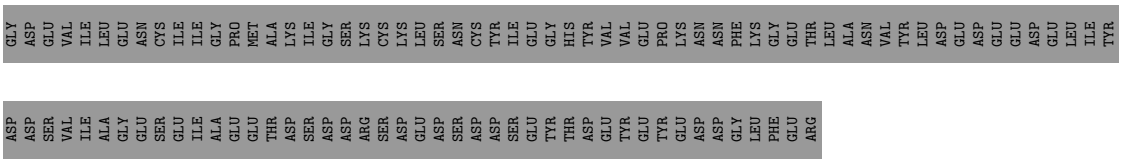
Chain I:



• Molecule 5: Translation initiation factor eIF-2B subunit gamma

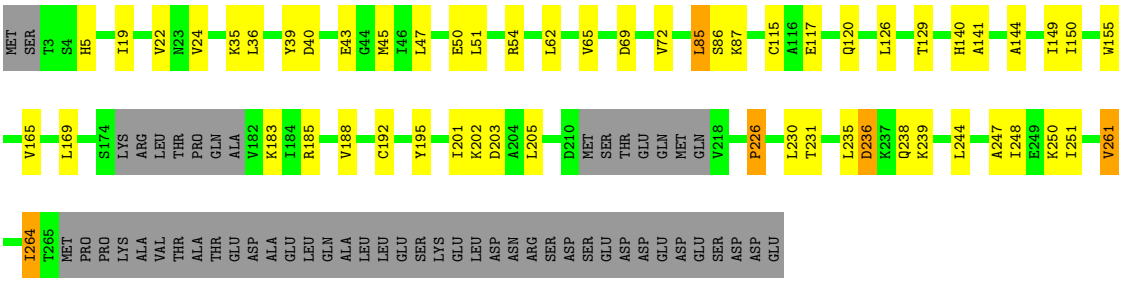
Chain J:





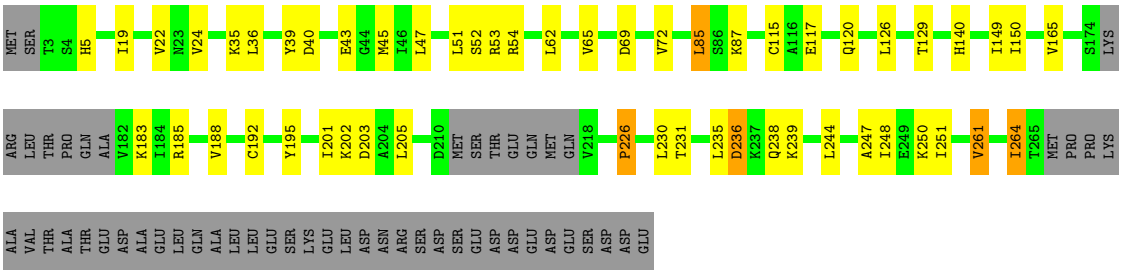
• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

Chain K:



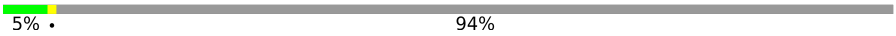
• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

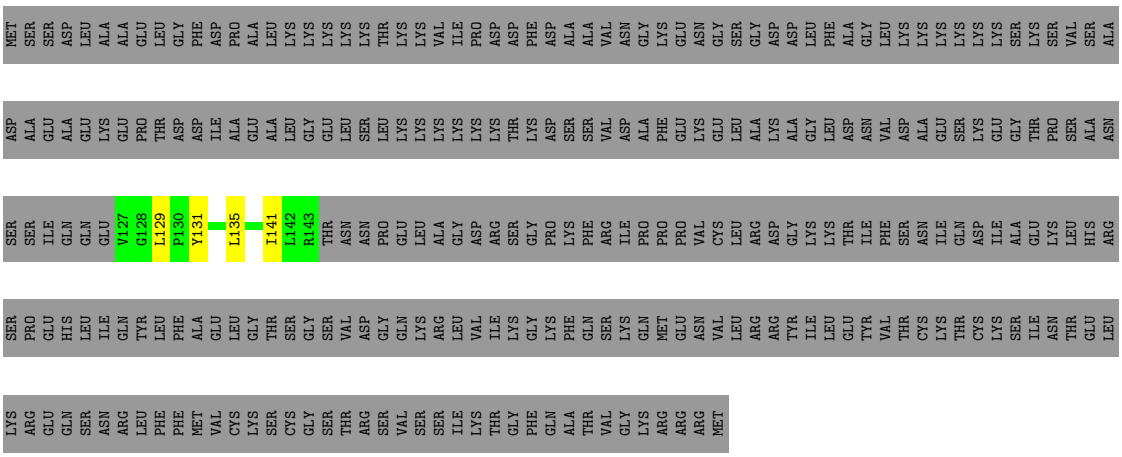
Chain L:



• Molecule 7: Eukaryotic translation initiation factor 2 subunit beta

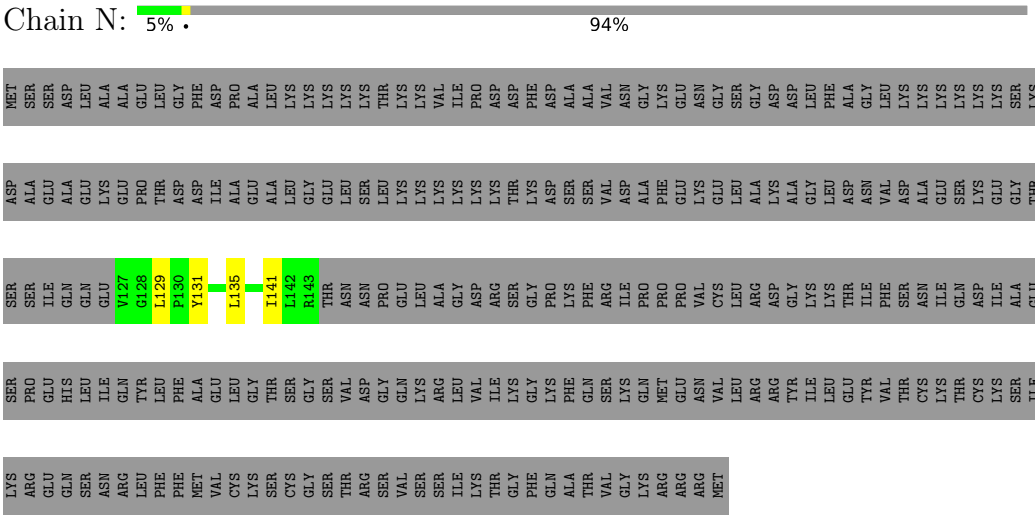
Chain M:





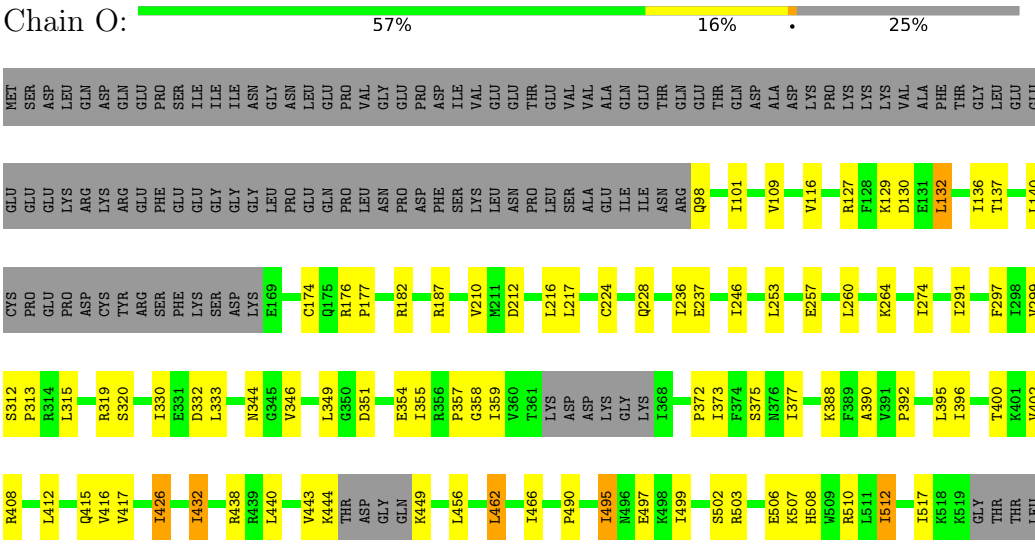
• Molecule 7: Eukaryotic translation initiation factor 2 subunit beta

Chain N:



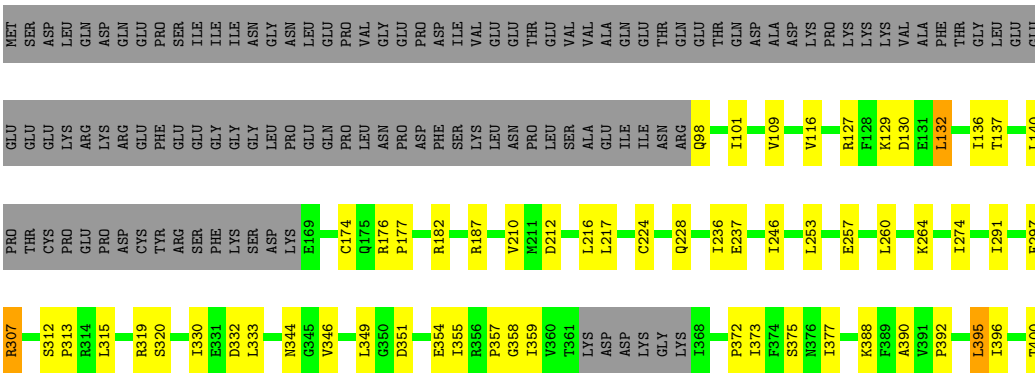
• Molecule 8: Eukaryotic translation initiation factor 2 subunit gamma

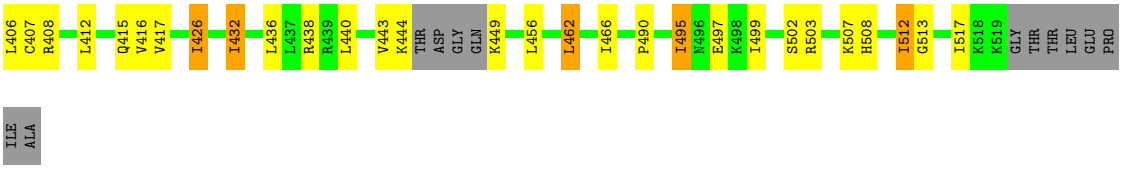
Chain O:



• Molecule 8: Eukaryotic translation initiation factor 2 subunit gamma

Chain P:




L406
C407
R408
L412
Q415
V416
V417
I426
I432
L436
L437
R438
R439
L440
V443
K444
THR
ASP
GLY
GLN
K449
L456
L462
I466
P490
I495
N496
E497
K498
I499
S502
R503
K507
H508
I512
G513
I517
K518
K519
GLY
THR
THR
LEU
GLU
PRO
ILE
ALA

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	64541	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF determination was performed per micrograph initially. After particle picking and initial reconstruction, per particle CTF determination was performed.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5500	Depositor
Magnification	37313	Depositor
Image detector	GATAN K2 QUANTUM (4k 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: SEP

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	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
1	A	0.34	0/2437	0.62	0/3304
1	B	0.34	0/2437	0.62	0/3304
2	C	0.33	0/2720	0.65	2/3685 (0.1%)
2	D	0.33	0/2720	0.65	2/3685 (0.1%)
3	E	0.35	0/2846	0.65	1/3857 (0.0%)
3	F	0.36	0/2846	0.65	1/3857 (0.0%)
4	G	0.35	0/3327	0.66	3/4512 (0.1%)
4	H	0.35	0/3327	0.66	3/4512 (0.1%)
5	I	0.32	0/2232	0.66	0/3015
5	J	0.32	0/2232	0.66	0/3015
6	K	0.37	0/2027	0.67	2/2726 (0.1%)
6	L	0.37	0/2027	0.67	2/2726 (0.1%)
7	M	0.53	0/146	0.71	0/196
7	N	0.53	0/146	0.71	0/196
8	O	0.47	0/3079	0.70	1/4157 (0.0%)
8	P	0.47	0/3079	0.70	1/4157 (0.0%)
All	All	0.37	0/37628	0.66	18/50904 (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
4	G	0	1
4	H	0	1
6	K	0	2
6	L	0	2
All	All	0	6

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	245	ASP	CB-CG-OD1	6.49	124.14	118.30
3	E	245	ASP	CB-CG-OD1	6.44	124.09	118.30
4	G	32	LEU	CA-CB-CG	6.05	129.21	115.30
4	H	32	LEU	CA-CB-CG	6.04	129.19	115.30
6	L	85	LEU	CA-CB-CG	5.99	129.07	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	178	ARG	Peptide
4	H	178	ARG	Peptide
6	K	140	HIS	Peptide
6	K	39	TYR	Peptide
6	L	39	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2393	0	2416	39	0
1	B	2393	0	2416	38	0
2	C	2677	0	2787	34	0
2	D	2677	0	2787	36	0
3	E	2797	0	2835	51	0
3	F	2797	0	2835	46	0
4	G	3265	0	3229	45	0
4	H	3265	0	3229	49	0
5	I	2187	0	2173	31	0
5	J	2187	0	2173	32	0
6	K	2010	0	2064	29	0
6	L	2010	0	2064	27	0
7	M	143	0	148	0	0
7	N	143	0	148	0	0
8	O	3034	0	3195	44	0
8	P	3034	0	3195	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	37012	0	37694	498	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 7.

The worst 5 of 498 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)
8:P:499:ILE:HD11	8:P:517:ILE:HG13	1.63	0.81
8:O:499:ILE:HD11	8:O:517:ILE:HG13	1.63	0.79
5:J:79:TYR:O	5:J:83:TRP:HB2	1.89	0.72
5:I:79:TYR:O	5:I:83:TRP:HB2	1.89	0.71
6:L:201:ILE:HG22	8:P:330:ILE:HG21	1.73	0.69

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	303/305 (99%)	264 (87%)	39 (13%)	0	100	100
1	B	303/305 (99%)	265 (88%)	38 (12%)	0	100	100
2	C	338/651 (52%)	303 (90%)	35 (10%)	0	100	100
2	D	338/651 (52%)	303 (90%)	35 (10%)	0	100	100
3	E	350/381 (92%)	327 (93%)	23 (7%)	0	100	100
3	F	350/381 (92%)	327 (93%)	23 (7%)	0	100	100
4	G	408/712 (57%)	364 (89%)	44 (11%)	0	100	100
4	H	408/712 (57%)	364 (89%)	44 (11%)	0	100	100
5	I	260/578 (45%)	214 (82%)	46 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	J	260/578 (45%)	215 (83%)	45 (17%)	0	100 100
6	K	242/304 (80%)	212 (88%)	29 (12%)	1 (0%)	36 74
6	L	242/304 (80%)	212 (88%)	29 (12%)	1 (0%)	36 74
7	M	15/285 (5%)	13 (87%)	1 (7%)	1 (7%)	1 20
7	N	15/285 (5%)	13 (87%)	1 (7%)	1 (7%)	1 20
8	O	388/527 (74%)	339 (87%)	43 (11%)	6 (2%)	11 50
8	P	388/527 (74%)	339 (87%)	43 (11%)	6 (2%)	11 50
All	All	4608/7486 (62%)	4074 (88%)	518 (11%)	16 (0%)	47 78

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	O	129	LYS
8	P	129	LYS
8	O	495	ILE
8	O	507	LYS
8	P	495	ILE

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	265/265 (100%)	264 (100%)	1 (0%)	92 96
1	B	265/265 (100%)	264 (100%)	1 (0%)	92 96
2	C	308/561 (55%)	307 (100%)	1 (0%)	93 96
2	D	308/561 (55%)	307 (100%)	1 (0%)	93 96
3	E	315/338 (93%)	314 (100%)	1 (0%)	93 96
3	F	315/338 (93%)	314 (100%)	1 (0%)	93 96
4	G	375/649 (58%)	375 (100%)	0	100 100
4	H	375/649 (58%)	375 (100%)	0	100 100
5	I	250/529 (47%)	249 (100%)	1 (0%)	92 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	J	250/529 (47%)	249 (100%)	1 (0%)	92 96
6	K	223/273 (82%)	211 (95%)	12 (5%)	24 59
6	L	223/273 (82%)	211 (95%)	12 (5%)	24 59
7	M	16/246 (6%)	13 (81%)	3 (19%)	1 12
7	N	16/246 (6%)	13 (81%)	3 (19%)	1 12
8	O	332/449 (74%)	306 (92%)	26 (8%)	14 47
8	P	332/449 (74%)	306 (92%)	26 (8%)	14 47
All	All	4168/6620 (63%)	4078 (98%)	90 (2%)	58 78

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	O	432	ILE
6	L	85	LEU
8	P	440	LEU
8	O	438	ARG
8	O	495	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
5	I	388	ASN
1	B	80	ASN
8	P	248	GLN
5	J	309	GLN
4	H	87	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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
6	SEP	K	52	6	9,9,10	1.55	1 (11%)	9,12,14	1.59	2 (22%)
6	SEP	L	52	6	9,9,10	1.56	2 (22%)	9,12,14	1.59	2 (22%)

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
6	SEP	K	52	6	-	5/5/8/10	-
6	SEP	L	52	6	-	5/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	52	SEP	P-O1P	3.24	1.61	1.50
6	K	52	SEP	P-O1P	3.23	1.61	1.50
6	L	52	SEP	CA-C	2.07	1.53	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	52	SEP	P-OG-CB	-3.19	109.50	118.30
6	L	52	SEP	P-OG-CB	-3.18	109.53	118.30
6	L	52	SEP	OG-CB-CA	2.80	110.87	108.14
6	K	52	SEP	OG-CB-CA	2.79	110.86	108.14

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	52	SEP	N-CA-CB-OG
6	L	52	SEP	CB-OG-P-O2P
6	K	52	SEP	N-CA-CB-OG
6	K	52	SEP	CB-OG-P-O2P
6	L	52	SEP	CB-OG-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	52	SEP	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.