wwPDB X-ray Structure Validation Summary Report (i)

Jun 25, 2024 – 09:49 AM EDT

PDB ID	:	6JLZ
Title	:	P-eIF2a - eIF2B complex
Authors	:	Kashiwagi, K.; Ito, T.
Deposited on	:	2019-03-07
Resolution	:	3.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp
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 (i)) were used in the production of this report:

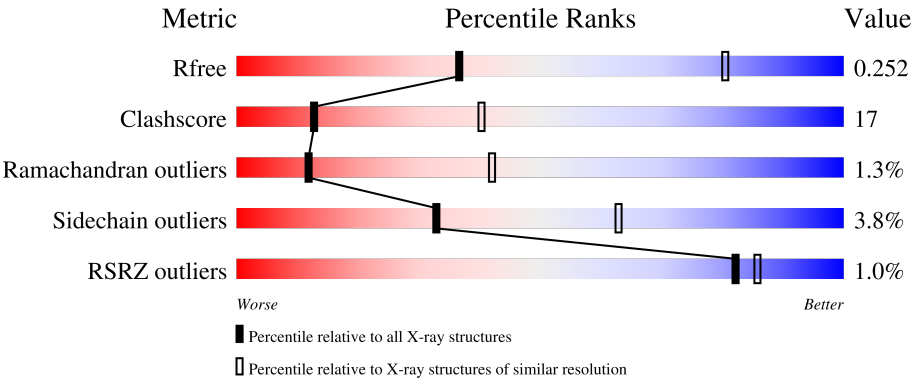
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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.



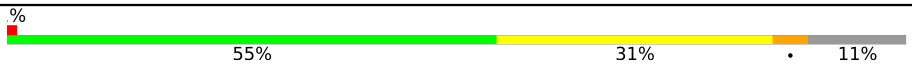
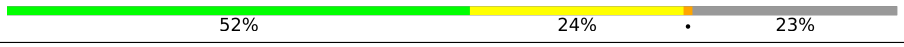
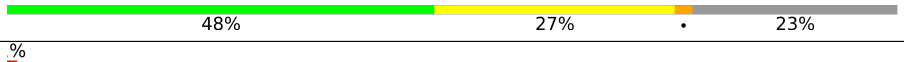
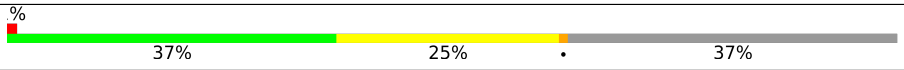
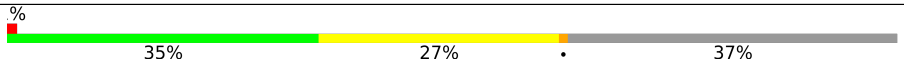
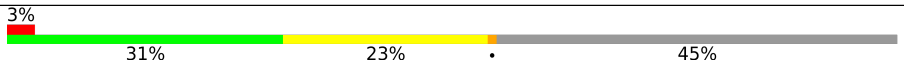
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	341	53% 38% · 7%
1	B	341	56% 34% · 8%
2	C	399	51% 32% · 16%
2	D	399	55% 30% 16%
3	E	458	55% 31% · 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	458	
4	G	467	
4	H	467	
5	I	678	
5	J	678	
6	L	304	
6	M	304	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	PO4	A	401	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 31826 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2476	1573	433	457	13			
1	B	315	Total	C	N	O	S	0	0	0
			2457	1562	428	454	13			

- Molecule 2 is a protein called Probable translation initiation factor eIF-2B subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	337	Total	C	N	O	S	0	0	0
			2609	1654	442	501	12			
2	D	337	Total	C	N	O	S	0	0	0
			2609	1654	442	501	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP Q9UT76
C	-4	PRO	-	expression tag	UNP Q9UT76
C	-3	ILE	-	expression tag	UNP Q9UT76
C	-2	SER	-	expression tag	UNP Q9UT76
C	-1	GLU	-	expression tag	UNP Q9UT76
C	0	PHE	-	expression tag	UNP Q9UT76
D	-5	GLY	-	expression tag	UNP Q9UT76
D	-4	PRO	-	expression tag	UNP Q9UT76
D	-3	ILE	-	expression tag	UNP Q9UT76
D	-2	SER	-	expression tag	UNP Q9UT76
D	-1	GLU	-	expression tag	UNP Q9UT76
D	0	PHE	-	expression tag	UNP Q9UT76

- Molecule 3 is a protein called Probable translation initiation factor eIF-2B subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	409	Total	C	N	O	S	0	0	0
			3178	2018	548	595	17			
3	F	409	Total	C	N	O	S	0	0	0
			3178	2018	548	595	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	157	TYR	ILE	conflict	UNP P56288
E	158	THR	TYR	conflict	UNP P56288
E	159	VAL	GLY	conflict	UNP P56288
F	157	TYR	ILE	conflict	UNP P56288
F	158	THR	TYR	conflict	UNP P56288
F	159	VAL	GLY	conflict	UNP P56288

- Molecule 4 is a protein called Probable translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	360	Total	C	N	O	S	0	0	0
			2845	1818	483	531	13			
4	H	361	Total	C	N	O	S	0	0	0
			2857	1827	484	533	13			

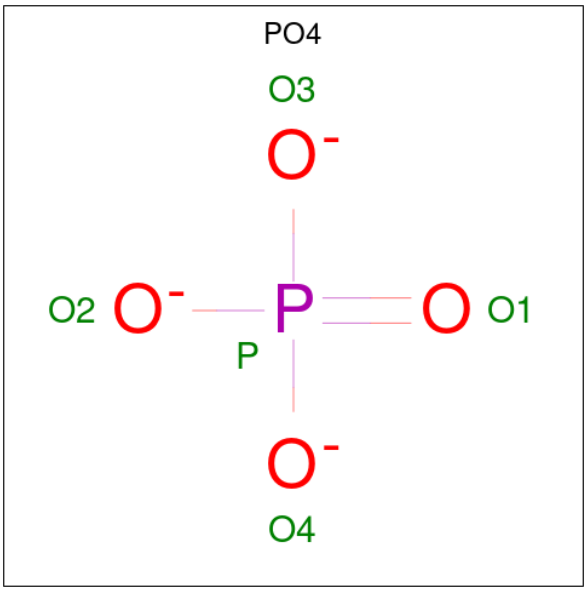
- Molecule 5 is a protein called Probable translation initiation factor eIF-2B subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	430	Total	C	N	O	S	0	0	0
			3393	2134	595	649	15			
5	J	428	Total	C	N	O	S	0	0	0
			3377	2123	592	647	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	L	167	Total	C	N	O	P	S	0	0	0
			1387	883	237	260	1	6			
6	M	169	Total	C	N	O	P	S	0	0	0
			1400	890	239	264	1	6			

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



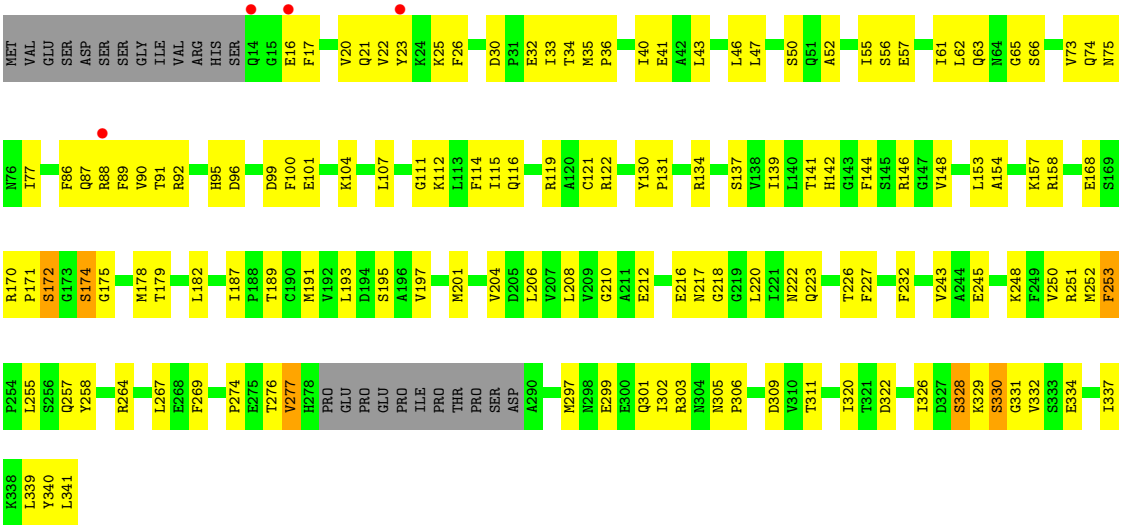
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O P 5 4 1	0	0
7	B	1	Total O P 5 4 1	0	0
7	C	1	Total O P 5 4 1	0	0
7	D	1	Total O P 5 4 1	0	0
7	E	1	Total O P 5 4 1	0	0
7	E	1	Total O P 5 4 1	0	0
7	F	1	Total O P 5 4 1	0	0
7	F	1	Total O P 5 4 1	0	0
7	G	1	Total O P 5 4 1	0	0
7	H	1	Total O P 5 4 1	0	0
7	I	1	Total O P 5 4 1	0	0
7	J	1	Total O P 5 4 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

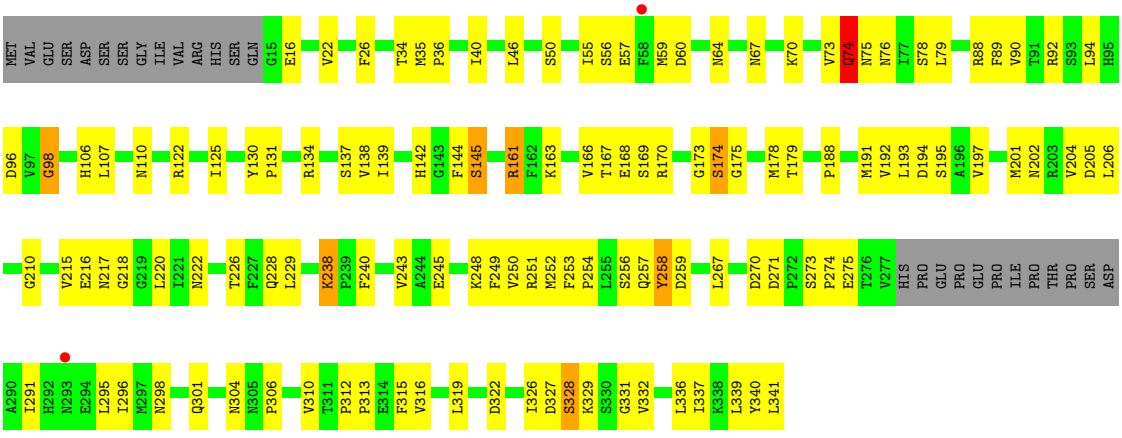
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain A:



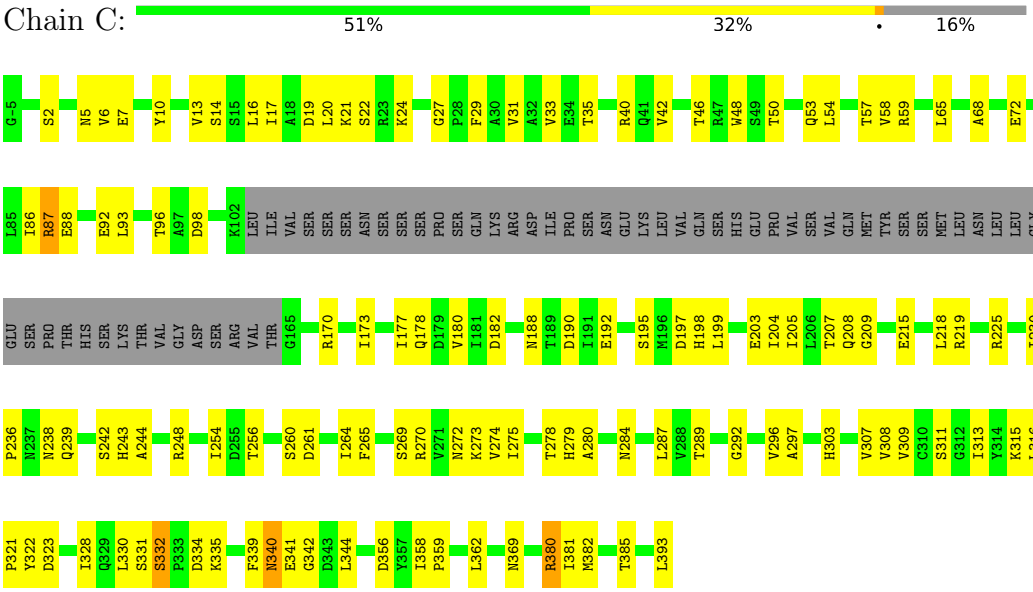
• Molecule 1: Translation initiation factor eIF-2B subunit alpha

Chain B:



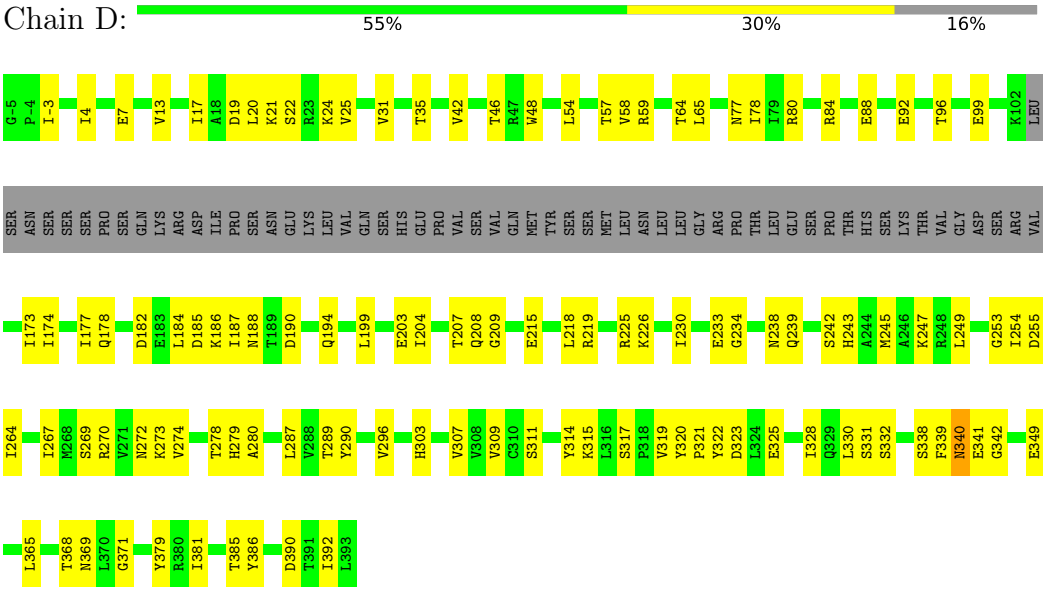
• Molecule 2: Probable translation initiation factor eIF-2B subunit beta

Chain C:



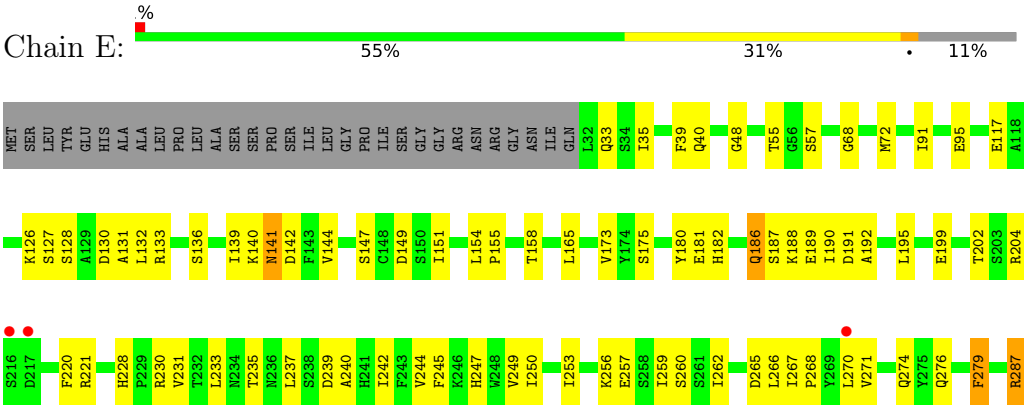
• Molecule 2: Probable translation initiation factor eIF-2B subunit beta

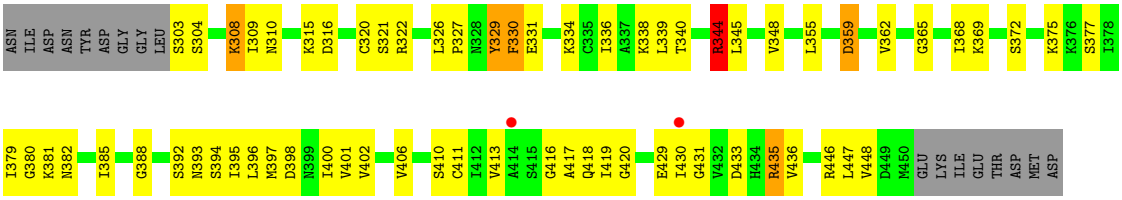
Chain D:



• Molecule 3: Probable translation initiation factor eIF-2B subunit gamma

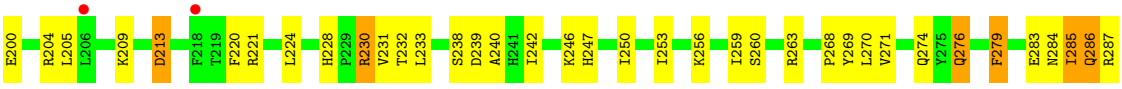
Chain E:

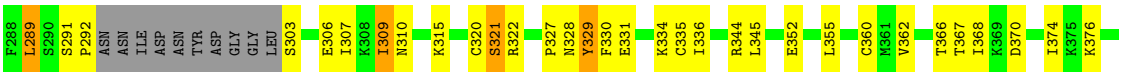


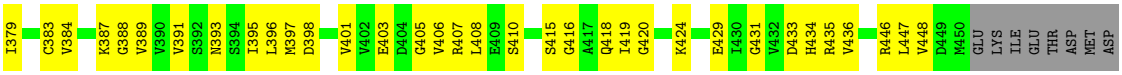


• Molecule 3: Probable translation initiation factor eIF-2B subunit gamma

Chain F:

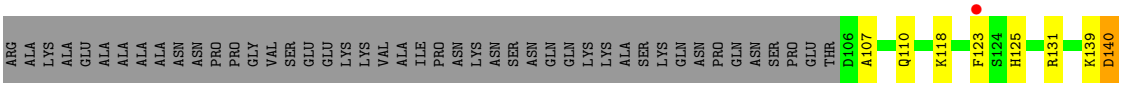


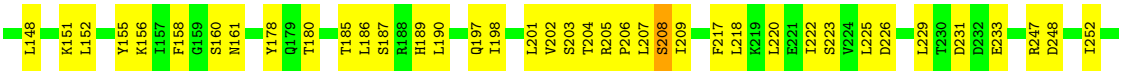




• Molecule 4: Probable translation initiation factor eIF-2B subunit delta

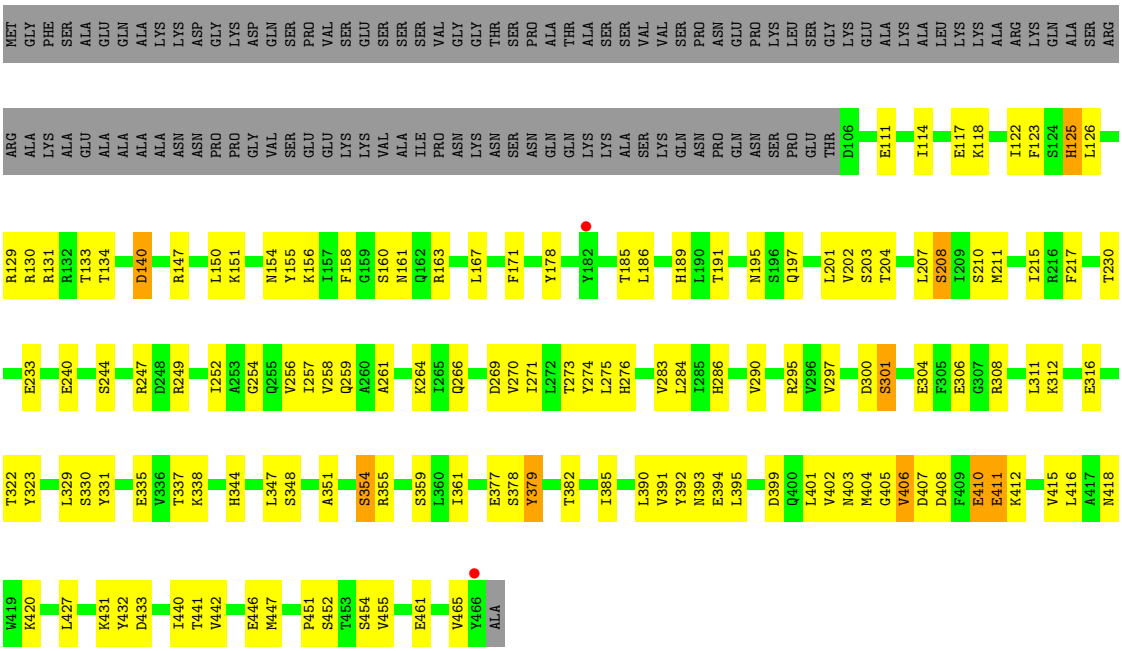
Chain G:



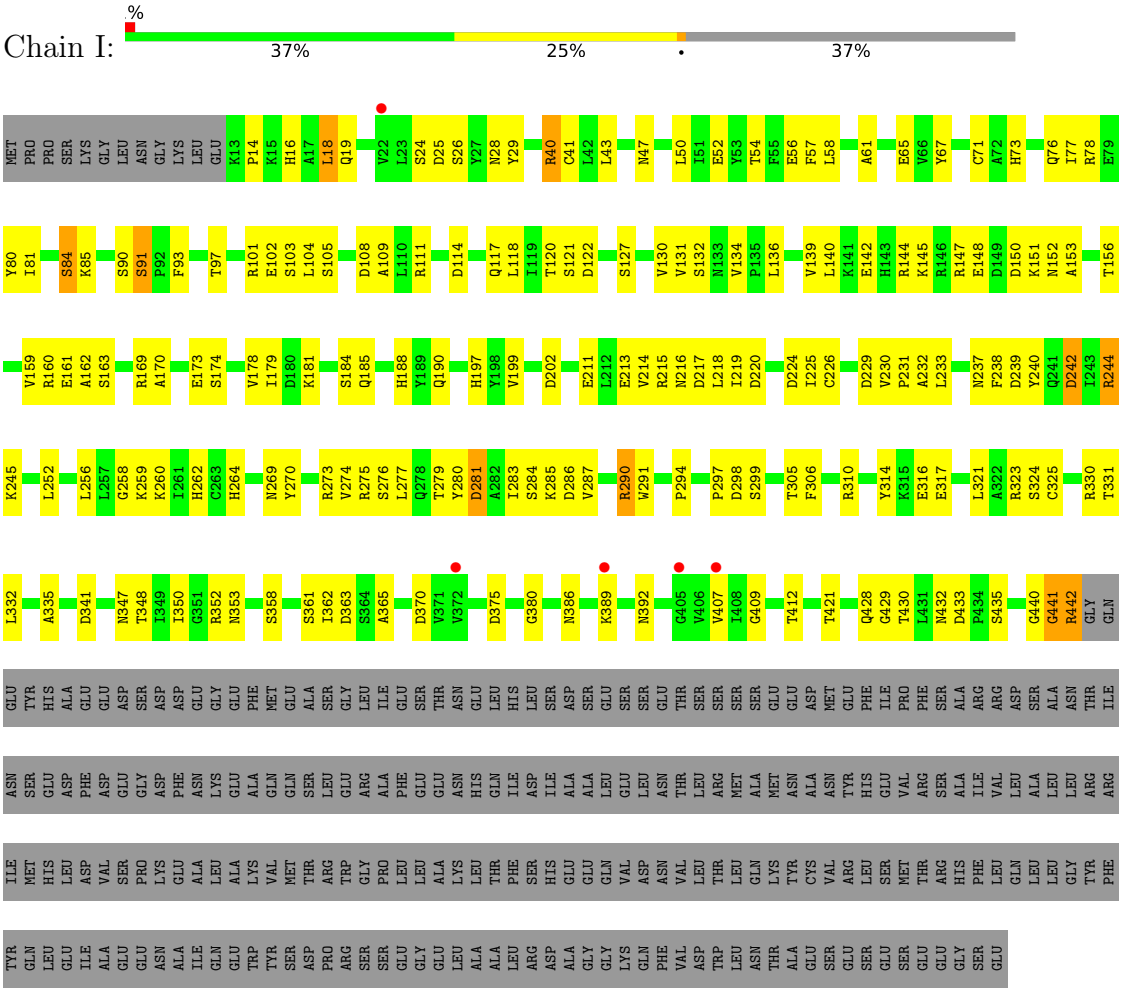


• Molecule 4: Probable translation initiation factor eIF-2B subunit delta

Chain H:

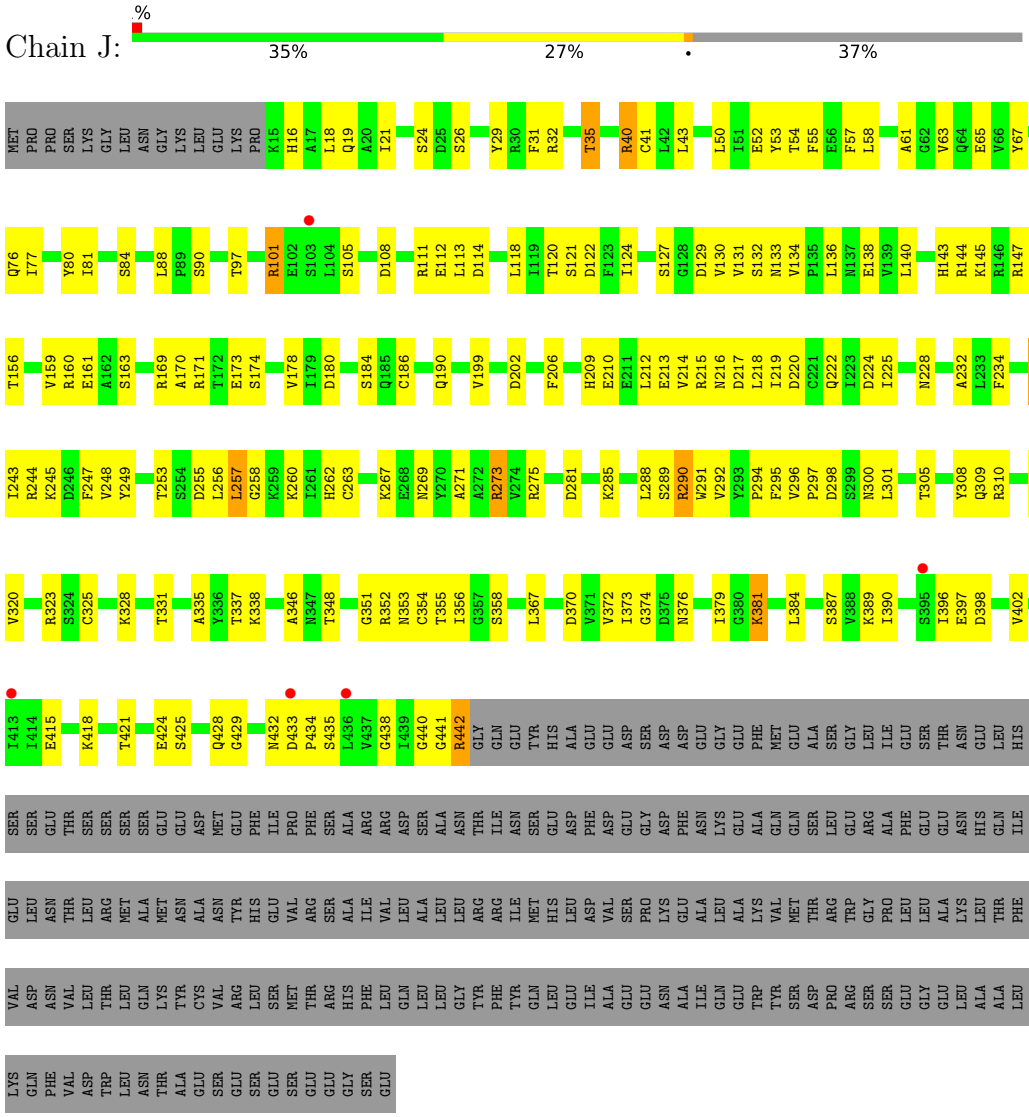


• Molecule 5: Probable translation initiation factor eIF-2B subunit epsilon



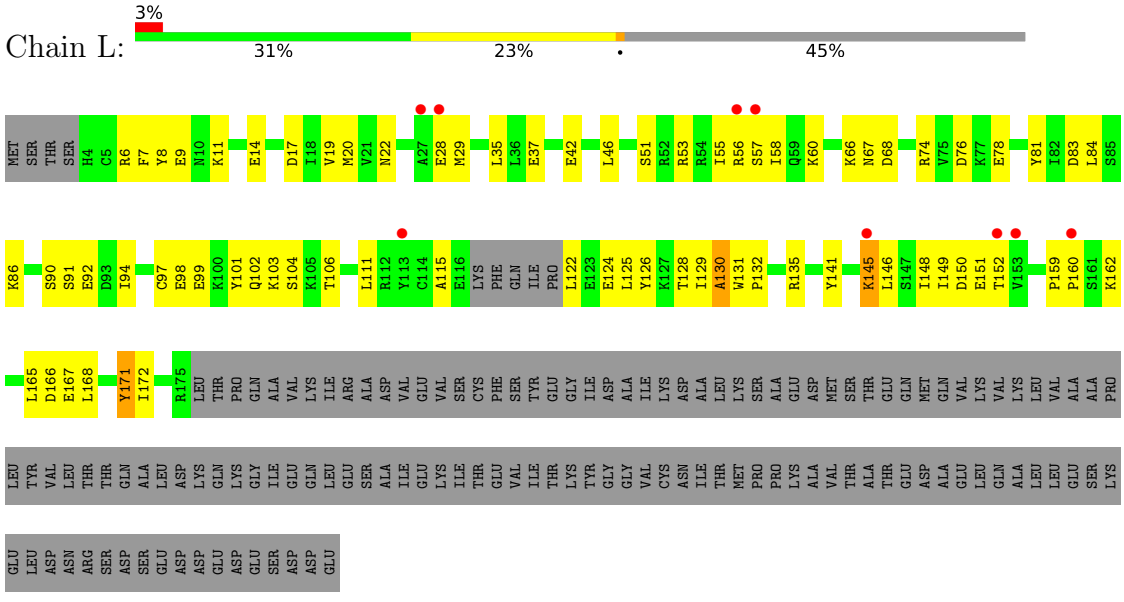
• Molecule 5: Probable translation initiation factor eIF-2B subunit epsilon

Chain J:



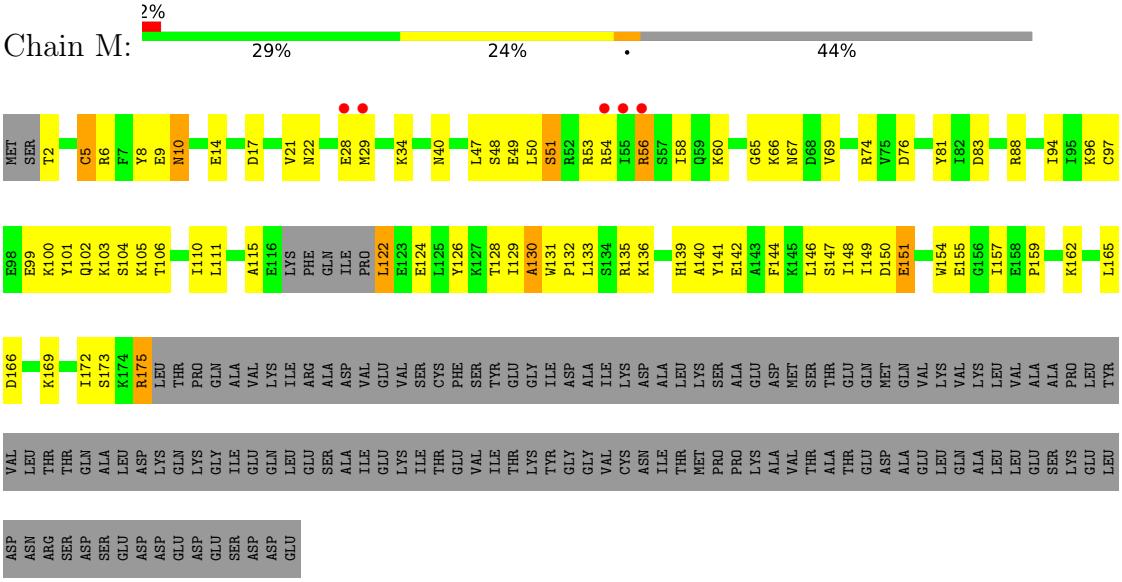
• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

Chain L:



• Molecule 6: Eukaryotic translation initiation factor 2 subunit alpha

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	155.58Å 207.71Å 155.74Å 90.00° 96.96° 90.00°	Depositor
Resolution (Å)	49.31 – 3.35 49.31 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.31-3.35) 89.6 (49.31-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.61 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.221 , 0.253 0.221 , 0.252	Depositor DCC
R_{free} test set	1982 reflections (1.43%)	wwPDB-VP
Wilson B-factor (Å^2)	98.9	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.408 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31826	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.34	0/2522	0.45	0/3411
1	B	0.34	0/2502	0.45	0/3384
2	C	0.37	0/2653	0.45	0/3600
2	D	0.38	0/2653	0.45	0/3600
3	E	0.36	0/3234	0.51	0/4376
3	F	0.36	0/3234	0.51	1/4376 (0.0%)
4	G	0.38	0/2892	0.46	0/3916
4	H	0.37	0/2905	0.45	0/3934
5	I	0.35	0/3454	0.48	0/4681
5	J	0.35	0/3437	0.48	0/4658
6	L	0.29	0/1398	0.44	0/1875
6	M	0.29	0/1411	0.44	0/1893
All	All	0.35	0/32295	0.47	1/43704 (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
3	E	0	2
3	F	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	289	LEU	CA-CB-CG	5.79	128.62	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	340	THR	Peptide
3	E	344	ARG	Peptide
3	F	344	ARG	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	2476	0	2498	109	0
1	B	2457	0	2483	102	0
2	C	2609	0	2642	92	0
2	D	2609	0	2642	81	0
3	E	3178	0	3239	99	0
3	F	3178	0	3239	106	1
4	G	2845	0	2937	80	0
4	H	2857	0	2946	91	0
5	I	3393	0	3381	126	0
5	J	3377	0	3361	143	0
6	L	1387	0	1415	61	1
6	M	1400	0	1425	64	0
7	A	5	0	0	2	0
7	B	5	0	0	0	0
7	C	5	0	0	1	0
7	D	5	0	0	0	0
7	E	10	0	0	0	0
7	F	10	0	0	1	0
7	G	5	0	0	1	0
7	H	5	0	0	0	0
7	I	5	0	0	0	0
7	J	5	0	0	0	0
All	All	31826	0	32208	1063	1

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 17.

The worst 5 of 1063 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)
6:L:68:ASP:OD2	6:L:86:LYS:HE2	1.39	1.19
5:I:290:ARG:NH1	5:I:298:ASP:OD2	1.90	1.05
1:A:216:GLU:OE2	1:A:251:ARG:NH1	1.93	1.01
5:J:242:ASP:OD1	5:J:245:LYS:N	1.99	0.95
3:E:230:ARG:NH2	5:J:213:GLU:OE2	2.01	0.94

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:367:THR:OG1	6:L:14:GLU:OE2[1_556]	2.03	0.17

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 X-ray entries followed by that with respect to entries of similar resolution.

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	313/341 (92%)	279 (89%)	30 (10%)	4 (1%)	12 42
1	B	311/341 (91%)	281 (90%)	25 (8%)	5 (2%)	9 38
2	C	333/399 (84%)	307 (92%)	25 (8%)	1 (0%)	41 73
2	D	333/399 (84%)	306 (92%)	24 (7%)	3 (1%)	17 51
3	E	405/458 (88%)	332 (82%)	66 (16%)	7 (2%)	9 36
3	F	405/458 (88%)	338 (84%)	61 (15%)	6 (2%)	10 39
4	G	358/467 (77%)	317 (88%)	38 (11%)	3 (1%)	19 53
4	H	359/467 (77%)	325 (90%)	28 (8%)	6 (2%)	9 36
5	I	428/678 (63%)	377 (88%)	46 (11%)	5 (1%)	13 44
5	J	426/678 (63%)	380 (89%)	39 (9%)	7 (2%)	9 38
6	L	162/304 (53%)	148 (91%)	13 (8%)	1 (1%)	25 59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	M	164/304 (54%)	146 (89%)	16 (10%)	2 (1%)	13 44
All	All	3997/5294 (76%)	3536 (88%)	411 (10%)	50 (1%)	12 42

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	356	ALA
1	A	74	GLN
1	A	255	LEU
1	B	98	GLY
2	D	255	ASP

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 X-ray entries followed by that with respect to entries of similar resolution.

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	275/298 (92%)	267 (97%)	8 (3%)	42 70
1	B	273/298 (92%)	262 (96%)	11 (4%)	31 62
2	C	290/350 (83%)	279 (96%)	11 (4%)	33 63
2	D	290/350 (83%)	284 (98%)	6 (2%)	53 77
3	E	355/395 (90%)	334 (94%)	21 (6%)	19 51
3	F	355/395 (90%)	336 (95%)	19 (5%)	22 54
4	G	324/408 (79%)	312 (96%)	12 (4%)	34 63
4	H	325/408 (80%)	311 (96%)	14 (4%)	29 60
5	I	381/596 (64%)	368 (97%)	13 (3%)	37 66
5	J	379/596 (64%)	368 (97%)	11 (3%)	42 70
6	L	153/273 (56%)	150 (98%)	3 (2%)	55 78
6	M	155/273 (57%)	148 (96%)	7 (4%)	27 59
All	All	3555/4640 (77%)	3419 (96%)	136 (4%)	33 63

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	J	40	ARG
5	J	242	ASP
6	M	10	ASN
3	E	257	GLU
3	E	228	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
5	I	303	ASN
5	J	117	GLN
3	F	328	ASN
4	H	176	GLN
4	H	400	GLN

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	L	51	6	8,9,10	1.48	1 (12%)	8,12,14	1.82	2 (25%)
6	SEP	M	51	6	8,9,10	1.50	1 (12%)	8,12,14	1.74	2 (25%)

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	L	51	6	-	3/5/8/10	-
6	SEP	M	51	6	-	1/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	51	SEP	P-O1P	3.31	1.61	1.50
6	L	51	SEP	P-O1P	3.25	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	51	SEP	P-OG-CB	-3.78	107.88	118.30
6	M	51	SEP	P-OG-CB	-3.46	108.76	118.30
6	M	51	SEP	OG-CB-CA	3.02	111.08	108.14
6	L	51	SEP	OG-CB-CA	2.97	111.03	108.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	51	SEP	CB-OG-P-O1P
6	L	51	SEP	CB-OG-P-O2P
6	L	51	SEP	CB-OG-P-O3P
6	M	51	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	51	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	$\#\|Z\| > 2$
7	PO4	D	401	-	4,4,4	1.14	0	6,6,6	0.39	0
7	PO4	F	502	-	4,4,4	1.04	0	6,6,6	0.44	0
7	PO4	G	501	-	4,4,4	1.10	0	6,6,6	0.53	0
7	PO4	B	401	-	4,4,4	1.00	0	6,6,6	0.41	0
7	PO4	C	401	-	4,4,4	1.11	0	6,6,6	0.44	0
7	PO4	E	501	-	4,4,4	1.19	0	6,6,6	0.51	0
7	PO4	F	501	-	4,4,4	1.22	0	6,6,6	0.44	0
7	PO4	E	502	-	4,4,4	1.03	0	6,6,6	0.41	0
7	PO4	H	501	-	4,4,4	1.14	0	6,6,6	0.42	0
7	PO4	I	701	-	4,4,4	1.10	0	6,6,6	0.47	0
7	PO4	A	401	-	4,4,4	1.03	0	6,6,6	0.41	0
7	PO4	J	701	-	4,4,4	1.03	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	502	PO4	1	0
7	G	501	PO4	1	0
7	C	401	PO4	1	0
7	A	401	PO4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	317/341 (92%)	-0.06	4 (1%)	77	80	76, 112, 160, 206	0
1	B	315/341 (92%)	0.00	2 (0%)	89	92	74, 110, 157, 180	0
2	C	337/399 (84%)	0.02	0	100	100	53, 90, 149, 189	0
2	D	337/399 (84%)	0.03	0	100	100	58, 90, 152, 208	0
3	E	409/458 (89%)	0.04	5 (1%)	79	82	66, 105, 169, 201	0
3	F	409/458 (89%)	-0.00	3 (0%)	87	91	69, 107, 170, 196	0
4	G	360/467 (77%)	0.04	1 (0%)	94	95	62, 89, 148, 183	0
4	H	361/467 (77%)	0.03	2 (0%)	89	92	62, 89, 151, 184	0
5	I	430/678 (63%)	0.00	5 (1%)	79	82	71, 108, 159, 199	0
5	J	428/678 (63%)	-0.00	5 (1%)	79	82	72, 108, 156, 194	0
6	L	166/304 (54%)	0.13	9 (5%)	25	28	87, 161, 204, 222	0
6	M	168/304 (55%)	0.04	5 (2%)	50	53	89, 159, 206, 215	0
All	All	4037/5294 (76%)	0.02	41 (1%)	82	86	53, 104, 175, 222	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	L	57	SER	5.1
6	L	56	ARG	4.7
6	M	55	ILE	4.1
5	J	103	SER	3.8
5	I	372	VAL	3.6

6.2 Non-standard residues in protein, DNA, RNA chains

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SEP	M	51	10/11	0.92	0.10	137,154,182,184	0
6	SEP	L	51	10/11	0.95	0.11	132,141,152,159	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PO4	B	401	5/5	0.81	0.13	137,161,171,193	0
7	PO4	I	701	5/5	0.82	0.40	111,124,146,169	0
7	PO4	J	701	5/5	0.85	0.95	136,141,152,185	0
7	PO4	A	401	5/5	0.86	0.15	149,154,168,180	0
7	PO4	D	401	5/5	0.91	0.23	56,91,105,123	0
7	PO4	H	501	5/5	0.91	0.23	91,93,111,124	0
7	PO4	F	501	5/5	0.92	0.23	84,99,115,117	0
7	PO4	C	401	5/5	0.93	0.18	63,115,116,137	0
7	PO4	E	502	5/5	0.93	0.20	114,130,143,164	0
7	PO4	E	501	5/5	0.94	0.32	61,91,121,127	0
7	PO4	F	502	5/5	0.94	0.17	131,139,155,167	0
7	PO4	G	501	5/5	0.94	0.23	81,92,120,121	0

6.5 Other polymers (i)

There are no such residues in this entry.