wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 02:51 PM EDT

PDB ID	:	5B04
Title	:	Crystal structure of the eukaryotic translation initiation factor 2B from Schizosaccharomyces pombe
Authors	:	Kashiwagi, K.; Ito, T.; Yokoyama, S.
Deposited on	:	2015-10-27
Resolution	:	2.99 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:

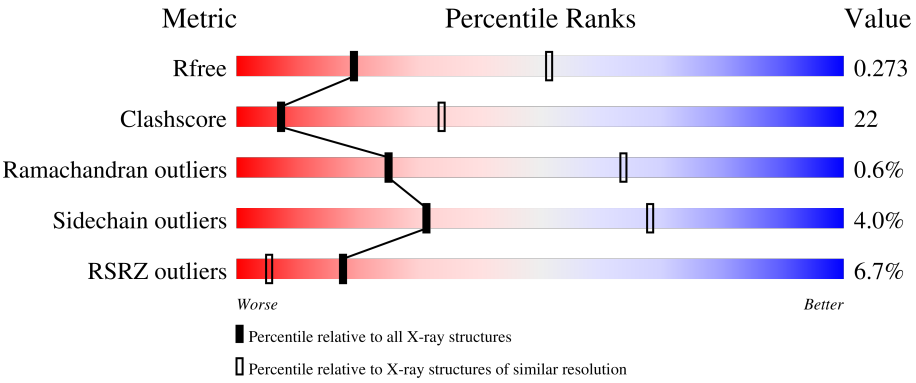
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.99 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.



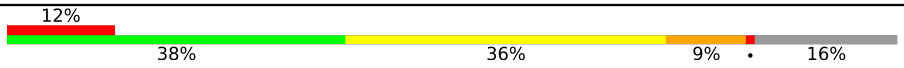
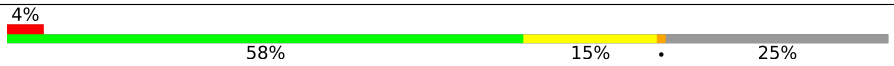
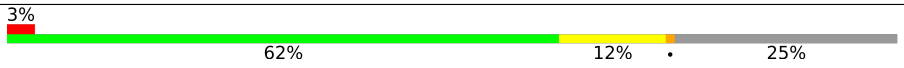
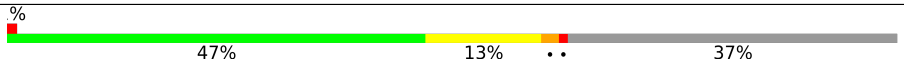
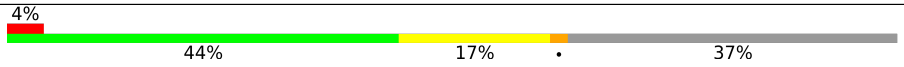
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	9% 59% 29% • 7%
1	B	341	5% 75% 17% • 6%
2	C	399	6% 66% 19% • 13%
2	D	399	3% 69% 17% • 13%
3	E	458	9% 45% 30% 7% • 16%

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	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 28584 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
			2472	1571	430	458	13			
1	B	319	Total	C	N	O	S	0	0	0
			2489	1582	434	460	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	349	Total	C	N	O	S	0	0	0
			2702	1714	459	515	14			
2	D	346	Total	C	N	O	S	0	0	0
			2674	1697	453	511	13			

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	384	Total	C	N	O	S	0	0	0
			2976	1895	511	553	17			
3	F	383	Total	C	N	O	S	0	0	0
			2967	1890	509	551	17			

There are 6 discrepancies between the modelled and reference sequences:

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

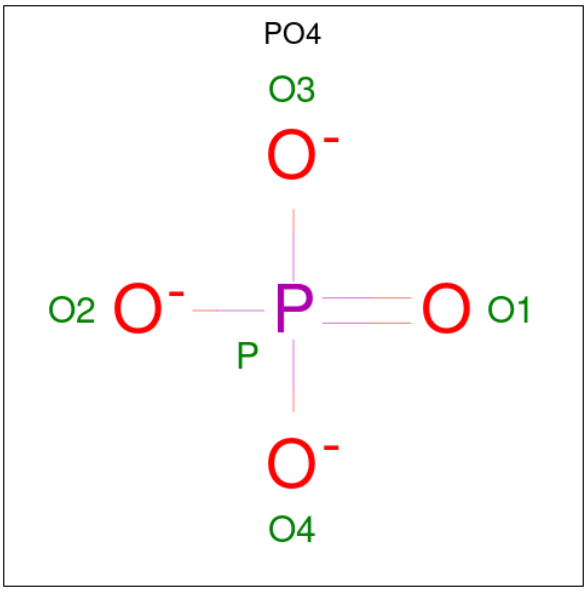
- Molecule 4 is a protein called Probable translation initiation factor eIF-2B subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	349	Total	C	N	O	S	0	0	0
			2755	1763	466	513	13			
4	H	349	Total	C	N	O	S	0	0	0
			2755	1763	466	513	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	428	Total	C	N	O	S	0	0	0
			3377	2123	592	647	15			
5	J	428	Total	C	N	O	S	0	0	0
			3372	2119	591	647	15			

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

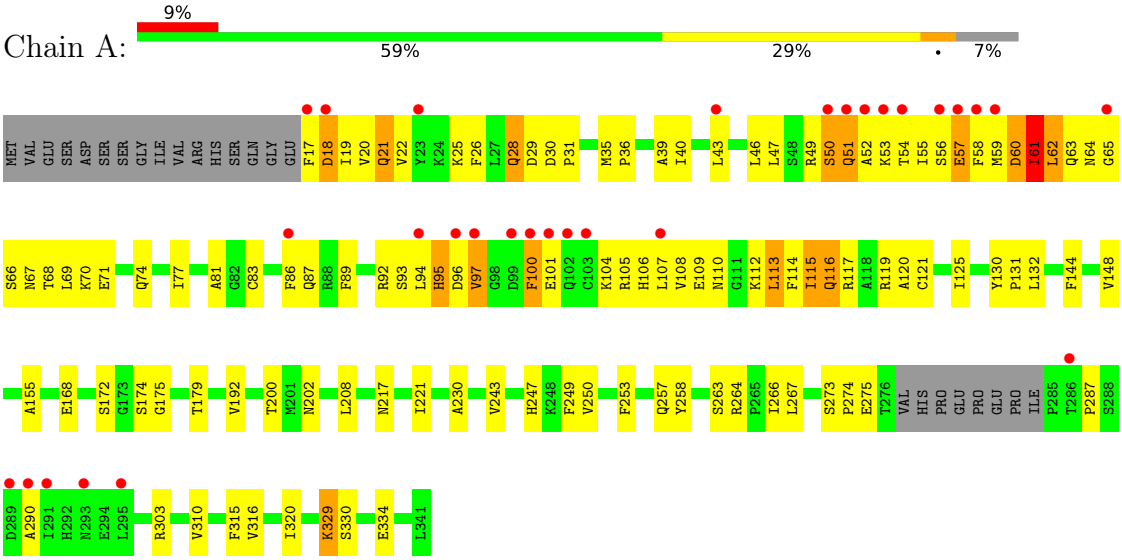


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	D	1	Total O P 5 4 1	0	0
6	G	1	Total O P 5 4 1	0	0
6	G	1	Total O P 5 4 1	0	0
6	H	1	Total O P 5 4 1	0	0
6	H	1	Total O P 5 4 1	0	0
6	I	1	Total O P 5 4 1	0	0

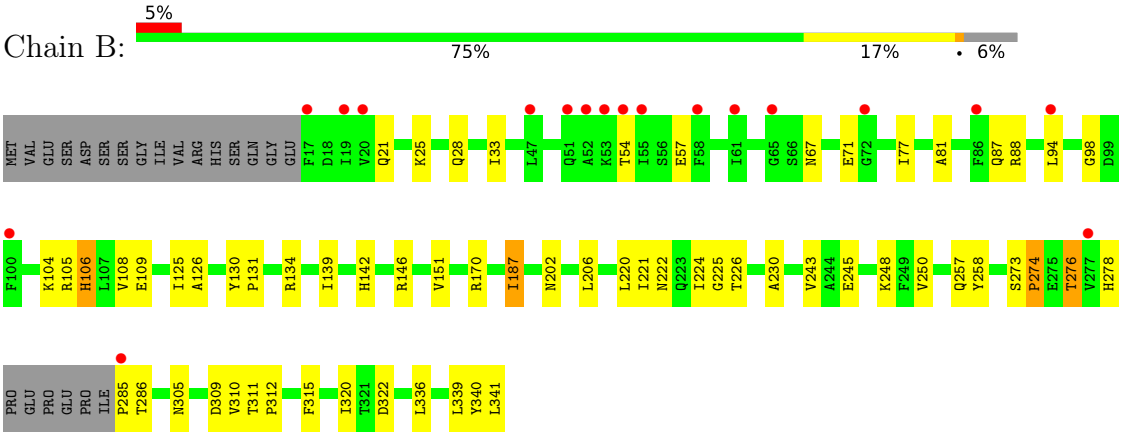
3 Residue-property plots (i)

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.

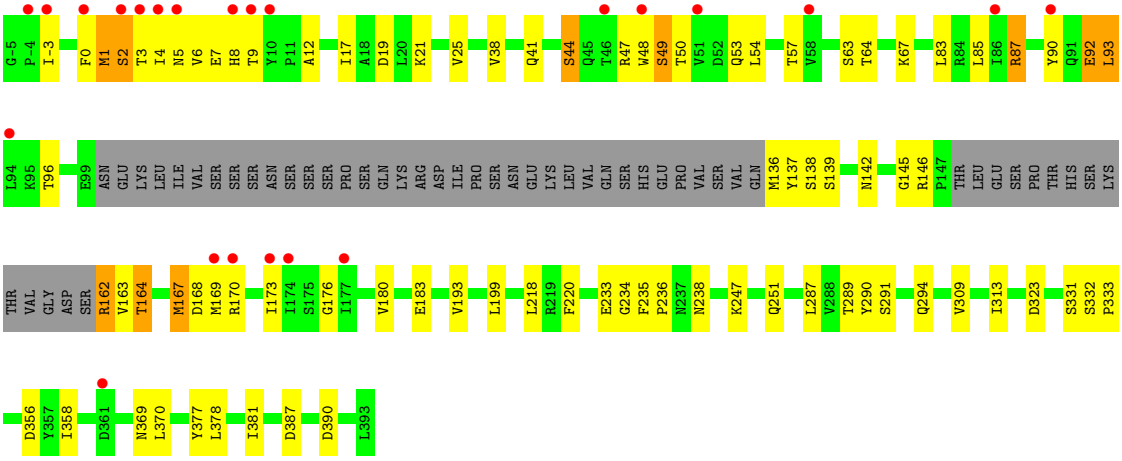
• Molecule 1: Translation initiation factor eIF-2B subunit alpha



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

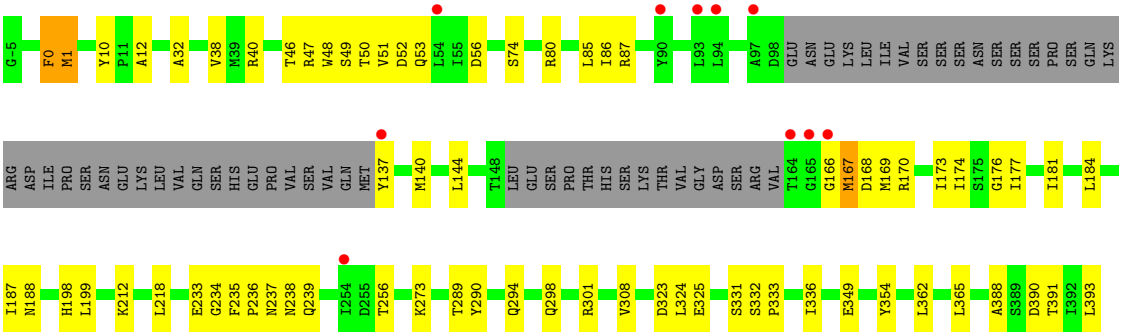


• Molecule 2: Probable translation initiation factor eIF-2B subunit beta



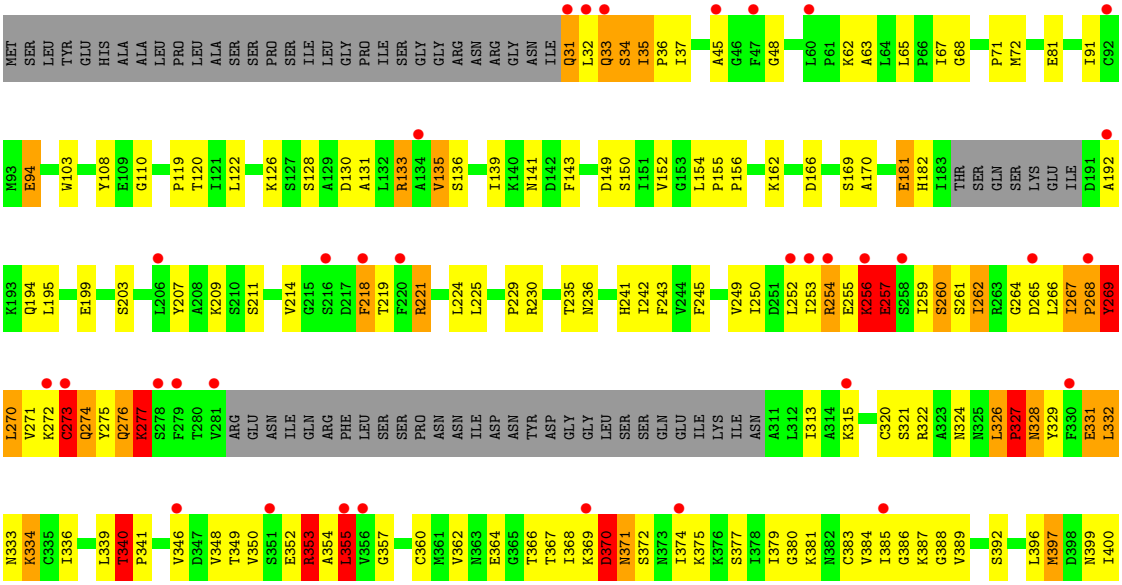
• Molecule 2: Probable translation initiation factor eIF-2B subunit beta

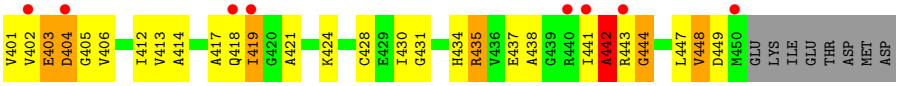
Chain D:



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

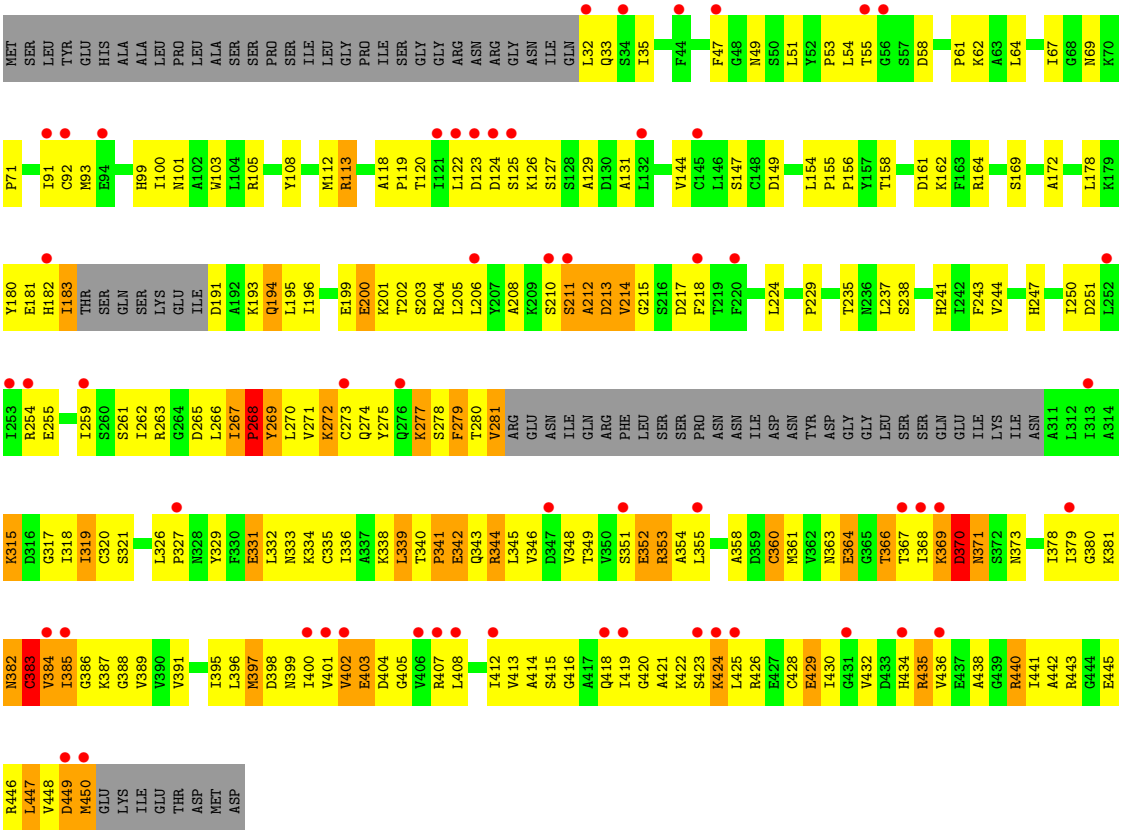
Chain E:





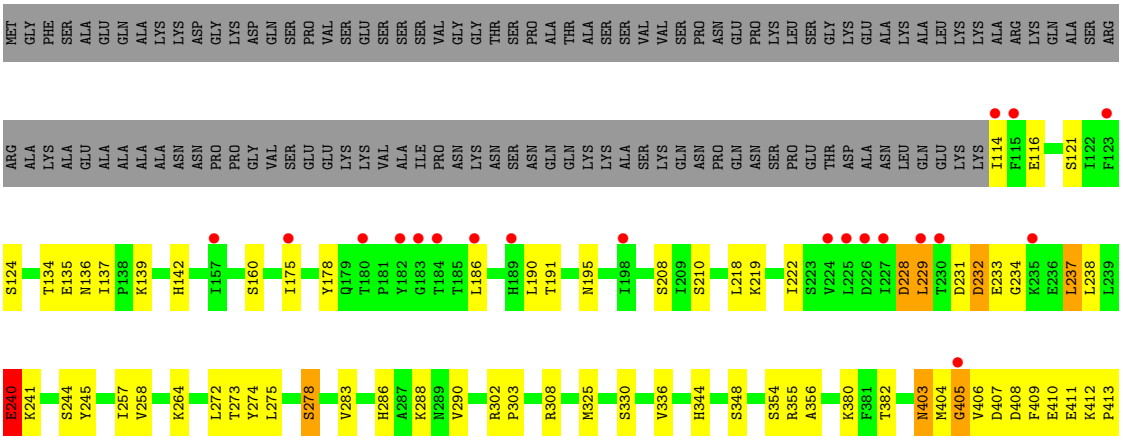
• Molecule 3: Probable translation initiation factor eIF-2B subunit gamma

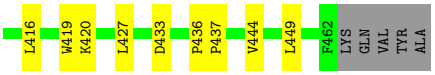
Chain F:



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

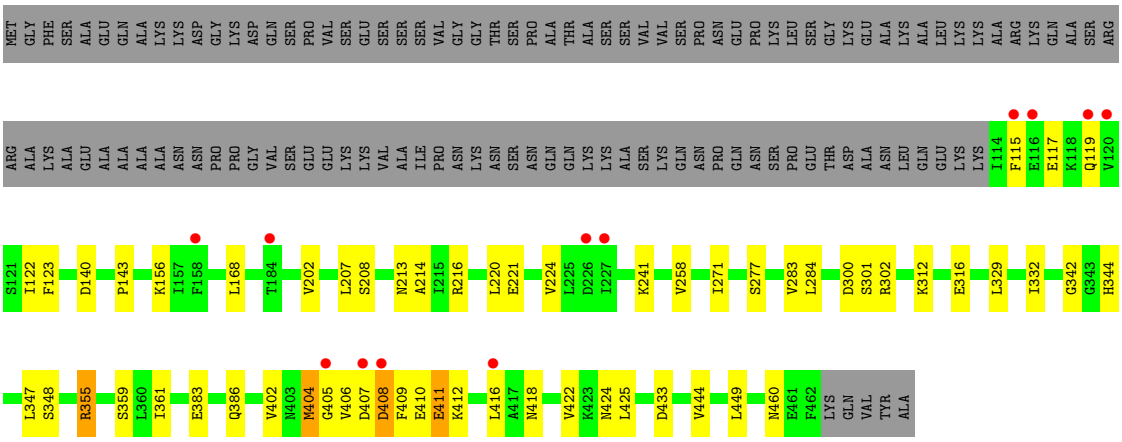
Chain G:





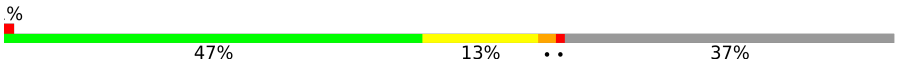
• Molecule 4: Probable translation initiation factor eIF-2B subunit delta

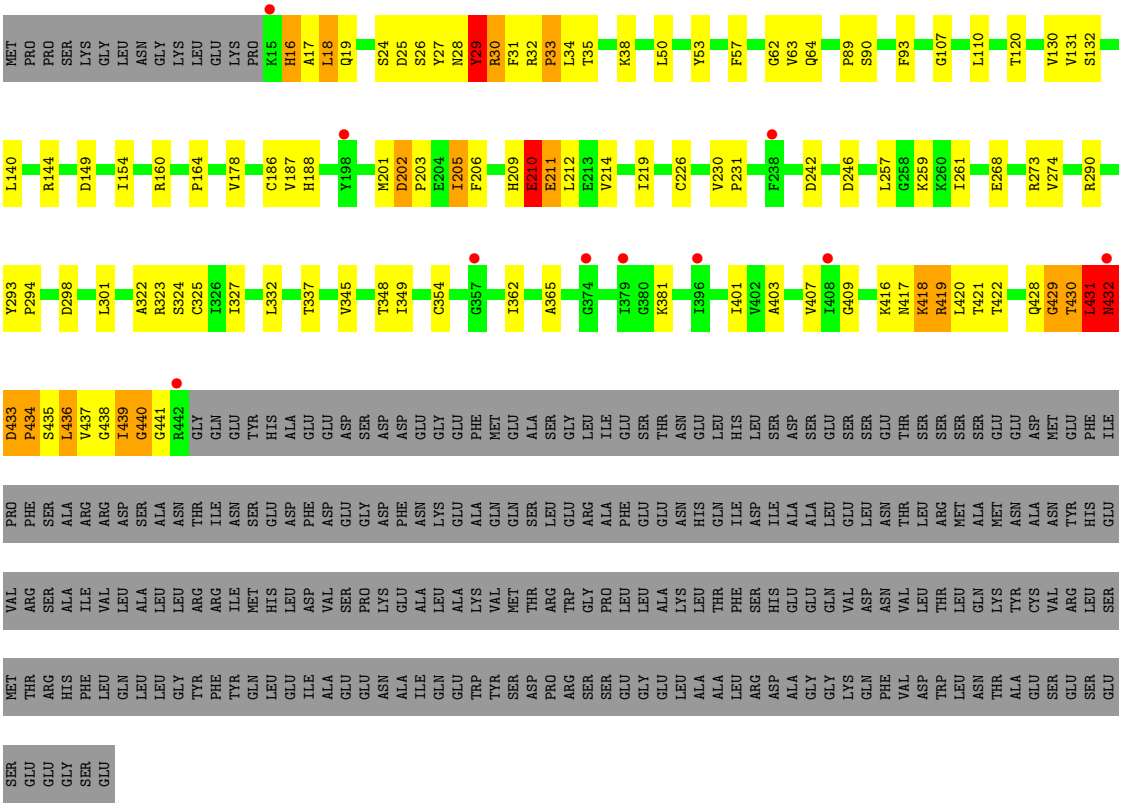
Chain H:



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

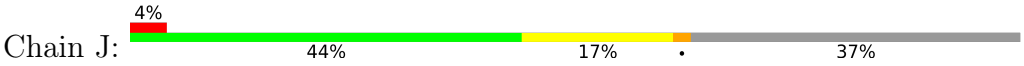
Chain I:

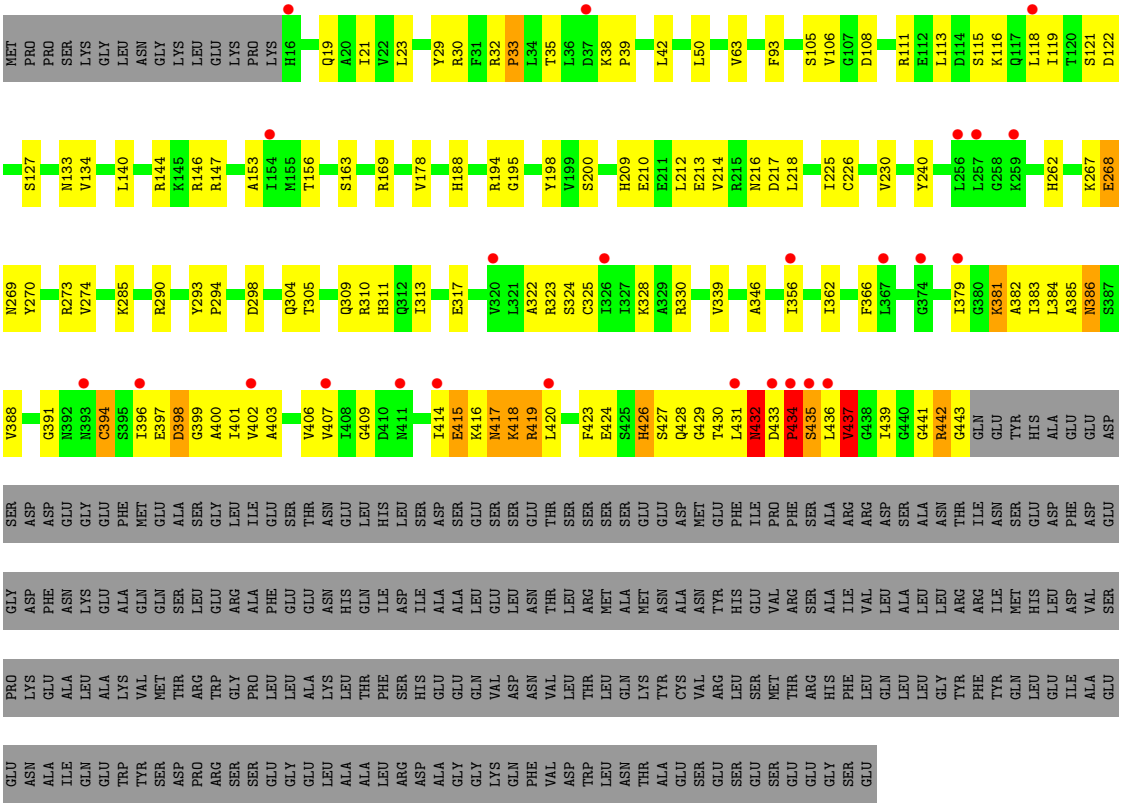




• Molecule 5: Probable translation initiation factor eIF-2B subunit epsilon

Chain J:


4%
44%
17%
37%


MET PRO PRO SER LYS GLY LEU ASN GLY LYS LEU GLU LYS PRO LYS H16 Q19 A20 I21 V22 L23 Y29 R30 F31 R32 P33 L34 T35 L36 D37 K38 P39 L42 L50 V63 F93 S105 V106 G107 D108 R111 E112 L113 D114 S115 K116 Q117 L118 I119 T120 S121 D122
S127 N133 V134 L140 R144 K145 R146 R147 A153 I154 M155 T156 S163 R169 V178 H188 R194 G195 Y198 V199 S200 H209 E210 E211 L212 E213 V214 R215 N216 D217 L218 I225 C226 V230 Y240 L256 L257 G258 K259 H262 K267 E268
N269 Y270 R273 V274 K285 R290 Y293 P294 D298 Q304 T305 Q309 R310 H311 Q312 I313 E317 V320 L321 A322 R323 S324 C325 I326 I327 K328 A329 R330 V339 A346 I356 I362 F366 L367 G374 I379 G380 K381 A382 I383 L384 A385 N386 S387
V388 G391 N392 N393 C394 S395 I396 E397 D398 G399 A400 I401 V402 A403 V406 V407 I408 G409 D410 N411 I414 E415 K416 N417 K418 R419 L420 F423 E424 S425 H426 S427 Q428 G429 T430 L431 N432 D433 P434 S435 L436 V437 G438 I439 G440 G441 R442 G443 GLN GLU TYR HIS ALA GLU GLU ASP
SER ASP ASP GLU GLY GLU PHE MET GLU ALA SER GLY LEU ILE GLU SER THR ASN GLU LEU HIS LEU SER ASP SER GLU SER SER GLU THR SER SER SER SER GLU GLU ASP MET GLU PHE ILE PRO PHE SER ALA ARG ASP SER ALA ASN THR ILE ASN SER GLU ASP PHE ASP GLU
GLY ASP PHE ASN LYS GLU ALA GLN GLN SER LEU GLU ARG ALA PHE GLU GLU ASN HIS GLN ILE ASP ILE ALA ALA LEU GLU LEU GLU ASN THR LEU ARG MET ALA MET ASN ALA ASN TYR HIS GLU VAL ARG SER ALA ILE VAL LEU ALA LEU LEU LEU GLY TYR PHE TYR GLN LEU LEU GLU ILE ALA GLU
PRO LYS GLU ALA LEU ALA LYS VAL MET THR ARG TRP GLY PRO LEU LEU ALA LYS LEU THR PHE SER HIS GLU GLU GLN VAL ASP ASN VAL LEU THR LEU GLN LYS TYR CYS VAL ARG LEU SER MET THR ARG HIS PHE LEU GLN LEU LEU LEU GLY TYR PHE TYR GLN LEU GLU ILE ALA GLU
GLU ASN ALA ILE GLN GLU TRP TYR SER ASP PRO ARG SER SER GLU GLY GLU LEU ALA ALA LEU ARG ASP ALA GLY GLY LYS GLN PHE VAL ASP TRP LEU ASN THR ALA GLU SER GLU SER GLU GLU GLY SER GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	144.50Å 209.23Å 223.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.99 49.29 – 2.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.29-2.99) 99.6 (49.29-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.222 , 0.271 0.227 , 0.273	Depositor DCC
R_{free} test set	6815 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	80.9	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 63.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	28584	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.32	0/2519	0.63	5/3409 (0.1%)
1	B	0.29	0/2537	0.48	2/3434 (0.1%)
2	C	0.31	0/2747	0.49	1/3726 (0.0%)
2	D	0.26	0/2719	0.46	2/3690 (0.1%)
3	E	0.57	2/3029 (0.1%)	0.91	21/4100 (0.5%)
3	F	0.51	3/3020 (0.1%)	1.08	30/4088 (0.7%)
4	G	0.38	1/2802 (0.0%)	0.58	3/3797 (0.1%)
4	H	0.27	0/2802	0.43	0/3797
5	I	0.46	1/3437 (0.0%)	0.77	14/4658 (0.3%)
5	J	0.45	2/3432 (0.1%)	0.63	5/4652 (0.1%)
All	All	0.40	9/29044 (0.0%)	0.69	83/39351 (0.2%)

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
1	A	0	2
3	E	0	5
3	F	0	6
4	H	0	1
5	I	0	1
5	J	0	1
All	All	0	16

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	268	PRO	N-CD	-13.76	1.28	1.47
5	J	434	PRO	N-CD	-9.39	1.34	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	33	PRO	N-CD	8.86	1.60	1.47
5	I	434	PRO	N-CD	7.20	1.57	1.47
3	E	257	GLU	CG-CD	-6.17	1.42	1.51

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	429	GLY	N-CA-C	16.66	154.74	113.10
3	F	370	ASP	N-CA-C	16.40	155.28	111.00
3	F	370	ASP	CB-CA-C	-15.86	78.69	110.40
5	I	432	ASN	CB-CA-C	-14.98	80.44	110.40
3	F	212	ALA	CB-CA-C	13.37	130.15	110.10

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	329	LYS	Peptide
1	A	60	ASP	Peptide
3	E	257	GLU	Peptide
3	E	260	SER	Peptide
3	E	269	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	2472	0	2492	150	0
1	B	2489	0	2512	52	0
2	C	2702	0	2744	95	0
2	D	2674	0	2714	52	1
3	E	2976	0	3032	265	0
3	F	2967	0	3022	325	7
4	G	2755	0	2841	91	0
4	H	2755	0	2841	45	0
5	I	3377	0	3361	140	1
5	J	3372	0	3351	134	7

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	1	0
6	G	10	0	0	1	0
6	H	10	0	0	0	0
6	I	5	0	0	1	0
All	All	28584	0	28910	1287	8

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 22.

The worst 5 of 1287 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)
3:F:218:PHE:CE2	5:I:203:PRO:HB3	1.37	1.58
3:F:368:ILE:HA	3:F:385:ILE:O	1.17	1.24
3:E:355:LEU:HD21	3:E:369:LYS:O	1.05	1.23
3:F:218:PHE:HE2	5:I:203:PRO:CB	1.54	1.21
3:F:265:ASP:O	3:F:268:PRO:HD2	1.35	1.21

The worst 5 of 8 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:113:ARG:NH2	5:J:443:GLY:C[2_555]	0.64	1.56
3:F:113:ARG:CZ	5:J:443:GLY:O[2_555]	0.66	1.54
3:F:113:ARG:NH2	5:J:443:GLY:O[2_555]	0.96	1.24
3:F:113:ARG:NH1	5:J:443:GLY:O[2_555]	1.51	0.69
3:F:113:ARG:CZ	5:J:443:GLY:C[2_555]	1.76	0.44

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%)	293 (94%)	17 (5%)	3 (1%)	15 53
1	B	315/341 (92%)	302 (96%)	12 (4%)	1 (0%)	41 76
2	C	343/399 (86%)	330 (96%)	13 (4%)	0	100 100
2	D	340/399 (85%)	327 (96%)	13 (4%)	0	100 100
3	E	378/458 (82%)	334 (88%)	36 (10%)	8 (2%)	7 33
3	F	377/458 (82%)	334 (89%)	40 (11%)	3 (1%)	19 57
4	G	347/467 (74%)	331 (95%)	15 (4%)	1 (0%)	41 76
4	H	347/467 (74%)	339 (98%)	8 (2%)	0	100 100
5	I	426/678 (63%)	400 (94%)	24 (6%)	2 (0%)	29 68
5	J	426/678 (63%)	385 (90%)	37 (9%)	4 (1%)	17 55
All	All	3612/4686 (77%)	3375 (93%)	215 (6%)	22 (1%)	25 64

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	262	ILE
3	E	442	ALA
3	E	270	LEU
3	E	277	LYS
5	J	432	ASN

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	276/298 (93%)	264 (96%)	12 (4%)	29 66
1	B	278/298 (93%)	274 (99%)	4 (1%)	67 88
2	C	301/350 (86%)	290 (96%)	11 (4%)	34 70
2	D	298/350 (85%)	295 (99%)	3 (1%)	76 91
3	E	330/395 (84%)	299 (91%)	31 (9%)	8 32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	F	329/395 (83%)	306 (93%)	23 (7%)	15 47
4	G	314/408 (77%)	307 (98%)	7 (2%)	52 81
4	H	314/408 (77%)	307 (98%)	7 (2%)	52 81
5	I	379/596 (64%)	363 (96%)	16 (4%)	30 66
5	J	378/596 (63%)	365 (97%)	13 (3%)	37 72
All	All	3197/4094 (78%)	3070 (96%)	127 (4%)	31 68

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	370	ASP
5	I	431	LEU
3	F	315	LYS
5	I	430	THR
5	J	417	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
5	I	347	ASN
5	J	393	ASN
5	J	428	GLN
5	J	417	ASN
3	E	276	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)

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)

9 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	$\#\|Z\| > 2$
6	PO4	A	401	-	4,4,4	0.93	0	6,6,6	0.43	0
6	PO4	H	502	-	4,4,4	0.93	0	6,6,6	0.46	0
6	PO4	G	502	-	4,4,4	0.91	0	6,6,6	0.42	0
6	PO4	H	501	-	4,4,4	0.91	0	6,6,6	0.45	0
6	PO4	D	401	-	4,4,4	0.92	0	6,6,6	0.43	0
6	PO4	G	501	-	4,4,4	0.91	0	6,6,6	0.43	0
6	PO4	I	701	-	4,4,4	0.90	0	6,6,6	0.42	0
6	PO4	B	401	-	4,4,4	0.94	0	6,6,6	0.45	0
6	PO4	C	401	-	4,4,4	0.90	0	6,6,6	0.42	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	401	PO4	1	0
6	G	501	PO4	1	0
6	I	701	PO4	1	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%)	0.60	30 (9%) 8 3	55, 86, 150, 173	0
1	B	319/341 (93%)	0.49	18 (5%) 24 8	49, 80, 123, 180	0
2	C	349/399 (87%)	0.46	23 (6%) 18 5	42, 68, 138, 165	0
2	D	346/399 (86%)	0.19	10 (2%) 51 23	41, 66, 111, 161	0
3	E	384/458 (83%)	0.67	42 (10%) 5 2	61, 99, 142, 163	0
3	F	383/458 (83%)	0.79	56 (14%) 2 1	66, 108, 153, 168	0
4	G	349/467 (74%)	0.45	20 (5%) 23 8	44, 75, 136, 167	0
4	H	349/467 (74%)	0.19	12 (3%) 45 19	44, 65, 116, 153	0
5	I	428/678 (63%)	0.23	10 (2%) 60 31	42, 73, 115, 148	0
5	J	428/678 (63%)	0.39	25 (5%) 23 7	50, 87, 122, 153	0
All	All	3652/4686 (77%)	0.44	246 (6%) 17 5	41, 80, 137, 180	0

The worst 5 of 246 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	423	SER	7.7
2	C	8	HIS	7.5
3	E	450	MET	6.5
4	G	226	ASP	6.0
2	C	4	ILE	5.7

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

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

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
6	PO4	G	501	5/5	0.88	0.17	91,94,118,136	0
6	PO4	G	502	5/5	0.89	0.18	62,67,102,104	0
6	PO4	H	501	5/5	0.89	0.17	81,85,101,134	0
6	PO4	I	701	5/5	0.90	0.15	101,102,127,141	0
6	PO4	H	502	5/5	0.95	0.20	71,82,90,98	0
6	PO4	D	401	5/5	0.97	0.22	50,53,72,73	0
6	PO4	A	401	5/5	0.98	0.16	70,71,84,89	0
6	PO4	B	401	5/5	0.98	0.19	63,67,86,93	0
6	PO4	C	401	5/5	0.99	0.18	51,53,68,70	0

6.5 Other polymers (i)

There are no such residues in this entry.