



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 03:08 PM EST

PDB ID : 1S0U
Title : eIF2gamma apo
Authors : Roll-Mecak, A.; Alone, P.; Cao, C.; Dever, T.E.; Burley, S.K.
Deposited on : 2004-01-04
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtrriage (Phenix) : 1.13
EDS : 2.16
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) : 2.16

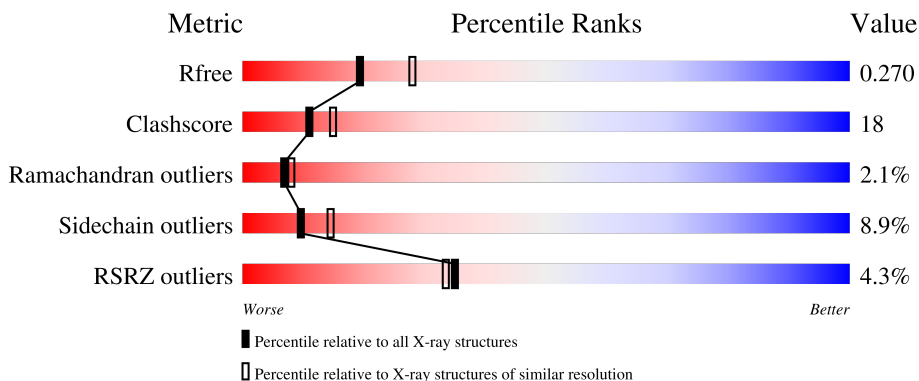
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	408	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3019 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 2 gamma subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	391	2836	1800	489	533	14	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	cloning artifact	UNP Q58657
A	31	PRO	-	cloning artifact	UNP Q58657
A	32	LEU	-	cloning artifact	UNP Q58657
A	33	GLY	-	cloning artifact	UNP Q58657
A	34	SER	-	cloning artifact	UNP Q58657

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

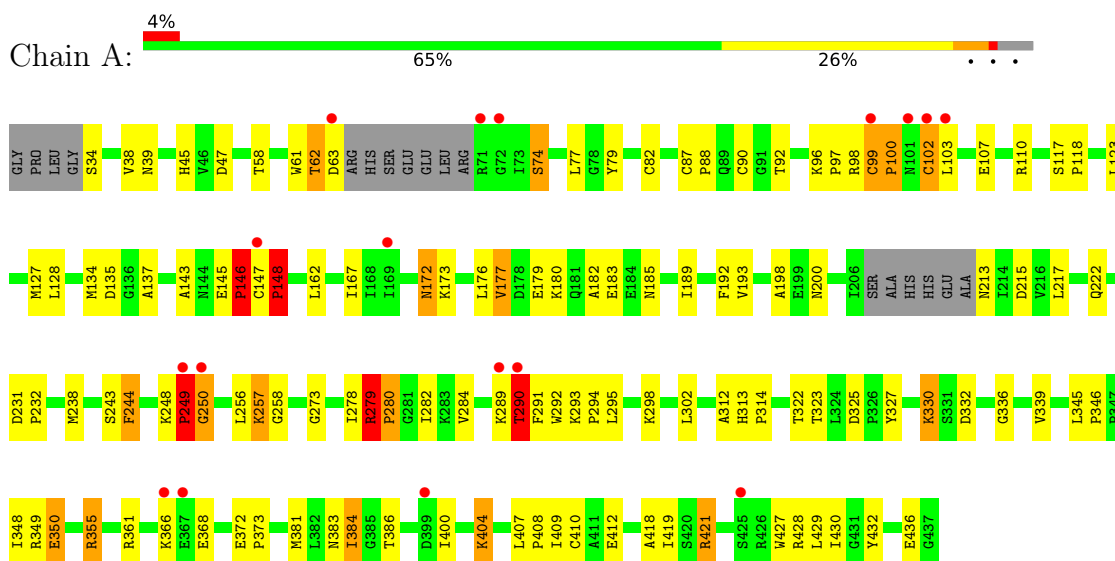
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	182	Total	O	0	0
			182	182		

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 2 gamma subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.84Å 52.49Å 74.13Å 90.00° 92.53° 90.00°	Depositor
Resolution (Å)	22.00 – 2.40 20.02 – 2.42	Depositor EDS
% Data completeness (in resolution range)	(Not available) (22.00-2.40) 98.6 (20.02-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.72 (at 2.41Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.212 , 0.264 0.217 , 0.270	Depositor DCC
R_{free} test set	1566 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l 0.011 for -k,-h,-l 0.033 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3019	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: ZN

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	0.49	2/2880 (0.1%)	1.05	13/3919 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	CYS	C-N	-7.89	1.19	1.34
1	A	147	CYS	CA-C	-5.05	1.39	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	ARG	C-N-CD	-22.06	72.07	120.60
1	A	147	CYS	C-N-CD	-17.86	81.30	120.60
1	A	148	PRO	CA-N-CD	-14.36	91.40	111.50
1	A	279	ARG	C-N-CA	13.63	179.26	122.00
1	A	147	CYS	C-N-CA	11.96	172.22	122.00
1	A	148	PRO	N-CA-CB	11.19	116.73	103.30
1	A	102	CYS	CA-CB-SG	10.65	133.18	114.00
1	A	148	PRO	N-CD-CG	9.26	117.08	103.20
1	A	90	CYS	CA-CB-SG	6.32	125.38	114.00
1	A	147	CYS	CA-C-N	-6.07	100.11	117.10
1	A	102	CYS	N-CA-C	-5.45	96.29	111.00
1	A	99	CYS	C-N-CD	-5.31	108.92	120.60
1	A	102	CYS	CB-CA-C	5.08	120.55	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2836	0	2848	103	0
2	A	1	0	0	0	0
3	A	182	0	0	8	0
All	All	3019	0	2848	103	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 18.

All (103) 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)
1:A:99:CYS:HB3	1:A:102:CYS:O	1.36	1.26
1:A:257:LYS:HE2	1:A:258:GLY:H	1.02	1.12
1:A:257:LYS:HE2	1:A:258:GLY:N	1.75	1.02
1:A:74:SER:OG	3:A:532:HOH:O	1.86	0.94
1:A:290:THR:O	1:A:290:THR:HG22	1.68	0.91
1:A:289:LYS:O	1:A:290:THR:HB	1.71	0.90
1:A:279:ARG:HE	1:A:348:ILE:HD11	1.35	0.90
1:A:346:PRO:HG2	1:A:410:CYS:SG	2.21	0.81
1:A:284:VAL:O	1:A:290:THR:HA	1.81	0.81
1:A:279:ARG:NE	1:A:348:ILE:HD11	1.96	0.79
1:A:118:PRO:HA	3:A:551:HOH:O	1.84	0.77
1:A:134:MET:CE	1:A:137:ALA:HB2	2.14	0.77
1:A:248:LYS:O	1:A:249:PRO:O	2.05	0.73
1:A:366:LYS:C	1:A:368:GLU:H	1.92	0.73
1:A:257:LYS:CE	1:A:258:GLY:H	1.94	0.71
1:A:290:THR:O	1:A:290:THR:CG2	2.38	0.71
1:A:134:MET:HE3	1:A:137:ALA:HB2	1.72	0.70
1:A:38:VAL:HG13	1:A:135:ASP:HB2	1.76	0.67
1:A:404:LYS:HB3	1:A:404:LYS:NZ	2.11	0.66
1:A:77:LEU:HB3	1:A:79:TYR:CE1	2.32	0.65
1:A:110:ARG:HE	1:A:222:GLN:HE22	1.44	0.65
1:A:99:CYS:CB	1:A:102:CYS:O	2.30	0.64
1:A:172:ASN:ND2	1:A:173:LYS:H	1.95	0.64
1:A:404:LYS:HB3	1:A:404:LYS:HZ2	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLU:C	1:A:146:PRO:O	2.38	0.61
1:A:361:ARG:HD3	1:A:428:ARG:NH2	2.16	0.61
1:A:176:LEU:O	1:A:177:VAL:HG22	2.02	0.59
1:A:383:ASN:ND2	3:A:453:HOH:O	2.36	0.58
1:A:408:PRO:O	1:A:409:ILE:HD12	2.03	0.58
1:A:117:SER:HB2	1:A:123:LEU:HB2	1.84	0.58
1:A:366:LYS:C	1:A:368:GLU:N	2.57	0.58
1:A:346:PRO:HB3	1:A:412:GLU:HG2	1.86	0.57
1:A:92:THR:HG21	1:A:99:CYS:SG	2.44	0.57
1:A:145:GLU:O	1:A:146:PRO:O	2.23	0.56
1:A:421:ARG:HD2	1:A:430:ILE:HG21	1.88	0.55
1:A:313:HIS:HB2	1:A:314:PRO:CD	2.37	0.55
1:A:349:ARG:HH11	1:A:349:ARG:HG2	1.72	0.54
1:A:355:ARG:HH12	1:A:400:ILE:HD11	1.72	0.54
1:A:419:ILE:O	1:A:429:LEU:HD12	2.07	0.54
1:A:244:PHE:N	1:A:244:PHE:CD1	2.75	0.53
1:A:96:LYS:HD2	1:A:100:PRO:HG3	1.90	0.53
1:A:182:ALA:O	1:A:183:GLU:CB	2.56	0.52
1:A:302:LEU:HD13	1:A:312:ALA:HB2	1.91	0.51
1:A:176:LEU:O	1:A:177:VAL:O	2.27	0.51
1:A:127:MET:HB3	1:A:162:LEU:HD11	1.91	0.51
1:A:325:ASP:OD1	1:A:327:TYR:HD2	1.93	0.51
1:A:92:THR:CG2	1:A:99:CYS:SG	2.99	0.51
1:A:248:LYS:O	1:A:249:PRO:C	2.45	0.50
1:A:98:ARG:O	1:A:100:PRO:HD3	2.12	0.50
1:A:384:ILE:HD12	3:A:440:HOH:O	2.11	0.50
1:A:325:ASP:OD1	1:A:327:TYR:CD2	2.65	0.50
1:A:189:ILE:O	1:A:193:VAL:HG22	2.12	0.50
1:A:248:LYS:C	1:A:249:PRO:O	2.49	0.50
1:A:313:HIS:HD2	1:A:314:PRO:O	1.95	0.49
1:A:172:ASN:HD22	1:A:173:LYS:H	1.60	0.49
1:A:45:HIS:HE1	1:A:47:ASP:OD2	1.95	0.49
1:A:381:MET:HB2	1:A:427:TRP:CE3	2.49	0.48
1:A:180:LYS:O	1:A:182:ALA:O	2.32	0.47
1:A:273:GLY:HA2	1:A:298:LYS:HE3	1.96	0.47
1:A:355:ARG:NH1	1:A:436:GLU:OE1	2.47	0.47
1:A:145:GLU:O	1:A:146:PRO:C	2.52	0.47
1:A:167:ILE:HD12	1:A:198:ALA:HB2	1.98	0.46
1:A:279:ARG:HG2	1:A:345:LEU:HD13	1.98	0.46
1:A:278:ILE:HB	1:A:295:LEU:HB2	1.98	0.46
1:A:291:PHE:CD2	1:A:291:PHE:N	2.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:VAL:CG1	1:A:39:ASN:N	2.79	0.45
1:A:292:TRP:CE2	1:A:408:PRO:HG2	2.52	0.45
1:A:238:MET:HB3	1:A:339:VAL:HB	1.99	0.45
1:A:34:SER:N	3:A:466:HOH:O	2.49	0.45
1:A:38:VAL:HG12	1:A:39:ASN:N	2.31	0.45
1:A:381:MET:HB2	1:A:427:TRP:CZ3	2.52	0.45
1:A:279:ARG:HB2	1:A:345:LEU:HD13	1.97	0.45
1:A:383:ASN:HB2	1:A:418:ALA:HB3	1.99	0.45
1:A:330:LYS:NZ	1:A:330:LYS:HB2	2.31	0.44
1:A:279:ARG:HA	1:A:279:ARG:HD2	1.24	0.44
1:A:250:GLY:C	3:A:492:HOH:O	2.56	0.44
1:A:313:HIS:HB2	1:A:314:PRO:HD2	1.99	0.44
1:A:282:ILE:HG22	3:A:522:HOH:O	2.18	0.43
1:A:292:TRP:NE1	1:A:408:PRO:HG2	2.33	0.43
1:A:292:TRP:CD1	1:A:408:PRO:HG2	2.53	0.43
1:A:349:ARG:NH1	1:A:349:ARG:HG2	2.33	0.43
1:A:62:THR:O	1:A:63:ASP:CB	2.66	0.43
1:A:293:LYS:HA	1:A:294:PRO:HD3	1.75	0.43
1:A:366:LYS:O	1:A:368:GLU:N	2.43	0.43
1:A:213:ASN:OD1	1:A:215:ASP:HB3	2.18	0.43
1:A:336:GLY:HA2	1:A:386:THR:C	2.39	0.43
1:A:302:LEU:HD13	1:A:312:ALA:CB	2.49	0.43
1:A:249:PRO:O	1:A:250:GLY:C	2.57	0.42
1:A:330:LYS:HB2	1:A:330:LYS:HZ3	1.85	0.42
1:A:58:THR:HG22	1:A:82:CYS:HB2	2.01	0.42
1:A:110:ARG:HH21	1:A:222:GLN:NE2	2.17	0.41
1:A:143:ALA:HA	1:A:185:ASN:ND2	2.35	0.41
1:A:258:GLY:HA3	1:A:322:THR:O	2.20	0.41
1:A:148:PRO:HG3	1:A:192:PHE:CD1	2.54	0.41
1:A:407:LEU:HA	1:A:408:PRO:HD3	1.93	0.41
1:A:123:LEU:HG	1:A:127:MET:CE	2.50	0.41
1:A:372:GLU:HA	1:A:373:PRO:HD3	1.85	0.41
1:A:61:TRP:HB3	3:A:488:HOH:O	2.21	0.41
1:A:128:LEU:HD13	1:A:432:TYR:HB3	2.03	0.41
1:A:355:ARG:NH1	1:A:400:ILE:HD11	2.35	0.41
1:A:350:GLU:H	1:A:350:GLU:HG2	1.73	0.41
1:A:243:SER:OG	1:A:332:ASP:HA	2.21	0.41
1:A:231:ASP:HA	1:A:232:PRO:HD3	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	385/408 (94%)	353 (92%)	24 (6%)	8 (2%)	7 8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	PRO
1	A	177	VAL
1	A	249	PRO
1	A	250	GLY
1	A	280	PRO
1	A	290	THR
1	A	146	PRO
1	A	62	THR

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	292/337 (87%)	266 (91%)	26 (9%)	9 14

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	SER
1	A	87	CYS
1	A	88	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	97	PRO
1	A	100	PRO
1	A	103	LEU
1	A	107	GLU
1	A	146	PRO
1	A	172	ASN
1	A	179	GLU
1	A	200	ASN
1	A	217	LEU
1	A	244	PHE
1	A	249	PRO
1	A	256	LEU
1	A	257	LYS
1	A	279	ARG
1	A	280	PRO
1	A	290	THR
1	A	323	THR
1	A	330	LYS
1	A	350	GLU
1	A	355	ARG
1	A	384	ILE
1	A	404	LYS
1	A	421	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	172	ASN
1	A	185	ASN
1	A	200	ASN
1	A	222	GLN
1	A	313	HIS
1	A	383	ASN

5.3.3 RNA

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	147:CYS	C	148:PRO	N	1.19

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	391/408 (95%)	0.13	17 (4%) 35 33	16, 27, 49, 62	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	PRO	5.7
1	A	250	GLY	4.5
1	A	425	SER	3.5
1	A	367	GLU	3.5
1	A	102	CYS	3.0
1	A	72	GLY	3.0
1	A	366	LYS	3.0
1	A	101	ASN	2.9
1	A	103	LEU	2.7
1	A	169	ILE	2.7
1	A	63	ASP	2.6
1	A	289	LYS	2.5
1	A	99	CYS	2.3
1	A	71	ARG	2.3
1	A	399	ASP	2.3
1	A	290	THR	2.2
1	A	147	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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, 95th 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
2	ZN	A	1	1/1	0.93	0.09	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.