



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 09:20 AM EDT

PDB ID : 2CCF / pdb_00002ccf
Title : Antiparallel Configuration of pLI E20S
Authors : Yadav, M.K.; Leman, L.J.; Price, D.J.; Brooks 3rd, C.L.; Stout, C.D.; Ghadiri, M.R.
Deposited on : 2006-01-16
Resolution : 1.70 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

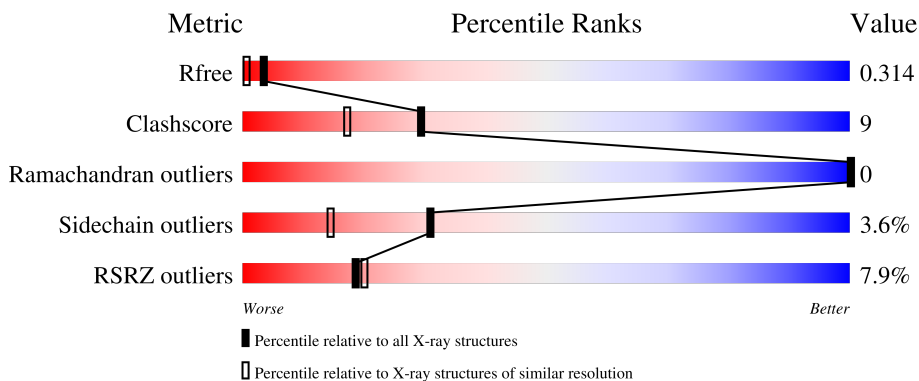
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	34	
1	B	34	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 558 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 General control protein GCN4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	31	253	163	43	46	1	0	0	0
1	B	32	255	163	43	49		0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ACE	-	acetylation	UNP P03069
A	5	ILE	LEU	engineered mutation	UNP P03069
A	9	LEU	VAL	engineered mutation	UNP P03069
A	12	ILE	LEU	engineered mutation	UNP P03069
A	16	LEU	ASN	engineered mutation	UNP P03069
A	19	ILE	LEU	engineered mutation	UNP P03069
A	20	SER	GLU	engineered mutation	UNP P03069
A	23	LEU	VAL	engineered mutation	UNP P03069
A	26	ILE	LEU	engineered mutation	UNP P03069
A	30	LEU	VAL	engineered mutation	UNP P03069
B	0	ACE	-	acetylation	UNP P03069
B	5	ILE	LEU	engineered mutation	UNP P03069
B	9	LEU	VAL	engineered mutation	UNP P03069
B	12	ILE	LEU	engineered mutation	UNP P03069
B	16	LEU	ASN	engineered mutation	UNP P03069
B	19	ILE	LEU	engineered mutation	UNP P03069
B	20	SER	GLU	engineered mutation	UNP P03069
B	23	LEU	VAL	engineered mutation	UNP P03069
B	26	ILE	LEU	engineered mutation	UNP P03069
B	30	LEU	VAL	engineered mutation	UNP P03069

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total 19	O 19	0	0
2	B	31	Total 31	O 31	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	35.39Å 35.39Å 104.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.13 – 1.70 52.12 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (52.13-1.70) 98.2 (52.12-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	12.67 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.245 , 0.316 0.242 , 0.314	Depositor DCC
R_{free} test set	355 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtrriage
Anisotropy	0.644	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	558	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.6072e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	3.74	42/254 (16.5%)	3.33	43/336 (12.8%)
1	B	3.90	50/256 (19.5%)	2.79	22/340 (6.5%)
All	All	3.82	92/510 (18.0%)	3.07	65/676 (9.6%)

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	14	SER	N-CA	15.12	1.65	1.46
1	B	4	GLN	CA-C	12.96	1.69	1.52
1	A	24	ALA	CA-CB	10.85	1.70	1.53
1	B	3	LYS	C-O	10.42	1.37	1.24
1	B	1	ARG	N-CA	10.27	1.65	1.46
1	A	25	ARG	CD-NE	10.07	1.60	1.46
1	A	4	GLN	CA-C	9.96	1.65	1.52
1	A	21	ASN	C-O	9.48	1.35	1.24
1	A	4	GLN	CG-CD	9.25	1.75	1.52
1	A	25	ARG	NE-CZ	9.21	1.43	1.33
1	B	7	ASP	CA-C	9.18	1.64	1.52
1	B	25	ARG	CZ-NH1	8.96	1.45	1.32
1	A	30	LEU	CA-C	8.91	1.64	1.52
1	B	21	ASN	C-O	8.90	1.34	1.24
1	B	24	ALA	C-O	8.75	1.34	1.24
1	B	25	ARG	CZ-NH2	8.56	1.44	1.33
1	B	15	LYS	C-O	8.54	1.34	1.24
1	A	28	LYS	CA-C	8.49	1.63	1.52
1	A	28	LYS	N-CA	8.23	1.55	1.46
1	B	28	LYS	N-CA	8.06	1.56	1.46
1	B	11	GLU	CA-CB	-7.79	1.41	1.53
1	A	6	GLU	CG-CD	7.77	1.71	1.52
1	A	19	ILE	N-CA	7.59	1.55	1.46
1	A	11	GLU	C-O	7.58	1.33	1.24
1	B	17	TYR	CG-CD2	7.57	1.55	1.39
1	A	10	GLU	C-O	7.53	1.32	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	25	ARG	N-CA	7.52	1.55	1.46
1	A	26	ILE	C-O	7.49	1.32	1.24
1	B	19	ILE	C-O	7.38	1.32	1.24
1	B	25	ARG	CA-C	7.34	1.62	1.52
1	B	25	ARG	CA-CB	-7.27	1.41	1.53
1	B	30	LEU	C-O	7.25	1.33	1.24
1	A	18	HIS	C-O	7.19	1.32	1.24
1	A	7	ASP	N-CA	-7.10	1.37	1.46
1	A	31	GLY	N-CA	7.06	1.56	1.45
1	B	29	LEU	C-O	6.99	1.32	1.24
1	B	28	LYS	CB-CG	6.80	1.72	1.52
1	B	30	LEU	N-CA	6.67	1.54	1.46
1	A	6	GLU	C-N	6.60	1.42	1.33
1	B	28	LYS	CD-CE	6.55	1.72	1.52
1	A	14	SER	C-O	6.51	1.32	1.24
1	A	22	GLU	N-CA	6.42	1.54	1.46
1	A	7	ASP	CG-OD2	6.37	1.37	1.25
1	A	4	GLN	N-CA	-6.35	1.38	1.46
1	A	20	SER	N-CA	-6.33	1.38	1.46
1	B	9	LEU	CA-C	-6.29	1.44	1.52
1	A	17	TYR	CZ-OH	6.26	1.51	1.38
1	B	11	GLU	CA-C	6.19	1.60	1.52
1	A	29	LEU	C-O	6.10	1.31	1.24
1	A	4	GLN	CD-OE1	6.10	1.35	1.23
1	B	1	ARG	CA-C	6.07	1.65	1.52
1	B	30	LEU	CG-CD2	6.06	1.72	1.52
1	B	6	GLU	CA-CB	-6.01	1.44	1.53
1	B	27	LYS	CG-CD	6.01	1.70	1.52
1	A	8	LYS	C-O	5.99	1.31	1.24
1	B	16	LEU	N-CA	5.98	1.54	1.46
1	B	10	GLU	CD-OE1	5.93	1.36	1.25
1	B	3	LYS	C-N	-5.91	1.26	1.33
1	B	17	TYR	CA-CB	5.88	1.62	1.53
1	A	13	LEU	C-N	5.86	1.42	1.34
1	B	16	LEU	CA-CB	5.83	1.62	1.53
1	B	32	GLU	CG-CD	5.77	1.66	1.52
1	A	17	TYR	CA-CB	5.73	1.62	1.53
1	A	16	LEU	C-O	5.71	1.30	1.24
1	B	18	HIS	C-O	-5.61	1.17	1.24
1	A	30	LEU	CG-CD1	-5.58	1.34	1.52
1	B	9	LEU	N-CA	5.53	1.53	1.46
1	A	25	ARG	CA-C	5.51	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	22	GLU	CA-CB	-5.50	1.44	1.53
1	A	6	GLU	C-O	5.43	1.30	1.24
1	B	30	LEU	CG-CD1	5.41	1.70	1.52
1	B	16	LEU	C-O	5.40	1.31	1.24
1	B	19	ILE	CB-CG1	5.38	1.64	1.53
1	B	10	GLU	CD-OE2	5.37	1.35	1.25
1	B	18	HIS	N-CA	5.36	1.53	1.46
1	B	30	LEU	CB-CG	-5.33	1.42	1.53
1	A	16	LEU	CG-CD2	5.33	1.70	1.52
1	A	9	LEU	CG-CD2	5.26	1.70	1.52
1	B	10	GLU	C-N	-5.25	1.26	1.33
1	A	14	SER	CB-OG	5.23	1.52	1.42
1	B	10	GLU	C-O	5.23	1.30	1.24
1	B	22	GLU	CD-OE2	5.22	1.35	1.25
1	A	27	LYS	CD-CE	5.18	1.68	1.52
1	B	28	LYS	CA-CB	5.16	1.61	1.53
1	B	6	GLU	C-O	5.15	1.30	1.24
1	A	29	LEU	CG-CD2	5.15	1.69	1.52
1	A	8	LYS	CA-C	5.15	1.59	1.52
1	A	4	GLN	CA-CB	-5.09	1.45	1.53
1	A	28	LYS	CB-CG	5.09	1.67	1.52
1	A	5	ILE	N-CA	5.08	1.52	1.46
1	B	23	LEU	N-CA	5.03	1.52	1.46
1	B	27	LYS	CD-CE	-5.01	1.37	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	LYS	N-CA-C	-11.33	98.93	111.28
1	A	31	GLY	N-CA-C	-10.66	82.39	113.30
1	A	17	TYR	CA-C-O	-9.20	111.16	120.82
1	A	2	MET	N-CA-C	-9.13	101.33	111.28
1	A	26	ILE	O-C-N	-9.04	112.49	121.90
1	B	26	ILE	N-CA-C	-9.04	102.04	110.53
1	B	22	GLU	N-CA-C	-8.57	101.44	112.23
1	B	4	GLN	N-CA-C	-8.45	102.03	111.07
1	B	25	ARG	N-CA-C	-8.22	102.40	111.36
1	A	22	GLU	N-CA-C	-8.15	102.35	111.07
1	A	14	SER	CA-CB-OG	-8.07	94.96	111.10
1	A	25	ARG	NE-CZ-NH1	7.99	129.49	121.50
1	A	26	ILE	N-CA-C	-7.65	103.34	110.53
1	A	28	LYS	CD-CE-NZ	-7.64	87.46	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	GLU	N-CA-C	-7.51	103.02	111.14
1	A	16	LEU	N-CA-CB	7.39	120.72	110.01
1	B	27	LYS	CG-CD-CE	-7.36	94.38	111.30
1	A	28	LYS	CA-C-N	7.14	130.19	120.54
1	A	28	LYS	C-N-CA	7.14	130.19	120.54
1	A	25	ARG	NH1-CZ-NH2	-7.05	110.14	119.30
1	A	10	GLU	CA-C-O	-6.99	113.14	120.55
1	B	29	LEU	N-CA-C	-6.87	103.87	111.36
1	A	29	LEU	CD1-CG-CD2	6.80	125.77	110.80
1	A	19	ILE	CB-CG1-CD1	-6.80	99.52	113.80
1	A	25	ARG	N-CA-C	-6.75	103.93	111.28
1	B	7	ASP	O-C-N	6.73	129.25	122.12
1	B	30	LEU	N-CA-C	-6.71	104.03	111.82
1	A	27	LYS	CA-C-O	-6.71	113.44	120.55
1	B	15	LYS	N-CA-C	-6.68	104.07	111.36
1	A	16	LEU	O-C-N	-6.67	115.20	122.07
1	A	21	ASN	CA-C-N	6.64	129.07	120.44
1	A	21	ASN	C-N-CA	6.64	129.07	120.44
1	B	16	LEU	N-CA-C	-6.61	103.90	112.23
1	B	12	ILE	O-C-N	-6.53	115.11	121.83
1	B	22	GLU	CB-CG-CD	6.43	123.53	112.60
1	A	8	LYS	N-CA-C	-6.39	104.40	111.36
1	A	25	ARG	CD-NE-CZ	6.39	133.34	124.40
1	B	10	GLU	CB-CG-CD	-6.33	101.84	112.60
1	A	2	MET	O-C-N	-6.18	115.56	122.12
1	A	9	LEU	CD1-CG-CD2	-6.16	97.25	110.80
1	A	19	ILE	N-CA-CB	-6.12	101.40	110.58
1	B	10	GLU	N-CA-C	-6.10	104.63	111.28
1	B	4	GLN	N-CA-CB	6.09	118.84	110.01
1	A	24	ALA	CA-C-O	-6.06	114.00	120.42
1	A	24	ALA	N-CA-C	-6.03	104.79	111.36
1	B	26	ILE	O-C-N	-5.95	115.71	121.90
1	B	5	ILE	CA-CB-CG1	-5.89	100.39	110.40
1	A	12	ILE	CA-CB-CG1	-5.88	100.41	110.40
1	A	20	SER	CA-C-N	-5.77	112.54	120.28
1	A	20	SER	C-N-CA	-5.77	112.54	120.28
1	A	17	TYR	N-CA-C	-5.64	105.03	111.07
1	B	29	LEU	CD1-CG-CD2	5.63	123.20	110.80
1	A	5	ILE	N-CA-C	-5.51	105.35	110.53
1	A	13	LEU	N-CA-C	-5.49	105.38	111.36
1	A	7	ASP	CB-CG-OD2	-5.49	105.78	118.40
1	B	10	GLU	CA-C-O	-5.33	114.89	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	SER	CA-C-O	-5.28	114.14	120.10
1	A	23	LEU	N-CA-CB	-5.21	101.91	110.40
1	A	17	TYR	N-CA-CB	-5.17	102.52	110.01
1	A	6	GLU	CA-CB-CG	-5.11	103.88	114.10
1	A	7	ASP	OD1-CG-OD2	5.11	135.16	122.90
1	A	8	LYS	CB-CA-C	-5.06	102.24	110.85
1	B	2	MET	CB-CA-C	-5.03	102.43	110.79
1	A	18	HIS	CA-C-N	-5.02	113.29	120.42
1	A	18	HIS	C-N-CA	-5.02	113.29	120.42

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	253	0	277	6	0
1	B	255	0	266	3	0
2	A	19	0	0	4	0
2	B	31	0	0	2	0
All	All	558	0	543	9	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 9.

All (9) 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:4:GLN:CD	1:A:4:GLN:CG	1.75	1.55
1:A:27:LYS:HE2	2:A:2019:HOH:O	1.71	0.89
1:A:27:LYS:CE	2:A:2019:HOH:O	2.24	0.84
1:B:22:GLU:OE1	2:B:2024:HOH:O	2.04	0.76
1:A:27:LYS:NZ	2:A:2019:HOH:O	2.26	0.69
1:B:18:HIS:NE2	2:B:2018:HOH:O	2.28	0.66
1:A:4:GLN:CD	1:A:4:GLN:CB	2.71	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:OE1	2:A:2003:HOH:O	2.17	0.58
1:B:18:HIS:O	1:B:22:GLU:HG3	2.16	0.46

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	29/34 (85%)	29 (100%)	0	0	100	100
1	B	30/34 (88%)	30 (100%)	0	0	100	100
All	All	59/68 (87%)	59 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

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	28/31 (90%)	28 (100%)	0	100	100
1	B	27/31 (87%)	25 (93%)	2 (7%)	13	3
All	All	55/62 (89%)	53 (96%)	2 (4%)	31	14

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	GLN
1	B	8	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS

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 oligosaccharides 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.

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	31/34 (91%)	0.67	2 (6%) 25 27	18, 26, 39, 42	0
1	B	32/34 (94%)	0.70	3 (9%) 14 14	18, 27, 37, 44	0
All	All	63/68 (92%)	0.69	5 (7%) 18 20	18, 27, 39, 44	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	GLY	5.0
1	B	2	MET	2.8
1	A	29	LEU	2.3
1	B	30	LEU	2.1
1	B	1	ARG	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.