



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:57 AM UTC

PDB ID : 6FLK / pdb_00006flk
Title : Crystal structure of Cep120 C2C domain
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Deposited on : 2018-01-26
Resolution : 1.60 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
Xtriage (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

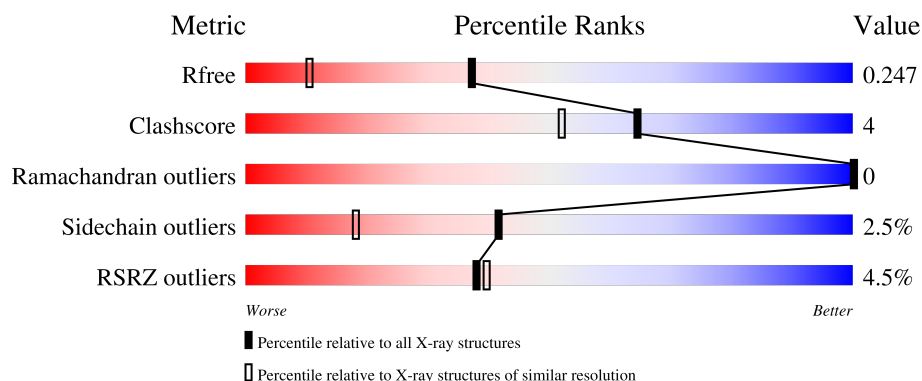
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	163	5% 72% 21% 6%
1	B	163	4% 71% 19% 5% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5464 atoms, of which 2520 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 Cep120.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	154	Total	C	H	N	O	S	0	3	0
			2521	822	1252	213	226	8			
1	B	154	Total	C	H	N	O	S	0	4	0
			2559	835	1268	220	228	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	448	GLY	-	expression tag	UNP Q8N960
A	449	PRO	-	expression tag	UNP Q8N960
B	448	GLY	-	expression tag	UNP Q8N960
B	449	PRO	-	expression tag	UNP Q8N960

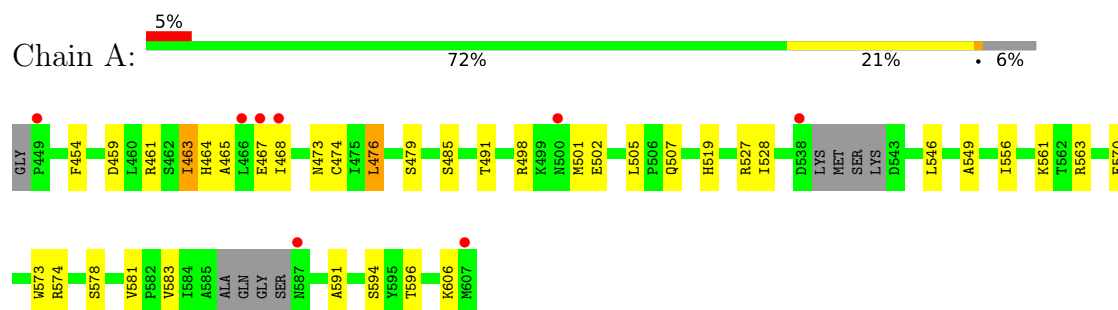
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	198	Total	O	0	0
			198	198		
2	B	186	Total	O	0	0
			186	186		

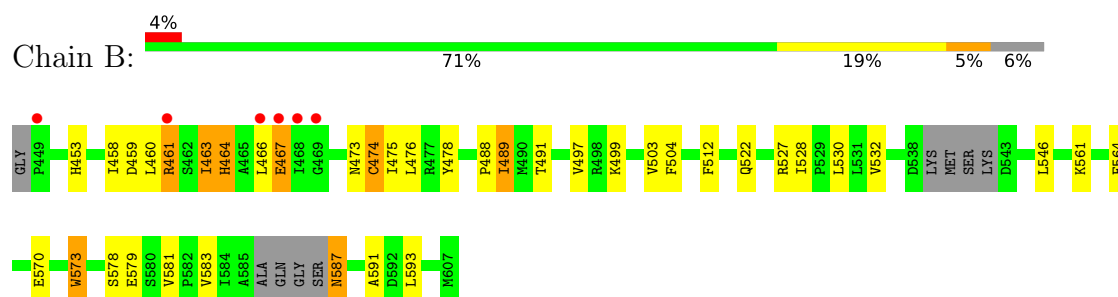
3 Residue-property plots

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: Cep120



• Molecule 1: Cep120



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	32.40Å 40.95Å 69.13Å 102.47° 98.07° 89.92°	Depositor
Resolution (Å)	39.97 – 1.60 39.97 – 1.60	Depositor EDS
% Data completeness (in resolution range)	75.9 (39.97-1.60) 93.8 (39.97-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 1.60Å)	Xtriage
Refinement program	PHENIX (dev_2863: ???)	Depositor
R, R_{free}	0.197 , 0.246 0.198 , 0.247	Depositor DCC
R_{free} test set	2127 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5464	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.91% 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

5.1 Standard geometry

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	1.38	13/1309 (1.0%)	1.48	27/1777 (1.5%)
1	B	1.69	24/1332 (1.8%)	1.67	36/1807 (2.0%)
All	All	1.54	37/2641 (1.4%)	1.58	63/3584 (1.8%)

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	B	0	1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	460	LEU	C-N	-11.25	1.19	1.33
1	B	522[A]	GLN	CA-C	10.52	1.66	1.52
1	B	522[B]	GLN	CA-C	10.52	1.66	1.52
1	B	522[A]	GLN	N-CA	10.05	1.58	1.46
1	B	522[B]	GLN	N-CA	10.05	1.58	1.46
1	B	573[A]	TRP	N-CA	9.77	1.58	1.46
1	B	573[B]	TRP	N-CA	9.77	1.58	1.46
1	B	573[A]	TRP	CA-C	8.46	1.63	1.52
1	B	573[B]	TRP	CA-C	8.46	1.63	1.52
1	A	528	ILE	C-N	7.92	1.43	1.33
1	A	454	PHE	N-CA	-7.64	1.36	1.45
1	A	581	VAL	C-N	7.62	1.43	1.33
1	B	463	ILE	C-N	-7.43	1.22	1.33
1	B	527	ARG	C-N	7.16	1.40	1.33
1	A	527	ARG	C-N	7.08	1.40	1.33
1	B	546	LEU	C-N	6.92	1.41	1.33
1	A	465	ALA	CA-C	-6.82	1.44	1.52
1	A	519	HIS	C-O	-6.61	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	594	SER	CA-C	-6.22	1.45	1.52
1	B	561	LYS	CA-C	-6.07	1.45	1.52
1	B	573[A]	TRP	C-O	5.97	1.31	1.24
1	B	573[B]	TRP	C-O	5.97	1.31	1.24
1	B	581	VAL	C-N	5.92	1.40	1.33
1	B	593	LEU	CA-C	-5.91	1.45	1.52
1	B	546	LEU	N-CA	-5.83	1.38	1.46
1	B	466	LEU	CA-C	-5.74	1.47	1.52
1	A	546	LEU	C-N	5.64	1.40	1.33
1	A	459	ASP	N-CA	-5.58	1.39	1.46
1	B	581	VAL	N-CA	-5.42	1.40	1.46
1	B	467	GLU	CA-C	-5.39	1.45	1.53
1	B	530	LEU	CA-C	-5.39	1.46	1.52
1	B	453	HIS	N-CA	-5.32	1.39	1.46
1	A	463	ILE	N-CA	-5.18	1.40	1.46
1	B	564	PHE	N-CA	-5.18	1.39	1.45
1	A	546	LEU	CA-C	-5.05	1.46	1.52
1	A	464	HIS	C-N	5.03	1.40	1.33
1	A	485	SER	CA-C	-5.02	1.46	1.52

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	THR	O-C-N	-9.29	112.26	122.85
1	A	528	ILE	N-CA-C	8.36	116.55	107.60
1	B	474	CYS	N-CA-C	8.25	122.87	109.59
1	A	468	ILE	N-CA-C	-7.63	97.28	108.87
1	B	528	ILE	N-CA-C	7.52	115.64	107.60
1	A	461	ARG	N-CA-C	7.31	118.89	111.07
1	A	474	CYS	N-CA-C	7.07	120.77	109.24
1	B	491	THR	N-CA-C	-7.00	101.10	110.55
1	B	579	GLU	O-C-N	-6.99	116.30	123.29
1	B	583	VAL	N-CA-C	-6.97	97.81	107.99
1	B	467	GLU	CA-C-N	6.93	131.78	123.19
1	B	467	GLU	C-N-CA	6.93	131.78	123.19
1	B	473	ASN	N-CA-C	-6.85	93.92	107.69
1	A	479	SER	CA-C-N	6.83	128.29	122.28
1	A	479	SER	C-N-CA	6.83	128.29	122.28
1	A	583	VAL	N-CA-C	-6.80	98.07	107.99
1	A	476	LEU	O-C-N	-6.74	114.65	123.21
1	A	491	THR	N-CA-C	-6.66	101.56	110.55
1	B	591	ALA	O-C-N	-6.55	116.74	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	ILE	O-C-N	-6.52	116.03	123.07
1	B	478	TYR	CA-C-N	6.46	132.70	122.62
1	B	478	TYR	C-N-CA	6.46	132.70	122.62
1	B	491	THR	O-C-N	-6.41	115.54	122.85
1	B	573[A]	TRP	CA-C-O	6.29	127.09	120.36
1	B	573[B]	TRP	CA-C-O	6.29	127.09	120.36
1	B	497	VAL	O-C-N	-6.25	116.45	123.20
1	B	461[A]	ARG	N-CA-C	6.14	117.64	111.07
1	B	461[B]	ARG	N-CA-C	6.14	117.64	111.07
1	B	461[C]	ARG	N-CA-C	6.14	117.64	111.07
1	A	549	ALA	CA-C-N	5.98	130.62	122.84
1	A	549	ALA	C-N-CA	5.98	130.62	122.84
1	B	522[A]	GLN	CA-C-O	5.89	126.80	120.55
1	B	522[B]	GLN	CA-C-O	5.89	126.80	120.55
1	A	591	ALA	O-C-N	-5.85	117.44	123.29
1	B	488	PRO	CA-C-N	5.84	131.84	122.50
1	B	488	PRO	C-N-CA	5.84	131.84	122.50
1	B	453	HIS	N-CA-C	-5.77	99.83	109.24
1	B	512	PHE	CA-C-N	5.73	130.63	122.72
1	B	512	PHE	C-N-CA	5.73	130.63	122.72
1	B	530	LEU	O-C-N	-5.72	116.55	123.13
1	B	532	VAL	CA-C-N	5.60	130.38	122.09
1	B	532	VAL	C-N-CA	5.60	130.38	122.09
1	A	473	ASN	N-CA-C	-5.52	97.49	107.75
1	A	464	HIS	CA-C-N	5.45	128.97	120.75
1	A	464	HIS	C-N-CA	5.45	128.97	120.75
1	B	564	PHE	O-C-N	-5.44	116.96	123.27
1	A	468	ILE	O-C-N	-5.40	116.57	122.83
1	A	463	ILE	N-CA-C	-5.36	100.34	108.17
1	A	596	THR	O-C-N	-5.33	116.76	123.27
1	A	583	VAL	CA-C-N	5.32	129.64	122.93
1	A	583	VAL	C-N-CA	5.32	129.64	122.93
1	B	503	VAL	CA-C-N	5.31	129.95	122.09
1	B	503	VAL	C-N-CA	5.31	129.95	122.09
1	B	578	SER	O-C-N	-5.27	116.84	123.27
1	A	501	MET	CA-C-N	5.27	129.99	122.72
1	A	501	MET	C-N-CA	5.27	129.99	122.72
1	A	561	LYS	O-C-N	-5.20	117.13	123.27
1	B	489	ILE	N-CA-C	-5.14	101.05	108.87
1	A	578	SER	O-C-N	-5.14	117.00	123.27
1	A	502	GLU	O-C-N	-5.08	117.53	123.27
1	B	504	PHE	O-C-N	-5.05	117.30	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	530	LEU	N-CA-C	-5.04	100.95	108.96
1	B	476	LEU	O-C-N	-5.02	116.83	123.21

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	464[A]	HIS	Mainchain

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	1269	1252	1254	10	1
1	B	1291	1268	1275	10	1
2	A	198	0	0	2	0
2	B	186	0	0	0	0
All	All	2944	2520	2529	20	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 4.

All (20) 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:606:LYS:HA	2:A:705:HOH:O	1.77	0.82
1:B:475:ILE:HD12	1:B:475:ILE:C	2.28	0.57
1:B:467:GLU:HG2	1:B:467:GLU:O	2.05	0.56
1:B:464[B]:HIS:ND1	1:B:464[B]:HIS:N	2.56	0.53
1:A:574:ARG:NH2	2:A:701:HOH:O	2.35	0.52
1:B:459:ASP:OD2	1:B:461[A]:ARG:NH2	2.43	0.52
1:B:587:ASN:N	1:B:587:ASN:OD1	2.42	0.52
1:A:476:LEU:HD22	1:A:505:LEU:HD13	1.93	0.49
1:A:563[B]:ARG:NH1	1:A:573[B]:TRP:CE2	2.81	0.48
1:A:570:GLU:OE1	1:A:606:LYS:NZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563[B]:ARG:HH11	1:A:573[B]:TRP:CD1	2.32	0.47
1:B:461[B]:ARG:HB3	1:B:461[B]:ARG:CZ	2.46	0.45
1:B:461[B]:ARG:CZ	1:B:461[B]:ARG:CB	2.98	0.42
1:A:463:ILE:O	1:A:463:ILE:HG23	2.19	0.42
1:A:467:GLU:O	1:A:467:GLU:HG3	2.20	0.41
1:A:507:GLN:HG2	1:A:507:GLN:O	2.21	0.40
1:A:463:ILE:O	1:A:463:ILE:CG2	2.70	0.40
1:B:461[A]:ARG:NH2	1:B:461[A]:ARG:HG2	2.35	0.40

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)
1:A:498:ARG:HH22	1:B:499:LYS:O[1_554]	1.58	0.02

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	151/163 (93%)	149 (99%)	2 (1%)	0	100	100
1	B	153/163 (94%)	151 (99%)	2 (1%)	0	100	100
All	All	304/326 (93%)	300 (99%)	4 (1%)	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	143/146 (98%)	142 (99%)	1 (1%)	76	63
1	B	145/146 (99%)	139 (96%)	6 (4%)	27	8
All	All	288/292 (99%)	281 (98%)	7 (2%)	42	19

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	556	ILE
1	B	458	ILE
1	B	463	ILE
1	B	474	CYS
1	B	489	ILE
1	B	570	GLU
1	B	587	ASN

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

Mol	Chain	Res	Type
1	B	552	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	460:LEU	C	461[C]:ARG	N	1.19
1	B	460:LEU	C	461[A]:ARG	N	1.19
1	B	460:LEU	C	461[B]:ARG	N	1.18

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	154/163 (94%)	0.02	8 (5%)	33 33	9, 19, 50, 72	3 (1%)
1	B	154/163 (94%)	0.05	6 (3%)	43 45	7, 19, 47, 65	4 (2%)
All	All	308/326 (94%)	0.04	14 (4%)	38 40	7, 19, 50, 72	7 (2%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	468	ILE	4.8
1	B	468	ILE	4.3
1	A	466	LEU	3.8
1	B	467	GLU	3.6
1	B	461[A]	ARG	3.2
1	B	466	LEU	3.1
1	B	469	GLY	2.8
1	A	467	GLU	2.8
1	A	587	ASN	2.6
1	A	607	MET	2.5
1	A	500	ASN	2.4
1	B	449	PRO	2.1
1	A	538	ASP	2.1
1	A	449	PRO	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.