



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:06 AM UTC

PDB ID : 5JSN / pdb_00005jsn
Title : Bcl2-inhibitor complex
Authors : Shen, B.W.; Stoddard, B.L.
Deposited on : 2016-05-09
Resolution : 2.10 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

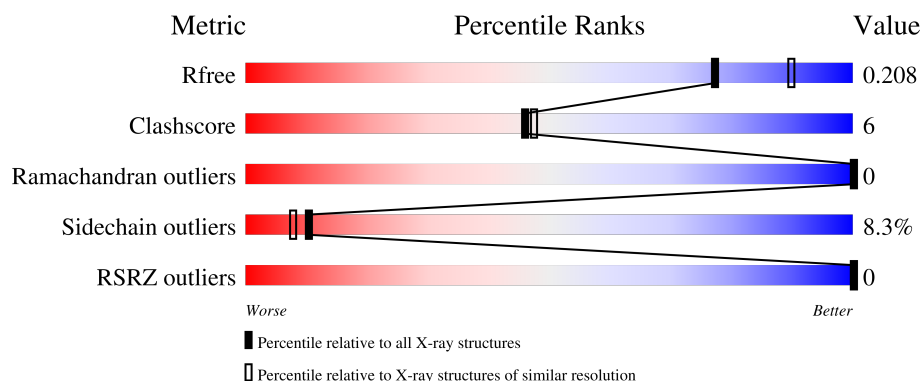
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

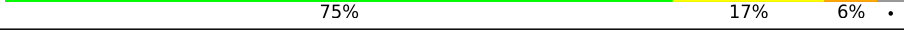
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	215	
1	C	215	
2	B	118	
2	D	118	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4540 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 Apoptosis regulator Bcl-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	0	0
			1234	788	218	221	7			
1	C	149	Total	C	N	O	S	0	1	0
			1237	790	218	222	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	LEU	-	expression tag	UNP P10415
A	209	GLU	-	expression tag	UNP P10415
A	210	HIS	-	expression tag	UNP P10415
A	211	HIS	-	expression tag	UNP P10415
A	212	HIS	-	expression tag	UNP P10415
A	213	HIS	-	expression tag	UNP P10415
A	214	HIS	-	expression tag	UNP P10415
A	215	HIS	-	expression tag	UNP P10415
C	208	LEU	-	expression tag	UNP P10415
C	209	GLU	-	expression tag	UNP P10415
C	210	HIS	-	expression tag	UNP P10415
C	211	HIS	-	expression tag	UNP P10415
C	212	HIS	-	expression tag	UNP P10415
C	213	HIS	-	expression tag	UNP P10415
C	214	HIS	-	expression tag	UNP P10415
C	215	HIS	-	expression tag	UNP P10415

- Molecule 2 is a protein called Bcl2 inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	115	Total	C	N	O	S	0	0	0
			953	592	178	182	1			
2	D	115	Total	C	N	O	S	0	1	0
			964	598	182	183	1			

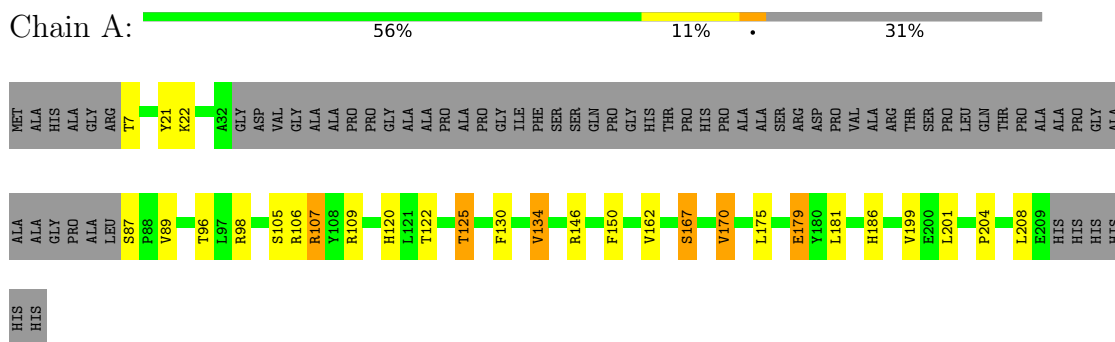
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total 50	O 50	0	0
3	B	19	Total 19	O 19	0	0
3	C	50	Total 50	O 50	0	0
3	D	33	Total 33	O 33	0	0

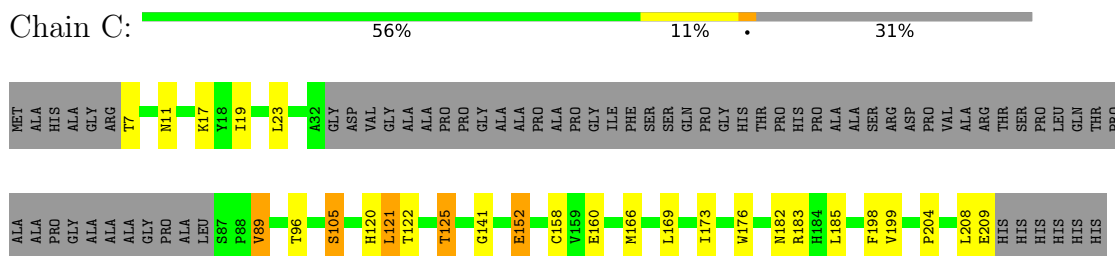
3 Residue-property plots

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.

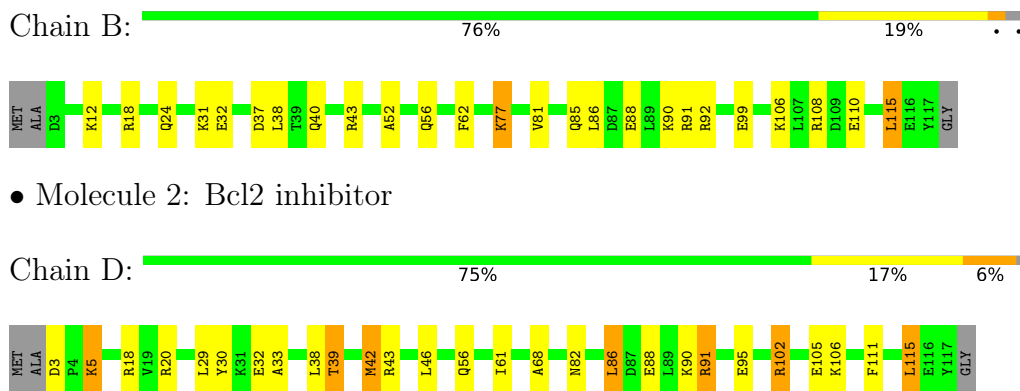
• Molecule 1: Apoptosis regulator Bcl-2



• Molecule 1: Apoptosis regulator Bcl-2



• Molecule 2: Bcl2 inhibitor



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	65.00Å 65.00Å 134.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.50 – 2.10 32.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (32.50-2.10) 99.0 (32.50-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.159 , 0.205 0.163 , 0.208	Depositor DCC
R_{free} test set	1650 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.305 for h,-k,-l	Xtriage
Reported twinning fraction	0.692 for H, K, L 0.308 for -H, K, -L	Depositor
Outliers	0 of 32173 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4540	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% 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	1.34	4/1269 (0.3%)	1.30	4/1719 (0.2%)
1	C	1.35	7/1275 (0.5%)	1.25	3/1727 (0.2%)
2	B	1.33	3/958 (0.3%)	1.35	1/1273 (0.1%)
2	D	1.34	2/969 (0.2%)	1.27	2/1287 (0.2%)
All	All	1.34	16/4471 (0.4%)	1.29	10/6006 (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
2	B	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	GLY	CA-C	-7.99	1.44	1.51
1	C	198	PHE	N-CA	-6.12	1.39	1.46
1	A	106	ARG	C-O	-5.99	1.17	1.24
1	A	167	SER	C-O	-5.92	1.18	1.24
2	B	108	ARG	N-CA	5.83	1.53	1.46
2	D	61	ILE	C-O	-5.83	1.17	1.24
1	C	158	CYS	N-CA	-5.56	1.39	1.46
2	B	52	ALA	C-O	5.53	1.30	1.24
1	C	152	GLU	C-O	-5.38	1.17	1.24
2	D	68	ALA	CA-C	5.30	1.59	1.52
1	A	107	ARG	C-O	-5.22	1.17	1.24
1	C	185	LEU	C-O	-5.21	1.17	1.23
2	B	108	ARG	CA-C	-5.14	1.46	1.52
1	A	146	ARG	N-CA	5.14	1.52	1.46
1	C	141	GLY	N-CA	5.11	1.50	1.45
1	C	19	ILE	C-O	5.07	1.30	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	HIS	N-CA-C	-6.53	98.62	109.46
1	C	120	HIS	N-CA-C	-6.49	98.69	109.46
1	A	186	HIS	N-CA-C	6.34	118.72	111.11
1	C	23	LEU	N-CA-C	5.71	117.17	111.07
1	C	89	VAL	N-CA-CB	5.58	119.02	111.21
2	B	77	LYS	CA-CB-CG	5.38	124.86	114.10
2	D	3	ASP	CA-C-N	5.30	125.11	119.28
2	D	3	ASP	C-N-CA	5.30	125.11	119.28
1	A	150	PHE	N-CA-C	5.24	117.40	111.11
1	A	22	LYS	CB-CG-CD	5.18	123.21	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	37	ASP	Peptide

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	1234	0	1172	11	0
1	C	1237	0	1177	14	0
2	B	953	0	995	13	0
2	D	964	0	1007	22	0
3	A	50	0	0	0	0
3	B	19	0	0	2	0
3	C	50	0	0	1	0
3	D	33	0	0	1	0
All	All	4540	0	4351	51	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 6.

All (51) 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)
2:D:39:THR:OG1	2:D:42:MET:HG3	1.79	0.80
2:B:24:GLN:OE1	2:D:20:ARG:NH1	2.17	0.78
2:B:43:ARG:HG3	2:B:115:LEU:HD23	1.65	0.77
2:D:43:ARG:HG3	2:D:115:LEU:HD23	1.72	0.70
2:B:18:ARG:NH2	2:B:56:GLN:HE21	1.90	0.69
1:C:208:LEU:HD21	2:D:90:LYS:HE2	1.76	0.68
2:D:18:ARG:NH2	2:D:56:GLN:OE1	2.27	0.67
2:D:102[A]:ARG:O	2:D:102[A]:ARG:HD2	1.98	0.64
2:D:102[A]:ARG:HD2	2:D:102[A]:ARG:C	2.25	0.62
2:B:18:ARG:HH21	2:B:56:GLN:HE21	1.46	0.61
2:D:33:ALA:HB2	2:D:46:LEU:HD13	1.81	0.61
1:A:175:LEU:O	1:A:179:GLU:HG3	2.02	0.59
2:B:56:GLN:NE2	3:B:201:HOH:O	2.28	0.56
1:C:105[B]:SER:OG	1:C:152:GLU:OE1	2.25	0.55
1:C:166:MET:HB3	1:C:169:LEU:HD13	1.89	0.54
1:C:183:ARG:NH2	3:C:302:HOH:O	2.33	0.54
2:B:106:LYS:HD2	3:B:205:HOH:O	2.07	0.54
2:B:40:GLN:HE22	2:B:43:ARG:NH1	2.07	0.53
1:A:167:SER:O	1:A:170:VAL:HG13	2.09	0.53
2:B:106:LYS:O	2:B:110:GLU:HG2	2.10	0.51
2:D:111:PHE:CZ	2:D:115:LEU:HD13	2.47	0.50
1:A:122:THR:OG1	1:A:125:THR:HB	2.13	0.49
1:A:107:ARG:HH11	2:B:62:PHE:HD1	1.61	0.48
1:C:204:PRO:O	1:C:208:LEU:HD13	2.14	0.48
1:A:96:THR:HG21	1:A:199:VAL:HA	1.96	0.47
1:C:122:THR:OG1	1:C:125:THR:HB	2.14	0.47
2:D:86:LEU:O	2:D:90:LYS:HG3	2.15	0.47
1:C:96:THR:HG21	1:C:199:VAL:HA	1.96	0.47
1:C:121:LEU:O	1:C:166:MET:HE1	2.14	0.47
1:A:204:PRO:O	1:A:208:LEU:HD13	2.14	0.47
1:C:208:LEU:HD11	2:D:90:LYS:NZ	2.30	0.47
1:A:107:ARG:NH1	2:B:62:PHE:CD1	2.84	0.46
2:D:86:LEU:CD1	2:D:90:LYS:HE3	2.46	0.45
1:A:130:PHE:O	1:A:134:VAL:HG13	2.17	0.45
1:C:208:LEU:HD21	2:D:90:LYS:CE	2.43	0.45
2:D:106:LYS:HE3	3:D:232:HOH:O	2.16	0.45
2:D:102[A]:ARG:NH1	2:D:105:GLU:OE1	2.50	0.44
2:B:81:VAL:HG22	2:B:85:GLN:HB2	1.99	0.44
2:D:5:LYS:HD3	2:D:5:LYS:HA	1.91	0.44
2:D:82:ASN:OD1	2:D:82:ASN:C	2.61	0.44
2:D:91:ARG:NH1	2:D:95:GLU:OE2	2.51	0.43
1:A:21:TYR:CE2	1:A:98:ARG:HB2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:88:GLU:OE2	2:D:91:ARG:NH2	2.45	0.42
1:C:208:LEU:HD11	2:D:90:LYS:HZ1	1.84	0.42
1:C:208:LEU:HD11	2:D:90:LYS:HE2	2.01	0.42
1:C:11:ASN:HD22	1:C:182:ASN:ND2	2.17	0.42
1:A:208:LEU:HD23	2:B:90:LYS:HD2	2.02	0.41
1:A:201:LEU:O	1:A:204:PRO:HD2	2.20	0.41
1:C:173:ILE:HD13	1:C:176:TRP:CZ3	2.55	0.41
2:B:88:GLU:O	2:B:92:ARG:HG2	2.20	0.41
2:D:30:TYR:N	2:D:111:PHE:HE1	2.19	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	145/215 (67%)	142 (98%)	3 (2%)	0	100	100
1	C	146/215 (68%)	142 (97%)	4 (3%)	0	100	100
2	B	113/118 (96%)	112 (99%)	1 (1%)	0	100	100
2	D	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
All	All	518/666 (78%)	508 (98%)	10 (2%)	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	130/172 (76%)	119 (92%)	11 (8%)	10	7
1	C	131/172 (76%)	122 (93%)	9 (7%)	14	12
2	B	98/99 (99%)	89 (91%)	9 (9%)	8	6
2	D	99/99 (100%)	88 (89%)	11 (11%)	6	3
All	All	458/542 (84%)	418 (91%)	40 (9%)	10	7

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	87	SER
1	A	89	VAL
1	A	105	SER
1	A	109	ARG
1	A	125	THR
1	A	134	VAL
1	A	162	VAL
1	A	170	VAL
1	A	179	GLU
1	A	181	LEU
2	B	12	LYS
2	B	31	LYS
2	B	32	GLU
2	B	38	LEU
2	B	77	LYS
2	B	86	LEU
2	B	91	ARG
2	B	99	GLU
2	B	115	LEU
1	C	7	THR
1	C	17	LYS
1	C	89	VAL
1	C	105[A]	SER
1	C	105[B]	SER
1	C	121	LEU
1	C	125	THR
1	C	160	GLU
1	C	209	GLU
2	D	5	LYS
2	D	29	LEU
2	D	32	GLU
2	D	38	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	39	THR
2	D	42	MET
2	D	86	LEU
2	D	91	ARG
2	D	102[A]	ARG
2	D	102[B]	ARG
2	D	115	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	GLN
2	B	40	GLN
2	B	56	GLN
2	B	58	ASN
1	C	11	ASN
1	C	20	HIS
1	C	163	ASN
1	C	172	ASN
1	C	182	ASN
1	C	186	HIS
1	C	192	ASN
2	D	85	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	149/215 (69%)	-1.02	0 100 100	30, 48, 73, 92	0
1	C	149/215 (69%)	-1.00	0 100 100	27, 48, 82, 109	1 (0%)
2	B	115/118 (97%)	-1.01	0 100 100	32, 58, 92, 121	0
2	D	115/118 (97%)	-1.11	0 100 100	26, 51, 87, 112	1 (0%)
All	All	528/666 (79%)	-1.03	0 100 100	26, 51, 87, 121	2 (0%)

There are no RSRZ outliers to report.

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.