



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:52 PM UTC

PDB ID : 7XFR / pdb_00007xfr
Title : Crystal structure of WIPI2b in complex with the second site of ATG16L1
Authors : Gong, X.Y.; Pan, L.F.
Deposited on : 2022-04-02
Resolution : 1.76 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

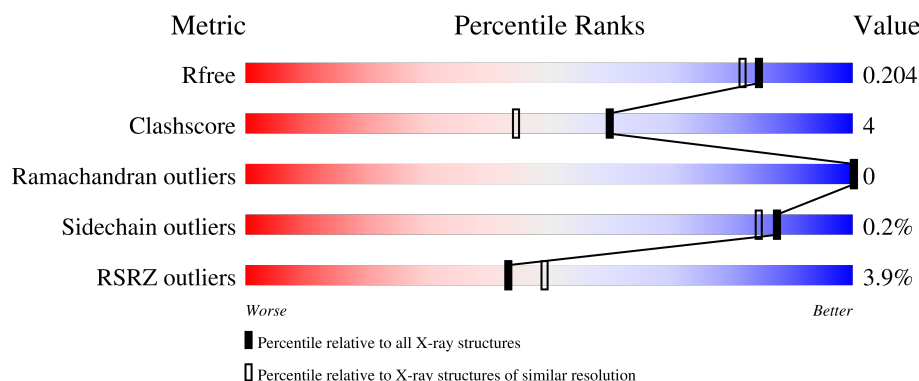
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	321	0% 94% 5%
1	C	321	3% 87% 12%
2	B	69	7% 94% 6%
2	D	69	14% 77% 13% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12359 atoms, of which 5928 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 Isoform 2 of WD repeat domain phosphoinositide-interacting protein 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	319	Total	C	H	N	O	S	0	4	0
			4969	1572	2489	424	465	19			
1	C	317	Total	C	H	N	O	S	0	5	0
			4865	1565	2394	422	464	20			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLY	-	expression tag	UNP Q9Y4P8-2
A	10	PRO	-	expression tag	UNP Q9Y4P8-2
A	11	GLY	-	expression tag	UNP Q9Y4P8-2
A	12	SER	-	expression tag	UNP Q9Y4P8-2
A	?	-	LYS	deletion	UNP Q9Y4P8-2
A	?	-	PRO	deletion	UNP Q9Y4P8-2
A	?	-	PRO	deletion	UNP Q9Y4P8-2
A	?	-	GLU	deletion	UNP Q9Y4P8-2
A	?	-	GLU	deletion	UNP Q9Y4P8-2
A	?	-	PRO	deletion	UNP Q9Y4P8-2
A	?	-	THR	deletion	UNP Q9Y4P8-2
A	?	-	THR	deletion	UNP Q9Y4P8-2
A	?	-	TRP	deletion	UNP Q9Y4P8-2
A	?	-	THR	deletion	UNP Q9Y4P8-2
A	?	-	GLY	deletion	UNP Q9Y4P8-2
A	?	-	TYR	deletion	UNP Q9Y4P8-2
A	?	-	PHE	deletion	UNP Q9Y4P8-2
A	?	-	GLY	deletion	UNP Q9Y4P8-2
A	?	-	LYS	deletion	UNP Q9Y4P8-2
A	?	-	VAL	deletion	UNP Q9Y4P8-2
A	?	-	LEU	deletion	UNP Q9Y4P8-2
A	?	-	MET	deletion	UNP Q9Y4P8-2
A	?	-	ALA	deletion	UNP Q9Y4P8-2
A	?	-	SER	deletion	UNP Q9Y4P8-2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP Q9Y4P8-2
A	?	-	SER	deletion	UNP Q9Y4P8-2
A	?	-	TYR	deletion	UNP Q9Y4P8-2
A	?	-	LEU	deletion	UNP Q9Y4P8-2
A	?	-	PRO	deletion	UNP Q9Y4P8-2
A	?	-	SER	deletion	UNP Q9Y4P8-2
A	?	-	GLN	deletion	UNP Q9Y4P8-2
A	?	-	VAL	deletion	UNP Q9Y4P8-2
A	?	-	THR	deletion	UNP Q9Y4P8-2
A	?	-	GLU	deletion	UNP Q9Y4P8-2
A	?	-	MET	deletion	UNP Q9Y4P8-2
A	?	-	PHE	deletion	UNP Q9Y4P8-2
A	?	-	ASN	deletion	UNP Q9Y4P8-2
C	9	GLY	-	expression tag	UNP Q9Y4P8-2
C	10	PRO	-	expression tag	UNP Q9Y4P8-2
C	11	GLY	-	expression tag	UNP Q9Y4P8-2
C	12	SER	-	expression tag	UNP Q9Y4P8-2
C	?	-	LYS	deletion	UNP Q9Y4P8-2
C	?	-	PRO	deletion	UNP Q9Y4P8-2
C	?	-	PRO	deletion	UNP Q9Y4P8-2
C	?	-	GLU	deletion	UNP Q9Y4P8-2
C	?	-	GLU	deletion	UNP Q9Y4P8-2
C	?	-	PRO	deletion	UNP Q9Y4P8-2
C	?	-	THR	deletion	UNP Q9Y4P8-2
C	?	-	THR	deletion	UNP Q9Y4P8-2
C	?	-	TRP	deletion	UNP Q9Y4P8-2
C	?	-	THR	deletion	UNP Q9Y4P8-2
C	?	-	GLY	deletion	UNP Q9Y4P8-2
C	?	-	TYR	deletion	UNP Q9Y4P8-2
C	?	-	PHE	deletion	UNP Q9Y4P8-2
C	?	-	GLY	deletion	UNP Q9Y4P8-2
C	?	-	LYS	deletion	UNP Q9Y4P8-2
C	?	-	VAL	deletion	UNP Q9Y4P8-2
C	?	-	LEU	deletion	UNP Q9Y4P8-2
C	?	-	MET	deletion	UNP Q9Y4P8-2
C	?	-	ALA	deletion	UNP Q9Y4P8-2
C	?	-	SER	deletion	UNP Q9Y4P8-2
C	?	-	THR	deletion	UNP Q9Y4P8-2
C	?	-	SER	deletion	UNP Q9Y4P8-2
C	?	-	TYR	deletion	UNP Q9Y4P8-2
C	?	-	LEU	deletion	UNP Q9Y4P8-2
C	?	-	PRO	deletion	UNP Q9Y4P8-2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP Q9Y4P8-2
C	?	-	GLN	deletion	UNP Q9Y4P8-2
C	?	-	VAL	deletion	UNP Q9Y4P8-2
C	?	-	THR	deletion	UNP Q9Y4P8-2
C	?	-	GLU	deletion	UNP Q9Y4P8-2
C	?	-	MET	deletion	UNP Q9Y4P8-2
C	?	-	PHE	deletion	UNP Q9Y4P8-2
C	?	-	ASN	deletion	UNP Q9Y4P8-2

- Molecule 2 is a protein called Autophagy-related protein 16-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	69	Total	C	H	N	O	S	0	2	0
			1113	339	557	95	117	5			
2	D	62	Total	C	H	N	O	S	0	3	0
			988	306	488	82	107	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	GLY	-	expression tag	UNP Q676U5
B	121	PRO	-	expression tag	UNP Q676U5
B	122	GLY	-	expression tag	UNP Q676U5
B	123	SER	-	expression tag	UNP Q676U5
D	120	GLY	-	expression tag	UNP Q676U5
D	121	PRO	-	expression tag	UNP Q676U5
D	122	GLY	-	expression tag	UNP Q676U5
D	123	SER	-	expression tag	UNP Q676U5

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	260	Total	O	0	0
			260	260		
3	B	25	Total	O	0	0
			25	25		
3	C	117	Total	O	0	0
			117	117		
3	D	22	Total	O	0	0
			22	22		

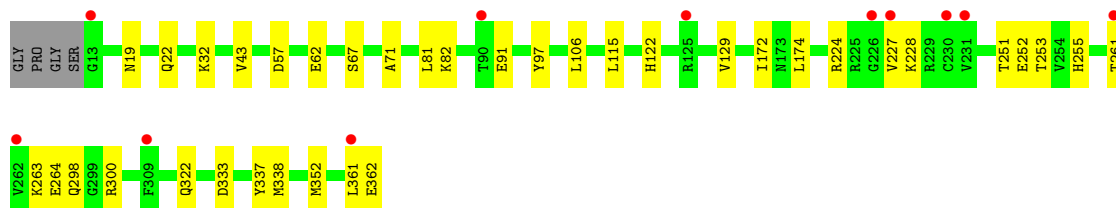
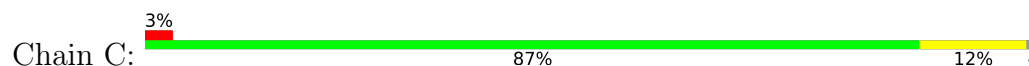
3 Residue-property plots [i](#)

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.

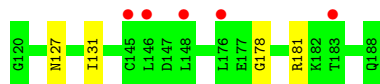
- Molecule 1: Isoform 2 of WD repeat domain phosphoinositide-interacting protein 2



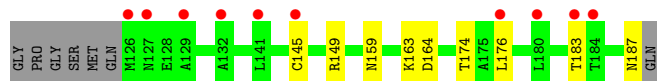
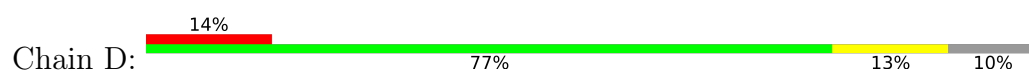
- Molecule 1: Isoform 2 of WD repeat domain phosphoinositide-interacting protein 2



- Molecule 2: Autophagy-related protein 16-1



- Molecule 2: Autophagy-related protein 16-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.20Å 80.63Å 76.75Å 90.00° 97.33° 90.00°	Depositor
Resolution (Å)	24.99 – 1.76 24.99 – 1.76	Depositor EDS
% Data completeness (in resolution range)	93.7 (24.99-1.76) 93.7 (24.99-1.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.165 , 0.193 (Not available) , 0.204	Depositor DCC
R_{free} test set	4061 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12359	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% 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](#)

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	0.47	0/2536	0.64	1/3425 (0.0%)
1	C	0.34	0/2526	0.53	0/3412
2	B	0.32	0/564	0.43	0/754
2	D	0.33	0/515	0.42	0/692
All	All	0.40	0/6141	0.56	1/8283 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	HIS	N-CA-C	-6.51	97.07	108.20

There are no chirality outliers.

There are no planarity outliers.

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	2480	2489	2507	14	0
1	C	2471	2394	2493	34	0
2	B	556	557	562	2	0
2	D	500	488	499	6	0
3	A	260	0	0	0	0
3	B	25	0	0	0	0
3	C	117	0	0	5	0
3	D	22	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6431	5928	6061	52	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 4.

All (52) 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:175:ARG:HH12	1:C:298:GLN:N	1.68	0.89
1:A:106:LEU:HD21	1:A:111:LEU:HD12	1.63	0.79
1:C:251:THR:HG22	1:C:253:THR:H	1.58	0.69
2:B:178:GLY:HA2	2:B:181:ARG:NH1	2.08	0.69
1:A:111:LEU:HD13	1:A:127:MET:HE1	1.77	0.67
1:C:263:LYS:H	1:C:298:GLN:HE22	1.46	0.64
1:C:352:MET:HE2	1:C:352:MET:HA	1.81	0.63
1:C:82:LYS:NZ	1:C:91:GLU:OE1	2.33	0.62
1:C:32:LYS:HD3	1:C:57:ASP:OD1	2.01	0.61
1:A:93:CYS:SG	1:A:95[B]:TYR:HE1	2.27	0.57
1:C:224:ARG:CZ	3:C:401:HOH:O	2.53	0.57
2:D:176:LEU:C	2:D:176:LEU:HD23	2.29	0.57
1:C:300:ARG:HA	3:C:401:HOH:O	2.04	0.56
2:D:183:THR:O	2:D:187:ASN:HB2	2.05	0.56
1:C:333:ASP:OD2	1:C:337:TYR:OH	2.20	0.56
1:C:263:LYS:H	1:C:298:GLN:NE2	2.05	0.55
1:A:71:ALA:HB1	1:A:81:LEU:HD11	1.89	0.55
1:A:93:CYS:SG	1:A:95[B]:TYR:CE1	3.01	0.54
1:C:261:THR:HG22	1:C:261:THR:O	2.06	0.53
1:C:19:ASN:HB3	3:C:484:HOH:O	2.07	0.53
1:C:71:ALA:HB1	1:C:81:LEU:HD11	1.91	0.53
1:C:263:LYS:N	1:C:298:GLN:HE22	2.09	0.50
1:C:224:ARG:NH2	3:C:401:HOH:O	2.44	0.49
1:C:172:ILE:O	1:C:174:LEU:HD22	2.14	0.48
1:C:263:LYS:O	1:C:298:GLN:NE2	2.47	0.47
1:A:305:VAL:HG13	1:A:339:TYR:CE2	2.49	0.47
1:A:111:LEU:C	1:A:111:LEU:HD23	2.39	0.47
1:C:43:VAL:HG12	1:C:338:MET:HE2	1.95	0.47
2:D:159:ASN:HD21	2:D:163:LYS:HE3	1.80	0.47
1:C:62:GLU:HG2	1:C:106:LEU:HG	1.97	0.46
1:C:263:LYS:N	1:C:298:GLN:NE2	2.63	0.46
1:C:22:GLN:NE2	1:C:106:LEU:HD12	2.31	0.44
2:B:127:ASN:O	2:B:131:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LYS:CD	1:C:57:ASP:OD1	2.66	0.43
2:D:174:THR:OG1	3:D:201:HOH:O	2.22	0.43
1:A:111:LEU:C	1:A:112:ILE:HD12	2.44	0.42
1:C:251:THR:CG2	1:C:252:GLU:N	2.82	0.42
1:C:43:VAL:HG22	1:C:322:GLN:OE1	2.19	0.42
1:C:97:TYR:HB3	1:C:115:LEU:HD11	2.00	0.42
1:C:227:VAL:HG12	1:C:228:LYS:N	2.34	0.42
1:C:361:LEU:O	1:C:362:GLU:C	2.63	0.42
1:A:115:LEU:HD22	1:A:120:TYR:HE1	1.84	0.42
1:A:175:ARG:HH12	1:C:298:GLN:H	1.57	0.42
1:A:175:ARG:HH12	1:C:264:GLU:C	2.26	0.41
1:C:122:HIS:CE1	1:C:129:VAL:HG22	2.55	0.41
1:A:173:ASN:O	1:A:175:ARG:HG2	2.21	0.41
1:A:68:SER:HA	1:A:86:PHE:CE2	2.55	0.41
1:C:251:THR:HG22	1:C:252:GLU:N	2.35	0.40
2:D:145:CYS:SG	2:D:149:ARG:NH1	2.94	0.40
1:C:67:SER:HB3	2:D:164:ASP:HB3	2.03	0.40
1:C:227:VAL:CG1	1:C:228:LYS:N	2.84	0.40
1:C:255:HIS:HD2	3:C:500:HOH:O	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	321/321 (100%)	317 (99%)	4 (1%)	0	100	100
1	C	320/321 (100%)	311 (97%)	9 (3%)	0	100	100
2	B	69/69 (100%)	69 (100%)	0	0	100	100
2	D	63/69 (91%)	63 (100%)	0	0	100	100
All	All	773/780 (99%)	760 (98%)	13 (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	276/274 (101%)	275 (100%)	1 (0%)	84	80
1	C	275/274 (100%)	275 (100%)	0	100	100
2	B	63/61 (103%)	63 (100%)	0	100	100
2	D	59/61 (97%)	59 (100%)	0	100	100
All	All	673/670 (100%)	672 (100%)	1 (0%)	87	85

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	150	ASN
1	A	173	ASN
2	B	160	GLN
2	B	170	GLN
1	C	152	ASN
1	C	255	HIS
1	C	298	GLN
2	D	159	ASN
2	D	160	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](#)

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, 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	319/321 (99%)	-0.29	4 (1%) 75 81	25, 36, 60, 89	4 (1%)
1	C	317/321 (98%)	0.25	11 (3%) 47 53	23, 49, 92, 129	5 (1%)
2	B	69/69 (100%)	0.57	5 (7%) 21 25	31, 58, 99, 116	2 (2%)
2	D	62/69 (89%)	0.74	10 (16%) 4 5	30, 64, 110, 126	2 (3%)
All	All	767/780 (98%)	0.09	30 (3%) 43 49	23, 43, 89, 129	13 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	262	VAL	7.4
1	C	361	LEU	6.6
2	B	145	CYS	3.9
1	C	309	PHE	3.8
2	D	129	ALA	3.8
2	D	126	MET	3.8
1	C	261	THR	3.4
1	C	90	THR	3.3
1	C	231	VAL	3.0
1	A	95[A]	TYR	3.0
1	C	230	CYS	3.0
1	A	12	SER	2.9
1	C	13	GLY	2.9
2	B	146	LEU	2.9
1	C	125[A]	ARG	2.7
2	D	176	LEU	2.7
1	C	227	VAL	2.5
2	B	176	LEU	2.5
1	A	262	VAL	2.5
2	D	132	ALA	2.4
1	C	226	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	148	LEU	2.4
2	D	127	ASN	2.3
2	D	183	THR	2.3
2	D	141	LEU	2.3
2	D	180	LEU	2.3
2	D	184	THR	2.2
1	A	227	VAL	2.0
2	D	145	CYS	2.0
2	B	183	THR	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 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.