



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 06:17 PM EDT

PDB ID : 6BCH
Title : I-LtrI E29D bound to cognate substrate (nicked complex)
Authors : Brown, C.; Zhang, K.; McMurrough, T.A.; Gloor, G.B.; Edgell, D.R.; Junop, M.
Deposited on : 2017-10-20
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

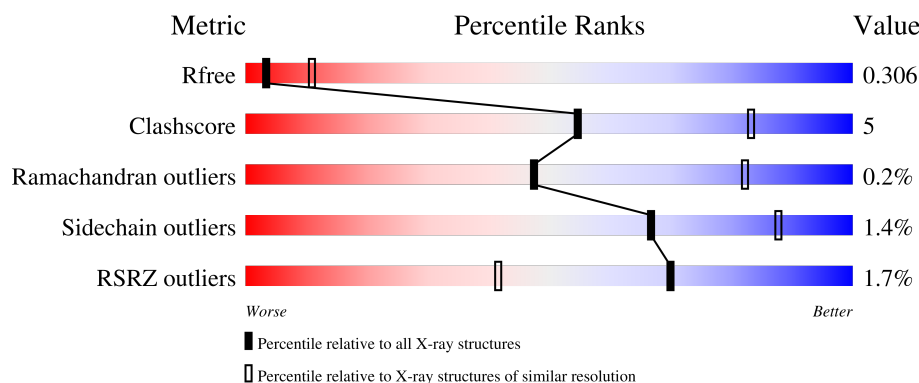
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



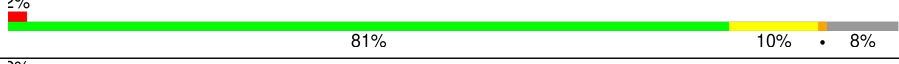


The reported resolution of this entry is 3.00 Å.

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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	315	
1	D	315	
1	H	315	
1	L	315	
2	B	16	

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Mol	Chain	Length	Quality of chain
2	E	16	 81% 12% 6%
2	I	16	 81% 19%
2	N	16	 81% 19%
3	C	26	 77% 19% .
3	F	26	 77% 19% .
3	J	26	 81% 19%
3	O	26	 77% 23%
4	G	11	 64% 18% 18%
4	K	11	 64% 18% 18%
4	P	11	 73% 9% 18%
4	X	11	 64% 18% 18%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12855 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 Ribosomal protein 3/homing endonuclease-like fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2158	1385	374	393	6			
1	D	289	Total	C	N	O	S	0	0	0
			2148	1377	369	396	6			
1	H	289	Total	C	N	O	S	0	0	0
			2139	1373	366	394	6			
1	L	289	Total	C	N	O	S	0	0	0
			2148	1377	369	396	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	ASP	GLU	engineered mutation	UNP C7SWF3
D	29	ASP	GLU	engineered mutation	UNP C7SWF3
H	29	ASP	GLU	engineered mutation	UNP C7SWF3
L	29	ASP	GLU	engineered mutation	UNP C7SWF3

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*GP*TP*CP*TP*AP*AP*AP*CP*GP*TP*CP*GP*TP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	16	Total	C	N	O	P	0	0	0
			310	147	57	91	15			
2	E	16	Total	C	N	O	P	0	0	0
			310	147	57	91	15			
2	I	16	Total	C	N	O	P	0	0	0
			310	147	57	91	15			
2	N	16	Total	C	N	O	P	0	0	0
			310	147	57	91	15			

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	26	Total 528	C 253	N 95	O 155	P 25	0	0	0
3	F	26	Total 528	C 253	N 95	O 155	P 25	0	0	0
3	J	26	Total 528	C 253	N 95	O 155	P 25	0	0	0
3	O	26	Total 528	C 253	N 95	O 155	P 25	0	0	0

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*AP*GP*GP*AP*GP*CP*AP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	X	11	Total 225	C 109	N 41	O 65	P 10	0	0	0
4	G	11	Total 225	C 109	N 41	O 65	P 10	0	0	0
4	K	11	Total 225	C 109	N 41	O 65	P 10	0	0	0
4	P	11	Total 225	C 109	N 41	O 65	P 10	0	0	0

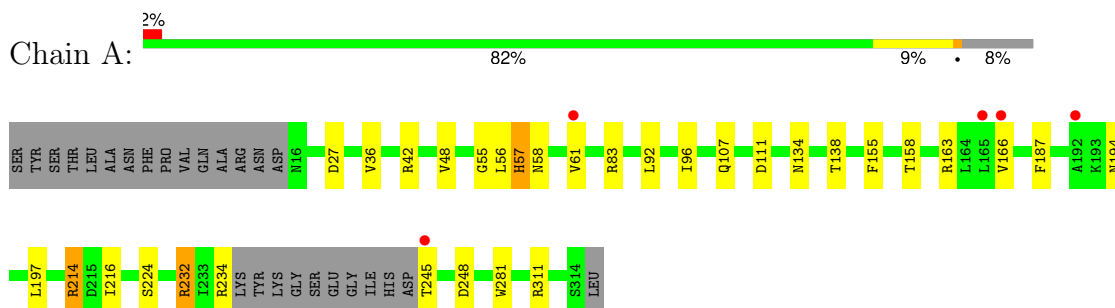
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	O 2	0	0
5	D	3	Total 3	O 3	0	0
5	H	2	Total 2	O 2	0	0
5	L	2	Total 2	O 2	0	0
5	P	1	Total 1	O 1	0	0

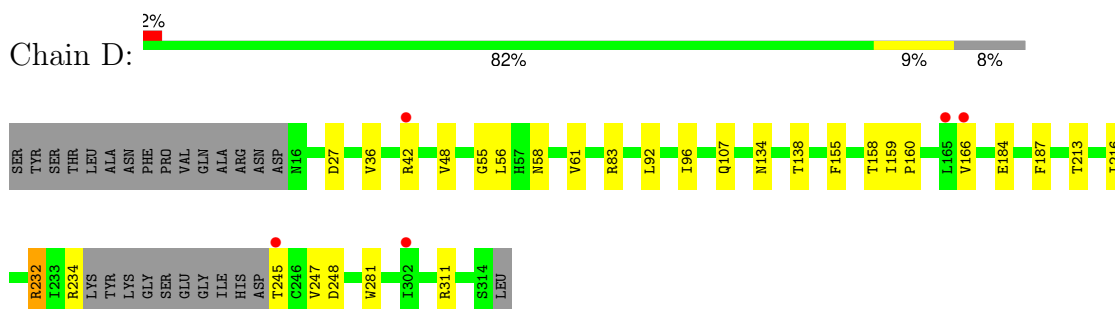
3 Residue-property plots [i](#)

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.

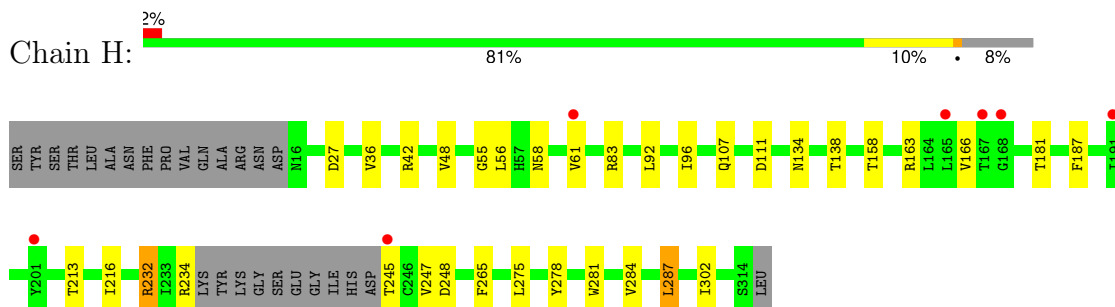
- Molecule 1: Ribosomal protein 3/homing endonuclease-like fusion protein



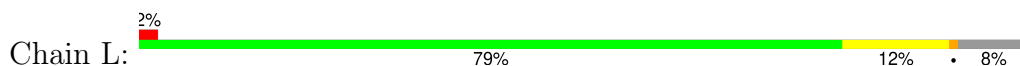
- Molecule 1: Ribosomal protein 3/homing endonuclease-like fusion protein

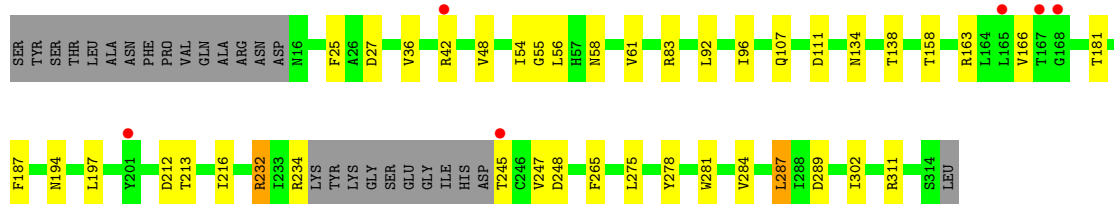


- Molecule 1: Ribosomal protein 3/homing endonuclease-like fusion protein



- Molecule 1: Ribosomal protein 3/homing endonuclease-like fusion protein

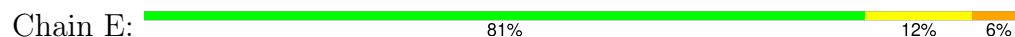




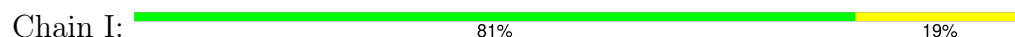
- Molecule 2: DNA (5'-D(*GP*GP*TP*CP*TP*AP*AP*AP*CP*GP*TP*CP*GP*TP*AP*T)-3')



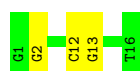
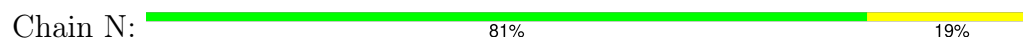
- Molecule 2: DNA (5'-D(*GP*GP*TP*CP*TP*AP*AP*AP*CP*GP*TP*CP*GP*TP*AP*T)-3')



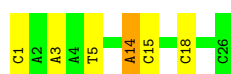
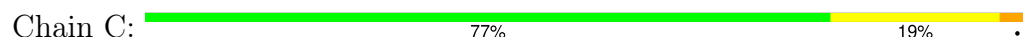
- Molecule 2: DNA (5'-D(*GP*GP*TP*CP*TP*AP*AP*AP*CP*GP*TP*CP*GP*TP*AP*T)-3')



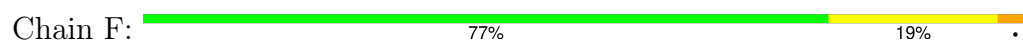
- Molecule 2: DNA (5'-D(*GP*GP*TP*CP*TP*AP*AP*AP*CP*GP*TP*CP*GP*TP*AP*T)-3')

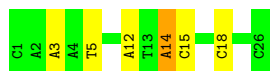


- Molecule 3: DNA (26-MER)

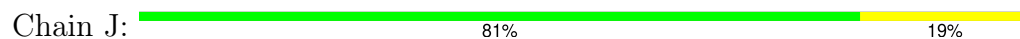


- Molecule 3: DNA (26-MER)

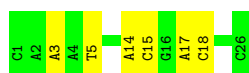
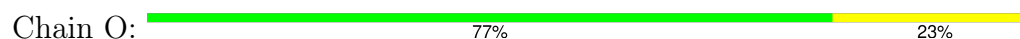




- Molecule 3: DNA (26-MER)



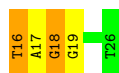
- Molecule 3: DNA (26-MER)



- Molecule 4: DNA (5'-D(*TP*AP*GP*GP*AP*GP*CP*AP*TP*TP*T)-3')



- Molecule 4: DNA (5'-D(*TP*AP*GP*GP*AP*GP*CP*AP*TP*TP*T)-3')



- Molecule 4: DNA (5'-D(*TP*AP*GP*GP*AP*GP*CP*AP*TP*TP*T)-3')



- Molecule 4: DNA (5'-D(*TP*AP*GP*GP*AP*GP*CP*AP*TP*TP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.76Å 66.31Å 169.92Å 90.03° 90.03° 90.22°	Depositor
Resolution (Å)	38.91 – 3.00 66.31 – 3.00	Depositor EDS
% Data completeness (in resolution range)	77.9 (38.91-3.00) 72.2 (66.31-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.254 , 0.306 0.258 , 0.306	Depositor DCC
R_{free} test set	1493 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	1.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.409 for h,-k,-l 0.409 for -h,k,-l 0.427 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12855	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% 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	0.28	0/2197	0.52	0/2995
1	D	0.28	0/2187	0.50	0/2985
1	H	0.26	0/2178	0.51	0/2974
1	L	0.27	0/2187	0.52	0/2985
2	B	0.57	0/347	1.01	0/535
2	E	0.65	0/347	1.09	1/535 (0.2%)
2	I	0.66	0/347	1.07	0/535
2	N	0.67	0/347	1.05	0/535
3	C	0.68	0/589	1.12	2/906 (0.2%)
3	F	0.68	0/589	1.11	2/906 (0.2%)
3	J	0.65	0/589	1.07	0/906
3	O	0.66	0/589	1.07	1/906 (0.1%)
4	G	1.01	2/252 (0.8%)	1.74	4/388 (1.0%)
4	K	1.02	2/252 (0.8%)	1.32	4/388 (1.0%)
4	P	0.76	1/252 (0.4%)	1.17	1/388 (0.3%)
4	X	1.04	2/252 (0.8%)	1.71	4/388 (1.0%)
All	All	0.49	7/13501 (0.1%)	0.83	19/19255 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	17	DA	O3'-P	-9.36	1.50	1.61
4	X	17	DA	O3'-P	-8.73	1.50	1.61
4	G	17	DA	O3'-P	-8.52	1.50	1.61
4	K	18	DG	O3'-P	-8.24	1.51	1.61
4	X	18	DG	O3'-P	-8.02	1.51	1.61

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	17	DA	OP1-P-OP2	-19.15	90.88	119.60
4	X	17	DA	OP1-P-OP2	-17.91	92.73	119.60
4	X	16	DT	OP2-P-O3'	17.87	144.51	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	16	DT	OP2-P-O3'	16.60	141.71	105.20
4	K	16	DT	OP2-P-O3'	9.44	125.97	105.20

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	2158	0	2064	24	0
1	D	2148	0	2036	24	0
1	H	2139	0	2023	24	0
1	L	2148	0	2036	27	0
2	B	310	0	170	5	0
2	E	310	0	170	3	0
2	I	310	0	170	2	0
2	N	310	0	170	2	0
3	C	528	0	295	8	0
3	F	528	0	295	8	0
3	J	528	0	295	7	0
3	O	528	0	295	7	0
4	G	225	0	127	6	0
4	K	225	0	127	6	0
4	P	225	0	127	2	0
4	X	225	0	127	4	0
5	A	2	0	0	0	0
5	D	3	0	0	1	0
5	H	2	0	0	0	0
5	L	2	0	0	0	0
5	P	1	0	0	0	0
All	All	12855	0	10527	122	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 5.

The worst 5 of 122 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:D:311:ARG:HH12	3:F:18:DC:H5'	1.28	0.97
1:A:311:ARG:HH12	3:C:18:DC:H5'	1.30	0.95
1:A:55:GLY:O	1:A:56:LEU:HD23	1.66	0.95
1:L:311:ARG:HH12	3:O:18:DC:H5'	1.29	0.93
3:F:14:DA:H2''	3:F:15:DC:H5''	1.61	0.82

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	285/315 (90%)	275 (96%)	8 (3%)	2 (1%)	22	60
1	D	285/315 (90%)	277 (97%)	8 (3%)	0	100	100
1	H	285/315 (90%)	277 (97%)	8 (3%)	0	100	100
1	L	285/315 (90%)	277 (97%)	8 (3%)	0	100	100
All	All	1140/1260 (90%)	1106 (97%)	32 (3%)	2 (0%)	47	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	214	ARG

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	215/282 (76%)	213 (99%)	2 (1%)	78	92
1	D	214/282 (76%)	212 (99%)	2 (1%)	78	92
1	H	212/282 (75%)	208 (98%)	4 (2%)	57	84
1	L	214/282 (76%)	210 (98%)	4 (2%)	57	84
All	All	855/1128 (76%)	843 (99%)	12 (1%)	67	88

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	287	LEU
1	L	27	ASP
1	L	287	LEU
1	L	158	THR
1	D	232	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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

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	289/315 (91%)	-0.03	5 (1%) 70 41	37, 70, 94, 117	0
1	D	289/315 (91%)	-0.01	5 (1%) 70 41	41, 69, 93, 121	0
1	H	289/315 (91%)	0.02	7 (2%) 59 30	41, 71, 97, 135	0
1	L	289/315 (91%)	0.02	6 (2%) 63 34	39, 69, 93, 120	0
2	B	16/16 (100%)	-0.09	0 100 100	50, 71, 109, 110	0
2	E	16/16 (100%)	-0.15	0 100 100	45, 72, 116, 120	0
2	I	16/16 (100%)	-0.18	0 100 100	56, 73, 112, 113	0
2	N	16/16 (100%)	-0.26	0 100 100	48, 68, 109, 112	0
3	C	26/26 (100%)	-0.04	0 100 100	39, 69, 85, 98	0
3	F	26/26 (100%)	-0.07	0 100 100	38, 68, 90, 101	0
3	J	26/26 (100%)	-0.05	0 100 100	44, 75, 88, 103	0
3	O	26/26 (100%)	-0.06	0 100 100	40, 69, 86, 103	0
4	G	11/11 (100%)	-0.45	0 100 100	44, 61, 70, 76	0
4	K	11/11 (100%)	-0.33	0 100 100	47, 60, 64, 68	0
4	P	11/11 (100%)	-0.39	0 100 100	47, 62, 70, 71	0
4	X	11/11 (100%)	-0.44	0 100 100	45, 60, 71, 75	0
All	All	1368/1472 (92%)	-0.03	23 (1%) 70 41	37, 69, 96, 135	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	168	GLY	7.7
1	H	167	THR	4.8
1	L	168	GLY	4.8
1	H	245	THR	3.6
1	L	201	TYR	3.4

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.