



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 07:11 PM UTC

PDB ID : 7BV6 / pdb_00007bv6
Title : Crystal structure of the autophagic STX17/SNAP29/VAMP8 SNARE complex
Authors : Li, Y.; Pan, L.F.
Deposited on : 2020-04-09
Resolution : 3.05 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	:	4-5-2 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

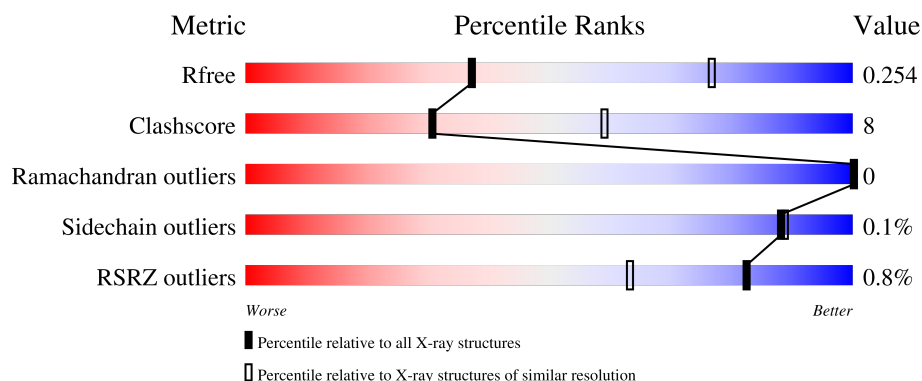
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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.



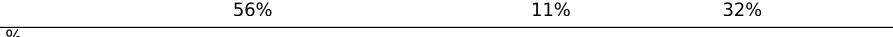
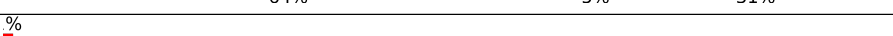
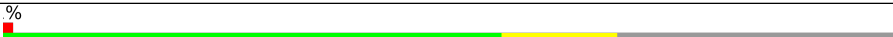
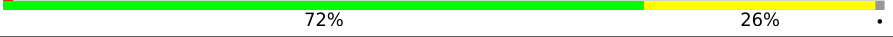
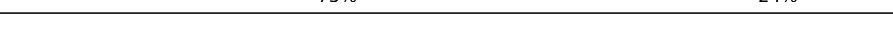
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	68	
1	E	68	
1	I	68	
1	M	68	
1	Q	68	

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Mol	Chain	Length	Quality of chain
1	U	68	
2	B	87	
2	F	87	
2	J	87	
2	N	87	
2	R	87	
2	V	87	
3	C	91	
3	G	91	
3	K	91	
3	O	91	
3	S	91	
3	W	91	
4	D	68	
4	H	68	
4	L	68	
4	P	68	
4	T	68	
4	X	68	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12345 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 Vesicle-associated membrane protein 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	66	Total	C	N	O	S	0	0	0
			547	336	106	104	1			
1	E	65	Total	C	N	O	S	0	0	0
			537	331	102	103	1			
1	I	66	Total	C	N	O	S	0	0	0
			537	330	102	104	1			
1	M	66	Total	C	N	O	S	0	0	0
			528	322	101	104	1			
1	Q	61	Total	C	N	O	S	0	0	0
			491	297	96	97	1			
1	U	66	Total	C	N	O	S	0	0	0
			539	330	104	104	1			

- Molecule 2 is a protein called Syntaxin-17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	61	Total	C	N	O	0	0	0
			459	285	75	99			
2	F	61	Total	C	N	O	0	0	0
			454	282	74	98			
2	J	59	Total	C	N	O	0	0	0
			441	272	72	97			
2	N	60	Total	C	N	O	0	0	0
			438	271	73	94			
2	R	55	Total	C	N	O	0	0	0
			413	255	67	91			
2	V	60	Total	C	N	O	0	0	0
			457	284	74	99			

- Molecule 3 is a protein called Synaptosomal-associated protein 29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	72	Total	C	N	O	S	0	0	0
			548	333	100	112	3			
3	G	74	Total	C	N	O	S	0	0	0
			560	342	102	113	3			
3	K	73	Total	C	N	O	S	0	0	0
			554	337	99	115	3			
3	O	73	Total	C	N	O	S	0	0	0
			555	336	103	113	3			
3	S	74	Total	C	N	O	S	0	0	0
			565	343	104	115	3			
3	W	72	Total	C	N	O	S	0	0	0
			541	329	97	112	3			

- Molecule 4 is a protein called Synaptosomal-associated protein 29.

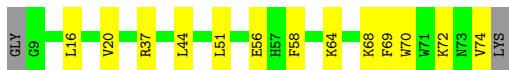
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	67	Total	C	N	O	S	0	0	0
			531	328	95	106	2			
4	H	68	Total	C	N	O	S	0	0	0
			539	332	95	110	2			
4	L	67	Total	C	N	O	S	0	0	0
			532	328	95	107	2			
4	P	65	Total	C	N	O	S	0	0	0
			525	323	94	106	2			
4	T	67	Total	C	N	O	S	0	0	0
			536	329	97	108	2			
4	X	65	Total	C	N	O	S	0	0	0
			518	319	93	104	2			

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: Vesicle-associated membrane protein 8

Chain A:  78% 19% .



- Molecule 1: Vesicle-associated membrane protein 8

Chain E:  85% 10% .



- Molecule 1: Vesicle-associated membrane protein 8

Chain I:  82% 15% .



- Molecule 1: Vesicle-associated membrane protein 8

Chain M:  75% 22% .



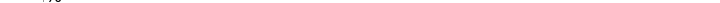
- Molecule 1: Vesicle-associated membrane protein 8

Chain Q:  71% 19% 10% .

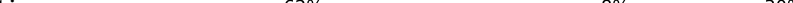


- Molecule 1: Vesicle-associated membrane protein 8

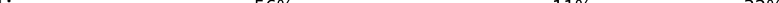
GLY
G9
E32
H43
L44
R45
N46
K47
T48
T54
S62
V74
LYS

Chain B:  %

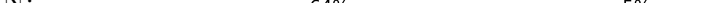
Category	Value	Color
HIS	168	Green
THR	169	Red
THR	172	Yellow
GLU	178	Dark Green
GLU	179	Dark Green
ALA	190	Yellow
GLU	191	Yellow
ALA	196	Yellow
ALA	197	Yellow
SER	209	Yellow
SER	210	Yellow
SER	211	Yellow
GLN	212	Yellow
LEU	213	Yellow
THR	214	Yellow
GLN	217	Yellow
GLN	217	Yellow
ASP	218	Yellow
GLN	219	Yellow
ASN	219	Yellow
A168	219	Green
A169	219	Red
W172	219	Yellow
D178	219	Dark Green
L179	219	Dark Green
S190	219	Yellow
L191	219	Yellow
Q196	219	Yellow
Q197	219	Yellow
S209	219	Yellow
A210	219	Yellow
A211	219	Yellow
V212	219	Yellow
N213	219	Yellow
V214	219	Yellow
G217	219	Yellow
V219	219	Yellow

Chain F:  3% 62% 8% 30%

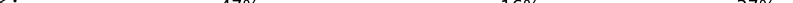
HIS	THR	THR	GLU	ALA	GLU	ALA	SER	SER	SER	GLN	LEU	THR	GLN	ILE	TYR	ALA	ALA	LEU	PRO	GLU	ILE	PRO	ASP	GLN	ASN	A168	E170	S171	M172	T174	S190	L191	Q196	I203	Y227	K228
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Chain J: 

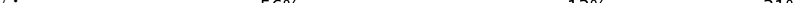
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THR	169	Red
THR	170	Yellow
GLU	171	Yellow
ALA	172	Yellow
GLU	173	Yellow
ALA	174	Yellow
ALA	175	Yellow
SER	176	Yellow
SER	177	Yellow
SER	178	Yellow
GLN	179	Yellow
SER	180	Yellow
THR	181	Yellow
THR	182	Yellow
GLN	183	Yellow
ILE	184	Yellow
ILE	185	Yellow
TYR	186	Yellow
ALA	187	Yellow
LEU	188	Yellow
LEU	189	Yellow
GLU	190	Yellow
GLU	191	Yellow
ILE	192	Yellow
ILE	193	Yellow
PRO	194	Yellow
GLN	195	Yellow
ASP	196	Yellow
GLN	197	Yellow
ASN	198	Yellow
A168	199	Green
A169	200	Red
E170	201	Yellow
T174	202	Yellow
E181	203	Yellow
V186	204	Yellow
S190	205	Yellow
K199	206	Yellow
I203	207	Yellow
A210	208	Yellow
V214	209	Yellow
N220	210	Yellow
K226	211	Red
TYR	212	Grey
YS	213	Grey

Chain N:  %

Label	Value	Color
HIS	1.00	Green
THR	0.99	Green
THR	0.99	Green
GLU	0.99	Green
ALA	0.99	Green
GLU	0.99	Green
ALA	0.99	Green
SER	0.99	Green
SER	0.99	Green
SER	0.99	Green
GLN	0.99	Green
SER	0.99	Green
THR	0.99	Green
THR	0.99	Green
GLN	0.99	Green
TYR	0.99	Green
LEU	0.99	Green
LEU	0.99	Green
PRO	0.99	Green
GLU	0.99	Green
ILE	0.99	Green
PRO	0.99	Green
GLN	0.99	Green
ASP	0.99	Green
GLN	0.99	Green
ASN	0.99	Green
A168	0.99	Green
A169	0.99	Green
D178	0.99	Green
L191	0.99	Green
Q197	0.99	Green
I203	0.99	Green
Y227	0.99	Green
LYS	0.99	Green

Chain R:  %

HIS	THR	THR	GLU	GLU	ALA	GLU	ALA	SER	SER	SER	GLN	SER	LEU	THR	GLN	ILE	TYR	ALA	ALA	LEU	PRO	GLU	ILE	PRO	GLN	ASP	ASN	ASN	A168	A169	E170	S171	W172	D178	E181	S190	V193	N194	S195	Q196	K199	V212	E215	E216	G217	G222	LYS	ALA	ALA	ALA	LYS	TYR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----

Chain V: 

HIS	THR	THR	GLU	ALA	GLU	ALA	SER	SER	SER	GLN	LEU	THR	GLN	ILE	TYR	ALA	ALA	LEU	PRO	GLU	GLU	ILE	PRO	GLN	ASP	GLN	ASN	A168	L191	L192	V193	N194	A195	Q196	S202	I203	A204	N208	S209	V212	G217	V227	I228
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- Molecule 3: Synaptosomal-associated protein 29

Chain C:  60% 19% 21%



- Molecule 3: Synaptosomal-associated protein 29

Chain G:  67% 14% 19%



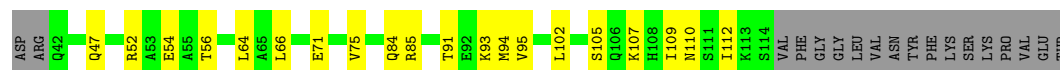
- Molecule 3: Synaptosomal-associated protein 29

Chain K:  65% 15% 20%



- Molecule 3: Synaptosomal-associated protein 29

Chain O:  58% 22% 20%



- Molecule 3: Synaptosomal-associated protein 29

Chain S:  70% 11% 19%



- Molecule 3: Synaptosomal-associated protein 29

Chain W:  65% 14% 21%



- Molecule 4: Synaptosomal-associated protein 29

Chain D:  76% 22% .



- Molecule 4: Synaptosomal-associated protein 29

Chain H:  71% 29%



• Molecule 4: Synaptosomal-associated protein 29

Chain L:  72% 26% .



• Molecule 4: Synaptosomal-associated protein 29

Chain P:  75% 21% .



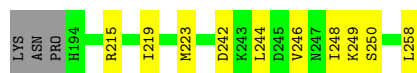
• Molecule 4: Synaptosomal-associated protein 29

Chain T:  75% 24% .



• Molecule 4: Synaptosomal-associated protein 29

Chain X:  81% 15% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.98Å 196.00Å 76.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 3.05 49.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.00-3.05) 99.8 (49.00-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.175 , 0.255 0.177 , 0.254	Depositor DCC
R_{free} test set	2088 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12345	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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	0/554	0.65	0/743
1	E	0.41	0/544	0.55	0/731
1	I	0.43	0/544	0.55	0/732
1	M	0.39	0/533	0.55	0/716
1	Q	0.37	0/494	0.56	0/660
1	U	0.38	0/546	0.54	0/735
2	B	0.41	0/463	0.57	0/627
2	F	0.41	0/458	0.56	0/623
2	J	0.41	0/444	0.54	0/603
2	N	0.41	0/441	0.56	0/600
2	R	0.39	0/416	0.58	0/566
2	V	0.41	0/461	0.61	0/625
3	C	0.43	0/549	0.61	0/733
3	G	0.44	0/562	0.58	0/752
3	K	0.40	0/556	0.61	0/744
3	O	0.42	0/556	0.59	0/743
3	S	0.43	0/567	0.60	0/758
3	W	0.42	0/542	0.53	0/725
4	D	0.42	0/534	0.65	0/715
4	H	0.41	0/542	0.60	0/726
4	L	0.41	0/535	0.55	0/716
4	P	0.42	0/527	0.59	0/703
4	T	0.39	0/539	0.55	0/722
4	X	0.37	0/520	0.60	0/695
All	All	0.41	0/12427	0.58	0/16693

There are no bond length outliers.

There are no bond angle outliers.

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	547	0	543	11	0
1	E	537	0	529	9	0
1	I	537	0	521	9	0
1	M	528	0	513	16	0
1	Q	491	0	489	14	0
1	U	539	0	521	8	0
2	B	459	0	442	16	0
2	F	454	0	431	7	0
2	J	441	0	424	9	0
2	N	438	0	418	6	0
2	R	413	0	395	17	0
2	V	457	0	444	9	0
3	C	548	0	553	16	0
3	G	560	0	555	17	0
3	K	554	0	543	17	0
3	O	555	0	555	16	0
3	S	565	0	558	6	0
3	W	541	0	537	12	0
4	D	531	0	539	15	0
4	H	539	0	542	18	0
4	L	532	0	539	19	0
4	P	525	0	538	16	0
4	T	536	0	542	11	0
4	X	518	0	528	11	0
All	All	12345	0	12199	203	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 8.

The worst 5 of 203 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)
3:K:67:MET:HE1	4:L:216:LEU:HD12	1.09	1.07
3:K:67:MET:HE1	4:L:216:LEU:CD1	1.86	1.05
3:K:67:MET:CE	4:L:216:LEU:HD12	1.98	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:67:MET:CE	4:L:216:LEU:CD1	2.55	0.82
3:K:95:VAL:HG13	4:L:244:LEU:HD12	1.64	0.78

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	64/68 (94%)	62 (97%)	2 (3%)	0	100	100
1	E	63/68 (93%)	62 (98%)	1 (2%)	0	100	100
1	I	64/68 (94%)	60 (94%)	4 (6%)	0	100	100
1	M	64/68 (94%)	62 (97%)	2 (3%)	0	100	100
1	Q	59/68 (87%)	58 (98%)	1 (2%)	0	100	100
1	U	64/68 (94%)	64 (100%)	0	0	100	100
2	B	59/87 (68%)	58 (98%)	1 (2%)	0	100	100
2	F	59/87 (68%)	57 (97%)	2 (3%)	0	100	100
2	J	57/87 (66%)	56 (98%)	1 (2%)	0	100	100
2	N	58/87 (67%)	55 (95%)	3 (5%)	0	100	100
2	R	53/87 (61%)	51 (96%)	2 (4%)	0	100	100
2	V	58/87 (67%)	57 (98%)	1 (2%)	0	100	100
3	C	70/91 (77%)	67 (96%)	3 (4%)	0	100	100
3	G	72/91 (79%)	72 (100%)	0	0	100	100
3	K	71/91 (78%)	71 (100%)	0	0	100	100
3	O	71/91 (78%)	68 (96%)	3 (4%)	0	100	100
3	S	72/91 (79%)	71 (99%)	1 (1%)	0	100	100
3	W	70/91 (77%)	69 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	65/68 (96%)	64 (98%)	1 (2%)	0	100	100
4	H	66/68 (97%)	63 (96%)	3 (4%)	0	100	100
4	L	65/68 (96%)	63 (97%)	2 (3%)	0	100	100
4	P	63/68 (93%)	63 (100%)	0	0	100	100
4	T	65/68 (96%)	63 (97%)	2 (3%)	0	100	100
4	X	63/68 (93%)	62 (98%)	1 (2%)	0	100	100
All	All	1535/1884 (82%)	1498 (98%)	37 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	60/61 (98%)	60 (100%)	0	100	100
1	E	59/61 (97%)	59 (100%)	0	100	100
1	I	58/61 (95%)	58 (100%)	0	100	100
1	M	57/61 (93%)	57 (100%)	0	100	100
1	Q	54/61 (88%)	54 (100%)	0	100	100
1	U	58/61 (95%)	58 (100%)	0	100	100
2	B	49/74 (66%)	49 (100%)	0	100	100
2	F	48/74 (65%)	48 (100%)	0	100	100
2	J	48/74 (65%)	48 (100%)	0	100	100
2	N	46/74 (62%)	46 (100%)	0	100	100
2	R	46/74 (62%)	46 (100%)	0	100	100
2	V	50/74 (68%)	50 (100%)	0	100	100
3	C	59/80 (74%)	59 (100%)	0	100	100
3	G	58/80 (72%)	58 (100%)	0	100	100
3	K	58/80 (72%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	59/80 (74%)	57 (97%)	2 (3%)	32	59
3	S	59/80 (74%)	59 (100%)	0	100	100
3	W	57/80 (71%)	57 (100%)	0	100	100
4	D	59/63 (94%)	59 (100%)	0	100	100
4	H	60/63 (95%)	60 (100%)	0	100	100
4	L	59/63 (94%)	59 (100%)	0	100	100
4	P	59/63 (94%)	59 (100%)	0	100	100
4	T	60/63 (95%)	60 (100%)	0	100	100
4	X	58/63 (92%)	58 (100%)	0	100	100
All	All	1338/1668 (80%)	1336 (100%)	2 (0%)	88	89

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

Mol	Chain	Res	Type
3	O	47	GLN
3	O	102	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	R	197	GLN
2	R	208	ASN
3	C	84	GLN
1	E	29	GLN
2	F	206	HIS

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 [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	66/68 (97%)	-0.56	0 100 100	25, 47, 97, 129	0
1	E	65/68 (95%)	-0.58	0 100 100	25, 50, 90, 124	0
1	I	66/68 (97%)	-0.30	1 (1%) 72 50	28, 52, 147, 184	0
1	M	66/68 (97%)	-0.32	1 (1%) 72 50	27, 59, 123, 147	0
1	Q	61/68 (89%)	-0.20	1 (1%) 70 47	30, 69, 144, 185	0
1	U	66/68 (97%)	-0.33	0 100 100	25, 62, 112, 153	0
2	B	61/87 (70%)	-0.65	1 (1%) 70 47	24, 38, 83, 148	0
2	F	61/87 (70%)	-0.49	3 (4%) 35 17	27, 42, 97, 177	0
2	J	59/87 (67%)	-0.39	2 (3%) 48 27	25, 46, 121, 124	0
2	N	60/87 (68%)	-0.50	1 (1%) 69 46	24, 47, 127, 180	0
2	R	55/87 (63%)	-0.28	1 (1%) 67 45	29, 54, 133, 182	0
2	V	60/87 (68%)	-0.49	1 (1%) 69 46	29, 50, 116, 151	0
3	C	72/91 (79%)	-0.58	0 100 100	29, 44, 98, 137	0
3	G	74/91 (81%)	-0.61	0 100 100	27, 44, 94, 106	0
3	K	73/91 (80%)	-0.45	0 100 100	26, 52, 124, 171	0
3	O	73/91 (80%)	-0.42	0 100 100	24, 53, 137, 157	0
3	S	74/91 (81%)	-0.22	0 100 100	30, 57, 156, 170	0
3	W	72/91 (79%)	-0.44	0 100 100	31, 52, 117, 133	0
4	D	67/68 (98%)	-0.69	0 100 100	28, 46, 74, 106	0
4	H	68/68 (100%)	-0.61	0 100 100	31, 49, 83, 114	0
4	L	67/68 (98%)	-0.60	1 (1%) 72 50	29, 51, 109, 140	0
4	P	65/68 (95%)	-0.58	0 100 100	28, 55, 115, 137	0
4	T	67/68 (98%)	-0.49	0 100 100	28, 54, 124, 152	0
4	X	65/68 (95%)	-0.45	0 100 100	31, 59, 109, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
All	All	1583/1884 (84%)	-0.47	13 (0%)	82 63	24, 51, 126, 185	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	169	ALA	3.0
2	F	169	ALA	3.0
2	F	170	GLU	2.8
1	Q	9	GLY	2.7
2	N	169	ALA	2.6

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.