



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 03:44 AM UTC

PDB ID : 5OSH / pdb\_00005osh  
Title : Structure of retromer VPS29-VPS35C subunits complexed with RidL N-terminal domain (1-236)  
Authors : Romano-Moreno, M.; Rojas, A.L.; Lucas, M.; Isupov, M.N.; Hierro, A.  
Deposited on : 2017-08-17  
Resolution : 4.30 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

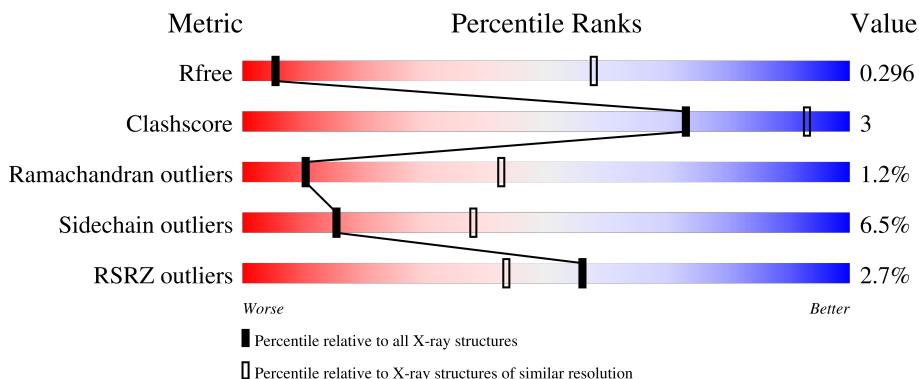
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.30 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	1052 (4.70-3.90)
Clashscore	190562	1097 (4.70-3.90)
Ramachandran outliers	187476	1001 (4.70-3.90)
Sidechain outliers	187428	1007 (4.72-3.88)
RSRZ outliers	180081	1049 (4.70-3.90)

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  $\geq 3$ , 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	182	 2% (red), 83% (green), 16% (yellow), . (grey)
1	D	182	 % (red), 79% (green), 21% (yellow)
1	G	182	 4% (red), 85% (green), 14% (yellow), . (grey)
1	J	182	 10% (red), 92% (green), 8% (yellow)
2	B	299	 % (red), 82% (green), 16% (yellow), . (grey)

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Mol	Chain	Length	Quality of chain
2	E	299	<p>2% 87% 10% ..</p>
2	H	299	<p>3% 87% 9% .</p>
2	K	299	<p>% 86% 10% ..</p>
3	C	223	<p>4% 83% 12% ..</p>
3	F	223	<p>2% 76% 17% . .</p>
3	I	223	<p>2% 85% 13% .</p>
3	L	223	<p>% 81% 11% . 6%</p>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 22276 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 Vacuolar protein sorting-associated protein 29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	182	1447	936	242	263	6	0	0	0
1	D	182	1447	936	242	263	6	0	0	0
1	G	182	1447	936	242	263	6	0	0	0
1	J	182	1447	936	242	263	6	0	0	0

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	299	2424	1539	423	452	10	0	0	0
2	E	294	2383	1514	418	441	10	0	0	0
2	H	290	2344	1491	408	435	10	0	0	0
2	K	293	2374	1509	417	438	10	0	0	0

- Molecule 3 is a protein called Interaptin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	217	1750	1103	299	344	4	0	0	0
3	F	214	1723	1085	294	340	4	0	0	0
3	I	223	1802	1135	306	356	5	0	0	0
3	L	209	1688	1062	288	334	4	0	0	0

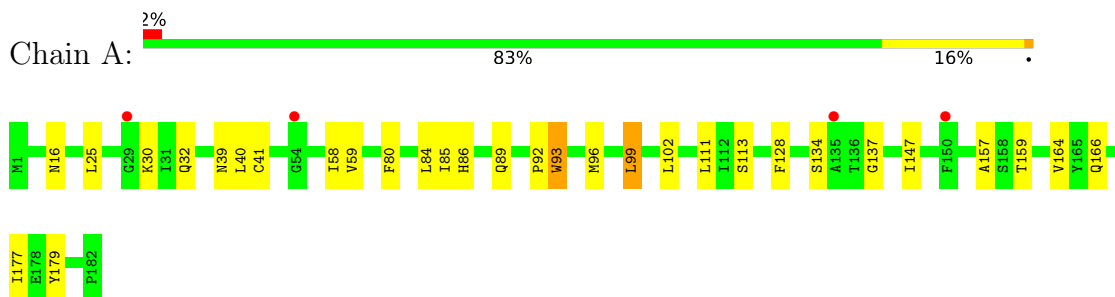
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP G8UZ99
C	2	ALA	-	expression tag	UNP G8UZ99
F	1	MET	-	initiating methionine	UNP G8UZ99
F	2	ALA	-	expression tag	UNP G8UZ99
I	1	MET	-	initiating methionine	UNP G8UZ99
I	2	ALA	-	expression tag	UNP G8UZ99
L	1	MET	-	initiating methionine	UNP G8UZ99
L	2	ALA	-	expression tag	UNP G8UZ99

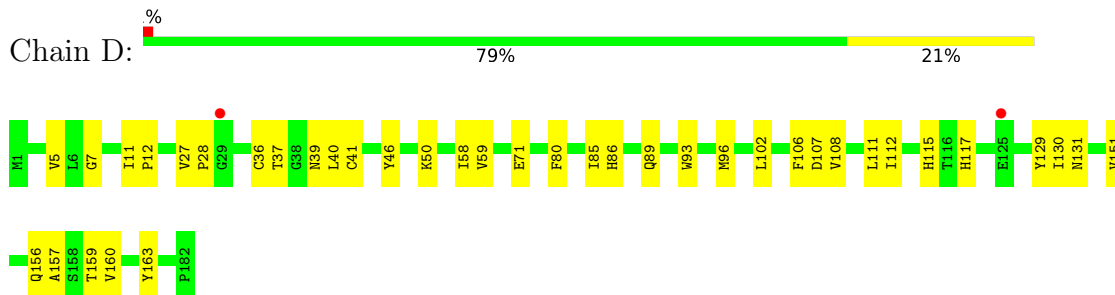
### 3 Residue-property plots [i](#)

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.

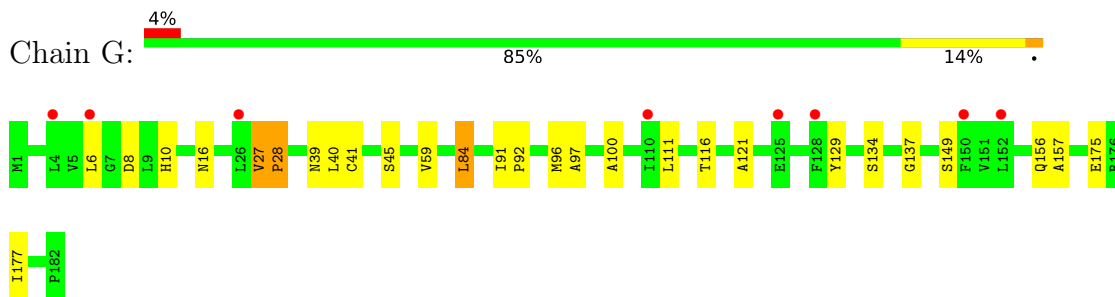
- Molecule 1: Vacuolar protein sorting-associated protein 29



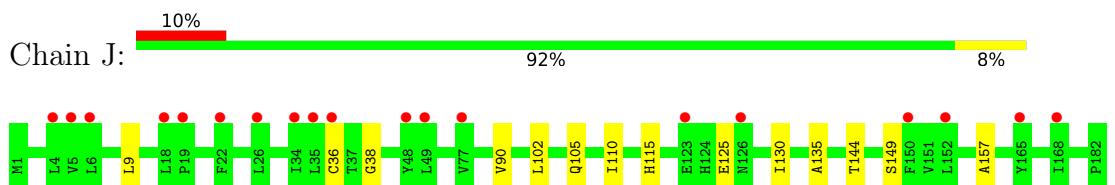
- Molecule 1: Vacuolar protein sorting-associated protein 29



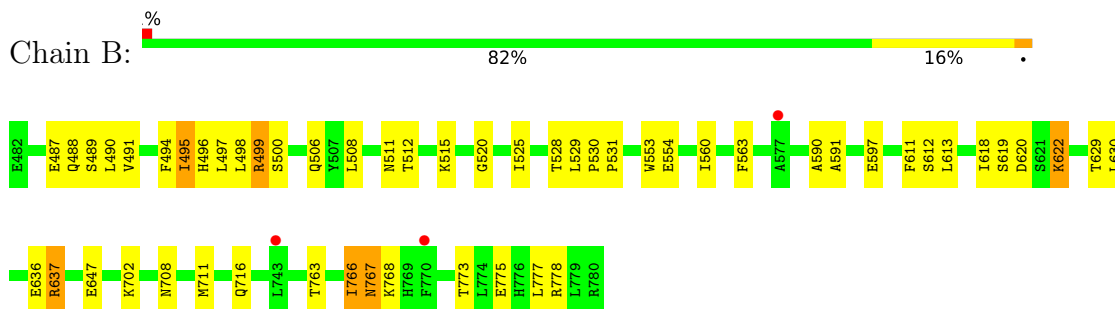
- Molecule 1: Vacuolar protein sorting-associated protein 29



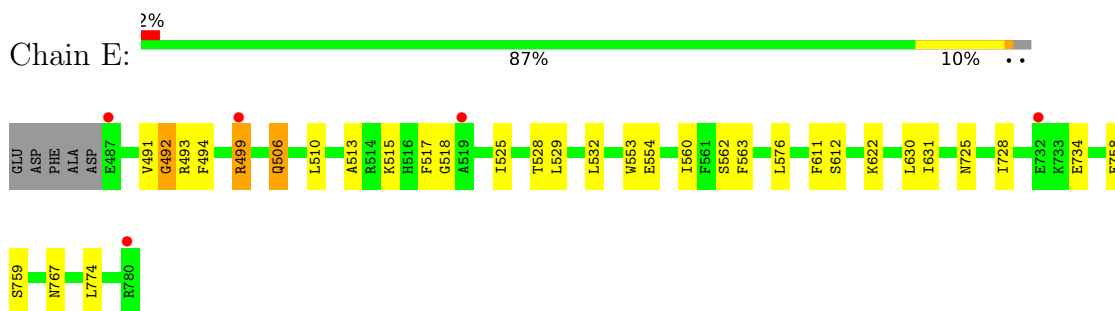
- Molecule 1: Vacuolar protein sorting-associated protein 29



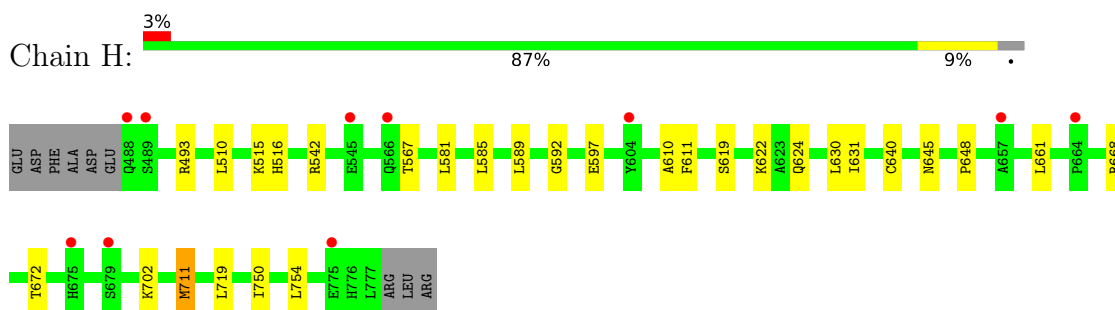
- Molecule 2: Vacuolar protein sorting-associated protein 35



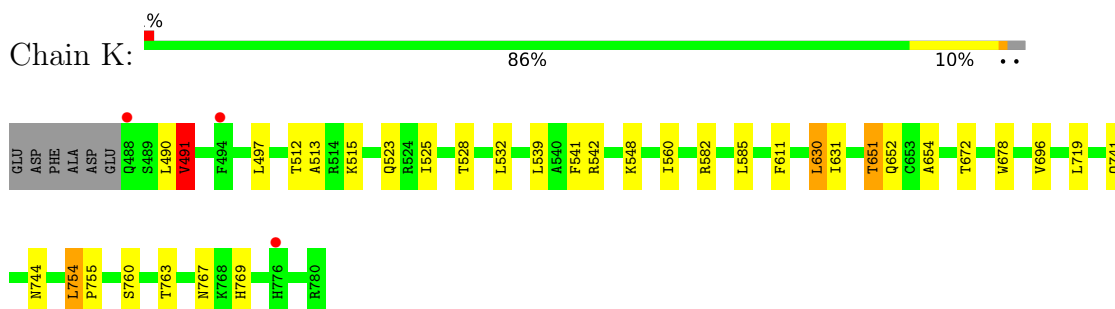
- Molecule 2: Vacuolar protein sorting-associated protein 35



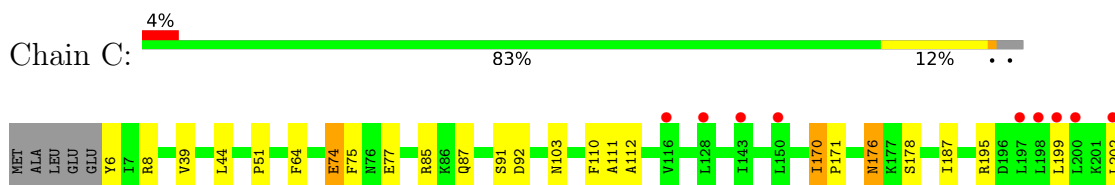
- Molecule 2: Vacuolar protein sorting-associated protein 35



- Molecule 2: Vacuolar protein sorting-associated protein 35

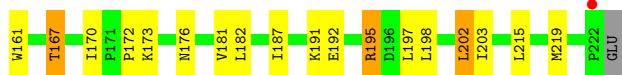
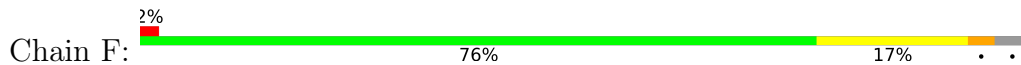


- Molecule 3: Interaptin

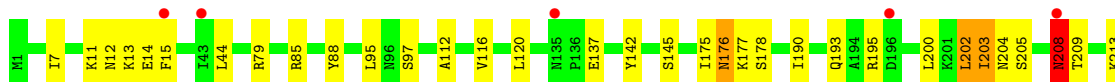
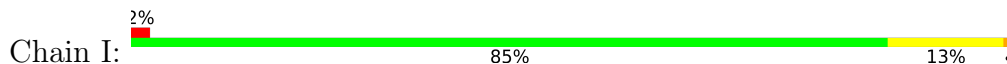




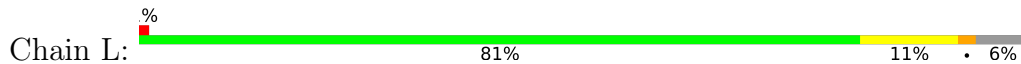
• Molecule 3: Interaptin



• Molecule 3: Interaptin



• Molecule 3: Interaptin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.20Å 173.24Å 445.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	222.89 – 4.30 222.89 – 4.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (222.89-4.30) 99.9 (222.89-4.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 4.30Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.254 , 0.311 0.249 , 0.296	Depositor DCC
$R_{free}$ test set	2460 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	216.4	Xtrriage
Anisotropy	0.285	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 405.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	22276	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	266.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.70	0/1481	0.95	1/2008 (0.0%)
1	D	0.76	1/1481 (0.1%)	1.02	0/2008
1	G	0.74	0/1481	0.93	2/2008 (0.1%)
1	J	0.65	0/1481	0.80	0/2008
2	B	0.76	0/2471	0.97	1/3327 (0.0%)
2	E	0.75	0/2429	0.94	0/3270
2	H	0.69	0/2390	0.95	0/3219
2	K	0.81	0/2420	0.89	0/3258
3	C	0.73	0/1783	1.00	5/2401 (0.2%)
3	F	0.77	0/1755	1.00	0/2362
3	I	0.83	0/1835	1.03	0/2469
3	L	0.75	0/1717	0.93	1/2311 (0.0%)
All	All	0.75	1/22724 (0.0%)	0.95	10/30649 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	159	THR	CA-CB	5.35	1.57	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	28	PRO	N-CA-C	6.47	121.40	111.11
3	C	171	PRO	N-CA-C	-6.21	103.13	110.70
1	G	27	VAL	CB-CA-C	6.13	115.34	109.33
3	L	203	ILE	CB-CA-C	-5.81	104.87	111.55
3	C	74	GLU	N-CA-C	5.76	118.42	110.35

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	1447	0	1459	13	0
1	D	1447	0	1459	17	0
1	G	1447	0	1459	10	0
1	J	1447	0	1459	7	0
2	B	2424	0	2407	21	0
2	E	2383	0	2379	11	0
2	H	2344	0	2336	9	0
2	K	2374	0	2373	18	0
3	C	1750	0	1726	8	0
3	F	1723	0	1704	21	0
3	I	1802	0	1783	15	0
3	L	1688	0	1673	7	0
All	All	22276	0	22217	141	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 3.

The worst 5 of 141 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:I:11:LYS:NZ	3:I:88:TYR:OH	2.19	0.75
3:L:176:ASN:ND2	3:L:178:SER:OG	2.26	0.69
1:A:134:SER:OG	1:A:137:GLY:N	2.30	0.64
1:G:27:VAL:HG22	1:G:28:PRO:HD2	1.84	0.60
3:L:58:VAL:HG21	3:L:95:LEU:HD11	1.83	0.59

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	180/182 (99%)	160 (89%)	17 (9%)	3 (2%)	7	35
1	D	180/182 (99%)	157 (87%)	21 (12%)	2 (1%)	11	45
1	G	180/182 (99%)	160 (89%)	18 (10%)	2 (1%)	11	45
1	J	180/182 (99%)	157 (87%)	20 (11%)	3 (2%)	7	35
2	B	297/299 (99%)	259 (87%)	34 (11%)	4 (1%)	9	41
2	E	292/299 (98%)	265 (91%)	25 (9%)	2 (1%)	18	55
2	H	288/299 (96%)	265 (92%)	20 (7%)	3 (1%)	12	47
2	K	291/299 (97%)	264 (91%)	25 (9%)	2 (1%)	18	55
3	C	215/223 (96%)	190 (88%)	24 (11%)	1 (0%)	24	62
3	F	212/223 (95%)	182 (86%)	26 (12%)	4 (2%)	6	32
3	I	221/223 (99%)	198 (90%)	19 (9%)	4 (2%)	6	33
3	L	205/223 (92%)	184 (90%)	19 (9%)	2 (1%)	12	47
All	All	2741/2816 (97%)	2441 (89%)	268 (10%)	32 (1%)	10	42

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ALA
2	B	496	HIS
1	D	157	ALA
3	F	50	ASP
3	F	71	SER

### 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	160/160 (100%)	151 (94%)	9 (6%)	19	42
1	D	160/160 (100%)	155 (97%)	5 (3%)	35	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	160/160 (100%)	151 (94%)	9 (6%)	19	42
1	J	160/160 (100%)	159 (99%)	1 (1%)	78	80
2	B	260/260 (100%)	235 (90%)	25 (10%)	8	26
2	E	256/260 (98%)	242 (94%)	14 (6%)	19	43
2	H	252/260 (97%)	240 (95%)	12 (5%)	23	45
2	K	255/260 (98%)	238 (93%)	17 (7%)	15	37
3	C	192/198 (97%)	174 (91%)	18 (9%)	8	27
3	F	190/198 (96%)	171 (90%)	19 (10%)	7	24
3	I	198/198 (100%)	186 (94%)	12 (6%)	17	39
3	L	187/198 (94%)	170 (91%)	17 (9%)	9	28
All	All	2430/2472 (98%)	2272 (94%)	158 (6%)	15	38

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	120	LEU
3	L	85	ARG
3	I	202	LEU
2	K	548	LYS
3	L	199	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	522	ASN
2	K	769	HIS
3	L	157	ASN
2	E	506	GLN
1	D	156	GLN

### 5.3.3 RNA

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	182/182 (100%)	0.08	4 (2%) 62 48	124, 191, 258, 292	0
1	D	182/182 (100%)	-0.15	2 (1%) 78 62	126, 182, 255, 298	0
1	G	182/182 (100%)	0.31	8 (4%) 39 34	185, 263, 320, 362	0
1	J	182/182 (100%)	0.44	19 (10%) 11 15	219, 314, 372, 462	0
2	B	299/299 (100%)	0.05	3 (1%) 79 64	140, 230, 338, 449	0
2	E	294/299 (98%)	-0.01	5 (1%) 69 54	121, 229, 313, 387	0
2	H	290/299 (96%)	0.18	10 (3%) 48 38	165, 275, 377, 435	0
2	K	293/299 (97%)	-0.05	3 (1%) 79 64	235, 343, 441, 539	0
3	C	217/223 (97%)	0.07	9 (4%) 41 35	132, 216, 314, 371	0
3	F	214/223 (95%)	0.08	4 (1%) 66 51	148, 226, 334, 438	0
3	I	223/223 (100%)	0.03	5 (2%) 62 48	210, 307, 384, 453	0
3	L	209/223 (93%)	0.07	3 (1%) 73 58	209, 315, 401, 451	0
All	All	2767/2816 (98%)	0.08	75 (2%) 56 43	121, 261, 385, 539	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	4	LEU	4.9
1	J	22	PHE	4.8
3	C	199	LEU	4.8
1	J	150	PHE	4.7
1	J	6	LEU	4.6

### 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.