



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2026 – 12:22 PM EDT

PDB ID : 9ZCS / pdb_00009zcs
Title : Crystal structure of HOPS subunits Vps33 and Vps16 in complex with the Nyv1 and Vam3 SNARE motifs
Authors : Stanton, A.E.; Jeffrey, P.D.; Hughson, F.M.
Deposited on : 2025-11-24
Resolution : 3.19 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

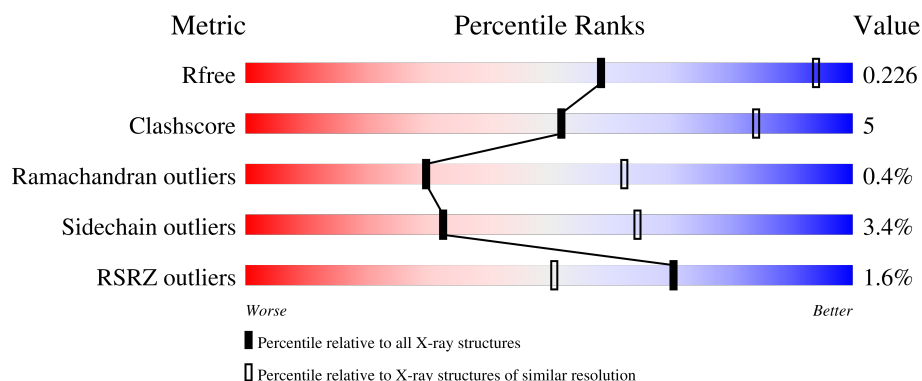
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	696	
2	B	274	
3	C	67	
4	D	51	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7455 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 Small conjugating protein ligase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	609	4798	3038	846	903	11	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	initiating methionine	UNP G0SCM5
A	-27	LYS	-	expression tag	UNP G0SCM5
A	-26	HIS	-	expression tag	UNP G0SCM5
A	-25	HIS	-	expression tag	UNP G0SCM5
A	-24	HIS	-	expression tag	UNP G0SCM5
A	-23	HIS	-	expression tag	UNP G0SCM5
A	-22	HIS	-	expression tag	UNP G0SCM5
A	-21	HIS	-	expression tag	UNP G0SCM5
A	-20	HIS	-	expression tag	UNP G0SCM5
A	-19	GLY	-	expression tag	UNP G0SCM5
A	-18	ALA	-	expression tag	UNP G0SCM5
A	-17	ALA	-	expression tag	UNP G0SCM5
A	-16	GLY	-	expression tag	UNP G0SCM5
A	-15	THR	-	expression tag	UNP G0SCM5
A	-14	SER	-	expression tag	UNP G0SCM5
A	-13	LEU	-	expression tag	UNP G0SCM5
A	-12	TYR	-	expression tag	UNP G0SCM5
A	-11	LYS	-	expression tag	UNP G0SCM5
A	-10	LYS	-	expression tag	UNP G0SCM5
A	-9	ALA	-	expression tag	UNP G0SCM5
A	-8	GLY	-	expression tag	UNP G0SCM5
A	-7	GLU	-	expression tag	UNP G0SCM5
A	-6	ASN	-	expression tag	UNP G0SCM5
A	-5	LEU	-	expression tag	UNP G0SCM5
A	-4	TYR	-	expression tag	UNP G0SCM5
A	-3	PHE	-	expression tag	UNP G0SCM5
A	-2	GLN	-	expression tag	UNP G0SCM5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP G0SCM5

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	265	Total	C	N	O	S	0	0	0
			2131	1344	381	397	9			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	518	MET	-	initiating methionine	UNP G0S6M7
B	519	GLY	-	expression tag	UNP G0S6M7
B	520	SER	-	expression tag	UNP G0S6M7
B	672	ARG	-	insertion	UNP G0S6M7
B	673	MET	-	insertion	UNP G0S6M7
B	674	GLN	-	insertion	UNP G0S6M7
B	675	GLU	-	insertion	UNP G0S6M7
B	676	THR	-	insertion	UNP G0S6M7
B	677	PHE	-	insertion	UNP G0S6M7
B	678	GLU	-	insertion	UNP G0S6M7
B	679	ARG	-	insertion	UNP G0S6M7
B	680	ASP	-	insertion	UNP G0S6M7
B	681	LEU	-	insertion	UNP G0S6M7
B	682	THR	-	insertion	UNP G0S6M7
B	683	ASP	-	insertion	UNP G0S6M7
B	684	SER	-	insertion	UNP G0S6M7
B	685	PHE	-	insertion	UNP G0S6M7
B	686	VAL	-	insertion	UNP G0S6M7
B	687	GLY	-	insertion	UNP G0S6M7
B	689	SER	-	insertion	UNP G0S6M7
B	690	VAL	-	insertion	UNP G0S6M7

- Molecule 3 is a protein called Nyv1 SNARE motif.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	37	Total	C	N	O	S	0	0	0
			285	173	57	54	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	146	GLY	-	expression tag	UNP G0S5G3
C	147	SER	-	expression tag	UNP G0S5G3

- Molecule 4 is a protein called SNAP receptor-like protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	33	Total	C	N	O	0	0	0
			241	151	39	51			

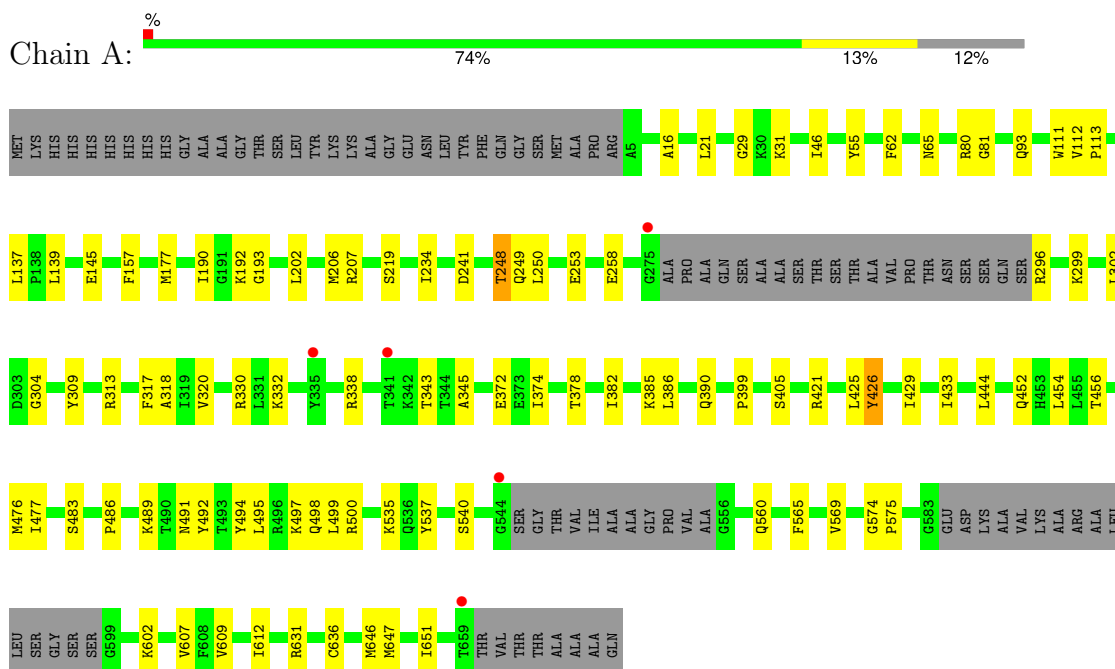
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	179	GLY	-	expression tag	UNP G0S236
D	180	SER	-	expression tag	UNP G0S236

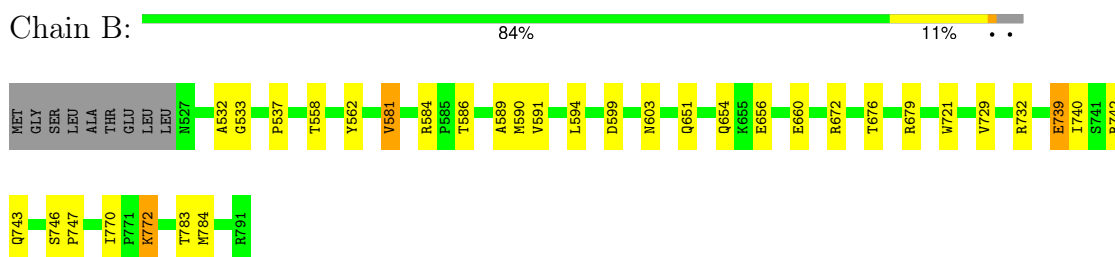
3 Residue-property plots

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.

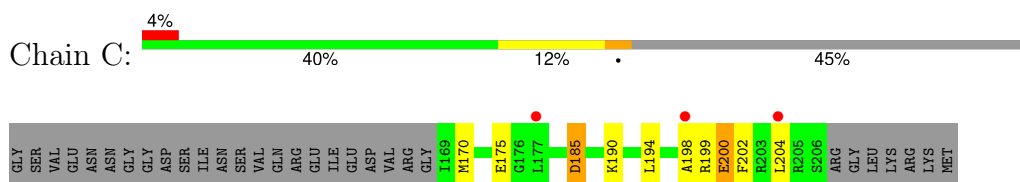
- Molecule 1: Small conjugating protein ligase-like protein



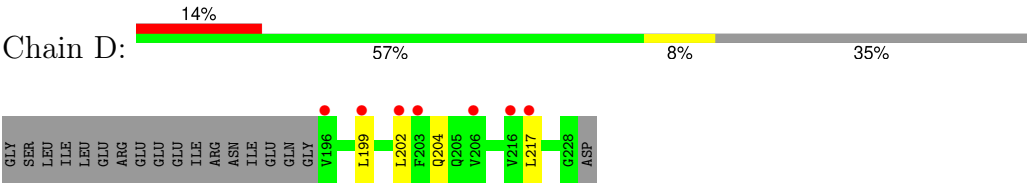
- Molecule 2: Vacuolar protein sorting-associated protein 16



- Molecule 3: Nyv1 SNARE motif



● Molecule 4: SNAP receptor-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	100.84Å 100.84Å 312.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 3.19 29.60 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.60-3.19) 99.7 (29.60-3.19)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.177 , 0.225 0.181 , 0.226	Depositor DCC
R_{free} test set	1416 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	76.0	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7455	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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	0.38	0/4873	0.58	0/6572
2	B	0.37	0/2170	0.58	0/2926
3	C	0.31	0/285	0.46	0/378
4	D	0.32	0/241	0.53	0/329
All	All	0.37	0/7569	0.58	0/10205

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 [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	4798	0	4858	55	0
2	B	2131	0	2139	19	0
3	C	285	0	286	8	0
4	D	241	0	233	1	0
All	All	7455	0	7516	77	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.

All (77) 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:607:VAL:HG22	1:A:636:CYS:HB2	1.67	0.76
1:A:177:MET:HE3	1:A:206:MET:HB2	1.67	0.73
1:A:299:LYS:HB3	4:D:217:LEU:HD21	1.70	0.72
1:A:456:THR:HG23	1:A:651:ILE:HA	1.74	0.69
2:B:739:GLU:OE2	2:B:742:ARG:NH2	2.28	0.65
2:B:770:ILE:HG12	2:B:784:MET:HE2	1.78	0.64
1:A:112:VAL:HG22	1:A:137:LEU:HB3	1.80	0.63
3:C:185:ASP:OD1	3:C:185:ASP:N	2.32	0.62
1:A:537:TYR:O	1:A:540:SER:HB3	2.00	0.62
1:A:21:LEU:HD13	1:A:55:TYR:CZ	2.37	0.60
1:A:29:GLY:O	1:A:31:LYS:NZ	2.34	0.59
1:A:145:GLU:OE2	1:A:304:GLY:N	2.33	0.59
2:B:558:THR:HB	2:B:590:MET:HE1	1.83	0.58
1:A:385:LYS:HE3	1:A:405:SER:HB3	1.87	0.57
1:A:253:GLU:HB2	1:A:313:ARG:HB2	1.89	0.55
1:A:426:TYR:CD1	1:A:433:ILE:HG12	2.42	0.54
2:B:651:GLN:HG2	2:B:654:GLN:NE2	2.24	0.53
1:A:62:PHE:HB2	1:A:65:ASN:ND2	2.22	0.53
1:A:374:ILE:O	1:A:378:THR:HG23	2.09	0.53
1:A:477:ILE:HG13	1:A:489:LYS:O	2.10	0.52
2:B:599:ASP:HB2	2:B:603:ASN:HB2	1.91	0.52
1:A:421:ARG:HG3	1:A:647:MET:HG3	1.91	0.52
1:A:302:LEU:HD22	1:A:309:TYR:CZ	2.46	0.51
2:B:676:THR:HG22	2:B:679:ARG:NH1	2.26	0.50
1:A:338:ARG:HE	3:C:175:GLU:HG2	1.76	0.50
1:A:372:GLU:OE1	3:C:190:LYS:NZ	2.43	0.49
2:B:581:VAL:HG21	2:B:591:VAL:HG21	1.95	0.49
1:A:476:MET:SD	1:A:491:ASN:HA	2.53	0.49
1:A:202:LEU:O	1:A:206:MET:HG3	2.13	0.48
2:B:586:THR:O	2:B:590:MET:HG2	2.13	0.48
1:A:193:GLY:C	1:A:575:PRO:HD2	2.37	0.48
2:B:672:ARG:O	2:B:676:THR:HG23	2.13	0.48
1:A:192:LYS:NZ	1:A:574:GLY:O	2.43	0.48
1:A:177:MET:HG2	1:A:206:MET:HE2	1.96	0.48
1:A:249:GLN:O	1:A:250:LEU:HD23	2.15	0.47
1:A:399:PRO:HB2	1:A:426:TYR:CZ	2.51	0.46
1:A:426:TYR:CD1	1:A:426:TYR:C	2.93	0.46
1:A:386:LEU:O	1:A:390:GLN:HG3	2.16	0.46
3:C:199:ARG:C	3:C:202:PHE:H	2.23	0.46
1:A:499:LEU:HA	1:A:499:LEU:HD23	1.70	0.46
2:B:729:VAL:O	2:B:732:ARG:NH2	2.48	0.46
1:A:80:ARG:HA	1:A:112:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ASP:HA	1:A:492:TYR:OH	2.16	0.46
1:A:157:PHE:CZ	1:A:646:MET:HG2	2.52	0.45
2:B:676:THR:HG22	2:B:679:ARG:HH12	1.80	0.45
2:B:533:GLY:O	2:B:537:PRO:HD3	2.17	0.45
2:B:599:ASP:CB	2:B:603:ASN:HB2	2.46	0.45
2:B:562:TYR:CE1	2:B:590:MET:HE3	2.51	0.45
1:A:81:GLY:HA2	1:A:111:TRP:CE3	2.53	0.44
2:B:721:TRP:CD2	2:B:747:PRO:HD2	2.53	0.44
1:A:137:LEU:HG	1:A:139:LEU:HG	2.00	0.44
1:A:248:THR:HA	1:A:258:GLU:OE2	2.17	0.43
1:A:426:TYR:CE1	1:A:433:ILE:HG12	2.53	0.43
1:A:317:PHE:HD1	1:A:320:VAL:HG21	1.84	0.43
1:A:192:LYS:HE2	1:A:569:VAL:HG12	2.01	0.42
2:B:740:ILE:O	2:B:743:GLN:HG3	2.18	0.42
1:A:343:THR:C	1:A:345:ALA:H	2.27	0.42
1:A:190:ILE:O	1:A:234:ILE:HA	2.20	0.42
1:A:338:ARG:NE	3:C:175:GLU:HG2	2.34	0.42
1:A:318:ALA:HB1	3:C:199:ARG:HG2	2.01	0.42
2:B:772:LYS:HB3	2:B:772:LYS:HE3	1.64	0.42
1:A:494:TYR:CZ	1:A:498:GLN:HG3	2.55	0.42
1:A:330:ARG:HD2	1:A:330:ARG:C	2.45	0.41
1:A:444:LEU:HA	1:A:444:LEU:HD23	1.76	0.41
3:C:190:LYS:O	3:C:194:LEU:HG	2.20	0.41
1:A:112:VAL:HA	1:A:113:PRO:HA	1.74	0.41
1:A:426:TYR:C	1:A:426:TYR:HD1	2.28	0.41
1:A:454:LEU:HD11	2:B:660:GLU:HG3	2.03	0.41
2:B:586:THR:O	2:B:589:ALA:HB3	2.21	0.41
1:A:425:LEU:O	1:A:429:ILE:HG22	2.20	0.41
1:A:495:LEU:HD22	1:A:499:LEU:HD12	2.02	0.40
3:C:198:ALA:C	3:C:200:GLU:H	2.29	0.40
1:A:565:PHE:O	1:A:569:VAL:HG23	2.22	0.40
1:A:16:ALA:HB1	1:A:46:ILE:HD12	2.04	0.40
1:A:497:LYS:HE3	1:A:498:GLN:NE2	2.36	0.40
1:A:499:LEU:O	1:A:500:ARG:C	2.64	0.40
1:A:535:LYS:HE3	1:A:560:GLN:HB3	2.02	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	601/696 (86%)	575 (96%)	23 (4%)	3 (0%)	24	59
2	B	263/274 (96%)	253 (96%)	9 (3%)	1 (0%)	30	62
3	C	35/67 (52%)	29 (83%)	6 (17%)	0	100	100
4	D	31/51 (61%)	27 (87%)	4 (13%)	0	100	100
All	All	930/1088 (86%)	884 (95%)	42 (4%)	4 (0%)	30	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	PRO
2	B	532	ALA
1	A	219	SER
1	A	483	SER

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	519/585 (89%)	507 (98%)	12 (2%)	44	70
2	B	228/235 (97%)	220 (96%)	8 (4%)	32	64
3	C	29/57 (51%)	25 (86%)	4 (14%)	3	18
4	D	26/44 (59%)	23 (88%)	3 (12%)	5	24
All	All	802/921 (87%)	775 (97%)	27 (3%)	32	64

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	207	ARG
1	A	248	THR
1	A	296	ARG
1	A	332	LYS
1	A	382	ILE
1	A	426	TYR
1	A	452	GLN
1	A	602	LYS
1	A	609	VAL
1	A	612	ILE
1	A	631	ARG
2	B	581	VAL
2	B	584	ARG
2	B	594	LEU
2	B	656	GLU
2	B	739	GLU
2	B	746	SER
2	B	772	LYS
2	B	783	THR
3	C	170	MET
3	C	185	ASP
3	C	200	GLU
3	C	204	LEU
4	D	199	LEU
4	D	202	LEU
4	D	204	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
1	A	418	GLN
1	A	581	GLN
2	B	654	GLN
4	D	205	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, 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	609/696 (87%)	-0.65	5 (0%) 82 67	36, 70, 170, 272	0
2	B	265/274 (96%)	-0.70	0 100 100	41, 75, 135, 200	0
3	C	37/67 (55%)	0.54	3 (8%) 18 11	143, 188, 249, 276	0
4	D	33/51 (64%)	0.96	7 (21%) 2 2	123, 209, 310, 323	0
All	All	944/1088 (86%)	-0.56	15 (1%) 70 51	36, 75, 208, 323	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	THR	3.3
4	D	217	LEU	3.0
4	D	206	VAL	2.9
4	D	216	VAL	2.9
1	A	275	GLY	2.7
3	C	204	LEU	2.6
3	C	177	LEU	2.5
1	A	335	TYR	2.5
4	D	196	VAL	2.5
3	C	198	ALA	2.3
4	D	202	LEU	2.2
4	D	203	PHE	2.1
1	A	544	GLY	2.1
4	D	199	LEU	2.0
1	A	659	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.