



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2018 – 06:58 PM EST

PDB ID : 5BUZ  
Title : Crystal Structure of a Complex Between the SNARE Vam3 and the HOPS Vps33-Vps16 subcomplex from *Chaetomium thermophilum*  
Authors : Baker, R.W.; Jeffrey, P.D.; Hughson, F.M.  
Deposited on : 2015-06-04  
Resolution : 3.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

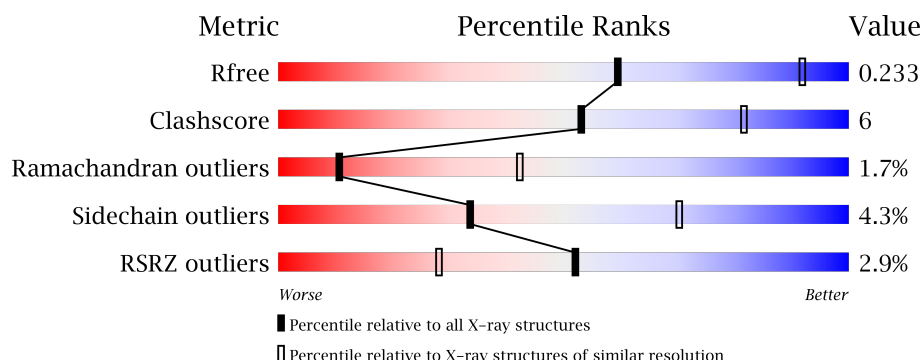
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	669	<div> <div>0.1%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>10%</div> </div> </div>
1	D	669	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>10%</div> </div> </div>
2	B	333	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>3%</div> </div> </div>
2	E	333	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>4%</div> </div> </div>
3	C	67	<div> <div>7%</div> <div> <div></div> <div>42%</div> <div>15%</div> <div>43%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	67	<p>3% 40% 18% 40%</p>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15276 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 SM (Sec1/Munc18-like) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	605	Total	C	N	O	S	0	0	0
			4770	3019	841	899	11			
1	D	605	Total	C	N	O	S	0	0	0
			4770	3019	841	899	11			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Putative vacuolar protein sorting-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	324	Total	C	N	O	S	0	0	0
			2583	1622	465	487	9			
2	E	324	Total	C	N	O	S	0	0	0
			2583	1622	465	487	9			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	502	MET	-	initiating methionine	UNP G0S6M7
B	503	GLY	-	expression tag	UNP G0S6M7
B	504	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	688	LEU	-	insertion	UNP G0S6M7
B	689	SER	-	insertion	UNP G0S6M7
B	690	VAL	LEU	engineered mutation	UNP G0S6M7
E	502	MET	-	initiating methionine	UNP G0S6M7
E	503	GLY	-	expression tag	UNP G0S6M7
E	504	SER	-	expression tag	UNP G0S6M7
E	672	ARG	-	insertion	UNP G0S6M7
E	673	MET	-	insertion	UNP G0S6M7
E	674	GLN	-	insertion	UNP G0S6M7
E	675	GLU	-	insertion	UNP G0S6M7
E	676	THR	-	insertion	UNP G0S6M7
E	677	PHE	-	insertion	UNP G0S6M7
E	678	GLU	-	insertion	UNP G0S6M7
E	679	ARG	-	insertion	UNP G0S6M7
E	680	ASP	-	insertion	UNP G0S6M7
E	681	LEU	-	insertion	UNP G0S6M7
E	682	THR	-	insertion	UNP G0S6M7
E	683	ASP	-	insertion	UNP G0S6M7
E	684	SER	-	insertion	UNP G0S6M7
E	685	PHE	-	insertion	UNP G0S6M7
E	686	VAL	-	insertion	UNP G0S6M7
E	687	GLY	-	insertion	UNP G0S6M7
E	688	LEU	-	insertion	UNP G0S6M7
E	689	SER	-	insertion	UNP G0S6M7
E	690	VAL	LEU	engineered mutation	UNP G0S6M7


- Molecule 3 is a protein called SNAP receptor-like protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	38	Total	C	N	O	0	0	0
			275	171	46	58			
3	F	40	Total	C	N	O	0	0	0
			295	182	51	62			

There are 4 discrepancies between the modelled and reference sequences:

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

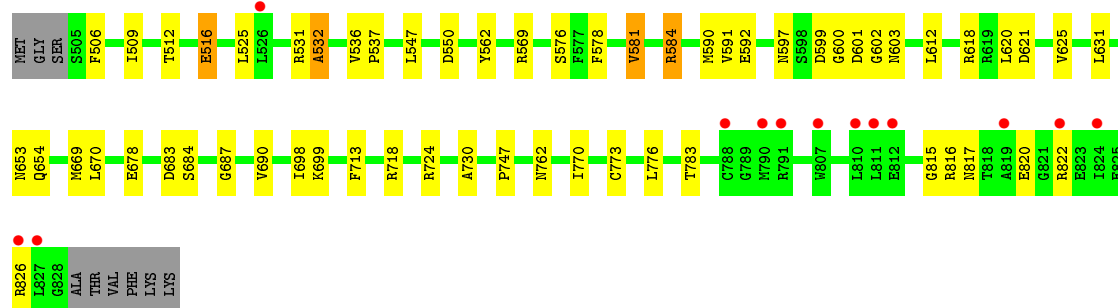
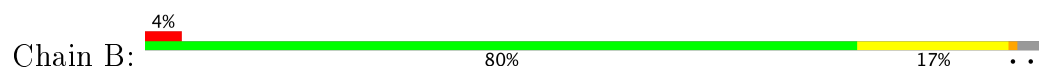
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ( $\text{RSRZ} > 2$ ). 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.

- Chain A: 
- | Residue | Percentage |
|---------|------------|
| T603    | 73%        |
| V604    | 73%        |
| F605    | 73%        |
| V606    | 73%        |
| V607    | 73%        |
| T615    | 73%        |
| L620    | 73%        |
| I623    | 73%        |
| C636    | 73%        |
| M647    | 73%        |
| I651    | 73%        |
| E652    | 73%        |
| T653    | 73%        |
| A654    | 73%        |
| T655    | 73%        |
| F656    | 73%        |
| E657    | 73%        |
| K658    | 73%        |
| THR     | 73%        |
| THR     | 73%        |
| VAL     | 73%        |
| ILE     | 73%        |
| ALA     | 73%        |
| THR     | 73%        |
| THR     | 73%        |
| ALA     | 73%        |
| ALA     | 73%        |
| ALA     | 73%        |
| ALA     | 73%        |
| GLN     | 73%        |
| A126    | 16%        |
| D131    | 16%        |
| L137    | 16%        |
| Y161    | 16%        |
| L162    | 16%        |
| G191    | 16%        |
| S219    | 16%        |
| D220    | 16%        |
| R221    | 16%        |
| A222    | 16%        |
| E231    | 16%        |
| E239    | 16%        |
| V269    | 16%        |
| V272    | 16%        |
| ILE     | 16%        |
| VAL     | 16%        |
| GLY     | 16%        |
| ALA     | 16%        |
| PRO     | 16%        |
| ALA     | 16%        |
| GLN     | 16%        |
| SER     | 16%        |
| ALA     | 16%        |
| ALA     | 16%        |
| SER     | 16%        |
| THR     | 16%        |
| SER     | 16%        |
| THR     | 16%        |
| VAL     | 16%        |
| PRO     | 16%        |
| THR     | 16%        |
| ASN     | 16%        |
| SER     | 16%        |
| SER     | 16%        |
| SER     | 16%        |
| GLN     | 16%        |
| SER     | 16%        |
| R296    | 16%        |
| K297    | 16%        |
| F317    | 16%        |
| V320    | 16%        |
| L324    | 16%        |
| R325    | 16%        |
| R329    | 16%        |
| L117    | 16%        |
| F118    | 16%        |
| R330    | 16%        |
| L331    | 16%        |
| V332    | 16%        |
| S333    | 10%        |
| D334    | 10%        |
| V335    | 10%        |
| E336    | 10%        |
| S337    | 10%        |
| R338    | 10%        |
| R339    | 10%        |
| T341    | 10%        |
| K342    | 10%        |
| T343    | 10%        |
| T344    | 10%        |
| A345    | 10%        |
| E346    | 10%        |
| L347    | 10%        |
| K348    | 10%        |
| E349    | 10%        |
| F350    | 10%        |
| V351    | 10%        |
| F355    | 10%        |
| Q358    | 10%        |
| Q361    | 10%        |
| Q362    | 10%        |
| S368    | 10%        |
| K369    | 10%        |
| L370    | 10%        |
| A371    | 10%        |
| L375    | 10%        |
| L382    | 10%        |
| L386    | 10%        |
| L409    | 10%        |
| T414    | 10%        |
| Q418    | 10%        |
| GLY     | 10%        |
| ASP     | 10%        |
| L422    | 10%        |
| Y426    | 10%        |
| L438    | 10%        |
| ALA     | 10%        |
| R443    | 10%        |
| ALA     | 10%        |
| LEU     | 10%        |
| LEU     | 10%        |
| SER     | 10%        |
| GLY     | 10%        |
| SER     | 10%        |
| SER     | 10%        |
| G454    | 10%        |
| G459    | 10%        |
| Q458    | 10%        |

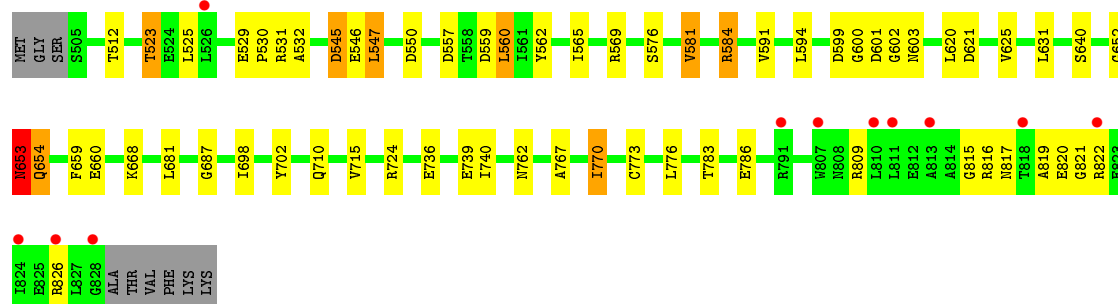
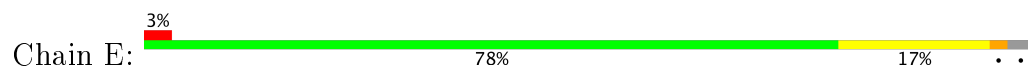
- Chain D:
- 
- 74% 3% 14% 10%
- | GLY  | SER  | MET  | ALA  | PRO  | ARG  | AS   | G6   | F7   | Q11  | K15  | D19  | V27  | K31  | D38  | G56  | N65  | K66  | N67  | T68  | G69 | T70 | S71 | Q72 | R73 | E82 | S83 | V84 | R85 | I90 | I94 | I97 | S101 | Q102 | H105 | V112 | P113 | T116 | L117 | F118 | E124 | F125 | A126 |     |      |      |      |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|-----|------|------|------|
| D131 | L137 | P138 | L139 | Y161 | L162 | L171 | H183 | I190 | G191 | E214 | S219 | D220 | R221 | A222 | E231 | I234 | E239 | V289 | V272 | I1E | VAL | GLY | ALA | PRO | ALA | GLN | SER | ALA | ALA | SER | THR | SER  | SER  | THR  | ALA  | VAL  | PRO  | THR  | ASN  | SER  | SER  | GLN  | GLW | R296 | K297 | I324 |



- Molecule 2: Putative vacuolar protein sorting-associated protein



- Molecule 2: Putative vacuolar protein sorting-associated protein



- Molecule 3: SNAP receptor-like protein



- Molecule 3: SNAP receptor-like protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.04Å 95.95Å 164.06Å 90.00° 99.12° 90.00°	Depositor
Resolution (Å)	47.98 – 3.10 47.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.98-3.10) 100.0 (47.98-3.10)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.194 , 0.233 0.194 , 0.233	Depositor DCC
$R_{free}$ test set	2640 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	89.9	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 59.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15276	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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

### 5.1 Standard geometry

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	0.22	0/4845	0.43	0/6535
1	D	0.23	0/4845	0.44	0/6535
2	B	0.23	0/2626	0.44	0/3543
2	E	0.23	0/2626	0.45	0/3543
3	C	0.22	0/275	0.47	0/375
3	F	0.22	0/295	0.48	0/401
All	All	0.23	0/15512	0.44	0/20932

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	4770	0	4819	61	0
1	D	4770	0	4819	62	0
2	B	2583	0	2581	29	0
2	E	2583	0	2581	44	0
3	C	275	0	254	7	0
3	F	295	0	273	7	0
All	All	15276	0	15327	191	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 6.

All (191) 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:500:ARG:O	1:A:527:ARG:NH1	2.20	0.74
2:B:599:ASP:H	2:B:600:GLY:HA2	1.53	0.74
1:D:500:ARG:O	1:D:527:ARG:NH1	2.24	0.70
1:A:484:GLY:O	1:A:488:GLN:NE2	2.26	0.67
1:A:65:ASN:HB3	1:A:67:ASN:OD1	1.96	0.66
1:A:70:THR:HB	1:A:102:GLN:HE22	1.61	0.66
1:A:654:ALA:HB3	2:B:631:LEU:HD13	1.78	0.66
1:A:351:VAL:HG12	3:C:206:VAL:HG21	1.78	0.66
1:D:272:VAL:HG13	1:D:369:ASN:HB2	1.80	0.64
1:A:438:LEU:HD22	1:A:468:SER:HB2	1.81	0.63
2:E:652:GLY:N	2:E:653:ASN:O	2.31	0.63
1:A:131:ASP:N	1:A:131:ASP:OD1	2.31	0.62
2:E:599:ASP:H	2:E:600:GLY:HA2	1.66	0.60
2:B:550:ASP:OD2	2:B:584:ARG:NH1	2.34	0.60
1:A:345:ALA:O	1:A:349:GLU:N	2.33	0.59
2:E:530:PRO:HB2	2:E:531:ARG:HE	1.67	0.59
1:A:443:ARG:NH1	2:B:713:PHE:O	2.35	0.59
1:D:355:PRO:HD3	3:F:206:VAL:HG13	1.84	0.59
1:D:324:LEU:HD21	1:D:368:SER:HA	1.86	0.58
1:D:131:ASP:N	1:D:131:ASP:OD1	2.36	0.58
1:D:654:ALA:HB3	2:E:631:LEU:HD13	1.86	0.58
3:F:219:THR:O	3:F:223:ASN:ND2	2.38	0.57
1:D:351:VAL:HG12	3:F:206:VAL:HG21	1.87	0.56
1:A:220:ASP:O	1:A:222:ALA:N	2.36	0.56
1:A:348:LYS:HG3	3:C:202:LEU:HD11	1.87	0.56
1:D:438:LEU:HD22	1:D:468:SER:HB2	1.86	0.56
1:D:341:THR:HG22	1:D:343:THR:HG22	1.88	0.55
1:D:386:LEU:HD13	1:D:418:GLN:HG2	1.89	0.55
1:D:325:ASN:O	1:D:329:ARG:N	2.35	0.55
1:D:348:LYS:O	1:D:352:LYS:HG2	2.08	0.54
1:A:358:GLN:OE1	3:C:213:GLN:NE2	2.39	0.54
1:A:97:ILE:O	1:A:101:SER:HB3	2.08	0.54
2:B:512:THR:O	2:B:516:GLU:HB2	2.09	0.53
1:A:116:THR:OG1	1:A:119:SER:OG	2.21	0.53
2:B:773:CYS:HB3	2:B:776:LEU:HD13	1.91	0.53
2:E:581:VAL:HG21	2:E:591:VAL:HG21	1.91	0.53
1:D:654:ALA:HB1	2:E:631:LEU:HB3	1.90	0.53
1:A:386:LEU:HD23	1:A:422:LEU:HD11	1.91	0.52
1:A:347:LEU:O	1:A:351:VAL:HG23	2.09	0.52
1:D:137:LEU:HD22	1:D:139:LEU:HG	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:VAL:HA	1:D:118:PHE:CE2	2.45	0.52
1:A:409:LEU:HD23	1:A:414:THR:HG21	1.92	0.52
3:F:201:VAL:O	3:F:205:GLN:HG2	2.10	0.52
2:E:550:ASP:OD2	2:E:584:ARG:NH1	2.43	0.51
1:D:220:ASP:O	1:D:222:ALA:N	2.40	0.51
2:E:601:ASP:O	2:E:603:ASN:N	2.43	0.51
2:B:698:ILE:HD13	2:B:724:ARG:HG3	1.92	0.51
2:E:822:ARG:O	2:E:826:ARG:N	2.35	0.51
1:A:53:ARG:NH2	3:C:223:ASN:OD1	2.44	0.51
1:D:85:ARG:HG3	2:E:600:GLY:HA3	1.92	0.50
1:A:526:ILE:HD12	1:A:620:LEU:HD13	1.93	0.50
2:B:599:ASP:HB2	2:B:603:ASN:HB2	1.93	0.50
1:D:442:ARG:HB3	2:E:659:PHE:CZ	2.47	0.50
1:D:409:LEU:HD23	1:D:414:THR:HG21	1.92	0.50
1:A:355:PRO:HD3	3:C:206:VAL:HG13	1.94	0.50
1:D:65:ASN:HB3	1:D:67:ASN:OD1	2.12	0.49
2:E:562:TYR:HD1	2:E:594:LEU:HD11	1.76	0.49
1:A:15:LYS:NZ	1:A:19:ASP:OD2	2.44	0.49
1:D:31:LYS:HD2	1:D:56:GLY:O	2.12	0.49
1:A:161:TYR:CE1	1:A:239:GLU:HB3	2.48	0.49
1:A:191:GLY:HA3	1:A:577:PHE:CZ	2.48	0.49
1:A:62:PHE:HB2	1:A:65:ASN:ND2	2.27	0.49
3:C:208:GLN:NE2	3:C:212:GLU:OE2	2.46	0.49
1:D:161:TYR:CE1	1:D:239:GLU:HB3	2.48	0.48
1:D:338:ARG:HD3	1:D:338:ARG:HA	1.57	0.48
1:D:409:LEU:O	1:D:414:THR:HG23	2.14	0.48
1:A:559:ALA:HB1	1:A:563:LYS:HD2	1.95	0.48
1:A:607:VAL:HG22	1:A:636:CYS:HB2	1.95	0.48
1:A:324:LEU:HD21	1:A:368:SER:HA	1.96	0.48
1:A:606:VAL:HG11	1:A:620:LEU:HD21	1.95	0.48
2:E:620:LEU:HD21	2:E:660:GLU:HG2	1.94	0.48
2:B:506:PHE:HA	2:B:509:ILE:HD12	1.94	0.47
1:D:191:GLY:HA3	1:D:577:PHE:CZ	2.49	0.47
1:A:386:LEU:HD13	1:A:418:GLN:HG2	1.95	0.47
1:A:495:LEU:HD22	1:A:499:LEU:HD12	1.97	0.47
2:E:640:SER:HB3	2:E:668:LYS:HE2	1.96	0.47
1:A:340:ASN:O	1:A:342:LYS:N	2.48	0.47
1:D:371:ALA:O	1:D:375:ILE:HG13	2.15	0.47
1:A:330:ARG:O	1:A:334:ASP:HB2	2.15	0.47
2:B:597:ASN:O	2:B:600:GLY:HA2	2.15	0.47
1:A:336:GLU:OE2	1:A:339:HIS:NE2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:621:ASP:O	2:E:625:VAL:HG23	2.15	0.47
1:A:231:GLU:HB3	1:A:604:VAL:HG22	1.96	0.47
1:D:90:ILE:O	1:D:94:ILE:HG13	2.15	0.47
1:D:15:LYS:NZ	1:D:19:ASP:OD2	2.48	0.47
2:E:815:GLY:O	2:E:817:ASN:N	2.48	0.47
3:F:196:VAL:O	3:F:200:ASN:HB2	2.15	0.47
1:D:386:LEU:HD23	1:D:422:LEU:HD11	1.97	0.46
1:D:340:ASN:O	1:D:342:LYS:N	2.48	0.46
1:A:272:VAL:O	1:A:369:ASN:ND2	2.45	0.46
2:B:599:ASP:N	2:B:600:GLY:HA2	2.21	0.46
1:A:494:TYR:CE2	1:A:498:GLN:HG3	2.51	0.46
1:D:27:VAL:HG13	1:D:31:LYS:HE2	1.96	0.46
1:D:655:THR:HG23	1:D:657:GLU:H	1.80	0.46
1:A:361:GLN:HE21	1:A:361:GLN:HB2	1.56	0.46
1:A:494:TYR:CZ	1:A:498:GLN:HG3	2.51	0.46
1:D:494:TYR:CZ	1:D:498:GLN:HG3	2.51	0.46
1:D:73:ARG:HG3	1:D:105:HIS:HA	1.98	0.46
1:A:269:VAL:O	1:A:297:LYS:HB2	2.16	0.45
2:B:683:ASP:OD1	2:B:684:SER:N	2.49	0.45
2:B:822:ARG:O	2:B:826:ARG:N	2.35	0.45
1:D:82:GLU:HG3	1:D:171:LEU:HD21	1.98	0.45
2:E:736:GLU:O	2:E:740:ILE:HG13	2.17	0.45
1:A:655:THR:HG23	1:A:657:GLU:H	1.82	0.45
2:E:773:CYS:HB3	2:E:776:LEU:HD13	1.97	0.45
1:A:409:LEU:O	1:A:414:THR:HG23	2.16	0.45
1:A:382:ILE:HD13	1:A:414:THR:HG22	1.99	0.45
1:D:336:GLU:OE2	1:D:339:HIS:NE2	2.48	0.45
2:E:736:GLU:HA	2:E:739:GLU:HB2	1.97	0.45
1:D:124:GLU:C	1:D:126:ALA:H	2.20	0.44
2:E:557:ASP:HB3	2:E:560:LEU:HB2	1.99	0.44
1:D:118:PHE:HD1	2:E:562:TYR:CE2	2.34	0.44
1:D:118:PHE:HD1	2:E:562:TYR:CZ	2.34	0.44
2:B:621:ASP:O	2:B:625:VAL:HG23	2.18	0.44
1:D:162:LEU:HB2	1:D:463:LEU:HD21	1.99	0.44
1:D:347:LEU:O	1:D:351:VAL:HG23	2.18	0.44
1:D:630:ARG:HG2	1:D:630:ARG:H	1.63	0.44
1:A:647:MET:O	1:A:651:ILE:HG13	2.17	0.44
2:B:601:ASP:O	2:B:603:ASN:N	2.51	0.44
3:C:196:VAL:O	3:C:200:ASN:HB2	2.17	0.44
2:E:620:LEU:HD23	2:E:620:LEU:HA	1.87	0.44
2:B:532:ALA:O	2:B:536:VAL:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:581:VAL:HG21	2:B:591:VAL:HG21	1.99	0.44
1:D:112:VAL:HA	1:D:113:PRO:HA	1.76	0.44
1:D:324:LEU:HD12	1:D:324:LEU:HA	1.87	0.43
1:D:484:GLY:O	1:D:488:GLN:NE2	2.51	0.43
1:D:657:GLU:HG2	2:E:687:GLY:HA3	2.00	0.43
2:E:786:GLU:OE2	2:E:809:ARG:NH1	2.45	0.43
1:A:112:VAL:HA	1:A:113:PRO:HA	1.74	0.43
2:E:815:GLY:C	2:E:817:ASN:H	2.20	0.43
1:D:116:THR:HB	2:E:559:ASP:CG	2.39	0.43
1:D:341:THR:O	1:D:346:GLU:HB3	2.18	0.43
2:E:565:ILE:HD13	2:E:591:VAL:HG23	2.01	0.43
1:A:317:PHE:HA	1:A:320:VAL:HG23	2.01	0.43
2:E:530:PRO:HB2	2:E:531:ARG:HA	1.99	0.43
2:E:599:ASP:HB2	2:E:603:ASN:HB2	1.99	0.43
2:E:786:GLU:CD	2:E:809:ARG:HH12	2.22	0.43
1:A:455:LEU:HD12	1:A:652:GLU:HG2	2.00	0.43
1:A:657:GLU:HG2	2:B:687:GLY:HA3	2.00	0.43
1:D:382:ILE:HD13	1:D:414:THR:HG22	2.00	0.43
1:D:600:ASP:OD1	1:D:600:ASP:N	2.48	0.43
2:E:545:ASP:O	2:E:547:LEU:N	2.42	0.43
1:D:601:LYS:HE3	1:D:632:ASN:OD1	2.19	0.43
2:E:698:ILE:HD13	2:E:724:ARG:HG3	2.01	0.43
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.87	0.42
2:B:620:LEU:HD23	2:B:620:LEU:HA	1.83	0.42
2:E:530:PRO:CB	2:E:531:ARG:HE	2.30	0.42
2:B:699:LYS:HE3	2:B:730:ALA:HB1	2.01	0.42
2:E:523:THR:C	2:E:525:LEU:H	2.22	0.42
2:E:653:ASN:HB3	2:E:654:GLN:H	1.35	0.42
1:A:371:ALA:O	1:A:375:ILE:HG13	2.19	0.42
1:D:620:LEU:HD12	1:D:620:LEU:HA	1.87	0.42
1:A:90:ILE:O	1:A:94:ILE:HG13	2.18	0.42
2:E:562:TYR:CD1	2:E:594:LEU:HD11	2.53	0.42
3:F:219:THR:OG1	3:F:220:ILE:N	2.53	0.42
1:A:654:ALA:HB1	2:B:631:LEU:HB3	2.01	0.42
2:B:562:TYR:HB2	2:B:590:MET:CE	2.49	0.42
1:D:538:LEU:HD12	1:D:538:LEU:HA	1.91	0.42
2:B:678:GLU:HG2	2:B:683:ASP:O	2.20	0.42
2:B:718:ARG:NH1	2:B:747:PRO:O	2.52	0.42
2:E:599:ASP:N	2:E:600:GLY:HA2	2.32	0.42
2:E:681:LEU:HD22	2:E:702:TYR:CE1	2.55	0.42
1:A:95:LYS:HE3	1:A:126:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASP:OD1	1:A:38:ASP:N	2.42	0.42
1:D:7:PHE:HA	1:D:183:HIS:CE1	2.54	0.42
2:E:660:GLU:OE1	2:E:660:GLU:N	2.45	0.42
2:B:536:VAL:HG22	2:B:537:PRO:HD3	2.01	0.41
2:B:578:PHE:CD1	2:B:612:LEU:HD13	2.55	0.41
2:B:815:GLY:O	2:B:817:ASN:N	2.52	0.41
1:D:522:ALA:HA	1:D:523:PRO:HD3	1.93	0.41
2:E:710:GLN:HG3	2:E:715:VAL:HB	2.02	0.41
2:B:592:GLU:OE2	2:B:618:ARG:NH2	2.54	0.41
1:D:269:VAL:O	1:D:297:LYS:HB2	2.19	0.41
3:F:193:GLU:O	3:F:196:VAL:HG12	2.20	0.41
1:A:73:ARG:HG3	1:A:105:HIS:HA	2.02	0.41
1:D:97:ILE:O	1:D:101:SER:HB3	2.20	0.41
1:D:190:ILE:O	1:D:234:ILE:HA	2.21	0.41
1:A:522:ALA:HA	1:A:523:PRO:HD3	1.93	0.41
1:A:103:THR:OG1	1:A:104:SER:N	2.54	0.41
1:D:456:THR:HG23	1:D:651:ILE:HA	2.03	0.41
2:E:767:ALA:O	2:E:770:ILE:HG13	2.21	0.41
1:A:454:LEU:HD12	1:A:454:LEU:HA	1.90	0.41
2:E:819:ALA:O	2:E:821:GLY:N	2.52	0.41
2:E:529:GLU:N	2:E:530:PRO:HD3	2.36	0.41
1:A:534:GLN:NE2	1:A:623:ILE:HG23	2.37	0.40
1:D:231:GLU:HB3	1:D:604:VAL:HG22	2.02	0.40
2:B:670:LEU:HD22	2:B:690:VAL:HG23	2.03	0.40
1:D:495:LEU:HD22	1:D:499:LEU:HD12	2.04	0.40
1:A:320:VAL:O	1:A:324:LEU:HB2	2.22	0.40
1:A:325:ASN:O	1:A:329:ARG:N	2.48	0.40
1:D:399:PRO:HB2	1:D:426:TYR:CZ	2.57	0.40

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	597/669 (89%)	551 (92%)	38 (6%)	8 (1%)	14	48
1	D	597/669 (89%)	545 (91%)	44 (7%)	8 (1%)	14	48
2	B	322/333 (97%)	286 (89%)	30 (9%)	6 (2%)	9	39
2	E	322/333 (97%)	288 (89%)	26 (8%)	8 (2%)	6	31
3	C	36/67 (54%)	30 (83%)	5 (14%)	1 (3%)	6	29
3	F	38/67 (57%)	34 (90%)	3 (8%)	1 (3%)	6	31
All	All	1912/2138 (89%)	1734 (91%)	146 (8%)	32 (2%)	11	42

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	340	ASN
2	B	532	ALA
2	B	653	ASN
2	B	654	GLN
3	C	215	GLU
1	D	340	ASN
2	E	532	ALA
2	E	545	ASP
2	E	602	GLY
2	E	653	ASN
1	A	341	THR
1	A	506	VAL
2	B	602	GLY
1	D	341	THR
2	E	654	GLN
3	F	215	GLU
1	A	71	SER
1	A	105	HIS
1	A	219	SER
1	A	344	THR
1	D	71	SER
1	D	105	HIS
1	D	219	SER
1	D	344	THR
2	E	820	GLU
1	A	221	ARG
2	B	820	GLU
2	E	546	GLU
2	E	816	ARG
1	D	221	ARG

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Mol	Chain	Res	Type
2	B	816	ARG
1	D	506	VAL

### 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	516/564 (92%)	494 (96%)	22 (4%)	33	70
1	D	516/564 (92%)	497 (96%)	19 (4%)	39	75
2	B	270/280 (96%)	258 (96%)	12 (4%)	33	69
2	E	270/280 (96%)	258 (96%)	12 (4%)	33	69
3	C	28/55 (51%)	27 (96%)	1 (4%)	40	75
3	F	30/55 (54%)	26 (87%)	4 (13%)	4	20
All	All	1630/1798 (91%)	1560 (96%)	70 (4%)	33	70

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	18	LYS
1	A	27	VAL
1	A	31	LYS
1	A	53	ARG
1	A	67	ASN
1	A	84	VAL
1	A	117	LEU
1	A	131	ASP
1	A	137	LEU
1	A	162	LEU
1	A	331	LEU
1	A	339	HIS
1	A	346	GLU
1	A	361	GLN
1	A	362	GLN

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Mol	Chain	Res	Type
1	A	426	TYR
1	A	504	ASP
1	A	533	LEU
1	A	603	THR
1	A	615	THR
1	A	620	LEU
2	B	516	GLU
2	B	525	LEU
2	B	531	ARG
2	B	547	LEU
2	B	569	ARG
2	B	576	SER
2	B	581	VAL
2	B	584	ARG
2	B	669	MET
2	B	762	ASN
2	B	770	ILE
2	B	783	THR
3	C	219	THR
1	D	11	GLN
1	D	27	VAL
1	D	31	LYS
1	D	38	ASP
1	D	84	VAL
1	D	102	GLN
1	D	131	ASP
1	D	137	LEU
1	D	331	LEU
1	D	339	HIS
1	D	346	GLU
1	D	362	GLN
1	D	426	TYR
1	D	504	ASP
1	D	533	LEU
1	D	603	THR
1	D	615	THR
1	D	620	LEU
1	D	630	ARG
2	E	512	THR
2	E	523	THR
2	E	547	LEU
2	E	560	LEU

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Mol	Chain	Res	Type
2	E	569	ARG
2	E	576	SER
2	E	581	VAL
2	E	584	ARG
2	E	653	ASN
2	E	762	ASN
2	E	770	ILE
2	E	783	THR
3	F	192	ILE
3	F	199	LEU
3	F	208	GLN
3	F	219	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	213	GLN

### 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 carbohydrates 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, 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	605/669 (90%)	-0.10	9 (1%) 74 54	52, 82, 174, 256	0
1	D	605/669 (90%)	-0.10	17 (2%) 53 29	50, 83, 187, 261	0
2	B	324/333 (97%)	0.12	13 (4%) 39 19	59, 116, 210, 260	0
2	E	324/333 (97%)	0.01	11 (3%) 46 23	59, 107, 201, 293	0
3	C	38/67 (56%)	0.49	5 (13%) 4 2	101, 147, 196, 229	0
3	F	40/67 (59%)	0.31	2 (5%) 30 13	104, 141, 182, 205	0
All	All	1936/2138 (90%)	-0.03	57 (2%) 52 28	50, 93, 196, 293	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	545	SER	8.5
1	D	556	GLY	7.6
2	B	824	ILE	6.2
1	D	557	GLY	6.1
1	A	337	SER	5.0
1	D	338	ARG	4.9
1	A	544	GLY	4.6
2	B	827	LEU	4.6
1	D	336	GLU	3.9
1	D	544	GLY	3.8
1	A	338	ARG	3.7
2	B	826	ARG	3.6
1	D	545	SER	3.4
2	B	810	LEU	3.4
2	B	788	CYS	3.3
2	B	790	MET	3.2
2	E	824	ILE	3.0
1	A	344	THR	3.0
2	B	526	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	102	GLN	2.9
1	D	543	LYS	2.9
2	B	791	ARG	2.7
1	A	336	GLU	2.7
1	D	329	ARG	2.7
2	E	818	THR	2.7
1	D	69	GLY	2.7
3	C	199	LEU	2.6
1	D	345	ALA	2.6
3	F	190	ARG	2.6
3	C	192	ILE	2.6
1	D	222	ALA	2.5
1	A	69	GLY	2.5
1	D	221	ARG	2.5
2	E	807	TRP	2.4
2	E	791	ARG	2.4
2	E	826	ARG	2.4
2	B	807	TRP	2.4
2	B	811	LEU	2.4
1	D	332	LYS	2.4
3	F	198	ASP	2.3
1	A	335	TYR	2.3
2	E	813	ALA	2.3
3	C	215	GLU	2.3
2	E	526	LEU	2.3
3	C	191	ASN	2.2
1	D	214	GLU	2.2
1	A	332	LYS	2.2
1	D	337	SER	2.2
2	E	828	GLY	2.2
2	E	810	LEU	2.1
2	B	819	ALA	2.1
2	B	822	ARG	2.1
2	B	812	GLU	2.1
3	C	196	VAL	2.1
1	D	341	THR	2.1
2	E	811	LEU	2.0
2	E	822	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.