



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:03 PM UTC

PDB ID : 5BUZ / pdb_00005buz
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

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

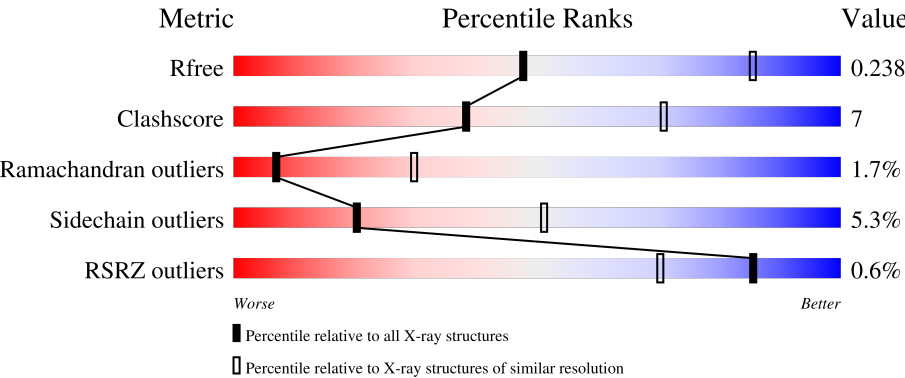
1 Overall quality at a glance i

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	669	71% 18% 10%
1	D	669	73% 15% 10%
2	B	333	79% 16% ...
2	E	333	76% 17% ...
3	C	67	42% 15% 43%

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Mol	Chain	Length	Quality of chain
3	F	67	40% 18% 40%

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.

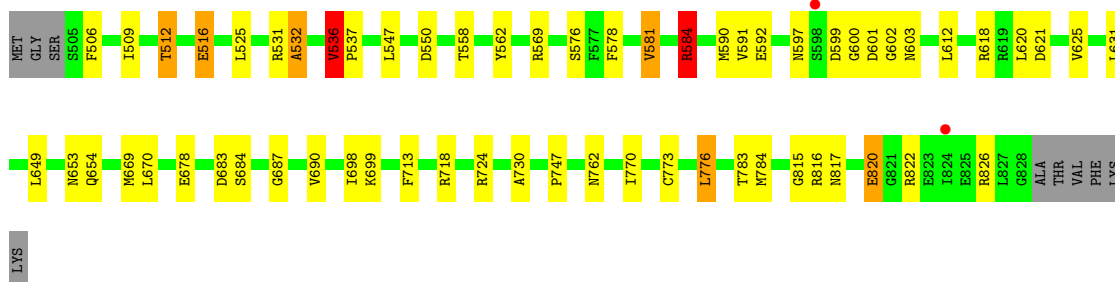
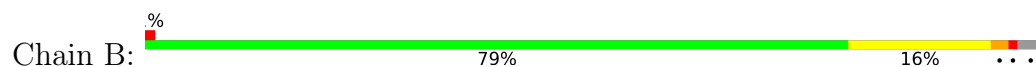
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	38	Total	C	N	O	0	0	0
			275	171	46	58			
3	F	40	Total	C	N	O	0	0	0
			295	182	51	62			

There are 4 discrepancies between the modelled and reference sequences:

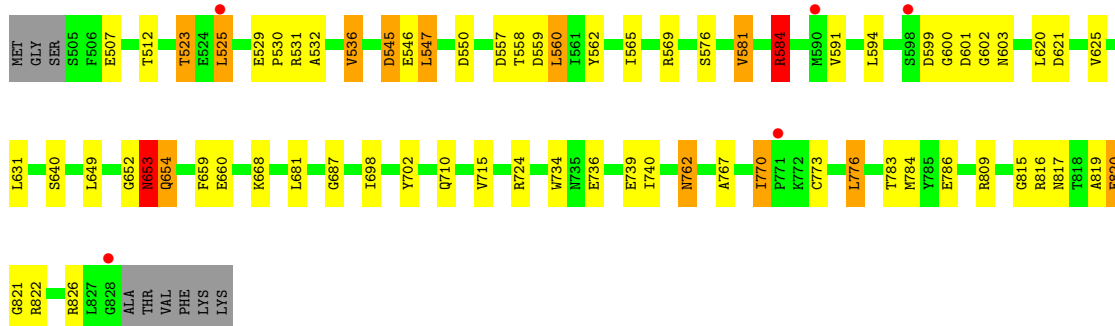
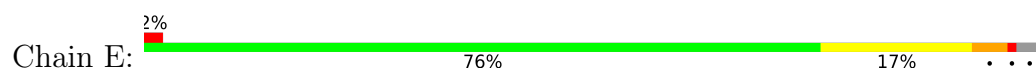
Chain	Residue	Modelled	Actual	Comment	Reference
C	179	GLY	-	expression tag	UNP G0S236
C	180	SER	-	expression tag	UNP G0S236
F	179	GLY	-	expression tag	UNP G0S236
F	180	SER	-	expression tag	UNP G0S236



- 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, α , β , γ	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) 99.9 (47.98-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.194 , 0.233 0.204 , 0.238	Depositor DCC
R_{free} test set	2639 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	89.9	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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	0.29	0/4845	0.77	4/6535 (0.1%)
1	D	0.29	0/4845	0.77	3/6535 (0.0%)
2	B	0.30	0/2626	0.79	4/3543 (0.1%)
2	E	0.31	0/2626	0.80	4/3543 (0.1%)
3	C	0.29	0/275	0.87	0/375
3	F	0.30	0/295	0.81	0/401
All	All	0.30	0/15512	0.78	15/20932 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	574	GLY	CA-C-N	6.87	126.63	119.76
1	D	574	GLY	C-N-CA	6.87	126.63	119.76
1	A	102	GLN	N-CA-C	-6.33	106.78	114.75
1	A	574	GLY	CA-C-N	6.05	125.81	119.76
1	A	574	GLY	C-N-CA	6.05	125.81	119.76
2	E	584	ARG	CA-C-N	6.02	125.50	119.24
2	E	584	ARG	C-N-CA	6.02	125.50	119.24
2	B	584	ARG	CA-C-N	5.75	125.22	119.24
2	B	584	ARG	C-N-CA	5.75	125.22	119.24
1	A	334	ASP	N-CA-C	-5.33	107.43	114.31
2	E	536	VAL	CA-C-N	-5.30	113.57	119.19
2	E	536	VAL	C-N-CA	-5.30	113.57	119.19
2	B	536	VAL	CA-C-N	-5.29	113.58	119.19
2	B	536	VAL	C-N-CA	-5.29	113.58	119.19
1	D	102	GLN	N-CA-C	-5.23	108.17	114.75

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	68	0
1	D	4770	0	4819	66	0
2	B	2583	0	2581	33	0
2	E	2583	0	2581	48	0
3	C	275	0	254	7	0
3	F	295	0	273	7	0
All	All	15276	0	15327	210	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 7.

All (210) 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
2:B:776:LEU:HD11	2:B:784:MET:HE1	1.78	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:776:LEU:HD11	2:E:784:MET:HE1	1.81	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
2:B:562:TYR:HB2	2:B:590:MET:HE1	1.83	0.60
1:D:177:MET:HE3	1:D:206:MET:HB2	1.84	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:654:ALA:HB3	2:E:631:LEU:HD13	1.86	0.58
1:D:131:ASP:N	1:D:131:ASP:OD1	2.36	0.58
1:A:177:MET:HE3	1:A:206:MET:HB2	1.86	0.57
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
1:D:654:ALA:HB1	2:E:631:LEU:HB3	1.90	0.53
2:E:581:VAL:HG21	2:E:591:VAL:HG21	1.91	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:84:VAL:HA	1:D:118:PHE:CE2	2.45	0.52
1:D:137:LEU:HD22	1:D:139:LEU:HG	1.90	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
1:D:124:GLU:C	1:D:126:ALA:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:62:PHE:HB2	1:A:65:ASN:ND2	2.27	0.49
1:A:191:GLY:HA3	1:A:577:PHE:CZ	2.48	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
2:E:815:GLY:C	2:E:817:ASN:H	2.20	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:D:116:THR:HB	2:E:559:ASP:CG	2.39	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
2:E:786:GLU:CD	2:E:809:ARG:HH12	2.22	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
1:A:336:GLU:OE2	1:A:339:HIS:NE2	2.45	0.47
2:B:597:ASN:O	2:B:600:GLY:HA2	2.15	0.47
2:E:523:THR:C	2:E:525:LEU:H	2.22	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:73:ARG:HG3	1:D:105:HIS:HA	1.98	0.46
1:D:494:TYR:CZ	1:D:498:GLN:HG3	2.51	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:A:177:MET:HG2	1:A:206:MET:HE2	1.99	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
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
1:A:115:ARG:HE	1:A:120:ASP:CG	2.25	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:177:MET:HG2	1:D:206:MET:HE2	1.98	0.44
1:D:347:LEU:O	1:D:351:VAL:HG23	2.18	0.44
1:A:174:ARG:HA	1:A:206:MET:HE1	1.98	0.44
1:D:630:ARG:H	1:D:630:ARG:HG2	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
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
1:A:343:THR:O	1:A:344:THR:C	2.61	0.43
1:A:124:GLU:C	1:A:126:ALA:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:815:GLY:C	2:B:817:ASN:H	2.27	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: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:B:820:GLU:C	2:B:822:ARG:H	2.27	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
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:38:ASP:OD1	1:A:38:ASP:N	2.42	0.42
1:A:95:LYS:HE3	1:A:126:ALA:HB1	2.02	0.42
1:D:7:PHE:HA	1:D:183:HIS:CE1	2.54	0.42
2:B:562:TYR:HB2	2:B:590:MET:CE	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:364:LEU:O	1:D:368:SER:OG	2.31	0.41
2:E:545:ASP:C	2:E:547:LEU:H	2.27	0.41
2:E:820:GLU:C	2:E:822:ARG:H	2.29	0.41
1:A:37:LYS:C	1:A:39:LEU:H	2.28	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:A:454:LEU:HD12	1:A:454:LEU:HA	1.90	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
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
1:D:343:THR:O	1:D:344:THR:C	2.63	0.40
2:B:670:LEU:HD22	2:B:690:VAL:HG23	2.03	0.40
2:E:734:TRP:CG	2:E:762:ASN:HD21	2.39	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

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	597/669 (89%)	551 (92%)	38 (6%)	8 (1%)	9	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	597/669 (89%)	545 (91%)	44 (7%)	8 (1%)	9	35
2	B	322/333 (97%)	286 (89%)	30 (9%)	6 (2%)	6	27
2	E	322/333 (97%)	288 (89%)	26 (8%)	8 (2%)	4	21
3	C	36/67 (54%)	30 (83%)	5 (14%)	1 (3%)	4	20
3	F	38/67 (57%)	34 (90%)	3 (8%)	1 (3%)	4	21
All	All	1912/2138 (89%)	1734 (91%)	146 (8%)	32 (2%)	7	30

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%)	492 (95%)	24 (5%)	23	55
1	D	516/564 (92%)	493 (96%)	23 (4%)	24	56
2	B	270/280 (96%)	253 (94%)	17 (6%)	16	45
2	E	270/280 (96%)	252 (93%)	18 (7%)	15	43
3	C	28/55 (51%)	27 (96%)	1 (4%)	31	62
3	F	30/55 (54%)	26 (87%)	4 (13%)	4	17
All	All	1630/1798 (91%)	1543 (95%)	87 (5%)	20	51

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	27	VAL
1	A	31	LYS
1	A	53	ARG
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
1	A	418	GLN
1	A	426	TYR

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Mol	Chain	Res	Type
1	A	440	HIS
1	A	504	ASP
1	A	533	LEU
1	A	538	LEU
1	A	567	GLU
1	A	603	THR
1	A	615	THR
1	A	620	LEU
2	B	512	THR
2	B	516	GLU
2	B	525	LEU
2	B	531	ARG
2	B	536	VAL
2	B	547	LEU
2	B	558	THR
2	B	569	ARG
2	B	576	SER
2	B	581	VAL
2	B	584	ARG
2	B	649	LEU
2	B	669	MET
2	B	762	ASN
2	B	770	ILE
2	B	776	LEU
2	B	783	THR
3	C	219	THR
1	D	27	VAL
1	D	31	LYS
1	D	38	ASP
1	D	84	VAL
1	D	93	GLN
1	D	131	ASP
1	D	137	LEU
1	D	162	LEU
1	D	323	LEU
1	D	331	LEU
1	D	339	HIS
1	D	418	GLN
1	D	426	TYR
1	D	429	ILE
1	D	452	GLN
1	D	504	ASP

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Mol	Chain	Res	Type
1	D	533	LEU
1	D	538	LEU
1	D	567	GLU
1	D	603	THR
1	D	615	THR
1	D	620	LEU
1	D	630	ARG
2	E	507	GLU
2	E	512	THR
2	E	523	THR
2	E	525	LEU
2	E	536	VAL
2	E	547	LEU
2	E	558	THR
2	E	560	LEU
2	E	569	ARG
2	E	576	SER
2	E	581	VAL
2	E	584	ARG
2	E	649	LEU
2	E	653	ASN
2	E	762	ASN
2	E	770	ILE
2	E	776	LEU
2	E	783	THR
3	F	192	ILE
3	F	199	LEU
3	F	208	GLN
3	F	219	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	59	ASN
1	A	86	ASN
1	A	102	GLN
1	A	195	ASN
1	A	249	GLN
1	A	362	GLN
1	A	392	ASN
1	A	451	HIS

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Mol	Chain	Res	Type
1	A	581	GLN
2	B	817	ASN
3	C	213	GLN
1	D	22	HIS
1	D	59	ASN
1	D	249	GLN
1	D	392	ASN
1	D	402	GLN
1	D	534	GLN
2	E	603	ASN
3	F	204	GLN
3	F	223	ASN

5.3.3 RNA [i](#)

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	605/669 (90%)	-0.48	4 (0%) 84 68	52, 82, 174, 256	0
1	D	605/669 (90%)	-0.45	0 100 100	50, 83, 187, 261	0
2	B	324/333 (97%)	-0.23	2 (0%) 85 70	59, 116, 210, 260	0
2	E	324/333 (97%)	-0.25	5 (1%) 72 52	59, 107, 201, 293	0
3	C	38/67 (56%)	-0.26	0 100 100	101, 147, 196, 229	0
3	F	40/67 (59%)	-0.02	0 100 100	104, 141, 182, 205	0
All	All	1936/2138 (90%)	-0.38	11 (0%) 85 70	50, 93, 196, 293	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	590	MET	2.7
2	B	824	ILE	2.7
1	A	271	ALA	2.5
1	A	272	VAL	2.4
2	E	525	LEU	2.3
2	E	771	PRO	2.3
2	B	598	SER	2.3
1	A	480	SER	2.2
2	E	828	GLY	2.1
1	A	599	GLY	2.1
2	E	598	SER	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.