Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:24 PM GMT

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)

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

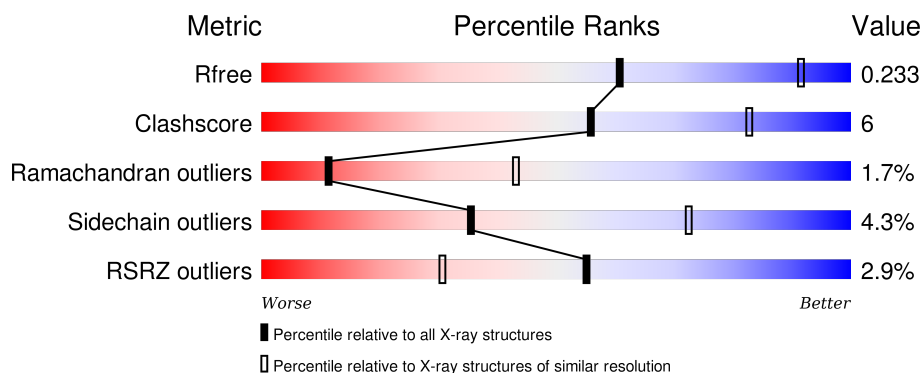|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 >=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 <=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	
1	D	669	
2	B	333	
2	E	333	
3	C	67	

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Mol	Chain	Length	Quality of chain
3	F	67	

2 Entry composition (i)

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 275	C 171	N 46	O 58	0	0	0
3	F	40	Total 295	C 182	N 51	O 62	0	0	0

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: SM (Sec1/Munc18-like) protein

- Molecule 1: SM (Sec1/Munc18-like) protein

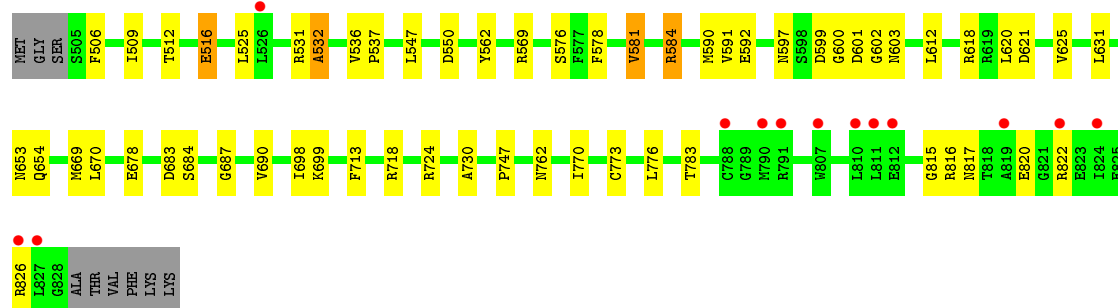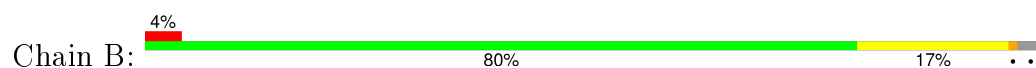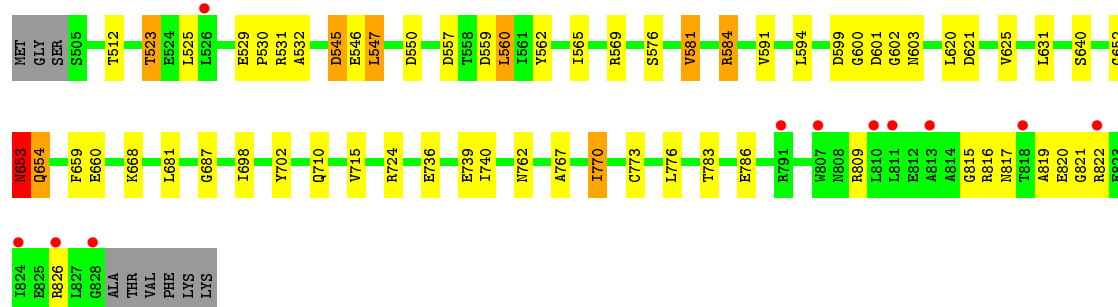G599 D600 K601 K602 T603 V604 T615 L620 R630 R631 N632 I651 A654 T655 F656 E657 K658 THR VAL THR THR ALA ALA GLN

• Molecule 2: Putative vacuolar protein sorting-associated protein

Chain B:

4%

80%   17%

MET GLY SER S505 F506 I509 T512 E516 L525 L526 R531 A532 V536 P537 L547 D550 Y562 R569 S576 F577 F578 V581 R584 M590 V591 E592 N597 S598 D599 G600 D601 G602 N603 L612 R618 R619 L620 D621 V625 L631

N653 Q654 M669 L670 E678 D683 S684 G687 V690 I698 K699 F713 R718 R724 A730 P747 N762 I770 C773 L776 T783 C788 G789 M790 R791 W807 L810 L811 E812 G815 R816 N817 T818 A819 E820 G821 R822 E823 I824 E825

R826 L827 G828 ALA THR VAL PHE LYS LYS

• Molecule 2: Putative vacuolar protein sorting-associated protein

Chain E:

3%

78%   17%

MET GLY SER S505 T512 T523 E524 L525 L526 E529 P530 R531 A532 D545 E546 L547 D550 D557 T558 D559 L560 I561 Y562 I565 R569 S576 V581 R584 V591 L594 D599 G600 D601 G602 N603 L620 D621 V625 L631 S640 G652

N653 Q654 F659 E660 K668 L681 G687 I698 Y702 Q710 V715 R724 E736 E739 I740 N762 A767 I770 C773 L776 T783 E786 R791 W807 N808 R809 L810 L811 E812 A813 A814 G815 R816 N817 T818 A819 E820 G821 R822 E823

I824 E825 R826 L827 G828 ALA THR VAL PHE LYS LYS

• Molecule 3: SNAP receptor-like protein

Chain C:

7%

42%   15%   43%

GLY SER LEU ILE LEU GLU ARG GLU GLU E188 N191 I192 V196 L199 N200 V201 L202 V206 A207 Q208 E212 Q213 G214 E215 T219 N223 V224 E225 ALA VAL GLY ASP ASP THR ARG GLY ALA ASP ARG GLU LEU ARG ALA ALA ALA ARG TYR GLN

• Molecule 3: SNAP receptor-like protein

Chain F:

3%

40%   18%   •   40%

GLY SER LEU ILE LEU GLU ARG E186 R190 N191 I192 E193 V196 S197 D198 L199 N200 V201 Q205 V206 A207 Q208 E215 T219 I220 N223 V224 E225 ALA VAL GLY ASP ASP THR ARG GLY ALA ASP ARG GLU LEU ARG ALA ALA ALA ARG TYR GLN

4 Data and refinement statistics (i)

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) 100.0 (47.98-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	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^2)	89.9	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 59.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 53146 reflections	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.22	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 (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	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:D:355:PRO:HD3	3:F:206:VAL:HG13	1.84	0.59
1:A:443:ARG:NH1	2:B:713:PHE:O	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:562:TYR:HD1	2:E:594:LEU:HD11	1.76	0.49
1:D:31:LYS:HD2	1:D:56:GLY:O	2.12	0.49
1:A:15:LYS:NZ	1:A:19:ASP:OD2	2.44	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
3:C:208:GLN:NE2	3:C:212:GLU:OE2	2.46	0.49
1:A:191:GLY:HA3	1:A:577:PHE:CZ	2.48	0.49
1:D:338:ARG:HD3	1:D:338:ARG:HA	1.57	0.48
1:D:161:TYR:CE1	1:D:239:GLU:HB3	2.48	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:606:VAL:HG11	1:A:620:LEU:HD21	1.95	0.48
1:A:324:LEU:HD21	1:A:368:SER:HA	1.96	0.48
2:E:620:LEU:HD21	2:E:660:GLU:HG2	1.94	0.48
1:D:191:GLY:HA3	1:D:577:PHE:CZ	2.49	0.47
2:B:506:PHE:HA	2:B:509:ILE:HD12	1.94	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:D:371:ALA:O	1:D:375:ILE:HG13	2.15	0.47
1:A:340:ASN:O	1:A:342:LYS:N	2.48	0.47
2:B:597:ASN:O	2:B:600:GLY:HA2	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

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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:D:27:VAL:HG13	1:D:31:LYS:HE2	1.96	0.46
1:A:494:TYR:CE2	1:A:498:GLN:HG3	2.51	0.46
1:D:655:THR:HG23	1:D:657:GLU:H	1.80	0.46
1:A:494:TYR:CZ	1:A:498:GLN:HG3	2.51	0.46
1:A:361:GLN:HE21	1:A:361:GLN:HB2	1.56	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
2:B:822:ARG:O	2:B:826:ARG:N	2.35	0.45
2:B:683:ASP:OD1	2:B:684:SER:N	2.49	0.45
1:A:269:VAL:O	1:A:297:LYS:HB2	2.16	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
2:E:736:GLU:HA	2:E:739:GLU:HB2	1.97	0.45
1:D:336:GLU:OE2	1:D:339:HIS:NE2	2.48	0.45
2:E:557:ASP:HB3	2:E:560:LEU:HB2	1.99	0.44
1:D:124:GLU:C	1:D:126:ALA:H	2.20	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:D:347:LEU:O	1:D:351:VAL:HG23	2.18	0.44
1:D:162:LEU:HB2	1:D:463:LEU:HD21	1.99	0.44
2:B:621:ASP:O	2:B:625:VAL:HG23	2.18	0.44
1:D:630:ARG:HG2	1:D:630:ARG:H	1.63	0.44
2:B:601:ASP:O	2:B:603:ASN:N	2.51	0.44
1:A:647:MET:O	1:A:651:ILE:HG13	2.17	0.44
2:E:620:LEU:HD23	2:E:620:LEU:HA	1.87	0.44
3:C:196:VAL:O	3:C:200:ASN:HB2	2.17	0.44
2:B:581:VAL:HG21	2:B:591:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:VAL:HA	1:D:113:PRO:HA	1.76	0.44
2:B:532:ALA:O	2:B:536:VAL:HG13	2.18	0.44
1:D:324:LEU:HD12	1:D:324:LEU:HA	1.87	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:D:484:GLY:O	1:D:488:GLN:NE2	2.51	0.43
2:E:815:GLY:C	2:E:817:ASN:H	2.20	0.43
1:A:112:VAL:HA	1:A:113:PRO:HA	1.74	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:599:ASP:HB2	2:E:603:ASN:HB2	1.99	0.43
2:E:530:PRO:HB2	2:E:531:ARG:HA	1.99	0.43
2:E:786:GLU:CD	2:E:809:ARG:HH12	2.22	0.43
1:D:382:ILE:HD13	1:D:414:THR:HG22	2.00	0.43
1:A:657:GLU:HG2	2:B:687:GLY:HA3	2.00	0.43
1:A:455:LEU:HD12	1:A:652:GLU:HG2	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:E:653:ASN:HB3	2:E:654:GLN:H	1.35	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
1:D:620:LEU:HD12	1:D:620:LEU:HA	1.87	0.42
1:A:371:ALA:O	1:A:375:ILE:HG13	2.19	0.42
3:F:219:THR:OG1	3:F:220:ILE:N	2.53	0.42
2:E:562:TYR:CD1	2:E:594:LEU:HD11	2.53	0.42
1:A:90:ILE:O	1:A:94:ILE:HG13	2.18	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:562:TYR:HB2	2:B:590:MET:CE	2.49	0.42
2:E:599:ASP:N	2:E:600:GLY:HA2	2.32	0.42
2:B:678:GLU:HG2	2:B:683:ASP:O	2.20	0.42
2:E:681:LEU:HD22	2:E:702:TYR:CE1	2.55	0.42
2:B:718:ARG:NH1	2:B:747:PRO:O	2.52	0.42
1:A:38:ASP:OD1	1:A:38:ASP:N	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:PHE:HA	1:D:183:HIS:CE1	2.54	0.42
1:A:95:LYS:HE3	1:A:126:ALA:HB1	2.02	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
3:F:193:GLU:O	3:F:196:VAL:HG12	2.20	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
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:D:231:GLU:HB3	1:D:604:VAL:HG22	2.02	0.40
1:A:534:GLN:NE2	1:A:623:ILE:HG23	2.37	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%)	15	50
1	D	597/669 (89%)	545 (91%)	44 (7%)	8 (1%)	15	50
2	B	322/333 (97%)	286 (89%)	30 (9%)	6 (2%)	10	40
2	E	322/333 (97%)	288 (89%)	26 (8%)	8 (2%)	7	32
3	C	36/67 (54%)	30 (83%)	5 (14%)	1 (3%)	6	30
3	F	38/67 (57%)	34 (90%)	3 (8%)	1 (3%)	7	32
All	All	1912/2138 (89%)	1734 (91%)	146 (8%)	32 (2%)	11	43

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 (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	516/564 (92%)	494 (96%)	22 (4%)	35	72
1	D	516/564 (92%)	497 (96%)	19 (4%)	41	76
2	B	270/280 (96%)	258 (96%)	12 (4%)	35	71
2	E	270/280 (96%)	258 (96%)	12 (4%)	35	71
3	C	28/55 (51%)	27 (96%)	1 (4%)	42	77
3	F	30/55 (54%)	26 (87%)	4 (13%)	5	20
All	All	1630/1798 (91%)	1560 (96%)	70 (4%)	35	72

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 (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 carbohydrates 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%)	-0.10	9 (1%)	76	58	52, 82, 174, 256	0
1	D	605/669 (90%)	-0.10	17 (2%)	56	32	50, 83, 187, 261	0
2	B	324/333 (97%)	0.12	13 (4%)	42	20	59, 116, 210, 260	0
2	E	324/333 (97%)	0.01	11 (3%)	49	24	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%)	32	13	104, 141, 182, 205	0
All	All	1936/2138 (90%)	-0.03	57 (2%)	55	31	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 (i)

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.