Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:12 AM GMT

PDB ID	:	2G3K
Title	:	Crystal structure of the C-terminal domain of Vps28
Authors	:	Pineda-Molina, E.; Belrhali, H.; Piefer, A.J.; Akula, I.; Bates, P.; Weissenhorn, W.
Deposited on	:	2006-02-20
Resolution	:	3.05 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

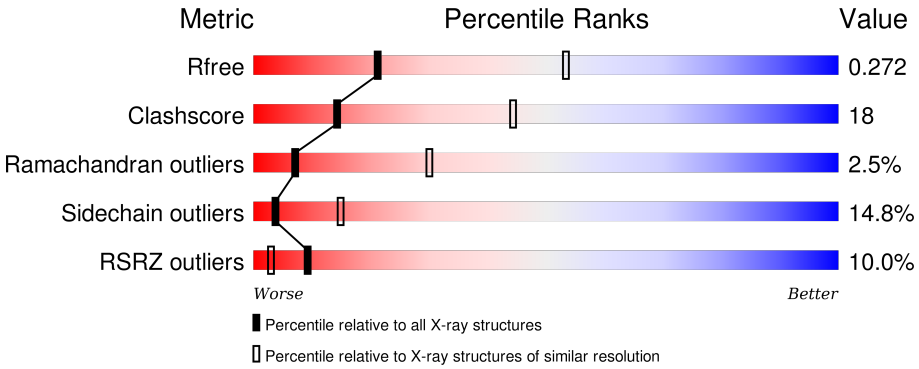
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.05 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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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	94	2% 70% 26% ·
1	B	94	15% 63% 34% ·
1	C	94	7% 51% 39% 9% ·
1	D	94	17% 54% 35% 11%
1	E	94	12% 53% 38% 9%

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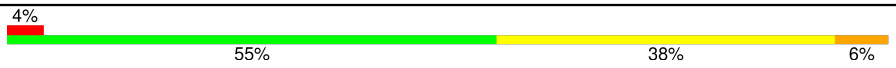
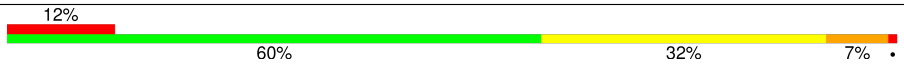
Mol	Chain	Length	Quality of chain
1	F	94	
1	G	94	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5446 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Vacuolar protein sorting-associated protein VPS28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	Se	0	0	0
			770	498	127	144	1			
1	B	94	Total	C	N	O	Se	0	0	0
			770	498	127	144	1			
1	C	94	Total	C	N	O	Se	0	0	0
			770	498	127	144	1			
1	D	94	Total	C	N	O	Se	0	0	0
			770	498	127	144	1			
1	E	94	Total	C	N	O	Se	0	0	0
			770	498	127	144	1			
1	F	94	Total	C	N	O	Se	0	0	0
			770	498	127	144	1			
1	G	94	Total	C	N	O	Se	0	0	0
			770	498	127	144	1			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	MSE	MET	MODIFIED RESIDUE	UNP Q02767
B	164	MSE	MET	MODIFIED RESIDUE	UNP Q02767
C	164	MSE	MET	MODIFIED RESIDUE	UNP Q02767
D	164	MSE	MET	MODIFIED RESIDUE	UNP Q02767
E	164	MSE	MET	MODIFIED RESIDUE	UNP Q02767
F	164	MSE	MET	MODIFIED RESIDUE	UNP Q02767
G	164	MSE	MET	MODIFIED RESIDUE	UNP Q02767

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total	O	0	0
			9	9		
2	B	5	Total	O	0	0
			5	5		

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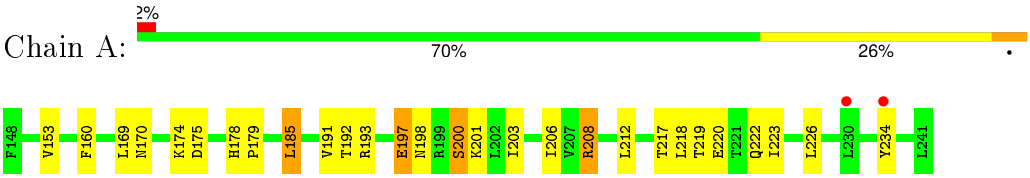
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	13	Total O 13 13	0	0
2	D	2	Total O 2 2	0	0
2	E	5	Total O 5 5	0	0
2	F	13	Total O 13 13	0	0
2	G	9	Total O 9 9	0	0

3 Residue-property plots (i)

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.

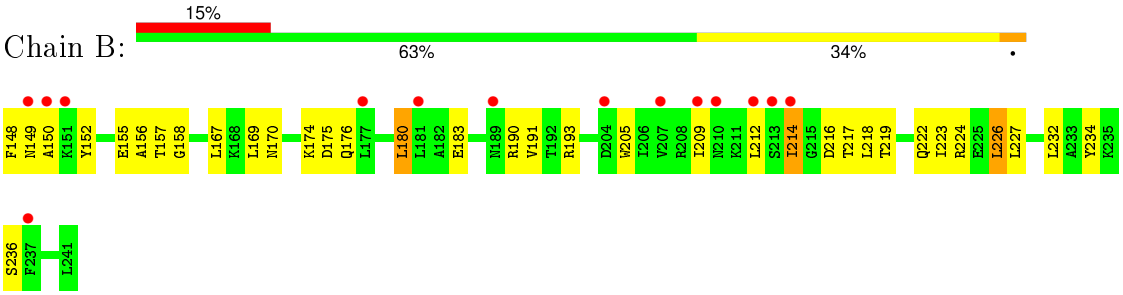
• Molecule 1: Vacuolar protein sorting-associated protein VPS28

Chain A:



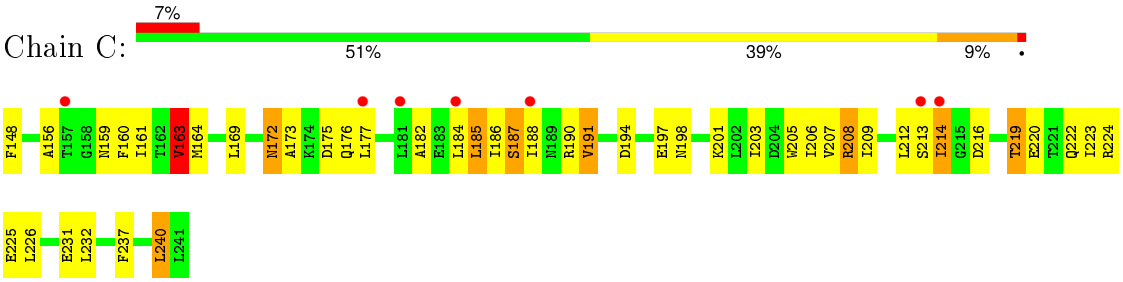
• Molecule 1: Vacuolar protein sorting-associated protein VPS28

Chain B:



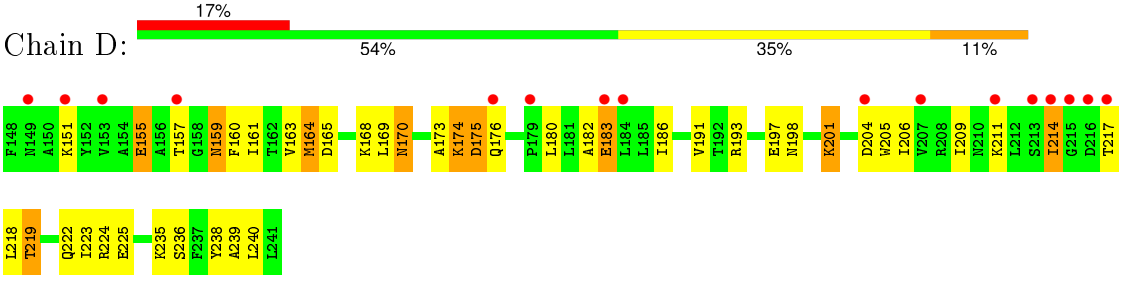
• Molecule 1: Vacuolar protein sorting-associated protein VPS28

Chain C:

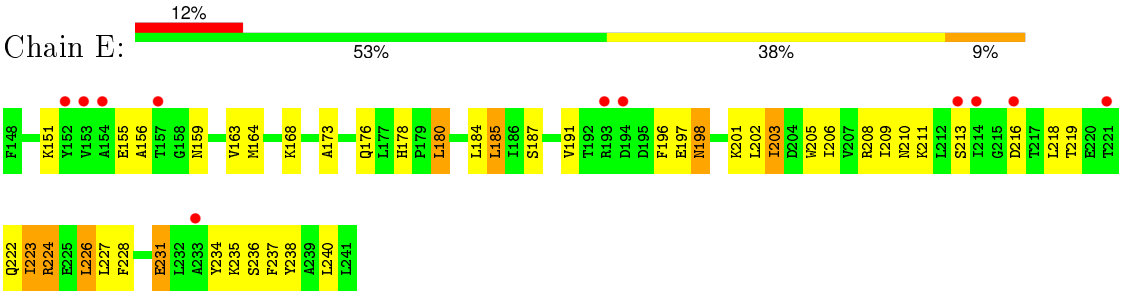


• Molecule 1: Vacuolar protein sorting-associated protein VPS28

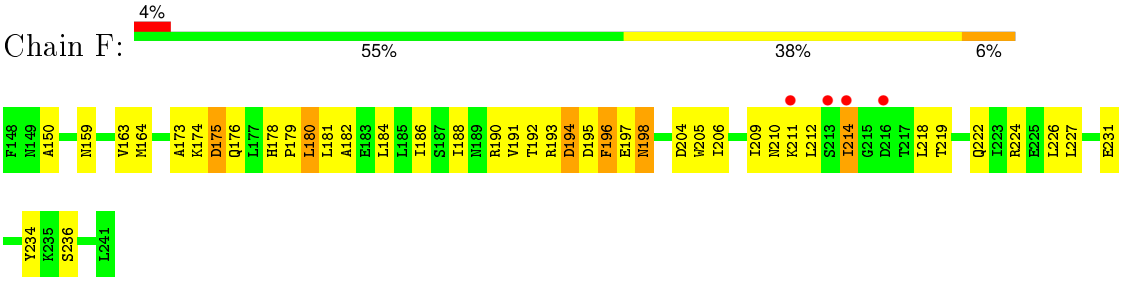
Chain D:



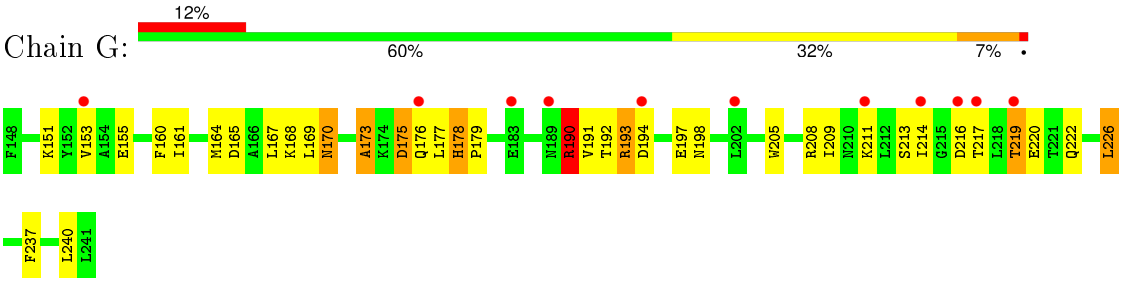
• Molecule 1: Vacuolar protein sorting-associated protein VPS28



• Molecule 1: Vacuolar protein sorting-associated protein VPS28



• Molecule 1: Vacuolar protein sorting-associated protein VPS28



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	117.58Å 117.58Å 294.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 3.05 19.94 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.94-3.05) 99.2 (19.94-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.50 (at 3.04Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.213 , 0.273 0.209 , 0.272	Depositor DCC
R_{free} test set	1205 reflections (5.40%)	DCC
Wilson B-factor (Å^2)	78.1	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 90.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 23506 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	5446	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.79	0/781	0.86	0/1054
1	B	0.68	0/781	0.79	0/1054
1	C	0.89	0/781	0.99	2/1054 (0.2%)
1	D	0.70	0/781	0.87	1/1054 (0.1%)
1	E	0.70	0/781	0.87	1/1054 (0.1%)
1	F	0.72	0/781	0.82	0/1054
1	G	0.71	0/781	0.90	2/1054 (0.2%)
All	All	0.75	0/5467	0.87	6/7378 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	190	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	C	185	LEU	CA-CB-CG	-5.78	102.01	115.30
1	C	163	VAL	CB-CA-C	-5.33	101.27	111.40
1	D	170	ASN	N-CA-C	5.12	124.82	111.00
1	E	226	LEU	CA-CB-CG	5.12	127.07	115.30
1	G	190	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	770	0	786	17	0
1	B	770	0	786	32	0
1	C	770	0	786	29	0
1	D	770	0	786	35	0
1	E	770	0	786	43	0
1	F	770	0	786	35	1
1	G	770	0	786	27	1
2	A	9	0	0	1	0
2	B	5	0	0	0	0
2	C	13	0	0	3	0
2	D	2	0	0	0	0
2	E	5	0	0	3	0
2	F	13	0	0	6	0
2	G	9	0	0	2	0
All	All	5446	0	5502	197	1

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 18.

All (197) 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:B:152:TYR:CZ	1:D:214:ILE:HD12	1.51	1.43
1:B:152:TYR:CE1	1:D:214:ILE:HD12	1.64	1.32
1:B:152:TYR:CE1	1:D:214:ILE:CD1	2.29	1.15
1:B:152:TYR:CZ	1:D:214:ILE:CD1	2.39	1.04
1:C:208:ARG:HD3	2:C:58:HOH:O	1.64	0.97
1:F:197:GLU:HB3	1:F:236:SER:OG	1.65	0.96
1:G:205:TRP:O	1:G:209:ILE:HG12	1.71	0.89
1:D:197:GLU:O	1:D:198:ASN:HB2	1.74	0.88
1:E:196:PHE:HD2	1:E:197:GLU:H	1.21	0.83
1:G:173:ALA:HB3	1:G:176:GLN:HG2	1.61	0.82
1:E:205:TRP:O	1:E:209:ILE:HG12	1.83	0.79
1:F:195:ASP:O	1:F:196:PHE:HB3	1.82	0.77
1:B:219:THR:H	1:B:222:GLN:HE21	1.30	0.76
1:D:201:LYS:O	1:D:204:ASP:HB3	1.85	0.76
1:C:220:GLU:HG2	2:C:79:HOH:O	1.85	0.76
1:D:205:TRP:HZ2	1:D:225:GLU:HG2	1.51	0.76
1:E:208:ARG:HD3	2:E:56:HOH:O	1.87	0.75
1:E:156:ALA:HA	1:E:187:SER:OG	1.86	0.74
1:G:167:LEU:O	1:G:170:ASN:N	2.21	0.73
1:G:190:ARG:HG2	1:G:190:ARG:HH11	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:PHE:O	1:G:164:MSE:HG3	1.88	0.72
1:C:173:ALA:HB3	1:C:176:GLN:HG3	1.72	0.72
1:E:159:ASN:HD22	1:E:187:SER:HB2	1.54	0.71
1:E:159:ASN:HD22	1:E:187:SER:CB	2.05	0.70
1:E:219:THR:HG22	1:E:222:GLN:HG2	1.72	0.70
1:F:164:MSE:HE3	1:F:231:GLU:HG2	1.74	0.69
1:E:159:ASN:ND2	1:E:187:SER:HB2	2.08	0.69
1:C:184:LEU:O	1:C:188:ILE:HG13	1.94	0.68
1:E:219:THR:CG2	1:E:222:GLN:HG2	2.24	0.67
1:G:173:ALA:HB3	1:G:176:GLN:CG	2.24	0.67
1:E:164:MSE:HE3	1:E:231:GLU:HG3	1.77	0.67
1:G:217:THR:HA	2:G:97:HOH:O	1.94	0.67
1:C:172:ASN:HD22	1:C:172:ASN:H	1.44	0.65
1:E:168:LYS:HD3	2:E:100:HOH:O	1.95	0.65
1:B:157:THR:HG23	1:B:234:TYR:HE1	1.61	0.65
1:D:218:LEU:HD23	1:D:223:ILE:HD13	1.79	0.64
1:C:173:ALA:H	1:C:176:GLN:HE21	1.45	0.64
1:G:190:ARG:HH11	1:G:190:ARG:CG	2.11	0.64
1:F:205:TRP:O	1:F:209:ILE:HG13	1.98	0.63
1:E:178:HIS:CD2	1:E:210:ASN:HD21	2.16	0.63
1:D:205:TRP:O	1:D:209:ILE:HG12	1.99	0.63
1:C:182:ALA:O	1:C:186:ILE:HG13	1.99	0.63
1:B:219:THR:OG1	1:B:222:GLN:HG3	1.97	0.62
1:B:152:TYR:CE1	1:D:214:ILE:HD11	2.31	0.62
1:D:219:THR:HG23	1:D:222:GLN:HG3	1.81	0.62
1:E:218:LEU:HB3	1:E:223:ILE:HD12	1.81	0.62
1:E:219:THR:H	1:E:222:GLN:HE21	1.46	0.62
1:C:205:TRP:O	1:C:209:ILE:HG12	2.01	0.61
1:E:196:PHE:CD2	1:E:197:GLU:N	2.67	0.61
1:F:190:ARG:HD2	2:F:52:HOH:O	2.00	0.61
1:G:167:LEU:HD11	1:G:226:LEU:HD13	1.81	0.61
1:C:203:ILE:O	1:C:207:VAL:HG23	2.01	0.60
1:B:183:GLU:OE2	1:B:183:GLU:HA	2.00	0.60
1:B:152:TYR:OH	1:D:214:ILE:HG21	2.02	0.60
1:E:218:LEU:HG	1:E:222:GLN:HG3	1.84	0.60
1:F:193:ARG:HG3	2:F:53:HOH:O	2.02	0.60
1:E:197:GLU:OE1	1:F:179:PRO:CG	2.50	0.59
1:E:164:MSE:CE	1:E:231:GLU:HG3	2.32	0.59
1:D:182:ALA:O	1:D:186:ILE:HG12	2.02	0.59
1:F:159:ASN:O	1:F:163:VAL:HG23	2.01	0.59
1:B:152:TYR:OH	1:D:214:ILE:CD1	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:THR:H	1:F:222:GLN:HE21	1.49	0.59
1:G:175:ASP:OD2	1:G:175:ASP:N	2.36	0.58
1:C:188:ILE:O	1:C:191:VAL:HG13	2.04	0.58
1:E:184:LEU:O	1:E:187:SER:HB3	2.03	0.58
1:F:192:THR:OG1	1:F:194:ASP:HB2	2.03	0.57
1:B:214:ILE:O	1:B:214:ILE:HG13	2.03	0.57
1:C:172:ASN:HB2	1:C:223:ILE:HD11	1.86	0.57
1:F:182:ALA:O	1:F:186:ILE:HG12	2.04	0.57
1:E:197:GLU:OE1	1:F:179:PRO:HG3	2.03	0.57
1:E:218:LEU:HB3	1:E:223:ILE:CD1	2.35	0.57
1:A:178:HIS:HD2	2:A:68:HOH:O	1.88	0.57
1:D:151:LYS:HG3	1:E:238:TYR:CE2	2.40	0.56
1:B:157:THR:HG23	1:B:234:TYR:CE1	2.41	0.56
1:E:219:THR:HG22	1:E:222:GLN:CG	2.35	0.56
1:F:181:LEU:HD13	1:F:206:ILE:HG23	1.88	0.56
1:F:190:ARG:NH1	2:F:64:HOH:O	2.39	0.55
1:E:198:ASN:O	1:E:202:LEU:HG	2.06	0.55
1:E:185:LEU:HD11	1:E:203:ILE:HG13	1.89	0.55
1:A:185:LEU:HD21	1:A:203:ILE:HG12	1.89	0.55
1:D:214:ILE:O	1:D:214:ILE:HG13	2.07	0.54
1:F:174:LYS:HG3	1:F:175:ASP:N	2.23	0.54
1:G:192:THR:OG1	1:G:194:ASP:OD2	2.25	0.54
1:B:152:TYR:OH	1:D:214:ILE:HD12	2.01	0.54
1:F:173:ALA:HB3	1:F:176:GLN:HB2	1.90	0.53
1:D:218:LEU:HD23	1:D:223:ILE:CD1	2.39	0.53
1:G:214:ILE:HG13	1:G:214:ILE:O	2.08	0.53
1:D:174:LYS:HB2	1:D:174:LYS:NZ	2.22	0.53
1:B:219:THR:HG23	1:B:222:GLN:HE21	1.72	0.53
1:E:228:PHE:HZ	1:F:180:LEU:HD21	1.74	0.53
1:G:161:ILE:HD13	1:G:164:MSE:HE2	1.91	0.52
1:E:231:GLU:O	1:E:234:TYR:HB3	2.09	0.52
1:E:213:SER:O	1:E:216:ASP:HB2	2.09	0.52
1:B:205:TRP:O	1:B:209:ILE:HG12	2.09	0.52
1:D:197:GLU:O	1:D:198:ASN:CB	2.51	0.52
1:F:181:LEU:HD12	1:F:209:ILE:HD12	1.92	0.52
1:B:174:LYS:HG3	1:B:175:ASP:N	2.25	0.51
1:B:219:THR:O	1:B:223:ILE:HG12	2.11	0.51
1:B:169:LEU:O	1:B:170:ASN:HB2	2.10	0.51
1:A:178:HIS:HB3	1:A:179:PRO:HD3	1.93	0.51
1:C:197:GLU:HG3	1:C:198:ASN:ND2	2.26	0.51
1:A:219:THR:HG22	1:A:222:GLN:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:MSE:HE3	1:C:231:GLU:HG2	1.93	0.51
1:G:208:ARG:HD3	2:G:55:HOH:O	2.11	0.51
1:F:164:MSE:CE	1:F:231:GLU:HG2	2.42	0.50
1:D:157:THR:O	1:D:160:PHE:HB2	2.12	0.50
1:C:172:ASN:ND2	1:C:172:ASN:H	2.08	0.50
1:G:197:GLU:O	1:G:198:ASN:HB2	2.10	0.50
1:G:219:THR:H	1:G:222:GLN:NE2	2.09	0.50
1:E:198:ASN:HD22	1:E:198:ASN:N	2.09	0.49
1:F:196:PHE:C	1:F:196:PHE:CD2	2.85	0.49
1:E:197:GLU:HB3	1:E:236:SER:CB	2.42	0.49
1:B:176:GLN:O	1:B:180:LEU:HB2	2.13	0.49
1:A:200:SER:HB3	1:B:155:GLU:OE1	2.13	0.49
1:C:172:ASN:HD22	1:C:172:ASN:N	2.08	0.49
1:D:151:LYS:HE2	1:E:238:TYR:HE2	1.77	0.49
1:D:236:SER:O	1:D:239:ALA:HB3	2.13	0.49
1:E:219:THR:HG22	1:E:222:GLN:CD	2.33	0.49
1:B:219:THR:HG23	1:B:222:GLN:NE2	2.28	0.48
1:B:218:LEU:HD23	1:B:223:ILE:HD13	1.94	0.48
1:F:214:ILE:HG13	1:F:214:ILE:O	2.13	0.48
1:B:219:THR:H	1:B:222:GLN:NE2	2.07	0.48
1:A:185:LEU:HD21	1:A:203:ILE:CG1	2.44	0.48
1:E:163:VAL:HG22	1:E:180:LEU:HB3	1.95	0.48
1:G:178:HIS:HB3	1:G:179:PRO:HD3	1.96	0.48
1:A:191:VAL:HG22	1:A:192:THR:HG22	1.95	0.48
1:A:197:GLU:O	1:A:198:ASN:HB2	2.14	0.47
1:E:173:ALA:H	1:E:176:GLN:NE2	2.12	0.47
1:E:173:ALA:H	1:E:176:GLN:HE21	1.61	0.47
1:F:197:GLU:HB3	1:F:236:SER:CB	2.43	0.47
1:F:197:GLU:CB	1:F:236:SER:OG	2.50	0.47
1:F:195:ASP:O	1:F:196:PHE:CB	2.54	0.47
1:G:193:ARG:H	1:G:193:ARG:HH11	1.63	0.47
1:C:212:LEU:HB3	1:C:216:ASP:HB3	1.96	0.47
1:A:160:PHE:CD2	1:A:234:TYR:HB2	2.49	0.47
1:A:169:LEU:O	1:A:170:ASN:HB2	2.14	0.47
1:B:216:ASP:OD1	1:B:217:THR:N	2.44	0.47
1:D:159:ASN:ND2	1:D:183:GLU:OE1	2.49	0.46
1:C:237:PHE:HA	1:C:240:LEU:HD22	1.96	0.46
1:E:219:THR:HG22	1:E:222:GLN:NE2	2.30	0.46
1:D:151:LYS:HE2	1:E:238:TYR:CE2	2.50	0.46
1:D:160:PHE:O	1:D:164:MSE:HG3	2.16	0.46
1:E:237:PHE:O	1:E:240:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:ALA:HB3	1:D:176:GLN:HE21	1.79	0.45
1:C:214:ILE:O	1:C:214:ILE:HG13	2.16	0.45
1:F:219:THR:OG1	1:F:222:GLN:HG3	2.16	0.45
1:D:163:VAL:HG22	1:D:180:LEU:HG	1.98	0.45
1:B:212:LEU:HD11	1:B:218:LEU:HD13	1.97	0.45
1:F:198:ASN:HA	2:F:72:HOH:O	2.15	0.45
1:F:184:LEU:O	1:F:188:ILE:HG13	2.17	0.44
1:C:159:ASN:HD22	1:C:187:SER:CB	2.29	0.44
1:A:201:LYS:HE2	1:A:208:ARG:HH22	1.81	0.44
1:C:156:ALA:HA	1:C:187:SER:OG	2.18	0.44
1:C:184:LEU:HD11	1:C:188:ILE:HD11	1.99	0.44
1:A:203:ILE:O	1:A:206:ILE:HG12	2.18	0.44
1:E:219:THR:HG23	1:E:222:GLN:HG2	2.00	0.43
1:G:173:ALA:O	1:G:177:LEU:HG	2.18	0.43
1:F:175:ASP:N	1:F:175:ASP:OD2	2.51	0.43
1:E:224:ARG:NH1	2:E:35:HOH:O	2.51	0.43
1:D:165:ASP:O	1:D:168:LYS:N	2.51	0.43
1:A:169:LEU:HD22	1:C:225:GLU:HG3	2.00	0.43
1:A:153:VAL:HG21	1:F:150:ALA:HB1	2.00	0.43
1:C:224:ARG:NH1	2:C:70:HOH:O	2.51	0.43
1:G:219:THR:HG23	1:G:222:GLN:NE2	2.34	0.43
1:A:174:LYS:HD2	1:A:212:LEU:O	2.19	0.43
1:C:219:THR:HG23	1:C:222:GLN:OE1	2.19	0.43
1:E:197:GLU:HB3	1:E:236:SER:HB2	2.00	0.42
1:E:197:GLU:HB3	1:E:236:SER:OG	2.19	0.42
1:G:219:THR:N	1:G:222:GLN:HE21	2.16	0.42
1:D:224:ARG:CD	1:G:169:LEU:HD23	2.50	0.42
1:F:178:HIS:CD2	1:F:210:ASN:OD1	2.72	0.42
1:B:155:GLU:O	1:B:156:ALA:C	2.58	0.42
1:F:227:LEU:HA	1:F:227:LEU:HD12	1.81	0.42
1:F:173:ALA:H	1:F:176:GLN:HE21	1.67	0.42
1:C:237:PHE:O	1:C:240:LEU:HB2	2.19	0.42
1:D:205:TRP:CZ2	1:D:225:GLU:HG2	2.41	0.42
1:G:193:ARG:H	1:G:193:ARG:NH1	2.16	0.42
1:G:165:ASP:O	1:G:169:LEU:HD12	2.18	0.42
1:G:237:PHE:O	1:G:240:LEU:HB2	2.20	0.42
1:G:190:ARG:HH11	1:G:190:ARG:CB	2.33	0.41
1:A:219:THR:HG22	1:A:222:GLN:CD	2.40	0.41
1:C:159:ASN:O	1:C:163:VAL:HG23	2.20	0.41
1:C:232:LEU:HA	1:C:232:LEU:HD23	1.83	0.41
1:D:175:ASP:OD2	1:D:175:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:TYR:CE1	1:E:151:LYS:HG3	2.55	0.41
1:A:206:ILE:HD11	1:B:158:GLY:O	2.21	0.41
1:F:190:ARG:CD	2:F:52:HOH:O	2.64	0.41
1:B:149:ASN:HB3	1:B:152:TYR:HB2	2.03	0.41
1:C:172:ASN:HA	1:C:177:LEU:HD11	2.03	0.41
1:B:167:LEU:HD11	1:B:226:LEU:HD13	2.02	0.41
1:B:214:ILE:CG1	1:B:214:ILE:O	2.68	0.41
1:D:164:MSE:O	1:D:168:LYS:HD2	2.21	0.40
1:C:172:ASN:N	1:C:172:ASN:ND2	2.68	0.40
1:F:212:LEU:HD11	1:F:218:LEU:HD13	2.03	0.40
1:G:151:LYS:O	1:G:153:VAL:N	2.55	0.40
1:B:152:TYR:OH	1:D:214:ILE:HD13	2.21	0.40
1:F:234:TYR:HE2	2:F:76:HOH:O	2.05	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:LYS:O	1:G:214:ILE:CD1[5_664]	2.11	0.09

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	92/94 (98%)	86 (94%)	5 (5%)	1 (1%)	17 53
1	B	92/94 (98%)	83 (90%)	7 (8%)	2 (2%)	8 34
1	C	92/94 (98%)	85 (92%)	5 (5%)	2 (2%)	8 34
1	D	92/94 (98%)	78 (85%)	12 (13%)	2 (2%)	8 34
1	E	92/94 (98%)	81 (88%)	11 (12%)	0	100 100
1	F	92/94 (98%)	85 (92%)	4 (4%)	3 (3%)	5 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	92/94 (98%)	76 (83%)	10 (11%)	6 (6%)	1 9
All	All	644/658 (98%)	574 (89%)	54 (8%)	16 (2%)	7 30

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	214	ILE
1	A	175	ASP
1	C	194	ASP
1	D	214	ILE
1	F	196	PHE
1	F	198	ASN
1	F	214	ILE
1	C	214	ILE
1	G	168	LYS
1	G	170	ASN
1	G	173	ALA
1	G	213	SER
1	B	150	ALA
1	G	211	LYS
1	D	155	GLU
1	G	178	HIS

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	84/83 (101%)	74 (88%)	10 (12%)	6 23
1	B	84/83 (101%)	74 (88%)	10 (12%)	6 23
1	C	84/83 (101%)	66 (79%)	18 (21%)	1 5
1	D	84/83 (101%)	66 (79%)	18 (21%)	1 5
1	E	84/83 (101%)	69 (82%)	15 (18%)	2 9
1	F	84/83 (101%)	77 (92%)	7 (8%)	14 44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	84/83 (101%)	75 (89%)	9 (11%)	8 30
All	All	588/581 (101%)	501 (85%)	87 (15%)	4 15

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

Mol	Chain	Res	Type
1	A	185	LEU
1	A	193	ARG
1	A	197	GLU
1	A	200	SER
1	A	208	ARG
1	A	217	THR
1	A	218	LEU
1	A	220	GLU
1	A	223	ILE
1	A	226	LEU
1	B	148	PHE
1	B	180	LEU
1	B	190	ARG
1	B	191	VAL
1	B	193	ARG
1	B	224	ARG
1	B	226	LEU
1	B	227	LEU
1	B	232	LEU
1	B	236	SER
1	C	148	PHE
1	C	160	PHE
1	C	161	ILE
1	C	163	VAL
1	C	169	LEU
1	C	172	ASN
1	C	175	ASP
1	C	185	LEU
1	C	187	SER
1	C	190	ARG
1	C	191	VAL
1	C	201	LYS
1	C	206	ILE
1	C	208	ARG
1	C	213	SER
1	C	219	THR

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Mol	Chain	Res	Type
1	C	226	LEU
1	C	240	LEU
1	D	155	GLU
1	D	159	ASN
1	D	161	ILE
1	D	164	MSE
1	D	169	LEU
1	D	170	ASN
1	D	174	LYS
1	D	175	ASP
1	D	183	GLU
1	D	191	VAL
1	D	193	ARG
1	D	201	LYS
1	D	206	ILE
1	D	211	LYS
1	D	217	THR
1	D	219	THR
1	D	235	LYS
1	D	240	LEU
1	E	155	GLU
1	E	180	LEU
1	E	185	LEU
1	E	191	VAL
1	E	198	ASN
1	E	201	LYS
1	E	203	ILE
1	E	206	ILE
1	E	211	LYS
1	E	223	ILE
1	E	224	ARG
1	E	226	LEU
1	E	227	LEU
1	E	231	GLU
1	E	235	LYS
1	F	175	ASP
1	F	180	LEU
1	F	191	VAL
1	F	194	ASP
1	F	204	ASP
1	F	224	ARG
1	F	226	LEU

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Mol	Chain	Res	Type
1	G	155	GLU
1	G	175	ASP
1	G	190	ARG
1	G	191	VAL
1	G	193	ARG
1	G	216	ASP
1	G	219	THR
1	G	220	GLU
1	G	226	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	HIS
1	A	210	ASN
1	B	176	GLN
1	B	222	GLN
1	C	176	GLN
1	C	198	ASN
1	D	170	ASN
1	E	159	ASN
1	E	176	GLN
1	E	198	ASN
1	E	210	ASN
1	E	222	GLN
1	F	176	GLN
1	F	178	HIS
1	F	222	GLN
1	G	198	ASN
1	G	222	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^{th} 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	93/94 (98%)	0.68	2 (2%) 65 40	61, 68, 76, 96	0
1	B	93/94 (98%)	1.04	14 (15%) 3 1	69, 77, 83, 96	0
1	C	93/94 (98%)	0.75	7 (7%) 17 6	49, 61, 75, 96	0
1	D	93/94 (98%)	1.10	16 (17%) 2 1	64, 75, 81, 97	0
1	E	93/94 (98%)	1.01	11 (11%) 6 2	76, 83, 89, 97	0
1	F	93/94 (98%)	0.85	4 (4%) 39 17	69, 76, 81, 97	0
1	G	93/94 (98%)	1.02	11 (11%) 6 2	72, 79, 88, 96	0
All	All	651/658 (98%)	0.92	65 (9%) 9 3	49, 76, 85, 97	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	214	ILE	7.0
1	D	214	ILE	4.6
1	E	214	ILE	4.6
1	G	214	ILE	4.2
1	C	214	ILE	4.0
1	G	176	GLN	4.0
1	G	189	ASN	3.9
1	B	213	SER	3.6
1	E	213	SER	3.6
1	B	150	ALA	3.5
1	F	213	SER	3.4
1	E	194	ASP	3.4
1	D	213	SER	3.4
1	D	179	PRO	3.3
1	G	216	ASP	3.2
1	D	204	ASP	3.2
1	E	221	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	216	ASP	3.1
1	G	211	LYS	2.9
1	B	149	ASN	2.9
1	F	211	LYS	2.8
1	C	188	ILE	2.7
1	D	215	GLY	2.7
1	B	177	LEU	2.7
1	B	214	ILE	2.7
1	D	157	THR	2.7
1	D	176	GLN	2.6
1	G	202	LEU	2.6
1	B	209	ILE	2.6
1	F	216	ASP	2.6
1	D	149	ASN	2.5
1	E	233	ALA	2.5
1	E	193	ARG	2.5
1	G	194	ASP	2.5
1	A	230	LEU	2.4
1	B	212	LEU	2.4
1	B	237	PHE	2.4
1	B	189	ASN	2.4
1	E	153	VAL	2.4
1	D	153	VAL	2.3
1	E	154	ALA	2.3
1	C	157	THR	2.3
1	D	211	LYS	2.2
1	B	181	LEU	2.2
1	C	181	LEU	2.2
1	E	152	TYR	2.2
1	E	216	ASP	2.2
1	C	213	SER	2.1
1	G	219	THR	2.1
1	B	151	LYS	2.1
1	A	234	TYR	2.1
1	D	207	VAL	2.1
1	C	177	LEU	2.1
1	B	207	VAL	2.1
1	D	217	THR	2.1
1	B	204	ASP	2.1
1	E	157	THR	2.1
1	C	184	LEU	2.1
1	D	183	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	183	GLU	2.1
1	D	151	LYS	2.0
1	B	210	ASN	2.0
1	G	153	VAL	2.0
1	D	184	LEU	2.0
1	G	217	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 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.