



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 09:47 PM 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 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/ValidationPDFNotes.html>

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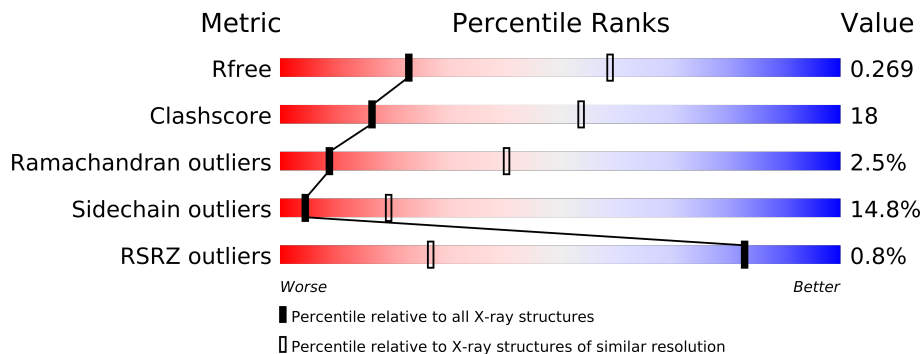
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2079 (3.12-3.00)
Clashscore	79885	2629 (3.12-3.00)
Ramachandran outliers	78287	2536 (3.12-3.00)
Sidechain outliers	78261	2539 (3.12-3.00)
RSRZ outliers	66119	2081 (3.12-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	94	
1	B	94	
1	C	94	
1	D	94	
1	E	94	
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 hydrogen and 0 are deuterium.

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 770	C 498	N 127	O 144	Se 1	0	0	0
1	B	94	Total 770	C 498	N 127	O 144	Se 1	0	0	0
1	C	94	Total 770	C 498	N 127	O 144	Se 1	0	0	0
1	D	94	Total 770	C 498	N 127	O 144	Se 1	0	0	0
1	E	94	Total 770	C 498	N 127	O 144	Se 1	0	0	0
1	F	94	Total 770	C 498	N 127	O 144	Se 1	0	0	0
1	G	94	Total 770	C 498	N 127	O 144	Se 1	0	0	0

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 9	O 9	0	0
2	B	5	Total 5	O 5	0	0

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

### 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: Vacuolar protein sorting-associated protein VPS28

Chain A: 



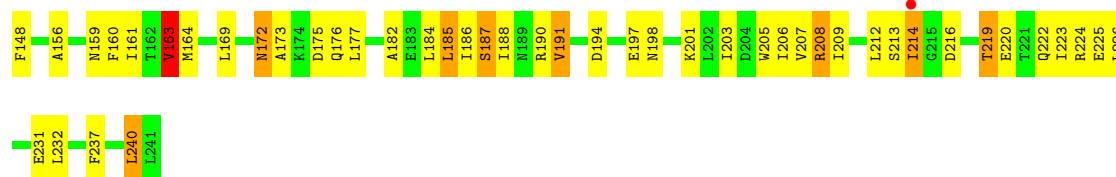
- Molecule 1: Vacuolar protein sorting-associated protein VPS28

Chain B: 



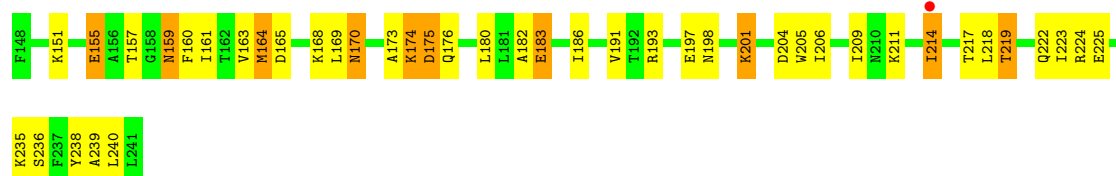
- Molecule 1: Vacuolar protein sorting-associated protein VPS28

Chain C: 



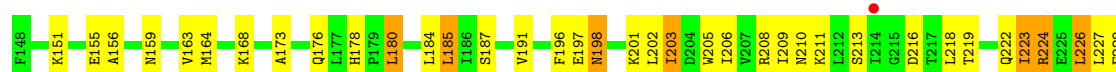
- Molecule 1: Vacuolar protein sorting-associated protein VPS28

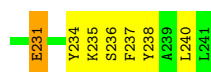
Chain D: 



- Molecule 1: Vacuolar protein sorting-associated protein VPS28

Chain E: 





- Molecule 1: Vacuolar protein sorting-associated protein VPS28

Chain F:



- Molecule 1: Vacuolar protein sorting-associated protein VPS28

Chain G:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.50 (at 3.04Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.213 , 0.273 0.213 , 0.269	Depositor DCC
$R_{free}$ test set	1203 reflections (5.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.1	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 107.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 23506 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.



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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (197) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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

## 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	92/94 (98%)	86 (94%)	5 (5%)	1 (1%)	21	66
1	B	92/94 (98%)	83 (90%)	7 (8%)	2 (2%)	10	44
1	C	92/94 (98%)	85 (92%)	5 (5%)	2 (2%)	10	44
1	D	92/94 (98%)	78 (85%)	12 (13%)	2 (2%)	10	44
1	E	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
1	F	92/94 (98%)	85 (92%)	4 (4%)	3 (3%)	6	32
1	G	92/94 (98%)	76 (83%)	10 (11%)	6 (6%)	2	12
All	All	644/658 (98%)	574 (89%)	54 (8%)	16 (2%)	9	40

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	214	ILE
1	A	175	ASP
1	C	194	ASP

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Mol	Chain	Res	Type
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 ⓘ

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%)	8	29
1	B	84/83 (101%)	74 (88%)	10 (12%)	8	29
1	C	84/83 (101%)	66 (79%)	18 (21%)	1	7
1	D	84/83 (101%)	66 (79%)	18 (21%)	1	7
1	E	84/83 (101%)	69 (82%)	15 (18%)	2	12
1	F	84/83 (101%)	77 (92%)	7 (8%)	16	52
1	G	84/83 (101%)	75 (89%)	9 (11%)	10	35
All	All	588/581 (101%)	501 (85%)	87 (15%)	4	19

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 chains 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	94/94 (100%)	-0.40	0 100 100	61, 68, 76, 96	0
1	B	94/94 (100%)	-0.30	1 (1%) 77 21	69, 77, 84, 96	0
1	C	94/94 (100%)	-0.30	1 (1%) 77 21	49, 61, 75, 96	0
1	D	94/94 (100%)	-0.13	1 (1%) 77 21	64, 76, 82, 97	0
1	E	94/94 (100%)	-0.25	1 (1%) 77 21	76, 83, 90, 97	0
1	F	94/94 (100%)	-0.42	0 100 100	69, 76, 82, 97	0
1	G	94/94 (100%)	-0.21	1 (1%) 77 21	72, 79, 88, 96	0
All	All	658/658 (100%)	-0.29	5 (0%) 83 27	49, 76, 86, 97	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	214	ILE	4.3
1	C	214	ILE	3.1
1	E	214	ILE	3.0
1	G	214	ILE	2.1
1	B	214	ILE	2.1

### 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.