



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2021 – 10:08 AM JST

PDB ID : 7VF4  
Title : Crystal structure of Vps75 from *Candida albicans*  
Authors : Wang, W.; Chen, X.; Yang, Z.; Chen, X.; Li, C.; Wang, M.  
Deposited on : 2021-09-10  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

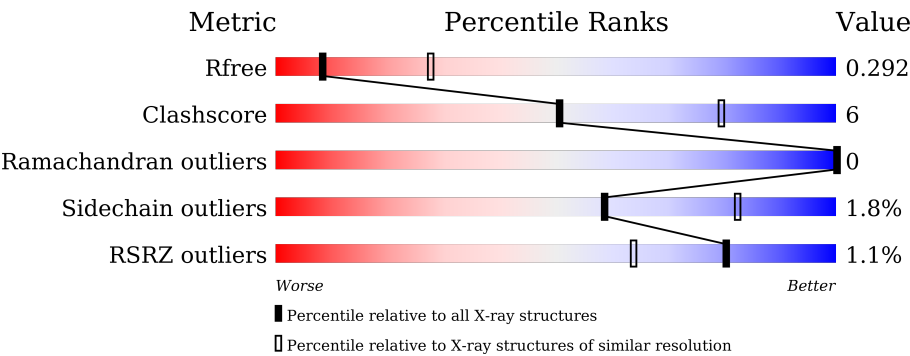
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

# 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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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  $\geq 3$ , 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	235	<div><div></div><div>83%11%6%</div></div>
1	B	235	<div><div>%</div><div>77%14%7%</div></div>
1	C	235	<div><div></div><div>83%11%6%</div></div>
1	D	235	<div><div>%</div><div>78%14%8%</div></div>
1	E	235	<div><div>%</div><div>76%17%6%</div></div>
1	F	235	<div><div>%</div><div>79%14%7%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	235	
1	H	235	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	E	301	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14715 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 Vps75.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1853	1203	296	350	4			
1	B	219	Total	C	N	O	S	0	0	0
			1835	1191	292	348	4			
1	C	222	Total	C	N	O	S	0	0	0
			1861	1209	297	351	4			
1	D	216	Total	C	N	O	S	0	0	0
			1816	1180	289	343	4			
1	E	220	Total	C	N	O	S	0	0	0
			1844	1198	295	347	4			
1	F	219	Total	C	N	O	S	0	0	0
			1838	1192	291	351	4			
1	G	219	Total	C	N	O	S	0	0	0
			1840	1196	294	346	4			
1	H	214	Total	C	N	O	S	0	0	0
			1796	1168	285	339	4			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A0A1D8PT39
A	227	LEU	-	expression tag	UNP A0A1D8PT39
A	228	GLU	-	expression tag	UNP A0A1D8PT39
A	229	HIS	-	expression tag	UNP A0A1D8PT39
A	230	HIS	-	expression tag	UNP A0A1D8PT39
A	231	HIS	-	expression tag	UNP A0A1D8PT39
A	232	HIS	-	expression tag	UNP A0A1D8PT39
A	233	HIS	-	expression tag	UNP A0A1D8PT39
A	234	HIS	-	expression tag	UNP A0A1D8PT39
B	0	MET	-	initiating methionine	UNP A0A1D8PT39
B	227	LEU	-	expression tag	UNP A0A1D8PT39
B	228	GLU	-	expression tag	UNP A0A1D8PT39
B	229	HIS	-	expression tag	UNP A0A1D8PT39

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Chain	Residue	Modelled	Actual	Comment	Reference
B	230	HIS	-	expression tag	UNP A0A1D8PT39
B	231	HIS	-	expression tag	UNP A0A1D8PT39
B	232	HIS	-	expression tag	UNP A0A1D8PT39
B	233	HIS	-	expression tag	UNP A0A1D8PT39
B	234	HIS	-	expression tag	UNP A0A1D8PT39
C	0	MET	-	initiating methionine	UNP A0A1D8PT39
C	227	LEU	-	expression tag	UNP A0A1D8PT39
C	228	GLU	-	expression tag	UNP A0A1D8PT39
C	229	HIS	-	expression tag	UNP A0A1D8PT39
C	230	HIS	-	expression tag	UNP A0A1D8PT39
C	231	HIS	-	expression tag	UNP A0A1D8PT39
C	232	HIS	-	expression tag	UNP A0A1D8PT39
C	233	HIS	-	expression tag	UNP A0A1D8PT39
C	234	HIS	-	expression tag	UNP A0A1D8PT39
D	0	MET	-	initiating methionine	UNP A0A1D8PT39
D	227	LEU	-	expression tag	UNP A0A1D8PT39
D	228	GLU	-	expression tag	UNP A0A1D8PT39
D	229	HIS	-	expression tag	UNP A0A1D8PT39
D	230	HIS	-	expression tag	UNP A0A1D8PT39
D	231	HIS	-	expression tag	UNP A0A1D8PT39
D	232	HIS	-	expression tag	UNP A0A1D8PT39
D	233	HIS	-	expression tag	UNP A0A1D8PT39
D	234	HIS	-	expression tag	UNP A0A1D8PT39
E	0	MET	-	initiating methionine	UNP A0A1D8PT39
E	227	LEU	-	expression tag	UNP A0A1D8PT39
E	228	GLU	-	expression tag	UNP A0A1D8PT39
E	229	HIS	-	expression tag	UNP A0A1D8PT39
E	230	HIS	-	expression tag	UNP A0A1D8PT39
E	231	HIS	-	expression tag	UNP A0A1D8PT39
E	232	HIS	-	expression tag	UNP A0A1D8PT39
E	233	HIS	-	expression tag	UNP A0A1D8PT39
E	234	HIS	-	expression tag	UNP A0A1D8PT39
F	0	MET	-	initiating methionine	UNP A0A1D8PT39
F	227	LEU	-	expression tag	UNP A0A1D8PT39
F	228	GLU	-	expression tag	UNP A0A1D8PT39
F	229	HIS	-	expression tag	UNP A0A1D8PT39
F	230	HIS	-	expression tag	UNP A0A1D8PT39
F	231	HIS	-	expression tag	UNP A0A1D8PT39
F	232	HIS	-	expression tag	UNP A0A1D8PT39
F	233	HIS	-	expression tag	UNP A0A1D8PT39
F	234	HIS	-	expression tag	UNP A0A1D8PT39
G	0	MET	-	initiating methionine	UNP A0A1D8PT39

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Chain	Residue	Modelled	Actual	Comment	Reference
G	227	LEU	-	expression tag	UNP A0A1D8PT39
G	228	GLU	-	expression tag	UNP A0A1D8PT39
G	229	HIS	-	expression tag	UNP A0A1D8PT39
G	230	HIS	-	expression tag	UNP A0A1D8PT39
G	231	HIS	-	expression tag	UNP A0A1D8PT39
G	232	HIS	-	expression tag	UNP A0A1D8PT39
G	233	HIS	-	expression tag	UNP A0A1D8PT39
G	234	HIS	-	expression tag	UNP A0A1D8PT39
H	0	MET	-	initiating methionine	UNP A0A1D8PT39
H	227	LEU	-	expression tag	UNP A0A1D8PT39
H	228	GLU	-	expression tag	UNP A0A1D8PT39
H	229	HIS	-	expression tag	UNP A0A1D8PT39
H	230	HIS	-	expression tag	UNP A0A1D8PT39
H	231	HIS	-	expression tag	UNP A0A1D8PT39
H	232	HIS	-	expression tag	UNP A0A1D8PT39
H	233	HIS	-	expression tag	UNP A0A1D8PT39
H	234	HIS	-	expression tag	UNP A0A1D8PT39

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cl 2 2	0	0
2	E	2	Total Cl 2 2	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	3	Total Na 3 3	0	0
3	C	2	Total Na 2 2	0	0
3	F	1	Total Na 1 1	0	0
3	G	1	Total Na 1 1	0	0
3	H	1	Total Na 1 1	0	0

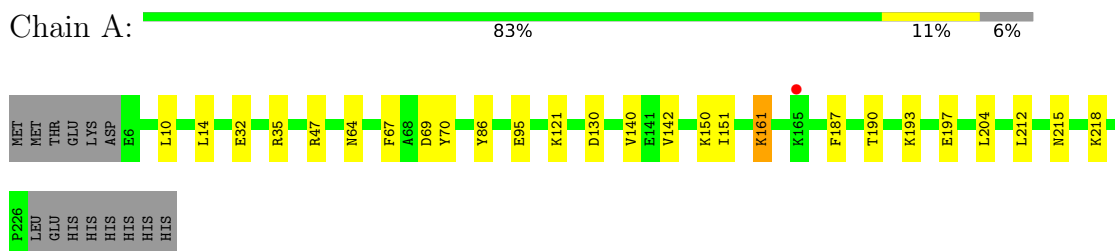
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	B	1	Total O 1 1	0	0
4	C	4	Total O 4 4	0	0
4	D	3	Total O 3 3	0	0
4	E	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0
4	G	4	Total O 4 4	0	0
4	H	2	Total O 2 2	0	0

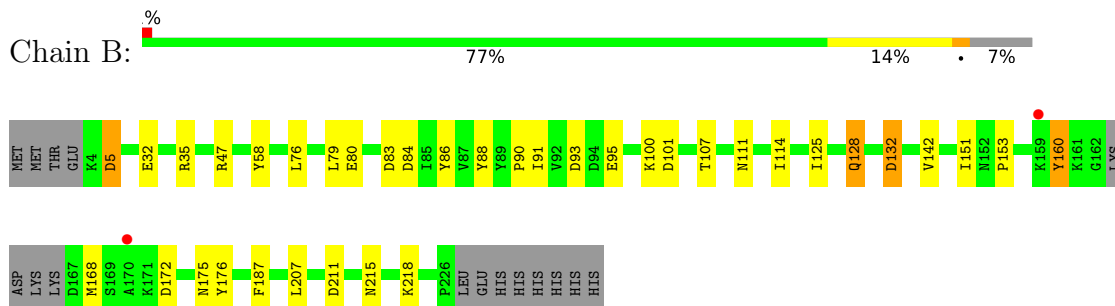
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

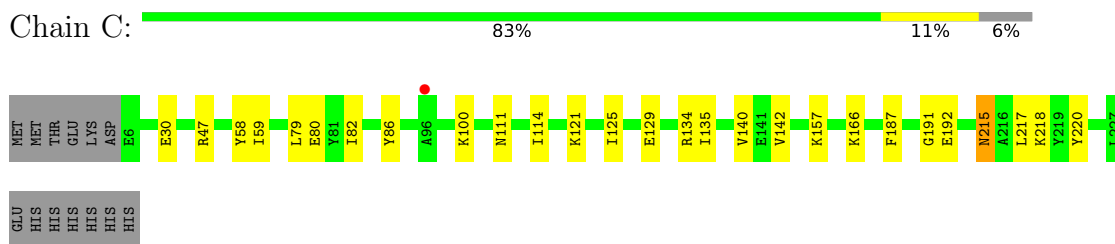
#### • Molecule 1: Vps75



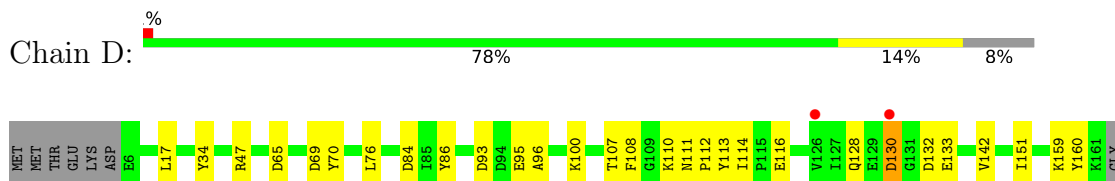
#### • Molecule 1: Vps75



#### • Molecule 1: Vps75



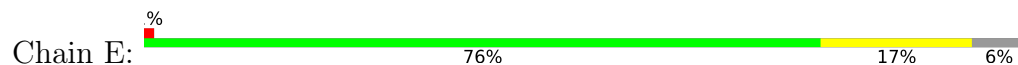
#### • Molecule 1: Vps75



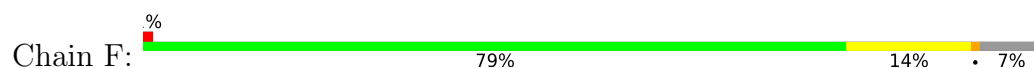




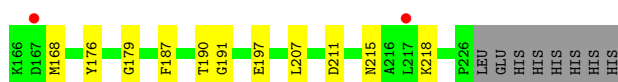
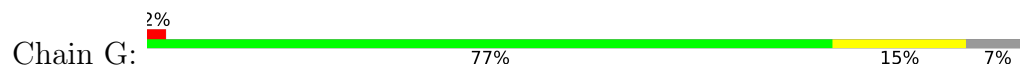
• Molecule 1: Vps75



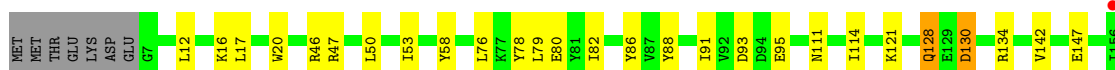
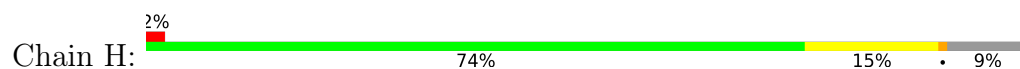
• Molecule 1: Vps75



• Molecule 1: Vps75



• Molecule 1: Vps75



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.61Å 137.17Å 226.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.75 – 3.10 37.75 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.75-3.10) 99.0 (37.75-3.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.244 , 0.292 0.240 , 0.292	Depositor DCC
$R_{free}$ test set	2420 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	80.2	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 32.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL

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	0.30	0/1899	0.46	0/2557
1	B	0.28	0/1880	0.44	0/2532
1	C	0.29	0/1907	0.46	0/2568
1	D	0.29	0/1860	0.44	0/2504
1	E	0.29	0/1890	0.46	0/2545
1	F	0.27	0/1883	0.43	0/2538
1	G	0.28	0/1886	0.44	0/2540
1	H	0.28	0/1841	0.44	0/2482
All	All	0.29	0/15046	0.45	0/20266

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	1853	0	1839	16	0
1	B	1835	0	1812	29	0
1	C	1861	0	1850	15	0
1	D	1816	0	1798	27	0
1	E	1844	0	1833	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1838	0	1809	17	0
1	G	1840	0	1830	22	0
1	H	1796	0	1773	25	0
2	A	2	0	0	1	0
2	E	2	0	0	3	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	4	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	3	0	0	1	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	4	0	0	0	0
4	H	2	0	0	0	0
All	All	14715	0	14544	166	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 (166) 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:F:128:GLN:HE21	1:F:134:ARG:HB2	1.49	0.76
1:B:111:ASN:HD21	1:B:114:ILE:HG22	1.54	0.73
1:E:164:ASP:HB2	1:E:167:ASP:HB2	1.70	0.73
1:A:193:LYS:NZ	1:C:192:GLU:OE1	2.23	0.71
1:D:69:ASP:HB3	1:E:199:ARG:HD2	1.74	0.69
1:H:88:TYR:OH	1:H:93:ASP:OD2	2.11	0.69
1:B:91:ILE:HD12	1:B:95:GLU:HA	1.77	0.66
1:C:166:LYS:NZ	1:G:63:GLU:O	2.30	0.65
1:E:121:LYS:HA	1:E:140:VAL:HG21	1.78	0.65
1:F:4:LYS:HA	1:F:8:LYS:HE3	1.79	0.65
1:A:47:ARG:HD2	1:A:86:TYR:CD1	2.31	0.65
1:E:78:TYR:OH	1:E:147:GLU:OE1	2.12	0.64
1:D:160:TYR:HE2	1:D:168:MET:HA	1.62	0.64
1:B:88:TYR:OH	1:B:93:ASP:OD2	2.16	0.62
1:D:69:ASP:O	1:E:181:LYS:NZ	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LEU:HD22	1:C:82:ILE:HD11	1.82	0.61
1:A:150:LYS:HG3	1:A:151:ILE:HG23	1.81	0.61
1:A:64:ASN:OD1	1:A:67:PHE:N	2.30	0.60
1:D:65:ASP:OD1	1:E:177:ARG:NH2	2.34	0.60
1:B:100:LYS:HB2	1:B:125:ILE:HG13	1.83	0.60
1:G:47:ARG:HD2	1:G:86:TYR:CD1	2.36	0.60
1:B:160:TYR:CE2	1:B:168:MET:HA	2.38	0.59
1:D:100:LYS:NZ	1:D:133:GLU:OE2	2.34	0.59
1:H:91:ILE:HD12	1:H:95:GLU:HA	1.84	0.59
1:G:190:THR:OG1	1:G:197:GLU:OE2	2.16	0.58
1:H:160:TYR:HE2	1:H:168:MET:HA	1.69	0.58
1:B:128:GLN:N	1:B:132:ASP:O	2.34	0.58
1:H:134:ARG:HH12	1:H:192:GLU:HG2	1.69	0.58
1:D:111:ASN:HD21	1:D:113:TYR:HB2	1.70	0.57
1:H:78:TYR:OH	1:H:147:GLU:OE1	2.12	0.57
1:C:47:ARG:HD2	1:C:86:TYR:CD1	2.41	0.56
1:B:215:ASN:OD1	1:B:218:LYS:NZ	2.36	0.56
1:G:164:ASP:OD1	1:G:164:ASP:N	2.38	0.56
1:E:142:VAL:HG21	1:E:187:PHE:CG	2.41	0.56
1:F:121:LYS:HA	1:F:140:VAL:HG21	1.88	0.55
1:C:217:LEU:HD13	1:D:17:LEU:HD13	1.89	0.55
1:F:142:VAL:HG21	1:F:187:PHE:CG	2.42	0.54
1:D:96:ALA:O	4:D:301:HOH:O	2.19	0.53
1:D:111:ASN:ND2	1:D:114:ILE:H	2.07	0.53
1:B:76:LEU:HD23	1:B:79:LEU:HD12	1.91	0.53
1:B:90:PRO:HD2	1:B:101:ASP:O	2.09	0.53
1:E:177:ARG:HG2	2:E:301:CL:CL	2.46	0.53
1:E:47:ARG:HD2	1:E:86:TYR:CD1	2.44	0.52
1:A:69:ASP:HB3	1:H:199:ARG:HD3	1.91	0.52
1:A:142:VAL:HG21	1:A:187:PHE:CG	2.44	0.52
1:B:58:TYR:CD1	1:B:80:GLU:HA	2.44	0.52
1:F:100:LYS:HB2	1:F:125:ILE:HG13	1.92	0.51
1:D:108:PHE:O	1:D:116:GLU:HG3	2.09	0.51
1:E:142:VAL:HG21	1:E:187:PHE:CD2	2.46	0.51
1:E:215:ASN:HB3	1:E:218:LYS:HD2	1.92	0.51
1:E:165:LYS:HE3	1:G:129:GLU:HA	1.94	0.49
1:E:94:ASP:O	1:G:161:LYS:NZ	2.42	0.49
1:F:207:LEU:HD12	1:F:211:ASP:HB3	1.93	0.49
1:E:79:LEU:HD22	1:E:82:ILE:HD11	1.95	0.49
1:B:151:ILE:HA	1:B:175:ASN:HB3	1.94	0.49
1:A:215:ASN:HB3	1:A:218:LYS:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:LEU:HD12	1:H:79:LEU:HD12	1.94	0.48
1:C:134:ARG:NH2	1:C:191:GLY:O	2.45	0.48
1:F:58:TYR:CG	1:F:80:GLU:HA	2.48	0.48
1:A:142:VAL:HG21	1:A:187:PHE:CD2	2.49	0.48
1:D:111:ASN:HD22	1:D:114:ILE:H	1.60	0.48
1:F:111:ASN:HD21	1:F:114:ILE:HG23	1.78	0.48
1:B:215:ASN:HB3	1:B:218:LYS:HD2	1.94	0.48
1:D:159:LYS:O	1:D:159:LYS:HD3	2.14	0.48
1:G:58:TYR:CG	1:G:80:GLU:HA	2.49	0.48
1:D:130:ASP:N	1:D:130:ASP:OD1	2.47	0.47
1:E:58:TYR:CD1	1:E:80:GLU:HA	2.49	0.47
1:F:24:MET:O	1:F:28:GLU:HG3	2.14	0.47
1:H:190:THR:OG1	1:H:197:GLU:OE2	2.19	0.47
1:A:190:THR:OG1	1:A:197:GLU:OE2	2.23	0.47
1:D:142:VAL:HG21	1:D:187:PHE:CD2	2.49	0.47
1:G:142:VAL:HG21	1:G:187:PHE:CD2	2.49	0.47
1:H:79:LEU:HD22	1:H:82:ILE:HD11	1.96	0.47
1:B:58:TYR:CG	1:B:80:GLU:HA	2.50	0.47
1:D:76:LEU:HD22	2:E:301:CL:CL	2.52	0.47
1:G:111:ASN:HD21	1:G:114:ILE:HG23	1.80	0.47
1:B:47:ARG:HD3	1:B:86:TYR:CD1	2.51	0.46
1:D:111:ASN:ND2	1:D:113:TYR:H	2.14	0.46
1:D:111:ASN:OD1	1:D:112:PRO:HD2	2.15	0.46
1:E:151:ILE:O	1:E:179:GLY:HA3	2.16	0.46
1:C:30:GLU:OE2	1:D:34:TYR:OH	2.21	0.46
1:H:47:ARG:HD2	1:H:86:TYR:CD1	2.50	0.46
1:E:64:ASN:ND2	1:E:212:LEU:HD21	2.31	0.46
1:G:46:ARG:HD3	1:H:20:TRP:CH2	2.51	0.46
1:G:42:MET:O	1:H:20:TRP:NE1	2.46	0.45
1:D:47:ARG:HD3	1:D:86:TYR:CD1	2.51	0.45
1:F:119:ILE:HD13	1:F:142:VAL:HG22	1.97	0.45
1:D:84:ASP:HB3	1:D:107:THR:OG1	2.16	0.45
1:H:46:ARG:NH2	1:H:213:TYR:O	2.33	0.45
1:H:58:TYR:CG	1:H:80:GLU:HA	2.51	0.45
1:A:161:LYS:H	1:A:161:LYS:HG3	1.54	0.45
1:H:128:GLN:HE22	1:H:134:ARG:HE	1.65	0.45
2:A:301:CL:CL	2:A:302:CL:CL	3.09	0.45
1:B:160:TYR:OH	1:B:172:ASP:OD2	2.21	0.44
1:G:134:ARG:NH2	1:G:191:GLY:O	2.51	0.44
1:H:168:MET:HB2	1:H:173:LYS:HG3	1.98	0.44
1:B:111:ASN:ND2	1:B:114:ILE:H	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:VAL:HG21	1:B:187:PHE:CG	2.53	0.44
1:C:215:ASN:HB3	1:C:218:LYS:HD2	2.00	0.44
1:G:153:PRO:HB3	1:G:176:TYR:CE1	2.52	0.44
1:H:130:ASP:OD1	1:H:130:ASP:N	2.51	0.44
1:E:93:ASP:HB2	1:E:95:GLU:HG2	1.98	0.44
1:B:153:PRO:HB3	1:B:176:TYR:CE1	2.53	0.43
1:D:160:TYR:CE2	1:D:168:MET:HA	2.47	0.43
1:E:165:LYS:HB3	1:E:165:LYS:HE2	1.94	0.43
1:F:142:VAL:HG21	1:F:187:PHE:CD2	2.53	0.43
1:B:47:ARG:HG3	1:B:84:ASP:OD1	2.19	0.43
1:F:59:ILE:HD12	1:F:220:TYR:HE1	1.83	0.43
1:B:160:TYR:HE2	1:B:168:MET:HA	1.82	0.43
1:D:142:VAL:HG21	1:D:187:PHE:CG	2.53	0.43
1:E:207:LEU:HD12	1:E:211:ASP:HB3	2.00	0.43
1:A:70:TYR:CD2	1:A:204:LEU:HB2	2.53	0.43
1:C:100:LYS:HB2	1:C:125:ILE:HG13	2.00	0.43
1:E:35:ARG:NH2	2:E:302:CL:CL	2.79	0.43
1:H:50:LEU:HA	1:H:53:ILE:HD12	2.00	0.43
1:A:47:ARG:HD2	1:A:86:TYR:CG	2.53	0.43
1:G:123:PHE:CD1	1:G:137:SER:HB2	2.53	0.43
1:C:111:ASN:ND2	1:C:114:ILE:O	2.52	0.43
1:F:196:LYS:HE3	1:F:196:LYS:HB3	1.93	0.43
1:B:153:PRO:HB3	1:B:176:TYR:HE1	1.84	0.43
1:E:37:LYS:HG2	1:E:92:VAL:HA	2.01	0.43
1:G:151:ILE:O	1:G:179:GLY:HA3	2.19	0.43
1:B:142:VAL:HG21	1:B:187:PHE:CD2	2.54	0.42
1:A:64:ASN:ND2	1:A:212:LEU:HD21	2.33	0.42
1:B:111:ASN:HD21	1:B:114:ILE:H	1.66	0.42
1:H:142:VAL:HG21	1:H:187:PHE:CD2	2.54	0.42
1:B:83:ASP:OD1	1:B:107:THR:OG1	2.31	0.42
1:F:160:TYR:HE2	1:F:168:MET:HA	1.84	0.42
1:G:121:LYS:HD2	1:G:187:PHE:HA	2.01	0.42
1:D:70:TYR:HA	1:E:199:ARG:NH1	2.34	0.42
1:C:59:ILE:HD12	1:C:220:TYR:HE1	1.85	0.42
1:C:121:LYS:HA	1:C:140:VAL:HG21	2.02	0.42
1:F:47:ARG:HD3	1:F:86:TYR:CD1	2.54	0.42
1:F:151:ILE:HA	1:F:175:ASN:HB3	2.01	0.42
1:D:93:ASP:HB2	1:D:95:GLU:HG3	2.01	0.42
1:E:90:PRO:HD2	1:E:101:ASP:O	2.20	0.42
1:H:17:LEU:HD23	1:H:17:LEU:HA	1.92	0.42
1:H:111:ASN:HD21	1:H:114:ILE:HG23	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LYS:HA	1:A:140:VAL:HG21	2.01	0.42
1:G:207:LEU:HD12	1:G:211:ASP:HB3	2.00	0.42
1:H:12:LEU:O	1:H:16:LYS:HG3	2.20	0.42
1:B:5:ASP:OD1	1:B:5:ASP:N	2.53	0.41
1:B:207:LEU:HD12	1:B:211:ASP:HB3	2.02	0.41
1:F:130:ASP:O	1:F:130:ASP:CG	2.58	0.41
1:H:208:LEU:O	1:H:213:TYR:HB2	2.20	0.41
1:E:130:ASP:O	1:E:130:ASP:CG	2.58	0.41
1:B:32:GLU:OE2	1:B:35:ARG:NH2	2.45	0.41
1:D:160:TYR:OH	1:D:172:ASP:OD2	2.22	0.41
1:G:108:PHE:O	1:G:116:GLU:HG3	2.21	0.41
1:G:160:TYR:CE2	1:G:168:MET:HA	2.56	0.41
1:B:84:ASP:HB3	1:B:107:THR:OG1	2.20	0.41
1:C:58:TYR:CG	1:C:80:GLU:HA	2.56	0.41
1:D:151:ILE:O	1:D:179:GLY:HA3	2.20	0.41
1:H:186:TRP:CD1	1:H:204:LEU:HD23	2.56	0.41
1:B:111:ASN:ND2	1:B:114:ILE:HG22	2.29	0.41
1:H:121:LYS:HD2	1:H:187:PHE:HA	2.03	0.41
1:D:110:LYS:HA	1:D:116:GLU:HB2	2.03	0.41
1:E:134:ARG:NH2	1:E:191:GLY:O	2.48	0.41
1:A:10:LEU:O	1:A:14:LEU:HG	2.21	0.40
1:A:32:GLU:OE2	1:A:35:ARG:NH2	2.47	0.40
1:G:215:ASN:HB3	1:G:218:LYS:HD2	2.01	0.40
1:C:142:VAL:HG21	1:C:187:PHE:CD2	2.56	0.40
1:C:157:LYS:HE3	1:C:157:LYS:HB2	1.84	0.40
1:E:23:GLU:O	1:E:27:VAL:HG23	2.21	0.40
1:G:57:TRP:CD1	1:G:84:ASP:HA	2.57	0.40
1:G:215:ASN:OD1	1:G:218:LYS:NZ	2.48	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	219/235 (93%)	214 (98%)	5 (2%)	0	100	100
1	B	215/235 (92%)	213 (99%)	2 (1%)	0	100	100
1	C	220/235 (94%)	214 (97%)	6 (3%)	0	100	100
1	D	212/235 (90%)	209 (99%)	3 (1%)	0	100	100
1	E	218/235 (93%)	213 (98%)	5 (2%)	0	100	100
1	F	215/235 (92%)	210 (98%)	5 (2%)	0	100	100
1	G	217/235 (92%)	214 (99%)	3 (1%)	0	100	100
1	H	210/235 (89%)	207 (99%)	3 (1%)	0	100	100
All	All	1726/1880 (92%)	1694 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	202/216 (94%)	199 (98%)	3 (2%)	65	85
1	B	200/216 (93%)	196 (98%)	4 (2%)	55	80
1	C	203/216 (94%)	200 (98%)	3 (2%)	65	85
1	D	198/216 (92%)	195 (98%)	3 (2%)	65	85
1	E	201/216 (93%)	198 (98%)	3 (2%)	65	85
1	F	201/216 (93%)	194 (96%)	7 (4%)	36	68
1	G	201/216 (93%)	198 (98%)	3 (2%)	65	85
1	H	196/216 (91%)	193 (98%)	3 (2%)	65	85
All	All	1602/1728 (93%)	1573 (98%)	29 (2%)	59	82

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	GLU
1	A	130	ASP

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Mol	Chain	Res	Type
1	A	161	LYS
1	B	5	ASP
1	B	128	GLN
1	B	132	ASP
1	B	160	TYR
1	C	129	GLU
1	C	135	ILE
1	C	215	ASN
1	D	128	GLN
1	D	130	ASP
1	D	132	ASP
1	E	130	ASP
1	E	150	LYS
1	E	168	MET
1	F	3	GLU
1	F	95	GLU
1	F	123	PHE
1	F	130	ASP
1	F	158	GLU
1	F	160	TYR
1	F	224	LEU
1	G	158	GLU
1	G	164	ASP
1	G	165	LYS
1	H	128	GLN
1	H	130	ASP
1	H	160	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	111	ASN
1	D	26	GLN
1	D	111	ASN
1	F	128	GLN
1	G	11	GLN

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

### 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	221/235 (94%)	-0.16	1 (0%) 91 81	34, 55, 101, 117	0
1	B	219/235 (93%)	0.15	2 (0%) 84 69	53, 91, 123, 134	0
1	C	222/235 (94%)	-0.19	1 (0%) 91 81	42, 62, 98, 120	0
1	D	216/235 (91%)	-0.08	3 (1%) 75 56	43, 68, 102, 129	0
1	E	220/235 (93%)	-0.17	2 (0%) 84 69	42, 66, 112, 124	0
1	F	219/235 (93%)	-0.06	2 (0%) 84 69	67, 90, 110, 128	0
1	G	219/235 (93%)	-0.03	5 (2%) 60 39	49, 79, 111, 121	0
1	H	214/235 (91%)	-0.02	4 (1%) 66 46	52, 82, 112, 133	0
All	All	1750/1880 (93%)	-0.07	20 (1%) 80 64	34, 75, 112, 134	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	ALA	5.4
1	A	165	LYS	4.3
1	C	96	ALA	4.0
1	G	167	ASP	3.5
1	F	157	LYS	3.4
1	E	165	LYS	2.8
1	E	9	ARG	2.7
1	G	164	ASP	2.5
1	H	160	TYR	2.4
1	G	163	LYS	2.3
1	G	95	GLU	2.3
1	D	126	VAL	2.2
1	B	159	LYS	2.2
1	F	156	ILE	2.1
1	G	217	LEU	2.1
1	D	221	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	130	ASP	2.1
1	H	158	GLU	2.0
1	H	156	ILE	2.0
1	H	172	ASP	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	E	302	1/1	0.50	0.17	68,68,68,68	0
3	NA	B	301	1/1	0.82	0.28	74,74,74,74	0
3	NA	F	301	1/1	0.83	0.42	53,53,53,53	0
2	CL	E	301	1/1	0.86	0.20	71,71,71,71	0
3	NA	G	301	1/1	0.87	0.35	74,74,74,74	0
3	NA	B	303	1/1	0.90	0.43	41,41,41,41	0
2	CL	A	302	1/1	0.91	0.19	50,50,50,50	0
3	NA	C	302	1/1	0.91	0.16	46,46,46,46	0
3	NA	C	301	1/1	0.94	0.36	75,75,75,75	0
2	CL	A	301	1/1	0.94	0.12	48,48,48,48	0
3	NA	H	301	1/1	0.94	0.12	72,72,72,72	0
3	NA	B	302	1/1	0.98	0.45	50,50,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.