



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:21 PM GMT

PDB ID : 3WXG  
Title : Crystal structure of CYLD USP domain (C596A) in complex with Lys63-linked diubiquitin  
Authors : Sato, Y.; Fukai, S.  
Deposited on : 2014-07-30  
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  
<http://wwpdb.org/validation/2016/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  
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

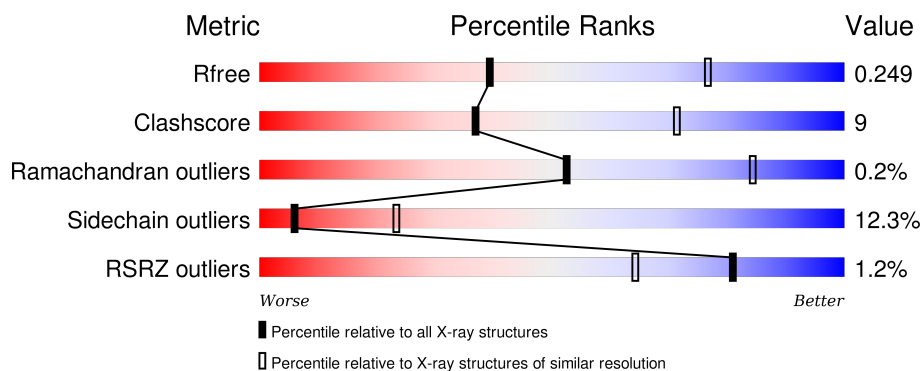
# 1 Overall quality at a glance

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  $\geq 3$ , 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  $\leq 5\%$ . 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	312	<div> <div style="width: 65%;"></div> <div style="width: 28%;"></div> <div style="width: 7%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div>
1	D	312	<div> <div style="width: 66%;"></div> <div style="width: 27%;"></div> <div style="width: 7%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div>
2	B	76	<div> <div style="width: 3%;"></div> <div style="width: 80%;"></div> <div style="width: 20%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div>
2	E	76	<div> <div style="width: 11%;"></div> <div style="width: 80%;"></div> <div style="width: 18%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div>
3	C	72	<div> <div style="width: 74%;"></div> <div style="width: 26%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div>

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Mol	Chain	Length	Quality of chain
3	F	72	 A horizontal bar chart showing the quality of chain F. The bar is divided into two segments: a green segment on the left representing 68% and a yellow segment on the right representing 31%. A small red dot is at the far right end of the bar.

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7218 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2432	1566	398	447	21			
1	D	300	Total	C	N	O	S	0	0	0
			2432	1566	398	447	21			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	SER	-	EXPRESSION TAG	UNP E7FEV5
A	576	HIS	-	EXPRESSION TAG	UNP E7FEV5
A	577	MET	-	EXPRESSION TAG	UNP E7FEV5
A	596	ALA	CYS	ENGINEERED MUTATION	UNP E7FEV5
A	781	LEU	-	LINKER	UNP E7FEV5
A	782	GLU	-	LINKER	UNP E7FEV5
A	783	GLY	-	LINKER	UNP E7FEV5
A	784	GLY	-	LINKER	UNP E7FEV5
D	575	SER	-	EXPRESSION TAG	UNP E7FEV5
D	576	HIS	-	EXPRESSION TAG	UNP E7FEV5
D	577	MET	-	EXPRESSION TAG	UNP E7FEV5
D	596	ALA	CYS	ENGINEERED MUTATION	UNP E7FEV5
D	781	LEU	-	LINKER	UNP E7FEV5
D	782	GLU	-	LINKER	UNP E7FEV5
D	783	GLY	-	LINKER	UNP E7FEV5
D	784	GLY	-	LINKER	UNP E7FEV5

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	0	0
			603	378	107	117	1			
2	E	76	Total	C	N	O	S	0	0	0
			603	378	107	117	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	63	ARG	LYS	ENGINEERED MUTATION	UNP P0CG50
E	63	ARG	LYS	ENGINEERED MUTATION	UNP P0CG50

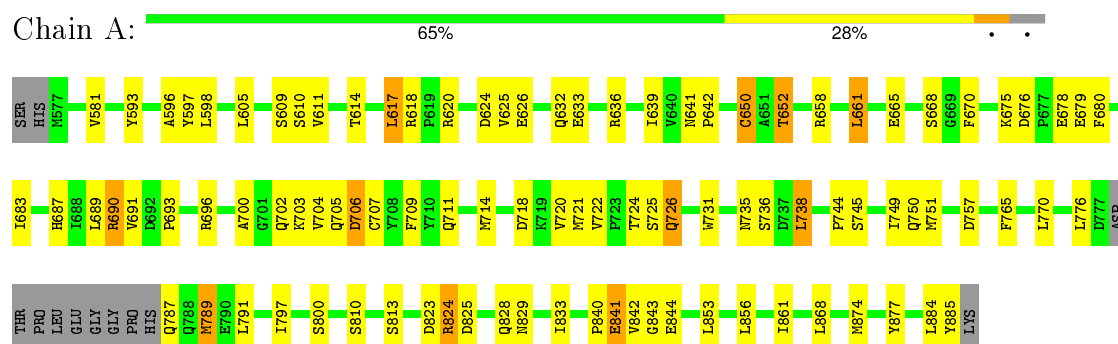
- Molecule 3 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	72	Total	C	N	O	S	0	0	0
			574	362	98	113	1			
3	F	72	Total	C	N	O	S	0	0	0
			574	362	98	113	1			

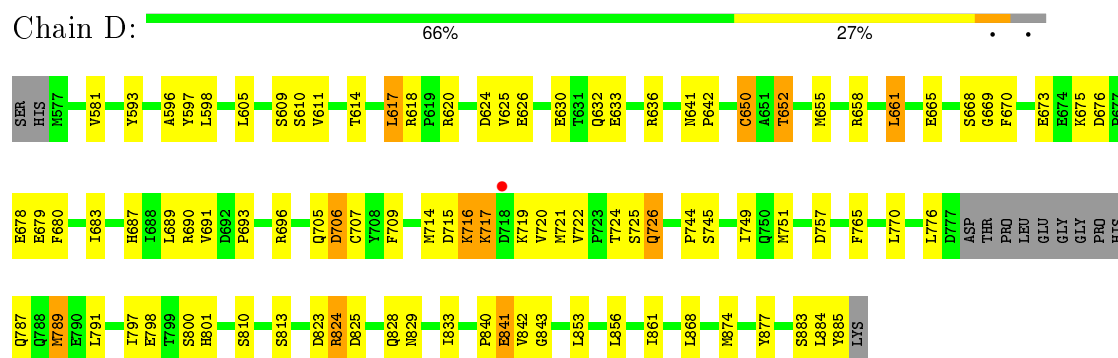
### 3 Residue-property plots [i](#)

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.

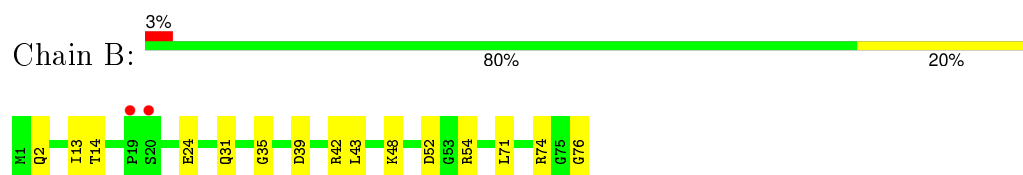
- Molecule 1: Uncharacterized protein



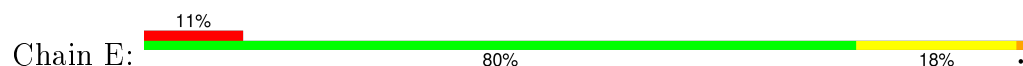
- Molecule 1: Uncharacterized protein



- Molecule 2: Ubiquitin



- Molecule 2: Ubiquitin





- Molecule 3: Ubiquitin



- Molecule 3: Ubiquitin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.02Å 65.66Å 69.82Å 103.49° 89.86° 90.61°	Depositor
Resolution (Å)	41.89 – 3.10 41.89 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.7 (41.89-3.10) 87.2 (41.89-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.188 , 0.246 0.193 , 0.249	Depositor DCC
$R_{free}$ test set	758 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 22.6	EDS
Estimated twinning fraction	0.337 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 15166 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% 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, 0.375 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	0.57	0/2486	0.75	0/3351
1	D	0.57	0/2486	0.75	0/3351
2	B	0.39	0/609	0.68	0/819
2	E	0.36	0/609	0.68	1/819 (0.1%)
3	C	0.43	0/580	0.71	0/781
3	F	0.42	0/580	0.68	0/781
All	All	0.52	0/7350	0.73	1/9902 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	42	ARG	NE-CZ-NH1	5.10	122.85	120.30

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	2432	0	2423	61	0
1	D	2432	0	2423	58	0
2	B	603	0	629	5	0
2	E	603	0	629	6	0
3	C	574	0	596	8	0
3	F	574	0	597	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7218	0	7297	136	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 9.

All (136) 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:736:SER:O	1:A:738:LEU:HG	1.58	1.03
1:A:665:GLU:HB3	1:A:668:SER:OG	1.76	0.86
1:D:665:GLU:HB3	1:D:668:SER:OG	1.77	0.85
1:D:632:GLN:OE1	1:D:636:ARG:NH1	2.12	0.81
1:A:632:GLN:OE1	1:A:636:ARG:NH1	2.13	0.81
1:D:689:LEU:O	1:D:691:VAL:HG23	1.82	0.78
1:D:800:SER:OG	3:F:1:MET:N	2.16	0.78
3:F:63:LYS:O	3:F:64:GLU:HB2	1.87	0.74
1:D:705:GLN:CD	2:E:48:LYS:HG3	2.15	0.67
1:D:798:GLU:HB3	3:F:16:GLU:OE1	1.99	0.63
1:A:593:TYR:O	1:A:658:ARG:NH2	2.32	0.62
1:A:665:GLU:HB3	1:A:668:SER:HG	1.62	0.62
1:D:593:TYR:O	1:D:658:ARG:NH2	2.32	0.62
1:D:842:VAL:HG13	1:D:868:LEU:HD22	1.81	0.62
1:D:689:LEU:O	1:D:691:VAL:N	2.33	0.61
1:A:689:LEU:O	1:A:690:ARG:C	2.39	0.61
1:A:665:GLU:CB	1:A:668:SER:OG	2.48	0.61
1:D:665:GLU:CB	1:D:668:SER:OG	2.48	0.61
1:A:689:LEU:O	1:A:691:VAL:HG23	2.01	0.61
1:A:842:VAL:HG13	1:A:868:LEU:HD22	1.83	0.60
1:D:665:GLU:HB3	1:D:668:SER:HG	1.63	0.60
1:D:716:LYS:HD2	1:D:717:LYS:N	2.17	0.60
1:D:650:CYS:HB2	1:D:652:THR:OG1	2.01	0.60
1:A:650:CYS:HB2	1:A:652:THR:OG1	2.01	0.59
1:A:658:ARG:NH1	1:A:670:PHE:O	2.35	0.59
1:A:791:LEU:HB2	1:A:877:TYR:CE2	2.37	0.58
1:D:791:LEU:HB2	1:D:877:TYR:CE2	2.39	0.57
1:D:658:ARG:NH1	1:D:670:PHE:O	2.37	0.57
1:D:801:HIS:N	3:F:16:GLU:OE2	2.38	0.56
1:A:736:SER:O	1:A:738:LEU:CG	2.46	0.55
1:A:720:VAL:HG22	1:A:721:MET:H	1.71	0.55
1:D:689:LEU:O	1:D:690:ARG:C	2.43	0.55
1:A:700:ALA:HB3	1:A:702:GLN:OE1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:THR:HG1	3:C:9:THR:HG1	1.55	0.54
3:F:7:THR:HG1	3:F:9:THR:HG1	1.55	0.54
1:D:724:THR:HA	1:D:765:PHE:O	2.08	0.54
1:D:842:VAL:HG13	1:D:868:LEU:CD2	2.37	0.54
1:A:683:ILE:O	1:A:687:HIS:HB2	2.07	0.54
1:A:724:THR:HA	1:A:765:PHE:O	2.09	0.53
1:D:720:VAL:HG22	1:D:721:MET:H	1.73	0.53
1:A:618:ARG:O	1:A:632:GLN:NE2	2.42	0.53
1:D:683:ILE:O	1:D:687:HIS:HB2	2.08	0.53
1:A:842:VAL:HG13	1:A:868:LEU:CD2	2.38	0.52
1:D:596:ALA:HB3	2:E:76:GLY:HA2	1.92	0.52
1:A:828:GLN:HG3	1:A:829:ASN:HD22	1.74	0.52
3:C:1:MET:O	3:C:1:MET:HG3	2.10	0.52
3:C:1:MET:HA	3:C:63:LYS:HD2	1.92	0.51
1:D:618:ARG:O	1:D:632:GLN:NE2	2.43	0.51
1:D:609:SER:OG	1:D:610:SER:N	2.44	0.51
1:A:609:SER:OG	1:A:610:SER:N	2.45	0.50
3:F:1:MET:HB3	3:F:17:VAL:O	2.12	0.50
1:D:828:GLN:HG3	1:D:829:ASN:HD22	1.77	0.49
1:D:823:ASP:O	1:D:833:ILE:N	2.45	0.49
1:A:823:ASP:O	1:A:833:ILE:N	2.45	0.49
1:A:597:TYR:CZ	1:A:675:LYS:HB2	2.47	0.49
1:D:884:LEU:O	1:D:885:TYR:HB3	2.12	0.48
1:D:706:ASP:N	1:D:706:ASP:OD1	2.45	0.48
1:D:618:ARG:NH1	1:D:624:ASP:OD1	2.47	0.48
3:F:2:GLN:H	3:F:63:LYS:HG3	1.78	0.48
1:A:718:ASP:OD1	1:A:718:ASP:N	2.46	0.48
1:A:596:ALA:HB3	2:B:76:GLY:HA2	1.95	0.48
1:D:597:TYR:CZ	1:D:675:LYS:HB2	2.49	0.47
1:A:618:ARG:NH1	1:A:624:ASP:OD1	2.48	0.47
1:D:726:GLN:HG2	1:D:770:LEU:HD12	1.95	0.47
1:D:840:PRO:O	1:D:843:GLY:N	2.48	0.47
1:D:625:VAL:HG12	1:D:626:GLU:H	1.79	0.47
1:A:706:ASP:N	1:A:706:ASP:OD1	2.47	0.47
1:A:884:LEU:O	1:A:885:TYR:HB3	2.15	0.47
2:E:31:GLN:O	2:E:35:GLY:N	2.45	0.47
1:A:617:LEU:O	1:A:618:ARG:C	2.53	0.47
1:A:726:GLN:HG2	1:A:770:LEU:HD12	1.96	0.47
1:D:597:TYR:CD1	1:D:597:TYR:C	2.88	0.46
1:D:715:ASP:C	1:D:715:ASP:OD1	2.53	0.46
1:A:641:ASN:HB2	1:A:642:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:823:ASP:OD1	1:D:824:ARG:N	2.48	0.46
2:B:31:GLN:O	2:B:35:GLY:N	2.46	0.46
1:A:625:VAL:HG12	1:A:626:GLU:H	1.81	0.46
1:A:693:PRO:CB	1:A:706:ASP:HB3	2.46	0.45
1:A:800:SER:OG	3:C:1:MET:N	2.33	0.45
3:C:1:MET:HB2	3:C:63:LYS:HB2	1.98	0.45
1:D:641:ASN:HB2	1:D:642:PRO:HD3	1.98	0.45
1:A:720:VAL:HG22	1:A:721:MET:N	2.31	0.45
1:A:597:TYR:CE2	1:A:675:LYS:HB2	2.51	0.45
1:D:625:VAL:HG12	1:D:626:GLU:N	2.32	0.45
1:D:617:LEU:O	1:D:618:ARG:C	2.55	0.45
1:A:597:TYR:CD1	1:A:597:TYR:C	2.90	0.45
3:C:63:LYS:O	3:C:64:GLU:CG	2.65	0.45
1:D:856:LEU:HD23	1:D:861:ILE:HG12	1.99	0.44
1:A:618:ARG:NH1	1:A:624:ASP:CG	2.71	0.44
1:A:714:MET:HE1	1:A:731:TRP:HE3	1.82	0.44
1:D:693:PRO:CB	1:D:706:ASP:HB3	2.48	0.44
1:A:625:VAL:HG12	1:A:626:GLU:N	2.33	0.44
1:D:842:VAL:CG1	1:D:868:LEU:HD22	2.46	0.44
1:D:658:ARG:O	1:D:661:LEU:HB2	2.18	0.44
1:A:705:GLN:OE1	1:A:705:GLN:HA	2.18	0.44
3:C:24:GLU:HG3	3:C:52:ASP:HB3	2.00	0.44
1:D:720:VAL:HG22	1:D:721:MET:N	2.33	0.44
3:F:24:GLU:HG3	3:F:52:ASP:HB3	2.00	0.44
1:D:705:GLN:OE1	2:E:48:LYS:HG3	2.18	0.43
1:A:658:ARG:O	1:A:661:LEU:HB2	2.18	0.43
1:A:744:PRO:O	1:A:789:MET:HE3	2.18	0.43
1:A:856:LEU:HD23	1:A:861:ILE:HG12	2.00	0.43
1:D:597:TYR:CE2	1:D:675:LYS:HB2	2.53	0.43
2:E:24:GLU:HG3	2:E:52:ASP:HB3	2.01	0.43
1:D:678:GLU:OE2	2:E:72:ARG:NE	2.44	0.43
1:D:598:LEU:CD1	1:D:680:PHE:CZ	3.02	0.43
1:A:618:ARG:NH1	1:A:624:ASP:OD2	2.52	0.43
1:D:678:GLU:HG2	1:D:709:PHE:HZ	1.83	0.43
1:A:823:ASP:OD1	1:A:824:ARG:N	2.50	0.43
1:D:840:PRO:O	1:D:841:GLU:C	2.57	0.42
1:D:618:ARG:NH1	1:D:624:ASP:CG	2.73	0.42
1:A:842:VAL:CG1	1:A:868:LEU:HD22	2.48	0.42
1:D:744:PRO:O	1:D:789:MET:HE3	2.19	0.42
1:A:840:PRO:O	1:A:841:GLU:C	2.58	0.42
1:D:813:SER:HB2	1:D:840:PRO:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:GLU:HG3	2:B:52:ASP:HB3	2.02	0.42
1:A:678:GLU:HG2	1:A:709:PHE:HZ	1.84	0.42
1:A:844:GLU:HG3	3:F:70:VAL:HG11	2.01	0.42
1:A:676:ASP:O	1:A:679:GLU:N	2.53	0.42
1:A:598:LEU:CD1	1:A:680:PHE:CZ	3.03	0.42
1:A:703:LYS:HE3	1:A:704:VAL:HG22	2.01	0.41
1:A:639:ILE:C	1:A:642:PRO:HD2	2.41	0.41
1:A:750:GLN:HE21	1:A:874:MET:CE	2.34	0.41
1:A:658:ARG:HD2	1:A:670:PHE:O	2.21	0.41
3:F:31:GLN:O	3:F:35:GLY:N	2.47	0.41
1:D:676:ASP:O	1:D:679:GLU:N	2.54	0.41
3:C:31:GLN:O	3:C:35:GLY:N	2.47	0.41
1:D:618:ARG:NH1	1:D:624:ASP:OD2	2.54	0.41
1:A:749:ILE:O	1:A:874:MET:HA	2.21	0.41
1:A:679:GLU:CD	2:B:74:ARG:HH11	2.24	0.41
1:D:749:ILE:O	1:D:874:MET:HA	2.21	0.40
1:A:840:PRO:O	1:A:843:GLY:N	2.49	0.40
1:D:655:MET:HA	1:D:658:ARG:HG3	2.03	0.40
1:D:669:GLY:O	1:D:673:GLU:HB2	2.21	0.40
1:A:813:SER:HB2	1:A:840:PRO:HB3	2.02	0.40
1:A:711:GLN:OE1	2:B:42:ARG:NH1	2.55	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	296/312 (95%)	263 (89%)	32 (11%)	1 (0%)	46	80
1	D	296/312 (95%)	265 (90%)	30 (10%)	1 (0%)	46	80
2	B	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
2	E	74/76 (97%)	73 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	70/72 (97%)	70 (100%)	0	0	100	100
3	F	70/72 (97%)	69 (99%)	1 (1%)	0	100	100
All	All	880/920 (96%)	813 (92%)	65 (7%)	2 (0%)	52	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	797	ILE
1	D	797	ILE

### 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	271/281 (96%)	241 (89%)	30 (11%)	8	29
1	D	271/281 (96%)	238 (88%)	33 (12%)	6	24
2	B	68/68 (100%)	60 (88%)	8 (12%)	6	25
2	E	68/68 (100%)	60 (88%)	8 (12%)	6	25
3	C	66/66 (100%)	56 (85%)	10 (15%)	3	14
3	F	66/66 (100%)	55 (83%)	11 (17%)	3	11
All	All	810/830 (98%)	710 (88%)	100 (12%)	6	23

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	581	VAL
1	A	605	LEU
1	A	611	VAL
1	A	614	THR
1	A	617	LEU
1	A	620	ARG
1	A	633	GLU
1	A	650	CYS

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Mol	Chain	Res	Type
1	A	652	THR
1	A	661	LEU
1	A	690	ARG
1	A	696	ARG
1	A	706	ASP
1	A	707	CYS
1	A	722	VAL
1	A	725	SER
1	A	726	GLN
1	A	735	ASN
1	A	738	LEU
1	A	745	SER
1	A	751	MET
1	A	757	ASP
1	A	776	LEU
1	A	787	GLN
1	A	789	MET
1	A	810	SER
1	A	824	ARG
1	A	825	ASP
1	A	841	GLU
1	A	853	LEU
2	B	2	GLN
2	B	13	ILE
2	B	14	THR
2	B	39	ASP
2	B	43	LEU
2	B	48	LYS
2	B	54	ARG
2	B	71	LEU
3	C	2	GLN
3	C	13	ILE
3	C	14	THR
3	C	39	ASP
3	C	42	ARG
3	C	43	LEU
3	C	48	LYS
3	C	54	ARG
3	C	71	LEU
3	C	72	ARG
1	D	581	VAL
1	D	605	LEU

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Mol	Chain	Res	Type
1	D	611	VAL
1	D	614	THR
1	D	617	LEU
1	D	620	ARG
1	D	630	GLU
1	D	633	GLU
1	D	650	CYS
1	D	652	THR
1	D	661	LEU
1	D	696	ARG
1	D	706	ASP
1	D	707	CYS
1	D	714	MET
1	D	716	LYS
1	D	717	LYS
1	D	719	LYS
1	D	722	VAL
1	D	725	SER
1	D	726	GLN
1	D	745	SER
1	D	751	MET
1	D	757	ASP
1	D	776	LEU
1	D	787	GLN
1	D	789	MET
1	D	810	SER
1	D	824	ARG
1	D	825	ASP
1	D	841	GLU
1	D	853	LEU
1	D	883	SER
2	E	2	GLN
2	E	13	ILE
2	E	14	THR
2	E	39	ASP
2	E	43	LEU
2	E	48	LYS
2	E	54	ARG
2	E	71	LEU
3	F	2	GLN
3	F	13	ILE
3	F	14	THR

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Mol	Chain	Res	Type
3	F	39	ASP
3	F	42	ARG
3	F	43	LEU
3	F	48	LYS
3	F	54	ARG
3	F	62	GLN
3	F	71	LEU
3	F	72	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	750	GLN
1	A	829	ASN
2	B	60	ASN
2	B	62	GLN
3	C	60	ASN
3	C	62	GLN
1	D	750	GLN
1	D	829	ASN
2	E	60	ASN
2	E	62	GLN
3	F	60	ASN
3	F	62	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<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	300/312 (96%)	-0.49	0 100 100	28, 48, 84, 116	0
1	D	300/312 (96%)	-0.48	1 (0%) 94 88	26, 49, 87, 119	0
2	B	76/76 (100%)	0.17	2 (2%) 59 35	60, 83, 113, 124	0
2	E	76/76 (100%)	0.67	8 (10%) 8 3	59, 96, 125, 136	0
3	C	72/72 (100%)	-0.34	0 100 100	36, 62, 82, 94	0
3	F	72/72 (100%)	-0.29	0 100 100	41, 63, 84, 91	0
All	All	896/920 (97%)	-0.30	11 (1%) 81 64	26, 56, 104, 136	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	10	GLY	3.2
2	B	20	SER	2.7
1	D	718	ASP	2.7
2	E	19	PRO	2.5
2	E	54	ARG	2.5
2	E	65	SER	2.5
2	E	3	ILE	2.4
2	B	19	PRO	2.3
2	E	25	ASN	2.3
2	E	59	TYR	2.2
2	E	45	PHE	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 [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.