



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 01:46 AM GMT

PDB ID : 1OSC  
Title : Crystal structure of rat CUTA1 at 2.15 Å resolution  
Authors : Arnesano, F.; Banci, L.; Benvenuti, M.; Bertini, I.; Calderone, V.; Mangani, S.; Viezzoli, M.S.; Structural Proteomics in Europe (SPINE)  
Deposited on : 2003-03-19  
Resolution : 2.15 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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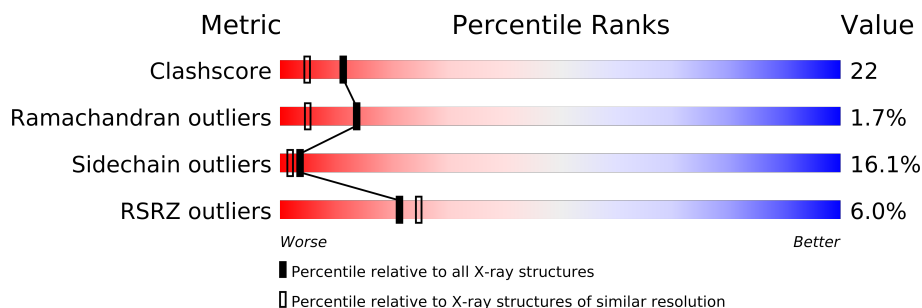
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.15 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))
Clashscore	79885	1299 (2.18-2.14)
Ramachandran outliers	78287	1272 (2.18-2.14)
Sidechain outliers	78261	1272 (2.18-2.14)
RSRZ outliers	66119	1094 (2.18-2.14)

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	126	
1	B	126	
1	C	126	
1	D	126	
1	E	126	
1	F	126	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5495 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 similar to divalent cation tolerant protein CUTA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	108	Total	C	N	O	S	0	0	0
			844	544	138	158	4			
1	B	109	Total	C	N	O	S	0	0	0
			852	549	139	160	4			
1	C	108	Total	C	N	O	S	0	0	0
			844	544	138	158	4			
1	D	109	Total	C	N	O	S	0	0	0
			848	546	139	159	4			
1	E	110	Total	C	N	O	S	0	0	0
			845	542	140	159	4			
1	F	111	Total	C	N	O	S	0	0	0
			857	551	141	161	4			

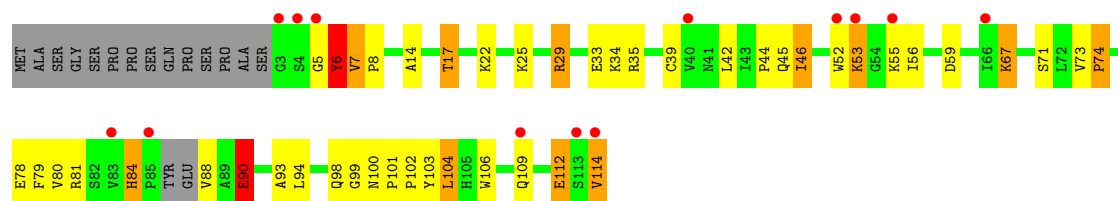
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	63	Total	O	0	0
			63	63		
2	B	85	Total	O	0	0
			85	85		
2	C	69	Total	O	0	0
			69	69		
2	D	69	Total	O	0	0
			69	69		
2	E	64	Total	O	0	0
			64	64		
2	F	55	Total	O	0	0
			55	55		



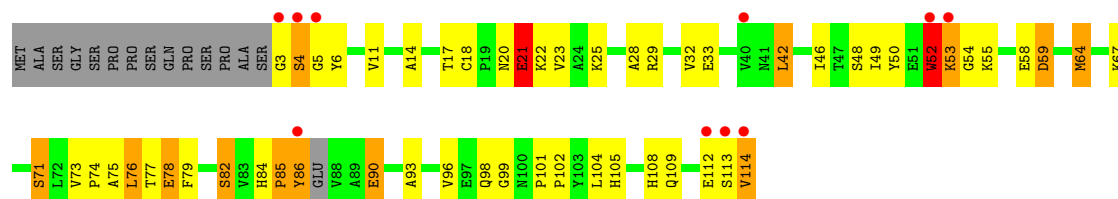
- Molecule 1: similar to divalent cation tolerant protein CUTA

Chain E: 



- Molecule 1: similar to divalent cation tolerant protein CUTA

Chain F: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.39Å 88.29Å 125.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.15 19.95 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.15) 100.0 (19.95-2.15)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.189 , 0.260 0.207 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	44.7	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 43312 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5495	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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	1.70	8/864 (0.9%)	1.65	9/1181 (0.8%)
1	B	1.67	7/872 (0.8%)	1.45	6/1191 (0.5%)
1	C	1.56	5/864 (0.6%)	1.38	10/1181 (0.8%)
1	D	1.64	11/868 (1.3%)	1.46	11/1186 (0.9%)
1	E	1.59	3/863 (0.3%)	1.36	6/1176 (0.5%)
1	F	1.56	5/876 (0.6%)	1.32	7/1194 (0.6%)
All	All	1.62	39/5207 (0.7%)	1.44	49/7109 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	3
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	3
All	All	0	14

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	6	TYR	C-N	20.41	1.81	1.34
1	A	84	HIS	C-N	-15.13	1.05	1.34
1	D	87	GLU	C-N	-11.54	1.07	1.34
1	B	87	GLU	C-N	-11.45	1.07	1.34
1	A	11	VAL	CB-CG2	8.07	1.69	1.52
1	B	91	VAL	CB-CG2	7.66	1.69	1.52
1	D	78	GLU	CD-OE1	7.60	1.34	1.25
1	A	73	VAL	CB-CG1	7.09	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	52	TRP	CB-CG	7.09	1.63	1.50
1	C	11	VAL	C-O	6.88	1.36	1.23
1	F	73	VAL	CB-CG1	6.72	1.67	1.52
1	F	11	VAL	CB-CG2	6.59	1.66	1.52
1	C	13	ALA	CA-CB	6.56	1.66	1.52
1	C	11	VAL	CB-CG2	6.45	1.66	1.52
1	A	103	TYR	CB-CG	-6.40	1.42	1.51
1	E	73	VAL	CB-CG2	6.26	1.66	1.52
1	D	34	LYS	CD-CE	6.11	1.66	1.51
1	A	58	GLU	CD-OE2	6.02	1.32	1.25
1	C	96	VAL	CB-CG1	-5.94	1.40	1.52
1	B	15	PHE	CD1-CE1	5.86	1.50	1.39
1	B	96	VAL	CB-CG1	5.77	1.65	1.52
1	A	6	TYR	N-CA	5.55	1.57	1.46
1	A	16	VAL	CB-CG1	-5.44	1.41	1.52
1	B	86	TYR	CE1-CZ	5.42	1.45	1.38
1	E	7	VAL	CB-CG1	5.41	1.64	1.52
1	C	6	TYR	CB-CG	5.37	1.59	1.51
1	D	96	VAL	CB-CG1	5.37	1.64	1.52
1	D	46	ILE	CB-CG2	5.35	1.69	1.52
1	A	73	VAL	CA-CB	-5.30	1.43	1.54
1	B	29	ARG	NE-CZ	5.28	1.40	1.33
1	D	78	GLU	CG-CD	5.28	1.59	1.51
1	D	90	GLU	CD-OE2	5.26	1.31	1.25
1	F	21	GLU	CD-OE1	5.26	1.31	1.25
1	D	109	GLN	CG-CD	5.22	1.63	1.51
1	D	14	ALA	CA-CB	5.15	1.63	1.52
1	F	6	TYR	CE2-CZ	-5.15	1.31	1.38
1	D	6	TYR	CE2-CZ	5.03	1.45	1.38
1	B	64	MET	CG-SD	5.02	1.94	1.81
1	F	90	GLU	CD-OE2	5.02	1.31	1.25

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	HIS	O-C-N	-24.76	74.05	121.10
1	B	87	GLU	O-C-N	-20.68	89.61	122.70
1	D	87	GLU	O-C-N	-19.70	91.18	122.70
1	A	84	HIS	CA-C-N	14.48	157.64	117.10
1	A	84	HIS	CA-CB-CG	14.15	137.65	113.60
1	E	6	TYR	CA-C-N	-14.06	86.27	117.20
1	B	87	GLU	CA-C-N	12.55	144.81	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	87	GLU	CA-C-N	11.68	142.89	117.20
1	E	6	TYR	O-C-N	11.43	140.99	122.70
1	F	64	MET	CG-SD-CE	-9.99	84.21	100.20
1	C	59	ASP	CB-CG-OD2	9.16	126.55	118.30
1	A	94	LEU	CA-CB-CG	-7.56	97.91	115.30
1	C	76	LEU	CA-CB-CG	7.42	132.37	115.30
1	A	59	ASP	CB-CG-OD2	7.41	124.97	118.30
1	A	84	HIS	N-CA-C	7.40	130.99	111.00
1	F	71	SER	CA-CB-OG	-6.95	92.42	111.20
1	C	87	GLU	O-C-N	-6.89	111.68	122.70
1	E	59	ASP	CB-CG-OD2	6.84	124.45	118.30
1	C	76	LEU	CB-CG-CD2	6.73	122.44	111.00
1	D	59	ASP	CB-CG-OD2	6.67	124.30	118.30
1	F	76	LEU	CB-CG-CD2	6.58	122.19	111.00
1	E	29	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	F	76	LEU	CA-CB-CG	6.24	129.65	115.30
1	A	104	LEU	CB-CG-CD1	6.08	121.33	111.00
1	D	11	VAL	CG1-CB-CG2	-5.88	101.48	110.90
1	D	104	LEU	CB-CG-CD1	5.88	121.00	111.00
1	A	104	LEU	CB-CG-CD2	5.85	120.95	111.00
1	F	82	SER	CB-CA-C	-5.76	99.16	110.10
1	F	59	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	76	LEU	CA-CB-CG	5.68	128.36	115.30
1	D	76	LEU	CA-CB-CG	5.67	128.34	115.30
1	D	87	GLU	C-N-CA	5.65	135.83	121.70
1	C	42	LEU	CB-CG-CD1	-5.56	101.55	111.00
1	F	59	ASP	CB-CG-OD1	-5.54	113.32	118.30
1	C	59	ASP	CB-CG-OD1	-5.53	113.33	118.30
1	C	91	VAL	CG1-CB-CG2	5.52	119.73	110.90
1	E	104	LEU	CB-CG-CD1	5.45	120.26	111.00
1	C	88	VAL	CA-CB-CG2	5.44	119.06	110.90
1	C	81	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	E	6	TYR	CB-CA-C	5.30	120.99	110.40
1	C	87	GLU	N-CA-CB	5.27	120.09	110.60
1	D	35	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	B	72	LEU	CB-CG-CD1	5.23	119.89	111.00
1	B	59	ASP	CB-CG-OD1	5.13	122.92	118.30
1	D	76	LEU	CB-CG-CD2	5.09	119.66	111.00
1	D	91	VAL	CG1-CB-CG2	-5.08	102.78	110.90
1	D	67	LYS	CB-CA-C	-5.06	100.28	110.40
1	B	17	THR	OG1-CB-CG2	-5.02	98.45	110.00
1	B	29	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	GLU	Peptide
1	A	83	VAL	Peptide
1	A	84	HIS	Mainchain
1	A	85	PRO	Peptide
1	B	112	GLU	Peptide
1	B	87	GLU	Mainchain,Peptide
1	C	87	GLU	Mainchain
1	C	88	VAL	Mainchain
1	D	87	GLU	Mainchain
1	E	84	HIS	Peptide
1	F	52	TRP	Peptide
1	F	77	THR	Peptide
1	F	85	PRO	Peptide

## 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	844	0	853	43	0
1	B	852	0	861	45	0
1	C	844	0	853	45	0
1	D	848	0	855	47	0
1	E	845	0	856	41	0
1	F	857	0	866	46	0
2	A	63	0	0	10	0
2	B	85	0	0	14	0
2	C	69	0	0	5	0
2	D	69	0	0	12	0
2	E	64	0	0	5	0
2	F	55	0	0	10	0
All	All	5495	0	5144	228	0

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 22.

All (228) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:6:TYR:C	1:E:7:VAL:N	1.81	1.34
1:F:114:VAL:HG21	2:F:168:HOH:O	1.40	1.20
1:D:29:ARG:HD3	2:D:166:HOH:O	1.45	1.15
1:D:53:LYS:HB3	1:D:53:LYS:NZ	1.61	1.12
1:D:53:LYS:HB3	1:D:53:LYS:HZ2	1.04	1.10
1:A:90:GLU:HG2	1:C:103:TYR:CE1	1.89	1.06
1:B:29:ARG:HD2	2:B:166:HOH:O	1.60	0.99
1:B:39:CYS:HB2	2:B:197:HOH:O	1.64	0.98
1:E:6:TYR:CA	1:E:7:VAL:N	2.29	0.95
1:A:39:CYS:HB2	2:A:174:HOH:O	1.65	0.95
1:E:6:TYR:HA	1:E:7:VAL:N	1.80	0.94
1:A:86:TYR:HD2	1:A:87:GLU:H	0.93	0.93
1:A:84:HIS:HD2	1:A:86:TYR:O	1.51	0.92
1:D:90:GLU:HG3	1:E:103:TYR:CZ	2.04	0.91
1:E:114:VAL:HG22	2:E:160:HOH:O	1.70	0.90
1:B:113:SER:HA	2:B:180:HOH:O	1.71	0.89
1:B:108:HIS:CE1	1:B:112:GLU:HG3	2.10	0.87
1:C:17:THR:HG22	1:C:90:GLU:CD	1.96	0.86
1:F:4:SER:HA	2:F:156:HOH:O	1.75	0.85
1:F:101:PRO:HD2	1:F:102:PRO:HD2	1.64	0.80
2:B:198:HOH:O	1:C:81:ARG:HD3	1.80	0.80
1:C:84:HIS:HD2	1:C:86:TYR:H	1.30	0.80
1:D:52:TRP:HD1	2:D:176:HOH:O	1.66	0.77
1:D:52:TRP:CD1	2:D:176:HOH:O	2.37	0.76
1:E:34:LYS:HE3	1:E:79:PHE:CE1	2.21	0.76
1:B:34:LYS:HE3	1:B:79:PHE:CE1	2.22	0.75
1:F:5:GLY:HA2	2:F:136:HOH:O	1.87	0.74
1:F:86:TYR:CD2	1:F:86:TYR:O	2.39	0.74
2:D:118:HOH:O	1:E:39:CYS:SG	2.44	0.74
1:D:45:GLN:HG2	2:D:172:HOH:O	1.87	0.74
1:B:84:HIS:HD2	1:B:86:TYR:H	1.36	0.74
1:B:39:CYS:CB	2:B:197:HOH:O	2.30	0.73
1:A:84:HIS:CD2	1:A:86:TYR:O	2.40	0.73
1:D:22:LYS:HD2	2:D:177:HOH:O	1.89	0.73
1:A:84:HIS:NE2	1:A:87:GLU:OE2	2.21	0.72
1:D:56:ILE:HD11	1:E:33:GLU:HB3	1.71	0.72
1:F:20:ASN:OD1	1:F:23:VAL:HG13	1.89	0.72
1:B:42:LEU:CD2	1:B:64:MET:HG2	2.19	0.72
1:B:86:TYR:O	1:B:87:GLU:HB2	1.87	0.72
1:D:21:GLU:HG2	1:D:62:VAL:HG21	1.72	0.71
1:A:90:GLU:CG	1:C:103:TYR:CE1	2.73	0.71
1:A:86:TYR:HD2	1:A:87:GLU:N	1.79	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:29:ARG:HD3	2:F:139:HOH:O	1.90	0.71
1:C:72:LEU:HD13	2:C:170:HOH:O	1.90	0.71
1:A:84:HIS:CE1	1:A:87:GLU:OE2	2.44	0.71
1:A:39:CYS:CB	2:A:174:HOH:O	2.29	0.71
1:D:53:LYS:CB	1:D:53:LYS:NZ	2.41	0.70
1:A:39:CYS:SG	2:A:174:HOH:O	2.48	0.69
1:F:86:TYR:HD2	1:F:86:TYR:O	1.75	0.69
1:C:17:THR:HG21	1:C:90:GLU:OE1	1.92	0.69
1:B:35:ARG:HG3	2:B:164:HOH:O	1.91	0.69
1:F:3:GLY:HA2	2:F:157:HOH:O	1.92	0.69
1:C:17:THR:CG2	1:C:90:GLU:OE1	2.42	0.68
1:B:78:GLU:OE2	1:B:81:ARG:NH1	2.26	0.68
1:C:113:SER:HA	2:C:182:HOH:O	1.93	0.68
1:E:44:PRO:O	1:E:45:GLN:HB2	1.94	0.68
1:D:67:LYS:HD3	1:D:67:LYS:N	2.08	0.67
1:E:94:LEU:HD21	1:F:96:VAL:HG22	1.77	0.66
1:B:17:THR:HG23	2:B:173:HOH:O	1.94	0.66
1:E:56:ILE:HD11	1:F:33:GLU:HB3	1.77	0.65
1:F:75:ALA:O	1:F:78:GLU:HB3	1.96	0.65
1:E:99:GLY:O	1:E:101:PRO:HD3	1.97	0.65
1:A:41:ASN:HB3	1:B:46:ILE:HD13	1.79	0.64
1:A:82:SER:O	1:A:83:VAL:HB	1.98	0.64
1:F:79:PHE:O	1:F:82:SER:HB2	1.97	0.64
1:A:90:GLU:HG2	1:C:103:TYR:HE1	1.57	0.64
1:D:52:TRP:CE3	2:D:169:HOH:O	2.50	0.63
1:E:100:ASN:ND2	1:E:102:PRO:HD2	2.13	0.63
1:D:103:TYR:CZ	1:F:90:GLU:HG3	2.33	0.63
1:D:41:ASN:HB3	1:F:46:ILE:HD12	1.80	0.62
1:A:86:TYR:CD2	1:A:87:GLU:N	2.60	0.62
1:B:81:ARG:HD3	2:B:176:HOH:O	1.99	0.62
1:A:22:LYS:O	1:A:26:GLU:HG3	2.00	0.62
1:B:106:TRP:NE1	1:B:110:VAL:HG11	2.14	0.62
1:E:80:VAL:O	1:E:84:HIS:HB2	2.00	0.61
1:B:73:VAL:N	1:B:74:PRO:CD	2.64	0.61
1:E:106:TRP:HA	1:E:109:GLN:HG2	1.82	0.61
1:D:34:LYS:HD3	2:D:171:HOH:O	2.01	0.60
1:D:18:CYS:O	1:D:61:GLU:HG2	2.02	0.60
1:F:29:ARG:CD	2:F:139:HOH:O	2.46	0.60
1:A:78:GLU:HB2	1:A:81:ARG:HH11	1.67	0.60
1:B:100:ASN:HB2	1:C:91:VAL:HG13	1.84	0.60
1:A:95:PRO:HD3	1:C:97:GLU:HG2	1.82	0.60
1:D:100:ASN:ND2	1:D:102:PRO:HD2	2.17	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:17:THR:CG2	1:C:90:GLU:CD	2.69	0.59
1:E:94:LEU:HD23	1:F:96:VAL:HA	1.84	0.59
1:A:113:SER:C	2:A:175:HOH:O	2.41	0.59
1:C:52:TRP:NE1	2:C:178:HOH:O	2.30	0.58
1:E:67:LYS:HE3	1:E:67:LYS:N	2.18	0.58
1:E:6:TYR:C	1:E:7:VAL:CA	2.70	0.58
1:B:87:GLU:HB3	2:B:170:HOH:O	2.03	0.58
1:A:81:ARG:HD3	1:C:100:ASN:HD21	1.69	0.58
1:D:41:ASN:HB3	1:F:46:ILE:CD1	2.34	0.57
1:A:91:VAL:HG13	1:C:100:ASN:HB2	1.85	0.57
1:F:101:PRO:CD	1:F:102:PRO:HD2	2.32	0.57
1:B:16:VAL:HG22	1:B:91:VAL:HG22	1.86	0.57
1:C:69:GLN:HB2	1:C:72:LEU:HD22	1.86	0.56
1:D:25:LYS:CE	2:F:161:HOH:O	2.53	0.56
1:D:28:ALA:O	1:D:32:VAL:HG13	2.04	0.56
1:F:28:ALA:O	1:F:32:VAL:HG13	2.06	0.56
1:A:113:SER:HB2	2:A:173:HOH:O	2.06	0.55
1:B:39:CYS:SG	2:B:197:HOH:O	2.58	0.55
1:A:58:GLU:OE1	1:C:25:LYS:CE	2.55	0.55
1:B:81:ARG:HD2	2:B:169:HOH:O	2.07	0.55
1:B:97:GLU:HG3	1:C:95:PRO:HG3	1.89	0.55
1:E:106:TRP:HA	1:E:109:GLN:CG	2.36	0.54
1:C:84:HIS:CD2	1:C:86:TYR:H	2.18	0.54
1:B:114:VAL:HB	2:B:161:HOH:O	2.06	0.54
1:D:21:GLU:O	1:D:25:LYS:HB2	2.06	0.54
1:A:41:ASN:ND2	2:A:129:HOH:O	2.41	0.54
1:F:84:HIS:CE1	1:F:86:TYR:HH	2.25	0.54
1:D:30:ALA:O	1:D:34:LYS:HG3	2.08	0.54
1:A:79:PHE:O	1:A:82:SER:O	2.25	0.53
1:C:84:HIS:CD2	1:C:86:TYR:HB2	2.44	0.53
1:E:55:LYS:HB2	2:E:162:HOH:O	2.07	0.53
1:A:45:GLN:HG3	1:C:44:PRO:HG3	1.90	0.53
1:D:103:TYR:CE2	1:F:90:GLU:HG3	2.44	0.53
1:D:98:GLN:HE22	1:F:74:PRO:HD3	1.73	0.53
1:B:33:GLU:HG2	1:B:34:LYS:N	2.24	0.53
1:E:101:PRO:HB2	1:E:102:PRO:HD3	1.91	0.53
1:F:49:ILE:HG13	1:F:58:GLU:HG2	1.89	0.52
1:F:101:PRO:HB2	1:F:102:PRO:HD3	1.90	0.52
1:B:41:ASN:HB3	1:C:46:ILE:HD13	1.90	0.52
1:B:29:ARG:HD3	2:B:171:HOH:O	2.08	0.52
1:A:113:SER:CB	2:A:173:HOH:O	2.57	0.52
1:D:90:GLU:HG3	1:E:103:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:112:GLU:OE2	1:E:112:GLU:HA	2.10	0.51
1:F:28:ALA:HB2	1:F:64:MET:HE1	1.93	0.51
1:C:30:ALA:O	1:C:34:LYS:HG3	2.11	0.51
1:D:17:THR:O	1:D:84:HIS:HE1	1.94	0.50
1:E:114:VAL:CG2	2:E:160:HOH:O	2.44	0.50
1:D:21:GLU:HG2	1:D:62:VAL:CG2	2.42	0.50
1:A:101:PRO:N	1:A:102:PRO:HD2	2.27	0.49
1:E:29:ARG:O	1:E:33:GLU:HG2	2.11	0.49
1:C:51:GLU:HG2	2:C:128:HOH:O	2.11	0.49
1:B:33:GLU:CG	1:B:34:LYS:N	2.73	0.49
1:F:90:GLU:HB2	2:F:122:HOH:O	2.13	0.48
1:E:7:VAL:HA	1:E:8:PRO:HD3	1.72	0.48
1:A:103:TYR:CZ	1:B:90:GLU:HB2	2.48	0.48
1:E:52:TRP:CD1	1:E:53:LYS:HE3	2.48	0.48
1:F:42:LEU:HD11	1:F:64:MET:CE	2.44	0.48
1:A:46:ILE:HD12	1:C:41:ASN:HB3	1.95	0.48
1:D:53:LYS:HD2	2:D:176:HOH:O	2.14	0.48
1:E:100:ASN:HD22	1:E:101:PRO:HD2	1.77	0.48
1:F:50:TYR:N	1:F:50:TYR:CD1	2.81	0.48
1:B:108:HIS:CE1	1:B:112:GLU:CG	2.91	0.48
1:B:29:ARG:HG2	1:C:56:ILE:HG21	1.96	0.48
1:B:106:TRP:O	1:B:107:VAL:C	2.52	0.48
1:E:74:PRO:HD3	1:F:98:GLN:HE22	1.78	0.48
1:A:95:PRO:HD3	1:C:97:GLU:CG	2.44	0.47
1:D:47:THR:HB	1:E:42:LEU:HD12	1.96	0.47
1:A:92:ILE:HG21	1:A:92:ILE:HD13	1.59	0.47
1:D:45:GLN:HG3	2:D:183:HOH:O	2.14	0.47
1:E:101:PRO:HB2	1:E:102:PRO:CD	2.44	0.47
1:B:28:ALA:HB3	1:C:49:ILE:HD12	1.97	0.47
1:A:18:CYS:O	1:A:61:GLU:HB3	2.14	0.47
1:C:31:VAL:HG23	1:C:37:ALA:HB3	1.97	0.47
1:C:42:LEU:HD22	1:C:64:MET:HG2	1.96	0.47
1:F:29:ARG:O	1:F:33:GLU:HG2	2.15	0.46
1:B:29:ARG:CD	2:B:166:HOH:O	2.40	0.46
1:F:99:GLY:HA3	1:F:104:LEU:HD11	1.97	0.46
1:A:25:LYS:O	1:A:29:ARG:HG3	2.16	0.46
1:C:100:ASN:ND2	1:C:102:PRO:HD2	2.32	0.45
1:F:52:TRP:HA	1:F:53:LYS:HA	1.62	0.45
1:A:84:HIS:NE2	1:A:87:GLU:HA	2.32	0.45
1:B:17:THR:OG1	1:B:90:GLU:HG2	2.17	0.44
1:B:50:TYR:CD1	1:B:50:TYR:N	2.84	0.44
1:C:6:TYR:CE1	1:C:104:LEU:HG	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:VAL:HG22	1:A:91:VAL:HB	1.99	0.44
1:F:105:HIS:O	1:F:109:GLN:HG3	2.17	0.44
1:A:6:TYR:O	1:A:8:PRO:HD3	2.18	0.44
1:F:53:LYS:HE3	1:F:53:LYS:HB3	1.80	0.44
1:B:14:ALA:HA	1:B:92:ILE:O	2.18	0.44
1:D:84:HIS:HD2	1:D:86:TYR:H	1.65	0.44
1:C:35:ARG:NH1	1:C:112:GLU:O	2.50	0.44
1:D:42:LEU:CD2	1:D:64:MET:HG2	2.47	0.44
1:B:17:THR:HG22	1:B:63:LEU:HD13	2.00	0.44
1:D:84:HIS:CD2	1:D:86:TYR:HB2	2.53	0.44
1:E:114:VAL:HA	2:E:165:HOH:O	2.16	0.44
1:E:46:ILE:HB	1:F:42:LEU:O	2.18	0.43
1:D:112:GLU:HA	1:D:112:GLU:OE1	2.18	0.43
1:C:17:THR:HG22	1:C:90:GLU:OE2	2.16	0.43
1:E:52:TRP:NE1	1:E:53:LYS:HE3	2.33	0.43
1:E:88:VAL:HG11	2:E:158:HOH:O	2.18	0.43
1:B:42:LEU:HD23	1:B:64:MET:HG2	1.98	0.43
1:E:14:ALA:HA	1:E:93:ALA:HA	2.01	0.43
1:B:94:LEU:HD23	1:C:94:LEU:HD23	2.01	0.43
1:D:50:TYR:OH	1:D:59:ASP:OD2	2.24	0.43
1:A:35:ARG:NH1	2:A:150:HOH:O	2.52	0.43
1:F:21:GLU:O	1:F:25:LYS:HG3	2.19	0.43
1:F:113:SER:HA	1:F:114:VAL:HA	1.72	0.42
1:F:14:ALA:HA	1:F:93:ALA:HA	2.01	0.42
1:F:108:HIS:NE2	1:F:112:GLU:CG	2.82	0.42
1:A:55:LYS:HA	2:A:126:HOH:O	2.19	0.42
1:D:67:LYS:NZ	1:F:90:GLU:OE2	2.52	0.42
1:D:78:GLU:HB2	2:D:163:HOH:O	2.18	0.42
1:B:100:ASN:HD22	1:B:101:PRO:HD2	1.85	0.42
1:E:17:THR:HG22	1:E:90:GLU:HB3	2.01	0.42
1:E:5:GLY:O	1:E:6:TYR:HB3	2.20	0.42
1:A:48:SER:O	1:A:58:GLU:HA	2.19	0.42
1:D:84:HIS:CD2	1:D:85:PRO:HD2	2.55	0.42
1:B:106:TRP:NE1	1:B:110:VAL:CG1	2.82	0.42
1:C:41:ASN:ND2	1:C:67:LYS:HE2	2.34	0.42
1:D:4:SER:N	2:D:178:HOH:O	2.53	0.42
1:D:74:PRO:HD3	1:E:98:GLN:HE22	1.85	0.42
1:C:94:LEU:HA	1:C:95:PRO:HD3	1.90	0.42
1:A:45:GLN:HG3	1:C:44:PRO:CG	2.49	0.41
1:D:17:THR:O	1:D:84:HIS:CE1	2.72	0.41
1:A:90:GLU:CG	1:C:103:TYR:CD1	3.03	0.41
1:D:62:VAL:HG12	1:D:63:LEU:N	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:94:LEU:CD2	1:F:96:VAL:HG22	2.48	0.41
1:D:53:LYS:CB	1:D:53:LYS:HZ3	2.27	0.41
1:F:85:PRO:O	1:F:86:TYR:CG	2.73	0.41
1:C:19:PRO:HA	1:C:61:GLU:HG2	2.03	0.41
1:C:14:ALA:HA	1:C:92:ILE:O	2.21	0.41
1:D:16:VAL:HA	1:D:90:GLU:O	2.21	0.41
1:F:48:SER:O	1:F:58:GLU:HA	2.20	0.41
1:C:45:GLN:HG2	2:C:181:HOH:O	2.20	0.41
1:B:100:ASN:HB3	1:B:103:TYR:HB3	2.02	0.41
1:D:100:ASN:HA	1:D:101:PRO:HD3	1.87	0.41
1:D:25:LYS:HE2	2:F:161:HOH:O	2.16	0.41
1:B:88:VAL:O	1:B:88:VAL:HG13	2.21	0.41
1:C:84:HIS:HD2	1:C:86:TYR:N	2.09	0.41
1:B:98:GLN:HE22	1:C:74:PRO:HD3	1.85	0.40
1:A:78:GLU:HG2	2:A:162:HOH:O	2.20	0.40
1:F:29:ARG:HD2	2:F:139:HOH:O	2.19	0.40
1:B:7:VAL:HG21	1:E:71:SER:HA	2.03	0.40
1:F:101:PRO:HB2	1:F:102:PRO:CD	2.51	0.40

There are no symmetry-related clashes.

## 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	106/126 (84%)	101 (95%)	3 (3%)	2 (2%)	12	4
1	B	107/126 (85%)	103 (96%)	3 (3%)	1 (1%)	25	15
1	C	106/126 (84%)	101 (95%)	2 (2%)	3 (3%)	8	1
1	D	107/126 (85%)	101 (94%)	5 (5%)	1 (1%)	25	15
1	E	106/126 (84%)	100 (94%)	4 (4%)	2 (2%)	12	4
1	F	107/126 (85%)	99 (92%)	6 (6%)	2 (2%)	12	4
All	All	639/756 (84%)	605 (95%)	23 (4%)	11 (2%)	14	5



All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	VAL
1	A	84	HIS
1	C	88	VAL
1	D	87	GLU
1	E	6	TYR
1	F	78	GLU
1	B	113	SER
1	C	87	GLU
1	C	112	GLU
1	E	90	GLU
1	F	54	GLY

### 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	95/108 (88%)	75 (79%)	20 (21%)	1	0
1	B	96/108 (89%)	81 (84%)	15 (16%)	4	2
1	C	95/108 (88%)	81 (85%)	14 (15%)	4	2
1	D	95/108 (88%)	81 (85%)	14 (15%)	4	2
1	E	95/108 (88%)	81 (85%)	14 (15%)	4	2
1	F	96/108 (89%)	81 (84%)	15 (16%)	4	2
All	All	572/648 (88%)	480 (84%)	92 (16%)	3	2

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	21	GLU
1	A	25	LYS
1	A	45	GLN
1	A	46	ILE
1	A	61	GLU
1	A	67	LYS
1	A	72	LEU

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Mol	Chain	Res	Type
1	A	76	LEU
1	A	78	GLU
1	A	82	SER
1	A	84	HIS
1	A	86	TYR
1	A	87	GLU
1	A	91	VAL
1	A	94	LEU
1	A	104	LEU
1	A	109	GLN
1	A	112	GLU
1	A	113	SER
1	B	33	GLU
1	B	46	ILE
1	B	51	GLU
1	B	53	LYS
1	B	55	LYS
1	B	67	LYS
1	B	72	LEU
1	B	76	LEU
1	B	78	GLU
1	B	100	ASN
1	B	104	LEU
1	B	111	THR
1	B	112	GLU
1	B	113	SER
1	B	114	VAL
1	C	17	THR
1	C	22	LYS
1	C	35	ARG
1	C	45	GLN
1	C	46	ILE
1	C	51	GLU
1	C	55	LYS
1	C	67	LYS
1	C	72	LEU
1	C	76	LEU
1	C	81	ARG
1	C	87	GLU
1	C	91	VAL
1	C	104	LEU
1	D	4	SER

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Mol	Chain	Res	Type
1	D	22	LYS
1	D	32	VAL
1	D	45	GLN
1	D	53	LYS
1	D	61	GLU
1	D	67	LYS
1	D	72	LEU
1	D	76	LEU
1	D	78	GLU
1	D	81	ARG
1	D	83	VAL
1	D	104	LEU
1	D	112	GLU
1	E	17	THR
1	E	22	LYS
1	E	25	LYS
1	E	35	ARG
1	E	46	ILE
1	E	53	LYS
1	E	67	LYS
1	E	74	PRO
1	E	78	GLU
1	E	81	ARG
1	E	90	GLU
1	E	104	LEU
1	E	112	GLU
1	E	114	VAL
1	F	4	SER
1	F	17	THR
1	F	18	CYS
1	F	21	GLU
1	F	22	LYS
1	F	42	LEU
1	F	52	TRP
1	F	53	LYS
1	F	55	LYS
1	F	59	ASP
1	F	67	LYS
1	F	71	SER
1	F	76	LEU
1	F	86	TYR
1	F	114	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	69	GLN
1	A	84	HIS
1	A	98	GLN
1	A	100	ASN
1	B	41	ASN
1	B	84	HIS
1	B	98	GLN
1	B	100	ASN
1	B	108	HIS
1	B	109	GLN
1	C	41	ASN
1	C	69	GLN
1	C	84	HIS
1	C	98	GLN
1	C	100	ASN
1	C	108	HIS
1	C	109	GLN
1	D	69	GLN
1	D	84	HIS
1	D	98	GLN
1	D	100	ASN
1	E	69	GLN
1	E	98	GLN
1	E	100	ASN
1	F	41	ASN
1	F	98	GLN
1	F	100	ASN

### 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	108/126 (85%)	0.11	5 (4%) 31 35	35, 49, 76, 99	0
1	B	109/126 (86%)	0.11	4 (3%) 39 43	35, 48, 73, 95	0
1	C	108/126 (85%)	0.05	4 (3%) 39 43	22, 51, 69, 87	0
1	D	109/126 (86%)	0.11	3 (2%) 50 55	37, 53, 70, 80	0
1	E	110/126 (87%)	0.52	13 (11%) 5 6	18, 56, 92, 103	0
1	F	111/126 (88%)	0.56	10 (9%) 10 11	39, 56, 90, 107	0
All	All	655/756 (86%)	0.25	39 (5%) 21 25	18, 52, 82, 107	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	113	SER	10.1
1	F	114	VAL	9.5
1	F	3	GLY	9.4
1	B	114	VAL	9.4
1	E	114	VAL	8.1
1	A	86	TYR	7.4
1	E	3	GLY	7.0
1	B	113	SER	6.1
1	F	4	SER	6.0
1	C	113	SER	5.9
1	E	113	SER	5.9
1	D	4	SER	5.5
1	A	113	SER	5.4
1	E	5	GLY	5.4
1	E	52	TRP	4.9
1	C	87	GLU	3.7
1	E	4	SER	3.7
1	F	53	LYS	3.7
1	F	52	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	112	GLU	3.6
1	B	52	TRP	3.2
1	E	85	PRO	3.2
1	A	85	PRO	2.9
1	E	109	GLN	2.8
1	C	112	GLU	2.6
1	D	109	GLN	2.6
1	A	40	VAL	2.6
1	E	55	LYS	2.5
1	B	86	TYR	2.5
1	A	112	GLU	2.4
1	F	86	TYR	2.3
1	E	40	VAL	2.3
1	F	5	GLY	2.3
1	E	53	LYS	2.2
1	C	55	LYS	2.1
1	F	40	VAL	2.0
1	E	83	VAL	2.0
1	D	66	ILE	2.0
1	E	66	ILE	2.0

## 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.