



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:23 PM 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 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

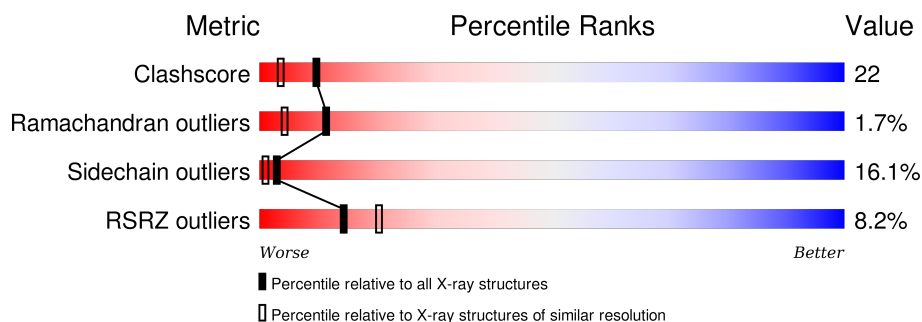
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	126	<div> <div>6%</div> <div> <div>49%</div> <div>21%</div> <div>14%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	126	<div> <div>6%</div> <div> <div>45%</div> <div>30%</div> <div>9%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	126	<div> <div>5%</div> <div> <div>47%</div> <div>26%</div> <div>10%</div> <div>•</div> <div>14%</div> </div> </div>
1	D	126	<div> <div>4%</div> <div> <div>45%</div> <div>29%</div> <div>10%</div> <div>•</div> <div>13%</div> </div> </div>
1	E	126	<div> <div>11%</div> <div> <div>51%</div> <div>26%</div> <div>9%</div> <div>•</div> <div>13%</div> </div> </div>
1	F	126	<div> <div>12%</div> <div> <div>44%</div> <div>33%</div> <div>10%</div> <div>•</div> <div>12%</div> </div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5495 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 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			

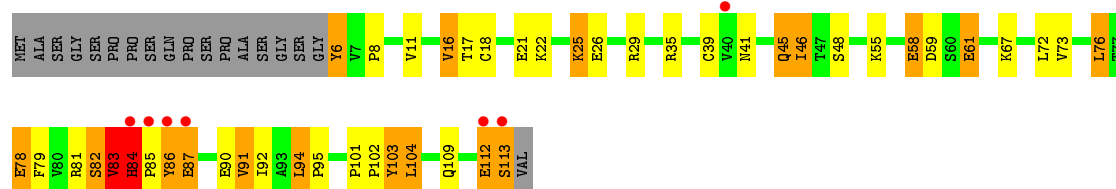
- Molecule 2 is water.

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		

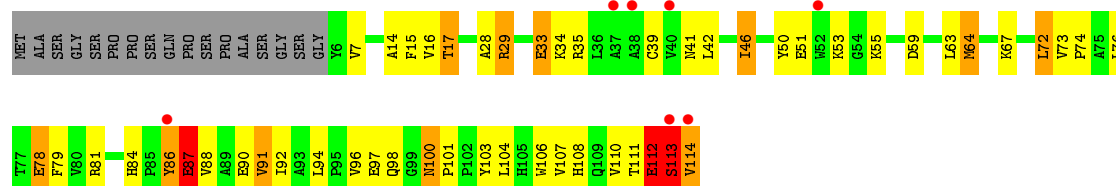
### 3 Residue-property plots [i](#)

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.

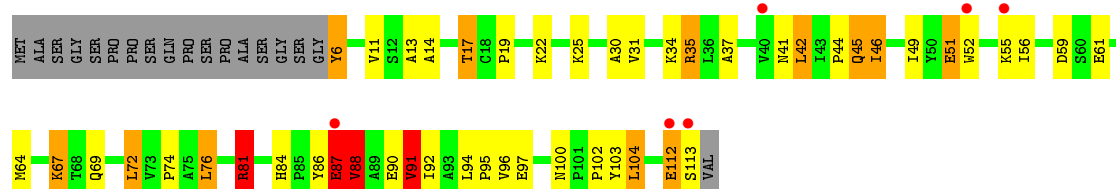
- Molecule 1: similar to divalent cation tolerant protein CUTA



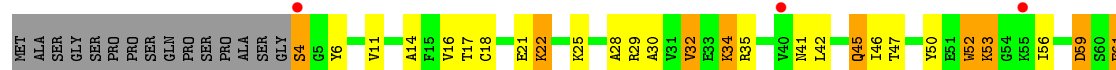
- Molecule 1: similar to divalent cation tolerant protein CUTA

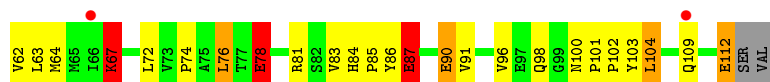


- Molecule 1: similar to divalent cation tolerant protein CUTA

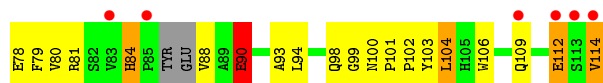


- Molecule 1: similar to divalent cation tolerant protein CUTA

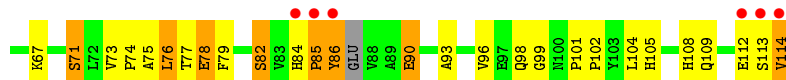




- Molecule 1: similar to divalent cation tolerant protein CUTA



- Molecule 1: similar to divalent cation tolerant protein CUTA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.39 Å 88.29 Å 125.85 Å 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 2.15 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.189 , 0.260 0.206 , (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> )	0.33 , 66.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	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.

<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 ⓘ

### 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 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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 22.

All (228) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:TYR:HD2	1:A:87:GLU:N	1.79	0.71
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [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	106/126 (84%)	101 (95%)	3 (3%)	2 (2%)	10 3
1	B	107/126 (85%)	103 (96%)	3 (3%)	1 (1%)	21 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	106/126 (84%)	101 (95%)	2 (2%)	3 (3%)	6	1
1	D	107/126 (85%)	101 (94%)	5 (5%)	1 (1%)	21	13
1	E	106/126 (84%)	100 (94%)	4 (4%)	2 (2%)	10	3
1	F	107/126 (85%)	99 (92%)	6 (6%)	2 (2%)	10	3
All	All	639/756 (84%)	605 (95%)	23 (4%)	11 (2%)	11	4

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%)	3	1
1	C	95/108 (88%)	81 (85%)	14 (15%)	4	1
1	D	95/108 (88%)	81 (85%)	14 (15%)	4	1
1	E	95/108 (88%)	81 (85%)	14 (15%)	4	1
1	F	96/108 (89%)	81 (84%)	15 (16%)	3	1
All	All	572/648 (88%)	480 (84%)	92 (16%)	3	1

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [i](#)

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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(Å²)	Q<0.9
1	A	108/126 (85%)	0.24	7 (6%)	22	31	35, 49, 76, 99	0
1	B	109/126 (86%)	0.19	7 (6%)	23	32	35, 48, 73, 95	0
1	C	108/126 (85%)	0.13	6 (5%)	28	38	22, 51, 69, 87	0
1	D	109/126 (86%)	0.21	5 (4%)	36	47	37, 53, 70, 80	0
1	E	110/126 (87%)	0.63	14 (12%)	5	8	18, 56, 92, 103	0
1	F	111/126 (88%)	0.69	15 (13%)	4	7	39, 56, 90, 107	0
All	All	655/756 (86%)	0.35	54 (8%)	14	20	18, 52, 82, 107	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	114	VAL	11.0
1	F	113	SER	10.9
1	F	3	GLY	10.6
1	B	114	VAL	10.1
1	A	86	TYR	9.7
1	E	114	VAL	9.2
1	E	3	GLY	8.2
1	E	52	TRP	7.3
1	E	113	SER	6.2
1	F	4	SER	6.2
1	A	113	SER	6.1
1	D	4	SER	5.9
1	B	113	SER	5.8
1	C	113	SER	5.8
1	E	5	GLY	5.0
1	F	52	TRP	4.9
1	F	53	LYS	4.2
1	F	112	GLU	4.2
1	C	87	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	52	TRP	4.0
1	E	4	SER	4.0
1	E	85	PRO	3.9
1	A	85	PRO	3.8
1	E	55	LYS	3.1
1	A	112	GLU	3.0
1	D	109	GLN	3.0
1	A	40	VAL	3.0
1	E	40	VAL	2.9
1	B	86	TYR	2.8
1	F	86	TYR	2.7
1	E	109	GLN	2.7
1	C	112	GLU	2.7
1	E	53	LYS	2.5
1	E	83	VAL	2.4
1	F	40	VAL	2.4
1	F	85	PRO	2.4
1	F	55	LYS	2.4
1	D	40	VAL	2.3
1	E	66	ILE	2.3
1	F	5	GLY	2.3
1	C	40	VAL	2.3
1	D	66	ILE	2.3
1	E	112	GLU	2.3
1	F	84	HIS	2.3
1	C	55	LYS	2.3
1	A	87	GLU	2.2
1	C	52	TRP	2.2
1	D	55	LYS	2.2
1	F	37	ALA	2.2
1	A	84	HIS	2.1
1	B	37	ALA	2.1
1	F	54	GLY	2.0
1	B	38	ALA	2.0
1	B	40	VAL	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 [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.