



# Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 06:56 AM GMT

PDB ID : 2D00  
Title : Subunit F of V-type ATPase/synthase  
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S.  
Deposited on : 2005-07-21  
Resolution : 2.20 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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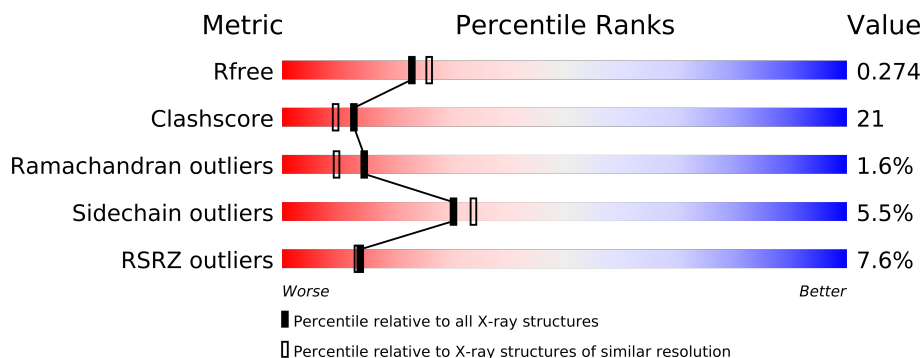
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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	109	
1	B	109	
1	C	109	
1	D	109	
1	E	109	
1	F	109	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5289 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 V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			833	527	144	158	4			
1	B	109	Total	C	N	O	S	0	0	0
			833	527	144	158	4			
1	C	109	Total	C	N	O	S	0	0	0
			833	527	144	158	4			
1	D	109	Total	C	N	O	S	0	0	0
			833	527	144	158	4			
1	E	109	Total	C	N	O	S	0	0	0
			833	527	144	158	4			
1	F	109	Total	C	N	O	S	0	0	0
			833	527	144	158	4			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP P74903
A	2	VAL	-	CLONING ARTIFACT	UNP P74903
A	3	PRO	-	CLONING ARTIFACT	UNP P74903
A	4	VAL	-	CLONING ARTIFACT	UNP P74903
A	5	ARG	-	CLONING ARTIFACT	UNP P74903
B	1	MET	-	CLONING ARTIFACT	UNP P74903
B	2	VAL	-	CLONING ARTIFACT	UNP P74903
B	3	PRO	-	CLONING ARTIFACT	UNP P74903
B	4	VAL	-	CLONING ARTIFACT	UNP P74903
B	5	ARG	-	CLONING ARTIFACT	UNP P74903
C	1	MET	-	CLONING ARTIFACT	UNP P74903
C	2	VAL	-	CLONING ARTIFACT	UNP P74903
C	3	PRO	-	CLONING ARTIFACT	UNP P74903
C	4	VAL	-	CLONING ARTIFACT	UNP P74903
C	5	ARG	-	CLONING ARTIFACT	UNP P74903
D	1	MET	-	CLONING ARTIFACT	UNP P74903
D	2	VAL	-	CLONING ARTIFACT	UNP P74903

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Chain	Residue	Modelled	Actual	Comment	Reference
D	3	PRO	-	CLONING ARTIFACT	UNP P74903
D	4	VAL	-	CLONING ARTIFACT	UNP P74903
D	5	ARG	-	CLONING ARTIFACT	UNP P74903
E	1	MET	-	CLONING ARTIFACT	UNP P74903
E	2	VAL	-	CLONING ARTIFACT	UNP P74903
E	3	PRO	-	CLONING ARTIFACT	UNP P74903
E	4	VAL	-	CLONING ARTIFACT	UNP P74903
E	5	ARG	-	CLONING ARTIFACT	UNP P74903
F	1	MET	-	CLONING ARTIFACT	UNP P74903
F	2	VAL	-	CLONING ARTIFACT	UNP P74903
F	3	PRO	-	CLONING ARTIFACT	UNP P74903
F	4	VAL	-	CLONING ARTIFACT	UNP P74903
F	5	ARG	-	CLONING ARTIFACT	UNP P74903

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Ca 2 2	0	0
2	D	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

- Molecule 3 is water.

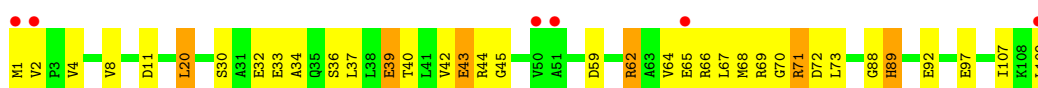
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	54	Total O 54 54	0	0
3	B	45	Total O 45 45	0	0
3	C	51	Total O 51 51	0	0
3	D	42	Total O 42 42	0	0
3	E	49	Total O 49 49	0	0
3	F	46	Total O 46 46	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

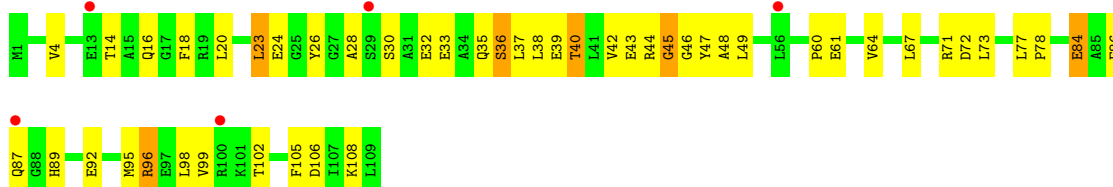
- Molecule 1: V-type ATP synthase subunit F

Chain A: 



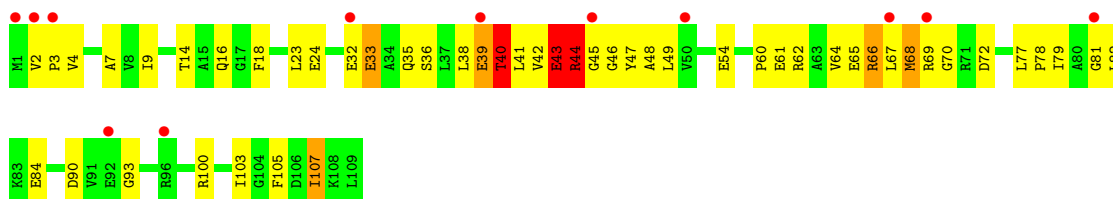
- Molecule 1: V-type ATP synthase subunit F

Chain B: 



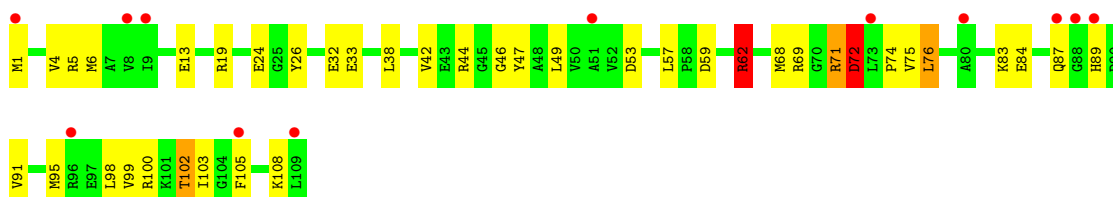
- Molecule 1: V-type ATP synthase subunit F

Chain C: 



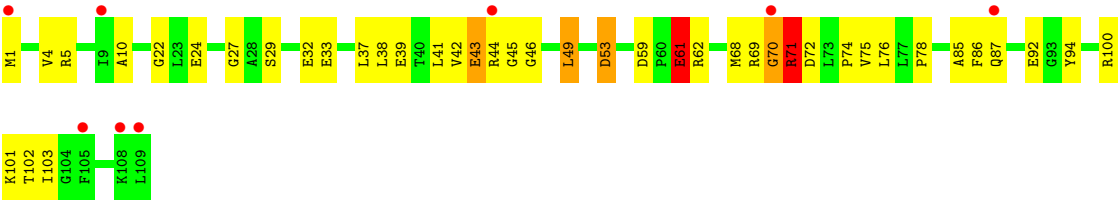
- Molecule 1: V-type ATP synthase subunit F

Chain D: 



- Molecule 1: V-type ATP synthase subunit F

Chain E: 



• Molecule 1: V-type ATP synthase subunit F

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.70Å 138.29Å 66.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 24.77 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.20) 99.4 (24.77-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.214 , 0.262 0.224 , 0.274	Depositor DCC
$R_{free}$ test set	1206 reflections (3.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 108.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 38526 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5289	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.46% 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

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

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	1.60	9/845 (1.1%)	1.29	7/1140 (0.6%)
1	B	1.32	2/845 (0.2%)	1.18	2/1140 (0.2%)
1	C	2.10	23/845 (2.7%)	1.38	6/1140 (0.5%)
1	D	1.51	7/845 (0.8%)	1.31	10/1140 (0.9%)
1	E	1.55	8/845 (0.9%)	1.32	7/1140 (0.6%)
1	F	1.72	12/845 (1.4%)	1.27	6/1140 (0.5%)
All	All	1.65	61/5070 (1.2%)	1.29	38/6840 (0.6%)

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	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	2
All	All	0	6

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	43	GLU	CD-OE1	26.75	1.55	1.25
1	F	97	GLU	CD-OE2	17.57	1.45	1.25
1	C	39	GLU	CD-OE2	15.09	1.42	1.25
1	C	39	GLU	CD-OE1	14.83	1.42	1.25
1	A	43	GLU	CG-CD	13.04	1.71	1.51
1	F	97	GLU	CD-OE1	11.60	1.38	1.25
1	C	44	ARG	C-N	10.87	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	45	GLY	C-N	10.84	1.52	1.33
1	A	39	GLU	C-O	10.58	1.43	1.23
1	E	24	GLU	CB-CG	-10.06	1.33	1.52
1	C	68	MET	CG-SD	10.06	2.07	1.81
1	C	39	GLU	C-O	9.35	1.41	1.23
1	E	33	GLU	CD-OE1	8.83	1.35	1.25
1	C	45	GLY	C-O	8.33	1.36	1.23
1	D	46	GLY	N-CA	8.24	1.58	1.46
1	A	45	GLY	C-O	8.15	1.36	1.23
1	E	29	SER	CB-OG	8.15	1.52	1.42
1	D	26	TYR	CD1-CE1	7.75	1.50	1.39
1	C	40	THR	CB-OG1	7.70	1.58	1.43
1	F	24	GLU	CG-CD	7.51	1.63	1.51
1	C	36	SER	CB-OG	7.46	1.51	1.42
1	D	13	GLU	CG-CD	7.45	1.63	1.51
1	E	43	GLU	CG-CD	7.14	1.62	1.51
1	C	45	GLY	N-CA	6.95	1.56	1.46
1	A	43	GLU	CD-OE1	6.88	1.33	1.25
1	C	24	GLU	CB-CG	-6.86	1.39	1.52
1	C	33	GLU	CG-CD	-6.82	1.41	1.51
1	C	18	PHE	CE2-CZ	-6.65	1.24	1.37
1	F	46	GLY	CA-C	6.58	1.62	1.51
1	F	46	GLY	N-CA	6.57	1.55	1.46
1	E	24	GLU	CD-OE1	6.54	1.32	1.25
1	F	15	ALA	CA-CB	-6.35	1.39	1.52
1	C	41	LEU	C-N	6.34	1.48	1.34
1	A	45	GLY	C-N	6.30	1.44	1.33
1	B	26	TYR	CB-CG	-6.26	1.42	1.51
1	C	42	VAL	C-O	6.26	1.35	1.23
1	F	33	GLU	CG-CD	6.22	1.61	1.51
1	D	72	ASP	N-CA	6.10	1.58	1.46
1	F	39	GLU	CB-CG	-5.95	1.40	1.52
1	F	61	GLU	CD-OE1	5.90	1.32	1.25
1	D	19	ARG	CD-NE	5.86	1.56	1.46
1	C	68	MET	C-O	5.84	1.34	1.23
1	E	61	GLU	CG-CD	5.70	1.60	1.51
1	C	16	GLN	CB-CG	-5.67	1.37	1.52
1	E	61	GLU	CB-CG	5.65	1.62	1.52
1	F	51	ALA	CA-CB	-5.64	1.40	1.52
1	C	70	GLY	N-CA	5.58	1.54	1.46
1	F	33	GLU	CD-OE1	5.56	1.31	1.25
1	A	30	SER	CA-CB	5.56	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	GLU	CG-CD	5.47	1.60	1.51
1	C	32	GLU	CG-CD	5.43	1.60	1.51
1	D	42	VAL	CB-CG1	-5.31	1.41	1.52
1	A	8	VAL	CB-CG2	5.31	1.64	1.52
1	E	43	GLU	CD-OE1	5.26	1.31	1.25
1	F	2	VAL	CB-CG2	5.24	1.63	1.52
1	B	92	GLU	CD-OE1	5.22	1.31	1.25
1	A	34	ALA	CA-CB	-5.21	1.41	1.52
1	C	32	GLU	CD-OE1	5.18	1.31	1.25
1	C	39	GLU	CB-CG	5.13	1.61	1.52
1	C	54	GLU	CB-CG	-5.12	1.42	1.52
1	D	42	VAL	CB-CG2	-5.04	1.42	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ASP	CB-CG-OD2	9.64	126.97	118.30
1	C	72	ASP	CB-CG-OD2	8.88	126.29	118.30
1	C	72	ASP	CB-CG-OD1	-8.58	110.58	118.30
1	C	68	MET	CG-SD-CE	-8.41	86.74	100.20
1	F	5	ARG	CG-CD-NE	-8.01	94.98	111.80
1	E	71	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	F	5	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	E	72	ASP	CB-CG-OD1	-7.02	111.98	118.30
1	A	72	ASP	CB-CG-OD1	-7.01	111.99	118.30
1	A	71	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	D	13	GLU	OE1-CD-OE2	-6.84	115.09	123.30
1	D	53	ASP	CB-CG-OD1	6.73	124.36	118.30
1	B	72	ASP	CB-CG-OD2	6.44	124.10	118.30
1	E	53	ASP	CB-CG-OD1	6.29	123.96	118.30
1	D	69	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	D	76	LEU	CA-CB-CG	6.11	129.34	115.30
1	E	24	GLU	OE1-CD-OE2	6.07	130.58	123.30
1	E	71	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	D	24	GLU	OE1-CD-OE2	5.82	130.28	123.30
1	A	89	HIS	N-CA-C	5.77	126.58	111.00
1	C	66	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	F	97	GLU	OE1-CD-OE2	5.56	129.98	123.30
1	C	39	GLU	OE1-CD-OE2	5.42	129.81	123.30
1	F	53	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	40	THR	CB-CA-C	-5.41	96.99	111.60
1	F	8	VAL	CG1-CB-CG2	-5.39	102.28	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	71	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	62	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	66	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	E	45	GLY	N-CA-C	5.24	126.20	113.10
1	A	59	ASP	CB-CG-OD1	5.24	123.02	118.30
1	E	49	LEU	CA-CB-CG	5.21	127.27	115.30
1	D	19	ARG	CG-CD-NE	5.15	122.61	111.80
1	B	45	GLY	N-CA-C	5.10	125.86	113.10
1	D	44	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	40	THR	CA-CB-CG2	-5.07	105.31	112.40
1	D	59	ASP	CB-CG-OD1	5.05	122.84	118.30
1	F	45	GLY	C-N-CA	-5.04	111.71	122.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	44	ARG	Peptide
1	C	44	ARG	Peptide
1	D	72	ASP	Peptide
1	E	71	ARG	Peptide
1	F	68	MET	Peptide
1	F	87	GLN	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	833	0	850	35	1
1	B	833	0	850	48	1
1	C	833	0	850	46	0
1	D	833	0	850	30	0
1	E	833	0	850	47	0
1	F	833	0	850	38	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	54	0	0	8	0
3	B	45	0	0	18	0
3	C	51	0	0	7	0
3	D	42	0	0	8	0
3	E	49	0	0	17	1
3	F	46	0	0	8	1
All	All	5289	0	5100	211	2

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 21.

All (211) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:68:MET:SD	1:C:68:MET:CG	2.07	1.41
1:A:37:LEU:HA	3:A:162:HOH:O	1.40	1.19
1:B:43:GLU:HG3	3:B:1043:HOH:O	1.48	1.14
1:F:32:GLU:HG3	3:F:117:HOH:O	1.58	1.02
1:C:39:GLU:HA	1:C:67:LEU:HD22	1.41	1.02
1:E:74:PRO:HD3	3:E:153:HOH:O	1.59	1.02
1:B:36:SER:OG	3:B:1046:HOH:O	1.71	1.01
1:C:64:VAL:O	3:C:1052:HOH:O	1.78	1.00
1:E:71:ARG:CG	3:E:156:HOH:O	2.10	0.98
1:E:59:ASP:OD1	1:E:61:GLU:OE1	1.80	0.97
1:B:24:GLU:OE1	1:B:47:TYR:HE1	1.47	0.97
1:E:71:ARG:HG2	3:E:156:HOH:O	1.63	0.95
1:B:105:PHE:CE1	3:E:154:HOH:O	2.22	0.92
1:B:24:GLU:OE1	1:B:47:TYR:CE1	2.24	0.90
1:D:103:ILE:HG23	1:D:105:PHE:HB2	1.55	0.89
1:C:39:GLU:CA	1:C:67:LEU:HD22	2.03	0.88
1:A:37:LEU:CA	3:A:162:HOH:O	2.10	0.87
1:C:39:GLU:HB3	3:C:1009:HOH:O	1.75	0.86
1:E:69:ARG:HG2	3:E:151:HOH:O	1.73	0.86
1:D:91:VAL:O	1:D:95:MET:HG2	1.78	0.84
1:A:33:GLU:O	1:A:36:SER:OG	1.94	0.83
1:B:35:GLN:HB3	3:B:1009:HOH:O	1.78	0.82
1:E:74:PRO:CD	3:E:153:HOH:O	2.23	0.81
1:B:105:PHE:HD2	3:E:138:HOH:O	1.63	0.81
1:A:70:GLY:HA3	3:D:1042:HOH:O	1.83	0.78
1:C:33:GLU:O	1:C:33:GLU:HG3	1.82	0.78
1:E:41:LEU:CD2	1:E:44:ARG:HH21	1.98	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:32:GLU:OE1	1:A:32:GLU:HA	1.83	0.77
1:A:70:GLY:CA	3:D:1042:HOH:O	2.32	0.77
1:D:71:ARG:O	3:D:1041:HOH:O	2.02	0.77
1:A:88:GLY:O	3:A:155:HOH:O	2.04	0.76
1:F:88:GLY:O	1:F:89:HIS:HD2	1.69	0.75
1:C:33:GLU:OE2	3:C:1011:HOH:O	2.04	0.74
1:D:99:VAL:O	1:D:103:ILE:HG22	1.88	0.74
1:A:71:ARG:HB3	1:F:68:MET:CE	2.17	0.74
1:B:42:VAL:CG2	3:B:1049:HOH:O	2.36	0.73
1:B:44:ARG:HG3	3:B:1043:HOH:O	1.88	0.73
1:B:105:PHE:CD2	3:E:138:HOH:O	2.39	0.72
1:B:105:PHE:HE1	3:E:154:HOH:O	1.68	0.71
1:B:44:ARG:CG	3:B:1043:HOH:O	2.37	0.71
1:C:67:LEU:HB2	3:C:1052:HOH:O	1.89	0.70
1:A:107:ILE:HG13	1:F:4:VAL:HG11	1.74	0.70
1:D:33:GLU:OE2	3:D:1042:HOH:O	2.08	0.70
1:A:71:ARG:HB3	1:F:68:MET:HE1	1.73	0.69
1:B:60:PRO:O	1:B:64:VAL:HG23	1.92	0.69
1:D:68:MET:HA	1:D:68:MET:HE2	1.74	0.69
1:E:41:LEU:HD23	1:E:44:ARG:HH21	1.57	0.69
1:A:4:VAL:HG11	1:F:107:ILE:HD12	1.75	0.69
1:F:68:MET:CE	1:F:68:MET:HA	2.22	0.69
1:C:44:ARG:O	1:C:46:GLY:N	2.21	0.69
1:F:88:GLY:O	1:F:89:HIS:CD2	2.45	0.69
1:C:68:MET:CB	1:C:68:MET:SD	2.81	0.69
1:E:71:ARG:CD	3:E:156:HOH:O	2.39	0.68
1:B:40:THR:OG1	3:B:1048:HOH:O	2.11	0.66
1:A:39:GLU:O	1:A:43:GLU:HG2	1.96	0.66
1:C:68:MET:CE	1:C:68:MET:CG	2.73	0.66
1:F:32:GLU:OE2	1:F:66:ARG:NH2	2.24	0.66
1:B:28:ALA:HB2	1:B:37:LEU:HD12	1.77	0.66
3:B:1046:HOH:O	1:E:32:GLU:CD	2.35	0.65
1:C:107:ILE:HD12	1:E:49:LEU:CD2	2.27	0.64
1:A:70:GLY:O	3:D:1042:HOH:O	2.15	0.64
1:C:107:ILE:HD12	1:E:49:LEU:HD22	1.80	0.64
1:B:44:ARG:O	1:B:46:GLY:N	2.27	0.64
1:F:68:MET:HA	1:F:68:MET:HE2	1.79	0.63
1:A:62:ARG:O	1:A:66:ARG:HG3	1.98	0.63
1:B:42:VAL:HG21	1:B:67:LEU:HD22	1.79	0.63
1:E:102:THR:HG22	1:E:103:ILE:HG23	1.80	0.63
1:B:4:VAL:HB	1:D:108:LYS:O	2.00	0.62
1:A:11:ASP:OD1	3:A:137:HOH:O	2.16	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:71:ARG:HB3	1:D:68:MET:HE2	1.83	0.61
1:F:94:TYR:CE2	1:F:98:LEU:HD12	2.36	0.61
1:E:69:ARG:NH2	3:E:139:HOH:O	2.34	0.60
1:B:84:GLU:HB3	3:B:1032:HOH:O	2.01	0.60
1:F:98:LEU:HD23	1:F:98:LEU:O	2.02	0.60
1:C:90:ASP:O	1:C:93:GLY:N	2.34	0.60
1:E:69:ARG:O	1:E:71:ARG:N	2.35	0.60
1:D:83:LYS:NZ	3:D:1030:HOH:O	2.32	0.59
1:B:71:ARG:HB3	1:D:68:MET:CE	2.32	0.59
1:D:100:ARG:HA	1:D:105:PHE:O	2.03	0.59
1:D:75:VAL:HG11	1:D:103:ILE:HD11	1.84	0.59
1:A:107:ILE:CD1	1:F:4:VAL:HG11	2.33	0.59
1:C:65:GLU:O	1:C:69:ARG:HD2	2.04	0.58
1:C:7:ALA:HB2	1:C:47:TYR:CE1	2.39	0.58
1:C:9:ILE:HD12	1:C:38:LEU:HD21	1.86	0.57
1:B:28:ALA:HB1	1:B:33:GLU:HG2	1.86	0.57
1:B:30:SER:HB2	1:B:32:GLU:OE1	2.04	0.57
1:C:40:THR:O	1:C:43:GLU:HG2	2.05	0.57
1:B:96:ARG:HD3	3:B:1022:HOH:O	2.05	0.57
1:E:75:VAL:HG11	1:E:103:ILE:HD13	1.87	0.56
1:B:87:GLN:HG3	3:B:1032:HOH:O	2.05	0.56
1:E:39:GLU:OE2	1:E:43:GLU:HG3	2.06	0.56
1:D:68:MET:CE	1:D:68:MET:HA	2.35	0.55
1:A:42:VAL:HG21	1:A:67:LEU:HD13	1.89	0.55
1:C:39:GLU:CA	1:C:67:LEU:CD2	2.83	0.55
1:A:32:GLU:HB3	1:D:32:GLU:HG3	1.89	0.55
1:A:107:ILE:CG1	1:F:4:VAL:HG11	2.36	0.55
1:B:77:LEU:HD11	1:B:102:THR:HG21	1.89	0.55
1:C:69:ARG:HD3	3:C:1040:HOH:O	2.07	0.55
1:C:100:ARG:HA	1:C:105:PHE:O	2.08	0.54
1:C:9:ILE:CD1	1:C:38:LEU:HD21	2.37	0.54
1:C:77:LEU:HD11	1:C:103:ILE:HG23	1.90	0.54
1:F:77:LEU:HD11	1:F:102:THR:HG21	1.90	0.54
1:B:42:VAL:HG11	1:B:67:LEU:HD13	1.90	0.54
1:A:107:ILE:HD11	1:F:4:VAL:CG1	2.38	0.53
1:B:60:PRO:HG2	1:B:61:GLU:OE2	2.08	0.53
1:C:107:ILE:HG12	1:E:4:VAL:HG11	1.90	0.53
1:F:97:GLU:O	1:F:101:LYS:HB2	2.09	0.53
1:C:14:THR:HG23	1:E:86:PHE:HE1	1.73	0.53
1:A:1:MET:HE2	3:A:151:HOH:O	2.09	0.53
1:C:81:GLY:HA3	1:C:84:GLU:OE1	2.09	0.53
1:C:39:GLU:O	1:C:43:GLU:HB3	2.08	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:16:GLN:O	1:B:20:LEU:HG	2.09	0.52
1:A:109:LEU:HD23	1:F:4:VAL:O	2.10	0.52
1:E:4:VAL:N	3:E:123:HOH:O	2.43	0.51
1:D:89:HIS:CD2	1:E:100:ARG:HH21	2.29	0.51
1:D:98:LEU:O	1:D:102:THR:OG1	2.24	0.51
1:D:62:ARG:NH2	3:D:1031:HOH:O	2.43	0.51
1:F:19:ARG:NH2	3:F:139:HOH:O	2.31	0.50
3:C:1014:HOH:O	1:E:68:MET:CE	2.59	0.50
1:C:64:VAL:O	1:C:68:MET:HG3	2.11	0.50
1:F:71:ARG:N	3:F:153:HOH:O	2.20	0.50
1:B:73:LEU:HG	1:D:68:MET:HE1	1.93	0.50
1:C:3:PRO:HD3	3:C:1044:HOH:O	2.11	0.50
3:B:1046:HOH:O	1:E:32:GLU:CG	2.59	0.50
1:C:65:GLU:HA	1:C:65:GLU:OE1	2.12	0.50
1:D:1:MET:HA	1:E:22:GLY:O	2.12	0.50
1:E:41:LEU:CD2	1:E:44:ARG:NH2	2.73	0.49
1:E:53:ASP:CG	3:E:149:HOH:O	2.50	0.49
1:B:23:LEU:HD23	1:B:23:LEU:N	2.28	0.49
1:D:75:VAL:HG11	1:D:103:ILE:CD1	2.42	0.49
1:F:64:VAL:O	1:F:68:MET:HG2	2.13	0.49
1:C:43:GLU:OE1	1:C:44:ARG:HD3	2.11	0.49
1:A:73:LEU:HD21	1:F:68:MET:HE3	1.95	0.49
1:E:38:LEU:O	1:E:42:VAL:HG23	2.12	0.49
1:C:33:GLU:CG	1:C:33:GLU:O	2.50	0.49
1:C:23:LEU:HD21	1:E:92:GLU:OE1	2.13	0.49
1:A:64:VAL:HG12	1:A:68:MET:HE2	1.95	0.49
1:B:98:LEU:HD13	3:B:1015:HOH:O	2.11	0.48
1:E:101:LYS:NZ	3:E:121:HOH:O	2.47	0.48
1:C:62:ARG:O	1:C:66:ARG:HG2	2.14	0.48
1:E:102:THR:HG21	3:E:150:HOH:O	2.14	0.48
1:C:65:GLU:HB3	1:C:69:ARG:NH1	2.29	0.48
1:D:84:GLU:O	1:D:87:GLN:HG3	2.13	0.48
1:A:37:LEU:HD23	3:A:162:HOH:O	2.13	0.47
1:F:68:MET:CE	1:F:68:MET:CA	2.92	0.47
1:B:28:ALA:CB	1:B:33:GLU:HG2	2.44	0.47
1:B:14:THR:HG22	1:B:18:PHE:CE1	2.49	0.47
1:A:64:VAL:HG12	1:A:68:MET:CE	2.44	0.47
1:A:32:GLU:CA	1:A:32:GLU:OE1	2.56	0.47
1:A:107:ILE:HD11	1:F:4:VAL:HG12	1.97	0.47
1:E:10:ALA:O	1:E:27:GLY:HA2	2.15	0.47
1:C:39:GLU:N	1:C:67:LEU:HD22	2.30	0.46
1:C:38:LEU:HD13	1:E:76:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:5:ARG:NH2	1:D:47:TYR:CZ	2.84	0.46
1:F:85:ALA:O	1:F:91:VAL:HG22	2.16	0.46
1:A:62:ARG:HD3	1:A:66:ARG:HD2	1.97	0.46
1:F:70:GLY:N	3:F:153:HOH:O	1.74	0.46
1:B:32:GLU:O	1:B:33:GLU:C	2.54	0.45
1:B:84:GLU:O	1:B:87:GLN:HG2	2.17	0.45
1:B:108:LYS:O	1:D:4:VAL:HB	2.16	0.45
1:C:39:GLU:HB2	1:C:67:LEU:HD23	1.98	0.45
1:C:81:GLY:O	1:C:84:GLU:OE1	2.35	0.45
1:B:95:MET:O	1:B:99:VAL:HG23	2.16	0.45
1:E:61:GLU:CD	1:E:61:GLU:H	2.20	0.45
1:C:9:ILE:CD1	1:C:38:LEU:CD2	2.95	0.45
1:F:32:GLU:CG	3:F:117:HOH:O	2.38	0.45
1:E:37:LEU:O	1:E:41:LEU:HG	2.17	0.45
3:B:1009:HOH:O	1:E:32:GLU:HG2	2.17	0.45
1:A:71:ARG:HB3	1:F:68:MET:HE2	1.97	0.44
1:A:73:LEU:HD21	1:F:68:MET:CE	2.47	0.44
1:B:38:LEU:HB3	1:B:67:LEU:HD11	1.99	0.44
1:C:78:PRO:O	1:C:79:ILE:HD13	2.17	0.44
1:B:73:LEU:HD21	1:D:68:MET:CE	2.47	0.44
1:E:85:ALA:HB2	1:E:94:TYR:CE2	2.53	0.44
1:F:100:ARG:HG2	3:F:126:HOH:O	2.16	0.44
3:B:1046:HOH:O	1:E:32:GLU:HG3	2.18	0.44
1:E:71:ARG:CB	3:E:156:HOH:O	2.56	0.44
1:D:38:LEU:HD23	1:D:38:LEU:HA	1.82	0.44
1:B:24:GLU:OE1	1:B:47:TYR:CZ	2.71	0.44
1:B:106:ASP:C	1:B:106:ASP:OD1	2.56	0.44
1:C:35:GLN:NE2	1:C:66:ARG:HB2	2.34	0.43
1:F:60:PRO:HD3	3:F:130:HOH:O	2.17	0.43
1:F:85:ALA:HB2	1:F:94:TYR:CE2	2.53	0.43
1:F:99:VAL:O	1:F:103:ILE:HG12	2.19	0.43
1:D:6:MET:HG3	1:D:49:LEU:HD23	2.00	0.43
1:A:97:GLU:HG2	3:A:148:HOH:O	2.20	0.42
1:F:68:MET:HE3	1:F:68:MET:HA	2.00	0.42
1:C:82:LEU:HD12	1:E:53:ASP:HB2	2.00	0.42
1:B:98:LEU:CD1	3:B:1015:HOH:O	2.68	0.42
1:B:48:ALA:O	1:D:74:PRO:HA	2.19	0.42
1:B:61:GLU:O	1:B:64:VAL:HB	2.20	0.42
1:F:104:GLY:O	1:F:105:PHE:HB2	2.20	0.42
1:E:5:ARG:HB3	1:E:46:GLY:O	2.19	0.42
1:D:5:ARG:HG2	3:D:1026:HOH:O	2.19	0.41
1:E:41:LEU:HD23	1:E:44:ARG:NH2	2.32	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:36:SER:C	3:A:139:HOH:O	2.59	0.41
1:F:43:GLU:HB3	3:F:119:HOH:O	2.21	0.41
1:E:85:ALA:HB2	1:E:94:TYR:CD2	2.55	0.41
1:C:4:VAL:HG13	1:C:48:ALA:HB3	2.02	0.41
1:C:60:PRO:HG3	1:E:78:PRO:HG3	2.03	0.41
1:B:78:PRO:HB3	1:D:57:LEU:HD23	2.02	0.41
1:A:20:LEU:O	1:B:4:VAL:HG21	2.21	0.41
1:D:74:PRO:O	1:D:76:LEU:HD23	2.21	0.41
1:F:65:GLU:O	1:F:69:ARG:HB3	2.20	0.41
1:C:61:GLU:O	1:C:65:GLU:HG2	2.21	0.41
1:E:70:GLY:O	1:E:71:ARG:C	2.59	0.40
3:B:1025:HOH:O	1:E:39:GLU:HG2	2.20	0.40
1:E:87:GLN:HB2	3:E:132:HOH:O	2.22	0.40
1:A:64:VAL:HG13	1:F:73:LEU:CD1	2.50	0.40
1:E:32:GLU:HA	1:E:32:GLU:OE1	2.21	0.40
1:B:106:ASP:HA	3:B:1012:HOH:O	2.20	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:92:GLU:OE2	3:E:157:HOH:O[2_665]	2.06	0.14
1:B:89:HIS:ND1	3:F:126:HOH:O[1_554]	2.08	0.12

## 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	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	25	21
1	B	107/109 (98%)	98 (92%)	6 (6%)	3 (3%)	8	3
1	C	107/109 (98%)	99 (92%)	7 (6%)	1 (1%)	25	21
1	D	107/109 (98%)	95 (89%)	11 (10%)	1 (1%)	25	21
1	E	107/109 (98%)	101 (94%)	4 (4%)	2 (2%)	12	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	107/109 (98%)	99 (92%)	6 (6%)	2 (2%)	12	7
All	All	642/654 (98%)	592 (92%)	40 (6%)	10 (2%)	14	9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	B	45	GLY
1	F	105	PHE
1	B	40	THR
1	C	40	THR
1	E	70	GLY
1	E	71	ARG
1	B	39	GLU
1	D	72	ASP
1	F	70	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	85/85 (100%)	81 (95%)	4 (5%)	36	42
1	B	85/85 (100%)	79 (93%)	6 (7%)	21	21
1	C	85/85 (100%)	81 (95%)	4 (5%)	36	42
1	D	85/85 (100%)	83 (98%)	2 (2%)	61	73
1	E	85/85 (100%)	82 (96%)	3 (4%)	48	57
1	F	85/85 (100%)	76 (89%)	9 (11%)	10	8
All	All	510/510 (100%)	482 (94%)	28 (6%)	30	34

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	20	LEU

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Mol	Chain	Res	Type
1	A	62	ARG
1	A	69	ARG
1	B	23	LEU
1	B	36	SER
1	B	49	LEU
1	B	84	GLU
1	B	86	PHE
1	B	96	ARG
1	C	2	VAL
1	C	43	GLU
1	C	49	LEU
1	C	107	ILE
1	D	62	ARG
1	D	102	THR
1	E	1	MET
1	E	61	GLU
1	E	62	ARG
1	F	12	PRO
1	F	62	ARG
1	F	68	MET
1	F	69	ARG
1	F	71	ARG
1	F	97	GLU
1	F	100	ARG
1	F	105	PHE
1	F	107	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	87	GLN
1	D	87	GLN
1	D	89	HIS
1	F	89	HIS

### 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 ⓘ

Of 4 ligands modelled in this entry, 4 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.

## 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	109/109 (100%)	0.23	6 (5%)	24 24	59, 68, 77, 83	0
1	B	109/109 (100%)	0.37	5 (4%)	31 31	58, 66, 78, 82	0
1	C	109/109 (100%)	0.42	12 (11%)	6 6	59, 68, 80, 84	0
1	D	109/109 (100%)	0.55	12 (11%)	6 6	53, 67, 76, 83	0
1	E	109/109 (100%)	0.31	8 (7%)	15 14	56, 66, 79, 84	0
1	F	109/109 (100%)	0.30	7 (6%)	19 18	53, 66, 80, 89	0
All	All	654/654 (100%)	0.36	50 (7%)	14 13	53, 67, 79, 89	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	88	GLY	5.8
1	E	1	MET	5.4
1	F	89	HIS	5.2
1	B	87	GLN	4.4
1	D	89	HIS	4.3
1	E	109	LEU	4.2
1	E	87	GLN	4.2
1	D	1	MET	4.0
1	F	108	LYS	3.8
1	F	88	GLY	3.6
1	C	69	ARG	3.5
1	D	109	LEU	3.5
1	F	87	GLN	3.5
1	D	87	GLN	3.3
1	C	92	GLU	3.2
1	D	80	ALA	3.1
1	D	105	PHE	3.1
1	F	2	VAL	3.0
1	C	2	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	70	GLY	2.8
1	C	39	GLU	2.7
1	C	1	MET	2.6
1	C	50	VAL	2.6
1	F	8	VAL	2.5
1	B	29	SER	2.4
1	A	109	LEU	2.4
1	D	51	ALA	2.4
1	C	32	GLU	2.4
1	C	45	GLY	2.4
1	A	1	MET	2.3
1	E	44	ARG	2.3
1	F	90	ASP	2.3
1	D	96	ARG	2.3
1	E	9	ILE	2.2
1	B	13	GLU	2.2
1	E	108	LYS	2.2
1	B	56	LEU	2.2
1	A	2	VAL	2.2
1	C	67	LEU	2.1
1	A	65	GLU	2.1
1	D	73	LEU	2.1
1	E	105	PHE	2.1
1	C	81	GLY	2.1
1	A	51	ALA	2.1
1	D	8	VAL	2.1
1	B	100	ARG	2.0
1	D	9	ILE	2.0
1	C	3	PRO	2.0
1	A	50	VAL	2.0
1	C	96	ARG	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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	C	1003	1/1	0.04	-1.31	53,53,53,53	0
2	CA	B	1004	1/1	0.03	-1.95	72,72,72,72	0
2	CA	B	1002	1/1	0.06	-2.23	67,67,67,67	0
2	CA	D	1001	1/1	0.03	-3.19	59,59,59,59	0

## 6.5 Other polymers

There are no such residues in this entry.