



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2023 – 08:07 PM JST

PDB ID : 8JLV  
Title : Beneficial flip of substrate orientation enable determine substrate specificity for zearalenone lactone hydrolase  
Authors : Xiang, L.; Wang, M.; Zhang, G.; Zhou, J.  
Deposited on : 2023-06-02  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

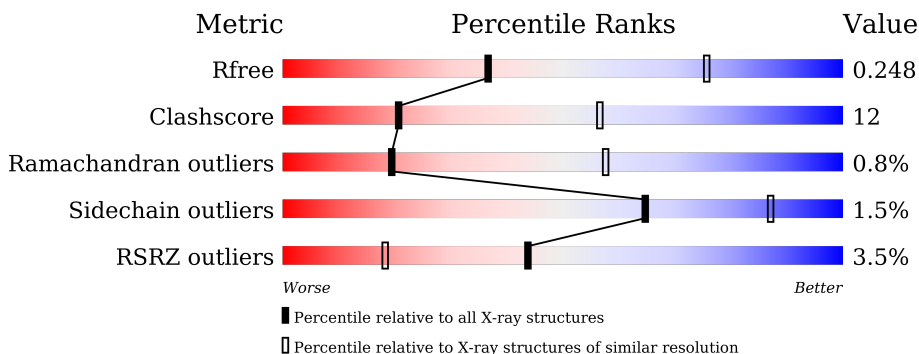
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	 2% 71% 28% .
1	B	264	 3% 74% 25% .
1	C	264	 2% 76% 23% .
1	D	264	 4% 78% 19% .
1	E	264	 7% 70% 27% ..
1	F	264	 3% 70% 27% .

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12360 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 AB hydrolase-1 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	264	2060	1313	340	394	13	0	0	0
1	A	264	2060	1313	340	394	13	0	0	0
1	C	264	2060	1313	340	394	13	0	0	0
1	D	264	2060	1313	340	394	13	0	0	0
1	E	264	2060	1313	340	394	13	0	0	0
1	F	264	2060	1313	340	394	13	0	0	0

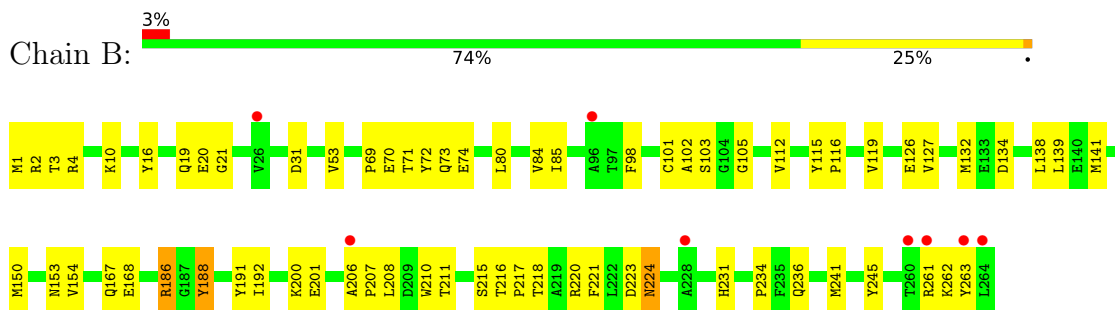
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	102	ALA	SER	conflict	UNP A0A072PAD1
A	102	ALA	SER	conflict	UNP A0A072PAD1
C	102	ALA	SER	conflict	UNP A0A072PAD1
D	102	ALA	SER	conflict	UNP A0A072PAD1
E	102	ALA	SER	conflict	UNP A0A072PAD1
F	102	ALA	SER	conflict	UNP A0A072PAD1

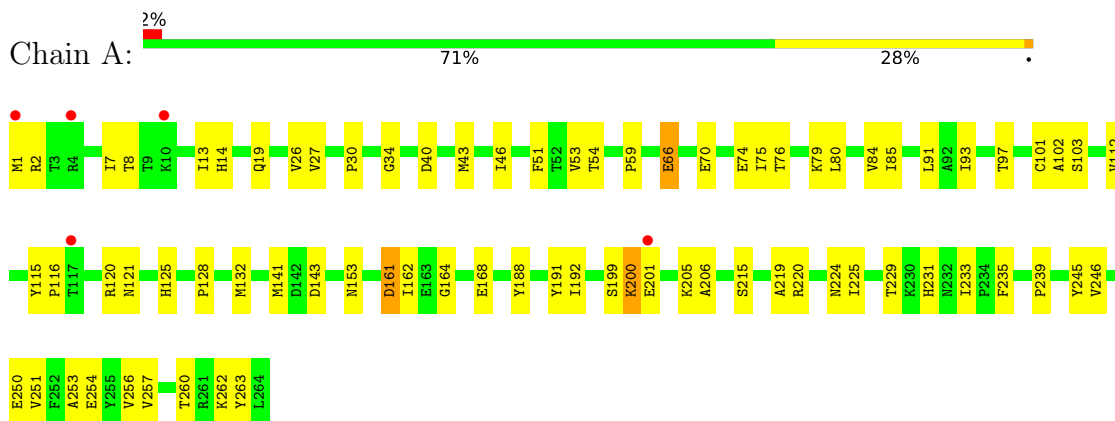
### 3 Residue-property plots [i](#)

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

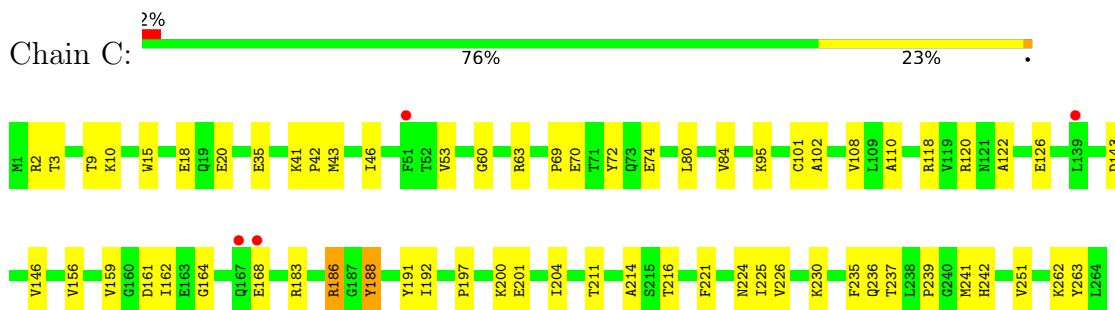
- Molecule 1: AB hydrolase-1 domain-containing protein



- Molecule 1: AB hydrolase-1 domain-containing protein



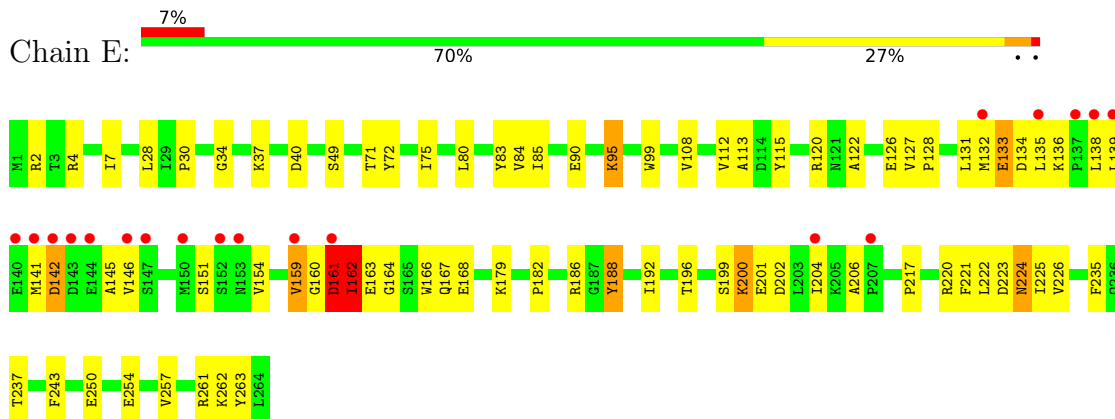
- Molecule 1: AB hydrolase-1 domain-containing protein



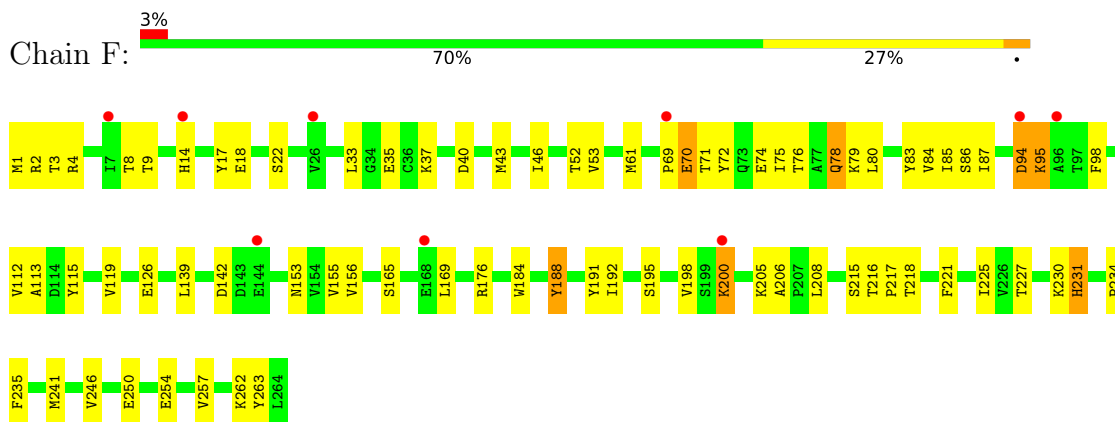
- Molecule 1: AB hydrolase-1 domain-containing protein



- Molecule 1: AB hydrolase-1 domain-containing protein



- Molecule 1: AB hydrolase-1 domain-containing protein



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.89Å 120.33Å 102.95Å 90.00° 97.42° 90.00°	Depositor
Resolution (Å)	42.70 – 3.00 44.74 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (42.70-3.00) 96.7 (44.74-3.00)	Depositor EDS
$R_{merge}$	0.32	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575, PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.204 , 0.247 0.205 , 0.248	Depositor DCC
$R_{free}$ test set	1833 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.5	Xtrriage
Anisotropy	0.019	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 20.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12360	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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	0.45	1/2117 (0.0%)	0.67	2/2887 (0.1%)
1	B	0.49	2/2117 (0.1%)	0.76	8/2887 (0.3%)
1	C	0.44	0/2117	0.65	2/2887 (0.1%)
1	D	0.50	2/2117 (0.1%)	0.85	12/2887 (0.4%)
1	E	0.42	0/2117	0.79	8/2887 (0.3%)
1	F	0.61	3/2117 (0.1%)	0.72	6/2887 (0.2%)
All	All	0.49	8/12702 (0.1%)	0.74	38/17322 (0.2%)

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	E	0	1
1	F	0	1
All	All	0	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	70	GLU	CD-OE2	-13.09	1.11	1.25
1	F	70	GLU	CG-CD	12.57	1.70	1.51
1	F	70	GLU	CD-OE1	-9.13	1.15	1.25
1	B	201	GLU	CG-CD	7.11	1.62	1.51
1	D	200	LYS	CB-CG	-6.74	1.34	1.52
1	B	201	GLU	CB-CG	6.13	1.63	1.52
1	A	1	MET	CB-CG	5.69	1.69	1.51
1	D	133	GLU	CD-OE2	5.32	1.31	1.25

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	7	ILE	CG1-CB-CG2	-12.67	83.53	111.40
1	E	162	ILE	CG1-CB-CG2	-11.51	86.07	111.40
1	E	161	ASP	CB-CG-OD1	-9.95	109.34	118.30
1	B	261	ARG	NE-CZ-NH1	-9.52	115.54	120.30
1	D	133	GLU	CA-C-O	-9.17	100.83	120.10
1	A	1	MET	N-CA-CB	9.15	127.06	110.60
1	C	41	LYS	CD-CE-NZ	-8.58	91.97	111.70
1	B	201	GLU	CA-CB-CG	8.54	132.20	113.40
1	B	261	ARG	CB-CG-CD	-8.38	89.83	111.60
1	F	70	GLU	CA-CB-CG	-8.23	95.28	113.40
1	E	161	ASP	CB-CG-OD2	7.90	125.41	118.30
1	D	200	LYS	CD-CE-NZ	-7.37	94.76	111.70
1	E	200	LYS	CD-CE-NZ	-7.36	94.77	111.70
1	E	159	VAL	CG1-CB-CG2	6.97	122.06	110.90
1	F	94	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	F	200	LYS	N-CA-CB	-6.68	98.57	110.60
1	D	94	ASP	CB-CA-C	-6.61	97.18	110.40
1	F	94	ASP	CB-CG-OD1	6.53	124.17	118.30
1	B	261	ARG	NE-CZ-NH2	6.45	123.53	120.30
1	D	132	MET	CG-SD-CE	6.43	110.48	100.20
1	D	133	GLU	CA-CB-CG	6.34	127.36	113.40
1	D	133	GLU	C-N-CA	6.31	137.47	121.70
1	D	94	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	E	160	GLY	C-N-CA	-6.21	106.17	121.70
1	D	132	MET	CB-CA-C	6.05	122.50	110.40
1	F	200	LYS	CD-CE-NZ	-5.96	97.98	111.70
1	F	200	LYS	CA-CB-CG	-5.83	100.56	113.40
1	E	95	LYS	CD-CE-NZ	5.66	124.72	111.70
1	D	133	GLU	CB-CA-C	-5.55	99.30	110.40
1	B	261	ARG	CD-NE-CZ	5.25	130.95	123.60
1	E	167	GLN	CB-CA-C	-5.25	99.90	110.40
1	B	201	GLU	CG-CD-OE2	5.18	128.66	118.30
1	A	161	ASP	C-N-CA	-5.12	108.90	121.70
1	D	133	GLU	CA-C-N	5.11	128.44	117.20
1	B	10	LYS	CA-CB-CG	-5.05	102.28	113.40
1	C	186	ARG	CA-CB-CG	5.05	124.51	113.40
1	D	133	GLU	O-C-N	5.01	130.72	122.70
1	B	10	LYS	CD-CE-NZ	5.01	123.21	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	66	GLU	Sidechain
1	E	161	ASP	Peptide
1	F	231	HIS	Sidechain

## 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	2060	0	2006	56	0
1	B	2060	0	2006	47	0
1	C	2060	0	2006	39	0
1	D	2060	0	2003	47	0
1	E	2060	0	2006	61	0
1	F	2060	0	2006	64	0
All	All	12360	0	12033	299	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 12.

All (299) 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:D:94:ASP:OD1	1:D:95:LYS:HB3	1.51	1.09
1:E:162:ILE:HD11	1:E:166:TRP:H	1.21	1.04
1:E:135:LEU:HB3	1:E:139:LEU:HD13	1.40	1.03
1:D:94:ASP:OD1	1:D:95:LYS:N	1.97	0.98
1:F:8:THR:OG1	1:F:14:HIS:ND1	1.99	0.96
1:B:218:THR:HA	1:F:218:THR:HG22	1.50	0.90
1:F:85:ILE:HG13	1:F:115:TYR:CD2	2.13	0.84
1:D:60:GLY:O	1:D:183:ARG:NH2	2.13	0.81
1:E:201:GLU:O	1:E:201:GLU:HG3	1.80	0.79
1:B:2:ARG:O	1:C:204:ILE:HD11	1.83	0.79
1:B:1:MET:HG2	1:B:21:GLY:H	1.46	0.79
1:D:94:ASP:OD1	1:D:95:LYS:CB	2.30	0.77
1:E:162:ILE:CD1	1:E:166:TRP:H	1.97	0.77
1:F:76:THR:OG1	1:F:78:GLN:NE2	2.18	0.77
1:B:168:GLU:HG2	1:B:168:GLU:O	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:LYS:O	1:D:140:GLU:HG3	1.86	0.74
1:A:200:LYS:HG3	1:A:231:HIS:NE2	2.04	0.71
1:F:69:PRO:HB2	1:F:70:GLU:OE1	1.91	0.70
1:A:164:GLY:O	1:A:168:GLU:HG3	1.92	0.70
1:B:134:ASP:OD1	1:B:220:ARG:NH2	2.25	0.69
1:D:2:ARG:HD3	1:D:20:GLU:HB2	1.73	0.68
1:C:9:THR:OG1	1:C:15:TRP:NE1	2.27	0.68
1:F:76:THR:HG23	1:F:79:LYS:H	1.60	0.67
1:A:19:GLN:HE21	1:A:91:LEU:HD13	1.59	0.67
1:D:125:HIS:ND1	1:D:211:THR:OG1	2.25	0.67
1:A:14:HIS:CE1	1:A:66:GLU:OE2	2.47	0.67
1:B:216:THR:O	1:F:218:THR:HG23	1.96	0.66
1:D:7:ILE:HD11	1:D:90:GLU:HB3	1.78	0.66
1:C:161:ASP:OD1	1:C:162:ILE:N	2.28	0.66
1:C:118:ARG:NH2	1:D:22:SER:OG	2.29	0.65
1:B:153:ASN:HB3	1:A:153:ASN:HD22	1.61	0.65
1:E:112:VAL:HG13	1:E:206:ALA:HB3	1.79	0.65
1:C:200:LYS:H	1:C:200:LYS:HE2	1.61	0.64
1:E:138:LEU:HD12	1:E:141:MET:HE3	1.79	0.64
1:C:108:VAL:HG13	1:C:122:ALA:HB1	1.79	0.64
1:B:216:THR:HG22	1:B:241:MET:HB3	1.79	0.64
1:E:131:LEU:HD11	1:E:135:LEU:HD22	1.79	0.64
1:A:112:VAL:HG13	1:A:206:ALA:HB3	1.80	0.63
1:C:9:THR:HG1	1:C:15:TRP:HE1	1.47	0.63
1:D:134:ASP:O	1:D:136:LYS:N	2.32	0.62
1:B:200:LYS:HD2	1:B:231:HIS:NE2	2.14	0.62
1:C:226:VAL:O	1:C:230:LYS:HG3	1.99	0.62
1:A:97:THR:HG23	1:A:120:ARG:HH11	1.65	0.62
1:A:80:LEU:O	1:A:84:VAL:HG23	2.01	0.61
1:C:126:GLU:OE2	1:C:216:THR:HG21	2.01	0.61
1:A:161:ASP:OD1	1:A:162:ILE:N	2.33	0.61
1:A:231:HIS:HB2	1:A:233:ILE:HD12	1.83	0.61
1:F:33:LEU:HD11	1:F:155:VAL:HG11	1.81	0.61
1:E:135:LEU:O	1:E:138:LEU:N	2.32	0.61
1:E:142:ASP:HB2	1:E:145:ALA:H	1.66	0.61
1:E:162:ILE:HG12	1:E:164:GLY:H	1.66	0.60
1:F:200:LYS:HD3	1:F:200:LYS:N	2.07	0.60
1:F:250:GLU:O	1:F:254:GLU:HG3	2.01	0.60
1:A:219:ALA:HB2	1:E:237:THR:HG21	1.82	0.60
1:D:230:LYS:HB3	1:D:231:HIS:CD2	2.36	0.60
1:E:2:ARG:HG2	1:E:4:ARG:NH1	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:MET:SD	1:A:162:ILE:HD11	2.42	0.59
1:A:97:THR:HG23	1:A:120:ARG:NH1	2.16	0.59
1:A:132:MET:SD	1:A:220:ARG:NH1	2.74	0.59
1:F:94:ASP:OD1	1:F:95:LYS:N	2.34	0.59
1:A:162:ILE:HG13	1:A:162:ILE:O	2.01	0.59
1:A:97:THR:HG22	1:A:121:ASN:HB3	1.85	0.59
1:D:262:LYS:HE2	1:D:263:TYR:CZ	2.37	0.58
1:E:161:ASP:OD1	1:E:161:ASP:O	2.19	0.58
1:F:69:PRO:HD2	1:F:70:GLU:OE1	2.03	0.58
1:B:132:MET:SD	1:B:220:ARG:NH1	2.76	0.58
1:A:199:SER:OG	1:A:201:GLU:OE1	2.20	0.58
1:F:98:PHE:HD1	1:F:119:VAL:HG23	1.69	0.58
1:A:201:GLU:OE1	1:A:201:GLU:N	2.34	0.58
1:C:188:TYR:O	1:C:192:ILE:HG22	2.04	0.58
1:B:112:VAL:HG13	1:B:206:ALA:HB3	1.84	0.57
1:D:200:LYS:HD3	1:D:231:HIS:CE1	2.39	0.57
1:A:43:MET:HG3	1:A:53:VAL:CG2	2.34	0.57
1:F:112:VAL:HG13	1:F:206:ALA:HB3	1.85	0.57
1:B:262:LYS:HE2	1:B:263:TYR:CZ	2.39	0.57
1:F:43:MET:HG3	1:F:53:VAL:HG11	1.87	0.57
1:D:80:LEU:O	1:D:84:VAL:HG23	2.04	0.56
1:D:75:ILE:HA	1:D:79:LYS:HE2	1.87	0.56
1:E:132:MET:O	1:E:133:GLU:C	2.43	0.56
1:D:94:ASP:OD1	1:D:95:LYS:CA	2.54	0.56
1:F:69:PRO:CB	1:F:70:GLU:OE1	2.53	0.56
1:B:141:MET:H	1:B:186:ARG:NH1	2.04	0.56
1:B:31:ASP:OD1	1:B:245:TYR:OH	2.23	0.56
1:A:13:ILE:HD13	1:A:59:PRO:HG3	1.89	0.55
1:B:126:GLU:HB3	1:B:221:PHE:CZ	2.42	0.55
1:D:155:VAL:HA	1:D:159:VAL:HB	1.88	0.55
1:F:69:PRO:HA	1:F:72:TYR:CZ	2.42	0.55
1:E:37:LYS:NZ	1:E:40:ASP:OD2	2.40	0.54
1:E:135:LEU:HB3	1:E:139:LEU:CD1	2.28	0.54
1:F:1:MET:HG3	1:F:2:ARG:N	2.23	0.54
1:F:69:PRO:CD	1:F:70:GLU:OE1	2.55	0.54
1:A:51:PHE:HE2	1:A:257:VAL:HG13	1.72	0.54
1:A:46:ILE:HG23	1:A:257:VAL:HG22	1.89	0.54
1:D:30:PRO:HB2	1:D:34:GLY:HA2	1.90	0.54
1:F:84:VAL:HA	1:F:87:ILE:HG22	1.90	0.53
1:F:85:ILE:HG13	1:F:115:TYR:HD2	1.68	0.53
1:E:162:ILE:CG1	1:E:164:GLY:H	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:PRO:HD2	1:F:70:GLU:CD	2.28	0.53
1:F:94:ASP:OD1	1:F:95:LYS:HG3	2.08	0.53
1:C:80:LEU:O	1:C:84:VAL:HG23	2.08	0.53
1:F:76:THR:CG2	1:F:79:LYS:HG3	2.39	0.53
1:F:98:PHE:CD1	1:F:119:VAL:HG23	2.44	0.52
1:F:200:LYS:NZ	1:F:227:THR:HG23	2.25	0.52
1:B:262:LYS:HE2	1:B:263:TYR:CE2	2.44	0.52
1:F:126:GLU:OE2	1:F:216:THR:HG21	2.09	0.52
1:B:3:THR:HG22	1:C:200:LYS:HB2	1.91	0.52
1:A:262:LYS:HE2	1:A:263:TYR:OH	2.09	0.52
1:F:37:LYS:NZ	1:F:40:ASP:OD2	2.41	0.52
1:B:217:PRO:HB3	1:F:215:SER:HA	1.92	0.52
1:E:49:SER:HB3	1:E:261:ARG:HH21	1.73	0.52
1:C:164:GLY:O	1:C:168:GLU:HG3	2.10	0.52
1:C:211:THR:HA	1:C:236:GLN:O	2.11	0.51
1:D:134:ASP:C	1:D:136:LYS:H	2.13	0.51
1:A:229:THR:HG21	1:E:226:VAL:HG13	1.92	0.51
1:C:262:LYS:HE2	1:C:263:TYR:CZ	2.45	0.51
1:E:223:ASP:OD1	1:E:224:ASN:ND2	2.43	0.51
1:A:225:ILE:HG12	1:A:235:PHE:CZ	2.46	0.51
1:E:95:LYS:HD3	1:E:120:ARG:HB2	1.92	0.51
1:D:26:VAL:HG22	1:D:97:THR:HB	1.93	0.51
1:D:230:LYS:C	1:D:231:HIS:CD2	2.84	0.51
1:F:188:TYR:O	1:F:192:ILE:HG22	2.11	0.50
1:E:113:ALA:HB2	1:E:202:ASP:HB3	1.93	0.50
1:B:150:MET:O	1:B:154:VAL:HG23	2.11	0.50
1:B:211:THR:HA	1:B:236:GLN:O	2.12	0.50
1:D:231:HIS:HB2	1:D:233:ILE:HD12	1.94	0.50
1:B:74:GLU:HA	1:B:191:TYR:CG	2.47	0.49
1:D:256:VAL:O	1:D:260:THR:HG22	2.11	0.49
1:F:200:LYS:HZ3	1:F:227:THR:HG23	1.77	0.49
1:B:103:SER:HB2	1:B:192:ILE:HD13	1.95	0.49
1:C:143:ASP:OD1	1:C:146:VAL:HG23	2.13	0.49
1:E:131:LEU:O	1:E:132:MET:HB2	2.12	0.49
1:B:85:ILE:HG13	1:B:115:TYR:CD2	2.47	0.49
1:A:85:ILE:HG13	1:A:115:TYR:CD2	2.48	0.49
1:F:216:THR:HG22	1:F:241:MET:HB3	1.95	0.49
1:E:186:ARG:HG2	1:E:186:ARG:HH21	1.77	0.49
1:A:97:THR:HA	1:A:121:ASN:O	2.13	0.49
1:A:19:GLN:NE2	1:A:91:LEU:HD13	2.27	0.48
1:A:51:PHE:CE2	1:A:257:VAL:HG13	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLU:HA	1:A:191:TYR:CG	2.48	0.48
1:E:162:ILE:HG13	1:E:163:GLU:N	2.28	0.48
1:F:85:ILE:HG13	1:F:115:TYR:CE2	2.47	0.48
1:B:69:PRO:HA	1:B:72:TYR:CZ	2.49	0.48
1:A:215:SER:HA	1:E:217:PRO:HB3	1.94	0.48
1:B:80:LEU:O	1:B:84:VAL:HG23	2.14	0.48
1:C:3:THR:O	1:C:18:GLU:HA	2.14	0.48
1:E:113:ALA:CB	1:E:202:ASP:HB3	2.44	0.48
1:F:76:THR:HG22	1:F:79:LYS:HG3	1.94	0.48
1:F:80:LEU:O	1:F:84:VAL:HG22	2.14	0.48
1:B:188:TYR:O	1:B:192:ILE:HG22	2.14	0.48
1:F:35:GLU:OE2	1:F:176:ARG:NH1	2.46	0.48
1:E:80:LEU:O	1:E:84:VAL:HG23	2.14	0.48
1:D:56:PHE:HZ	1:D:84:VAL:HG13	1.79	0.47
1:E:138:LEU:HD11	1:E:146:VAL:HG13	1.97	0.47
1:E:142:ASP:O	1:E:146:VAL:HG23	2.14	0.47
1:F:2:ARG:HG3	1:F:4:ARG:NE	2.29	0.47
1:F:198:VAL:O	1:F:200:LYS:HE2	2.13	0.47
1:E:126:GLU:HB3	1:E:221:PHE:CZ	2.50	0.47
1:B:2:ARG:O	1:C:201:GLU:OE2	2.33	0.47
1:A:262:LYS:HE2	1:A:263:TYR:CZ	2.48	0.47
1:F:74:GLU:HG2	1:F:191:TYR:CE1	2.48	0.47
1:A:162:ILE:HD12	1:A:162:ILE:HA	1.66	0.47
1:C:216:THR:HG22	1:C:241:MET:HB3	1.95	0.47
1:E:154:VAL:HG22	1:E:159:VAL:HG23	1.97	0.47
1:A:76:THR:OG1	1:A:79:LYS:HG3	2.15	0.47
1:D:262:LYS:HE2	1:D:263:TYR:OH	2.15	0.47
1:E:71:THR:HG22	1:E:83:TYR:CZ	2.50	0.47
1:F:43:MET:HG3	1:F:53:VAL:CG1	2.45	0.47
1:E:162:ILE:HD11	1:E:166:TRP:N	2.06	0.47
1:F:46:ILE:HG23	1:F:257:VAL:HG12	1.96	0.47
1:A:43:MET:HG3	1:A:53:VAL:HG23	1.97	0.47
1:D:75:ILE:HA	1:D:79:LYS:CE	2.45	0.47
1:D:56:PHE:CZ	1:D:84:VAL:HG13	2.50	0.46
1:F:71:THR:HG22	1:F:83:TYR:CZ	2.50	0.46
1:D:159:VAL:HG22	1:D:243:PHE:CD1	2.49	0.46
1:A:43:MET:HG3	1:A:53:VAL:HG21	1.96	0.46
1:C:108:VAL:CG1	1:C:122:ALA:HB1	2.44	0.46
1:B:4:ARG:HG3	1:B:16:TYR:CE2	2.51	0.46
1:E:162:ILE:CD1	1:E:166:TRP:CB	2.93	0.46
1:F:139:LEU:HA	1:F:139:LEU:HD23	1.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:GLU:O	1:D:254:GLU:HG3	2.16	0.46
1:A:253:ALA:O	1:A:257:VAL:HG23	2.16	0.46
1:F:208:LEU:O	1:F:234:PRO:HD2	2.15	0.46
1:B:70:GLU:HG2	1:B:71:THR:N	2.31	0.45
1:A:70:GLU:O	1:A:79:LYS:NZ	2.32	0.45
1:C:156:VAL:HA	1:C:159:VAL:HG23	1.97	0.45
1:F:113:ALA:O	1:F:205:LYS:NZ	2.40	0.45
1:B:223:ASP:OD1	1:B:224:ASN:ND2	2.48	0.45
1:E:159:VAL:HA	1:E:243:PHE:HD1	1.81	0.45
1:C:239:PRO:HG2	1:C:251:VAL:HG11	1.97	0.45
1:F:165:SER:HB2	1:F:246:VAL:O	2.16	0.45
1:B:101:CYS:SG	1:B:102:ALA:N	2.90	0.45
1:C:9:THR:HG22	1:C:10:LYS:N	2.31	0.45
1:D:112:VAL:HG13	1:D:206:ALA:HB3	1.99	0.45
1:B:216:THR:HG22	1:B:241:MET:CB	2.47	0.45
1:C:2:ARG:HA	1:C:20:GLU:HB2	1.99	0.45
1:E:250:GLU:O	1:E:254:GLU:HG3	2.17	0.45
1:D:75:ILE:HD11	1:D:188:TYR:CD2	2.51	0.45
1:D:41:LYS:O	1:D:45:LEU:HD12	2.17	0.45
1:D:108:VAL:CG1	1:D:122:ALA:HB1	2.47	0.44
1:A:27:VAL:HG22	1:A:54:THR:HG23	1.99	0.44
1:C:214:ALA:HB2	1:C:237:THR:CG2	2.47	0.44
1:D:232:ASN:O	1:D:232:ASN:ND2	2.49	0.44
1:F:126:GLU:HB3	1:F:221:PHE:CZ	2.53	0.44
1:D:126:GLU:OE2	1:D:242:HIS:ND1	2.32	0.44
1:D:135:LEU:N	1:D:135:LEU:HD22	2.32	0.44
1:A:102:ALA:HA	1:A:128:PRO:HD3	1.99	0.44
1:C:110:ALA:HA	1:C:197:PRO:HG3	2.00	0.44
1:C:226:VAL:HG12	1:C:230:LYS:HD2	1.98	0.44
1:F:262:LYS:NZ	1:F:263:TYR:OH	2.51	0.44
1:A:2:ARG:NH2	1:A:40:ASP:O	2.51	0.44
1:A:239:PRO:HG2	1:A:251:VAL:HG11	1.99	0.44
1:D:134:ASP:C	1:D:136:LYS:N	2.71	0.44
1:E:201:GLU:O	1:E:204:ILE:HG22	2.18	0.44
1:B:207:PRO:HB3	1:B:263:TYR:CE1	2.53	0.44
1:C:70:GLU:H	1:C:70:GLU:HG3	1.49	0.43
1:A:116:PRO:HG2	1:A:205:LYS:HZ2	1.83	0.43
1:C:60:GLY:O	1:C:183:ARG:NH2	2.51	0.43
1:C:69:PRO:HA	1:C:72:TYR:CZ	2.53	0.43
1:D:162:ILE:HD12	1:D:162:ILE:HA	1.85	0.43
1:A:256:VAL:O	1:A:260:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:PRO:HB3	1:E:132:MET:CE	2.48	0.43
1:E:188:TYR:O	1:E:192:ILE:HG22	2.18	0.43
1:F:153:ASN:HA	1:F:156:VAL:HG12	2.00	0.43
1:F:22:SER:HA	1:F:52:THR:OG1	2.18	0.43
1:B:167:GLN:HB2	1:A:143:ASP:OD1	2.19	0.43
1:E:108:VAL:HG13	1:E:122:ALA:HB1	1.99	0.43
1:E:141:MET:HB2	1:E:142:ASP:H	1.69	0.43
1:F:61:MET:HE1	1:F:184:TRP:HB2	2.01	0.43
1:F:225:ILE:HG12	1:F:235:PHE:CZ	2.54	0.43
1:D:230:LYS:O	1:D:231:HIS:HD2	2.02	0.43
1:B:138:LEU:HD11	1:B:154:VAL:HG21	2.01	0.43
1:E:199:SER:HB3	1:E:202:ASP:OD2	2.19	0.43
1:E:220:ARG:HG2	1:E:221:PHE:CE2	2.53	0.43
1:A:75:ILE:HG22	1:A:192:ILE:HD12	1.99	0.42
1:F:227:THR:O	1:F:231:HIS:CD2	2.72	0.42
1:D:135:LEU:O	1:D:138:LEU:N	2.52	0.42
1:E:162:ILE:HD13	1:E:162:ILE:HG21	1.72	0.42
1:A:54:THR:HG21	1:A:93:ILE:CD1	2.49	0.42
1:C:126:GLU:OE1	1:C:242:HIS:ND1	2.30	0.42
1:D:75:ILE:HD12	1:D:75:ILE:O	2.20	0.42
1:E:30:PRO:HB2	1:E:34:GLY:HA2	2.01	0.42
1:F:3:THR:O	1:F:18:GLU:HA	2.19	0.42
1:B:69:PRO:HB3	1:B:73:GLN:NE2	2.34	0.42
1:D:7:ILE:HD13	1:D:7:ILE:HG21	1.45	0.42
1:A:103:SER:HB2	1:A:192:ILE:HD13	2.00	0.42
1:C:126:GLU:HB3	1:C:221:PHE:CZ	2.54	0.42
1:E:7:ILE:CD1	1:E:90:GLU:HB3	2.50	0.42
1:E:72:TYR:CA	1:E:75:ILE:HD11	2.48	0.42
1:E:262:LYS:HE2	1:E:263:TYR:OH	2.18	0.42
1:A:7:ILE:HD12	1:A:8:THR:H	1.83	0.42
1:C:43:MET:HG3	1:C:53:VAL:HG11	2.01	0.42
1:D:101:CYS:SG	1:D:102:ALA:N	2.93	0.42
1:B:105:GLY:HA3	1:B:127:VAL:HG12	2.01	0.42
1:A:26:VAL:O	1:A:53:VAL:HA	2.20	0.42
1:A:74:GLU:HA	1:A:191:TYR:CD2	2.54	0.42
1:E:164:GLY:O	1:E:168:GLU:HG3	2.20	0.42
1:F:74:GLU:HA	1:F:191:TYR:CG	2.55	0.42
1:B:98:PHE:CE1	1:B:119:VAL:HG12	2.55	0.42
1:B:112:VAL:O	1:B:116:PRO:HG3	2.20	0.42
1:D:125:HIS:HD1	1:D:211:THR:HG1	1.59	0.42
1:D:159:VAL:HG12	1:D:160:GLY:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:VAL:CG1	1:E:122:ALA:HB1	2.50	0.41
1:A:97:THR:HG21	1:A:260:THR:HG22	2.02	0.41
1:C:74:GLU:HA	1:C:191:TYR:CG	2.56	0.41
1:E:131:LEU:HD12	1:E:134:ASP:HA	2.02	0.41
1:F:230:LYS:HB2	1:F:231:HIS:NE2	2.35	0.41
1:B:150:MET:HA	1:A:153:ASN:ND2	2.35	0.41
1:D:94:ASP:O	1:D:118:ARG:NE	2.38	0.41
1:B:2:ARG:HA	1:B:20:GLU:HB2	2.03	0.41
1:D:225:ILE:HG12	1:D:235:PHE:CZ	2.55	0.41
1:E:85:ILE:HG13	1:E:115:TYR:CD2	2.54	0.41
1:B:127:VAL:HG22	1:B:210:TRP:HZ2	1.85	0.41
1:A:101:CYS:HA	1:A:125:HIS:O	2.20	0.41
1:C:42:PRO:O	1:C:46:ILE:HG13	2.21	0.41
1:E:28:LEU:HD23	1:E:99:TRP:HB3	2.03	0.41
1:B:208:LEU:O	1:B:234:PRO:HD2	2.20	0.41
1:B:215:SER:HA	1:F:217:PRO:HB3	2.02	0.41
1:F:69:PRO:CG	1:F:70:GLU:OE1	2.69	0.41
1:A:30:PRO:HB2	1:A:34:GLY:HA2	2.03	0.41
1:C:101:CYS:SG	1:C:102:ALA:N	2.94	0.41
1:C:120:ARG:HH11	1:C:120:ARG:HD2	1.76	0.41
1:E:127:VAL:HG11	1:E:196:THR:HG21	2.02	0.41
1:E:162:ILE:CG1	1:E:163:GLU:N	2.84	0.41
1:F:70:GLU:CD	1:F:70:GLU:H	1.96	0.41
1:F:71:THR:C	1:F:75:ILE:HD11	2.41	0.41
1:E:222:LEU:O	1:E:226:VAL:HG23	2.20	0.41
1:E:257:VAL:O	1:E:261:ARG:HG3	2.21	0.41
1:F:76:THR:HG1	1:F:195:SER:CB	2.33	0.41
1:F:169:LEU:HD23	1:F:169:LEU:HA	1.92	0.41
1:C:35:GLU:OE2	1:C:63:ARG:NH2	2.54	0.40
1:E:72:TYR:HA	1:E:75:ILE:HD11	2.03	0.40
1:F:9:THR:HG21	1:F:86:SER:OG	2.20	0.40
1:A:250:GLU:O	1:A:254:GLU:HG3	2.21	0.40
1:B:19:GLN:HA	1:B:53:VAL:O	2.21	0.40
1:B:139:LEU:HD23	1:B:139:LEU:HA	1.67	0.40
1:C:225:ILE:HG12	1:C:235:PHE:CZ	2.57	0.40
1:E:179:LYS:O	1:E:182:PRO:HD2	2.22	0.40
1:E:225:ILE:HG12	1:E:235:PHE:CZ	2.55	0.40
1:F:35:GLU:CD	1:F:176:ARG:HH11	2.25	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	262/264 (99%)	250 (95%)	11 (4%)	1 (0%)	34	72
1	B	262/264 (99%)	247 (94%)	14 (5%)	1 (0%)	34	72
1	C	262/264 (99%)	249 (95%)	12 (5%)	1 (0%)	34	72
1	D	262/264 (99%)	244 (93%)	14 (5%)	4 (2%)	10	42
1	E	262/264 (99%)	242 (92%)	16 (6%)	4 (2%)	10	42
1	F	262/264 (99%)	250 (95%)	11 (4%)	1 (0%)	34	72
All	All	1572/1584 (99%)	1482 (94%)	78 (5%)	12 (1%)	19	57

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	135	LEU
1	E	133	GLU
1	E	162	ILE
1	D	133	GLU
1	A	188	TYR
1	E	136	LYS
1	B	188	TYR
1	D	134	ASP
1	D	188	TYR
1	C	188	TYR
1	E	188	TYR
1	F	188	TYR

### 5.3.2 Protein sidechains [i](#)

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	224/224 (100%)	219 (98%)	5 (2%)	52	81
1	B	224/224 (100%)	222 (99%)	2 (1%)	78	92
1	C	224/224 (100%)	221 (99%)	3 (1%)	69	89
1	D	224/224 (100%)	222 (99%)	2 (1%)	78	92
1	E	224/224 (100%)	220 (98%)	4 (2%)	59	85
1	F	224/224 (100%)	220 (98%)	4 (2%)	59	85
All	All	1344/1344 (100%)	1324 (98%)	20 (2%)	65	87

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	186	ARG
1	B	224	ASN
1	A	141	MET
1	A	200	LYS
1	A	224	ASN
1	A	245	TYR
1	A	246	VAL
1	C	95	LYS
1	C	186	ARG
1	C	224	ASN
1	D	22	SER
1	D	82	SER
1	E	142	ASP
1	E	151	SER
1	E	200	LYS
1	E	224	ASN
1	F	17	TYR
1	F	78	GLN
1	F	95	LYS
1	F	142	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	19	GLN
1	A	153	ASN

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Mol	Chain	Res	Type
1	D	73	GLN
1	D	231	HIS
1	E	121	ASN
1	F	78	GLN

### 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 monosaccharides 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(Å <sup>2</sup> )	Q<0.9
1	A	264/264 (100%)	0.15	5 (1%) 66 37	36, 46, 58, 87	0
1	B	264/264 (100%)	0.12	8 (3%) 50 22	37, 47, 58, 79	0
1	C	264/264 (100%)	0.10	4 (1%) 73 46	37, 49, 61, 73	0
1	D	264/264 (100%)	0.18	11 (4%) 36 14	38, 48, 78, 105	0
1	E	264/264 (100%)	0.34	19 (7%) 15 4	42, 52, 78, 102	0
1	F	264/264 (100%)	0.38	9 (3%) 45 19	43, 62, 76, 86	0
All	All	1584/1584 (100%)	0.21	56 (3%) 44 18	36, 50, 72, 105	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	141	MET	5.0
1	E	161	ASP	4.4
1	D	134	ASP	4.4
1	D	132	MET	4.2
1	E	146	VAL	3.9
1	E	137	PRO	3.9
1	F	144	GLU	3.6
1	E	152	SER	3.6
1	C	168	GLU	3.5
1	E	138	LEU	3.5
1	E	153	ASN	3.4
1	A	1	MET	3.4
1	B	264	LEU	3.2
1	A	201	GLU	3.2
1	D	135	LEU	3.2
1	F	94	ASP	2.9
1	A	4	ARG	2.9
1	E	139	LEU	2.9
1	B	261	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	138	LEU	2.9
1	B	228	ALA	2.8
1	F	200	LYS	2.8
1	E	207	PRO	2.8
1	D	133	GLU	2.8
1	E	132	MET	2.8
1	E	150	MET	2.7
1	B	26	VAL	2.7
1	F	69	PRO	2.7
1	D	130	TYR	2.7
1	E	141	MET	2.7
1	E	159	VAL	2.6
1	E	140	GLU	2.6
1	D	139	LEU	2.5
1	E	144	GLU	2.5
1	A	10	LYS	2.5
1	E	135	LEU	2.5
1	F	26	VAL	2.4
1	C	167	GLN	2.4
1	D	161	ASP	2.4
1	C	51	PHE	2.3
1	F	7	ILE	2.3
1	B	206	ALA	2.3
1	F	14	HIS	2.3
1	E	143	ASP	2.2
1	D	137	PRO	2.2
1	F	168	GLU	2.2
1	A	117	THR	2.2
1	E	142	ASP	2.2
1	D	169	LEU	2.2
1	B	263	TYR	2.2
1	E	204	ILE	2.1
1	B	260	THR	2.1
1	B	96	ALA	2.1
1	C	139	LEU	2.0
1	F	96	ALA	2.0
1	E	147	SER	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 monosaccharides 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.