



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 11:28 AM BST

PDB ID : 6M36  
Title : The crystal structure of B. subtilis RsbV/RsbW complex in the monoclinic crystal form  
Authors : Pathak, D.; Kwon, E.; Kim, D.Y.  
Deposited on : 2020-03-02  
Resolution : 3.40 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.

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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	:	2.13.1
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)	:	2.13.1

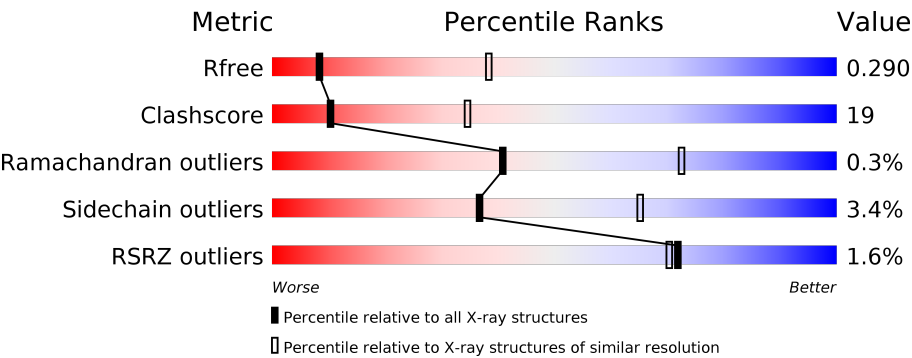
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 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	141	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>51%21%•27%</div></div>
1	C	141	<div><div></div><div></div><div></div><div></div><div></div></div> <div>39%33%•26%</div>
1	E	141	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>41%29%•29%</div></div>
1	G	141	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>45%26%•26%</div></div>
1	I	141	<div><div></div><div></div><div></div><div></div><div></div></div> <div>43%28%•26%</div>
1	K	141	<div><div></div><div></div><div></div><div></div><div></div></div> <div>46%27%27%</div>

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Mol	Chain	Length	Quality of chain
1	M	141	<div><div><div></div><div></div><div></div></div><div>4%</div><div>38%</div><div>35%</div><div>26%</div><div></div></div>
1	O	141	<div><div><div></div><div></div><div></div></div><div>2%</div><div>30%</div><div>37%</div><div>30%</div><div></div></div>
2	B	103	<div><div><div></div><div></div><div></div></div><div>2%</div><div>67%</div><div>29%</div><div></div><div></div></div>
2	D	103	<div><div><div></div><div></div><div></div></div><div>2%</div><div>63%</div><div>30%</div><div></div><div></div><div></div></div>
2	F	103	<div><div><div></div><div></div><div></div></div><div>5%</div><div>65%</div><div>26%</div><div>8%</div><div></div></div>
2	H	103	<div><div><div></div><div></div><div></div></div><div>%</div><div>65%</div><div>32%</div><div></div><div></div></div>
2	J	103	<div><div><div></div><div></div><div></div></div><div>3%</div><div>48%</div><div>48%</div><div></div><div></div></div>
2	L	103	<div><div><div></div><div></div><div></div></div><div></div><div>55%</div><div>43%</div><div></div></div>
2	N	103	<div><div><div></div><div></div><div></div></div><div></div><div>57%</div><div>37%</div><div></div><div></div></div>
2	P	103	<div><div><div></div><div></div><div></div></div><div>%</div><div>55%</div><div>41%</div><div></div><div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12580 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 Serine-protein kinase RsbW.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	0	0
			802	508	131	157	6			
1	C	105	Total	C	N	O	S	0	0	0
			824	524	133	161	6			
1	E	100	Total	C	N	O	S	0	0	0
			777	493	124	154	6			
1	G	104	Total	C	N	O	S	0	0	0
			814	517	132	159	6			
1	I	104	Total	C	N	O	S	0	0	0
			808	511	132	159	6			
1	K	103	Total	C	N	O	S	0	0	0
			802	508	131	157	6			
1	M	105	Total	C	N	O	S	0	0	0
			824	524	133	161	6			
1	O	98	Total	C	N	O	S	0	0	0
			760	483	123	148	6			

- Molecule 2 is a protein called Anti-sigma-B factor antagonist.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			774	490	130	151	3			
2	D	99	Total	C	N	O	S	0	0	0
			768	487	129	149	3			
2	F	95	Total	C	N	O	S	0	0	0
			742	471	124	144	3			
2	H	101	Total	C	N	O	S	0	0	0
			779	493	131	152	3			
2	J	100	Total	C	N	O	S	0	0	0
			774	490	130	151	3			
2	L	101	Total	C	N	O	S	0	0	0
			779	493	131	152	3			

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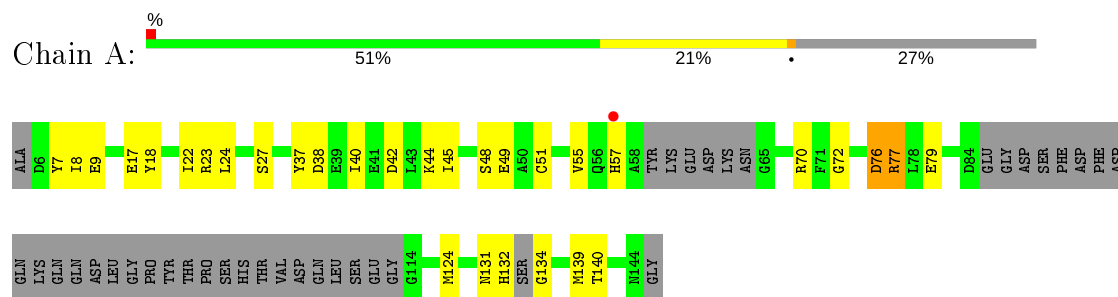
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	101	Total	C	N	O	S	0	0	0
			779	493	131	152	3			
2	P	100	Total	C	N	O	S	0	0	0
			774	490	130	151	3			

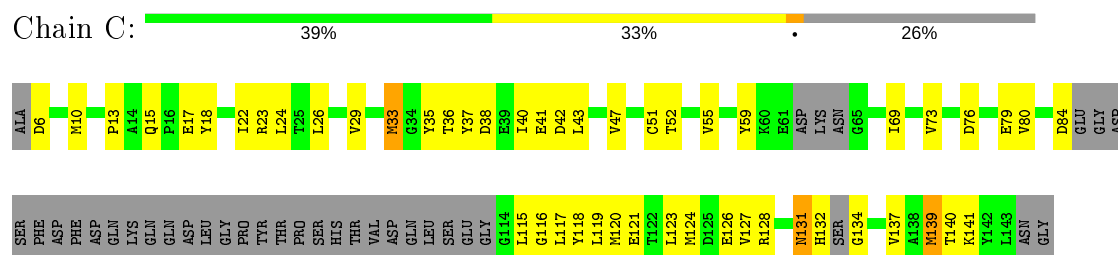
### 3 Residue-property plots [i](#)

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.

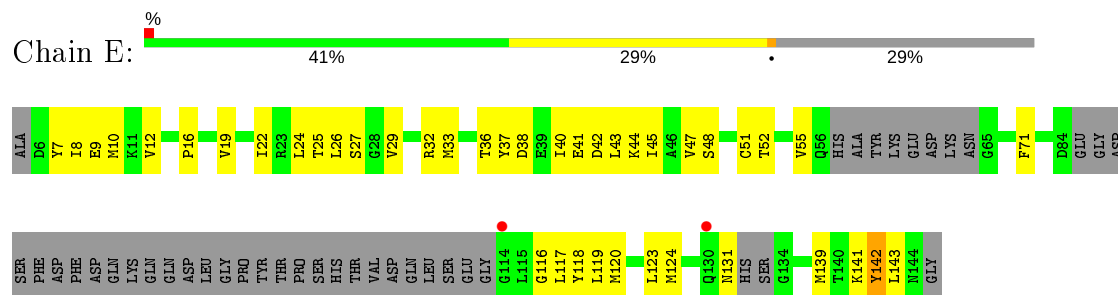
- Molecule 1: Serine-protein kinase RsbW



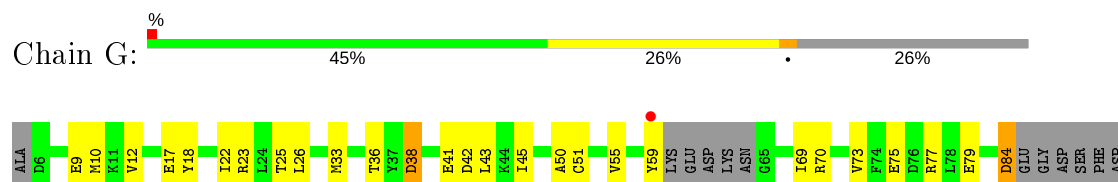
- Molecule 1: Serine-protein kinase RsbW

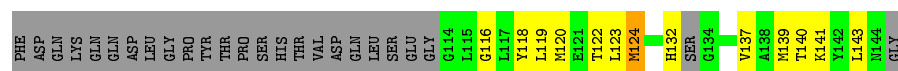


- Molecule 1: Serine-protein kinase RsbW

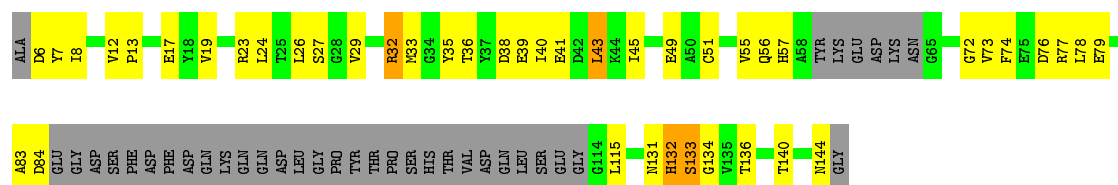


- Molecule 1: Serine-protein kinase RsbW

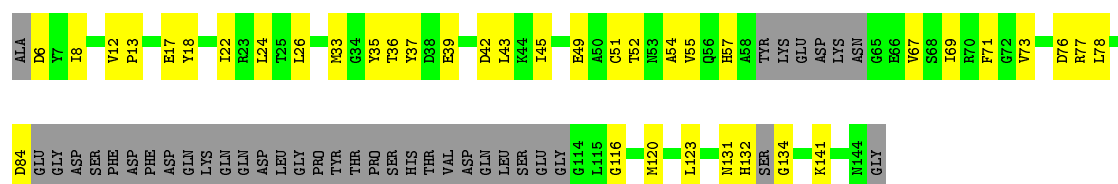




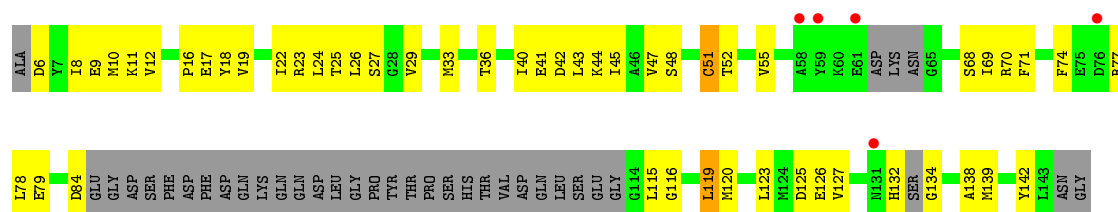
- Molecule 1: Serine-protein kinase RsbW



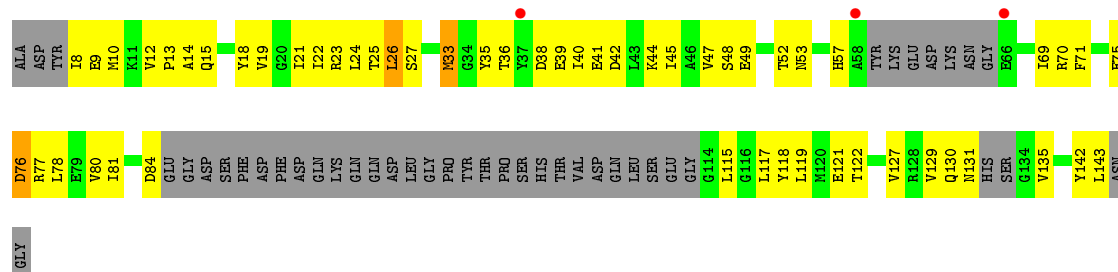
- Molecule 1: Serine-protein kinase RsbW



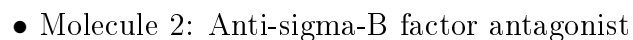
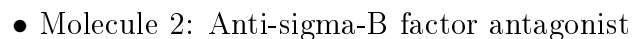
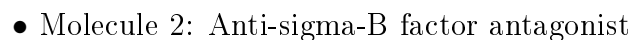
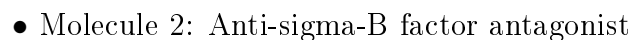
- Molecule 1: Serine-protein kinase RsbW

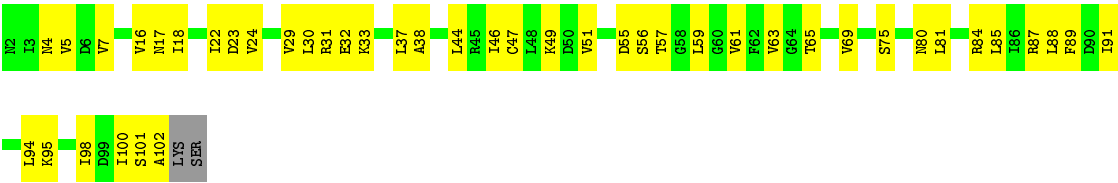


- Molecule 1: Serine-protein kinase RsbW

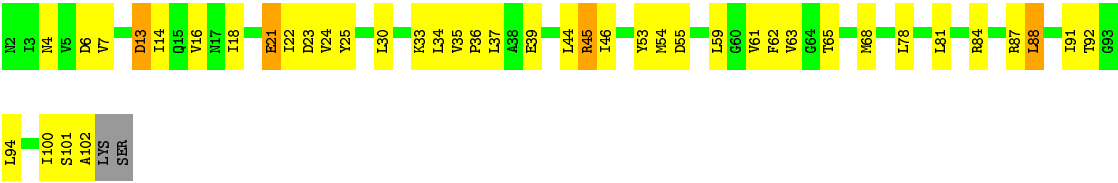


- Molecule 2: Anti-sigma-B factor antagonist

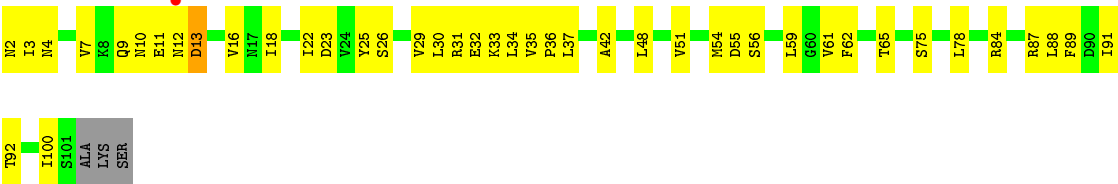




● Molecule 2: Anti-sigma-B factor antagonist



● Molecule 2: Anti-sigma-B factor antagonist



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.23Å 70.94Å 137.68Å 90.00° 105.35° 90.00°	Depositor
Resolution (Å)	29.79 – 3.40 29.79 – 3.40	Depositor EDS
% Data completeness (in resolution range)	96.1 (29.79-3.40) 96.1 (29.79-3.40)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 3.39Å)	Xtriage
Refinement program	PHENIX dev_3051	Depositor
R, $R_{free}$	0.207 , 0.290 0.207 , 0.290	Depositor DCC
$R_{free}$ test set	1465 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.2	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12580	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 4.45% 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

### 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	0.59	0/810	0.81	0/1092
1	C	0.58	0/833	0.80	0/1122
1	E	0.50	0/783	0.74	0/1055
1	G	0.50	0/823	0.77	2/1110 (0.2%)
1	I	0.59	0/817	0.84	1/1103 (0.1%)
1	K	0.57	0/810	0.74	0/1092
1	M	0.48	0/833	0.74	0/1122
1	O	0.52	0/766	0.76	1/1032 (0.1%)
2	B	0.59	0/780	0.82	1/1050 (0.1%)
2	D	0.52	0/774	0.81	2/1042 (0.2%)
2	F	0.48	0/747	0.73	0/1004
2	H	0.54	0/785	0.82	0/1057
2	J	0.57	0/780	0.81	1/1050 (0.1%)
2	L	0.49	0/785	0.71	0/1057
2	N	0.63	1/785 (0.1%)	0.80	1/1057 (0.1%)
2	P	0.53	0/780	0.83	0/1050
All	All	0.54	1/12691 (0.0%)	0.78	9/17095 (0.1%)

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	C	0	1
2	P	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	21	GLU	CG-CD	5.39	1.60	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	34	LEU	CA-CB-CG	7.06	131.53	115.30
2	B	85	LEU	CA-CB-CG	-6.78	99.71	115.30
2	N	88	LEU	CA-CB-CG	6.46	130.17	115.30
1	I	43	LEU	CA-CB-CG	6.35	129.90	115.30
1	G	143	LEU	CA-CB-CG	6.30	129.78	115.30
1	G	124	MET	CA-CB-CG	-6.29	102.61	113.30
2	J	81	LEU	CA-CB-CG	5.41	127.75	115.30
1	O	26	LEU	CB-CG-CD1	-5.33	101.94	111.00
2	D	44	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	33	MET	Peptide
2	P	9	GLN	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	802	0	795	26	0
1	C	824	0	817	41	0
1	E	777	0	776	34	0
1	G	814	0	804	36	0
1	I	808	0	801	39	0
1	K	802	0	795	32	0
1	M	824	0	817	44	0
1	O	760	0	766	54	0
2	B	774	0	804	19	0
2	D	768	0	799	26	0
2	F	742	0	771	21	0
2	H	779	0	809	31	0
2	J	774	0	804	40	0
2	L	779	0	809	35	0
2	N	779	0	809	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	774	0	804	35	0
All	All	12580	0	12780	473	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 19.

All (473) 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)
2:F:31:ARG:HG3	2:F:61:VAL:HG23	1.22	1.11
1:I:8:ILE:HG12	1:K:12:VAL:HG12	1.48	0.94
1:M:12:VAL:HG11	1:M:18:TYR:HB3	1.53	0.90
1:G:42:ASP:OD1	2:H:84:ARG:NH1	2.08	0.87
1:E:45:ILE:HD11	2:F:84:ARG:HH11	1.42	0.84
1:O:131:ASN:HB3	1:O:135:VAL:HG22	1.62	0.81
1:O:42:ASP:OD1	2:P:84:ARG:NH1	2.13	0.81
2:J:14:ILE:HG21	2:J:37:LEU:HD22	1.62	0.81
2:B:33:LYS:NZ	2:H:7:VAL:O	2.16	0.79
1:E:45:ILE:HD11	2:F:84:ARG:NH1	1.97	0.79
1:G:118:TYR:O	1:G:122:THR:OG1	2.01	0.78
2:J:4:ASN:ND2	2:P:4:ASN:OD1	2.15	0.78
1:C:42:ASP:OD1	2:D:84:ARG:NH1	2.16	0.78
2:F:31:ARG:CG	2:F:61:VAL:HG23	2.09	0.76
2:H:7:VAL:HG12	2:H:16:VAL:HG22	1.64	0.76
2:H:6:ASP:OD2	2:H:8:LYS:NZ	2.19	0.76
1:A:79:GLU:HG3	1:A:140:THR:HG22	1.67	0.76
1:I:33:MET:SD	1:I:78:LEU:HD23	2.26	0.76
2:J:7:VAL:HG12	2:J:16:VAL:HG12	1.67	0.75
2:L:31:ARG:HD3	2:L:61:VAL:HG12	1.68	0.75
1:M:8:ILE:HG23	1:M:71:PHE:HB2	1.69	0.75
1:O:23:ARG:NH2	2:P:23:ASP:OD2	2.18	0.74
2:J:48:LEU:HD12	2:J:81:LEU:HD13	1.70	0.74
2:J:30:LEU:HD21	2:J:62:PHE:HE1	1.53	0.73
1:A:132:HIS:CE1	1:I:134:GLY:HA2	2.23	0.72
1:G:120:MET:HB3	1:G:139:MET:HE1	1.71	0.72
2:B:95:LYS:HG3	2:B:100:ILE:HD12	1.72	0.72
1:M:17:GLU:HG3	2:N:25:TYR:CE2	2.24	0.71
2:H:14:ILE:HD13	2:H:37:LEU:HD22	1.72	0.71
2:N:16:VAL:HB	2:N:46:ILE:HG22	1.73	0.71
1:G:50:ALA:HB2	1:G:120:MET:HE1	1.74	0.70
1:I:26:LEU:HD21	1:I:43:LEU:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:GLU:HG3	2:B:80:ASN:N	2.07	0.69
1:M:16:PRO:O	1:M:19:VAL:HG22	1.92	0.69
1:I:133:SER:H	1:I:134:GLY:C	1.95	0.69
1:C:124:MET:HE2	1:C:139:MET:HG3	1.75	0.68
2:L:56:SER:HA	2:L:59:LEU:HD12	1.76	0.68
1:G:26:LEU:HD21	1:G:43:LEU:HB3	1.74	0.68
1:G:123:LEU:O	1:G:141:LYS:HE2	1.93	0.68
1:I:79:GLU:HB2	1:I:140:THR:HG22	1.76	0.68
2:N:14:ILE:HB	2:N:44:LEU:HD23	1.76	0.68
2:N:87:ARG:O	2:N:91:ILE:HG13	1.94	0.67
2:B:35:VAL:HG12	2:B:36:PRO:HD3	1.76	0.67
2:P:87:ARG:HE	2:P:91:ILE:HD11	1.60	0.67
1:A:42:ASP:OD1	2:B:84:ARG:NH1	2.28	0.67
2:F:16:VAL:HB	2:F:46:ILE:HG12	1.76	0.67
2:P:35:VAL:HG12	2:P:36:PRO:HD3	1.76	0.67
2:F:66:PHE:HD2	2:F:76:LEU:HD23	1.60	0.66
1:O:41:GLU:HB3	2:P:84:ARG:CZ	2.24	0.66
2:D:90:ASP:HA	2:D:95:LYS:HB2	1.77	0.66
2:N:35:VAL:HG12	2:N:36:PRO:HD3	1.78	0.66
2:J:83:GLU:HG3	2:J:84:ARG:N	2.12	0.65
1:E:123:LEU:O	1:E:141:LYS:NZ	2.24	0.65
2:H:69:VAL:HG11	2:H:75:SER:O	1.96	0.65
1:C:116:GLY:O	1:C:120:MET:HG3	1.96	0.65
2:F:38:ALA:HB1	2:F:68:MET:HB3	1.79	0.65
1:M:48:SER:O	1:M:52:THR:OG1	2.15	0.65
1:C:132:HIS:CD2	1:K:134:GLY:N	2.65	0.64
2:J:81:LEU:HD12	2:J:85:LEU:HB3	1.79	0.64
2:L:7:VAL:O	2:N:33:LYS:NZ	2.31	0.64
2:J:53:TYR:OH	2:J:55:ASP:OD1	2.15	0.64
1:K:13:PRO:HG2	1:K:18:TYR:CD2	2.31	0.64
2:N:14:ILE:HG21	2:N:37:LEU:HD22	1.79	0.64
1:G:124:MET:HE3	1:G:141:LYS:HB2	1.79	0.64
2:J:16:VAL:HG23	2:J:46:ILE:HG23	1.79	0.64
1:K:84:ASP:OD1	1:K:84:ASP:N	2.31	0.64
2:J:54:MET:HE3	2:J:85:LEU:HD11	1.79	0.63
1:O:70:ARG:HB3	1:O:81:ILE:HB	1.79	0.63
1:K:36:THR:OG1	1:K:39:GLU:HG2	1.98	0.63
1:M:74:PHE:HB2	1:M:77:ARG:O	1.98	0.63
2:H:54:MET:HE1	2:H:62:PHE:CE2	2.34	0.63
1:A:132:HIS:CE1	1:I:134:GLY:CA	2.81	0.62
2:L:4:ASN:OD1	2:N:4:ASN:HB3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:116:GLY:O	1:G:120:MET:HG3	1.99	0.62
2:J:87:ARG:O	2:J:91:ILE:HG13	1.99	0.62
1:A:24:LEU:HD11	1:C:24:LEU:HD11	1.82	0.62
2:D:49:LYS:HD3	2:D:50:ASP:OD1	2.00	0.62
2:D:6:ASP:OD2	2:D:8:LYS:NZ	2.23	0.61
2:D:34:LEU:HA	2:D:37:LEU:HD13	1.81	0.61
2:L:16:VAL:HB	2:L:46:ILE:HG23	1.82	0.61
1:A:45:ILE:HD13	2:B:88:LEU:HD21	1.82	0.61
2:H:54:MET:HE1	2:H:62:PHE:HE2	1.65	0.61
1:O:33:MET:SD	1:O:78:LEU:HD21	2.41	0.61
2:N:46:ILE:HD12	2:N:62:PHE:CE1	2.36	0.61
2:J:22:ILE:HD12	2:J:54:MET:HE2	1.83	0.60
2:H:94:LEU:HD13	2:H:97:ILE:HD12	1.83	0.60
1:A:49:GLU:OE2	2:B:56:SER:OG	2.19	0.60
1:O:49:GLU:OE2	2:P:55:ASP:HB2	2.02	0.60
1:I:133:SER:H	1:I:134:GLY:CA	2.13	0.60
1:K:12:VAL:HG23	1:K:67:VAL:HG13	1.84	0.60
1:C:76:ASP:OD1	1:C:76:ASP:N	2.29	0.60
1:E:124:MET:HG3	1:E:139:MET:SD	2.41	0.60
2:B:58:GLY:O	2:B:61:VAL:HG12	2.02	0.59
2:L:55:ASP:OD1	2:L:57:THR:OG1	2.19	0.59
1:G:43:LEU:CD1	1:G:141:LYS:HD3	2.32	0.59
2:L:51:VAL:CG1	2:L:85:LEU:HD11	2.32	0.59
1:M:25:THR:OG1	1:O:25:THR:OG1	1.97	0.59
1:G:43:LEU:HD11	1:G:141:LYS:HD3	1.84	0.59
2:N:61:VAL:O	2:N:65:THR:HG23	2.02	0.59
1:O:35:TYR:HB3	1:O:39:GLU:HB2	1.83	0.59
2:F:96:ASP:OD1	2:F:97:ILE:HG13	2.02	0.59
1:M:12:VAL:HG11	1:M:18:TYR:CB	2.29	0.59
2:J:6:ASP:OD1	2:P:33:LYS:HE2	2.03	0.59
2:H:37:LEU:HB3	2:H:44:LEU:HD21	1.84	0.59
1:E:116:GLY:HA2	1:E:119:LEU:HD13	1.83	0.59
1:E:32:ARG:HH22	2:H:2:ASN:N	2.00	0.59
1:C:120:MET:HE1	1:C:137:VAL:HG11	1.84	0.58
1:E:8:ILE:HB	1:E:71:PHE:HB2	1.83	0.58
1:K:13:PRO:HG2	1:K:18:TYR:CE2	2.39	0.58
2:P:89:PHE:CD2	2:P:100:ILE:HD11	2.38	0.58
2:B:97:ILE:HG13	2:B:98:ILE:HD12	1.86	0.58
1:G:12:VAL:HG21	1:G:22:ILE:HD11	1.85	0.58
2:J:31:ARG:HG3	2:J:61:VAL:HG23	1.86	0.58
1:I:115:LEU:HD11	2:J:92:THR:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:GLU:HA	2:H:25:TYR:CD2	2.38	0.57
1:O:115:LEU:HD12	2:P:56:SER:HB2	1.86	0.57
1:E:44:LYS:O	1:E:48:SER:OG	2.15	0.57
1:M:22:ILE:HG21	1:M:69:ILE:HD13	1.86	0.57
1:O:69:ILE:HA	1:O:81:ILE:O	2.03	0.57
1:C:84:ASP:OD1	1:C:84:ASP:N	2.35	0.57
1:O:118:TYR:CE1	1:O:122:THR:HG21	2.40	0.57
1:O:53:ASN:O	1:O:57:HIS:HB2	2.05	0.57
1:O:22:ILE:HG21	1:O:69:ILE:HD13	1.86	0.57
1:E:10:MET:HA	1:G:9:GLU:O	2.05	0.56
1:G:123:LEU:HD21	2:H:87:ARG:HH22	1.70	0.56
1:O:10:MET:CE	1:O:71:PHE:HE2	2.19	0.56
1:O:35:TYR:HE1	1:O:78:LEU:HD11	1.70	0.56
1:K:49:GLU:OE2	2:L:55:ASP:HB2	2.05	0.56
1:O:75:GLU:OE2	1:O:76:ASP:HB2	2.06	0.56
2:N:87:ARG:CZ	2:N:91:ILE:HD11	2.36	0.56
1:A:76:ASP:OD1	1:A:77:ARG:NE	2.39	0.56
1:G:9:GLU:HG2	1:G:70:ARG:HG3	1.87	0.56
1:K:123:LEU:O	1:K:141:LYS:NZ	2.35	0.56
2:L:33:LYS:HE3	2:N:6:ASP:OD1	2.05	0.56
2:P:42:ALA:O	2:P:75:SER:N	2.25	0.56
1:C:51:CYS:O	1:C:55:VAL:HG23	2.05	0.55
1:O:12:VAL:HG11	1:O:22:ILE:HD11	1.87	0.55
1:I:36:THR:O	1:I:40:ILE:HG22	2.06	0.55
2:N:18:ILE:HG21	2:N:22:ILE:HD11	1.89	0.55
1:K:8:ILE:HB	1:K:71:PHE:HB2	1.88	0.55
2:L:49:LYS:HG3	2:L:80:ASN:HB3	1.88	0.55
1:I:6:ASP:HB2	1:I:73:VAL:HG13	1.89	0.55
2:N:7:VAL:HG12	2:N:16:VAL:HG22	1.88	0.55
1:C:134:GLY:HA2	1:K:132:HIS:NE2	2.21	0.55
1:O:48:SER:O	1:O:52:THR:HG23	2.07	0.55
2:H:77:LYS:NZ	2:H:99:ASP:OD2	2.39	0.54
1:K:26:LEU:HD21	1:K:43:LEU:HB3	1.87	0.54
2:P:62:PHE:CD2	2:P:78:LEU:HD21	2.43	0.54
1:A:124:MET:HE3	1:A:139:MET:HB2	1.88	0.54
1:I:13:PRO:HG2	1:K:6:ASP:HB3	1.90	0.54
1:M:6:ASP:OD1	1:M:6:ASP:N	2.38	0.54
1:G:50:ALA:HB2	1:G:120:MET:CE	2.37	0.54
1:C:33:MET:SD	1:C:73:VAL:HG23	2.48	0.54
2:H:89:PHE:CD2	2:H:100:ILE:HD11	2.43	0.54
1:G:123:LEU:CD2	2:H:87:ARG:HH22	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:LEU:HD22	1:E:47:VAL:HG21	1.89	0.54
2:F:55:ASP:OD1	2:F:57:THR:OG1	2.26	0.54
1:K:33:MET:SD	1:K:73:VAL:HG23	2.48	0.54
1:I:84:ASP:N	1:I:84:ASP:OD1	2.39	0.54
1:I:29:VAL:O	1:I:33:MET:HG3	2.07	0.54
1:A:23:ARG:NH1	1:A:48:SER:OG	2.40	0.54
1:E:142:TYR:HD1	1:E:143:LEU:H	1.56	0.54
1:K:42:ASP:OD1	2:L:84:ARG:NH1	2.41	0.54
2:P:7:VAL:HG12	2:P:16:VAL:HG22	1.90	0.54
1:I:41:GLU:HG2	2:J:84:ARG:NH2	2.23	0.53
1:O:27:SER:OG	1:O:44:LYS:HD3	2.08	0.53
2:P:29:VAL:O	2:P:32:GLU:HG2	2.09	0.53
1:A:37:TYR:O	1:A:40:ILE:HG22	2.08	0.53
1:C:23:ARG:NH2	2:D:21:GLU:OE1	2.33	0.53
1:E:16:PRO:O	1:E:19:VAL:HG23	2.08	0.53
1:M:45:ILE:HG12	2:N:53:TYR:HE1	1.72	0.53
1:I:51:CYS:O	1:I:55:VAL:HG23	2.08	0.53
1:C:132:HIS:HD2	1:K:134:GLY:N	2.06	0.53
2:P:61:VAL:O	2:P:65:THR:HG23	2.09	0.53
2:D:44:LEU:HD11	2:D:76:LEU:HD23	1.90	0.53
1:O:36:THR:O	1:O:40:ILE:HG22	2.09	0.53
1:M:33:MET:HE1	1:M:78:LEU:HD13	1.90	0.52
1:I:24:LEU:HD11	1:K:24:LEU:HD11	1.92	0.52
2:N:59:LEU:O	2:N:63:VAL:HG12	2.09	0.52
2:B:34:LEU:HD23	2:B:65:THR:HG21	1.91	0.52
1:E:32:ARG:NH2	2:H:2:ASN:HB2	2.24	0.52
2:L:37:LEU:HB3	2:L:44:LEU:HD21	1.92	0.52
2:N:59:LEU:HD22	2:N:94:LEU:HD22	1.92	0.52
1:A:8:ILE:HD11	1:C:18:TYR:CD2	2.44	0.52
1:G:124:MET:CE	1:G:141:LYS:HB2	2.39	0.52
1:K:33:MET:HE2	1:K:35:TYR:HE1	1.74	0.52
1:O:33:MET:HG2	1:O:78:LEU:HD21	1.91	0.52
2:N:78:LEU:HB2	2:N:100:ILE:HG22	1.90	0.52
1:G:22:ILE:HG21	1:G:69:ILE:HD13	1.92	0.52
1:E:32:ARG:HH21	2:H:2:ASN:HB2	1.75	0.52
1:O:129:VAL:O	1:O:130:GLN:HG3	2.09	0.51
1:C:37:TYR:O	1:C:40:ILE:HG12	2.10	0.51
1:C:22:ILE:HG21	1:C:69:ILE:HD13	1.92	0.51
1:G:84:ASP:N	1:G:84:ASP:OD1	2.40	0.51
1:M:115:LEU:O	1:M:119:LEU:HD23	2.10	0.51
1:M:23:ARG:NH1	1:M:48:SER:OG	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:94:LEU:O	2:L:98:ILE:HG12	2.09	0.51
1:M:127:VAL:HG13	1:M:139:MET:HG2	1.92	0.51
1:I:132:HIS:O	1:I:132:HIS:ND1	2.36	0.51
1:C:17:GLU:HB3	2:D:25:TYR:CE1	2.45	0.51
2:J:34:LEU:HA	2:J:37:LEU:HD12	1.91	0.51
2:L:59:LEU:HD11	2:L:88:LEU:HD11	1.92	0.51
2:N:35:VAL:O	2:N:39:GLU:HG3	2.10	0.51
1:E:116:GLY:O	1:E:119:LEU:N	2.42	0.51
1:G:51:CYS:O	1:G:55:VAL:HG23	2.10	0.51
2:J:48:LEU:O	2:J:51:VAL:HG22	2.10	0.51
2:B:4:ASN:OD1	2:H:6:ASP:HB2	2.10	0.51
1:M:24:LEU:O	1:M:27:SER:OG	2.21	0.51
1:O:18:TYR:O	1:O:22:ILE:HG12	2.08	0.51
1:A:44:LYS:O	1:A:48:SER:HB2	2.11	0.51
2:P:48:LEU:HD22	2:P:51:VAL:HG21	1.93	0.51
2:P:62:PHE:HD2	2:P:78:LEU:HD21	1.75	0.51
2:B:79:GLU:HG3	2:B:80:ASN:H	1.74	0.51
2:J:61:VAL:O	2:J:65:THR:HG23	2.12	0.50
1:M:26:LEU:HD21	1:M:43:LEU:HB3	1.93	0.50
2:F:23:ASP:OD1	2:F:25:TYR:N	2.42	0.50
2:J:40:GLN:N	2:J:41:GLY:HA2	2.26	0.50
2:J:49:LYS:HB2	2:J:80:ASN:HB3	1.92	0.50
1:C:36:THR:O	1:C:40:ILE:HG23	2.11	0.50
1:E:124:MET:SD	1:E:141:LYS:HB2	2.52	0.50
1:G:132:HIS:ND1	1:G:132:HIS:O	2.44	0.50
2:L:24:VAL:HA	2:L:57:THR:HG21	1.93	0.50
1:I:83:ALA:HB1	1:I:136:THR:HG22	1.93	0.50
1:O:14:ALA:O	1:O:15:GLN:NE2	2.42	0.50
1:I:77:ARG:HB3	1:I:77:ARG:CZ	2.41	0.50
1:K:22:ILE:HG23	1:K:69:ILE:HD13	1.93	0.50
2:L:87:ARG:O	2:L:91:ILE:HG12	2.12	0.50
1:O:44:LYS:O	1:O:48:SER:OG	2.29	0.50
1:I:83:ALA:CB	1:I:136:THR:HG22	2.42	0.49
2:D:44:LEU:CD1	2:D:76:LEU:HD23	2.42	0.49
2:L:18:ILE:HG21	2:L:22:ILE:HD11	1.95	0.49
1:M:77:ARG:NH1	1:M:79:GLU:OE2	2.45	0.49
1:C:26:LEU:HD21	1:C:43:LEU:HB3	1.94	0.49
2:D:6:ASP:OD1	2:F:33:LYS:NZ	2.44	0.49
1:C:47:VAL:HG22	1:C:80:VAL:HG11	1.93	0.49
1:M:47:VAL:HG22	1:M:139:MET:HE3	1.95	0.49
1:C:115:LEU:O	1:C:118:TYR:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:31:ARG:HG3	2:H:61:VAL:HG23	1.93	0.49
1:K:51:CYS:O	1:K:55:VAL:HG23	2.13	0.49
1:O:77:ARG:HG2	1:O:142:TYR:CE1	2.47	0.49
1:O:41:GLU:HB3	2:P:84:ARG:NH1	2.28	0.49
2:L:51:VAL:HG11	2:L:85:LEU:HD11	1.94	0.49
2:H:24:VAL:HA	2:H:57:THR:HG21	1.94	0.49
2:L:38:ALA:HB2	2:L:65:THR:HG23	1.95	0.49
1:O:117:LEU:O	1:O:121:GLU:HG3	2.13	0.48
1:E:117:LEU:HG	1:E:120:MET:HE3	1.96	0.48
1:K:45:ILE:O	1:K:49:GLU:HG2	2.14	0.48
2:F:66:PHE:CD2	2:F:98:ILE:HG23	2.48	0.48
2:H:39:GLU:HG2	2:H:68:MET:CE	2.44	0.48
1:I:17:GLU:HG2	2:J:25:TYR:CZ	2.48	0.48
2:P:33:LYS:O	2:P:37:LEU:HD13	2.14	0.48
1:C:115:LEU:HD11	2:D:92:THR:HG22	1.95	0.48
2:F:87:ARG:O	2:F:91:ILE:HG13	2.14	0.48
1:O:75:GLU:O	1:O:77:ARG:HG3	2.13	0.48
2:B:87:ARG:O	2:B:91:ILE:HG13	2.14	0.48
1:C:120:MET:CE	1:C:137:VAL:HG11	2.43	0.47
1:C:29:VAL:O	1:C:33:MET:HG2	2.14	0.47
1:K:12:VAL:HG21	1:K:22:ILE:HD11	1.96	0.47
1:C:17:GLU:HG3	1:C:18:TYR:CE1	2.49	0.47
2:L:17:ASN:HD22	2:L:47:CYS:HB3	1.80	0.47
2:B:82:SER:O	2:B:86:ILE:HD12	2.14	0.47
1:A:9:GLU:O	1:C:10:MET:HA	2.14	0.47
1:A:27:SER:HA	1:A:40:ILE:HD11	1.96	0.47
1:C:17:GLU:HG3	1:C:18:TYR:CD1	2.49	0.47
1:M:17:GLU:OE1	1:M:17:GLU:N	2.40	0.47
1:O:121:GLU:HA	1:O:127:VAL:HG21	1.96	0.47
2:P:87:ARG:O	2:P:91:ILE:HG13	2.15	0.47
1:C:79:GLU:HG3	1:C:140:THR:HG22	1.97	0.47
2:H:65:THR:O	2:H:69:VAL:HG23	2.13	0.47
1:M:11:LYS:HG2	1:M:68:SER:HA	1.97	0.47
1:C:117:LEU:HD12	1:C:120:MET:SD	2.54	0.47
1:G:36:THR:HG22	1:G:38:ASP:H	1.79	0.47
2:J:59:LEU:HD11	2:J:88:LEU:CD2	2.45	0.47
1:A:70:ARG:HH21	1:A:70:ARG:HG2	1.80	0.47
1:I:133:SER:HB2	1:I:136:THR:HG23	1.97	0.47
2:J:53:TYR:CZ	2:J:55:ASP:OD1	2.67	0.46
1:K:8:ILE:HB	1:K:71:PHE:HD2	1.80	0.46
1:M:24:LEU:HD11	1:O:24:LEU:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:47:VAL:HG13	1:O:80:VAL:HG11	1.96	0.46
2:B:7:VAL:O	2:H:33:LYS:NZ	2.49	0.46
2:D:2:ASN:HB3	2:D:3:ILE:H	1.45	0.46
2:J:95:LYS:HG3	2:J:100:ILE:HG21	1.97	0.46
1:M:51:CYS:O	1:M:55:VAL:HG23	2.15	0.46
2:B:98:ILE:HG22	2:B:99:ASP:O	2.16	0.46
1:K:33:MET:SD	1:K:78:LEU:HD13	2.55	0.46
2:J:16:VAL:HG22	2:J:46:ILE:HG12	1.98	0.46
2:L:7:VAL:HG11	2:L:37:LEU:HD11	1.98	0.46
1:M:17:GLU:HG3	2:N:25:TYR:HE2	1.78	0.46
1:M:33:MET:CE	1:M:78:LEU:HD13	2.46	0.46
2:D:66:PHE:HD2	2:D:98:ILE:HG23	1.79	0.46
2:J:85:LEU:HD13	2:J:85:LEU:HA	1.77	0.46
1:O:45:ILE:O	1:O:49:GLU:HG2	2.16	0.46
2:P:35:VAL:CG1	2:P:36:PRO:HD3	2.44	0.46
1:M:9:GLU:O	1:O:10:MET:HA	2.16	0.46
1:O:13:PRO:HB2	1:O:18:TYR:HE2	1.80	0.46
2:D:59:LEU:O	2:D:63:VAL:HG12	2.15	0.46
2:P:22:ILE:HD12	2:P:54:MET:HE2	1.97	0.46
1:C:13:PRO:O	1:C:15:GLN:N	2.48	0.46
1:E:52:THR:HG22	2:F:24:VAL:CG1	2.46	0.46
1:G:36:THR:HG22	1:G:38:ASP:N	2.32	0.45
1:O:26:LEU:HD12	1:O:47:VAL:HG11	1.98	0.45
1:O:76:ASP:O	1:O:142:TYR:HA	2.16	0.45
1:A:37:TYR:HA	1:A:40:ILE:HG22	1.98	0.45
1:E:48:SER:O	1:E:52:THR:HG23	2.16	0.45
2:J:10:ASN:OD1	2:J:11:GLU:N	2.49	0.45
1:A:51:CYS:O	1:A:55:VAL:HG23	2.15	0.45
2:F:90:ASP:O	2:F:93:GLY:N	2.42	0.45
2:P:10:ASN:HB3	2:P:13:ASP:O	2.16	0.45
2:F:34:LEU:HD21	2:F:46:ILE:CD1	2.46	0.45
2:H:37:LEU:HA	2:H:40:GLN:OE1	2.17	0.45
1:O:8:ILE:HB	1:O:71:PHE:HB2	1.99	0.45
2:H:14:ILE:HB	2:H:44:LEU:HD23	1.99	0.45
2:J:34:LEU:HD23	2:J:37:LEU:HD12	1.97	0.45
1:E:51:CYS:O	1:E:55:VAL:HG22	2.17	0.45
1:I:12:VAL:HG12	1:K:8:ILE:HD12	1.99	0.45
1:O:77:ARG:HG2	1:O:142:TYR:HE1	1.82	0.45
1:I:56:GLN:HG3	1:I:57:HIS:ND1	2.31	0.45
2:J:30:LEU:HD21	2:J:62:PHE:CE1	2.43	0.45
2:J:35:VAL:HB	2:J:36:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:75:GLU:HG3	1:G:75:GLU:H	1.48	0.44
2:H:92:THR:OG1	2:H:94:LEU:HD23	2.18	0.44
1:I:7:TYR:HD1	1:I:72:GLY:HA2	1.81	0.44
1:M:125:ASP:O	1:M:126:GLU:HG3	2.17	0.44
1:M:132:HIS:HB2	1:M:134:GLY:HA2	1.98	0.44
1:M:29:VAL:HG22	1:O:21:ILE:HD13	1.99	0.44
1:I:19:VAL:HG12	1:I:23:ARG:HH21	1.81	0.44
2:P:59:LEU:HD11	2:P:88:LEU:CD2	2.47	0.44
2:H:81:LEU:HD22	2:H:100:ILE:HG23	1.99	0.44
1:C:52:THR:HG23	2:D:24:VAL:HB	2.00	0.44
2:D:69:VAL:HG11	2:D:75:SER:O	2.18	0.44
1:E:48:SER:OG	2:F:53:TYR:OH	2.31	0.44
1:G:41:GLU:O	1:G:45:ILE:HG13	2.18	0.44
1:O:76:ASP:OD1	1:O:143:LEU:N	2.49	0.44
2:P:10:ASN:OD1	2:P:11:GLU:N	2.50	0.44
2:L:80:ASN:H	2:L:102:ALA:HA	1.83	0.44
1:O:35:TYR:CE2	1:O:143:LEU:HD23	2.52	0.44
1:O:115:LEU:HD21	2:P:92:THR:HG22	1.99	0.44
1:O:22:ILE:CG2	1:O:69:ILE:HD13	2.47	0.44
1:E:36:THR:O	1:E:40:ILE:HG23	2.18	0.44
2:J:6:ASP:O	2:J:16:VAL:HA	2.18	0.44
2:L:81:LEU:HD21	2:L:89:PHE:CE2	2.52	0.44
1:M:84:ASP:OD1	1:M:84:ASP:N	2.50	0.44
1:G:17:GLU:HG2	2:H:25:TYR:CE1	2.53	0.44
2:N:21:GLU:HG2	2:N:53:TYR:HB3	2.00	0.44
1:A:134:GLY:HA2	1:I:132:HIS:CE1	2.53	0.44
2:L:84:ARG:HB3	2:L:84:ARG:NH2	2.33	0.44
2:N:81:LEU:H	2:N:102:ALA:HA	1.81	0.44
1:O:19:VAL:O	1:O:23:ARG:HG2	2.18	0.44
1:I:33:MET:CE	1:I:73:VAL:HG23	2.48	0.43
1:M:17:GLU:H	1:M:17:GLU:CD	2.20	0.43
1:A:7:TYR:HD1	1:A:72:GLY:HA2	1.82	0.43
2:B:48:LEU:HD11	2:B:62:PHE:HE2	1.84	0.43
1:G:139:MET:HB3	1:G:139:MET:HE3	1.83	0.43
2:H:85:LEU:HD23	2:H:85:LEU:HA	1.87	0.43
1:I:133:SER:N	1:I:134:GLY:CA	2.80	0.43
1:I:45:ILE:O	1:I:49:GLU:HG2	2.19	0.43
1:I:56:GLN:HE21	1:I:57:HIS:CE1	2.35	0.43
1:I:23:ARG:NH1	2:J:21:GLU:OE1	2.52	0.43
1:C:119:LEU:HD23	1:C:119:LEU:HA	1.59	0.43
2:J:43:ASP:HA	2:J:75:SER:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:23:ASP:OD1	2:L:24:VAL:N	2.42	0.43
1:E:26:LEU:HD21	1:E:43:LEU:HB3	1.99	0.43
1:G:119:LEU:HD12	1:G:119:LEU:HA	1.64	0.43
1:K:116:GLY:O	1:K:120:MET:HG3	2.18	0.43
1:K:54:ALA:O	1:K:57:HIS:HB3	2.18	0.43
1:E:42:ASP:OD1	1:E:123:LEU:HB3	2.18	0.43
1:C:126:GLU:OE2	1:C:128:ARG:NH1	2.51	0.43
1:G:120:MET:HE2	1:G:137:VAL:HG11	2.00	0.43
1:I:74:PHE:HB2	1:I:77:ARG:NH1	2.33	0.43
1:O:8:ILE:N	1:O:71:PHE:O	2.51	0.43
1:M:10:MET:HA	1:O:9:GLU:O	2.18	0.43
2:D:5:VAL:HB	2:D:33:LYS:HD3	2.01	0.43
1:I:27:SER:HA	1:I:40:ILE:HD11	2.00	0.43
2:P:30:LEU:O	2:P:34:LEU:HB2	2.19	0.43
1:K:52:THR:HG23	2:L:24:VAL:HG21	2.01	0.43
1:M:132:HIS:HA	1:M:134:GLY:O	2.19	0.43
1:C:131:ASN:HA	1:C:132:HIS:HA	1.71	0.42
1:M:120:MET:HE3	1:M:127:VAL:HG11	2.00	0.42
1:M:52:THR:HG23	2:N:24:VAL:HB	2.01	0.42
1:C:6:ASP:O	1:C:73:VAL:HG12	2.19	0.42
2:D:18:ILE:HG21	2:D:22:ILE:HD11	2.01	0.42
1:E:24:LEU:O	1:E:27:SER:OG	2.28	0.42
1:E:29:VAL:O	1:E:33:MET:HE2	2.18	0.42
1:K:69:ILE:O	1:K:69:ILE:HG13	2.18	0.42
1:M:41:GLU:HG2	2:N:84:ARG:CD	2.49	0.42
2:P:23:ASP:OD1	2:P:25:TYR:N	2.50	0.42
1:C:33:MET:HG3	1:C:35:TYR:CE1	2.55	0.42
1:E:43:LEU:CD1	1:E:141:LYS:HD3	2.50	0.42
2:J:2:ASN:HB3	2:J:3:ILE:H	1.77	0.42
1:M:36:THR:O	1:M:40:ILE:HG22	2.19	0.42
2:N:78:LEU:HD22	2:N:100:ILE:HG22	2.01	0.42
2:N:39:GLU:HG2	2:N:68:MET:CE	2.49	0.42
2:D:54:MET:HE1	2:D:85:LEU:HD22	2.01	0.42
1:I:35:TYR:HB3	1:I:39:GLU:HB2	2.02	0.42
2:P:88:LEU:HD23	2:P:88:LEU:O	2.19	0.42
1:E:52:THR:HG22	2:F:24:VAL:HB	2.01	0.42
2:L:29:VAL:O	2:L:32:GLU:HG2	2.20	0.42
2:N:13:ASP:HB3	2:N:45:ARG:HH21	1.84	0.42
1:E:41:GLU:O	1:E:45:ILE:HG13	2.20	0.42
1:M:40:ILE:O	1:M:44:LYS:HG3	2.19	0.42
1:O:33:MET:CG	1:O:78:LEU:HD21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:TYR:O	1:A:22:ILE:HG12	2.19	0.42
1:I:56:GLN:HG3	1:I:57:HIS:CE1	2.55	0.42
1:M:42:ASP:CG	1:M:123:LEU:HD22	2.40	0.42
1:O:119:LEU:HA	1:O:119:LEU:HD23	1.81	0.42
1:G:12:VAL:HG11	1:G:18:TYR:HB3	2.00	0.42
2:J:46:ILE:HB	2:J:78:LEU:HD23	2.01	0.42
2:N:23:ASP:OD1	2:N:25:TYR:N	2.49	0.42
2:D:31:ARG:HG3	2:D:61:VAL:HG23	2.02	0.42
2:D:33:LYS:HB3	2:D:33:LYS:HE2	1.94	0.42
2:F:31:ARG:CA	2:F:61:VAL:HG21	2.50	0.42
1:M:127:VAL:HA	1:M:138:ALA:O	2.20	0.42
2:P:11:GLU:HA	2:P:12:ASN:HA	1.43	0.42
1:O:13:PRO:HB2	1:O:18:TYR:CE2	2.54	0.41
1:A:57:HIS:NE2	1:A:134:GLY:HA2	2.35	0.41
1:G:79:GLU:HG3	1:G:140:THR:HG22	2.01	0.41
1:K:131:ASN:N	1:K:131:ASN:OD1	2.53	0.41
2:L:59:LEU:O	2:L:63:VAL:HG12	2.21	0.41
2:P:3:ILE:HG21	2:P:26:SER:HB2	2.02	0.41
2:N:30:LEU:HD23	2:N:61:VAL:HG11	2.03	0.41
1:C:123:LEU:HA	1:C:123:LEU:HD23	1.73	0.41
1:G:33:MET:SD	1:G:73:VAL:HG13	2.60	0.41
1:I:32:ARG:H	1:I:32:ARG:HG2	1.43	0.41
1:M:116:GLY:O	1:M:120:MET:HG3	2.20	0.41
2:N:30:LEU:HG	2:N:34:LEU:HD12	2.02	0.41
1:C:121:GLU:HA	1:C:127:VAL:HG21	2.02	0.41
1:E:43:LEU:HD11	1:E:141:LYS:HD3	2.01	0.41
1:E:25:THR:CG2	1:G:25:THR:OG1	2.68	0.41
1:I:17:GLU:HG3	1:I:17:GLU:H	1.60	0.41
2:N:14:ILE:HD13	2:N:37:LEU:HD22	2.02	0.41
1:O:26:LEU:HD11	1:O:47:VAL:HG21	2.02	0.41
1:A:70:ARG:NH2	1:A:70:ARG:HG2	2.36	0.41
2:D:56:SER:HA	2:D:59:LEU:HD12	2.02	0.41
1:C:124:MET:CE	1:C:141:LYS:HB2	2.51	0.41
2:D:31:ARG:HB3	2:D:31:ARG:CZ	2.51	0.41
2:B:49:LYS:HE3	1:E:37:TYR:CE1	2.55	0.41
2:H:39:GLU:HG2	2:H:68:MET:HE2	2.01	0.41
2:J:67:LYS:O	2:J:71:LYS:HG3	2.21	0.41
2:L:95:LYS:HG3	2:L:100:ILE:CD1	2.51	0.41
2:N:55:ASP:OD1	2:N:55:ASP:N	2.54	0.41
2:P:2:ASN:HB3	2:P:3:ILE:H	1.59	0.41
1:C:41:GLU:HB3	2:D:84:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:43:ASP:HA	2:J:75:SER:H	1.85	0.41
1:M:77:ARG:HB2	1:M:142:TYR:HD1	1.85	0.41
2:N:22:ILE:HD12	2:N:54:MET:HE2	2.03	0.41
1:O:35:TYR:HB3	1:O:39:GLU:CB	2.50	0.41
1:A:17:GLU:H	1:A:17:GLU:HG3	1.33	0.41
2:D:79:GLU:HA	2:D:80:ASN:HA	1.36	0.41
1:G:26:LEU:HD11	1:G:43:LEU:HD23	2.02	0.41
2:J:8:LYS:CE	2:P:33:LYS:HZ3	2.34	0.41
2:B:77:LYS:HA	2:B:99:ASP:HB3	2.03	0.41
1:E:12:VAL:HG11	1:E:22:ILE:HD11	2.03	0.41
2:J:88:LEU:O	2:J:92:THR:OG1	2.39	0.41
2:L:5:VAL:HB	2:L:33:LYS:HD2	2.02	0.41
2:P:22:ILE:HA	2:P:26:SER:OG	2.21	0.41
1:K:17:GLU:H	1:K:17:GLU:HG3	1.64	0.41
2:L:30:LEU:HA	2:L:30:LEU:HD12	1.85	0.41
1:K:37:TYR:CE2	2:L:84:ARG:HD2	2.56	0.41
1:M:16:PRO:HB3	2:N:24:VAL:HG13	2.03	0.41
2:P:18:ILE:HG21	2:P:22:ILE:HD11	2.03	0.41
2:L:101:SER:OG	2:L:102:ALA:N	2.53	0.40
2:L:69:VAL:HG11	2:L:75:SER:O	2.21	0.40
2:L:95:LYS:HG3	2:L:100:ILE:HD13	2.02	0.40
1:O:35:TYR:CE1	1:O:78:LEU:HD11	2.54	0.40
2:F:97:ILE:HG21	2:F:97:ILE:HD13	1.86	0.40
1:M:70:ARG:HH11	1:M:70:ARG:HG2	1.86	0.40
1:A:7:TYR:CD1	1:A:72:GLY:HA2	2.55	0.40
2:D:66:PHE:CD1	2:D:66:PHE:C	2.95	0.40
1:E:9:GLU:O	1:G:10:MET:HA	2.22	0.40
2:N:88:LEU:O	2:N:92:THR:OG1	2.35	0.40
1:A:131:ASN:O	1:A:132:HIS:HB3	2.22	0.40
1:C:126:GLU:O	1:C:139:MET:HA	2.21	0.40
2:F:65:THR:O	2:F:69:VAL:HG23	2.22	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	95/141 (67%)	94 (99%)	1 (1%)	0	100	100
1	C	97/141 (69%)	93 (96%)	4 (4%)	0	100	100
1	E	92/141 (65%)	90 (98%)	2 (2%)	0	100	100
1	G	96/141 (68%)	92 (96%)	3 (3%)	1 (1%)	15	46
1	I	98/141 (70%)	93 (95%)	4 (4%)	1 (1%)	15	46
1	K	95/141 (67%)	94 (99%)	1 (1%)	0	100	100
1	M	97/141 (69%)	95 (98%)	2 (2%)	0	100	100
1	O	90/141 (64%)	88 (98%)	2 (2%)	0	100	100
2	B	98/103 (95%)	93 (95%)	4 (4%)	1 (1%)	15	46
2	D	97/103 (94%)	93 (96%)	4 (4%)	0	100	100
2	F	91/103 (88%)	86 (94%)	4 (4%)	1 (1%)	14	44
2	H	99/103 (96%)	95 (96%)	4 (4%)	0	100	100
2	J	98/103 (95%)	93 (95%)	5 (5%)	0	100	100
2	L	99/103 (96%)	98 (99%)	1 (1%)	0	100	100
2	N	99/103 (96%)	94 (95%)	5 (5%)	0	100	100
2	P	98/103 (95%)	88 (90%)	10 (10%)	0	100	100
All	All	1539/1952 (79%)	1479 (96%)	56 (4%)	4 (0%)	41	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	77	ARG
2	B	41	GLY
2	F	74	GLY
1	I	133	SER

### 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	87/120 (72%)	84 (97%)	3 (3%)	37	65
1	C	89/120 (74%)	85 (96%)	4 (4%)	27	58
1	E	85/120 (71%)	80 (94%)	5 (6%)	19	49
1	G	88/120 (73%)	84 (96%)	4 (4%)	27	58
1	I	88/120 (73%)	82 (93%)	6 (7%)	16	45
1	K	87/120 (72%)	85 (98%)	2 (2%)	50	74
1	M	89/120 (74%)	87 (98%)	2 (2%)	52	75
1	O	83/120 (69%)	79 (95%)	4 (5%)	25	56
2	B	88/90 (98%)	85 (97%)	3 (3%)	37	65
2	D	87/90 (97%)	85 (98%)	2 (2%)	50	74
2	F	85/90 (94%)	83 (98%)	2 (2%)	49	74
2	H	88/90 (98%)	86 (98%)	2 (2%)	50	74
2	J	88/90 (98%)	84 (96%)	4 (4%)	27	58
2	L	88/90 (98%)	88 (100%)	0	100	100
2	N	88/90 (98%)	85 (97%)	3 (3%)	37	65
2	P	88/90 (98%)	86 (98%)	2 (2%)	50	74
All	All	1396/1680 (83%)	1348 (97%)	48 (3%)	37	65

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	76	ASP
1	A	77	ARG
2	B	68	MET
2	B	87	ARG
2	B	101	SER
1	C	38	ASP
1	C	59	TYR
1	C	131	ASN
1	C	139	MET
2	D	34	LEU
2	D	49	LYS
1	E	7	TYR
1	E	38	ASP
1	E	118	TYR
1	E	131	ASN

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Mol	Chain	Res	Type
1	E	142	TYR
2	F	39	GLU
2	F	84	ARG
1	G	23	ARG
1	G	38	ASP
1	G	59	TYR
1	G	84	ASP
2	H	13	ASP
2	H	75	SER
1	I	32	ARG
1	I	38	ASP
1	I	76	ASP
1	I	131	ASN
1	I	132	HIS
1	I	144	ASN
2	J	44	LEU
2	J	50	ASP
2	J	68	MET
2	J	84	ARG
1	K	76	ASP
1	K	77	ARG
1	M	51	CYS
1	M	119	LEU
2	N	13	ASP
2	N	45	ARG
2	N	101	SER
1	O	33	MET
1	O	38	ASP
1	O	76	ASP
1	O	84	ASP
2	P	13	ASP
2	P	31	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	C	57	HIS
1	C	132	HIS
1	I	57	HIS
2	P	80	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 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	103/141 (73%)	-0.43	1 (0%) 82 81	30, 50, 79, 87	0
1	C	105/141 (74%)	-0.40	0 100 100	34, 48, 76, 100	0
1	E	100/141 (70%)	-0.01	2 (2%) 65 64	58, 86, 105, 110	0
1	G	104/141 (73%)	-0.07	1 (0%) 82 81	54, 70, 89, 104	0
1	I	104/141 (73%)	-0.35	0 100 100	33, 49, 74, 84	0
1	K	103/141 (73%)	-0.32	0 100 100	45, 66, 84, 91	0
1	M	105/141 (74%)	0.04	5 (4%) 30 31	48, 75, 101, 125	0
1	O	98/141 (69%)	-0.10	3 (3%) 49 48	50, 75, 98, 110	0
2	B	100/103 (97%)	-0.30	2 (2%) 65 64	40, 65, 93, 116	0
2	D	99/103 (96%)	-0.19	2 (2%) 65 64	42, 72, 104, 141	0
2	F	95/103 (92%)	0.07	5 (5%) 26 27	63, 91, 118, 131	0
2	H	101/103 (98%)	-0.29	1 (0%) 82 81	42, 57, 82, 118	0
2	J	100/103 (97%)	-0.32	3 (3%) 50 49	39, 58, 89, 116	0
2	L	101/103 (98%)	-0.22	0 100 100	47, 71, 94, 113	0
2	N	101/103 (98%)	-0.40	0 100 100	41, 58, 83, 118	0
2	P	100/103 (97%)	-0.29	1 (1%) 82 81	40, 60, 94, 110	0
All	All	1619/1952 (82%)	-0.23	26 (1%) 72 70	30, 66, 100, 141	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	114	GLY	4.1
2	F	10	ASN	3.3
2	B	96	ASP	3.2
2	J	74	GLY	3.0
1	M	59	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	12	ASN	2.9
2	H	12	ASN	2.6
2	F	43	ASP	2.5
2	D	11	GLU	2.4
2	P	12	ASN	2.4
2	D	12	ASN	2.3
1	M	58	ALA	2.3
1	M	131	ASN	2.3
2	F	75	SER	2.2
1	E	130	GLN	2.2
2	F	12	ASN	2.2
1	M	61	GLU	2.2
2	J	96	ASP	2.1
2	J	97	ILE	2.1
1	G	59	TYR	2.1
2	F	96	ASP	2.1
1	O	58	ALA	2.1
1	M	76	ASP	2.1
1	A	57	HIS	2.1
1	O	66	GLU	2.1
1	O	37	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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.