



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 08:59 AM UTC

PDB ID : 8BLM / pdb\_00008blm  
Title : Structure of RutB  
Authors : Rajendran, C.  
Deposited on : 2022-11-09  
Resolution : 1.90 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 : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

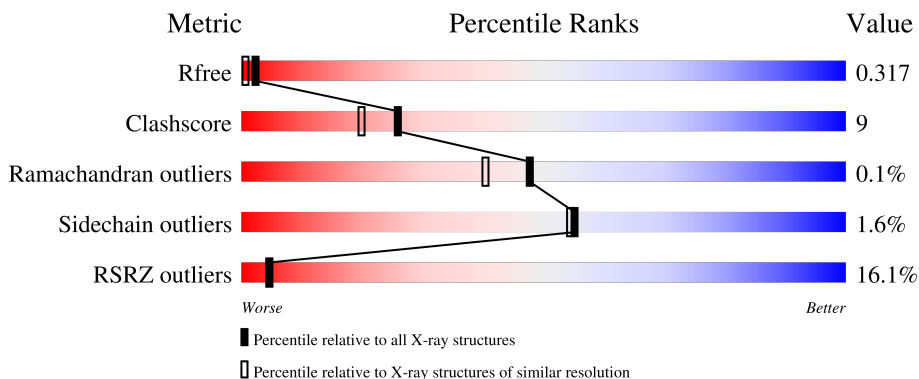
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

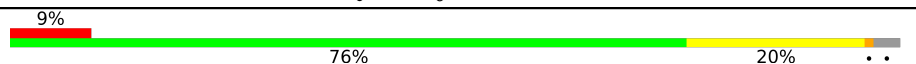




The reported resolution of this entry is 1.90 Å.

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))
$R_{free}$	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	230	
1	B	230	
1	C	230	
1	D	230	
1	E	230	

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Mol	Chain	Length	Quality of chain
1	F	230	
1	G	230	
1	H	230	
1	I	230	
1	J	230	
1	K	230	
1	L	230	
1	M	230	
1	N	230	
1	O	230	
1	P	230	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28516 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 Ureidoacrylate amidohydrolase RutB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	222	Total 1709	C 1098	N 285	O 321	S 5	0	0	0
1	B	222	Total 1715	C 1104	N 285	O 321	S 5	0	0	0
1	C	222	Total 1715	C 1104	N 285	O 321	S 5	0	0	0
1	D	220	Total 1702	C 1096	N 283	O 318	S 5	0	0	0
1	E	222	Total 1703	C 1098	N 283	O 317	S 5	0	0	0
1	F	220	Total 1694	C 1092	N 282	O 315	S 5	0	0	0
1	G	222	Total 1711	C 1101	N 284	O 321	S 5	0	0	0
1	H	222	Total 1715	C 1104	N 285	O 321	S 5	0	0	0
1	I	222	Total 1708	C 1099	N 285	O 319	S 5	0	0	0
1	J	222	Total 1696	C 1091	N 281	O 319	S 5	0	0	0
1	K	220	Total 1692	C 1091	N 282	O 314	S 5	0	0	0
1	L	220	Total 1702	C 1096	N 283	O 318	S 5	0	0	0
1	M	222	Total 1713	C 1103	N 285	O 320	S 5	0	0	0
1	N	222	Total 1711	C 1102	N 284	O 320	S 5	0	0	0
1	O	222	Total 1715	C 1104	N 285	O 321	S 5	0	0	0
1	P	220	Total 1683	C 1085	N 279	O 314	S 5	0	0	0

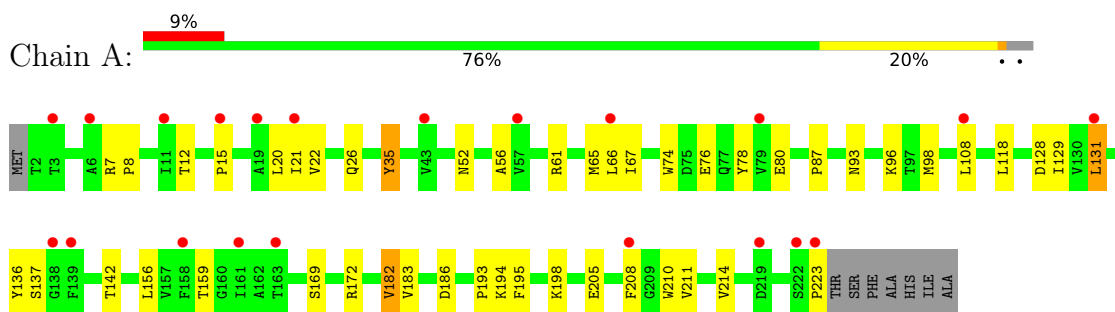
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	95	Total O 95 95	0	0
2	B	87	Total O 87 87	0	0
2	C	96	Total O 96 96	0	0
2	D	81	Total O 81 81	0	0
2	E	78	Total O 78 78	0	0
2	F	70	Total O 70 70	0	0
2	G	78	Total O 78 78	0	0
2	H	81	Total O 81 81	0	0
2	I	93	Total O 93 93	0	0
2	J	84	Total O 84 84	0	0
2	K	71	Total O 71 71	0	0
2	L	82	Total O 82 82	0	0
2	M	68	Total O 68 68	0	0
2	N	48	Total O 48 48	0	0
2	O	62	Total O 62 62	0	0
2	P	58	Total O 58 58	0	0

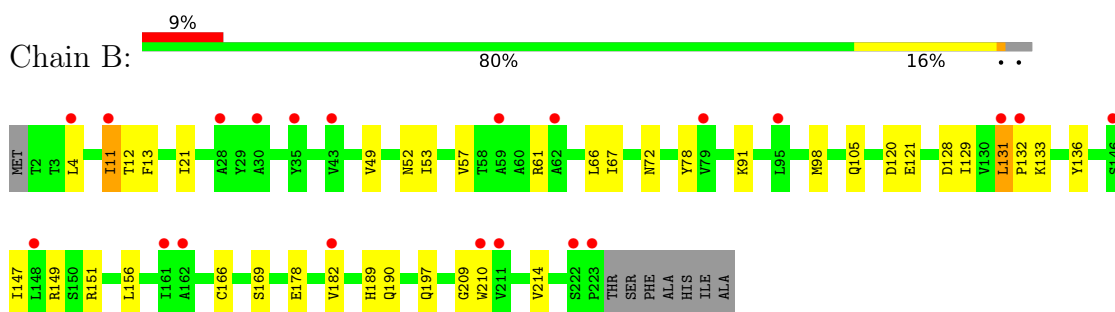
### 3 Residue-property plots [i](#)

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.

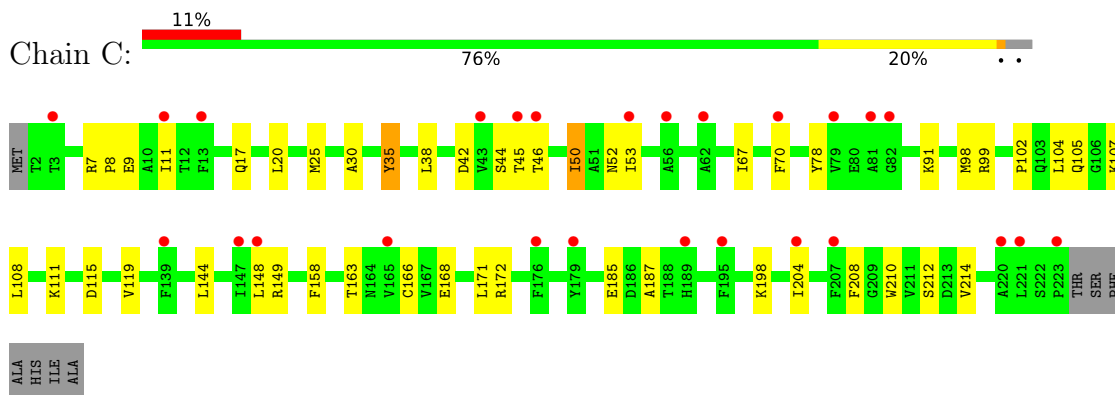
- Molecule 1: Ureidoacrylate amidohydrolase RutB



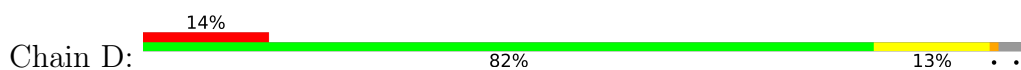
- Molecule 1: Ureidoacrylate amidohydrolase RutB

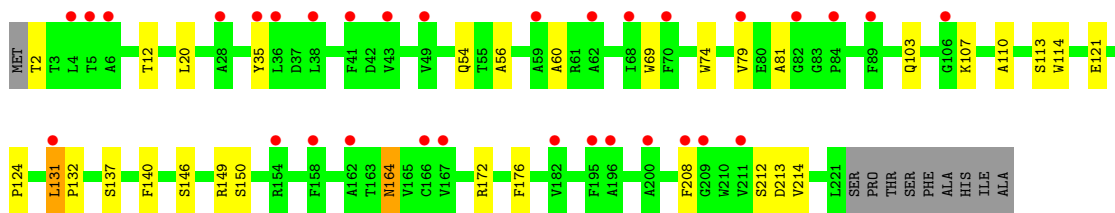


- Molecule 1: Ureidoacrylate amidohydrolase RutB

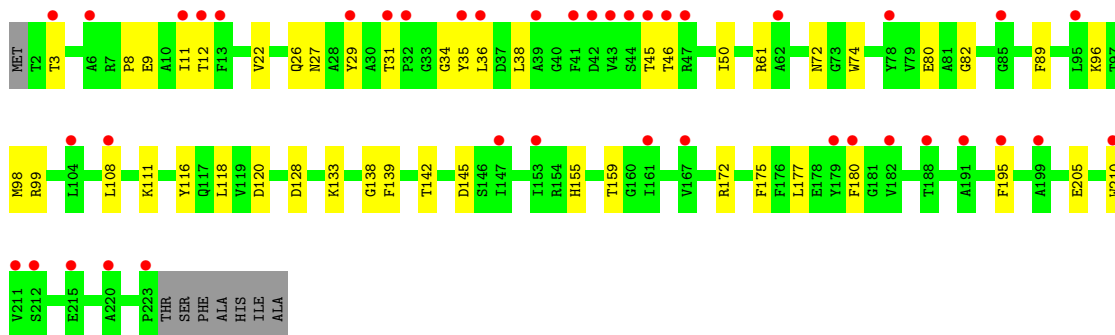
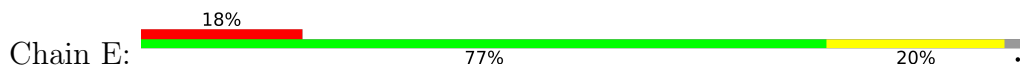


- Molecule 1: Ureidoacrylate amidohydrolase RutB

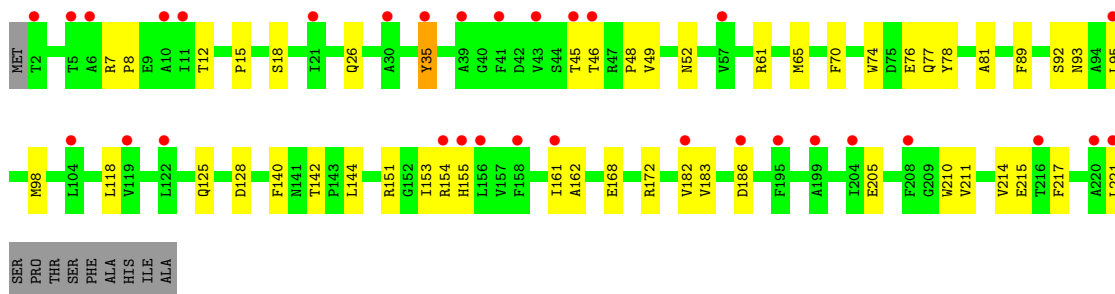
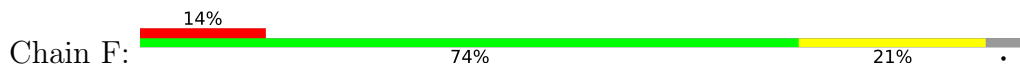




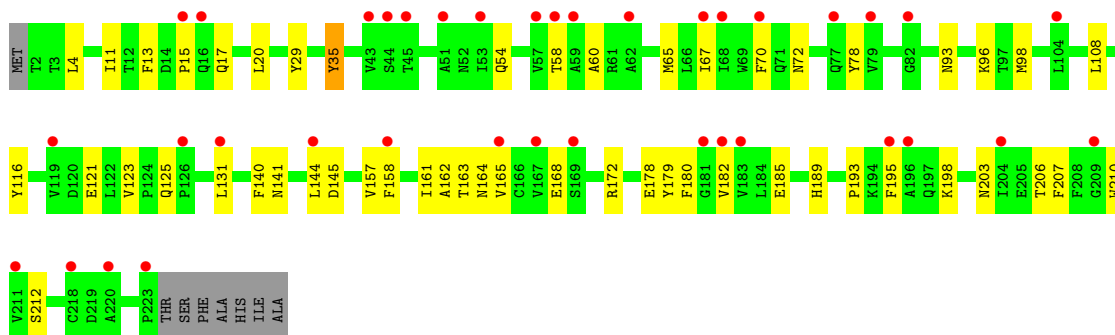
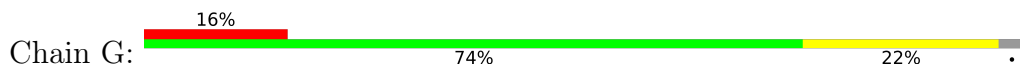
● Molecule 1: Ureidoacrylate amidohydrolase RutB



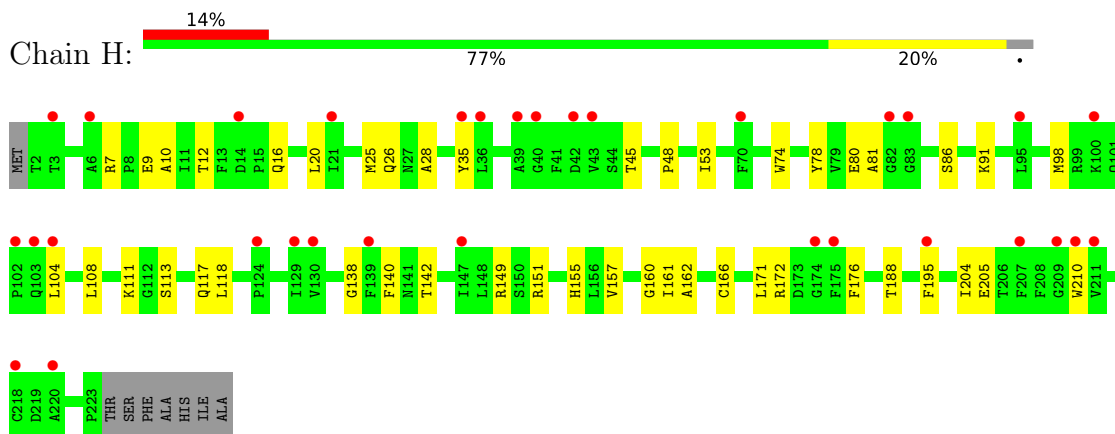
● Molecule 1: Ureidoacrylate amidohydrolase RutB



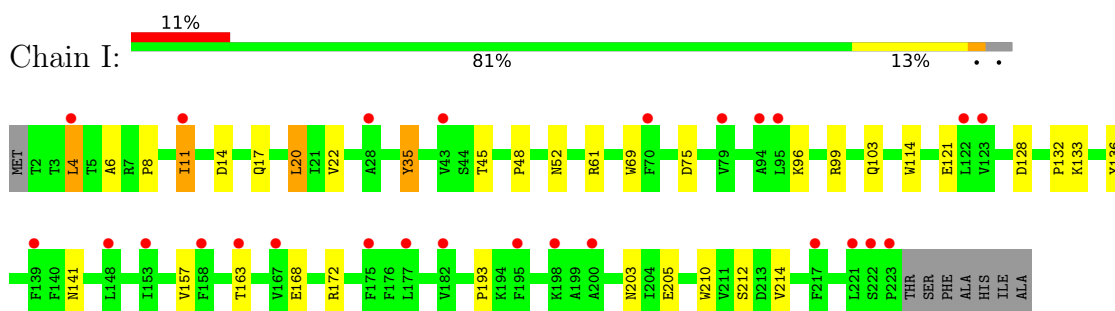
● Molecule 1: Ureidoacrylate amidohydrolase RutB



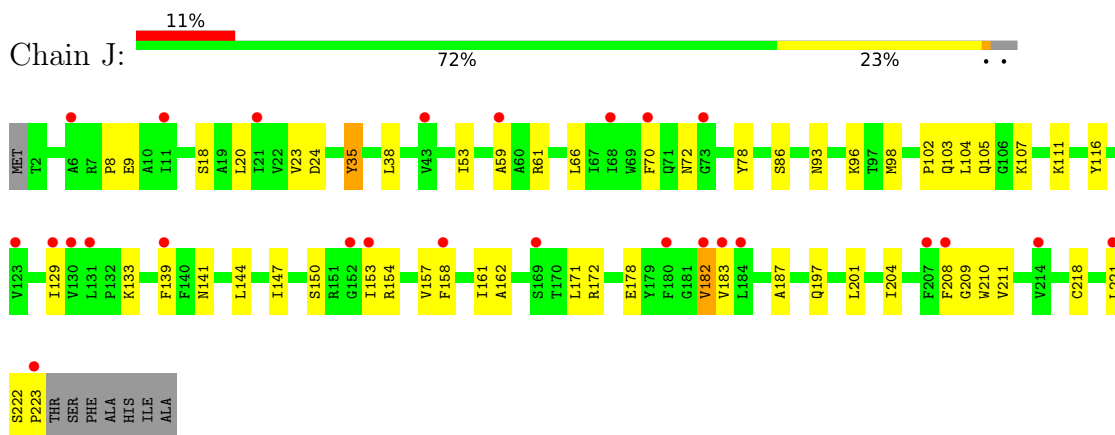
● Molecule 1: Ureidoacrylate amidohydrolase RutB



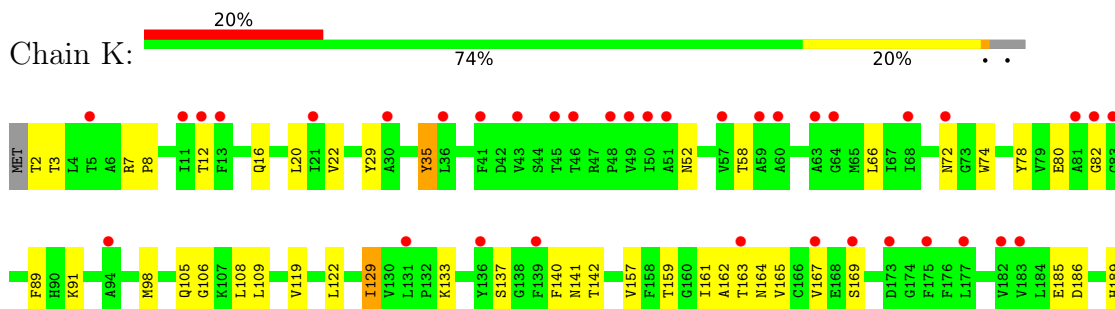
- Molecule 1: Ureidoacrylate amidohydrolase RutB

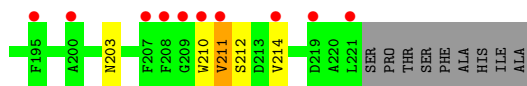


- Molecule 1: Ureidoacrylate amidohydrolase RutB

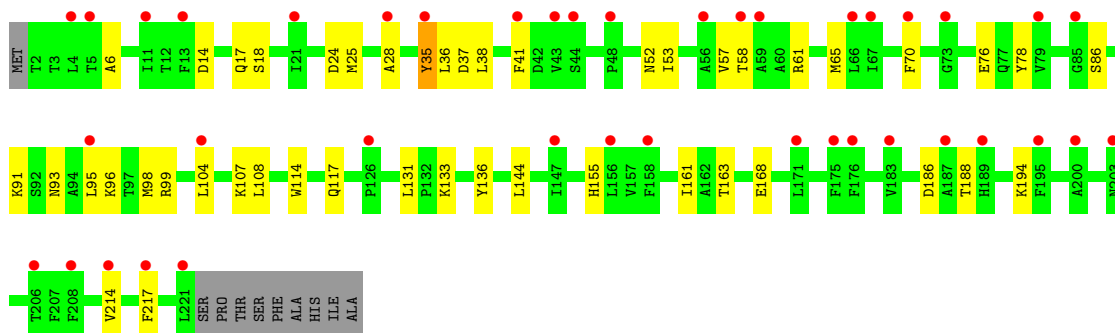
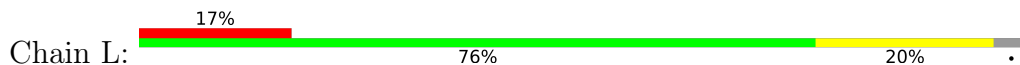


- Molecule 1: Ureidoacrylate amidohydrolase RutB

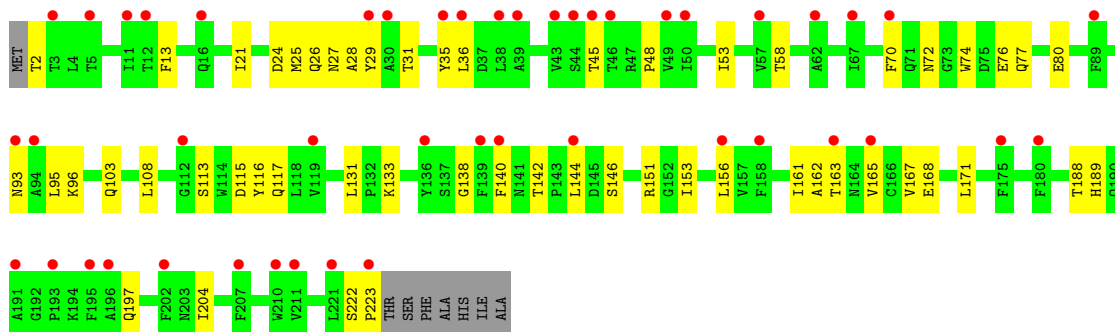
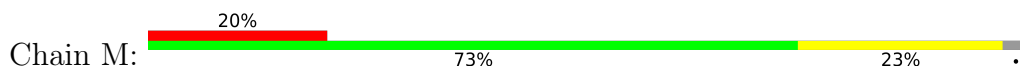




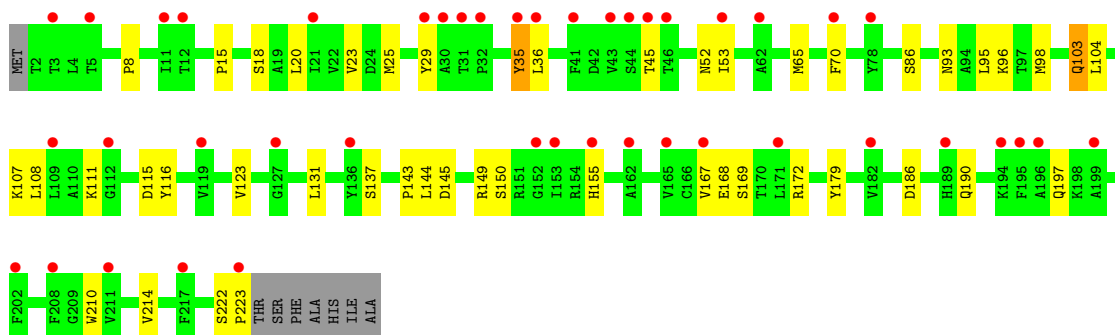
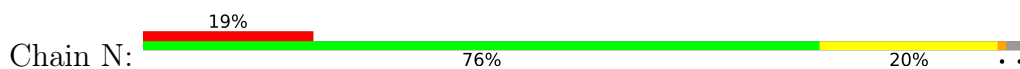
- Molecule 1: Ureidoacrylate amidohydrolase RutB



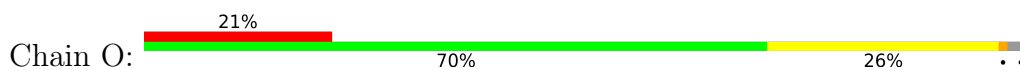
- Molecule 1: Ureidoacrylate amidohydrolase RutB

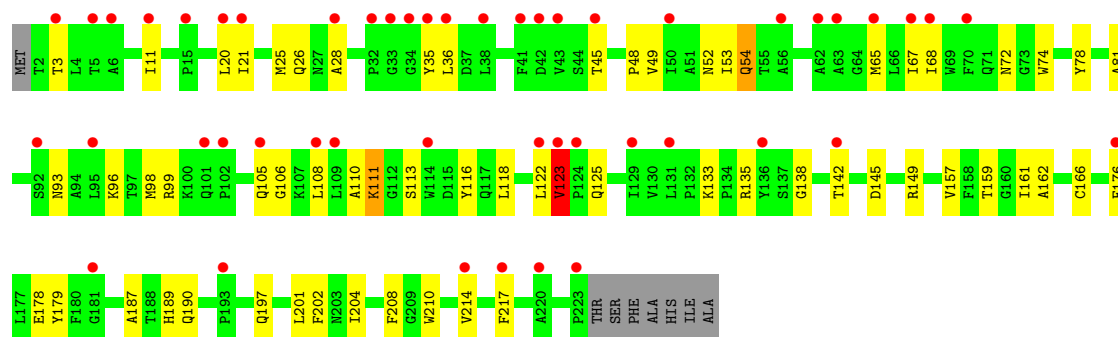


- Molecule 1: Ureidoacrylate amidohydrolase RutB

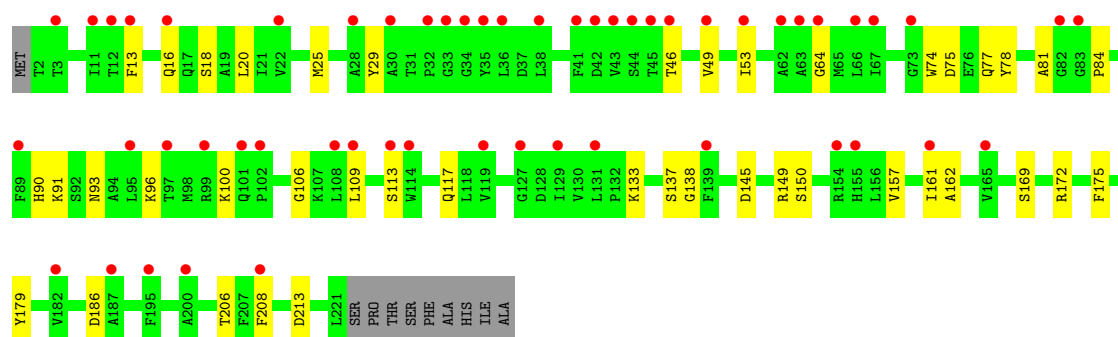
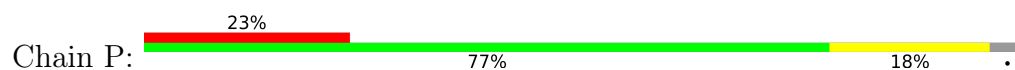


- Molecule 1: Ureidoacrylate amidohydrolase RutB





• Molecule 1: Ureidoacrylate amidohydrolase RutB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.59Å 110.89Å 128.71Å 90.00° 99.13° 90.00°	Depositor
Resolution (Å)	47.67 – 1.90 47.67 – 1.90	Depositor EDS
% Data completeness (in resolution range)	81.3 (47.67-1.90) 85.6 (47.67-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.95 (at 1.94Å)	Xtrriage
Refinement program	PHENIX 1.13-2998	Depositor
R, $R_{free}$	0.263 , 0.318 0.265 , 0.317	Depositor DCC
$R_{free}$ test set	11083 reflections (4.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtrriage
Anisotropy	0.561	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 28.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	28516	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6160e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.40	0/1753	0.62	0/2392
1	B	0.42	0/1760	0.64	0/2401
1	C	0.44	0/1760	0.68	0/2401
1	D	0.44	0/1746	0.63	0/2381
1	E	0.38	0/1748	0.59	0/2386
1	F	0.37	0/1738	0.60	0/2371
1	G	0.41	0/1756	0.62	0/2397
1	H	0.39	0/1760	0.60	0/2401
1	I	0.42	0/1753	0.64	0/2392
1	J	0.41	0/1741	0.62	0/2379
1	K	0.42	0/1736	0.66	0/2369
1	L	0.41	1/1746 (0.1%)	0.60	0/2381
1	M	0.37	0/1758	0.59	0/2398
1	N	0.41	0/1756	0.61	0/2396
1	O	0.36	0/1760	0.58	1/2401 (0.0%)
1	P	0.34	0/1727	0.56	0/2359
All	All	0.40	1/27998 (0.0%)	0.62	1/38205 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	6	ALA	C-N	-5.35	1.22	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	123	VAL	O-C-N	-5.21	115.16	121.10

There are no chirality outliers.

There are no planarity outliers.

## 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	1709	0	1668	36	0
1	B	1715	0	1675	35	1
1	C	1715	0	1675	37	0
1	D	1702	0	1663	28	0
1	E	1703	0	1659	28	0
1	F	1694	0	1653	32	0
1	G	1711	0	1664	40	0
1	H	1715	0	1675	35	0
1	I	1708	0	1662	25	0
1	J	1696	0	1632	42	1
1	K	1692	0	1648	40	0
1	L	1702	0	1663	28	1
1	M	1713	0	1670	40	0
1	N	1711	0	1669	29	0
1	O	1715	0	1675	45	0
1	P	1683	0	1627	23	1
2	A	95	0	0	1	0
2	B	87	0	0	5	0
2	C	96	0	0	5	0
2	D	81	0	0	7	0
2	E	78	0	0	6	0
2	F	70	0	0	1	0
2	G	78	0	0	4	0
2	H	81	0	0	7	0
2	I	93	0	0	5	0
2	J	84	0	0	5	0
2	K	71	0	0	6	0
2	L	82	0	0	3	0
2	M	68	0	0	3	0
2	N	48	0	0	1	0
2	O	62	0	0	4	0
2	P	58	0	0	1	0
All	All	28516	0	26578	510	2

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 9.

All (510) 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:J:72:ASN:HD22	1:J:133:LYS:NZ	1.57	1.03
1:J:72:ASN:ND2	1:J:133:LYS:HZ2	1.57	1.01
1:K:98:MET:HE3	1:K:105:GLN:HA	1.52	0.92
1:M:163:THR:HG22	1:M:188:THR:HB	1.53	0.90
1:I:172:ARG:NH2	2:I:301:HOH:O	2.11	0.82
1:F:15:PRO:HB3	1:F:65:MET:HE2	1.61	0.81
1:K:7:ARG:HB2	1:K:211:VAL:HG13	1.61	0.80
1:J:72:ASN:HD22	1:J:133:LYS:HZ2	0.79	0.76
1:G:123:VAL:HG13	1:G:125:GLN:NE2	2.00	0.76
1:D:140:PHE:N	2:D:301:HOH:O	2.15	0.75
1:B:178:GLU:OE2	1:D:146:SER:OG	2.05	0.74
1:C:52:ASN:HB3	1:C:214:VAL:HG21	1.69	0.73
1:B:61:ARG:NH1	2:B:303:HOH:O	2.21	0.73
1:D:149:ARG:NH2	2:D:302:HOH:O	2.14	0.72
1:I:203:ASN:ND2	2:I:301:HOH:O	2.22	0.72
1:G:78:TYR:O	2:G:301:HOH:O	2.08	0.72
1:E:8:PRO:HD2	1:E:210:TRP:CD1	2.25	0.71
1:O:98:MET:HE3	1:O:105:GLN:HA	1.73	0.70
1:N:103:GLN:HG3	1:N:104:LEU:HD22	1.74	0.69
1:N:70:PHE:HZ	1:N:144:LEU:HD22	1.58	0.69
1:I:121:GLU:N	1:I:121:GLU:OE1	2.24	0.69
1:K:161:ILE:O	2:K:301:HOH:O	2.10	0.69
1:F:186:ASP:OD2	2:F:301:HOH:O	2.10	0.68
1:I:52:ASN:HB3	1:I:214:VAL:HG21	1.76	0.68
1:K:16:GLN:NE2	2:K:302:HOH:O	2.13	0.68
1:B:72:ASN:HD22	1:B:133:LYS:NZ	1.92	0.68
1:O:96:LYS:HG2	1:O:99:ARG:HH21	1.59	0.67
1:H:10:ALA:O	2:H:301:HOH:O	2.12	0.67
1:K:98:MET:HE3	1:K:106:GLY:H	1.60	0.67
1:C:98:MET:HE2	1:C:105:GLN:HA	1.77	0.67
1:J:66:LEU:HD21	1:J:129:ILE:HD12	1.77	0.67
1:L:37:ASP:OD1	2:L:302:HOH:O	2.13	0.67
1:K:78:TYR:CZ	1:K:98:MET:HE1	2.30	0.67
1:K:20:LEU:HD12	1:K:157:VAL:HB	1.77	0.67
1:E:99:ARG:NH1	2:E:304:HOH:O	2.27	0.66
1:I:75:ASP:OD2	2:I:302:HOH:O	2.13	0.66
1:B:209:GLY:O	1:H:91:LYS:NZ	2.26	0.66
1:G:17:GLN:NE2	2:G:303:HOH:O	2.25	0.66
1:H:78:TYR:OH	1:H:98:MET:HE1	1.95	0.66
1:D:137:SER:O	2:D:301:HOH:O	2.11	0.66
1:D:56:ALA:HB2	1:D:214:VAL:HG13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:72:ASN:HD22	1:M:133:LYS:HG3	1.61	0.66
1:C:78:TYR:OH	1:C:98:MET:HE1	1.96	0.66
1:E:3:THR:OG1	2:E:301:HOH:O	2.14	0.65
1:A:131:LEU:HD11	1:A:142:THR:HB	1.78	0.65
1:J:70:PHE:HZ	1:J:144:LEU:HD22	1.62	0.64
1:K:137:SER:HB2	1:K:169:SER:OG	1.97	0.64
1:N:70:PHE:CZ	1:N:144:LEU:HD22	2.32	0.64
1:G:98:MET:HE2	1:G:108:LEU:HB2	1.79	0.64
1:G:54:GLN:O	1:G:58:THR:HG22	1.98	0.63
1:G:70:PHE:HZ	1:G:144:LEU:HD22	1.63	0.63
1:M:72:ASN:ND2	1:M:133:LYS:NZ	2.46	0.63
1:O:93:ASN:ND2	2:O:307:HOH:O	2.32	0.63
1:L:76:GLU:OE1	2:L:303:HOH:O	2.15	0.62
1:P:93:ASN:HA	1:P:96:LYS:HB2	1.81	0.62
1:L:93:ASN:HA	1:L:96:LYS:HB2	1.81	0.62
1:J:72:ASN:ND2	1:J:133:LYS:NZ	2.30	0.62
1:F:151:ARG:HB2	1:F:153:ILE:HD12	1.81	0.62
1:J:20:LEU:HD12	1:J:157:VAL:HG23	1.82	0.61
1:C:30:ALA:O	1:C:46:THR:HG21	2.01	0.61
1:P:145:ASP:OD1	1:P:179:TYR:OH	2.18	0.61
1:M:2:THR:N	2:M:308:HOH:O	2.34	0.61
1:F:8:PRO:HD2	1:F:210:TRP:CD1	2.35	0.61
1:H:45:THR:O	1:H:48:PRO:HD2	2.00	0.61
1:O:78:TYR:CE2	1:O:98:MET:HE1	2.35	0.61
1:K:203:ASN:ND2	2:K:303:HOH:O	2.22	0.60
1:B:52:ASN:HB3	1:B:214:VAL:HG21	1.82	0.60
1:J:129:ILE:HD13	1:J:147:ILE:HG21	1.83	0.60
1:G:70:PHE:CZ	1:G:144:LEU:HD22	2.37	0.60
1:E:138:GLY:O	1:E:142:THR:OG1	2.19	0.60
1:A:74:TRP:HB3	1:A:80:GLU:HB2	1.84	0.59
1:M:76:GLU:OE1	1:M:77:GLN:NE2	2.28	0.59
1:A:8:PRO:HD2	1:A:210:TRP:CD1	2.38	0.59
1:L:86:SER:HB2	1:P:150:SER:OG	2.02	0.59
1:N:98:MET:HE2	1:N:108:LEU:HB2	1.84	0.59
1:B:61:ARG:NH2	1:B:128:ASP:OD2	2.35	0.59
1:C:98:MET:HE3	1:C:108:LEU:H	1.66	0.59
1:H:140:PHE:O	1:H:142:THR:HG23	2.03	0.59
1:E:120:ASP:OD2	2:E:302:HOH:O	2.17	0.59
1:N:96:LYS:NZ	2:N:302:HOH:O	2.29	0.58
1:G:15:PRO:O	1:G:65:MET:HG2	2.03	0.58
1:J:154:ARG:NH1	2:J:306:HOH:O	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LYS:NZ	1:H:205:GLU:O	2.33	0.58
1:B:66:LEU:HD21	1:B:129:ILE:HD12	1.85	0.58
1:A:195:PHE:CE2	1:G:198:LYS:HE2	2.38	0.58
1:O:20:LEU:HB3	1:O:67:ILE:HD13	1.85	0.58
1:E:96:LYS:NZ	2:E:305:HOH:O	2.27	0.58
1:K:78:TYR:OH	1:K:98:MET:HE1	2.04	0.58
1:B:12:THR:HG21	1:F:12:THR:HG21	1.86	0.58
1:D:74:TRP:CD2	1:D:81:ALA:HB2	2.38	0.58
1:G:35:TYR:HB2	1:G:108:LEU:HD13	1.86	0.58
1:A:61:ARG:NH2	1:A:128:ASP:OD2	2.36	0.58
1:C:158:PHE:CD2	1:C:171:LEU:HD12	2.39	0.58
1:C:25:MET:HG3	1:C:53:ILE:HD13	1.86	0.57
1:H:149:ARG:NE	2:H:312:HOH:O	2.37	0.57
1:J:59:ALA:HB1	1:J:221:LEU:HD12	1.87	0.57
1:M:72:ASN:HD22	1:M:133:LYS:NZ	2.03	0.57
1:K:7:ARG:NH1	2:K:307:HOH:O	2.26	0.57
1:F:61:ARG:NH1	1:F:125:GLN:HG3	2.20	0.57
1:N:18:SER:HB3	1:N:65:MET:HE3	1.87	0.57
1:H:98:MET:HE3	1:H:108:LEU:H	1.70	0.56
1:M:171:LEU:HD22	1:M:204:ILE:HG12	1.87	0.56
1:C:8:PRO:HG2	1:C:9:GLU:OE1	2.05	0.56
1:C:172:ARG:HG2	1:C:208:PHE:CE1	2.40	0.56
1:G:123:VAL:HG13	1:G:123:VAL:O	2.04	0.56
1:H:98:MET:CE	1:H:108:LEU:H	2.18	0.56
1:A:195:PHE:HA	1:A:198:LYS:HE2	1.87	0.56
1:C:171:LEU:HD22	1:C:204:ILE:HG12	1.86	0.56
1:J:38:LEU:HD13	1:J:104:LEU:HD13	1.87	0.56
1:J:197:GLN:HE21	1:J:201:LEU:HD11	1.70	0.56
1:M:138:GLY:O	1:M:142:THR:OG1	2.22	0.56
1:A:66:LEU:HD11	1:A:129:ILE:HD12	1.87	0.56
1:O:138:GLY:O	1:O:142:THR:OG1	2.18	0.56
1:C:17:GLN:O	2:C:301:HOH:O	2.18	0.56
1:O:74:TRP:CD2	1:O:81:ALA:HB2	2.40	0.56
1:G:4:LEU:HB2	1:G:13:PHE:HE1	1.69	0.56
1:M:72:ASN:HD22	1:M:133:LYS:HZ2	1.51	0.56
1:O:98:MET:CE	1:O:106:GLY:H	2.18	0.56
1:L:57:VAL:HG12	1:L:61:ARG:HH12	1.71	0.55
1:F:89:PHE:HA	1:F:95:LEU:HD12	1.88	0.55
1:M:116:TYR:OH	2:M:301:HOH:O	2.11	0.55
1:P:96:LYS:O	1:P:100:LYS:HG3	2.07	0.55
1:M:163:THR:HG23	1:M:189:HIS:C	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:ASN:HB3	1:F:214:VAL:HG21	1.89	0.55
1:K:52:ASN:HB3	1:K:214:VAL:HG21	1.89	0.55
1:K:7:ARG:HB2	1:K:211:VAL:CG1	2.32	0.54
1:K:78:TYR:CE2	1:K:98:MET:HE1	2.42	0.54
1:C:70:PHE:HZ	1:C:144:LEU:HD22	1.72	0.54
1:H:98:MET:HE2	1:H:104:LEU:O	2.08	0.54
1:M:72:ASN:ND2	1:M:133:LYS:HZ2	2.06	0.54
1:I:136:TYR:HB2	1:O:176:PHE:CZ	2.43	0.54
1:K:8:PRO:HD2	1:K:210:TRP:CD1	2.43	0.54
1:C:149:ARG:HD3	2:C:351:HOH:O	2.07	0.54
1:G:145:ASP:OD1	1:G:179:TYR:OH	2.25	0.53
1:H:26:GLN:HA	1:H:118:LEU:HA	1.90	0.53
1:H:9:GLU:OE2	1:H:210:TRP:NE1	2.33	0.53
1:O:45:THR:O	1:O:48:PRO:HD2	2.07	0.53
1:O:98:MET:SD	1:O:108:LEU:HB2	2.49	0.53
1:B:72:ASN:HD22	1:B:133:LYS:HZ2	1.57	0.53
1:E:82:GLY:O	1:E:89:PHE:HB2	2.09	0.53
1:L:52:ASN:HB3	1:L:214:VAL:HG21	1.90	0.53
1:M:163:THR:HG21	1:M:197:GLN:OE1	2.09	0.53
1:J:111:LYS:HA	1:J:116:TYR:CD2	2.44	0.53
2:B:370:HOH:O	1:D:149:ARG:HG2	2.09	0.53
1:O:123:VAL:HG22	1:O:125:GLN:OE1	2.09	0.52
1:B:72:ASN:ND2	1:B:133:LYS:NZ	2.56	0.52
1:N:25:MET:HE2	1:N:53:ILE:HD12	1.92	0.52
1:C:20:LEU:HB3	1:C:67:ILE:HD13	1.92	0.51
1:M:25:MET:HG3	1:M:53:ILE:HD13	1.92	0.51
1:G:161:ILE:HG12	1:G:189:HIS:HB3	1.93	0.51
1:A:12:THR:OG1	1:E:3:THR:HG22	2.10	0.51
1:M:103:GLN:CD	1:M:103:GLN:H	2.19	0.51
1:B:120:ASP:OD1	2:B:302:HOH:O	2.18	0.51
1:C:166:CYS:SG	2:C:367:HOH:O	2.56	0.51
1:D:110:ALA:O	1:D:113:SER:OG	2.24	0.51
1:K:22:VAL:HA	1:K:159:THR:OG1	2.11	0.51
1:M:113:SER:O	1:M:117:GLN:HG3	2.11	0.51
1:O:74:TRP:O	1:O:111:LYS:HG2	2.11	0.51
1:D:20:LEU:HD22	1:D:60:ALA:HB2	1.92	0.51
1:L:114:TRP:HA	1:L:117:GLN:HG3	1.93	0.51
1:K:98:MET:CE	1:K:105:GLN:HA	2.35	0.51
1:K:162:ALA:HA	1:K:189:HIS:O	2.10	0.51
1:M:146:SER:OG	1:O:178:GLU:OE2	2.24	0.51
1:F:18:SER:OG	1:F:155:HIS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:18:SER:OG	1:L:155:HIS:HB2	2.12	0.50
1:J:59:ALA:HB2	1:J:218:CYS:SG	2.50	0.50
1:E:195:PHE:O	2:E:303:HOH:O	2.18	0.50
1:H:113:SER:O	1:H:117:GLN:HG3	2.12	0.50
1:O:98:MET:HE3	1:O:106:GLY:H	1.77	0.50
1:P:46:THR:HG22	1:P:46:THR:O	2.12	0.50
1:P:75:ASP:OD2	1:P:77:GLN:HG3	2.11	0.50
1:J:35:TYR:CD1	1:J:35:TYR:C	2.89	0.50
1:E:29:TYR:HA	1:E:36:LEU:HD12	1.93	0.50
1:M:74:TRP:HB3	1:M:80:GLU:HB2	1.93	0.50
1:O:54:GLN:HG3	1:O:122:LEU:CD2	2.41	0.50
1:A:87:PRO:HD2	1:G:178:GLU:OE1	2.12	0.50
1:C:111:LYS:NZ	2:C:321:HOH:O	2.44	0.50
1:F:140:PHE:O	1:F:142:THR:HG23	2.12	0.50
1:G:116:TYR:OH	2:G:302:HOH:O	2.11	0.50
1:E:72:ASN:OD1	1:E:133:LYS:NZ	2.32	0.49
1:J:86:SER:HB2	1:N:150:SER:OG	2.11	0.49
1:O:25:MET:HE2	1:O:53:ILE:HD12	1.93	0.49
1:O:28:ALA:HB1	1:O:35:TYR:HB3	1.94	0.49
1:A:21:ILE:HD12	1:A:156:LEU:HB3	1.94	0.49
1:A:137:SER:HB2	1:A:169:SER:HB3	1.93	0.49
1:L:35:TYR:C	1:L:35:TYR:CD1	2.91	0.49
1:A:98:MET:HE2	1:A:108:LEU:HB2	1.94	0.49
1:M:70:PHE:HZ	1:M:144:LEU:HD22	1.77	0.49
1:M:163:THR:HA	1:M:167:VAL:HB	1.93	0.49
1:D:176:PHE:O	2:D:303:HOH:O	2.20	0.49
1:E:26:GLN:HA	1:E:118:LEU:HA	1.94	0.49
1:E:61:ARG:NH2	1:E:128:ASP:OD2	2.34	0.49
1:D:103:GLN:O	1:J:107:LYS:HE2	2.12	0.49
1:O:72:ASN:HD22	1:O:133:LYS:HZ2	1.60	0.49
1:B:78:TYR:CZ	1:B:98:MET:HE1	2.48	0.49
1:B:129:ILE:HD13	1:B:147:ILE:HG21	1.95	0.49
1:J:154:ARG:NH2	1:J:178:GLU:O	2.43	0.49
1:O:72:ASN:HD22	1:O:133:LYS:NZ	2.11	0.49
1:A:78:TYR:OH	1:A:98:MET:SD	2.70	0.49
1:A:182:VAL:HG13	1:A:210:TRP:HB2	1.95	0.49
1:N:145:ASP:OD1	1:N:179:TYR:OH	2.27	0.49
1:E:46:THR:O	1:E:50:ILE:HG13	2.13	0.48
1:F:183:VAL:HG12	1:F:211:VAL:HG22	1.95	0.48
1:L:98:MET:HG3	1:L:108:LEU:HD12	1.94	0.48
1:C:98:MET:SD	1:C:108:LEU:HB2	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:TYR:C	1:G:35:TYR:CD1	2.91	0.48
1:N:8:PRO:HD2	1:N:210:TRP:CD1	2.48	0.48
1:L:95:LEU:O	1:L:99:ARG:HG3	2.13	0.48
1:N:168:GLU:OE2	1:N:172:ARG:NH2	2.36	0.48
1:F:74:TRP:CD2	1:F:81:ALA:HB2	2.48	0.48
1:M:80:GLU:HG2	2:M:362:HOH:O	2.12	0.48
1:A:35:TYR:CD1	1:A:35:TYR:C	2.92	0.48
1:J:23:VAL:HA	1:J:70:PHE:HB2	1.95	0.48
1:K:74:TRP:HB3	1:K:80:GLU:HB2	1.95	0.48
1:O:26:GLN:HA	1:O:118:LEU:HA	1.96	0.48
1:F:70:PHE:CZ	1:F:144:LEU:HD22	2.49	0.48
1:G:185:GLU:HG2	1:G:212:SER:O	2.14	0.48
1:J:18:SER:HA	1:J:153:ILE:HG23	1.95	0.48
1:N:15:PRO:HA	1:N:18:SER:HB2	1.96	0.48
1:P:113:SER:HB3	2:P:341:HOH:O	2.12	0.48
1:H:80:GLU:OE1	1:H:111:LYS:NZ	2.42	0.48
1:L:14:ASP:OD2	1:L:17:GLN:HG2	2.13	0.48
1:L:25:MET:HG3	1:L:53:ILE:HD13	1.95	0.48
1:L:65:MET:HE1	1:L:217:PHE:CZ	2.49	0.48
1:N:18:SER:OG	1:N:155:HIS:HB2	2.13	0.48
1:K:72:ASN:O	1:K:109:LEU:HD22	2.14	0.48
1:C:42:ASP:OD1	1:C:44:SER:OG	2.32	0.48
1:F:76:GLU:OE2	1:F:77:GLN:NE2	2.47	0.47
1:I:136:TYR:HB2	1:O:176:PHE:HZ	1.79	0.47
1:M:70:PHE:CZ	1:M:144:LEU:HD22	2.49	0.47
1:O:21:ILE:HD13	1:O:68:ILE:HB	1.96	0.47
1:F:7:ARG:HB3	1:F:205:GLU:CD	2.39	0.47
1:H:91:LYS:HA	1:H:91:LYS:HD2	1.60	0.47
1:N:111:LYS:HG2	1:N:116:TYR:CE2	2.49	0.47
1:E:74:TRP:HB3	1:E:80:GLU:HB2	1.95	0.47
1:F:26:GLN:HA	1:F:118:LEU:HA	1.96	0.47
1:M:21:ILE:HD12	1:M:156:LEU:HB3	1.97	0.47
1:A:22:VAL:HA	1:A:159:THR:OG1	2.15	0.47
1:A:136:TYR:OH	1:G:207:PHE:O	2.20	0.47
1:H:35:TYR:CD1	1:H:35:TYR:C	2.92	0.47
1:L:95:LEU:HD23	1:L:99:ARG:NH2	2.29	0.47
1:M:35:TYR:OH	1:M:93:ASN:HB2	2.14	0.47
1:M:35:TYR:HA	1:M:108:LEU:HD13	1.95	0.47
1:A:87:PRO:HA	1:G:180:PHE:CE2	2.50	0.47
1:B:4:LEU:HD22	1:B:13:PHE:HE1	1.79	0.47
1:C:185:GLU:HG2	1:C:212:SER:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:THR:O	1:G:168:GLU:HB2	2.15	0.47
1:J:8:PRO:HG2	1:J:9:GLU:OE1	2.15	0.47
1:J:158:PHE:CD2	1:J:171:LEU:HD12	2.50	0.47
1:M:29:TYR:HA	1:M:36:LEU:HD12	1.97	0.47
1:B:61:ARG:HH21	1:B:128:ASP:CG	2.23	0.47
1:I:22:VAL:HG11	1:I:69:TRP:CZ3	2.50	0.47
1:H:7:ARG:NH2	2:H:320:HOH:O	2.48	0.47
1:F:217:PHE:O	1:F:221:LEU:HG	2.15	0.47
1:J:172:ARG:HD3	1:J:208:PHE:CZ	2.49	0.47
1:K:185:GLU:HG2	1:K:212:SER:O	2.15	0.47
1:O:65:MET:HE1	1:O:217:PHE:CZ	2.50	0.47
1:O:166:CYS:SG	2:O:345:HOH:O	2.60	0.47
1:B:49:VAL:O	1:B:53:ILE:HG13	2.16	0.46
1:B:151:ARG:HG3	1:B:151:ARG:HH11	1.79	0.46
1:G:123:VAL:HG13	1:G:125:GLN:HE21	1.80	0.46
1:I:11:ILE:HG21	1:I:210:TRP:CE2	2.50	0.46
1:I:163:THR:O	1:I:168:GLU:HB2	2.15	0.46
1:N:137:SER:HB2	1:N:169:SER:HB3	1.95	0.46
1:F:61:ARG:NH2	1:F:128:ASP:OD2	2.48	0.46
1:J:182:VAL:HA	1:J:210:TRP:O	2.15	0.46
1:I:205:GLU:OE1	2:I:303:HOH:O	2.21	0.46
1:B:169:SER:OG	1:H:172:ARG:HD3	2.16	0.46
1:L:186:ASP:OD2	2:L:304:HOH:O	2.21	0.46
1:O:98:MET:HE3	1:O:106:GLY:N	2.30	0.46
1:F:46:THR:O	1:F:49:VAL:HG22	2.15	0.46
1:M:72:ASN:ND2	1:M:133:LYS:HZ3	2.13	0.46
1:B:149:ARG:HD3	1:D:149:ARG:CZ	2.46	0.46
1:G:140:PHE:O	1:G:141:ASN:HB2	2.15	0.46
1:I:20:LEU:HD22	1:I:157:VAL:O	2.16	0.46
1:N:35:TYR:OH	1:N:93:ASN:HB2	2.15	0.46
1:O:96:LYS:CG	1:O:99:ARG:HH21	2.26	0.46
1:C:38:LEU:HD13	1:C:104:LEU:HD13	1.97	0.46
1:I:132:PRO:HB2	2:I:377:HOH:O	2.14	0.46
1:J:96:LYS:NZ	2:J:305:HOH:O	2.29	0.46
1:J:171:LEU:HD13	1:J:204:ILE:HD13	1.98	0.46
1:C:35:TYR:CD1	1:C:35:TYR:C	2.94	0.46
1:M:222:SER:HB2	1:M:223:PRO:HD3	1.98	0.45
1:C:8:PRO:HD2	1:C:210:TRP:CD1	2.51	0.45
1:P:161:ILE:HA	1:P:162:ALA:HA	1.72	0.45
1:A:7:ARG:HB3	1:A:205:GLU:OE2	2.16	0.45
1:A:61:ARG:HH21	1:A:128:ASP:CG	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ASP:HB2	1:I:103:GLN:OE1	2.16	0.45
1:D:164:ASN:OD1	1:D:164:ASN:N	2.49	0.45
1:G:54:GLN:NE2	1:G:121:GLU:HB3	2.30	0.45
1:L:91:LYS:HA	1:L:91:LYS:HD2	1.77	0.45
1:P:137:SER:HB2	1:P:169:SER:HB3	1.99	0.45
1:B:149:ARG:NH1	2:B:315:HOH:O	2.41	0.45
1:C:45:THR:HG22	1:C:45:THR:O	2.17	0.45
1:G:123:VAL:HG13	1:G:125:GLN:HE22	1.78	0.45
1:C:50:ILE:HD12	1:C:119:VAL:HG21	1.99	0.45
1:E:98:MET:HE2	1:E:108:LEU:HB2	1.99	0.45
1:E:139:PHE:CD1	1:E:177:LEU:HD12	2.51	0.45
1:I:4:LEU:HD23	1:I:6:ALA:HB2	1.99	0.45
1:K:98:MET:HE3	1:K:106:GLY:N	2.27	0.45
1:P:78:TYR:CE2	1:P:106:GLY:HA2	2.51	0.45
1:K:98:MET:HE3	1:K:105:GLN:CA	2.37	0.45
1:A:96:LYS:NZ	2:A:304:HOH:O	2.32	0.45
1:G:158:PHE:N	1:G:182:VAL:O	2.47	0.45
1:A:15:PRO:HB3	1:A:65:MET:HG2	1.98	0.45
1:D:140:PHE:HB2	2:D:301:HOH:O	2.17	0.45
1:J:139:PHE:O	2:J:301:HOH:O	2.21	0.45
1:A:195:PHE:CZ	1:G:198:LYS:HE2	2.52	0.45
1:C:198:LYS:HZ1	1:F:215:GLU:CD	2.24	0.45
1:D:137:SER:C	2:D:301:HOH:O	2.57	0.45
1:D:150:SER:OG	1:H:86:SER:HB2	2.17	0.45
1:F:168:GLU:OE2	1:F:172:ARG:NH2	2.35	0.45
1:G:93:ASN:HA	1:G:96:LYS:HB2	1.98	0.45
1:M:24:ASP:O	1:M:26:GLN:N	2.45	0.45
1:P:13:PHE:HD2	1:P:18:SER:OG	2.00	0.45
1:A:12:THR:HG21	1:E:12:THR:HG21	1.99	0.45
1:D:2:THR:O	1:D:12:THR:HA	2.17	0.45
1:D:172:ARG:HD3	1:D:208:PHE:CZ	2.52	0.45
1:F:92:SER:HB3	1:F:95:LEU:HB2	1.98	0.45
1:K:186:ASP:N	1:K:186:ASP:OD1	2.47	0.45
1:M:131:LEU:HD23	1:M:131:LEU:HA	1.87	0.45
1:O:20:LEU:HD12	1:O:157:VAL:O	2.16	0.45
1:D:74:TRP:CG	1:D:81:ALA:HB2	2.52	0.44
1:H:74:TRP:CD2	1:H:81:ALA:HB2	2.52	0.44
1:H:151:ARG:NE	2:H:321:HOH:O	2.48	0.44
1:J:183:VAL:CG1	1:J:211:VAL:HG22	2.47	0.44
1:K:2:THR:O	1:K:12:THR:HA	2.16	0.44
1:L:78:TYR:CZ	1:L:98:MET:HE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:172:ARG:O	1:P:175:PHE:HB3	2.18	0.44
1:C:91:LYS:NZ	1:E:205:GLU:O	2.45	0.44
1:F:35:TYR:OH	1:F:93:ASN:HB2	2.16	0.44
1:J:78:TYR:OH	1:J:98:MET:SD	2.73	0.44
1:K:122:LEU:HD23	1:K:122:LEU:HA	1.71	0.44
1:K:98:MET:CE	1:K:106:GLY:H	2.27	0.44
1:A:76:GLU:H	1:A:76:GLU:CD	2.25	0.44
1:J:222:SER:HB2	1:J:223:PRO:HD3	1.99	0.44
1:K:119:VAL:HB	2:K:332:HOH:O	2.17	0.44
1:O:35:TYR:OH	1:O:93:ASN:HB2	2.18	0.44
1:P:16:GLN:HG2	1:P:64:GLY:O	2.17	0.44
1:D:35:TYR:CD1	1:D:35:TYR:C	2.94	0.44
1:J:61:ARG:HG3	2:J:335:HOH:O	2.18	0.44
1:N:131:LEU:HA	1:N:131:LEU:HD23	1.73	0.44
1:A:223:PRO:HA	1:C:99:ARG:CD	2.47	0.44
1:B:182:VAL:HA	1:B:210:TRP:O	2.17	0.44
1:M:151:ARG:HB2	1:M:153:ILE:HD12	1.99	0.44
1:O:190:GLN:HB3	1:O:197:GLN:HB2	2.00	0.44
1:M:45:THR:O	1:M:48:PRO:HD2	2.17	0.44
1:A:20:LEU:HD23	1:A:67:ILE:HD12	1.98	0.44
1:C:144:LEU:O	1:C:148:LEU:HG	2.18	0.44
1:E:27:ASN:HA	1:E:31:THR:OG1	2.18	0.44
1:F:70:PHE:CE2	1:F:144:LEU:HD22	2.53	0.44
1:N:190:GLN:HB3	1:N:197:GLN:HB2	1.99	0.44
1:A:193:PRO:HG2	1:A:195:PHE:CE2	2.53	0.43
1:B:49:VAL:HG21	1:B:189:HIS:HB2	2.00	0.43
1:K:133:LYS:HB2	2:K:339:HOH:O	2.17	0.43
1:L:70:PHE:HZ	1:L:144:LEU:HD22	1.83	0.43
1:O:49:VAL:HG21	1:O:189:HIS:HB2	2.00	0.43
1:E:11:ILE:HG21	1:E:210:TRP:CE2	2.53	0.43
1:M:72:ASN:HB2	1:M:133:LYS:HZ2	1.83	0.43
1:N:107:LYS:HE3	1:N:115:ASP:HB2	2.00	0.43
1:P:113:SER:O	1:P:117:GLN:HG3	2.18	0.43
1:O:197:GLN:O	1:O:201:LEU:HG	2.18	0.43
1:B:166:CYS:SG	2:B:366:HOH:O	2.46	0.43
1:G:195:PHE:CD1	1:G:195:PHE:C	2.97	0.43
1:F:183:VAL:CG1	1:F:211:VAL:HG22	2.47	0.43
1:A:35:TYR:OH	1:A:93:ASN:HB2	2.18	0.43
1:M:140:PHE:O	1:M:142:THR:HG23	2.18	0.43
1:O:53:ILE:HG12	1:O:187:ALA:HB1	2.01	0.43
1:O:135:ARG:NH2	2:O:319:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:186:ASP:OD2	1:P:213:ASP:HB2	2.19	0.43
1:I:8:PRO:HD2	1:I:210:TRP:CD1	2.54	0.43
1:N:52:ASN:HB3	1:N:214:VAL:HG21	2.01	0.43
1:O:11:ILE:HG21	1:O:210:TRP:CE2	2.54	0.43
1:O:116:TYR:OH	2:O:301:HOH:O	2.20	0.43
1:D:54:GLN:NE2	1:D:121:GLU:HB3	2.34	0.43
1:H:20:LEU:HD12	1:H:157:VAL:HB	2.00	0.43
1:K:3:THR:HB	1:O:3:THR:HB	2.00	0.43
1:K:29:TYR:OH	1:K:72:ASN:ND2	2.51	0.43
1:B:57:VAL:HG13	1:B:67:ILE:HD12	2.01	0.43
1:B:190:GLN:HB3	1:B:197:GLN:HE21	1.84	0.43
1:C:53:ILE:HG13	1:C:187:ALA:HB1	1.99	0.43
1:D:114:TRP:CG	1:J:102:PRO:HB2	2.54	0.43
1:E:22:VAL:HA	1:E:159:THR:OG1	2.19	0.43
1:I:45:THR:O	1:I:48:PRO:HD2	2.19	0.43
1:A:26:GLN:HA	1:A:118:LEU:HA	2.00	0.43
1:A:52:ASN:HB3	1:A:214:VAL:HG21	1.99	0.43
1:H:155:HIS:ND1	2:H:309:HOH:O	2.33	0.43
1:I:133:LYS:NZ	1:I:136:TYR:O	2.50	0.43
1:J:24:ASP:OD2	1:J:72:ASN:HB2	2.18	0.43
1:K:66:LEU:HD11	1:K:129:ILE:CG1	2.48	0.43
1:P:133:LYS:HD3	1:P:138:GLY:HA2	2.01	0.43
1:B:72:ASN:ND2	1:B:133:LYS:HZ1	2.17	0.42
1:E:172:ARG:O	1:E:175:PHE:HB3	2.18	0.42
1:F:45:THR:O	1:F:48:PRO:HD2	2.19	0.42
1:P:20:LEU:HD12	1:P:157:VAL:O	2.19	0.42
1:A:183:VAL:CG1	1:A:211:VAL:HG22	2.49	0.42
1:H:28:ALA:HB1	1:H:35:TYR:HB3	2.01	0.42
1:M:28:ALA:HA	1:M:115:ASP:OD1	2.18	0.42
1:N:29:TYR:HA	1:N:36:LEU:HD12	2.01	0.42
1:O:161:ILE:HA	1:O:162:ALA:HA	1.74	0.42
1:A:172:ARG:HG2	1:A:208:PHE:CD1	2.54	0.42
1:E:34:GLY:O	1:E:38:LEU:HG	2.19	0.42
1:E:155:HIS:HA	1:E:180:PHE:O	2.19	0.42
1:G:164:ASN:OD1	1:G:164:ASN:N	2.52	0.42
1:G:60:ALA:HB3	1:G:67:ILE:HD11	2.00	0.42
1:G:180:PHE:HD2	1:G:210:TRP:CH2	2.38	0.42
1:J:111:LYS:HG2	1:J:116:TYR:CZ	2.54	0.42
1:K:140:PHE:O	1:K:142:THR:HG23	2.18	0.42
1:P:172:ARG:HG2	1:P:208:PHE:CD1	2.54	0.42
1:E:11:ILE:HG21	1:E:210:TRP:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:24:ASP:HB2	1:L:161:ILE:O	2.20	0.42
1:L:194:LYS:HB2	1:L:194:LYS:HE2	1.80	0.42
1:P:49:VAL:O	1:P:53:ILE:HG13	2.19	0.42
1:B:21:ILE:HD12	1:B:156:LEU:HB3	2.02	0.42
1:H:138:GLY:O	1:H:142:THR:OG1	2.32	0.42
1:H:161:ILE:HA	1:H:162:ALA:HA	1.79	0.42
1:I:14:ASP:HB3	1:I:17:GLN:HB2	2.01	0.42
1:M:163:THR:O	1:M:168:GLU:HB2	2.20	0.42
1:C:102:PRO:HB2	1:I:114:TRP:CG	2.54	0.42
1:C:163:THR:O	1:C:168:GLU:HB2	2.19	0.42
1:G:203:ASN:ND2	2:G:309:HOH:O	2.42	0.42
1:I:35:TYR:CD1	1:I:35:TYR:C	2.97	0.42
1:D:131:LEU:HA	1:D:131:LEU:HD23	1.72	0.42
1:H:16:GLN:OE1	2:H:302:HOH:O	2.22	0.42
1:K:163:THR:HA	1:K:167:VAL:HB	2.01	0.42
1:N:36:LEU:HD23	1:N:36:LEU:HA	1.91	0.42
1:A:194:LYS:HB2	1:A:194:LYS:HE2	1.76	0.42
1:F:154:ARG:HA	1:F:154:ARG:HD2	1.96	0.42
1:F:161:ILE:HA	1:F:162:ALA:HA	1.73	0.42
1:G:168:GLU:O	1:G:172:ARG:HG3	2.20	0.42
1:L:163:THR:OG1	1:L:188:THR:HB	2.20	0.42
1:J:161:ILE:HA	1:J:162:ALA:HA	1.79	0.42
1:O:53:ILE:HG12	1:O:159:THR:HB	2.01	0.42
1:B:4:LEU:HB3	1:B:11:ILE:HG12	2.01	0.41
1:H:160:GLY:O	1:H:188:THR:HA	2.21	0.41
1:H:195:PHE:CD1	1:H:195:PHE:C	2.98	0.41
1:I:4:LEU:HD21	1:I:212:SER:HB2	2.02	0.41
1:J:53:ILE:HG12	1:J:187:ALA:HB1	2.01	0.41
1:J:93:ASN:HA	1:J:96:LYS:HB2	2.02	0.41
1:K:7:ARG:NH2	1:K:211:VAL:HG21	2.35	0.41
1:P:25:MET:HG3	1:P:53:ILE:HD12	2.02	0.41
1:I:193:PRO:HD3	1:O:202:PHE:CZ	2.55	0.41
1:O:36:LEU:HD23	1:O:36:LEU:HA	1.79	0.41
1:B:136:TYR:HB2	1:H:176:PHE:CE1	2.55	0.41
1:C:11:ILE:HG21	1:C:210:TRP:CE2	2.55	0.41
1:E:145:ASP:HB2	2:E:318:HOH:O	2.20	0.41
1:G:193:PRO:HG2	1:G:195:PHE:CE2	2.55	0.41
1:J:141:ASN:HB3	1:N:143:PRO:HB3	2.02	0.41
1:K:35:TYR:CD1	1:K:35:TYR:C	2.98	0.41
1:K:98:MET:SD	1:K:108:LEU:HB2	2.60	0.41
1:N:95:LEU:HD23	1:N:98:MET:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:186:ASP:OD1	1:N:186:ASP:N	2.49	0.41
1:O:145:ASP:OD1	1:O:179:TYR:OH	2.31	0.41
1:A:56:ALA:HB2	1:A:214:VAL:HG13	2.02	0.41
1:K:91:LYS:HB3	1:K:91:LYS:HE3	1.83	0.41
1:N:222:SER:HB2	1:N:223:PRO:HD3	2.02	0.41
1:G:11:ILE:HG21	1:G:210:TRP:CE2	2.56	0.41
1:H:25:MET:HE2	1:H:53:ILE:HD12	2.02	0.41
1:L:38:LEU:HD13	1:L:104:LEU:HD13	2.01	0.41
1:M:2:THR:HB	1:M:13:PHE:O	2.21	0.41
1:N:23:VAL:HB	1:N:167:VAL:HG22	2.02	0.41
1:O:110:ALA:O	1:O:113:SER:OG	2.32	0.41
1:G:206:THR:HB	1:G:207:PHE:CD2	2.55	0.41
1:J:105:GLN:HB3	2:J:357:HOH:O	2.21	0.41
1:L:163:THR:O	1:L:168:GLU:HB2	2.21	0.41
1:P:74:TRP:CD2	1:P:81:ALA:HB2	2.55	0.41
1:P:84:PRO:O	1:P:90:HIS:NE2	2.50	0.41
1:C:20:LEU:HB3	1:C:67:ILE:CD1	2.50	0.41
1:C:172:ARG:HG2	1:C:208:PHE:CD1	2.55	0.41
1:D:131:LEU:HD22	1:D:132:PRO:HD2	2.03	0.41
1:B:136:TYR:HB2	1:H:176:PHE:CZ	2.56	0.41
1:B:149:ARG:HG3	2:D:302:HOH:O	2.20	0.41
1:D:20:LEU:HD12	1:D:20:LEU:HA	1.90	0.41
1:E:111:LYS:HA	1:E:116:TYR:CD2	2.56	0.41
1:F:217:PHE:CZ	1:F:221:LEU:HD11	2.55	0.41
1:G:161:ILE:HA	1:G:162:ALA:HA	1.76	0.41
1:J:150:SER:OG	1:N:86:SER:HB2	2.21	0.41
1:L:28:ALA:HA	1:L:35:TYR:H	1.86	0.41
1:N:98:MET:CE	1:N:108:LEU:HB2	2.49	0.41
1:O:204:ILE:HA	1:O:208:PHE:HB2	2.02	0.41
1:G:29:TYR:OH	1:G:72:ASN:ND2	2.54	0.41
1:K:164:ASN:OD1	1:K:164:ASN:N	2.52	0.41
1:L:36:LEU:HD22	1:L:41:PHE:CD2	2.56	0.41
1:A:186:ASP:OD1	1:A:214:VAL:HG23	2.22	0.40
1:B:121:GLU:OE1	1:B:121:GLU:N	2.48	0.40
1:C:107:LYS:NZ	2:C:302:HOH:O	2.20	0.40
1:L:133:LYS:NZ	1:L:136:TYR:O	2.54	0.40
1:M:35:TYR:CD1	1:M:35:TYR:C	2.99	0.40
1:C:91:LYS:HD2	1:C:91:LYS:HA	1.64	0.40
1:F:35:TYR:CD1	1:F:35:TYR:C	2.99	0.40
1:F:78:TYR:CZ	1:F:98:MET:HE1	2.56	0.40
1:H:166:CYS:SG	2:H:374:HOH:O	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:144:LEU:HA	1:J:147:ILE:HD12	2.03	0.40
1:M:27:ASN:HA	1:M:31:THR:OG1	2.22	0.40
1:D:69:TRP:CD1	1:D:124:PRO:HB3	2.57	0.40
1:D:212:SER:OG	1:D:213:ASP:N	2.54	0.40
1:F:168:GLU:O	1:F:172:ARG:HG3	2.21	0.40
1:G:20:LEU:HD12	1:G:157:VAL:HB	2.03	0.40
1:B:61:ARG:HH11	1:B:61:ARG:HD2	1.71	0.40
1:B:131:LEU:HA	1:B:132:PRO:HD2	2.00	0.40
1:L:131:LEU:HD23	1:L:131:LEU:HA	1.89	0.40
1:M:161:ILE:HA	1:M:162:ALA:HA	1.77	0.40
1:P:29:TYR:CE2	1:P:109:LEU:HD21	2.57	0.40
1:D:107:LYS:NZ	1:J:103:GLN:O	2.53	0.40
1:H:74:TRP:O	1:H:111:LYS:HG3	2.21	0.40
1:H:171:LEU:HD13	1:H:204:ILE:HD13	2.02	0.40
1:I:61:ARG:NH2	1:I:128:ASP:OD2	2.54	0.40
1:I:96:LYS:HG2	1:I:99:ARG:HH21	1.86	0.40
1:K:82:GLY:O	1:K:89:PHE:HB2	2.22	0.40
1:O:52:ASN:HB3	1:O:214:VAL:HG21	2.03	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	Interatomic distance (Å)	Clash overlap (Å)
1:J:209:GLY:O	1:P:91:LYS:NZ[2_656]	2.04	0.16
1:B:105:GLN:O	1:L:107:LYS:NZ[2_556]	2.11	0.09

## 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	220/230 (96%)	214 (97%)	6 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	220/230 (96%)	211 (96%)	9 (4%)	0	100	100
1	C	220/230 (96%)	213 (97%)	6 (3%)	1 (0%)	24	16
1	D	218/230 (95%)	211 (97%)	7 (3%)	0	100	100
1	E	220/230 (96%)	213 (97%)	7 (3%)	0	100	100
1	F	218/230 (95%)	210 (96%)	8 (4%)	0	100	100
1	G	220/230 (96%)	212 (96%)	7 (3%)	1 (0%)	24	16
1	H	220/230 (96%)	210 (96%)	10 (4%)	0	100	100
1	I	220/230 (96%)	211 (96%)	9 (4%)	0	100	100
1	J	220/230 (96%)	213 (97%)	7 (3%)	0	100	100
1	K	218/230 (95%)	205 (94%)	12 (6%)	1 (0%)	24	16
1	L	218/230 (95%)	210 (96%)	8 (4%)	0	100	100
1	M	220/230 (96%)	212 (96%)	7 (3%)	1 (0%)	24	16
1	N	220/230 (96%)	211 (96%)	9 (4%)	0	100	100
1	O	220/230 (96%)	211 (96%)	9 (4%)	0	100	100
1	P	218/230 (95%)	210 (96%)	8 (4%)	0	100	100
All	All	3510/3680 (95%)	3377 (96%)	129 (4%)	4 (0%)	48	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	35	TYR
1	K	165	VAL
1	G	165	VAL
1	M	165	VAL

### 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	180/188 (96%)	177 (98%)	3 (2%)	53	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	181/188 (96%)	179 (99%)	2 (1%)	65	67
1	C	181/188 (96%)	179 (99%)	2 (1%)	65	67
1	D	179/188 (95%)	176 (98%)	3 (2%)	53	52
1	E	178/188 (95%)	175 (98%)	3 (2%)	53	52
1	F	177/188 (94%)	175 (99%)	2 (1%)	65	67
1	G	180/188 (96%)	178 (99%)	2 (1%)	65	67
1	H	181/188 (96%)	180 (99%)	1 (1%)	78	81
1	I	179/188 (95%)	174 (97%)	5 (3%)	38	32
1	J	176/188 (94%)	174 (99%)	2 (1%)	65	67
1	K	176/188 (94%)	171 (97%)	5 (3%)	38	32
1	L	179/188 (95%)	177 (99%)	2 (1%)	65	67
1	M	180/188 (96%)	177 (98%)	3 (2%)	53	52
1	N	180/188 (96%)	174 (97%)	6 (3%)	33	26
1	O	181/188 (96%)	177 (98%)	4 (2%)	45	42
1	P	174/188 (93%)	172 (99%)	2 (1%)	65	67
All	All	2862/3008 (95%)	2815 (98%)	47 (2%)	55	54

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	TYR
1	A	131	LEU
1	A	182	VAL
1	B	11	ILE
1	B	131	LEU
1	C	7	ARG
1	C	50	ILE
1	D	79	VAL
1	D	131	LEU
1	D	164	ASN
1	E	9	GLU
1	E	35	TYR
1	E	45	THR
1	F	35	TYR
1	F	182	VAL
1	G	35	TYR
1	G	131	LEU

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Mol	Chain	Res	Type
1	H	12	THR
1	I	4	LEU
1	I	11	ILE
1	I	20	LEU
1	I	35	TYR
1	I	141	ASN
1	J	35	TYR
1	J	182	VAL
1	K	35	TYR
1	K	58	THR
1	K	129	ILE
1	K	141	ASN
1	K	211	VAL
1	L	35	TYR
1	L	58	THR
1	M	58	THR
1	M	95	LEU
1	M	96	LYS
1	N	20	LEU
1	N	35	TYR
1	N	45	THR
1	N	103	GLN
1	N	123	VAL
1	N	149	ARG
1	O	54	GLN
1	O	111	LYS
1	O	123	VAL
1	O	149	ARG
1	P	149	ARG
1	P	206	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	77	GLN
1	A	125	GLN
1	A	189	HIS
1	B	27	ASN
1	B	72	ASN
1	B	197	GLN
1	C	54	GLN

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Mol	Chain	Res	Type
1	C	72	ASN
1	D	125	GLN
1	E	71	GLN
1	F	27	ASN
1	F	54	GLN
1	F	101	GLN
1	G	77	GLN
1	G	125	GLN
1	H	105	GLN
1	I	77	GLN
1	I	101	GLN
1	I	125	GLN
1	I	141	ASN
1	J	72	ASN
1	J	93	ASN
1	L	72	ASN
1	L	103	GLN
1	L	125	GLN
1	M	16	GLN
1	M	72	ASN
1	M	125	GLN
1	M	141	ASN
1	M	155	HIS
1	M	189	HIS
1	N	27	ASN
1	N	101	GLN
1	N	125	GLN
1	N	141	ASN
1	O	72	ASN
1	O	103	GLN
1	O	141	ASN
1	O	155	HIS
1	P	93	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 oligosaccharides 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	222/230 (96%)	1.16	21 (9%) 14 14	21, 27, 36, 44	0
1	B	222/230 (96%)	1.14	21 (9%) 14 14	18, 27, 36, 44	0
1	C	222/230 (96%)	1.23	26 (11%) 9 10	19, 28, 37, 53	0
1	D	220/230 (95%)	1.29	32 (14%) 6 6	19, 28, 37, 48	0
1	E	222/230 (96%)	1.40	41 (18%) 3 3	18, 31, 44, 57	0
1	F	220/230 (95%)	1.27	32 (14%) 6 6	21, 30, 40, 46	0
1	G	222/230 (96%)	1.39	37 (16%) 4 4	20, 30, 39, 48	0
1	H	222/230 (96%)	1.29	32 (14%) 6 6	19, 29, 41, 51	0
1	I	222/230 (96%)	1.10	26 (11%) 9 10	19, 27, 37, 47	0
1	J	222/230 (96%)	1.19	26 (11%) 9 10	19, 28, 36, 42	0
1	K	220/230 (95%)	1.43	47 (21%) 2 2	21, 30, 41, 46	0
1	L	220/230 (95%)	1.41	40 (18%) 3 3	21, 31, 40, 48	0
1	M	222/230 (96%)	1.50	46 (20%) 2 2	21, 34, 46, 55	0
1	N	222/230 (96%)	1.47	43 (19%) 3 3	21, 34, 49, 62	0
1	O	222/230 (96%)	1.48	48 (21%) 2 2	20, 32, 48, 61	0
1	P	220/230 (95%)	1.50	54 (24%) 2 1	21, 33, 48, 62	0
All	All	3542/3680 (96%)	1.33	572 (16%) 4 4	18, 29, 43, 62	0

All (572) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	LEU	4.8
1	N	223	PRO	4.5
1	N	43	VAL	4.4
1	K	167	VAL	4.3
1	G	82	GLY	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	196	ALA	4.3
1	A	11	ILE	4.2
1	N	30	ALA	4.2
1	L	21	ILE	4.2
1	G	211	VAL	4.2
1	I	223	PRO	4.2
1	G	70	PHE	4.1
1	C	11	ILE	4.1
1	N	199	ALA	4.1
1	C	223	PRO	4.1
1	E	3	THR	4.1
1	G	62	ALA	4.1
1	M	156	LEU	4.1
1	J	73	GLY	4.0
1	O	33	GLY	4.0
1	O	41	PHE	4.0
1	M	211	VAL	4.0
1	O	223	PRO	4.0
1	M	43	VAL	3.8
1	F	156	LEU	3.8
1	G	195	PHE	3.7
1	L	28	ALA	3.7
1	N	3	THR	3.7
1	B	131	LEU	3.6
1	M	46	THR	3.6
1	P	12	THR	3.6
1	P	182	VAL	3.5
1	O	34	GLY	3.5
1	J	223	PRO	3.5
1	M	223	PRO	3.5
1	B	62	ALA	3.5
1	E	161	ILE	3.4
1	O	123	VAL	3.4
1	M	191	ALA	3.4
1	F	221	LEU	3.4
1	K	208	PHE	3.4
1	K	221	LEU	3.4
1	L	4	LEU	3.4
1	E	223	PRO	3.4
1	K	183	VAL	3.4
1	J	6	ALA	3.4
1	M	30	ALA	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	P	41	PHE	3.4
1	D	5	THR	3.3
1	F	11	ILE	3.3
1	P	62	ALA	3.3
1	N	32	PRO	3.3
1	O	50	ILE	3.3
1	K	200	ALA	3.3
1	G	209	GLY	3.3
1	O	70	PHE	3.2
1	L	44	SER	3.2
1	M	11	ILE	3.2
1	B	223	PRO	3.2
1	D	211	VAL	3.2
1	E	182	VAL	3.2
1	M	45	THR	3.2
1	B	146	SER	3.2
1	J	70	PHE	3.2
1	K	175	PHE	3.2
1	C	204	ILE	3.2
1	C	45	THR	3.2
1	N	36	LEU	3.2
1	O	42	ASP	3.2
1	O	45	THR	3.1
1	D	89	PHE	3.1
1	E	195	PHE	3.1
1	O	217	PHE	3.1
1	H	6	ALA	3.1
1	N	196	ALA	3.1
1	G	53	ILE	3.1
1	M	67	ILE	3.1
1	L	183	VAL	3.1
1	G	158	PHE	3.1
1	K	207	PHE	3.1
1	P	195	PHE	3.1
1	N	46	THR	3.1
1	O	11	ILE	3.1
1	K	21	ILE	3.0
1	P	30	ALA	3.0
1	L	221	LEU	3.0
1	M	221	LEU	3.0
1	P	38	LEU	3.0
1	C	43	VAL	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	208	PHE	3.0
1	G	44	SER	3.0
1	K	41	PHE	3.0
1	L	70	PHE	3.0
1	I	94	ALA	3.0
1	C	221	LEU	3.0
1	M	38	LEU	3.0
1	P	66	LEU	3.0
1	P	108	LEU	3.0
1	K	182	VAL	2.9
1	N	167	VAL	2.9
1	F	216	THR	2.9
1	A	223	PRO	2.9
1	H	195	PHE	2.9
1	B	11	ILE	2.9
1	B	161	ILE	2.9
1	O	68	ILE	2.9
1	D	38	LEU	2.9
1	H	103	GLN	2.9
1	F	154	ARG	2.9
1	K	219	ASP	2.9
1	E	43	VAL	2.9
1	H	211	VAL	2.9
1	M	119	VAL	2.9
1	K	46	THR	2.9
1	K	82	GLY	2.9
1	P	46	THR	2.9
1	B	182	VAL	2.9
1	N	182	VAL	2.9
1	E	45	THR	2.9
1	L	126	PRO	2.9
1	L	13	PHE	2.9
1	M	158	PHE	2.9
1	E	6	ALA	2.9
1	D	131	LEU	2.9
1	E	104	LEU	2.9
1	O	122	LEU	2.9
1	D	82	GLY	2.9
1	J	59	ALA	2.8
1	J	180	PHE	2.8
1	L	195	PHE	2.8
1	M	94	ALA	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	M	50	ILE	2.8
1	O	67	ILE	2.8
1	N	152	GLY	2.8
1	N	45	THR	2.8
1	O	105	GLN	2.8
1	C	81	ALA	2.8
1	D	70	PHE	2.8
1	N	44	SER	2.8
1	G	104	LEU	2.8
1	O	108	LEU	2.8
1	M	3	THR	2.8
1	C	165	VAL	2.8
1	D	182	VAL	2.8
1	E	211	VAL	2.8
1	N	211	VAL	2.8
1	M	35	TYR	2.8
1	K	169	SER	2.8
1	O	220	ALA	2.8
1	J	158	PHE	2.8
1	B	95	LEU	2.8
1	H	104	LEU	2.8
1	C	147	ILE	2.8
1	G	182	VAL	2.8
1	L	59	ALA	2.7
1	E	41	PHE	2.7
1	H	70	PHE	2.7
1	J	21	ILE	2.7
1	G	167	VAL	2.7
1	I	167	VAL	2.7
1	A	6	ALA	2.7
1	O	35	TYR	2.7
1	E	85	GLY	2.7
1	G	218	CYS	2.7
1	K	12	THR	2.7
1	M	5	THR	2.7
1	G	131	LEU	2.7
1	J	68	ILE	2.7
1	B	79	VAL	2.7
1	K	43	VAL	2.7
1	P	119	VAL	2.7
1	E	220	ALA	2.7
1	L	187	ALA	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	176	PHE	2.7
1	D	84	PRO	2.7
1	E	44	SER	2.7
1	E	212	SER	2.7
1	H	102	PRO	2.7
1	P	44	SER	2.7
1	E	153	ILE	2.7
1	N	62	ALA	2.6
1	C	195	PHE	2.6
1	I	139	PHE	2.6
1	P	45	THR	2.6
1	E	108	LEU	2.6
1	P	161	ILE	2.6
1	D	209	GLY	2.6
1	H	40	GLY	2.6
1	P	22	VAL	2.6
1	G	58	THR	2.6
1	K	195	PHE	2.6
1	B	132	PRO	2.6
1	E	191	ALA	2.6
1	F	30	ALA	2.6
1	K	59	ALA	2.6
1	K	214	VAL	2.6
1	A	3	THR	2.6
1	F	2	THR	2.6
1	G	169	SER	2.6
1	O	136	TYR	2.6
1	G	15	PRO	2.6
1	C	70	PHE	2.6
1	P	208	PHE	2.6
1	I	95	LEU	2.6
1	P	154	ARG	2.6
1	G	77	GLN	2.6
1	E	11	ILE	2.6
1	L	11	ILE	2.6
1	L	67	ILE	2.6
1	N	11	ILE	2.6
1	P	34	GLY	2.6
1	H	100	LYS	2.6
1	E	167	VAL	2.6
1	G	165	VAL	2.6
1	H	130	VAL	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	M	165	VAL	2.6
1	D	154	ARG	2.5
1	N	78	TYR	2.5
1	L	176	PHE	2.5
1	M	195	PHE	2.5
1	P	42	ASP	2.5
1	E	210	TRP	2.5
1	K	83	GLY	2.5
1	K	81	ALA	2.5
1	I	222	SER	2.5
1	G	183	VAL	2.5
1	I	182	VAL	2.5
1	N	31	THR	2.5
1	D	208	PHE	2.5
1	E	95	LEU	2.5
1	O	38	LEU	2.5
1	F	155	HIS	2.5
1	M	44	SER	2.5
1	B	28	ALA	2.5
1	C	220	ALA	2.5
1	D	62	ALA	2.5
1	F	10	ALA	2.5
1	F	39	ALA	2.5
1	A	79	VAL	2.5
1	C	46	THR	2.5
1	K	173	ASP	2.5
1	N	29	TYR	2.5
1	P	35	TYR	2.5
1	B	148	LEU	2.5
1	D	195	PHE	2.5
1	F	41	PHE	2.5
1	F	122	LEU	2.5
1	I	70	PHE	2.5
1	K	139	PHE	2.5
1	L	175	PHE	2.5
1	N	41	PHE	2.5
1	O	109	LEU	2.5
1	F	204	ILE	2.5
1	O	92	SER	2.5
1	P	11	ILE	2.5
1	P	53	ILE	2.5
1	F	57	VAL	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	119	VAL	2.5
1	N	119	VAL	2.5
1	N	194	LYS	2.5
1	J	152	GLY	2.4
1	K	209	GLY	2.4
1	E	78	TYR	2.4
1	H	95	LEU	2.4
1	K	13	PHE	2.4
1	M	139	PHE	2.4
1	P	67	ILE	2.4
1	D	59	ALA	2.4
1	G	45	THR	2.4
1	G	59	ALA	2.4
1	L	200	ALA	2.4
1	P	63	ALA	2.4
1	L	43	VAL	2.4
1	P	43	VAL	2.4
1	E	47	ARG	2.4
1	J	131	LEU	2.4
1	J	169	SER	2.4
1	K	136	TYR	2.4
1	K	177	LEU	2.4
1	M	29	TYR	2.4
1	H	207	PHE	2.4
1	I	195	PHE	2.4
1	J	129	ILE	2.4
1	O	21	ILE	2.4
1	O	129	ILE	2.4
1	E	31	THR	2.4
1	P	114	TRP	2.4
1	M	93	ASN	2.4
1	H	174	GLY	2.4
1	P	33	GLY	2.4
1	D	35	TYR	2.4
1	A	139	PHE	2.4
1	E	180	PHE	2.4
1	F	195	PHE	2.4
1	C	3	THR	2.4
1	E	147	ILE	2.4
1	G	68	ILE	2.4
1	G	204	ILE	2.4
1	K	63	ALA	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	223	PRO	2.4
1	O	32	PRO	2.4
1	F	43	VAL	2.4
1	G	43	VAL	2.4
1	G	57	VAL	2.4
1	I	123	VAL	2.4
1	B	222	SER	2.4
1	F	104	LEU	2.3
1	N	109	LEU	2.3
1	C	179	TYR	2.3
1	D	158	PHE	2.3
1	H	175	PHE	2.3
1	L	208	PHE	2.3
1	M	180	PHE	2.3
1	N	195	PHE	2.3
1	N	208	PHE	2.3
1	O	101	GLN	2.3
1	F	161	ILE	2.3
1	K	11	ILE	2.3
1	N	162	ALA	2.3
1	E	32	PRO	2.3
1	K	57	VAL	2.3
1	L	214	VAL	2.3
1	H	42	ASP	2.3
1	B	210	TRP	2.3
1	O	114	TRP	2.3
1	I	177	LEU	2.3
1	O	36	LEU	2.3
1	O	95	LEU	2.3
1	L	35	TYR	2.3
1	M	12	THR	2.3
1	M	163	THR	2.3
1	D	41	PHE	2.3
1	I	158	PHE	2.3
1	J	139	PHE	2.3
1	L	41	PHE	2.3
1	M	202	PHE	2.3
1	N	35	TYR	2.3
1	B	30	ALA	2.3
1	G	196	ALA	2.3
1	I	28	ALA	2.3
1	P	200	ALA	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	N	21	ILE	2.3
1	O	15	PRO	2.3
1	O	193	PRO	2.3
1	D	106	GLY	2.3
1	O	181	GLY	2.3
1	D	166	CYS	2.3
1	K	131	LEU	2.3
1	K	45	THR	2.3
1	P	97	THR	2.3
1	P	89	PHE	2.3
1	B	162	ALA	2.3
1	D	162	ALA	2.3
1	H	39	ALA	2.3
1	H	82	GLY	2.3
1	K	50	ILE	2.3
1	K	68	ILE	2.3
1	A	43	VAL	2.3
1	J	183	VAL	2.3
1	H	218	CYS	2.3
1	P	155	HIS	2.3
1	A	163	THR	2.3
1	E	12	THR	2.3
1	F	95	LEU	2.3
1	K	5	THR	2.3
1	M	36	LEU	2.3
1	O	131	LEU	2.3
1	P	95	LEU	2.3
1	C	207	PHE	2.2
1	E	215	GLU	2.2
1	K	60	ALA	2.2
1	P	13	PHE	2.2
1	P	73	GLY	2.2
1	D	68	ILE	2.2
1	H	21	ILE	2.2
1	G	16	GLN	2.2
1	K	211	VAL	2.2
1	F	5	THR	2.2
1	H	3	THR	2.2
1	L	156	LEU	2.2
1	O	20	LEU	2.2
1	G	126	PRO	2.2
1	M	193	PRO	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	6	ALA	2.2
1	D	28	ALA	2.2
1	F	199	ALA	2.2
1	F	220	ALA	2.2
1	L	56	ALA	2.2
1	E	29	TYR	2.2
1	F	158	PHE	2.2
1	H	35	TYR	2.2
1	M	70	PHE	2.2
1	I	153	ILE	2.2
1	N	153	ILE	2.2
1	C	79	VAL	2.2
1	J	214	VAL	2.2
1	K	49	VAL	2.2
1	M	49	VAL	2.2
1	P	165	VAL	2.2
1	F	46	THR	2.2
1	K	163	THR	2.2
1	L	5	THR	2.2
1	L	58	THR	2.2
1	C	148	LEU	2.2
1	D	36	LEU	2.2
1	J	221	LEU	2.2
1	K	36	LEU	2.2
1	M	144	LEU	2.2
1	P	131	LEU	2.2
1	K	64	GLY	2.2
1	P	82	GLY	2.2
1	B	59	ALA	2.2
1	C	56	ALA	2.2
1	K	94	ALA	2.2
1	M	62	ALA	2.2
1	E	13	PHE	2.2
1	I	175	PHE	2.2
1	N	202	PHE	2.2
1	A	21	ILE	2.2
1	J	11	ILE	2.2
1	J	153	ILE	2.2
1	L	189	HIS	2.2
1	L	203	ASN	2.2
1	N	155	HIS	2.2
1	B	211	VAL	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	167	VAL	2.2
1	I	79	VAL	2.2
1	J	123	VAL	2.2
1	L	79	VAL	2.2
1	O	43	VAL	2.2
1	P	16	GLN	2.2
1	E	42	ASP	2.2
1	B	4	LEU	2.2
1	E	36	LEU	2.2
1	G	144	LEU	2.2
1	L	104	LEU	2.2
1	L	171	LEU	2.2
1	K	48	PRO	2.2
1	P	102	PRO	2.2
1	E	39	ALA	2.2
1	G	220	ALA	2.2
1	M	196	ALA	2.2
1	O	56	ALA	2.2
1	O	63	ALA	2.2
1	N	189	HIS	2.1
1	A	158	PHE	2.1
1	H	139	PHE	2.1
1	L	217	PHE	2.1
1	M	140	PHE	2.1
1	E	35	TYR	2.1
1	G	67	ILE	2.1
1	H	147	ILE	2.1
1	M	16	GLN	2.1
1	E	46	THR	2.1
1	E	188	THR	2.1
1	F	182	VAL	2.1
1	A	222	SER	2.1
1	G	181	GLY	2.1
1	I	4	LEU	2.1
1	I	148	LEU	2.1
1	I	221	LEU	2.1
1	P	36	LEU	2.1
1	A	19	ALA	2.1
1	E	199	ALA	2.1
1	K	30	ALA	2.1
1	M	39	ALA	2.1
1	O	28	ALA	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	P	28	ALA	2.1
1	C	139	PHE	2.1
1	L	158	PHE	2.1
1	M	175	PHE	2.1
1	N	70	PHE	2.1
1	P	101	GLN	2.1
1	B	35	TYR	2.1
1	L	147	ILE	2.1
1	F	45	THR	2.1
1	I	163	THR	2.1
1	K	210	TRP	2.1
1	L	206	THR	2.1
1	N	5	THR	2.1
1	A	57	VAL	2.1
1	A	138	GLY	2.1
1	D	49	VAL	2.1
1	N	127	GLY	2.1
1	P	83	GLY	2.1
1	H	36	LEU	2.1
1	I	122	LEU	2.1
1	L	95	LEU	2.1
1	N	171	LEU	2.1
1	O	102	PRO	2.1
1	E	62	ALA	2.1
1	F	6	ALA	2.1
1	K	51	ALA	2.1
1	O	6	ALA	2.1
1	O	62	ALA	2.1
1	J	207	PHE	2.1
1	J	208	PHE	2.1
1	M	89	PHE	2.1
1	A	161	ILE	2.1
1	F	186	ASP	2.1
1	H	14	ASP	2.1
1	H	129	ILE	2.1
1	I	11	ILE	2.1
1	N	53	ILE	2.1
1	N	136	TYR	2.1
1	P	113	SER	2.1
1	N	12	THR	2.1
1	O	5	THR	2.1
1	H	83	GLY	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	L	85	GLY	2.1
1	M	112	GLY	2.1
1	C	189	HIS	2.1
1	D	43	VAL	2.1
1	J	130	VAL	2.1
1	M	210	TRP	2.1
1	O	214	VAL	2.1
1	P	49	VAL	2.1
1	A	15	PRO	2.1
1	O	124	PRO	2.1
1	A	108	LEU	2.1
1	D	4	LEU	2.1
1	J	184	LEU	2.1
1	L	66	LEU	2.1
1	P	109	LEU	2.1
1	G	51	ALA	2.1
1	H	220	ALA	2.1
1	I	200	ALA	2.1
1	A	219	ASP	2.1
1	C	53	ILE	2.0
1	F	21	ILE	2.0
1	I	217	PHE	2.0
1	N	217	PHE	2.0
1	E	179	TYR	2.0
1	F	35	TYR	2.0
1	M	136	TYR	2.0
1	L	73	GLY	2.0
1	N	112	GLY	2.0
1	P	64	GLY	2.0
1	P	127	GLY	2.0
1	B	43	VAL	2.0
1	H	43	VAL	2.0
1	N	165	VAL	2.0
1	A	66	LEU	2.0
1	H	210	TRP	2.0
1	C	62	ALA	2.0
1	D	200	ALA	2.0
1	P	99	ARG	2.0
1	P	187	ALA	2.0
1	I	198	LYS	2.0
1	O	65	MET	2.0
1	A	208	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	13	PHE	2.0
1	M	207	PHE	2.0
1	O	176	PHE	2.0
1	P	129	ILE	2.0
1	P	139	PHE	2.0
1	C	82	GLY	2.0
1	H	209	GLY	2.0
1	O	3	THR	2.0
1	O	142	THR	2.0
1	P	3	THR	2.0
1	K	72	ASN	2.0
1	H	124	PRO	2.0
1	L	48	PRO	2.0
1	P	32	PRO	2.0
1	D	79	VAL	2.0
1	F	119	VAL	2.0
1	G	79	VAL	2.0
1	I	43	VAL	2.0
1	J	43	VAL	2.0
1	J	182	VAL	2.0
1	M	57	VAL	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 oligosaccharides 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.