



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:48 PM GMT

PDB ID : 4W6R  
Title : Crystal Structure of Full-Length Split GFP Mutant D102C Disulfide Dimer,  
P 1 Space Group  
Authors : Leibly, D.J.; Waldo, G.S.; Yeates, T.O.  
Deposited on : 2014-08-20  
Resolution : 3.47 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

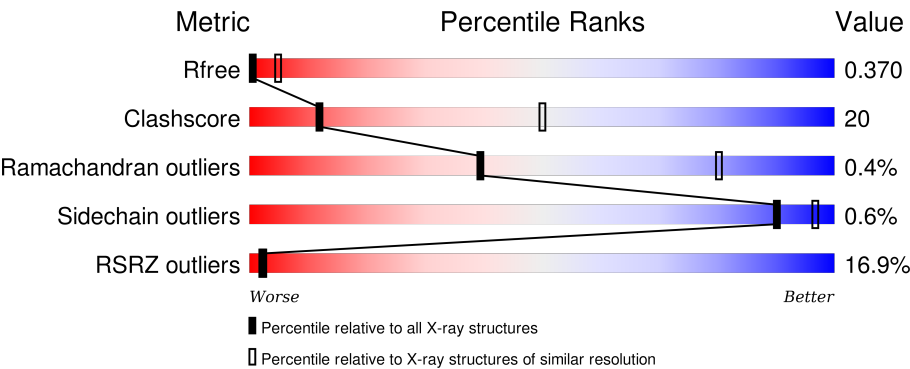
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.47 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 <sub>free</sub>	91344	1173 (3.60-3.36)
Clashscore	102246	1010 (3.58-3.38)
Ramachandran outliers	100387	1245 (3.60-3.36)
Sidechain outliers	100360	1246 (3.60-3.36)
RSRZ outliers	91569	1180 (3.60-3.36)

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

Mol	Chain	Length	Quality of chain
1	A	234	<div><div>14%</div><div><div></div><div>59%</div><div>31%</div><div>• 8%</div></div></div>
1	B	234	<div><div>11%</div><div><div></div><div>58%</div><div>29%</div><div>• 12%</div></div></div>
1	C	234	<div><div>15%</div><div><div></div><div>59%</div><div>29%</div><div>12%</div></div></div>
1	D	234	<div><div>9%</div><div><div></div><div>53%</div><div>28%</div><div>• 17%</div></div></div>
1	E	234	<div><div>10%</div><div><div></div><div>66%</div><div>23%</div><div>11%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	234	
1	G	234	
1	H	234	
1	I	234	
1	J	234	
1	K	234	
1	L	234	
1	M	234	
1	N	234	
1	O	234	
1	P	234	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25002 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.

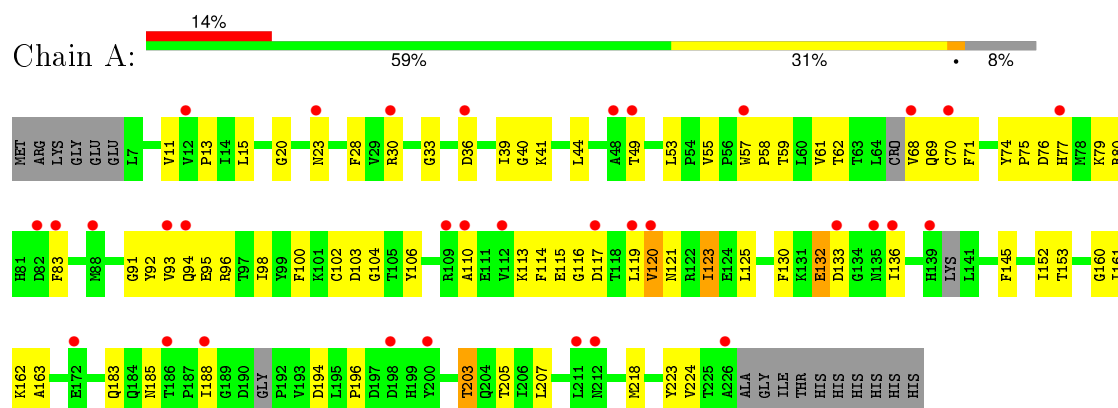
- Molecule 1 is a protein called fluorescent protein D102C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1721	1098	291	327	5			
1	B	205	Total	C	N	O	S	0	0	0
			1649	1052	280	313	4			
1	C	207	Total	C	N	O	S	0	0	0
			1643	1052	277	309	5			
1	D	194	Total	C	N	O	S	0	0	0
			1552	993	261	293	5			
1	E	208	Total	C	N	O	S	0	0	0
			1661	1059	280	317	5			
1	F	201	Total	C	N	O	S	0	0	0
			1600	1020	270	307	3			
1	G	188	Total	C	N	O	S	0	0	0
			1497	949	262	282	4			
1	H	191	Total	C	N	O	S	0	0	0
			1537	980	264	289	4			
1	I	209	Total	C	N	O	S	0	0	0
			1671	1065	285	316	5			
1	J	184	Total	C	N	O	S	0	0	0
			1459	931	247	278	3			
1	K	175	Total	C	N	O	S	0	0	0
			1391	896	229	263	3			
1	L	197	Total	C	N	O	S	0	0	0
			1573	1002	269	298	4			
1	M	168	Total	C	N	O	S	0	0	0
			1352	864	233	251	4			
1	N	174	Total	C	N	O	S	0	0	0
			1387	876	235	273	3			
1	O	213	Total	C	N	O	S	0	0	0
			1677	1065	286	322	4			
1	P	204	Total	C	N	O	S	0	0	0
			1632	1038	281	308	5			

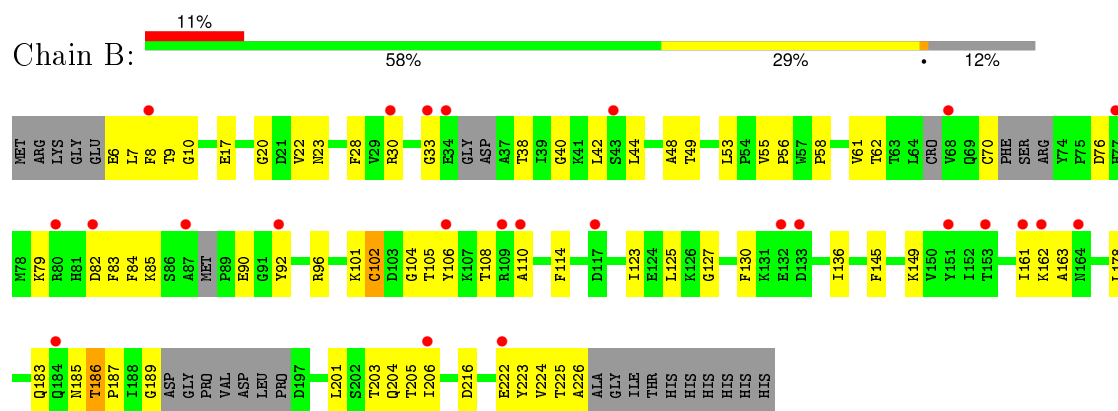
### 3 Residue-property plots

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

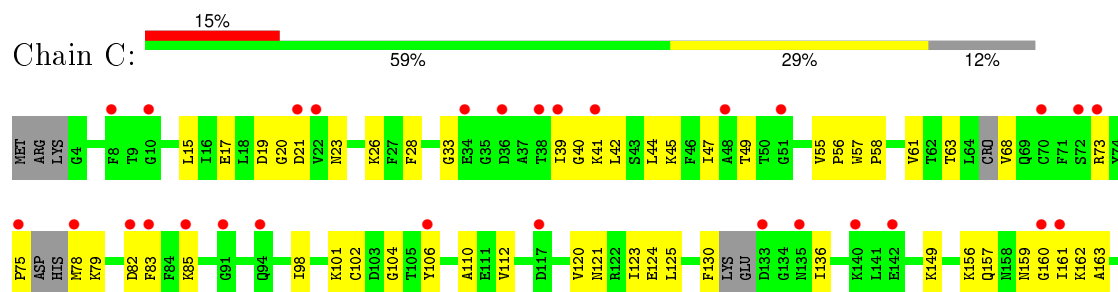
#### • Molecule 1: fluorescent protein D102C

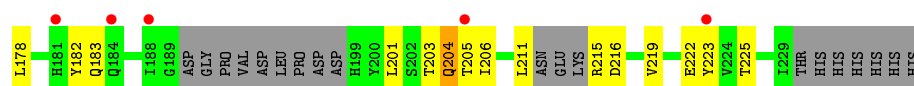


#### • Molecule 1: fluorescent protein D102C



#### • Molecule 1: fluorescent protein D102C

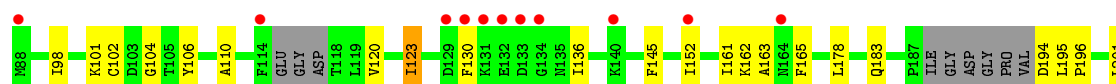




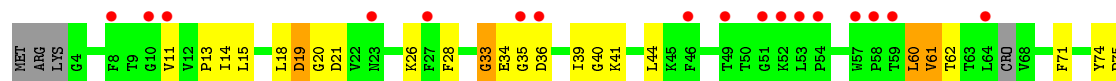
• Molecule 1: fluorescent protein D102C



• Molecule 1: fluorescent protein D102C



• Molecule 1: fluorescent protein D102C

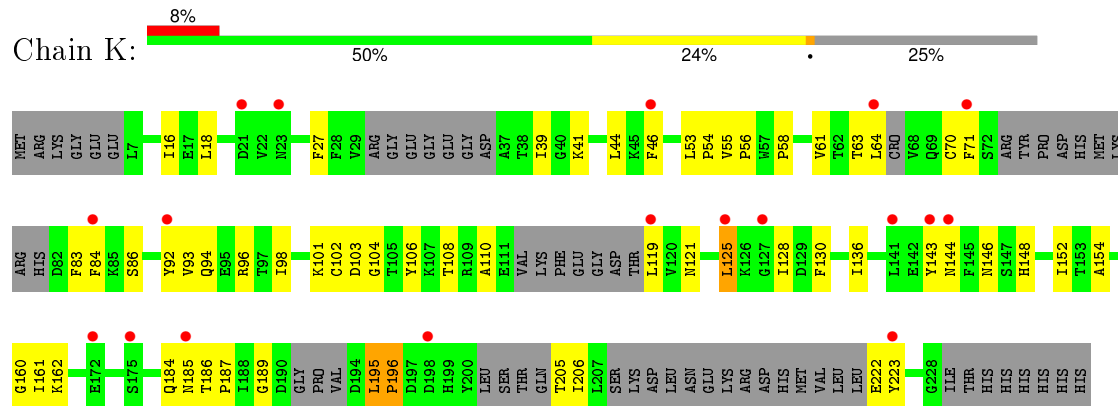


• Molecule 1: fluorescent protein D102C

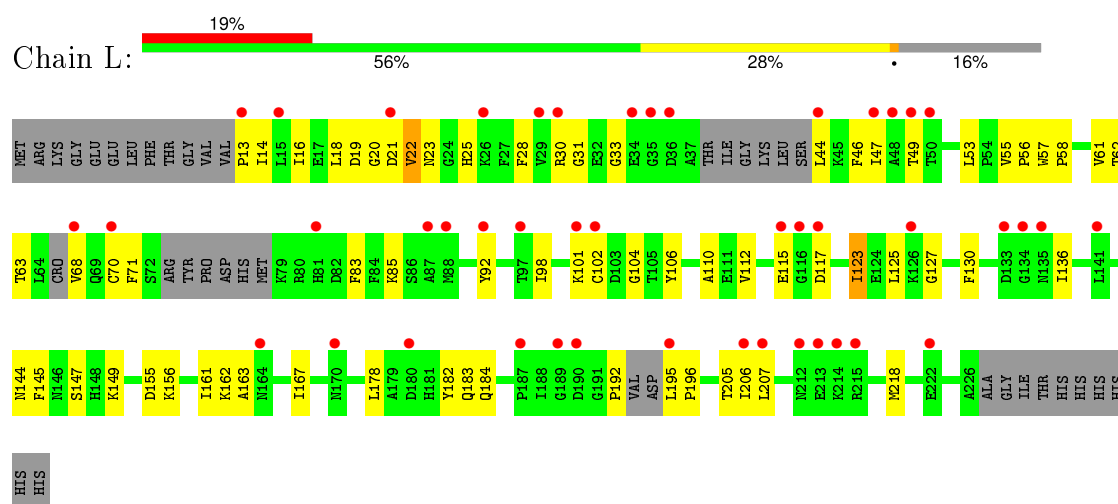




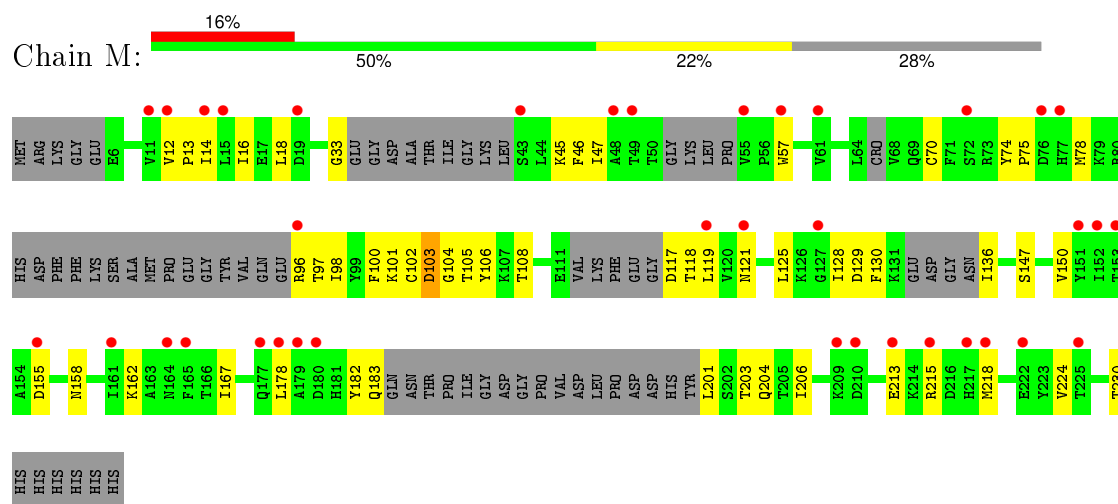
- Molecule 1: fluorescent protein D102C



- Molecule 1: fluorescent protein D102C



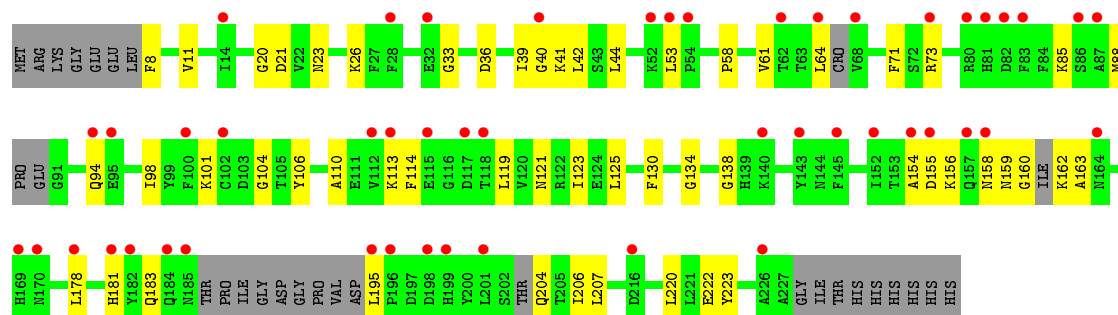
- Molecule 1: fluorescent protein D102C



- Molecule 1: fluorescent protein D102C







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.42Å 92.56Å 124.53Å 94.94° 96.17° 102.25°	Depositor
Resolution (Å)	89.88 – 3.47 89.88 – 3.47	Depositor EDS
% Data completeness (in resolution range)	89.4 (89.88-3.47) 83.9 (89.88-3.47)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 3.49Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1555)	Depositor
R, $R_{free}$	0.307 , 0.357 0.326 , 0.370	Depositor DCC
$R_{free}$ test set	4609 reflections (10.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	101.2	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 40.0	EDS
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 46082 reflections	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	25002	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.38	0/1758	0.82	3/2375 (0.1%)
1	B	0.34	0/1681	0.77	1/2265 (0.0%)
1	C	0.33	0/1675	0.80	1/2258 (0.0%)
1	D	0.38	0/1579	0.89	3/2121 (0.1%)
1	E	0.33	0/1694	0.78	4/2287 (0.2%)
1	F	0.36	0/1631	0.81	2/2199 (0.1%)
1	G	0.35	0/1524	0.82	0/2053
1	H	0.34	0/1567	0.82	4/2112 (0.2%)
1	I	0.35	0/1705	0.84	4/2302 (0.2%)
1	J	0.35	0/1483	0.82	0/1998
1	K	0.41	0/1417	0.81	2/1912 (0.1%)
1	L	0.33	0/1605	0.76	1/2164 (0.0%)
1	M	0.31	0/1373	0.84	0/1847
1	N	0.33	0/1410	0.86	3/1899 (0.2%)
1	O	0.40	0/1712	0.81	1/2314 (0.0%)
1	P	0.33	0/1663	0.79	1/2239 (0.0%)
All	All	0.35	0/25477	0.81	30/34345 (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	D	0	1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	15	LEU	CA-CB-CG	7.89	133.45	115.30
1	D	125	LEU	CA-CB-CG	7.63	132.85	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	220	LEU	CA-CB-CG	7.57	132.72	115.30
1	A	203	THR	N-CA-C	7.12	130.21	111.00
1	H	203	THR	N-CA-C	6.86	129.52	111.00
1	K	195	LEU	C-N-CD	-6.75	105.75	120.60
1	N	136	ILE	CG1-CB-CG2	-6.53	97.05	111.40
1	E	26	LYS	N-CA-C	6.47	128.46	111.00
1	N	125	LEU	CA-CB-CG	6.41	130.04	115.30
1	F	33	GLY	N-CA-C	-6.06	97.95	113.10
1	I	195	LEU	C-N-CD	-5.87	107.69	120.60
1	I	20	GLY	N-CA-C	5.83	127.66	113.10
1	L	18	LEU	CA-CB-CG	5.79	128.61	115.30
1	P	162	LYS	N-CA-CB	-5.73	100.29	110.60
1	E	220	LEU	CA-CB-CG	5.66	128.32	115.30
1	H	117	ASP	CB-CA-C	-5.51	99.38	110.40
1	A	69	GLN	O-C-N	5.50	131.51	122.70
1	H	204	GLN	N-CA-C	5.50	125.85	111.00
1	I	120	VAL	CB-CA-C	-5.29	101.34	111.40
1	C	211	LEU	N-CA-C	5.29	125.28	111.00
1	E	195	LEU	C-N-CD	-5.27	109.01	120.60
1	K	125	LEU	CA-CB-CG	5.26	127.40	115.30
1	D	142	GLU	N-CA-C	5.22	125.10	111.00
1	I	82	ASP	CB-CA-C	5.21	120.83	110.40
1	O	194	ASP	N-CA-C	-5.17	97.03	111.00
1	D	133	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	102	CYS	CA-CB-SG	5.17	123.30	114.00
1	A	132	GLU	N-CA-C	-5.14	97.12	111.00
1	F	60	LEU	N-CA-C	-5.10	97.24	111.00
1	E	165	PHE	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	111	GLU	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	1721	0	1680	100	0
1	B	1649	0	1615	84	0
1	C	1643	0	1611	59	1
1	D	1552	0	1511	61	1
1	E	1661	0	1623	38	0
1	F	1600	0	1557	47	1
1	G	1497	0	1460	86	0
1	H	1537	0	1487	56	0
1	I	1671	0	1633	95	0
1	J	1459	0	1431	58	1
1	K	1391	0	1359	51	0
1	L	1573	0	1532	60	0
1	M	1352	0	1339	46	0
1	N	1387	0	1351	40	0
1	O	1677	0	1616	102	0
1	P	1632	0	1586	42	0
All	All	25002	0	24391	986	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 20.

All (986) 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:I:28:PHE:CE2	1:I:30:ARG:HG3	1.44	1.51
1:A:152:ILE:O	1:A:153:THR:HG22	1.19	1.34
1:D:15:LEU:O	1:D:15:LEU:HD12	1.31	1.30
1:B:106:TYR:CE1	1:B:130:PHE:CE1	2.24	1.24
1:G:44:LEU:O	1:G:219:VAL:HG13	1.36	1.24
1:E:28:PHE:CE2	1:E:30:ARG:HG3	1.71	1.24
1:I:42:LEU:HD21	1:I:71:PHE:CB	1.69	1.23
1:O:104:GLY:HA3	1:O:130:PHE:CD1	1.74	1.20
1:O:185:ASN:O	1:O:186:THR:HG22	1.00	1.16
1:O:185:ASN:O	1:O:186:THR:CG2	1.92	1.16
1:O:74:TYR:CD2	1:O:82:ASP:HB2	1.80	1.16
1:G:7:LEU:CG	1:G:8:PHE:H	1.57	1.15
1:I:42:LEU:HD21	1:I:71:PHE:CG	1.81	1.15
1:A:102:CYS:SG	1:N:102:CYS:HB3	1.88	1.13
1:H:203:THR:CG2	1:H:224:VAL:HG13	1.78	1.13
1:G:7:LEU:HG	1:G:8:PHE:N	1.59	1.12
1:B:106:TYR:CE1	1:B:130:PHE:CZ	2.37	1.12
1:B:9:THR:HG23	1:B:10:GLY:H	1.02	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:GLU:HG3	1:B:7:LEU:H	0.97	1.09
1:I:28:PHE:CE2	1:I:30:ARG:CG	2.36	1.08
1:I:43:SER:HB3	1:I:221:LEU:HD23	1.21	1.08
1:E:86:SER:HG	1:E:194:ASP:N	1.51	1.08
1:A:203:THR:HG22	1:A:224:VAL:HG13	1.15	1.08
1:H:203:THR:HG22	1:H:224:VAL:HG13	1.33	1.06
1:F:33:GLY:HA3	1:F:44:LEU:HD23	1.35	1.06
1:E:28:PHE:HE2	1:E:30:ARG:HG3	1.02	1.06
1:H:203:THR:HG22	1:H:224:VAL:CG1	1.88	1.03
1:I:28:PHE:CZ	1:I:30:ARG:HG3	1.93	1.02
1:A:152:ILE:O	1:A:153:THR:CG2	2.08	1.01
1:G:61:VAL:CG1	1:G:220:LEU:HD11	1.91	1.00
1:A:15:LEU:HB2	1:A:120:VAL:HG22	1.40	1.00
1:G:7:LEU:HG	1:G:8:PHE:H	0.87	1.00
1:A:102:CYS:SG	1:N:102:CYS:CB	2.49	1.00
1:A:119:LEU:O	1:A:120:VAL:HG23	1.62	1.00
1:I:43:SER:CB	1:I:221:LEU:HD23	1.91	1.00
1:A:203:THR:CG2	1:A:224:VAL:HG13	1.91	1.00
1:O:74:TYR:CE2	1:O:82:ASP:CG	2.34	0.99
1:N:103:ASP:OD2	1:N:136:ILE:HD13	1.62	0.99
1:A:203:THR:HG22	1:A:224:VAL:CG1	1.93	0.98
1:A:93:VAL:HG23	1:A:188:ILE:HG13	1.44	0.98
1:J:43:SER:HB2	1:J:220:LEU:O	1.63	0.98
1:A:94:GLN:HG3	1:A:185:ASN:OD1	1.64	0.97
1:G:61:VAL:HG13	1:G:220:LEU:HD11	1.46	0.97
1:G:207:LEU:HD22	1:G:219:VAL:O	1.64	0.96
1:O:104:GLY:CA	1:O:130:PHE:CD1	2.47	0.96
1:B:6:GLU:HG3	1:B:7:LEU:N	1.74	0.96
1:G:61:VAL:HG13	1:G:220:LEU:CD1	1.96	0.96
1:H:203:THR:HG22	1:H:224:VAL:HG22	1.49	0.95
1:B:9:THR:HG23	1:B:10:GLY:N	1.80	0.95
1:I:28:PHE:HD2	1:I:49:THR:OG1	1.50	0.95
1:O:104:GLY:HA3	1:O:130:PHE:CG	2.02	0.95
1:I:103:ASP:OD2	1:I:136:ILE:HD13	1.67	0.94
1:B:22:VAL:HG11	1:B:106:TYR:OH	1.67	0.94
1:O:74:TYR:CD2	1:O:82:ASP:CB	2.50	0.94
1:I:135:ASN:C	1:I:136:ILE:HD12	1.87	0.94
1:G:207:LEU:HD13	1:G:218:MET:CE	1.99	0.93
1:N:33:GLY:HA3	1:N:44:LEU:HD23	1.48	0.93
1:H:203:THR:HG22	1:H:224:VAL:CG2	1.99	0.92
1:P:88:MET:HE1	1:P:113:LYS:HA	1.48	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:33:GLY:HA3	1:I:44:LEU:HD23	1.52	0.91
1:B:106:TYR:HE1	1:B:130:PHE:CE1	1.88	0.91
1:B:9:THR:CG2	1:B:10:GLY:H	1.82	0.90
1:I:28:PHE:HE2	1:I:30:ARG:CG	1.79	0.90
1:G:61:VAL:HG22	1:G:220:LEU:CD1	2.01	0.90
1:A:28:PHE:HD2	1:A:49:THR:HG1	1.12	0.90
1:G:205:THR:HG23	1:G:220:LEU:HD23	1.50	0.90
1:G:103:ASP:OD1	1:G:104:GLY:N	2.04	0.90
1:D:15:LEU:O	1:D:15:LEU:CD1	2.20	0.89
1:F:33:GLY:CA	1:F:44:LEU:HD23	2.02	0.89
1:O:104:GLY:O	1:O:130:PHE:CE1	2.26	0.89
1:C:203:THR:O	1:C:204:GLN:HG3	1.73	0.89
1:A:15:LEU:O	1:A:121:ASN:N	2.05	0.88
1:C:47:ILE:HD13	1:C:215:ARG:NH2	1.88	0.88
1:M:128:ILE:HG22	1:M:129:ASP:CG	1.94	0.88
1:L:23:ASN:HD21	1:L:130:PHE:N	1.71	0.88
1:K:83:PHE:CE2	1:K:161:ILE:HG13	2.09	0.88
1:A:100:PHE:HB2	1:A:103:ASP:HB3	1.57	0.87
1:D:104:GLY:HA3	1:D:130:PHE:HD1	1.37	0.86
1:H:13:PRO:HD2	1:H:117:ASP:O	1.75	0.86
1:G:199:HIS:HB2	1:G:228:GLY:HA2	1.56	0.86
1:F:20:GLY:HA2	1:F:125:LEU:O	1.76	0.85
1:I:28:PHE:CZ	1:I:30:ARG:CG	2.58	0.85
1:E:163:ALA:HB3	1:E:183:GLN:HB3	1.56	0.85
1:A:15:LEU:O	1:A:120:VAL:HA	1.77	0.85
1:I:42:LEU:HD21	1:I:71:PHE:HB3	1.56	0.85
1:C:110:ALA:HB2	1:C:123:ILE:HG12	1.59	0.85
1:O:74:TYR:HE2	1:O:82:ASP:CG	1.78	0.85
1:B:106:TYR:CE1	1:B:127:GLY:HA3	2.12	0.84
1:B:22:VAL:CG1	1:B:106:TYR:OH	2.24	0.84
1:D:104:GLY:HA3	1:D:130:PHE:CD1	2.11	0.84
1:G:205:THR:HG23	1:G:220:LEU:CD2	2.07	0.83
1:A:100:PHE:CB	1:A:103:ASP:HB3	2.08	0.83
1:P:88:MET:CE	1:P:113:LYS:HA	2.08	0.83
1:B:6:GLU:CG	1:B:7:LEU:H	1.85	0.83
1:J:43:SER:CB	1:J:220:LEU:O	2.27	0.83
1:G:207:LEU:HD13	1:G:218:MET:HE2	1.60	0.83
1:I:135:ASN:HB2	1:I:136:ILE:HD12	1.61	0.82
1:G:61:VAL:HG22	1:G:220:LEU:HD12	1.60	0.82
1:O:127:GLY:CA	1:O:130:PHE:HE2	1.92	0.82
1:G:44:LEU:O	1:G:219:VAL:CG1	2.26	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:42:LEU:CD2	1:I:71:PHE:CG	2.62	0.82
1:O:106:TYR:CE1	1:O:130:PHE:CZ	2.68	0.82
1:D:109:ARG:O	1:D:123:ILE:HG23	1.79	0.81
1:I:28:PHE:HE2	1:I:30:ARG:HG3	1.01	0.81
1:I:135:ASN:HB2	1:I:136:ILE:CD1	2.11	0.81
1:G:205:THR:HG22	1:G:206:ILE:N	1.96	0.81
1:O:104:GLY:C	1:O:130:PHE:CE1	2.55	0.80
1:A:68:VAL:CG2	1:A:71:PHE:CD2	2.65	0.79
1:G:208:SER:HB2	1:G:219:VAL:HB	1.64	0.79
1:O:127:GLY:HA3	1:O:130:PHE:HE2	1.47	0.79
1:K:162:LYS:HG2	1:K:184:GLN:HG2	1.64	0.79
1:F:18:LEU:HD23	1:F:19:ASP:O	1.81	0.79
1:E:28:PHE:CE2	1:E:30:ARG:CG	2.62	0.79
1:L:23:ASN:HD21	1:L:130:PHE:H	1.31	0.79
1:O:14:ILE:CD1	1:O:42:LEU:HD22	2.13	0.79
1:A:93:VAL:CG2	1:A:188:ILE:CG1	2.61	0.79
1:B:106:TYR:CD1	1:B:130:PHE:CE1	2.70	0.79
1:B:106:TYR:CD1	1:B:130:PHE:CZ	2.70	0.78
1:O:74:TYR:CE2	1:O:82:ASP:CB	2.65	0.78
1:F:14:ILE:HB	1:F:33:GLY:O	1.83	0.78
1:H:203:THR:HG23	1:H:224:VAL:HG13	1.64	0.78
1:A:15:LEU:HD12	1:A:120:VAL:HG22	1.64	0.77
1:E:39:ILE:HG23	1:E:41:LYS:HG3	1.64	0.77
1:G:61:VAL:CG2	1:G:220:LEU:HD11	2.14	0.77
1:L:110:ALA:HB2	1:L:123:ILE:HG23	1.66	0.77
1:C:47:ILE:HD13	1:C:215:ARG:HH21	1.50	0.77
1:M:98:ILE:HB	1:M:106:TYR:HB2	1.66	0.77
1:K:108:THR:HG22	1:K:125:LEU:HD23	1.67	0.77
1:A:15:LEU:CB	1:A:120:VAL:HG22	2.15	0.77
1:I:135:ASN:CB	1:I:136:ILE:HD12	2.15	0.77
1:A:102:CYS:HG	1:N:102:CYS:HG	1.32	0.76
1:F:102:CYS:N	1:O:102:CYS:SG	2.51	0.76
1:I:28:PHE:HD2	1:I:49:THR:HG1	0.77	0.76
1:D:83:PHE:CZ	1:D:161:ILE:HG21	2.21	0.75
1:M:104:GLY:HA3	1:M:130:PHE:CD1	2.20	0.75
1:O:106:TYR:CD1	1:O:130:PHE:HZ	2.04	0.75
1:E:28:PHE:HE2	1:E:30:ARG:CG	1.91	0.75
1:A:68:VAL:HG21	1:A:71:PHE:CE2	2.21	0.75
1:N:110:ALA:HB2	1:N:123:ILE:HG23	1.69	0.75
1:H:141:LEU:HD23	1:H:142:GLU:O	1.86	0.75
1:L:33:GLY:HA3	1:L:44:LEU:HD23	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:HG22	1:A:71:PHE:CD2	2.22	0.74
1:G:83:PHE:HB2	1:G:161:ILE:HD12	1.69	0.74
1:H:203:THR:CG2	1:H:224:VAL:CG1	2.56	0.74
1:D:107:LYS:O	1:D:108:THR:OG1	2.06	0.74
1:A:93:VAL:CG2	1:A:188:ILE:HG13	2.18	0.74
1:I:42:LEU:HD21	1:I:71:PHE:HB2	1.69	0.74
1:A:93:VAL:HG23	1:A:188:ILE:CG1	2.15	0.74
1:O:74:TYR:CD2	1:O:82:ASP:CG	2.61	0.73
1:H:203:THR:HG22	1:H:224:VAL:CB	2.18	0.73
1:F:98:ILE:HB	1:F:106:TYR:HB2	1.70	0.73
1:C:15:LEU:HD12	1:C:120:VAL:HG13	1.69	0.73
1:O:35:GLY:HA2	1:O:42:LEU:HD23	1.71	0.73
1:N:100:PHE:CD2	1:N:130:PHE:HE1	2.07	0.72
1:H:40:GLY:O	1:H:223:TYR:HA	1.88	0.72
1:O:100:PHE:HD2	1:O:104:GLY:O	1.70	0.72
1:P:39:ILE:HG23	1:P:41:LYS:HG3	1.71	0.72
1:H:110:ALA:HB2	1:H:123:ILE:HG23	1.72	0.72
1:P:39:ILE:HD13	1:P:41:LYS:HE3	1.72	0.72
1:B:185:ASN:O	1:B:186:THR:HB	1.88	0.72
1:M:75:PRO:HD2	1:M:78:MET:HB2	1.72	0.72
1:E:28:PHE:HD2	1:E:49:THR:HG1	1.35	0.72
1:I:136:ILE:HD12	1:I:136:ILE:N	2.03	0.71
1:I:18:LEU:HD23	1:I:19:ASP:O	1.90	0.71
1:A:163:ALA:HB3	1:A:183:GLN:HB3	1.73	0.71
1:I:42:LEU:O	1:I:44:LEU:HG	1.90	0.71
1:E:39:ILE:HD13	1:E:41:LYS:HE3	1.71	0.71
1:G:207:LEU:HD21	1:G:220:LEU:HG	1.71	0.71
1:H:203:THR:HA	1:H:223:TYR:O	1.91	0.71
1:A:15:LEU:HB2	1:A:120:VAL:CG2	2.19	0.71
1:D:128:ILE:HD12	1:D:129:ASP:CG	2.11	0.71
1:I:39:ILE:HG21	1:I:41:LYS:HE3	1.73	0.70
1:I:43:SER:HB3	1:I:221:LEU:CD2	2.11	0.70
1:O:185:ASN:C	1:O:186:THR:HG22	2.04	0.70
1:A:68:VAL:CG2	1:A:71:PHE:HD2	2.05	0.70
1:K:70:CYS:SG	1:K:84:PHE:HB3	2.31	0.70
1:G:207:LEU:HD23	1:G:220:LEU:HA	1.74	0.70
1:I:28:PHE:CD2	1:I:49:THR:OG1	2.34	0.70
1:H:204:GLN:O	1:H:205:THR:OG1	2.10	0.69
1:A:68:VAL:HG21	1:A:71:PHE:CD2	2.26	0.69
1:E:110:ALA:HB2	1:E:123:ILE:HG23	1.73	0.69
1:E:57:TRP:HB3	1:E:218:MET:SD	2.33	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:ILE:HD12	1:D:129:ASP:OD2	1.93	0.69
1:O:14:ILE:HD11	1:O:42:LEU:CD2	2.22	0.69
1:A:93:VAL:CG2	1:A:188:ILE:HG12	2.23	0.68
1:J:93:VAL:O	1:J:185:ASN:HB3	1.93	0.68
1:A:102:CYS:HG	1:N:102:CYS:CB	2.00	0.68
1:J:162:LYS:HE2	1:J:184:GLN:HG3	1.74	0.68
1:E:102:CYS:SG	1:J:102:CYS:N	2.66	0.68
1:F:62:THR:O	1:F:96:ARG:NH1	2.27	0.68
1:N:100:PHE:HD2	1:N:130:PHE:HE1	1.42	0.68
1:A:39:ILE:HG21	1:A:41:LYS:HE3	1.75	0.68
1:G:39:ILE:HG21	1:G:41:LYS:HE3	1.76	0.68
1:B:6:GLU:CG	1:B:7:LEU:N	2.47	0.68
1:J:33:GLY:HA3	1:J:44:LEU:HD23	1.76	0.68
1:A:15:LEU:CD1	1:A:120:VAL:HG22	2.23	0.67
1:A:152:ILE:C	1:A:153:THR:HG22	2.11	0.67
1:E:28:PHE:HD2	1:E:49:THR:OG1	1.76	0.67
1:G:61:VAL:HG13	1:G:220:LEU:HD13	1.76	0.67
1:K:98:ILE:HB	1:K:106:TYR:HB2	1.76	0.67
1:H:203:THR:CG2	1:H:224:VAL:HG22	2.21	0.67
1:G:61:VAL:CG2	1:G:220:LEU:CD1	2.72	0.67
1:N:100:PHE:HD2	1:N:130:PHE:CE1	2.12	0.67
1:G:83:PHE:O	1:G:84:PHE:CB	2.43	0.67
1:B:106:TYR:CZ	1:B:130:PHE:CZ	2.83	0.66
1:B:7:LEU:O	1:B:9:THR:HG22	1.93	0.66
1:J:110:ALA:HB2	1:J:123:ILE:HG23	1.77	0.66
1:I:43:SER:CB	1:I:221:LEU:CD2	2.70	0.66
1:D:111:GLU:O	1:D:112:VAL:HG13	1.95	0.66
1:A:15:LEU:HD12	1:A:120:VAL:CG2	2.25	0.66
1:C:215:ARG:O	1:C:215:ARG:HG3	1.94	0.66
1:I:33:GLY:HA3	1:I:44:LEU:CD2	2.24	0.66
1:H:206:ILE:HG13	1:L:206:ILE:HG13	1.78	0.66
1:C:73:ARG:HD3	1:C:225:THR:HG22	1.78	0.66
1:O:106:TYR:CD1	1:O:130:PHE:CZ	2.84	0.65
1:H:102:CYS:N	1:M:102:CYS:SG	2.69	0.65
1:I:18:LEU:CD2	1:I:19:ASP:O	2.44	0.65
1:G:7:LEU:CD1	1:G:8:PHE:H	2.09	0.65
1:I:83:PHE:HB3	1:I:161:ILE:HD11	1.78	0.65
1:I:135:ASN:CA	1:I:136:ILE:HD12	2.25	0.65
1:M:100:PHE:CG	1:M:136:ILE:HD11	2.32	0.65
1:C:149:LYS:HE3	1:I:142:GLU:OE2	1.96	0.65
1:J:145:PHE:HB3	1:J:205:THR:OG1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:THR:HG22	1:G:206:ILE:H	1.60	0.65
1:G:7:LEU:CG	1:G:8:PHE:N	2.31	0.65
1:A:15:LEU:O	1:A:120:VAL:CA	2.45	0.64
1:O:104:GLY:CA	1:O:130:PHE:CE1	2.79	0.64
1:J:222:GLU:OE2	1:J:224:VAL:CG2	2.46	0.64
1:G:13:PRO:HB2	1:G:118:THR:HG22	1.78	0.64
1:A:13:PRO:HD2	1:A:117:ASP:O	1.98	0.64
1:F:206:ILE:HG13	1:P:206:ILE:HG13	1.80	0.64
1:I:135:ASN:C	1:I:136:ILE:CD1	2.65	0.64
1:H:141:LEU:HD11	1:H:169:HIS:HB3	1.80	0.64
1:J:183:GLN:NE2	1:J:185:ASN:HD21	1.95	0.64
1:G:205:THR:CG2	1:G:220:LEU:CD2	2.76	0.64
1:A:15:LEU:HB2	1:A:120:VAL:HA	1.80	0.64
1:N:62:THR:O	1:N:96:ARG:NH1	2.30	0.64
1:P:159:ASN:O	1:P:195:LEU:HD21	1.97	0.63
1:O:14:ILE:HD11	1:O:42:LEU:HD22	1.81	0.63
1:O:145:PHE:HB3	1:O:205:THR:OG1	1.97	0.63
1:D:73:ARG:NH1	1:D:74:TYR:O	2.30	0.63
1:F:110:ALA:HB2	1:F:123:ILE:HG23	1.80	0.63
1:I:72:SER:HA	1:I:224:VAL:HG13	1.79	0.63
1:K:83:PHE:CZ	1:K:161:ILE:HG13	2.34	0.63
1:I:56:PRO:HD3	1:I:136:ILE:O	1.99	0.62
1:P:88:MET:SD	1:P:114:PHE:N	2.72	0.62
1:I:110:ALA:HB2	1:I:123:ILE:HG23	1.80	0.62
1:M:104:GLY:HA3	1:M:130:PHE:HD1	1.62	0.62
1:C:39:ILE:HG21	1:C:41:LYS:HE3	1.81	0.62
1:B:186:THR:HG22	1:B:187:PRO:N	2.15	0.62
1:J:16:ILE:CD1	1:J:44:LEU:HD13	2.30	0.62
1:N:100:PHE:CD2	1:N:130:PHE:CE1	2.87	0.62
1:A:119:LEU:O	1:A:120:VAL:CG2	2.44	0.62
1:M:167:ILE:O	1:M:178:LEU:HD23	1.99	0.62
1:A:132:GLU:HG2	1:P:156:LYS:HD3	1.82	0.62
1:J:11:VAL:HG22	1:J:36:ASP:OD1	2.00	0.62
1:O:22:VAL:HG13	1:O:130:PHE:CD2	2.35	0.62
1:H:76:ASP:HA	1:H:79:LYS:HE3	1.82	0.62
1:I:119:LEU:HD23	1:I:119:LEU:O	2.00	0.62
1:C:68:VAL:O	1:C:68:VAL:HG23	2.00	0.62
1:K:160:GLY:O	1:K:161:ILE:HD13	2.00	0.61
1:I:83:PHE:CZ	1:I:160:GLY:HA2	2.36	0.61
1:N:35:GLY:HA3	1:N:42:LEU:HD23	1.81	0.61
1:I:135:ASN:CB	1:I:136:ILE:CD1	2.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ILE:CD1	1:C:215:ARG:HH21	2.14	0.61
1:D:28:PHE:N	1:D:50:THR:OG1	2.26	0.61
1:P:110:ALA:HB2	1:P:123:ILE:HG23	1.81	0.61
1:P:58:PRO:HA	1:P:61:VAL:HG23	1.81	0.61
1:O:127:GLY:HA3	1:O:130:PHE:CE2	2.32	0.61
1:M:150:VAL:O	1:M:201:LEU:N	2.34	0.61
1:P:98:ILE:HB	1:P:106:TYR:HB2	1.82	0.61
1:B:70:CYS:HB3	1:B:84:PHE:HB2	1.82	0.60
1:G:148:HIS:CE1	1:G:168:ARG:H	2.19	0.60
1:O:14:ILE:HD12	1:O:42:LEU:HD22	1.83	0.60
1:D:73:ARG:HB3	1:D:225:THR:HA	1.83	0.60
1:N:36:ASP:OD2	1:N:39:ILE:HG22	2.01	0.60
1:H:205:THR:O	1:H:206:ILE:HG13	2.01	0.60
1:B:76:ASP:HA	1:B:79:LYS:HE3	1.82	0.60
1:G:199:HIS:CB	1:G:228:GLY:HA2	2.28	0.60
1:F:18:LEU:CD2	1:F:19:ASP:O	2.49	0.60
1:C:102:CYS:SG	1:D:102:CYS:N	2.74	0.60
1:J:76:ASP:O	1:J:77:HIS:HB3	2.01	0.60
1:C:182:TYR:OH	1:L:156:LYS:HD2	2.01	0.60
1:J:168:ARG:HG2	1:J:178:LEU:HD23	1.83	0.60
1:B:8:PHE:C	1:B:9:THR:HG22	2.22	0.60
1:F:198:ASP:O	1:F:199:HIS:ND1	2.34	0.60
1:C:110:ALA:CB	1:C:123:ILE:HG12	2.32	0.60
1:E:73:ARG:HH21	1:E:225:THR:HG21	1.66	0.60
1:D:105:THR:O	1:D:127:GLY:HA2	2.01	0.60
1:A:100:PHE:HB3	1:A:103:ASP:HB3	1.84	0.59
1:D:17:GLU:HB2	1:D:122:ARG:HA	1.83	0.59
1:A:76:ASP:HA	1:A:79:LYS:HE3	1.84	0.59
1:K:41:LYS:HG2	1:K:223:TYR:CE2	2.36	0.59
1:I:43:SER:CB	1:I:221:LEU:HA	2.32	0.59
1:E:76:ASP:HA	1:E:79:LYS:HE3	1.84	0.59
1:A:98:ILE:HB	1:A:106:TYR:HB2	1.84	0.59
1:H:215:ARG:HB2	1:H:217:HIS:NE2	2.16	0.59
1:L:98:ILE:HB	1:L:106:TYR:HB2	1.85	0.59
1:B:8:PHE:O	1:B:9:THR:C	2.39	0.59
1:M:117:ASP:CG	1:M:118:THR:H	2.05	0.59
1:B:185:ASN:O	1:B:186:THR:CB	2.50	0.59
1:C:203:THR:C	1:C:204:GLN:HG3	2.21	0.59
1:K:104:GLY:HA3	1:K:130:PHE:CD1	2.38	0.59
1:O:104:GLY:HA3	1:O:130:PHE:CE1	2.34	0.59
1:A:68:VAL:C	1:A:70:CYS:H	2.04	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:143:TYR:O	1:N:143:TYR:HD1	1.86	0.59
1:G:147:SER:CB	1:O:144:ASN:HD22	2.14	0.59
1:O:74:TYR:CD2	1:O:82:ASP:OD2	2.56	0.59
1:G:207:LEU:HD13	1:G:218:MET:HE3	1.84	0.59
1:B:92:TYR:HB2	1:B:186:THR:O	2.03	0.58
1:B:201:LEU:HA	1:B:226:ALA:HB2	1.84	0.58
1:B:106:TYR:CD1	1:B:127:GLY:CA	2.87	0.58
1:O:92:TYR:HB2	1:O:186:THR:O	2.04	0.58
1:O:33:GLY:HA3	1:O:44:LEU:HD23	1.85	0.58
1:O:76:ASP:HA	1:O:79:LYS:HE3	1.85	0.58
1:A:83:PHE:CZ	1:A:160:GLY:HA2	2.39	0.58
1:A:68:VAL:C	1:A:70:CYS:N	2.56	0.58
1:M:108:THR:HG22	1:M:125:LEU:HD23	1.83	0.58
1:D:108:THR:O	1:D:123:ILE:CG2	2.51	0.58
1:I:88:MET:CE	1:I:119:LEU:HD12	2.34	0.58
1:M:70:CYS:SG	1:M:119:LEU:HD11	2.43	0.58
1:C:104:GLY:HA3	1:C:130:PHE:CD1	2.38	0.58
1:L:104:GLY:HA3	1:L:130:PHE:CD1	2.39	0.58
1:J:12:VAL:HG13	1:J:71:PHE:HE1	1.69	0.58
1:C:20:GLY:HA2	1:C:125:LEU:O	2.03	0.58
1:I:43:SER:HB3	1:I:221:LEU:HA	1.85	0.58
1:B:83:PHE:CD2	1:B:161:ILE:HD11	2.38	0.58
1:C:163:ALA:HB3	1:C:183:GLN:HB3	1.85	0.58
1:J:94:GLN:HA	1:J:185:ASN:OD1	2.02	0.58
1:B:110:ALA:HB2	1:B:123:ILE:HG23	1.86	0.58
1:D:111:GLU:HA	1:D:111:GLU:OE1	2.04	0.57
1:O:205:THR:HG22	1:O:222:GLU:HG2	1.86	0.57
1:B:203:THR:HG22	1:B:224:VAL:HG13	1.85	0.57
1:H:104:GLY:HA3	1:H:130:PHE:CD1	2.39	0.57
1:B:33:GLY:HA3	1:B:44:LEU:HD23	1.85	0.57
1:A:110:ALA:HB2	1:A:123:ILE:HG23	1.86	0.57
1:A:145:PHE:HB3	1:A:205:THR:OG1	2.04	0.57
1:N:100:PHE:O	1:N:101:LYS:C	2.38	0.57
1:D:98:ILE:HB	1:D:106:TYR:HB2	1.85	0.57
1:J:149:LYS:HA	1:J:201:LEU:O	2.05	0.57
1:L:28:PHE:HE2	1:L:30:ARG:HG3	1.69	0.57
1:O:28:PHE:HD2	1:O:49:THR:HG1	1.50	0.57
1:O:81:HIS:O	1:O:196:PRO:HB3	2.04	0.57
1:L:28:PHE:CE2	1:L:30:ARG:HG3	2.40	0.57
1:P:104:GLY:HA3	1:P:130:PHE:CD1	2.39	0.57
1:F:39:ILE:HG21	1:F:41:LYS:HE3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:C	1:A:120:VAL:HG23	2.25	0.57
1:J:36:ASP:O	1:J:40:GLY:N	2.37	0.57
1:A:33:GLY:HA3	1:A:44:LEU:HD23	1.87	0.57
1:F:60:LEU:O	1:F:61:VAL:HB	2.05	0.57
1:D:121:ASN:HD21	1:D:123:ILE:HD11	1.70	0.57
1:M:150:VAL:HB	1:M:201:LEU:HB2	1.87	0.57
1:D:106:TYR:CE1	1:D:130:PHE:HZ	2.23	0.57
1:D:121:ASN:ND2	1:D:123:ILE:HD11	2.20	0.57
1:J:27:PHE:HA	1:J:50:THR:HG21	1.87	0.57
1:J:73:ARG:HG2	1:J:75:PRO:HD3	1.86	0.56
1:F:36:ASP:HB2	1:F:41:LYS:HB2	1.86	0.56
1:C:79:LYS:NZ	1:M:230:THR:OG1	2.23	0.56
1:B:105:THR:HG23	1:B:105:THR:O	2.04	0.56
1:B:8:PHE:O	1:B:10:GLY:N	2.37	0.56
1:J:43:SER:CA	1:J:220:LEU:O	2.52	0.56
1:B:48:ALA:HB3	1:B:216:ASP:HB3	1.88	0.56
1:K:83:PHE:HA	1:K:86:SER:HB2	1.87	0.56
1:I:76:ASP:HA	1:I:79:LYS:HE3	1.88	0.56
1:E:33:GLY:HA3	1:E:44:LEU:HD23	1.87	0.56
1:K:94:GLN:HB3	1:K:110:ALA:HB3	1.87	0.56
1:E:145:PHE:HB3	1:E:205:THR:OG1	2.05	0.56
1:H:90:GLU:OE2	1:H:189:GLY:HA2	2.06	0.56
1:K:83:PHE:CD2	1:K:161:ILE:HG13	2.40	0.56
1:D:108:THR:O	1:D:109:ARG:O	2.23	0.56
1:M:14:ILE:H	1:M:33:GLY:C	2.09	0.56
1:L:57:TRP:HB3	1:L:218:MET:HE1	1.86	0.56
1:H:31:GLY:HA3	1:H:46:PHE:CD1	2.41	0.56
1:I:83:PHE:CB	1:I:161:ILE:HD11	2.35	0.56
1:H:144:ASN:HD22	1:L:147:SER:CB	2.18	0.56
1:B:101:LYS:HD2	1:B:178:LEU:HD12	1.86	0.56
1:D:155:ASP:O	1:D:156:LYS:HB2	2.06	0.56
1:C:203:THR:O	1:C:204:GLN:CG	2.52	0.55
1:P:11:VAL:HG22	1:P:36:ASP:OD1	2.05	0.55
1:B:186:THR:HG23	1:B:187:PRO:HD2	1.88	0.55
1:L:163:ALA:HB3	1:L:183:GLN:HB3	1.87	0.55
1:L:58:PRO:HA	1:L:61:VAL:HG23	1.88	0.55
1:D:55:VAL:HG21	1:D:106:TYR:OH	2.07	0.55
1:K:71:PHE:HE2	1:K:119:LEU:HD22	1.72	0.55
1:A:104:GLY:HA3	1:A:130:PHE:CD1	2.42	0.55
1:M:155:ASP:HB2	1:M:162:LYS:HG3	1.88	0.55
1:O:163:ALA:HB3	1:O:183:GLN:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ASP:OD2	1:B:85:LYS:HD2	2.06	0.55
1:N:18:LEU:HD12	1:N:123:ILE:HD13	1.88	0.55
1:H:141:LEU:CD1	1:H:169:HIS:HB3	2.35	0.55
1:N:143:TYR:CD1	1:N:143:TYR:O	2.60	0.55
1:J:130:PHE:HE2	1:J:136:ILE:HG12	1.71	0.55
1:I:41:LYS:O	1:I:42:LEU:HG	2.06	0.55
1:G:207:LEU:CD2	1:G:220:LEU:HG	2.36	0.55
1:B:28:PHE:CE2	1:B:30:ARG:HG3	2.41	0.55
1:C:206:ILE:HG13	1:I:206:ILE:HG13	1.89	0.55
1:N:145:PHE:HB3	1:N:205:THR:OG1	2.06	0.54
1:L:23:ASN:ND2	1:L:130:PHE:H	2.01	0.54
1:F:98:ILE:HG12	1:F:181:HIS:CD2	2.42	0.54
1:J:56:PRO:HD3	1:J:136:ILE:O	2.07	0.54
1:L:22:VAL:HG12	1:L:23:ASN:N	2.22	0.54
1:H:58:PRO:HA	1:H:61:VAL:HG23	1.89	0.54
1:B:104:GLY:HA3	1:B:130:PHE:CD1	2.43	0.54
1:K:18:LEU:HD21	1:K:125:LEU:HD12	1.89	0.54
1:J:162:LYS:HE2	1:J:184:GLN:CG	2.36	0.54
1:I:145:PHE:HB3	1:I:205:THR:OG1	2.06	0.54
1:H:161:ILE:HD11	1:H:196:PRO:HG3	1.88	0.54
1:B:106:TYR:CD1	1:B:127:GLY:HA2	2.43	0.54
1:J:16:ILE:HD11	1:J:44:LEU:HD13	1.89	0.54
1:O:224:VAL:HG12	1:O:225:THR:N	2.22	0.54
1:G:171:VAL:HG12	1:G:173:ASP:H	1.72	0.54
1:J:28:PHE:CE2	1:J:30:ARG:HG3	2.41	0.54
1:D:128:ILE:CD1	1:D:129:ASP:OD2	2.55	0.54
1:N:94:GLN:HG3	1:N:185:ASN:OD1	2.08	0.54
1:K:102:CYS:N	1:L:102:CYS:SG	2.80	0.54
1:B:42:LEU:HB2	1:B:222:GLU:HB3	1.89	0.54
1:A:68:VAL:CG2	1:A:70:CYS:SG	2.96	0.54
1:H:33:GLY:HA3	1:H:44:LEU:HD23	1.89	0.54
1:I:101:LYS:HD2	1:I:178:LEU:HD12	1.88	0.54
1:C:101:LYS:HD2	1:C:178:LEU:HD12	1.90	0.54
1:D:33:GLY:HA3	1:D:44:LEU:HD23	1.90	0.54
1:B:106:TYR:CD1	1:B:127:GLY:HA3	2.42	0.54
1:H:98:ILE:HB	1:H:106:TYR:HB2	1.88	0.54
1:H:41:LYS:HE2	1:H:223:TYR:OH	2.08	0.53
1:K:70:CYS:SG	1:K:92:TYR:HE2	2.31	0.53
1:N:163:ALA:HB3	1:N:183:GLN:HE21	1.73	0.53
1:G:98:ILE:HB	1:G:106:TYR:HB2	1.90	0.53
1:P:88:MET:CE	1:P:113:LYS:CA	2.85	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ILE:HD13	1:C:215:ARG:CZ	2.38	0.53
1:D:38:THR:O	1:D:73:ARG:HD3	2.08	0.53
1:I:11:VAL:HG22	1:I:36:ASP:OD1	2.08	0.53
1:J:14:ILE:HB	1:J:44:LEU:HD21	1.89	0.53
1:O:104:GLY:O	1:O:130:PHE:HE1	1.82	0.53
1:C:47:ILE:CD1	1:C:215:ARG:NH2	2.65	0.53
1:E:39:ILE:HA	1:E:73:ARG:HD3	1.91	0.53
1:B:186:THR:CG2	1:B:187:PRO:N	2.72	0.53
1:F:112:VAL:HG22	1:F:121:ASN:OD1	2.09	0.53
1:G:208:SER:HB2	1:G:219:VAL:CB	2.37	0.53
1:B:90:GLU:HG2	1:B:189:GLY:HA3	1.90	0.53
1:J:74:TYR:O	1:J:74:TYR:CD1	2.61	0.53
1:H:82:ASP:OD2	1:H:85:LYS:HD2	2.09	0.53
1:K:187:PRO:HB2	1:K:189:GLY:O	2.08	0.53
1:G:7:LEU:O	1:G:8:PHE:HB2	2.07	0.53
1:E:40:GLY:N	1:E:73:ARG:HB2	2.24	0.53
1:J:183:GLN:HE21	1:J:185:ASN:ND2	2.05	0.53
1:F:11:VAL:HG22	1:F:36:ASP:OD1	2.08	0.53
1:A:207:LEU:HD13	1:A:218:MET:HE2	1.89	0.53
1:E:101:LYS:HD2	1:E:178:LEU:HD12	1.90	0.53
1:A:59:THR:HG21	1:A:136:ILE:HD12	1.90	0.53
1:B:58:PRO:HA	1:B:61:VAL:HG23	1.91	0.53
1:G:205:THR:CG2	1:G:220:LEU:HD21	2.39	0.53
1:A:93:VAL:O	1:A:93:VAL:HG12	2.09	0.53
1:D:130:PHE:CE2	1:D:136:ILE:HG21	2.44	0.53
1:F:207:LEU:O	1:P:204:GLN:NE2	2.39	0.53
1:P:33:GLY:HA3	1:P:44:LEU:HD23	1.91	0.53
1:N:100:PHE:HB3	1:N:103:ASP:HB3	1.91	0.53
1:P:114:PHE:HE1	1:P:119:LEU:HD12	1.74	0.53
1:M:104:GLY:HA3	1:M:130:PHE:CE1	2.43	0.53
1:J:71:PHE:CE2	1:J:119:LEU:HD23	2.44	0.53
1:O:11:VAL:HG22	1:O:36:ASP:OD1	2.09	0.53
1:G:70:CYS:SG	1:G:119:LEU:HD11	2.49	0.53
1:O:58:PRO:HA	1:O:61:VAL:HG23	1.90	0.53
1:L:28:PHE:HD2	1:L:49:THR:HG1	1.57	0.52
1:I:42:LEU:CD2	1:I:71:PHE:CD2	2.93	0.52
1:O:127:GLY:CA	1:O:130:PHE:CE2	2.84	0.52
1:A:132:GLU:O	1:A:133:ASP:HB3	2.08	0.52
1:C:157:GLN:HE22	1:L:184:GLN:NE2	2.07	0.52
1:F:145:PHE:HB3	1:F:205:THR:OG1	2.09	0.52
1:F:163:ALA:HB3	1:F:183:GLN:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:TYR:HD1	1:A:92:TYR:O	1.92	0.52
1:O:74:TYR:HE2	1:O:82:ASP:OD1	1.92	0.52
1:I:88:MET:HE2	1:I:119:LEU:HD12	1.89	0.52
1:K:16:ILE:HD13	1:K:64:LEU:O	2.09	0.52
1:N:21:ASP:HB3	1:N:26:LYS:HG2	1.92	0.52
1:A:115:GLU:HG2	1:A:115:GLU:O	2.09	0.52
1:K:161:ILE:HG22	1:K:162:LYS:N	2.25	0.52
1:O:35:GLY:CA	1:O:42:LEU:HD23	2.38	0.52
1:L:70:CYS:O	1:L:85:LYS:NZ	2.39	0.52
1:G:144:ASN:OD1	1:O:204:GLN:NE2	2.42	0.52
1:G:220:LEU:O	1:G:222:GLU:HG3	2.10	0.52
1:D:142:GLU:HG2	1:D:172:GLU:OE2	2.10	0.52
1:B:106:TYR:HD1	1:B:127:GLY:HA2	1.75	0.52
1:G:33:GLY:HA3	1:G:44:LEU:HD23	1.91	0.52
1:A:68:VAL:HG22	1:A:71:PHE:HD2	1.65	0.52
1:K:18:LEU:HD11	1:K:125:LEU:HD11	1.91	0.52
1:O:101:LYS:O	1:O:102:CYS:HB2	2.10	0.52
1:I:198:ASP:O	1:I:199:HIS:ND1	2.43	0.52
1:O:100:PHE:CD2	1:O:104:GLY:O	2.59	0.52
1:P:64:LEU:O	1:P:121:ASN:ND2	2.42	0.52
1:M:100:PHE:CD2	1:M:136:ILE:HD11	2.44	0.52
1:K:161:ILE:HD11	1:K:196:PRO:HD2	1.91	0.52
1:K:143:TYR:O	1:K:144:ASN:ND2	2.43	0.51
1:P:36:ASP:HB3	1:P:39:ILE:HG22	1.91	0.51
1:P:41:LYS:HE2	1:P:223:TYR:OH	2.10	0.51
1:L:56:PRO:HD3	1:L:136:ILE:O	2.11	0.51
1:O:199:HIS:ND1	1:O:227:ALA:O	2.42	0.51
1:H:21:ASP:OD1	1:H:26:LYS:HG2	2.11	0.51
1:J:62:THR:HG21	1:J:167:ILE:HG13	1.93	0.51
1:A:68:VAL:HG13	1:A:68:VAL:O	2.09	0.51
1:D:16:ILE:HG21	1:D:64:LEU:HD23	1.92	0.51
1:E:104:GLY:HA3	1:E:130:PHE:CD1	2.45	0.51
1:I:83:PHE:HB3	1:I:161:ILE:CD1	2.40	0.51
1:G:147:SER:HB2	1:O:144:ASN:HD22	1.75	0.51
1:D:145:PHE:HB3	1:D:205:THR:HB	1.90	0.51
1:C:63:THR:O	1:C:123:ILE:HD11	2.11	0.51
1:O:74:TYR:CE2	1:O:82:ASP:OD2	2.64	0.51
1:E:38:THR:O	1:E:73:ARG:HG3	2.11	0.51
1:L:101:LYS:HD2	1:L:178:LEU:HD12	1.93	0.51
1:D:149:LYS:HA	1:D:201:LEU:O	2.10	0.51
1:B:145:PHE:HB3	1:B:205:THR:OG1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:PHE:O	1:B:9:THR:CG2	2.59	0.51
1:K:83:PHE:CZ	1:K:84:PHE:CE1	2.99	0.51
1:K:93:VAL:N	1:K:186:THR:O	2.35	0.51
1:C:57:TRP:HE1	1:C:216:ASP:CG	2.14	0.51
1:B:183:GLN:HE21	1:B:185:ASN:HD21	1.58	0.51
1:J:28:PHE:HD2	1:J:49:THR:OG1	1.94	0.51
1:H:15:LEU:CD1	1:H:120:VAL:HG22	2.41	0.51
1:P:155:ASP:O	1:P:160:GLY:N	2.44	0.51
1:G:123:ILE:HG22	1:G:124:GLU:O	2.11	0.51
1:K:146:ASN:HB2	1:K:148:HIS:CE1	2.45	0.51
1:M:147:SER:OG	1:M:203:THR:O	2.21	0.51
1:D:11:VAL:HG22	1:D:36:ASP:OD1	2.11	0.51
1:M:128:ILE:HG22	1:M:129:ASP:OD2	2.11	0.50
1:D:97:THR:HA	1:D:106:TYR:O	2.11	0.50
1:D:17:GLU:O	1:D:123:ILE:HG13	2.11	0.50
1:B:106:TYR:CE1	1:B:127:GLY:CA	2.91	0.50
1:L:22:VAL:HA	1:L:127:GLY:O	2.11	0.50
1:G:11:VAL:HG22	1:G:36:ASP:OD1	2.11	0.50
1:H:144:ASN:HD22	1:L:147:SER:HB2	1.77	0.50
1:K:144:ASN:HD22	1:M:204:GLN:NE2	2.08	0.50
1:O:100:PHE:CB	1:O:103:ASP:CB	2.90	0.50
1:L:30:ARG:O	1:L:47:ILE:N	2.37	0.50
1:N:34:GLU:O	1:N:43:SER:O	2.29	0.50
1:E:36:ASP:CG	1:E:39:ILE:HG22	2.32	0.50
1:L:22:VAL:HG12	1:L:23:ASN:H	1.77	0.50
1:E:73:ARG:HE	1:E:225:THR:HG22	1.77	0.50
1:B:9:THR:CG2	1:B:10:GLY:N	2.52	0.50
1:J:162:LYS:HE2	1:J:184:GLN:CD	2.30	0.50
1:C:203:THR:O	1:C:223:TYR:O	2.29	0.50
1:C:73:ARG:HH21	1:I:211:LEU:HD21	1.76	0.50
1:A:161:ILE:HD11	1:A:196:PRO:HG3	1.93	0.50
1:I:36:ASP:HB2	1:I:41:LYS:HB2	1.94	0.50
1:L:22:VAL:HA	1:L:127:GLY:CA	2.42	0.50
1:A:68:VAL:HG22	1:A:70:CYS:SG	2.52	0.50
1:F:21:ASP:HB3	1:F:26:LYS:HG2	1.93	0.50
1:L:145:PHE:HB3	1:L:205:THR:OG1	2.11	0.49
1:B:8:PHE:C	1:B:9:THR:CG2	2.80	0.49
1:J:183:GLN:HE21	1:J:185:ASN:HD21	1.60	0.49
1:G:93:VAL:HG13	1:G:110:ALA:O	2.13	0.49
1:K:63:THR:HG21	1:K:125:LEU:HD21	1.94	0.49
1:H:83:PHE:HB2	1:H:196:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ARG:O	1:C:216:ASP:C	2.49	0.49
1:M:128:ILE:CG2	1:M:129:ASP:N	2.76	0.49
1:H:215:ARG:HB2	1:H:217:HIS:CE1	2.48	0.49
1:I:62:THR:HB	1:I:96:ARG:HH12	1.78	0.49
1:E:98:ILE:HB	1:E:106:TYR:HB2	1.93	0.49
1:E:152:ILE:HG23	1:E:161:ILE:HG23	1.94	0.49
1:D:75:PRO:HD2	1:D:78:MET:HB2	1.94	0.49
1:B:104:GLY:HA3	1:B:130:PHE:CE1	2.48	0.49
1:F:19:ASP:N	1:F:19:ASP:OD1	2.44	0.49
1:L:83:PHE:CD1	1:L:196:PRO:HD3	2.47	0.49
1:G:101:LYS:HG2	1:G:102:CYS:SG	2.52	0.49
1:G:205:THR:CG2	1:G:220:LEU:HD23	2.32	0.49
1:O:100:PHE:HB2	1:O:103:ASP:CB	2.42	0.49
1:L:23:ASN:ND2	1:L:130:PHE:O	2.46	0.49
1:A:11:VAL:HG22	1:A:36:ASP:OD1	2.13	0.49
1:F:21:ASP:HB3	1:F:26:LYS:HA	1.95	0.49
1:N:46:PHE:O	1:N:217:HIS:HB2	2.12	0.49
1:O:23:ASN:ND2	1:O:130:PHE:O	2.45	0.49
1:F:20:GLY:CA	1:F:125:LEU:O	2.55	0.49
1:A:83:PHE:HB2	1:A:196:PRO:HD3	1.95	0.49
1:F:98:ILE:HG12	1:F:181:HIS:HD2	1.78	0.49
1:C:123:ILE:CG2	1:C:124:GLU:N	2.76	0.49
1:G:208:SER:CB	1:G:219:VAL:HB	2.40	0.48
1:B:6:GLU:OE1	1:B:6:GLU:HA	2.13	0.48
1:H:141:LEU:HD11	1:H:169:HIS:CG	2.48	0.48
1:F:35:GLY:HA3	1:F:71:PHE:CE1	2.48	0.48
1:G:219:VAL:HG12	1:G:220:LEU:H	1.78	0.48
1:M:18:LEU:HD11	1:M:125:LEU:HD11	1.93	0.48
1:L:57:TRP:HB3	1:L:218:MET:CE	2.43	0.48
1:O:162:LYS:HA	1:O:183:GLN:O	2.13	0.48
1:G:140:LYS:O	1:G:171:VAL:HG13	2.13	0.48
1:P:98:ILE:HG23	1:P:181:HIS:CD2	2.48	0.48
1:H:47:ILE:HG12	1:H:217:HIS:ND1	2.28	0.48
1:L:19:ASP:O	1:L:125:LEU:N	2.41	0.48
1:G:103:ASP:CG	1:G:104:GLY:N	2.66	0.48
1:M:128:ILE:HG22	1:M:129:ASP:N	2.28	0.48
1:F:19:ASP:HA	1:F:28:PHE:HD1	1.78	0.48
1:G:13:PRO:HD2	1:G:117:ASP:O	2.14	0.48
1:C:79:LYS:HZ2	1:M:230:THR:HG1	1.57	0.48
1:A:62:THR:O	1:A:96:ARG:NH1	2.46	0.48
1:A:153:THR:O	1:A:161:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:THR:HG23	1:G:220:LEU:HD21	1.92	0.48
1:O:74:TYR:HD2	1:O:82:ASP:OD2	1.97	0.48
1:K:58:PRO:HA	1:K:61:VAL:HG23	1.94	0.48
1:J:15:LEU:HD22	1:J:120:VAL:HG23	1.96	0.48
1:I:42:LEU:HD21	1:I:71:PHE:CD2	2.43	0.48
1:G:55:VAL:HG11	1:G:106:TYR:OH	2.13	0.48
1:P:20:GLY:HA2	1:P:125:LEU:O	2.13	0.48
1:G:205:THR:CG2	1:G:206:ILE:H	2.22	0.48
1:I:41:LYS:HG2	1:I:223:TYR:CE1	2.48	0.48
1:D:102:CYS:O	1:D:131:LYS:HE3	2.13	0.48
1:K:130:PHE:CE2	1:K:136:ILE:HG21	2.49	0.48
1:B:102:CYS:SG	1:I:102:CYS:N	2.86	0.48
1:I:41:LYS:C	1:I:42:LEU:HG	2.34	0.48
1:A:15:LEU:O	1:A:120:VAL:C	2.52	0.48
1:D:17:GLU:N	1:D:121:ASN:O	2.38	0.48
1:A:68:VAL:HG21	1:A:71:PHE:HE2	1.73	0.48
1:D:100:PHE:HE1	1:D:106:TYR:CD1	2.32	0.48
1:D:56:PRO:HD3	1:D:136:ILE:O	2.14	0.48
1:L:21:ASP:O	1:L:25:HIS:O	2.32	0.48
1:A:94:GLN:HG2	1:A:95:GLU:N	2.29	0.47
1:A:68:VAL:O	1:A:70:CYS:N	2.46	0.47
1:N:20:GLY:HA3	1:N:125:LEU:HG	1.96	0.47
1:I:58:PRO:HA	1:I:61:VAL:HG23	1.95	0.47
1:J:33:GLY:CA	1:J:44:LEU:HD23	2.42	0.47
1:A:80:ARG:O	1:A:194:ASP:HB3	2.13	0.47
1:G:61:VAL:CB	1:G:220:LEU:HD11	2.42	0.47
1:N:100:PHE:O	1:N:102:CYS:N	2.47	0.47
1:M:100:PHE:O	1:M:101:LYS:C	2.51	0.47
1:D:16:ILE:CG2	1:D:64:LEU:HD23	2.44	0.47
1:M:45:LYS:NZ	1:M:213:GLU:OE2	2.40	0.47
1:M:167:ILE:O	1:M:178:LEU:CD2	2.62	0.47
1:C:102:CYS:SG	1:D:101:LYS:HG2	2.54	0.47
1:I:28:PHE:HE2	1:I:30:ARG:CD	2.26	0.47
1:O:21:ASP:OD1	1:O:26:LYS:HG2	2.14	0.47
1:B:106:TYR:CD1	1:B:130:PHE:HZ	2.31	0.47
1:P:101:LYS:HD2	1:P:178:LEU:HD12	1.96	0.47
1:G:207:LEU:CD2	1:G:219:VAL:O	2.48	0.47
1:J:18:LEU:HB2	1:J:123:ILE:HD12	1.96	0.47
1:L:55:VAL:HG22	1:L:136:ILE:HG22	1.97	0.47
1:L:144:ASN:CA	1:L:207:LEU:HD12	2.44	0.47
1:N:87:ALA:HB3	1:N:92:TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:128:ILE:HG22	1:O:129:ASP:CG	2.35	0.47
1:K:154:ALA:HB1	1:K:195:LEU:HD23	1.96	0.47
1:C:21:ASP:OD1	1:C:26:LYS:HG2	2.15	0.47
1:H:71:PHE:HE2	1:H:119:LEU:HD23	1.79	0.47
1:G:205:THR:O	1:G:206:ILE:CB	2.63	0.47
1:I:161:ILE:CG2	1:I:162:LYS:N	2.77	0.47
1:D:209:LYS:HE3	1:D:218:MET:HE1	1.97	0.47
1:M:100:PHE:CD2	1:M:136:ILE:CD1	2.98	0.47
1:B:225:THR:O	1:B:226:ALA:HB3	2.15	0.47
1:K:206:ILE:HG13	1:M:206:ILE:HG13	1.97	0.47
1:O:7:LEU:HD13	1:O:114:PHE:CE2	2.50	0.47
1:C:58:PRO:HA	1:C:61:VAL:HG23	1.97	0.47
1:L:155:ASP:OD2	1:L:162:LYS:HE2	2.15	0.47
1:O:207:LEU:HB3	1:O:218:MET:SD	2.55	0.47
1:A:152:ILE:HG22	1:A:153:THR:N	2.29	0.46
1:G:207:LEU:CD2	1:G:220:LEU:HA	2.42	0.46
1:B:40:GLY:O	1:B:223:TYR:HA	2.15	0.46
1:C:75:PRO:HD2	1:C:78:MET:HB2	1.96	0.46
1:F:104:GLY:HA3	1:F:130:PHE:CD1	2.50	0.46
1:E:56:PRO:HD3	1:E:136:ILE:O	2.15	0.46
1:L:16:ILE:HG21	1:L:46:PHE:HE1	1.81	0.46
1:B:106:TYR:CD1	1:B:130:PHE:HE1	2.30	0.46
1:C:157:GLN:HE22	1:L:184:GLN:HE22	1.62	0.46
1:J:167:ILE:HB	1:J:179:ALA:HB3	1.97	0.46
1:G:31:GLY:HA3	1:G:46:PHE:CD1	2.51	0.46
1:I:44:LEU:N	1:I:220:LEU:O	2.49	0.46
1:I:135:ASN:HD22	1:I:177:GLN:NE2	2.13	0.46
1:D:161:ILE:HD13	1:D:196:PRO:HG3	1.98	0.46
1:P:220:LEU:HD21	1:P:222:GLU:HB2	1.98	0.46
1:F:74:TYR:HA	1:F:75:PRO:HD2	1.76	0.46
1:E:28:PHE:CZ	1:E:30:ARG:HG3	2.37	0.46
1:B:28:PHE:HD2	1:B:49:THR:OG1	1.98	0.46
1:E:74:TYR:OH	1:E:84:PHE:HD2	1.99	0.46
1:M:100:PHE:CD1	1:M:136:ILE:HD11	2.50	0.46
1:A:58:PRO:HA	1:A:61:VAL:HG23	1.98	0.46
1:F:15:LEU:HD22	1:F:120:VAL:HG13	1.98	0.46
1:I:28:PHE:CE2	1:I:30:ARG:CD	2.98	0.46
1:A:15:LEU:HB2	1:A:120:VAL:CA	2.45	0.46
1:P:40:GLY:HA2	1:P:71:PHE:O	2.15	0.46
1:E:42:LEU:HB2	1:E:222:GLU:HB3	1.97	0.46
1:A:68:VAL:O	1:A:68:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:HG23	1:A:70:CYS:SG	2.54	0.46
1:J:222:GLU:OE2	1:J:224:VAL:HG21	2.16	0.46
1:O:224:VAL:O	1:O:225:THR:CG2	2.64	0.46
1:H:15:LEU:HD11	1:H:120:VAL:HG22	1.98	0.46
1:B:206:ILE:HG13	1:D:206:ILE:HG13	1.98	0.46
1:B:204:GLN:NE2	1:D:207:LEU:O	2.48	0.46
1:B:22:VAL:HG13	1:B:106:TYR:OH	2.14	0.46
1:L:55:VAL:HG13	1:L:56:PRO:HD2	1.98	0.46
1:A:15:LEU:C	1:A:120:VAL:HA	2.37	0.46
1:O:14:ILE:HD11	1:O:42:LEU:HD21	1.95	0.46
1:G:147:SER:HB2	1:G:203:THR:O	2.16	0.46
1:I:76:ASP:O	1:I:79:LYS:HG3	2.16	0.46
1:O:20:GLY:HA2	1:O:125:LEU:O	2.15	0.46
1:N:108:THR:HA	1:N:124:GLU:O	2.17	0.46
1:O:36:ASP:HB3	1:O:39:ILE:HG22	1.98	0.45
1:C:33:GLY:HA3	1:C:44:LEU:HD23	1.97	0.45
1:C:82:ASP:OD2	1:C:85:LYS:HD2	2.16	0.45
1:I:104:GLY:HA3	1:I:130:PHE:CD1	2.51	0.45
1:H:75:PRO:HD2	1:H:78:MET:HB2	1.98	0.45
1:B:20:GLY:HA2	1:B:125:LEU:O	2.16	0.45
1:C:40:GLY:HA3	1:C:73:ARG:HB2	1.97	0.45
1:C:149:LYS:HA	1:C:201:LEU:O	2.16	0.45
1:A:55:VAL:HG11	1:A:106:TYR:OH	2.17	0.45
1:A:57:TRP:HB3	1:A:218:MET:CE	2.46	0.45
1:M:96:ARG:NE	1:M:183:GLN:OE1	2.46	0.45
1:H:100:PHE:O	1:H:101:LYS:C	2.50	0.45
1:F:161:ILE:CG2	1:F:162:LYS:N	2.80	0.45
1:C:63:THR:O	1:C:123:ILE:CD1	2.65	0.45
1:I:100:PHE:HE2	1:I:106:TYR:CE2	2.35	0.45
1:K:55:VAL:HG13	1:K:56:PRO:HD2	1.99	0.45
1:O:224:VAL:O	1:O:225:THR:HG23	2.16	0.45
1:J:58:PRO:HA	1:J:61:VAL:HG23	1.99	0.45
1:F:203:THR:HG22	1:F:224:VAL:HG13	1.97	0.45
1:A:113:LYS:O	1:A:119:LEU:HA	2.17	0.45
1:L:23:ASN:HD21	1:L:130:PHE:CA	2.28	0.45
1:B:70:CYS:HB3	1:B:84:PHE:CB	2.47	0.45
1:A:20:GLY:HA2	1:A:125:LEU:O	2.16	0.45
1:B:149:LYS:HA	1:B:201:LEU:O	2.17	0.45
1:B:163:ALA:HB3	1:B:183:GLN:HB3	1.99	0.45
1:K:16:ILE:HG12	1:K:121:ASN:HB3	1.99	0.45
1:L:62:THR:HG21	1:L:167:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:100:PHE:HB3	1:O:103:ASP:CB	2.47	0.45
1:M:18:LEU:HD21	1:M:125:LEU:HD12	1.99	0.45
1:B:161:ILE:CG2	1:B:162:LYS:N	2.80	0.45
1:O:224:VAL:CG1	1:O:225:THR:N	2.80	0.45
1:A:92:TYR:CD1	1:A:92:TYR:O	2.70	0.45
1:H:15:LEU:HD12	1:H:120:VAL:HG13	1.98	0.45
1:J:20:GLY:HA2	1:J:125:LEU:O	2.17	0.45
1:K:161:ILE:CG2	1:K:162:LYS:N	2.80	0.44
1:M:98:ILE:O	1:M:105:THR:HA	2.17	0.44
1:O:28:PHE:HD2	1:O:49:THR:OG1	2.00	0.44
1:K:93:VAL:O	1:K:185:ASN:HA	2.18	0.44
1:I:23:ASN:OD1	1:I:130:PHE:HB2	2.17	0.44
1:A:36:ASP:HB2	1:A:41:LYS:HB2	2.00	0.44
1:L:92:TYR:CZ	1:L:112:VAL:HG11	2.52	0.44
1:H:163:ALA:HB3	1:H:183:GLN:HB3	1.98	0.44
1:C:205:THR:CG2	1:C:222:GLU:OE1	2.65	0.44
1:J:162:LYS:HE2	1:J:184:GLN:NE2	2.32	0.44
1:I:88:MET:CE	1:I:119:LEU:CD1	2.95	0.44
1:J:98:ILE:O	1:J:105:THR:HA	2.18	0.44
1:P:8:PHE:CE1	1:P:85:LYS:HB3	2.53	0.44
1:P:94:GLN:HE21	1:P:183:GLN:NE2	2.16	0.44
1:A:83:PHE:CD2	1:A:161:ILE:HD12	2.53	0.44
1:O:22:VAL:HG13	1:O:130:PHE:CE2	2.52	0.44
1:N:101:LYS:HB2	1:N:178:LEU:HB2	1.99	0.44
1:J:12:VAL:HG13	1:J:71:PHE:CE1	2.51	0.44
1:I:142:GLU:OE1	1:I:170:ASN:HB3	2.17	0.44
1:C:19:ASP:O	1:C:125:LEU:N	2.45	0.44
1:K:93:VAL:HB	1:K:186:THR:OG1	2.18	0.44
1:I:28:PHE:HZ	1:I:30:ARG:CG	2.24	0.44
1:I:43:SER:HA	1:I:220:LEU:O	2.17	0.44
1:A:68:VAL:CG2	1:A:71:PHE:CE2	2.91	0.44
1:O:14:ILE:HG21	1:O:44:LEU:HD21	2.00	0.44
1:H:113:LYS:O	1:H:119:LEU:HD12	2.18	0.44
1:F:86:SER:HB2	1:F:192:PRO:O	2.17	0.44
1:M:97:THR:OG1	1:M:182:TYR:HB2	2.17	0.44
1:O:55:VAL:HG21	1:O:106:TYR:OH	2.18	0.44
1:M:101:LYS:N	1:M:178:LEU:O	2.23	0.44
1:O:220:LEU:HD21	1:O:222:GLU:CD	2.37	0.44
1:M:155:ASP:OD2	1:M:158:ASN:ND2	2.51	0.44
1:D:133:ASP:OD2	1:L:192:PRO:HA	2.17	0.44
1:J:16:ILE:HD12	1:J:44:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:53:LEU:HD23	1:I:53:LEU:HA	1.79	0.44
1:N:56:PRO:HD2	1:N:136:ILE:HG23	1.99	0.44
1:E:15:LEU:HB2	1:E:120:VAL:HG22	1.99	0.44
1:P:40:GLY:N	1:P:73:ARG:HB3	2.33	0.43
1:C:42:LEU:HB2	1:C:222:GLU:HB3	2.00	0.43
1:D:100:PHE:CD2	1:D:136:ILE:HD11	2.53	0.43
1:L:63:THR:HG21	1:L:125:LEU:HD12	2.00	0.43
1:N:98:ILE:HB	1:N:106:TYR:HB2	1.99	0.43
1:F:136:ILE:C	1:F:138:GLY:H	2.21	0.43
1:H:141:LEU:HD11	1:H:169:HIS:CB	2.47	0.43
1:G:83:PHE:CZ	1:G:160:GLY:HA2	2.53	0.43
1:K:130:PHE:HE2	1:K:136:ILE:HG21	1.83	0.43
1:H:100:PHE:HB2	1:H:103:ASP:HB3	2.00	0.43
1:F:204:GLN:NE2	1:P:207:LEU:O	2.49	0.43
1:G:53:LEU:HD23	1:G:53:LEU:HA	1.81	0.43
1:O:104:GLY:N	1:O:130:PHE:CD1	2.86	0.43
1:E:41:LYS:HE2	1:E:223:TYR:OH	2.19	0.43
1:M:12:VAL:HA	1:M:13:PRO:HD3	1.90	0.43
1:G:205:THR:CG2	1:G:206:ILE:N	2.65	0.43
1:A:94:GLN:CG	1:A:185:ASN:OD1	2.52	0.43
1:I:197:ASP:OD1	1:I:198:ASP:N	2.52	0.43
1:I:209:LYS:HG3	1:I:217:HIS:CE1	2.54	0.43
1:M:47:ILE:HD13	1:M:215:ARG:NH2	2.34	0.43
1:K:27:PHE:CD2	1:K:54:PRO:HD3	2.53	0.43
1:D:103:ASP:OD2	1:D:177:GLN:NE2	2.49	0.43
1:A:23:ASN:ND2	1:A:130:PHE:O	2.51	0.43
1:L:144:ASN:HA	1:L:207:LEU:HD12	1.99	0.43
1:P:134:GLY:O	1:P:138:GLY:HA3	2.18	0.43
1:F:14:ILE:N	1:F:33:GLY:O	2.50	0.43
1:P:154:ALA:HB1	1:P:195:LEU:HD13	2.00	0.43
1:O:161:ILE:CG2	1:O:162:LYS:N	2.81	0.43
1:L:161:ILE:HD11	1:L:196:PRO:HG3	2.00	0.43
1:O:108:THR:HA	1:O:124:GLU:O	2.19	0.43
1:G:220:LEU:O	1:G:221:LEU:C	2.57	0.43
1:A:91:GLY:HA3	1:A:188:ILE:HD12	2.00	0.43
1:P:114:PHE:CE1	1:P:119:LEU:HD12	2.53	0.43
1:P:71:PHE:CE2	1:P:119:LEU:HD13	2.54	0.43
1:C:204:GLN:O	1:C:222:GLU:HG3	2.18	0.43
1:C:204:GLN:HE21	1:I:144:ASN:HB3	1.84	0.43
1:G:36:ASP:HB2	1:G:41:LYS:HB2	2.01	0.43
1:O:163:ALA:N	1:O:183:GLN:O	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:20:GLY:O	1:L:21:ASP:OD1	2.36	0.43
1:D:53:LEU:HD12	1:D:57:TRP:CE2	2.53	0.43
1:H:56:PRO:HD3	1:H:136:ILE:O	2.19	0.43
1:F:13:PRO:HA	1:F:34:GLU:HG3	2.01	0.43
1:A:203:THR:HG22	1:A:224:VAL:HG22	2.01	0.43
1:O:14:ILE:HG13	1:O:34:GLU:HA	2.01	0.43
1:N:98:ILE:O	1:N:105:THR:HA	2.18	0.43
1:O:213:GLU:OE2	1:O:215:ARG:HD3	2.17	0.43
1:O:23:ASN:OD1	1:O:130:PHE:HD2	2.01	0.43
1:P:88:MET:HE1	1:P:113:LYS:CA	2.35	0.43
1:J:147:SER:HA	1:J:203:THR:O	2.18	0.43
1:E:203:THR:HG22	1:E:224:VAL:HG13	2.00	0.43
1:P:21:ASP:OD1	1:P:26:LYS:HG2	2.19	0.43
1:L:53:LEU:HA	1:L:53:LEU:HD23	1.84	0.43
1:D:57:TRP:CE2	1:D:218:MET:HG2	2.54	0.43
1:F:191:GLY:HA2	1:F:192:PRO:HD3	1.86	0.43
1:H:59:THR:HG21	1:H:136:ILE:HD12	2.01	0.43
1:O:84:PHE:HE1	1:O:185:ASN:ND2	2.17	0.42
1:D:143:TYR:OH	1:D:218:MET:SD	2.72	0.42
1:J:199:HIS:CE1	1:J:228:GLY:HA2	2.53	0.42
1:I:18:LEU:HD23	1:I:19:ASP:C	2.39	0.42
1:J:14:ILE:HG12	1:J:71:PHE:CZ	2.54	0.42
1:M:178:LEU:HA	1:M:178:LEU:HD23	1.80	0.42
1:J:40:GLY:HA3	1:J:73:ARG:HB2	2.01	0.42
1:K:103:ASP:OD2	1:K:136:ILE:HD13	2.19	0.42
1:H:161:ILE:CG2	1:H:162:LYS:N	2.82	0.42
1:O:111:GLU:O	1:O:121:ASN:HA	2.19	0.42
1:J:154:ALA:N	1:J:198:ASP:OD1	2.53	0.42
1:K:205:THR:HA	1:K:222:GLU:HA	2.01	0.42
1:B:22:VAL:CG2	1:B:106:TYR:CZ	3.02	0.42
1:I:42:LEU:CD2	1:I:71:PHE:CB	2.64	0.42
1:F:14:ILE:CB	1:F:33:GLY:O	2.60	0.42
1:J:12:VAL:CG1	1:J:71:PHE:HE1	2.32	0.42
1:P:158:ASN:O	1:P:159:ASN:CB	2.68	0.42
1:L:55:VAL:HG11	1:L:106:TYR:OH	2.19	0.42
1:K:56:PRO:HD3	1:K:136:ILE:O	2.20	0.42
1:B:224:VAL:O	1:B:225:THR:C	2.57	0.42
1:G:61:VAL:HG11	1:G:220:LEU:HD11	1.92	0.42
1:I:43:SER:HB2	1:I:220:LEU:O	2.18	0.42
1:O:127:GLY:C	1:O:130:PHE:HE2	2.23	0.42
1:K:70:CYS:HG	1:K:92:TYR:HE2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:VAL:HA	1:G:13:PRO:HD3	1.84	0.42
1:O:7:LEU:HD13	1:O:114:PHE:HE2	1.83	0.42
1:N:149:LYS:HA	1:N:201:LEU:O	2.19	0.42
1:I:97:THR:HG22	1:I:107:LYS:HG2	2.00	0.42
1:A:152:ILE:O	1:A:162:LYS:O	2.37	0.42
1:O:74:TYR:CE2	1:O:82:ASP:HA	2.54	0.42
1:B:9:THR:O	1:B:38:THR:HG23	2.19	0.42
1:L:22:VAL:CG1	1:L:23:ASN:N	2.81	0.42
1:D:103:ASP:HB3	1:D:104:GLY:H	1.64	0.42
1:B:62:THR:O	1:B:96:ARG:NH1	2.51	0.42
1:O:98:ILE:HB	1:O:106:TYR:HB2	2.02	0.42
1:G:71:PHE:CE2	1:G:119:LEU:HD13	2.54	0.42
1:P:163:ALA:HB3	1:P:183:GLN:HB3	2.02	0.42
1:J:198:ASP:HB3	1:J:199:HIS:H	1.71	0.42
1:M:16:ILE:HD13	1:M:46:PHE:HE1	1.85	0.42
1:D:215:ARG:O	1:D:217:HIS:N	2.52	0.42
1:I:36:ASP:O	1:I:40:GLY:N	2.53	0.42
1:K:83:PHE:CZ	1:K:161:ILE:CG1	3.02	0.42
1:G:168:ARG:HG2	1:G:178:LEU:HD23	2.02	0.42
1:N:39:ILE:HD12	1:N:39:ILE:HA	1.87	0.42
1:H:46:PHE:CD2	1:H:64:LEU:HD13	2.54	0.42
1:G:124:GLU:HG2	1:G:125:LEU:H	1.85	0.42
1:F:40:GLY:HA2	1:F:71:PHE:O	2.19	0.42
1:L:14:ILE:HD13	1:L:68:VAL:HG21	2.01	0.42
1:A:203:THR:HA	1:A:223:TYR:O	2.18	0.42
1:M:103:ASP:HB3	1:M:104:GLY:H	1.57	0.42
1:I:161:ILE:HG22	1:I:162:LYS:N	2.34	0.42
1:C:23:ASN:OD1	1:C:130:PHE:HB2	2.20	0.42
1:K:101:LYS:HG3	1:L:102:CYS:SG	2.60	0.42
1:O:121:ASN:CG	1:O:123:ILE:HD11	2.40	0.42
1:I:12:VAL:HA	1:I:13:PRO:HD3	1.92	0.42
1:B:55:VAL:HG13	1:B:56:PRO:HD2	2.01	0.42
1:B:56:PRO:HD3	1:B:136:ILE:O	2.19	0.42
1:I:52:LYS:HD2	1:I:216:ASP:OD2	2.18	0.42
1:I:28:PHE:HZ	1:I:30:ARG:HE	1.68	0.42
1:A:161:ILE:CG2	1:A:162:LYS:N	2.83	0.42
1:H:203:THR:CB	1:H:224:VAL:HG22	2.50	0.42
1:A:36:ASP:O	1:A:40:GLY:N	2.53	0.42
1:H:55:VAL:HG13	1:H:56:PRO:HD2	2.02	0.42
1:C:156:LYS:HD2	1:L:182:TYR:OH	2.18	0.42
1:C:161:ILE:CG2	1:C:162:LYS:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:18:LEU:HB2	1:N:123:ILE:HD12	2.00	0.42
1:C:55:VAL:HG13	1:C:56:PRO:HD2	2.02	0.42
1:C:98:ILE:HB	1:C:106:TYR:HB2	2.02	0.42
1:E:28:PHE:CZ	1:E:30:ARG:CG	3.01	0.41
1:A:15:LEU:HD22	1:A:30:ARG:NH2	2.35	0.41
1:C:40:GLY:CA	1:C:73:ARG:HB2	2.51	0.41
1:F:136:ILE:O	1:F:138:GLY:N	2.53	0.41
1:G:52:LYS:HG2	1:G:216:ASP:OD2	2.20	0.41
1:G:141:LEU:HD23	1:G:141:LEU:HA	1.85	0.41
1:M:57:TRP:HB3	1:M:218:MET:HE1	2.02	0.41
1:B:106:TYR:HE1	1:B:127:GLY:HA3	1.74	0.41
1:B:7:LEU:HD22	1:B:114:PHE:CD2	2.55	0.41
1:F:33:GLY:N	1:F:44:LEU:HD23	2.34	0.41
1:K:96:ARG:HB2	1:K:108:THR:OG1	2.20	0.41
1:I:211:LEU:HD23	1:I:211:LEU:HA	1.76	0.41
1:O:143:TYR:OH	1:O:208:SER:O	2.37	0.41
1:O:149:LYS:HA	1:O:201:LEU:O	2.20	0.41
1:J:211:LEU:HD23	1:J:211:LEU:HA	1.90	0.41
1:I:28:PHE:CZ	1:I:30:ARG:HG2	2.50	0.41
1:H:142:GLU:OE2	1:L:149:LYS:HE3	2.21	0.41
1:O:114:PHE:CE1	1:O:119:LEU:HD12	2.55	0.41
1:C:112:VAL:HG22	1:C:121:ASN:OD1	2.21	0.41
1:I:149:LYS:HA	1:I:201:LEU:O	2.21	0.41
1:A:114:PHE:CD1	1:A:116:GLY:O	2.73	0.41
1:N:100:PHE:CB	1:N:103:ASP:HB3	2.50	0.41
1:O:205:THR:CG2	1:O:222:GLU:HG2	2.50	0.41
1:L:31:GLY:HA2	1:L:46:PHE:HA	2.02	0.41
1:K:195:LEU:HA	1:K:196:PRO:HD2	1.77	0.41
1:G:36:ASP:O	1:G:40:GLY:N	2.54	0.41
1:P:42:LEU:HB2	1:P:222:GLU:HB3	2.02	0.41
1:G:149:LYS:HA	1:G:201:LEU:O	2.21	0.41
1:K:53:LEU:HD23	1:K:53:LEU:HA	1.88	0.41
1:B:23:ASN:OD1	1:B:130:PHE:HB2	2.20	0.41
1:L:23:ASN:ND2	1:L:130:PHE:HB2	2.36	0.41
1:F:18:LEU:HD23	1:F:19:ASP:C	2.39	0.41
1:G:83:PHE:CB	1:G:161:ILE:HD12	2.46	0.41
1:I:161:ILE:HD13	1:I:161:ILE:HG21	1.90	0.41
1:O:195:LEU:HA	1:O:196:PRO:HD2	1.92	0.41
1:D:143:TYR:CZ	1:D:218:MET:SD	3.14	0.41
1:O:123:ILE:CG2	1:O:124:GLU:N	2.83	0.41
1:E:58:PRO:HA	1:E:61:VAL:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:13:PRO:HD2	1:L:117:ASP:O	2.21	0.41
1:D:162:LYS:HZ3	1:D:184:GLN:CB	2.33	0.41
1:E:152:ILE:CD1	1:E:201:LEU:HD11	2.51	0.41
1:D:47:ILE:HD11	1:D:215:ARG:HG3	2.03	0.41
1:C:56:PRO:HD3	1:C:136:ILE:O	2.21	0.41
1:C:45:LYS:HD3	1:C:219:VAL:HG22	2.01	0.41
1:C:83:PHE:CZ	1:C:160:GLY:HA2	2.55	0.41
1:N:58:PRO:HA	1:N:61:VAL:HG23	2.02	0.41
1:A:53:LEU:HA	1:A:53:LEU:HD23	1.87	0.41
1:N:57:TRP:CG	1:N:218:MET:HG2	2.55	0.41
1:D:108:THR:O	1:D:123:ILE:HG23	2.21	0.41
1:P:36:ASP:HB2	1:P:41:LYS:HB2	2.03	0.41
1:J:12:VAL:HA	1:J:13:PRO:HD3	1.95	0.41
1:D:112:VAL:O	1:D:113:LYS:HB3	2.21	0.41
1:H:15:LEU:HG	1:H:120:VAL:HG22	2.02	0.41
1:M:203:THR:HG22	1:M:224:VAL:HG13	2.02	0.41
1:G:205:THR:HG22	1:G:206:ILE:O	2.21	0.41
1:I:43:SER:CA	1:I:220:LEU:O	2.69	0.41
1:O:35:GLY:CA	1:O:42:LEU:CD2	2.99	0.41
1:F:41:LYS:HE2	1:F:223:TYR:OH	2.21	0.41
1:K:71:PHE:CE2	1:K:119:LEU:HD22	2.54	0.41
1:B:17:GLU:OE2	1:B:30:ARG:NH2	2.54	0.41
1:D:47:ILE:HD11	1:D:215:ARG:CB	2.51	0.41
1:I:128:ILE:HD12	1:I:129:ASP:OD2	2.20	0.41
1:F:108:THR:HA	1:F:124:GLU:O	2.21	0.41
1:O:13:PRO:HD2	1:O:117:ASP:O	2.20	0.41
1:P:53:LEU:HA	1:P:53:LEU:HD23	1.80	0.41
1:B:53:LEU:HA	1:B:53:LEU:HD23	1.87	0.41
1:N:102:CYS:O	1:N:102:CYS:SG	2.79	0.41
1:K:152:ILE:HG23	1:K:161:ILE:CG2	2.51	0.41
1:J:76:ASP:HB3	1:J:77:HIS:H	1.51	0.41
1:B:33:GLY:CA	1:B:44:LEU:HD23	2.51	0.41
1:B:28:PHE:HE2	1:B:30:ARG:HG3	1.86	0.41
1:G:55:VAL:HG13	1:G:56:PRO:HD2	2.03	0.41
1:E:161:ILE:CG2	1:E:162:LYS:N	2.84	0.41
1:G:94:GLN:HB2	1:G:185:ASN:ND2	2.35	0.41
1:M:74:TYR:HA	1:M:75:PRO:HD3	1.87	0.40
1:P:23:ASN:OD1	1:P:130:PHE:HB2	2.21	0.40
1:O:114:PHE:HE1	1:O:119:LEU:HD12	1.86	0.40
1:F:161:ILE:HD11	1:F:196:PRO:HG3	2.03	0.40
1:A:77:HIS:ND1	1:A:77:HIS:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:101:LYS:CB	1:M:178:LEU:HB2	2.52	0.40
1:L:156:LYS:HG2	1:L:195:LEU:HD12	2.04	0.40
1:A:55:VAL:HG22	1:A:136:ILE:HG22	2.04	0.40
1:I:104:GLY:HA3	1:I:130:PHE:CG	2.57	0.40
1:K:44:LEU:HD13	1:K:46:PHE:CZ	2.56	0.40
1:K:39:ILE:O	1:K:39:ILE:HG22	2.21	0.40
1:B:22:VAL:HG22	1:B:106:TYR:CZ	2.55	0.40
1:O:39:ILE:HG23	1:O:41:LYS:HB2	2.03	0.40
1:L:14:ILE:HD11	1:L:71:PHE:CE2	2.57	0.40
1:G:81:HIS:CE1	1:G:197:ASP:HB2	2.55	0.40
1:B:23:ASN:ND2	1:B:130:PHE:O	2.55	0.40
1:B:9:THR:O	1:B:38:THR:CG2	2.69	0.40
1:C:123:ILE:HG22	1:C:124:GLU:N	2.35	0.40
1:J:98:ILE:HB	1:J:106:TYR:HB2	2.04	0.40
1:A:74:TYR:HA	1:A:75:PRO:HD3	1.95	0.40
1:G:15:LEU:HB2	1:G:120:VAL:HG22	2.03	0.40
1:J:10:GLY:HA3	1:L:115:GLU:O	2.21	0.40
1:J:53:LEU:HD23	1:J:53:LEU:HA	1.87	0.40
1:E:211:LEU:HD23	1:E:211:LEU:HA	1.83	0.40
1:A:40:GLY:HA2	1:A:71:PHE:O	2.21	0.40
1:O:205:THR:CB	1:O:222:GLU:HG2	2.51	0.40
1:O:76:ASP:O	1:O:79:LYS:HG3	2.22	0.40
1:O:128:ILE:HG22	1:O:129:ASP:N	2.36	0.40
1:C:28:PHE:HD2	1:C:49:THR:CG2	2.34	0.40
1:O:53:LEU:HD23	1:O:53:LEU:HA	1.80	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:D:157:GLN:OE1	1:F:184:GLN:NE2[1_445]	2.14	0.06
1:C:17:GLU:OE2	1:J:50:THR:OG1[1_455]	2.17	0.03

## 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	207/234 (88%)	195 (94%)	11 (5%)	1 (0%)	34	77
1	B	193/234 (82%)	184 (95%)	8 (4%)	1 (0%)	34	77
1	C	195/234 (83%)	188 (96%)	6 (3%)	1 (0%)	34	77
1	D	174/234 (74%)	161 (92%)	12 (7%)	1 (1%)	30	74
1	E	198/234 (85%)	191 (96%)	6 (3%)	1 (0%)	34	77
1	F	187/234 (80%)	180 (96%)	6 (3%)	1 (0%)	34	77
1	G	176/234 (75%)	167 (95%)	8 (4%)	1 (1%)	30	74
1	H	175/234 (75%)	169 (97%)	6 (3%)	0	100	100
1	I	199/234 (85%)	192 (96%)	6 (3%)	1 (0%)	34	77
1	J	168/234 (72%)	163 (97%)	5 (3%)	0	100	100
1	K	159/234 (68%)	154 (97%)	4 (2%)	1 (1%)	30	74
1	L	187/234 (80%)	181 (97%)	5 (3%)	1 (0%)	34	77
1	M	152/234 (65%)	149 (98%)	2 (1%)	1 (1%)	26	72
1	N	162/234 (69%)	159 (98%)	3 (2%)	0	100	100
1	O	207/234 (88%)	198 (96%)	7 (3%)	2 (1%)	19	65
1	P	192/234 (82%)	186 (97%)	6 (3%)	0	100	100
All	All	2931/3744 (78%)	2817 (96%)	101 (3%)	13 (0%)	39	80

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	VAL
1	F	61	VAL
1	G	206	ILE
1	D	196	PRO
1	C	204	GLN
1	E	196	PRO
1	L	22	VAL
1	K	196	PRO
1	M	103	ASP
1	O	75	PRO
1	B	186	THR
1	I	196	PRO
1	O	186	THR

### 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	189/204 (93%)	188 (100%)	1 (0%)	92	97
1	B	181/204 (89%)	180 (99%)	1 (1%)	90	97
1	C	178/204 (87%)	177 (99%)	1 (1%)	90	97
1	D	170/204 (83%)	170 (100%)	0	100	100
1	E	182/204 (89%)	181 (100%)	1 (0%)	92	97
1	F	175/204 (86%)	174 (99%)	1 (1%)	90	97
1	G	163/204 (80%)	162 (99%)	1 (1%)	90	97
1	H	168/204 (82%)	166 (99%)	2 (1%)	78	91
1	I	183/204 (90%)	181 (99%)	2 (1%)	80	92
1	J	160/204 (78%)	159 (99%)	1 (1%)	90	97
1	K	152/204 (74%)	151 (99%)	1 (1%)	88	95
1	L	171/204 (84%)	170 (99%)	1 (1%)	90	97
1	M	149/204 (73%)	148 (99%)	1 (1%)	88	95
1	N	153/204 (75%)	152 (99%)	1 (1%)	88	95
1	O	179/204 (88%)	178 (99%)	1 (1%)	90	97
1	P	177/204 (87%)	177 (100%)	0	100	100
All	All	2730/3264 (84%)	2714 (99%)	16 (1%)	90	97

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ILE
1	B	108	THR
1	C	159	ASN
1	E	123	ILE
1	F	19	ASP
1	G	123	ILE
1	H	123	ILE
1	H	204	GLN

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Mol	Chain	Res	Type
1	I	119	LEU
1	I	159	ASN
1	J	76	ASP
1	K	128	ILE
1	L	123	ILE
1	M	121	ASN
1	N	102	CYS
1	O	102	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	B	94	GLN
1	B	185	ASN
1	C	204	GLN
1	D	121	ASN
1	F	94	GLN
1	H	94	GLN
1	I	135	ASN
1	J	183	GLN
1	K	144	ASN
1	L	23	ASN
1	L	69	GLN
1	L	94	GLN
1	L	184	GLN
1	N	164	ASN
1	O	139	HIS
1	P	94	GLN
1	P	181	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	215/234 (91%)	1.01	33 (15%) 3 3	50, 80, 148, 324	0
1	B	205/234 (87%)	0.78	25 (12%) 5 6	51, 87, 175, 274	0
1	C	207/234 (88%)	0.93	34 (16%) 2 2	55, 91, 164, 338	0
1	D	194/234 (82%)	0.62	20 (10%) 9 8	57, 92, 169, 237	0
1	E	208/234 (88%)	0.70	23 (11%) 7 7	64, 96, 157, 204	0
1	F	201/234 (85%)	0.94	30 (14%) 3 3	69, 106, 174, 357	0
1	G	188/234 (80%)	0.98	37 (19%) 1 2	52, 103, 181, 284	0
1	H	191/234 (81%)	1.13	40 (20%) 1 1	69, 102, 172, 382	0
1	I	209/234 (89%)	0.68	19 (9%) 11 10	64, 98, 165, 249	0
1	J	184/234 (78%)	0.63	19 (10%) 9 8	51, 95, 166, 270	0
1	K	175/234 (74%)	0.68	18 (10%) 9 8	73, 102, 181, 323	0
1	L	197/234 (84%)	1.19	45 (22%) 1 1	67, 114, 206, 293	0
1	M	168/234 (71%)	1.30	37 (22%) 1 1	75, 119, 203, 375	0
1	N	174/234 (74%)	1.27	45 (25%) 1 1	72, 130, 219, 388	0
1	O	213/234 (91%)	1.53	56 (26%) 1 1	54, 126, 205, 302	0
1	P	204/234 (87%)	1.25	49 (24%) 1 1	73, 134, 217, 464	0
All	All	3133/3744 (83%)	0.98	530 (16%) 2 2	50, 104, 188, 464	0

All (530) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	164	ASN	11.6
1	M	164	ASN	9.9
1	O	86	SER	9.4
1	M	76	ASP	9.2
1	O	223	TYR	9.0

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Mol	Chain	Res	Type	RSRZ
1	L	49	THR	8.2
1	G	49	THR	7.8
1	H	194	ASP	7.8
1	O	118	THR	7.7
1	N	117	ASP	7.4
1	M	152	ILE	7.3
1	B	117	ASP	7.0
1	P	185	ASN	6.8
1	O	224	VAL	6.8
1	E	133	ASP	6.8
1	O	222	GLU	6.8
1	O	76	ASP	6.7
1	O	196	PRO	6.4
1	P	117	ASP	6.4
1	H	121	ASN	6.2
1	L	180	ASP	6.2
1	O	8	PHE	6.2
1	H	144	ASN	6.1
1	J	117	ASP	6.0
1	P	182	TYR	6.0
1	M	153	THR	6.0
1	O	85	LYS	6.0
1	L	213	GLU	5.8
1	F	139	HIS	5.7
1	H	110	ALA	5.7
1	N	116	GLY	5.7
1	D	36	ASP	5.6
1	N	218	MET	5.5
1	H	122	ARG	5.5
1	O	87	ALA	5.5
1	P	158	ASN	5.5
1	O	225	THR	5.5
1	A	49	THR	5.4
1	C	34	GLU	5.4
1	K	71	PHE	5.4
1	M	151	TYR	5.4
1	M	72	SER	5.4
1	I	32	GLU	5.3
1	N	214	LYS	5.3
1	L	115	GLU	5.3
1	M	12	VAL	5.2
1	A	133	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	N	213	GLU	5.1
1	O	114	PHE	5.1
1	D	196	PRO	5.0
1	O	117	ASP	5.0
1	L	212	ASN	5.0
1	L	133	ASP	4.9
1	O	53	LEU	4.9
1	L	117	ASP	4.9
1	P	184	GLN	4.9
1	P	86	SER	4.8
1	D	72	SER	4.8
1	F	49	THR	4.8
1	B	153	THR	4.8
1	O	151	TYR	4.7
1	M	48	ALA	4.7
1	O	197	ASP	4.7
1	F	10	GLY	4.6
1	O	150	VAL	4.5
1	L	134	GLY	4.5
1	B	106	TYR	4.5
1	G	50	THR	4.5
1	H	117	ASP	4.5
1	M	11	VAL	4.5
1	C	41	LYS	4.4
1	I	116	GLY	4.4
1	C	51	GLY	4.4
1	O	81	HIS	4.4
1	C	38	THR	4.4
1	O	75	PRO	4.4
1	G	217	HIS	4.4
1	A	70	CYS	4.4
1	L	141	LEU	4.4
1	F	58	PRO	4.3
1	A	112	VAL	4.3
1	G	223	TYR	4.3
1	L	44	LEU	4.3
1	O	200	TYR	4.3
1	C	188	ILE	4.3
1	E	6	GLU	4.3
1	H	195	LEU	4.2
1	G	57	TRP	4.2
1	O	125	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	G	118	THR	4.2
1	H	92	TYR	4.2
1	H	34	GLU	4.2
1	P	216	ASP	4.2
1	J	36	ASP	4.1
1	P	82	ASP	4.1
1	A	136	ILE	4.1
1	M	178	LEU	4.1
1	P	157	GLN	4.1
1	G	117	ASP	4.1
1	N	115	GLU	4.1
1	F	51	GLY	4.1
1	K	185	ASN	4.0
1	B	82	ASP	4.0
1	O	115	GLU	4.0
1	P	112	VAL	4.0
1	G	218	MET	4.0
1	F	53	LEU	4.0
1	P	181	HIS	3.9
1	A	82	ASP	3.9
1	L	34	GLU	3.9
1	L	190	ASP	3.9
1	B	30	ARG	3.9
1	O	74	TYR	3.8
1	P	53	LEU	3.8
1	L	187	PRO	3.8
1	H	57	TRP	3.8
1	N	196	PRO	3.8
1	L	26	LYS	3.8
1	O	143	TYR	3.8
1	B	80	ARG	3.8
1	C	21	ASP	3.8
1	I	4	GLY	3.8
1	A	198	ASP	3.7
1	I	117	ASP	3.7
1	G	110	ALA	3.7
1	N	86	SER	3.7
1	I	7	LEU	3.7
1	O	201	LEU	3.7
1	P	68	VAL	3.7
1	F	54	PRO	3.7
1	M	217	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	L	47	ILE	3.7
1	C	10	GLY	3.6
1	H	109	ARG	3.6
1	N	131	LYS	3.6
1	B	110	ALA	3.6
1	E	76	ASP	3.6
1	A	30	ARG	3.6
1	P	32	GLU	3.6
1	B	34	GLU	3.6
1	A	139	HIS	3.6
1	O	90	GLU	3.6
1	H	70	CYS	3.6
1	A	186	THR	3.6
1	J	102	CYS	3.6
1	P	140	LYS	3.5
1	A	68	VAL	3.5
1	I	52	LYS	3.5
1	G	208	SER	3.5
1	O	83	PHE	3.5
1	G	111	GLU	3.5
1	M	179	ALA	3.5
1	F	23	ASN	3.5
1	B	43	SER	3.5
1	L	195	LEU	3.5
1	P	152	ILE	3.5
1	E	227	ALA	3.4
1	P	52	LYS	3.4
1	C	73	ARG	3.4
1	F	192	PRO	3.4
1	J	180	ASP	3.4
1	H	15	LEU	3.4
1	O	141	LEU	3.4
1	M	77	HIS	3.4
1	O	9	THR	3.4
1	A	83	PHE	3.4
1	I	8	PHE	3.4
1	P	169	HIS	3.4
1	E	134	GLY	3.4
1	G	48	ALA	3.4
1	D	7	LEU	3.4
1	L	21	ASP	3.4
1	H	35	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	N	163	ALA	3.4
1	B	109	ARG	3.4
1	O	84	PHE	3.4
1	G	141	LEU	3.4
1	O	170	ASN	3.3
1	F	35	GLY	3.3
1	E	222	GLU	3.3
1	O	88	MET	3.3
1	L	222	GLU	3.3
1	P	196	PRO	3.3
1	M	155	ASP	3.3
1	K	92	TYR	3.3
1	G	40	GLY	3.3
1	G	83	PHE	3.3
1	K	64	LEU	3.3
1	E	5	GLU	3.3
1	N	103	ASP	3.3
1	C	8	PHE	3.2
1	D	83	PHE	3.2
1	H	218	MET	3.2
1	K	119	LEU	3.2
1	J	146	ASN	3.2
1	O	134	GLY	3.2
1	F	153	THR	3.2
1	N	119	LEU	3.2
1	P	95	GLU	3.2
1	H	90	GLU	3.2
1	P	198	ASP	3.2
1	H	37	ALA	3.2
1	F	82	ASP	3.1
1	H	161	ILE	3.1
1	O	116	GLY	3.1
1	F	46	PHE	3.1
1	H	120	VAL	3.1
1	P	81	HIS	3.1
1	H	43	SER	3.1
1	C	70	CYS	3.1
1	N	45	LYS	3.1
1	H	124	GLU	3.1
1	F	84	PHE	3.1
1	M	57	TRP	3.1
1	I	53	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	126	LYS	3.1
1	L	36	ASP	3.1
1	O	89	PRO	3.1
1	C	160	GLY	3.1
1	I	102	CYS	3.0
1	H	44	LEU	3.0
1	B	77	HIS	3.0
1	D	116	GLY	3.0
1	N	57	TRP	3.0
1	N	36	ASP	3.0
1	C	161	ILE	3.0
1	L	116	GLY	3.0
1	F	92	TYR	3.0
1	M	49	THR	3.0
1	P	155	ASP	3.0
1	M	218	MET	3.0
1	C	75	PRO	3.0
1	I	36	ASP	3.0
1	O	54	PRO	3.0
1	C	82	ASP	3.0
1	A	212	ASN	3.0
1	L	214	LYS	3.0
1	J	133	ASP	2.9
1	H	111	GLU	2.9
1	O	57	TRP	2.9
1	O	92	TYR	2.9
1	A	48	ALA	2.9
1	A	110	ALA	2.9
1	P	14	ILE	2.9
1	E	131	LYS	2.9
1	H	68	VAL	2.9
1	M	180	ASP	2.9
1	B	164	ASN	2.9
1	D	195	LEU	2.9
1	L	70	CYS	2.9
1	B	151	TYR	2.9
1	N	161	ILE	2.9
1	O	108	THR	2.9
1	G	26	LYS	2.9
1	H	118	THR	2.9
1	O	42	LEU	2.9
1	G	11	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	182	TYR	2.9
1	G	121	ASN	2.9
1	F	57	TRP	2.9
1	N	223	TYR	2.9
1	P	54	PRO	2.8
1	P	94	GLN	2.8
1	G	209	LYS	2.8
1	L	102	CYS	2.8
1	L	170	ASN	2.8
1	H	24	GLY	2.8
1	N	145	PHE	2.8
1	P	164	ASN	2.8
1	A	93	VAL	2.8
1	P	143	TYR	2.8
1	M	14	ILE	2.8
1	G	60	LEU	2.8
1	O	137	LEU	2.8
1	P	100	PHE	2.8
1	A	23	ASN	2.8
1	J	185	ASN	2.8
1	D	78	MET	2.8
1	G	112	VAL	2.8
1	M	121	ASN	2.8
1	M	161	ILE	2.8
1	O	40	GLY	2.8
1	B	161	ILE	2.8
1	D	10	GLY	2.8
1	N	92	TYR	2.8
1	F	11	VAL	2.8
1	H	217	HIS	2.8
1	M	177	GLN	2.8
1	O	14	ILE	2.8
1	L	68	VAL	2.8
1	L	88	MET	2.8
1	F	36	ASP	2.8
1	A	188	ILE	2.8
1	C	72	SER	2.8
1	P	64	LEU	2.8
1	P	170	ASN	2.8
1	F	64	LEU	2.7
1	O	119	LEU	2.7
1	G	17	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	68	VAL	2.7
1	H	153	THR	2.7
1	I	21	ASP	2.7
1	L	215	ARG	2.7
1	N	200	TYR	2.7
1	L	30	ARG	2.7
1	E	129	ASP	2.7
1	A	226	ALA	2.7
1	J	71	PHE	2.7
1	N	180	ASP	2.7
1	E	130	PHE	2.7
1	L	35	GLY	2.7
1	O	32	GLU	2.7
1	B	162	LYS	2.7
1	I	39	ILE	2.7
1	H	12	VAL	2.7
1	G	220	LEU	2.7
1	N	44	LEU	2.7
1	N	48	ALA	2.7
1	C	78	MET	2.7
1	E	88	MET	2.7
1	G	120	VAL	2.7
1	C	91	GLY	2.7
1	E	10	GLY	2.7
1	J	7	LEU	2.7
1	C	85	LYS	2.6
1	J	184	GLN	2.6
1	P	113	LYS	2.6
1	H	163	ALA	2.6
1	H	71	PHE	2.6
1	O	163	ALA	2.6
1	A	135	ASN	2.6
1	I	214	LYS	2.6
1	M	210	ASP	2.6
1	O	102	CYS	2.6
1	N	46	PHE	2.6
1	D	115	GLU	2.6
1	E	132	GLU	2.6
1	L	48	ALA	2.6
1	L	101	LYS	2.6
1	G	145	PHE	2.6
1	E	164	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	21	ASP	2.5
1	C	22	VAL	2.5
1	M	222	GLU	2.5
1	J	13	PRO	2.5
1	P	102	CYS	2.5
1	D	152	ILE	2.5
1	L	206	ILE	2.5
1	N	128	ILE	2.5
1	F	161	ILE	2.5
1	M	213	GLU	2.5
1	G	138	GLY	2.5
1	H	83	PHE	2.5
1	C	48	ALA	2.5
1	G	180	ASP	2.5
1	B	206	ILE	2.5
1	A	94	GLN	2.5
1	L	15	LEU	2.5
1	N	102	CYS	2.5
1	G	27	PHE	2.5
1	N	19	ASP	2.5
1	H	102	CYS	2.5
1	L	135	ASN	2.5
1	L	189	GLY	2.5
1	J	44	LEU	2.5
1	B	8	PHE	2.5
1	E	114	PHE	2.5
1	F	27	PHE	2.5
1	B	133	ASP	2.4
1	D	15	LEU	2.4
1	A	57	TRP	2.4
1	D	79	LYS	2.4
1	K	172	GLU	2.4
1	M	215	ARG	2.4
1	B	222	GLU	2.4
1	P	80	ARG	2.4
1	B	87	ALA	2.4
1	C	142	GLU	2.4
1	K	127	GLY	2.4
1	O	205	THR	2.4
1	O	152	ILE	2.4
1	F	159	ASN	2.4
1	P	83	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	140	LYS	2.4
1	P	73	ARG	2.4
1	E	213	GLU	2.4
1	E	9	THR	2.4
1	E	152	ILE	2.4
1	O	43	SER	2.4
1	P	178	LEU	2.4
1	C	39	ILE	2.4
1	L	92	TYR	2.4
1	O	145	PHE	2.4
1	L	81	HIS	2.4
1	A	120	VAL	2.4
1	F	164	ASN	2.4
1	F	163	ALA	2.4
1	H	152	ILE	2.4
1	M	119	LEU	2.4
1	N	151	TYR	2.4
1	I	216	ASP	2.3
1	I	14	ILE	2.3
1	B	68	VAL	2.3
1	N	47	ILE	2.3
1	K	175	SER	2.3
1	L	50	THR	2.3
1	C	133	ASP	2.3
1	H	84	PHE	2.3
1	H	123	ILE	2.3
1	C	106	TYR	2.3
1	M	127	GLY	2.3
1	A	119	LEU	2.3
1	G	15	LEU	2.3
1	N	190	ASP	2.3
1	L	13	PRO	2.3
1	P	195	LEU	2.3
1	C	135	ASN	2.3
1	D	6	GLU	2.3
1	N	63	THR	2.3
1	G	144	ASN	2.3
1	N	212	ASN	2.3
1	I	208	SER	2.3
1	C	181	HIS	2.3
1	C	205	THR	2.3
1	O	82	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	28	PHE	2.3
1	N	155	ASP	2.3
1	H	72	SER	2.3
1	J	39	ILE	2.3
1	D	37	ALA	2.2
1	J	163	ALA	2.2
1	M	96	ARG	2.2
1	A	211	LEU	2.2
1	C	83	PHE	2.2
1	H	47	ILE	2.2
1	N	222	GLU	2.2
1	G	53	LEU	2.2
1	K	84	PHE	2.2
1	F	107	LYS	2.2
1	B	92	TYR	2.2
1	G	116	GLY	2.2
1	K	141	LEU	2.2
1	G	36	ASP	2.2
1	E	77	HIS	2.2
1	O	226	ALA	2.2
1	P	115	GLU	2.2
1	I	73	ARG	2.2
1	N	100	PHE	2.2
1	N	165	PHE	2.2
1	A	88	MET	2.2
1	M	209	LYS	2.2
1	H	25	HIS	2.2
1	D	68	VAL	2.2
1	G	39	ILE	2.2
1	J	207	LEU	2.2
1	N	37	ALA	2.2
1	N	54	PRO	2.2
1	N	99	TYR	2.2
1	D	75	PRO	2.2
1	A	77	HIS	2.2
1	D	84	PHE	2.2
1	F	8	PHE	2.2
1	N	61	VAL	2.2
1	A	200	TYR	2.2
1	C	184	GLN	2.2
1	G	46	PHE	2.2
1	K	125	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	O	36	ASP	2.2
1	P	145	PHE	2.2
1	P	40	GLY	2.2
1	C	36	ASP	2.2
1	B	132	GLU	2.1
1	B	184	GLN	2.1
1	H	69	GLN	2.1
1	M	165	PHE	2.1
1	P	87	ALA	2.1
1	M	19	ASP	2.1
1	E	72	SER	2.1
1	J	58	PRO	2.1
1	L	29	VAL	2.1
1	A	36	ASP	2.1
1	K	198	ASP	2.1
1	N	198	ASP	2.1
1	F	52	LYS	2.1
1	K	144	ASN	2.1
1	O	164	ASN	2.1
1	I	27	PHE	2.1
1	P	226	ALA	2.1
1	K	23	ASN	2.1
1	L	97	THR	2.1
1	P	199	HIS	2.1
1	L	164	ASN	2.1
1	M	15	LEU	2.1
1	N	132	GLU	2.1
1	A	109	ARG	2.1
1	A	172	GLU	2.1
1	C	94	GLN	2.1
1	J	46	PHE	2.1
1	G	122	ARG	2.1
1	P	201	LEU	2.1
1	C	223	TYR	2.1
1	E	52	LYS	2.1
1	E	79	LYS	2.1
1	F	176	VAL	2.1
1	M	43	SER	2.1
1	M	55	VAL	2.1
1	N	118	THR	2.1
1	K	46	PHE	2.1
1	J	43	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	59	THR	2.1
1	G	222	GLU	2.1
1	A	12	VAL	2.1
1	O	133	ASP	2.0
1	E	140	LYS	2.0
1	B	33	GLY	2.0
1	F	196	PRO	2.0
1	L	87	ALA	2.0
1	D	114	PHE	2.0
1	N	211	LEU	2.0
1	C	117	ASP	2.0
1	D	74	TYR	2.0
1	K	143	TYR	2.0
1	K	223	TYR	2.0
1	M	61	VAL	2.0
1	M	225	THR	2.0
1	P	62	THR	2.0
1	P	118	THR	2.0
1	A	117	ASP	2.0
1	P	154	ALA	2.0
1	L	207	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.