



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:07 PM GMT

PDB ID : 4UV3  
Title : Structure of the curli transport lipoprotein CsgG in its membrane- bound conformation  
Authors : Goyal, P.; Krasteva, P.V.; Gerven, N.V.; Gubellini, F.; Broeck, I.V.D.; Troupiotis-Tsailaki, A.; Jonckheere, W.; Pehau-Arnaudet, G.; Pinkner, J.S.; Chapman, M.R.; Hultgren, S.J.; Howorka, S.; Fronzes, R.; Remaut, H.  
Deposited on : 2014-08-04  
Resolution : 3.59 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

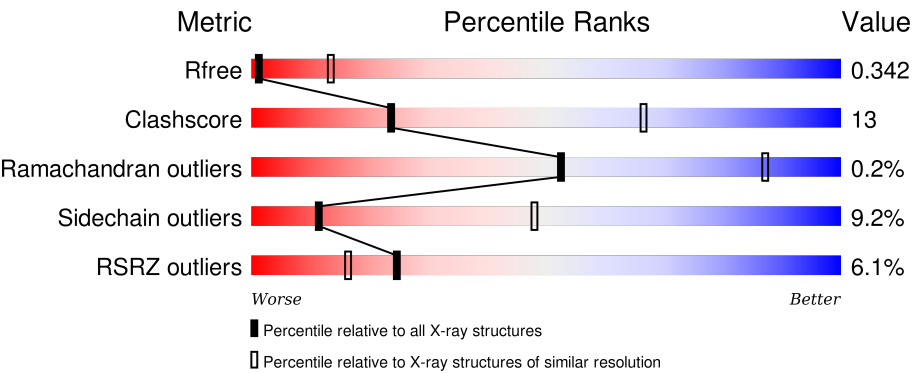
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.59 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	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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	262	<div><div>2%</div><div>66%</div><div>26%</div><div>• 5%</div></div>
1	B	262	<div><div>2%</div><div>66%</div><div>26%</div><div>• 5%</div></div>
1	C	262	<div><div>7%</div><div>66%</div><div>27%</div><div>• 6%</div></div>
1	D	262	<div><div>11%</div><div>66%</div><div>25%</div><div>• 5%</div></div>
1	E	262	<div><div>13%</div><div>62%</div><div>30%</div><div>• 6%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	262	
1	G	262	
1	H	262	
1	I	262	
1	J	262	
1	K	262	
1	L	262	
1	M	262	
1	N	262	
1	O	262	
1	P	262	
1	Q	262	
1	R	262	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 34255 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 CURLI PRODUCTION ASSEMBLY/TRANSPORT COMPONENT CSGG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1911	1204	333	367	7			
1	B	248	Total	C	N	O	S	0	0	0
			1911	1204	333	367	7			
1	C	247	Total	C	N	O	S	0	0	0
			1900	1198	329	366	7			
1	D	248	Total	C	N	O	S	0	0	0
			1911	1204	333	367	7			
1	E	247	Total	C	N	O	S	0	0	0
			1900	1198	329	366	7			
1	F	247	Total	C	N	O	S	0	0	0
			1900	1198	329	366	7			
1	G	247	Total	C	N	O	S	0	0	0
			1900	1198	329	366	7			
1	H	248	Total	C	N	O	S	0	0	0
			1911	1204	333	367	7			
1	I	247	Total	C	N	O	S	0	0	0
			1900	1198	329	366	7			
1	J	248	Total	C	N	O	S	0	0	0
			1911	1204	333	367	7			
1	K	247	Total	C	N	O	S	0	0	0
			1900	1198	329	366	7			
1	L	247	Total	C	N	O	S	0	0	0
			1900	1198	329	366	7			
1	M	247	Total	C	N	O	S	0	0	0
			1900	1198	329	366	7			
1	N	247	Total	C	N	O	S	0	0	0
			1900	1198	329	366	7			
1	O	247	Total	C	N	O	S	0	0	0
			1900	1198	329	366	7			
1	P	247	Total	C	N	O	S	0	0	0
			1900	1198	329	366	7			

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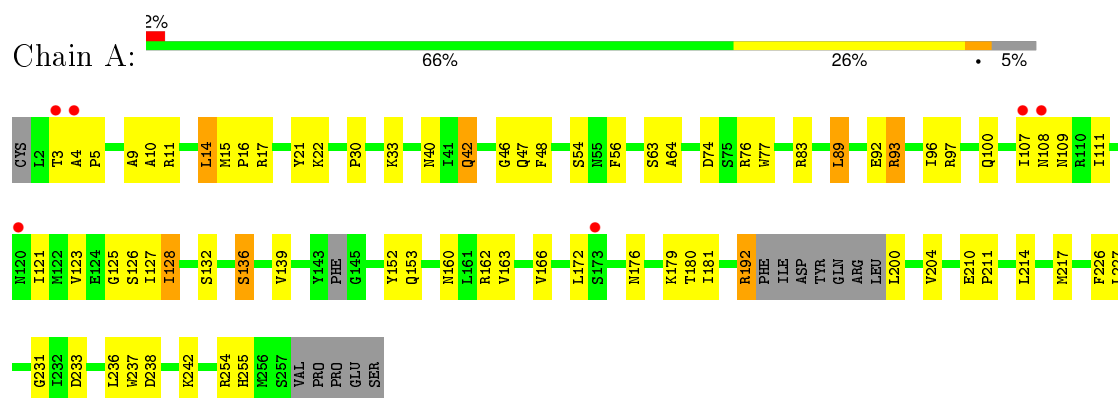
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	247	Total	C	N	O	S	0	0	0
			1900	1198	329	366	7			
1	R	247	Total	C	N	O	S	0	0	0
			1900	1198	329	366	7			

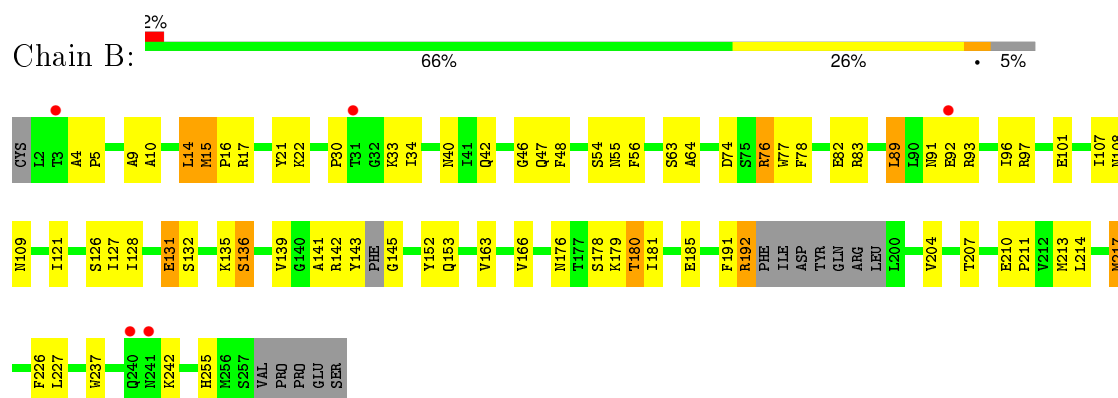
### 3 Residue-property plots [i](#)

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.

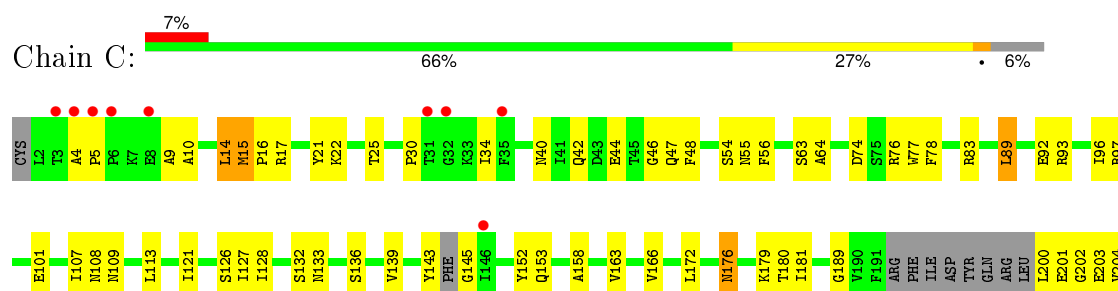
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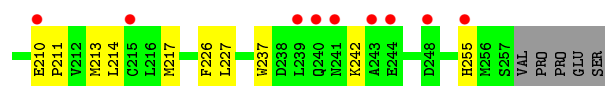


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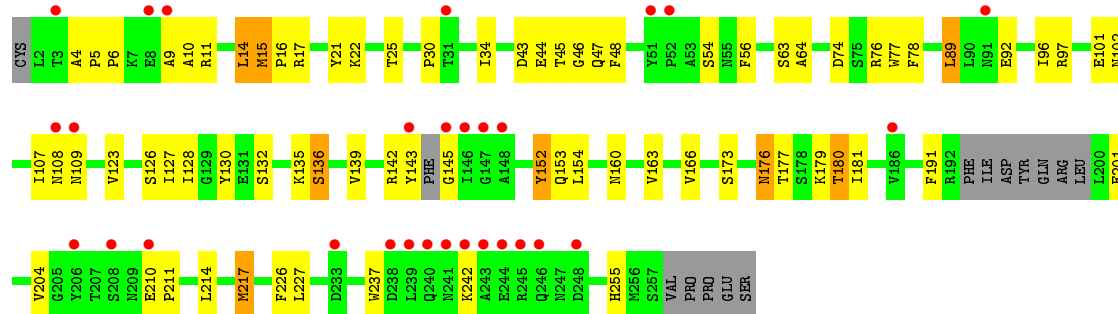


#### • Molecule 1: CURLI PRODUCTION ASSEMBLY/TRANSPORT COMPONENT CSGG

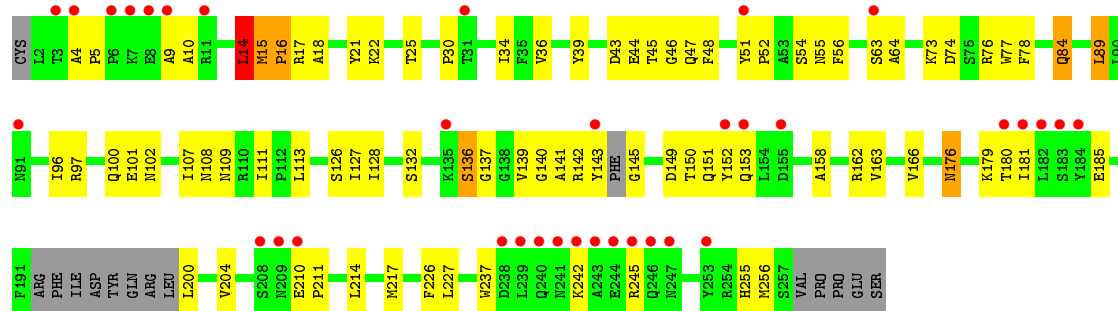




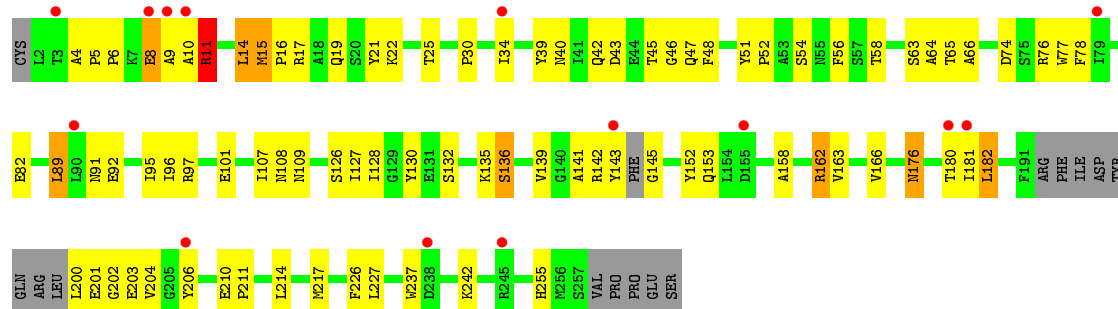
• Molecule 1: CURLI PRODUCTION ASSEMBLY/TRANSPORT COMPONENT CSGG



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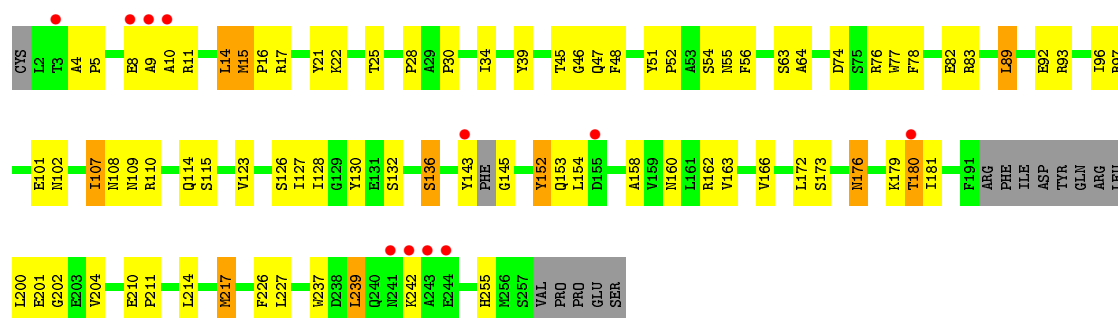


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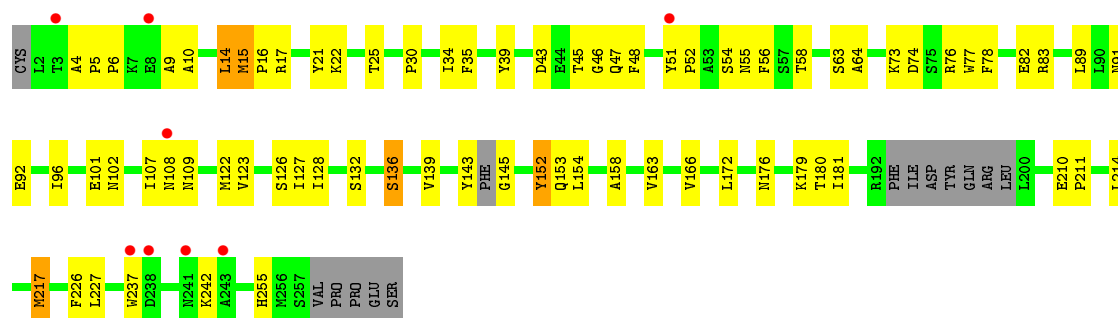


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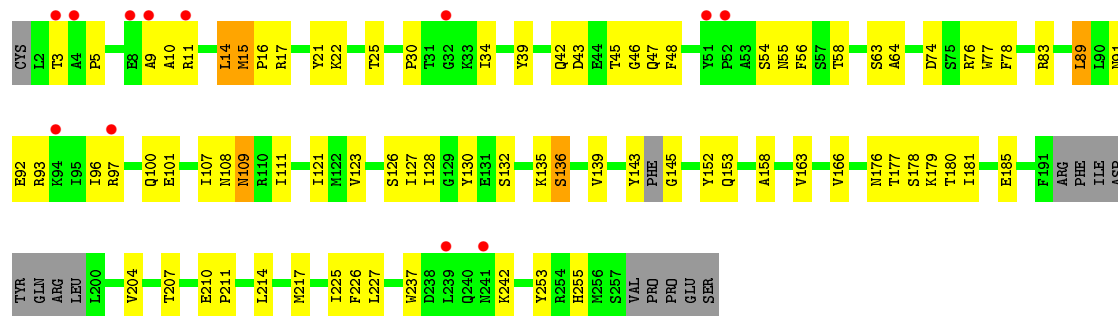




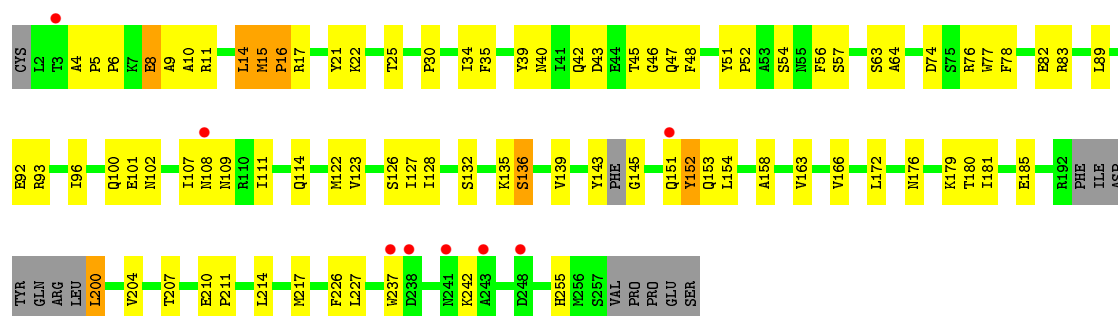
- Molecule 1: CURLI PRODUCTION ASSEMBLY/TRANSPORT COMPONENT CSGG



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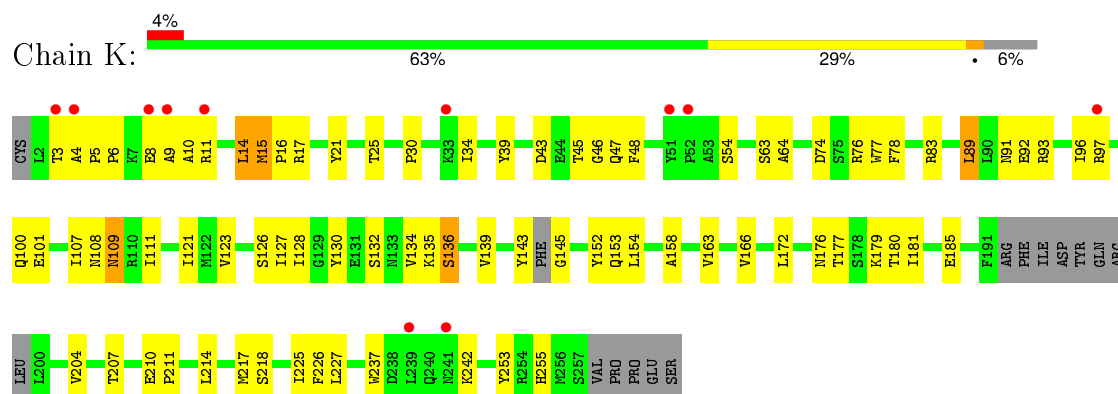


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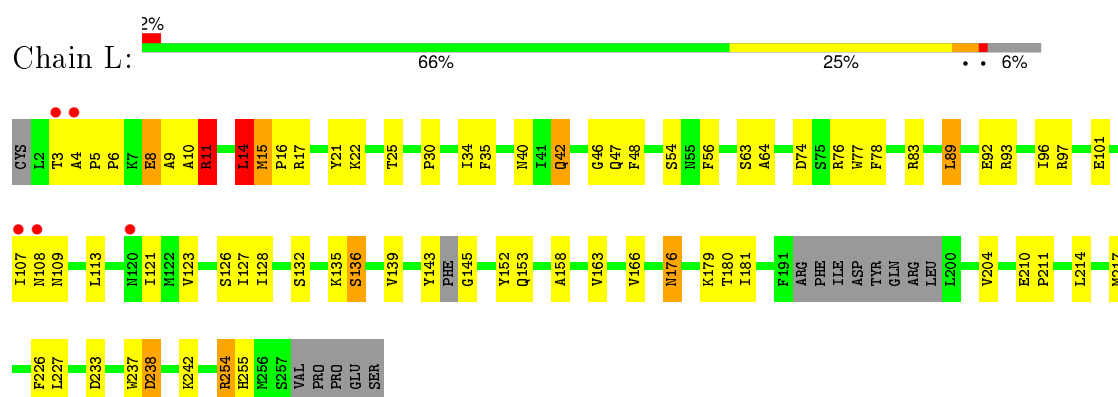




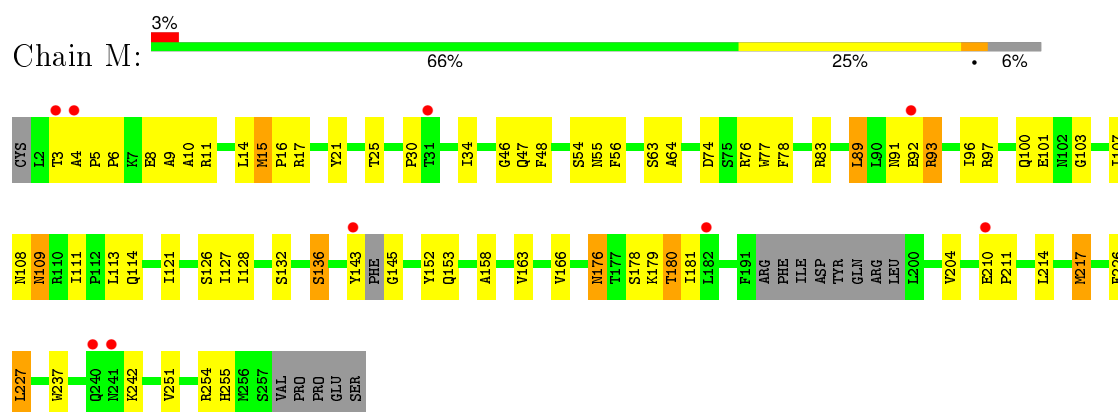
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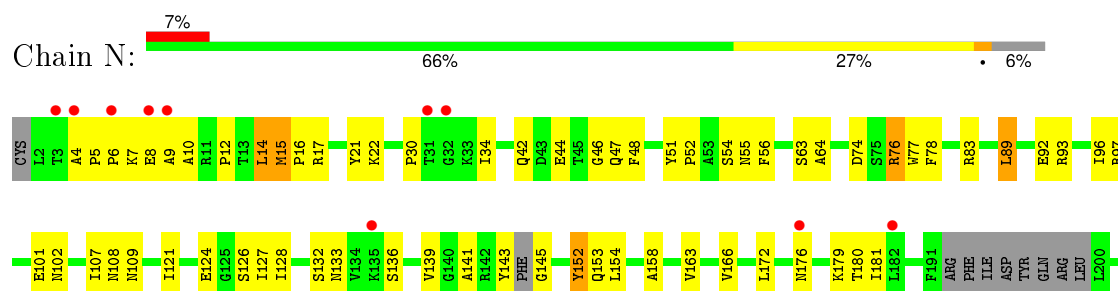
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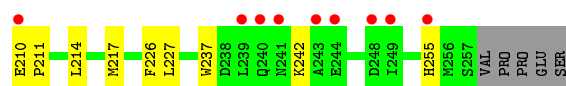


• Molecule 1: CURLI PRODUCTION ASSEMBLY/TRANSPORT COMPONENT CSGG

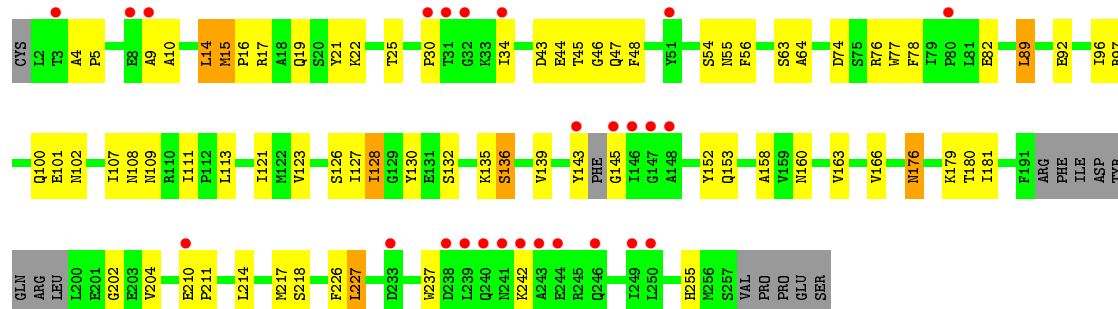


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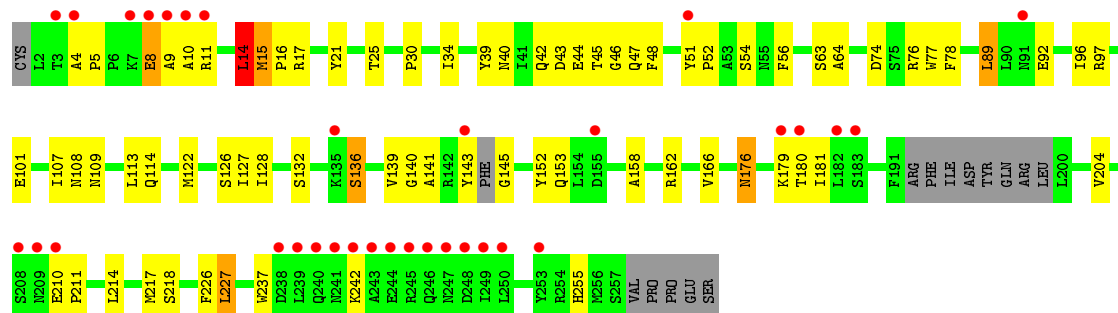




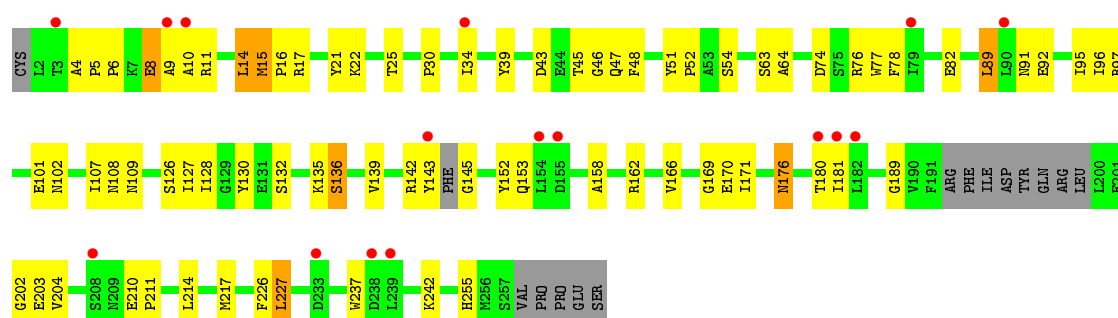
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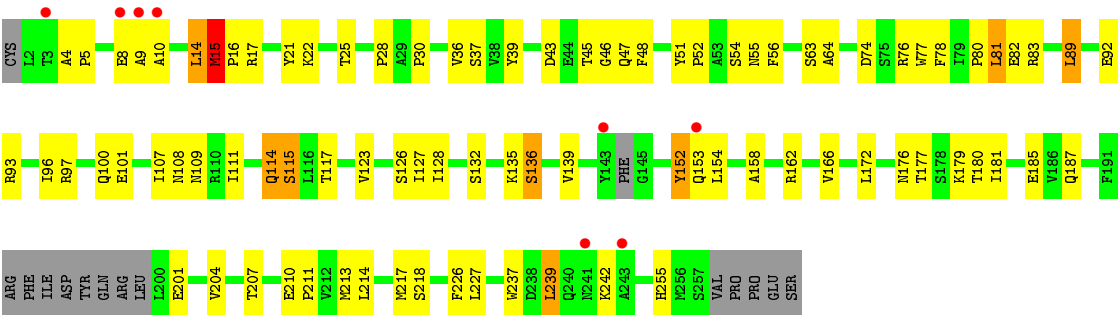


• Molecule 1: CURLI PRODUCTION ASSEMBLY/TRANSPORT COMPONENT CSGG



• Molecule 1: CURLI PRODUCTION ASSEMBLY/TRANSPORT COMPONENT CSGG





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.93Å 372.85Å 161.97Å 90.00° 92.90° 90.00°	Depositor
Resolution (Å)	30.00 – 3.59 43.85 – 3.59	Depositor EDS
% Data completeness (in resolution range)	91.5 (30.00-3.59) 91.6 (43.85-3.59)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.297 , 0.349 0.293 , 0.342	Depositor DCC
$R_{free}$ test set	5104 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	101.0	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 91.0	EDS
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	3 of 102130 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	34255	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.94 % 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 3.9236e-05. 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.62	0/1941	0.75	1/2633 (0.0%)
1	B	0.57	0/1941	0.74	1/2633 (0.0%)
1	C	0.53	0/1930	0.70	0/2619
1	D	0.52	0/1941	0.68	0/2633
1	E	0.59	0/1930	0.73	0/2619
1	F	0.58	0/1930	0.74	3/2619 (0.1%)
1	G	0.58	0/1930	0.73	0/2619
1	H	0.56	0/1941	0.71	0/2633
1	I	0.55	0/1930	0.70	0/2619
1	J	0.56	0/1941	0.69	0/2633
1	K	0.56	0/1930	0.70	0/2619
1	L	0.62	0/1930	0.77	3/2619 (0.1%)
1	M	0.57	0/1930	0.74	2/2619 (0.1%)
1	N	0.52	0/1930	0.70	0/2619
1	O	0.51	0/1930	0.70	1/2619 (0.0%)
1	P	0.56	0/1930	0.71	0/2619
1	Q	0.57	0/1930	0.71	0/2619
1	R	0.64	2/1930 (0.1%)	0.76	1/2619 (0.0%)
All	All	0.57	2/34795 (0.0%)	0.72	12/47212 (0.0%)

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	E	0	1
1	L	0	1
1	P	0	1
1	R	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	115	SER	C-O	-5.42	1.13	1.23
1	R	15	MET	CG-SD	-5.03	1.68	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	81	LEU	C-N-CA	5.73	136.02	121.70
1	O	128	ILE	CB-CA-C	-5.68	100.24	111.60
1	F	11	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	L	11	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	L	238	ASP	CB-CG-OD1	5.53	123.27	118.30
1	L	238	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	F	162	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	A	93	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	76	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	F	182	LEU	CA-CB-CG	5.05	126.92	115.30
1	M	8	GLU	OE1-CD-OE2	-5.03	117.26	123.30
1	M	93	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	14	LEU	Peptide
1	L	14	LEU	Peptide
1	P	14	LEU	Peptide
1	R	78	PHE	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	1911	0	1930	70	0
1	B	1911	0	1930	60	0
1	C	1900	0	1917	63	0
1	D	1911	0	1930	67	0
1	E	1900	0	1917	82	0
1	F	1900	0	1917	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1900	0	1917	86	0
1	H	1911	0	1930	85	0
1	I	1900	0	1917	68	0
1	J	1911	0	1930	90	0
1	K	1900	0	1917	71	0
1	L	1900	0	1917	83	0
1	M	1900	0	1917	68	0
1	N	1900	0	1917	67	0
1	O	1900	0	1917	69	0
1	P	1900	0	1917	67	0
1	Q	1900	0	1917	67	0
1	R	1900	0	1917	80	0
All	All	34255	0	34571	909	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (909) 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:F:107:ILE:HD13	1:N:107:ILE:HD13	1.33	1.09
1:E:107:ILE:HD13	1:O:107:ILE:HD13	1.38	1.05
1:E:84:GLN:HG3	1:E:84:GLN:O	1.57	0.99
1:D:107:ILE:HD13	1:P:107:ILE:HD13	1.44	0.99
1:F:182:LEU:HD22	1:G:9:ALA:HB1	1.43	0.99
1:C:107:ILE:HD13	1:Q:107:ILE:HD13	1.46	0.96
1:J:54:SER:HB3	1:R:48:PHE:HB2	1.49	0.94
1:A:107:ILE:HD13	1:J:107:ILE:HD13	1.49	0.94
1:N:226:PHE:CZ	1:O:14:LEU:HD22	2.05	0.92
1:F:182:LEU:HD22	1:G:9:ALA:CB	1.98	0.92
1:J:200:LEU:HD23	1:J:200:LEU:O	1.69	0.92
1:F:162:ARG:NH2	1:G:82:GLU:OE1	2.03	0.92
1:C:226:PHE:CZ	1:D:14:LEU:HD22	2.06	0.90
1:L:233:ASP:OD2	1:L:254:ARG:NH2	2.03	0.90
1:H:107:ILE:HD13	1:L:107:ILE:HD13	1.54	0.90
1:J:48:PHE:HB2	1:K:54:SER:HB3	1.55	0.89
1:G:48:PHE:HB2	1:H:54:SER:HB3	1.54	0.89
1:G:128:ILE:HD11	1:G:160:ASN:HB2	1.55	0.89
1:D:226:PHE:CZ	1:E:14:LEU:HD22	2.08	0.88
1:O:128:ILE:HD11	1:O:160:ASN:HB2	1.58	0.86
1:A:14:LEU:HD22	1:I:226:PHE:CZ	2.11	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:36:VAL:HG12	1:R:80:PRO:HA	1.58	0.86
1:K:3:THR:HA	1:R:154:LEU:HD22	1.58	0.85
1:N:16:PRO:HG3	1:O:5:PRO:HG3	1.58	0.84
1:M:55:ASN:ND2	1:N:56:PHE:CE2	2.46	0.83
1:H:16:PRO:HG3	1:I:5:PRO:HG3	1.61	0.82
1:B:107:ILE:HD13	1:R:107:ILE:HD13	1.61	0.82
1:K:226:PHE:CZ	1:L:14:LEU:HD22	2.15	0.82
1:H:48:PHE:HB2	1:I:54:SER:HB3	1.59	0.81
1:J:154:LEU:HD22	1:L:3:THR:HB	1.63	0.80
1:O:226:PHE:CZ	1:P:14:LEU:HD22	2.17	0.80
1:Q:189:GLY:HA3	1:Q:203:GLU:OE2	1.82	0.80
1:A:92:GLU:OE2	1:I:83:ARG:NE	2.14	0.79
1:Q:171:ILE:HG13	1:R:82:GLU:HB2	1.65	0.78
1:J:14:LEU:HD22	1:R:226:PHE:CZ	2.18	0.78
1:B:145:GLY:N	1:B:191:PHE:O	2.18	0.77
1:E:48:PHE:HB2	1:F:54:SER:HB3	1.65	0.77
1:Q:226:PHE:CZ	1:R:14:LEU:HD22	2.20	0.76
1:A:3:THR:O	1:H:180:THR:HG21	1.86	0.76
1:I:107:ILE:HD13	1:K:107:ILE:HD13	1.67	0.76
1:J:152:TYR:CE2	1:L:3:THR:HG22	2.21	0.75
1:N:48:PHE:HB2	1:O:54:SER:HB3	1.69	0.75
1:C:16:PRO:HG3	1:D:5:PRO:HG3	1.67	0.75
1:J:48:PHE:HB2	1:K:54:SER:CB	2.17	0.74
1:G:226:PHE:CZ	1:H:14:LEU:HD22	2.21	0.74
1:J:54:SER:CB	1:R:48:PHE:HB2	2.17	0.74
1:A:226:PHE:CZ	1:B:14:LEU:HD22	2.22	0.74
1:F:226:PHE:CZ	1:G:14:LEU:HD22	2.23	0.74
1:F:139:VAL:HG22	1:G:204:VAL:HG22	1.70	0.73
1:M:226:PHE:CZ	1:N:14:LEU:HD22	2.23	0.73
1:D:48:PHE:HB2	1:E:54:SER:HB3	1.70	0.73
1:D:128:ILE:HG23	1:E:63:SER:OG	1.89	0.72
1:P:136:SER:HB2	1:P:153:GLN:HG3	1.71	0.72
1:P:48:PHE:HB2	1:Q:54:SER:HB3	1.70	0.72
1:M:210:GLU:OE1	1:N:9:ALA:HB3	1.90	0.72
1:K:83:ARG:NE	1:L:92:GLU:OE2	2.18	0.72
1:D:136:SER:HB2	1:D:153:GLN:HG3	1.72	0.72
1:B:226:PHE:CZ	1:C:14:LEU:HD22	2.25	0.71
1:E:136:SER:HB2	1:E:153:GLN:HG3	1.71	0.71
1:R:28:PRO:HB2	1:R:239:LEU:HD21	1.73	0.71
1:O:136:SER:HB2	1:O:153:GLN:HG3	1.73	0.70
1:G:136:SER:HB2	1:G:153:GLN:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:136:SER:HB2	1:R:153:GLN:HG2	1.74	0.70
1:L:226:PHE:CE2	1:M:14:LEU:HG	2.27	0.70
1:G:28:PRO:HB2	1:G:239:LEU:HD21	1.72	0.70
1:C:48:PHE:HB2	1:D:54:SER:HB3	1.72	0.70
1:F:136:SER:HB2	1:F:153:GLN:HG2	1.74	0.70
1:D:191:PHE:HD1	1:D:201:GLU:HG3	1.56	0.70
1:G:48:PHE:HB2	1:H:54:SER:CB	2.22	0.70
1:O:48:PHE:HB2	1:P:54:SER:HB3	1.74	0.70
1:H:136:SER:HB2	1:H:153:GLN:HG2	1.74	0.69
1:M:136:SER:HB2	1:M:153:GLN:HG2	1.72	0.69
1:J:136:SER:HB2	1:J:153:GLN:HG2	1.74	0.69
1:I:136:SER:HB2	1:I:153:GLN:HG2	1.75	0.69
1:A:136:SER:HB2	1:A:153:GLN:HG2	1.74	0.69
1:Q:48:PHE:HB2	1:R:54:SER:HB3	1.73	0.69
1:Q:136:SER:HB2	1:Q:153:GLN:HG2	1.74	0.69
1:B:16:PRO:HG3	1:C:5:PRO:HG3	1.72	0.68
1:B:136:SER:HB2	1:B:153:GLN:HG2	1.74	0.68
1:N:226:PHE:CZ	1:O:14:LEU:CD2	2.76	0.68
1:G:107:ILE:HG21	1:M:107:ILE:HD13	1.74	0.68
1:O:16:PRO:HG3	1:P:5:PRO:HG3	1.76	0.68
1:N:55:ASN:ND2	1:O:56:PHE:CE2	2.62	0.67
1:E:139:VAL:HG22	1:F:204:VAL:HG22	1.77	0.67
1:L:136:SER:HB2	1:L:153:GLN:HG2	1.74	0.67
1:K:136:SER:HB2	1:K:153:GLN:HG2	1.75	0.67
1:L:176:ASN:O	1:M:15:MET:HB2	1.95	0.67
1:F:48:PHE:HB2	1:G:54:SER:HB3	1.77	0.67
1:R:81:LEU:HD11	1:R:117:THR:HG22	1.77	0.66
1:A:176:ASN:O	1:B:15:MET:HB2	1.95	0.66
1:H:226:PHE:CZ	1:I:14:LEU:HD22	2.30	0.66
1:B:55:ASN:ND2	1:C:56:PHE:CE2	2.64	0.66
1:A:3:THR:HA	1:H:154:LEU:CD2	2.25	0.66
1:O:218:SER:HB2	1:P:8:GLU:OE2	1.95	0.66
1:E:84:GLN:CG	1:E:84:GLN:O	2.38	0.66
1:E:141:ALA:HA	1:F:202:GLY:HA2	1.77	0.66
1:D:128:ILE:HD12	1:D:160:ASN:HB2	1.78	0.65
1:P:139:VAL:HG22	1:Q:204:VAL:HG22	1.77	0.65
1:F:182:LEU:CD2	1:G:9:ALA:HB1	2.23	0.65
1:O:139:VAL:HG22	1:P:204:VAL:HG22	1.77	0.65
1:K:3:THR:HA	1:R:154:LEU:CD2	2.26	0.65
1:R:15:MET:CE	1:R:213:MET:HE3	2.26	0.65
1:C:133:ASN:OD1	1:C:153:GLN:CD	2.34	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:PHE:CZ	1:D:14:LEU:CD2	2.80	0.65
1:D:143:TYR:O	1:D:145:GLY:N	2.30	0.64
1:C:40:ASN:OD1	1:C:42:GLN:NE2	2.30	0.64
1:J:152:TYR:HE2	1:L:3:THR:HG22	1.60	0.64
1:H:48:PHE:HB2	1:I:54:SER:CB	2.26	0.64
1:R:185:GLU:OE2	1:R:187:GLN:NE2	2.31	0.63
1:J:226:PHE:CZ	1:K:14:LEU:HD22	2.33	0.63
1:H:39:TYR:HE1	1:I:92:GLU:HG2	1.63	0.63
1:L:233:ASP:CG	1:L:254:ARG:HH22	2.01	0.63
1:N:176:ASN:O	1:O:15:MET:HB2	1.98	0.63
1:Q:139:VAL:HG22	1:R:204:VAL:HG22	1.79	0.63
1:M:251:VAL:HG12	1:M:254:ARG:NH2	2.14	0.63
1:L:143:TYR:O	1:L:145:GLY:N	2.31	0.62
1:D:16:PRO:HG3	1:E:5:PRO:HG3	1.81	0.62
1:K:166:VAL:HA	1:L:89:LEU:HD21	1.82	0.62
1:K:176:ASN:O	1:L:15:MET:N	2.31	0.62
1:J:56:PHE:CE2	1:R:55:ASN:ND2	2.68	0.62
1:O:166:VAL:HG11	1:P:96:ILE:CD1	2.29	0.62
1:K:48:PHE:HB2	1:L:54:SER:HB3	1.82	0.62
1:A:166:VAL:HG11	1:B:96:ILE:HD11	1.82	0.61
1:J:39:TYR:HE1	1:K:92:GLU:HG2	1.66	0.61
1:N:143:TYR:O	1:N:145:GLY:N	2.34	0.60
1:N:139:VAL:HG22	1:O:204:VAL:HG22	1.83	0.60
1:B:176:ASN:O	1:C:15:MET:HB2	2.01	0.60
1:Q:143:TYR:O	1:Q:145:GLY:N	2.35	0.60
1:F:19:GLN:HB2	1:G:8:GLU:OE2	2.02	0.60
1:G:16:PRO:HG3	1:H:5:PRO:HG3	1.84	0.60
1:A:233:ASP:OD1	1:A:254:ARG:NH2	2.33	0.60
1:A:204:VAL:HG22	1:I:139:VAL:HG22	1.83	0.60
1:D:166:VAL:HG11	1:E:96:ILE:CD1	2.31	0.60
1:A:166:VAL:HG11	1:B:96:ILE:CD1	2.32	0.60
1:O:166:VAL:HG11	1:P:96:ILE:HD11	1.82	0.60
1:F:143:TYR:O	1:F:145:GLY:N	2.35	0.60
1:A:46:GLY:O	1:A:47:GLN:NE2	2.34	0.60
1:L:46:GLY:O	1:L:47:GLN:NE2	2.35	0.59
1:K:139:VAL:HG22	1:L:204:VAL:HG22	1.84	0.59
1:A:3:THR:CA	1:H:154:LEU:HD22	2.33	0.59
1:G:15:MET:HE1	1:G:217:MET:HG3	1.83	0.59
1:M:176:ASN:O	1:N:15:MET:HB2	2.02	0.59
1:H:154:LEU:HD13	1:H:180:THR:CG2	2.33	0.59
1:D:4:ALA:HB1	1:D:5:PRO:CD	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:143:TYR:O	1:O:145:GLY:N	2.35	0.59
1:J:154:LEU:HD13	1:J:180:THR:CG2	2.32	0.59
1:J:154:LEU:HD22	1:L:3:THR:O	2.02	0.59
1:D:180:THR:HG21	1:F:4:ALA:HA	1.85	0.59
1:F:176:ASN:O	1:G:15:MET:HB2	2.02	0.58
1:L:166:VAL:HG11	1:M:96:ILE:CD1	2.33	0.58
1:L:128:ILE:HG22	1:M:63:SER:HB2	1.85	0.58
1:D:226:PHE:CZ	1:E:14:LEU:CD2	2.83	0.58
1:P:16:PRO:HG3	1:Q:5:PRO:HG3	1.85	0.58
1:O:56:PHE:CE1	1:P:56:PHE:CE2	2.92	0.58
1:O:4:ALA:HB1	1:O:5:PRO:CD	2.34	0.58
1:C:176:ASN:O	1:D:15:MET:HB2	2.03	0.58
1:M:15:MET:HE1	1:M:217:MET:HG3	1.86	0.58
1:O:176:ASN:O	1:P:15:MET:HB2	2.03	0.58
1:A:163:VAL:HG23	1:A:227:LEU:HD22	1.86	0.58
1:G:4:ALA:HB1	1:G:5:PRO:CD	2.34	0.58
1:A:89:LEU:HD21	1:I:166:VAL:HA	1.84	0.57
1:A:15:MET:CE	1:A:214:LEU:HD12	2.34	0.57
1:A:15:MET:N	1:I:176:ASN:O	2.34	0.57
1:L:226:PHE:CZ	1:M:14:LEU:HG	2.40	0.57
1:M:166:VAL:HG11	1:N:96:ILE:CD1	2.34	0.57
1:A:4:ALA:HB1	1:A:5:PRO:CD	2.34	0.57
1:A:14:LEU:CD2	1:I:226:PHE:CZ	2.86	0.57
1:K:177:THR:HA	1:L:14:LEU:HA	1.87	0.57
1:B:166:VAL:HA	1:C:89:LEU:HD21	1.85	0.57
1:L:4:ALA:HB1	1:L:5:PRO:CD	2.35	0.57
1:D:166:VAL:HG11	1:E:96:ILE:HD11	1.85	0.57
1:L:166:VAL:HG11	1:M:96:ILE:HD11	1.85	0.57
1:C:189:GLY:HA3	1:C:203:GLU:OE2	2.04	0.57
1:H:4:ALA:HB1	1:H:5:PRO:CD	2.35	0.57
1:K:154:LEU:HD13	1:K:180:THR:CG2	2.35	0.57
1:L:163:VAL:HG23	1:L:227:LEU:HD22	1.87	0.57
1:N:166:VAL:HA	1:O:89:LEU:HD21	1.86	0.57
1:M:4:ALA:HB1	1:M:5:PRO:CD	2.34	0.57
1:R:4:ALA:HB1	1:R:5:PRO:CD	2.34	0.57
1:F:162:ARG:HH21	1:G:82:GLU:CD	2.08	0.57
1:R:37:SER:HA	1:R:81:LEU:O	2.05	0.57
1:C:139:VAL:HG22	1:D:204:VAL:HG22	1.86	0.57
1:J:176:ASN:O	1:K:15:MET:HB2	2.05	0.57
1:J:154:LEU:HD22	1:L:3:THR:CB	2.34	0.57
1:D:46:GLY:O	1:D:47:GLN:NE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:VAL:HG23	1:B:227:LEU:HD22	1.87	0.57
1:E:139:VAL:O	1:E:149:ASP:OD1	2.23	0.56
1:J:4:ALA:HB1	1:J:5:PRO:CD	2.35	0.56
1:C:46:GLY:O	1:C:47:GLN:NE2	2.38	0.56
1:A:128:ILE:HG22	1:B:63:SER:HB2	1.87	0.56
1:D:15:MET:HE3	1:D:217:MET:HG3	1.87	0.56
1:H:176:ASN:O	1:I:15:MET:HB2	2.05	0.56
1:P:46:GLY:O	1:P:47:GLN:NE2	2.38	0.56
1:Q:4:ALA:HB1	1:Q:5:PRO:CD	2.35	0.56
1:K:64:ALA:HB2	1:K:127:ILE:HD11	1.88	0.56
1:C:4:ALA:HB1	1:C:5:PRO:CD	2.35	0.56
1:L:64:ALA:HB2	1:L:127:ILE:HD11	1.88	0.56
1:D:176:ASN:O	1:E:15:MET:HB2	2.06	0.56
1:B:166:VAL:HG11	1:C:96:ILE:CD1	2.36	0.56
1:B:4:ALA:HB1	1:B:5:PRO:CD	2.36	0.56
1:G:83:ARG:NE	1:H:92:GLU:OE2	2.30	0.56
1:P:226:PHE:CZ	1:Q:14:LEU:HD22	2.41	0.56
1:C:143:TYR:O	1:C:145:GLY:N	2.39	0.56
1:B:46:GLY:O	1:B:47:GLN:NE2	2.38	0.56
1:K:4:ALA:HB1	1:K:5:PRO:CD	2.36	0.56
1:N:176:ASN:O	1:O:15:MET:N	2.38	0.56
1:K:30:PRO:HB3	1:K:77:TRP:CZ3	2.41	0.56
1:A:48:PHE:HB2	1:B:54:SER:HB3	1.87	0.56
1:M:166:VAL:HA	1:N:89:LEU:HD21	1.87	0.55
1:I:64:ALA:HB2	1:I:127:ILE:HD11	1.88	0.55
1:G:107:ILE:CG2	1:M:107:ILE:HD13	2.36	0.55
1:H:166:VAL:HG11	1:I:96:ILE:CD1	2.36	0.55
1:E:176:ASN:O	1:F:15:MET:HB2	2.06	0.55
1:F:135:LYS:HE3	1:H:6:PRO:HD3	1.86	0.55
1:F:4:ALA:HB1	1:F:5:PRO:CD	2.36	0.55
1:R:25:THR:O	1:R:76:ARG:NH2	2.37	0.55
1:M:46:GLY:O	1:M:47:GLN:NE2	2.39	0.55
1:F:176:ASN:O	1:G:15:MET:N	2.38	0.55
1:I:30:PRO:HB3	1:I:77:TRP:CZ3	2.42	0.55
1:G:180:THR:HG21	1:I:3:THR:O	2.06	0.55
1:M:143:TYR:O	1:M:145:GLY:N	2.38	0.55
1:G:128:ILE:HG23	1:H:63:SER:OG	2.06	0.55
1:M:180:THR:HG23	1:N:10:ALA:HB3	1.89	0.55
1:C:166:VAL:HA	1:D:89:LEU:HD21	1.88	0.55
1:B:64:ALA:HB2	1:B:127:ILE:HD11	1.89	0.55
1:O:46:GLY:O	1:O:47:GLN:NE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:143:TYR:O	1:I:145:GLY:N	2.39	0.55
1:N:4:ALA:HB1	1:N:5:PRO:CD	2.37	0.55
1:J:166:VAL:HG11	1:K:96:ILE:CD1	2.36	0.55
1:N:30:PRO:HB3	1:N:77:TRP:CZ3	2.42	0.55
1:E:4:ALA:HB1	1:E:5:PRO:CD	2.37	0.55
1:I:15:MET:HG2	1:I:16:PRO:HD2	1.89	0.55
1:K:143:TYR:O	1:K:145:GLY:N	2.39	0.55
1:N:128:ILE:HG22	1:O:63:SER:HB2	1.89	0.55
1:J:54:SER:HB3	1:R:48:PHE:CB	2.31	0.55
1:A:3:THR:HB	1:H:154:LEU:HD22	1.89	0.55
1:M:15:MET:HG2	1:M:16:PRO:HD2	1.89	0.55
1:H:128:ILE:HG22	1:I:63:SER:HB2	1.89	0.55
1:M:30:PRO:HB3	1:M:77:TRP:CZ3	2.41	0.55
1:P:4:ALA:HB1	1:P:5:PRO:CD	2.37	0.55
1:D:64:ALA:HB2	1:D:127:ILE:HD11	1.89	0.55
1:L:15:MET:HG2	1:L:16:PRO:HD2	1.90	0.54
1:L:48:PHE:HB2	1:M:54:SER:HB3	1.89	0.54
1:K:180:THR:HG21	1:M:3:THR:O	2.07	0.54
1:B:128:ILE:HG22	1:C:63:SER:HB2	1.90	0.54
1:Q:64:ALA:HB2	1:Q:127:ILE:HD11	1.89	0.54
1:A:64:ALA:HB2	1:A:127:ILE:HD11	1.88	0.54
1:F:142:ARG:O	1:G:201:GLU:N	2.31	0.54
1:D:48:PHE:HB2	1:E:54:SER:CB	2.37	0.54
1:F:16:PRO:HG3	1:G:5:PRO:HG3	1.89	0.54
1:G:166:VAL:HG11	1:H:96:ILE:CD1	2.37	0.54
1:O:64:ALA:HB2	1:O:127:ILE:HD11	1.88	0.54
1:J:64:ALA:HB2	1:J:127:ILE:HD11	1.89	0.54
1:E:101:GLU:HB2	1:O:97:ARG:HG2	1.89	0.54
1:C:64:ALA:HB2	1:C:127:ILE:HD11	1.89	0.54
1:D:135:LYS:HE3	1:F:6:PRO:HD3	1.89	0.54
1:B:30:PRO:HB3	1:B:77:TRP:CZ3	2.42	0.54
1:J:5:PRO:HG3	1:R:16:PRO:HG3	1.90	0.54
1:A:54:SER:HB3	1:I:48:PHE:HB2	1.89	0.54
1:E:143:TYR:O	1:E:145:GLY:N	2.41	0.54
1:N:64:ALA:HB2	1:N:127:ILE:HD11	1.90	0.54
1:F:15:MET:HG2	1:F:16:PRO:HD2	1.89	0.54
1:P:143:TYR:O	1:P:145:GLY:N	2.41	0.54
1:F:64:ALA:HB2	1:F:127:ILE:HD11	1.89	0.54
1:L:83:ARG:NE	1:M:92:GLU:OE2	2.36	0.54
1:G:39:TYR:HE1	1:H:92:GLU:HG2	1.73	0.54
1:M:64:ALA:HB2	1:M:127:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:30:PRO:HB3	1:Q:77:TRP:CZ3	2.42	0.54
1:H:30:PRO:HB3	1:H:77:TRP:CZ3	2.43	0.54
1:H:46:GLY:O	1:H:47:GLN:NE2	2.41	0.54
1:D:128:ILE:HG12	1:E:63:SER:HB2	1.89	0.54
1:F:141:ALA:HA	1:G:202:GLY:HA2	1.90	0.54
1:E:143:TYR:HD1	1:F:200:LEU:CD1	2.21	0.54
1:I:163:VAL:HG23	1:I:227:LEU:HD22	1.89	0.54
1:H:64:ALA:HB2	1:H:127:ILE:HD11	1.89	0.54
1:N:46:GLY:O	1:N:47:GLN:NE2	2.41	0.54
1:F:163:VAL:HG23	1:F:227:LEU:HD22	1.90	0.54
1:Q:15:MET:HG2	1:Q:16:PRO:HD2	1.89	0.53
1:J:96:ILE:CD1	1:R:166:VAL:HG11	2.38	0.53
1:H:163:VAL:HG23	1:H:227:LEU:HD22	1.90	0.53
1:J:163:VAL:HG23	1:J:227:LEU:HD22	1.90	0.53
1:E:30:PRO:HB3	1:E:77:TRP:CZ3	2.43	0.53
1:F:166:VAL:HG11	1:G:96:ILE:CD1	2.38	0.53
1:E:149:ASP:OD1	1:E:150:THR:N	2.41	0.53
1:N:163:VAL:HG23	1:N:227:LEU:HD22	1.91	0.53
1:O:128:ILE:O	1:O:158:ALA:HB3	2.08	0.53
1:H:39:TYR:CE1	1:I:92:GLU:HG2	2.43	0.53
1:L:30:PRO:HB3	1:L:77:TRP:CZ3	2.44	0.53
1:J:54:SER:CB	1:R:48:PHE:CB	2.86	0.53
1:P:176:ASN:O	1:Q:15:MET:HB2	2.07	0.53
1:C:128:ILE:HG22	1:D:63:SER:HB2	1.90	0.53
1:F:30:PRO:HB3	1:F:77:TRP:CZ3	2.43	0.53
1:R:36:VAL:CG1	1:R:80:PRO:HA	2.35	0.53
1:E:139:VAL:HG13	1:F:204:VAL:HG22	1.91	0.53
1:J:15:MET:N	1:R:176:ASN:O	2.38	0.53
1:R:64:ALA:HB2	1:R:127:ILE:HD11	1.91	0.53
1:K:226:PHE:CZ	1:L:14:LEU:CD2	2.90	0.53
1:J:166:VAL:HA	1:K:89:LEU:HD21	1.91	0.53
1:H:154:LEU:HD13	1:H:180:THR:HG23	1.91	0.52
1:O:30:PRO:HB3	1:O:77:TRP:CZ3	2.44	0.52
1:G:162:ARG:HH21	1:H:82:GLU:CD	2.13	0.52
1:J:92:GLU:OE2	1:R:83:ARG:NE	2.28	0.52
1:E:64:ALA:HB2	1:E:127:ILE:HD11	1.91	0.52
1:E:163:VAL:HG23	1:E:227:LEU:HD22	1.91	0.52
1:J:154:LEU:HD13	1:J:180:THR:HG23	1.90	0.52
1:J:39:TYR:CE1	1:K:92:GLU:HG2	2.44	0.52
1:C:30:PRO:HB3	1:C:77:TRP:CZ3	2.44	0.52
1:F:46:GLY:O	1:F:47:GLN:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:141:ALA:HA	1:Q:202:GLY:HA2	1.92	0.52
1:K:163:VAL:HG23	1:K:227:LEU:HD22	1.90	0.52
1:G:93:ARG:HH22	1:G:115:SER:HA	1.75	0.52
1:A:56:PHE:CE1	1:B:56:PHE:HE2	2.28	0.52
1:A:15:MET:HB2	1:I:176:ASN:O	2.10	0.52
1:N:83:ARG:NE	1:O:92:GLU:OE2	2.34	0.52
1:J:25:THR:O	1:J:76:ARG:NH2	2.42	0.52
1:R:93:ARG:HH22	1:R:115:SER:HA	1.75	0.52
1:D:163:VAL:HG23	1:D:227:LEU:HD22	1.92	0.52
1:J:30:PRO:HB3	1:J:77:TRP:CZ3	2.44	0.52
1:C:128:ILE:O	1:C:158:ALA:HB3	2.10	0.52
1:C:163:VAL:HG23	1:C:227:LEU:HD22	1.91	0.52
1:M:128:ILE:HG22	1:N:63:SER:HB2	1.90	0.52
1:P:30:PRO:HB3	1:P:77:TRP:CZ3	2.45	0.52
1:G:64:ALA:HB2	1:G:127:ILE:HD11	1.91	0.52
1:L:139:VAL:HG22	1:M:204:VAL:HG22	1.91	0.52
1:H:143:TYR:O	1:H:145:GLY:N	2.42	0.52
1:E:97:ARG:HG2	1:O:101:GLU:HB2	1.91	0.52
1:J:15:MET:HB2	1:R:176:ASN:O	2.10	0.52
1:L:25:THR:O	1:L:76:ARG:NH2	2.42	0.52
1:G:25:THR:O	1:G:76:ARG:NH2	2.40	0.52
1:D:30:PRO:HB3	1:D:77:TRP:CZ3	2.45	0.52
1:J:204:VAL:HG22	1:R:139:VAL:HG22	1.92	0.52
1:A:30:PRO:HB3	1:A:77:TRP:CZ3	2.44	0.52
1:E:18:ALA:HB3	1:F:8:GLU:HG3	1.91	0.52
1:E:25:THR:O	1:E:76:ARG:NH2	2.42	0.52
1:H:102:ASN:OD1	1:L:97:ARG:NH1	2.42	0.51
1:Q:176:ASN:O	1:R:15:MET:N	2.41	0.51
1:J:46:GLY:O	1:J:47:GLN:NE2	2.43	0.51
1:I:45:THR:OG1	1:I:130:TYR:N	2.43	0.51
1:B:181:ILE:HG23	1:B:210:GLU:HB3	1.93	0.51
1:P:166:VAL:HA	1:Q:89:LEU:HD21	1.92	0.51
1:G:163:VAL:HG23	1:G:227:LEU:HD22	1.92	0.51
1:G:56:PHE:CE1	1:H:56:PHE:CE2	2.98	0.51
1:N:76:ARG:O	1:N:76:ARG:HG3	2.10	0.51
1:M:181:ILE:HG23	1:M:210:GLU:HB3	1.92	0.51
1:L:226:PHE:CE1	1:M:14:LEU:HD11	2.45	0.51
1:J:83:ARG:NE	1:K:92:GLU:OE2	2.25	0.51
1:D:25:THR:O	1:D:76:ARG:NH2	2.40	0.51
1:M:25:THR:O	1:M:76:ARG:NH2	2.43	0.51
1:H:83:ARG:NE	1:I:92:GLU:OE2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:128:ILE:O	1:H:158:ALA:HB3	2.11	0.51
1:A:56:PHE:CE1	1:B:56:PHE:CE2	2.98	0.51
1:G:55:ASN:ND2	1:H:56:PHE:CE2	2.78	0.51
1:E:46:GLY:O	1:E:47:GLN:NE2	2.43	0.51
1:R:15:MET:SD	1:R:213:MET:HE3	2.50	0.51
1:A:93:ARG:NH1	1:A:97:ARG:HH22	2.09	0.51
1:R:46:GLY:O	1:R:47:GLN:NE2	2.44	0.51
1:E:142:ARG:N	1:F:201:GLU:O	2.30	0.51
1:P:25:THR:O	1:P:76:ARG:NH2	2.40	0.51
1:J:128:ILE:O	1:J:158:ALA:HB3	2.11	0.51
1:G:176:ASN:O	1:H:15:MET:HB2	2.10	0.51
1:K:15:MET:HG2	1:K:16:PRO:HD2	1.93	0.51
1:N:128:ILE:O	1:N:158:ALA:HB3	2.11	0.51
1:E:39:TYR:HE1	1:F:92:GLU:HG2	1.76	0.51
1:Q:171:ILE:CG1	1:R:82:GLU:HB2	2.38	0.51
1:A:3:THR:HA	1:H:154:LEU:HD22	1.90	0.50
1:M:128:ILE:O	1:M:158:ALA:HB3	2.11	0.50
1:D:142:ARG:O	1:E:200:LEU:HD12	2.11	0.50
1:K:25:THR:O	1:K:76:ARG:NH2	2.42	0.50
1:J:154:LEU:CD2	1:L:3:THR:HA	2.41	0.50
1:P:64:ALA:HB2	1:P:127:ILE:HD11	1.92	0.50
1:J:35:PHE:HE2	1:K:109:ASN:OD1	1.92	0.50
1:G:15:MET:HG2	1:G:16:PRO:HD2	1.92	0.50
1:A:63:SER:HB2	1:I:128:ILE:HG22	1.92	0.50
1:G:46:GLY:O	1:G:47:GLN:NE2	2.44	0.50
1:Q:25:THR:O	1:Q:76:ARG:NH2	2.40	0.50
1:G:128:ILE:O	1:G:158:ALA:HB3	2.11	0.50
1:H:166:VAL:HG11	1:I:96:ILE:HD11	1.93	0.50
1:P:16:PRO:HG3	1:Q:5:PRO:CG	2.42	0.50
1:A:5:PRO:HG3	1:I:16:PRO:HG3	1.94	0.50
1:K:154:LEU:HD13	1:K:180:THR:HG23	1.92	0.50
1:D:135:LYS:HE3	1:F:6:PRO:CD	2.41	0.50
1:E:166:VAL:HG11	1:F:96:ILE:CD1	2.42	0.50
1:Q:128:ILE:O	1:Q:158:ALA:HB3	2.11	0.50
1:M:166:VAL:HG11	1:N:96:ILE:HD11	1.94	0.50
1:L:135:LYS:HE3	1:N:6:PRO:HD3	1.93	0.50
1:N:226:PHE:CE1	1:O:14:LEU:HD22	2.47	0.50
1:O:128:ILE:HG23	1:P:63:SER:OG	2.11	0.50
1:B:166:VAL:HG11	1:C:96:ILE:HD11	1.94	0.50
1:J:139:VAL:HG22	1:K:204:VAL:HG22	1.94	0.50
1:O:48:PHE:HB2	1:P:54:SER:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:6:PRO:HD3	1:Q:135:LYS:HE3	1.92	0.50
1:A:17:ARG:NH1	1:A:74:ASP:OD2	2.45	0.50
1:R:128:ILE:O	1:R:158:ALA:HB3	2.12	0.50
1:H:166:VAL:HA	1:I:89:LEU:HD21	1.93	0.50
1:J:128:ILE:HG22	1:K:63:SER:HB2	1.94	0.50
1:G:30:PRO:HB3	1:G:77:TRP:CZ3	2.46	0.50
1:D:176:ASN:O	1:E:15:MET:N	2.44	0.50
1:G:17:ARG:NH1	1:G:74:ASP:OD2	2.44	0.50
1:A:181:ILE:HG23	1:A:210:GLU:HB3	1.94	0.50
1:L:181:ILE:HG23	1:L:210:GLU:HB3	1.93	0.50
1:E:15:MET:HG2	1:E:16:PRO:HD2	1.93	0.49
1:C:25:THR:O	1:C:76:ARG:NH2	2.43	0.49
1:Q:166:VAL:HG11	1:R:96:ILE:CD1	2.42	0.49
1:J:14:LEU:CD2	1:R:226:PHE:CZ	2.94	0.49
1:J:166:VAL:HG11	1:K:96:ILE:HD11	1.93	0.49
1:A:15:MET:HE3	1:A:214:LEU:HD12	1.93	0.49
1:G:181:ILE:HG23	1:G:210:GLU:HB3	1.94	0.49
1:E:181:ILE:HG23	1:E:210:GLU:HB3	1.95	0.49
1:C:17:ARG:NH1	1:C:74:ASP:OD2	2.45	0.49
1:F:128:ILE:O	1:F:158:ALA:HB3	2.12	0.49
1:N:9:ALA:O	1:N:10:ALA:HB3	2.13	0.49
1:O:16:PRO:HG3	1:P:5:PRO:CG	2.40	0.49
1:Q:128:ILE:HG22	1:R:63:SER:HB2	1.94	0.49
1:I:128:ILE:O	1:I:158:ALA:HB3	2.12	0.49
1:C:181:ILE:HG23	1:C:210:GLU:HB3	1.94	0.49
1:G:166:VAL:HG11	1:H:96:ILE:HD11	1.93	0.49
1:P:128:ILE:HG22	1:Q:63:SER:HB2	1.94	0.49
1:G:162:ARG:NH2	1:H:82:GLU:OE2	2.44	0.49
1:L:211:PRO:HB2	1:L:214:LEU:HB2	1.94	0.49
1:B:4:ALA:O	1:I:135:LYS:HE3	2.13	0.49
1:I:128:ILE:HG13	1:I:128:ILE:O	2.13	0.49
1:K:45:THR:OG1	1:K:130:TYR:N	2.46	0.49
1:E:128:ILE:HG22	1:F:63:SER:HB2	1.94	0.49
1:H:15:MET:HG2	1:H:16:PRO:HD2	1.95	0.49
1:C:15:MET:HG2	1:C:16:PRO:HD2	1.94	0.49
1:L:17:ARG:NH1	1:L:74:ASP:OD2	2.45	0.49
1:D:139:VAL:HG22	1:E:204:VAL:HG22	1.95	0.49
1:K:128:ILE:HG22	1:L:63:SER:HB2	1.94	0.49
1:I:25:THR:O	1:I:76:ARG:NH2	2.43	0.49
1:J:48:PHE:CB	1:K:54:SER:CB	2.90	0.49
1:G:48:PHE:CB	1:H:54:SER:HB3	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:39:TYR:CE1	1:R:92:GLU:HG2	2.48	0.49
1:C:55:ASN:ND2	1:D:56:PHE:CE2	2.81	0.49
1:N:93:ARG:NH1	1:N:97:ARG:HH22	2.11	0.49
1:A:40:ASN:ND2	1:A:42:GLN:HG3	2.28	0.49
1:J:96:ILE:HD11	1:R:166:VAL:HG11	1.95	0.48
1:Q:128:ILE:HG13	1:Q:128:ILE:O	2.13	0.48
1:P:15:MET:HG2	1:P:16:PRO:HD2	1.94	0.48
1:A:93:ARG:HH12	1:A:97:ARG:HH22	1.62	0.48
1:K:128:ILE:O	1:K:128:ILE:HG13	2.12	0.48
1:R:181:ILE:HG23	1:R:210:GLU:HB3	1.93	0.48
1:G:39:TYR:CE1	1:H:92:GLU:HG2	2.48	0.48
1:M:128:ILE:HG13	1:M:128:ILE:O	2.13	0.48
1:K:128:ILE:O	1:K:158:ALA:HB3	2.13	0.48
1:R:17:ARG:NH1	1:R:74:ASP:OD2	2.45	0.48
1:P:211:PRO:HB2	1:P:214:LEU:HB2	1.95	0.48
1:O:25:THR:O	1:O:76:ARG:NH2	2.41	0.48
1:I:181:ILE:HG23	1:I:210:GLU:HB3	1.95	0.48
1:A:14:LEU:HA	1:I:177:THR:HA	1.94	0.48
1:L:128:ILE:O	1:L:158:ALA:HB3	2.13	0.48
1:H:9:ALA:O	1:H:10:ALA:HB3	2.13	0.48
1:J:82:GLU:CD	1:R:162:ARG:HH21	2.16	0.48
1:B:192:ARG:HA	1:B:192:ARG:HD3	1.61	0.48
1:H:181:ILE:HG23	1:H:210:GLU:HB3	1.95	0.48
1:G:9:ALA:O	1:G:10:ALA:HB3	2.14	0.48
1:J:154:LEU:HD22	1:L:3:THR:CA	2.44	0.48
1:H:10:ALA:HB2	1:I:3:THR:OG1	2.13	0.48
1:D:97:ARG:HG2	1:P:101:GLU:HB2	1.96	0.48
1:N:17:ARG:NH1	1:N:74:ASP:OD2	2.46	0.48
1:J:143:TYR:O	1:J:145:GLY:N	2.47	0.48
1:R:30:PRO:HB3	1:R:77:TRP:CZ3	2.49	0.48
1:P:17:ARG:NH1	1:P:74:ASP:OD2	2.46	0.48
1:E:17:ARG:NH1	1:E:74:ASP:OD2	2.46	0.48
1:J:43:ASP:C	1:J:45:THR:H	2.17	0.48
1:N:15:MET:HG2	1:N:16:PRO:HD2	1.96	0.48
1:F:9:ALA:O	1:F:10:ALA:HB3	2.14	0.48
1:E:36:VAL:CG1	1:E:78:PHE:CD1	2.97	0.48
1:I:17:ARG:NH1	1:I:74:ASP:OD2	2.47	0.48
1:A:226:PHE:CZ	1:B:14:LEU:CD2	2.96	0.48
1:O:176:ASN:O	1:P:15:MET:N	2.44	0.48
1:A:211:PRO:HB2	1:A:214:LEU:HB2	1.96	0.48
1:C:166:VAL:HG11	1:D:96:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:128:ILE:O	1:P:158:ALA:HB3	2.14	0.48
1:E:128:ILE:O	1:E:158:ALA:HB3	2.13	0.48
1:Q:46:GLY:O	1:Q:47:GLN:NE2	2.46	0.48
1:K:134:VAL:HG12	1:M:6:PRO:CD	2.44	0.48
1:J:154:LEU:CD2	1:L:3:THR:CA	2.91	0.48
1:M:83:ARG:NE	1:N:92:GLU:OE2	2.44	0.48
1:K:9:ALA:O	1:K:10:ALA:HB3	2.14	0.48
1:Q:169:GLY:O	1:R:82:GLU:HB3	2.13	0.48
1:J:15:MET:HG2	1:J:16:PRO:HD2	1.95	0.48
1:Q:181:ILE:HG23	1:Q:210:GLU:HB3	1.95	0.48
1:I:46:GLY:O	1:I:47:GLN:NE2	2.47	0.48
1:K:15:MET:HB3	1:K:15:MET:HE2	1.77	0.48
1:E:39:TYR:CE1	1:F:92:GLU:HG2	2.48	0.48
1:A:83:ARG:NE	1:B:92:GLU:OE2	2.38	0.48
1:M:17:ARG:NH1	1:M:74:ASP:OD2	2.47	0.48
1:F:181:ILE:HG23	1:F:210:GLU:HB3	1.94	0.48
1:P:181:ILE:HG23	1:P:210:GLU:HB3	1.96	0.48
1:O:19:GLN:HG2	1:P:11:ARG:HH21	1.78	0.48
1:B:48:PHE:HB2	1:C:54:SER:HB3	1.96	0.48
1:E:128:ILE:HG13	1:E:128:ILE:O	2.14	0.47
1:H:17:ARG:NH1	1:H:74:ASP:OD2	2.47	0.47
1:B:180:THR:HG23	1:C:10:ALA:HB3	1.94	0.47
1:E:140:GLY:O	1:F:203:GLU:N	2.33	0.47
1:L:93:ARG:NH1	1:L:97:ARG:HH22	2.11	0.47
1:P:128:ILE:HG13	1:P:128:ILE:O	2.14	0.47
1:C:9:ALA:O	1:C:10:ALA:HB3	2.14	0.47
1:L:40:ASN:ND2	1:L:42:GLN:HG3	2.29	0.47
1:D:181:ILE:HG23	1:D:210:GLU:HB3	1.95	0.47
1:H:25:THR:O	1:H:76:ARG:NH2	2.43	0.47
1:R:36:VAL:O	1:R:81:LEU:N	2.47	0.47
1:L:226:PHE:CD2	1:M:14:LEU:HD21	2.49	0.47
1:F:25:THR:O	1:F:76:ARG:NH2	2.41	0.47
1:E:48:PHE:HB2	1:F:54:SER:CB	2.40	0.47
1:Q:226:PHE:CZ	1:R:14:LEU:CD2	2.95	0.47
1:N:128:ILE:HG13	1:N:128:ILE:O	2.15	0.47
1:H:128:ILE:HG13	1:H:128:ILE:O	2.15	0.47
1:E:55:ASN:ND2	1:F:56:PHE:CE2	2.82	0.47
1:F:65:THR:HG23	1:F:66:ALA:N	2.30	0.47
1:P:39:TYR:HE1	1:Q:92:GLU:HG2	1.78	0.47
1:A:3:THR:HG22	1:H:152:TYR:HE2	1.80	0.47
1:B:176:ASN:O	1:C:15:MET:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:ASN:O	1:D:15:MET:N	2.47	0.47
1:H:176:ASN:O	1:I:15:MET:N	2.44	0.47
1:J:128:ILE:HG13	1:J:128:ILE:O	2.15	0.47
1:R:128:ILE:HG13	1:R:128:ILE:O	2.15	0.47
1:B:17:ARG:NH1	1:B:74:ASP:OD2	2.47	0.47
1:F:17:ARG:NH1	1:F:74:ASP:OD2	2.48	0.47
1:C:211:PRO:HB2	1:C:214:LEU:HB2	1.97	0.47
1:E:9:ALA:O	1:E:10:ALA:HB3	2.15	0.47
1:K:17:ARG:NH1	1:K:74:ASP:OD2	2.48	0.47
1:H:15:MET:HE1	1:H:217:MET:HG3	1.97	0.47
1:J:176:ASN:O	1:K:15:MET:N	2.42	0.47
1:N:76:ARG:O	1:N:76:ARG:CG	2.63	0.47
1:M:9:ALA:O	1:M:10:ALA:HB3	2.15	0.47
1:M:227:LEU:HA	1:M:227:LEU:HD12	1.73	0.47
1:Q:39:TYR:HE1	1:R:92:GLU:HG2	1.79	0.47
1:R:9:ALA:O	1:R:10:ALA:HB3	2.14	0.47
1:K:46:GLY:O	1:K:47:GLN:NE2	2.48	0.47
1:A:9:ALA:O	1:A:10:ALA:HB3	2.15	0.47
1:Q:9:ALA:O	1:Q:10:ALA:HB3	2.14	0.47
1:H:43:ASP:C	1:H:45:THR:H	2.18	0.47
1:E:151:GLN:HB2	1:E:185:GLU:HG3	1.96	0.47
1:H:16:PRO:HG3	1:I:5:PRO:CG	2.39	0.47
1:F:19:GLN:HG2	1:G:11:ARG:NH2	2.29	0.47
1:H:47:GLN:NE2	1:I:58:THR:O	2.44	0.47
1:J:9:ALA:O	1:J:10:ALA:HB3	2.14	0.47
1:A:76:ARG:HA	1:A:76:ARG:HH11	1.80	0.47
1:O:181:ILE:HG23	1:O:210:GLU:HB3	1.96	0.47
1:B:40:ASN:ND2	1:B:42:GLN:HG3	2.30	0.47
1:G:176:ASN:O	1:H:15:MET:N	2.41	0.46
1:B:135:LYS:HE3	1:D:6:PRO:HD3	1.96	0.46
1:D:9:ALA:O	1:D:10:ALA:HB3	2.15	0.46
1:O:9:ALA:O	1:O:10:ALA:HB3	2.14	0.46
1:J:40:ASN:ND2	1:J:42:GLN:HG3	2.30	0.46
1:J:154:LEU:HD21	1:L:3:THR:HA	1.96	0.46
1:A:3:THR:O	1:H:154:LEU:HD13	2.15	0.46
1:O:15:MET:HE2	1:O:15:MET:HB3	1.76	0.46
1:P:166:VAL:HG11	1:Q:96:ILE:CD1	2.45	0.46
1:K:17:ARG:HB3	1:K:21:TYR:HB2	1.97	0.46
1:C:93:ARG:NH1	1:C:97:ARG:HH22	2.12	0.46
1:D:17:ARG:NH1	1:D:74:ASP:OD2	2.48	0.46
1:E:15:MET:HB3	1:E:15:MET:HE2	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:ILE:HG13	1:F:128:ILE:O	2.14	0.46
1:E:102:ASN:O	1:O:113:LEU:N	2.34	0.46
1:E:211:PRO:HB2	1:E:214:LEU:HB2	1.96	0.46
1:A:3:THR:CB	1:H:154:LEU:HD22	2.45	0.46
1:A:3:THR:HA	1:H:154:LEU:HD21	1.96	0.46
1:C:15:MET:HB3	1:C:15:MET:HE2	1.79	0.46
1:K:39:TYR:CE1	1:L:92:GLU:HG2	2.51	0.46
1:O:15:MET:HG2	1:O:16:PRO:HD2	1.98	0.46
1:K:176:ASN:O	1:L:15:MET:HB2	2.16	0.46
1:P:39:TYR:CE1	1:Q:92:GLU:HG2	2.50	0.46
1:K:181:ILE:HG23	1:K:210:GLU:HB3	1.96	0.46
1:J:17:ARG:NH1	1:J:74:ASP:OD2	2.49	0.46
1:D:128:ILE:HG23	1:E:63:SER:CB	2.45	0.46
1:D:15:MET:HG2	1:D:16:PRO:HD2	1.96	0.46
1:L:15:MET:HB3	1:L:15:MET:HE2	1.75	0.46
1:C:128:ILE:O	1:C:128:ILE:HG13	2.15	0.46
1:N:133:ASN:OD1	1:N:153:GLN:NE2	2.48	0.46
1:G:48:PHE:CB	1:H:54:SER:CB	2.91	0.46
1:O:226:PHE:CZ	1:P:14:LEU:CD2	2.92	0.46
1:A:92:GLU:HG2	1:I:39:TYR:CE1	2.50	0.46
1:M:143:TYR:C	1:M:145:GLY:N	2.69	0.46
1:F:40:ASN:ND2	1:F:42:GLN:HG3	2.30	0.46
1:M:211:PRO:HB2	1:M:214:LEU:HB2	1.98	0.46
1:J:181:ILE:HG23	1:J:210:GLU:HB3	1.96	0.46
1:A:176:ASN:HB3	1:B:15:MET:HB2	1.97	0.46
1:P:17:ARG:HB3	1:P:21:TYR:HB2	1.98	0.46
1:D:101:GLU:HB2	1:P:97:ARG:HG2	1.98	0.46
1:N:211:PRO:HB2	1:N:214:LEU:HB2	1.97	0.46
1:F:166:VAL:HG11	1:G:96:ILE:HD11	1.96	0.46
1:J:82:GLU:OE2	1:R:162:ARG:NH2	2.48	0.46
1:F:43:ASP:C	1:F:45:THR:H	2.19	0.46
1:I:9:ALA:O	1:I:10:ALA:HB3	2.16	0.46
1:P:9:ALA:O	1:P:10:ALA:HB3	2.15	0.46
1:A:92:GLU:HG2	1:I:39:TYR:HE1	1.81	0.46
1:C:97:ARG:HG2	1:Q:101:GLU:HB2	1.97	0.46
1:L:128:ILE:O	1:L:128:ILE:HG13	2.15	0.45
1:F:15:MET:HB3	1:F:15:MET:HE2	1.80	0.45
1:E:143:TYR:HD1	1:F:200:LEU:HD12	1.80	0.45
1:C:113:LEU:N	1:Q:102:ASN:O	2.42	0.45
1:L:9:ALA:O	1:L:10:ALA:HB3	2.16	0.45
1:O:17:ARG:NH1	1:O:74:ASP:OD2	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:181:ILE:HG23	1:N:210:GLU:HB3	1.97	0.45
1:R:211:PRO:HB2	1:R:214:LEU:HB2	1.98	0.45
1:F:107:ILE:HD13	1:N:107:ILE:CD1	2.24	0.45
1:F:162:ARG:NH2	1:G:82:GLU:CD	2.65	0.45
1:J:154:LEU:CD2	1:L:3:THR:O	2.65	0.45
1:L:17:ARG:HB3	1:L:21:TYR:HB2	1.97	0.45
1:A:33:LYS:HE2	1:A:76:ARG:HH22	1.81	0.45
1:B:211:PRO:HB2	1:B:214:LEU:HB2	1.97	0.45
1:L:11:ARG:O	1:L:11:ARG:HG2	2.15	0.45
1:C:83:ARG:NE	1:D:92:GLU:OE2	2.34	0.45
1:O:211:PRO:HB2	1:O:214:LEU:HB2	1.99	0.45
1:G:211:PRO:HB2	1:G:214:LEU:HB2	1.98	0.45
1:Q:17:ARG:NH1	1:Q:74:ASP:OD2	2.49	0.45
1:Q:211:PRO:HB2	1:Q:214:LEU:HB2	1.98	0.45
1:A:15:MET:HG3	1:I:178:SER:HB2	1.97	0.45
1:Q:16:PRO:HG3	1:R:5:PRO:HG3	1.98	0.45
1:B:17:ARG:HB3	1:B:21:TYR:HB2	1.99	0.45
1:A:162:ARG:HH21	1:B:82:GLU:CD	2.20	0.45
1:D:173:SER:HA	1:E:73:LYS:NZ	2.31	0.45
1:D:211:PRO:HB2	1:D:214:LEU:HB2	1.98	0.45
1:O:166:VAL:HA	1:P:89:LEU:HD21	1.98	0.45
1:I:211:PRO:HB2	1:I:214:LEU:HB2	1.99	0.45
1:F:211:PRO:HB2	1:F:214:LEU:HB2	1.98	0.45
1:M:166:VAL:HG11	1:N:96:ILE:HD12	1.98	0.45
1:I:15:MET:HB3	1:I:15:MET:HE2	1.77	0.45
1:A:16:PRO:HG3	1:B:5:PRO:HG3	1.99	0.45
1:E:17:ARG:HB3	1:E:21:TYR:HB2	1.98	0.45
1:F:17:ARG:HB3	1:F:21:TYR:HB2	1.99	0.45
1:Q:17:ARG:HB3	1:Q:21:TYR:HB2	1.99	0.45
1:F:97:ARG:HG2	1:N:101:GLU:HB2	1.98	0.45
1:Q:162:ARG:NH2	1:R:82:GLU:OE2	2.49	0.45
1:O:166:VAL:HG11	1:P:96:ILE:HD12	1.99	0.45
1:C:92:GLU:O	1:C:96:ILE:HG13	2.17	0.45
1:E:143:TYR:C	1:E:145:GLY:N	2.70	0.45
1:E:166:VAL:HA	1:F:89:LEU:HD21	1.97	0.45
1:O:128:ILE:HG23	1:P:63:SER:CB	2.47	0.45
1:L:121:ILE:HD13	1:L:163:VAL:HG13	1.99	0.45
1:A:17:ARG:HB3	1:A:21:TYR:HB2	1.97	0.45
1:F:101:GLU:HB2	1:N:97:ARG:HG2	1.98	0.45
1:M:17:ARG:HB3	1:M:21:TYR:HB2	1.99	0.45
1:B:142:ARG:O	1:C:201:GLU:N	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:100:GLN:NE2	1:K:111:ILE:O	2.32	0.45
1:B:93:ARG:NH1	1:B:97:ARG:HH22	2.15	0.45
1:J:8:GLU:OE2	1:R:218:SER:HB2	2.16	0.45
1:O:56:PHE:CE1	1:P:56:PHE:HE2	2.35	0.45
1:K:135:LYS:HE3	1:M:4:ALA:O	2.17	0.45
1:A:97:ARG:NH1	1:J:102:ASN:OD1	2.50	0.45
1:B:139:VAL:HG22	1:C:204:VAL:HG22	1.99	0.45
1:J:211:PRO:HB2	1:J:214:LEU:HB2	1.99	0.45
1:C:101:GLU:HB2	1:Q:97:ARG:HG2	1.98	0.45
1:H:211:PRO:HB2	1:H:214:LEU:HB2	1.99	0.45
1:K:166:VAL:HG11	1:L:96:ILE:CD1	2.47	0.45
1:N:143:TYR:C	1:N:145:GLY:N	2.70	0.45
1:Q:166:VAL:HA	1:R:89:LEU:HD21	1.99	0.45
1:K:218:SER:HB2	1:L:8:GLU:OE2	2.17	0.45
1:K:179:LYS:NZ	1:L:8:GLU:CG	2.80	0.45
1:B:141:ALA:HA	1:C:202:GLY:HA2	1.98	0.45
1:Q:43:ASP:C	1:Q:45:THR:H	2.21	0.45
1:K:211:PRO:HB2	1:K:214:LEU:HB2	1.99	0.45
1:A:100:GLN:NE2	1:A:111:ILE:O	2.34	0.45
1:H:55:ASN:ND2	1:I:56:PHE:CE2	2.85	0.45
1:N:56:PHE:CE1	1:O:56:PHE:CE2	3.05	0.44
1:I:17:ARG:HB3	1:I:21:TYR:HB2	1.98	0.44
1:D:143:TYR:C	1:D:145:GLY:N	2.71	0.44
1:B:131:GLU:OE1	1:C:213:MET:HB2	2.18	0.44
1:B:9:ALA:O	1:B:10:ALA:HB3	2.17	0.44
1:L:143:TYR:C	1:L:145:GLY:N	2.70	0.44
1:P:176:ASN:O	1:Q:15:MET:N	2.50	0.44
1:G:143:TYR:C	1:G:145:GLY:N	2.71	0.44
1:G:110:ARG:NH1	1:M:103:GLY:HA2	2.31	0.44
1:Q:170:GLU:HA	1:R:81:LEU:HD23	1.99	0.44
1:Q:189:GLY:HA3	1:Q:203:GLU:CD	2.36	0.44
1:Q:166:VAL:HG11	1:R:96:ILE:HD11	2.00	0.44
1:G:152:TYR:CE2	1:G:154:LEU:HD23	2.52	0.44
1:E:43:ASP:C	1:E:45:THR:H	2.20	0.44
1:N:48:PHE:HB2	1:O:54:SER:CB	2.43	0.44
1:P:143:TYR:C	1:P:145:GLY:N	2.71	0.44
1:F:97:ARG:NH1	1:N:102:ASN:OD1	2.51	0.44
1:L:16:PRO:HG3	1:M:5:PRO:HG3	1.99	0.44
1:K:43:ASP:C	1:K:45:THR:H	2.21	0.44
1:P:218:SER:HB2	1:Q:8:GLU:OE2	2.17	0.44
1:F:166:VAL:HA	1:G:89:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:ARG:HH21	1:F:82:GLU:CD	2.21	0.44
1:P:40:ASN:ND2	1:P:42:GLN:HG3	2.33	0.44
1:C:48:PHE:HB2	1:D:54:SER:CB	2.43	0.44
1:E:176:ASN:O	1:F:15:MET:N	2.50	0.44
1:P:43:ASP:C	1:P:45:THR:H	2.21	0.44
1:F:143:TYR:HA	1:G:200:LEU:HA	1.99	0.44
1:E:226:PHE:CZ	1:F:14:LEU:HD22	2.53	0.44
1:Q:143:TYR:C	1:Q:145:GLY:N	2.72	0.43
1:O:143:TYR:C	1:O:145:GLY:N	2.72	0.43
1:F:39:TYR:CE1	1:G:92:GLU:HG2	2.53	0.43
1:E:51:TYR:CG	1:E:52:PRO:HA	2.53	0.43
1:O:55:ASN:ND2	1:P:56:PHE:CE2	2.86	0.43
1:J:154:LEU:CD2	1:L:3:THR:HB	2.40	0.43
1:E:47:GLN:NE2	1:F:58:THR:O	2.45	0.43
1:Q:45:THR:OG1	1:Q:130:TYR:N	2.51	0.43
1:E:137:GLY:HA2	1:F:206:TYR:HA	1.99	0.43
1:M:178:SER:HB2	1:N:15:MET:HG3	2.00	0.43
1:N:166:VAL:HG11	1:O:96:ILE:CD1	2.48	0.43
1:D:17:ARG:HB3	1:D:21:TYR:HB2	2.00	0.43
1:B:143:TYR:HA	1:C:200:LEU:HA	2.00	0.43
1:J:154:LEU:HD13	1:L:3:THR:O	2.18	0.43
1:A:176:ASN:O	1:B:15:MET:N	2.38	0.43
1:L:166:VAL:HA	1:M:89:LEU:HD21	2.00	0.43
1:R:152:TYR:CE2	1:R:154:LEU:HD23	2.53	0.43
1:G:56:PHE:CD1	1:H:56:PHE:CE2	3.07	0.43
1:C:93:ARG:HH12	1:C:97:ARG:HH22	1.67	0.43
1:F:45:THR:OG1	1:F:130:TYR:N	2.52	0.43
1:D:166:VAL:HA	1:E:89:LEU:HD21	1.99	0.43
1:B:166:VAL:HG11	1:C:96:ILE:HD12	2.00	0.43
1:E:36:VAL:HG11	1:E:78:PHE:CD1	2.53	0.43
1:Q:227:LEU:HA	1:Q:227:LEU:HD12	1.77	0.43
1:R:185:GLU:HG3	1:R:207:THR:HG22	2.01	0.43
1:J:63:SER:HB2	1:R:128:ILE:HG22	2.00	0.43
1:F:128:ILE:HG22	1:G:63:SER:HB2	1.99	0.43
1:R:17:ARG:HB3	1:R:21:TYR:HB2	2.01	0.43
1:D:43:ASP:C	1:D:45:THR:H	2.22	0.43
1:N:8:GLU:OE2	1:N:12:PRO:HD3	2.19	0.43
1:G:128:ILE:HG23	1:H:63:SER:CB	2.48	0.43
1:M:55:ASN:ND2	1:N:56:PHE:HE2	2.12	0.43
1:P:139:VAL:HG13	1:Q:204:VAL:HG22	2.00	0.43
1:L:93:ARG:HH12	1:L:97:ARG:HH22	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:ARG:HG2	1:M:101:GLU:HB2	2.01	0.43
1:P:227:LEU:HD12	1:P:227:LEU:HA	1.78	0.43
1:C:14:LEU:HD23	1:C:14:LEU:H	1.83	0.43
1:N:92:GLU:O	1:N:96:ILE:HG13	2.18	0.43
1:J:15:MET:HB3	1:J:15:MET:HE2	1.79	0.43
1:J:92:GLU:HG2	1:R:39:TYR:HE1	1.83	0.43
1:K:121:ILE:HD13	1:K:163:VAL:HG13	2.01	0.43
1:I:179:LYS:NZ	1:I:210:GLU:OE2	2.51	0.43
1:K:179:LYS:NZ	1:K:210:GLU:OE2	2.51	0.43
1:D:173:SER:HA	1:E:73:LYS:HZ1	1.83	0.43
1:N:141:ALA:HA	1:O:202:GLY:HA2	2.00	0.43
1:Q:34:ILE:O	1:Q:78:PHE:HA	2.19	0.43
1:I:185:GLU:HG3	1:I:207:THR:HG22	2.01	0.43
1:H:179:LYS:NZ	1:H:210:GLU:OE2	2.52	0.43
1:L:56:PHE:CE1	1:M:56:PHE:HE2	2.36	0.43
1:A:192:ARG:N	1:A:200:LEU:O	2.50	0.43
1:J:57:SER:HG	1:R:48:PHE:H	1.60	0.42
1:I:100:GLN:NE2	1:I:111:ILE:O	2.32	0.42
1:F:162:ARG:CZ	1:G:82:GLU:OE1	2.67	0.42
1:K:39:TYR:HE1	1:L:92:GLU:HG2	1.83	0.42
1:F:143:TYR:C	1:F:145:GLY:N	2.72	0.42
1:I:43:ASP:C	1:I:45:THR:H	2.23	0.42
1:L:179:LYS:NZ	1:L:210:GLU:OE2	2.52	0.42
1:O:17:ARG:HB3	1:O:21:TYR:HB2	2.00	0.42
1:F:14:LEU:H	1:F:14:LEU:HD23	1.84	0.42
1:P:51:TYR:CG	1:P:52:PRO:HA	2.55	0.42
1:G:34:ILE:O	1:G:78:PHE:HA	2.19	0.42
1:J:34:ILE:O	1:J:78:PHE:HA	2.18	0.42
1:R:43:ASP:C	1:R:45:THR:H	2.22	0.42
1:K:185:GLU:HG3	1:K:207:THR:HG22	2.01	0.42
1:R:100:GLN:NE2	1:R:111:ILE:O	2.32	0.42
1:B:185:GLU:HG3	1:B:207:THR:HG22	2.00	0.42
1:J:200:LEU:C	1:J:200:LEU:HD23	2.35	0.42
1:F:142:ARG:N	1:G:201:GLU:O	2.50	0.42
1:I:121:ILE:HD13	1:I:163:VAL:HG13	2.02	0.42
1:B:179:LYS:NZ	1:B:210:GLU:OE2	2.52	0.42
1:A:179:LYS:NZ	1:A:210:GLU:OE2	2.52	0.42
1:N:93:ARG:HH12	1:N:97:ARG:HH22	1.67	0.42
1:E:34:ILE:O	1:E:78:PHE:HA	2.19	0.42
1:I:101:GLU:HA	1:K:101:GLU:HA	2.00	0.42
1:N:14:LEU:H	1:N:14:LEU:HD23	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:92:GLU:O	1:O:96:ILE:HG13	2.19	0.42
1:J:92:GLU:HG2	1:R:39:TYR:CE1	2.54	0.42
1:N:179:LYS:NZ	1:N:210:GLU:OE2	2.52	0.42
1:B:97:ARG:HG2	1:R:101:GLU:HB2	2.01	0.42
1:R:51:TYR:CG	1:R:52:PRO:HA	2.55	0.42
1:A:139:VAL:HG22	1:B:204:VAL:HG22	2.02	0.42
1:H:34:ILE:O	1:H:78:PHE:HA	2.20	0.42
1:M:180:THR:HG23	1:N:10:ALA:CB	2.49	0.42
1:H:92:GLU:O	1:H:96:ILE:HG13	2.19	0.42
1:J:16:PRO:HG3	1:K:5:PRO:HG3	2.01	0.42
1:A:56:PHE:CE2	1:I:55:ASN:ND2	2.87	0.42
1:R:92:GLU:O	1:R:96:ILE:HG13	2.18	0.42
1:E:179:LYS:NZ	1:E:210:GLU:OE2	2.52	0.42
1:C:17:ARG:HB3	1:C:21:TYR:HB2	1.99	0.42
1:N:17:ARG:HB3	1:N:21:TYR:HB2	2.01	0.42
1:F:34:ILE:O	1:F:78:PHE:HA	2.19	0.42
1:N:51:TYR:CG	1:N:52:PRO:HA	2.55	0.42
1:D:166:VAL:HG11	1:E:96:ILE:HD12	2.01	0.42
1:N:124:GLU:OE2	1:O:82:GLU:OE2	2.38	0.42
1:I:93:ARG:NH1	1:I:97:ARG:HH22	2.17	0.42
1:D:152:TYR:CE2	1:D:154:LEU:HD23	2.55	0.42
1:G:102:ASN:O	1:M:113:LEU:N	2.47	0.42
1:O:43:ASP:C	1:O:45:THR:H	2.22	0.42
1:J:14:LEU:H	1:J:14:LEU:HD23	1.84	0.42
1:B:178:SER:HB2	1:C:15:MET:HG3	2.02	0.42
1:H:166:VAL:HG11	1:I:96:ILE:HD12	2.02	0.42
1:Q:14:LEU:H	1:Q:14:LEU:HD23	1.84	0.42
1:D:179:LYS:NZ	1:D:210:GLU:OE2	2.53	0.42
1:D:102:ASN:OD1	1:P:97:ARG:NH1	2.53	0.42
1:E:256:MET:O	1:F:14:LEU:HD21	2.19	0.42
1:O:135:LYS:HE3	1:Q:6:PRO:HD3	2.01	0.42
1:M:48:PHE:HB2	1:N:54:SER:HB3	2.02	0.42
1:A:96:ILE:CD1	1:I:166:VAL:HG11	2.49	0.42
1:M:179:LYS:NZ	1:M:210:GLU:OE2	2.53	0.42
1:G:17:ARG:HB3	1:G:21:TYR:HB2	2.00	0.42
1:I:34:ILE:O	1:I:78:PHE:HA	2.20	0.42
1:M:34:ILE:O	1:M:78:PHE:HA	2.20	0.42
1:H:35:PHE:HE2	1:I:109:ASN:OD1	2.02	0.42
1:L:176:ASN:O	1:M:15:MET:N	2.46	0.42
1:C:121:ILE:HD13	1:C:163:VAL:HG13	2.02	0.42
1:Q:51:TYR:CG	1:Q:52:PRO:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:TYR:CG	1:F:52:PRO:HA	2.55	0.42
1:K:93:ARG:NH1	1:K:97:ARG:HH22	2.17	0.42
1:K:6:PRO:HD3	1:R:135:LYS:HE3	2.02	0.42
1:M:93:ARG:NH1	1:M:97:ARG:HH22	2.18	0.42
1:G:107:ILE:HG21	1:M:107:ILE:CD1	2.47	0.42
1:F:39:TYR:HE1	1:G:92:GLU:HG2	1.85	0.42
1:N:121:ILE:HD13	1:N:163:VAL:HG13	2.02	0.42
1:P:179:LYS:NZ	1:P:210:GLU:OE2	2.52	0.42
1:O:179:LYS:NZ	1:O:210:GLU:OE2	2.52	0.42
1:O:100:GLN:NE2	1:O:111:ILE:O	2.34	0.42
1:P:34:ILE:O	1:P:78:PHE:HA	2.20	0.42
1:D:34:ILE:O	1:D:78:PHE:HA	2.20	0.42
1:D:14:LEU:H	1:D:14:LEU:HD23	1.85	0.41
1:Q:158:ALA:CB	1:R:15:MET:SD	3.08	0.41
1:L:135:LYS:CE	1:N:6:PRO:HD3	2.51	0.41
1:E:151:GLN:HB2	1:E:185:GLU:CG	2.50	0.41
1:H:51:TYR:CG	1:H:52:PRO:HA	2.55	0.41
1:E:107:ILE:CD1	1:O:107:ILE:HD13	2.28	0.41
1:F:226:PHE:CZ	1:G:14:LEU:CD2	2.98	0.41
1:K:166:VAL:HG11	1:L:96:ILE:HD11	2.03	0.41
1:L:56:PHE:CE1	1:M:56:PHE:CE2	3.08	0.41
1:B:121:ILE:HD13	1:B:163:VAL:HG13	2.02	0.41
1:C:166:VAL:HG11	1:D:96:ILE:HD11	2.01	0.41
1:H:139:VAL:HG22	1:I:204:VAL:HG22	2.02	0.41
1:J:152:TYR:CE2	1:J:154:LEU:HD23	2.54	0.41
1:A:121:ILE:HD13	1:A:163:VAL:HG13	2.02	0.41
1:K:143:TYR:C	1:K:145:GLY:N	2.74	0.41
1:G:92:GLU:O	1:G:96:ILE:HG13	2.20	0.41
1:H:17:ARG:HB3	1:H:21:TYR:HB2	2.01	0.41
1:M:93:ARG:NH2	1:M:114:GLN:O	2.53	0.41
1:G:101:GLU:HB2	1:M:97:ARG:HG2	2.02	0.41
1:P:92:GLU:O	1:P:96:ILE:HG13	2.20	0.41
1:P:15:MET:HE2	1:P:15:MET:HB3	1.82	0.41
1:K:225:ILE:HG21	1:K:253:TYR:CD2	2.56	0.41
1:G:51:TYR:CG	1:G:52:PRO:HA	2.55	0.41
1:F:19:GLN:HG2	1:G:11:ARG:CZ	2.51	0.41
1:D:92:GLU:O	1:D:96:ILE:HG13	2.20	0.41
1:R:179:LYS:NZ	1:R:210:GLU:OE2	2.54	0.41
1:P:14:LEU:HD23	1:P:14:LEU:H	1.86	0.41
1:H:14:LEU:H	1:H:14:LEU:HD23	1.85	0.41
1:L:226:PHE:CZ	1:M:14:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:MET:CE	1:B:217:MET:HG3	2.51	0.41
1:F:130:TYR:CD1	1:F:130:TYR:C	2.93	0.41
1:M:100:GLN:NE2	1:M:111:ILE:O	2.36	0.41
1:J:14:LEU:HA	1:R:177:THR:HA	2.03	0.41
1:L:92:GLU:O	1:L:96:ILE:HG13	2.20	0.41
1:G:47:GLN:NE2	1:H:58:THR:O	2.49	0.41
1:E:166:VAL:HG11	1:F:96:ILE:HD11	2.01	0.41
1:G:179:LYS:NZ	1:G:210:GLU:OE2	2.54	0.41
1:D:56:PHE:CE1	1:E:56:PHE:CE2	3.09	0.41
1:L:34:ILE:O	1:L:78:PHE:HA	2.21	0.41
1:P:162:ARG:HH21	1:Q:82:GLU:CD	2.24	0.41
1:O:227:LEU:HD12	1:O:227:LEU:HA	1.75	0.41
1:P:140:GLY:O	1:Q:203:GLU:N	2.47	0.41
1:G:226:PHE:CZ	1:H:14:LEU:CD2	2.98	0.41
1:J:56:PHE:CE2	1:R:56:PHE:CE1	3.09	0.41
1:C:143:TYR:C	1:C:145:GLY:N	2.74	0.41
1:R:93:ARG:NH2	1:R:114:GLN:O	2.54	0.41
1:J:179:LYS:NZ	1:J:210:GLU:OE2	2.53	0.41
1:M:121:ILE:HD13	1:M:163:VAL:HG13	2.02	0.41
1:A:125:GLY:HA3	1:A:160:ASN:O	2.21	0.41
1:G:45:THR:OG1	1:G:130:TYR:N	2.54	0.41
1:P:113:LEU:HD23	1:P:113:LEU:HA	1.97	0.41
1:O:130:TYR:C	1:O:130:TYR:CD1	2.94	0.41
1:E:113:LEU:N	1:O:102:ASN:O	2.39	0.41
1:A:231:GLY:HA2	1:A:236:LEU:HD13	2.03	0.41
1:O:121:ILE:HD13	1:O:163:VAL:HG13	2.03	0.41
1:N:152:TYR:CE2	1:N:154:LEU:HD23	2.56	0.41
1:Q:91:ASN:O	1:Q:95:ILE:HG13	2.21	0.41
1:J:185:GLU:HG3	1:J:207:THR:HG22	2.01	0.41
1:H:48:PHE:CB	1:I:54:SER:CB	2.96	0.41
1:J:135:LYS:HE3	1:L:6:PRO:HD3	2.02	0.41
1:G:166:VAL:HG11	1:H:96:ILE:HD12	2.02	0.41
1:F:56:PHE:CE1	1:G:56:PHE:HE2	2.38	0.41
1:J:100:GLN:NE2	1:J:111:ILE:O	2.34	0.41
1:E:100:GLN:NE2	1:E:111:ILE:O	2.34	0.41
1:K:34:ILE:O	1:K:78:PHE:HA	2.21	0.41
1:O:34:ILE:O	1:O:78:PHE:HA	2.20	0.41
1:G:173:SER:HA	1:H:73:LYS:NZ	2.36	0.41
1:E:14:LEU:HD23	1:E:14:LEU:H	1.86	0.40
1:J:180:THR:HG21	1:L:3:THR:O	2.21	0.40
1:A:166:VAL:HA	1:B:89:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ARG:NE	1:C:92:GLU:OE2	2.46	0.40
1:J:135:LYS:HE3	1:L:4:ALA:O	2.21	0.40
1:J:51:TYR:CG	1:J:52:PRO:HA	2.55	0.40
1:B:101:GLU:HB2	1:R:97:ARG:HG2	2.02	0.40
1:N:34:ILE:O	1:N:78:PHE:HA	2.21	0.40
1:H:15:MET:HE3	1:H:15:MET:HB3	1.91	0.40
1:F:91:ASN:O	1:F:95:ILE:HG13	2.21	0.40
1:C:34:ILE:O	1:C:78:PHE:HA	2.21	0.40
1:F:11:ARG:HB3	1:F:11:ARG:HH11	1.86	0.40
1:B:34:ILE:O	1:B:78:PHE:HA	2.21	0.40
1:R:36:VAL:O	1:R:81:LEU:O	2.39	0.40
1:A:92:GLU:O	1:A:96:ILE:HG13	2.22	0.40
1:I:92:GLU:O	1:I:96:ILE:HG13	2.22	0.40
1:J:166:VAL:HG11	1:K:96:ILE:HD12	2.02	0.40
1:I:143:TYR:C	1:I:145:GLY:N	2.75	0.40
1:I:225:ILE:HG21	1:I:253:TYR:CD2	2.57	0.40
1:F:48:PHE:HB2	1:G:54:SER:CB	2.50	0.40
1:K:92:GLU:O	1:K:96:ILE:HG13	2.21	0.40
1:J:93:ARG:NH2	1:J:114:GLN:O	2.55	0.40
1:L:35:PHE:HE2	1:M:109:ASN:OD1	2.04	0.40
1:D:177:THR:HA	1:E:14:LEU:HA	2.02	0.40
1:H:102:ASN:O	1:L:113:LEU:N	2.43	0.40
1:A:97:ARG:HG2	1:J:101:GLU:HB2	2.03	0.40
1:J:17:ARG:HB3	1:J:21:TYR:HB2	2.02	0.40
1:H:101:GLU:HA	1:L:101:GLU:HA	2.04	0.40
1:Q:142:ARG:O	1:R:201:GLU:N	2.39	0.40
1:D:130:TYR:CD1	1:D:130:TYR:C	2.95	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/262 (92%)	225 (93%)	16 (7%)	1 (0%)	39	80
1	B	242/262 (92%)	227 (94%)	15 (6%)	0	100	100
1	C	241/262 (92%)	225 (93%)	15 (6%)	1 (0%)	39	80
1	D	242/262 (92%)	227 (94%)	14 (6%)	1 (0%)	39	80
1	E	241/262 (92%)	226 (94%)	13 (5%)	2 (1%)	24	69
1	F	241/262 (92%)	228 (95%)	13 (5%)	0	100	100
1	G	241/262 (92%)	227 (94%)	14 (6%)	0	100	100
1	H	242/262 (92%)	226 (93%)	16 (7%)	0	100	100
1	I	241/262 (92%)	229 (95%)	12 (5%)	0	100	100
1	J	242/262 (92%)	225 (93%)	16 (7%)	1 (0%)	39	80
1	K	241/262 (92%)	227 (94%)	14 (6%)	0	100	100
1	L	241/262 (92%)	226 (94%)	15 (6%)	0	100	100
1	M	241/262 (92%)	226 (94%)	15 (6%)	0	100	100
1	N	241/262 (92%)	224 (93%)	16 (7%)	1 (0%)	39	80
1	O	241/262 (92%)	226 (94%)	14 (6%)	1 (0%)	39	80
1	P	241/262 (92%)	227 (94%)	13 (5%)	1 (0%)	39	80
1	Q	241/262 (92%)	228 (95%)	13 (5%)	0	100	100
1	R	241/262 (92%)	225 (93%)	16 (7%)	0	100	100
All	All	4343/4716 (92%)	4074 (94%)	260 (6%)	9 (0%)	52	87

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	44	GLU
1	O	44	GLU
1	P	44	GLU
1	C	44	GLU
1	D	44	GLU
1	E	16	PRO
1	N	44	GLU
1	A	128	ILE
1	J	16	PRO

### 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	209/223 (94%)	189 (90%)	20 (10%)	10	45
1	B	209/223 (94%)	188 (90%)	21 (10%)	9	43
1	C	208/223 (93%)	190 (91%)	18 (9%)	13	51
1	D	209/223 (94%)	191 (91%)	18 (9%)	13	51
1	E	208/223 (93%)	190 (91%)	18 (9%)	13	51
1	F	208/223 (93%)	190 (91%)	18 (9%)	13	51
1	G	208/223 (93%)	187 (90%)	21 (10%)	9	43
1	H	209/223 (94%)	191 (91%)	18 (9%)	13	51
1	I	208/223 (93%)	189 (91%)	19 (9%)	12	48
1	J	209/223 (94%)	188 (90%)	21 (10%)	9	43
1	K	208/223 (93%)	190 (91%)	18 (9%)	13	51
1	L	208/223 (93%)	186 (89%)	22 (11%)	8	40
1	M	208/223 (93%)	191 (92%)	17 (8%)	14	53
1	N	208/223 (93%)	189 (91%)	19 (9%)	12	48
1	O	208/223 (93%)	190 (91%)	18 (9%)	13	51
1	P	208/223 (93%)	189 (91%)	19 (9%)	12	48
1	Q	208/223 (93%)	189 (91%)	19 (9%)	12	48
1	R	208/223 (93%)	187 (90%)	21 (10%)	9	43
All	All	3749/4014 (93%)	3404 (91%)	345 (9%)	11	48

All (345) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	14	LEU
1	A	22	LYS
1	A	42	GLN
1	A	89	LEU
1	A	108	ASN

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Mol	Chain	Res	Type
1	A	109	ASN
1	A	123	VAL
1	A	126	SER
1	A	132	SER
1	A	136	SER
1	A	152	TYR
1	A	172	LEU
1	A	180	THR
1	A	192	ARG
1	A	217	MET
1	A	237	TRP
1	A	238	ASP
1	A	242	LYS
1	A	255	HIS
1	B	14	LEU
1	B	15	MET
1	B	22	LYS
1	B	33	LYS
1	B	76	ARG
1	B	89	LEU
1	B	91	ASN
1	B	108	ASN
1	B	109	ASN
1	B	126	SER
1	B	131	GLU
1	B	132	SER
1	B	136	SER
1	B	152	TYR
1	B	180	THR
1	B	192	ARG
1	B	213	MET
1	B	217	MET
1	B	237	TRP
1	B	242	LYS
1	B	255	HIS
1	C	14	LEU
1	C	15	MET
1	C	22	LYS
1	C	89	LEU
1	C	108	ASN
1	C	109	ASN
1	C	126	SER

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Mol	Chain	Res	Type
1	C	132	SER
1	C	136	SER
1	C	152	TYR
1	C	172	LEU
1	C	176	ASN
1	C	179	LYS
1	C	180	THR
1	C	217	MET
1	C	237	TRP
1	C	242	LYS
1	C	255	HIS
1	D	11	ARG
1	D	14	LEU
1	D	15	MET
1	D	22	LYS
1	D	89	LEU
1	D	108	ASN
1	D	109	ASN
1	D	123	VAL
1	D	126	SER
1	D	132	SER
1	D	136	SER
1	D	152	TYR
1	D	176	ASN
1	D	180	THR
1	D	217	MET
1	D	237	TRP
1	D	242	LYS
1	D	255	HIS
1	E	14	LEU
1	E	15	MET
1	E	22	LYS
1	E	84	GLN
1	E	89	LEU
1	E	108	ASN
1	E	109	ASN
1	E	126	SER
1	E	132	SER
1	E	136	SER
1	E	152	TYR
1	E	176	ASN
1	E	180	THR

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Mol	Chain	Res	Type
1	E	217	MET
1	E	237	TRP
1	E	242	LYS
1	E	245	ARG
1	E	255	HIS
1	F	8	GLU
1	F	11	ARG
1	F	14	LEU
1	F	15	MET
1	F	22	LYS
1	F	89	LEU
1	F	108	ASN
1	F	109	ASN
1	F	126	SER
1	F	132	SER
1	F	136	SER
1	F	152	TYR
1	F	176	ASN
1	F	180	THR
1	F	217	MET
1	F	237	TRP
1	F	242	LYS
1	F	255	HIS
1	G	14	LEU
1	G	15	MET
1	G	22	LYS
1	G	89	LEU
1	G	107	ILE
1	G	108	ASN
1	G	109	ASN
1	G	114	GLN
1	G	123	VAL
1	G	126	SER
1	G	132	SER
1	G	136	SER
1	G	152	TYR
1	G	172	LEU
1	G	176	ASN
1	G	180	THR
1	G	217	MET
1	G	237	TRP
1	G	239	LEU

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Mol	Chain	Res	Type
1	G	242	LYS
1	G	255	HIS
1	H	14	LEU
1	H	15	MET
1	H	22	LYS
1	H	89	LEU
1	H	91	ASN
1	H	108	ASN
1	H	109	ASN
1	H	122	MET
1	H	123	VAL
1	H	126	SER
1	H	132	SER
1	H	136	SER
1	H	152	TYR
1	H	172	LEU
1	H	217	MET
1	H	237	TRP
1	H	242	LYS
1	H	255	HIS
1	I	11	ARG
1	I	14	LEU
1	I	15	MET
1	I	22	LYS
1	I	42	GLN
1	I	89	LEU
1	I	91	ASN
1	I	108	ASN
1	I	109	ASN
1	I	123	VAL
1	I	126	SER
1	I	132	SER
1	I	136	SER
1	I	152	TYR
1	I	180	THR
1	I	217	MET
1	I	237	TRP
1	I	242	LYS
1	I	255	HIS
1	J	8	GLU
1	J	11	ARG
1	J	14	LEU

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Mol	Chain	Res	Type
1	J	15	MET
1	J	22	LYS
1	J	89	LEU
1	J	108	ASN
1	J	109	ASN
1	J	122	MET
1	J	123	VAL
1	J	126	SER
1	J	132	SER
1	J	136	SER
1	J	151	GLN
1	J	152	TYR
1	J	172	LEU
1	J	200	LEU
1	J	217	MET
1	J	237	TRP
1	J	242	LYS
1	J	255	HIS
1	K	8	GLU
1	K	11	ARG
1	K	14	LEU
1	K	15	MET
1	K	89	LEU
1	K	91	ASN
1	K	108	ASN
1	K	109	ASN
1	K	123	VAL
1	K	126	SER
1	K	132	SER
1	K	136	SER
1	K	152	TYR
1	K	172	LEU
1	K	217	MET
1	K	237	TRP
1	K	242	LYS
1	K	255	HIS
1	L	8	GLU
1	L	11	ARG
1	L	14	LEU
1	L	15	MET
1	L	22	LYS
1	L	42	GLN

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Mol	Chain	Res	Type
1	L	89	LEU
1	L	108	ASN
1	L	109	ASN
1	L	123	VAL
1	L	126	SER
1	L	132	SER
1	L	136	SER
1	L	152	TYR
1	L	176	ASN
1	L	180	THR
1	L	217	MET
1	L	237	TRP
1	L	238	ASP
1	L	242	LYS
1	L	254	ARG
1	L	255	HIS
1	M	11	ARG
1	M	15	MET
1	M	89	LEU
1	M	91	ASN
1	M	108	ASN
1	M	109	ASN
1	M	126	SER
1	M	132	SER
1	M	136	SER
1	M	152	TYR
1	M	176	ASN
1	M	180	THR
1	M	217	MET
1	M	227	LEU
1	M	237	TRP
1	M	242	LYS
1	M	255	HIS
1	N	7	LYS
1	N	14	LEU
1	N	15	MET
1	N	22	LYS
1	N	42	GLN
1	N	76	ARG
1	N	89	LEU
1	N	108	ASN
1	N	109	ASN

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Mol	Chain	Res	Type
1	N	126	SER
1	N	132	SER
1	N	136	SER
1	N	152	TYR
1	N	172	LEU
1	N	180	THR
1	N	217	MET
1	N	237	TRP
1	N	242	LYS
1	N	255	HIS
1	O	14	LEU
1	O	15	MET
1	O	22	LYS
1	O	89	LEU
1	O	108	ASN
1	O	109	ASN
1	O	123	VAL
1	O	126	SER
1	O	132	SER
1	O	136	SER
1	O	152	TYR
1	O	176	ASN
1	O	180	THR
1	O	217	MET
1	O	227	LEU
1	O	237	TRP
1	O	242	LYS
1	O	255	HIS
1	P	8	GLU
1	P	14	LEU
1	P	15	MET
1	P	89	LEU
1	P	108	ASN
1	P	109	ASN
1	P	114	GLN
1	P	122	MET
1	P	126	SER
1	P	132	SER
1	P	136	SER
1	P	152	TYR
1	P	176	ASN
1	P	180	THR

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Mol	Chain	Res	Type
1	P	217	MET
1	P	227	LEU
1	P	237	TRP
1	P	242	LYS
1	P	255	HIS
1	Q	8	GLU
1	Q	11	ARG
1	Q	14	LEU
1	Q	15	MET
1	Q	22	LYS
1	Q	89	LEU
1	Q	108	ASN
1	Q	109	ASN
1	Q	126	SER
1	Q	132	SER
1	Q	136	SER
1	Q	152	TYR
1	Q	176	ASN
1	Q	180	THR
1	Q	217	MET
1	Q	227	LEU
1	Q	237	TRP
1	Q	242	LYS
1	Q	255	HIS
1	R	8	GLU
1	R	14	LEU
1	R	15	MET
1	R	22	LYS
1	R	89	LEU
1	R	108	ASN
1	R	109	ASN
1	R	114	GLN
1	R	123	VAL
1	R	126	SER
1	R	132	SER
1	R	136	SER
1	R	152	TYR
1	R	172	LEU
1	R	180	THR
1	R	217	MET
1	R	227	LEU
1	R	237	TRP

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Mol	Chain	Res	Type
1	R	239	LEU
1	R	242	LYS
1	R	255	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	114	GLN
1	B	40	ASN
1	B	187	GLN
1	C	42	GLN
1	C	176	ASN
1	D	176	ASN
1	E	114	GLN
1	E	151	GLN
1	E	176	ASN
1	E	187	GLN
1	F	40	ASN
1	F	160	ASN
1	F	176	ASN
1	G	176	ASN
1	H	187	GLN
1	I	114	GLN
1	J	40	ASN
1	J	120	ASN
1	K	187	GLN
1	L	40	ASN
1	L	114	GLN
1	L	176	ASN
1	M	176	ASN
1	N	153	GLN
1	O	176	ASN
1	P	40	ASN
1	P	151	GLN
1	P	176	ASN
1	Q	160	ASN
1	Q	176	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 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	248/262 (94%)	-0.12	6 (2%) 62 47	38, 94, 165, 213	0
1	B	248/262 (94%)	-0.02	5 (2%) 68 54	45, 99, 162, 200	0
1	C	247/262 (94%)	0.37	18 (7%) 18 12	49, 119, 181, 226	0
1	D	248/262 (94%)	0.61	29 (11%) 6 5	58, 120, 186, 224	0
1	E	247/262 (94%)	0.64	35 (14%) 4 3	52, 118, 183, 230	0
1	F	247/262 (94%)	0.26	14 (5%) 27 19	53, 117, 184, 233	0
1	G	247/262 (94%)	0.20	11 (4%) 37 26	53, 117, 174, 236	0
1	H	248/262 (94%)	0.16	8 (3%) 51 37	57, 112, 174, 249	0
1	I	247/262 (94%)	0.09	12 (4%) 33 23	43, 105, 167, 258	0
1	J	248/262 (94%)	0.14	8 (3%) 51 37	58, 112, 184, 238	0
1	K	247/262 (94%)	0.05	11 (4%) 37 26	38, 107, 168, 229	0
1	L	247/262 (94%)	-0.15	5 (2%) 68 54	29, 92, 155, 227	0
1	M	247/262 (94%)	0.05	9 (3%) 46 33	41, 102, 158, 205	0
1	N	247/262 (94%)	0.33	19 (7%) 16 11	42, 115, 173, 212	0
1	O	247/262 (94%)	0.58	26 (10%) 8 6	57, 123, 185, 229	0
1	P	247/262 (94%)	0.59	33 (13%) 4 4	51, 120, 188, 248	0
1	Q	247/262 (94%)	0.29	16 (6%) 22 14	50, 121, 184, 240	0
1	R	247/262 (94%)	0.15	8 (3%) 51 37	50, 116, 176, 204	0
All	All	4451/4716 (94%)	0.23	273 (6%) 25 16	29, 111, 179, 258	0

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	143	TYR	7.4
1	D	143	TYR	7.0
1	F	9	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
1	E	208	SER	6.6
1	P	243	ALA	6.5
1	P	208	SER	6.2
1	C	243	ALA	5.9
1	D	239	LEU	5.9
1	O	239	LEU	5.8
1	D	238	ASP	5.7
1	D	242	LYS	5.6
1	D	233	ASP	5.5
1	E	143	TYR	5.5
1	E	3	THR	5.5
1	G	9	ALA	5.3
1	Q	9	ALA	5.3
1	R	3	THR	5.2
1	E	182	LEU	5.1
1	E	238	ASP	5.1
1	Q	155	ASP	5.0
1	E	239	LEU	4.9
1	E	243	ALA	4.8
1	N	243	ALA	4.8
1	O	242	LYS	4.8
1	P	143	TYR	4.8
1	I	8	GLU	4.8
1	O	238	ASP	4.8
1	C	241	ASN	4.7
1	N	240	GLN	4.7
1	E	242	LYS	4.7
1	P	242	LYS	4.7
1	P	239	LEU	4.6
1	B	3	THR	4.6
1	D	241	ASN	4.6
1	K	3	THR	4.6
1	P	9	ALA	4.6
1	P	3	THR	4.4
1	G	8	GLU	4.4
1	N	210	GLU	4.4
1	Q	34	ILE	4.3
1	C	240	GLN	4.3
1	N	241	ASN	4.2
1	O	9	ALA	4.2
1	R	9	ALA	4.2
1	I	51	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	N	32	GLY	4.1
1	K	8	GLU	4.1
1	E	9	ALA	4.1
1	P	244	GLU	4.0
1	G	3	THR	4.0
1	E	7	LYS	4.0
1	C	4	ALA	4.0
1	O	233	ASP	4.0
1	G	241	ASN	4.0
1	P	241	ASN	3.9
1	F	34	ILE	3.9
1	J	3	THR	3.9
1	K	51	TYR	3.9
1	A	108	ASN	3.8
1	E	6	PRO	3.8
1	Q	10	ALA	3.8
1	K	9	ALA	3.7
1	C	32	GLY	3.7
1	F	10	ALA	3.7
1	N	255	HIS	3.7
1	O	241	ASN	3.7
1	L	120	ASN	3.7
1	E	241	ASN	3.6
1	O	8	GLU	3.6
1	E	180	THR	3.6
1	N	4	ALA	3.6
1	N	6	PRO	3.5
1	N	182	LEU	3.5
1	A	3	THR	3.5
1	G	10	ALA	3.5
1	P	238	ASP	3.4
1	H	3	THR	3.4
1	E	183	SER	3.4
1	I	3	THR	3.4
1	N	239	LEU	3.4
1	L	108	ASN	3.4
1	K	4	ALA	3.4
1	P	248	ASP	3.3
1	P	8	GLU	3.3
1	H	8	GLU	3.3
1	D	240	GLN	3.3
1	C	6	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	244	GLU	3.2
1	F	155	ASP	3.2
1	D	244	GLU	3.2
1	Q	79	ILE	3.2
1	P	246	GLN	3.2
1	O	244	GLU	3.2
1	K	239	LEU	3.2
1	P	247	ASN	3.2
1	C	239	LEU	3.2
1	E	245	ARG	3.2
1	D	246	GLN	3.2
1	I	11	ARG	3.1
1	P	183	SER	3.1
1	A	4	ALA	3.1
1	Q	3	THR	3.1
1	E	210	GLU	3.1
1	P	182	LEU	3.1
1	O	240	GLN	3.1
1	C	255	HIS	3.1
1	D	146	ILE	3.1
1	I	239	LEU	3.1
1	E	244	GLU	3.1
1	O	210	GLU	3.1
1	F	8	GLU	3.0
1	J	241	ASN	3.0
1	N	3	THR	3.0
1	P	51	TYR	3.0
1	O	32	GLY	3.0
1	O	51	TYR	3.0
1	C	3	THR	3.0
1	D	248	ASP	3.0
1	Q	182	LEU	3.0
1	R	10	ALA	3.0
1	F	180	THR	3.0
1	I	9	ALA	3.0
1	O	31	THR	3.0
1	F	143	TYR	2.9
1	P	4	ALA	2.9
1	G	180	THR	2.9
1	E	181	ILE	2.9
1	D	9	ALA	2.9
1	Q	181	ILE	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	51	TYR	2.8
1	E	246	GLN	2.8
1	M	3	THR	2.8
1	L	4	ALA	2.8
1	P	210	GLU	2.8
1	E	135	LYS	2.8
1	E	155	ASP	2.8
1	H	241	ASN	2.8
1	I	4	ALA	2.8
1	O	145	GLY	2.8
1	D	243	ALA	2.8
1	O	243	ALA	2.8
1	A	120	ASN	2.8
1	E	247	ASN	2.8
1	Q	180	THR	2.8
1	E	184	TYR	2.8
1	P	11	ARG	2.8
1	E	4	ALA	2.8
1	O	246	GLN	2.8
1	D	148	ALA	2.7
1	E	253	TYR	2.7
1	C	146	ILE	2.7
1	J	243	ALA	2.7
1	R	241	ASN	2.7
1	F	206	TYR	2.7
1	D	8	GLU	2.7
1	F	3	THR	2.7
1	M	182	LEU	2.7
1	O	146	ILE	2.7
1	J	238	ASP	2.7
1	P	7	LYS	2.7
1	P	240	GLN	2.6
1	E	91	ASN	2.6
1	D	186	VAL	2.6
1	F	181	ILE	2.6
1	P	253	TYR	2.6
1	K	241	ASN	2.6
1	P	10	ALA	2.6
1	Q	143	TYR	2.6
1	M	92	GLU	2.5
1	E	240	GLN	2.5
1	F	79	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	176	ASN	2.5
1	O	3	THR	2.5
1	G	243	ALA	2.5
1	E	51	TYR	2.5
1	K	33	LYS	2.5
1	O	147	GLY	2.5
1	O	148	ALA	2.5
1	R	243	ALA	2.5
1	I	241	ASN	2.5
1	J	108	ASN	2.5
1	C	8	GLU	2.5
1	Q	238	ASP	2.5
1	C	5	PRO	2.4
1	D	145	GLY	2.4
1	B	241	ASN	2.4
1	D	208	SER	2.4
1	E	8	GLU	2.4
1	Q	208	SER	2.4
1	L	3	THR	2.4
1	H	237	TRP	2.4
1	B	92	GLU	2.4
1	I	52	PRO	2.4
1	R	143	TYR	2.4
1	Q	90	LEU	2.4
1	Q	233	ASP	2.4
1	R	8	GLU	2.4
1	H	108	ASN	2.4
1	P	91	ASN	2.4
1	A	107	ILE	2.4
1	N	8	GLU	2.4
1	J	237	TRP	2.3
1	N	244	GLU	2.3
1	O	250	LEU	2.3
1	P	155	ASP	2.3
1	D	31	THR	2.3
1	M	31	THR	2.3
1	C	210	GLU	2.3
1	O	34	ILE	2.3
1	N	249	ILE	2.3
1	D	245	ARG	2.3
1	K	97	ARG	2.3
1	P	180	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	11	ARG	2.3
1	E	152	TYR	2.3
1	D	210	GLU	2.3
1	B	240	GLN	2.3
1	F	90	LEU	2.3
1	A	173	SER	2.2
1	B	31	THR	2.2
1	E	11	ARG	2.2
1	G	143	TYR	2.2
1	D	108	ASN	2.2
1	G	155	ASP	2.2
1	N	248	ASP	2.2
1	R	153	GLN	2.2
1	J	248	ASP	2.2
1	H	238	ASP	2.2
1	O	80	PRO	2.2
1	F	238	ASP	2.2
1	M	143	TYR	2.2
1	D	91	ASN	2.2
1	M	241	ASN	2.2
1	C	215	CYS	2.2
1	D	206	TYR	2.2
1	I	97	ARG	2.2
1	K	52	PRO	2.2
1	C	31	THR	2.2
1	G	244	GLU	2.2
1	C	35	PHE	2.2
1	J	151	GLN	2.2
1	N	31	THR	2.1
1	D	147	GLY	2.1
1	O	30	PRO	2.1
1	F	245	ARG	2.1
1	D	3	THR	2.1
1	P	179	LYS	2.1
1	M	4	ALA	2.1
1	P	245	ARG	2.1
1	D	52	PRO	2.1
1	Q	154	LEU	2.1
1	D	109	ASN	2.1
1	N	135	LYS	2.1
1	P	135	LYS	2.1
1	I	32	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	249	ILE	2.1
1	E	153	GLN	2.1
1	H	243	ALA	2.1
1	I	94	LYS	2.1
1	M	240	GLN	2.1
1	L	107	ILE	2.1
1	P	209	ASN	2.1
1	Q	239	LEU	2.0
1	M	210	GLU	2.0
1	E	31	THR	2.0
1	G	242	LYS	2.0
1	H	51	TYR	2.0
1	E	209	ASN	2.0
1	C	248	ASP	2.0
1	N	9	ALA	2.0
1	E	63	SER	2.0
1	P	250	LEU	2.0
1	O	249	ILE	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 carbohydrates 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.