



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:37 am BST

PDB ID : 5TBK  
Title : Crystal structure of human importin  $\alpha 3$  bound to RCC1  
Authors : Sankhala, R.S.; Lokareddy, R.K.; Pumroy, R.A.; Cingolani, G.  
Deposited on : 2016-09-12  
Resolution : 3.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

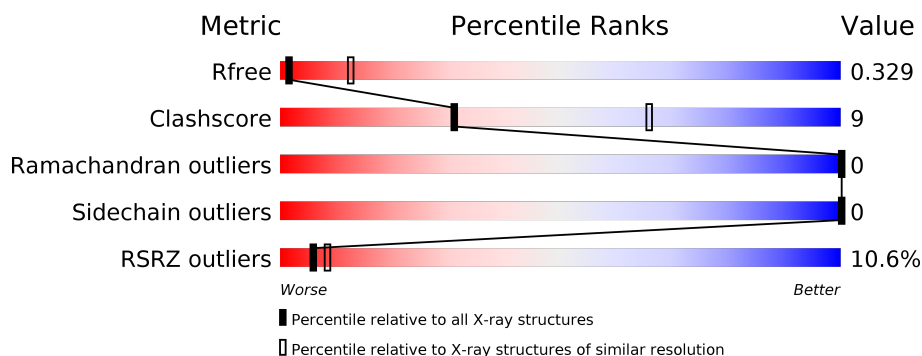
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	521	
1	B	521	
1	C	521	
1	D	521	
1	E	521	
1	F	521	

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Mol	Chain	Length	Quality of chain
1	G	521	
1	H	521	
2	I	421	
2	J	421	
2	K	421	
2	L	421	
2	M	421	
2	N	421	
2	O	421	
2	P	421	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 50677 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 Importin subunit alpha-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3219	2043	545	618	13			
1	B	415	Total	C	N	O	S	0	0	0
			3187	2024	541	609	13			
1	C	417	Total	C	N	O	S	0	0	0
			3200	2031	543	613	13			
1	D	415	Total	C	N	O	S	0	0	0
			3206	2036	543	614	13			
1	E	416	Total	C	N	O	S	0	0	0
			3194	2028	542	611	13			
1	F	416	Total	C	N	O	S	0	0	0
			3194	2028	542	611	13			
1	G	417	Total	C	N	O	S	0	0	0
			3200	2031	543	613	13			
1	H	417	Total	C	N	O	S	0	0	0
			3200	2031	543	613	13			

- Molecule 2 is a protein called Regulator of chromosome condensation.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	419	Total	C	N	O	S	0	0	0
			3139	1954	562	604	19			
2	K	418	Total	C	N	O	S	0	0	0
			3132	1949	561	603	19			
2	L	418	Total	C	N	O	S	0	0	0
			3132	1949	561	603	19			
2	M	419	Total	C	N	O	S	0	0	0
			3139	1954	562	604	19			
2	N	418	Total	C	N	O	S	0	0	0
			3132	1949	561	603	19			
2	O	418	Total	C	N	O	S	0	0	0
			3132	1949	561	603	19			

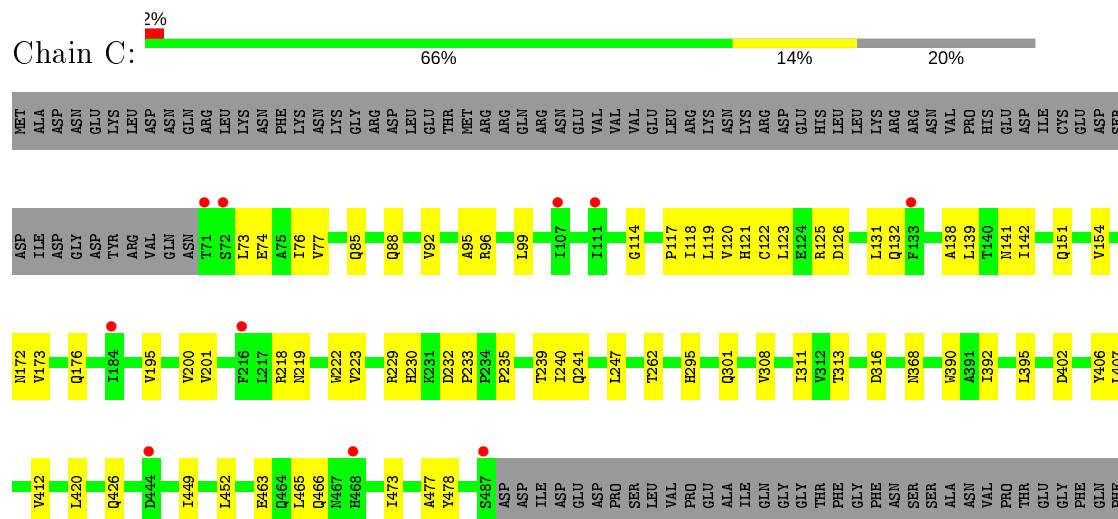
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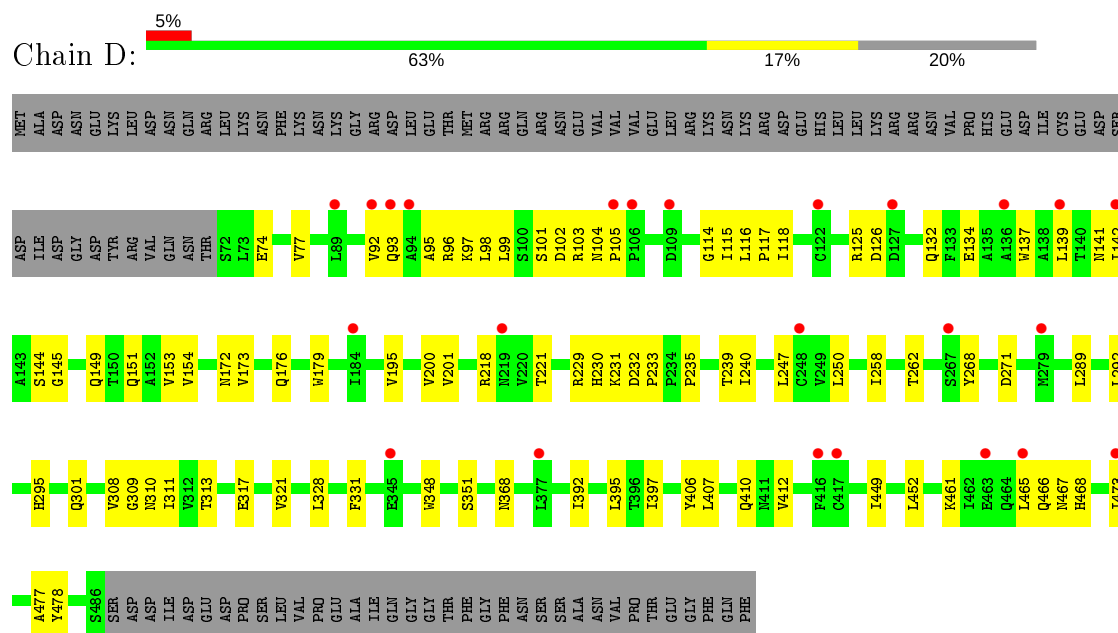
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	419	Total	C	N	O	S	0	0	0
			3139	1954	562	604	19			
2	J	418	Total	C	N	O	S	0	0	0
			3132	1949	561	603	19			



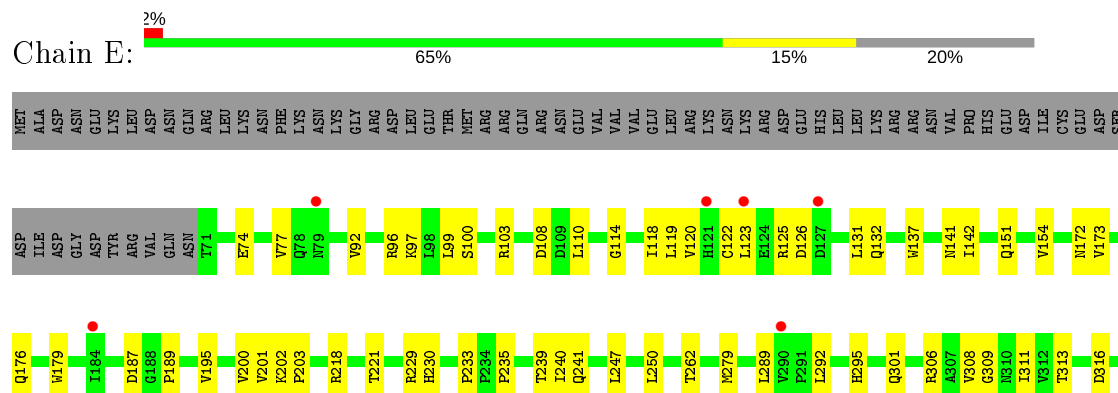
- Molecule 1: Importin subunit alpha-3

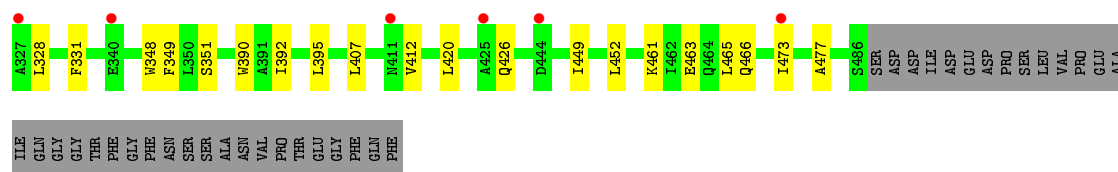


- Molecule 1: Importin subunit alpha-3

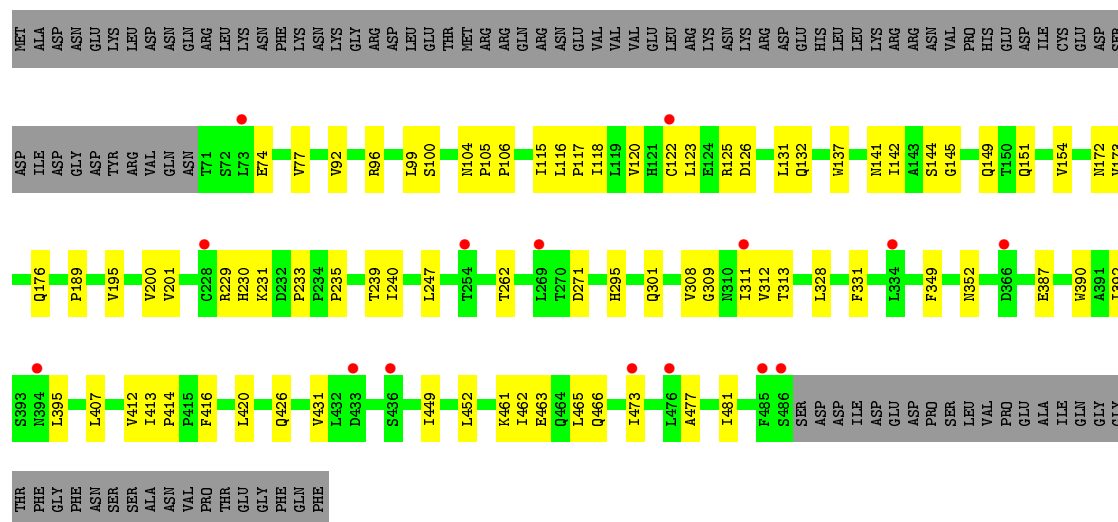


- Molecule 1: Importin subunit alpha-3

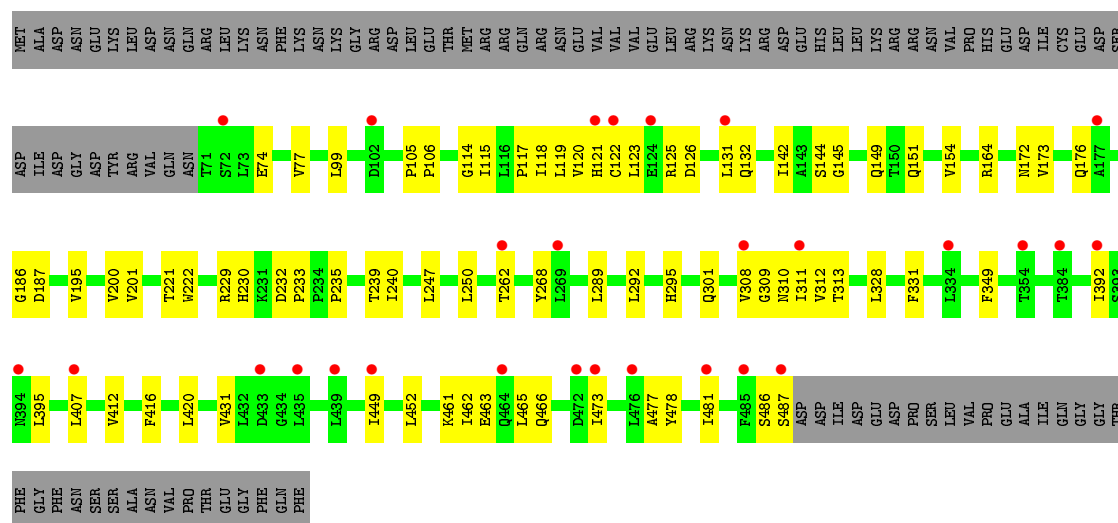




• Molecule 1: Importin subunit alpha-3



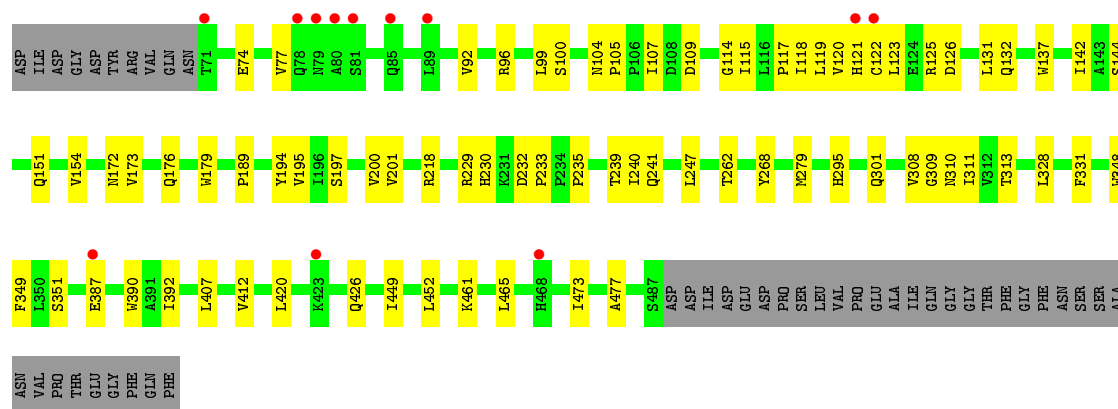
• Molecule 1: Importin subunit alpha-3



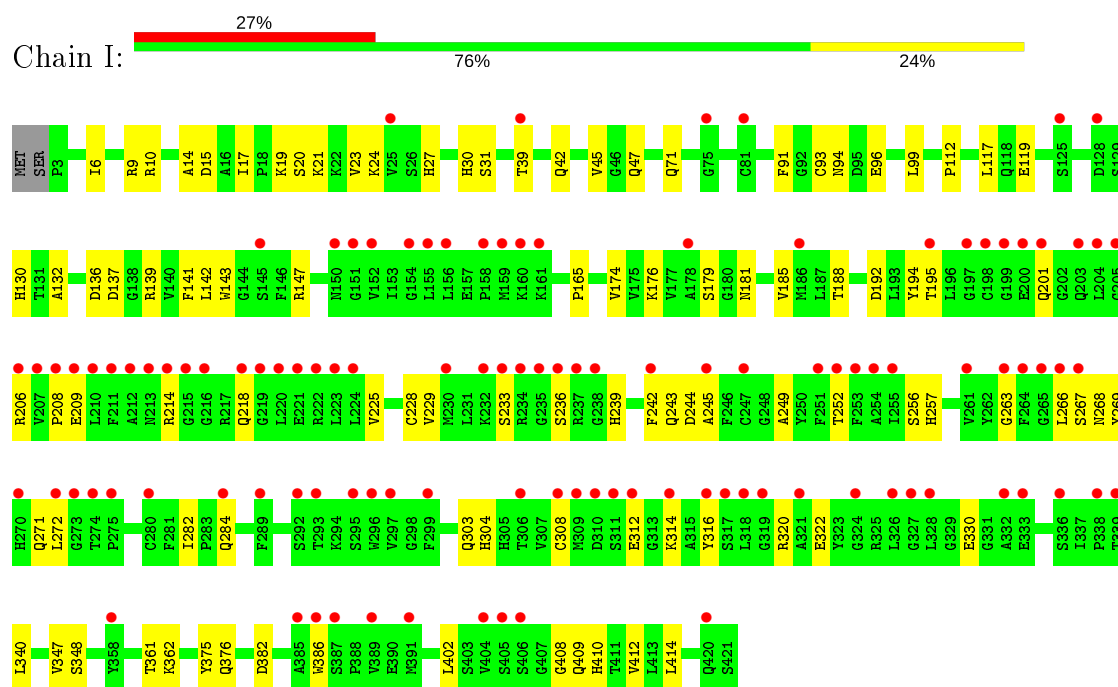
• Molecule 1: Importin subunit alpha-3



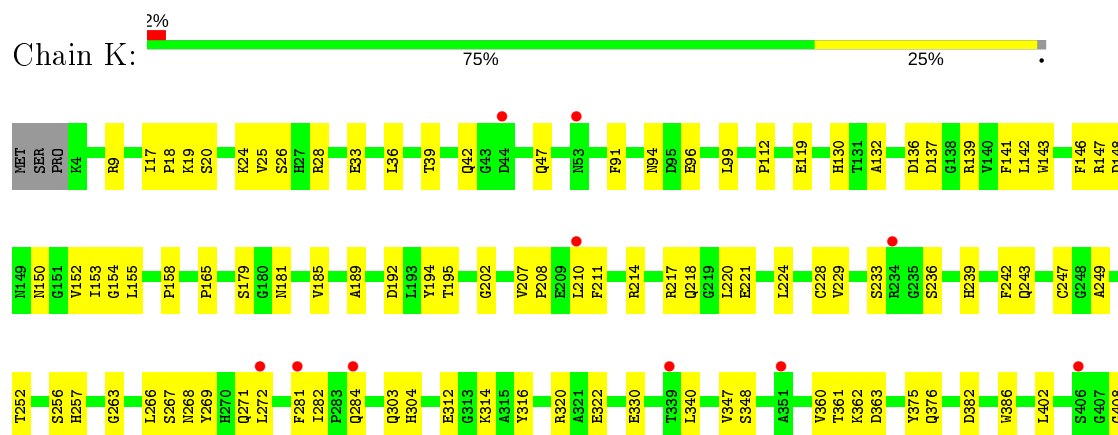




• Molecule 2: Regulator of chromosome condensation

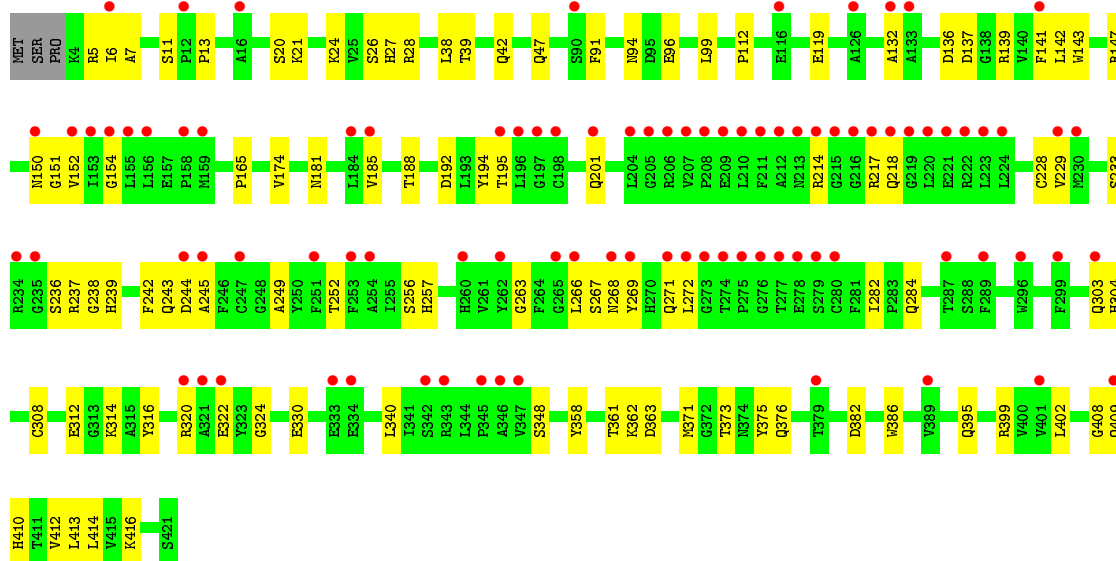
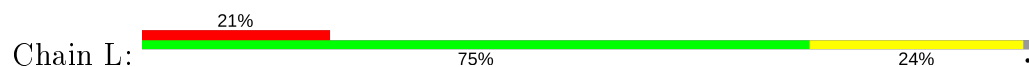


• Molecule 2: Regulator of chromosome condensation

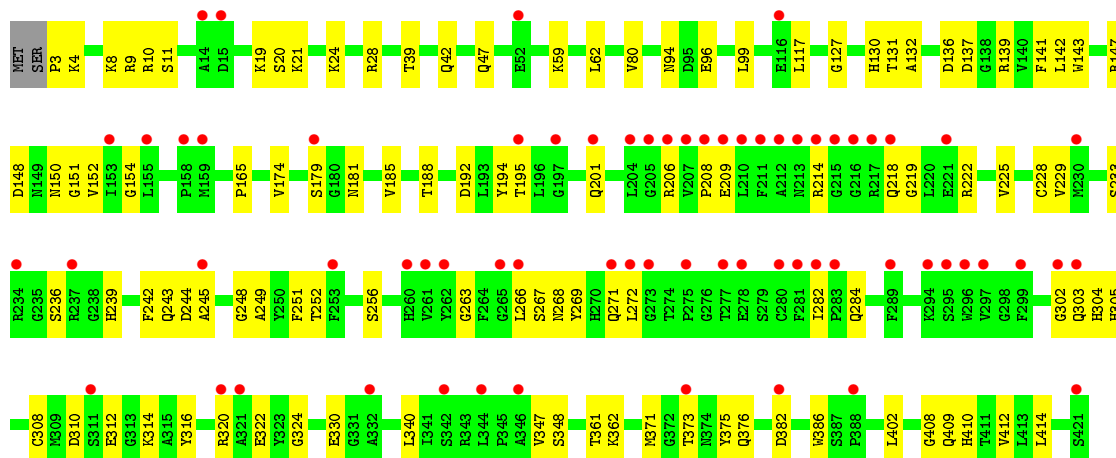
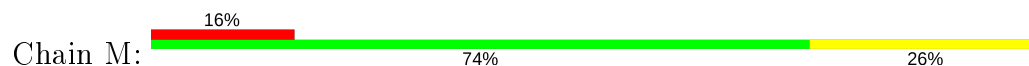




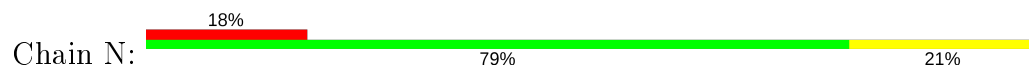
• Molecule 2: Regulator of chromosome condensation



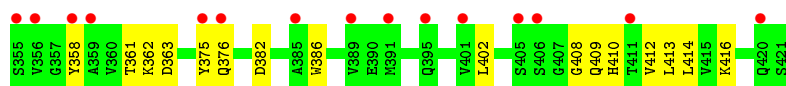
• Molecule 2: Regulator of chromosome condensation



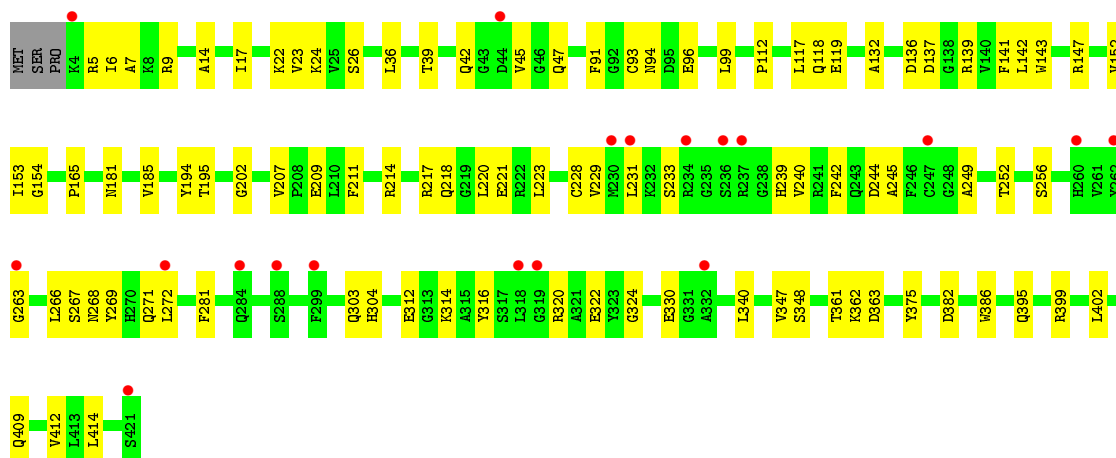
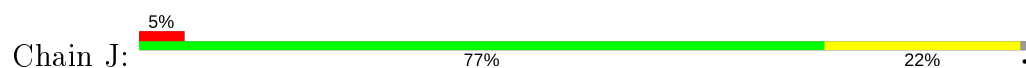
• Molecule 2: Regulator of chromosome condensation







- Molecule 2: Regulator of chromosome condensation



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.40 Å 162.49 Å 161.59 Å 75.65° 85.63° 72.17°	Depositor
Resolution (Å)	19.99 – 3.45 49.33 – 3.44	Depositor EDS
% Data completeness (in resolution range)	75.5 (19.99-3.45) 79.7 (49.33-3.44)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 3.40 Å)	Xtriage
Refinement program	PHENIX 1.10.1-2155	Depositor
R, $R_{free}$	0.278 , 0.296 0.309 , 0.329	Depositor DCC
$R_{free}$ test set	2000 reflections (1.39%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	85.6	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 19.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	50677	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	129.0	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 24.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7376e-03.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.38	0/3279	0.51	0/4481
1	B	0.32	0/3247	0.46	0/4439
1	C	0.36	0/3260	0.50	0/4457
1	D	0.33	0/3266	0.48	0/4463
1	E	0.28	0/3254	0.45	0/4449
1	F	0.31	0/3254	0.46	0/4449
1	G	0.31	0/3260	0.47	0/4457
1	H	0.30	0/3260	0.45	0/4457
2	I	0.27	0/3198	0.49	0/4313
2	J	0.31	0/3190	0.50	0/4302
2	K	0.32	0/3190	0.50	0/4302
2	L	0.27	0/3190	0.48	0/4302
2	M	0.29	0/3198	0.48	0/4313
2	N	0.27	0/3190	0.47	0/4302
2	O	0.28	0/3190	0.49	0/4302
2	P	0.27	0/3198	0.50	0/4313
All	All	0.31	0/51624	0.48	0/70101

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3219	0	3241	80	0
1	B	3187	0	3192	61	0
1	C	3200	0	3204	54	0
1	D	3206	0	3229	77	0
1	E	3194	0	3199	59	0
1	F	3194	0	3199	50	0
1	G	3200	0	3204	55	0
1	H	3200	0	3204	55	0
2	I	3139	0	3110	71	0
2	J	3132	0	3102	72	0
2	K	3132	0	3102	74	0
2	L	3132	0	3102	73	0
2	M	3139	0	3110	66	0
2	N	3132	0	3102	54	0
2	O	3132	0	3102	67	0
2	P	3139	0	3110	79	0
All	All	50677	0	50512	925	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 9.

All (925) 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:A:80:ALA:CA	1:A:88:GLN:HE22	1.36	1.38
1:A:80:ALA:HA	1:A:88:GLN:NE2	1.38	1.32
1:D:95:ALA:O	1:D:98:LEU:HG	1.38	1.20
1:B:226:ASN:OD1	2:I:20:SER:HB2	1.47	1.14
1:D:99:LEU:HD11	2:P:24:LYS:O	1.50	1.11
2:J:233:SER:HB3	2:J:240:VAL:HG23	1.19	1.09
1:A:95:ALA:O	1:A:98:LEU:HG	1.52	1.08
1:B:229:ARG:HH21	2:I:20:SER:HB3	1.15	1.04
1:B:229:ARG:NH2	2:I:20:SER:HB3	1.71	1.04
2:J:211:PHE:HB3	2:J:214:ARG:HD3	1.36	1.01
2:J:233:SER:CB	2:J:240:VAL:HG23	1.99	0.92
1:A:99:LEU:HD11	2:K:24:LYS:O	1.73	0.89
2:P:6:ILE:HG22	2:P:7:ALA:N	1.88	0.88
2:J:233:SER:HB3	2:J:240:VAL:CG2	2.05	0.86
2:K:137:ASP:OD2	2:K:139:ARG:NH1	2.09	0.84
1:A:82:SER:N	1:A:88:GLN:OE1	2.12	0.82
1:A:80:ALA:HA	1:A:88:GLN:HE22	0.66	0.82
1:A:98:LEU:HA	1:A:101:SER:HB2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:137:ASP:OD2	2:J:139:ARG:NH1	2.14	0.81
2:P:209:GLU:O	2:P:214:ARG:NH2	2.13	0.81
2:P:6:ILE:HG22	2:P:7:ALA:O	1.80	0.81
1:D:99:LEU:CD1	2:P:24:LYS:O	2.28	0.80
1:A:368:ASN:OD1	2:J:217:ARG:NH1	2.15	0.80
2:L:137:ASP:OD2	2:L:139:ARG:NH1	2.16	0.79
1:E:137:TRP:HE1	2:L:26:SER:HB2	1.47	0.78
2:M:137:ASP:OD2	2:M:139:ARG:NH1	2.17	0.77
2:N:137:ASP:OD2	2:N:139:ARG:NH1	2.17	0.77
2:M:42:GLN:HB2	2:M:409:GLN:HB3	1.67	0.76
1:B:218:ARG:NH1	2:I:119:GLU:OE2	2.18	0.76
1:D:99:LEU:HD12	2:P:26:SER:N	1.99	0.76
1:E:218:ARG:NH1	2:L:119:GLU:OE2	2.18	0.76
2:O:137:ASP:OD2	2:O:139:ARG:NH1	2.19	0.75
1:A:80:ALA:C	1:A:88:GLN:HE22	1.89	0.75
2:J:233:SER:CB	2:J:240:VAL:CG2	2.64	0.74
1:B:226:ASN:OD1	2:I:20:SER:CB	2.33	0.74
1:D:144:SER:O	2:P:21:LYS:HD3	1.88	0.74
1:A:99:LEU:HD21	1:A:141:ASN:CG	2.08	0.73
1:G:115:ILE:O	1:G:119:LEU:HG	1.87	0.73
2:I:209:GLU:O	2:I:214:ARG:NH2	2.21	0.72
1:B:222:TRP:HE1	2:I:20:SER:HA	1.52	0.72
1:G:144:SER:HA	2:N:21:LYS:HD2	1.72	0.72
2:I:137:ASP:OD2	2:I:139:ARG:NH1	2.23	0.72
1:E:235:PRO:HG2	1:E:240:ILE:HD11	1.72	0.71
1:D:99:LEU:HD21	1:D:141:ASN:HB3	1.72	0.71
2:I:42:GLN:HB2	2:I:409:GLN:HB3	1.73	0.71
2:P:6:ILE:CG2	2:P:7:ALA:N	2.54	0.71
1:A:487:SER:HB3	2:M:62:LEU:HB3	1.73	0.71
1:D:114:GLY:O	1:D:117:PRO:HD2	1.89	0.71
1:G:99:LEU:HD13	1:G:142:ILE:HD11	1.72	0.71
1:H:218:ARG:NH1	2:O:119:GLU:OE2	2.24	0.70
1:G:122:CYS:HB2	1:G:131:LEU:HD21	1.73	0.70
2:M:151:GLY:H	2:O:150:ASN:HA	1.56	0.70
1:A:99:LEU:HD21	1:A:141:ASN:HB3	1.72	0.70
1:A:88:GLN:HA	1:A:88:GLN:HE21	1.57	0.70
1:C:402:ASP:HB3	2:K:214:ARG:HH21	1.57	0.69
1:B:295:HIS:O	1:B:301:GLN:NE2	2.25	0.69
2:P:137:ASP:OD2	2:P:139:ARG:NH1	2.24	0.69
1:F:99:LEU:HD13	1:F:142:ILE:HD11	1.75	0.69
2:O:209:GLU:O	2:O:214:ARG:NH2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:237:ARG:HG2	2:L:238:GLY:H	1.56	0.69
1:H:117:PRO:O	1:H:121:HIS:ND1	2.24	0.69
1:C:313:THR:O	1:C:313:THR:HG22	1.92	0.69
1:A:218:ARG:NH1	2:K:119:GLU:OE2	2.25	0.69
1:H:295:HIS:O	1:H:301:GLN:NE2	2.25	0.68
2:L:42:GLN:HB2	2:L:409:GLN:HB3	1.75	0.68
2:P:42:GLN:HB2	2:P:409:GLN:HB3	1.75	0.68
1:C:218:ARG:NH1	2:J:119:GLU:OE2	2.26	0.68
1:D:229:ARG:NH1	2:P:19:LYS:HB3	2.09	0.68
1:F:312:VAL:O	2:M:8:LYS:NZ	2.26	0.68
1:E:295:HIS:O	1:E:301:GLN:NE2	2.25	0.68
2:N:42:GLN:HB2	2:N:409:GLN:HB3	1.74	0.68
1:D:295:HIS:O	1:D:301:GLN:NE2	2.26	0.68
1:C:235:PRO:HG2	1:C:240:ILE:HD11	1.76	0.67
2:O:233:SER:HB3	2:O:236:SER:HA	1.76	0.67
1:H:122:CYS:HB2	1:H:131:LEU:HD21	1.75	0.67
1:E:99:LEU:HD13	1:E:142:ILE:HD11	1.76	0.67
2:O:42:GLN:HB2	2:O:409:GLN:HB3	1.77	0.67
1:G:235:PRO:HG2	1:G:240:ILE:HD11	1.74	0.67
2:J:96:GLU:OE2	2:J:147:ARG:NH2	2.28	0.67
1:H:348:TRP:CZ2	2:O:11:SER:HB3	2.30	0.67
1:D:218:ARG:NH1	2:P:119:GLU:OE2	2.28	0.66
1:H:235:PRO:HG2	1:H:240:ILE:HD11	1.78	0.66
1:A:99:LEU:HD21	1:A:141:ASN:CB	2.25	0.66
1:C:99:LEU:HD13	1:C:142:ILE:HD11	1.76	0.66
2:M:209:GLU:O	2:M:214:ARG:NH2	2.29	0.66
1:A:478:TYR:OH	2:M:59:LYS:N	2.26	0.66
1:A:402:ASP:HB2	2:J:214:ARG:HH22	1.59	0.66
2:K:42:GLN:HB2	2:K:409:GLN:HB3	1.78	0.65
1:D:99:LEU:CD1	2:P:25:VAL:HA	2.27	0.65
1:H:99:LEU:HD13	1:H:142:ILE:HD11	1.76	0.65
2:L:233:SER:HB3	2:L:236:SER:HA	1.79	0.65
1:A:99:LEU:HD12	2:K:26:SER:H	1.62	0.65
1:A:88:GLN:HA	1:A:88:GLN:NE2	2.12	0.65
2:I:27:HIS:HB3	2:I:30:HIS:CE1	2.31	0.65
1:B:99:LEU:HD13	1:B:142:ILE:HD11	1.79	0.65
1:F:295:HIS:O	1:F:301:GLN:NE2	2.29	0.65
1:B:273:GLY:HA2	2:I:10:ARG:HH22	1.62	0.64
1:A:406:TYR:HB2	2:J:218:GLN:HG3	1.79	0.64
1:B:466:GLN:HG3	1:B:466:GLN:O	1.97	0.64
1:A:295:HIS:O	1:A:301:GLN:NE2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:TYR:HE2	2:O:59:LYS:HB2	1.62	0.64
2:I:42:GLN:O	2:I:47:GLN:NE2	2.31	0.64
1:A:471:GLU:HA	1:A:474:TYR:CE2	2.33	0.63
2:M:42:GLN:O	2:M:47:GLN:NE2	2.31	0.63
1:A:80:ALA:CA	1:A:88:GLN:NE2	2.21	0.63
2:J:42:GLN:HB2	2:J:409:GLN:HB3	1.80	0.63
2:N:312:GLU:OE1	2:N:314:LYS:NZ	2.31	0.63
2:K:96:GLU:OE2	2:K:147:ARG:NH2	2.31	0.63
2:K:39:THR:HG22	2:K:412:VAL:HG22	1.79	0.63
1:A:99:LEU:HD12	2:K:26:SER:N	2.14	0.62
2:J:312:GLU:OE1	2:J:314:LYS:NZ	2.32	0.62
2:L:39:THR:HG22	2:L:412:VAL:HG22	1.81	0.62
1:B:122:CYS:HB2	1:B:131:LEU:HD21	1.81	0.62
1:F:235:PRO:HG2	1:F:240:ILE:HD11	1.81	0.62
1:B:247:LEU:HD22	1:B:262:THR:HG23	1.79	0.62
2:P:6:ILE:HG22	2:P:7:ALA:H	1.62	0.62
2:O:42:GLN:O	2:O:47:GLN:NE2	2.32	0.62
2:N:96:GLU:OE2	2:N:147:ARG:NH2	2.32	0.62
2:N:42:GLN:O	2:N:47:GLN:NE2	2.32	0.62
1:D:116:LEU:HD21	1:D:142:ILE:HD13	1.81	0.62
2:L:151:GLY:O	2:L:217:ARG:NH2	2.32	0.62
2:M:96:GLU:OE2	2:M:147:ARG:NH2	2.33	0.62
2:P:42:GLN:O	2:P:47:GLN:NE2	2.32	0.62
1:A:116:LEU:HD21	1:A:142:ILE:HD13	1.80	0.62
2:J:153:ILE:HB	2:J:220:LEU:HD21	1.81	0.62
2:K:312:GLU:OE1	2:K:314:LYS:NZ	2.33	0.62
1:D:95:ALA:O	1:D:98:LEU:CG	2.32	0.62
1:D:98:LEU:O	1:D:102:ASP:N	2.31	0.62
2:J:211:PHE:CB	2:J:214:ARG:HD3	2.21	0.62
2:P:96:GLU:OE2	2:P:147:ARG:NH2	2.33	0.62
2:L:312:GLU:OE1	2:L:314:LYS:NZ	2.32	0.61
2:M:233:SER:HB3	2:M:236:SER:HA	1.82	0.61
2:P:312:GLU:OE1	2:P:314:LYS:NZ	2.33	0.61
1:B:392:ILE:HG23	1:B:407:LEU:HD21	1.83	0.61
2:O:39:THR:HG22	2:O:412:VAL:HG22	1.81	0.61
1:A:235:PRO:HG2	1:A:240:ILE:HD11	1.81	0.61
1:B:229:ARG:NH2	2:I:20:SER:CB	2.58	0.61
1:D:99:LEU:HD12	2:P:26:SER:H	1.63	0.61
2:J:231:LEU:O	2:J:239:HIS:HB2	2.00	0.61
2:N:233:SER:HB3	2:N:236:SER:HA	1.81	0.61
1:G:312:VAL:O	2:N:8:LYS:NZ	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:229:ARG:NH1	1:G:268:TYR:OH	2.33	0.61
1:D:98:LEU:HA	1:D:101:SER:HB2	1.82	0.61
2:J:211:PHE:HE1	2:J:223:LEU:HD21	1.65	0.61
1:A:99:LEU:CD2	1:A:141:ASN:HB3	2.31	0.61
1:C:126:ASP:OD1	1:C:132:GLN:NE2	2.27	0.61
2:I:96:GLU:OE2	2:I:147:ARG:NH2	2.33	0.60
1:E:316:ASP:OD2	2:L:5:ARG:NH2	2.33	0.60
1:C:295:HIS:O	1:C:301:GLN:NE2	2.32	0.60
2:J:217:ARG:O	2:J:221:GLU:HB2	2.02	0.60
1:C:368:ASN:OD1	2:K:217:ARG:NH2	2.33	0.60
1:H:247:LEU:HD22	1:H:262:THR:HG23	1.84	0.60
1:E:122:CYS:HB2	1:E:131:LEU:HD21	1.82	0.60
2:I:192:ASP:OD1	2:I:239:HIS:NE2	2.35	0.60
2:I:312:GLU:OE1	2:I:314:LYS:NZ	2.32	0.60
2:I:19:LYS:HB3	2:I:21:LYS:HE3	1.84	0.60
2:J:42:GLN:O	2:J:47:GLN:NE2	2.35	0.60
2:M:214:ARG:NH1	2:M:218:GLN:OE1	2.34	0.60
1:A:80:ALA:C	1:A:88:GLN:NE2	2.53	0.60
2:K:28:ARG:HH22	2:K:243:GLN:HG2	1.66	0.60
2:L:96:GLU:OE2	2:L:147:ARG:NH2	2.35	0.60
1:G:74:GLU:O	1:G:77:VAL:HG22	2.02	0.60
1:B:229:ARG:HH21	2:I:20:SER:CB	2.03	0.59
1:C:117:PRO:O	1:C:121:HIS:ND1	2.29	0.59
1:G:295:HIS:O	1:G:301:GLN:NE2	2.33	0.59
2:N:181:ASN:ND2	2:N:249:ALA:HB1	2.17	0.59
2:P:208:PRO:HB3	2:P:282:ILE:HD11	1.83	0.59
2:I:320:ARG:NH2	2:I:322:GLU:OE1	2.36	0.59
2:I:94:ASN:HB2	2:I:99:LEU:HD12	1.83	0.59
2:P:181:ASN:ND2	2:P:249:ALA:HB1	2.18	0.59
1:D:93:GLN:HG2	1:D:134:GLU:CD	2.22	0.59
2:N:320:ARG:NH2	2:N:322:GLU:OE1	2.36	0.59
1:E:126:ASP:OD1	1:E:132:GLN:NE2	2.33	0.59
1:F:247:LEU:HD22	1:F:262:THR:HG23	1.84	0.59
2:J:266:LEU:O	2:J:271:GLN:NE2	2.36	0.59
2:L:42:GLN:O	2:L:47:GLN:NE2	2.36	0.59
1:D:126:ASP:OD1	1:D:132:GLN:NE2	2.32	0.58
1:E:247:LEU:HD22	1:E:262:THR:HG23	1.85	0.58
2:O:96:GLU:OE2	2:O:147:ARG:NH2	2.36	0.58
1:E:348:TRP:CD2	2:L:11:SER:HB2	2.38	0.58
2:I:181:ASN:ND2	2:I:249:ALA:HB1	2.18	0.58
2:O:320:ARG:NH2	2:O:322:GLU:OE1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:320:ARG:NH2	2:J:322:GLU:OE1	2.37	0.58
2:L:267:SER:HB2	2:L:272:LEU:HD12	1.85	0.58
1:A:80:ALA:C	1:A:88:GLN:OE1	2.42	0.58
1:C:119:LEU:HD22	1:C:139:LEU:HG	1.86	0.58
2:O:181:ASN:ND2	2:O:249:ALA:HB1	2.19	0.58
1:E:392:ILE:HG23	1:E:407:LEU:HD21	1.85	0.58
1:F:122:CYS:HB2	1:F:131:LEU:HD21	1.85	0.58
2:J:143:TRP:HB3	2:J:165:PRO:HA	1.85	0.58
1:C:96:ARG:NH2	2:J:26:SER:OG	2.37	0.58
1:A:318:GLN:NE2	1:B:275:GLU:OE1	2.37	0.58
1:B:126:ASP:OD1	1:B:132:GLN:NE2	2.32	0.57
1:C:201:VAL:HG21	1:C:239:THR:HG23	1.85	0.57
2:M:39:THR:HG22	2:M:412:VAL:HG22	1.86	0.57
2:O:130:HIS:HE1	2:O:179:SER:HB3	1.68	0.57
2:P:6:ILE:CG2	2:P:7:ALA:H	2.14	0.57
1:B:137:TRP:CH2	2:I:24:LYS:HE2	2.39	0.57
1:D:392:ILE:HG23	1:D:407:LEU:HD21	1.86	0.57
2:I:266:LEU:O	2:I:271:GLN:NE2	2.38	0.57
2:M:192:ASP:OD1	2:M:239:HIS:NE2	2.37	0.57
1:D:235:PRO:HG2	1:D:240:ILE:HD11	1.86	0.57
2:I:39:THR:HG22	2:I:412:VAL:HG22	1.86	0.57
2:J:209:GLU:HG3	2:J:281:PHE:CD2	2.40	0.57
2:J:39:THR:HG22	2:J:412:VAL:HG22	1.86	0.57
2:L:181:ASN:ND2	2:L:249:ALA:HB1	2.19	0.57
2:P:375:TYR:CZ	2:P:382:ASP:HB3	2.39	0.57
1:G:392:ILE:HG23	1:G:407:LEU:HD21	1.86	0.57
2:I:130:HIS:HE1	2:I:179:SER:HB3	1.68	0.57
2:K:153:ILE:HB	2:K:220:LEU:HD21	1.85	0.57
2:O:267:SER:HB2	2:O:272:LEU:HD12	1.86	0.57
2:P:320:ARG:NH2	2:P:322:GLU:OE1	2.38	0.57
1:D:461:LYS:O	1:D:465:LEU:HB2	2.03	0.57
1:F:392:ILE:HG23	1:F:407:LEU:HD21	1.86	0.57
2:I:242:PHE:HA	2:I:256:SER:HA	1.86	0.57
2:L:192:ASP:OD1	2:L:239:HIS:NE2	2.38	0.57
2:O:94:ASN:HB2	2:O:99:LEU:HD12	1.86	0.57
1:G:395:LEU:HD22	1:G:407:LEU:HD22	1.87	0.57
2:K:217:ARG:O	2:K:221:GLU:HB2	2.04	0.57
2:N:39:THR:HG22	2:N:412:VAL:HG22	1.84	0.57
2:M:130:HIS:HE1	2:M:179:SER:HB3	1.68	0.57
2:P:266:LEU:O	2:P:271:GLN:NE2	2.37	0.57
2:P:94:ASN:HB2	2:P:99:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ASP:OD1	1:A:132:GLN:NE2	2.27	0.57
2:K:192:ASP:OD1	2:K:239:HIS:NE2	2.38	0.57
2:M:267:SER:HB2	2:M:272:LEU:HD12	1.87	0.57
2:P:143:TRP:HB3	2:P:165:PRO:HA	1.87	0.57
1:A:310:ASN:O	1:A:313:THR:OG1	2.21	0.57
2:M:312:GLU:OE1	2:M:314:LYS:NZ	2.34	0.56
2:N:94:ASN:HB2	2:N:99:LEU:HD12	1.87	0.56
1:C:73:LEU:HD12	1:C:74:GLU:HB2	1.87	0.56
2:K:266:LEU:O	2:K:271:GLN:NE2	2.38	0.56
2:O:192:ASP:OD1	2:O:239:HIS:NE2	2.38	0.56
1:A:392:ILE:HG23	1:A:407:LEU:HD21	1.86	0.56
1:D:104:ASN:HB2	1:D:105:PRO:HD3	1.86	0.56
2:M:320:ARG:NH2	2:M:322:GLU:OE1	2.38	0.56
2:M:94:ASN:HB2	2:M:99:LEU:HD12	1.87	0.56
2:K:228:CYS:SG	2:K:229:VAL:N	2.79	0.56
2:L:266:LEU:O	2:L:271:GLN:NE2	2.38	0.56
1:E:108:ASP:O	1:E:110:LEU:N	2.38	0.56
1:H:308:VAL:HA	1:H:311:ILE:HD12	1.87	0.56
1:H:392:ILE:HG23	1:H:407:LEU:HD21	1.87	0.56
2:L:320:ARG:NH2	2:L:322:GLU:OE1	2.38	0.56
2:O:312:GLU:OE1	2:O:314:LYS:NZ	2.34	0.56
1:C:141:ASN:OD1	2:J:23:VAL:HG13	2.05	0.56
2:O:143:TRP:HB3	2:O:165:PRO:HA	1.87	0.56
1:C:122:CYS:HB2	1:C:131:LEU:HD21	1.87	0.56
2:L:143:TRP:HB3	2:L:165:PRO:HA	1.88	0.56
2:P:242:PHE:HA	2:P:256:SER:HA	1.88	0.56
1:A:103:ARG:NH1	2:K:189:ALA:O	2.35	0.56
2:K:181:ASN:ND2	2:K:249:ALA:HB1	2.20	0.56
2:K:33:GLU:OE2	2:K:416:LYS:HE2	2.06	0.56
2:N:266:LEU:O	2:N:271:GLN:NE2	2.39	0.56
2:J:233:SER:HB2	2:J:240:VAL:HG22	1.88	0.55
2:L:228:CYS:SG	2:L:229:VAL:N	2.79	0.55
2:M:266:LEU:O	2:M:271:GLN:NE2	2.39	0.55
1:F:387:GLU:OE1	2:M:9:ARG:NH2	2.39	0.55
1:F:473:ILE:O	1:F:477:ALA:HB2	2.06	0.55
1:G:115:ILE:CG2	1:G:119:LEU:HD11	2.36	0.55
1:C:406:TYR:HB2	2:K:218:GLN:HG3	1.86	0.55
2:M:143:TRP:HB3	2:M:165:PRO:HA	1.88	0.55
1:G:186:GLY:HA3	2:N:20:SER:OG	2.07	0.55
2:P:192:ASP:OD1	2:P:239:HIS:NE2	2.40	0.55
1:C:229:ARG:HG2	1:C:230:HIS:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:267:SER:HB2	2:I:272:LEU:HD12	1.89	0.55
2:I:143:TRP:HB3	2:I:165:PRO:HA	1.87	0.55
1:E:137:TRP:NE1	2:L:26:SER:HB2	2.21	0.55
1:E:96:ARG:NH2	2:L:26:SER:OG	2.40	0.55
1:G:176:GLN:HE22	2:N:24:LYS:HD3	1.71	0.55
1:A:122:CYS:HB2	1:A:131:LEU:HD21	1.89	0.55
1:G:117:PRO:O	1:G:121:HIS:ND1	2.25	0.55
1:E:187:ASP:HA	2:L:21:LYS:NZ	2.22	0.55
2:K:94:ASN:HB2	2:K:99:LEU:HD12	1.88	0.55
1:E:308:VAL:HA	1:E:311:ILE:HD12	1.89	0.54
2:I:375:TYR:CZ	2:I:382:ASP:HB3	2.42	0.54
2:J:211:PHE:CE1	2:J:223:LEU:HD21	2.43	0.54
1:A:96:ARG:NH1	2:K:26:SER:OG	2.40	0.54
2:L:28:ARG:HH22	2:L:243:GLN:HG2	1.72	0.54
2:M:181:ASN:ND2	2:M:249:ALA:HB1	2.21	0.54
2:N:143:TRP:HB3	2:N:165:PRO:HA	1.88	0.54
1:A:115:ILE:HA	1:A:118:ILE:HD12	1.90	0.54
1:E:189:PRO:HB2	1:E:233:PRO:HG2	1.90	0.54
1:G:115:ILE:HG22	1:G:119:LEU:CD1	2.38	0.54
1:G:120:VAL:O	1:G:123:LEU:HB3	2.07	0.54
1:C:392:ILE:HG23	1:C:407:LEU:HD21	1.88	0.54
2:J:267:SER:HB2	2:J:272:LEU:HD12	1.89	0.54
2:N:192:ASP:OD1	2:N:239:HIS:NE2	2.40	0.54
2:N:267:SER:HB2	2:N:272:LEU:HD12	1.90	0.54
2:O:266:LEU:O	2:O:271:GLN:NE2	2.40	0.54
1:H:126:ASP:OD1	1:H:132:GLN:NE2	2.33	0.54
1:A:195:VAL:HG12	1:A:200:VAL:HG11	1.90	0.54
2:J:233:SER:HB2	2:J:240:VAL:CG2	2.38	0.54
1:A:366:ASP:O	2:J:217:ARG:NH2	2.40	0.54
1:B:144:SER:HB2	2:I:23:VAL:HG22	1.90	0.54
1:B:351:SER:OG	2:I:9:ARG:NH2	2.41	0.54
2:K:42:GLN:O	2:K:47:GLN:NE2	2.40	0.54
2:L:94:ASN:HB2	2:L:99:LEU:HD12	1.89	0.54
2:O:228:CYS:SG	2:O:229:VAL:N	2.81	0.54
1:B:222:TRP:CZ2	2:I:20:SER:O	2.61	0.53
1:B:235:PRO:HG2	1:B:240:ILE:HD11	1.89	0.53
1:D:96:ARG:HG2	1:D:137:TRP:CD1	2.43	0.53
1:H:328:LEU:HA	1:H:331:PHE:HD2	1.72	0.53
1:B:387:GLU:OE1	2:I:9:ARG:NH2	2.37	0.53
2:N:228:CYS:SG	2:N:229:VAL:N	2.82	0.53
2:O:185:VAL:HG12	2:O:195:THR:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:420:LEU:HB3	1:G:465:LEU:HD11	1.90	0.53
2:K:267:SER:HB2	2:K:272:LEU:HD12	1.91	0.53
2:P:39:THR:HG22	2:P:412:VAL:HG22	1.89	0.53
1:A:282:ASP:OD1	1:B:241:GLN:NE2	2.42	0.53
2:I:228:CYS:SG	2:I:229:VAL:N	2.82	0.53
1:A:402:ASP:HB2	2:J:214:ARG:NH2	2.24	0.53
2:I:15:ASP:O	2:I:17:ILE:N	2.39	0.53
2:M:228:CYS:SG	2:M:229:VAL:N	2.81	0.53
1:H:348:TRP:CH2	2:O:11:SER:HB3	2.44	0.53
2:I:233:SER:HB3	2:I:236:SER:HA	1.91	0.53
2:I:316:TYR:HE1	2:I:340:LEU:HD13	1.74	0.53
2:K:148:ASP:C	2:K:150:ASN:H	2.12	0.53
1:F:229:ARG:NH2	2:M:20:SER:OG	2.42	0.53
2:J:132:ALA:HB2	2:J:142:LEU:HD13	1.91	0.53
2:K:17:ILE:HB	2:K:18:PRO:HD3	1.90	0.53
2:L:316:TYR:HE1	2:L:340:LEU:HD13	1.74	0.53
2:M:316:TYR:HE1	2:M:340:LEU:HD13	1.74	0.53
2:O:214:ARG:NH1	2:O:218:GLN:OE1	2.42	0.53
2:P:228:CYS:SG	2:P:229:VAL:N	2.81	0.53
1:F:74:GLU:O	1:F:77:VAL:HG22	2.09	0.53
1:H:105:PRO:O	1:H:107:ILE:N	2.41	0.53
2:K:185:VAL:HG12	2:K:195:THR:HG22	1.91	0.53
2:J:228:CYS:SG	2:J:229:VAL:N	2.82	0.52
1:A:201:VAL:HG21	1:A:239:THR:HG23	1.91	0.52
1:D:229:ARG:CZ	2:P:19:LYS:HB3	2.40	0.52
2:O:316:TYR:HE1	2:O:340:LEU:HD13	1.75	0.52
1:E:97:LYS:HE3	2:L:28:ARG:HA	1.90	0.52
1:C:218:ARG:NH1	2:J:118:GLN:O	2.42	0.52
2:K:143:TRP:HB3	2:K:165:PRO:HA	1.91	0.52
1:B:229:ARG:HG2	1:B:230:HIS:H	1.74	0.52
1:C:313:THR:O	1:C:313:THR:CG2	2.58	0.52
1:H:179:TRP:CE2	2:O:24:LYS:HG3	2.44	0.52
1:C:473:ILE:O	1:C:477:ALA:CB	2.58	0.52
1:D:229:ARG:HG2	1:D:230:HIS:H	1.74	0.52
1:G:247:LEU:HD22	1:G:262:THR:HG23	1.91	0.52
2:N:316:TYR:HE1	2:N:340:LEU:HD13	1.73	0.52
1:D:368:ASN:OD1	2:I:214:ARG:HA	2.09	0.52
1:E:420:LEU:HB3	1:E:465:LEU:HD11	1.92	0.52
2:P:267:SER:HB2	2:P:272:LEU:HD12	1.91	0.52
1:G:473:ILE:O	1:G:477:ALA:HB2	2.09	0.52
2:J:242:PHE:HA	2:J:256:SER:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:ILE:O	1:C:477:ALA:HB2	2.09	0.52
2:J:181:ASN:ND2	2:J:249:ALA:HB1	2.25	0.52
2:K:320:ARG:NH2	2:K:322:GLU:OE1	2.39	0.52
1:B:449:ILE:HA	1:B:452:LEU:HD12	1.90	0.52
2:M:185:VAL:HG12	2:M:195:THR:HG22	1.92	0.52
2:O:28:ARG:HH22	2:O:243:GLN:HG2	1.74	0.52
2:J:217:ARG:O	2:J:221:GLU:CB	2.58	0.51
2:J:316:TYR:HE1	2:J:340:LEU:HD13	1.75	0.51
1:B:189:PRO:HB2	1:B:233:PRO:HG2	1.92	0.51
1:A:92:VAL:HG11	1:A:131:LEU:HD12	1.93	0.51
2:J:252:THR:O	2:J:263:GLY:HA2	2.10	0.51
1:C:402:ASP:CB	2:K:214:ARG:HH21	2.23	0.51
1:D:116:LEU:CD2	1:D:142:ILE:HD13	2.41	0.51
1:A:99:LEU:CD1	2:K:25:VAL:HA	2.40	0.51
1:A:229:ARG:HG2	1:A:230:HIS:H	1.74	0.51
1:H:229:ARG:HG2	1:H:268:TYR:CE2	2.45	0.51
2:K:316:TYR:HE1	2:K:340:LEU:HD13	1.75	0.51
1:A:96:ARG:HG2	1:A:137:TRP:CD1	2.46	0.51
1:F:420:LEU:HB3	1:F:465:LEU:HD11	1.91	0.51
2:P:151:GLY:O	2:P:217:ARG:NH2	2.44	0.51
2:K:158:PRO:HG3	2:K:224:LEU:HD12	1.92	0.51
2:L:185:VAL:HG12	2:L:195:THR:HG22	1.91	0.51
2:K:252:THR:O	2:K:263:GLY:HA2	2.11	0.51
1:D:74:GLU:O	1:D:77:VAL:HG22	2.11	0.51
2:P:358:TYR:OH	2:P:376:GLN:O	2.23	0.51
1:B:309:GLY:O	1:B:313:THR:HG23	2.10	0.51
1:C:92:VAL:HG11	1:C:131:LEU:HD12	1.92	0.51
1:C:247:LEU:HD22	1:C:262:THR:HG23	1.93	0.50
1:E:328:LEU:HA	1:E:331:PHE:HD2	1.77	0.50
2:P:10:ARG:HG2	2:P:11:SER:H	1.76	0.50
1:C:395:LEU:HD22	1:C:407:LEU:HD22	1.94	0.50
1:F:229:ARG:HG2	1:F:230:HIS:H	1.76	0.50
1:G:172:ASN:OD1	1:G:173:VAL:N	2.44	0.50
1:E:141:ASN:ND2	2:L:24:LYS:O	2.31	0.50
2:P:316:TYR:HE1	2:P:340:LEU:HD13	1.76	0.50
1:C:114:GLY:O	1:C:118:ILE:HG12	2.11	0.50
1:F:104:ASN:N	1:F:105:PRO:HD3	2.25	0.50
2:K:375:TYR:CZ	2:K:382:ASP:HB3	2.46	0.50
1:A:247:LEU:HD22	1:A:262:THR:HG23	1.93	0.50
1:E:229:ARG:HG2	1:E:230:HIS:H	1.77	0.50
1:E:407:LEU:HG	1:E:412:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:TRP:CZ2	2:P:22:LYS:HE3	2.47	0.50
1:B:473:ILE:O	1:B:477:ALA:HB2	2.11	0.50
1:E:461:LYS:O	1:E:465:LEU:HG	2.12	0.50
1:F:126:ASP:OD1	1:F:132:GLN:NE2	2.33	0.50
2:L:214:ARG:NH1	2:L:218:GLN:OE1	2.38	0.50
2:M:28:ARG:HH22	2:M:243:GLN:HG2	1.76	0.50
1:B:222:TRP:HZ2	2:I:20:SER:O	1.94	0.50
1:C:466:GLN:HB2	2:O:58:LYS:HZ1	1.76	0.50
2:M:252:THR:O	2:M:263:GLY:HA2	2.12	0.50
1:B:410:GLN:OE1	2:P:214:ARG:NH1	2.44	0.50
1:E:195:VAL:HG12	1:E:200:VAL:HG11	1.93	0.50
1:G:229:ARG:HG2	1:G:230:HIS:H	1.76	0.50
2:N:28:ARG:HH22	2:N:243:GLN:HG2	1.76	0.50
2:P:185:VAL:HG12	2:P:195:THR:HG22	1.94	0.50
1:E:473:ILE:O	1:E:477:ALA:HB2	2.11	0.50
2:N:185:VAL:HG12	2:N:195:THR:HG22	1.94	0.50
1:H:407:LEU:HG	1:H:412:VAL:HG11	1.92	0.49
1:H:473:ILE:O	1:H:477:ALA:HB2	2.12	0.49
1:A:104:ASN:HB2	1:A:105:PRO:HD3	1.95	0.49
1:H:420:LEU:HB3	1:H:465:LEU:HD11	1.94	0.49
2:J:94:ASN:HB2	2:J:99:LEU:HD12	1.94	0.49
2:P:132:ALA:HB2	2:P:142:LEU:HD13	1.94	0.49
1:G:328:LEU:HA	1:G:331:PHE:HD2	1.78	0.49
1:H:195:VAL:HG12	1:H:200:VAL:HG11	1.94	0.49
2:I:252:THR:O	2:I:263:GLY:HA2	2.12	0.49
1:D:247:LEU:HD22	1:D:262:THR:HG23	1.94	0.49
1:D:397:ILE:HG21	2:P:6:ILE:HD11	1.93	0.49
1:D:449:ILE:HA	1:D:452:LEU:HD12	1.95	0.49
1:G:478:TYR:OH	2:P:58:LYS:N	2.44	0.49
1:B:407:LEU:HG	1:B:412:VAL:HG11	1.94	0.49
1:D:99:LEU:HD21	1:D:141:ASN:CB	2.40	0.49
1:F:473:ILE:O	1:F:477:ALA:CB	2.60	0.49
2:I:185:VAL:HG12	2:I:195:THR:HG22	1.94	0.49
2:I:268:ASN:OD1	2:I:269:TYR:N	2.46	0.49
1:E:176:GLN:OE1	2:L:24:LYS:HE2	2.12	0.49
1:A:407:LEU:HG	1:A:412:VAL:HG11	1.94	0.49
1:B:473:ILE:O	1:B:477:ALA:CB	2.60	0.49
1:E:74:GLU:O	1:E:77:VAL:HG22	2.12	0.49
1:A:309:GLY:O	1:A:313:THR:HG23	2.12	0.49
1:D:99:LEU:HD13	2:P:25:VAL:HA	1.93	0.49
1:F:390:TRP:HZ2	1:F:426:GLN:HE21	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:402:LEU:N	2:L:414:LEU:O	2.45	0.49
2:P:376:GLN:NE2	2:P:408:GLY:O	2.46	0.49
1:A:88:GLN:CA	1:A:88:GLN:HE21	2.18	0.49
1:B:74:GLU:O	1:B:77:VAL:HG22	2.12	0.49
1:G:126:ASP:OD1	1:G:132:GLN:NE2	2.36	0.49
1:H:172:ASN:OD1	1:H:173:VAL:N	2.45	0.49
1:D:473:ILE:O	1:D:477:ALA:HB2	2.13	0.49
1:G:201:VAL:HG21	1:G:239:THR:HG23	1.95	0.49
1:H:390:TRP:HZ2	1:H:426:GLN:HE21	1.61	0.49
2:I:132:ALA:HB2	2:I:142:LEU:HD13	1.95	0.49
2:J:268:ASN:OD1	2:J:269:TYR:N	2.46	0.49
2:P:252:THR:O	2:P:263:GLY:HA2	2.13	0.49
1:G:195:VAL:HG12	1:G:200:VAL:HG11	1.95	0.48
2:N:151:GLY:O	2:N:217:ARG:NH2	2.44	0.48
1:A:172:ASN:OD1	1:A:173:VAL:N	2.46	0.48
1:H:114:GLY:O	1:H:118:ILE:HG12	2.13	0.48
1:H:449:ILE:HA	1:H:452:LEU:HD12	1.95	0.48
1:H:473:ILE:O	1:H:477:ALA:CB	2.61	0.48
2:L:252:THR:O	2:L:263:GLY:HA2	2.13	0.48
1:H:107:ILE:C	1:H:109:ASP:H	2.16	0.48
1:F:144:SER:HA	2:M:21:LYS:CG	2.43	0.48
1:F:120:VAL:O	1:F:123:LEU:HB3	2.13	0.48
1:G:473:ILE:O	1:G:477:ALA:CB	2.62	0.48
1:H:125:ARG:O	1:H:132:GLN:NE2	2.45	0.48
2:N:252:THR:O	2:N:263:GLY:HA2	2.13	0.48
2:N:402:LEU:N	2:N:414:LEU:O	2.45	0.48
2:P:119:GLU:HG3	2:P:141:PHE:HE2	1.78	0.48
1:C:449:ILE:HA	1:C:452:LEU:HD12	1.96	0.48
1:D:473:ILE:O	1:D:477:ALA:CB	2.62	0.48
1:G:232:ASP:HB3	1:G:233:PRO:HD3	1.95	0.48
2:J:375:TYR:CZ	2:J:382:ASP:HB3	2.48	0.48
2:O:252:THR:O	2:O:263:GLY:HA2	2.13	0.48
1:F:308:VAL:HG12	1:F:349:PHE:HE1	1.79	0.48
1:A:95:ALA:O	1:A:97:LYS:N	2.47	0.48
1:D:328:LEU:HA	1:D:331:PHE:HD2	1.77	0.48
1:C:172:ASN:OD1	1:C:173:VAL:N	2.46	0.48
1:E:241:GLN:NE2	1:E:279:MET:SD	2.84	0.48
2:M:132:ALA:HB2	2:M:142:LEU:HD13	1.95	0.48
1:B:328:LEU:HA	1:B:331:PHE:HD2	1.78	0.48
1:E:151:GLN:HA	1:E:154:VAL:HG22	1.95	0.48
1:E:92:VAL:HG11	1:E:131:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:387:GLU:OE1	2:O:9:ARG:NH2	2.46	0.48
2:M:242:PHE:HA	2:M:256:SER:HA	1.96	0.48
2:M:347:VAL:HA	2:M:361:THR:HA	1.95	0.48
2:N:375:TYR:CZ	2:N:382:ASP:HB3	2.49	0.48
1:B:195:VAL:HG12	1:B:200:VAL:HG11	1.95	0.48
1:E:395:LEU:HD22	1:E:407:LEU:HD22	1.96	0.48
1:H:104:ASN:N	1:H:105:PRO:HD3	2.28	0.48
1:H:232:ASP:HB3	1:H:233:PRO:HD3	1.95	0.48
2:J:14:ALA:HB3	2:J:17:ILE:CG1	2.44	0.48
2:O:347:VAL:HA	2:O:361:THR:HA	1.96	0.48
2:O:402:LEU:N	2:O:414:LEU:O	2.43	0.48
2:I:214:ARG:HD2	2:I:218:GLN:OE1	2.14	0.47
2:J:207:VAL:HB	2:J:211:PHE:CZ	2.49	0.47
1:A:137:TRP:CZ3	2:K:24:LYS:HE3	2.49	0.47
2:L:150:ASN:HB2	2:L:217:ARG:HH21	1.79	0.47
2:M:19:LYS:O	2:M:21:LYS:N	2.47	0.47
2:O:47:GLN:HG3	2:O:410:HIS:ND1	2.28	0.47
2:P:402:LEU:N	2:P:414:LEU:O	2.45	0.47
1:D:172:ASN:OD1	1:D:173:VAL:N	2.48	0.47
1:E:108:ASP:C	1:E:110:LEU:N	2.68	0.47
1:F:189:PRO:HB2	1:F:233:PRO:HG2	1.96	0.47
1:H:309:GLY:HA3	1:H:348:TRP:CZ3	2.48	0.47
1:E:308:VAL:HG12	1:E:349:PHE:HE1	1.79	0.47
1:E:390:TRP:HZ2	1:E:426:GLN:HE21	1.63	0.47
2:P:208:PRO:HB3	2:P:282:ILE:CD1	2.44	0.47
1:A:241:GLN:NE2	1:A:279:MET:SD	2.84	0.47
1:B:231:LYS:HD3	1:B:271:ASP:OD2	2.14	0.47
1:E:473:ILE:O	1:E:477:ALA:CB	2.62	0.47
2:J:244:ASP:OD1	2:J:245:ALA:N	2.46	0.47
2:J:402:LEU:N	2:J:414:LEU:O	2.46	0.47
2:K:91:PHE:HB3	2:K:112:PRO:HA	1.96	0.47
2:K:242:PHE:HA	2:K:256:SER:HA	1.96	0.47
2:O:361:THR:OG1	2:O:363:ASP:OD1	2.21	0.47
2:P:244:ASP:OD1	2:P:245:ALA:N	2.46	0.47
1:B:172:ASN:OD1	1:B:173:VAL:N	2.47	0.47
1:C:195:VAL:HG12	1:C:200:VAL:HG11	1.95	0.47
1:D:176:GLN:HE22	2:P:24:LYS:HD3	1.80	0.47
2:I:402:LEU:N	2:I:414:LEU:O	2.42	0.47
2:M:268:ASN:OD1	2:M:269:TYR:N	2.48	0.47
2:O:132:ALA:HB2	2:O:142:LEU:HD13	1.96	0.47
2:P:268:ASN:OD1	2:P:269:TYR:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:TYR:O	1:D:410:GLN:HG2	2.14	0.47
2:N:132:ALA:HB2	2:N:142:LEU:HD13	1.95	0.47
2:O:376:GLN:NE2	2:O:408:GLY:O	2.48	0.47
2:P:119:GLU:HG3	2:P:141:PHE:CE2	2.50	0.47
1:B:289:LEU:HD12	1:B:292:LEU:HD12	1.96	0.47
2:J:209:GLU:HG3	2:J:281:PHE:HD2	1.76	0.47
1:A:449:ILE:HA	1:A:452:LEU:HD12	1.97	0.47
1:E:309:GLY:O	1:E:313:THR:HG23	2.15	0.47
2:I:176:LYS:NZ	2:I:244:ASP:OD1	2.40	0.47
2:I:47:GLN:HG3	2:I:410:HIS:ND1	2.29	0.47
2:K:402:LEU:N	2:K:414:LEU:O	2.45	0.47
2:L:194:TYR:HE1	2:L:228:CYS:HB2	1.79	0.47
1:C:151:GLN:HA	1:C:154:VAL:HG22	1.96	0.47
1:E:189:PRO:HB3	1:E:230:HIS:HB3	1.97	0.47
1:F:201:VAL:HG21	1:F:239:THR:HG23	1.95	0.47
1:C:316:ASP:OD1	2:J:5:ARG:NH2	2.48	0.47
1:D:231:LYS:HD3	1:D:271:ASP:OD2	2.15	0.47
1:E:201:VAL:HG21	1:E:239:THR:HG23	1.97	0.47
1:G:222:TRP:HZ2	2:N:20:SER:O	1.97	0.47
2:N:94:ASN:ND2	2:N:103:THR:OG1	2.42	0.47
2:P:176:LYS:NZ	2:P:244:ASP:OD1	2.40	0.47
1:F:328:LEU:HA	1:F:331:PHE:HD2	1.79	0.47
2:L:132:ALA:HB2	2:L:142:LEU:HD13	1.97	0.47
1:G:125:ARG:O	1:G:132:GLN:NE2	2.48	0.46
2:I:194:TYR:HE1	2:I:228:CYS:HB2	1.80	0.46
2:K:136:ASP:OD1	2:K:137:ASP:N	2.48	0.46
2:K:268:ASN:OD1	2:K:269:TYR:N	2.48	0.46
1:D:232:ASP:HB3	1:D:233:PRO:HD3	1.96	0.46
1:F:309:GLY:O	1:F:313:THR:HG23	2.14	0.46
1:G:289:LEU:HD12	1:G:292:LEU:HD12	1.97	0.46
1:H:92:VAL:HG11	1:H:131:LEU:HD12	1.97	0.46
2:M:402:LEU:N	2:M:414:LEU:O	2.46	0.46
1:A:74:GLU:O	1:A:77:VAL:HG22	2.14	0.46
1:D:467:ASN:OD1	1:D:468:HIS:N	2.48	0.46
2:L:268:ASN:OD1	2:L:269:TYR:N	2.48	0.46
2:M:47:GLN:HG3	2:M:410:HIS:ND1	2.30	0.46
2:N:268:ASN:OD1	2:N:269:TYR:N	2.48	0.46
1:H:328:LEU:HA	1:H:331:PHE:CD2	2.50	0.46
2:J:185:VAL:HG12	2:J:195:THR:HG22	1.97	0.46
2:O:268:ASN:OD1	2:O:269:TYR:N	2.48	0.46
1:E:172:ASN:OD1	1:E:173:VAL:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:229:ARG:HH22	2:O:18:PRO:HG2	1.80	0.46
1:H:461:LYS:O	1:H:465:LEU:HG	2.16	0.46
2:J:119:GLU:HG3	2:J:141:PHE:HE2	1.81	0.46
2:K:130:HIS:HE1	2:K:179:SER:HB3	1.81	0.46
2:O:242:PHE:HA	2:O:256:SER:HA	1.98	0.46
1:F:463:GLU:O	1:F:466:GLN:HG2	2.15	0.46
2:M:244:ASP:OD1	2:M:245:ALA:N	2.45	0.46
2:O:375:TYR:CZ	2:O:382:ASP:HB3	2.50	0.46
1:G:105:PRO:N	1:G:106:PRO:CD	2.79	0.46
1:G:308:VAL:HA	1:G:311:ILE:HD12	1.97	0.46
1:A:103:ARG:HD3	2:K:189:ALA:O	2.16	0.46
2:K:361:THR:OG1	2:K:363:ASP:OD1	2.22	0.46
2:L:242:PHE:HA	2:L:256:SER:HA	1.97	0.46
1:C:74:GLU:O	1:C:77:VAL:HG22	2.16	0.46
2:J:91:PHE:HB3	2:J:112:PRO:HA	1.98	0.46
2:K:233:SER:OG	2:K:236:SER:HB3	2.16	0.46
1:A:473:ILE:O	1:A:477:ALA:HB2	2.16	0.46
1:C:229:ARG:HG2	1:C:230:HIS:N	2.31	0.46
1:G:461:LYS:O	1:G:465:LEU:HG	2.16	0.46
2:I:31:SER:HB2	2:I:71:GLN:HB2	1.98	0.46
1:B:92:VAL:HG11	1:B:131:LEU:HD12	1.98	0.45
1:F:151:GLN:HA	1:F:154:VAL:HG22	1.98	0.45
2:J:136:ASP:OD1	2:J:137:ASP:N	2.49	0.45
2:L:375:TYR:CZ	2:L:382:ASP:HB3	2.51	0.45
2:L:6:ILE:HG22	2:L:7:ALA:N	2.31	0.45
1:C:402:ASP:HB3	2:K:214:ARG:NH2	2.27	0.45
1:D:309:GLY:O	1:D:313:THR:HG23	2.17	0.45
1:G:308:VAL:HG12	1:G:349:PHE:HE1	1.81	0.45
1:E:306:ARG:HH12	2:L:13:PRO:HA	1.81	0.45
1:H:96:ARG:NH2	2:O:26:SER:OG	2.50	0.45
1:A:232:ASP:HB3	1:A:233:PRO:HD3	1.98	0.45
1:A:88:GLN:CA	1:A:88:GLN:NE2	2.77	0.45
1:D:139:LEU:HD22	1:D:153:VAL:HG13	1.97	0.45
2:I:376:GLN:NE2	2:I:408:GLY:O	2.50	0.45
2:P:214:ARG:NH1	2:P:218:GLN:OE1	2.50	0.45
1:D:310:ASN:O	1:D:313:THR:OG1	2.27	0.45
1:E:308:VAL:HG12	1:E:349:PHE:CE1	2.51	0.45
1:H:189:PRO:HB3	1:H:230:HIS:HB3	1.99	0.45
1:D:103:ARG:HD3	2:P:189:ALA:O	2.17	0.45
2:P:361:THR:OG1	2:P:363:ASP:OD1	2.23	0.45
1:A:116:LEU:HB2	1:A:117:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125:ARG:O	1:F:132:GLN:NE2	2.47	0.45
2:M:148:ASP:C	2:M:150:ASN:H	2.19	0.45
1:B:151:GLN:HA	1:B:154:VAL:HG22	1.98	0.45
1:D:99:LEU:CD2	1:D:141:ASN:HB3	2.45	0.45
1:D:407:LEU:HG	1:D:412:VAL:HG11	1.97	0.45
1:F:176:GLN:HE22	2:M:24:LYS:HD3	1.80	0.45
1:G:308:VAL:HG12	1:G:349:PHE:CE1	2.51	0.45
2:I:303:GLN:HG3	2:I:304:HIS:ND1	2.32	0.45
2:J:361:THR:OG1	2:J:363:ASP:OD1	2.22	0.45
2:L:395:GLN:OE1	2:L:399:ARG:NH1	2.50	0.45
2:P:330:GLU:HA	2:P:386:TRP:HB3	1.98	0.45
2:P:347:VAL:HA	2:P:361:THR:HA	1.98	0.45
1:F:407:LEU:HG	1:F:412:VAL:HG11	1.98	0.45
1:G:114:GLY:O	1:G:118:ILE:HG12	2.16	0.45
1:H:151:GLN:HA	1:H:154:VAL:HG22	1.98	0.45
2:K:347:VAL:HA	2:K:361:THR:HA	1.99	0.45
1:G:313:THR:HA	2:N:8:LYS:HE2	1.98	0.45
1:D:201:VAL:HG21	1:D:239:THR:HG23	1.98	0.45
1:D:95:ALA:O	1:D:98:LEU:N	2.49	0.45
1:E:119:LEU:HA	1:E:122:CYS:SG	2.57	0.45
1:E:187:ASP:HA	2:L:21:LYS:HZ3	1.80	0.45
2:M:136:ASP:OD1	2:M:137:ASP:N	2.50	0.45
2:M:80:VAL:HG21	2:M:131:THR:HG21	1.98	0.45
2:N:308:CYS:SG	2:N:316:TYR:HB2	2.57	0.45
2:O:244:ASP:OD1	2:O:245:ALA:N	2.46	0.45
2:O:358:TYR:OH	2:O:376:GLN:O	2.27	0.45
1:F:308:VAL:HA	1:F:311:ILE:HD12	1.98	0.45
1:F:462:ILE:HG22	1:F:481:ILE:HD11	1.99	0.45
1:E:103:ARG:HD3	2:L:257:HIS:ND1	2.32	0.45
2:M:194:TYR:HE1	2:M:228:CYS:HB2	1.82	0.45
2:N:214:ARG:NH1	2:N:218:GLN:OE1	2.48	0.45
1:D:96:ARG:O	1:D:96:ARG:HD2	2.17	0.45
1:E:114:GLY:O	1:E:118:ILE:HG12	2.17	0.45
1:F:145:GLY:HA3	1:F:149:GLN:OE1	2.17	0.45
1:H:74:GLU:O	1:H:77:VAL:HG22	2.16	0.45
1:B:222:TRP:NE1	2:I:20:SER:HA	2.28	0.45
2:K:194:TYR:HE1	2:K:228:CYS:HB2	1.81	0.45
2:K:36:LEU:O	2:K:414:LEU:HD12	2.17	0.45
2:L:119:GLU:HG3	2:L:141:PHE:HE2	1.82	0.45
2:N:244:ASP:OD1	2:N:245:ALA:N	2.47	0.45
2:P:47:GLN:HG3	2:P:410:HIS:ND1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:HA	1:B:122:CYS:SG	2.58	0.44
1:D:308:VAL:HA	1:D:311:ILE:HD12	1.99	0.44
1:H:194:TYR:O	1:H:197:SER:OG	2.29	0.44
1:H:309:GLY:O	1:H:313:THR:HG23	2.17	0.44
2:I:174:VAL:HA	2:I:188:THR:HA	1.99	0.44
2:L:376:GLN:NE2	2:L:408:GLY:O	2.50	0.44
2:N:347:VAL:HA	2:N:361:THR:HA	1.99	0.44
2:O:136:ASP:OD1	2:O:137:ASP:N	2.50	0.44
1:C:119:LEU:HD11	1:C:138:ALA:HB3	1.99	0.44
1:D:144:SER:O	2:P:21:LYS:CD	2.62	0.44
1:D:466:GLN:OE1	1:D:478:TYR:HD1	2.01	0.44
1:F:116:LEU:HB2	1:F:117:PRO:HD3	1.99	0.44
1:F:172:ASN:OD1	1:F:173:VAL:N	2.50	0.44
1:H:119:LEU:HA	1:H:122:CYS:SG	2.58	0.44
2:I:330:GLU:HA	2:I:386:TRP:HB3	1.98	0.44
2:L:119:GLU:HG3	2:L:141:PHE:CE2	2.51	0.44
2:N:242:PHE:HA	2:N:256:SER:HA	1.99	0.44
1:B:410:GLN:HE22	2:P:214:ARG:NE	2.15	0.44
1:E:120:VAL:O	1:E:123:LEU:HB3	2.17	0.44
1:G:145:GLY:HA3	1:G:149:GLN:OE1	2.16	0.44
2:K:211:PHE:HB2	2:K:214:ARG:HD2	1.99	0.44
2:O:36:LEU:O	2:O:414:LEU:HD12	2.17	0.44
2:P:136:ASP:OD1	2:P:137:ASP:N	2.49	0.44
1:E:100:SER:OG	2:L:26:SER:HB3	2.17	0.44
1:G:478:TYR:CE2	2:P:58:LYS:HB2	2.52	0.44
1:D:289:LEU:HD12	1:D:292:LEU:HD12	1.99	0.44
2:N:330:GLU:HA	2:N:386:TRP:HB3	2.00	0.44
2:N:376:GLN:NE2	2:N:408:GLY:O	2.50	0.44
2:P:194:TYR:HE1	2:P:228:CYS:HB2	1.83	0.44
1:B:308:VAL:HA	1:B:311:ILE:HD12	2.00	0.44
1:D:95:ALA:C	1:D:98:LEU:HG	2.26	0.44
1:F:395:LEU:HD22	1:F:407:LEU:HD22	1.99	0.44
2:N:119:GLU:HG3	2:N:141:PHE:HE2	1.83	0.44
1:A:308:VAL:HG12	1:A:349:PHE:HE1	1.82	0.44
1:B:201:VAL:HG21	1:B:239:THR:HG23	1.98	0.44
1:B:306:ARG:NH1	2:I:14:ALA:HB2	2.33	0.44
1:C:222:TRP:CE2	2:J:22:LYS:HD3	2.53	0.44
1:D:395:LEU:HD22	1:D:407:LEU:HD22	2.00	0.44
1:G:187:ASP:HA	2:N:21:LYS:NZ	2.33	0.44
2:J:330:GLU:HA	2:J:386:TRP:HB3	1.99	0.44
1:B:310:ASN:O	1:B:313:THR:OG1	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:GLN:HA	1:D:154:VAL:HG22	2.00	0.44
1:H:176:GLN:HE22	2:O:24:LYS:HD3	1.83	0.44
2:K:211:PHE:CB	2:K:214:ARG:HD2	2.47	0.44
2:L:348:SER:HB3	2:L:362:LYS:HA	1.99	0.44
2:N:348:SER:HB3	2:N:362:LYS:HA	2.00	0.44
1:C:308:VAL:HA	1:C:311:ILE:HD12	1.99	0.44
1:G:309:GLY:O	1:G:313:THR:HG23	2.17	0.44
1:B:397:ILE:HD13	2:I:6:ILE:HG13	2.00	0.43
1:D:221:THR:HG22	1:D:250:LEU:HD13	2.00	0.43
2:L:27:HIS:ND1	2:L:28:ARG:N	2.66	0.43
2:M:308:CYS:SG	2:M:316:TYR:HB2	2.58	0.43
2:M:375:TYR:CZ	2:M:382:ASP:HB3	2.53	0.43
2:N:194:TYR:HE1	2:N:228:CYS:HB2	1.83	0.43
2:O:148:ASP:C	2:O:150:ASN:H	2.20	0.43
2:M:150:ASN:HA	2:O:151:GLY:N	2.33	0.43
1:E:463:GLU:O	1:E:466:GLN:HG2	2.18	0.43
1:F:308:VAL:HG12	1:F:349:PHE:CE1	2.53	0.43
1:A:321:VAL:HG21	1:B:237:MET:HG2	2.01	0.43
1:F:449:ILE:HA	1:F:452:LEU:HD12	2.00	0.43
2:L:27:HIS:CE1	2:L:28:ARG:HG2	2.53	0.43
2:M:376:GLN:NE2	2:M:408:GLY:O	2.52	0.43
1:A:98:LEU:O	1:A:102:ASP:N	2.41	0.43
1:C:463:GLU:O	1:C:466:GLN:HG2	2.19	0.43
1:G:151:GLN:HA	1:G:154:VAL:HG22	2.00	0.43
1:H:348:TRP:O	1:H:351:SER:OG	2.23	0.43
2:K:119:GLU:HG3	2:K:141:PHE:HE2	1.83	0.43
2:K:303:GLN:HG3	2:K:304:HIS:ND1	2.33	0.43
2:N:150:ASN:HB2	2:N:217:ARG:HH21	1.84	0.43
1:F:189:PRO:HB3	1:F:230:HIS:HB3	2.00	0.43
1:G:486:SER:O	1:G:487:SER:OG	2.31	0.43
1:H:310:ASN:O	1:H:313:THR:OG1	2.27	0.43
2:I:136:ASP:OD1	2:I:137:ASP:N	2.51	0.43
2:I:244:ASP:OD1	2:I:245:ALA:N	2.48	0.43
1:A:176:GLN:OE1	2:K:24:LYS:HE2	2.18	0.43
2:K:348:SER:N	2:K:360:VAL:O	2.50	0.43
2:O:302:GLY:HA3	2:O:305:HIS:CE1	2.53	0.43
1:C:219:ASN:O	1:C:223:VAL:HG23	2.18	0.43
1:F:416:PHE:CZ	1:F:431:VAL:HA	2.54	0.43
2:J:119:GLU:HG3	2:J:141:PHE:CE2	2.53	0.43
2:O:194:TYR:HE1	2:O:228:CYS:HB2	1.84	0.43
2:P:206:ARG:HB3	2:P:229:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LEU:HA	1:A:331:PHE:HD2	1.84	0.43
1:B:467:ASN:OD1	1:B:468:HIS:HB2	2.19	0.43
1:C:407:LEU:HG	1:C:412:VAL:HG11	2.00	0.43
1:C:85:GLN:HA	1:C:88:GLN:HB2	2.00	0.43
1:H:120:VAL:O	1:H:123:LEU:HB3	2.19	0.43
1:H:201:VAL:HG21	1:H:239:THR:HG23	2.00	0.43
2:I:91:PHE:HB3	2:I:112:PRO:HA	2.00	0.43
2:N:136:ASP:OD1	2:N:137:ASP:N	2.51	0.43
1:A:309:GLY:HA3	1:A:348:TRP:CZ3	2.54	0.43
1:A:96:ARG:O	1:A:96:ARG:HD2	2.19	0.43
1:D:145:GLY:HA3	1:D:149:GLN:OE1	2.18	0.43
1:D:195:VAL:HG12	1:D:200:VAL:HG11	2.00	0.43
1:E:449:ILE:HA	1:E:452:LEU:HD12	2.01	0.43
2:K:185:VAL:HG22	2:K:247:CYS:SG	2.59	0.43
1:E:179:TRP:NE1	2:L:24:LYS:HB2	2.34	0.43
2:M:219:GLY:O	2:M:222:ARG:N	2.51	0.43
1:E:125:ARG:O	1:E:132:GLN:NE2	2.51	0.43
1:G:126:ASP:OD2	1:G:164:ARG:NH2	2.52	0.43
2:J:117:LEU:HD11	2:J:141:PHE:CE2	2.54	0.43
2:M:324:GLY:HA2	2:M:386:TRP:CE3	2.54	0.43
1:H:241:GLN:NE2	1:H:279:MET:SD	2.91	0.43
2:N:303:GLN:HG3	2:N:304:HIS:ND1	2.34	0.43
1:D:92:VAL:O	1:D:95:ALA:HB3	2.19	0.42
1:G:221:THR:HG22	1:G:250:LEU:HD13	2.00	0.42
1:H:309:GLY:HA3	1:H:348:TRP:HZ3	1.84	0.42
2:J:303:GLN:HG3	2:J:304:HIS:ND1	2.34	0.42
2:L:136:ASP:OD1	2:L:137:ASP:N	2.51	0.42
1:B:93:GLN:O	1:B:97:LYS:HG2	2.19	0.42
1:C:120:VAL:O	1:C:123:LEU:HB3	2.19	0.42
1:D:317:GLU:O	1:D:321:VAL:HG23	2.19	0.42
1:A:123:LEU:HD11	1:A:165:LEU:HD11	2.02	0.42
1:D:93:GLN:O	1:D:96:ARG:N	2.53	0.42
2:J:152:VAL:HG12	2:J:154:GLY:H	1.84	0.42
2:L:308:CYS:SG	2:L:316:TYR:HB2	2.59	0.42
2:L:324:GLY:HA2	2:L:386:TRP:CE3	2.55	0.42
2:M:152:VAL:HG12	2:M:154:GLY:H	1.84	0.42
2:M:348:SER:HB3	2:M:362:LYS:HA	2.00	0.42
2:N:402:LEU:HD11	2:N:416:LYS:HB2	2.02	0.42
2:P:174:VAL:HA	2:P:188:THR:HA	2.00	0.42
2:P:91:PHE:HB3	2:P:112:PRO:HA	2.02	0.42
1:A:151:GLN:HA	1:A:154:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:ASP:HB3	1:C:233:PRO:HD3	2.00	0.42
1:E:108:ASP:C	1:E:110:LEU:H	2.22	0.42
2:J:194:TYR:HE1	2:J:228:CYS:HB2	1.84	0.42
2:K:330:GLU:HA	2:K:386:TRP:HB3	2.01	0.42
2:L:361:THR:OG1	2:L:363:ASP:OD1	2.21	0.42
2:O:348:SER:HB3	2:O:362:LYS:HA	2.00	0.42
1:A:116:LEU:CD2	1:A:142:ILE:HD13	2.47	0.42
1:E:221:THR:HG22	1:E:250:LEU:HD13	2.02	0.42
2:I:208:PRO:HB3	2:I:282:ILE:HD11	2.01	0.42
2:J:395:GLN:OE1	2:J:399:ARG:NH1	2.52	0.42
2:O:303:GLN:HG3	2:O:304:HIS:ND1	2.35	0.42
2:P:36:LEU:O	2:P:414:LEU:HD12	2.20	0.42
1:D:229:ARG:NH1	1:D:268:TYR:OH	2.53	0.42
1:D:348:TRP:O	1:D:351:SER:OG	2.25	0.42
1:F:195:VAL:HG12	1:F:200:VAL:HG11	2.00	0.42
2:K:119:GLU:HG3	2:K:141:PHE:CE2	2.54	0.42
2:P:117:LEU:HD11	2:P:141:PHE:CE2	2.55	0.42
1:E:289:LEU:HD12	1:E:292:LEU:HD12	2.00	0.42
1:F:461:LYS:O	1:F:465:LEU:HG	2.19	0.42
1:G:463:GLU:O	1:G:466:GLN:HG2	2.18	0.42
1:H:308:VAL:HG12	1:H:349:PHE:HE1	1.84	0.42
1:E:348:TRP:O	1:E:351:SER:OG	2.26	0.42
1:G:310:ASN:O	1:G:313:THR:OG1	2.27	0.42
1:G:449:ILE:HA	1:G:452:LEU:HD12	2.02	0.42
1:A:390:TRP:CE3	2:K:9:ARG:HD2	2.55	0.42
2:O:330:GLU:HA	2:O:386:TRP:HB3	2.01	0.42
1:G:462:ILE:HG22	1:G:481:ILE:HD11	2.02	0.42
2:L:174:VAL:HA	2:L:188:THR:HA	2.01	0.42
2:L:330:GLU:HA	2:L:386:TRP:HB3	2.01	0.42
2:M:117:LEU:HD11	2:M:141:PHE:CE2	2.55	0.42
1:H:137:TRP:HE1	2:O:26:SER:HB2	1.85	0.42
2:P:10:ARG:HG2	2:P:11:SER:N	2.34	0.42
2:P:176:LYS:NZ	2:P:245:ALA:O	2.48	0.42
2:P:348:SER:HB3	2:P:362:LYS:HA	2.01	0.42
1:A:104:ASN:OD1	2:K:257:HIS:CD2	2.72	0.42
1:A:289:LEU:HD12	1:A:292:LEU:HD12	2.01	0.42
1:F:105:PRO:N	1:F:106:PRO:CD	2.83	0.42
1:F:231:LYS:HD3	1:F:271:ASP:OD2	2.20	0.42
2:I:206:ARG:HB3	2:I:229:VAL:HG22	2.02	0.42
1:C:390:TRP:CE3	2:J:9:ARG:HD2	2.54	0.42
2:K:152:VAL:HG12	2:K:154:GLY:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:302:GLY:HA3	2:M:305:HIS:CE1	2.54	0.42
2:K:207:VAL:HB	2:K:211:PHE:CE1	2.54	0.41
2:M:208:PRO:HB3	2:M:282:ILE:HD11	2.01	0.41
2:M:3:PRO:HB2	2:M:4:LYS:H	1.65	0.41
2:P:402:LEU:HD11	2:P:416:LYS:HB2	2.01	0.41
1:A:256:VAL:O	1:A:260:VAL:HG23	2.20	0.41
1:A:308:VAL:HA	1:A:311:ILE:HD12	2.02	0.41
1:G:407:LEU:HG	1:G:412:VAL:HG11	2.02	0.41
2:L:201:GLN:HB3	2:L:266:LEU:HB2	2.01	0.41
2:L:402:LEU:HD11	2:L:416:LYS:HB2	2.01	0.41
2:N:302:GLY:HA3	2:N:305:HIS:CE1	2.55	0.41
2:O:248:GLY:HA3	2:O:251:PHE:CE2	2.55	0.41
2:O:324:GLY:HA2	2:O:386:TRP:CE3	2.54	0.41
1:C:76:ILE:HG21	1:C:95:ALA:HB2	2.01	0.41
1:D:125:ARG:O	1:D:132:GLN:NE2	2.48	0.41
1:D:96:ARG:HG2	1:D:137:TRP:CG	2.55	0.41
1:G:328:LEU:HA	1:G:331:PHE:CD2	2.56	0.41
2:I:348:SER:HB3	2:I:362:LYS:HA	2.01	0.41
2:K:132:ALA:HB2	2:K:142:LEU:HD13	2.02	0.41
2:L:152:VAL:HG12	2:L:154:GLY:H	1.86	0.41
2:L:358:TYR:OH	2:L:376:GLN:O	2.29	0.41
2:M:10:ARG:HG3	2:M:11:SER:H	1.85	0.41
2:M:248:GLY:HA3	2:M:251:PHE:CE2	2.55	0.41
2:M:371:MET:HG2	2:M:373:THR:H	1.85	0.41
1:F:352:ASN:O	2:M:8:LYS:HE3	2.19	0.41
2:O:174:VAL:HA	2:O:188:THR:HA	2.01	0.41
1:A:420:LEU:HB3	1:A:465:LEU:HD11	2.02	0.41
1:B:120:VAL:O	1:B:123:LEU:HB3	2.20	0.41
1:B:232:ASP:HB3	1:B:233:PRO:CD	2.50	0.41
1:D:95:ALA:O	1:D:97:LYS:N	2.53	0.41
2:J:347:VAL:HA	2:J:361:THR:HA	2.02	0.41
2:J:324:GLY:HA2	2:J:386:TRP:CE3	2.55	0.41
1:E:229:ARG:NH2	2:L:20:SER:HB3	2.36	0.41
2:L:244:ASP:OD1	2:L:245:ALA:N	2.49	0.41
2:M:330:GLU:HA	2:M:386:TRP:HB3	2.02	0.41
2:N:174:VAL:HA	2:N:188:THR:HA	2.01	0.41
1:C:466:GLN:OE1	2:O:58:LYS:NZ	2.53	0.41
2:J:36:LEU:O	2:J:414:LEU:HD12	2.21	0.41
2:K:19:LYS:O	2:K:20:SER:HB3	2.20	0.41
2:K:202:GLY:HA3	2:K:281:PHE:CD1	2.56	0.41
2:K:376:GLN:NE2	2:K:408:GLY:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:47:GLN:HG3	2:K:410:HIS:ND1	2.36	0.41
2:L:371:MET:HG2	2:L:373:THR:H	1.86	0.41
2:L:47:GLN:HG3	2:L:410:HIS:ND1	2.35	0.41
2:N:47:GLN:HG3	2:N:410:HIS:ND1	2.36	0.41
2:P:38:LEU:HB2	2:P:413:LEU:HB2	2.03	0.41
1:F:115:ILE:HA	1:F:118:ILE:HG12	2.02	0.41
2:I:347:VAL:HA	2:I:361:THR:HA	2.02	0.41
2:K:348:SER:HB3	2:K:362:LYS:HA	2.02	0.41
2:L:38:LEU:HB2	2:L:413:LEU:HB2	2.02	0.41
2:M:310:ASP:OD1	2:M:314:LYS:N	2.54	0.41
2:O:119:GLU:HG3	2:O:141:PHE:CE2	2.55	0.41
1:B:416:PHE:CZ	1:B:431:VAL:HA	2.55	0.41
2:K:208:PRO:C	2:K:210:LEU:H	2.24	0.41
1:E:328:LEU:HA	1:E:331:PHE:CD2	2.55	0.41
1:H:115:ILE:HG22	1:H:119:LEU:HD23	2.03	0.41
2:J:14:ALA:HB3	2:J:17:ILE:HG13	2.03	0.41
2:L:6:ILE:HG22	2:L:7:ALA:H	1.86	0.41
2:M:127:GLY:HA3	2:M:130:HIS:NE2	2.35	0.41
2:N:119:GLU:HG3	2:N:141:PHE:CE2	2.56	0.41
2:N:282:ILE:O	2:N:284:GLN:N	2.54	0.41
2:O:119:GLU:HG3	2:O:141:PHE:HE2	1.85	0.41
1:H:144:SER:HB2	2:O:23:VAL:HG22	2.03	0.41
1:D:99:LEU:HD12	2:P:25:VAL:HA	2.02	0.41
1:B:461:LYS:O	1:B:465:LEU:HG	2.21	0.41
1:D:115:ILE:HA	1:D:118:ILE:HD12	2.03	0.41
1:F:92:VAL:HG11	1:F:131:LEU:HD12	2.02	0.41
2:I:45:VAL:HG21	2:I:93:CYS:HB2	2.03	0.41
2:P:303:GLN:HG3	2:P:304:HIS:ND1	2.35	0.41
1:B:126:ASP:OD2	1:B:164:ARG:NH2	2.53	0.41
1:F:96:ARG:HD2	1:F:137:TRP:CG	2.56	0.41
2:J:6:ILE:HG22	2:J:7:ALA:N	2.36	0.41
2:J:45:VAL:HG21	2:J:93:CYS:HB2	2.03	0.41
1:A:137:TRP:CH2	2:K:24:LYS:HE3	2.56	0.41
2:M:174:VAL:HA	2:M:188:THR:HA	2.03	0.41
2:N:201:GLN:HB3	2:N:266:LEU:HB2	2.02	0.41
1:C:420:LEU:HB3	1:C:465:LEU:HD11	2.02	0.41
1:D:229:ARG:HG2	1:D:230:HIS:N	2.36	0.41
2:I:201:GLN:HB3	2:I:266:LEU:HB2	2.03	0.41
2:I:243:GLN:HE21	2:I:257:HIS:HA	1.86	0.41
2:N:152:VAL:HG12	2:N:154:GLY:H	1.84	0.41
2:O:282:ILE:O	2:O:284:GLN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:91:PHE:HB3	2:O:112:PRO:HA	2.02	0.41
2:P:201:GLN:HB3	2:P:266:LEU:HB2	2.02	0.41
1:A:80:ALA:C	1:A:88:GLN:CD	2.80	0.40
1:C:176:GLN:HE22	2:J:24:LYS:HD3	1.86	0.40
1:C:390:TRP:HZ2	1:C:426:GLN:HE21	1.67	0.40
1:D:328:LEU:HA	1:D:331:PHE:CD2	2.55	0.40
1:F:229:ARG:HG2	1:F:230:HIS:N	2.36	0.40
2:O:402:LEU:HD11	2:O:416:LYS:HB2	2.03	0.40
1:H:387:GLU:CD	2:O:9:ARG:HH22	2.25	0.40
1:B:241:GLN:NE2	1:B:279:MET:SD	2.93	0.40
1:D:96:ARG:HB2	1:D:134:GLU:OE1	2.21	0.40
2:I:206:ARG:NH2	2:I:225:VAL:O	2.54	0.40
2:J:202:GLY:HA3	2:J:281:PHE:CD1	2.56	0.40
2:K:402:LEU:HD11	2:K:416:LYS:HB2	2.03	0.40
2:L:91:PHE:HB3	2:L:112:PRO:HA	2.03	0.40
2:M:282:ILE:O	2:M:284:GLN:N	2.53	0.40
2:M:303:GLN:HG3	2:M:304:HIS:ND1	2.36	0.40
2:N:38:LEU:HB2	2:N:413:LEU:HB2	2.02	0.40
1:D:221:THR:HG21	1:D:258:ILE:HG23	2.03	0.40
1:G:115:ILE:CG2	1:G:119:LEU:CD1	2.99	0.40
1:B:144:SER:CB	2:I:23:VAL:HG22	2.52	0.40
2:K:146:PHE:CE2	2:K:155:LEU:HD12	2.56	0.40
2:L:194:TYR:CE1	2:L:228:CYS:HB2	2.56	0.40
2:L:233:SER:N	2:L:236:SER:OG	2.28	0.40
2:M:201:GLN:HB3	2:M:266:LEU:HB2	2.02	0.40
1:H:100:SER:OG	2:O:26:SER:HB3	2.22	0.40
1:B:115:ILE:O	1:B:119:LEU:HG	2.22	0.40
1:C:241:GLN:HA	1:C:241:GLN:OE1	2.22	0.40
1:D:99:LEU:HD21	1:D:141:ASN:CG	2.42	0.40
1:F:100:SER:HB2	1:F:141:ASN:HD22	1.86	0.40
1:G:416:PHE:CZ	1:G:431:VAL:HA	2.56	0.40
2:I:308:CYS:SG	2:I:316:TYR:HB2	2.62	0.40
2:J:348:SER:HB3	2:J:362:LYS:HA	2.03	0.40
2:K:282:ILE:O	2:K:284:GLN:N	2.55	0.40
2:L:303:GLN:HG3	2:L:304:HIS:ND1	2.36	0.40
2:O:308:CYS:SG	2:O:316:TYR:HB2	2.62	0.40
1:B:395:LEU:HD22	1:B:407:LEU:HD22	2.03	0.40
1:C:125:ARG:O	1:C:132:GLN:NE2	2.53	0.40
1:E:202:LYS:HB3	1:E:203:PRO:HD3	2.04	0.40
1:F:413:ILE:HB	1:F:414:PRO:HD3	2.03	0.40
2:I:117:LEU:HD11	2:I:141:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:282:ILE:O	2:I:284:GLN:N	2.54	0.40
2:L:282:ILE:O	2:L:284:GLN:N	2.54	0.40
2:M:206:ARG:NH2	2:M:225:VAL:O	2.54	0.40
2:P:152:VAL:HG12	2:P:154:GLY:H	1.87	0.40
2:P:206:ARG:NH2	2:P:225:VAL:O	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	415/521 (80%)	404 (97%)	11 (3%)	0	100	100
1	B	413/521 (79%)	400 (97%)	13 (3%)	0	100	100
1	C	415/521 (80%)	402 (97%)	13 (3%)	0	100	100
1	D	413/521 (79%)	406 (98%)	7 (2%)	0	100	100
1	E	414/521 (80%)	401 (97%)	13 (3%)	0	100	100
1	F	414/521 (80%)	400 (97%)	14 (3%)	0	100	100
1	G	415/521 (80%)	404 (97%)	11 (3%)	0	100	100
1	H	415/521 (80%)	403 (97%)	12 (3%)	0	100	100
2	I	417/421 (99%)	396 (95%)	21 (5%)	0	100	100
2	J	416/421 (99%)	394 (95%)	22 (5%)	0	100	100
2	K	416/421 (99%)	395 (95%)	21 (5%)	0	100	100
2	L	416/421 (99%)	395 (95%)	21 (5%)	0	100	100
2	M	417/421 (99%)	396 (95%)	21 (5%)	0	100	100
2	N	416/421 (99%)	396 (95%)	20 (5%)	0	100	100
2	O	416/421 (99%)	394 (95%)	22 (5%)	0	100	100
2	P	417/421 (99%)	394 (94%)	23 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6645/7536 (88%)	6380 (96%)	265 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	365/460 (79%)	365 (100%)	0	100	100
1	B	357/460 (78%)	357 (100%)	0	100	100
1	C	359/460 (78%)	359 (100%)	0	100	100
1	D	363/460 (79%)	363 (100%)	0	100	100
1	E	358/460 (78%)	358 (100%)	0	100	100
1	F	358/460 (78%)	358 (100%)	0	100	100
1	G	359/460 (78%)	359 (100%)	0	100	100
1	H	359/460 (78%)	359 (100%)	0	100	100
2	I	339/341 (99%)	339 (100%)	0	100	100
2	J	338/341 (99%)	338 (100%)	0	100	100
2	K	338/341 (99%)	338 (100%)	0	100	100
2	L	338/341 (99%)	338 (100%)	0	100	100
2	M	339/341 (99%)	339 (100%)	0	100	100
2	N	338/341 (99%)	338 (100%)	0	100	100
2	O	338/341 (99%)	338 (100%)	0	100	100
2	P	339/341 (99%)	339 (100%)	0	100	100
All	All	5585/6408 (87%)	5585 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	417/521 (80%)	0.05	7 (1%) 70 67	23, 67, 143, 273	0
1	B	415/521 (79%)	0.15	17 (4%) 37 36	38, 103, 178, 245	0
1	C	417/521 (80%)	0.08	10 (2%) 59 56	30, 76, 142, 224	0
1	D	415/521 (79%)	0.29	24 (5%) 23 23	52, 105, 196, 263	0
1	E	416/521 (79%)	0.11	12 (2%) 51 49	54, 108, 196, 292	0
1	F	416/521 (79%)	0.05	15 (3%) 42 41	57, 92, 162, 213	0
1	G	417/521 (80%)	0.17	28 (6%) 17 19	64, 103, 170, 241	0
1	H	417/521 (80%)	0.14	12 (2%) 51 49	58, 106, 211, 289	0
2	I	419/421 (99%)	1.56	113 (26%) 0 0	88, 157, 289, 394	0
2	J	418/421 (99%)	0.29	19 (4%) 33 32	61, 102, 169, 241	0
2	K	418/421 (99%)	0.23	10 (2%) 59 56	60, 108, 170, 220	0
2	L	418/421 (99%)	1.09	90 (21%) 0 1	89, 175, 288, 361	0
2	M	419/421 (99%)	0.73	67 (15%) 1 3	63, 129, 277, 346	0
2	N	418/421 (99%)	0.97	75 (17%) 1 2	85, 155, 274, 342	0
2	O	418/421 (99%)	0.92	82 (19%) 1 1	54, 154, 279, 341	0
2	P	419/421 (99%)	1.61	127 (30%) 0 0	90, 169, 296, 368	0
All	All	6677/7536 (88%)	0.53	708 (10%) 6 8	23, 116, 246, 394	0

All (708) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	223	LEU	15.2
2	N	272	LEU	15.2
2	P	215	GLY	13.6
2	N	212	ALA	13.3
2	N	266	LEU	12.6

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Mol	Chain	Res	Type	RSRZ
2	O	272	LEU	11.4
2	I	272	LEU	11.4
2	P	151	GLY	11.3
2	P	209	GLU	11.1
2	N	211	PHE	10.8
2	N	155	LEU	10.7
2	I	199	GLY	10.3
2	I	203	GLN	10.2
2	P	222	ARG	10.0
2	P	223	LEU	10.0
2	I	224	LEU	9.9
2	P	203	GLN	9.9
2	M	296	TRP	9.8
2	L	155	LEU	9.2
2	P	197	GLY	9.0
2	L	272	LEU	8.9
2	M	272	LEU	8.8
2	P	224	LEU	8.7
2	I	222	ARG	8.7
2	N	214	ARG	8.7
2	L	216	GLY	8.6
2	I	212	ALA	8.5
2	L	197	GLY	8.5
2	N	204	LEU	8.4
2	I	201	GLN	8.3
2	M	204	LEU	8.1
2	I	266	LEU	8.0
2	O	155	LEU	7.8
2	I	209	GLU	7.8
2	I	205	GLY	7.8
2	P	155	LEU	7.7
2	P	328	LEU	7.7
2	N	197	GLY	7.7
2	I	220	LEU	7.6
2	I	265	GLY	7.6
2	L	346	ALA	7.5
2	L	218	GLN	7.5
2	P	212	ALA	7.5
2	I	218	GLN	7.4
2	O	266	LEU	7.4
2	I	216	GLY	7.3
2	I	200	GLU	7.3

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Mol	Chain	Res	Type	RSRZ
2	M	205	GLY	7.3
2	I	273	GLY	7.2
2	P	295	SER	7.2
2	L	208	PRO	7.2
2	I	210	LEU	7.1
2	M	265	GLY	7.1
2	P	208	PRO	7.1
2	P	210	LEU	7.0
2	L	133	ALA	7.0
2	N	216	GLY	7.0
2	L	204	LEU	7.0
2	M	211	PHE	6.8
2	N	215	GLY	6.8
2	I	292	SER	6.8
2	P	198	CYS	6.8
2	I	158	PRO	6.8
2	I	297	VAL	6.7
2	J	237	ARG	6.7
1	D	105	PRO	6.6
2	O	223	LEU	6.6
2	I	208	PRO	6.5
2	P	204	LEU	6.5
2	I	312	GLU	6.5
1	F	122	CYS	6.5
2	I	327	GLY	6.4
2	M	266	LEU	6.4
2	O	205	GLY	6.4
2	I	270	HIS	6.3
2	I	161	LYS	6.3
2	I	204	LEU	6.1
2	I	215	GLY	6.1
2	P	201	GLN	6.1
2	O	204	LEU	6.1
2	O	296	TRP	6.1
2	I	155	LEU	6.0
2	P	213	ASN	6.0
2	N	213	ASN	6.0
2	P	199	GLY	6.0
2	P	220	LEU	5.9
2	P	267	SER	5.9
2	N	280	CYS	5.9
2	N	230	MET	5.9

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Mol	Chain	Res	Type	RSRZ
2	O	154	GLY	5.9
2	P	270	HIS	5.8
2	O	244	ASP	5.8
2	L	215	GLY	5.8
2	N	271	GLN	5.8
2	N	218	GLN	5.7
2	L	277	THR	5.7
2	P	277	THR	5.6
2	O	215	GLY	5.6
2	P	216	GLY	5.5
2	I	234	ARG	5.5
2	P	200	GLU	5.5
2	O	271	GLN	5.5
2	L	195	THR	5.4
2	L	214	ARG	5.4
2	L	280	CYS	5.4
2	N	265	GLY	5.3
2	P	205	GLY	5.3
2	I	338	PRO	5.3
2	O	216	GLY	5.3
2	P	161	LYS	5.3
2	P	211	PHE	5.3
2	P	358	TYR	5.2
2	L	211	PHE	5.2
2	O	214	ARG	5.2
2	L	278	GLU	5.2
2	N	199	GLY	5.1
2	L	220	LEU	5.1
2	N	217	ARG	5.1
2	P	159	MET	5.1
2	I	154	GLY	5.1
2	L	245	ALA	5.0
2	P	214	ARG	5.0
2	N	154	GLY	5.0
2	O	265	GLY	5.0
2	I	317	SER	5.0
2	I	198	CYS	4.9
2	L	266	LEU	4.9
2	L	299	PHE	4.9
2	L	156	LEU	4.9
2	N	346	ALA	4.9
2	L	273	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
2	O	319	GLY	4.8
1	E	127	ASP	4.8
2	N	223	LEU	4.8
2	I	247	CYS	4.8
2	M	388	PRO	4.8
2	O	208	PRO	4.8
2	P	95	ASP	4.8
2	P	299	PHE	4.7
2	O	211	PHE	4.7
2	L	296	TRP	4.7
2	P	154	GLY	4.7
2	L	275	PRO	4.6
2	P	158	PRO	4.6
2	O	276	GLY	4.6
2	P	385	ALA	4.6
2	I	267	SER	4.6
2	I	264	PHE	4.6
1	F	433	ASP	4.6
2	I	221	GLU	4.6
2	P	207	VAL	4.6
2	N	159	MET	4.5
2	O	277	THR	4.5
2	N	421	SER	4.5
2	M	213	ASN	4.5
2	N	279	SER	4.5
2	P	317	SER	4.5
2	I	293	THR	4.5
2	L	342	SER	4.5
2	P	150	ASN	4.5
2	P	263	GLY	4.5
2	O	218	GLN	4.4
2	L	159	MET	4.4
1	G	122	CYS	4.4
2	I	230	MET	4.4
2	I	219	GLY	4.4
2	I	242	PHE	4.4
2	M	216	GLY	4.4
2	I	311	SER	4.4
2	N	333	GLU	4.4
2	N	342	SER	4.4
2	P	391	MET	4.4
2	P	25	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
2	M	280	CYS	4.3
2	M	261	VAL	4.3
2	M	282	ILE	4.3
2	I	296	TRP	4.3
2	M	295	SER	4.3
2	L	132	ALA	4.2
2	L	265	GLY	4.2
2	O	209	GLU	4.2
2	M	210	LEU	4.2
2	N	160	LYS	4.2
1	D	93	GLN	4.2
2	P	266	LEU	4.1
2	M	209	GLU	4.1
2	O	217	ARG	4.1
2	L	276	GLY	4.1
2	I	275	PRO	4.1
2	P	338	PRO	4.1
2	M	155	LEU	4.1
2	L	201	GLN	4.1
2	N	221	GLU	4.1
2	N	261	VAL	4.1
2	O	321	ALA	4.1
2	L	262	TYR	4.1
2	M	271	GLN	4.0
2	N	205	GLY	4.0
2	N	208	PRO	4.0
2	P	219	GLY	4.0
1	G	121	HIS	4.0
2	I	251	PHE	4.0
2	P	251	PHE	4.0
1	F	394	ASN	4.0
2	I	213	ASN	4.0
2	P	297	VAL	4.0
2	I	306	THR	4.0
2	I	299	PHE	4.0
2	M	297	VAL	4.0
2	O	421	SER	4.0
2	I	253	PHE	4.0
2	K	284	GLN	4.0
2	I	387	SER	4.0
1	D	377	LEU	4.0
2	I	319	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
2	P	359	ALA	4.0
1	G	464	GLN	3.9
2	L	347	VAL	3.9
2	I	274	THR	3.9
2	I	284	GLN	3.9
2	I	295	SER	3.9
1	B	416	PHE	3.9
2	I	151	GLY	3.9
2	N	296	TRP	3.9
2	L	244	ASP	3.9
2	M	212	ALA	3.9
2	P	234	ARG	3.9
2	L	196	LEU	3.9
2	P	24	LYS	3.9
2	O	197	GLY	3.9
1	A	468	HIS	3.9
1	F	73	LEU	3.9
2	N	222	ARG	3.9
2	I	333	GLU	3.9
2	M	218	GLN	3.9
2	L	154	GLY	3.9
2	L	209	GLU	3.8
2	M	158	PRO	3.8
2	P	293	THR	3.8
2	I	289	PHE	3.8
1	D	109	ASP	3.8
2	O	219	GLY	3.8
1	G	433	ASP	3.8
2	L	207	VAL	3.8
2	L	253	PHE	3.8
2	O	280	CYS	3.8
2	L	217	ARG	3.8
2	O	206	ARG	3.8
2	L	303	GLN	3.8
2	P	178	ALA	3.7
2	M	273	GLY	3.7
2	I	159	MET	3.7
2	L	251	PHE	3.7
2	L	401	VAL	3.7
2	M	320	ARG	3.7
2	N	161	LYS	3.7
2	N	198	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
2	N	388	PRO	3.7
1	D	122	CYS	3.7
2	L	213	ASN	3.7
2	P	333	GLU	3.7
2	M	221	GLU	3.7
2	N	201	GLN	3.7
2	N	262	TYR	3.6
2	N	344	LEU	3.6
2	P	253	PHE	3.6
2	P	389	VAL	3.6
1	H	80	ALA	3.6
2	N	184	LEU	3.6
2	I	308	CYS	3.6
2	M	262	TYR	3.6
2	L	210	LEU	3.6
1	A	72	SER	3.6
2	I	318	LEU	3.6
2	L	206	ARG	3.6
2	O	273	GLY	3.6
2	M	303	GLN	3.6
2	J	236	SER	3.6
2	I	245	ALA	3.6
2	P	275	PRO	3.6
2	I	386	TRP	3.6
2	L	322	GLU	3.6
1	C	468	HIS	3.6
2	P	152	VAL	3.5
2	N	210	LEU	3.5
2	I	235	GLY	3.5
2	O	220	LEU	3.5
2	L	16	ALA	3.5
2	I	309	MET	3.5
2	L	158	PRO	3.5
2	M	237	ARG	3.5
1	G	131	LEU	3.5
2	M	275	PRO	3.5
2	M	346	ALA	3.5
1	H	71	THR	3.4
2	I	328	LEU	3.4
2	M	421	SER	3.4
2	M	299	PHE	3.4
2	N	235	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
2	O	267	SER	3.4
2	K	234	ARG	3.4
2	L	116	GLU	3.4
2	I	156	LEU	3.4
2	P	218	GLN	3.4
2	P	242	PHE	3.4
2	P	318	LEU	3.4
2	P	149	ASN	3.4
2	I	238	GLY	3.4
2	O	198	CYS	3.4
2	P	110	MET	3.4
2	I	332	ALA	3.4
2	N	335	LYS	3.3
2	O	201	GLN	3.3
2	M	289	PHE	3.3
2	N	253	PHE	3.3
2	P	221	GLU	3.3
2	I	197	GLY	3.3
2	O	318	LEU	3.3
2	P	195	THR	3.3
2	I	211	PHE	3.3
2	P	312	GLU	3.3
2	M	230	MET	3.3
2	N	219	GLY	3.3
2	O	161	LYS	3.3
2	J	263	GLY	3.3
2	P	206	ARG	3.3
2	P	269	TYR	3.3
2	P	160	LYS	3.3
2	O	186	MET	3.2
2	P	339	THR	3.2
1	A	109	ASP	3.2
2	L	230	MET	3.2
1	C	444	ASP	3.2
2	P	177	VAL	3.2
2	I	280	CYS	3.2
2	O	222	ARG	3.2
2	P	405	SER	3.2
1	D	416	PHE	3.2
2	I	152	VAL	3.2
2	M	253	PHE	3.2
2	O	268	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
2	L	219	GLY	3.2
2	M	281	PHE	3.2
2	N	209	GLU	3.2
2	J	288	SER	3.2
2	O	221	GLU	3.2
2	P	311	SER	3.2
1	G	354	THR	3.2
2	P	272	LEU	3.2
2	L	229	VAL	3.2
2	P	247	CYS	3.2
1	C	72	SER	3.1
2	I	261	VAL	3.1
2	P	292	SER	3.1
2	M	159	MET	3.1
2	L	409	GLN	3.1
2	P	128	ASP	3.1
2	O	153	ILE	3.1
2	O	199	GLY	3.1
2	L	247	CYS	3.1
2	M	116	GLU	3.1
2	I	206	ARG	3.1
2	O	229	VAL	3.1
2	P	284	GLN	3.1
1	E	121	HIS	3.1
2	L	321	ALA	3.1
2	M	201	GLN	3.1
2	M	217	ARG	3.1
1	D	473	ILE	3.0
2	L	205	GLY	3.0
2	P	306	THR	3.0
2	P	81	CYS	3.0
2	I	236	SER	3.0
1	B	417	CYS	3.0
2	K	272	LEU	3.0
2	M	283	PRO	3.0
2	O	158	PRO	3.0
2	O	195	THR	3.0
2	M	208	PRO	3.0
1	E	340	GLU	3.0
2	M	153	ILE	3.0
2	I	389	VAL	3.0
2	I	324	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	M	332	ALA	2.9
2	P	294	LYS	2.9
1	B	373	ILE	2.9
1	A	105	PRO	2.9
1	D	142	ILE	2.9
2	O	212	ALA	2.9
1	F	311	ILE	2.9
2	J	318	LEU	2.9
2	L	289	PHE	2.9
2	M	52	GLU	2.9
2	L	345	PRO	2.9
2	I	195	THR	2.9
2	P	308	CYS	2.9
1	E	411	ASN	2.9
1	C	71	THR	2.9
2	N	149	ASN	2.9
2	I	326	LEU	2.9
2	J	272	LEU	2.9
1	E	425	ALA	2.9
2	P	420	GLN	2.9
1	E	79	ASN	2.9
2	O	177	VAL	2.9
2	P	356	VAL	2.9
2	L	212	ALA	2.9
2	O	270	HIS	2.9
1	F	473	ILE	2.8
2	N	367	PHE	2.8
2	P	179	SER	2.8
2	I	263	GLY	2.8
1	H	121	HIS	2.8
2	I	214	ARG	2.8
1	H	85	GLN	2.8
2	P	278	GLU	2.8
2	M	344	LEU	2.8
2	O	156	LEU	2.8
2	I	405	SER	2.8
2	O	289	PHE	2.8
2	O	392	MET	2.8
2	P	329	GLY	2.8
2	P	307	VAL	2.8
2	O	190	ASP	2.8
2	I	254	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	P	39	THR	2.8
2	L	260	HIS	2.8
1	D	92	VAL	2.8
2	P	406	SER	2.8
2	L	268	ASN	2.8
1	H	468	HIS	2.8
2	O	314	LYS	2.8
2	J	4	LYS	2.8
2	J	262	TYR	2.8
2	O	248	GLY	2.7
2	L	333	GLU	2.7
2	O	373	THR	2.7
2	M	215	GLY	2.7
2	O	389	VAL	2.7
2	J	284	GLN	2.7
2	L	287	THR	2.7
2	N	196	LEU	2.7
2	O	15	ASP	2.7
2	O	210	LEU	2.7
2	P	217	ARG	2.7
2	P	326	LEU	2.7
1	B	462	ILE	2.7
2	P	337	ILE	2.7
1	D	139	LEU	2.7
2	O	149	ASN	2.7
2	J	231	LEU	2.7
1	H	79	ASN	2.7
2	O	293	THR	2.7
2	I	420	GLN	2.7
2	O	185	VAL	2.7
1	F	476	LEU	2.7
1	D	465	LEU	2.7
2	L	254	ALA	2.7
2	N	332	ALA	2.7
2	N	331	GLY	2.6
2	N	116	GLU	2.6
2	P	395	GLN	2.6
2	L	234	ARG	2.6
2	L	269	TYR	2.6
2	P	250	TYR	2.6
2	M	277	THR	2.6
2	N	267	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	L	222	ARG	2.6
1	D	417	CYS	2.6
1	A	487	SER	2.6
2	L	221	GLU	2.6
2	N	319	GLY	2.6
2	I	310	ASP	2.6
1	G	269	LEU	2.6
1	G	392	ILE	2.6
1	G	407	LEU	2.6
2	I	25	VAL	2.6
2	O	207	VAL	2.6
1	D	127	ASP	2.6
2	N	207	VAL	2.6
1	G	435	LEU	2.6
1	D	136	ALA	2.6
1	C	107	ILE	2.6
1	E	327	ALA	2.6
1	B	461	LYS	2.6
2	N	185	VAL	2.6
2	N	347	VAL	2.6
2	P	235	GLY	2.6
1	E	290	VAL	2.5
2	N	152	VAL	2.5
2	J	234	ARG	2.5
1	F	269	LEU	2.5
2	L	274	THR	2.5
2	M	245	ALA	2.5
2	L	223	LEU	2.5
2	N	334	GLU	2.5
1	G	177	ALA	2.5
2	L	198	CYS	2.5
1	A	110	LEU	2.5
2	I	125	SER	2.5
1	G	472	ASP	2.5
2	O	245	ALA	2.5
2	O	299	PHE	2.5
2	P	265	GLY	2.5
2	O	251	PHE	2.5
1	F	436	SER	2.5
2	P	26	SER	2.5
1	B	166	LEU	2.5
1	G	262	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	P	40	LEU	2.5
2	P	274	THR	2.5
2	O	253	PHE	2.5
1	E	184	ILE	2.5
2	O	213	ASN	2.4
2	I	385	ALA	2.4
2	I	406	SER	2.4
2	O	344	LEU	2.4
1	B	184	ILE	2.4
2	L	235	GLY	2.4
2	P	355	SER	2.4
2	M	382	ASP	2.4
2	I	160	LYS	2.4
2	I	255	ILE	2.4
2	O	116	GLU	2.4
1	C	111	ILE	2.4
2	K	53	ASN	2.4
2	M	373	THR	2.4
1	B	121	HIS	2.4
1	G	449	ILE	2.4
2	P	347	VAL	2.4
2	I	150	ASN	2.4
2	I	252	THR	2.4
2	P	74	ALA	2.4
2	P	245	ALA	2.4
1	H	89	LEU	2.4
2	L	224	LEU	2.4
2	I	404	VAL	2.4
1	B	122	CYS	2.4
1	G	124	GLU	2.4
2	I	321	ALA	2.4
2	M	278	GLU	2.4
1	H	122	CYS	2.4
2	O	315	ALA	2.4
2	I	207	VAL	2.3
2	P	273	GLY	2.3
2	J	319	GLY	2.3
1	C	133	PHE	2.3
2	I	186	MET	2.3
2	J	44	ASP	2.3
2	M	342	SER	2.3
2	N	278	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	N	156	LEU	2.3
2	L	152	VAL	2.3
1	D	345	GLU	2.3
2	N	200	GLU	2.3
1	G	384	THR	2.3
2	P	376	GLN	2.3
1	D	89	LEU	2.3
1	E	123	LEU	2.3
1	G	476	LEU	2.3
2	L	6	ILE	2.3
2	I	233	SER	2.3
2	N	345	PRO	2.3
2	I	391	MET	2.3
2	O	184	LEU	2.3
2	N	229	VAL	2.3
2	O	242	PHE	2.3
2	N	275	PRO	2.3
2	P	238	GLY	2.3
1	D	279	MET	2.3
2	P	411	THR	2.3
2	M	207	VAL	2.3
2	J	299	PHE	2.3
2	P	75	GLY	2.3
1	C	487	SER	2.3
2	O	279	SER	2.3
1	G	308	VAL	2.3
2	I	316	TYR	2.3
2	N	340	LEU	2.3
2	I	339	THR	2.3
2	I	232	LYS	2.3
2	P	116	GLU	2.3
2	P	132	ALA	2.3
2	K	339	THR	2.2
2	O	320	ARG	2.2
2	J	230	MET	2.2
1	G	481	ILE	2.2
2	L	141	PHE	2.2
2	J	247	CYS	2.2
2	L	389	VAL	2.2
2	K	406	SER	2.2
2	N	220	LEU	2.2
1	D	248	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	P	153	ILE	2.2
2	N	249	ALA	2.2
2	I	145	SER	2.2
2	L	90	SER	2.2
1	F	485	PHE	2.2
2	K	351	ALA	2.2
2	M	321	ALA	2.2
2	P	33	GLU	2.2
1	G	439	LEU	2.2
2	N	289	PHE	2.2
2	J	421	SER	2.2
1	D	94	ALA	2.2
2	L	271	GLN	2.2
2	L	379	THR	2.2
2	P	252	THR	2.2
2	P	288	SER	2.2
1	A	403	GLN	2.2
2	L	153	ILE	2.2
2	O	6	ILE	2.2
1	B	420	LEU	2.2
2	M	214	ARG	2.2
2	O	401	VAL	2.2
2	P	375	TYR	2.2
2	J	332	ALA	2.2
1	D	106	PRO	2.2
1	D	219	ASN	2.2
2	O	230	MET	2.2
2	P	401	VAL	2.2
2	O	5	ARG	2.2
2	L	184	LEU	2.2
2	I	336	SER	2.2
2	O	16	ALA	2.2
2	L	12	PRO	2.2
2	M	15	ASP	2.2
2	I	39	THR	2.2
2	I	178	ALA	2.1
2	N	251	PHE	2.1
2	P	125	SER	2.1
1	E	444	ASP	2.1
1	B	80	ALA	2.1
1	G	487	SER	2.1
2	M	179	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	P	236	SER	2.1
2	I	358	TYR	2.1
1	C	216	PHE	2.1
2	L	126	ALA	2.1
2	I	237	ARG	2.1
2	M	294	LYS	2.1
1	B	377	LEU	2.1
2	P	231	LEU	2.1
2	L	150	ASN	2.1
2	M	14	ALA	2.1
1	G	473	ILE	2.1
1	B	228	CYS	2.1
1	H	78	GLN	2.1
1	B	303	ALA	2.1
2	P	310	ASP	2.1
2	P	56	GLU	2.1
2	M	195	THR	2.1
2	I	75	GLY	2.1
1	F	366	ASP	2.1
1	D	184	ILE	2.1
2	K	210	LEU	2.1
2	O	196	LEU	2.1
2	P	271	GLN	2.1
1	G	394	ASN	2.1
2	N	254	ALA	2.1
1	G	72	SER	2.1
2	N	366	VAL	2.1
2	O	152	VAL	2.1
2	K	281	PHE	2.1
1	D	267	SER	2.1
1	F	334	LEU	2.1
2	P	336	SER	2.1
2	P	148	ASP	2.1
2	L	320	ARG	2.1
2	O	294	LYS	2.1
2	L	185	VAL	2.1
1	G	311	ILE	2.1
2	M	197	GLY	2.1
1	F	228	CYS	2.0
1	H	387	GLU	2.0
2	L	343	ARG	2.0
1	F	486	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	I	314	LYS	2.0
2	M	311	SER	2.0
2	N	325	ARG	2.0
2	J	260	HIS	2.0
2	M	302	GLY	2.0
2	P	232	LYS	2.0
2	N	242	PHE	2.0
1	B	100	SER	2.0
1	D	463	GLU	2.0
1	G	102	ASP	2.0
1	H	81	SER	2.0
1	B	225	VAL	2.0
2	N	315	ALA	2.0
2	P	350	VAL	2.0
1	E	473	ILE	2.0
1	F	254	THR	2.0
2	L	334	GLU	2.0
2	I	128	ASP	2.0
2	K	44	ASP	2.0
2	M	260	HIS	2.0
1	C	184	ILE	2.0
1	G	485	PHE	2.0
2	O	275	PRO	2.0
2	I	81	CYS	2.0
1	H	423	LYS	2.0
1	B	304	ALA	2.0
1	G	334	LEU	2.0
2	L	279	SER	2.0
2	P	130	HIS	2.0
2	M	206	ARG	2.0
2	M	234	ARG	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 [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.