



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2017 – 08:35 AM EDT

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 : unknown
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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

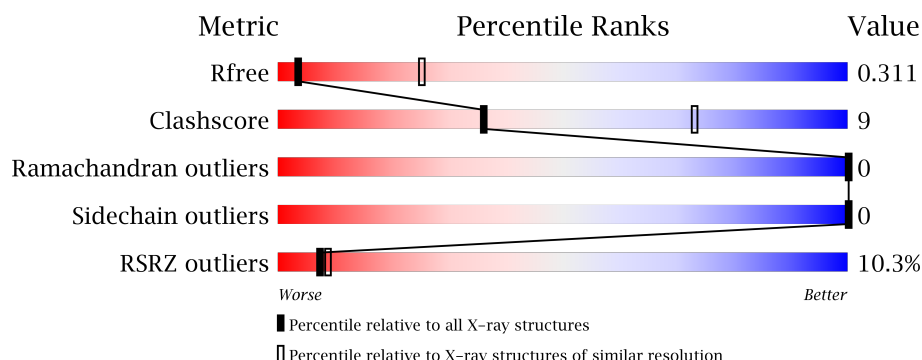
1 Overall quality at a glance

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}	100719	1135 (3.56-3.36)
Clashscore	112137	1040 (3.52-3.40)
Ramachandran outliers	110173	1009 (3.52-3.40)
Sidechain outliers	110143	1010 (3.52-3.40)
RSRZ outliers	101464	1017 (3.54-3.38)

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 ≥ 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	521	<div> <div>0.5%</div> <div>64% 16% 20%</div> </div>
1	B	521	<div> <div>3%</div> <div>65% 15% 20%</div> </div>
1	C	521	<div> <div>2%</div> <div>66% 14% 20%</div> </div>
1	D	521	<div> <div>5%</div> <div>63% 17% 20%</div> </div>
1	E	521	<div> <div>2%</div> <div>65% 15% 20%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	521	
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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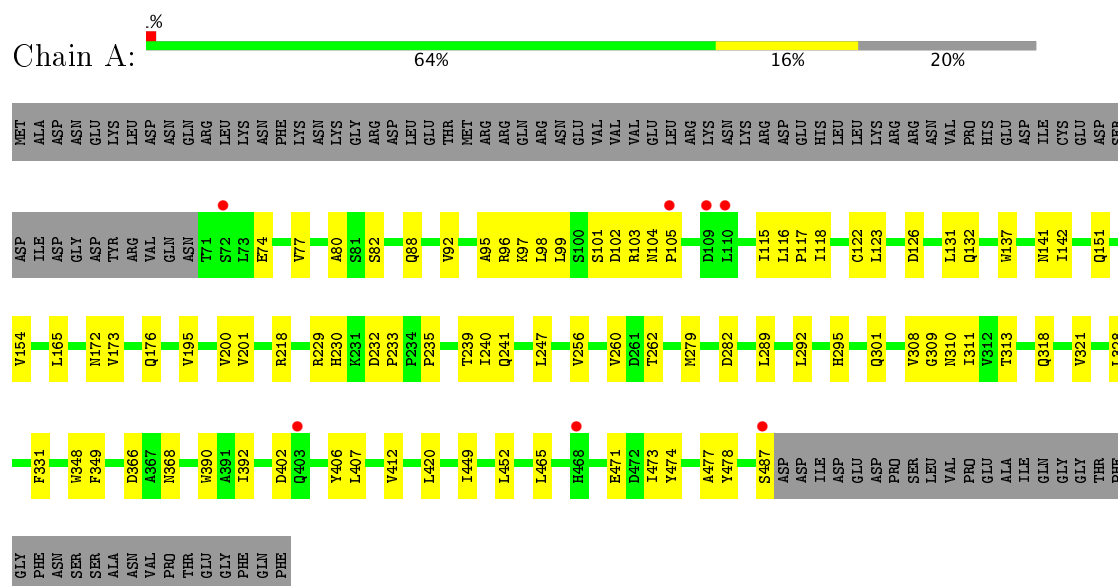
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	419	Total	C	N	O	S	0	0	0
			3139	1954	562	604	19			
2	J	418	Total	C	N	O	S	0	0	0
			3132	1949	561	603	19			

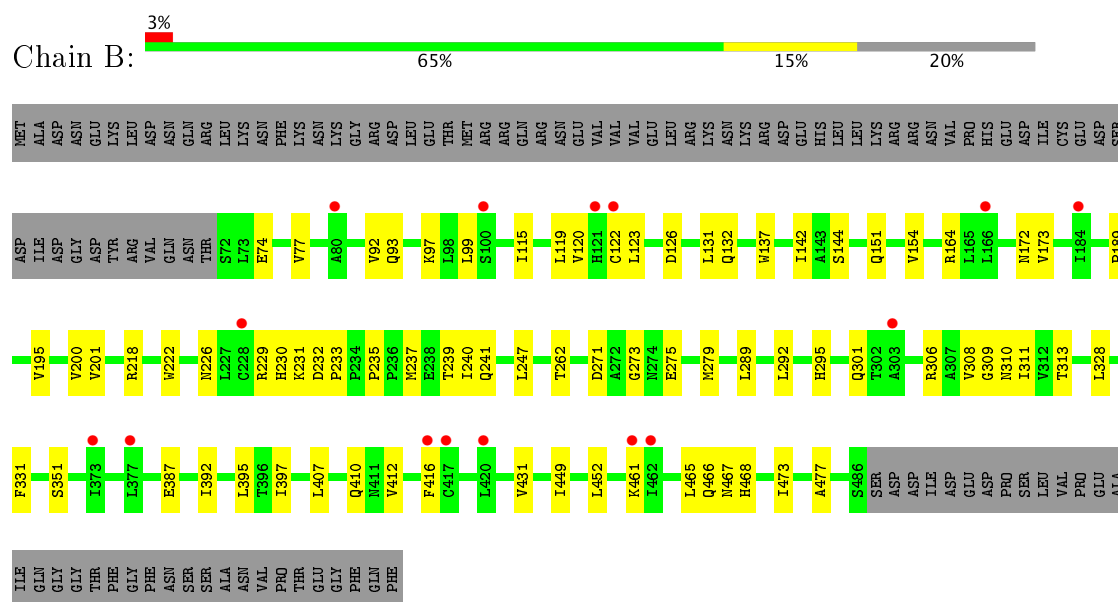
3 Residue-property plots [i](#)

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

• Molecule 1: Importin subunit alpha-3



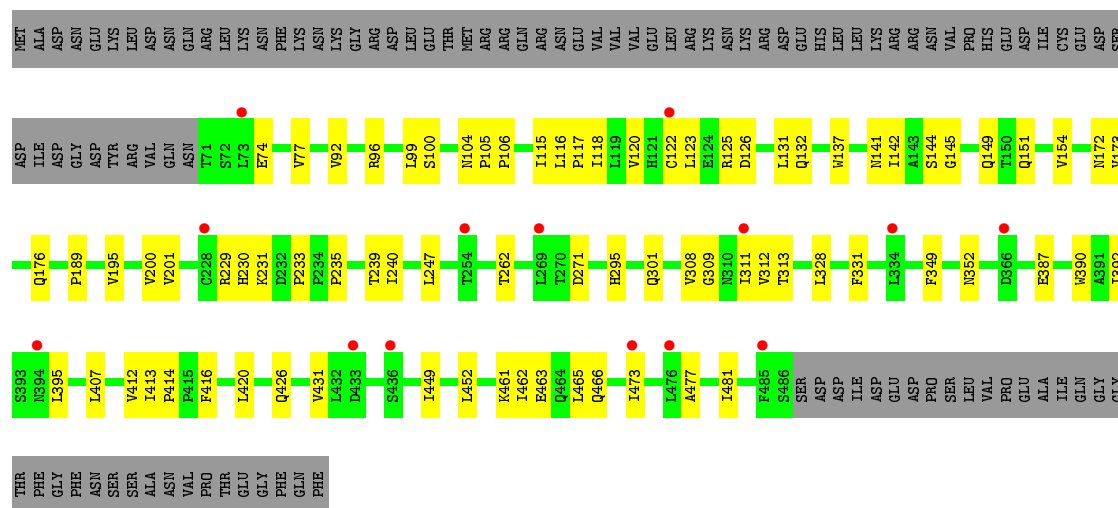
• Molecule 1: Importin subunit alpha-3



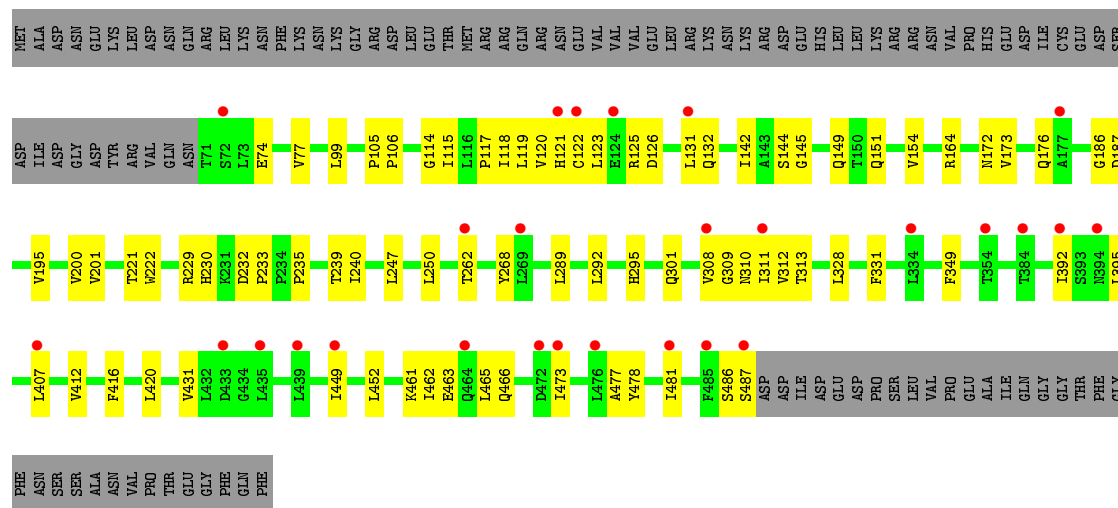
• Molecule 1: Importin subunit alpha-3

ILE
GLN
GLY
GLY
THR
PHE
GLY
PHE
ASN
SER
SER
ALA
ASN
VAL
PRO
THR
GLU
GLY
PHE
PHE

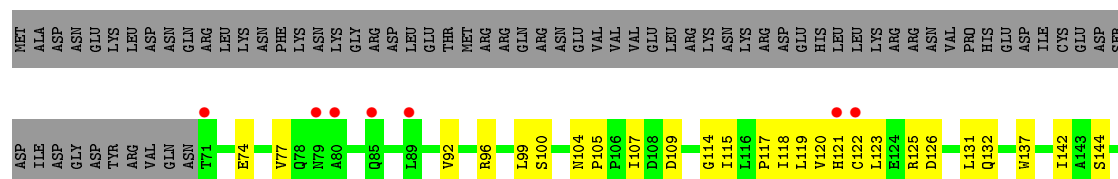
• Molecule 1: Importin subunit alpha-3

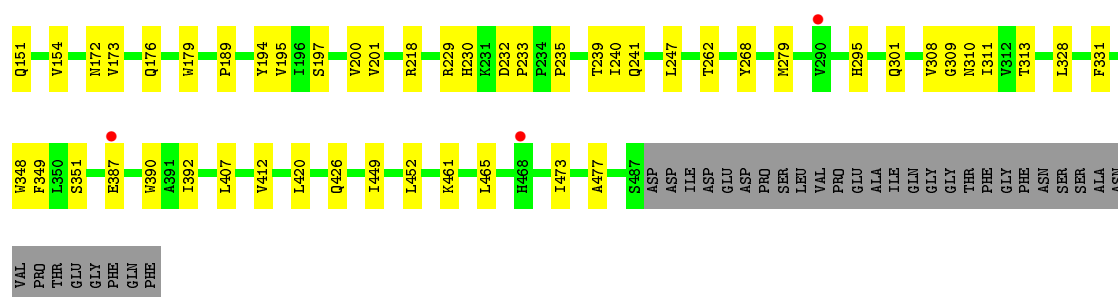


• Molecule 1: Importin subunit alpha-3

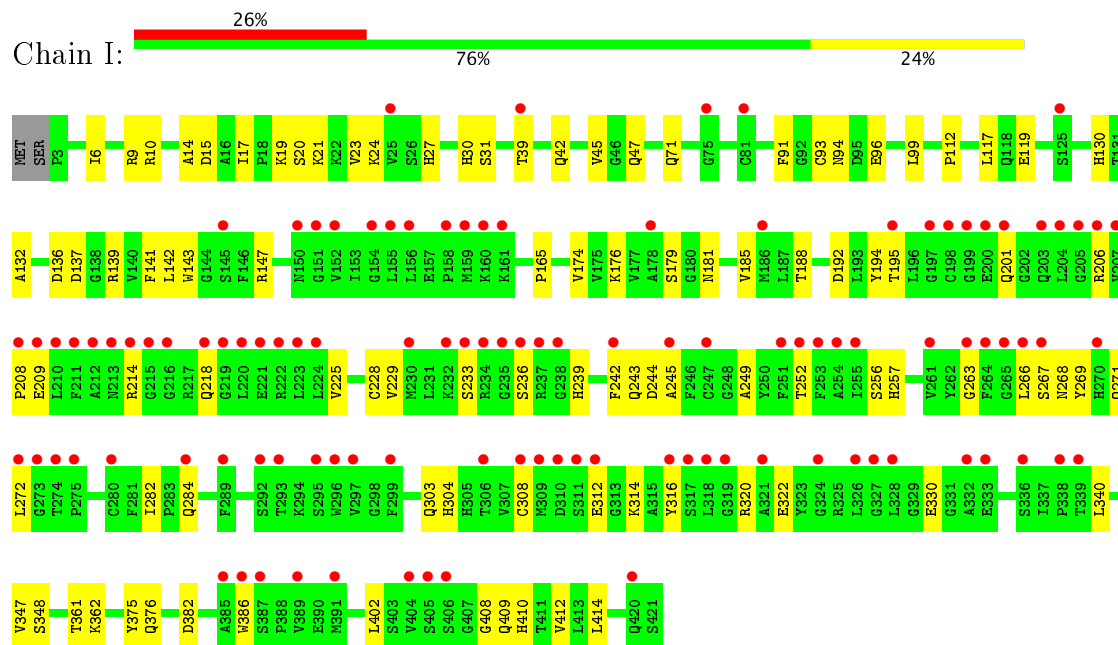


• Molecule 1: Importin subunit alpha-3

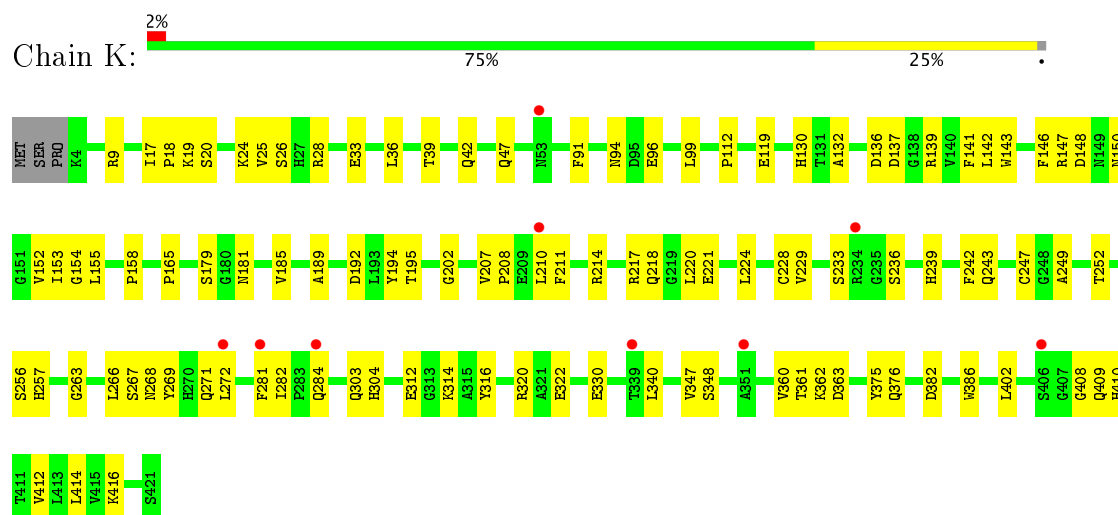




• Molecule 2: Regulator of chromosome condensation

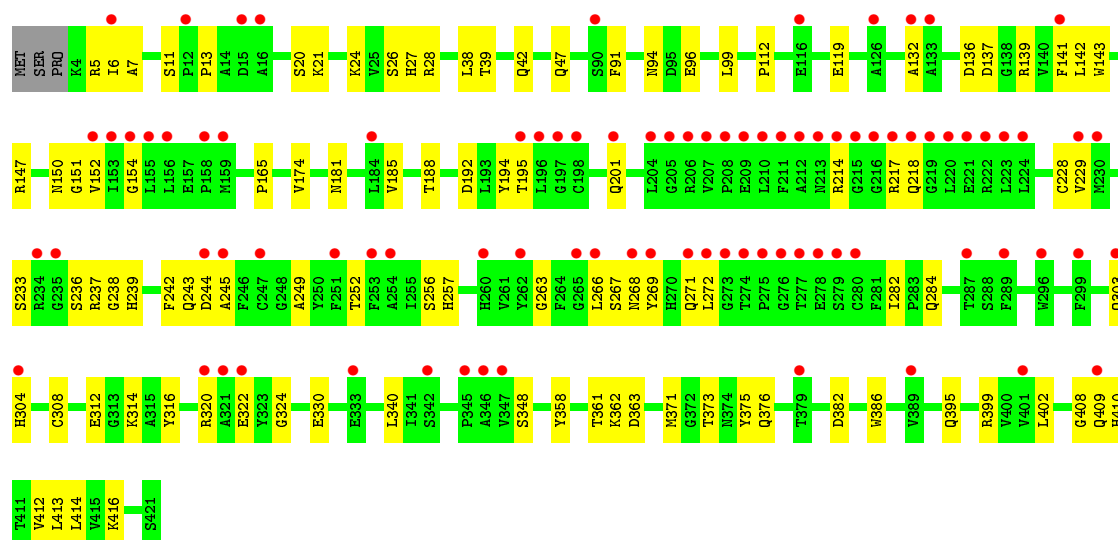


• Molecule 2: Regulator of chromosome condensation

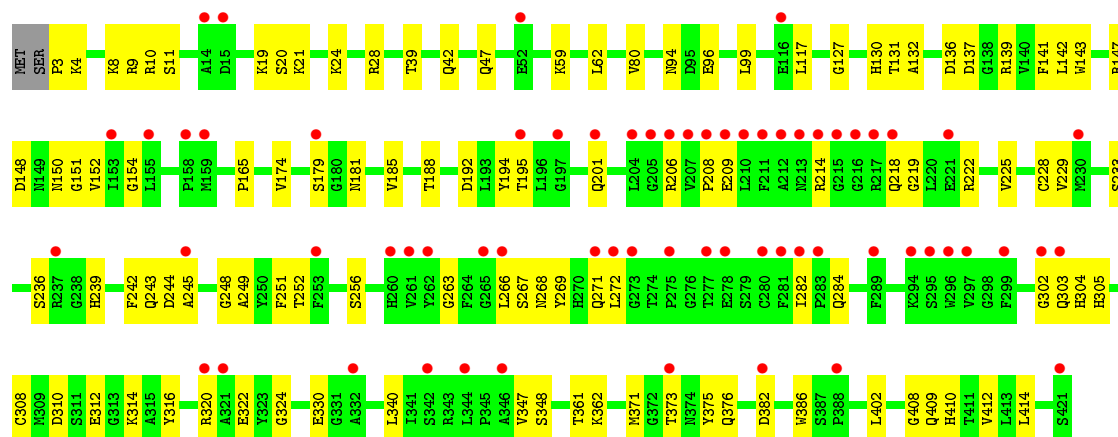
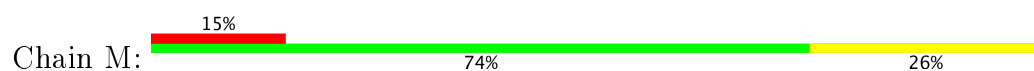


• Molecule 2: Regulator of chromosome condensation

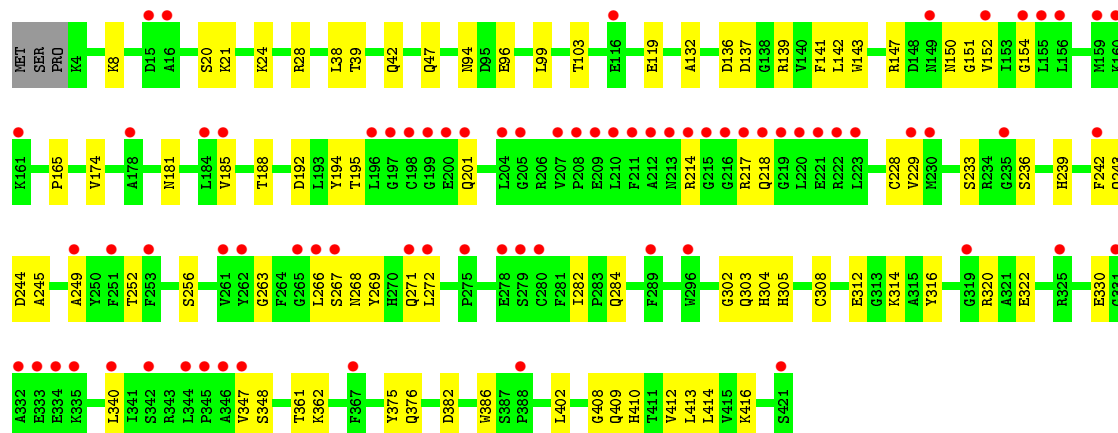
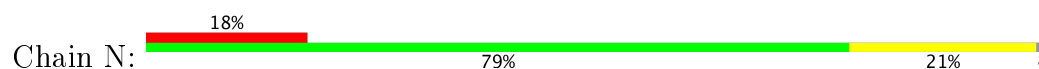




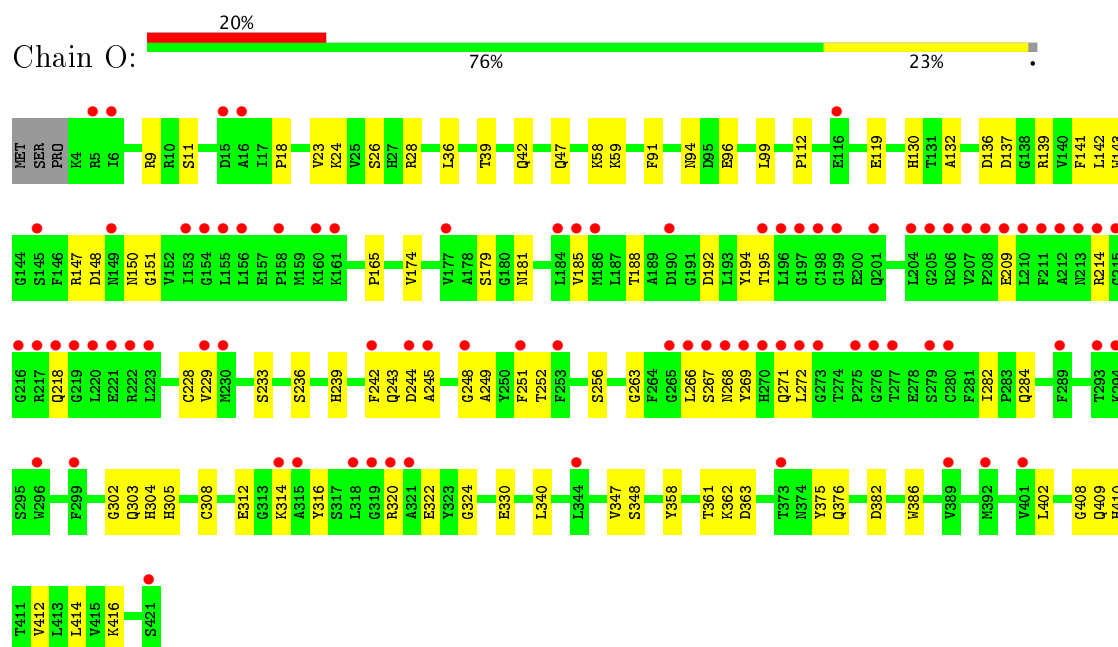
• Molecule 2: Regulator of chromosome condensation



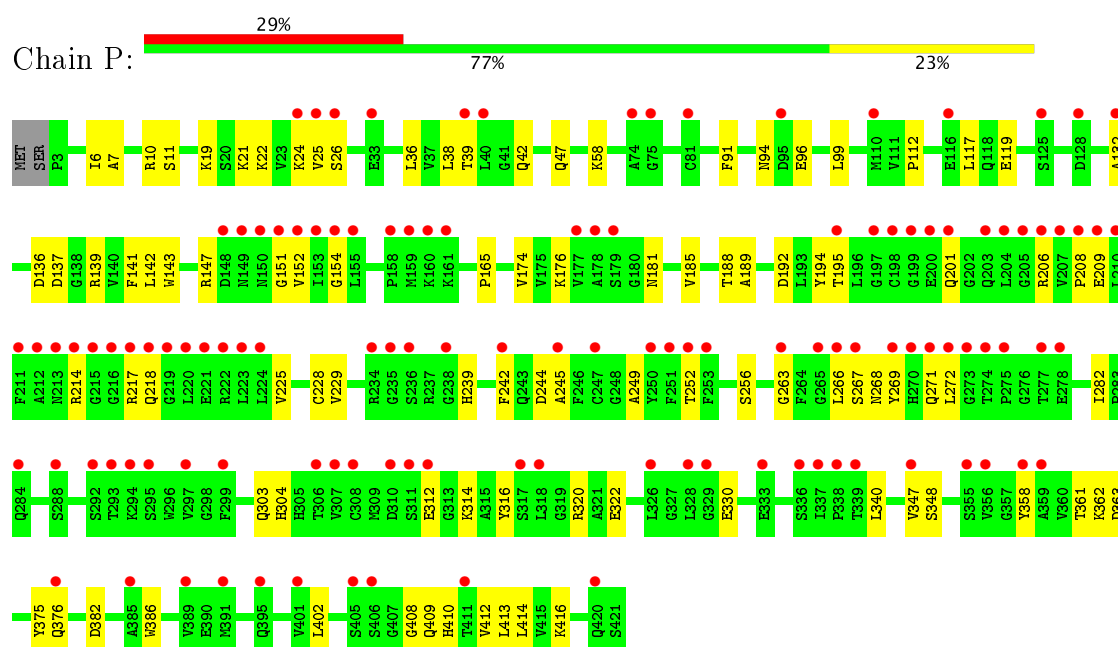
• Molecule 2: Regulator of chromosome condensation



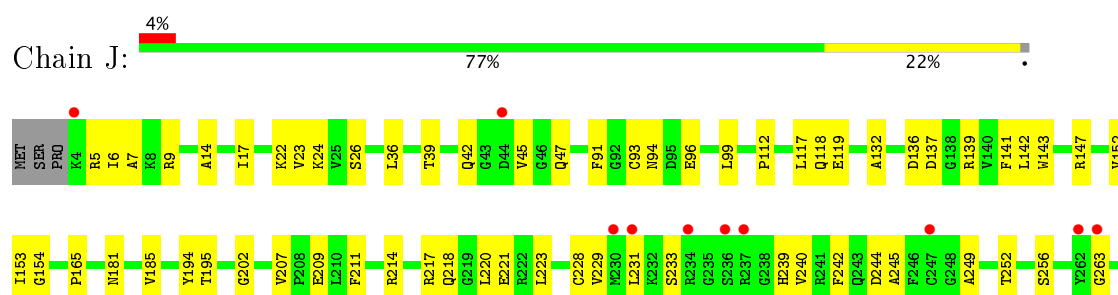
• Molecule 2: Regulator of chromosome condensation

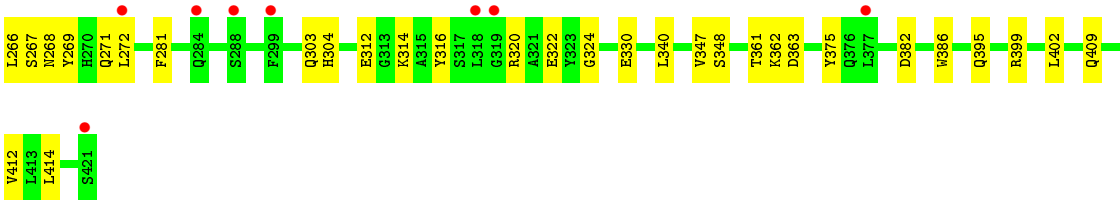


• Molecule 2: Regulator of chromosome condensation



• Molecule 2: Regulator of chromosome condensation





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 74.5 (49.33-3.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.40 Å)	Xtrriage
Refinement program	PHENIX 1.10.1-2155	Depositor
R, R_{free}	0.278 , 0.296 0.295 , 0.311	Depositor DCC
R_{free} test set	1729 reflections (1.37%)	DCC
Wilson B-factor (Å ²)	88.3	Xtrriage
Anisotropy	0.244	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 26.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	50677	wwPDB-VP
Average B, all atoms (Å ²)	129.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.36 % 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 3.8894e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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
1:B:222:TRP:HE1	2:I:20:SER:HA	1.52	0.72
2:I:209:GLU:O	2:I:214:ARG:NH2	2.21	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:D:114:GLY:O	1:D:117:PRO:HD2	1.89	0.71
1:A:487:SER:HB3	2:M:62:LEU:HB3	1.73	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:D:229:ARG:NH1	2:P:19:LYS:HB3	2.09	0.68
1:C:218:ARG:NH1	2:J:119:GLU:OE2	2.26	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:D:392:ILE:HG23	1:D:407:LEU:HD21	1.86	0.57
1:B:137:TRP:CH2	2:I:24:LYS:HE2	2.39	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
2:K:181:ASN:ND2	2:K:249:ALA:HB1	2.20	0.56
1:A:103:ARG:NH1	2:K:189:ALA:O	2.35	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
1:G:176:GLN:HE22	2:N:24:LYS:HD3	1.71	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: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
2:K:94:ASN:HB2	2:K:99:LEU:HD12	1.88	0.55
1:E:187:ASP:HA	2:L:21:LYS:NZ	2.22	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: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
1:A:366:ASP:O	2:J:217:ARG:NH2	2.40	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:F:229:ARG:NH2	2:M:20:SER:OG	2.42	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
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
2:O:316:TYR:HE1	2:O:340:LEU:HD13	1.75	0.52
1:D:229:ARG:CZ	2:P:19:LYS:HB3	2.40	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:E:97:LYS:HE3	2:L:28:ARG:HA	1.90	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:C:466:GLN:HB2	2:O:58:LYS:HZ1	1.76	0.50
1:B:222:TRP:HZ2	2:I:20:SER:O	1.94	0.50
2:M:252:THR:O	2:M:263:GLY:HA2	2.12	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:B:410:GLN:OE1	2:P:214:ARG:NH1	2.44	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: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:D:397:ILE:HG21	2:P:6:ILE:HD11	1.93	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:E:176:GLN:OE1	2:L:24:LYS:HE2	2.12	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: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:F:390:TRP:HZ2	1:F:426:GLN:HE21	1.61	0.49
2:L:402:LEU:N	2:L:414:LEU:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:LEU:HD13	2:P:25:VAL:HA	1.93	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:F:144:SER:HA	2:M:21:LYS:CG	2.43	0.48
1:H:107:ILE:C	1:H:109:ASP:H	2.16	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:92:VAL:HG11	1:E:131:LEU:HD12	1.96	0.48
1:E:151:GLN:HA	1:E:154:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:387:GLU:OE1	2:O:9:ARG:NH2	2.46	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: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:C:316:ASP:OD1	2:J:5:ARG:NH2	2.48	0.47
2:N:94:ASN:ND2	2:N:103:THR:OG1	2.42	0.47
1:G:222:TRP:HZ2	2:N:20:SER:O	1.97	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: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
1:H:229:ARG:HH22	2:O:18:PRO:HG2	1.80	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:A:103:ARG:HD3	2:K:189:ALA:O	2.16	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
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:E:306:ARG:HH12	2:L:13:PRO:HA	1.81	0.45
1:G:308:VAL:HG12	1:G:349:PHE:HE1	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:103:ARG:HD3	2:P:189:ALA:O	2.17	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
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: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
1:F:176:GLN:HE22	2:M:24:LYS:HD3	1.80	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:E:103:ARG:HD3	2:L:257:HIS:ND1	2.32	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
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:B:410:GLN:HE22	2:P:214:ARG:NE	2.15	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: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:G:478:TYR:CE2	2:P:58:LYS:HB2	2.52	0.44
1:E:100:SER:OG	2:L:26:SER:HB3	2.17	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: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
1:B:306:ARG:NH1	2:I:14:ALA:HB2	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:D:221:THR:HG22	1:D:250:LEU:HD13	2.00	0.43
1:B:397:ILE:HD13	2:I:6:ILE:HG13	2.00	0.43
2:L:27:HIS:ND1	2:L:28:ARG:N	2.66	0.43
2:M:150:ASN:HA	2:O:151:GLY:N	2.33	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
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:A:390:TRP:CE3	2:K:9:ARG:HD2	2.55	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
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
1:H:137:TRP:HE1	2:O:26:SER:HB2	1.85	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
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: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
1:A:104:ASN:OD1	2:K:257:HIS:CD2	2.72	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:324:GLY:HA2	2:J:386:TRP:CE3	2.55	0.41
2:J:347:VAL:HA	2:J:361:THR:HA	2.02	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:45:VAL:HG21	2:J:93:CYS:HB2	2.03	0.41
2:J:6:ILE:HG22	2:J:7:ALA:N	2.36	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:243:GLN:HE21	2:I:257:HIS:HA	1.86	0.41
2:I:201:GLN:HB3	2:I:266:LEU:HB2	2.03	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, 95th 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 ²)	Q<0.9
1	A	417/521 (80%)	0.04	7 (1%) 70 64	23, 67, 143, 273	0
1	B	415/521 (79%)	0.14	15 (3%) 43 39	38, 103, 178, 245	0
1	C	417/521 (80%)	0.07	11 (2%) 56 49	30, 76, 142, 224	0
1	D	415/521 (79%)	0.27	25 (6%) 23 21	52, 105, 196, 263	0
1	E	416/521 (79%)	0.10	12 (2%) 52 45	54, 108, 196, 292	0
1	F	416/521 (79%)	0.04	14 (3%) 46 40	57, 92, 162, 213	0
1	G	417/521 (80%)	0.15	27 (6%) 20 18	64, 103, 170, 241	0
1	H	417/521 (80%)	0.12	10 (2%) 59 52	58, 106, 211, 289	0
2	I	419/421 (99%)	1.54	110 (26%) 1 1	88, 157, 289, 394	0
2	J	418/421 (99%)	0.28	18 (4%) 36 31	61, 102, 169, 241	0
2	K	418/421 (99%)	0.22	9 (2%) 62 55	60, 108, 170, 220	0
2	L	418/421 (99%)	1.07	88 (21%) 1 1	89, 175, 288, 361	0
2	M	419/421 (99%)	0.73	65 (15%) 2 3	63, 129, 277, 346	0
2	N	418/421 (99%)	0.96	75 (17%) 2 2	85, 155, 274, 342	0
2	O	418/421 (99%)	0.90	84 (20%) 1 1	54, 154, 279, 341	0
2	P	419/421 (99%)	1.59	121 (28%) 1 1	90, 169, 296, 368	0
All	All	6677/7536 (88%)	0.51	691 (10%) 7 9	23, 116, 246, 394	0

All (691) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	223	LEU	15.7
2	N	272	LEU	15.0
2	P	215	GLY	13.7
2	N	212	ALA	12.8
2	N	266	LEU	12.4

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Mol	Chain	Res	Type	RSRZ
2	I	272	LEU	11.5
2	P	151	GLY	11.3
2	P	209	GLU	11.3
2	O	272	LEU	11.1
2	N	155	LEU	10.7
2	N	211	PHE	10.5
2	I	224	LEU	10.3
2	I	203	GLN	9.9
2	P	222	ARG	9.9
2	P	203	GLN	9.8
2	P	223	LEU	9.8
2	I	199	GLY	9.8
2	M	296	TRP	9.4
2	L	155	LEU	9.3
2	L	272	LEU	9.1
2	P	197	GLY	9.0
2	P	224	LEU	8.8
2	I	222	ARG	8.8
2	M	272	LEU	8.7
2	N	214	ARG	8.6
2	N	204	LEU	8.5
2	M	204	LEU	8.4
2	L	216	GLY	8.2
2	I	201	GLN	8.1
2	N	197	GLY	7.9
2	L	346	ALA	7.9
2	I	212	ALA	7.9
2	P	212	ALA	7.8
2	O	155	LEU	7.8
2	P	155	LEU	7.8
2	I	220	LEU	7.7
2	I	266	LEU	7.7
2	L	197	GLY	7.6
2	I	209	GLU	7.5
2	I	205	GLY	7.4
2	O	266	LEU	7.4
2	L	218	GLN	7.4
2	I	216	GLY	7.4
2	P	328	LEU	7.4
2	P	208	PRO	7.3
2	M	205	GLY	7.3
2	P	210	LEU	7.1

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Mol	Chain	Res	Type	RSRZ
2	I	218	GLN	7.1
2	I	210	LEU	7.1
2	L	133	ALA	7.1
2	I	265	GLY	7.1
2	I	273	GLY	7.1
2	I	200	GLU	7.0
2	M	265	GLY	7.0
2	P	295	SER	7.0
2	L	208	PRO	6.9
2	N	216	GLY	6.9
2	I	292	SER	6.8
2	I	297	VAL	6.8
2	L	204	LEU	6.8
2	N	215	GLY	6.8
2	P	204	LEU	6.7
2	M	211	PHE	6.6
2	I	208	PRO	6.6
1	D	105	PRO	6.6
2	O	223	LEU	6.6
2	I	158	PRO	6.6
2	I	204	LEU	6.5
2	J	237	ARG	6.5
2	P	198	CYS	6.5
2	I	312	GLU	6.4
2	I	161	LYS	6.3
1	F	122	CYS	6.3
2	M	266	LEU	6.3
2	I	270	HIS	6.2
2	O	205	GLY	6.2
2	I	327	GLY	6.1
2	P	201	GLN	6.0
2	I	215	GLY	6.0
2	I	155	LEU	6.0
2	O	296	TRP	6.0
2	O	204	LEU	6.0
2	N	213	ASN	5.9
2	N	280	CYS	5.9
2	P	270	HIS	5.9
2	N	230	MET	5.8
2	P	220	LEU	5.8
2	P	267	SER	5.8
2	L	277	THR	5.7

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Mol	Chain	Res	Type	RSRZ
2	N	218	GLN	5.7
2	P	213	ASN	5.7
2	N	271	GLN	5.7
2	P	277	THR	5.7
2	I	234	ARG	5.6
2	O	154	GLY	5.5
2	P	199	GLY	5.5
2	L	278	GLU	5.4
2	O	271	GLN	5.4
2	L	280	CYS	5.4
2	O	244	ASP	5.4
2	P	216	GLY	5.4
2	L	195	THR	5.4
2	P	161	LYS	5.3
2	O	215	GLY	5.3
2	P	205	GLY	5.3
2	P	200	GLU	5.3
2	I	338	PRO	5.2
2	L	245	ALA	5.2
2	N	154	GLY	5.2
2	N	265	GLY	5.2
2	L	215	GLY	5.2
2	L	214	ARG	5.2
2	P	211	PHE	5.2
2	P	358	TYR	5.1
2	O	214	ARG	5.1
2	L	211	PHE	5.1
2	I	154	GLY	5.0
2	O	216	GLY	5.0
2	O	265	GLY	5.0
2	L	220	LEU	5.0
2	P	159	MET	5.0
2	N	217	ARG	4.9
2	P	214	ARG	4.9
2	N	199	GLY	4.9
2	N	346	ALA	4.9
2	M	388	PRO	4.9
2	I	247	CYS	4.9
2	L	299	PHE	4.8
2	N	333	GLU	4.8
2	L	156	LEU	4.8
1	E	127	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
2	I	221	GLU	4.8
2	L	275	PRO	4.8
2	N	223	LEU	4.8
2	O	208	PRO	4.7
2	P	299	PHE	4.7
2	O	319	GLY	4.7
2	I	198	CYS	4.7
2	L	273	GLY	4.7
2	P	95	ASP	4.7
2	P	158	PRO	4.6
2	I	317	SER	4.6
2	I	267	SER	4.6
2	L	266	LEU	4.6
2	O	218	GLN	4.6
2	I	242	PHE	4.6
2	P	154	GLY	4.5
2	P	150	ASN	4.5
2	P	207	VAL	4.5
2	M	213	ASN	4.5
1	F	433	ASP	4.5
2	L	296	TRP	4.5
2	I	264	PHE	4.5
2	O	277	THR	4.5
2	I	219	GLY	4.5
2	M	280	CYS	4.5
2	I	293	THR	4.4
2	N	159	MET	4.4
2	N	279	SER	4.4
2	P	266	LEU	4.4
2	O	211	PHE	4.4
2	P	385	ALA	4.4
2	L	342	SER	4.4
2	I	311	SER	4.4
2	N	421	SER	4.4
2	O	276	GLY	4.4
2	P	263	GLY	4.4
2	I	230	MET	4.3
2	P	391	MET	4.3
2	L	159	MET	4.3
2	M	282	ILE	4.3
2	P	317	SER	4.3
1	G	122	CYS	4.3

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Mol	Chain	Res	Type	RSRZ
2	M	261	VAL	4.2
2	L	262	TYR	4.2
2	M	216	GLY	4.2
2	M	155	LEU	4.2
1	D	93	GLN	4.2
2	I	275	PRO	4.2
2	M	209	GLU	4.2
2	L	132	ALA	4.1
2	M	210	LEU	4.1
2	I	296	TRP	4.1
2	N	160	LYS	4.1
2	N	342	SER	4.1
2	M	297	VAL	4.1
2	I	151	GLY	4.1
2	L	347	VAL	4.1
2	N	261	VAL	4.1
2	I	213	ASN	4.1
2	O	217	ARG	4.1
2	I	387	SER	4.1
2	N	205	GLY	4.1
2	O	209	GLU	4.1
2	P	297	VAL	4.0
2	M	295	SER	4.0
2	M	271	GLN	4.0
2	I	306	THR	4.0
2	P	338	PRO	4.0
2	N	222	ARG	4.0
2	N	221	GLU	4.0
2	P	359	ALA	4.0
2	L	244	ASP	4.0
2	I	251	PHE	4.0
2	M	212	ALA	4.0
2	I	284	GLN	3.9
2	L	303	GLN	3.9
2	L	201	GLN	3.9
1	D	377	LEU	3.9
1	F	394	ASN	3.9
2	O	197	GLY	3.9
2	O	321	ALA	3.9
2	I	299	PHE	3.9
2	O	280	CYS	3.9
2	L	265	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
2	I	253	PHE	3.9
2	I	274	THR	3.9
1	G	121	HIS	3.9
2	P	251	PHE	3.9
2	M	158	PRO	3.9
2	L	276	GLY	3.9
1	A	468	HIS	3.9
2	I	295	SER	3.9
2	M	218	GLN	3.9
2	P	234	ARG	3.9
2	O	421	SER	3.8
2	N	198	CYS	3.8
2	P	178	ALA	3.8
1	B	416	PHE	3.8
2	L	154	GLY	3.8
2	N	208	PRO	3.8
2	P	219	GLY	3.8
2	P	293	THR	3.8
2	I	289	PHE	3.8
2	L	196	LEU	3.8
1	D	109	ASP	3.8
2	N	296	TRP	3.8
2	I	319	GLY	3.7
2	L	253	PHE	3.7
2	M	303	GLN	3.7
2	N	161	LYS	3.7
1	G	464	GLN	3.7
2	L	213	ASN	3.7
1	A	72	SER	3.7
1	F	73	LEU	3.7
2	M	320	ARG	3.7
2	K	284	GLN	3.7
2	P	25	VAL	3.7
2	O	206	ARG	3.7
1	D	122	CYS	3.7
2	O	219	GLY	3.7
2	J	236	SER	3.7
2	I	159	MET	3.7
2	I	333	GLU	3.7
2	L	209	GLU	3.7
2	P	275	PRO	3.6
2	P	333	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
2	L	217	ARG	3.6
2	L	322	GLU	3.6
2	P	152	VAL	3.6
2	L	251	PHE	3.6
2	M	262	TYR	3.6
2	N	262	TYR	3.6
2	I	245	ALA	3.6
2	L	401	VAL	3.6
2	N	201	GLN	3.6
2	I	238	GLY	3.6
2	P	253	PHE	3.6
2	M	273	GLY	3.6
2	L	16	ALA	3.5
2	L	207	VAL	3.5
2	N	388	PRO	3.5
2	I	235	GLY	3.5
2	L	210	LEU	3.5
2	M	346	ALA	3.5
2	P	24	LYS	3.5
2	I	156	LEU	3.5
2	I	386	TRP	3.5
2	P	389	VAL	3.5
2	O	267	SER	3.5
1	G	433	ASP	3.5
2	N	184	LEU	3.5
2	M	237	ARG	3.5
2	N	335	LYS	3.5
2	L	158	PRO	3.5
2	M	221	GLU	3.5
2	M	275	PRO	3.5
2	O	273	GLY	3.5
2	P	149	ASN	3.4
2	O	220	LEU	3.4
2	N	210	LEU	3.4
2	L	206	ARG	3.4
1	G	131	LEU	3.4
2	P	269	TYR	3.4
2	O	161	LYS	3.4
2	N	344	LEU	3.4
1	C	468	HIS	3.4
2	M	421	SER	3.4
1	H	80	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	M	299	PHE	3.4
2	I	309	MET	3.4
2	M	289	PHE	3.3
1	C	444	ASP	3.3
2	M	230	MET	3.3
2	L	116	GLU	3.3
2	N	253	PHE	3.3
2	P	318	LEU	3.3
1	H	71	THR	3.3
2	K	234	ARG	3.3
2	L	230	MET	3.3
2	O	198	CYS	3.3
2	I	328	LEU	3.3
2	I	318	LEU	3.3
2	P	195	THR	3.3
2	P	242	PHE	3.3
2	I	152	VAL	3.3
2	I	308	CYS	3.3
2	M	201	GLN	3.3
2	P	206	ARG	3.3
2	P	221	GLU	3.3
2	P	292	SER	3.3
2	O	318	LEU	3.3
2	P	177	VAL	3.3
2	P	160	LYS	3.2
2	P	339	THR	3.2
2	O	186	MET	3.2
2	P	110	MET	3.2
2	N	235	GLY	3.2
2	I	197	GLY	3.2
2	N	219	GLY	3.2
2	O	268	ASN	3.2
2	P	312	GLU	3.2
1	C	72	SER	3.2
1	A	109	ASP	3.2
2	P	272	LEU	3.2
2	I	332	ALA	3.2
2	M	281	PHE	3.2
1	D	416	PHE	3.2
2	O	201	GLN	3.2
1	E	121	HIS	3.2
2	L	247	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	P	81	CYS	3.2
2	I	280	CYS	3.2
2	J	263	GLY	3.1
2	M	116	GLU	3.1
2	P	247	CYS	3.1
2	M	253	PHE	3.1
2	O	222	ARG	3.1
2	J	288	SER	3.1
2	I	261	VAL	3.1
1	G	354	THR	3.1
2	I	211	PHE	3.1
2	O	158	PRO	3.1
2	I	236	SER	3.1
2	P	128	ASP	3.1
2	L	205	GLY	3.1
2	P	218	GLN	3.1
2	I	389	VAL	3.1
2	I	405	SER	3.1
2	I	206	ARG	3.1
2	L	229	VAL	3.1
2	L	321	ALA	3.1
2	P	311	SER	3.1
2	P	405	SER	3.1
2	O	221	GLU	3.1
1	A	105	PRO	3.0
1	D	473	ILE	3.0
2	L	409	GLN	3.0
2	N	209	GLU	3.0
1	B	417	CYS	3.0
2	M	217	ARG	3.0
2	O	293	THR	3.0
2	L	219	GLY	3.0
2	L	345	PRO	3.0
1	H	468	HIS	3.0
2	M	159	MET	3.0
2	O	229	VAL	3.0
2	O	199	GLY	3.0
2	O	212	ALA	3.0
2	L	289	PHE	3.0
2	P	306	THR	3.0
2	N	332	ALA	2.9
2	M	208	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
2	O	195	THR	2.9
2	L	212	ALA	2.9
2	K	272	LEU	2.9
1	E	340	GLU	2.9
2	L	260	HIS	2.9
2	P	294	LYS	2.9
2	N	149	ASN	2.9
2	L	287	THR	2.9
2	O	314	LYS	2.9
2	P	284	GLN	2.9
2	P	420	GLN	2.9
2	M	153	ILE	2.9
2	I	214	ARG	2.9
2	P	179	SER	2.9
2	O	270	HIS	2.9
2	O	289	PHE	2.9
1	B	373	ILE	2.8
2	O	153	ILE	2.8
1	D	142	ILE	2.8
2	O	15	ASP	2.8
1	E	411	ASN	2.8
1	A	487	SER	2.8
2	N	367	PHE	2.8
2	P	307	VAL	2.8
2	M	52	GLU	2.8
2	O	156	LEU	2.8
2	P	356	VAL	2.8
1	H	121	HIS	2.8
2	I	324	GLY	2.8
2	L	268	ASN	2.8
1	E	425	ALA	2.8
2	M	332	ALA	2.8
2	P	395	GLN	2.8
1	E	79	ASN	2.8
1	F	311	ILE	2.8
2	P	278	GLU	2.8
1	H	79	ASN	2.8
2	O	190	ASP	2.8
2	O	248	GLY	2.7
2	I	195	THR	2.7
2	J	318	LEU	2.7
1	D	92	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	462	ILE	2.7
2	M	277	THR	2.7
2	O	373	THR	2.7
1	F	473	ILE	2.7
2	J	272	LEU	2.7
2	L	333	GLU	2.7
2	I	254	ALA	2.7
1	H	85	GLN	2.7
2	P	39	THR	2.7
2	J	4	LYS	2.7
2	M	283	PRO	2.7
2	P	308	CYS	2.7
2	I	326	LEU	2.7
2	P	406	SER	2.7
1	C	71	THR	2.7
2	M	344	LEU	2.7
2	P	217	ARG	2.7
2	I	263	GLY	2.7
2	O	392	MET	2.7
2	O	389	VAL	2.7
2	I	420	GLN	2.7
2	O	185	VAL	2.7
2	P	329	GLY	2.7
2	J	262	TYR	2.6
2	N	196	LEU	2.6
2	O	210	LEU	2.6
1	C	107	ILE	2.6
1	G	269	LEU	2.6
2	L	269	TYR	2.6
2	L	198	CYS	2.6
2	N	331	GLY	2.6
2	O	177	VAL	2.6
1	D	139	LEU	2.6
2	M	215	GLY	2.6
2	N	116	GLU	2.6
1	D	465	LEU	2.6
2	J	284	GLN	2.6
2	L	254	ALA	2.6
2	N	267	SER	2.6
2	L	234	ARG	2.6
2	J	234	ARG	2.6
2	P	337	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	127	ASP	2.6
2	L	222	ARG	2.6
2	N	152	VAL	2.6
2	J	231	LEU	2.6
2	O	207	VAL	2.5
2	O	149	ASN	2.5
2	O	251	PHE	2.5
2	N	185	VAL	2.5
2	L	221	GLU	2.5
2	M	245	ALA	2.5
2	N	334	GLU	2.5
1	A	110	LEU	2.5
2	O	299	PHE	2.5
2	P	74	ALA	2.5
2	I	25	VAL	2.5
2	P	40	LEU	2.5
2	I	125	SER	2.5
1	E	290	VAL	2.5
2	N	347	VAL	2.5
2	P	250	TYR	2.5
2	L	274	THR	2.5
1	G	392	ILE	2.5
1	B	121	HIS	2.5
1	E	327	ALA	2.5
1	G	407	LEU	2.5
2	I	160	LYS	2.5
1	G	435	LEU	2.5
2	P	326	LEU	2.5
2	N	319	GLY	2.5
1	B	461	LYS	2.5
1	E	123	LEU	2.5
1	F	476	LEU	2.5
2	P	235	GLY	2.5
2	I	310	ASP	2.5
2	P	265	GLY	2.5
2	I	406	SER	2.5
2	N	278	GLU	2.5
1	F	269	LEU	2.4
2	O	253	PHE	2.4
2	P	245	ALA	2.4
2	I	145	SER	2.4
1	B	166	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	I	404	VAL	2.4
2	P	274	THR	2.4
2	L	235	GLY	2.4
1	D	417	CYS	2.4
2	O	245	ALA	2.4
2	M	342	SER	2.4
2	L	223	LEU	2.4
2	O	213	ASN	2.4
1	D	136	ALA	2.4
1	G	177	ALA	2.4
2	N	207	VAL	2.4
2	M	382	ASP	2.4
2	O	315	ALA	2.4
1	B	184	ILE	2.4
1	F	436	SER	2.4
2	I	385	ALA	2.4
2	M	278	GLU	2.4
2	N	249	ALA	2.4
2	L	224	LEU	2.4
2	N	156	LEU	2.4
2	P	26	SER	2.4
2	I	255	ILE	2.4
2	O	344	LEU	2.4
1	C	487	SER	2.3
1	D	94	ALA	2.3
1	E	184	ILE	2.3
1	D	248	CYS	2.3
2	I	150	ASN	2.3
2	J	247	CYS	2.3
1	G	449	ILE	2.3
2	M	373	THR	2.3
1	D	279	MET	2.3
2	O	116	GLU	2.3
2	M	14	ALA	2.3
2	N	345	PRO	2.3
2	I	186	MET	2.3
2	I	252	THR	2.3
1	C	111	ILE	2.3
2	P	132	ALA	2.3
2	N	275	PRO	2.3
2	J	230	MET	2.3
1	G	472	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	O	184	LEU	2.3
1	F	485	PHE	2.3
2	J	319	GLY	2.3
2	P	355	SER	2.3
1	G	262	THR	2.3
2	I	316	TYR	2.3
2	L	6	ILE	2.3
2	O	16	ALA	2.3
2	P	347	VAL	2.3
2	J	421	SER	2.3
2	O	320	ARG	2.3
2	I	391	MET	2.3
1	G	476	LEU	2.3
2	I	336	SER	2.3
1	D	345	GLU	2.3
2	M	15	ASP	2.3
1	B	122	CYS	2.3
2	I	178	ALA	2.3
2	P	411	THR	2.3
2	K	406	SER	2.3
2	L	141	PHE	2.3
2	M	207	VAL	2.3
2	N	289	PHE	2.3
2	P	116	GLU	2.2
1	H	122	CYS	2.2
2	K	53	ASN	2.2
2	N	340	LEU	2.2
2	O	275	PRO	2.2
2	J	299	PHE	2.2
1	D	89	LEU	2.2
2	L	271	GLN	2.2
2	P	75	GLY	2.2
2	P	238	GLY	2.2
1	G	487	SER	2.2
2	N	220	LEU	2.2
2	O	242	PHE	2.2
2	N	229	VAL	2.2
2	L	126	ALA	2.2
2	P	376	GLN	2.2
2	P	125	SER	2.2
1	G	308	VAL	2.2
1	G	481	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	P	288	SER	2.2
2	L	152	VAL	2.2
2	L	389	VAL	2.2
2	M	321	ALA	2.2
2	N	200	GLU	2.2
2	J	44	ASP	2.2
2	I	232	LYS	2.2
2	I	321	ALA	2.2
2	N	16	ALA	2.2
2	N	178	ALA	2.2
1	B	420	LEU	2.2
2	K	339	THR	2.2
1	D	230	HIS	2.2
2	O	279	SER	2.2
1	B	80	ALA	2.2
1	D	106	PRO	2.2
1	G	384	THR	2.2
2	O	230	MET	2.2
2	O	401	VAL	2.2
1	B	100	SER	2.2
1	G	72	SER	2.2
1	E	444	ASP	2.2
1	G	124	GLU	2.2
2	I	207	VAL	2.2
2	P	153	ILE	2.2
2	M	206	ARG	2.2
1	C	133	PHE	2.2
2	N	251	PHE	2.2
2	O	6	ILE	2.2
2	P	33	GLU	2.2
2	P	252	THR	2.2
2	P	236	SER	2.1
1	F	228	CYS	2.1
2	P	310	ASP	2.1
2	L	320	ARG	2.1
2	M	294	LYS	2.1
2	O	294	LYS	2.1
2	P	336	SER	2.1
1	F	366	ASP	2.1
2	K	210	LEU	2.1
2	P	401	VAL	2.1
2	M	179	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	P	273	GLY	2.1
2	L	184	LEU	2.1
2	I	39	THR	2.1
2	I	339	THR	2.1
1	A	403	GLN	2.1
2	M	302	GLY	2.1
1	C	216	PHE	2.1
1	H	89	LEU	2.1
2	N	325	ARG	2.1
1	H	387	GLU	2.1
1	B	377	LEU	2.1
2	L	379	THR	2.1
1	G	473	ILE	2.1
2	L	15	ASP	2.1
1	G	439	LEU	2.1
1	B	228	CYS	2.1
2	I	237	ARG	2.1
2	N	15	ASP	2.1
1	F	254	THR	2.1
1	B	303	ALA	2.1
2	L	153	ILE	2.1
2	P	148	ASP	2.1
2	L	90	SER	2.1
2	K	281	PHE	2.0
2	P	271	GLN	2.0
2	I	81	CYS	2.0
2	O	5	ARG	2.0
2	K	351	ALA	2.0
2	M	195	THR	2.0
2	I	75	GLY	2.0
2	M	214	ARG	2.0
1	D	115	ILE	2.0
1	F	334	LEU	2.0
2	J	377	LEU	2.0
2	N	242	PHE	2.0
1	C	402	ASP	2.0
1	D	267	SER	2.0
2	L	304	HIS	2.0
2	M	260	HIS	2.0
2	O	145	SER	2.0
1	G	311	ILE	2.0
2	O	196	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	394	ASN	2.0
1	D	83	ASP	2.0
2	I	233	SER	2.0
2	L	279	SER	2.0
2	O	269	TYR	2.0
1	E	473	ILE	2.0
1	G	334	LEU	2.0
2	M	197	GLY	2.0
1	G	485	PHE	2.0
1	D	219	ASN	2.0
1	C	78	GLN	2.0
2	O	160	LYS	2.0
2	L	12	PRO	2.0
1	H	290	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.