



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 04:43 PM JST

PDB ID : 5XJX  
Title : Pre-formed plant receptor ERL1-TMM complex  
Authors : Chai, J.; Lin, G.; Zhang, L.; Han, Z.; Yang, X.; Liu, W.; Qi, Y.; Chang, J.;  
Li, E.  
Deposited on : 2017-05-04  
Resolution : 3.06 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

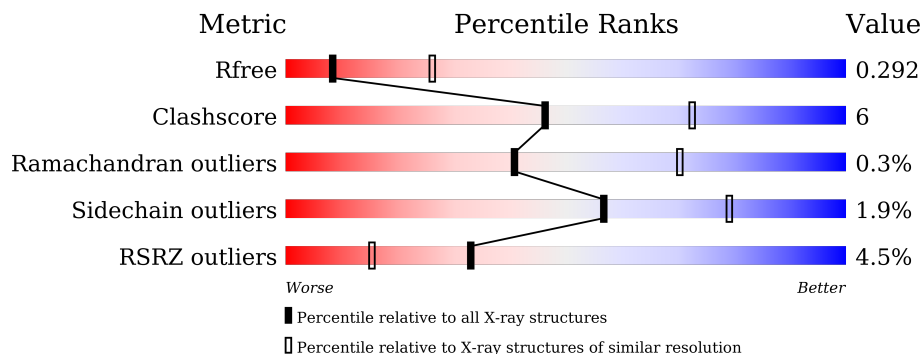
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.06 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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

Mol	Chain	Length	Quality of chain
1	C	433	 % 69% 15% 16%
1	D	433	 2% 70% 14% 16%
1	F	433	 2% 67% 17% 16%
1	H	433	 % 69% 15% 16%
1	J	433	 % 71% 13% 16%
1	L	433	 5% 68% 15% 16%

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Mol	Chain	Length	Quality of chain
2	A	556	
2	B	556	
2	E	556	
2	G	556	
2	I	556	
2	K	556	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 41970 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 Protein TOO MANY MOUTHS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	365	2840	1792	513	524	11	0	0	0
1	F	365	2840	1792	513	524	11	0	0	0
1	D	365	2840	1792	513	524	11	0	0	0
1	L	365	2840	1792	513	524	11	0	0	0
1	H	365	2840	1792	513	524	11	0	0	0
1	J	365	2840	1792	513	524	11	0	0	0

- Molecule 2 is a protein called LRR receptor-like serine/threonine-protein kinase ERL1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	K	544	4155	2641	705	791	18	0	0	0
2	G	544	4155	2641	705	791	18	0	0	0
2	A	544	4155	2641	705	791	18	0	0	0
2	I	544	4155	2641	705	791	18	0	0	0
2	B	544	4155	2641	705	791	18	0	0	0
2	E	544	4155	2641	705	791	18	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	574	HIS	-	expression tag	UNP C0L6W6

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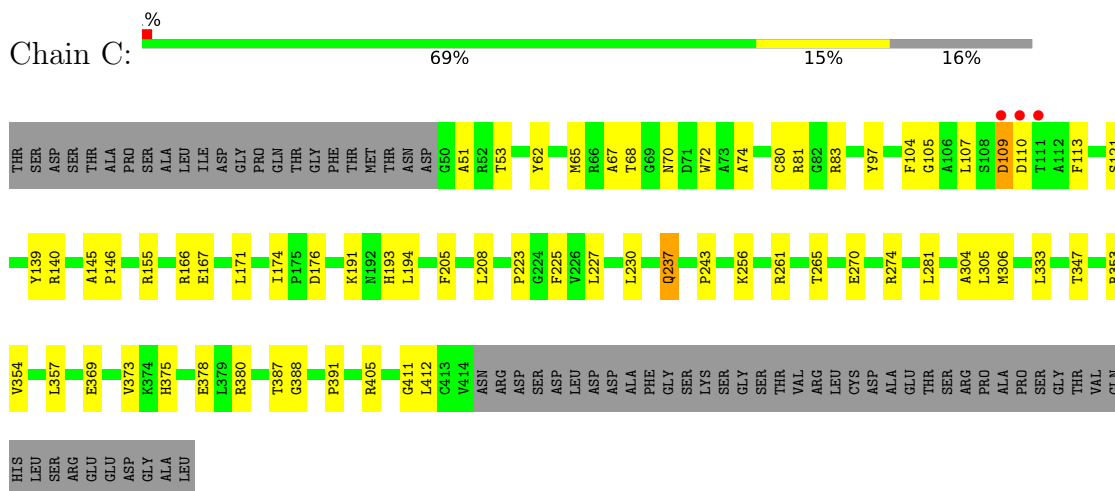
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Chain	Residue	Modelled	Actual	Comment	Reference
K	575	HIS	-	expression tag	UNP C0LGW6
K	576	HIS	-	expression tag	UNP C0LGW6
K	577	HIS	-	expression tag	UNP C0LGW6
K	578	HIS	-	expression tag	UNP C0LGW6
K	579	HIS	-	expression tag	UNP C0LGW6
G	574	HIS	-	expression tag	UNP C0LGW6
G	575	HIS	-	expression tag	UNP C0LGW6
G	576	HIS	-	expression tag	UNP C0LGW6
G	577	HIS	-	expression tag	UNP C0LGW6
G	578	HIS	-	expression tag	UNP C0LGW6
G	579	HIS	-	expression tag	UNP C0LGW6
A	574	HIS	-	expression tag	UNP C0LGW6
A	575	HIS	-	expression tag	UNP C0LGW6
A	576	HIS	-	expression tag	UNP C0LGW6
A	577	HIS	-	expression tag	UNP C0LGW6
A	578	HIS	-	expression tag	UNP C0LGW6
A	579	HIS	-	expression tag	UNP C0LGW6
I	574	HIS	-	expression tag	UNP C0LGW6
I	575	HIS	-	expression tag	UNP C0LGW6
I	576	HIS	-	expression tag	UNP C0LGW6
I	577	HIS	-	expression tag	UNP C0LGW6
I	578	HIS	-	expression tag	UNP C0LGW6
I	579	HIS	-	expression tag	UNP C0LGW6
B	574	HIS	-	expression tag	UNP C0LGW6
B	575	HIS	-	expression tag	UNP C0LGW6
B	576	HIS	-	expression tag	UNP C0LGW6
B	577	HIS	-	expression tag	UNP C0LGW6
B	578	HIS	-	expression tag	UNP C0LGW6
B	579	HIS	-	expression tag	UNP C0LGW6
E	574	HIS	-	expression tag	UNP C0LGW6
E	575	HIS	-	expression tag	UNP C0LGW6
E	576	HIS	-	expression tag	UNP C0LGW6
E	577	HIS	-	expression tag	UNP C0LGW6
E	578	HIS	-	expression tag	UNP C0LGW6
E	579	HIS	-	expression tag	UNP C0LGW6

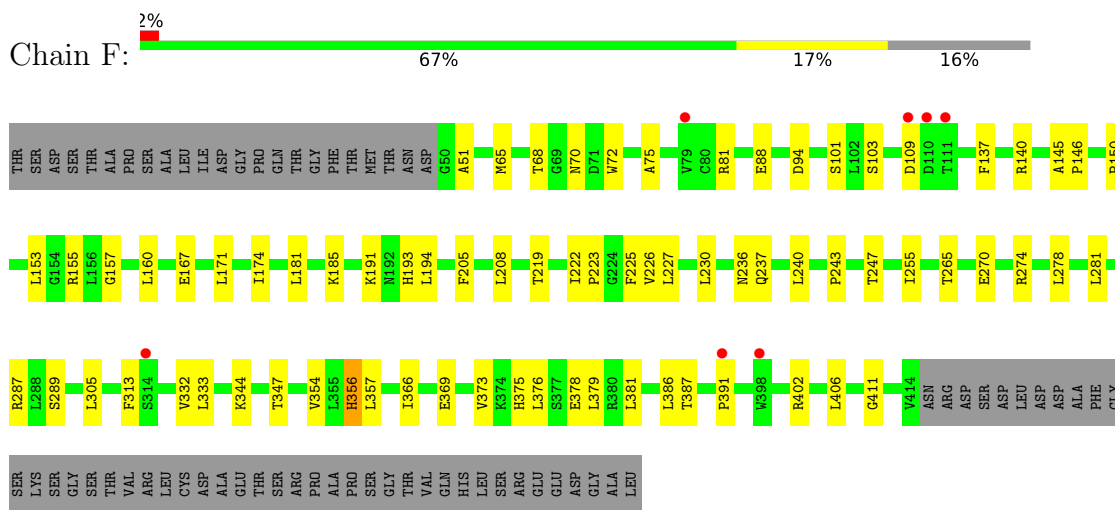
### 3 Residue-property plots [i](#)

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

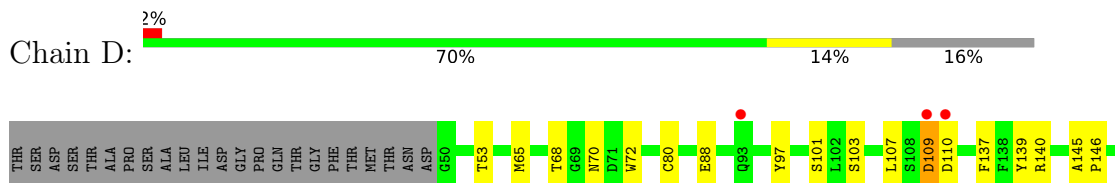
#### • Molecule 1: Protein TOO MANY MOUTHS

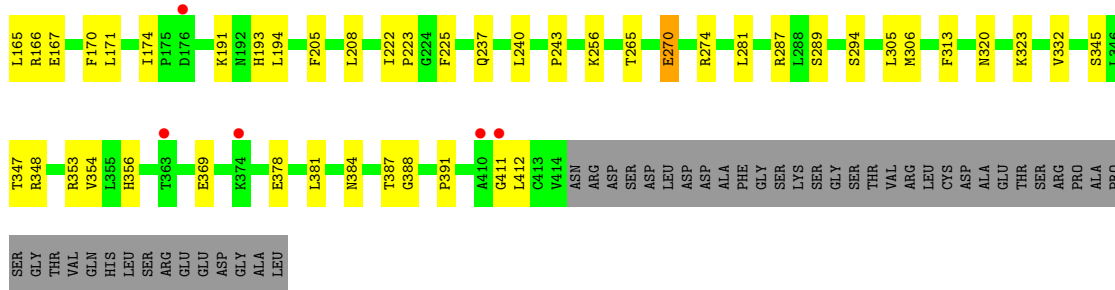


#### • Molecule 1: Protein TOO MANY MOUTHS

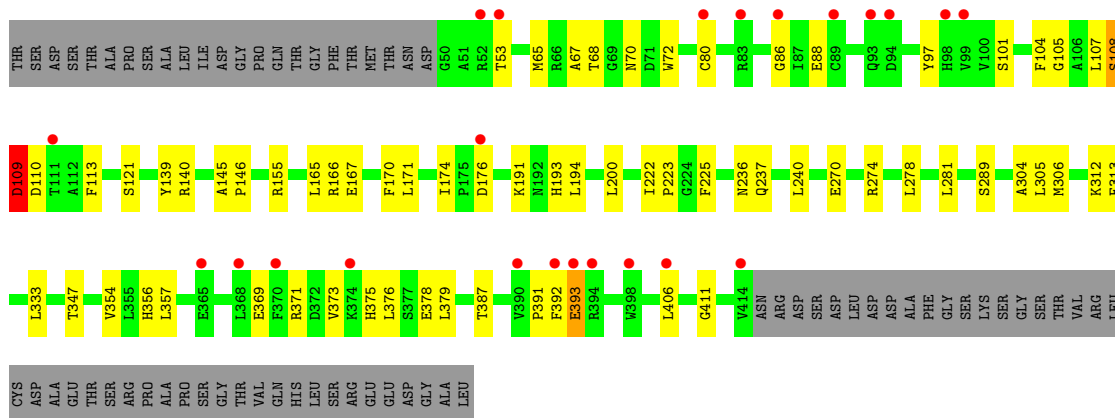


#### • Molecule 1: Protein TOO MANY MOUTHS

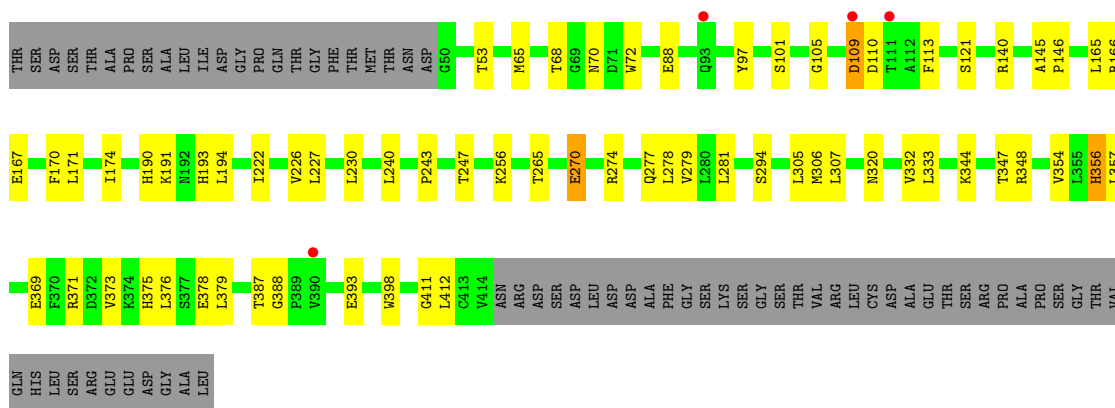




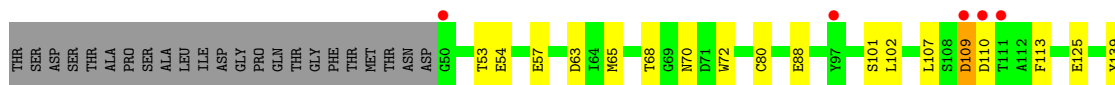
● Molecule 1: Protein TOO MANY MOUTHS

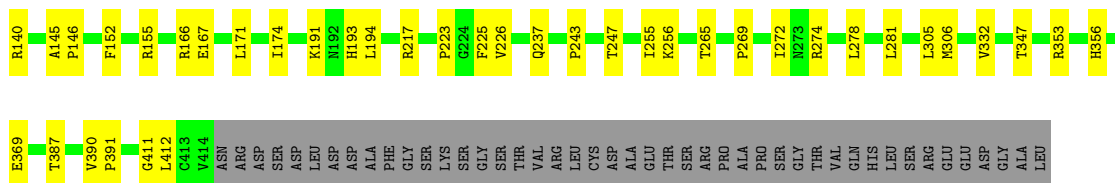


● Molecule 1: Protein TOO MANY MOUTHS

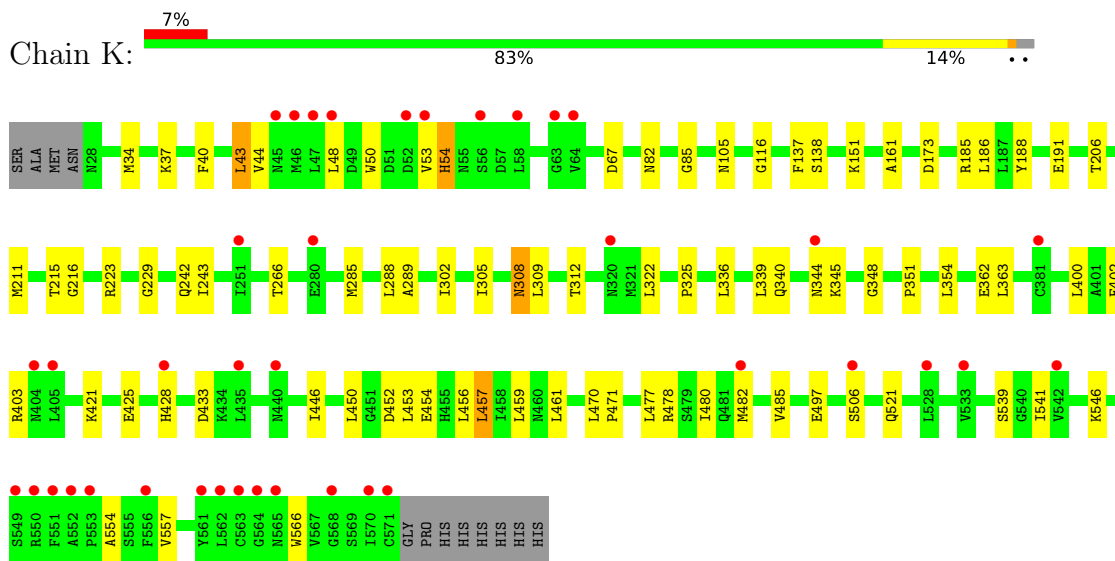


● Molecule 1: Protein TOO MANY MOUTHS

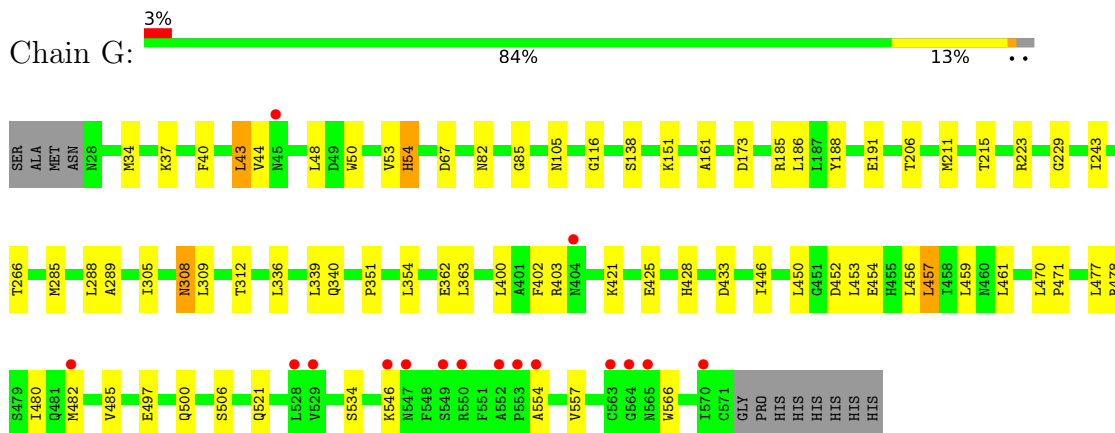




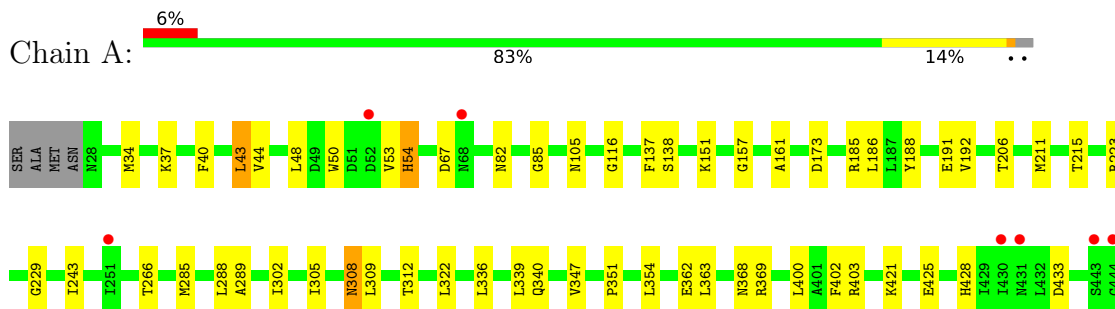
• Molecule 2: LRR receptor-like serine/threonine-protein kinase ERL1



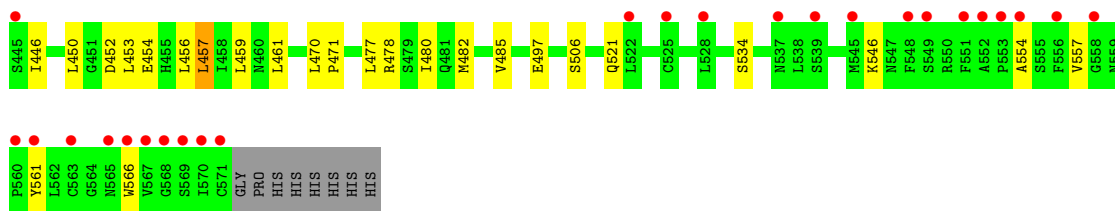
• Molecule 2: LRR receptor-like serine/threonine-protein kinase ERL1



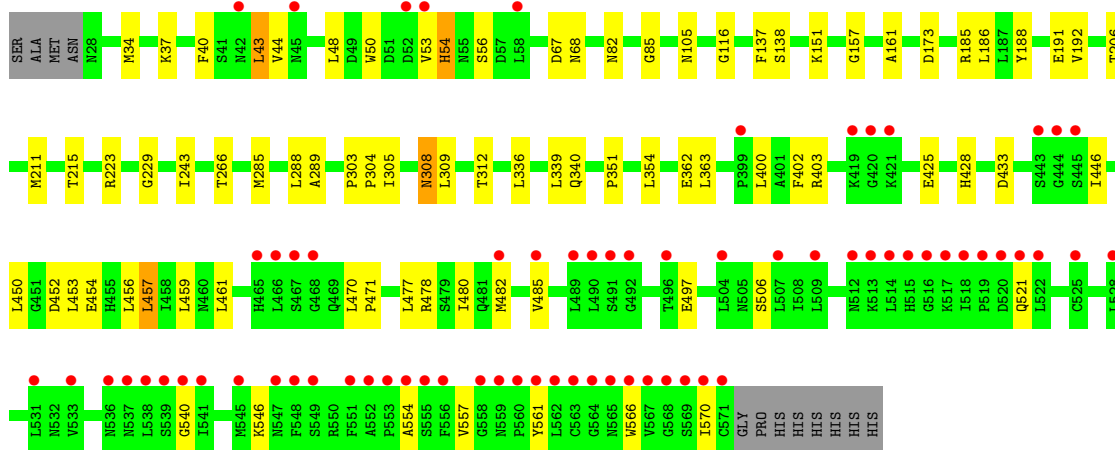
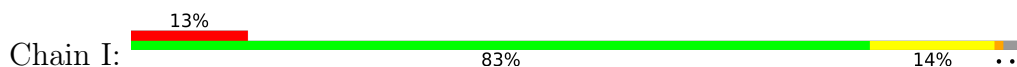
• Molecule 2: LRR receptor-like serine/threonine-protein kinase ERL1



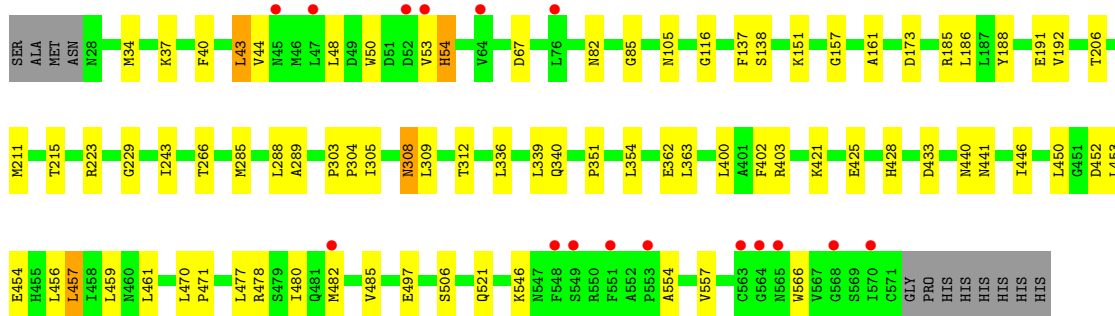
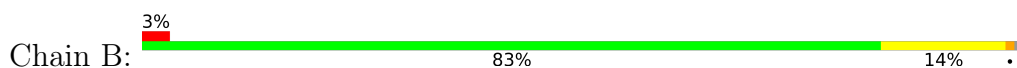




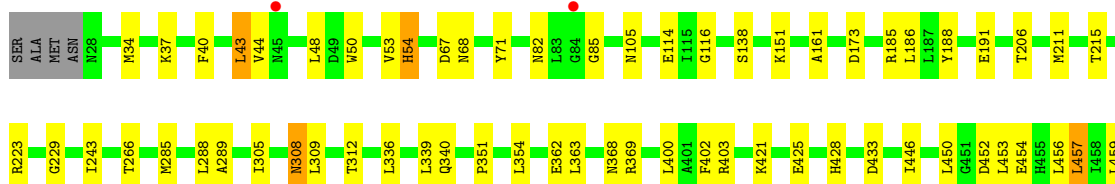
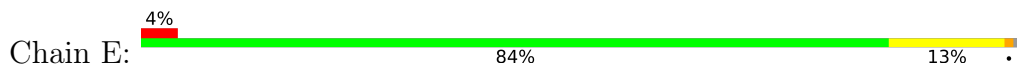
● Molecule 2: LRR receptor-like serine/threonine-protein kinase ERL1

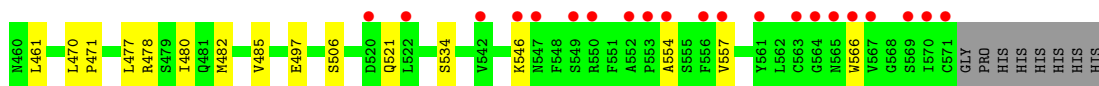


● Molecule 2: LRR receptor-like serine/threonine-protein kinase ERL1



● Molecule 2: LRR receptor-like serine/threonine-protein kinase ERL1





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.17Å 114.39Å 191.95Å 89.57° 90.46° 59.86°	Depositor
Resolution (Å)	43.25 – 3.06 49.87 – 3.06	Depositor EDS
% Data completeness (in resolution range)	97.6 (43.25-3.06) 97.6 (49.87-3.06)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.59 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.254 , 0.276 0.279 , 0.292	Depositor DCC
$R_{free}$ test set	7889 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.8	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 14.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,-h+k,l 0.000 for h-k,h,l 0.011 for -h+k,-h,l 0.011 for -k,h-k,l 0.087 for -h+k,k,-l 0.016 for -k,-h,-l 0.002 for -h,-k,l 0.002 for -h,-h+k,-l 0.031 for h,h-k,-l 0.000 for h-k,-k,-l 0.001 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	41970	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	C	0.27	0/2896	0.50	0/3933
1	D	0.26	0/2896	0.50	0/3933
1	F	0.26	0/2896	0.50	0/3933
1	H	0.31	0/2896	0.52	0/3933
1	J	0.26	0/2896	0.50	0/3933
1	L	0.34	0/2896	0.54	2/3933 (0.1%)
2	A	0.27	0/4231	0.51	0/5758
2	B	0.27	0/4231	0.51	0/5758
2	E	0.27	0/4231	0.51	0/5758
2	G	0.27	0/4231	0.51	0/5758
2	I	0.27	0/4231	0.51	0/5758
2	K	0.27	0/4231	0.51	0/5758
All	All	0.28	0/42762	0.51	2/58146 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	108	SER	C-N-CA	5.12	134.49	121.70
1	L	109	ASP	N-CA-CB	5.04	119.68	110.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	C	2840	0	2889	39	3
1	D	2840	0	2889	43	0
1	F	2840	0	2889	46	0
1	H	2840	0	2889	43	0
1	J	2840	0	2889	38	1
1	L	2840	0	2889	44	0
2	A	4155	0	4195	56	1
2	B	4155	0	4195	52	0
2	E	4155	0	4195	53	0
2	G	4155	0	4195	51	0
2	I	4155	0	4195	52	3
2	K	4155	0	4195	58	0
All	All	41970	0	42504	534	4

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 6.

All (534) 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)
2:K:242:GLN:HG3	1:L:110:ASP:OD2	1.21	1.29
2:K:242:GLN:CG	1:L:110:ASP:OD2	2.12	0.98
2:G:454:GLU:OE1	2:G:478:ARG:NH1	1.97	0.97
2:A:454:GLU:OE1	2:A:478:ARG:NH1	1.97	0.97
2:I:454:GLU:OE1	2:I:478:ARG:NH1	1.97	0.97
2:E:454:GLU:OE1	2:E:478:ARG:NH1	1.97	0.97
2:K:454:GLU:OE1	2:K:478:ARG:NH1	1.97	0.96
2:B:454:GLU:OE1	2:B:478:ARG:NH1	1.97	0.96
2:G:340:GLN:NE2	2:G:362:GLU:OE2	2.03	0.92
2:K:340:GLN:NE2	2:K:362:GLU:OE2	2.03	0.92
2:B:340:GLN:NE2	2:B:362:GLU:OE2	2.03	0.92
2:I:340:GLN:NE2	2:I:362:GLU:OE2	2.03	0.91
2:E:340:GLN:NE2	2:E:362:GLU:OE2	2.03	0.90
2:A:340:GLN:NE2	2:A:362:GLU:OE2	2.03	0.90
1:J:70:ASN:HD22	1:J:72:TRP:HE1	1.21	0.88
1:L:68:THR:HG21	1:L:104:PHE:HE1	1.39	0.87
1:L:68:THR:HG21	1:L:104:PHE:CE1	2.11	0.85
2:K:400:LEU:HD22	1:J:125:GLU:HB3	1.59	0.84
1:C:70:ASN:HD22	1:C:72:TRP:HE1	1.23	0.84
1:D:70:ASN:HD22	1:D:72:TRP:HE1	1.27	0.82
2:E:116:GLY:HA3	2:E:138:SER:HB2	1.62	0.82
2:K:116:GLY:HA3	2:K:138:SER:HB2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:116:GLY:HA3	2:G:138:SER:HB2	1.62	0.82
2:B:116:GLY:HA3	2:B:138:SER:HB2	1.62	0.81
2:A:116:GLY:HA3	2:A:138:SER:HB2	1.62	0.81
2:I:482:MET:HG2	2:I:506:SER:HB2	1.63	0.81
2:B:482:MET:HG2	2:B:506:SER:HB2	1.63	0.81
2:I:116:GLY:HA3	2:I:138:SER:HB2	1.62	0.81
2:E:482:MET:HG2	2:E:506:SER:HB2	1.63	0.80
2:G:482:MET:HG2	2:G:506:SER:HB2	1.63	0.80
2:K:482:MET:HG2	2:K:506:SER:HB2	1.63	0.80
1:H:145:ALA:HB1	1:H:146:PRO:HD2	1.65	0.79
1:F:145:ALA:HB1	1:F:146:PRO:HD2	1.66	0.78
2:A:482:MET:HG2	2:A:506:SER:HB2	1.63	0.78
2:G:433:ASP:HB2	2:G:457:LEU:HD22	1.66	0.77
2:A:433:ASP:HB2	2:A:457:LEU:HD22	1.67	0.77
2:E:433:ASP:HB2	2:E:457:LEU:HD22	1.67	0.77
2:I:433:ASP:HB2	2:I:457:LEU:HD22	1.67	0.77
2:B:433:ASP:HB2	2:B:457:LEU:HD22	1.67	0.77
2:K:433:ASP:HB2	2:K:457:LEU:HD22	1.66	0.77
2:I:351:PRO:HG2	2:I:354:LEU:HD13	1.68	0.76
2:B:351:PRO:HG2	2:B:354:LEU:HD13	1.68	0.76
2:E:351:PRO:HG2	2:E:354:LEU:HD13	1.68	0.76
2:K:351:PRO:HG2	2:K:354:LEU:HD13	1.68	0.76
1:J:145:ALA:HB1	1:J:146:PRO:HD2	1.68	0.75
2:A:351:PRO:HG2	2:A:354:LEU:HD13	1.68	0.75
2:K:325:PRO:HB3	1:D:320:ASN:OD1	1.86	0.75
2:G:351:PRO:HG2	2:G:354:LEU:HD13	1.68	0.75
1:C:145:ALA:HB1	1:C:146:PRO:HD2	1.68	0.75
2:K:497:GLU:OE2	2:K:497:GLU:N	2.20	0.75
2:A:497:GLU:OE2	2:A:497:GLU:N	2.20	0.74
2:B:497:GLU:N	2:B:497:GLU:OE2	2.20	0.74
2:I:497:GLU:N	2:I:497:GLU:OE2	2.20	0.74
2:E:497:GLU:N	2:E:497:GLU:OE2	2.20	0.73
1:J:387:THR:HA	1:J:411:GLY:HA3	1.70	0.73
1:L:70:ASN:HD22	1:L:72:TRP:HE1	1.35	0.72
1:L:145:ALA:HB1	1:L:146:PRO:HD2	1.71	0.71
2:G:497:GLU:N	2:G:497:GLU:OE2	2.20	0.71
1:D:145:ALA:HB1	1:D:146:PRO:HD2	1.71	0.71
1:C:387:THR:HA	1:C:411:GLY:HA3	1.73	0.70
1:F:70:ASN:HD22	1:F:72:TRP:HE1	1.40	0.69
1:H:70:ASN:HD22	1:H:72:TRP:HE1	1.39	0.69
1:H:320:ASN:ND2	2:A:347:VAL:HG23	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:GLU:OE2	1:D:294:SER:OG	2.11	0.68
1:D:387:THR:HA	1:D:411:GLY:HA3	1.76	0.67
1:F:387:THR:HA	1:F:411:GLY:HA3	1.77	0.66
2:G:206:THR:HG23	2:G:229:GLY:HA3	1.79	0.65
2:K:541:ILE:HG23	1:F:75:ALA:HB1	1.79	0.65
2:G:500:GLN:NE2	2:E:521:GLN:HE21	1.94	0.65
2:A:206:THR:HG23	2:A:229:GLY:HA3	1.79	0.65
2:K:206:THR:HG23	2:K:229:GLY:HA3	1.79	0.64
2:E:206:THR:HG23	2:E:229:GLY:HA3	1.79	0.64
2:I:206:THR:HG23	2:I:229:GLY:HA3	1.79	0.63
2:B:206:THR:HG23	2:B:229:GLY:HA3	1.79	0.63
1:H:387:THR:HA	1:H:411:GLY:HA3	1.79	0.63
1:D:171:LEU:HD23	1:D:193:HIS:HB2	1.79	0.62
1:L:387:THR:HA	1:L:411:GLY:HA3	1.82	0.60
1:C:274:ARG:HG2	1:C:274:ARG:HH11	1.67	0.60
2:B:305:ILE:O	2:B:308:ASN:ND2	2.36	0.59
1:F:174:ILE:HG12	1:F:194:LEU:HD13	1.85	0.59
2:K:305:ILE:O	2:K:308:ASN:ND2	2.36	0.59
1:L:289:SER:HA	1:L:313:PHE:HA	1.85	0.59
2:G:305:ILE:O	2:G:308:ASN:ND2	2.36	0.58
2:A:305:ILE:O	2:A:308:ASN:ND2	2.36	0.58
1:F:332:VAL:HA	1:F:356:HIS:HB2	1.85	0.58
1:C:53:THR:HB	1:C:80:CYS:HB2	1.85	0.58
2:E:305:ILE:O	2:E:308:ASN:ND2	2.36	0.58
1:L:171:LEU:HD23	1:L:193:HIS:HB2	1.85	0.58
1:H:274:ARG:HG2	1:H:274:ARG:HH11	1.69	0.58
2:I:185:ARG:HA	2:I:188:TYR:HD2	1.69	0.57
2:B:185:ARG:HA	2:B:188:TYR:HD2	1.69	0.57
2:K:185:ARG:HA	2:K:188:TYR:HD2	1.69	0.57
1:J:274:ARG:HG2	1:J:274:ARG:HH11	1.68	0.57
2:A:425:GLU:HA	2:A:428:HIS:HD2	1.70	0.57
1:H:226:VAL:HG22	1:H:247:THR:HB	1.85	0.57
2:G:185:ARG:HA	2:G:188:TYR:HD2	1.69	0.57
1:D:347:THR:HG21	1:D:369:GLU:HB3	1.87	0.57
1:H:88:GLU:HB2	1:H:101:SER:HB3	1.86	0.57
1:F:51:ALA:O	1:F:81:ARG:NH1	2.36	0.57
2:A:53:VAL:HG13	2:A:54:HIS:ND1	2.20	0.57
2:A:185:ARG:HA	2:A:188:TYR:HD2	1.69	0.57
1:D:88:GLU:HB2	1:D:101:SER:HB3	1.86	0.56
2:E:185:ARG:HA	2:E:188:TYR:HD2	1.69	0.56
2:G:53:VAL:HG13	2:G:54:HIS:ND1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:LEU:HD23	1:F:193:HIS:HB2	1.87	0.56
1:D:222:ILE:HG12	1:D:240:LEU:HD13	1.87	0.56
1:D:289:SER:HA	1:D:313:PHE:HA	1.87	0.56
1:D:306:MET:HE2	2:B:137:PHE:HE1	1.70	0.56
2:G:425:GLU:HA	2:G:428:HIS:HD2	1.70	0.56
2:E:425:GLU:HA	2:E:428:HIS:HD2	1.70	0.56
2:I:53:VAL:HG13	2:I:54:HIS:ND1	2.20	0.56
1:C:171:LEU:HD23	1:C:193:HIS:HB2	1.86	0.56
2:A:185:ARG:HA	2:A:188:TYR:CD2	2.41	0.56
2:E:185:ARG:HA	2:E:188:TYR:CD2	2.41	0.56
1:D:274:ARG:HG2	1:D:274:ARG:HH11	1.70	0.56
2:B:425:GLU:HA	2:B:428:HIS:HD2	1.70	0.56
2:K:40:PHE:HA	2:K:85:GLY:HA3	1.88	0.56
2:G:40:PHE:HA	2:G:85:GLY:HA3	1.88	0.56
2:I:470:LEU:HD12	2:I:471:PRO:HD2	1.88	0.56
2:B:470:LEU:HD12	2:B:471:PRO:HD2	1.88	0.56
2:K:53:VAL:HG13	2:K:54:HIS:ND1	2.20	0.56
1:F:274:ARG:HG2	1:F:274:ARG:HH11	1.70	0.56
2:G:185:ARG:HA	2:G:188:TYR:CD2	2.41	0.56
2:I:425:GLU:HA	2:I:428:HIS:HD2	1.70	0.56
2:E:40:PHE:HA	2:E:85:GLY:HA3	1.88	0.56
1:D:167:GLU:HG2	1:D:191:LYS:HB3	1.88	0.56
2:A:40:PHE:HA	2:A:85:GLY:HA3	1.88	0.56
2:B:53:VAL:HG13	2:B:54:HIS:ND1	2.20	0.56
2:B:185:ARG:HA	2:B:188:TYR:CD2	2.41	0.56
1:C:167:GLU:HG2	1:C:191:LYS:HB3	1.88	0.55
1:L:200:LEU:HD23	1:L:223:PRO:HB3	1.88	0.55
1:H:174:ILE:HG12	1:H:194:LEU:HD13	1.88	0.55
2:I:185:ARG:HA	2:I:188:TYR:CD2	2.41	0.55
2:B:40:PHE:HA	2:B:85:GLY:HA3	1.88	0.55
2:K:185:ARG:HA	2:K:188:TYR:CD2	2.41	0.55
1:H:347:THR:HG21	1:H:369:GLU:HB3	1.88	0.55
2:E:53:VAL:HG13	2:E:54:HIS:ND1	2.20	0.55
2:K:325:PRO:HG3	1:D:323:LYS:HD2	1.87	0.55
2:K:425:GLU:HA	2:K:428:HIS:HD2	1.70	0.55
2:E:470:LEU:HD12	2:E:471:PRO:HD2	1.88	0.55
1:L:274:ARG:HH11	1:L:274:ARG:HG2	1.71	0.55
2:G:470:LEU:HD12	2:G:471:PRO:HD2	1.88	0.55
2:I:40:PHE:HA	2:I:85:GLY:HA3	1.88	0.55
2:A:470:LEU:HD12	2:A:471:PRO:HD2	1.88	0.55
2:I:305:ILE:O	2:I:308:ASN:ND2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:347:THR:HG21	1:J:369:GLU:HB3	1.89	0.55
2:K:453:LEU:HD12	2:K:456:LEU:HD22	1.89	0.55
2:I:453:LEU:HD12	2:I:456:LEU:HD22	1.89	0.55
2:K:470:LEU:HD12	2:K:471:PRO:HD2	1.88	0.54
2:G:453:LEU:HD12	2:G:456:LEU:HD22	1.89	0.54
2:B:453:LEU:HD12	2:B:456:LEU:HD22	1.89	0.54
1:F:193:HIS:CE1	2:I:68:ASN:O	2.60	0.54
1:H:320:ASN:CG	2:A:347:VAL:HG23	2.28	0.54
2:I:521:GLN:N	2:I:521:GLN:OE1	2.40	0.54
1:C:174:ILE:HG12	1:C:194:LEU:HD13	1.89	0.54
1:F:354:VAL:HG13	1:F:378:GLU:HB2	1.90	0.54
2:A:521:GLN:OE1	2:A:521:GLN:N	2.40	0.54
2:E:453:LEU:HD12	2:E:456:LEU:HD22	1.89	0.54
2:A:453:LEU:HD12	2:A:456:LEU:HD22	1.89	0.54
1:J:174:ILE:HG12	1:J:194:LEU:HD13	1.88	0.54
1:D:174:ILE:HG12	1:D:194:LEU:HD13	1.90	0.53
2:K:137:PHE:HE1	1:L:306:MET:HE2	1.73	0.53
1:H:227:LEU:HD12	1:H:230:LEU:HD22	1.91	0.53
1:J:139:TYR:HD1	1:J:166:ARG:HB3	1.74	0.53
2:G:82:ASN:HA	2:G:105:ASN:HA	1.90	0.53
2:G:433:ASP:HA	2:G:456:LEU:HA	1.90	0.53
2:A:433:ASP:HA	2:A:456:LEU:HA	1.90	0.53
2:E:521:GLN:OE1	2:E:521:GLN:N	2.40	0.53
2:A:82:ASN:HA	2:A:105:ASN:HA	1.91	0.53
1:C:227:LEU:HD12	1:C:230:LEU:HD22	1.90	0.53
1:F:167:GLU:HG2	1:F:191:LYS:HB3	1.90	0.53
1:H:171:LEU:HD23	1:H:193:HIS:HB2	1.90	0.52
1:L:53:THR:HB	1:L:80:CYS:HB2	1.91	0.52
1:L:166:ARG:HG2	1:L:167:GLU:HG3	1.91	0.52
2:I:433:ASP:HA	2:I:456:LEU:HA	1.90	0.52
1:C:65:MET:O	1:C:68:THR:HG22	2.10	0.52
1:H:167:GLU:HG2	1:H:191:LYS:HB3	1.89	0.52
1:C:70:ASN:HB3	1:C:72:TRP:NE1	2.25	0.52
1:H:270:GLU:OE2	1:H:294:SER:OG	2.16	0.52
1:H:320:ASN:CG	2:A:347:VAL:CG2	2.78	0.52
1:C:347:THR:HG21	1:C:369:GLU:HB3	1.92	0.52
1:L:88:GLU:HB2	1:L:101:SER:HB3	1.92	0.52
2:B:82:ASN:HA	2:B:105:ASN:HA	1.90	0.52
2:I:82:ASN:HA	2:I:105:ASN:HA	1.90	0.52
1:F:402:ARG:NH1	2:E:114:GLU:OE2	2.37	0.52
1:C:353:ARG:NH2	2:A:157:GLY:HA2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:289:ALA:HA	2:I:312:THR:HA	1.93	0.51
1:D:139:TYR:HD1	1:D:166:ARG:HB3	1.75	0.51
2:B:433:ASP:HA	2:B:456:LEU:HA	1.90	0.51
2:E:289:ALA:HA	2:E:312:THR:HA	1.93	0.51
2:K:433:ASP:HA	2:K:456:LEU:HA	1.90	0.51
2:A:289:ALA:HA	2:A:312:THR:HA	1.93	0.51
2:K:82:ASN:HA	2:K:105:ASN:HA	1.91	0.51
2:B:289:ALA:HA	2:B:312:THR:HA	1.93	0.51
2:E:433:ASP:HA	2:E:456:LEU:HA	1.90	0.51
1:C:146:PRO:HB3	1:C:171:LEU:HD12	1.92	0.51
1:J:171:LEU:HD23	1:J:193:HIS:HB2	1.92	0.51
1:H:222:ILE:HG12	1:H:240:LEU:HD13	1.93	0.51
2:E:82:ASN:HA	2:E:105:ASN:HA	1.90	0.51
2:K:289:ALA:HA	2:K:312:THR:HA	1.93	0.51
2:G:289:ALA:HA	2:G:312:THR:HA	1.93	0.51
2:K:428:HIS:NE2	1:J:63:ASP:OD1	2.44	0.51
1:D:306:MET:HE2	2:B:137:PHE:CE1	2.45	0.51
1:L:174:ILE:HG12	1:L:194:LEU:HD13	1.92	0.51
1:J:353:ARG:NH2	2:I:157:GLY:HA2	2.26	0.51
2:K:521:GLN:OE1	2:K:521:GLN:N	2.40	0.50
1:F:146:PRO:HB3	1:F:171:LEU:HD12	1.93	0.50
2:G:500:GLN:HE22	2:E:521:GLN:NE2	2.10	0.50
1:F:255:ILE:HA	1:F:278:LEU:HA	1.93	0.50
1:F:347:THR:HG21	1:F:369:GLU:HB3	1.94	0.50
1:D:107:LEU:HD21	2:B:192:VAL:HA	1.93	0.50
2:K:188:TYR:CD1	2:K:211:MET:HA	2.47	0.50
1:H:256:LYS:HB2	2:G:186:LEU:HD11	1.94	0.50
2:G:521:GLN:OE1	2:G:521:GLN:N	2.40	0.50
2:K:539:SER:HB2	1:F:72:TRP:HB3	1.94	0.50
1:F:88:GLU:HB2	1:F:101:SER:HB3	1.93	0.50
2:E:188:TYR:CD1	2:E:211:MET:HA	2.47	0.50
1:L:165:LEU:HB3	1:L:170:PHE:HE2	1.77	0.49
1:J:88:GLU:HB2	1:J:101:SER:HB3	1.93	0.49
1:J:65:MET:O	1:J:68:THR:HG22	2.12	0.49
2:A:188:TYR:CD1	2:A:211:MET:HA	2.47	0.49
1:H:281:LEU:HD23	1:H:305:LEU:HD13	1.95	0.49
2:G:188:TYR:CD1	2:G:211:MET:HA	2.47	0.49
2:I:188:TYR:CD1	2:I:211:MET:HA	2.47	0.49
1:F:205:PHE:HB3	1:F:208:LEU:HB2	1.95	0.49
1:L:347:THR:HG21	1:L:369:GLU:HB3	1.95	0.49
2:B:188:TYR:CD1	2:B:211:MET:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:281:LEU:HD23	1:J:305:LEU:HD13	1.95	0.49
2:G:477:LEU:HB3	2:G:480:ILE:HB	1.95	0.48
1:C:281:LEU:HD23	1:C:305:LEU:HD13	1.95	0.48
1:J:369:GLU:OE1	1:J:369:GLU:N	2.43	0.48
2:A:477:LEU:HB3	2:A:480:ILE:HB	1.95	0.48
2:B:477:LEU:HB3	2:B:480:ILE:HB	1.95	0.48
2:E:477:LEU:HB3	2:E:480:ILE:HB	1.95	0.48
1:C:369:GLU:OE1	1:C:369:GLU:N	2.41	0.48
1:F:222:ILE:HG12	1:F:240:LEU:HD13	1.95	0.48
2:A:34:MET:HE1	2:A:37:LYS:HD3	1.94	0.48
2:I:477:LEU:HB3	2:I:480:ILE:HB	1.95	0.48
1:C:304:ALA:HB1	1:C:306:MET:HE1	1.95	0.48
2:K:216:GLY:O	1:L:109:ASP:OD1	2.32	0.48
1:L:65:MET:O	1:L:68:THR:HG22	2.14	0.48
1:J:306:MET:HE2	2:I:137:PHE:HE1	1.79	0.48
1:D:146:PRO:HB3	1:D:171:LEU:HD12	1.94	0.48
2:G:500:GLN:NE2	2:E:521:GLN:NE2	2.61	0.48
1:C:140:ARG:HA	1:C:167:GLU:O	2.14	0.48
2:B:34:MET:HE3	2:B:50:TRP:HB3	1.95	0.48
1:L:140:ARG:HA	1:L:167:GLU:O	2.14	0.48
1:L:167:GLU:HG2	1:L:191:LYS:HB3	1.94	0.48
1:J:226:VAL:HG22	1:J:247:THR:HB	1.95	0.48
2:K:477:LEU:HB3	2:K:480:ILE:HB	1.95	0.48
1:F:376:LEU:HD23	1:F:379:LEU:HB2	1.95	0.48
1:H:369:GLU:OE1	1:H:369:GLU:N	2.44	0.48
1:H:371:ARG:HG3	1:H:393:GLU:HG3	1.96	0.48
2:B:521:GLN:OE1	2:B:521:GLN:N	2.40	0.48
1:F:157:GLY:HA2	1:F:181:LEU:HD23	1.96	0.47
2:K:461:LEU:HB2	2:K:485:VAL:HG12	1.96	0.47
1:F:65:MET:O	1:F:68:THR:HG22	2.14	0.47
1:H:146:PRO:HB3	1:H:171:LEU:HD12	1.96	0.47
2:K:191:GLU:HA	2:K:215:THR:HG22	1.97	0.47
1:D:65:MET:O	1:D:68:THR:HG22	2.15	0.47
1:D:332:VAL:HA	1:D:356:HIS:HB2	1.96	0.47
1:H:243:PRO:HA	1:H:265:THR:O	2.14	0.47
1:J:146:PRO:HB3	1:J:171:LEU:HD12	1.96	0.47
2:E:461:LEU:HB2	2:E:485:VAL:HG12	1.96	0.47
2:E:191:GLU:HA	2:E:215:THR:HG22	1.97	0.47
1:D:53:THR:HB	1:D:80:CYS:HB2	1.97	0.47
2:A:191:GLU:HA	2:A:215:THR:HG22	1.97	0.47
2:A:461:LEU:HB2	2:A:485:VAL:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:34:MET:CE	2:E:50:TRP:HB3	2.45	0.47
2:K:37:LYS:HB2	2:K:50:TRP:CE3	2.50	0.47
1:L:376:LEU:HD23	1:L:379:LEU:HB2	1.97	0.47
2:K:34:MET:HE1	2:K:37:LYS:HD3	1.97	0.46
2:K:34:MET:CE	2:K:50:TRP:HB3	2.45	0.46
2:G:161:ALA:HB1	2:G:186:LEU:HD23	1.97	0.46
1:L:371:ARG:HG3	1:L:393:GLU:CG	2.45	0.46
1:H:332:VAL:HA	1:H:356:HIS:HB2	1.97	0.46
2:G:37:LYS:HB2	2:G:50:TRP:CE3	2.50	0.46
2:A:37:LYS:HB2	2:A:50:TRP:CE3	2.51	0.46
2:I:461:LEU:HB2	2:I:485:VAL:HG12	1.96	0.46
2:E:34:MET:HE3	2:E:50:TRP:HB3	1.98	0.46
1:J:193:HIS:CE1	2:E:68:ASN:O	2.69	0.46
2:A:34:MET:CE	2:A:50:TRP:HB3	2.45	0.46
2:E:37:LYS:HB2	2:E:50:TRP:CE3	2.50	0.46
1:D:53:THR:HA	1:D:97:TYR:HB2	1.98	0.46
2:G:34:MET:CE	2:G:50:TRP:HB3	2.45	0.46
2:I:34:MET:CE	2:I:50:TRP:HB3	2.45	0.46
2:B:37:LYS:HB2	2:B:50:TRP:CE3	2.50	0.46
2:B:461:LEU:HB2	2:B:485:VAL:HG12	1.96	0.46
1:J:274:ARG:HG2	1:J:274:ARG:NH1	2.31	0.46
2:G:461:LEU:HB2	2:G:485:VAL:HG12	1.96	0.46
2:B:34:MET:CE	2:B:50:TRP:HB3	2.45	0.46
2:K:37:LYS:HD2	2:K:50:TRP:HB2	1.98	0.46
1:F:223:PRO:HB2	1:F:225:PHE:CZ	2.51	0.46
1:F:373:VAL:HG13	1:F:375:HIS:CE1	2.50	0.46
1:L:105:GLY:HA3	1:L:139:TYR:O	2.16	0.46
1:C:105:GLY:O	1:C:113:PHE:HB2	2.16	0.46
2:K:161:ALA:HB1	2:K:186:LEU:HD23	1.97	0.46
1:L:223:PRO:HB2	1:L:225:PHE:CZ	2.50	0.46
2:B:191:GLU:HA	2:B:215:THR:HG22	1.97	0.46
1:H:65:MET:O	1:H:68:THR:HG22	2.16	0.46
2:G:37:LYS:HD2	2:G:50:TRP:HB2	1.98	0.46
2:B:37:LYS:HE2	2:B:43:LEU:HD22	1.98	0.46
1:C:107:LEU:HD21	2:A:192:VAL:HA	1.97	0.46
1:F:140:ARG:HA	1:F:167:GLU:O	2.15	0.46
1:L:333:LEU:HB2	1:L:357:LEU:HD23	1.97	0.46
1:H:347:THR:HG22	1:H:348:ARG:HD2	1.97	0.46
2:B:161:ALA:HB1	2:B:186:LEU:HD23	1.97	0.46
2:E:37:LYS:HE2	2:E:43:LEU:HD22	1.99	0.46
2:A:37:LYS:HD2	2:A:50:TRP:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:37:LYS:HB2	2:I:50:TRP:CE3	2.50	0.45
2:I:161:ALA:HB1	2:I:186:LEU:HD23	1.97	0.45
2:I:400:LEU:HD12	2:I:400:LEU:HA	1.73	0.45
1:J:107:LEU:HD21	2:I:192:VAL:HA	1.97	0.45
2:I:191:GLU:HA	2:I:215:THR:HG22	1.97	0.45
1:H:354:VAL:HG13	1:H:378:GLU:HB2	1.99	0.45
2:A:161:ALA:HB1	2:A:186:LEU:HD23	1.97	0.45
2:I:37:LYS:HE2	2:I:43:LEU:HD22	1.98	0.45
2:E:37:LYS:HD2	2:E:50:TRP:HB2	1.98	0.45
2:K:37:LYS:HE2	2:K:43:LEU:HD22	1.99	0.45
1:D:205:PHE:HB3	1:D:208:LEU:HB2	1.98	0.45
2:G:151:LYS:HB2	2:G:173:ASP:OD1	2.17	0.45
1:C:53:THR:HA	1:C:97:TYR:HB2	1.98	0.45
2:K:403:ARG:HB3	2:K:425:GLU:HB3	1.99	0.45
1:F:227:LEU:HD12	1:F:230:LEU:HD22	1.97	0.45
1:L:278:LEU:HD21	1:L:281:LEU:HB2	1.98	0.45
1:H:278:LEU:HD21	1:H:281:LEU:HB2	1.97	0.45
2:E:403:ARG:HB3	2:E:425:GLU:HB3	1.99	0.45
1:F:369:GLU:OE1	1:F:369:GLU:N	2.46	0.45
2:G:37:LYS:HE2	2:G:43:LEU:HD22	1.99	0.45
2:B:37:LYS:HD2	2:B:50:TRP:HB2	1.98	0.45
1:C:68:THR:HG21	1:C:104:PHE:CE1	2.51	0.45
1:F:281:LEU:HD23	1:F:305:LEU:HD13	1.99	0.45
1:H:165:LEU:HB3	1:H:170:PHE:HE2	1.82	0.45
2:A:37:LYS:HE2	2:A:43:LEU:HD22	1.99	0.45
2:I:37:LYS:HD2	2:I:50:TRP:HB2	1.98	0.45
1:F:265:THR:HG22	1:F:287:ARG:HB2	1.99	0.45
1:L:354:VAL:HG13	1:L:378:GLU:HB2	1.99	0.45
1:H:140:ARG:HA	1:H:167:GLU:O	2.17	0.45
2:E:161:ALA:HB1	2:E:186:LEU:HD23	1.97	0.45
1:L:373:VAL:HG13	1:L:375:HIS:CE1	2.52	0.45
1:H:279:VAL:HB	2:G:186:LEU:HD22	1.99	0.45
1:H:376:LEU:HD23	1:H:379:LEU:HB2	1.99	0.45
2:G:53:VAL:HG13	2:G:54:HIS:CE1	2.52	0.45
2:G:191:GLU:HA	2:G:215:THR:HG22	1.97	0.45
2:I:151:LYS:HB2	2:I:173:ASP:OD1	2.17	0.45
2:B:400:LEU:HD12	2:B:400:LEU:HA	1.73	0.45
2:G:34:MET:HE3	2:G:50:TRP:HB3	1.99	0.44
2:B:151:LYS:HB2	2:B:173:ASP:OD1	2.17	0.44
2:B:403:ARG:HB3	2:B:425:GLU:HB3	1.99	0.44
2:K:151:LYS:HB2	2:K:173:ASP:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:GLY:O	1:D:412:LEU:HA	2.15	0.44
1:H:105:GLY:O	1:H:113:PHE:HB2	2.18	0.44
1:H:306:MET:O	1:H:307:LEU:HD23	2.18	0.44
2:I:34:MET:HE1	2:I:37:LYS:HD3	2.00	0.44
2:K:53:VAL:HG13	2:K:54:HIS:CE1	2.52	0.44
1:D:274:ARG:HG2	1:D:274:ARG:NH1	2.32	0.44
1:D:353:ARG:NH2	2:B:157:GLY:HA2	2.31	0.44
2:G:400:LEU:HD12	2:G:400:LEU:HA	1.73	0.44
2:G:403:ARG:HB3	2:G:425:GLU:HB3	1.99	0.44
2:A:53:VAL:HG13	2:A:54:HIS:CE1	2.52	0.44
2:E:53:VAL:HG13	2:E:54:HIS:CE1	2.52	0.44
1:C:205:PHE:HB3	1:C:208:LEU:HB2	1.98	0.44
1:D:140:ARG:HA	1:D:167:GLU:O	2.17	0.44
1:J:243:PRO:HA	1:J:265:THR:O	2.17	0.44
2:A:151:LYS:HB2	2:A:173:ASP:OD1	2.17	0.44
2:A:403:ARG:HB3	2:A:425:GLU:HB3	1.99	0.44
2:E:151:LYS:HB2	2:E:173:ASP:OD1	2.17	0.44
1:C:243:PRO:HA	1:C:265:THR:O	2.17	0.44
1:D:165:LEU:HB3	1:D:170:PHE:HE2	1.82	0.44
2:I:403:ARG:HB3	2:I:425:GLU:HB3	1.99	0.44
1:J:223:PRO:HB2	1:J:225:PHE:CZ	2.53	0.44
2:K:344:ASN:HB3	2:K:345:LYS:H	1.72	0.44
1:F:150:PRO:HG2	1:F:153:LEU:HG	2.00	0.44
1:D:223:PRO:HB2	1:D:225:PHE:CZ	2.52	0.44
2:E:368:ASN:HB3	2:E:369:ARG:H	1.71	0.44
1:F:344:LYS:O	1:F:347:THR:HB	2.18	0.44
2:I:53:VAL:HG13	2:I:54:HIS:CE1	2.52	0.44
1:C:139:TYR:HD1	1:C:166:ARG:HB3	1.83	0.44
1:J:255:ILE:HA	1:J:278:LEU:HA	2.00	0.44
1:J:332:VAL:HA	1:J:356:HIS:HB2	1.99	0.44
1:C:274:ARG:HG2	1:C:274:ARG:NH1	2.29	0.43
1:L:108:SER:HB3	1:L:109:ASP:H	1.59	0.43
1:L:369:GLU:OE1	1:L:369:GLU:N	2.45	0.43
2:G:339:LEU:HD23	2:G:363:LEU:HD13	2.00	0.43
2:K:400:LEU:HD12	2:K:400:LEU:HA	1.73	0.43
2:B:53:VAL:HG13	2:B:54:HIS:CE1	2.52	0.43
1:L:392:PHE:CE2	1:L:406:LEU:HD11	2.53	0.43
1:C:62:TYR:CD2	1:C:74:ALA:HA	2.53	0.43
1:C:380:ARG:CZ	1:C:405:ARG:NH1	2.81	0.43
1:D:223:PRO:HB2	1:D:225:PHE:CE1	2.54	0.43
1:L:146:PRO:HB3	1:L:171:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ASP:HB3	1:C:110:ASP:H	1.70	0.43
1:F:70:ASN:HB3	1:F:72:TRP:NE1	2.33	0.43
1:H:344:LYS:O	1:H:347:THR:HB	2.19	0.43
2:I:34:MET:HE3	2:I:50:TRP:HB3	2.01	0.43
2:B:339:LEU:HD23	2:B:363:LEU:HD13	2.00	0.43
1:D:243:PRO:HA	1:D:265:THR:O	2.18	0.43
1:L:274:ARG:HG2	1:L:274:ARG:NH1	2.32	0.43
1:J:255:ILE:HG13	2:I:186:LEU:HD13	2.00	0.43
2:K:421:LYS:HB3	2:K:421:LYS:HE2	1.81	0.43
1:D:347:THR:HG22	1:D:348:ARG:HD2	2.00	0.43
1:L:281:LEU:HD23	1:L:305:LEU:HD13	2.01	0.43
2:I:303:PRO:HA	2:I:304:PRO:HD3	1.94	0.43
1:D:265:THR:HG22	1:D:287:ARG:HB2	2.01	0.43
1:H:53:THR:HA	1:H:97:TYR:HB2	2.01	0.43
1:H:166:ARG:HG3	1:H:190:HIS:HB3	2.00	0.43
2:G:285:MET:O	2:G:288:LEU:HB2	2.19	0.43
2:G:446:ILE:HG23	2:G:450:LEU:HD22	2.01	0.43
1:C:51:ALA:O	1:C:81:ARG:NH1	2.46	0.43
2:A:339:LEU:HD23	2:A:363:LEU:HD13	2.00	0.43
2:I:339:LEU:HD23	2:I:363:LEU:HD13	2.00	0.43
2:E:285:MET:O	2:E:288:LEU:HB2	2.19	0.43
1:F:219:THR:HG22	2:I:56:SER:HB2	2.01	0.43
2:B:285:MET:O	2:B:288:LEU:HB2	2.19	0.43
1:F:160:LEU:HD23	1:F:181:LEU:HD13	2.00	0.42
1:H:277:GLN:OE1	2:G:185:ARG:NH2	2.52	0.42
2:G:336:LEU:HD21	2:G:339:LEU:HD13	2.01	0.42
2:A:400:LEU:O	2:A:403:ARG:HG2	2.19	0.42
2:A:446:ILE:HG23	2:A:450:LEU:HD22	2.01	0.42
2:E:421:LYS:H	2:E:421:LYS:HG2	1.70	0.42
2:K:336:LEU:HD21	2:K:339:LEU:HD13	2.01	0.42
1:F:289:SER:HA	1:F:313:PHE:HA	2.02	0.42
1:F:381:LEU:HB2	1:F:406:LEU:HD23	2.02	0.42
2:A:368:ASN:HB3	2:A:369:ARG:H	1.71	0.42
2:K:285:MET:O	2:K:288:LEU:HB2	2.19	0.42
2:K:400:LEU:O	2:K:403:ARG:HG2	2.19	0.42
1:F:274:ARG:HG2	1:F:274:ARG:NH1	2.32	0.42
1:H:388:GLY:O	1:H:412:LEU:HA	2.20	0.42
2:G:400:LEU:O	2:G:403:ARG:HG2	2.19	0.42
2:I:285:MET:O	2:I:288:LEU:HB2	2.19	0.42
2:B:336:LEU:HD21	2:B:339:LEU:HD13	2.01	0.42
2:E:336:LEU:HD21	2:E:339:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:421:LYS:HB3	2:E:421:LYS:HE2	1.81	0.42
1:L:107:LEU:HD13	1:L:107:LEU:O	2.20	0.42
1:J:217:ARG:HD3	2:E:71:TYR:CE2	2.53	0.42
2:I:400:LEU:O	2:I:403:ARG:HG2	2.19	0.42
2:E:339:LEU:HD23	2:E:363:LEU:HD13	2.00	0.42
2:E:400:LEU:HA	2:E:400:LEU:HD12	1.73	0.42
1:J:269:PRO:O	1:J:272:ILE:HG12	2.20	0.42
2:K:137:PHE:CE1	1:L:306:MET:HE2	2.54	0.42
1:J:167:GLU:HG2	1:J:191:LYS:HB3	2.01	0.42
2:E:446:ILE:HG23	2:E:450:LEU:HD22	2.01	0.42
1:H:109:ASP:HB3	1:H:110:ASP:H	1.71	0.42
1:J:53:THR:HB	1:J:80:CYS:HB2	2.01	0.42
1:J:140:ARG:HA	1:J:167:GLU:O	2.20	0.42
2:G:309:LEU:HD23	2:G:312:THR:HG21	2.02	0.42
2:A:336:LEU:HD21	2:A:339:LEU:HD13	2.01	0.42
2:A:421:LYS:H	2:A:421:LYS:HG2	1.70	0.42
2:B:446:ILE:HG23	2:B:450:LEU:HD22	2.01	0.42
2:K:339:LEU:HD23	2:K:363:LEU:HD13	2.00	0.42
1:F:243:PRO:HA	1:F:265:THR:O	2.18	0.42
1:J:54:GLU:HG3	1:J:57:GLU:H	1.84	0.42
1:J:256:LYS:HB2	2:I:186:LEU:HD11	2.02	0.42
2:A:285:MET:O	2:A:288:LEU:HB2	2.19	0.42
2:A:309:LEU:HD23	2:A:312:THR:HG21	2.02	0.42
2:I:336:LEU:HD21	2:I:339:LEU:HD13	2.01	0.42
2:B:421:LYS:H	2:B:421:LYS:HG2	1.70	0.42
2:B:421:LYS:HE2	2:B:421:LYS:HB3	1.81	0.42
1:C:306:MET:HE2	2:A:137:PHE:HE1	1.85	0.42
2:A:400:LEU:HA	2:A:400:LEU:HD12	1.73	0.42
2:B:400:LEU:O	2:B:403:ARG:HG2	2.19	0.42
1:C:354:VAL:HG13	1:C:378:GLU:HB2	2.02	0.42
1:F:226:VAL:HG22	1:F:247:THR:HB	2.01	0.42
1:L:53:THR:HA	1:L:97:TYR:HB2	2.02	0.42
2:B:440:ASN:HB3	2:B:441:ASN:H	1.75	0.42
2:E:400:LEU:O	2:E:403:ARG:HG2	2.19	0.42
1:C:223:PRO:HB2	1:C:225:PHE:CZ	2.55	0.41
1:C:333:LEU:HB2	1:C:357:LEU:HD23	2.02	0.41
2:K:554:ALA:HA	2:K:557:VAL:HG23	2.02	0.41
2:I:554:ALA:HA	2:I:557:VAL:HG23	2.02	0.41
2:B:303:PRO:HA	2:B:304:PRO:HD3	1.94	0.41
2:E:554:ALA:HA	2:E:557:VAL:HG23	2.02	0.41
1:C:67:ALA:O	1:C:121:SER:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:GLY:O	1:C:412:LEU:HA	2.20	0.41
2:K:446:ILE:HG23	2:K:450:LEU:HD22	2.01	0.41
1:F:333:LEU:HB2	1:F:357:LEU:HD23	2.02	0.41
1:J:125:GLU:HG3	1:J:152:PHE:CG	2.55	0.41
2:I:446:ILE:HG23	2:I:450:LEU:HD22	2.01	0.41
2:K:348:GLY:HA3	1:D:320:ASN:CG	2.40	0.41
1:F:222:ILE:H	1:F:222:ILE:HG13	1.69	0.41
1:D:103:SER:HA	1:D:137:PHE:HB2	2.02	0.41
1:H:373:VAL:HG13	1:H:375:HIS:CE1	2.55	0.41
2:E:309:LEU:HD23	2:E:312:THR:HG21	2.02	0.41
2:K:456:LEU:HD21	2:K:459:LEU:HD13	2.03	0.41
1:H:274:ARG:HG2	1:H:274:ARG:NH1	2.32	0.41
2:A:554:ALA:HA	2:A:557:VAL:HG23	2.02	0.41
1:C:373:VAL:HG13	1:C:375:HIS:CE1	2.56	0.41
1:F:185:LYS:HA	1:F:208:LEU:HA	2.01	0.41
1:J:109:ASP:HB3	1:J:110:ASP:H	1.73	0.41
1:J:194:LEU:HD23	1:J:194:LEU:HA	1.90	0.41
2:I:456:LEU:HD21	2:I:459:LEU:HD13	2.03	0.41
2:B:309:LEU:HD23	2:B:312:THR:HG21	2.02	0.41
2:K:309:LEU:HD23	2:K:312:THR:HG21	2.02	0.41
1:F:366:ILE:HG12	1:F:386:LEU:HD13	2.03	0.41
1:H:320:ASN:HB2	2:A:347:VAL:HG21	2.03	0.41
1:J:102:LEU:HD12	1:J:102:LEU:HA	1.91	0.41
2:E:456:LEU:HD21	2:E:459:LEU:HD13	2.03	0.41
1:D:323:LYS:HE2	1:D:345:SER:HB3	2.03	0.41
1:C:256:LYS:HB2	2:A:186:LEU:HD11	2.02	0.41
1:F:103:SER:HA	1:F:137:PHE:HB2	2.03	0.41
2:G:421:LYS:HB3	2:G:421:LYS:HE2	1.81	0.41
2:G:534:SER:HB2	2:G:557:VAL:O	2.21	0.41
2:A:421:LYS:HB3	2:A:421:LYS:HE2	1.81	0.41
2:A:534:SER:HB2	2:A:557:VAL:O	2.21	0.41
2:B:456:LEU:HD21	2:B:459:LEU:HD13	2.03	0.41
2:B:554:ALA:HA	2:B:557:VAL:HG23	2.02	0.41
1:D:281:LEU:HD23	1:D:305:LEU:HD13	2.03	0.41
1:D:381:LEU:O	1:D:384:ASN:ND2	2.49	0.41
2:I:243:ILE:HG12	2:I:266:THR:HB	2.03	0.41
1:D:354:VAL:HG13	1:D:378:GLU:HB2	2.03	0.40
1:L:312:LYS:HD3	1:L:312:LYS:HA	1.91	0.40
1:H:333:LEU:HB2	1:H:357:LEU:HD23	2.03	0.40
2:G:554:ALA:HA	2:G:557:VAL:HG23	2.02	0.40
2:B:243:ILE:HG12	2:B:266:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:GLN:HG3	1:C:261:ARG:HD2	2.04	0.40
2:K:243:ILE:HG12	2:K:266:THR:HB	2.03	0.40
1:L:222:ILE:HG12	1:L:240:LEU:HD13	2.03	0.40
1:L:304:ALA:HB1	1:L:306:MET:CE	2.51	0.40
2:A:243:ILE:HG12	2:A:266:THR:HB	2.03	0.40
2:I:309:LEU:HD23	2:I:312:THR:HG21	2.02	0.40
2:E:243:ILE:HG12	2:E:266:THR:HB	2.03	0.40
1:D:109:ASP:HB3	1:D:110:ASP:H	1.75	0.40
1:D:369:GLU:OE1	1:D:369:GLU:N	2.47	0.40
1:L:86:GLY:HA2	1:L:113:PHE:CD1	2.56	0.40
1:J:390:VAL:HG12	1:J:412:LEU:HD13	2.04	0.40
2:A:302:ILE:HG12	2:A:322:LEU:HD13	2.04	0.40
2:K:302:ILE:HG12	2:K:322:LEU:HD13	2.04	0.40
1:D:256:LYS:HB2	2:B:186:LEU:HD11	2.04	0.40
2:A:456:LEU:HD21	2:A:459:LEU:HD13	2.03	0.40
2:E:534:SER:HB2	2:E:557:VAL:O	2.21	0.40
1:F:194:LEU:HD23	1:F:194:LEU:HA	1.88	0.40
1:L:67:ALA:O	1:L:121:SER:HA	2.22	0.40
2:G:243:ILE:HG12	2:G:266:THR:HB	2.03	0.40
2:G:456:LEU:HD21	2:G:459:LEU:HD13	2.03	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ARG:O	2:I:570:ILE:O[1_546]	1.93	0.27
1:C:113:PHE:O	2:I:561:TYR:OH[1_546]	1.96	0.24
1:C:72:TRP:CB	2:I:540:GLY:CA[1_546]	2.16	0.04
1:J:113:PHE:O	2:A:561:TYR:OH[1_554]	2.19	0.01

## 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	C	363/433 (84%)	334 (92%)	27 (7%)	2 (1%)	25	55
1	D	363/433 (84%)	333 (92%)	28 (8%)	2 (1%)	25	55
1	F	363/433 (84%)	333 (92%)	28 (8%)	2 (1%)	25	55
1	H	363/433 (84%)	334 (92%)	28 (8%)	1 (0%)	41	70
1	J	363/433 (84%)	332 (92%)	29 (8%)	2 (1%)	25	55
1	L	363/433 (84%)	334 (92%)	27 (7%)	2 (1%)	25	55
2	A	542/556 (98%)	485 (90%)	56 (10%)	1 (0%)	47	77
2	B	542/556 (98%)	484 (89%)	57 (10%)	1 (0%)	47	77
2	E	542/556 (98%)	485 (90%)	56 (10%)	1 (0%)	47	77
2	G	542/556 (98%)	485 (90%)	56 (10%)	1 (0%)	47	77
2	I	542/556 (98%)	485 (90%)	56 (10%)	1 (0%)	47	77
2	K	542/556 (98%)	485 (90%)	56 (10%)	1 (0%)	47	77
All	All	5430/5934 (92%)	4909 (90%)	504 (9%)	17 (0%)	41	70

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	109	ASP
1	F	109	ASP
1	D	109	ASP
1	L	109	ASP
1	H	109	ASP
1	J	109	ASP
1	C	391	PRO
1	F	391	PRO
1	J	391	PRO
1	D	391	PRO
2	K	44	VAL
2	G	44	VAL
2	A	44	VAL
2	I	44	VAL
2	B	44	VAL
2	E	44	VAL
1	L	391	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	322/378 (85%)	318 (99%)	4 (1%)	71	87
1	D	322/378 (85%)	320 (99%)	2 (1%)	86	93
1	F	322/378 (85%)	316 (98%)	6 (2%)	57	79
1	H	322/378 (85%)	318 (99%)	4 (1%)	71	87
1	J	322/378 (85%)	320 (99%)	2 (1%)	86	93
1	L	322/378 (85%)	315 (98%)	7 (2%)	52	76
2	A	476/486 (98%)	465 (98%)	11 (2%)	50	75
2	B	476/486 (98%)	465 (98%)	11 (2%)	50	75
2	E	476/486 (98%)	465 (98%)	11 (2%)	50	75
2	G	476/486 (98%)	465 (98%)	11 (2%)	50	75
2	I	476/486 (98%)	465 (98%)	11 (2%)	50	75
2	K	476/486 (98%)	465 (98%)	11 (2%)	50	75
All	All	4788/5184 (92%)	4697 (98%)	91 (2%)	57	79

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	155	ARG
1	C	176	ASP
1	C	237	GLN
1	C	270	GLU
2	K	43	LEU
2	K	48	LEU
2	K	54	HIS
2	K	67	ASP
2	K	223	ARG
2	K	308	ASN
2	K	402	PHE
2	K	452	ASP
2	K	457	LEU
2	K	546	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	K	566	TRP
1	F	94	ASP
1	F	155	ARG
1	F	236	ASN
1	F	237	GLN
1	F	270	GLU
1	F	356	HIS
1	D	237	GLN
1	D	270	GLU
1	L	155	ARG
1	L	176	ASP
1	L	236	ASN
1	L	237	GLN
1	L	270	GLU
1	L	356	HIS
1	L	393	GLU
1	H	121	SER
1	H	270	GLU
1	H	356	HIS
1	H	398	TRP
1	J	155	ARG
1	J	237	GLN
2	G	43	LEU
2	G	48	LEU
2	G	54	HIS
2	G	67	ASP
2	G	223	ARG
2	G	308	ASN
2	G	402	PHE
2	G	452	ASP
2	G	457	LEU
2	G	546	LYS
2	G	566	TRP
2	A	43	LEU
2	A	48	LEU
2	A	54	HIS
2	A	67	ASP
2	A	223	ARG
2	A	308	ASN
2	A	402	PHE
2	A	452	ASP
2	A	457	LEU

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Mol	Chain	Res	Type
2	A	546	LYS
2	A	566	TRP
2	I	43	LEU
2	I	48	LEU
2	I	54	HIS
2	I	67	ASP
2	I	223	ARG
2	I	308	ASN
2	I	402	PHE
2	I	452	ASP
2	I	457	LEU
2	I	546	LYS
2	I	566	TRP
2	B	43	LEU
2	B	48	LEU
2	B	54	HIS
2	B	67	ASP
2	B	223	ARG
2	B	308	ASN
2	B	402	PHE
2	B	452	ASP
2	B	457	LEU
2	B	546	LYS
2	B	566	TRP
2	E	43	LEU
2	E	48	LEU
2	E	54	HIS
2	E	67	ASP
2	E	223	ARG
2	E	308	ASN
2	E	402	PHE
2	E	452	ASP
2	E	457	LEU
2	E	546	LYS
2	E	566	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	70	ASN
1	F	70	ASN
1	D	70	ASN

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Mol	Chain	Res	Type
1	L	70	ASN
1	H	70	ASN
1	J	70	ASN
2	G	428	HIS
2	G	500	GLN
2	A	428	HIS
2	I	428	HIS
2	B	428	HIS
2	E	428	HIS

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	C	365/433 (84%)	-0.24	3 (0%) 86 70	30, 42, 66, 85	0
1	D	365/433 (84%)	-0.08	8 (2%) 62 38	31, 51, 79, 91	0
1	F	365/433 (84%)	-0.01	7 (1%) 66 43	29, 51, 75, 91	0
1	H	365/433 (84%)	-0.02	4 (1%) 80 60	30, 50, 84, 100	0
1	J	365/433 (84%)	-0.17	5 (1%) 75 53	29, 43, 70, 90	0
1	L	365/433 (84%)	0.24	23 (6%) 20 8	30, 61, 99, 112	0
2	A	544/556 (97%)	0.41	32 (5%) 22 9	40, 61, 84, 109	0
2	B	544/556 (97%)	0.17	16 (2%) 51 26	40, 61, 84, 109	0
2	E	544/556 (97%)	0.31	23 (4%) 36 17	40, 61, 84, 109	0
2	G	544/556 (97%)	0.16	16 (2%) 51 26	40, 61, 84, 109	0
2	I	544/556 (97%)	0.84	71 (13%) 3 1	40, 61, 84, 109	0
2	K	544/556 (97%)	0.36	39 (7%) 15 5	40, 61, 84, 109	0
All	All	5454/5934 (91%)	0.21	247 (4%) 33 15	29, 58, 84, 112	0

All (247) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	569	SER	14.0
2	I	563	CYS	12.6
2	I	548	PHE	12.1
2	A	568	GLY	11.5
2	I	568	GLY	11.3
2	A	570	ILE	10.8
2	I	571	CYS	10.7
2	I	570	ILE	9.4
2	I	549	SER	8.7
2	I	560	PRO	8.2
2	A	563	CYS	7.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	E	553	PRO	7.2
2	I	567	VAL	6.9
2	I	537	ASN	6.6
2	A	569	SER	6.4
2	I	551	PHE	6.2
2	B	563	CYS	6.0
2	A	537	ASN	5.9
2	E	571	CYS	5.9
2	I	533	VAL	5.8
2	A	548	PHE	5.7
2	A	567	VAL	5.6
2	I	539	SER	5.6
2	I	525	CYS	5.4
2	I	443	SER	5.4
2	E	567	VAL	5.4
2	A	553	PRO	5.3
2	I	561	TYR	5.3
2	I	556	PHE	5.2
2	A	571	CYS	5.1
2	I	522	LEU	5.0
2	G	553	PRO	4.8
2	I	553	PRO	4.7
2	I	489	LEU	4.7
2	G	552	ALA	4.7
2	E	563	CYS	4.7
1	L	398	TRP	4.6
2	K	568	GLY	4.6
1	L	83	ARG	4.6
2	E	566	TRP	4.5
2	I	492	GLY	4.5
2	I	565	ASN	4.5
2	I	554	ALA	4.5
1	L	98	HIS	4.5
2	I	520	ASP	4.5
2	I	547	ASN	4.5
2	E	569	SER	4.4
2	B	549	SER	4.4
2	I	545	MET	4.4
2	I	465	HIS	4.4
2	A	549	SER	4.4
2	I	566	TRP	4.3
2	E	554	ALA	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	G	547	ASN	4.2
2	E	565	ASN	4.1
2	I	536	ASN	4.1
1	L	414	VAL	4.1
2	A	554	ALA	4.0
2	G	550	ARG	3.9
2	A	551	PHE	3.9
2	K	563	CYS	3.9
2	I	514	LEU	3.9
2	K	564	GLY	3.9
2	A	525	CYS	3.9
2	E	552	ALA	3.8
2	K	570	ILE	3.8
1	J	109	ASP	3.8
2	G	549	SER	3.8
2	A	561	TYR	3.7
1	L	53	THR	3.7
2	I	515	HIS	3.7
2	I	467	SER	3.7
2	B	564	GLY	3.7
2	I	509	LEU	3.7
2	I	52	ASP	3.7
2	I	491	SER	3.7
2	K	52	ASP	3.6
2	I	513	LYS	3.6
2	K	56	SER	3.6
2	G	528	LEU	3.6
2	I	519	PRO	3.5
2	E	570	ILE	3.5
2	E	550	ARG	3.5
2	I	528	LEU	3.5
1	C	109	ASP	3.5
2	K	553	PRO	3.5
2	G	529	VAL	3.5
2	I	540	GLY	3.5
2	A	566	TRP	3.5
1	H	390	VAL	3.4
1	L	390	VAL	3.3
2	A	522	LEU	3.3
2	I	504	LEU	3.3
2	I	541	ILE	3.3
2	K	482	MET	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	111	THR	3.3
2	A	556	PHE	3.2
2	K	53	VAL	3.2
2	I	538	LEU	3.2
1	D	109	ASP	3.2
1	L	89	CYS	3.2
2	G	404	ASN	3.2
2	I	444	GLY	3.2
2	G	564	GLY	3.1
2	K	344	ASN	3.1
2	I	420	GLY	3.1
2	E	564	GLY	3.1
1	F	391	PRO	3.1
2	B	570	ILE	3.0
1	J	110	ASP	3.0
2	K	404	ASN	3.0
2	B	548	PHE	3.0
1	F	110	ASP	3.0
1	H	111	THR	3.0
2	A	560	PRO	3.0
1	L	368	LEU	2.9
1	F	109	ASP	2.9
2	I	445	SER	2.9
2	K	565	ASN	2.9
2	B	52	ASP	2.9
2	I	564	GLY	2.9
2	K	571	CYS	2.8
2	B	47	LEU	2.8
2	K	64	VAL	2.8
2	K	556	PHE	2.8
2	K	58	LEU	2.8
2	I	490	LEU	2.8
2	I	421	LYS	2.8
1	F	79	VAL	2.8
2	I	419	LYS	2.8
2	E	549	SER	2.8
2	E	522	LEU	2.8
2	A	565	ASN	2.8
2	K	47	LEU	2.7
2	K	549	SER	2.7
2	K	528	LEU	2.7
1	L	370	PHE	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	L	392	PHE	2.7
2	E	556	PHE	2.7
1	D	93	GLN	2.7
2	K	561	TYR	2.7
2	K	320	ASN	2.7
2	I	558	GLY	2.6
2	E	84	GLY	2.6
2	A	539	SER	2.6
1	H	93	GLN	2.6
2	K	440	ASN	2.6
2	K	542	VAL	2.6
2	E	547	ASN	2.6
1	F	398	TRP	2.6
1	D	176	ASP	2.6
2	I	468	GLY	2.6
2	I	559	ASN	2.5
1	F	314	SER	2.5
1	J	111	THR	2.5
2	A	444	GLY	2.5
2	K	251	ILE	2.5
2	G	563	CYS	2.5
2	A	430	ILE	2.5
2	I	518	ILE	2.5
2	I	45	ASN	2.5
1	D	363	THR	2.5
1	L	393	GLU	2.5
2	K	552	ALA	2.5
2	A	552	ALA	2.5
2	A	545	MET	2.5
2	B	551	PHE	2.5
1	L	52	ARG	2.5
2	A	52	ASP	2.5
2	A	431	ASN	2.4
2	I	521	GLN	2.4
1	L	94	ASP	2.4
2	I	512	ASN	2.4
1	C	111	THR	2.4
2	I	496	THR	2.4
2	K	562	LEU	2.4
2	A	443	SER	2.4
1	L	111	THR	2.4
2	K	46	MET	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	553	PRO	2.4
2	K	381	CYS	2.4
2	I	466	LEU	2.4
2	I	531	LEU	2.4
2	E	520	ASP	2.3
2	B	64	VAL	2.3
1	D	110	ASP	2.3
2	I	562	LEU	2.3
2	K	551	PHE	2.3
2	K	428	HIS	2.3
1	D	374	LYS	2.3
2	E	542	VAL	2.3
2	K	533	VAL	2.3
1	D	411	GLY	2.3
1	L	80	CYS	2.3
2	G	565	ASN	2.3
2	I	517	LYS	2.3
2	K	405	LEU	2.3
2	G	554	ALA	2.3
2	G	546	LYS	2.3
2	I	485	VAL	2.3
2	I	42	ASN	2.3
2	I	555	SER	2.3
1	L	176	ASP	2.2
1	L	406	LEU	2.2
2	I	58	LEU	2.2
2	A	558	GLY	2.2
2	G	482	MET	2.2
2	K	435	LEU	2.2
2	I	552	ALA	2.2
2	K	550	ARG	2.2
1	L	99	VAL	2.2
2	G	570	ILE	2.2
2	A	445	SER	2.2
2	K	506	SER	2.2
2	B	76	LEU	2.2
2	K	45	ASN	2.2
1	C	110	ASP	2.2
2	I	482	MET	2.2
1	L	365	GLU	2.2
2	I	399	PRO	2.1
1	L	86	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	45	ASN	2.1
1	D	410	ALA	2.1
1	J	97	TYR	2.1
2	E	561	TYR	2.1
2	B	53	VAL	2.1
1	J	50	GLY	2.1
2	A	251	ILE	2.1
2	I	507	LEU	2.1
2	B	565	ASN	2.1
2	I	53	VAL	2.1
2	B	568	GLY	2.1
2	E	45	ASN	2.1
2	K	280	GLU	2.1
2	B	45	ASN	2.1
2	K	48	LEU	2.1
2	I	516	GLY	2.1
2	E	557	VAL	2.0
2	K	63	GLY	2.0
2	A	68	ASN	2.0
2	B	482	MET	2.0
1	L	374	LYS	2.0
2	A	528	LEU	2.0
1	H	109	ASP	2.0
2	E	546	LYS	2.0
1	L	93	GLN	2.0
1	L	394	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

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

## 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides 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.