



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2017 – 03:45 AM EDT

PDB ID : 4XMM  
Title : Structure of the yeast coat nucleoporin complex, space group C2  
Authors : Stuwe, T.; Correia, A.R.; Lin, D.H.; Paduch, M.; Lu, V.T.; Kossiakoff, A.A.;  
Hoelz, A.  
Deposited on : unknown  
Resolution : 7.38 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
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-20029824

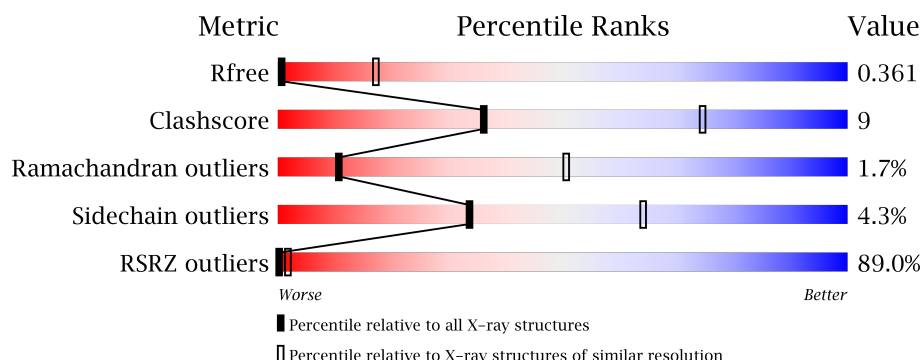
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 7.38 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	1100 (10.00-3.70)
Clashscore	112137	1035 (10.00-3.80)
Ramachandran outliers	110173	1003 (10.00-3.76)
Sidechain outliers	110143	1098 (10.00-3.70)
RSRZ outliers	101464	1003 (10.00-3.72)

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

Mol	Chain	Length	Quality of chain
1	A	297	<div> <div>92%</div> <div> <div>64%</div> <div>25%</div> <div>8%</div> </div> </div>
2	B	652	<div> <div>70%</div> <div> <div>56%</div> <div>19%</div> <div>22%</div> </div> </div>
3	C	349	<div> <div>83%</div> <div> <div>61%</div> <div>26%</div> <div>12%</div> </div> </div>
4	D	715	<div> <div>81%</div> <div> <div>66%</div> <div>19%</div> <div>13%</div> </div> </div>
5	E	1045	<div> <div>69%</div> <div> <div>71%</div> <div>14%</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
6	F	454	<div><div>82%</div><div><div></div><div></div><div></div><div></div></div><div>68%21%8%</div></div>
7	H	271	<div><div>70%</div><div><div></div><div></div><div></div><div></div></div><div>71%8%20%</div></div>
8	L	217	<div><div>85%</div><div><div></div><div></div><div></div><div></div></div><div>86%10%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 26139 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 transport protein SEC13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			

- Molecule 2 is a protein called Nucleoporin NUP145.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	511	Total	C	N	O	S	0	0	0
			3805	2417	648	730	10			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	61	MET	-	initiating methionine	UNP P49687
B	62	GLY	-	expression tag	UNP P49687
B	63	SER	-	expression tag	UNP P49687
B	64	SER	-	expression tag	UNP P49687
B	65	HIS	-	expression tag	UNP P49687
B	66	HIS	-	expression tag	UNP P49687
B	67	HIS	-	expression tag	UNP P49687
B	68	HIS	-	expression tag	UNP P49687
B	69	HIS	-	expression tag	UNP P49687
B	70	HIS	-	expression tag	UNP P49687
B	71	SER	-	expression tag	UNP P49687
B	72	ASP	-	expression tag	UNP P49687
B	73	GLN	-	expression tag	UNP P49687
B	74	PRO	-	expression tag	UNP P49687

- Molecule 3 is a protein called Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	307	Total	C	N	O	S	0	0	0
			2438	1543	422	462	11			

- Molecule 4 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	620	Total	C	N	O	S	0	0	0
			4535	2884	753	877	21			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	30	MET	-	initiating methionine	UNP P46673
D	31	GLY	-	expression tag	UNP P46673
D	32	SER	-	expression tag	UNP P46673
D	33	SER	-	expression tag	UNP P46673
D	34	HIS	-	expression tag	UNP P46673
D	35	HIS	-	expression tag	UNP P46673
D	36	HIS	-	expression tag	UNP P46673
D	37	HIS	-	expression tag	UNP P46673
D	38	HIS	-	expression tag	UNP P46673
D	39	HIS	-	expression tag	UNP P46673
D	40	SER	-	expression tag	UNP P46673
D	41	ASP	-	expression tag	UNP P46673
D	42	GLN	-	expression tag	UNP P46673
D	43	PRO	-	expression tag	UNP P46673

- Molecule 5 is a protein called Nucleoporin NUP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	896	Total	C	N	O	S	0	0	0
			6622	4232	1099	1275	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	MET	-	initiating methionine	UNP P35729
E	-6	HIS	-	expression tag	UNP P35729
E	-5	HIS	-	expression tag	UNP P35729
E	-4	HIS	-	expression tag	UNP P35729
E	-3	HIS	-	expression tag	UNP P35729
E	-2	HIS	-	expression tag	UNP P35729
E	-1	HIS	-	expression tag	UNP P35729
E	0	SER	-	expression tag	UNP P35729
E	1	THR	-	expression tag	UNP P35729

- Molecule 6 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	419	Total	C	N	O	S	0	0	0
			3404	2178	557	657	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P52891
F	-1	PRO	-	expression tag	UNP P52891
F	0	HIS	-	expression tag	UNP P52891

- Molecule 7 is a protein called Antibody 57 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	217	Total	C	N	O	S	0	0	0
			1576	988	267	315	6			

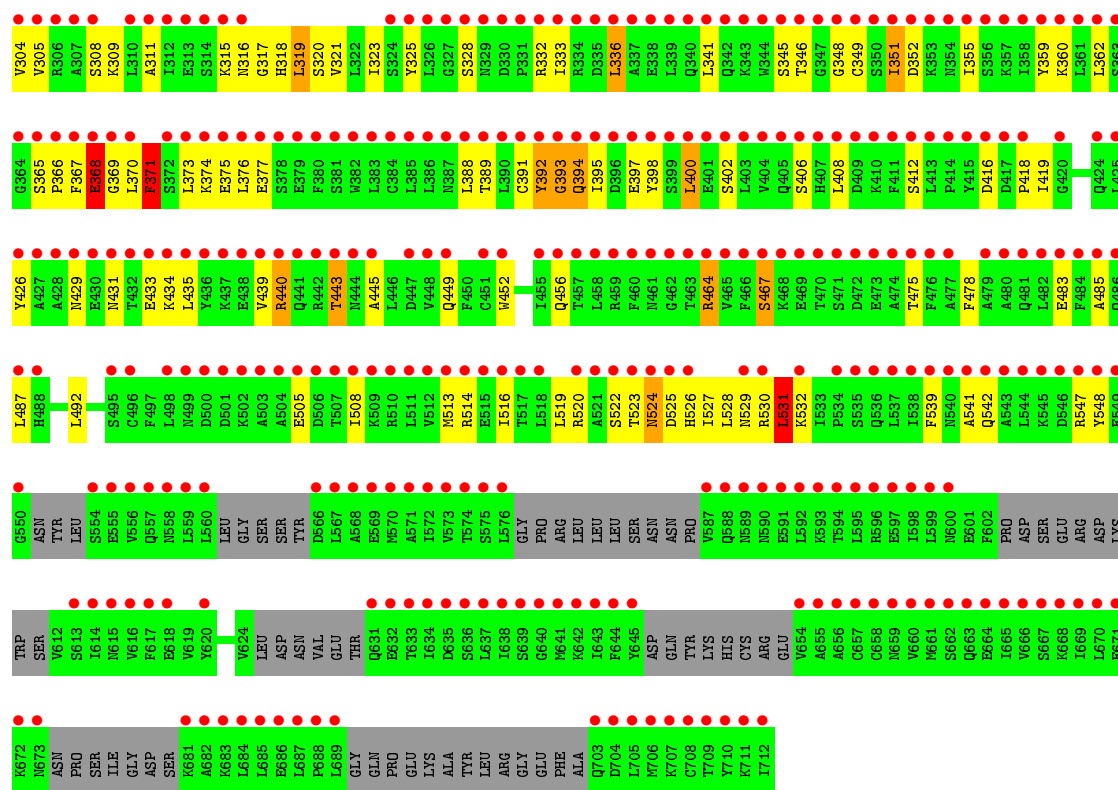
- Molecule 8 is a protein called Antibody 57 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	L	210	Total	C	N	O	S	0	0	0
			1599	996	270	327	6			

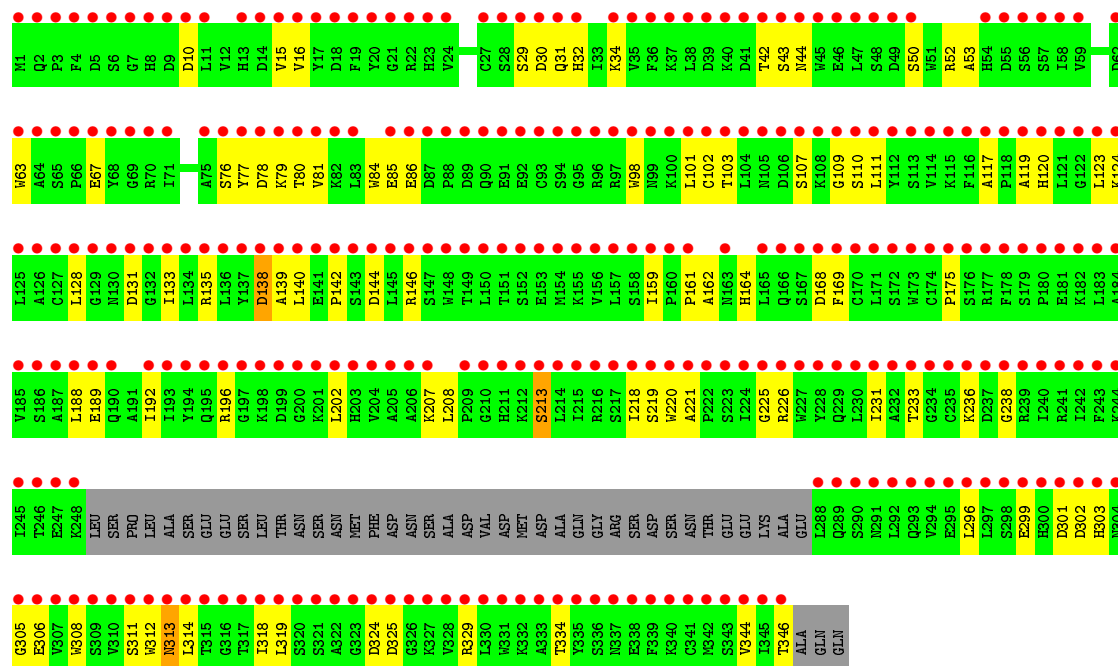
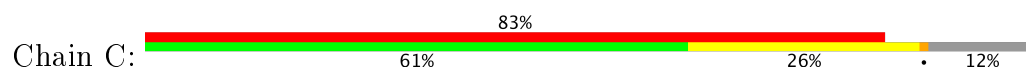
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

- [illegible]

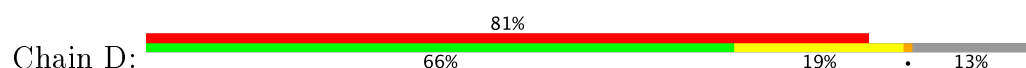
- Chain B:



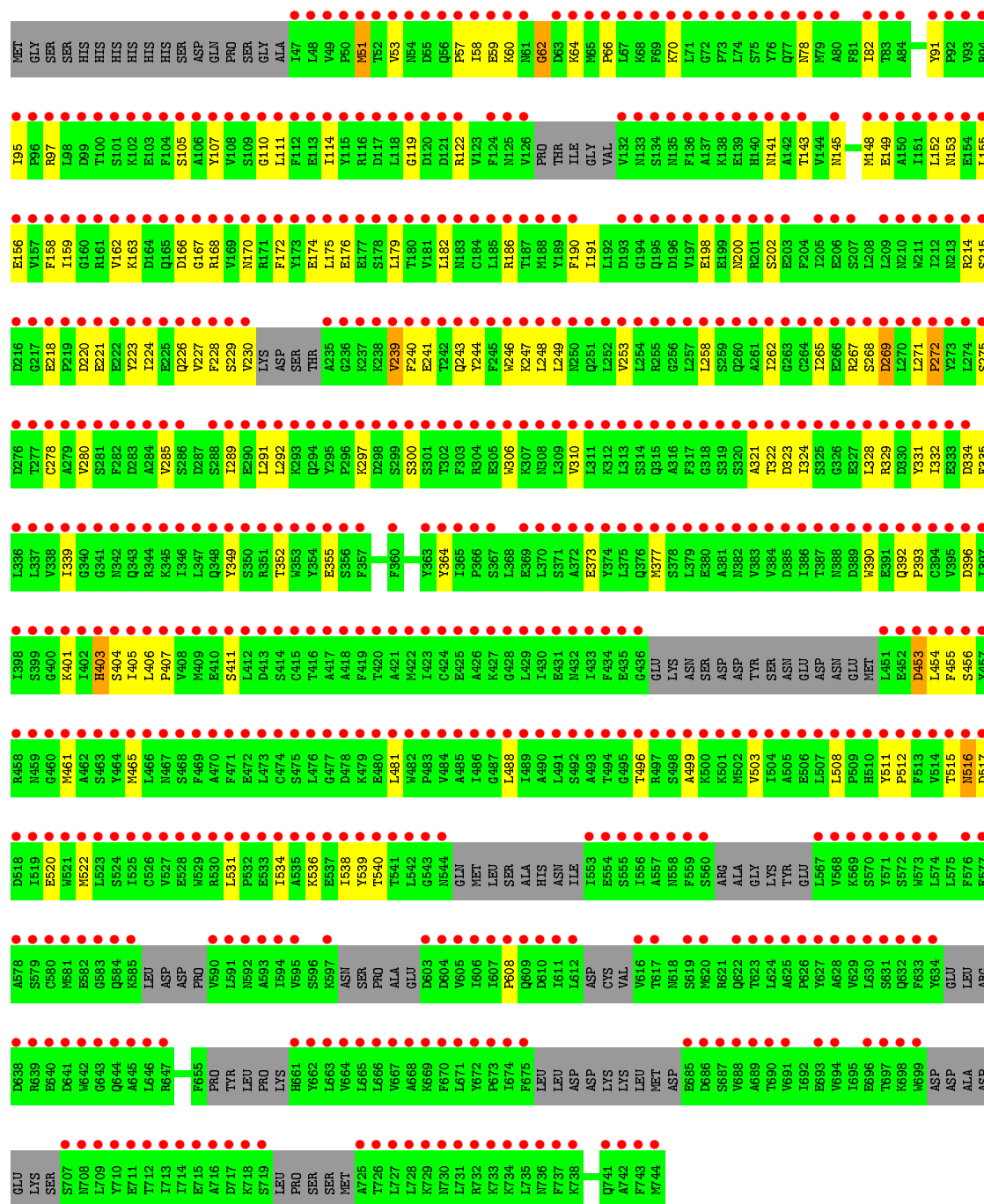
### • Molecule 3: Nucleoporin SEH1



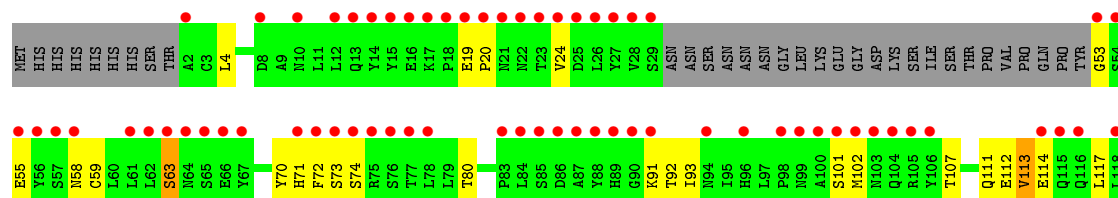
### • Molecule 4: Nucleoporin NUP85







• Molecule 5: Nucleoporin NUP120

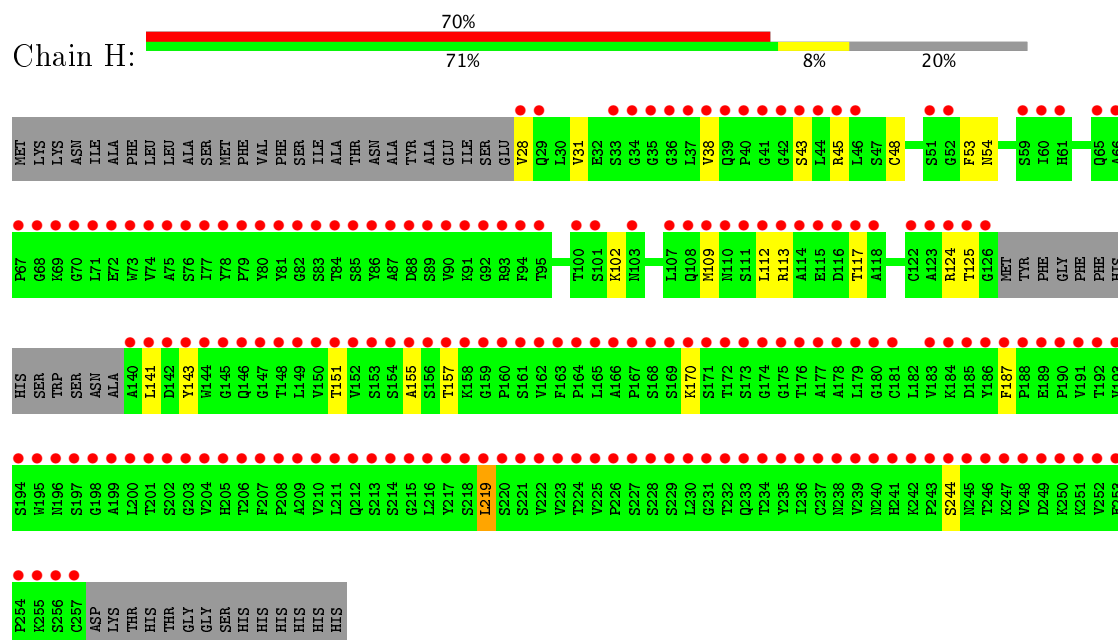




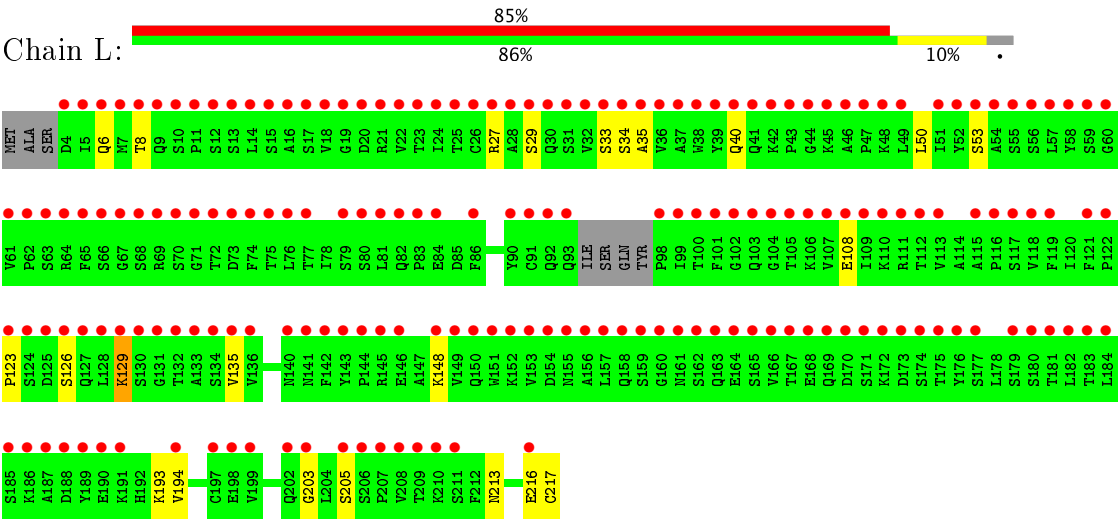
- Molecule 6: Nucleoporin NUP84



- Molecule 7: Antibody 57 heavy chain



● Molecule 8: Antibody 57 light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.65Å 186.30Å 199.57Å 90.00° 100.85° 90.00°	Depositor
Resolution (Å)	67.52 – 7.38 68.01 – 7.38	Depositor EDS
% Data completeness (in resolution range)	99.5 (67.52-7.38) 99.7 (68.01-7.38)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 7.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1809)	Depositor
R, $R_{free}$	0.330 , 0.353 0.328 , 0.361	Depositor DCC
$R_{free}$ test set	1021 reflections (9.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	734.6	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.50 , -10.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.75	EDS
Total number of atoms	26139	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	716.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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

### 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	0.32	0/2220	0.62	0/3028
2	B	0.37	0/3860	0.66	2/5224 (0.0%)
3	C	0.28	0/2499	0.64	0/3388
4	D	0.30	0/4602	0.58	2/6246 (0.0%)
5	E	0.33	0/6730	0.55	1/9158 (0.0%)
6	F	0.35	0/3472	0.64	2/4714 (0.0%)
7	H	0.31	0/1610	0.62	1/2194 (0.0%)
8	L	0.29	0/1631	0.60	0/2210
All	All	0.32	0/26624	0.60	8/36162 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
5	E	0	2
6	F	0	1
All	All	0	5

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	167	GLY	N-CA-C	-6.40	97.09	113.10
4	D	608	PRO	N-CA-CB	6.10	110.62	103.30
2	B	187	ASP	CB-CG-OD2	6.04	123.73	118.30
7	H	219	LEU	CA-CB-CG	6.04	129.19	115.30
5	E	818	PRO	N-CA-CB	5.78	110.23	103.30
2	B	260	LEU	CB-CG-CD2	-5.54	101.58	111.00
6	F	24	ILE	N-CA-C	5.49	125.83	111.00
6	F	24	ILE	CG1-CB-CG2	5.04	122.48	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	371	PHE	Peptide
2	B	392	TYR	Peptide
5	E	190	ASP	Mainchain
5	E	264	ASP	Sidechain
6	F	151	GLY	Mainchain

## 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	2160	0	2096	60	0
2	B	3805	0	3499	106	0
3	C	2438	0	2378	56	0
4	D	4535	0	4073	104	0
5	E	6622	0	5907	80	0
6	F	3404	0	3378	77	2
7	H	1576	0	1532	13	0
8	L	1599	0	1554	9	2
All	All	26139	0	24417	462	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (462) 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)
5:E:537:THR:HG22	5:E:743:ASN:HA	1.54	0.86
5:E:293:LEU:HD13	5:E:297:LEU:HD12	1.59	0.85
4:D:517:ASP:OD1	7:H:54:ASN:N	2.10	0.85
4:D:159:ILE:HG12	4:D:175:LEU:HB3	1.59	0.84
4:D:156:GLU:OE2	4:D:214:ARG:NH1	2.13	0.81
6:F:314:ILE:HG22	6:F:315:LEU:HG	1.64	0.80
4:D:155:LEU:O	4:D:159:ILE:HG13	1.82	0.80
1:A:18:ASP:OD2	2:B:548:TYR:OH	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:113:VAL:HG23	5:E:114:GLU:H	1.49	0.77
4:D:141:ASN:O	4:D:145:ASN:ND2	2.18	0.76
2:B:416:ASP:HA	2:B:443:THR:HG21	1.66	0.76
2:B:292:ILE:H	2:B:292:ILE:HD12	1.52	0.75
2:B:317:GLY:HA3	6:F:250:LEU:HD13	1.70	0.74
6:F:70:LEU:HD22	6:F:343:ILE:HD11	1.68	0.74
3:C:329:ARG:HG2	3:C:344:VAL:HG22	1.70	0.73
4:D:152:LEU:HD21	4:D:182:LEU:HB3	1.70	0.72
4:D:241:GLU:HG2	4:D:328:LEU:HD13	1.71	0.71
1:A:12:ILE:HD12	2:B:170:GLY:HA3	1.73	0.71
6:F:62:VAL:HG12	6:F:66:LYS:HE3	1.73	0.71
8:L:126:SER:O	8:L:129:LYS:HB3	1.91	0.70
5:E:404:VAL:HG11	5:E:438:GLU:HA	1.74	0.70
2:B:315:LYS:HG3	6:F:162:LEU:HB3	1.74	0.70
2:B:367:PHE:O	2:B:369:GLY:N	2.26	0.69
4:D:454:LEU:O	4:D:456:SER:N	2.26	0.69
2:B:483:GLU:CD	2:B:514:ARG:HH22	1.96	0.69
4:D:163:LYS:HB2	4:D:172:PHE:CD1	2.29	0.68
3:C:220:TRP:HA	3:C:231:ILE:HG22	1.76	0.67
3:C:102:CYS:SG	3:C:103:THR:N	2.67	0.67
3:C:161:PRO:HB2	3:C:164:HIS:CD2	2.30	0.67
8:L:193:LYS:HE3	8:L:213:ASN:HB3	1.76	0.67
3:C:306:GLU:N	3:C:324:ASP:OD2	2.27	0.66
2:B:152:ALA:HB1	2:B:160:LEU:HD11	1.78	0.66
5:E:335:VAL:HG13	5:E:352:ILE:HB	1.77	0.66
2:B:209:PRO:HB3	2:B:532:LYS:HB2	1.78	0.66
8:L:33:SER:O	8:L:35:ALA:N	2.29	0.65
4:D:119:GLY:O	4:D:122:ARG:HG2	1.97	0.65
2:B:305:VAL:HG22	6:F:242:LEU:HD22	1.78	0.65
3:C:221:ALA:HB2	3:C:312:TRP:CE2	2.31	0.65
5:E:63:SER:OG	5:E:112:GLU:OE1	2.15	0.64
6:F:8:GLN:C	6:F:10:GLU:H	1.99	0.64
6:F:13:THR:O	6:F:17:ASP:N	2.24	0.64
6:F:20:LYS:O	6:F:24:ILE:HG12	1.97	0.64
5:E:55:GLU:HB2	5:E:74:SER:HA	1.78	0.64
1:A:227:GLN:HA	1:A:256:VAL:HG13	1.79	0.63
1:A:180:ASN:HA	1:A:207:VAL:HG23	1.79	0.63
7:H:109:MET:HB3	7:H:112:LEU:HD21	1.79	0.63
3:C:85:GLU:HB2	3:C:101:LEU:HD11	1.80	0.63
2:B:318:HIS:NE2	6:F:260:GLU:OE2	2.29	0.63
3:C:313:ASN:HB2	3:C:318:ILE:H	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:829:SER:HA	5:E:841:ALA:HB1	1.81	0.62
3:C:81:VAL:HG23	3:C:111:LEU:HD13	1.81	0.62
8:L:216:GLU:O	8:L:217:CYS:HB2	1.98	0.62
4:D:265:ILE:HG21	4:D:289:ILE:HD11	1.81	0.61
2:B:300:LEU:HD23	2:B:388:LEU:HD21	1.82	0.61
4:D:170:ASN:O	4:D:174:GLU:HG3	2.00	0.61
2:B:332:ARG:NH1	6:F:213:CYS:SG	2.73	0.61
3:C:42:THR:O	3:C:44:ASN:N	2.31	0.61
5:E:119:VAL:HB	5:E:131:LEU:HB2	1.82	0.61
4:D:515:THR:HG22	4:D:516:ASN:H	1.65	0.61
4:D:148:MET:HE3	4:D:152:LEU:HG	1.83	0.60
4:D:240:PHE:O	4:D:241:GLU:HG3	2.01	0.60
2:B:297:LEU:HD23	2:B:300:LEU:HD12	1.84	0.60
2:B:519:LEU:O	2:B:529:ASN:ND2	2.34	0.60
4:D:244:TYR:O	4:D:248:LEU:HG	2.02	0.59
6:F:207:SER:HA	6:F:210:MET:HE3	1.83	0.59
2:B:525:ASP:O	2:B:528:LEU:HB2	2.02	0.59
5:E:609:GLY:O	5:E:613:ILE:HG22	2.02	0.59
2:B:426:TYR:O	2:B:464:ARG:NH2	2.36	0.59
5:E:596:PHE:CZ	5:E:704:SER:HA	2.38	0.59
5:E:91:LYS:NZ	5:E:142:ALA:O	2.30	0.59
4:D:162:VAL:O	4:D:166:ASP:HB3	2.03	0.59
2:B:152:ALA:HB1	2:B:160:LEU:CD1	2.32	0.59
1:A:217:LEU:HD22	1:A:218:LEU:H	1.69	0.58
4:D:258:LEU:HD22	4:D:292:LEU:HD22	1.85	0.58
4:D:534:ILE:O	4:D:538:ILE:HG12	2.02	0.58
3:C:123:LEU:HB2	3:C:139:ALA:HB3	1.86	0.58
4:D:163:LYS:HD2	4:D:172:PHE:CZ	2.39	0.58
4:D:520:GLU:OE2	7:H:54:ASN:ND2	2.37	0.58
2:B:321:VAL:HG11	6:F:211:ILE:HG23	1.85	0.58
5:E:185:GLY:O	5:E:196:PRO:HA	2.04	0.58
1:A:205:ASP:HB3	1:A:227:GLN:HB3	1.85	0.57
2:B:180:LEU:HD21	2:B:185:LEU:HD13	1.85	0.57
5:E:245:ILE:HB	5:E:255:GLN:HB2	1.84	0.57
6:F:280:SER:HB2	6:F:284:SER:HB3	1.86	0.57
3:C:225:GLY:O	4:D:453:ASP:HB3	2.04	0.57
6:F:433:ALA:HB1	6:F:439:SER:OG	2.05	0.57
5:E:329:TRP:HB3	5:E:355:TRP:HB3	1.85	0.57
3:C:238:GLY:HA2	3:C:305:GLY:O	2.05	0.57
5:E:342:LEU:HD13	5:E:379:ILE:HD12	1.86	0.57
5:E:101:SER:HA	5:E:123:LEU:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:343:ILE:HD13	6:F:344:ARG:N	2.19	0.57
6:F:71:GLU:OE1	6:F:75:TRP:NE1	2.36	0.57
1:A:117:LEU:HB2	1:A:153:TRP:NE1	2.20	0.56
2:B:199:THR:HB	2:B:213:GLU:HB2	1.87	0.56
4:D:159:ILE:HG22	4:D:172:PHE:CE1	2.39	0.56
4:D:145:ASN:OD1	4:D:190:PHE:HA	2.04	0.56
4:D:271:LEU:O	4:D:275:SER:HB3	2.04	0.56
5:E:659:TYR:OH	5:E:744:VAL:HA	2.05	0.56
4:D:508:LEU:HG	4:D:522:MET:HE3	1.87	0.56
5:E:288:VAL:HG12	5:E:300:MET:HB3	1.88	0.56
2:B:156:THR:HG22	2:B:514:ARG:HD2	1.88	0.56
5:E:537:THR:CG2	5:E:743:ASN:HA	2.31	0.56
4:D:536:LYS:O	4:D:540:THR:OG1	2.20	0.56
7:H:157:THR:HG22	7:H:244:SER:HB3	1.87	0.56
1:A:49:LEU:HB3	1:A:82:TRP:CZ3	2.42	0.56
6:F:34:ASP:HB3	6:F:35:PRO:HD3	1.88	0.55
4:D:159:ILE:HG21	4:D:176:GLU:HG2	1.87	0.55
2:B:256:VAL:HA	6:F:222:VAL:CG1	2.36	0.55
2:B:359:TYR:HA	2:B:362:LEU:HD12	1.86	0.55
6:F:237:ILE:HD11	6:F:240:HIS:HA	1.87	0.55
6:F:410:SER:HA	6:F:436:LEU:HD11	1.88	0.55
2:B:433:GLU:OE1	2:B:467:SER:OG	2.20	0.55
1:A:200:LEU:HD11	1:A:243:TRP:CD1	2.41	0.55
2:B:180:LEU:HD11	2:B:478:PHE:HE1	1.71	0.55
2:B:292:ILE:HD11	6:F:163:ARG:HD3	1.88	0.55
5:E:245:ILE:HG21	5:E:311:LEU:HD23	1.88	0.55
8:L:33:SER:C	8:L:35:ALA:H	2.09	0.55
1:A:95:HIS:CE1	1:A:97:VAL:HG22	2.42	0.55
4:D:163:LYS:HB2	4:D:172:PHE:CE1	2.41	0.55
3:C:15:VAL:O	4:D:70:LYS:HD2	2.07	0.55
1:A:236:GLN:HB2	1:A:243:TRP:CE3	2.42	0.55
4:D:461:MET:O	4:D:465:MET:HG3	2.07	0.55
6:F:350:VAL:HG22	6:F:355:LEU:HD22	1.90	0.54
4:D:328:LEU:O	4:D:332:ILE:HG13	2.08	0.54
1:A:212:TRP:HA	1:A:222:LEU:HD23	1.90	0.54
1:A:9:ASN:OD1	1:A:12:ILE:HD11	2.08	0.54
2:B:351:ILE:HA	6:F:155:SER:HA	1.88	0.54
2:B:525:ASP:HA	2:B:528:LEU:HD12	1.90	0.54
4:D:186:ARG:HA	4:D:190:PHE:HB2	1.90	0.54
4:D:280:VAL:HG21	4:D:321:ALA:HB3	1.89	0.54
2:B:520:ARG:NH2	2:B:542:GLN:HE21	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:102:MET:HB3	5:E:107:THR:HG21	1.89	0.54
1:A:64:PRO:HB3	2:B:548:TYR:HB2	1.90	0.54
1:A:275:ASP:OD1	1:A:275:ASP:N	2.41	0.53
6:F:341:HIS:CE1	6:F:343:ILE:HD12	2.43	0.53
4:D:265:ILE:C	4:D:267:ARG:H	2.12	0.53
2:B:186:PHE:HD1	2:B:487:LEU:HD11	1.74	0.53
3:C:128:LEU:HD23	3:C:169:PHE:HB3	1.89	0.53
3:C:53:ALA:HB1	3:C:84:TRP:CZ2	2.44	0.52
2:B:345:SER:HB3	2:B:371:PHE:CE2	2.43	0.52
2:B:520:ARG:HH21	2:B:542:GLN:HE21	1.58	0.52
2:B:336:LEU:HB3	6:F:206:ILE:HG23	1.91	0.52
2:B:256:VAL:HA	6:F:222:VAL:HG12	1.90	0.52
5:E:232:ARG:NE	5:E:249:THR:OG1	2.39	0.52
3:C:324:ASP:HB3	4:D:64:LYS:HB3	1.90	0.52
4:D:227:VAL:C	4:D:229:SER:H	2.12	0.52
1:A:178:ALA:HB1	1:A:206:TRP:CE2	2.44	0.52
1:A:154:ALA:HB2	1:A:212:TRP:CE3	2.44	0.52
6:F:431:ILE:HD12	6:F:431:ILE:H	1.74	0.52
2:B:524:ASN:O	2:B:528:LEU:HG	2.10	0.52
2:B:355:ILE:HG21	6:F:157:ASP:HB3	1.92	0.52
4:D:517:ASP:CG	7:H:53:PHE:HA	2.31	0.52
2:B:178:THR:HG21	2:B:485:ALA:HB2	1.91	0.51
5:E:739:PHE:O	5:E:743:ASN:N	2.36	0.51
1:A:117:LEU:HB2	1:A:153:TRP:HE1	1.75	0.51
1:A:214:PRO:HG2	1:A:264:LEU:HA	1.93	0.51
3:C:29:SER:C	3:C:31:GLN:H	2.13	0.51
1:A:261:SER:CB	2:B:153:LYS:HA	2.41	0.51
5:E:258:ASP:OD1	5:E:260:VAL:HG22	2.11	0.51
5:E:500:GLU:HB2	5:E:507:PHE:CZ	2.45	0.51
5:E:531:LYS:HB3	5:E:553:ILE:HG12	1.93	0.51
1:A:62:ALA:HB2	1:A:107:TRP:CE2	2.46	0.51
5:E:58:ASN:HB3	5:E:70:TYR:CZ	2.46	0.51
2:B:315:LYS:NZ	6:F:254:ALA:O	2.40	0.51
4:D:152:LEU:O	4:D:156:GLU:HG3	2.11	0.51
1:A:259:ARG:HB2	1:A:272:SER:HB2	1.93	0.51
2:B:281:ILE:HB	2:B:301:LEU:HD21	1.93	0.51
2:B:435:LEU:O	2:B:439:VAL:HG23	2.11	0.51
5:E:70:TYR:HA	5:E:80:THR:O	2.10	0.51
3:C:308:TRP:CD1	4:D:66:PRO:HA	2.46	0.51
5:E:190:ASP:OD2	5:E:191:GLY:N	2.44	0.51
2:B:186:PHE:CD1	2:B:487:LEU:HD11	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:156:GLU:HG2	4:D:179:LEU:CD2	2.41	0.50
6:F:50:ALA:HB1	6:F:69:GLU:HG3	1.93	0.50
2:B:397:GLU:N	2:B:397:GLU:OE1	2.40	0.50
3:C:117:ALA:HB3	3:C:124:LYS:HB3	1.93	0.50
4:D:107:TYR:CZ	4:D:111:LEU:HD11	2.47	0.50
5:E:288:VAL:HG13	5:E:336:LEU:HD22	1.94	0.50
2:B:374:LYS:O	2:B:377:GLU:HB2	2.11	0.50
6:F:354:SER:O	6:F:358:VAL:HG23	2.11	0.50
2:B:389:THR:O	2:B:393:GLY:HA3	2.10	0.50
3:C:10:ASP:HB3	3:C:29:SER:HB2	1.92	0.50
3:C:218:ILE:HG22	3:C:233:THR:HG22	1.94	0.50
4:D:218:GLU:HA	4:D:220:ASP:N	2.27	0.50
4:D:306:TRP:O	4:D:310:VAL:HG23	2.12	0.50
5:E:466:TYR:HB3	5:E:470:ILE:HB	1.92	0.50
1:A:57:TRP:HD1	1:A:102:VAL:O	1.94	0.50
5:E:125:ASP:OD1	5:E:127:SER:OG	2.17	0.50
3:C:67:GLU:OE1	3:C:119:ALA:HB1	2.12	0.49
4:D:110:GLY:O	4:D:114:ILE:HG13	2.12	0.49
4:D:158:PHE:O	4:D:162:VAL:HG23	2.12	0.49
6:F:233:THR:HG22	6:F:234:GLN:O	2.12	0.49
8:L:40:GLN:HB2	8:L:50:LEU:HD11	1.93	0.49
1:A:138:PRO:HB2	1:A:140:ILE:HD11	1.93	0.49
6:F:379:ILE:HG13	6:F:385:LEU:HD23	1.94	0.49
2:B:523:THR:HA	2:B:526:HIS:HB2	1.95	0.49
4:D:60:LYS:C	4:D:62:GLY:H	2.14	0.49
1:A:174:VAL:HA	1:A:183:LYS:O	2.13	0.49
4:D:278:CYS:SG	4:D:323:ASP:HB2	2.53	0.49
5:E:53:GLY:HA2	5:E:73:SER:HA	1.94	0.49
1:A:181:LEU:HD23	1:A:201:GLU:HG2	1.95	0.49
2:B:317:GLY:O	2:B:320:SER:HB3	2.13	0.49
2:B:483:GLU:OE2	2:B:514:ARG:NH2	2.35	0.49
1:A:229:ARG:HB2	1:A:229:ARG:HH11	1.78	0.48
1:A:272:SER:OG	2:B:152:ALA:HB3	2.13	0.48
3:C:77:TYR:HA	3:C:110:SER:HB3	1.95	0.48
1:A:118:VAL:O	1:A:125:VAL:HA	2.14	0.48
2:B:182:ARG:HD2	2:B:449:GLN:OE1	2.13	0.48
5:E:160:VAL:HG23	5:E:161:ARG:N	2.28	0.48
5:E:522:ASN:O	5:E:526:ARG:HG3	2.12	0.48
2:B:173:ILE:H	2:B:173:ILE:HD12	1.78	0.48
5:E:967:PHE:HA	5:E:978:ALA:HB2	1.95	0.48
6:F:349:SER:OG	6:F:358:VAL:HG21	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:ASP:OD1	3:C:32:HIS:HB2	2.13	0.48
4:D:228:PHE:HE2	4:D:267:ARG:HB3	1.77	0.48
3:C:311:SER:O	3:C:319:LEU:HD12	2.13	0.48
3:C:312:TRP:CZ3	3:C:319:LEU:HB2	2.48	0.48
1:A:38:VAL:O	1:A:39:GLU:HG3	2.14	0.48
4:D:262:ILE:HG12	4:D:289:ILE:HG23	1.96	0.48
5:E:24:VAL:HG11	5:E:143:ASN:HA	1.95	0.48
5:E:233:TYR:CG	5:E:311:LEU:HD22	2.49	0.47
2:B:262:LYS:NZ	2:B:398:TYR:O	2.36	0.47
5:E:188:LYS:HE2	5:E:191:GLY:HA2	1.95	0.47
5:E:247:ASP:O	5:E:251:PHE:N	2.47	0.47
3:C:324:ASP:HB3	4:D:64:LYS:HD3	1.95	0.47
1:A:43:HIS:CD2	2:B:173:ILE:HD11	2.50	0.47
3:C:34:LYS:HG2	3:C:50:SER:HB2	1.95	0.47
4:D:152:LEU:HD22	4:D:179:LEU:HD12	1.97	0.47
3:C:159:ILE:O	3:C:161:PRO:HD3	2.15	0.47
5:E:160:VAL:HG23	5:E:161:ARG:H	1.79	0.47
5:E:24:VAL:HG23	5:E:93:ILE:HG23	1.95	0.47
6:F:431:ILE:N	6:F:431:ILE:HD12	2.30	0.47
6:F:293:ILE:HD11	6:F:327:VAL:HG21	1.97	0.47
7:H:31:VAL:O	7:H:48:CYS:HA	2.14	0.47
3:C:312:TRP:CE2	3:C:319:LEU:HD13	2.50	0.47
4:D:186:ARG:HG3	4:D:190:PHE:HB2	1.97	0.47
4:D:392:GLN:HB3	4:D:393:PRO:HD3	1.96	0.47
5:E:163:PRO:HA	5:E:178:LEU:HA	1.95	0.47
2:B:270:THR:OG1	2:B:391:CYS:SG	2.72	0.47
6:F:157:ASP:OD1	6:F:163:ARG:NH2	2.46	0.47
4:D:249:LEU:O	4:D:253:VAL:HG23	2.15	0.47
6:F:86:ASN:OD1	6:F:400:ASN:ND2	2.48	0.47
2:B:304:VAL:HG13	2:B:323:ILE:HG22	1.97	0.47
3:C:219:SER:HG	3:C:312:TRP:HD1	1.61	0.47
5:E:570:LEU:O	5:E:574:LEU:HB2	2.15	0.47
6:F:207:SER:O	6:F:211:ILE:HG13	2.15	0.47
6:F:431:ILE:H	6:F:431:ILE:CD1	2.28	0.47
3:C:140:LEU:O	3:C:142:PRO:HD3	2.15	0.46
1:A:227:GLN:OE1	1:A:256:VAL:HG11	2.15	0.46
3:C:236:LYS:HG3	3:C:306:GLU:OE1	2.15	0.46
2:B:256:VAL:HG13	6:F:222:VAL:O	2.15	0.46
2:B:309:LYS:HE3	6:F:314:ILE:HD12	1.98	0.46
1:A:12:ILE:HA	1:A:28:SER:HA	1.96	0.46
2:B:319:LEU:HB2	6:F:159:ASP:OD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:VAL:HG12	3:C:63:TRP:HD1	1.81	0.46
3:C:196:ARG:HH11	3:C:202:LEU:HD21	1.78	0.46
2:B:431:ASN:HB2	2:B:434:LYS:HB3	1.96	0.46
4:D:226:GLN:O	4:D:230:VAL:HG23	2.15	0.46
1:A:12:ILE:HG23	1:A:27:CYS:O	2.15	0.46
4:D:223:TYR:HA	4:D:226:GLN:HB2	1.96	0.46
6:F:8:GLN:O	6:F:10:GLU:N	2.48	0.46
2:B:156:THR:HG22	2:B:514:ARG:CD	2.45	0.46
5:E:490:VAL:HG22	5:E:590:GLN:HG3	1.97	0.46
1:A:16:VAL:HG21	1:A:59:VAL:O	2.16	0.46
1:A:259:ARG:NH1	2:B:151:PHE:HB2	2.30	0.46
5:E:177:PHE:CD1	5:E:183:LEU:HD22	2.51	0.46
2:B:526:HIS:C	2:B:528:LEU:N	2.68	0.46
1:A:116:LEU:O	1:A:127:VAL:HA	2.16	0.46
1:A:95:HIS:NE2	1:A:138:PRO:HB3	2.31	0.46
2:B:360:LYS:HG3	2:B:366:PRO:HA	1.97	0.46
2:B:526:HIS:C	2:B:530:ARG:HD2	2.36	0.46
3:C:208:LEU:HD11	3:C:231:ILE:CD1	2.46	0.46
4:D:268:SER:HB2	4:D:269:ASP:OD1	2.17	0.45
4:D:97:ARG:HB3	4:D:97:ARG:NH1	2.32	0.45
2:B:325:TYR:OH	6:F:210:MET:O	2.21	0.45
6:F:433:ALA:O	6:F:435:PHE:N	2.44	0.45
6:F:219:LEU:HD22	6:F:227:ILE:HG12	1.98	0.45
4:D:97:ARG:NH2	4:D:411:SER:O	2.50	0.45
8:L:123:PRO:HD3	8:L:135:VAL:HG22	1.98	0.45
2:B:492:LEU:HD12	2:B:508:ILE:HD13	1.96	0.45
4:D:152:LEU:CD2	4:D:182:LEU:HB3	2.44	0.45
4:D:453:ASP:OD1	4:D:499:ALA:HB1	2.17	0.45
7:H:43:SER:HA	7:H:109:MET:O	2.16	0.45
2:B:178:THR:HG22	2:B:180:LEU:H	1.81	0.45
2:B:352:ASP:HB3	2:B:355:ILE:HD13	1.98	0.45
3:C:124:LYS:HG3	3:C:138:ASP:OD1	2.17	0.45
5:E:291:LEU:HA	5:E:292:PRO:HD3	1.76	0.45
5:E:643:ASP:OD2	5:E:646:ILE:HG13	2.17	0.45
6:F:144:TRP:CH2	6:F:158:LEU:HA	2.51	0.45
1:A:16:VAL:HG23	1:A:59:VAL:HG23	1.98	0.45
4:D:153:ASN:HA	4:D:156:GLU:OE1	2.16	0.45
5:E:4:LEU:HB2	5:E:381:SER:HB2	1.96	0.45
2:B:393:GLY:O	2:B:394:GLN:HB2	2.17	0.45
3:C:208:LEU:HD11	3:C:231:ILE:HD11	1.97	0.45
6:F:284:SER:O	6:F:288:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:513:MET:HG2	2:B:541:ALA:HB2	1.99	0.45
4:D:198:GLU:HG2	4:D:300:SER:CB	2.47	0.45
4:D:268:SER:O	4:D:272:PRO:HG2	2.16	0.45
5:E:436:HIS:NE2	5:E:438:GLU:HB2	2.31	0.45
1:A:18:ASP:OD1	1:A:18:ASP:N	2.46	0.45
5:E:130:THR:O	5:E:150:PHE:HA	2.17	0.45
6:F:143:LYS:HG3	6:F:144:TRP:N	2.32	0.45
4:D:322:THR:HG23	4:D:329:ARG:HD3	1.97	0.44
1:A:43:HIS:HD2	2:B:173:ILE:HD11	1.82	0.44
3:C:296:LEU:HD21	3:C:299:GLU:HG3	1.98	0.44
7:H:155:ALA:HB3	7:H:187:PHE:CE1	2.52	0.44
5:E:623:LEU:HA	5:E:623:LEU:HD23	1.74	0.44
6:F:116:LEU:O	6:F:119:ILE:HB	2.17	0.44
6:F:264:TYR:O	6:F:268:SER:OG	2.34	0.44
6:F:81:LEU:HD13	6:F:85:ARG:NH2	2.32	0.44
4:D:285:VAL:O	4:D:289:ILE:HG13	2.18	0.44
4:D:406:LEU:HB2	4:D:407:PRO:HD3	1.98	0.44
6:F:8:GLN:C	6:F:10:GLU:N	2.68	0.44
7:H:28:VAL:HG11	7:H:143:TYR:CE1	2.53	0.44
3:C:31:GLN:OE1	3:C:52:ARG:NH1	2.50	0.44
4:D:202:SER:HA	4:D:297:LYS:O	2.18	0.44
5:E:247:ASP:HB2	5:E:254:ILE:HG13	1.98	0.44
1:A:257:LEU:HA	1:A:273:GLY:HA2	1.98	0.44
5:E:352:ILE:HD13	5:E:471:ILE:HG12	1.99	0.44
5:E:658:HIS:HA	5:E:661:GLN:OE1	2.18	0.44
1:A:35:ILE:HB	1:A:47:ASP:HB2	2.00	0.44
2:B:391:CYS:O	2:B:395:ILE:HD11	2.17	0.44
5:E:534:ASP:HA	5:E:537:THR:OG1	2.18	0.44
4:D:141:ASN:N	4:D:141:ASN:HD22	2.16	0.44
5:E:668:TYR:CZ	5:E:672:LYS:HE3	2.53	0.44
7:H:125:THR:HG23	7:H:141:LEU:HD23	1.99	0.44
2:B:256:VAL:HG22	6:F:222:VAL:O	2.18	0.44
2:B:392:TYR:O	2:B:394:GLN:N	2.44	0.44
3:C:107:SER:HA	3:C:135:ARG:HH21	1.83	0.44
5:E:218:SER:OG	5:E:219:ASP:N	2.50	0.44
5:E:427:LEU:HD13	5:E:442:TYR:CE1	2.53	0.44
2:B:311:ALA:HB1	2:B:316:ASN:O	2.18	0.43
4:D:328:LEU:HA	4:D:331:TYR:HB2	2.00	0.43
6:F:106:GLU:O	6:F:110:MET:HG2	2.18	0.43
2:B:394:GLN:HG2	2:B:397:GLU:HB2	2.00	0.43
6:F:385:LEU:O	6:F:389:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:297:LEU:HA	5:E:297:LEU:HD23	1.88	0.43
2:B:333:ILE:HG23	6:F:210:MET:SD	2.59	0.43
1:A:52:HIS:CE1	1:A:80:LEU:HD12	2.53	0.43
2:B:319:LEU:N	6:F:159:ASP:OD2	2.29	0.43
6:F:390:THR:O	6:F:394:ILE:HG12	2.19	0.43
2:B:309:LYS:CE	6:F:314:ILE:HD12	2.48	0.43
4:D:221:GLU:HA	4:D:224:ILE:HG13	2.00	0.43
4:D:58:ILE:HG22	4:D:59:GLU:N	2.33	0.43
5:E:736:ASN:C	5:E:738:ARG:H	2.21	0.43
8:L:6:GLN:HB2	8:L:29:SER:HB3	2.01	0.43
1:A:63:HIS:CD2	1:A:64:PRO:HD2	2.53	0.43
2:B:400:LEU:HB3	2:B:426:TYR:OH	2.18	0.43
3:C:303:HIS:HA	3:C:325:ASP:OD2	2.19	0.43
5:E:508:LYS:O	5:E:512:THR:HG23	2.19	0.43
6:F:109:LEU:HD23	6:F:298:ILE:HG13	2.00	0.43
4:D:243:GLN:O	4:D:247:LYS:HG3	2.19	0.43
4:D:390:TRP:C	4:D:393:PRO:HD2	2.39	0.43
6:F:82:LEU:HD23	6:F:82:LEU:HA	1.87	0.43
8:L:194:VAL:HG22	8:L:213:ASN:ND2	2.34	0.43
3:C:131:ASP:OD2	3:C:135:ARG:NH2	2.51	0.43
4:D:511:TYR:HA	4:D:512:PRO:HD3	1.73	0.43
6:F:77:LEU:HG	6:F:125:TRP:CD2	2.54	0.43
7:H:117:THR:HG23	7:H:151:THR:HA	2.01	0.43
4:D:335:PHE:O	4:D:339:ILE:HG13	2.19	0.43
4:D:215:SER:HB2	4:D:390:TRP:CH2	2.54	0.43
4:D:215:SER:HB2	4:D:390:TRP:CZ2	2.53	0.43
5:E:627:TYR:HA	5:E:661:GLN:OE1	2.19	0.43
1:A:261:SER:HB2	2:B:153:LYS:HA	2.01	0.42
1:A:45:LEU:HB2	2:B:168:LYS:HE2	2.01	0.42
1:A:280:LEU:HB2	1:A:292:ALA:O	2.19	0.42
2:B:345:SER:HB3	2:B:371:PHE:HE2	1.84	0.42
2:B:531:LEU:O	2:B:532:LYS:HG2	2.19	0.42
6:F:227:ILE:C	6:F:229:ASN:H	2.22	0.42
6:F:293:ILE:HD11	6:F:327:VAL:CG2	2.49	0.42
6:F:86:ASN:C	6:F:88:ASP:H	2.23	0.42
2:B:208:TYR:CE2	2:B:505:GLU:HG3	2.54	0.42
2:B:247:TYR:CE2	2:B:260:LEU:HD13	2.54	0.42
2:B:513:MET:HA	2:B:541:ALA:HB1	2.02	0.42
3:C:313:ASN:HA	3:C:313:ASN:HD22	1.61	0.42
4:D:454:LEU:HD21	4:D:503:VAL:HG21	2.01	0.42
2:B:418:PRO:HB3	2:B:445:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:295:ASN:ND2	5:E:329:TRP:O	2.52	0.42
6:F:341:HIS:HA	6:F:342:PRO:HD3	1.89	0.42
5:E:180:ASP:HA	5:E:220:TYR:CD1	2.55	0.42
5:E:177:PHE:HD1	5:E:183:LEU:HD22	1.84	0.42
2:B:203:ARG:NE	2:B:210:GLN:HB2	2.34	0.42
4:D:168:ARG:HD3	4:D:170:ASN:HB3	2.02	0.42
5:E:53:GLY:HA3	5:E:71:HIS:HB3	2.02	0.42
5:E:92:THR:HG21	5:E:479:TYR:OH	2.19	0.42
3:C:76:SER:HB3	3:C:78:ASP:OD1	2.19	0.42
4:D:149:GLU:HG3	4:D:186:ARG:NE	2.34	0.42
4:D:159:ILE:HD13	4:D:176:GLU:HA	2.01	0.42
5:E:386:LEU:HD23	5:E:621:GLN:HA	2.01	0.42
2:B:365:SER:HB3	2:B:368:GLU:HB2	2.01	0.42
2:B:452:TRP:CD1	2:B:475:THR:HA	2.54	0.42
3:C:189:GLU:HA	3:C:213:SER:O	2.20	0.42
4:D:57:PRO:HB3	4:D:91:TYR:OH	2.19	0.42
5:E:111:GLN:HG3	5:E:168:TYR:CG	2.55	0.42
1:A:222:LEU:O	1:A:233:ILE:HA	2.20	0.42
3:C:192:ILE:HG22	3:C:207:LYS:HG2	2.02	0.42
5:E:436:HIS:CD2	5:E:438:GLU:H	2.37	0.42
6:F:23:LYS:HD2	6:F:434:THR:HG21	2.01	0.42
1:A:60:ASP:H	1:A:70:LEU:CD1	2.33	0.42
5:E:153:GLN:OE1	5:E:193:HIS:HA	2.20	0.42
5:E:59:CYS:HB2	5:E:464:THR:OG1	2.19	0.42
5:E:287:LEU:O	5:E:300:MET:HA	2.20	0.41
6:F:22:PHE:CG	6:F:38:ILE:HD11	2.54	0.41
4:D:269:ASP:N	4:D:269:ASP:OD1	2.53	0.41
4:D:78:ASN:HD21	4:D:95:ILE:HG13	1.85	0.41
6:F:104:LEU:HG	6:F:224:ASP:HB3	2.02	0.41
6:F:359:ILE:HD13	6:F:389:VAL:HG13	2.02	0.41
7:H:102:LYS:HB3	7:H:102:LYS:HE2	1.87	0.41
2:B:216:LEU:O	2:B:217:LEU:HD23	2.19	0.41
3:C:77:TYR:HD1	3:C:110:SER:HB3	1.86	0.41
3:C:131:ASP:O	3:C:133:ILE:HG13	2.20	0.41
3:C:175:PRO:HD3	3:C:220:TRP:HB3	2.02	0.41
5:E:117:LEU:HA	5:E:117:LEU:HD23	1.90	0.41
7:H:38:VAL:HG11	7:H:112:LEU:HD13	2.02	0.41
1:A:191:ALA:C	1:A:193:THR:H	2.23	0.41
2:B:162:THR:HG22	2:B:163:LYS:N	2.35	0.41
2:B:373:LEU:HB3	2:B:376:LEU:HD12	2.02	0.41
3:C:79:LYS:HG2	3:C:109:GLY:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:SER:HB3	2:B:159:MET:H	1.85	0.41
1:A:285:LEU:HD22	2:B:440:ARG:HB3	2.02	0.41
4:D:152:LEU:HA	4:D:152:LEU:HD23	1.85	0.41
3:C:346:THR:C	4:D:51:MET:HB3	2.41	0.41
5:E:186:LEU:HA	5:E:186:LEU:HD12	1.91	0.41
6:F:81:LEU:HD12	6:F:350:VAL:HG12	2.00	0.41
4:D:141:ASN:C	4:D:145:ASN:HD22	2.24	0.41
4:D:396:ASP:OD1	4:D:401:LYS:HE3	2.20	0.41
2:B:263:LYS:HA	2:B:263:LYS:HD3	1.75	0.41
3:C:144:ASP:C	3:C:146:ARG:H	2.24	0.41
4:D:141:ASN:C	4:D:145:ASN:ND2	2.74	0.41
4:D:373:GLU:O	4:D:377:MET:HG3	2.21	0.41
4:D:57:PRO:HB2	4:D:82:ILE:HD11	2.03	0.41
5:E:167:PHE:O	5:E:174:SER:HB2	2.21	0.41
2:B:247:TYR:CZ	2:B:260:LEU:HD13	2.56	0.41
4:D:403:HIS:O	4:D:405:ILE:HG23	2.20	0.41
1:A:223:ALA:HB2	1:A:262:TRP:CZ2	2.55	0.41
2:B:375:GLU:C	2:B:377:GLU:H	2.24	0.41
1:A:63:HIS:HD2	1:A:65:LYS:H	1.68	0.41
4:D:240:PHE:CD1	4:D:268:SER:HB3	2.56	0.41
5:E:169:VAL:HG13	5:E:228:LEU:HD22	2.03	0.41
1:A:261:SER:HB2	2:B:153:LYS:HG2	2.03	0.40
3:C:86:GLU:HB2	3:C:98:TRP:CZ2	2.56	0.40
4:D:145:ASN:OD1	4:D:190:PHE:CA	2.69	0.40
4:D:159:ILE:HG12	4:D:175:LEU:CB	2.40	0.40
4:D:531:LEU:HB3	4:D:534:ILE:CG1	2.51	0.40
6:F:13:THR:O	6:F:17:ASP:HB2	2.21	0.40
1:A:217:LEU:HD13	1:A:218:LEU:N	2.36	0.40
1:A:225:VAL:CG2	1:A:271:LEU:HD22	2.51	0.40
4:D:291:LEU:HD13	4:D:310:VAL:HG22	2.03	0.40
4:D:246:TRP:CD1	4:D:331:TYR:CD2	3.09	0.40
6:F:425:LEU:HD23	6:F:425:LEU:HA	1.90	0.40
1:A:17:LEU:HG	2:B:161:LEU:HD11	2.03	0.40
3:C:16:VAL:HG12	3:C:63:TRP:CD1	2.55	0.40
4:D:105:SER:HB2	4:D:481:LEU:HD21	2.03	0.40
4:D:97:ARG:HB3	4:D:97:ARG:HH11	1.86	0.40
5:E:19:GLU:HA	5:E:20:PRO:HD3	1.99	0.40
1:A:59:VAL:HB	1:A:70:LEU:HD11	2.03	0.40
1:A:23:ARG:NH1	1:A:84:GLU:OE1	2.54	0.40
2:B:187:ASP:OD1	2:B:187:ASP:C	2.60	0.40
4:D:352:THR:OG1	4:D:355:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:LEU:HD11	2:B:508:ILE:HG23	2.04	0.40
4:D:334:ASP:HB3	4:D:349:TYR:HE2	1.86	0.40
6:F:343:ILE:HD13	6:F:344:ARG:H	1.85	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:233:THR:OG1	8:L:203:GLY:O[4_455]	2.05	0.15
6:F:232:ASN:O	8:L:205:SER:N[4_455]	2.08	0.12

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	270/297 (91%)	228 (84%)	36 (13%)	6 (2%)	8	44
2	B	491/652 (75%)	451 (92%)	30 (6%)	10 (2%)	9	46
3	C	303/349 (87%)	266 (88%)	31 (10%)	6 (2%)	9	46
4	D	592/715 (83%)	532 (90%)	50 (8%)	10 (2%)	11	50
5	E	858/1045 (82%)	798 (93%)	49 (6%)	11 (1%)	14	56
6	F	413/454 (91%)	368 (89%)	34 (8%)	11 (3%)	6	40
7	H	213/271 (79%)	206 (97%)	7 (3%)	0	100	100
8	L	206/217 (95%)	198 (96%)	6 (3%)	2 (1%)	18	61
All	All	3346/4000 (84%)	3047 (91%)	243 (7%)	56 (2%)	11	50

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	158	SER

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Mol	Chain	Res	Type
2	B	368	GLU
2	B	371	PHE
2	B	394	GLN
3	C	43	SER
4	D	272	PRO
4	D	403	HIS
4	D	455	PHE
6	F	9	THR
6	F	11	ARG
6	F	138	ASN
6	F	165	ASN
8	L	34	SER
1	A	218	LEU
2	B	180	LEU
2	B	348	GLY
2	B	429	ASN
2	B	527	ILE
3	C	162	ALA
3	C	302	ASP
4	D	62	GLY
4	D	239	VAL
5	E	113	VAL
5	E	598	LYS
5	E	602	ILE
6	F	8	GLN
6	F	55	ASN
6	F	141	THR
6	F	354	SER
8	L	129	LYS
3	C	120	HIS
4	D	404	SER
5	E	264	ASP
6	F	434	THR
6	F	440	ASP
2	B	531	LEU
3	C	213	SER
5	E	284	ASN
5	E	346	ALA
6	F	87	ALA
1	A	114	PRO
1	A	131	LYS
4	D	53	VAL

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Mol	Chain	Res	Type
4	D	200	ASN
4	D	364	TYR
5	E	190	ASP
5	E	600	ASP
1	A	247	LEU
3	C	188	LEU
5	E	231	GLU
5	E	500	GLU
2	B	393	GLY
5	E	737	ILE
1	A	202	GLY
4	D	191	ILE
1	A	97	VAL

### 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	233/252 (92%)	224 (96%)	9 (4%)	37	66
2	B	367/594 (62%)	332 (90%)	35 (10%)	10	36
3	C	269/305 (88%)	261 (97%)	8 (3%)	46	72
4	D	424/642 (66%)	414 (98%)	10 (2%)	54	78
5	E	639/980 (65%)	616 (96%)	23 (4%)	40	68
6	F	387/418 (93%)	367 (95%)	20 (5%)	27	59
7	H	175/224 (78%)	170 (97%)	5 (3%)	48	73
8	L	184/191 (96%)	179 (97%)	5 (3%)	50	74
All	All	2678/3606 (74%)	2563 (96%)	115 (4%)	33	64

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	22	LYS

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Mol	Chain	Res	Type
1	A	43	HIS
1	A	46	ILE
1	A	47	ASP
1	A	225	VAL
1	A	227	GLN
1	A	229	ARG
1	A	275	ASP
2	B	160	LEU
2	B	175	ARG
2	B	214	SER
2	B	216	LEU
2	B	225	MET
2	B	234	LEU
2	B	251	THR
2	B	308	SER
2	B	319	LEU
2	B	328	SER
2	B	336	LEU
2	B	341	LEU
2	B	346	THR
2	B	349	CYS
2	B	351	ILE
2	B	368	GLU
2	B	370	LEU
2	B	371	PHE
2	B	400	LEU
2	B	402	SER
2	B	406	SER
2	B	408	LEU
2	B	412	SER
2	B	419	ILE
2	B	440	ARG
2	B	443	THR
2	B	456	GLN
2	B	464	ARG
2	B	467	SER
2	B	516	ILE
2	B	522	SER
2	B	524	ASN
2	B	531	LEU
2	B	539	PHE
2	B	547	ARG

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Mol	Chain	Res	Type
3	C	80	THR
3	C	138	ASP
3	C	168	ASP
3	C	226	ARG
3	C	301	ASP
3	C	313	ASN
3	C	314	LEU
3	C	334	THR
4	D	51	MET
4	D	143	THR
4	D	239	VAL
4	D	269	ASP
4	D	324	ILE
4	D	453	ASP
4	D	488	LEU
4	D	496	THR
4	D	516	ASN
4	D	539	TYR
5	E	63	SER
5	E	72	PHE
5	E	127	SER
5	E	172	GLN
5	E	183	LEU
5	E	209	THR
5	E	230	HIS
5	E	270	PHE
5	E	280	LEU
5	E	305	VAL
5	E	314	THR
5	E	335	VAL
5	E	338	ARG
5	E	370	ASP
5	E	408	PHE
5	E	422	ARG
5	E	590	GLN
5	E	600	ASP
5	E	628	ARG
5	E	638	VAL
5	E	644	THR
5	E	703	ASP
5	E	706	ASN
6	F	17	ASP

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Mol	Chain	Res	Type
6	F	26	GLN
6	F	58	ASP
6	F	71	GLU
6	F	77	LEU
6	F	86	ASN
6	F	88	ASP
6	F	118	GLN
6	F	141	THR
6	F	166	THR
6	F	237	ILE
6	F	268	SER
6	F	274	GLN
6	F	284	SER
6	F	343	ILE
6	F	357	SER
6	F	365	MET
6	F	403	SER
6	F	422	LEU
6	F	431	ILE
7	H	45	ARG
7	H	113	ARG
7	H	124	ARG
7	H	170	LYS
7	H	219	LEU
8	L	8	THR
8	L	27	ARG
8	L	53	SER
8	L	108	GLU
8	L	148	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	43	HIS
1	A	63	HIS
2	B	210	GLN
2	B	329	ASN
2	B	536	GLN
2	B	542	GLN
3	C	313	ASN
4	D	467	ASN

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Mol	Chain	Res	Type
5	E	255	GLN
5	E	284	ASN
5	E	295	ASN
5	E	350	ASN
5	E	575	ASN
5	E	588	ASN
6	F	97	HIS
8	L	213	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	274/297 (92%)	15.07	272 (99%) 0 1	629, 712, 763, 800	0
2	B	511/652 (78%)	9.33	459 (89%) 0 2	374, 655, 746, 784	0
3	C	307/349 (87%)	10.24	290 (94%) 0 1	631, 756, 814, 905	0
4	D	620/715 (86%)	9.98	581 (93%) 0 1	388, 746, 989, 1000	0
5	E	896/1045 (85%)	8.87	726 (81%) 0 2	422, 725, 816, 883	0
6	F	419/454 (92%)	12.15	373 (89%) 0 2	545, 699, 803, 877	0
7	H	217/271 (80%)	8.87	189 (87%) 0 2	528, 677, 821, 884	0
8	L	210/217 (96%)	8.38	185 (88%) 0 2	526, 676, 756, 791	0
All	All	3454/4000 (86%)	10.12	3075 (89%) 0 2	374, 711, 890, 1000	0

All (3075) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	ASP	75.7
5	E	519	THR	62.9
1	A	27	CYS	59.4
1	A	100	ALA	58.7
2	B	153	LYS	56.3
1	A	15	ALA	54.0
1	A	12	ILE	51.9
6	F	356	PRO	49.0
1	A	228	ASP	48.3
1	A	104	SER	47.3
1	A	102	VAL	46.0
4	D	467	ASN	45.7
6	F	357	SER	44.6
6	F	359	ILE	44.2
4	D	219	PRO	43.7
5	E	608	ASP	43.4

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Mol	Chain	Res	Type	RSRZ
5	E	689	GLY	43.2
6	F	15	PHE	42.9
1	A	77	GLY	42.8
2	B	432	THR	42.8
7	H	185	ASP	42.6
1	A	103	ASN	42.4
7	H	186	TYR	41.8
5	E	518	SER	41.8
4	D	73	PRO	41.4
5	E	604	ALA	40.2
4	D	495	GLY	39.1
6	F	355	LEU	39.1
1	A	150	SER	39.1
3	C	229	GLN	37.9
3	C	21	GLY	37.6
2	B	428	ALA	37.4
1	A	28	SER	37.3
6	F	68	TRP	37.2
7	H	110	ASN	37.0
1	A	229	ARG	37.0
1	A	101	SER	36.8
5	E	563	GLU	36.8
6	F	50	ALA	36.7
4	D	459	ASN	36.7
6	F	360	HIS	36.6
5	E	517	ALA	36.3
8	L	130	SER	35.3
1	A	149	ASN	35.3
5	E	522	ASN	34.9
6	F	100	ASN	34.7
1	A	252	LYS	33.9
1	A	255	ASP	33.7
7	H	160	PRO	33.6
6	F	67	ASP	33.4
6	F	349	SER	33.4
1	A	151	ALA	33.4
3	C	130	ASN	33.3
6	F	49	LEU	33.2
1	A	253	PHE	33.2
6	F	404	VAL	32.9
3	C	292	LEU	32.8
1	A	32	THR	32.4

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Mol	Chain	Res	Type	RSRZ
6	F	46	ALA	32.3
1	A	256	VAL	32.1
6	F	350	VAL	32.0
5	E	690	VAL	31.9
1	A	95	HIS	31.7
3	C	195	GLN	31.4
4	D	463	SER	31.4
4	D	631	SER	31.3
4	D	238	LYS	31.3
5	E	876	LEU	31.3
4	D	673	PRO	31.2
4	D	320	SER	31.1
6	F	358	VAL	31.1
4	D	72	GLY	31.0
1	A	121	SER	30.9
5	E	849	ALA	30.9
1	A	98	HIS	30.8
1	A	74	SER	30.8
4	D	460	GLY	30.8
6	F	397	ASP	30.6
5	E	514	ASN	30.4
6	F	339	SER	30.4
3	C	223	SER	30.4
1	A	76	ASP	30.3
5	E	691	LYS	30.3
6	F	19	LEU	30.3
5	E	757	GLU	30.2
4	D	242	THR	30.1
3	C	246	THR	29.8
1	A	230	THR	29.8
5	E	743	ASN	29.8
6	F	42	PHE	29.8
6	F	354	SER	29.7
6	F	71	GLU	29.7
4	D	632	GLN	29.6
5	E	396	ASP	29.6
5	E	572	ASP	29.6
2	B	151	PHE	29.5
4	D	714	ILE	29.5
1	A	204	SER	29.5
5	E	520	LEU	29.3
8	L	54	ALA	29.3

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Mol	Chain	Res	Type	RSRZ
6	F	362	SER	29.3
1	A	227	GLN	29.1
2	B	472	ASP	29.0
4	D	500	LYS	28.9
2	B	171	VAL	28.7
1	A	26	THR	28.7
6	F	402	GLY	28.6
6	F	86	ASN	28.6
1	A	249	LYS	28.2
6	F	69	GLU	28.1
2	B	499	ASN	27.9
6	F	361	SER	27.9
3	C	18	ASP	27.9
5	E	397	ILE	27.8
2	B	278	GLY	27.8
6	F	39	ILE	27.7
1	A	56	VAL	27.6
8	L	128	LEU	27.4
5	E	541	PRO	27.3
1	A	147	GLY	27.3
4	D	394	CYS	27.2
6	F	364	GLU	27.2
6	F	53	LEU	27.2
1	A	120	SER	27.0
6	F	148	ILE	27.0
4	D	468	SER	26.9
5	E	549	LYS	26.9
1	A	58	ARG	26.7
6	F	431	ILE	26.7
6	F	432	TYR	26.6
2	B	158	SER	26.6
5	E	875	LEU	26.6
2	B	170	GLY	26.5
2	B	471	SER	26.5
6	F	403	SER	26.5
3	C	65	SER	26.5
2	B	349	CYS	26.4
6	F	363	VAL	26.3
7	H	218	SER	26.3
2	B	152	ALA	26.2
4	D	321	ALA	26.2
5	E	848	SER	26.2

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Mol	Chain	Res	Type	RSRZ
5	E	536	ILE	26.1
5	E	515	GLY	26.1
5	E	966	CYS	26.0
2	B	541	ALA	25.9
5	E	537	THR	25.9
3	C	316	GLY	25.8
1	A	263	SER	25.8
1	A	259	ARG	25.7
2	B	544	LEU	25.7
5	E	561	GLN	25.6
4	D	220	ASP	25.6
6	F	72	ALA	25.5
5	E	548	GLU	25.5
5	E	566	ASN	25.4
7	H	111	SER	25.4
7	H	159	GLY	25.4
5	E	452	ASP	25.3
4	D	454	LEU	25.3
5	E	968	ARG	25.2
3	C	17	TYR	25.2
6	F	52	ASP	25.1
1	A	79	VAL	25.1
1	A	106	GLN	25.0
6	F	55	ASN	25.0
4	D	540	THR	24.9
1	A	205	ASP	24.9
6	F	400	ASN	24.9
2	B	642	LYS	24.7
3	C	67	GLU	24.6
1	A	226	SER	24.6
6	F	150	SER	24.6
5	E	841	ALA	24.6
6	F	75	TRP	24.6
7	H	217	TYR	24.6
2	B	155	SER	24.4
6	F	36	PHE	24.4
4	D	162	VAL	24.4
4	D	300	SER	24.3
4	D	494	THR	24.2
4	D	496	THR	24.2
8	L	10	SER	24.2
3	C	182	LYS	24.1

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Mol	Chain	Res	Type	RSRZ
5	E	603	SER	24.1
6	F	401	PRO	24.1
3	C	176	SER	24.1
1	A	248	LEU	24.1
4	D	456	SER	24.0
6	F	275	GLU	24.0
4	D	541	THR	24.0
5	E	562	PHE	24.0
4	D	391	GLU	23.9
5	E	709	VAL	23.8
6	F	221	PRO	23.8
1	A	29	SER	23.8
4	D	239	VAL	23.8
5	E	521	SER	23.8
1	A	31	LYS	23.8
1	A	257	LEU	23.7
4	D	350	SER	23.7
6	F	433	ALA	23.7
6	F	65	SER	23.7
2	B	427	ALA	23.6
2	B	470	THR	23.6
1	A	57	TRP	23.5
5	E	580	PRO	23.5
6	F	395	CYS	23.4
5	E	565	THR	23.4
5	E	760	PHE	23.4
4	D	382	ASN	23.4
5	E	540	LEU	23.4
8	L	124	SER	23.4
5	E	840	PHE	23.4
4	D	180	THR	23.3
4	D	78	ASN	23.3
4	D	229	SER	23.3
8	L	53	SER	23.3
2	B	665	ILE	23.2
5	E	564	ILE	23.2
1	A	109	PRO	23.2
5	E	535	ILE	23.2
3	C	228	TYR	23.2
5	E	551	THR	23.2
4	D	74	LEU	23.1
5	E	659	TYR	23.1

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Mol	Chain	Res	Type	RSRZ
5	E	398	VAL	23.0
3	C	291	ASN	23.0
5	E	843	LYS	23.0
6	F	224	ASP	22.9
6	F	11	ARG	22.9
7	H	173	SER	22.9
1	A	231	CYS	22.9
2	B	157	GLY	22.9
6	F	16	SER	22.9
6	F	35	PRO	22.9
6	F	64	SER	22.8
2	B	178	THR	22.8
3	C	110	SER	22.8
2	B	543	ALA	22.8
5	E	399	THR	22.8
6	F	54	ALA	22.8
4	D	260	GLN	22.7
2	B	506	ASP	22.7
5	E	207	SER	22.7
2	B	510	ARG	22.6
6	F	384	TYR	22.6
5	E	736	ASN	22.6
4	D	236	GLY	22.6
4	D	216	ASP	22.5
5	E	687	SER	22.5
6	F	23	LYS	22.4
8	L	126	SER	22.4
1	A	246	THR	22.4
5	E	201	ASP	22.4
4	D	116	ARG	22.4
1	A	265	SER	22.3
7	H	252	VAL	22.3
5	E	662	PHE	22.3
4	D	497	ARG	22.2
4	D	77	GLN	22.2
2	B	156	THR	22.2
1	A	99	SER	22.2
3	C	181	GLU	22.2
4	D	453	ASP	22.1
5	E	648	GLY	22.1
5	E	877	ILE	22.1
4	D	538	ILE	22.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	E	208	LEU	22.1
6	F	396	LEU	22.0
4	D	241	GLU	22.0
6	F	70	LEU	22.0
5	E	560	ASN	22.0
4	D	112	PHE	22.0
3	C	225	GLY	22.0
4	D	259	SER	22.0
1	A	78	LYS	21.9
1	A	148	VAL	21.9
6	F	12	PHE	21.9
4	D	218	GLU	21.9
4	D	499	ALA	21.9
5	E	607	PHE	21.9
6	F	220	ASN	21.8
1	A	290	GLU	21.8
1	A	119	ALA	21.8
4	D	529	TRP	21.7
2	B	664	GLU	21.7
4	D	165	GLN	21.5
6	F	38	ILE	21.5
1	A	250	GLU	21.5
3	C	149	THR	21.5
3	C	324	ASP	21.4
5	E	568	LYS	21.4
5	E	552	ASP	21.3
3	C	226	ARG	21.3
3	C	245	ILE	21.3
6	F	277	LEU	21.3
5	E	538	GLY	21.3
3	C	293	GLN	21.3
5	E	542	ASP	21.3
4	D	213	ASN	21.3
2	B	281	ILE	21.2
5	E	652	SER	21.2
3	C	119	ALA	21.2
5	E	545	THR	21.2
7	H	216	LEU	21.2
1	A	251	GLU	21.2
8	L	6	GLN	21.1
8	L	123	PRO	21.1
2	B	169	SER	21.1

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Mol	Chain	Res	Type	RSRZ
1	A	110	HIS	21.0
6	F	387	ARG	21.0
6	F	229	ASN	21.0
7	H	241	HIS	21.0
1	A	55	PRO	20.9
5	E	533	LEU	20.8
7	H	221	SER	20.8
4	D	711	GLU	20.8
8	L	5	ILE	20.8
5	E	575	ASN	20.7
6	F	333	SER	20.7
5	E	403	ASP	20.7
4	D	237	LYS	20.7
1	A	13	HIS	20.6
4	D	712	THR	20.6
2	B	393	GLY	20.6
1	A	54	GLY	20.6
3	C	68	TYR	20.6
5	E	723	PHE	20.5
5	E	842	LEU	20.5
5	E	645	GLU	20.5
2	B	285	ILE	20.4
2	B	668	LYS	20.4
6	F	22	PHE	20.4
2	B	431	ASN	20.4
6	F	435	PHE	20.4
3	C	122	GLY	20.4
1	A	289	TRP	20.3
4	D	319	SER	20.3
3	C	102	CYS	20.3
2	B	337	ALA	20.2
4	D	301	SER	20.1
6	F	18	THR	20.1
3	C	196	ARG	20.1
2	B	500	ASP	20.1
6	F	146	ASN	20.1
2	B	274	VAL	20.0
1	A	96	ALA	20.0
4	D	322	THR	20.0
6	F	43	ARG	20.0
6	F	321	ALA	20.0
6	F	272	PRO	19.9

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Mol	Chain	Res	Type	RSRZ
3	C	222	PRO	19.9
1	A	129	GLU	19.9
5	E	627	TYR	19.9
6	F	56	SER	19.9
2	B	162	THR	19.9
4	D	176	GLU	19.8
1	A	118	VAL	19.8
5	E	851	TYR	19.8
6	F	326	GLU	19.8
3	C	174	CYS	19.8
2	B	542	GLN	19.7
4	D	498	SER	19.7
5	E	546	THR	19.7
5	E	682	ASP	19.7
1	A	178	ALA	19.7
5	E	85	SER	19.7
5	E	221	ASP	19.7
5	E	720	PHE	19.6
6	F	391	HIS	19.6
3	C	221	ALA	19.6
1	A	113	GLY	19.6
4	D	717	ASP	19.5
5	E	952	ASN	19.5
2	B	340	GLN	19.5
2	B	391	CYS	19.5
7	H	220	SER	19.5
4	D	352	THR	19.4
3	C	216	ARG	19.4
5	E	658	HIS	19.4
5	E	739	PHE	19.4
2	B	270	THR	19.4
2	B	503	ALA	19.4
6	F	40	ARG	19.4
2	B	435	LEU	19.4
1	A	284	ASN	19.4
3	C	103	THR	19.4
4	D	217	GLY	19.3
5	E	708	ASN	19.3
5	E	213	SER	19.3
4	D	501	LYS	19.3
4	D	326	GLY	19.3
4	D	224	ILE	19.3

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Mol	Chain	Res	Type	RSRZ
6	F	274	GLN	19.3
5	E	544	MET	19.3
2	B	443	THR	19.3
6	F	415	THR	19.3
1	A	51	GLY	19.3
5	E	143	ASN	19.3
4	D	277	THR	19.2
7	H	41	GLY	19.2
1	A	52	HIS	19.2
5	E	646	ILE	19.2
6	F	336	PRO	19.2
4	D	177	GLU	19.2
8	L	131	GLY	19.1
1	A	137	SER	19.1
6	F	73	ARG	19.1
7	H	112	LEU	19.1
7	H	42	GLY	19.0
5	E	76	SER	19.0
6	F	47	GLY	19.0
3	C	118	PRO	19.0
4	D	318	GLY	19.0
5	E	404	VAL	19.0
6	F	329	ASN	18.9
1	A	292	ALA	18.9
3	C	313	ASN	18.9
2	B	345	SER	18.9
5	E	222	SER	18.9
8	L	71	GLY	18.9
6	F	82	LEU	18.9
3	C	314	LEU	18.8
4	D	110	GLY	18.8
6	F	439	SER	18.7
7	H	233	GLN	18.7
4	D	710	TYR	18.7
4	D	299	SER	18.7
4	D	475	SER	18.7
2	B	363	SER	18.6
5	E	737	ILE	18.6
2	B	284	LYS	18.6
2	B	505	GLU	18.6
6	F	78	VAL	18.6
6	F	399	ILE	18.6

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Mol	Chain	Res	Type	RSRZ
8	L	185	SER	18.6
2	B	347	GLY	18.6
4	D	215	SER	18.5
3	C	64	ALA	18.5
4	D	223	TYR	18.5
8	L	34	SER	18.5
1	A	291	PRO	18.5
4	D	539	TYR	18.5
5	E	965	TYR	18.5
4	D	455	PHE	18.5
4	D	526	CYS	18.4
5	E	878	HIS	18.4
6	F	165	ASN	18.4
5	E	906	GLN	18.4
2	B	210	GLN	18.4
2	B	348	GLY	18.4
6	F	393	ALA	18.4
5	E	653	THR	18.4
7	H	40	PRO	18.3
5	E	539	GLU	18.3
4	D	230	VAL	18.3
7	H	113	ARG	18.3
4	D	713	ILE	18.3
8	L	132	THR	18.3
3	C	150	LEU	18.3
6	F	434	THR	18.3
4	D	327	GLU	18.3
4	D	135	ASN	18.3
6	F	347	MET	18.2
4	D	276	ASP	18.2
8	L	36	VAL	18.2
4	D	214	ARG	18.2
4	D	160	GLY	18.2
5	E	141	SER	18.2
1	A	215	THR	18.2
8	L	125	ASP	18.1
7	H	210	VAL	18.1
6	F	337	SER	18.1
1	A	266	GLY	18.1
2	B	163	LYS	18.1
2	B	404	VAL	18.1
3	C	244	LYS	18.1

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Mol	Chain	Res	Type	RSRZ
1	A	108	ALA	18.1
4	D	583	GLY	18.1
5	E	982	TYR	18.1
7	H	158	LYS	18.0
5	E	683	SER	18.0
8	L	55	SER	18.0
3	C	179	SER	18.0
1	A	112	TYR	18.0
1	A	73	CYS	18.0
6	F	222	VAL	18.0
5	E	209	THR	17.9
5	E	978	ALA	17.9
6	F	341	HIS	17.9
6	F	430	PRO	17.9
5	E	181	GLY	17.9
6	F	278	GLN	17.9
4	D	225	GLU	17.9
1	A	247	LEU	17.9
5	E	874	ASN	17.9
5	E	410	ASN	17.8
6	F	332	ALA	17.8
6	F	273	ASN	17.8
5	E	850	GLU	17.8
5	E	180	ASP	17.8
2	B	469	GLU	17.8
8	L	93	GLN	17.8
1	A	208	ARG	17.8
4	D	582	GLU	17.8
5	E	656	ASP	17.8
1	A	105	VAL	17.7
5	E	707	SER	17.7
6	F	416	TYR	17.7
6	F	414	THR	17.7
5	E	650	HIS	17.7
2	B	282	GLU	17.7
6	F	340	GLU	17.7
7	H	191	VAL	17.7
1	A	206	TRP	17.7
5	E	706	ASN	17.6
5	E	504	SER	17.6
4	D	715	GLU	17.6
1	A	209	ASP	17.6

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Mol	Chain	Res	Type	RSRZ
2	B	288	SER	17.6
1	A	261	SER	17.6
2	B	333	ILE	17.6
6	F	66	LYS	17.6
8	L	8	THR	17.6
3	C	151	THR	17.6
5	E	661	GLN	17.5
1	A	282	LYS	17.5
5	E	142	ALA	17.5
6	F	79	GLU	17.5
5	E	963	LYS	17.5
5	E	969	MET	17.4
2	B	338	GLU	17.4
4	D	179	LEU	17.4
4	D	351	ARG	17.4
5	E	657	LEU	17.4
4	D	570	SER	17.4
6	F	236	GLY	17.4
3	C	109	GLY	17.4
5	E	202	ASN	17.4
5	E	910	GLN	17.3
5	E	666	ASN	17.3
5	E	710	TYR	17.3
1	A	254	PRO	17.3
2	B	154	PHE	17.3
6	F	87	ALA	17.3
6	F	37	ASN	17.3
1	A	264	LEU	17.3
3	C	131	ASP	17.2
3	C	217	SER	17.2
7	H	235	TYR	17.2
4	D	393	PRO	17.2
6	F	83	VAL	17.2
5	E	852	SER	17.2
3	C	308	TRP	17.2
3	C	315	THR	17.2
2	B	433	GLU	17.2
6	F	151	GLY	17.2
5	E	759	MET	17.1
2	B	405	GLN	17.1
4	D	464	TYR	17.1
3	C	312	TRP	17.1

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Mol	Chain	Res	Type	RSRZ
5	E	593	PRO	17.1
3	C	230	LEU	17.1
4	D	71	LEU	17.1
7	H	246	THR	17.1
6	F	59	GLU	17.1
1	A	136	THR	17.1
6	F	99	TYR	17.1
5	E	950	SER	17.1
4	D	257	LEU	17.1
4	D	672	TYR	17.1
4	D	166	ASP	17.1
8	L	7	MET	17.1
2	B	669	ILE	17.1
8	L	48	LYS	17.0
7	H	212	GLN	17.0
5	E	844	CYS	17.0
4	D	75	SER	17.0
4	D	243	GLN	17.0
2	B	160	LEU	16.9
5	E	893	HIS	16.9
2	B	501	ASP	16.9
6	F	428	ASN	16.9
6	F	164	GLU	16.9
3	C	205	ALA	16.9
6	F	147	SER	16.9
7	H	206	THR	16.9
5	E	722	THR	16.9
1	A	97	VAL	16.9
2	B	266	HIS	16.8
4	D	471	PHE	16.8
3	C	180	PRO	16.8
5	E	200	ASN	16.8
4	D	390	TRP	16.8
4	D	381	ALA	16.8
2	B	639	SER	16.8
8	L	186	LYS	16.8
1	A	94	VAL	16.7
6	F	62	VAL	16.7
2	B	303	ASP	16.7
4	D	235	ALA	16.7
2	B	466	PHE	16.7
6	F	170	ASP	16.7

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Mol	Chain	Res	Type	RSRZ
6	F	20	LYS	16.7
1	A	288	LYS	16.6
8	L	162	SER	16.6
2	B	661	MET	16.6
4	D	641	ASP	16.6
8	L	32	VAL	16.6
2	B	514	ARG	16.6
8	L	100	THR	16.6
5	E	742	GLU	16.6
1	A	30	ASP	16.5
3	C	175	PRO	16.5
2	B	330	ASP	16.5
6	F	436	LEU	16.5
5	E	655	LEU	16.5
5	E	763	THR	16.5
3	C	203	HIS	16.5
4	D	181	VAL	16.5
2	B	504	ALA	16.5
2	B	459	ARG	16.4
6	F	429	ILE	16.4
8	L	28	ALA	16.4
1	A	146	ILE	16.4
5	E	569	ILE	16.4
1	A	260	ALA	16.3
2	B	662	SER	16.3
3	C	247	GLU	16.3
5	E	409	CYS	16.3
5	E	921	THR	16.3
3	C	144	ASP	16.3
4	D	226	GLN	16.3
2	B	408	LEU	16.3
6	F	228	ALA	16.3
2	B	159	MET	16.2
6	F	113	ASN	16.2
5	E	741	LEU	16.2
4	D	329	ARG	16.2
1	A	16	VAL	16.2
5	E	644	THR	16.2
6	F	408	ASP	16.2
8	L	163	GLN	16.2
1	A	9	ASN	16.1
4	D	315	GLN	16.1

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Mol	Chain	Res	Type	RSRZ
5	E	879	PHE	16.1
2	B	346	THR	16.1
6	F	322	LEU	16.1
4	D	156	GLU	16.1
4	D	458	ARG	16.1
6	F	111	GLN	16.1
1	A	171	ARG	16.1
5	E	719	PHE	16.1
2	B	394	GLN	16.1
5	E	516	PHE	16.1
5	E	775	GLU	16.0
8	L	29	SER	16.0
5	E	523	ASP	16.0
2	B	206	ASN	16.0
7	H	152	VAL	16.0
2	B	467	SER	16.0
3	C	214	LEU	16.0
1	A	214	PRO	16.0
4	D	388	ASN	16.0
2	B	708	CYS	16.0
8	L	67	GLY	16.0
5	E	740	PHE	16.0
7	H	209	ALA	16.0
6	F	58	ASP	16.0
5	E	581	VAL	16.0
6	F	223	ILE	16.0
5	E	534	ASP	16.0
2	B	179	GLU	15.9
2	B	364	GLY	15.9
2	B	441	GLN	15.9
2	B	641	MET	15.9
6	F	420	LEU	15.9
5	E	967	PHE	15.9
4	D	96	PRO	15.9
7	H	187	PHE	15.9
3	C	309	SER	15.9
2	B	334	ARG	15.9
1	A	122	ASP	15.8
3	C	317	THR	15.8
3	C	79	LYS	15.8
2	B	640	GLY	15.8
5	E	437	ASN	15.8

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Mol	Chain	Res	Type	RSRZ
2	B	498	LEU	15.8
4	D	502	MET	15.8
6	F	152	GLY	15.8
1	A	75	TYR	15.8
6	F	270	ALA	15.8
8	L	69	ARG	15.8
6	F	353	ASP	15.8
5	E	198	LEU	15.7
8	L	72	THR	15.7
5	E	953	LEU	15.7
1	A	155	PRO	15.7
6	F	394	ILE	15.7
4	D	424	CYS	15.7
2	B	660	VAL	15.7
3	C	202	LEU	15.7
4	D	228	PHE	15.7
2	B	328	SER	15.6
4	D	171	ARG	15.6
5	E	249	THR	15.6
4	D	133	ASN	15.6
4	D	178	SER	15.6
5	E	73	SER	15.6
5	E	724	PHE	15.6
4	D	504	ILE	15.6
2	B	545	LYS	15.6
2	B	256	VAL	15.6
2	B	208	TYR	15.6
7	H	155	ALA	15.5
4	D	240	PHE	15.5
4	D	584	GLN	15.5
5	E	571	PHE	15.5
4	D	221	GLU	15.5
5	E	559	GLU	15.5
4	D	644	GLN	15.5
7	H	215	GLY	15.5
3	C	311	SER	15.5
4	D	222	GLU	15.5
8	L	127	GLN	15.5
2	B	329	ASN	15.4
5	E	951	GLN	15.4
2	B	280	GLU	15.4
3	C	227	TRP	15.4

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Mol	Chain	Res	Type	RSRZ
5	E	686	PHE	15.4
8	L	70	SER	15.4
4	D	378	SER	15.4
5	E	981	LEU	15.4
2	B	406	SER	15.4
4	D	347	LEU	15.3
6	F	149	THR	15.3
2	B	203	ARG	15.3
4	D	537	GLU	15.3
5	E	526	ARG	15.3
5	E	567	LEU	15.3
1	A	59	VAL	15.3
7	H	237	CYS	15.3
6	F	45	ALA	15.3
5	E	606	LYS	15.3
6	F	57	GLY	15.3
2	B	290	ASN	15.3
7	H	93	ARG	15.3
4	D	275	SER	15.2
6	F	85	ARG	15.2
4	D	634	TYR	15.2
4	D	114	ILE	15.2
5	E	845	ILE	15.2
2	B	343	LYS	15.2
4	D	183	ASN	15.2
4	D	302	THR	15.2
5	E	846	SER	15.2
5	E	556	ASN	15.1
4	D	325	SER	15.1
6	F	406	GLU	15.1
3	C	152	SER	15.1
5	E	219	ASP	15.1
3	C	138	ASP	15.1
5	E	663	LEU	15.1
6	F	76	HIS	15.1
6	F	409	LYS	15.1
3	C	238	GLY	15.1
6	F	8	GLN	15.1
6	F	61	ASN	15.1
5	E	100	ALA	15.0
6	F	438	GLU	15.0
5	E	903	ASN	15.0

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Mol	Chain	Res	Type	RSRZ
1	A	117	LEU	15.0
3	C	188	LEU	15.0
1	A	93	ALA	15.0
5	E	448	THR	15.0
5	E	16	GLU	15.0
5	E	15	TYR	15.0
5	E	716	GLU	15.0
4	D	492	SER	15.0
5	E	210	ARG	14.9
5	E	555	LYS	14.9
2	B	663	GLN	14.9
5	E	407	GLY	14.9
4	D	413	ASP	14.9
3	C	94	SER	14.9
6	F	383	PRO	14.9
6	F	410	SER	14.9
2	B	243	ASP	14.9
4	D	466	LEU	14.9
1	A	245	LYS	14.9
5	E	609	GLY	14.8
6	F	413	ILE	14.8
3	C	20	TYR	14.8
4	D	392	GLN	14.8
2	B	540	ASN	14.8
4	D	716	ALA	14.8
8	L	11	PRO	14.8
5	E	66	GLU	14.8
5	E	912	ASP	14.8
6	F	153	LEU	14.8
6	F	112	ASP	14.8
5	E	979	GLU	14.8
5	E	1030	LEU	14.8
5	E	405	GLU	14.8
3	C	306	GLU	14.8
5	E	891	LEU	14.7
1	A	50	THR	14.7
6	F	379	ILE	14.7
5	E	371	GLU	14.6
7	H	166	ALA	14.6
2	B	486	GLN	14.6
2	B	484	PHE	14.6
1	A	283	GLU	14.6

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Mol	Chain	Res	Type	RSRZ
4	D	687	SER	14.6
2	B	344	TRP	14.6
5	E	212	PHE	14.6
2	B	314	SER	14.5
1	A	281	TRP	14.5
4	D	113	GLU	14.5
4	D	172	PHE	14.5
1	A	235	THR	14.5
8	L	73	ASP	14.5
2	B	342	GLN	14.5
3	C	120	HIS	14.5
2	B	507	THR	14.5
1	A	138	PRO	14.5
6	F	348	ALA	14.5
8	L	68	SER	14.4
8	L	165	SER	14.4
6	F	417	ILE	14.4
6	F	84	PHE	14.4
5	E	717	ASN	14.4
5	E	250	SER	14.3
5	E	326	SER	14.3
4	D	474	CYS	14.3
4	D	525	ILE	14.3
5	E	761	ALA	14.3
4	D	580	CYS	14.3
5	E	196	PRO	14.3
4	D	708	ASN	14.3
6	F	237	ILE	14.3
1	A	213	SER	14.2
2	B	176	LEU	14.2
5	E	773	SER	14.2
5	E	394	ASP	14.2
6	F	172	LYS	14.2
1	A	258	TRP	14.2
7	H	167	PRO	14.2
2	B	229	SER	14.2
1	A	267	ASN	14.2
3	C	290	SER	14.2
5	E	584	ASN	14.2
5	E	524	VAL	14.2
4	D	514	VAL	14.2
6	F	334	ARG	14.2

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Mol	Chain	Res	Type	RSRZ
5	E	205	LEU	14.2
5	E	602	ILE	14.1
2	B	277	ILE	14.1
7	H	208	PRO	14.1
7	H	244	SER	14.1
4	D	134	SER	14.1
2	B	424	GLN	14.1
6	F	226	GLN	14.1
4	D	99	ASP	14.0
5	E	726	SER	14.0
2	B	659	ASN	14.0
2	B	161	LEU	14.0
1	A	270	ALA	14.0
4	D	294	GLN	14.0
3	C	343	SER	14.0
4	D	93	VAL	14.0
3	C	224	ILE	13.9
1	A	202	GLY	13.9
2	B	468	LYS	13.9
4	D	304	ARG	13.9
6	F	97	HIS	13.9
3	C	90	GLN	13.9
5	E	670	GLN	13.9
3	C	210	GLY	13.9
8	L	187	ALA	13.9
5	E	588	ASN	13.9
5	E	413	SER	13.8
1	A	203	HIS	13.8
8	L	25	THR	13.8
5	E	745	GLU	13.8
2	B	407	HIS	13.8
3	C	136	LEU	13.8
5	E	190	ASP	13.8
6	F	225	THR	13.8
4	D	462	ALA	13.8
6	F	330	ARG	13.8
2	B	473	GLU	13.8
5	E	1029	ASP	13.7
7	H	154	SER	13.7
2	B	485	ALA	13.7
5	E	764	LEU	13.7
7	H	238	ASN	13.7

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Mol	Chain	Res	Type	RSRZ
5	E	947	SER	13.7
6	F	25	GLU	13.7
1	A	274	GLY	13.7
3	C	310	VAL	13.7
4	D	470	ALA	13.7
7	H	87	ALA	13.7
4	D	669	LYS	13.7
4	D	726	THR	13.7
7	H	214	SER	13.7
4	D	105	SER	13.6
8	L	35	ALA	13.6
7	H	184	LYS	13.6
7	H	189	GLU	13.6
5	E	673	CYS	13.6
4	D	278	CYS	13.6
2	B	149	TYR	13.6
5	E	438	GLU	13.6
7	H	156	SER	13.6
1	A	90	SER	13.6
2	B	341	LEU	13.6
2	B	389	THR	13.6
6	F	94	MET	13.6
5	E	203	SER	13.5
1	A	126	SER	13.5
2	B	667	SER	13.5
5	E	432	ILE	13.5
4	D	66	PRO	13.5
6	F	167	ASN	13.5
8	L	164	GLU	13.5
5	E	660	LYS	13.5
4	D	324	ILE	13.5
5	E	503	GLY	13.5
5	E	902	THR	13.5
1	A	91	GLN	13.5
5	E	204	TYR	13.5
5	E	905	LEU	13.5
7	H	114	ALA	13.5
2	B	403	LEU	13.5
5	E	756	GLN	13.5
5	E	839	GLU	13.4
4	D	581	MET	13.4
6	F	365	MET	13.4

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Mol	Chain	Res	Type	RSRZ
5	E	964	LEU	13.4
3	C	213	SER	13.4
4	D	95	ILE	13.4
3	C	121	LEU	13.4
5	E	780	HIS	13.4
4	D	293	LYS	13.4
5	E	455	THR	13.4
8	L	66	SER	13.4
2	B	657	CYS	13.4
4	D	248	LEU	13.4
5	E	772	GLN	13.4
3	C	237	ASP	13.4
1	A	220	SER	13.4
5	E	55	GLU	13.4
7	H	43	SER	13.4
5	E	649	GLN	13.4
6	F	96	LEU	13.4
4	D	477	GLY	13.3
6	F	14	LYS	13.3
5	E	140	SER	13.3
6	F	88	ASP	13.3
5	E	406	ARG	13.3
4	D	725	ALA	13.3
4	D	323	ASP	13.3
5	E	468	ASP	13.3
2	B	177	PRO	13.3
4	D	628	ALA	13.2
6	F	366	LEU	13.2
7	H	161	SER	13.2
2	B	464	ARG	13.2
6	F	101	SER	13.2
5	E	680	LEU	13.2
1	A	152	SER	13.1
1	A	128	VAL	13.1
1	A	153	TRP	13.1
1	A	60	ASP	13.1
5	E	847	LYS	13.1
3	C	197	GLY	13.1
1	A	154	ALA	13.1
6	F	41	GLU	13.1
2	B	434	LYS	13.1
5	E	592	LYS	13.1

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Mol	Chain	Res	Type	RSRZ
4	D	718	LYS	13.1
3	C	117	ALA	13.0
3	C	307	VAL	13.0
4	D	115	TYR	13.0
6	F	234	GLN	13.0
1	A	175	THR	13.0
7	H	251	LYS	13.0
8	L	4	ASP	13.0
4	D	489	ILE	13.0
5	E	688	PHE	13.0
4	D	629	VAL	13.0
4	D	111	LEU	13.0
4	D	630	LEU	13.0
5	E	412	LYS	13.0
5	E	447	GLU	13.0
6	F	271	ILE	12.9
5	E	738	ARG	12.9
4	D	92	PRO	12.9
6	F	405	GLU	12.9
6	F	124	VAL	12.9
2	B	395	ILE	12.9
5	E	776	ILE	12.9
5	E	744	VAL	12.9
4	D	709	LEU	12.9
5	E	971	ASN	12.9
5	E	573	GLU	12.8
4	D	94	ARG	12.8
2	B	614	ILE	12.8
2	B	350	SER	12.8
6	F	21	GLU	12.8
6	F	307	GLN	12.8
6	F	427	GLU	12.8
5	E	725	ARG	12.8
3	C	168	ASP	12.8
1	A	233	ILE	12.8
4	D	530	ARG	12.7
5	E	647	PHE	12.7
6	F	77	LEU	12.7
5	E	554	PHE	12.7
5	E	948	ILE	12.7
2	B	546	ASP	12.7
4	D	106	ALA	12.7

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Mol	Chain	Res	Type	RSRZ
8	L	47	PRO	12.7
4	D	298	ASP	12.7
1	A	242	PRO	12.7
4	D	210	ASN	12.6
7	H	88	ASP	12.6
5	E	430	ASN	12.6
1	A	271	LEU	12.6
2	B	265	ARG	12.6
3	C	173	TRP	12.6
3	C	235	CYS	12.6
2	B	335	ASP	12.6
4	D	159	ILE	12.6
2	B	173	ILE	12.6
4	D	640	GLU	12.6
1	A	145	ALA	12.6
7	H	116	ASP	12.6
4	D	531	LEU	12.6
6	F	276	VAL	12.6
7	H	253	GLU	12.5
6	F	17	ASP	12.5
3	C	330	LEU	12.5
5	E	681	LYS	12.5
5	E	57	SER	12.5
4	D	247	LYS	12.5
6	F	24	ILE	12.5
6	F	227	ILE	12.5
3	C	204	VAL	12.5
4	D	461	MET	12.5
5	E	576	SER	12.5
5	E	557	CYS	12.5
6	F	392	LEU	12.4
2	B	509	LYS	12.4
4	D	174	GLU	12.4
4	D	395	VAL	12.4
5	E	578	ASP	12.4
4	D	536	LYS	12.4
7	H	153	SER	12.4
5	E	458	ASN	12.4
3	C	19	PHE	12.4
5	E	502	ASP	12.4
2	B	523	THR	12.4
4	D	528	GLU	12.4

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Mol	Chain	Res	Type	RSRZ
6	F	81	LEU	12.3
5	E	25	ASP	12.3
4	D	633	PHE	12.3
4	D	432	ASN	12.3
1	A	80	LEU	12.3
4	D	117	ASP	12.3
5	E	543	SER	12.3
6	F	345	VAL	12.3
2	B	429	ASN	12.3
3	C	325	ASP	12.3
2	B	150	THR	12.3
4	D	227	VAL	12.3
5	E	172	GLN	12.3
6	F	296	THR	12.3
1	A	84	GLU	12.3
7	H	234	THR	12.3
4	D	273	TYR	12.3
2	B	513	MET	12.3
5	E	771	ASP	12.2
2	B	396	ASP	12.2
6	F	34	ASP	12.2
5	E	721	MET	12.2
4	D	674	ILE	12.2
5	E	927	ASN	12.2
6	F	269	GLY	12.2
5	E	624	SER	12.2
7	H	202	SER	12.2
3	C	345	ILE	12.2
5	E	206	LYS	12.2
1	A	135	THR	12.2
6	F	233	THR	12.2
2	B	202	ALA	12.2
6	F	175	GLU	12.2
5	E	918	PHE	12.1
5	E	654	LEU	12.1
4	D	56	GLN	12.1
3	C	124	LYS	12.1
4	D	406	LEU	12.1
7	H	195	TRP	12.1
5	E	525	LEU	12.1
2	B	352	ASP	12.1
2	B	286	ARG	12.1

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Mol	Chain	Res	Type	RSRZ
5	E	684	SER	12.1
3	C	92	GLU	12.1
3	C	234	GLY	12.1
5	E	56	TYR	12.0
8	L	9	GLN	12.0
2	B	291	GLU	12.0
2	B	331	PRO	12.0
4	D	109	SER	12.0
6	F	51	LEU	12.0
4	D	465	MET	12.0
4	D	154	GLU	12.0
3	C	326	GLY	12.0
6	F	74	PHE	12.0
4	D	153	ASN	12.0
5	E	611	THR	12.0
2	B	259	ALA	12.0
7	H	179	LEU	11.9
3	C	141	GLU	11.9
4	D	76	TYR	11.9
5	E	591	MET	11.9
4	D	568	VAL	11.9
7	H	207	PHE	11.9
3	C	333	ALA	11.9
1	A	240	GLN	11.9
4	D	101	SER	11.9
5	E	1036	GLY	11.9
5	E	907	LEU	11.9
5	E	99	ASN	11.9
8	L	103	GLN	11.9
5	E	433	ILE	11.9
1	A	177	GLY	11.9
1	A	279	THR	11.8
5	E	529	SER	11.8
2	B	93	TRP	11.8
4	D	328	LEU	11.8
7	H	89	SER	11.8
5	E	160	VAL	11.8
2	B	481	GLN	11.8
6	F	411	LYS	11.8
7	H	178	ALA	11.8
4	D	57	PRO	11.7
2	B	709	THR	11.7

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Mol	Chain	Res	Type	RSRZ
6	F	173	ASP	11.7
2	B	251	THR	11.7
6	F	344	ARG	11.7
4	D	103	GLU	11.7
7	H	222	VAL	11.7
8	L	98	PRO	11.7
4	D	255	ARG	11.7
5	E	161	ARG	11.7
6	F	219	LEU	11.7
7	H	157	THR	11.7
1	A	39	GLU	11.7
6	F	117	TYR	11.7
3	C	294	VAL	11.6
4	D	544	ASN	11.6
5	E	917	ASP	11.6
6	F	231	PHE	11.6
8	L	161	ASN	11.6
1	A	186	LYS	11.6
6	F	201	LYS	11.6
8	L	27	ARG	11.6
1	A	241	GLY	11.6
2	B	615	ASN	11.6
5	E	400	LYS	11.6
4	D	384	VAL	11.6
5	E	325	ALA	11.6
5	E	779	LEU	11.6
1	A	188	ASN	11.6
2	B	283	GLU	11.6
5	E	623	LEU	11.6
2	B	643	ILE	11.5
4	D	397	ILE	11.5
5	E	669	ARG	11.5
4	D	385	ASP	11.5
1	A	11	LEU	11.5
4	D	488	LEU	11.5
6	F	98	PRO	11.5
3	C	66	PRO	11.5
5	E	665	LEU	11.5
4	D	70	LYS	11.5
6	F	171	VAL	11.5
6	F	60	SER	11.5
3	C	1	MET	11.5

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Mol	Chain	Res	Type	RSRZ
1	A	25	ALA	11.5
1	A	262	TRP	11.5
4	D	503	VAL	11.5
4	D	161	ARG	11.5
8	L	30	GLN	11.5
4	D	251	GLN	11.5
5	E	778	GLN	11.5
4	D	396	ASP	11.5
5	E	962	LYS	11.5
5	E	451	ARG	11.5
6	F	26	GLN	11.4
4	D	642	TRP	11.4
2	B	638	ILE	11.4
3	C	305	GLY	11.4
5	E	453	VAL	11.4
6	F	323	THR	11.4
5	E	220	TYR	11.4
4	D	472	GLU	11.4
4	D	675	PHE	11.4
4	D	567	LEU	11.4
1	A	232	ILE	11.4
5	E	1031	ARG	11.4
8	L	188	ASP	11.4
2	B	666	VAL	11.4
4	D	244	TYR	11.4
1	A	187	TYR	11.4
4	D	55	ASP	11.3
4	D	104	PHE	11.3
1	A	10	GLU	11.3
2	B	475	THR	11.3
6	F	202	LEU	11.3
3	C	206	ALA	11.3
5	E	240	ASN	11.3
3	C	44	ASN	11.3
4	D	164	ASP	11.3
5	E	77	THR	11.3
6	F	426	TYR	11.3
4	D	534	ILE	11.3
5	E	983	GLN	11.3
3	C	194	TYR	11.3
3	C	346	THR	11.3
3	C	236	LYS	11.3

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Mol	Chain	Res	Type	RSRZ
1	A	278	VAL	11.3
4	D	579	SER	11.3
6	F	398	ILE	11.2
3	C	137	TYR	11.2
4	D	518	ASP	11.2
5	E	239	GLN	11.2
4	D	410	GLU	11.2
6	F	203	SER	11.2
1	A	225	VAL	11.2
3	C	299	GLU	11.2
4	D	505	ALA	11.2
4	D	527	VAL	11.2
3	C	108	LYS	11.2
6	F	385	LEU	11.2
5	E	594	GLY	11.2
6	F	319	SER	11.2
6	F	418	SER	11.2
5	E	439	ASP	11.2
2	B	263	LYS	11.2
5	E	414	ARG	11.2
6	F	419	LEU	11.2
5	E	685	GLU	11.2
8	L	129	LYS	11.1
4	D	108	VAL	11.1
4	D	662	TYR	11.1
4	D	375	LEU	11.1
1	A	111	GLU	11.1
3	C	23	HIS	11.1
5	E	774	TYR	11.1
6	F	421	LYS	11.1
4	D	252	LEU	11.1
6	F	44	SER	11.1
5	E	733	SER	11.1
4	D	198	GLU	11.1
6	F	13	THR	11.1
2	B	688	PRO	11.1
6	F	9	THR	11.1
7	H	219	LEU	11.1
1	A	40	GLY	11.1
4	D	506	GLU	11.1
5	E	216	SER	11.1
3	C	40	LYS	11.0

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Mol	Chain	Res	Type	RSRZ
5	E	651	ILE	11.0
4	D	184	CYS	11.0
7	H	201	THR	11.0
1	A	293	GLY	11.0
2	B	92	ASP	11.0
7	H	236	ILE	11.0
1	A	176	GLY	11.0
6	F	423	GLN	11.0
4	D	414	SER	11.0
2	B	476	PHE	11.0
5	E	101	SER	11.0
4	D	58	ILE	11.0
4	D	175	LEU	11.0
5	E	920	SER	10.9
3	C	212	LYS	10.9
2	B	502	LYS	10.9
5	E	445	ASN	10.9
3	C	157	LEU	10.9
3	C	318	ILE	10.9
8	L	141	ASN	10.9
8	L	155	ASN	10.9
3	C	153	GLU	10.9
4	D	476	LEU	10.9
5	E	985	ILE	10.9
1	A	64	PRO	10.9
2	B	228	THR	10.9
4	D	377	MET	10.9
4	D	524	SER	10.9
5	E	911	GLU	10.9
5	E	718	SER	10.9
5	E	1032	ASP	10.9
2	B	279	PRO	10.9
5	E	626	HIS	10.9
4	D	535	ALA	10.9
6	F	10	GLU	10.8
5	E	136	SER	10.8
1	A	63	HIS	10.8
6	F	300	ASN	10.8
5	E	746	CYS	10.8
3	C	96	ARG	10.8
5	E	970	LEU	10.8
2	B	175	ARG	10.8

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Mol	Chain	Res	Type	RSRZ
7	H	190	PRO	10.8
1	A	83	LYS	10.8
5	E	215	SER	10.8
4	D	409	MET	10.8
5	E	977	ALA	10.8
2	B	658	CYS	10.8
3	C	337	ASN	10.8
2	B	483	GLU	10.8
2	B	327	GLY	10.8
2	B	571	ALA	10.8
1	A	285	LEU	10.8
8	L	56	SER	10.7
5	E	182	GLY	10.7
6	F	424	GLY	10.7
4	D	348	GLN	10.7
1	A	19	TYR	10.7
2	B	294	GLN	10.7
1	A	114	PRO	10.7
7	H	188	PRO	10.7
3	C	43	SER	10.7
5	E	904	PHE	10.7
2	B	275	SER	10.7
6	F	285	ASP	10.7
5	E	467	GLY	10.7
6	F	154	LYS	10.7
2	B	671	GLU	10.7
2	B	387	ASN	10.7
3	C	189	GLU	10.7
4	D	512	PRO	10.7
8	L	102	GLY	10.7
6	F	325	GLN	10.7
4	D	685	GLU	10.7
5	E	901	ARG	10.7
5	E	1033	GLU	10.6
5	E	89	HIS	10.6
3	C	87	ASP	10.6
3	C	158	SER	10.6
7	H	250	LYS	10.6
5	E	558	LEU	10.6
2	B	440	ARG	10.6
2	B	397	GLU	10.6
5	E	832	PHE	10.6

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Mol	Chain	Res	Type	RSRZ
2	B	438	GLU	10.6
7	H	180	GLY	10.6
5	E	949	LEU	10.6
2	B	402	SER	10.6
3	C	143	SER	10.6
5	E	980	VAL	10.6
4	D	169	VAL	10.5
5	E	425	GLN	10.5
6	F	440	ASP	10.5
8	L	15	SER	10.5
2	B	293	GLU	10.5
2	B	260	LEU	10.5
1	A	156	ALA	10.5
1	A	33	ILE	10.5
2	B	268	ARG	10.5
8	L	176	TYR	10.5
5	E	909	LEU	10.5
1	A	180	ASN	10.5
7	H	196	ASN	10.5
4	D	52	THR	10.5
3	C	140	LEU	10.5
5	E	890	ARG	10.5
6	F	342	PRO	10.5
4	D	469	PHE	10.5
6	F	407	VAL	10.5
2	B	413	LEU	10.5
4	D	523	LEU	10.4
5	E	601	PHE	10.4
6	F	382	LYS	10.4
3	C	147	SER	10.4
7	H	109	MET	10.4
6	F	63	ILE	10.4
1	A	238	ASN	10.4
8	L	172	LYS	10.3
4	D	379	LEU	10.3
4	D	627	TYR	10.3
2	B	463	THR	10.3
8	L	177	SER	10.3
3	C	199	ASP	10.3
4	D	353	TRP	10.3
2	B	209	PRO	10.3
2	B	480	ALA	10.3

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Mol	Chain	Res	Type	RSRZ
5	E	179	GLU	10.2
1	A	127	VAL	10.2
1	A	131	LYS	10.2
3	C	3	PRO	10.2
4	D	521	TRP	10.2
4	D	643	GLY	10.2
5	E	758	PHE	10.2
6	F	230	GLU	10.2
5	E	500	GLU	10.2
2	B	465	VAL	10.2
2	B	522	SER	10.2
8	L	160	GLY	10.2
5	E	853	LEU	10.2
3	C	177	ARG	10.2
3	C	159	ILE	10.2
4	D	421	ALA	10.2
2	B	377	GLU	10.1
5	E	547	VAL	10.1
2	B	304	VAL	10.1
6	F	198	GLU	10.1
1	A	170	SER	10.1
3	C	220	TRP	10.1
1	A	144	HIS	10.1
5	E	587	ILE	10.1
6	F	343	ILE	10.1
2	B	416	ASP	10.1
2	B	635	ASP	10.1
4	D	571	TYR	10.1
7	H	199	ALA	10.1
3	C	78	ASP	10.1
1	A	287	GLY	10.1
5	E	417	THR	10.1
6	F	235	GLN	10.1
5	E	590	GLN	10.1
3	C	145	LEU	10.0
6	F	442	LEU	10.0
8	L	209	THR	10.0
5	E	191	GLY	10.0
6	F	306	ASN	10.0
1	A	268	VAL	10.0
2	B	711	LYS	10.0
4	D	457	TYR	10.0

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Mol	Chain	Res	Type	RSRZ
6	F	258	PRO	10.0
2	B	226	GLU	10.0
6	F	289	HIS	10.0
2	B	672	LYS	10.0
1	A	92	ILE	10.0
6	F	335	HIS	10.0
2	B	425	LEU	9.9
4	D	405	ILE	9.9
8	L	33	SER	9.9
5	E	162	VAL	9.9
1	A	207	VAL	9.9
7	H	108	GLN	9.9
4	D	343	GLN	9.9
7	H	183	VAL	9.9
5	E	570	LEU	9.9
5	E	14	TYR	9.9
2	B	437	LYS	9.9
8	L	31	SER	9.9
2	B	201	GLU	9.9
2	B	458	LEU	9.9
5	E	589	ASN	9.9
7	H	45	ARG	9.9
5	E	211	PHE	9.8
2	B	444	ASN	9.8
4	D	606	ILE	9.8
8	L	75	THR	9.8
8	L	74	PHE	9.8
2	B	262	LYS	9.8
3	C	344	VAL	9.8
5	E	275	ALA	9.8
3	C	298	SER	9.8
5	E	838	GLN	9.8
7	H	231	GLY	9.8
8	L	181	THR	9.8
5	E	677	GLU	9.8
3	C	339	PHE	9.8
6	F	437	ASN	9.8
5	E	444	ALA	9.8
5	E	671	ASP	9.8
2	B	707	LYS	9.8
1	A	221	TYR	9.8
2	B	656	ALA	9.8

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Mol	Chain	Res	Type	RSRZ
2	B	354	ASN	9.8
7	H	197	SER	9.8
4	D	355	GLU	9.8
1	A	139	ILE	9.8
1	A	17	LEU	9.7
5	E	88	TYR	9.7
1	A	179	ASP	9.7
6	F	308	VAL	9.7
5	E	531	LYS	9.7
5	E	434	MET	9.7
5	E	765	PHE	9.7
5	E	667	LEU	9.7
3	C	99	ASN	9.7
3	C	93	CYS	9.6
4	D	136	PHE	9.6
2	B	239	SER	9.6
5	E	928	ALA	9.6
3	C	178	PHE	9.6
2	B	548	TYR	9.6
2	B	569	GLU	9.6
2	B	426	TYR	9.6
2	B	474	ALA	9.6
3	C	242	ILE	9.6
4	D	542	LEU	9.6
6	F	92	ASP	9.6
3	C	319	LEU	9.6
4	D	125	ASN	9.6
8	L	133	ALA	9.6
3	C	91	GLU	9.6
6	F	213	CYS	9.6
2	B	442	ARG	9.5
1	A	53	GLU	9.5
3	C	80	THR	9.5
2	B	634	ILE	9.5
4	D	569	LYS	9.5
5	E	151	HIS	9.5
5	E	770	PHE	9.5
4	D	272	PRO	9.5
5	E	674	LEU	9.5
3	C	45	TRP	9.5
7	H	91	LYS	9.5
5	E	454	LYS	9.5

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Mol	Chain	Res	Type	RSRZ
7	H	205	HIS	9.5
5	E	449	ILE	9.5
3	C	123	LEU	9.5
1	A	130	PHE	9.5
6	F	293	ILE	9.5
8	L	80	SER	9.5
7	H	232	THR	9.5
5	E	192	VAL	9.4
5	E	284	ASN	9.4
6	F	163	ARG	9.4
5	E	954	ARG	9.4
8	L	44	GLY	9.4
4	D	661	HIS	9.4
5	E	643	ASP	9.4
7	H	243	PRO	9.4
6	F	232	ASN	9.4
1	A	172	LYS	9.4
4	D	173	TYR	9.4
6	F	292	GLN	9.4
6	F	320	HIS	9.4
1	A	20	TYR	9.4
1	A	239	GLU	9.4
3	C	320	SER	9.4
2	B	414	PRO	9.4
2	B	292	ILE	9.4
2	B	591	GLU	9.4
3	C	332	LYS	9.4
2	B	287	ASN	9.4
2	B	375	GLU	9.4
6	F	95	GLU	9.4
5	E	960	CYS	9.4
5	E	214	ARG	9.3
2	B	547	ARG	9.3
3	C	104	LEU	9.3
5	E	429	GLU	9.3
4	D	719	SER	9.3
3	C	200	GLY	9.3
3	C	48	SER	9.3
8	L	26	CYS	9.3
4	D	728	LEU	9.3
5	E	892	GLY	9.3
6	F	305	ASN	9.3

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Mol	Chain	Res	Type	RSRZ
4	D	100	THR	9.3
5	E	664	LEU	9.3
6	F	145	LEU	9.3
6	F	279	TYR	9.3
2	B	332	ARG	9.3
8	L	168	GLU	9.3
4	D	163	LYS	9.3
5	E	21	ASN	9.3
5	E	711	ASN	9.3
4	D	344	ARG	9.3
2	B	247	TYR	9.2
5	E	147	GLY	9.2
4	D	138	LYS	9.2
5	E	1008	SER	9.2
2	B	339	LEU	9.2
5	E	550	PHE	9.2
3	C	323	GLY	9.2
2	B	673	ASN	9.2
7	H	239	VAL	9.2
2	B	411	PHE	9.2
1	A	38	VAL	9.2
1	A	41	GLU	9.2
1	A	280	LEU	9.2
5	E	961	PHE	9.2
2	B	302	ASN	9.2
8	L	37	ALA	9.2
6	F	331	VAL	9.1
3	C	239	ARG	9.1
4	D	520	GLU	9.1
4	D	316	ALA	9.1
5	E	64	ASN	9.1
4	D	522	MET	9.1
5	E	285	ASN	9.1
3	C	170	CYS	9.1
4	D	452	GLU	9.1
4	D	609	GLN	9.1
8	L	20	ASP	9.1
3	C	100	LYS	9.1
2	B	415	TYR	9.1
5	E	231	GLU	9.1
6	F	338	GLU	9.1
5	E	86	ASP	9.1

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Mol	Chain	Res	Type	RSRZ
5	E	401	THR	9.1
7	H	245	ASN	9.1
8	L	91	CYS	9.1
5	E	527	SER	9.0
5	E	1035	ARG	9.0
8	L	175	THR	9.0
2	B	439	VAL	9.0
5	E	27	TYR	9.0
5	E	919	PHE	9.0
3	C	172	SER	9.0
5	E	1006	VAL	9.0
2	B	685	LEU	9.0
4	D	264	CYS	9.0
4	D	296	PRO	9.0
6	F	48	GLN	9.0
5	E	930	SER	9.0
4	D	430	ILE	9.0
7	H	115	GLU	9.0
7	H	117	THR	9.0
4	D	317	PHE	9.0
3	C	46	GLU	9.0
4	D	170	ASN	9.0
2	B	537	LEU	9.0
8	L	79	SER	9.0
2	B	242	PHE	9.0
6	F	390	THR	9.0
3	C	300	HIS	9.0
4	D	102	LYS	9.0
8	L	167	THR	9.0
4	D	516	ASN	9.0
2	B	400	LEU	8.9
4	D	354	TYR	8.9
1	A	65	LYS	8.9
3	C	328	VAL	8.9
2	B	455	ILE	8.9
6	F	388	ILE	8.9
4	D	638	ASP	8.9
5	E	443	LEU	8.9
6	F	389	VAL	8.9
5	E	436	HIS	8.9
1	A	42	THR	8.9
2	B	613	SER	8.9

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Mol	Chain	Res	Type	RSRZ
1	A	275	ASP	8.9
4	D	274	LEU	8.9
3	C	297	LEU	8.9
2	B	188	ASP	8.8
4	D	585	LYS	8.8
5	E	612	SER	8.8
4	D	167	GLY	8.8
5	E	1026	THR	8.8
4	D	281	SER	8.8
7	H	92	GLY	8.8
1	A	72	SER	8.8
1	A	244	LYS	8.8
5	E	913	ILE	8.8
5	E	931	ASP	8.8
2	B	572	ILE	8.8
2	B	712	ILE	8.8
6	F	425	LEU	8.8
6	F	386	LEU	8.8
7	H	68	GLY	8.7
5	E	395	LEU	8.7
6	F	441	CYS	8.7
7	H	248	VAL	8.7
5	E	585	ASP	8.7
3	C	77	TYR	8.7
7	H	142	ASP	8.7
3	C	295	GLU	8.7
5	E	693	PHE	8.7
3	C	107	SER	8.7
6	F	80	LEU	8.7
2	B	594	THR	8.7
4	D	297	LYS	8.7
4	D	261	ALA	8.7
7	H	211	LEU	8.7
2	B	398	TYR	8.7
2	B	538	ILE	8.7
5	E	512	THR	8.7
1	A	272	SER	8.7
3	C	142	PRO	8.7
7	H	181	CYS	8.7
5	E	1028	THR	8.7
7	H	249	ASP	8.7
6	F	128	GLU	8.6

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Mol	Chain	Res	Type	RSRZ
6	F	156	CYS	8.6
8	L	57	LEU	8.6
6	F	168	VAL	8.6
2	B	636	SER	8.6
8	L	180	SER	8.6
2	B	686	GLU	8.6
8	L	52	TYR	8.6
3	C	303	HIS	8.6
2	B	207	PRO	8.6
1	A	125	VAL	8.6
5	E	248	LEU	8.6
2	B	390	LEU	8.6
5	E	65	SER	8.6
5	E	157	ASP	8.6
2	B	301	LEU	8.6
5	E	150	PHE	8.6
5	E	461	SER	8.6
5	E	507	PHE	8.6
4	D	49	VAL	8.6
5	E	178	LEU	8.6
5	E	976	ALA	8.6
1	A	198	SER	8.6
5	E	929	HIS	8.6
7	H	230	LEU	8.6
4	D	137	ALA	8.6
5	E	762	MET	8.6
2	B	410	LYS	8.6
7	H	151	THR	8.6
2	B	436	TYR	8.6
3	C	335	TYR	8.5
2	B	539	PHE	8.5
3	C	146	ARG	8.5
5	E	440	GLU	8.5
3	C	187	ALA	8.5
5	E	26	LEU	8.5
2	B	644	PHE	8.5
5	E	428	SER	8.5
8	L	159	SER	8.5
5	E	995	ARG	8.5
2	B	417	ASP	8.5
5	E	999	CYS	8.5
8	L	17	SER	8.5

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Mol	Chain	Res	Type	RSRZ
2	B	244	PRO	8.4
1	A	134	GLY	8.4
3	C	101	LEU	8.4
5	E	605	ILE	8.4
1	A	140	ILE	8.4
2	B	516	ILE	8.4
5	E	149	TRP	8.4
4	D	349	TYR	8.4
1	A	85	GLU	8.4
2	B	710	TYR	8.4
6	F	129	ASN	8.4
5	E	72	PHE	8.4
8	L	140	ASN	8.4
5	E	1005	ASN	8.4
1	A	216	VAL	8.4
4	D	727	LEU	8.4
8	L	62	PRO	8.4
7	H	85	SER	8.4
2	B	240	ILE	8.3
5	E	553	ILE	8.3
6	F	141	THR	8.3
5	E	505	GLU	8.3
5	E	402	GLY	8.3
2	B	461	ASN	8.3
4	D	389	ASP	8.3
5	E	188	LYS	8.3
8	L	104	GLY	8.3
6	F	114	LYS	8.3
6	F	352	LEU	8.3
3	C	97	ARG	8.3
5	E	17	LYS	8.3
5	E	946	ASP	8.3
5	E	193	HIS	8.3
4	D	519	ILE	8.3
5	E	387	VAL	8.3
5	E	766	SER	8.3
4	D	303	PHE	8.3
5	E	620	HIS	8.3
5	E	1003	VAL	8.3
6	F	108	LYS	8.3
7	H	194	SER	8.2
8	L	150	GLN	8.2

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Mol	Chain	Res	Type	RSRZ
2	B	336	LEU	8.2
2	B	187	ASP	8.2
2	B	392	TYR	8.2
2	B	219	LYS	8.2
6	F	412	LEU	8.2
1	A	236	GLN	8.2
8	L	92	GLN	8.2
2	B	401	GLU	8.2
8	L	13	SER	8.2
2	B	212	SER	8.2
5	E	735	LYS	8.2
3	C	116	PHE	8.2
4	D	603	ASP	8.2
4	D	374	TYR	8.2
5	E	416	GLY	8.2
5	E	498	HIS	8.2
3	C	321	SER	8.2
3	C	148	TRP	8.2
2	B	271	SER	8.1
1	A	88	ARG	8.1
2	B	670	LEU	8.1
6	F	93	GLU	8.1
2	B	379	GLU	8.1
4	D	245	PHE	8.1
5	E	218	SER	8.1
1	A	201	GLU	8.1
2	B	616	VAL	8.1
8	L	19	GLY	8.1
7	H	164	PRO	8.1
5	E	497	MET	8.1
4	D	69	PHE	8.1
4	D	67	LEU	8.1
8	L	205	SER	8.1
5	E	232	ARG	8.1
5	E	90	GLY	8.1
4	D	305	GLU	8.1
7	H	213	SER	8.0
5	E	22	ASN	8.0
5	E	372	SER	8.0
2	B	456	GLN	8.0
7	H	39	GLN	8.0
7	H	229	SER	8.0

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Mol	Chain	Res	Type	RSRZ
4	D	513	PHE	8.0
6	F	218	TYR	8.0
5	E	884	GLU	8.0
6	F	176	GLU	8.0
5	E	144	THR	8.0
7	H	83	SER	8.0
5	E	894	GLU	8.0
1	A	107	TRP	8.0
5	E	1004	ILE	8.0
5	E	955	SER	8.0
1	A	81	ILE	8.0
2	B	227	LYS	8.0
5	E	435	ALA	7.9
2	B	704	ASP	7.9
4	D	139	GLU	7.9
4	D	515	THR	7.9
2	B	267	CYS	7.9
3	C	37	LYS	7.9
4	D	671	LEU	7.9
4	D	98	LEU	7.9
5	E	148	GLU	7.9
7	H	44	LEU	7.9
1	A	18	ASP	7.9
4	D	608	PRO	7.9
5	E	53	GLY	7.9
7	H	170	LYS	7.9
4	D	258	LEU	7.9
7	H	80	TYR	7.9
2	B	172	SER	7.9
1	A	269	LEU	7.9
3	C	49	ASP	7.9
4	D	604	ASP	7.9
2	B	687	LEU	7.9
2	B	255	GLN	7.9
5	E	678	VAL	7.9
4	D	263	GLY	7.8
4	D	665	LEU	7.8
2	B	325	TYR	7.8
2	B	369	GLY	7.8
6	F	155	SER	7.8
2	B	409	ASP	7.8
5	E	273	VAL	7.8

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Mol	Chain	Res	Type	RSRZ
2	B	381	SER	7.8
1	A	34	LYS	7.8
3	C	126	ALA	7.8
2	B	378	SER	7.8
7	H	240	ASN	7.8
2	B	257	LYS	7.8
5	E	908	LEU	7.8
6	F	280	SER	7.8
3	C	289	GLN	7.8
4	D	532	PRO	7.8
4	D	624	LEU	7.7
5	E	924	ARG	7.7
4	D	543	GLY	7.7
3	C	341	CYS	7.7
8	L	24	ILE	7.7
7	H	78	TYR	7.7
3	C	186	SER	7.7
4	D	605	VAL	7.7
5	E	1027	LEU	7.7
1	A	68	THR	7.7
3	C	342	MET	7.7
1	A	22	LYS	7.7
6	F	297	GLU	7.7
5	E	984	TYR	7.7
5	E	1034	LEU	7.7
4	D	732	ARG	7.7
5	E	579	ILE	7.7
4	D	490	ALA	7.7
3	C	135	ARG	7.7
6	F	204	ASP	7.7
3	C	169	PHE	7.7
8	L	99	ILE	7.6
3	C	331	TRP	7.6
2	B	276	GLN	7.6
5	E	426	ILE	7.6
1	A	286	GLU	7.6
2	B	570	MET	7.6
2	B	180	LEU	7.6
4	D	152	LEU	7.6
5	E	755	VAL	7.6
5	E	734	HIS	7.6
3	C	69	GLY	7.6

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Mol	Chain	Res	Type	RSRZ
3	C	160	PRO	7.6
4	D	269	ASP	7.6
5	E	628	ARG	7.6
2	B	316	ASN	7.6
8	L	206	SER	7.6
3	C	193	ILE	7.6
5	E	1000	TYR	7.6
4	D	51	MET	7.6
1	A	115	LEU	7.6
2	B	549	GLU	7.6
4	D	402	ILE	7.6
3	C	329	ARG	7.6
4	D	698	LYS	7.6
5	E	104	GLN	7.6
2	B	264	GLU	7.6
3	C	139	ALA	7.6
2	B	261	LEU	7.6
6	F	216	GLN	7.6
5	E	238	THR	7.5
4	D	158	PHE	7.5
8	L	198	GLU	7.5
5	E	704	SER	7.5
2	B	245	VAL	7.5
3	C	296	LEU	7.5
4	D	331	TYR	7.5
6	F	116	LEU	7.5
3	C	125	LEU	7.5
4	D	591	LEU	7.5
6	F	90	ASP	7.5
7	H	73	TRP	7.5
2	B	631	GLN	7.5
1	A	24	LEU	7.5
3	C	22	ARG	7.5
7	H	81	TYR	7.5
4	D	151	ILE	7.5
5	E	251	PHE	7.5
2	B	324	SER	7.4
4	D	493	ALA	7.4
4	D	697	THR	7.4
7	H	69	LYS	7.4
5	E	159	THR	7.4
7	H	193	VAL	7.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	380	PHE	7.4
2	B	524	ASN	7.4
7	H	165	LEU	7.4
4	D	54	ASN	7.4
2	B	706	MET	7.4
4	D	312	LYS	7.4
8	L	90	TYR	7.4
5	E	777	PHE	7.4
7	H	192	THR	7.4
4	D	473	LEU	7.4
5	E	808	TRP	7.4
4	D	383	VAL	7.3
7	H	94	PHE	7.3
1	A	21	GLY	7.3
8	L	169	GLN	7.3
4	D	150	ALA	7.3
4	D	290	GLU	7.3
5	E	475	CYS	7.3
5	E	582	VAL	7.3
2	B	592	LEU	7.3
5	E	185	GLY	7.3
3	C	201	LYS	7.3
6	F	303	LEU	7.3
5	E	596	PHE	7.3
4	D	573	TRP	7.3
8	L	83	PRO	7.3
3	C	322	ALA	7.3
8	L	108	GLU	7.3
1	A	237	ASP	7.3
2	B	249	TYR	7.3
6	F	110	MET	7.3
3	C	301	ASP	7.2
6	F	194	ASP	7.2
4	D	157	VAL	7.2
5	E	630	THR	7.2
4	D	271	LEU	7.2
2	B	557	GLN	7.2
4	D	330	ASP	7.2
6	F	380	ILE	7.2
7	H	171	SER	7.2
3	C	89	ASP	7.2
5	E	619	LEU	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	219	ARG	7.2
1	A	197	GLU	7.2
3	C	327	LYS	7.2
2	B	515	GLU	7.2
5	E	754	GLU	7.2
5	E	260	VAL	7.2
5	E	459	GLU	7.2
7	H	163	PHE	7.2
5	E	511	ARG	7.2
6	F	127	LYS	7.2
2	B	174	LYS	7.2
6	F	104	LEU	7.2
5	E	530	LYS	7.1
3	C	132	GLY	7.1
8	L	179	SER	7.1
4	D	572	SER	7.1
5	E	456	ALA	7.1
2	B	412	SER	7.1
4	D	279	ALA	7.1
1	A	8	HIS	7.1
5	E	411	LEU	7.1
4	D	107	TYR	7.1
4	D	626	PRO	7.1
1	A	48	THR	7.1
8	L	117	SER	7.1
1	A	66	PHE	7.0
3	C	129	GLY	7.0
5	E	58	ASN	7.0
5	E	74	SER	7.0
5	E	441	GLU	7.0
2	B	595	LEU	7.0
5	E	499	SER	7.0
6	F	328	LEU	7.0
2	B	511	LEU	7.0
5	E	269	HIS	7.0
6	F	254	ALA	7.0
2	B	703	GLN	7.0
5	E	139	PHE	7.0
7	H	198	GLY	7.0
5	E	75	ARG	7.0
5	E	370	ASP	7.0
5	E	462	SER	7.0

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Mol	Chain	Res	Type	RSRZ
8	L	23	THR	6.9
5	E	705	LEU	6.9
4	D	686	ASP	6.9
2	B	573	VAL	6.9
5	E	600	ASP	6.9
2	B	368	GLU	6.9
7	H	76	SER	6.9
2	B	382	TRP	6.9
1	A	173	PHE	6.9
4	D	707	SER	6.9
5	E	715	THR	6.9
7	H	228	SER	6.9
5	E	258	ASP	6.9
2	B	633	THR	6.9
8	L	183	THR	6.9
2	B	534	PRO	6.9
7	H	162	VAL	6.9
4	D	168	ARG	6.9
3	C	240	ILE	6.9
4	D	412	LEU	6.9
4	D	744	MET	6.9
5	E	13	GLN	6.8
3	C	241	ARG	6.8
8	L	189	TYR	6.8
1	A	210	VAL	6.8
5	E	164	HIS	6.8
8	L	18	VAL	6.8
7	H	70	GLY	6.8
6	F	255	GLY	6.8
7	H	71	LEU	6.8
7	H	90	VAL	6.7
3	C	63	TRP	6.7
2	B	164	ASP	6.7
5	E	369	ASN	6.7
3	C	215	ILE	6.7
2	B	273	ILE	6.7
1	A	234	TRP	6.7
2	B	246	SER	6.7
5	E	63	SER	6.7
5	E	632	GLN	6.7
1	A	224	SER	6.7
5	E	54	SER	6.7

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Mol	Chain	Res	Type	RSRZ
5	E	29	SER	6.7
2	B	289	SER	6.7
2	B	199	THR	6.7
5	E	1007	LEU	6.7
2	B	186	PHE	6.7
5	E	828	LEU	6.7
3	C	2	GLN	6.7
3	C	29	SER	6.7
2	B	252	ASP	6.7
1	A	133	ASN	6.7
5	E	28	VAL	6.7
3	C	219	SER	6.7
4	D	688	VAL	6.6
7	H	172	THR	6.6
1	A	37	GLU	6.6
4	D	308	ASN	6.6
7	H	149	LEU	6.6
8	L	82	GLN	6.6
1	A	82	TRP	6.6
2	B	682	ALA	6.6
4	D	314	SER	6.6
8	L	12	SER	6.6
8	L	166	VAL	6.6
5	E	457	PHE	6.6
7	H	67	PRO	6.6
6	F	253	GLN	6.6
6	F	166	THR	6.6
4	D	280	VAL	6.6
5	E	153	GLN	6.6
5	E	577	PHE	6.6
4	D	50	PRO	6.5
5	E	480	ASN	6.5
5	E	833	ASP	6.5
6	F	121	ILE	6.5
5	E	272	LYS	6.5
8	L	63	SER	6.5
6	F	422	LEU	6.5
5	E	508	LYS	6.5
5	E	885	VAL	6.5
6	F	174	LYS	6.5
3	C	190	GLN	6.5
3	C	154	MET	6.5

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Mol	Chain	Res	Type	RSRZ
8	L	105	THR	6.5
8	L	59	SER	6.5
3	C	71	ILE	6.5
1	A	174	VAL	6.5
4	D	517	ASP	6.5
2	B	215	SER	6.5
4	D	729	LYS	6.5
4	D	267	ARG	6.4
2	B	253	ASN	6.4
2	B	365	SER	6.4
5	E	230	HIS	6.4
4	D	356	SER	6.4
5	E	887	ASP	6.4
6	F	257	ASP	6.4
2	B	315	LYS	6.4
5	E	338	ARG	6.4
6	F	304	GLU	6.4
7	H	242	LYS	6.4
3	C	50	SER	6.4
3	C	76	SER	6.4
6	F	238	LYS	6.4
7	H	168	SER	6.4
7	H	86	TYR	6.4
4	D	451	LEU	6.3
5	E	146	ASN	6.3
3	C	106	ASP	6.3
1	A	116	LEU	6.3
2	B	399	SER	6.3
2	B	637	LEU	6.3
4	D	510	HIS	6.3
4	D	417	ALA	6.3
5	E	415	TYR	6.3
1	A	185	TRP	6.3
4	D	201	ARG	6.3
4	D	486	ILE	6.3
1	A	223	ALA	6.3
2	B	558	ASN	6.3
2	B	457	THR	6.3
4	D	120	ASP	6.3
4	D	590	VAL	6.3
5	E	532	PHE	6.3
3	C	16	VAL	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	23	ARG	6.3
5	E	359	THR	6.3
8	L	40	GLN	6.3
6	F	160	PHE	6.2
2	B	297	LEU	6.2
4	D	211	TRP	6.2
3	C	302	ASP	6.2
2	B	189	VAL	6.2
5	E	888	VAL	6.2
7	H	150	VAL	6.2
4	D	479	LYS	6.2
8	L	14	LEU	6.2
7	H	140	ALA	6.2
3	C	171	LEU	6.2
4	D	250	ASN	6.2
8	L	16	ALA	6.2
4	D	625	ALA	6.2
3	C	183	LEU	6.2
5	E	703	ASP	6.2
5	E	598	LYS	6.2
2	B	430	GLU	6.2
1	A	124	LYS	6.2
4	D	663	LEU	6.2
5	E	156	TYR	6.2
8	L	86	PHE	6.2
3	C	59	VAL	6.2
4	D	268	SER	6.2
5	E	408	PHE	6.1
2	B	205	SER	6.1
5	E	322	ASN	6.1
6	F	282	TRP	6.1
4	D	370	LEU	6.1
8	L	154	ASP	6.1
5	E	135	LEU	6.1
5	E	872	TYR	6.1
6	F	105	PHE	6.1
6	F	346	LEU	6.1
3	C	167	SER	6.1
5	E	195	GLU	6.1
8	L	134	SER	6.1
6	F	120	TRP	6.1
4	D	647	ARG	6.1

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Mol	Chain	Res	Type	RSRZ
2	B	307	ALA	6.1
4	D	434	PHE	6.1
7	H	72	GLU	6.1
3	C	38	LEU	6.1
7	H	174	GLY	6.1
8	L	43	PRO	6.1
6	F	367	LEU	6.1
4	D	149	GLU	6.1
1	A	87	GLY	6.1
4	D	420	THR	6.0
2	B	181	GLN	6.0
5	E	994	ILE	6.0
1	A	273	GLY	6.0
4	D	487	GLY	6.0
7	H	247	LYS	6.0
4	D	668	ALA	6.0
4	D	333	GLU	6.0
2	B	183	LYS	6.0
5	E	163	PRO	6.0
2	B	568	ALA	6.0
4	D	483	PRO	6.0
4	D	670	PHE	6.0
5	E	115	GLN	6.0
1	A	189	SER	6.0
5	E	357	SER	6.0
3	C	304	ASN	6.0
4	D	429	LEU	6.0
5	E	615	SER	6.0
3	C	13	HIS	6.0
4	D	282	PHE	6.0
1	A	199	THR	5.9
3	C	288	LEU	5.9
4	D	743	PHE	5.9
2	B	590	ASN	5.9
3	C	105	ASN	5.9
6	F	89	LEU	5.9
4	D	607	ILE	5.9
5	E	323	LEU	5.9
2	B	574	THR	5.9
2	B	520	ARG	5.9
5	E	199	PHE	5.9
3	C	39	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
2	B	167	GLY	5.9
5	E	996	LYS	5.9
5	E	171	PRO	5.9
3	C	95	GLY	5.9
4	D	639	ARG	5.9
4	D	623	THR	5.9
5	E	241	CYS	5.9
5	E	360	ALA	5.9
8	L	118	VAL	5.9
6	F	381	ASP	5.9
5	E	672	LYS	5.9
2	B	536	GLN	5.9
2	B	705	LEU	5.9
6	F	309	GLY	5.8
2	B	517	THR	5.8
2	B	460	PHE	5.8
3	C	334	THR	5.8
2	B	477	ALA	5.8
4	D	558	ASN	5.8
5	E	130	THR	5.8
5	E	781	ASP	5.8
2	B	359	TYR	5.8
5	E	574	LEU	5.8
4	D	380	GLU	5.8
6	F	310	THR	5.8
2	B	94	VAL	5.8
2	B	248	PRO	5.8
2	B	617	PHE	5.8
4	D	387	THR	5.8
6	F	327	VAL	5.8
8	L	156	ALA	5.8
4	D	345	LYS	5.8
6	F	142	SER	5.8
2	B	298	TYR	5.8
5	E	466	TYR	5.8
1	A	86	ASN	5.8
1	A	200	LEU	5.8
5	E	676	ALA	5.7
2	B	353	LYS	5.7
4	D	371	SER	5.7
4	D	415	CYS	5.7
4	D	478	ASP	5.7

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Mol	Chain	Res	Type	RSRZ
4	D	511	TYR	5.7
5	E	829	SER	5.7
7	H	177	ALA	5.7
8	L	158	GLN	5.7
4	D	185	LEU	5.7
2	B	306	ARG	5.7
2	B	535	SER	5.7
4	D	182	LEU	5.7
5	E	78	LEU	5.7
5	E	889	LEU	5.7
5	E	442	TYR	5.7
2	B	645	TYR	5.6
4	D	555	SER	5.6
8	L	106	LYS	5.6
4	D	306	TRP	5.6
4	D	386	ILE	5.6
2	B	258	MET	5.6
4	D	735	LEU	5.6
5	E	640	PHE	5.6
2	B	214	SER	5.6
5	E	393	HIS	5.6
8	L	101	PHE	5.6
7	H	225	VAL	5.6
6	F	123	MET	5.6
8	L	157	LEU	5.6
5	E	328	ILE	5.5
4	D	398	ILE	5.5
4	D	253	VAL	5.5
5	E	583	LEU	5.5
4	D	79	MET	5.5
6	F	125	TRP	5.5
2	B	168	LYS	5.5
5	E	155	PRO	5.5
5	E	427	LEU	5.5
6	F	301	TYR	5.5
4	D	620	MET	5.5
2	B	684	LEU	5.5
5	E	925	LEU	5.5
3	C	115	LYS	5.5
8	L	109	ILE	5.5
5	E	18	PRO	5.5
4	D	731	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
5	E	986	LEU	5.5
6	F	140	PRO	5.5
8	L	191	LYS	5.5
7	H	200	LEU	5.5
6	F	302	LEU	5.5
5	E	194	TYR	5.4
1	A	61	TRP	5.4
1	A	243	TRP	5.4
1	A	184	ILE	5.4
8	L	42	LYS	5.4
2	B	230	SER	5.4
7	H	82	GLY	5.4
3	C	133	ILE	5.4
4	D	262	ILE	5.4
5	E	327	ALA	5.4
2	B	356	SER	5.4
6	F	378	ASP	5.4
2	B	272	TRP	5.4
5	E	631	LEU	5.4
8	L	152	LYS	5.4
5	E	324	SER	5.4
4	D	342	ASN	5.4
5	E	639	LEU	5.4
4	D	425	GLU	5.4
5	E	668	TYR	5.4
8	L	77	THR	5.4
2	B	233	ASN	5.4
4	D	577	GLU	5.3
2	B	269	LEU	5.3
6	F	109	LEU	5.3
7	H	226	PRO	5.3
7	H	224	THR	5.3
2	B	462	GLY	5.3
8	L	51	ILE	5.3
5	E	528	ILE	5.3
8	L	65	PHE	5.3
2	B	683	LYS	5.3
1	A	132	GLU	5.3
4	D	332	ILE	5.3
8	L	142	PHE	5.3
3	C	166	GLN	5.3
3	C	55	ASP	5.3

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Mol	Chain	Res	Type	RSRZ
8	L	170	ASP	5.3
5	E	19	GLU	5.3
4	D	65	MET	5.3
7	H	176	THR	5.3
5	E	152	LEU	5.3
5	E	189	VAL	5.3
8	L	171	SER	5.3
4	D	401	LYS	5.3
5	E	186	LEU	5.3
4	D	419	PHE	5.3
3	C	338	GLU	5.3
5	E	197	LEU	5.3
3	C	42	THR	5.2
4	D	212	ILE	5.2
5	E	873	LEU	5.2
8	L	46	ALA	5.2
2	B	232	TYR	5.2
5	E	390	GLN	5.2
5	E	103	ASN	5.2
3	C	47	LEU	5.2
3	C	248	LYS	5.2
2	B	374	LYS	5.2
4	D	484	VAL	5.2
5	E	895	CYS	5.2
4	D	742	ALA	5.2
5	E	638	VAL	5.2
4	D	83	THR	5.2
1	A	89	TRP	5.2
3	C	88	PRO	5.2
4	D	508	LEU	5.2
4	D	366	PRO	5.2
4	D	610	ASP	5.2
2	B	351	ILE	5.2
4	D	292	LEU	5.2
8	L	58	TYR	5.1
2	B	554	SER	5.1
2	B	575	SER	5.1
4	D	554	GLU	5.1
4	D	435	GLU	5.1
4	D	509	PRO	5.1
5	E	421	GLU	5.1
8	L	122	PRO	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	143	ALA	5.1
5	E	460	ALA	5.1
8	L	45	LYS	5.1
2	B	689	LEU	5.1
7	H	254	PRO	5.1
4	D	592	ASN	5.1
4	D	699	TRP	5.1
4	D	690	THR	5.1
3	C	7	GLY	5.1
1	A	217	LEU	5.1
6	F	288	ILE	5.1
7	H	143	TYR	5.1
6	F	118	GLN	5.1
6	F	268	SER	5.1
5	E	431	LYS	5.0
2	B	593	LYS	5.0
4	D	407	PRO	5.0
2	B	254	ASP	5.0
6	F	91	LEU	5.0
4	D	256	GLY	5.0
8	L	84	GLU	5.0
6	F	210	MET	5.0
4	D	423	ILE	5.0
4	D	311	LEU	5.0
5	E	102	MET	5.0
1	A	183	LYS	5.0
4	D	209	LEU	5.0
4	D	346	ILE	5.0
4	D	155	LEU	5.0
6	F	107	LYS	4.9
8	L	38	TRP	4.9
5	E	474	ASN	4.9
5	E	943	LYS	4.9
1	A	43	HIS	4.9
6	F	178	HIS	4.9
5	E	173	PHE	4.9
4	D	399	SER	4.9
6	F	214	GLY	4.9
5	E	1025	VAL	4.9
3	C	340	LYS	4.9
5	E	361	SER	4.9
1	A	211	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	212	TRP	4.9
4	D	666	LEU	4.9
7	H	74	VAL	4.9
2	B	655	ALA	4.9
7	H	126	GLY	4.9
3	C	111	LEU	4.8
2	B	311	ALA	4.8
4	D	140	HIS	4.8
3	C	10	ASP	4.8
5	E	926	CYS	4.8
3	C	198	LYS	4.8
4	D	612	LEU	4.8
8	L	190	GLU	4.8
4	D	291	LEU	4.8
3	C	85	GLU	4.8
8	L	64	ARG	4.8
3	C	98	TRP	4.8
5	E	266	ASP	4.8
1	A	49	LEU	4.8
4	D	411	SER	4.8
4	D	254	LEU	4.8
8	L	110	LYS	4.8
4	D	480	GLU	4.8
6	F	169	LEU	4.8
3	C	30	ASP	4.8
5	E	477	GLN	4.7
5	E	422	ARG	4.7
7	H	66	ALA	4.7
5	E	268	SER	4.7
5	E	595	ILE	4.7
1	A	47	ASP	4.7
2	B	362	LEU	4.7
6	F	291	ASN	4.7
5	E	476	PHE	4.7
5	E	24	VAL	4.7
2	B	204	LYS	4.7
3	C	70	ARG	4.7
5	E	124	LYS	4.7
2	B	521	ALA	4.7
4	D	645	ALA	4.7
2	B	384	CYS	4.7
4	D	533	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
7	H	84	THR	4.7
5	E	625	ILE	4.7
4	D	422	MET	4.7
5	E	132	GLN	4.7
3	C	11	LEU	4.7
2	B	224	TYR	4.7
7	H	204	VAL	4.7
1	A	62	ALA	4.6
5	E	513	LEU	4.6
8	L	184	LEU	4.6
4	D	307	LYS	4.6
3	C	57	SER	4.6
5	E	12	LEU	4.6
2	B	479	ALA	4.6
4	D	295	TYR	4.6
2	B	597	GLU	4.6
2	B	620	TYR	4.6
2	B	313	GLU	4.6
4	D	199	GLU	4.6
5	E	10	ASN	4.6
5	E	267	PRO	4.6
2	B	97	LEU	4.6
6	F	265	SER	4.6
1	A	123	GLY	4.6
2	B	360	LYS	4.6
5	E	388	ASP	4.6
5	E	586	LEU	4.6
6	F	252	GLN	4.5
5	E	87	ALA	4.5
2	B	355	ILE	4.5
4	D	246	TRP	4.5
5	E	283	TYR	4.5
3	C	5	ASP	4.5
4	D	436	GLY	4.5
6	F	239	LYS	4.5
3	C	4	PHE	4.5
4	D	559	PHE	4.5
6	F	115	GLN	4.5
5	E	261	SER	4.5
8	L	210	LYS	4.5
2	B	576	LEU	4.5
2	B	550	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
4	D	132	VAL	4.5
6	F	313	LEU	4.5
1	A	194	TYR	4.5
7	H	101	SER	4.5
4	D	118	LEU	4.5
4	D	491	LEU	4.5
3	C	28	SER	4.5
4	D	372	ALA	4.5
5	E	629	ILE	4.5
2	B	236	LYS	4.5
1	A	71	ALA	4.5
8	L	197	CYS	4.5
5	E	501	THR	4.5
7	H	123	ALA	4.4
1	A	46	ILE	4.4
2	B	250	LYS	4.4
3	C	41	ASP	4.4
4	D	736	ASN	4.4
2	B	182	ARG	4.4
3	C	209	PRO	4.4
7	H	125	THR	4.4
5	E	1002	MET	4.4
3	C	62	ASP	4.4
8	L	151	TRP	4.4
8	L	116	PRO	4.4
2	B	310	LEU	4.4
5	E	679	LEU	4.4
4	D	408	VAL	4.4
2	B	654	VAL	4.4
4	D	646	LEU	4.4
4	D	696	GLU	4.4
8	L	121	PHE	4.4
2	B	165	ILE	4.4
5	E	305	VAL	4.4
5	E	821	HIS	4.4
2	B	241	LEU	4.4
5	E	96	HIS	4.4
4	D	97	ARG	4.4
4	D	53	VAL	4.4
5	E	450	LEU	4.4
5	E	264	ASP	4.4
5	E	356	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
5	E	358	GLY	4.3
2	B	213	GLU	4.3
4	D	68	LYS	4.3
8	L	143	TYR	4.3
5	E	71	HIS	4.3
8	L	144	PRO	4.3
5	E	105	ARG	4.3
4	D	80	ALA	4.3
8	L	41	GLN	4.3
4	D	141	ASN	4.3
7	H	36	GLY	4.3
7	H	124	ARG	4.3
5	E	98	PRO	4.3
2	B	451	CYS	4.3
7	H	223	VAL	4.3
6	F	7	TYR	4.3
1	A	69	ILE	4.3
2	B	632	GLU	4.3
4	D	206	GLU	4.3
3	C	24	VAL	4.3
2	B	376	LEU	4.2
5	E	154	ASN	4.2
7	H	227	SER	4.2
2	B	589	ASN	4.2
4	D	616	VAL	4.2
5	E	675	LEU	4.2
4	D	360	PHE	4.2
4	D	373	GLU	4.2
5	E	91	LYS	4.2
2	B	588	GLN	4.2
4	D	376	GLN	4.2
2	B	96	GLN	4.2
5	E	418	GLN	4.2
6	F	135	ARG	4.1
5	E	692	PHE	4.1
7	H	144	TRP	4.1
3	C	155	LYS	4.1
5	E	145	LEU	4.1
4	D	64	LYS	4.1
2	B	223	ASP	4.1
4	D	91	TYR	4.1
2	B	295	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
5	E	599	LYS	4.1
5	E	997	ARG	4.1
1	A	182	VAL	4.1
7	H	203	GLY	4.1
6	F	251	SER	4.1
5	E	83	PRO	4.1
4	D	556	ILE	4.1
5	E	294	GLU	4.1
5	E	187	LYS	4.1
4	D	431	GLU	4.1
2	B	184	PHE	4.1
3	C	207	LYS	4.1
5	E	217	LYS	4.1
2	B	555	GLU	4.1
7	H	77	ILE	4.1
5	E	391	SER	4.0
5	E	831	LEU	4.0
2	B	388	LEU	4.0
2	B	372	SER	4.0
2	B	567	LEU	4.0
5	E	242	HIS	4.0
4	D	594	ILE	4.0
4	D	578	ALA	4.0
4	D	593	ALA	4.0
4	D	482	TRP	4.0
4	D	59	GLU	4.0
4	D	560	SER	4.0
5	E	223	VAL	4.0
3	C	185	VAL	4.0
2	B	197	LYS	4.0
3	C	82	LYS	4.0
5	E	312	THR	4.0
5	E	827	GLN	3.9
3	C	8	HIS	3.9
7	H	38	VAL	3.9
4	D	266	GLU	3.9
5	E	270	PHE	3.9
1	A	141	ILE	3.9
3	C	9	ASP	3.9
3	C	233	THR	3.9
7	H	75	ALA	3.9
7	H	148	THR	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	326	LEU	3.9
4	D	730	ASN	3.9
4	D	249	LEU	3.9
5	E	618	SER	3.9
8	L	21	ARG	3.9
2	B	525	ASP	3.9
6	F	261	ARG	3.9
5	E	329	TRP	3.9
8	L	203	GLY	3.9
2	B	526	HIS	3.9
1	A	192	GLN	3.9
5	E	617	GLU	3.9
4	D	737	PHE	3.9
1	A	222	LEU	3.9
5	E	137	PHE	3.9
5	E	622	LEU	3.9
6	F	318	PRO	3.9
2	B	385	LEU	3.9
4	D	485	ALA	3.8
1	A	35	ILE	3.8
3	C	81	VAL	3.8
5	E	944	ILE	3.8
6	F	195	GLU	3.8
8	L	119	PHE	3.8
2	B	495	SER	3.8
4	D	369	GLU	3.8
8	L	149	VAL	3.8
4	D	557	ALA	3.8
7	H	79	PRO	3.8
5	E	616	LEU	3.8
4	D	741	GLN	3.8
8	L	49	LEU	3.8
2	B	308	SER	3.8
4	D	416	THR	3.8
6	F	316	PRO	3.8
4	D	202	SER	3.8
4	D	207	SER	3.8
3	C	56	SER	3.8
6	F	199	GLU	3.8
3	C	83	LEU	3.8
5	E	1001	LEU	3.8
5	E	23	THR	3.7

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Mol	Chain	Res	Type	RSRZ
4	D	334	ASP	3.7
6	F	134	GLU	3.7
1	A	276	ASN	3.7
6	F	295	GLN	3.7
3	C	86	GLU	3.7
3	C	27	CYS	3.7
6	F	197	LEU	3.7
3	C	112	TYR	3.7
5	E	362	LYS	3.7
6	F	161	PRO	3.7
8	L	76	LEU	3.7
4	D	576	PHE	3.7
2	B	220	ASP	3.7
5	E	817	VAL	3.7
1	A	190	ASP	3.7
5	E	809	LYS	3.7
5	E	506	LEU	3.7
4	D	142	ALA	3.7
8	L	39	TYR	3.7
2	B	305	VAL	3.7
4	D	427	LYS	3.7
2	B	452	TRP	3.7
5	E	830	LEU	3.6
3	C	336	SER	3.6
7	H	256	SER	3.6
6	F	294	LEU	3.6
7	H	29	GLN	3.6
5	E	496	ASN	3.6
3	C	134	LEU	3.6
4	D	197	VAL	3.6
5	E	510	LEU	3.6
8	L	208	VAL	3.6
2	B	420	GLY	3.6
4	D	126	VAL	3.6
5	E	263	SER	3.6
4	D	574	LEU	3.6
5	E	377	GLU	3.6
5	E	123	LEU	3.6
6	F	248	TYR	3.5
8	L	173	ASP	3.5
5	E	694	ASN	3.5
8	L	182	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
8	L	202	GLN	3.5
4	D	400	GLY	3.5
8	L	81	LEU	3.5
4	D	338	VAL	3.5
7	H	146	GLN	3.5
6	F	351	ILE	3.5
3	C	184	ALA	3.5
5	E	621	GLN	3.5
4	D	194	GLY	3.5
5	E	446	LEU	3.5
8	L	135	VAL	3.5
5	E	348	TYR	3.5
5	E	635	LEU	3.5
3	C	156	VAL	3.5
1	A	142	ASP	3.5
7	H	255	LYS	3.4
8	L	61	VAL	3.4
3	C	192	ILE	3.4
3	C	218	ILE	3.4
8	L	60	GLY	3.4
4	D	187	THR	3.4
4	D	611	ILE	3.4
5	E	224	ILE	3.4
5	E	274	GLU	3.4
5	E	922	LEU	3.4
6	F	312	GLU	3.4
5	E	478	PRO	3.4
6	F	241	SER	3.4
7	H	169	SER	3.4
5	E	702	ILE	3.4
6	F	139	VAL	3.4
2	B	366	PRO	3.4
2	B	512	VAL	3.4
4	D	553	ILE	3.4
5	E	125	ASP	3.4
7	H	103	ASN	3.4
5	E	265	SER	3.3
1	A	181	LEU	3.3
2	B	185	LEU	3.3
7	H	95	THR	3.3
3	C	127	CYS	3.3
2	B	447	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
4	D	196	ASP	3.3
4	D	200	ASN	3.3
1	A	36	PHE	3.3
5	E	184	LEU	3.3
7	H	35	GLY	3.3
5	E	271	ARG	3.3
2	B	445	ALA	3.3
2	B	556	VAL	3.3
4	D	689	ALA	3.3
3	C	32	HIS	3.3
7	H	60	ILE	3.3
4	D	186	ARG	3.3
2	B	192	ASP	3.3
4	D	363	TYR	3.3
5	E	330	SER	3.3
4	D	404	SER	3.3
4	D	285	VAL	3.2
5	E	131	LEU	3.2
5	E	170	SER	3.2
2	B	193	LYS	3.2
6	F	259	TYR	3.2
5	E	634	LEU	3.2
7	H	61	HIS	3.2
4	D	48	LEU	3.2
6	F	217	GLU	3.2
5	E	375	ASN	3.2
6	F	284	SER	3.2
6	F	138	ASN	3.2
2	B	600	ASN	3.2
5	E	347	SER	3.2
1	A	70	LEU	3.2
1	A	277	LYS	3.2
4	D	667	VAL	3.2
7	H	59	SER	3.2
2	B	598	ILE	3.2
7	H	141	LEU	3.1
2	B	448	VAL	3.1
6	F	245	ARG	3.1
3	C	58	ILE	3.1
3	C	6	SER	3.1
3	C	31	GLN	3.1
4	D	195	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
4	D	664	VAL	3.1
6	F	144	TRP	3.1
2	B	225	MET	3.1
4	D	288	SER	3.1
8	L	145	ARG	3.1
1	A	196	LEU	3.1
2	B	200	ILE	3.1
2	B	681	LYS	3.1
4	D	364	TYR	3.1
5	E	343	ASN	3.1
5	E	392	GLU	3.1
5	E	987	MET	3.1
2	B	383	LEU	3.0
4	D	403	HIS	3.0
4	D	691	VAL	3.0
4	D	310	VAL	3.0
4	D	507	LEU	3.0
7	H	145	GLY	3.0
2	B	361	LEU	3.0
4	D	270	LEU	3.0
6	F	162	LEU	3.0
6	F	191	GLY	3.0
1	A	195	VAL	3.0
2	B	222	LEU	3.0
2	B	449	GLN	3.0
5	E	610	PHE	3.0
5	E	810	ASP	3.0
5	E	94	ASN	3.0
8	L	216	GLU	3.0
7	H	122	CYS	3.0
2	B	508	ILE	3.0
6	F	281	ASP	3.0
5	E	818	PRO	3.0
5	E	822	SER	3.0
4	D	284	ALA	3.0
5	E	701	TYR	2.9
4	D	597	LYS	2.9
6	F	102	ARG	2.9
3	C	15	VAL	2.9
4	D	82	ILE	2.9
8	L	174	SER	2.9
2	B	386	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	693	GLU	2.9
5	E	341	GLU	2.9
6	F	249	SER	2.9
4	D	733	LYS	2.9
5	E	346	ALA	2.9
2	B	596	ARG	2.9
8	L	112	THR	2.9
2	B	367	PHE	2.9
5	E	62	LEU	2.9
7	H	118	ALA	2.9
4	D	365	ILE	2.9
3	C	54	HIS	2.9
1	A	218	LEU	2.9
4	D	428	GLY	2.9
4	D	694	VAL	2.9
5	E	252	THR	2.9
4	D	619	SER	2.9
8	L	22	VAL	2.9
5	E	20	PRO	2.9
2	B	358	ILE	2.9
2	B	559	LEU	2.9
5	E	177	PHE	2.9
4	D	148	MET	2.9
4	D	357	PHE	2.9
4	D	481	LEU	2.9
2	B	370	LEU	2.9
4	D	121	ASP	2.9
5	E	509	TYR	2.9
5	E	998	LYS	2.9
5	E	114	GLU	2.8
5	E	871	HIS	2.8
2	B	217	LEU	2.8
5	E	355	TRP	2.8
3	C	165	LEU	2.8
6	F	177	ASP	2.8
4	D	119	GLY	2.8
8	L	199	VAL	2.8
5	E	384	LYS	2.8
2	B	618	GLU	2.8
2	B	496	CYS	2.8
5	E	247	ASP	2.8
3	C	128	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	34	LYS	2.8
4	D	367	SER	2.8
5	E	423	ALA	2.8
4	D	418	ALA	2.8
2	B	530	ARG	2.8
6	F	103	GLY	2.8
4	D	289	ILE	2.8
7	H	65	GLN	2.7
3	C	211	HIS	2.7
4	D	337	LEU	2.7
5	E	469	GLU	2.7
3	C	231	ILE	2.7
2	B	357	LYS	2.7
2	B	95	GLU	2.7
4	D	47	ILE	2.7
4	D	622	GLN	2.7
4	D	340	GLY	2.7
5	E	228	LEU	2.7
2	B	231	ASP	2.7
5	E	825	TYR	2.7
2	B	312	ILE	2.7
3	C	35	VAL	2.7
6	F	283	GLU	2.7
8	L	146	GLU	2.7
8	L	153	VAL	2.7
5	E	637	PHE	2.7
5	E	256	ASP	2.7
5	E	61	LEU	2.7
7	H	51	SER	2.7
7	H	28	VAL	2.7
5	E	67	TYR	2.7
7	H	147	GLY	2.7
6	F	299	GLU	2.7
6	F	119	ILE	2.6
7	H	34	GLY	2.6
2	B	373	LEU	2.6
3	C	75	ALA	2.6
5	E	344	VAL	2.6
2	B	532	LYS	2.6
4	D	63	ASP	2.6
4	D	283	ASP	2.6
7	H	107	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
8	L	148	LYS	2.6
5	E	320	PRO	2.6
5	E	134	PRO	2.6
3	C	232	ALA	2.5
4	D	122	ARG	2.5
4	D	426	ALA	2.5
5	E	642	LEU	2.5
2	B	299	LEU	2.5
5	E	886	LEU	2.5
3	C	163	ASN	2.5
2	B	190	TYR	2.5
8	L	107	VAL	2.5
2	B	211	ILE	2.5
8	L	211	SER	2.5
1	A	67	GLY	2.5
4	D	60	LYS	2.5
4	D	734	LYS	2.5
5	E	869	HIS	2.5
6	F	324	VAL	2.5
4	D	595	VAL	2.5
3	C	14	ASP	2.5
5	E	276	VAL	2.5
4	D	61	ASN	2.5
6	F	205	ASN	2.5
7	H	46	LEU	2.5
7	H	175	GLY	2.5
6	F	200	ALA	2.5
8	L	207	PRO	2.5
4	D	190	PHE	2.5
2	B	566	ASP	2.5
4	D	313	LEU	2.5
6	F	287	HIS	2.4
5	E	636	THR	2.4
2	B	300	LEU	2.4
4	D	336	LEU	2.4
5	E	424	GLN	2.4
1	A	157	THR	2.4
1	A	193	THR	2.4
4	D	188	MET	2.4
4	D	433	ILE	2.4
6	F	262	ALA	2.4
4	D	339	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	488	HIS	2.4
6	F	256	LEU	2.4
5	E	633	VAL	2.4
5	E	339	PRO	2.4
4	D	265	ILE	2.4
4	D	203	GLU	2.4
8	L	136	VAL	2.4
6	F	215	ILE	2.4
5	E	304	LEU	2.3
2	B	482	LEU	2.3
5	E	641	ASP	2.3
6	F	315	LEU	2.3
4	D	145	ASN	2.3
4	D	205	ILE	2.3
3	C	36	PHE	2.3
3	C	243	PHE	2.3
7	H	33	SER	2.3
5	E	380	GLU	2.3
6	F	143	LYS	2.3
6	F	317	LEU	2.3
7	H	257	CYS	2.3
2	B	418	PRO	2.3
4	D	189	TYR	2.3
5	E	945	VAL	2.3
3	C	114	VAL	2.3
4	D	309	LEU	2.3
5	E	116	GLN	2.3
4	D	286	SER	2.3
5	E	807	ILE	2.3
4	D	341	GLY	2.3
7	H	37	LEU	2.3
4	D	193	ASP	2.2
6	F	136	PRO	2.2
5	E	597	TRP	2.2
5	E	862	GLN	2.2
7	H	100	THR	2.2
8	L	111	ARG	2.2
8	L	115	ALA	2.2
8	L	194	VAL	2.2
5	E	321	THR	2.2
5	E	826	TYR	2.2
6	F	244	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	529	ASN	2.2
3	C	113	SER	2.2
4	D	617	THR	2.2
5	E	613	ILE	2.2
7	H	52	GLY	2.2
4	D	124	PHE	2.2
5	E	233	TYR	2.2
2	B	587	VAL	2.1
5	E	8	ASP	2.1
2	B	560	LEU	2.1
6	F	242	LEU	2.1
5	E	814	THR	2.1
2	B	296	PHE	2.1
5	E	84	LEU	2.1
5	E	183	LEU	2.1
5	E	118	LEU	2.1
3	C	161	PRO	2.1
5	E	385	SER	2.1
2	B	518	LEU	2.1
5	E	293	LEU	2.1
1	A	45	LEU	2.1
2	B	487	LEU	2.1
4	D	738	LYS	2.1
5	E	262	GLN	2.1
4	D	84	ALA	2.1
5	E	106	TYR	2.1
6	F	209	CYS	2.0
5	E	2	ALA	2.0
5	E	813	CYS	2.0
2	B	599	LEU	2.0
8	L	113	VAL	2.0
5	E	493	TRP	2.0
2	B	218	PHE	2.0
4	D	143	THR	2.0
5	E	129	LEU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.