



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 11:01 pm GMT

PDB ID : 4NQX  
Title : Crystal Structure of HLA A\*0101 in complex with NP44-S7N, an 9-mer influenza epitope  
Authors : Rossjohn, J.; Gras, S.  
Deposited on : 2013-11-26  
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

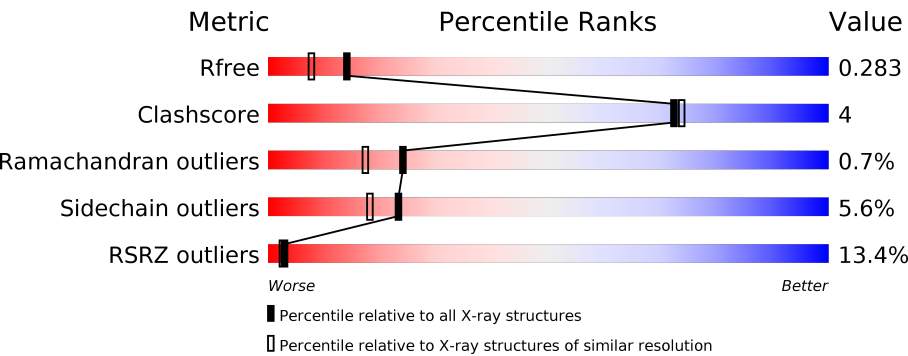
MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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	284	<div><div>4%</div><div>87%</div><div>8%</div><div>• •</div></div>
1	C	284	<div><div>10%</div><div>87%</div><div>9%</div><div>• •</div></div>
1	E	284	<div><div>8%</div><div>83%</div><div>12%</div><div>• •</div></div>
1	G	284	<div><div>12%</div><div>85%</div><div>10%</div><div>• •</div></div>
1	I	284	<div><div>9%</div><div>85%</div><div>11%</div><div>• •</div></div>
1	K	284	<div><div>18%</div><div>86%</div><div>10%</div><div>• •</div></div>

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Mol	Chain	Length	Quality of chain
2	B	100	
2	D	100	
2	F	100	
2	H	100	
2	J	100	
2	L	100	
3	M	9	
3	N	9	
3	O	9	
3	P	9	
3	Q	9	
3	R	9	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19771 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 HLA class I histocompatibility antigen, A-1 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	3	0
			2255	1399	416	430	10			
1	C	275	Total	C	N	O	S	0	1	0
			2245	1394	411	430	10			
1	E	275	Total	C	N	O	S	0	2	0
			2256	1399	415	432	10			
1	G	274	Total	C	N	O	S	0	2	0
			2248	1395	415	428	10			
1	I	274	Total	C	N	O	S	0	2	0
			2247	1394	413	430	10			
1	K	275	Total	C	N	O	S	0	1	0
			2243	1392	410	431	10			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	1	0
			845	539	142	160	4			
2	D	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	F	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	H	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	J	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	L	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	EXPRESSION TAG	UNP P61769

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	EXPRESSION TAG	UNP P61769
F	0	MET	-	EXPRESSION TAG	UNP P61769
H	0	MET	-	EXPRESSION TAG	UNP P61769
J	0	MET	-	EXPRESSION TAG	UNP P61769
L	0	MET	-	EXPRESSION TAG	UNP P61769

- Molecule 3 is a protein called NP44-S7N mutant peptide, CTELKLNDY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			
3	N	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			
3	O	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			
3	P	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			
3	Q	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			
3	R	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	116	Total	O	0	0
			116	116		
4	B	49	Total	O	0	0
			49	49		
4	C	110	Total	O	0	0
			110	110		
4	D	51	Total	O	0	0
			51	51		
4	E	90	Total	O	0	0
			90	90		
4	F	43	Total	O	0	0
			43	43		
4	G	70	Total	O	0	0
			70	70		
4	H	34	Total	O	0	0
			34	34		
4	I	55	Total	O	0	0
			55	55		

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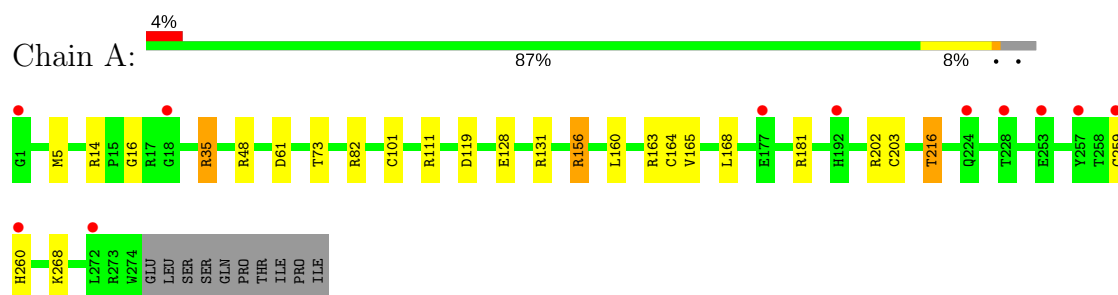
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	27	Total 27	O 27	0	0
4	K	97	Total 97	O 97	0	0
4	L	32	Total 32	O 32	0	0
4	M	7	Total 7	O 7	0	0
4	N	5	Total 5	O 5	0	0
4	O	2	Total 2	O 2	0	0
4	P	4	Total 4	O 4	0	0
4	Q	3	Total 3	O 3	0	0
4	R	4	Total 4	O 4	0	0

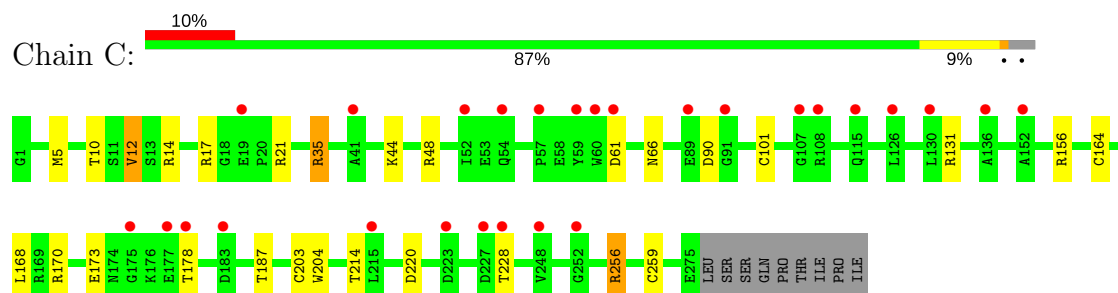
### 3 Residue-property plots [i](#)

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

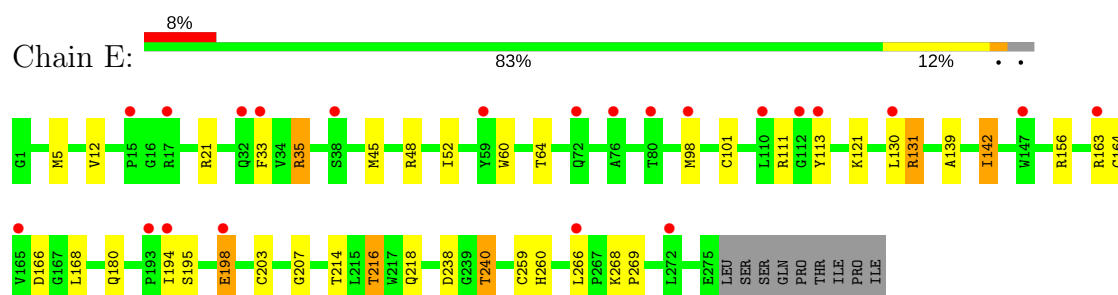
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



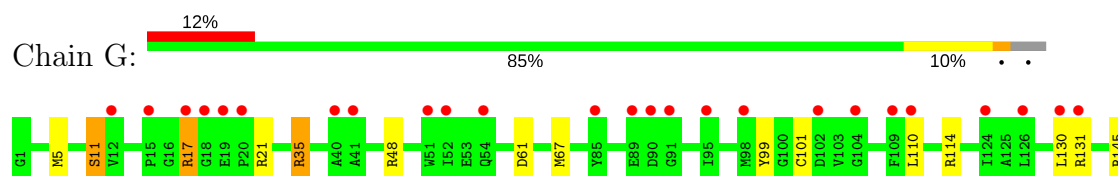
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain

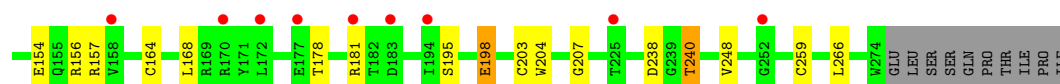


- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain

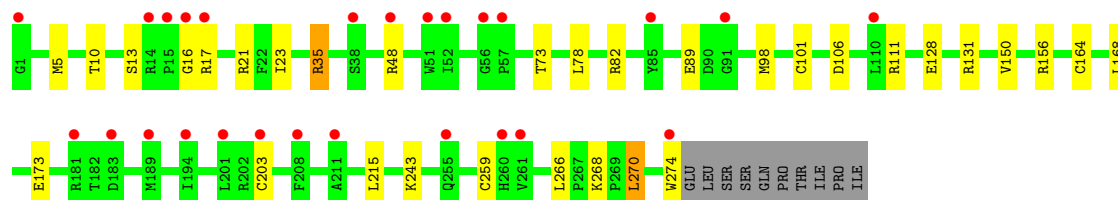
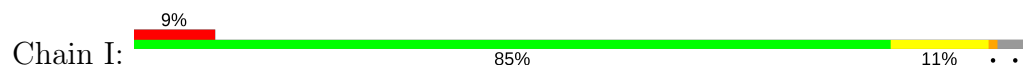


- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain

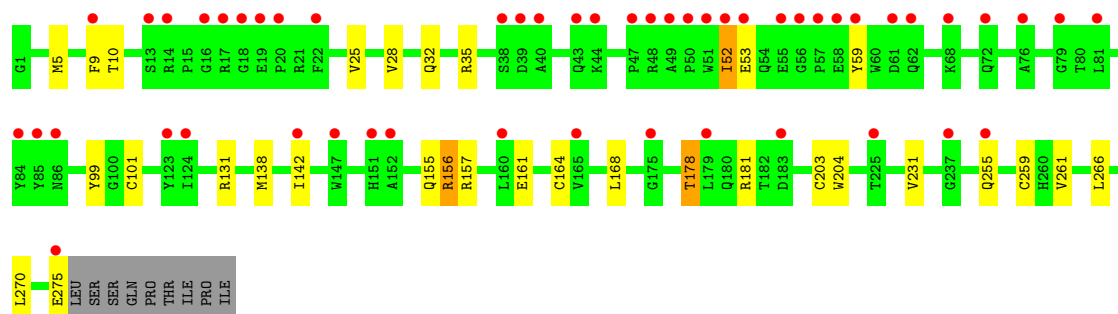
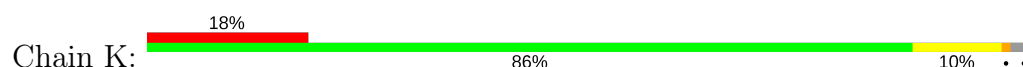




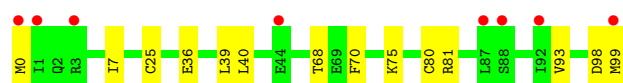
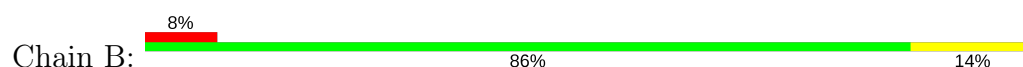
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



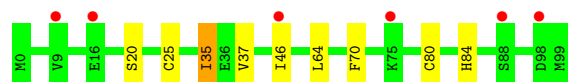
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



- Molecule 2: Beta-2-microglobulin



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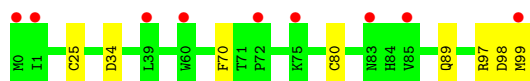
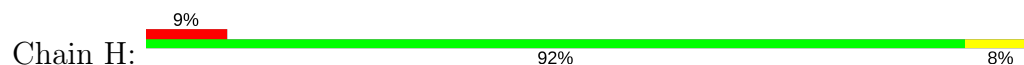
- Molecule 2: Beta-2-microglobulin



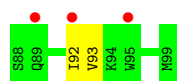
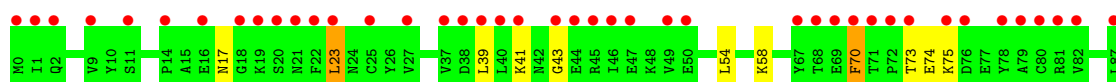
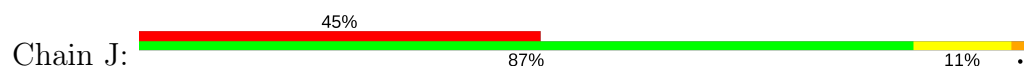




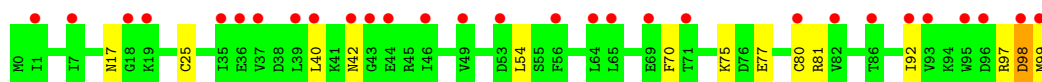
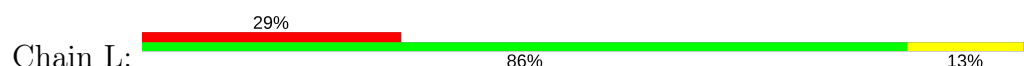
- Molecule 2: Beta-2-microglobulin



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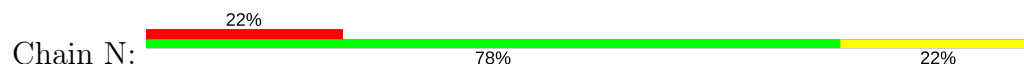
- Molecule 2: Beta-2-microglobulin



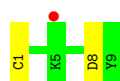
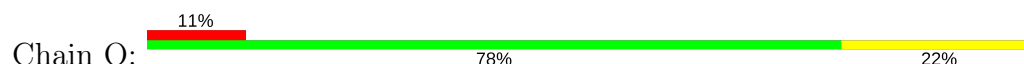
- Molecule 3: NP44-S7N mutant peptide, CTELKLNDY



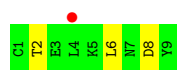
- Molecule 3: NP44-S7N mutant peptide, CTELKLNDY



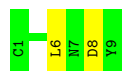
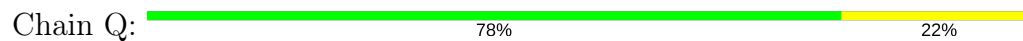
- Molecule 3: NP44-S7N mutant peptide, CTELKLNDY



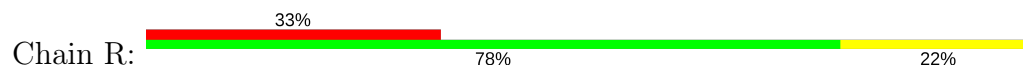
- Molecule 3: NP44-S7N mutant peptide, CTELKLNDY



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- Molecule 3: NP44-S7N mutant peptide, CTELKLNDY



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	264.61Å 81.41Å 140.29Å 90.00° 121.82° 90.00°	Depositor
Resolution (Å)	45.75 – 2.00 45.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (45.75-2.00) 96.2 (45.75-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 2.00Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.10.0	Depositor
R, $R_{free}$	0.270 , 0.283 0.275 , 0.283	Depositor DCC
$R_{free}$ test set	8305 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 32.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.077 for -h-2*1,-k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	19771	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6027e-05.*

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

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

## 5 Model quality [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.37	0/2316	0.58	0/3140
1	C	0.38	0/2305	0.58	0/3125
1	E	0.39	0/2316	0.61	0/3139
1	G	0.37	0/2309	0.59	0/3131
1	I	0.35	0/2307	0.58	0/3127
1	K	0.38	0/2303	0.61	0/3123
2	B	0.38	0/868	0.64	0/1173
2	D	0.37	0/860	0.63	0/1162
2	F	0.45	0/852	0.83	2/1152 (0.2%)
2	H	0.39	0/860	0.63	0/1162
2	J	0.40	0/860	0.61	0/1162
2	L	0.37	0/860	0.63	0/1162
3	M	0.35	0/76	0.63	0/100
3	N	0.35	0/76	0.57	0/100
3	O	0.33	0/76	0.54	0/100
3	P	0.38	0/76	0.83	0/100
3	Q	0.31	0/76	0.61	0/100
3	R	0.36	0/76	0.51	0/100
All	All	0.38	0/19472	0.61	2/26358 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	85	VAL	C-N-CA	9.21	144.74	121.70
2	F	74	GLU	C-N-CA	5.33	135.03	121.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2255	0	2114	14	0
1	C	2245	0	2109	13	0
1	E	2256	0	2115	24	0
1	G	2248	0	2109	18	0
1	I	2247	0	2107	14	0
1	K	2243	0	2102	16	0
2	B	845	0	815	8	0
2	D	837	0	805	5	0
2	F	829	0	796	18	0
2	H	837	0	805	3	0
2	J	837	0	805	4	0
2	L	837	0	805	9	0
3	M	76	0	74	1	0
3	N	76	0	74	2	0
3	O	76	0	74	1	0
3	P	76	0	74	3	0
3	Q	76	0	74	1	0
3	R	76	0	74	0	0
4	A	116	0	0	2	0
4	B	49	0	0	0	0
4	C	110	0	0	0	0
4	D	51	0	0	1	0
4	E	90	0	0	0	0
4	F	43	0	0	0	0
4	G	70	0	0	0	0
4	H	34	0	0	0	0
4	I	55	0	0	0	0
4	J	27	0	0	0	0
4	K	97	0	0	2	0
4	L	32	0	0	0	0
4	M	7	0	0	0	0
4	N	5	0	0	0	0
4	O	2	0	0	0	0
4	P	4	0	0	0	0
4	Q	3	0	0	0	0
4	R	4	0	0	0	0
All	All	19771	0	17931	132	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ILE:HD11	2:B:25:CYS:SG	2.05	0.96
1:E:45:MET:H	1:E:64:THR:HG22	1.38	0.87
1:G:67:MET:CE	3:P:2:THR:HG21	2.15	0.77
1:A:216:THR:HG23	1:A:260[A]:HIS:HB3	1.66	0.76
2:D:35:ILE:HD11	2:D:64:LEU:HD12	1.67	0.76
1:C:66:ASN:HD22	3:N:2:THR:HG23	1.52	0.74
2:H:25:CYS:HG	2:H:80:CYS:HG	0.86	0.71
1:E:60:TRP:O	1:E:64:THR:HG23	1.90	0.71
2:L:25:CYS:HG	2:L:80:CYS:HG	0.71	0.69
1:I:10:THR:HG21	2:J:54:LEU:HD23	1.74	0.69
1:E:268:LYS:HG3	1:E:269:PRO:HD2	1.75	0.69
1:E:207:GLY:HA2	1:E:240:THR:HG21	1.74	0.68
2:D:35:ILE:HG23	2:D:84:HIS:HD2	1.59	0.68
1:G:207:GLY:HA2	1:G:240:THR:HG21	1.75	0.66
1:K:10[A]:THR:HG21	2:L:54:LEU:HD23	1.77	0.66
1:A:203:CYS:HG	1:A:259:CYS:HG	1.43	0.65
1:E:139:ALA:O	1:E:142:ILE:HG12	1.98	0.63
1:K:9:PHE:HE1	1:K:99:TYR:CE2	2.17	0.62
1:K:161:GLU:HB2	4:K:333:HOH:O	2.00	0.60
1:E:33:PHE:HD2	1:E:52:ILE:HD12	1.66	0.60
1:G:207:GLY:HA2	1:G:240:THR:CG2	2.33	0.59
1:I:203:CYS:HG	1:I:259:CYS:HG	1.47	0.59
1:E:207:GLY:HA2	1:E:240:THR:CG2	2.32	0.59
1:K:203:CYS:HG	1:K:259:CYS:HG	1.47	0.58
1:C:203:CYS:HG	1:C:259:CYS:HG	1.47	0.58
1:G:67:MET:HE1	3:P:2:THR:HG21	1.83	0.57
1:K:157:ARG:NH1	4:K:333:HOH:O	2.38	0.57
1:I:215:LEU:HD13	1:I:243:LYS:HD3	1.87	0.57
1:G:5:MET:HB2	1:G:168:LEU:HD13	1.88	0.56
1:E:101:CYS:HG	1:E:164:CYS:HG	1.51	0.56
2:F:25:CYS:HB2	2:F:80:CYS:SG	2.45	0.56
1:G:99:TYR:OH	3:P:2:THR:HG23	2.06	0.56
1:G:203:CYS:HG	1:G:259:CYS:HG	1.50	0.56
1:A:101:CYS:HG	1:A:164:CYS:HG	1.51	0.53
1:A:111:ARG:HD3	1:A:128:GLU:HG3	1.91	0.53
2:F:84:HIS:HB3	2:F:86:THR:CG2	2.39	0.53
2:D:35:ILE:HG23	2:D:84:HIS:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.91	0.53
1:C:5:MET:HB2	1:C:168:LEU:HD13	1.90	0.52
2:L:40:LEU:HD11	2:L:81:ARG:HE	1.74	0.52
1:K:5:MET:HB2	1:K:168:LEU:HD13	1.92	0.52
1:I:111:ARG:HE	1:I:128:GLU:HG3	1.73	0.52
1:I:5:MET:HB2	1:I:168:LEU:HD13	1.92	0.52
1:C:101:CYS:HG	1:C:164:CYS:HG	1.50	0.51
1:I:266:LEU:HD22	1:I:270:LEU:HD13	1.91	0.51
1:C:187:THR:HG23	1:C:204:TRP:O	2.11	0.51
1:K:204:TRP:HZ2	2:L:99:MET:HB2	1.75	0.51
1:A:216:THR:HG23	1:A:260[B]:HIS:HB2	1.93	0.50
1:C:203:CYS:SG	1:C:259:CYS:SG	3.03	0.50
2:F:78:TYR:HB2	2:F:95:TRP:HD1	1.77	0.50
1:E:45:MET:N	1:E:64:THR:HG22	2.18	0.50
1:K:178:THR:HA	1:K:181:ARG:HE	1.77	0.50
2:F:51:HIS:O	2:F:64:LEU:HD22	2.12	0.50
1:I:73:THR:HG21	3:Q:6:LEU:HB3	1.92	0.50
2:F:37:VAL:HB	2:F:82:VAL:HG22	1.94	0.50
2:F:84:HIS:HB3	2:F:86:THR:HG21	1.93	0.50
1:G:203:CYS:SG	1:G:259:CYS:SG	3.06	0.49
1:G:204:TRP:HH2	2:H:99:MET:HG2	1.76	0.49
2:B:39:LEU:HD13	2:B:68:THR:HG22	1.95	0.49
2:F:40:LEU:HD12	2:F:46:ILE:HB	1.93	0.49
1:A:160:LEU:O	1:A:165:VAL:HG23	2.13	0.49
1:E:98:MET:HB3	1:E:113:TYR:HE2	1.77	0.48
2:B:7:ILE:CD1	2:B:25:CYS:SG	2.92	0.48
1:C:14:ARG:HB2	1:C:17:ARG:HB2	1.96	0.48
1:K:101:CYS:SG	1:K:164:CYS:SG	3.06	0.48
1:I:13:SER:HB3	1:I:78:LEU:HD13	1.95	0.48
1:E:163:ARG:HG3	3:O:1:CYS:SG	2.53	0.48
2:F:74:GLU:CA	2:F:75:LYS:HB3	2.44	0.47
1:E:5:MET:HB2	1:E:168:LEU:HD13	1.96	0.47
1:I:203:CYS:SG	1:I:259:CYS:SG	3.03	0.47
2:F:39:LEU:H	2:F:45:ARG:HG3	1.79	0.47
1:K:155:GLN:HE21	1:K:156:ARG:HH12	1.61	0.47
1:G:204:TRP:CH2	2:H:99:MET:HG2	2.50	0.47
2:J:23:LEU:HB3	2:J:70:PHE:CZ	2.50	0.47
1:E:98:MET:HG3	2:F:56:PHE:HE1	1.79	0.47
1:K:101:CYS:HG	1:K:164:CYS:HG	1.52	0.46
2:J:17:ASN:HB2	2:J:73:THR:HA	1.96	0.46
1:E:203:CYS:HG	1:E:259:CYS:HG	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:THR:HG23	1:E:260:HIS:HB2	1.97	0.46
1:I:101:CYS:HG	1:I:164:CYS:HG	1.60	0.46
2:D:25:CYS:CB	2:D:80:CYS:HG	2.24	0.45
1:C:101:CYS:SG	1:C:164:CYS:SG	3.06	0.45
1:C:66:ASN:HD22	3:N:2:THR:CG2	2.27	0.45
1:A:163:ARG:NH2	4:A:310:HOH:O	2.49	0.45
1:E:101:CYS:SG	1:E:164:CYS:SG	3.10	0.45
1:E:131:ARG:HH22	2:L:92:ILE:H	1.65	0.44
2:F:50:GLU:HG2	2:F:67:TYR:CZ	2.52	0.44
2:D:20:SER:HB3	1:I:106:ASP:HA	1.98	0.44
1:C:12:VAL:HG23	1:C:21:ARG:HB3	1.98	0.44
1:E:35:ARG:HE	1:E:48:ARG:HH11	1.65	0.44
1:I:35:ARG:HE	1:I:48:ARG:HH11	1.65	0.44
1:K:261:VAL:HG13	1:K:270:LEU:HB2	1.99	0.44
1:C:35:ARG:HE	1:C:48:ARG:HH11	1.65	0.44
1:G:35:ARG:HE	1:G:48:ARG:HH11	1.66	0.44
1:A:35:ARG:HE	1:A:48:ARG:HH11	1.65	0.43
1:E:98:MET:HG3	2:F:56:PHE:CE1	2.54	0.43
1:G:101:CYS:HG	1:G:164:CYS:HG	1.54	0.43
1:K:255:GLN:CD	1:K:255:GLN:H	2.22	0.43
1:C:220:ASP:OD1	1:C:256:ARG:HG3	2.18	0.43
2:F:39:LEU:HD22	2:F:81:ARG:HD3	2.00	0.43
1:G:195:SER:OG	1:G:198:GLU:HG2	2.19	0.43
2:B:40:LEU:HD11	2:B:81:ARG:HB2	2.01	0.43
1:E:194:ILE:HD12	1:G:145:ARG:HB3	2.01	0.43
1:K:204:TRP:CZ2	2:L:99:MET:HB2	2.53	0.43
1:E:98:MET:HB3	1:E:113:TYR:CE2	2.53	0.43
1:G:178:THR:HA	1:G:181:ARG:HH21	1.84	0.43
1:E:238:ASP:OD1	1:E:240:THR:HG22	2.18	0.43
2:F:74:GLU:N	2:F:75:LYS:HB3	2.34	0.42
1:A:73:THR:HG21	3:M:6:LEU:HB3	2.01	0.42
2:F:89:GLN:HB3	2:F:90:PRO:C	2.40	0.42
1:I:10:THR:CG2	1:I:23:ILE:HB	2.49	0.42
2:F:85:VAL:N	2:F:86:THR:HB	2.34	0.42
1:A:156:ARG:NH2	4:A:314:HOH:O	2.53	0.42
2:B:7:ILE:HG23	2:B:93:VAL:HG21	2.02	0.42
2:B:7:ILE:CG2	2:B:93:VAL:HG21	2.49	0.42
1:G:154:GLU:HG3	1:G:157[A]:ARG:HH12	1.84	0.42
1:G:238:ASP:OD1	1:G:240:THR:HG22	2.20	0.42
2:F:51:HIS:O	2:F:64:LEU:CD2	2.68	0.41
2:L:42:ASN:HB2	2:L:77:GLU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:41:LYS:C	2:J:43:GLY:H	2.24	0.41
1:K:52:ILE:HB	1:K:53:GLU:H	1.59	0.41
1:C:10:THR:HG23	4:D:146:HOH:O	2.19	0.41
1:A:268:LYS:HZ3	1:I:268:LYS:HB3	1.85	0.41
1:K:25:VAL:HG13	1:K:32:GLN:HG3	2.02	0.41
1:A:119:ASP:HB3	2:B:0:MET:SD	2.61	0.41
1:E:195:SER:OG	1:E:198:GLU:HG2	2.21	0.41
2:F:5:PRO:HB3	2:F:30:PHE:HB3	2.03	0.41
2:L:97:ARG:HG2	2:L:98:ASP:H	1.85	0.40
1:A:202:ARG:CZ	2:B:99:MET:O	2.69	0.40
1:E:12:VAL:HG13	1:E:21:ARG:HB3	2.03	0.40
1:G:11:SER:HA	1:G:21:ARG:O	2.22	0.40
2:L:97:ARG:HG2	2:L:98:ASP:N	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	275/284 (97%)	270 (98%)	4 (2%)	1 (0%)	36	31
1	C	274/284 (96%)	268 (98%)	6 (2%)	0	100	100
1	E	275/284 (97%)	269 (98%)	6 (2%)	0	100	100
1	G	274/284 (96%)	269 (98%)	4 (2%)	1 (0%)	36	31
1	I	274/284 (96%)	270 (98%)	3 (1%)	1 (0%)	36	31
1	K	274/284 (96%)	262 (96%)	11 (4%)	1 (0%)	36	31
2	B	99/100 (99%)	98 (99%)	0	1 (1%)	17	10
2	D	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	F	97/100 (97%)	79 (81%)	8 (8%)	10 (10%)	0	0
2	H	98/100 (98%)	94 (96%)	3 (3%)	1 (1%)	17	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
2	L	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
3	M	7/9 (78%)	7 (100%)	0	0	100	100
3	N	7/9 (78%)	7 (100%)	0	0	100	100
3	O	7/9 (78%)	7 (100%)	0	0	100	100
3	P	7/9 (78%)	7 (100%)	0	0	100	100
3	Q	7/9 (78%)	7 (100%)	0	0	100	100
3	R	7/9 (78%)	7 (100%)	0	0	100	100
All	All	2276/2358 (96%)	2204 (97%)	56 (2%)	16 (1%)	24	17

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	15	ALA
2	F	61	SER
2	F	62	PHE
2	F	86	THR
1	G	17	ARG
2	H	98	ASP
2	F	52	SER
2	F	89	GLN
2	B	98	ASP
2	F	41	LYS
2	F	75	LYS
2	F	16	GLU
2	F	53	ASP
1	K	52	ILE
1	A	16	GLY
1	I	16	GLY

### 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	234/241 (97%)	226 (97%)	8 (3%)	40	38
1	C	233/241 (97%)	220 (94%)	13 (6%)	23	18
1	E	234/241 (97%)	218 (93%)	16 (7%)	17	12
1	G	233/241 (97%)	220 (94%)	13 (6%)	23	18
1	I	233/241 (97%)	221 (95%)	12 (5%)	25	21
1	K	233/241 (97%)	222 (95%)	11 (5%)	29	24
2	B	96/95 (101%)	92 (96%)	4 (4%)	32	29
2	D	95/95 (100%)	91 (96%)	4 (4%)	32	29
2	F	94/95 (99%)	85 (90%)	9 (10%)	9	5
2	H	95/95 (100%)	91 (96%)	4 (4%)	32	29
2	J	95/95 (100%)	87 (92%)	8 (8%)	12	7
2	L	95/95 (100%)	91 (96%)	4 (4%)	32	29
3	M	9/9 (100%)	9 (100%)	0	100	100
3	N	9/9 (100%)	8 (89%)	1 (11%)	7	3
3	O	9/9 (100%)	8 (89%)	1 (11%)	7	3
3	P	9/9 (100%)	7 (78%)	2 (22%)	1	0
3	Q	9/9 (100%)	8 (89%)	1 (11%)	7	3
3	R	9/9 (100%)	7 (78%)	2 (22%)	1	0
All	All	2024/2070 (98%)	1911 (94%)	113 (6%)	23	18

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	35	ARG
1	A	61	ASP
1	A	82	ARG
1	A	131	ARG
1	A	156	ARG
1	A	181	ARG
1	A	216	THR
2	B	36	GLU
2	B	70	PHE
2	B	75	LYS
2	B	80	CYS
1	C	12	VAL
1	C	35	ARG

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Mol	Chain	Res	Type
1	C	44	LYS
1	C	61	ASP
1	C	90	ASP
1	C	131	ARG
1	C	156	ARG
1	C	170	ARG
1	C	173	GLU
1	C	178	THR
1	C	214	THR
1	C	228	THR
1	C	256	ARG
2	D	35	ILE
2	D	37	VAL
2	D	46	ILE
2	D	70	PHE
1	E	35	ARG
1	E	111	ARG
1	E	121	LYS
1	E	130	LEU
1	E	131	ARG
1	E	142	ILE
1	E	156[A]	ARG
1	E	156[B]	ARG
1	E	166	ASP
1	E	180	GLN
1	E	198	GLU
1	E	214	THR
1	E	216	THR
1	E	218	GLN
1	E	240	THR
1	E	266	LEU
2	F	1	ILE
2	F	19	LYS
2	F	37	VAL
2	F	40	LEU
2	F	70	PHE
2	F	74	GLU
2	F	86	THR
2	F	87	LEU
2	F	95	TRP
1	G	11	SER
1	G	17	ARG

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Mol	Chain	Res	Type
1	G	35	ARG
1	G	61	ASP
1	G	110	LEU
1	G	114	ARG
1	G	130	LEU
1	G	131	ARG
1	G	156	ARG
1	G	198	GLU
1	G	240	THR
1	G	248	VAL
1	G	266	LEU
2	H	34	ASP
2	H	70	PHE
2	H	89	GLN
2	H	97	ARG
1	I	17	ARG
1	I	21	ARG
1	I	35	ARG
1	I	82	ARG
1	I	89	GLU
1	I	98	MET
1	I	131	ARG
1	I	150	VAL
1	I	156	ARG
1	I	173	GLU
1	I	270	LEU
1	I	274	TRP
2	J	23	LEU
2	J	39	LEU
2	J	58	LYS
2	J	70	PHE
2	J	74	GLU
2	J	75	LYS
2	J	92	ILE
2	J	93	VAL
1	K	28	VAL
1	K	35	ARG
1	K	59	TYR
1	K	131	ARG
1	K	138	MET
1	K	142	ILE
1	K	156	ARG

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Mol	Chain	Res	Type
1	K	178	THR
1	K	231	VAL
1	K	266	LEU
1	K	275	GLU
2	L	17	ASN
2	L	70	PHE
2	L	75	LYS
2	L	98	ASP
3	N	5	LYS
3	O	8	ASP
3	P	6	LEU
3	P	8	ASP
3	Q	8	ASP
3	R	5	LYS
3	R	8	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	32	GLN
1	C	54	GLN
1	C	62	GLN
1	C	66	ASN
1	C	192	HIS
1	E	96	GLN
2	F	2	GLN
1	G	96	GLN
1	K	127	ASN
1	K	155	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	274/284 (96%)	0.56	11 (4%) 38 38	19, 38, 61, 79	0
1	C	275/284 (96%)	0.93	27 (9%) 7 7	26, 42, 70, 82	0
1	E	275/284 (96%)	0.90	22 (8%) 12 12	27, 41, 64, 93	0
1	G	274/284 (96%)	1.04	34 (12%) 4 3	26, 45, 73, 95	0
1	I	274/284 (96%)	0.96	26 (9%) 8 8	24, 49, 81, 109	0
1	K	275/284 (96%)	1.29	51 (18%) 1 1	28, 47, 90, 119	0
2	B	100/100 (100%)	0.77	8 (8%) 12 12	20, 36, 58, 64	0
2	D	100/100 (100%)	0.68	6 (6%) 22 21	25, 36, 62, 70	0
2	F	99/100 (99%)	1.97	34 (34%) 0 0	25, 53, 89, 99	0
2	H	100/100 (100%)	0.75	9 (9%) 9 9	27, 39, 61, 67	0
2	J	100/100 (100%)	2.16	45 (45%) 0 0	26, 57, 95, 104	0
2	L	100/100 (100%)	1.39	29 (29%) 0 0	32, 49, 77, 84	0
3	M	9/9 (100%)	0.09	0 100 100	21, 27, 30, 43	0
3	N	9/9 (100%)	1.25	2 (22%) 0 0	35, 42, 48, 61	0
3	O	9/9 (100%)	0.91	1 (11%) 5 5	31, 40, 44, 58	0
3	P	9/9 (100%)	1.30	1 (11%) 5 5	38, 43, 45, 60	0
3	Q	9/9 (100%)	0.19	0 100 100	31, 35, 39, 49	0
3	R	9/9 (100%)	1.66	3 (33%) 0 0	40, 47, 62, 63	0
All	All	2300/2358 (97%)	1.03	309 (13%) 3 2	19, 43, 76, 119	0

All (309) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	82	VAL	11.1
1	K	53	GLU	8.5
2	J	18	GLY	8.4

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Mol	Chain	Res	Type	RSRZ
2	J	80	CYS	8.0
2	F	40	LEU	7.6
2	J	0	MET	7.3
2	J	71	THR	7.3
2	F	49	VAL	6.8
1	E	113	TYR	6.7
2	J	22	PHE	6.6
2	F	73	THR	6.6
1	G	17	ARG	6.4
1	K	56	GLY	6.4
1	K	49	ALA	6.4
1	K	52	ILE	6.3
1	I	16	GLY	6.3
2	F	75	LYS	6.2
2	B	0	MET	6.2
2	H	0	MET	6.1
2	J	79	ALA	6.0
2	J	20	SER	5.9
1	E	194	ILE	5.9
2	J	45	ARG	5.8
1	G	15	PRO	5.7
2	J	72	PRO	5.6
1	K	38	SER	5.5
1	I	15	PRO	5.4
2	J	41	LYS	5.4
1	K	51	TRP	5.4
1	K	59	TYR	5.2
2	J	21	ASN	5.1
2	F	80	CYS	5.1
1	K	17	ARG	5.1
1	C	107	GLY	5.1
2	F	76	ASP	5.1
1	G	91	GLY	5.0
1	I	17	ARG	4.9
2	F	74	GLU	4.9
2	F	20	SER	4.7
1	C	130	LEU	4.7
1	C	91	GLY	4.7
2	L	98	ASP	4.7
1	G	110	LEU	4.6
1	K	18	GLY	4.6
1	C	41	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
2	J	81	ARG	4.6
2	F	51	HIS	4.5
2	J	1	ILE	4.4
1	K	48	ARG	4.3
1	G	54	GLN	4.3
2	D	75	LYS	4.3
1	G	18	GLY	4.3
2	F	41	LYS	4.3
2	L	82	VAL	4.2
2	F	98	ASP	4.2
1	K	44	LYS	4.2
1	K	84	TYR	4.2
2	B	99	MET	4.1
1	C	177	GLU	4.1
2	J	68	THR	4.1
1	K	85	TYR	4.0
2	F	88	SER	4.0
2	F	52	SER	3.9
2	J	70	PHE	3.9
2	J	78	TYR	3.9
2	J	40	LEU	3.8
1	G	181	ARG	3.8
3	O	5	LYS	3.8
2	L	95	TRP	3.8
1	I	194	ILE	3.8
1	K	62	GLN	3.8
2	H	99	MET	3.7
2	L	43	GLY	3.7
1	G	41	ALA	3.7
1	I	1	GLY	3.7
1	I	201	LEU	3.6
1	G	126	LEU	3.6
2	F	39	LEU	3.6
2	J	19	LYS	3.6
2	B	1	ILE	3.5
2	L	35	ILE	3.5
1	G	90	ASP	3.5
1	E	17	ARG	3.5
2	D	16	GLU	3.5
1	K	72	GLN	3.5
2	J	75	LYS	3.5
2	F	68	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	172	LEU	3.4
2	J	67	TYR	3.4
1	G	12	VAL	3.4
2	J	69	GLU	3.4
1	K	9	PHE	3.4
1	G	131	ARG	3.4
1	G	19	GLU	3.3
1	C	227	ASP	3.3
3	R	8	ASP	3.3
1	A	192	HIS	3.3
1	E	38	SER	3.3
2	F	37	VAL	3.3
2	F	87	LEU	3.3
2	J	82	VAL	3.3
2	J	23	LEU	3.2
2	D	98	ASP	3.2
2	J	73	THR	3.2
1	K	50	PRO	3.2
1	I	203	CYS	3.2
1	K	275	GLU	3.2
2	F	1	ILE	3.2
2	J	49	VAL	3.2
1	K	124	ILE	3.2
2	H	75	LYS	3.2
3	P	4	LEU	3.1
1	I	48	ARG	3.1
1	K	81	LEU	3.1
1	K	58	GLU	3.1
1	K	152	ALA	3.1
1	A	1	GLY	3.1
2	J	87	LEU	3.1
1	K	123	TYR	3.1
2	J	46	ILE	3.1
2	J	76	ASP	3.1
1	I	57	PRO	3.1
2	L	99	MET	3.0
2	F	43	GLY	3.0
1	A	253	GLU	3.0
1	A	272	LEU	3.0
1	E	15	PRO	3.0
2	L	71	THR	3.0
1	C	152	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	15	ALA	3.0
1	A	177	GLU	2.9
1	C	61	ASP	2.9
1	K	39	ASP	2.9
2	J	14	PRO	2.9
1	K	225	THR	2.9
1	G	124	ILE	2.9
1	E	193	PRO	2.9
2	J	89	GLN	2.9
1	K	40	ALA	2.9
2	F	81	ARG	2.9
1	I	51	TRP	2.9
1	G	98	MET	2.9
2	L	92	ILE	2.8
2	L	80	CYS	2.8
1	A	257	TYR	2.8
2	J	38	ASP	2.8
2	L	18	GLY	2.8
2	H	60	TRP	2.8
2	D	88	SER	2.8
1	K	76	ALA	2.7
1	C	183	ASP	2.7
2	J	43	GLY	2.7
1	C	108	ARG	2.7
2	L	69	GLU	2.7
1	E	59	TYR	2.7
1	K	20	PRO	2.7
1	C	178	THR	2.7
1	G	194	ILE	2.7
2	H	1	ILE	2.7
2	J	92	ILE	2.7
1	K	19	GLU	2.7
2	F	16	GLU	2.7
2	J	44	GLU	2.7
1	K	68	LYS	2.7
1	A	224	GLN	2.7
2	F	99	MET	2.7
2	F	85	VAL	2.6
2	J	16	GLU	2.6
2	F	89	GLN	2.6
1	G	158	VAL	2.6
1	I	274	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	85	VAL	2.6
1	K	237	GLY	2.6
1	C	57	PRO	2.6
1	C	52	ILE	2.6
1	I	91	GLY	2.6
1	K	55	GLU	2.6
1	E	130	LEU	2.6
2	L	64	LEU	2.6
1	I	14	ARG	2.6
1	K	14	ARG	2.6
1	I	260	HIS	2.6
1	K	147	TRP	2.6
1	K	86	ASN	2.6
1	K	165	VAL	2.5
1	I	85	TYR	2.5
1	G	177	GLU	2.5
1	C	54	GLN	2.5
1	K	47	PRO	2.5
1	K	160	LEU	2.5
1	E	165	VAL	2.5
2	D	9	VAL	2.5
2	L	19	LYS	2.5
1	E	98	MET	2.5
1	G	130	LEU	2.5
1	K	79	GLY	2.5
1	K	255	GLN	2.5
2	J	37	VAL	2.5
2	L	44	GLU	2.5
1	I	181	ARG	2.5
1	G	89	GLU	2.5
2	B	88	SER	2.5
2	L	7	ILE	2.5
2	L	40	LEU	2.4
2	F	78	TYR	2.4
2	L	1	ILE	2.4
1	A	260[A]	HIS	2.4
1	K	151	HIS	2.4
1	C	252	GLY	2.4
1	G	252	GLY	2.4
1	C	60	TRP	2.4
1	G	51	TRP	2.4
1	E	76	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	72	PRO	2.4
1	I	208	PHE	2.4
2	H	39	LEU	2.4
1	G	52	ILE	2.4
2	J	9	VAL	2.4
2	F	95	TRP	2.4
1	C	59	TYR	2.4
3	N	1	CYS	2.4
1	I	110	LEU	2.4
1	C	228	THR	2.4
2	L	96	ASP	2.4
2	F	42	ASN	2.3
2	H	83	ASN	2.3
2	J	27	VAL	2.3
1	I	211	ALA	2.3
2	J	11	SER	2.3
2	B	92	ILE	2.3
1	G	85	TYR	2.3
1	I	52	ILE	2.3
3	N	9	TYR	2.3
1	E	272	LEU	2.3
1	G	109	PHE	2.3
2	L	86	THR	2.3
1	K	13	SER	2.3
3	R	9	TYR	2.3
1	C	115	GLN	2.3
1	E	163	ARG	2.3
2	J	95	TRP	2.3
2	F	46	ILE	2.3
2	L	42	ASN	2.3
1	I	255	GLN	2.3
1	E	147	TRP	2.3
1	K	183	ASP	2.3
1	E	112	GLY	2.3
1	G	104	GLY	2.3
1	A	228[A]	THR	2.2
1	E	80	THR	2.2
1	E	110	LEU	2.2
1	K	179	LEU	2.2
2	L	93	VAL	2.2
1	I	56	GLY	2.2
1	I	183	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	36	GLU	2.2
1	G	40	ALA	2.2
1	E	266	LEU	2.2
2	F	14	PRO	2.2
2	L	37	VAL	2.2
1	G	225	THR	2.2
1	A	18	GLY	2.2
2	J	47	GLU	2.2
1	G	170	ARG	2.2
1	G	95	ILE	2.2
2	B	87	LEU	2.2
2	L	65	LEU	2.2
2	B	3	ARG	2.2
2	J	2	GLN	2.2
1	C	248	VAL	2.2
2	B	44	GLU	2.2
1	C	136	ALA	2.2
1	K	142	ILE	2.1
1	C	215	LEU	2.1
1	I	38	SER	2.1
2	F	70	PHE	2.1
2	L	56	PHE	2.1
1	K	175	GLY	2.1
1	K	61	ASP	2.1
2	J	39	LEU	2.1
1	C	19	GLU	2.1
2	J	25	CYS	2.1
1	C	223	ASP	2.1
1	G	183	ASP	2.1
1	C	175	GLY	2.1
2	L	39	LEU	2.1
1	I	189	MET	2.1
2	F	91	LYS	2.1
1	G	102	ASP	2.1
1	E	72	GLN	2.1
1	E	198	GLU	2.1
1	K	57	PRO	2.1
1	K	43	GLN	2.1
1	A	259	CYS	2.1
1	C	126	LEU	2.0
2	L	46	ILE	2.0
2	L	53	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
3	R	5	LYS	2.0
1	K	22	PHE	2.0
1	C	89	GLU	2.0
1	K	16	GLY	2.0
2	J	50	GLU	2.0
2	F	38	ASP	2.0
1	E	33	PHE	2.0
1	E	32[A]	GLN	2.0
1	G	20	PRO	2.0
2	D	46	ILE	2.0
1	I	261	VAL	2.0
2	L	49	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.