



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:33 AM UTC

PDB ID : 8DNT / pdb\_00008dnt  
Title : SARS-CoV-2 specific T cell receptor  
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Deposited on : 2022-07-11  
Resolution : 3.18 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

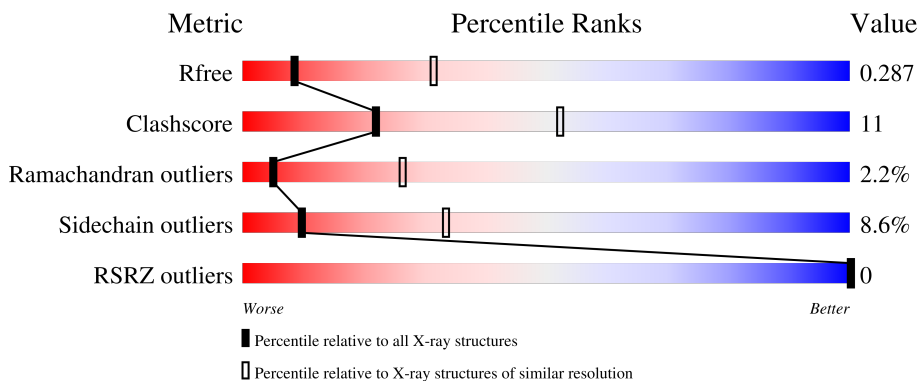
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.18 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))
$R_{free}$	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	203	 69% 27% ..
1	H	203	 64% 28% 5% .
1	M	203	 70% 25% ..
1	V	203	 69% 27% ..
2	B	244	 61% 35% ..

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Mol	Chain	Length	Quality of chain
2	I	244	71% 26% ..
2	P	244	74% 21% ..
2	W	244	71% 26% ..
3	D	9	56% 44%
3	J	9	56% 33% 11%
3	Q	9	33% 33% 33%
3	X	9	78% 22%
4	E	279	72% 24% ..
4	K	279	65% 33% ..
4	R	279	68% 29% .
4	Y	279	68% 29% ..
5	F	100	69% 29% .
5	L	100	58% 34% 8%
5	T	100	64% 35% .
5	Z	100	74% 23% .

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 26210 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 T-cell receptor alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	199	1548	964	260	316	8	0	0	0
1	H	198	1543	961	259	315	8	0	0	0
1	M	198	1543	961	259	315	8	0	0	0
1	V	198	1539	958	258	315	8	0	0	0

- Molecule 2 is a protein called T-cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	242	1894	1189	328	372	5	0	0	0
2	I	242	1881	1180	327	369	5	0	0	0
2	P	242	1897	1190	330	372	5	0	0	0
2	W	242	1894	1189	328	372	5	0	0	0

- Molecule 3 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	9	77	49	14	14	0	0	0
3	J	9	77	49	14	14	0	0	0
3	Q	9	77	49	14	14	0	0	0
3	X	9	77	49	14	14	0	0	0

- Molecule 4 is a protein called MHC class I antigen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	275	Total	C	N	O	S	0	0	0
			2239	1399	408	423	9			
4	K	276	Total	C	N	O	S	0	0	0
			2236	1398	403	426	9			
4	R	278	Total	C	N	O	S	0	0	0
			2241	1400	408	424	9			
4	Y	274	Total	C	N	O	S	0	0	0
			2196	1380	395	413	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	MET	-	initiating methionine	UNP U5YKE0
E	276	GLY	-	expression tag	UNP U5YKE0
E	277	GLY	-	expression tag	UNP U5YKE0
E	278	GLY	-	expression tag	UNP U5YKE0
K	0	MET	-	initiating methionine	UNP U5YKE0
K	276	GLY	-	expression tag	UNP U5YKE0
K	277	GLY	-	expression tag	UNP U5YKE0
K	278	GLY	-	expression tag	UNP U5YKE0
R	0	MET	-	initiating methionine	UNP U5YKE0
R	276	GLY	-	expression tag	UNP U5YKE0
R	277	GLY	-	expression tag	UNP U5YKE0
R	278	GLY	-	expression tag	UNP U5YKE0
Y	0	MET	-	initiating methionine	UNP U5YKE0
Y	276	GLY	-	expression tag	UNP U5YKE0
Y	277	GLY	-	expression tag	UNP U5YKE0
Y	278	GLY	-	expression tag	UNP U5YKE0

- Molecule 5 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	100	Total	C	N	O	S	0	0	0
			813	518	137	154	4			
5	L	100	Total	C	N	O	S	0	0	0
			822	525	139	154	4			
5	T	100	Total	C	N	O	S	0	0	0
			804	516	135	150	3			
5	Z	100	Total	C	N	O	S	0	0	0
			812	519	138	152	3			

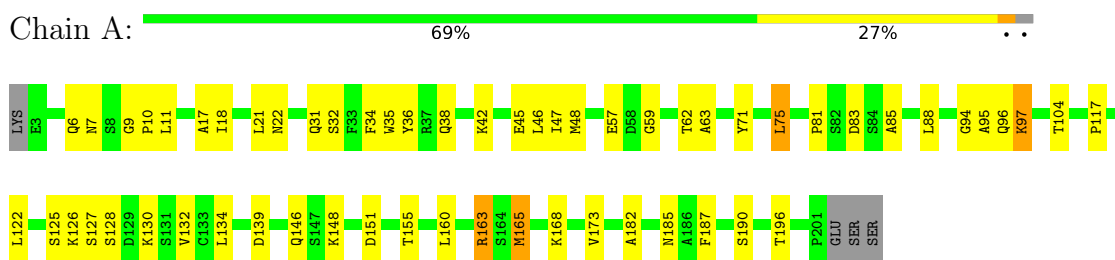
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	initiating methionine	UNP P61769
L	1	MET	-	initiating methionine	UNP P61769
T	1	MET	-	initiating methionine	UNP P61769
Z	1	MET	-	initiating methionine	UNP P61769

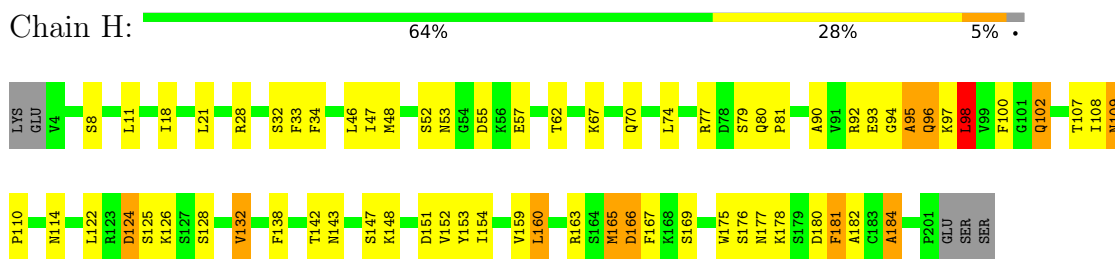
### 3 Residue-property plots [i](#)

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

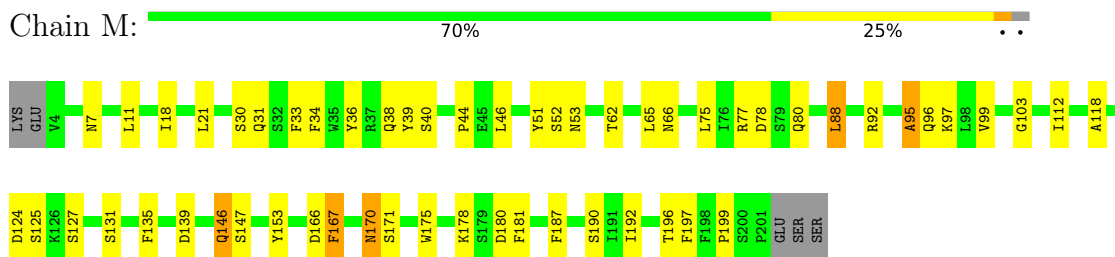
- Molecule 1: T-cell receptor alpha chain



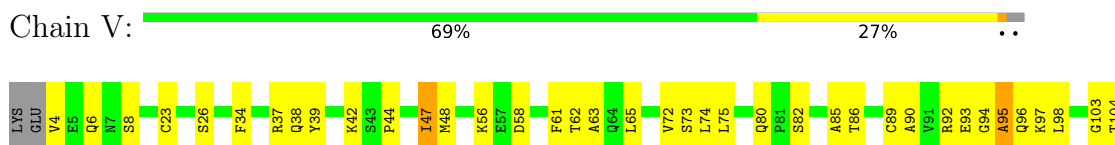
- Molecule 1: T-cell receptor alpha chain



- Molecule 1: T-cell receptor alpha chain

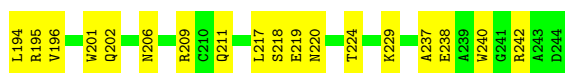


- Molecule 1: T-cell receptor alpha chain

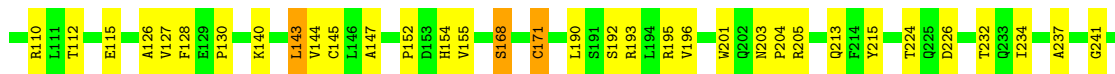
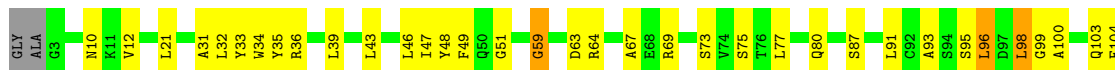




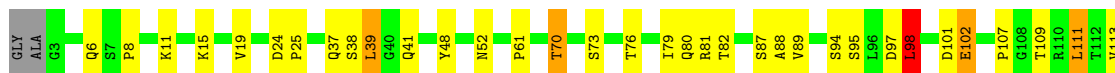
- Molecule 2: T-cell receptor beta chain



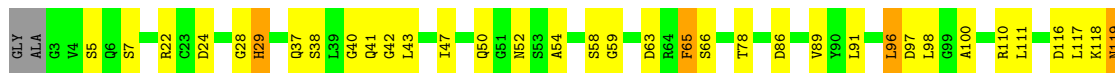
- Molecule 2: T-cell receptor beta chain



- Molecule 2: T-cell receptor beta chain



- Molecule 2: T-cell receptor beta chain



D244

- Molecule 3: Nucleoprotein

Chain D: 56% 44%

- Molecule 3: Nucleoprotein

Chain J: 56% 33% 11%

- Molecule 3: Nucleoprotein

Chain Q: 33% 33% 33%

- Molecule 3: Nucleoprotein

Chain X: 78% 22%

- Molecule 4: MHC class I antigen alpha chain

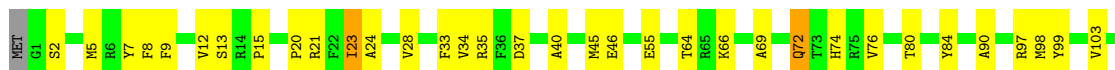
Chain E: 72% 24% ..

- Molecule 4: MHC class I antigen alpha chain

Chain K: 65% 33% ..



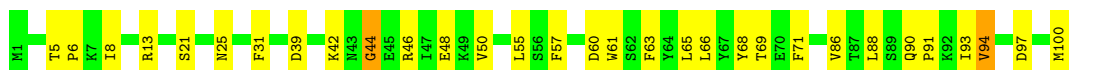
• Molecule 4: MHC class I antigen alpha chain



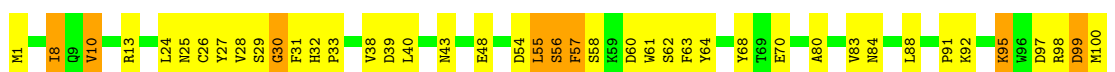
• Molecule 4: MHC class I antigen alpha chain



• Molecule 5: Beta-2-microglobulin

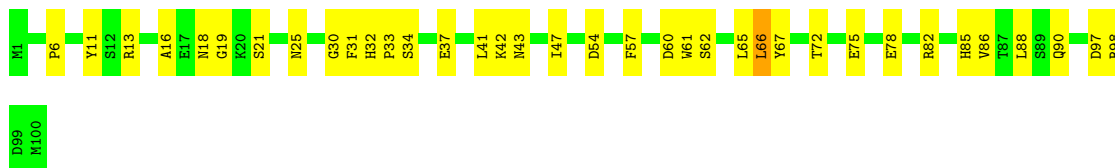


• Molecule 5: Beta-2-microglobulin



• Molecule 5: Beta-2-microglobulin





- Molecule 5: Beta-2-microglobulin

Chain Z: 74% 23%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.16Å 121.83Å 210.56Å 90.00° 100.02° 90.00°	Depositor
Resolution (Å)	30.00 – 3.18 30.00 – 3.18	Depositor EDS
% Data completeness (in resolution range)	74.7 (30.00-3.18) 74.3 (30.00-3.18)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 3.18Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.221 , 0.313 (Not available) , 0.287	Depositor DCC
$R_{free}$ test set	2857 reflections (3.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	107.6	Xtrriage
Anisotropy	0.249	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 78.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	26210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	155.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.45	0/1581	0.82	0/2143
1	H	0.46	0/1576	0.84	0/2136
1	M	0.45	0/1576	0.84	0/2136
1	V	0.44	0/1572	0.85	0/2132
2	B	0.44	0/1942	0.83	0/2643
2	I	0.45	0/1929	0.82	0/2629
2	P	0.44	0/1945	0.84	0/2647
2	W	0.45	0/1942	0.83	0/2643
3	D	0.37	0/76	0.78	0/100
3	J	0.36	0/76	1.01	0/100
3	Q	0.39	0/76	0.99	0/100
3	X	0.36	0/76	0.71	0/100
4	E	0.44	0/2304	0.90	3/3129 (0.1%)
4	K	0.44	0/2301	0.92	1/3126 (0.0%)
4	R	0.44	0/2306	0.93	1/3132 (0.0%)
4	Y	0.44	0/2258	0.91	0/3069
5	F	0.42	0/836	0.86	1/1137 (0.1%)
5	L	0.44	0/845	0.90	0/1146
5	T	0.45	0/827	0.81	0/1125
5	Z	0.42	0/835	0.81	0/1135
All	All	0.44	0/26879	0.86	6/36508 (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
3	D	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	5	THR	CB-CA-C	8.61	119.66	109.85
4	K	178	THR	N-CA-C	-7.45	106.13	114.62
4	E	64	THR	CB-CA-C	5.53	116.30	109.16
4	R	200	THR	CB-CA-C	5.06	118.89	110.74
4	E	64	THR	N-CA-C	-5.05	108.38	114.75
4	E	65	ARG	N-CA-C	-5.04	107.13	113.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	5	ARG	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1548	0	1460	39	0
1	H	1543	0	1458	44	0
1	M	1543	0	1458	44	0
1	V	1539	0	1447	32	0
2	B	1894	0	1796	46	0
2	I	1881	0	1769	45	0
2	P	1897	0	1801	28	0
2	W	1894	0	1796	35	0
3	D	77	0	88	1	0
3	J	77	0	88	3	0
3	Q	77	0	88	8	0
3	X	77	0	88	2	0
4	E	2239	0	2083	45	0
4	K	2236	0	2070	66	0
4	R	2241	0	2077	57	0
4	Y	2196	0	2025	43	0
5	F	813	0	753	13	0
5	L	822	0	777	24	0
5	T	804	0	746	19	0
5	Z	812	0	757	14	0
All	All	26210	0	24625	542	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 11.

All (542) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:46:LEU:HB3	2:P:102:GLU:HG3	1.23	1.09
4:R:230:LEU:HD11	4:R:243:LYS:HE3	1.43	1.01
1:M:96:GLN:HE22	3:Q:6:LEU:HB3	1.23	0.98
2:W:41:GLN:HG2	2:W:42:GLY:H	1.29	0.98
4:K:127:LYS:HD3	4:K:128:GLU:H	1.29	0.96
1:M:96:GLN:NE2	3:Q:6:LEU:HB3	1.80	0.94
1:A:95:ALA:HB2	4:E:66:LYS:HA	1.48	0.93
1:M:46:LEU:HB3	2:P:102:GLU:CG	1.99	0.91
1:H:97:LYS:O	1:H:98:LEU:HB2	1.69	0.90
1:M:95:ALA:HB1	4:R:69:ALA:HB2	1.54	0.87
4:Y:6:ARG:HD3	4:Y:98:MET:HE2	1.56	0.87
1:A:96:GLN:HG2	2:B:98:LEU:HG	1.57	0.85
1:M:46:LEU:HD22	2:P:102:GLU:HB2	1.61	0.82
4:R:230:LEU:HD13	4:R:245:ALA:HB2	1.64	0.80
1:H:96:GLN:HG2	2:I:98:LEU:HG	1.62	0.80
1:H:147:SER:HA	1:H:154:ILE:HD12	1.64	0.80
5:F:97:ASP:HB3	5:F:100:MET:HB3	1.63	0.79
2:I:21:LEU:HB2	2:I:77:LEU:HB3	1.63	0.79
1:M:88:LEU:HD12	1:M:103:GLY:HA2	1.63	0.79
4:R:35:ARG:HH21	4:R:37:ASP:HB2	1.47	0.78
4:K:74:HIS:CE1	4:K:97:ARG:HD2	2.19	0.78
1:V:90:ALA:HB1	1:V:98:LEU:HD11	1.66	0.77
4:E:106:ASP:O	4:E:107:TRP:HB2	1.85	0.76
2:P:97:ASP:O	2:P:98:LEU:HB2	1.84	0.76
1:H:80:GLN:HG2	1:H:81:PRO:HD2	1.68	0.75
4:R:202:ARG:HD3	4:R:246:ALA:HB2	1.67	0.75
4:K:74:HIS:HE1	4:K:97:ARG:HD2	1.50	0.74
1:H:79:SER:HB3	1:H:108:ILE:HD12	1.69	0.74
4:K:74:HIS:HA	4:K:77:ASP:HB2	1.69	0.73
4:E:52:ILE:HD13	4:E:171:TYR:HE1	1.53	0.73
2:P:87:SER:HB3	2:P:113:VAL:H	1.52	0.73
4:K:8:PHE:HD1	5:L:57:PHE:CE1	2.07	0.73
1:H:167:PHE:HE2	1:H:169:SER:HB3	1.54	0.72
4:K:81:LEU:HD13	4:K:118:TYR:CD1	2.25	0.72
1:V:62:THR:HB	1:V:75:LEU:HB2	1.72	0.71
5:L:38:VAL:HG22	5:L:83:VAL:HG22	1.72	0.71
1:H:34:PHE:HB2	1:H:90:ALA:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:56:SER:OG	5:L:57:PHE:N	2.20	0.70
1:H:92:ARG:HD3	1:H:96:GLN:HG3	1.73	0.70
5:F:50:VAL:HG22	5:F:69:THR:HB	1.75	0.69
1:A:75:LEU:HD21	1:M:75:LEU:HD21	1.75	0.69
4:K:9:PHE:HD1	4:K:22:PHE:HZ	1.40	0.69
1:H:110:PRO:HG3	1:H:159:VAL:HG11	1.76	0.68
1:H:165:MET:O	1:H:166:ASP:HB2	1.92	0.68
2:B:53:SER:O	2:B:55:PRO:HD3	1.93	0.68
4:R:35:ARG:NH2	4:R:37:ASP:HB2	2.08	0.68
4:R:98:MET:HE1	4:R:113:TYR:HD1	1.58	0.68
1:H:167:PHE:CE2	1:H:169:SER:HB3	2.29	0.67
4:K:9:PHE:HE2	4:K:99:TYR:CE2	2.13	0.67
1:H:178:LYS:HE2	1:H:180:ASP:HB2	1.77	0.66
4:K:106:ASP:O	4:K:107:TRP:HB2	1.95	0.66
1:M:30:SER:HB2	1:M:33:PHE:CZ	2.29	0.66
1:A:62:THR:HB	1:A:75:LEU:HB2	1.78	0.66
1:H:124:ASP:HA	2:I:128:PHE:HD2	1.60	0.66
2:B:117:LEU:HD22	2:B:217:LEU:HD21	1.78	0.66
2:P:25:PRO:HG2	2:P:73:SER:HB2	1.78	0.65
2:W:97:ASP:HB2	2:W:100:ALA:HB2	1.78	0.65
1:M:62:THR:HB	1:M:75:LEU:HB2	1.77	0.65
2:I:110:ARG:HG2	2:I:154:HIS:CE1	2.31	0.65
4:E:51:TRP:CZ2	4:E:179:LEU:HD21	2.32	0.65
4:K:234:ARG:HG2	4:K:242:GLN:O	1.96	0.65
1:H:97:LYS:O	1:H:98:LEU:CB	2.45	0.65
4:K:9:PHE:HD1	4:K:22:PHE:CZ	2.14	0.65
2:B:4:VAL:HG22	2:B:26:ILE:HG13	1.79	0.64
4:K:9:PHE:CD1	4:K:22:PHE:HZ	2.15	0.64
5:T:30:GLY:HA2	5:T:62:SER:HB2	1.80	0.64
4:Y:81:LEU:HD13	4:Y:118:TYR:CD1	2.31	0.64
1:M:46:LEU:HD13	2:P:102:GLU:HA	1.80	0.64
2:I:21:LEU:HD22	2:I:77:LEU:HD23	1.79	0.64
2:B:162:ASN:HD21	2:B:206:ASN:HA	1.62	0.64
1:V:34:PHE:HB2	1:V:90:ALA:HB3	1.80	0.63
4:R:72:GLN:HA	4:R:72:GLN:NE2	2.13	0.63
2:W:209:ARG:HG3	2:W:238:GLU:HG2	1.82	0.62
2:P:25:PRO:HB3	2:P:94:SER:HB3	1.82	0.62
4:Y:81:LEU:HD21	4:Y:123:TYR:CE1	2.35	0.62
1:A:38:GLN:O	1:A:85:ALA:HB1	2.00	0.62
4:R:123:TYR:HD2	4:R:124:ILE:HG22	1.63	0.62
4:R:208:PHE:HD1	4:R:263:HIS:NE2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:187:THR:HA	4:K:204:TRP:O	1.99	0.62
2:W:41:GLN:HG2	2:W:42:GLY:N	2.08	0.62
4:R:99:TYR:HB3	4:R:114:HIS:CD2	2.35	0.61
4:K:5:MET:HB2	4:K:168:LEU:HD13	1.80	0.61
4:E:167:TRP:O	4:E:171:TYR:HD2	1.84	0.61
4:Y:202:ARG:HD3	4:Y:244:TRP:CE3	2.35	0.61
4:K:14:ARG:HB2	4:K:17:ARG:HB2	1.83	0.61
5:L:60:ASP:O	5:L:61:TRP:HB2	2.01	0.61
2:I:31:ALA:HB3	2:I:95:SER:HB2	1.83	0.61
5:L:26:CYS:HB2	5:L:40:LEU:HD21	1.82	0.61
1:A:81:PRO:HG3	1:A:168:LYS:HE2	1.83	0.60
4:E:5:MET:HB2	4:E:168:LEU:HD13	1.82	0.60
5:T:19:GLY:HA2	5:T:72:THR:HG22	1.83	0.60
1:H:34:PHE:HZ	1:H:92:ARG:HH21	1.49	0.60
1:H:92:ARG:NH2	2:I:100:ALA:O	2.35	0.60
4:K:69:ALA:HA	4:K:72:GLN:HB2	1.83	0.60
4:R:253:GLN:O	4:R:256:ARG:HG3	2.01	0.60
1:M:118:ALA:HA	1:M:197:PHE:HB3	1.83	0.60
5:F:25:ASN:HB3	5:F:66:LEU:HD11	1.84	0.59
2:P:52:ASN:HB2	2:P:70:THR:HG22	1.84	0.59
1:V:4:VAL:N	1:V:26:SER:HG	2.00	0.59
4:E:185:PRO:HD2	4:E:266:LEU:HD11	1.84	0.59
4:E:167:TRP:O	4:E:171:TYR:CD2	2.56	0.59
2:I:12:VAL:HG11	2:I:152:PRO:HG3	1.85	0.59
2:I:130:PRO:HD2	2:I:201:TRP:CZ2	2.38	0.59
1:V:39:TYR:HB2	1:V:42:LYS:HB2	1.84	0.59
4:R:210:PRO:HD2	4:R:264:GLU:HG3	1.83	0.59
2:B:97:ASP:HB2	2:B:100:ALA:HB2	1.84	0.59
1:M:30:SER:C	1:M:31:GLN:HG2	2.28	0.59
4:R:204:TRP:HE3	4:R:206:LEU:HD11	1.67	0.59
4:E:106:ASP:O	4:E:107:TRP:CB	2.50	0.59
4:R:128:GLU:O	4:R:130:LEU:HD12	2.03	0.59
2:I:192:SER:O	2:I:193:ARG:HG3	2.03	0.59
4:K:202:ARG:HG2	4:K:204:TRP:HE1	1.67	0.59
2:I:127:VAL:HG23	2:I:237:ALA:HB3	1.85	0.58
1:A:22:ASN:HD21	1:A:71:TYR:HD2	1.51	0.58
4:K:156:LEU:C	4:K:158:ALA:H	2.10	0.58
4:R:9:PHE:CD1	4:R:24:ALA:HB1	2.38	0.58
1:V:48:MET:HE2	1:V:63:ALA:HB3	1.85	0.58
4:K:202:ARG:HG2	4:K:204:TRP:NE1	2.19	0.58
2:P:117:LEU:HD22	2:P:217:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:67:VAL:HA	4:E:70:HIS:HB2	1.85	0.58
4:R:188:HIS:CE1	4:R:190:THR:HG23	2.39	0.58
4:Y:207:SER:HA	4:Y:240:THR:HB	1.86	0.58
4:R:72:GLN:HA	4:R:72:GLN:HE21	1.68	0.58
1:V:197:PHE:O	1:V:199:PRO:HD3	2.04	0.57
4:K:229:GLU:HB2	4:K:246:ALA:HB3	1.87	0.57
4:E:7:TYR:O	4:E:98:MET:HA	2.03	0.57
4:K:127:LYS:HD3	4:K:128:GLU:N	2.10	0.57
5:Z:14:HIS:O	5:Z:15:PRO:C	2.47	0.57
4:E:236:ALA:HB1	5:F:13:ARG:HG3	1.86	0.57
2:I:33:TYR:CD2	2:I:48:TYR:HB2	2.39	0.57
5:L:58:SER:C	5:L:60:ASP:H	2.12	0.57
4:Y:224:GLN:HE21	4:Y:227:ASP:H	1.53	0.57
4:R:9:PHE:HD1	4:R:24:ALA:CB	2.17	0.57
5:Z:42:LYS:C	5:Z:44:GLY:H	2.13	0.57
4:K:47:PRO:HB3	4:K:60:TRP:CH2	2.40	0.57
5:Z:30:GLY:HA2	5:Z:62:SER:HB2	1.86	0.57
2:B:69:ARG:HD2	2:B:75:SER:HB2	1.87	0.56
4:K:207:SER:HA	4:K:240:THR:HB	1.87	0.56
2:B:143:LEU:HB2	2:B:194:LEU:HB3	1.87	0.56
5:L:8:ILE:HG23	5:L:28:VAL:HG12	1.87	0.56
1:H:124:ASP:HA	2:I:128:PHE:CD2	2.39	0.56
4:Y:87:GLN:HE21	5:Z:1:MET:HE1	1.71	0.56
1:A:95:ALA:CB	4:E:66:LYS:HA	2.31	0.56
4:K:52:ILE:C	4:K:54:GLN:H	2.14	0.56
1:M:197:PHE:HD2	1:M:199:PRO:HD3	1.71	0.56
5:T:6:PRO:HB3	5:T:31:PHE:HB3	1.88	0.56
2:P:137:HIS:HD2	2:P:138:THR:HG23	1.69	0.56
1:V:92:ARG:HA	1:V:98:LEU:HA	1.88	0.56
1:M:88:LEU:CD1	1:M:103:GLY:HA2	2.35	0.56
1:V:37:ARG:O	1:V:44:PRO:HA	2.06	0.56
4:R:218:GLN:NE2	4:R:221:GLY:O	2.38	0.56
4:E:14:ARG:HB2	4:E:17:ARG:HD2	1.86	0.56
4:E:253:GLN:HE22	4:Y:121:LYS:HB2	1.70	0.56
4:R:188:HIS:HE1	4:R:190:THR:HG23	1.71	0.56
1:H:57:GLU:HG2	1:H:62:THR:HG23	1.88	0.55
1:M:18:ILE:HG13	1:M:77:ARG:HA	1.88	0.55
2:P:146:LEU:HD22	2:P:148:THR:HG23	1.88	0.55
1:H:47:ILE:HG13	1:H:48:MET:HG2	1.88	0.55
2:I:32:LEU:HA	2:I:93:ALA:O	2.06	0.55
3:J:6:LEU:CD1	3:J:6:LEU:N	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:96:GLN:OE1	2:W:98:LEU:HD23	2.07	0.55
4:E:11:SER:HB2	4:E:95:VAL:HG12	1.88	0.55
4:E:20:PRO:HD2	4:E:75:ARG:HD2	1.88	0.55
4:K:156:LEU:C	4:K:158:ALA:N	2.60	0.55
2:W:5:SER:HB3	2:W:24:ASP:HB3	1.87	0.55
4:E:52:ILE:HD13	4:E:171:TYR:CE1	2.37	0.55
1:H:53:ASN:HD21	1:H:67:LYS:HB2	1.71	0.55
4:Y:133:TRP:HB2	4:Y:144:LYS:HE2	1.89	0.55
4:Y:202:ARG:HG2	4:Y:204:TRP:NE1	2.22	0.55
1:H:21:LEU:HB2	1:H:74:LEU:HB3	1.89	0.55
1:A:117:PRO:HB2	1:A:196:THR:HG23	1.90	0.54
4:R:208:PHE:HD1	4:R:263:HIS:HE2	1.52	0.54
1:H:128:SER:HB2	2:I:126:ALA:HB2	1.88	0.54
1:M:125:SER:C	1:M:127:SER:H	2.13	0.54
5:F:6:PRO:HB3	5:F:31:PHE:HB3	1.88	0.54
4:R:97:ARG:NH1	4:R:116:TYR:OH	2.40	0.54
1:V:97:LYS:O	1:V:98:LEU:HB3	2.07	0.54
4:E:214:THR:HB	4:E:262:GLN:HB2	1.88	0.54
1:H:160:LEU:HB3	2:I:171:CYS:HB3	1.88	0.54
1:V:6:GLN:HG3	1:V:23:CYS:HB3	1.89	0.54
1:H:152:VAL:HG13	1:H:176:SER:HB2	1.90	0.54
2:W:7:SER:HB3	2:W:22:ARG:HB3	1.89	0.54
1:A:96:GLN:O	1:A:97:LYS:HB2	2.08	0.54
4:E:187:THR:HB	4:E:272:LEU:HD11	1.88	0.54
4:K:67:VAL:HA	4:K:70:HIS:HB2	1.88	0.54
1:H:33:PHE:C	1:H:34:PHE:HD1	2.16	0.54
5:F:42:LYS:C	5:F:44:GLY:H	2.16	0.54
1:M:95:ALA:HA	4:R:66:LYS:HA	1.88	0.54
4:E:59:TYR:O	4:E:63:GLU:HG2	2.08	0.53
4:E:213:ILE:HG13	4:E:262:GLN:O	2.08	0.53
1:V:48:MET:HE2	1:V:63:ALA:CB	2.38	0.53
1:V:62:THR:HG22	1:V:63:ALA:N	2.23	0.53
2:W:89:VAL:HG22	2:W:110:ARG:HE	1.73	0.53
1:A:48:MET:HE2	1:A:63:ALA:H	1.73	0.53
2:P:157:LEU:HG	2:P:212:VAL:HG22	1.90	0.53
5:F:88:LEU:HB3	5:F:90:GLN:O	2.09	0.53
1:A:81:PRO:HG3	1:A:168:LYS:CE	2.38	0.53
4:K:9:PHE:CE2	4:K:99:TYR:CE2	2.95	0.53
4:R:13:SER:HA	4:R:20:PRO:HB3	1.91	0.53
3:J:6:LEU:HD23	4:K:73:THR:OG1	2.08	0.53
4:Y:59:TYR:O	4:Y:63:GLU:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:T:65:LEU:HD13	5:T:67:TYR:CE1	2.44	0.53
4:E:51:TRP:HB3	4:E:175:GLY:HA3	1.90	0.53
4:K:159:TYR:O	4:K:163:THR:N	2.42	0.53
4:R:34:VAL:HB	4:R:45:MET:HE2	1.90	0.53
4:Y:127:LYS:HG3	4:Y:134:THR:OG1	2.09	0.53
4:E:52:ILE:CD1	4:E:171:TYR:HE1	2.19	0.53
4:R:37:ASP:HB3	4:R:40:ALA:HB2	1.90	0.52
2:W:132:GLU:HA	2:W:135:ILE:HD12	1.91	0.52
1:M:53:ASN:HD22	1:M:53:ASN:H	1.57	0.52
4:K:9:PHE:CE2	4:K:99:TYR:HE2	2.27	0.52
4:R:261:VAL:HB	4:R:270:LEU:HB2	1.91	0.52
2:W:110:ARG:HG2	2:W:154:HIS:NE2	2.25	0.52
2:B:38:SER:O	2:B:39:LEU:C	2.53	0.52
4:R:21:ARG:HH12	4:R:23:ILE:HD12	1.74	0.52
3:X:6:LEU:HD22	4:Y:97:ARG:HH22	1.75	0.52
1:V:38:GLN:O	1:V:85:ALA:HB1	2.09	0.52
2:W:117:LEU:HD22	2:W:217:LEU:HD21	1.92	0.52
4:Y:100:GLY:O	4:Y:160:LEU:HD22	2.10	0.52
4:K:44:ARG:HH21	4:K:61:ASP:HA	1.75	0.52
4:Y:227:ASP:O	4:Y:247:VAL:HA	2.10	0.52
5:T:30:GLY:HA2	5:T:62:SER:CB	2.40	0.51
4:Y:74:HIS:HA	4:Y:77:ASP:HB2	1.92	0.51
4:K:236:ALA:HB1	5:L:13:ARG:HG2	1.93	0.51
2:P:6:GLN:HB2	2:P:107:PRO:HG2	1.93	0.51
3:Q:8:GLN:HE22	4:R:76:VAL:HB	1.75	0.51
2:B:157:LEU:HD23	2:B:158:SER:N	2.26	0.51
2:P:79:ILE:HG22	2:P:82:THR:HG22	1.92	0.51
4:R:12:VAL:HG21	5:T:34:SER:OG	2.09	0.51
2:W:223:TRP:CE2	2:W:225:GLN:HB2	2.45	0.51
4:Y:60:TRP:O	4:Y:64:THR:HB	2.10	0.51
2:I:213:GLN:HG2	2:I:215:TYR:CZ	2.45	0.51
1:A:95:ALA:HB2	4:E:66:LYS:HG3	1.92	0.51
1:V:122:LEU:HG	2:W:129:GLU:O	2.11	0.51
2:I:147:ALA:HB3	2:I:190:LEU:HB3	1.92	0.51
1:A:36:TYR:CE2	1:A:46:LEU:HB2	2.46	0.50
1:A:97:LYS:HA	2:B:33:TYR:HE2	1.76	0.50
2:B:160:TRP:HE1	2:B:211:GLN:HB3	1.76	0.50
3:X:8:GLN:HG3	4:Y:73:THR:HG23	1.93	0.50
1:A:18:ILE:HG21	1:A:75:LEU:HD23	1.92	0.50
1:A:134:LEU:HD12	1:A:173:VAL:HG22	1.91	0.50
5:L:29:SER:O	5:L:30:GLY:C	2.53	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:95:ALA:O	1:H:96:GLN:NE2	2.43	0.50
4:K:9:PHE:HE2	4:K:99:TYR:HE2	1.60	0.50
1:M:51:TYR:HB3	3:Q:5:ARG:NH1	2.27	0.50
5:T:43:ASN:HA	5:T:78:GLU:HB2	1.93	0.50
4:E:35:ARG:HH21	4:E:37:ASP:HB2	1.76	0.50
1:A:122:LEU:HD13	1:A:132:VAL:HG12	1.93	0.50
2:B:37:GLN:HB2	2:B:43:LEU:HA	1.93	0.50
4:E:111:ARG:HH11	4:E:128:GLU:HG3	1.77	0.50
1:V:8:SER:HA	1:V:103:GLY:O	2.12	0.50
1:V:118:ALA:HB2	1:V:197:PHE:HB3	1.94	0.50
2:W:130:PRO:HG2	2:W:141:ALA:HB1	1.94	0.50
4:R:80:THR:HG22	4:R:84:TYR:CE1	2.46	0.49
4:Y:253:GLN:HB3	4:Y:256:ARG:HE	1.77	0.49
4:E:35:ARG:HG3	4:E:46:GLU:HB2	1.94	0.49
5:Z:41:LEU:HD11	5:Z:82:ARG:HD2	1.94	0.49
2:B:89:VAL:HG22	2:B:110:ARG:HG2	1.95	0.49
1:A:96:GLN:CG	2:B:98:LEU:HG	2.36	0.49
4:K:207:SER:CA	4:K:240:THR:HB	2.43	0.49
2:W:157:LEU:HD23	2:W:158:SER:N	2.27	0.49
2:I:33:TYR:HD2	2:I:48:TYR:HB2	1.75	0.49
2:I:215:TYR:HA	2:I:232:THR:HG23	1.95	0.49
4:R:8:PHE:HD1	5:T:57:PHE:CE1	2.31	0.49
1:V:95:ALA:HB1	4:Y:69:ALA:HB2	1.93	0.49
5:L:29:SER:O	5:L:31:PHE:HD1	1.95	0.49
5:L:58:SER:C	5:L:60:ASP:N	2.71	0.49
4:E:210:PRO:HD2	4:E:263:HIS:HE1	1.78	0.49
2:P:145:CYS:HB2	2:P:159:TRP:CZ2	2.48	0.49
4:K:25:VAL:HG21	5:L:54:ASP:HB3	1.95	0.48
5:F:46:ARG:O	5:F:48:GLU:HG3	2.13	0.48
1:H:163:ARG:HB2	2:I:168:SER:OG	2.13	0.48
4:Y:231:VAL:HG22	4:Y:244:TRP:O	2.13	0.48
1:A:130:LYS:HE2	2:B:148:THR:HG21	1.94	0.48
4:Y:8:PHE:O	4:Y:24:ALA:HA	2.13	0.48
4:Y:116:TYR:CE1	4:Y:147:TRP:HH2	2.32	0.48
2:I:47:ILE:HD13	2:I:67:ALA:HB3	1.95	0.48
2:W:116:ASP:HB2	2:W:118:LYS:HE2	1.95	0.48
4:Y:19:GLU:HB3	4:Y:20:PRO:HD2	1.94	0.48
2:B:206:ASN:O	2:B:240:TRP:HA	2.13	0.48
1:H:80:GLN:HG2	1:H:81:PRO:CD	2.41	0.48
4:R:219:ARG:O	4:R:221:GLY:N	2.46	0.48
5:F:60:ASP:O	5:F:61:TRP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:SER:HA	2:B:111:LEU:HD23	1.94	0.48
4:K:168:LEU:O	4:K:172:LEU:HD12	2.13	0.48
4:R:230:LEU:CD1	4:R:243:LYS:HE3	2.29	0.48
2:W:43:LEU:HD11	2:W:91:LEU:HD12	1.96	0.48
1:A:95:ALA:HB2	4:E:66:LYS:CA	2.31	0.48
1:M:65:LEU:HD12	1:M:66:ASN:H	1.78	0.48
4:Y:141:GLN:HA	4:Y:144:LYS:HB2	1.95	0.48
4:K:8:PHE:CE1	4:K:98:MET:HG3	2.49	0.47
2:P:37:GLN:O	2:P:88:ALA:HB1	2.13	0.47
4:R:9:PHE:CD1	4:R:24:ALA:CB	2.96	0.47
4:Y:123:TYR:HD2	4:Y:124:ILE:HG22	1.79	0.47
1:H:153:TYR:HD2	1:H:175:TRP:NE1	2.12	0.47
1:A:31:GLN:NE2	3:D:4:ASP:HB2	2.30	0.47
2:P:130:PRO:HD2	2:P:201:TRP:CZ2	2.50	0.47
4:K:133:TRP:CD1	4:K:133:TRP:H	2.32	0.47
1:M:170:ASN:N	1:M:170:ASN:HD22	2.13	0.47
4:R:35:ARG:HG3	4:R:46:GLU:HB2	1.96	0.47
2:B:194:LEU:HG	2:B:195:ARG:N	2.29	0.47
2:I:128:PHE:O	2:I:143:LEU:HD23	2.15	0.47
4:K:206:LEU:HD23	4:K:242:GLN:HG2	1.96	0.47
4:R:99:TYR:HB3	4:R:114:HIS:HD2	1.79	0.47
1:V:48:MET:SD	1:V:58:ASP:HB2	2.54	0.47
4:R:138:MET:O	4:R:141:GLN:HB2	2.13	0.47
5:Z:3:GLN:HB3	5:Z:87:THR:HG22	1.97	0.47
1:M:39:TYR:O	1:M:40:SER:C	2.58	0.47
4:R:202:ARG:HB3	4:R:204:TRP:HE1	1.80	0.47
2:W:130:PRO:HD2	2:W:201:TRP:CH2	2.50	0.47
4:Y:81:LEU:HA	4:Y:84:TYR:HB2	1.96	0.47
1:H:100:PHE:CD1	2:I:43:LEU:HD23	2.50	0.47
1:H:182:ALA:O	1:H:184:ALA:N	2.40	0.47
4:Y:23:ILE:HG21	5:Z:55:LEU:HB3	1.97	0.47
4:E:23:ILE:HG21	5:F:55:LEU:HB3	1.96	0.46
1:M:31:GLN:O	3:Q:5:ARG:NH1	2.48	0.46
4:Y:99:TYR:HB3	4:Y:114:HIS:HD2	1.80	0.46
5:Z:18:ASN:HA	5:Z:73:PRO:HG2	1.97	0.46
1:A:95:ALA:HB3	4:E:69:ALA:HB3	1.96	0.46
2:B:127:VAL:HG23	2:B:237:ALA:HB3	1.97	0.46
5:L:80:ALA:CB	5:L:95:LYS:HA	2.44	0.46
1:V:173:VAL:HG23	2:W:193:ARG:HE	1.80	0.46
5:Z:25:ASN:HB3	5:Z:66:LEU:HD11	1.96	0.46
4:E:11:SER:HB2	4:E:95:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:35:TYR:OH	2:I:103:GLN:NE2	2.41	0.46
2:B:123:PRO:HB2	2:B:147:ALA:HB1	1.98	0.46
4:E:116:TYR:HB2	4:E:124:ILE:HG22	1.97	0.46
2:I:145:CYS:HB3	2:I:192:SER:HB3	1.96	0.46
1:A:11:LEU:HD13	1:A:104:THR:HG21	1.97	0.46
1:A:35:TRP:N	1:A:48:MET:O	2.46	0.46
4:K:111:ARG:HD2	4:K:128:GLU:HG3	1.98	0.46
4:K:239:GLY:O	4:K:240:THR:C	2.58	0.46
1:M:197:PHE:CD2	1:M:199:PRO:HD3	2.48	0.46
4:R:133:TRP:HE1	4:R:153:ALA:HB2	1.81	0.46
1:M:118:ALA:HA	1:M:197:PHE:CB	2.46	0.46
5:T:16:ALA:HB1	5:T:98:ARG:HE	1.81	0.46
1:V:86:THR:HA	1:V:104:THR:O	2.15	0.46
2:W:119:ASN:HD21	2:W:187:ARG:HD2	1.81	0.46
4:K:78:LEU:HD23	4:K:95:VAL:HG23	1.97	0.46
2:B:145:CYS:HB2	2:B:159:TRP:CZ2	2.51	0.46
1:A:57:GLU:HG2	1:A:62:THR:HG23	1.97	0.46
2:B:52:ASN:HB2	2:B:70:THR:HG22	1.98	0.46
1:H:124:ASP:C	1:H:126:LYS:H	2.24	0.46
2:I:192:SER:C	2:I:193:ARG:HG3	2.41	0.46
5:L:55:LEU:HD11	5:L:63:PHE:HB3	1.98	0.46
2:W:65:PHE:N	2:W:65:PHE:CD1	2.84	0.46
1:M:31:GLN:HE22	3:Q:1:LEU:HD21	1.81	0.45
2:W:123:PRO:HB3	2:W:150:PHE:HB3	1.98	0.45
1:A:187:PHE:HB3	1:A:190:SER:HB2	1.97	0.45
2:B:67:ALA:HB2	2:B:77:LEU:HD12	1.97	0.45
4:K:73:THR:O	4:K:77:ASP:OD1	2.34	0.45
1:M:38:GLN:HB2	1:M:44:PRO:HB3	1.97	0.45
2:P:38:SER:O	2:P:39:LEU:C	2.60	0.45
5:T:32:HIS:ND1	5:T:33:PRO:HA	2.32	0.45
1:A:17:ALA:HB2	1:M:7:ASN:HD21	1.81	0.45
4:R:15:PRO:HG2	4:R:90:ALA:HA	1.98	0.45
4:R:123:TYR:CZ	4:R:140:ALA:HA	2.51	0.45
2:B:180:GLN:HG3	2:B:183:LEU:HD13	1.98	0.45
4:E:3:HIS:HB2	4:E:103:VAL:HG23	1.98	0.45
1:H:132:VAL:HG11	2:I:144:VAL:HG11	1.99	0.45
2:I:49:PHE:CD2	2:I:69:ARG:HB3	2.51	0.45
2:B:143:LEU:HD13	2:B:194:LEU:HD23	1.97	0.45
5:T:25:ASN:HB3	5:T:66:LEU:HD11	1.99	0.45
2:B:48:TYR:O	2:B:55:PRO:HD2	2.17	0.45
2:I:51:GLY:O	2:I:69:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:93:ALA:HB1	2:I:103:GLN:HG2	1.99	0.45
2:W:38:SER:C	2:W:40:GLY:H	2.25	0.45
2:B:218:SER:C	2:B:220:ASN:H	2.25	0.45
4:R:217:TRP:CE2	4:R:247:VAL:HG12	2.52	0.45
2:B:30:THR:O	2:B:30:THR:HG22	2.16	0.45
2:B:31:ALA:HB3	2:B:95:SER:HB3	1.99	0.45
2:B:116:ASP:HB2	2:B:118:LYS:HB2	1.98	0.45
5:F:50:VAL:HG13	5:F:68:TYR:O	2.16	0.45
2:P:184:ASN:HD22	2:P:184:ASN:HA	1.59	0.45
4:K:7:TYR:O	4:K:98:MET:HA	2.16	0.45
2:W:210:CYS:HB3	2:W:237:ALA:HB3	1.98	0.45
1:A:35:TRP:HB2	1:A:48:MET:HB2	1.99	0.45
1:H:138:PHE:HD1	1:H:142:THR:HB	1.82	0.45
4:K:10:THR:O	4:K:22:PHE:HA	2.17	0.45
2:P:11:LYS:HE2	2:P:19:VAL:HG12	1.99	0.44
4:Y:74:HIS:CE1	4:Y:97:ARG:HE	2.34	0.44
1:A:163:ARG:C	1:A:165:MET:H	2.24	0.44
5:T:60:ASP:O	5:T:61:TRP:HB2	2.18	0.44
5:T:65:LEU:HD23	5:T:65:LEU:HA	1.81	0.44
2:W:47:ILE:HD11	2:W:54:ALA:HB1	1.99	0.44
2:W:122:PRO:HD3	2:W:230:PRO:HB3	1.98	0.44
5:L:24:LEU:O	5:L:68:TYR:HA	2.17	0.44
4:Y:78:LEU:O	4:Y:82:ARG:HG3	2.17	0.44
2:I:43:LEU:HD12	2:I:43:LEU:HA	1.90	0.44
4:K:209:TYR:CD2	4:K:210:PRO:HA	2.52	0.44
1:H:107:THR:HG22	1:H:109:ASN:OD1	2.18	0.44
1:M:36:TYR:CE1	1:M:46:LEU:HD12	2.52	0.44
4:K:160:LEU:C	4:K:162:GLY:H	2.25	0.44
4:R:203:CYS:O	4:R:244:TRP:HA	2.17	0.44
2:W:66:SER:HB3	2:W:78:THR:H	1.83	0.44
4:Y:12:VAL:HG22	4:Y:94:THR:HG23	1.99	0.44
2:B:219:GLU:HA	2:B:229:LYS:NZ	2.33	0.44
1:H:96:GLN:OE1	2:I:99:GLY:HA2	2.18	0.44
1:H:176:SER:HB3	1:H:181:PHE:CD2	2.53	0.44
4:Y:123:TYR:CD2	4:Y:124:ILE:HG22	2.53	0.44
4:E:11:SER:HA	4:E:21:ARG:O	2.18	0.43
4:K:81:LEU:HD13	4:K:118:TYR:HD1	1.81	0.43
1:M:92:ARG:HD2	1:M:96:GLN:HG3	2.00	0.43
1:H:8:SER:HB3	1:H:102:GLN:HE22	1.83	0.43
2:I:10:ASN:OD1	2:I:110:ARG:HB3	2.17	0.43
4:K:44:ARG:NH2	4:K:61:ASP:HA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:184:ALA:HA	4:K:185:PRO:HD3	1.91	0.43
4:Y:35:ARG:HD3	4:Y:48:ARG:HD3	2.01	0.43
4:E:124:ILE:HA	4:E:134:THR:O	2.19	0.43
4:K:74:HIS:NE2	4:K:97:ARG:NH2	2.55	0.43
1:M:135:PHE:HB3	1:M:187:PHE:CZ	2.53	0.43
4:R:235:PRO:O	5:T:11:TYR:OH	2.27	0.43
1:V:124:ASP:C	1:V:126:LYS:H	2.26	0.43
4:E:19:GLU:H	4:E:19:GLU:HG3	1.65	0.43
4:K:44:ARG:O	4:K:46:GLU:HG3	2.18	0.43
4:K:202:ARG:NH2	5:L:99:ASP:OD2	2.52	0.43
2:W:29:HIS:CE1	2:W:96:LEU:HD23	2.53	0.43
2:I:46:LEU:HA	2:I:59:GLY:O	2.18	0.43
4:R:264:GLU:H	4:R:264:GLU:HG2	1.51	0.43
1:A:125:SER:O	1:A:127:SER:N	2.51	0.43
4:E:9:PHE:HB2	4:E:97:ARG:HB3	2.01	0.43
2:I:203:ASN:C	2:I:205:ARG:H	2.26	0.43
2:I:34:TRP:HZ2	2:I:75:SER:HB3	1.84	0.43
2:I:93:ALA:HA	2:I:104:PHE:O	2.19	0.43
2:I:204:PRO:HA	2:I:241:GLY:O	2.18	0.43
5:Z:58:SER:C	5:Z:60:ASP:H	2.27	0.43
2:B:130:PRO:HD2	2:B:201:TRP:CZ2	2.53	0.43
5:L:32:HIS:ND1	5:L:33:PRO:HA	2.34	0.43
1:M:178:LYS:HG2	1:M:180:ASP:H	1.83	0.43
4:E:104:GLY:O	4:E:105:SER:C	2.62	0.43
1:M:153:TYR:HD2	1:M:175:TRP:NE1	2.16	0.43
2:W:50:GLN:NE2	4:Y:72:GLN:HB3	2.34	0.43
2:W:215:TYR:HA	2:W:232:THR:HG23	2.01	0.43
4:Y:123:TYR:HD2	4:Y:124:ILE:N	2.16	0.43
4:K:202:ARG:O	4:K:204:TRP:HD1	2.02	0.42
2:P:8:PRO:O	2:P:109:THR:HG23	2.19	0.42
2:B:178:LYS:HG2	2:B:188:TYR:CE1	2.53	0.42
5:F:55:LEU:HD13	5:F:65:LEU:HD21	2.00	0.42
1:V:58:ASP:N	1:V:61:PHE:O	2.51	0.42
4:Y:170:ARG:CA	4:Y:170:ARG:CG	2.97	0.42
4:E:3:HIS:O	4:E:102:ASP:HA	2.20	0.42
2:I:140:LYS:HD3	2:I:195:ARG:HE	1.82	0.42
4:K:133:TRP:CD1	4:K:133:TRP:N	2.87	0.42
1:A:47:ILE:HD12	1:A:47:ILE:HA	1.94	0.42
4:E:103:VAL:HG12	4:E:108:ARG:C	2.44	0.42
2:I:95:SER:O	2:I:96:LEU:C	2.62	0.42
1:A:6:GLN:HG3	1:A:22:ASN:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:ARG:HG3	2:B:238:GLU:HG2	2.01	0.42
1:H:34:PHE:HZ	1:H:92:ARG:NH2	2.14	0.42
2:P:80:GLN:O	2:P:81:ARG:C	2.62	0.42
2:P:176:PRO:HB3	2:P:190:LEU:HD12	2.01	0.42
1:V:147:SER:HB2	1:V:154:ILE:HG13	2.02	0.42
2:W:129:GLU:HG2	2:W:201:TRP:HH2	1.83	0.42
2:W:176:PRO:HB3	2:W:190:LEU:HB2	2.01	0.42
4:Y:9:PHE:HB2	4:Y:97:ARG:HB3	2.02	0.42
2:B:202:GLN:HA	2:B:242:ARG:O	2.19	0.42
1:M:34:PHE:HE1	1:M:92:ARG:HB2	1.84	0.42
4:R:2:SER:HB2	4:R:103:VAL:O	2.20	0.42
4:R:122:ASP:OD1	4:R:122:ASP:N	2.52	0.42
2:B:15:LYS:HD2	2:B:84:GLN:HG3	2.02	0.42
2:I:34:TRP:CZ3	2:I:77:LEU:HD22	2.54	0.42
4:K:106:ASP:O	4:K:107:TRP:CB	2.66	0.42
1:M:166:ASP:O	1:M:167:PHE:C	2.63	0.42
4:R:5:MET:HE3	4:R:7:TYR:HE2	1.84	0.42
1:A:9:GLY:HA3	1:A:10:PRO:C	2.45	0.42
2:B:38:SER:O	2:B:41:GLN:N	2.53	0.42
5:F:57:PHE:HA	5:F:63:PHE:HA	2.02	0.42
1:V:155:THR:HG22	2:W:177:LEU:HD21	2.01	0.42
2:B:11:LYS:HE3	2:B:13:THR:HB	2.01	0.42
1:H:95:ALA:HA	4:K:66:LYS:HA	2.02	0.42
3:J:1:LEU:HD22	4:K:167:TRP:NE1	2.34	0.42
3:Q:9:LEU:HD22	4:R:143:THR:HG21	2.02	0.42
5:T:88:LEU:HB3	5:T:90:GLN:O	2.20	0.42
5:Z:42:LYS:C	5:Z:44:GLY:N	2.78	0.42
1:A:128:SER:C	1:A:130:LYS:H	2.27	0.42
1:M:52:SER:C	1:M:65:LEU:HD23	2.44	0.42
1:V:6:GLN:NE2	1:V:89:CYS:HB3	2.34	0.42
1:V:96:GLN:OE1	4:Y:69:ALA:HB1	2.20	0.42
4:K:81:LEU:C	4:K:83:GLY:N	2.75	0.41
1:A:46:LEU:CD2	2:B:102:GLU:HA	2.50	0.41
2:I:64:ARG:HD2	2:I:80:GLN:O	2.20	0.41
2:I:87:SER:HA	2:I:112:THR:HA	2.03	0.41
4:K:52:ILE:C	4:K:54:GLN:N	2.75	0.41
4:K:147:TRP:CD1	4:K:152:VAL:HG21	2.56	0.41
4:R:5:MET:HB2	4:R:168:LEU:HD13	2.02	0.41
5:T:30:GLY:CA	5:T:62:SER:HB2	2.48	0.41
5:Z:50:VAL:HG22	5:Z:69:THR:HB	2.02	0.41
1:A:32:SER:HB3	1:A:34:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:2:SER:HA	4:E:104:GLY:HA2	2.03	0.41
2:I:130:PRO:HD2	2:I:201:TRP:CE2	2.54	0.41
5:L:27:TYR:CE2	5:L:29:SER:HB3	2.54	0.41
5:L:88:LEU:HD22	5:L:92:LYS:HE3	2.03	0.41
4:Y:231:VAL:HG11	4:Y:244:TRP:CZ2	2.56	0.41
4:E:230:LEU:HD12	4:E:245:ALA:HB2	2.01	0.41
1:M:36:TYR:HE1	1:M:46:LEU:HD12	1.86	0.41
4:R:139:ALA:C	4:R:141:GLN:H	2.29	0.41
5:L:84:ASN:HD22	5:L:91:PRO:HG3	1.86	0.41
4:R:74:HIS:CE1	4:R:97:ARG:HB2	2.55	0.41
1:A:182:ALA:H	1:A:185:ASN:HD21	1.69	0.41
4:E:197:HIS:HB3	5:Z:1:MET:N	2.36	0.41
5:L:97:ASP:CG	5:L:99:ASP:HB2	2.46	0.41
3:Q:3:LEU:HD22	4:R:97:ARG:NH2	2.35	0.41
5:T:42:LYS:HB3	5:T:47:ILE:HD11	2.03	0.41
1:V:65:LEU:HD13	1:V:72:VAL:HB	2.02	0.41
1:V:126:LYS:HA	1:V:126:LYS:HD3	1.85	0.41
4:Y:99:TYR:HB3	4:Y:114:HIS:CD2	2.56	0.41
2:B:181:PRO:HB2	2:B:182:ALA:H	1.72	0.41
2:B:219:GLU:HA	2:B:229:LYS:HZ1	1.86	0.41
1:H:114:ASN:O	1:H:114:ASN:ND2	2.54	0.41
1:M:18:ILE:N	1:M:18:ILE:HD12	2.36	0.41
1:M:146:GLN:HB3	1:M:147:SER:H	1.72	0.41
2:P:11:LYS:HG2	2:P:111:LEU:HD12	2.02	0.41
4:R:9:PHE:HD1	4:R:24:ALA:HB2	1.84	0.41
1:V:150:SER:HB2	2:W:181:PRO:HG3	2.01	0.41
2:W:37:GLN:HB2	2:W:43:LEU:HD12	2.03	0.41
4:Y:97:ARG:HG3	4:Y:98:MET:N	2.36	0.41
4:Y:111:ARG:NH2	4:Y:113:TYR:HD2	2.19	0.41
5:Z:30:GLY:HA2	5:Z:62:SER:CB	2.49	0.41
1:A:155:THR:HG21	2:B:191:SER:HB3	2.02	0.41
4:K:119:ASP:HB3	5:L:1:MET:HA	2.02	0.41
2:P:157:LEU:HD23	2:P:157:LEU:C	2.45	0.41
5:T:41:LEU:HD11	5:T:82:ARG:HB2	2.02	0.41
5:L:10:VAL:HG13	5:L:25:ASN:O	2.20	0.40
1:V:47:ILE:HD12	1:V:47:ILE:HA	1.78	0.40
1:H:18:ILE:HG12	1:H:77:ARG:HA	2.04	0.40
4:K:35:ARG:HG2	4:K:48:ARG:HG3	2.03	0.40
5:L:30:GLY:HA2	5:L:62:SER:HB2	2.03	0.40
2:B:23:CYS:O	2:B:25:PRO:HD3	2.22	0.40
1:M:131:SER:HB2	1:M:181:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:28:VAL:HG23	4:R:33:PHE:CD1	2.55	0.40
2:B:62:SER:OG	2:B:63:ASP:N	2.54	0.40
2:B:173:ASP:O	2:B:190:LEU:HD11	2.22	0.40
1:H:28:ARG:HG3	1:H:70:GLN:NE2	2.36	0.40
4:K:9:PHE:HB2	4:K:97:ARG:HB3	2.03	0.40
2:P:139:GLN:O	2:P:198:ALA:HB2	2.20	0.40
5:T:85:HIS:CD2	5:T:86:VAL:H	2.40	0.40
1:H:95:ALA:H	4:K:65:ARG:HB3	1.87	0.40
4:K:11:SER:HB3	4:K:95:VAL:HB	2.04	0.40
1:M:53:ASN:H	1:M:53:ASN:ND2	2.18	0.40
1:M:112:ILE:HG21	1:M:139:ASP:HA	2.04	0.40
1:M:190:SER:HB2	1:M:192:ILE:HG23	2.04	0.40
2:P:196:VAL:HB	2:P:197:SER:H	1.79	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	197/203 (97%)	157 (80%)	33 (17%)	7 (4%)	2	17
1	H	196/203 (97%)	162 (83%)	28 (14%)	6 (3%)	3	19
1	M	196/203 (97%)	161 (82%)	30 (15%)	5 (3%)	4	23
1	V	196/203 (97%)	167 (85%)	26 (13%)	3 (2%)	8	35
2	B	240/244 (98%)	203 (85%)	31 (13%)	6 (2%)	4	24
2	I	240/244 (98%)	195 (81%)	42 (18%)	3 (1%)	9	38
2	P	240/244 (98%)	200 (83%)	33 (14%)	7 (3%)	3	21
2	W	240/244 (98%)	201 (84%)	34 (14%)	5 (2%)	5	27
3	D	7/9 (78%)	7 (100%)	0	0	100	100
3	J	7/9 (78%)	7 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	7/9 (78%)	7 (100%)	0	0	100	100
3	X	7/9 (78%)	7 (100%)	0	0	100	100
4	E	273/279 (98%)	240 (88%)	28 (10%)	5 (2%)	6	31
4	K	274/279 (98%)	233 (85%)	36 (13%)	5 (2%)	6	31
4	R	276/279 (99%)	243 (88%)	31 (11%)	2 (1%)	18	50
4	Y	272/279 (98%)	247 (91%)	19 (7%)	6 (2%)	5	26
5	F	98/100 (98%)	85 (87%)	10 (10%)	3 (3%)	3	19
5	L	98/100 (98%)	87 (89%)	9 (9%)	2 (2%)	6	28
5	T	98/100 (98%)	87 (89%)	8 (8%)	3 (3%)	3	19
5	Z	98/100 (98%)	84 (86%)	10 (10%)	4 (4%)	2	15
All	All	3260/3340 (98%)	2780 (85%)	408 (12%)	72 (2%)	5	26

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	LYS
1	A	126	LYS
2	B	39	LEU
2	B	181	PRO
4	E	107	TRP
5	F	91	PRO
1	H	95	ALA
1	H	98	LEU
1	H	166	ASP
5	L	30	GLY
1	M	95	ALA
2	P	101	ASP
1	V	95	ALA
5	Z	75	GLU
1	A	42	LYS
2	B	101	ASP
2	B	176	PRO
4	E	207	SER
1	H	94	GLY
2	I	98	LEU
4	K	267	PRO
1	M	124	ASP
2	P	15	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	P	39	LEU
2	P	98	LEU
4	R	207	SER
4	R	220	ASP
1	V	94	GLY
4	Y	267	PRO
5	Z	53	SER
1	A	146	GLN
1	H	148	LYS
1	H	184	ALA
2	I	39	LEU
4	K	226	GLN
5	L	48	GLU
1	M	78	ASP
1	M	146	GLN
1	M	167	PHE
5	T	21	SER
2	W	59	GLY
2	W	86	ASP
4	Y	220	ASP
4	Y	223	ASP
1	A	148	LYS
4	E	265	GLY
4	K	107	TRP
4	K	176	LYS
4	K	221	GLY
5	T	13	ARG
2	W	58	SER
4	Y	252	GLY
5	Z	44	GLY
4	E	226	GLN
2	P	41	GLN
5	T	75	GLU
1	V	190	SER
2	W	96	LEU
4	Y	29	ASP
4	Y	269	PRO
1	A	94	GLY
5	F	94	VAL
2	P	163	GLY
2	W	28	GLY
5	F	44	GLY

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Mol	Chain	Res	Type
2	P	61	PRO
1	A	59	GLY
2	B	149	GLY
2	I	59	GLY
5	Z	15	PRO
2	B	8	PRO
4	E	210	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	176/181 (97%)	165 (94%)	11 (6%)	16	45
1	H	176/181 (97%)	156 (89%)	20 (11%)	5	22
1	M	176/181 (97%)	167 (95%)	9 (5%)	21	51
1	V	175/181 (97%)	160 (91%)	15 (9%)	10	33
2	B	206/208 (99%)	188 (91%)	18 (9%)	9	33
2	I	203/208 (98%)	189 (93%)	14 (7%)	14	42
2	P	207/208 (100%)	186 (90%)	21 (10%)	7	27
2	W	206/208 (99%)	193 (94%)	13 (6%)	16	45
3	D	9/9 (100%)	7 (78%)	2 (22%)	1	5
3	J	9/9 (100%)	6 (67%)	3 (33%)	0	1
3	Q	9/9 (100%)	6 (67%)	3 (33%)	0	1
3	X	9/9 (100%)	9 (100%)	0	100	100
4	E	229/232 (99%)	214 (93%)	15 (7%)	15	43
4	K	228/232 (98%)	204 (90%)	24 (10%)	6	25
4	R	227/232 (98%)	208 (92%)	19 (8%)	10	35
4	Y	218/232 (94%)	194 (89%)	24 (11%)	6	24
5	F	89/95 (94%)	82 (92%)	7 (8%)	11	37
5	L	91/95 (96%)	78 (86%)	13 (14%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	T	86/95 (90%)	81 (94%)	5 (6%)	18	47
5	Z	88/95 (93%)	83 (94%)	5 (6%)	18	48
All	All	2817/2900 (97%)	2576 (91%)	241 (9%)	10	33

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	21	LEU
1	A	45	GLU
1	A	75	LEU
1	A	83	ASP
1	A	88	LEU
1	A	139	ASP
1	A	151	ASP
1	A	160	LEU
1	A	163	ARG
1	A	165	MET
2	B	4	VAL
2	B	19	VAL
2	B	21	LEU
2	B	32	LEU
2	B	43	LEU
2	B	76	THR
2	B	89	VAL
2	B	92	CYS
2	B	96	LEU
2	B	109	THR
2	B	112	THR
2	B	155	VAL
2	B	177	LEU
2	B	180	GLN
2	B	183	LEU
2	B	184	ASN
2	B	196	VAL
2	B	224	THR
3	D	6	LEU
3	D	7	ASN
4	E	19	GLU
4	E	30	ASP
4	E	37	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	E	65	ARG
4	E	70	HIS
4	E	121	LYS
4	E	166	GLU
4	E	178	THR
4	E	202	ARG
4	E	203	CYS
4	E	215	LEU
4	E	223	ASP
4	E	256	ARG
4	E	260	HIS
4	E	270	LEU
5	F	8	ILE
5	F	21	SER
5	F	39	ASP
5	F	71	PHE
5	F	86	VAL
5	F	93	ILE
5	F	94	VAL
1	H	11	LEU
1	H	32	SER
1	H	46	LEU
1	H	52	SER
1	H	55	ASP
1	H	93	GLU
1	H	96	GLN
1	H	98	LEU
1	H	102	GLN
1	H	109	ASN
1	H	122	LEU
1	H	124	ASP
1	H	125	SER
1	H	132	VAL
1	H	143	ASN
1	H	151	ASP
1	H	160	LEU
1	H	165	MET
1	H	177	ASN
1	H	181	PHE
2	I	36	ARG
2	I	63	ASP
2	I	73	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	I	91	LEU
2	I	96	LEU
2	I	115	GLU
2	I	143	LEU
2	I	155	VAL
2	I	168	SER
2	I	171	CYS
2	I	196	VAL
2	I	224	THR
2	I	226	ASP
2	I	234	ILE
3	J	3	LEU
3	J	6	LEU
3	J	8	GLN
4	K	12	VAL
4	K	19	GLU
4	K	61	ASP
4	K	81	LEU
4	K	82	ARG
4	K	102	ASP
4	K	113	TYR
4	K	129	ASP
4	K	133	TRP
4	K	145	HIS
4	K	146	LYS
4	K	148	GLU
4	K	182	THR
4	K	190	THR
4	K	203	CYS
4	K	215	LEU
4	K	222	GLU
4	K	223	ASP
4	K	228	THR
4	K	258	THR
4	K	259	CYS
4	K	260	HIS
4	K	271	THR
4	K	272	LEU
5	L	8	ILE
5	L	10	VAL
5	L	39	ASP
5	L	43	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	L	55	LEU
5	L	56	SER
5	L	57	PHE
5	L	64	TYR
5	L	70	GLU
5	L	95	LYS
5	L	98	ARG
5	L	99	ASP
5	L	100	MET
1	M	11	LEU
1	M	21	LEU
1	M	80	GLN
1	M	88	LEU
1	M	97	LYS
1	M	99	VAL
1	M	170	ASN
1	M	171	SER
1	M	196	THR
2	P	24	ASP
2	P	48	TYR
2	P	70	THR
2	P	76	THR
2	P	89	VAL
2	P	95	SER
2	P	98	LEU
2	P	102	GLU
2	P	111	LEU
2	P	135	ILE
2	P	138	THR
2	P	143	LEU
2	P	144	VAL
2	P	146	LEU
2	P	171	CYS
2	P	177	LEU
2	P	184	ASN
2	P	190	LEU
2	P	196	VAL
2	P	200	PHE
2	P	222	GLU
3	Q	1	LEU
3	Q	6	LEU
3	Q	8	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	R	23	ILE
4	R	55	GLU
4	R	64	THR
4	R	72	GLN
4	R	110	LEU
4	R	122	ASP
4	R	130	LEU
4	R	134	THR
4	R	141	GLN
4	R	145	HIS
4	R	155	GLN
4	R	163	THR
4	R	177	GLU
4	R	183	ASP
4	R	189	MET
4	R	207	SER
4	R	248	VAL
4	R	258	THR
4	R	264	GLU
5	T	18	ASN
5	T	37	GLU
5	T	54	ASP
5	T	66	LEU
5	T	97	ASP
1	V	47	ILE
1	V	56	LYS
1	V	73	SER
1	V	74	LEU
1	V	80	GLN
1	V	82	SER
1	V	93	GLU
1	V	113	GLN
1	V	124	ASP
1	V	137	ASP
1	V	142	THR
1	V	146	GLN
1	V	177	ASN
1	V	185	ASN
1	V	196	THR
2	W	29	HIS
2	W	52	ASN
2	W	63	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	W	65	PHE
2	W	111	LEU
2	W	119	ASN
2	W	127	VAL
2	W	148	THR
2	W	155	VAL
2	W	177	LEU
2	W	185	ASP
2	W	200	PHE
2	W	236	SER
4	Y	4	SER
4	Y	44	ARG
4	Y	64	THR
4	Y	65	ARG
4	Y	75	ARG
4	Y	80	THR
4	Y	107	TRP
4	Y	113	TYR
4	Y	137	ASP
4	Y	156	LEU
4	Y	163	THR
4	Y	177	GLU
4	Y	178	THR
4	Y	182	THR
4	Y	183	ASP
4	Y	200	THR
4	Y	214	THR
4	Y	215	LEU
4	Y	216	THR
4	Y	232	GLU
4	Y	256	ARG
4	Y	258	THR
4	Y	261	VAL
4	Y	266	LEU
5	Z	14	HIS
5	Z	22	ASN
5	Z	28	VAL
5	Z	65	LEU
5	Z	71	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	38	GLN
1	A	64	GLN
1	A	66	ASN
1	A	111	ASN
1	A	121	GLN
1	A	170	ASN
1	A	185	ASN
2	B	37	GLN
2	B	119	ASN
2	B	139	GLN
2	B	180	GLN
2	B	184	ASN
2	B	202	GLN
2	B	225	GLN
4	E	32	GLN
4	E	70	HIS
4	E	115	GLN
4	E	155	GLN
4	E	191	HIS
4	E	197	HIS
4	E	218	GLN
4	E	224	GLN
4	E	242	GLN
5	F	90	GLN
1	H	6	GLN
1	H	22	ASN
1	H	53	ASN
1	H	64	GLN
1	H	102	GLN
1	H	121	GLN
1	H	141	GLN
1	H	143	ASN
1	H	188	ASN
2	I	50	GLN
2	I	84	GLN
2	I	139	GLN
2	I	184	ASN
2	I	202	GLN
2	I	211	GLN
3	J	8	GLN
4	K	32	GLN
4	K	43	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	K	70	HIS
4	K	72	GLN
4	K	93	HIS
4	K	115	GLN
4	K	197	HIS
5	L	84	ASN
1	M	31	GLN
1	M	38	GLN
1	M	64	GLN
1	M	66	ASN
1	M	70	GLN
1	M	114	ASN
1	M	143	ASN
1	M	177	ASN
1	M	189	ASN
2	P	10	ASN
2	P	37	GLN
2	P	41	GLN
2	P	84	GLN
2	P	119	ASN
2	P	139	GLN
2	P	167	HIS
2	P	184	ASN
3	Q	7	ASN
3	Q	8	GLN
4	R	3	HIS
4	R	115	GLN
4	R	188	HIS
4	R	218	GLN
5	T	9	GLN
5	T	14	HIS
1	V	6	GLN
1	V	7	ASN
1	V	64	GLN
1	V	80	GLN
2	W	29	HIS
2	W	37	GLN
2	W	50	GLN
2	W	83	GLN
2	W	84	GLN
2	W	103	GLN
2	W	119	ASN

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Mol	Chain	Res	Type
2	W	139	GLN
2	W	154	HIS
2	W	167	HIS
2	W	175	GLN
2	W	180	GLN
3	X	8	GLN
4	Y	32	GLN
4	Y	70	HIS
4	Y	87	GLN
4	Y	93	HIS
4	Y	180	GLN
4	Y	191	HIS
4	Y	224	GLN

### 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 oligosaccharides in this entry.

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

There are no ligands in this entry.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	199/203 (98%)	-0.90	0 100 100	116, 171, 247, 291	0
1	H	198/203 (97%)	-0.89	0 100 100	99, 160, 250, 281	0
1	M	198/203 (97%)	-0.84	0 100 100	89, 159, 236, 307	0
1	V	198/203 (97%)	-0.89	0 100 100	94, 161, 253, 288	0
2	B	242/244 (99%)	-0.93	0 100 100	116, 187, 247, 278	0
2	I	242/244 (99%)	-0.93	0 100 100	111, 159, 215, 273	0
2	P	242/244 (99%)	-0.96	0 100 100	87, 147, 207, 234	0
2	W	242/244 (99%)	-0.96	0 100 100	116, 156, 193, 221	0
3	D	9/9 (100%)	-0.58	0 100 100	135, 141, 181, 188	0
3	J	9/9 (100%)	-0.71	0 100 100	101, 111, 134, 151	0
3	Q	9/9 (100%)	-0.52	0 100 100	88, 109, 141, 153	0
3	X	9/9 (100%)	-0.78	0 100 100	116, 125, 171, 174	0
4	E	275/279 (98%)	-1.10	0 100 100	104, 157, 200, 226	0
4	K	276/279 (98%)	-1.02	0 100 100	77, 127, 161, 191	0
4	R	278/279 (99%)	-1.03	0 100 100	77, 128, 164, 187	0
4	Y	274/279 (98%)	-0.97	0 100 100	106, 147, 186, 220	0
5	F	100/100 (100%)	-0.86	0 100 100	128, 177, 232, 255	0
5	L	100/100 (100%)	-0.94	0 100 100	86, 123, 157, 182	0
5	T	100/100 (100%)	-0.95	0 100 100	93, 127, 168, 177	0
5	Z	100/100 (100%)	-0.94	0 100 100	116, 154, 196, 238	0
All	All	3300/3340 (98%)	-0.95	0 100 100	77, 151, 222, 307	0

There are no RSRZ outliers to report.

## 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 oligosaccharides 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.