



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 10:12 PM EDT

PDB ID : 1S7W  
Title : Crystal structures of the murine class I major histocompatibility complex H-2Db in complex with LCMV-derived gp33 index peptide and three of its escape variants  
Authors : Velloso, L.M.; Michaelsson, J.; Ljunggren, H.G.; Schneider, G.; Achour, A.  
Deposited on : 2004-01-30  
Resolution : 2.40 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:

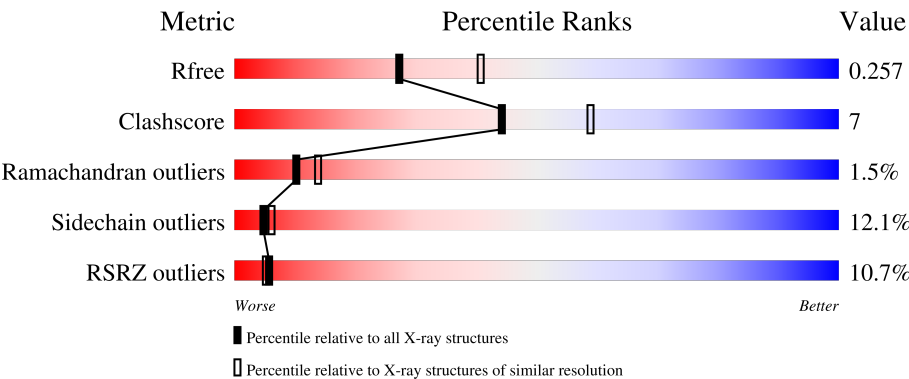
MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

# 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 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	338	<div><div>10%</div><div>60%16%18%</div></div>
1	D	338	<div><div>9%</div><div>64%13%18%</div></div>
1	G	338	<div><div>12%</div><div>65%13%18%</div></div>
1	J	338	<div><div>14%</div><div>67%11%18%</div></div>
2	B	99	<div><div>%</div><div>73%20%5%</div></div>

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Mol	Chain	Length	Quality of chain
2	E	99	<div><div></div><div>2%</div><div>79%</div><div>18%</div><div>••</div></div>
2	H	99	<div><div></div><div>%</div><div>76%</div><div>23%</div><div>•</div></div>
2	K	99	<div><div></div><div>4%</div><div>76%</div><div>24%</div><div></div></div>
3	C	9	<div><div></div><div></div><div>78%</div><div>22%</div><div></div></div>
3	F	9	<div><div></div><div></div><div>89%</div><div>11%</div><div></div></div>
3	I	9	<div><div></div><div>11%</div><div>67%</div><div>33%</div><div></div></div>
3	L	9	<div><div></div><div></div><div>89%</div><div>11%</div><div></div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13148 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 H-2 class I histocompatibility antigen, D-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	1	0
			2269	1432	401	427	9			
1	D	276	Total	C	N	O	S	0	0	0
			2264	1430	400	425	9			
1	G	276	Total	C	N	O	S	0	0	0
			2264	1430	400	425	9			
1	J	276	Total	C	N	O	S	0	0	0
			2264	1430	400	425	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			812	519	137	150	6			
2	E	99	Total	C	N	O	S	0	0	0
			818	523	138	151	6			
2	H	99	Total	C	N	O	S	0	0	0
			818	523	138	151	6			
2	K	99	Total	C	N	O	S	0	0	0
			818	523	138	151	6			

- Molecule 3 is a protein called Glycoprotein 9-residue peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			74	49	11	13	1			
3	F	9	Total	C	N	O	S	0	0	0
			74	49	11	13	1			
3	I	9	Total	C	N	O	S	0	0	0
			74	49	11	13	1			
3	L	9	Total	C	N	O	S	0	0	0
			74	49	11	13	1			

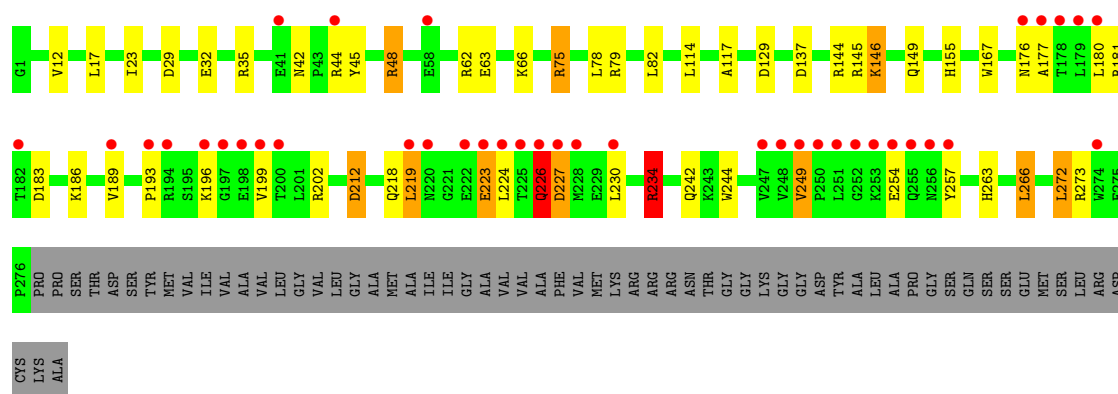
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	LEU	VAL	engineered mutation	UNP P07399
C	9	MET	CYS	SEE REMARK 999	UNP P07399
F	3	LEU	VAL	engineered mutation	UNP P07399
F	9	MET	CYS	SEE REMARK 999	UNP P07399
I	3	LEU	VAL	engineered mutation	UNP P07399
I	9	MET	CYS	SEE REMARK 999	UNP P07399
L	3	LEU	VAL	engineered mutation	UNP P07399
L	9	MET	CYS	SEE REMARK 999	UNP P07399

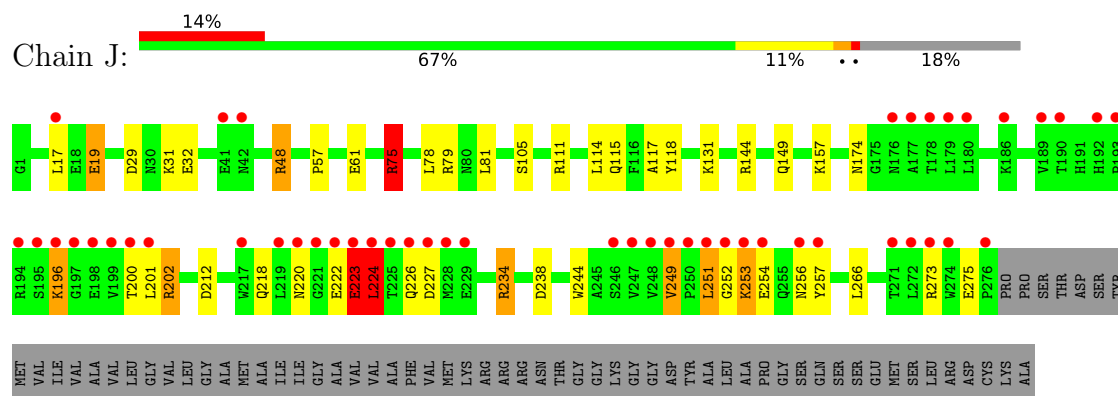
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	87	Total O 87 87	0	0
4	B	57	Total O 57 57	0	0
4	C	2	Total O 2 2	0	0
4	D	80	Total O 80 80	0	0
4	E	35	Total O 35 35	0	0
4	F	3	Total O 3 3	0	0
4	G	84	Total O 84 84	0	0
4	H	44	Total O 44 44	0	0
4	I	2	Total O 2 2	0	0
4	J	83	Total O 83 83	0	0
4	K	44	Total O 44 44	0	0
4	L	4	Total O 4 4	0	0

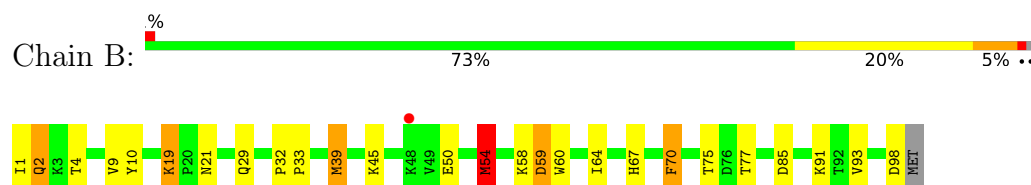




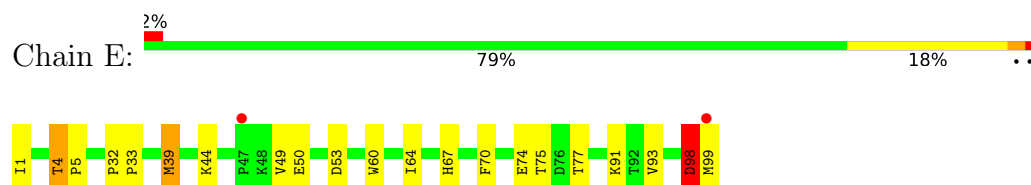
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



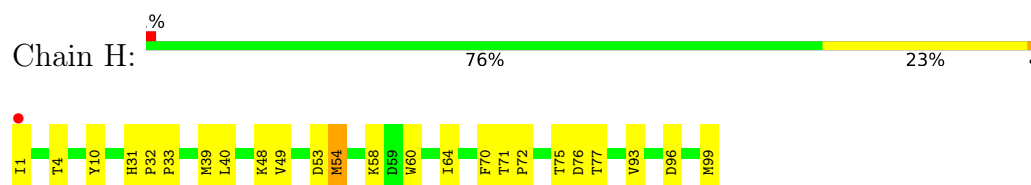
- Molecule 2: Beta-2-microglobulin



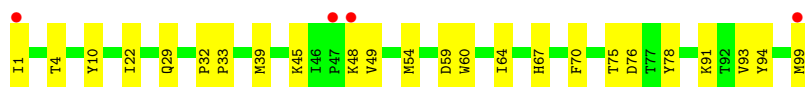
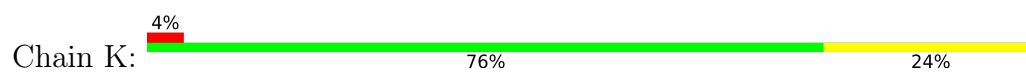
- Molecule 2: Beta-2-microglobulin



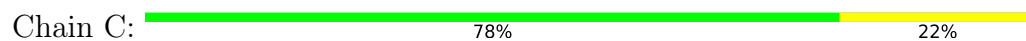
- Molecule 2: Beta-2-microglobulin



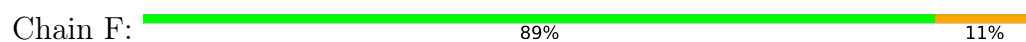
- Molecule 2: Beta-2-microglobulin



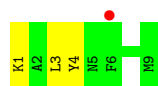
- Molecule 3: Glycoprotein 9-residue peptide



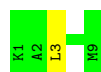
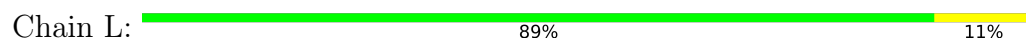
- Molecule 3: Glycoprotein 9-residue peptide



- Molecule 3: Glycoprotein 9-residue peptide



- Molecule 3: Glycoprotein 9-residue peptide





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.25Å 123.30Å 99.30Å 90.00° 103.13° 90.00°	Depositor
Resolution (Å)	19.84 – 2.40 38.05 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.84-2.40) 99.9 (38.05-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.31 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.199 , 0.246 0.213 , 0.257	Depositor DCC
$R_{free}$ test set	1689 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13148	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.15% 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	0.68	0/2337	0.87	8/3174 (0.3%)
1	D	0.67	0/2331	0.87	9/3166 (0.3%)
1	G	0.69	1/2331 (0.0%)	0.85	11/3166 (0.3%)
1	J	0.64	0/2331	0.85	5/3166 (0.2%)
2	B	0.78	2/838 (0.2%)	0.94	3/1138 (0.3%)
2	E	0.78	1/844 (0.1%)	0.85	2/1146 (0.2%)
2	H	0.77	0/844	0.88	3/1146 (0.3%)
2	K	0.73	0/844	0.87	2/1146 (0.2%)
3	C	0.95	0/75	1.01	0/98
3	F	0.85	0/75	0.95	0/98
3	I	0.95	0/75	0.92	0/98
3	L	0.81	0/75	0.95	0/98
All	All	0.70	4/13000 (0.0%)	0.87	43/17640 (0.2%)

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
1	A	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	39	MET	SD-CE	-6.21	1.43	1.77
2	B	39	MET	SD-CE	-5.56	1.46	1.77
2	B	54	MET	CG-SD	5.52	1.95	1.81
1	G	146	LYS	CE-NZ	5.48	1.62	1.49

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	98	ASP	CB-CG-OD2	8.08	125.57	118.30
1	A	35	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	G	129	ASP	CB-CG-OD2	7.46	125.01	118.30
1	D	35	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	29	ASP	CB-CG-OD2	7.32	124.89	118.30
1	D	234	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	234	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	G	212	ASP	CB-CG-OD2	6.89	124.50	118.30
1	G	146	LYS	CD-CE-NZ	6.61	126.89	111.70
1	A	234	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	D	234	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	J	212	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	35	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	H	53	ASP	CB-CG-OD2	6.20	123.88	118.30
1	G	29	ASP	CB-CG-OD2	6.15	123.83	118.30
2	E	53	ASP	CB-CG-OD2	6.12	123.81	118.30
1	D	238	ASP	CB-CG-OD2	6.04	123.73	118.30
1	D	35	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	227	ASP	CB-CG-OD2	5.99	123.69	118.30
1	J	238	ASP	CB-CG-OD2	5.95	123.65	118.30
1	G	183	ASP	CB-CG-OD2	5.92	123.63	118.30
1	D	29	ASP	CB-CG-OD2	5.88	123.59	118.30
1	G	35	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	G	144	ARG	NE-CZ-NH1	5.73	123.16	120.30
2	K	59	ASP	CB-CG-OD2	5.71	123.44	118.30
1	J	75	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	G	234	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	G	35	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	183	ASP	CB-CG-OD2	5.42	123.18	118.30
1	D	129	ASP	CB-CG-OD2	5.40	123.16	118.30
2	H	96	ASP	CB-CG-OD2	5.35	123.11	118.30
2	B	85	ASP	CB-CG-OD2	5.30	123.07	118.30
1	J	227	ASP	CB-CG-OD2	5.29	123.07	118.30
1	J	29	ASP	CB-CG-OD2	5.28	123.05	118.30
1	G	137	ASP	CB-CG-OD2	5.21	122.98	118.30
1	D	106	ASP	CB-CG-OD1	5.19	122.97	118.30
2	H	76	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	101	CYS	N-CA-C	5.16	124.94	111.00
2	K	76	ASP	CB-CG-OD2	5.10	122.89	118.30
1	G	234	ARG	NE-CZ-NH2	-5.06	117.77	120.30
2	B	59	ASP	CB-CG-OD2	5.05	122.84	118.30
1	D	227	ASP	CB-CG-OD2	5.05	122.84	118.30
2	E	98	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	6	ARG	Peptide
1	A	98	MET	Mainchain
1	A	99[B]	SER	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	2269	0	2138	45	0
1	D	2264	0	2136	36	0
1	G	2264	0	2136	26	0
1	J	2264	0	2136	20	0
2	B	812	0	787	13	0
2	E	818	0	791	9	0
2	H	818	0	791	11	0
2	K	818	0	791	14	0
3	C	74	0	76	2	0
3	F	74	0	76	5	0
3	I	74	0	76	3	0
3	L	74	0	76	0	0
4	A	87	0	0	7	0
4	B	57	0	0	0	0
4	C	2	0	0	0	0
4	D	80	0	0	3	0
4	E	35	0	0	1	0
4	F	3	0	0	0	0
4	G	84	0	0	7	0
4	H	44	0	0	3	0
4	I	2	0	0	0	0
4	J	83	0	0	3	0
4	K	44	0	0	4	0
4	L	4	0	0	0	0
All	All	13148	0	12010	163	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 7.

All (163) 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)
4:G:347:HOH:O	2:H:99:MET:CG	2.01	1.09
1:D:219:LEU:HD13	1:D:257:TYR:OH	1.48	1.09
1:J:144:ARG:HD2	4:J:404:HOH:O	1.62	1.00
1:A:99[A]:SER:OG	1:A:100:GLY:N	1.91	0.96
1:D:219:LEU:HB2	1:D:257:TYR:CE1	2.09	0.87
1:D:219:LEU:CD1	1:D:257:TYR:OH	2.22	0.87
1:A:99[A]:SER:HA	4:A:413:HOH:O	1.83	0.78
1:A:99[B]:SER:HA	4:A:413:HOH:O	1.83	0.77
2:H:31:HIS:ND1	4:H:140:HOH:O	2.17	0.77
1:A:1:GLY:N	1:A:2:PRO:HD2	2.00	0.76
1:D:219:LEU:CD1	1:D:257:TYR:CZ	2.69	0.75
1:D:219:LEU:HD13	1:D:257:TYR:CZ	2.22	0.75
1:A:1:GLY:N	1:A:2:PRO:CD	2.51	0.74
1:J:75:ARG:HH11	1:J:75:ARG:HG3	1.53	0.72
2:H:77:THR:HG22	4:H:139:HOH:O	1.88	0.71
1:A:99[A]:SER:O	1:A:113:TYR:O	2.10	0.69
2:K:78:TYR:OH	4:K:143:HOH:O	2.09	0.69
1:D:194:ARG:O	1:D:198:GLU:O	2.11	0.69
1:J:234:ARG:HD3	2:K:10:TYR:CE2	2.29	0.67
1:D:219:LEU:CB	1:D:257:TYR:CE1	2.78	0.66
1:D:54:GLN:HE22	1:D:174:ASN:HB3	1.62	0.65
1:A:1:GLY:H3	1:A:2:PRO:CD	2.09	0.64
1:D:66:LYS:HZ2	3:F:1:LYS:HE3	1.63	0.64
1:J:249:VAL:HG22	1:J:257:TYR:CZ	2.31	0.63
1:A:6:ARG:HD3	1:A:99[A]:SER:OG	1.99	0.62
1:G:32:GLU:OE2	1:G:48:ARG:HD2	2.00	0.61
2:K:54:MET:HA	4:K:100:HOH:O	2.00	0.61
1:D:142:ILE:HG13	4:D:398:HOH:O	2.01	0.61
1:D:256:ASN:C	1:D:256:ASN:HD22	2.05	0.59
1:A:219:LEU:HD13	1:A:257:TYR:CZ	2.38	0.59
1:D:66:LYS:NZ	3:F:1:LYS:HE3	2.17	0.59
1:A:193:PRO:HA	1:A:199:VAL:HG12	1.85	0.59
1:D:219:LEU:HD12	1:D:257:TYR:CZ	2.38	0.59
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.38	0.58
1:A:99[B]:SER:O	4:A:413:HOH:O	2.11	0.58
1:A:1:GLY:H3	1:A:2:PRO:HD2	1.66	0.58
1:G:249:VAL:HG12	1:G:257:TYR:CZ	2.39	0.58
1:J:75:ARG:HH11	1:J:75:ARG:CG	2.17	0.58
1:D:66:LYS:HZ2	3:F:1:LYS:CE	2.17	0.57
1:G:145:ARG:O	1:G:149:GLN:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLY:H2	1:A:2:PRO:HD2	1.69	0.57
1:G:189:VAL:HG23	1:G:272:LEU:HD11	1.88	0.56
1:G:263:HIS:HB3	1:G:266:LEU:HD22	1.88	0.56
1:D:66:LYS:NZ	3:F:1:LYS:CE	2.68	0.55
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.42	0.55
1:G:146:LYS:CE	4:G:355:HOH:O	2.53	0.55
1:D:234:ARG:HD2	1:D:242:GLN:HB2	1.89	0.55
2:E:98:ASP:O	2:E:99:MET:C	2.44	0.55
1:G:62:ARG:NH2	3:I:1:LYS:HD2	2.21	0.55
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.42	0.55
2:K:39:MET:HE3	2:K:49:VAL:HG13	1.89	0.55
1:G:176:ASN:OD1	1:G:180:LEU:HD13	2.06	0.54
1:J:202:ARG:HD2	1:J:244:TRP:CE3	2.42	0.54
1:A:6:ARG:HA	1:A:99[A]:SER:OG	2.08	0.54
1:G:63:GLU:O	1:G:66:LYS:HB2	2.07	0.54
1:G:146:LYS:HE3	4:G:355:HOH:O	2.07	0.54
2:E:4:THR:HG22	4:E:101:HOH:O	2.06	0.54
2:E:39:MET:CE	2:E:49:VAL:HG13	2.38	0.53
1:D:32:GLU:OE2	1:D:48:ARG:HD2	2.09	0.53
2:H:39:MET:HE2	2:H:49:VAL:HG13	1.91	0.53
1:A:30:ASN:ND2	4:A:416:HOH:O	2.42	0.52
1:D:256:ASN:ND2	1:D:257:TYR:CD2	2.77	0.52
1:J:75:ARG:HG3	1:J:75:ARG:NH1	2.21	0.52
1:A:219:LEU:C	1:A:221:GLY:N	2.64	0.51
1:J:19:GLU:HG3	1:J:75:ARG:CZ	2.40	0.51
1:J:249:VAL:HG22	1:J:257:TYR:CE2	2.45	0.51
1:A:199:VAL:HG11	1:A:251:LEU:HD12	1.91	0.51
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.46	0.51
1:A:224:LEU:HD23	1:A:247:VAL:HG21	1.93	0.51
1:J:32:GLU:OE2	1:J:48:ARG:CD	2.58	0.51
1:D:194:ARG:O	1:D:195:SER:O	2.29	0.51
1:J:32:GLU:OE2	1:J:48:ARG:HD2	2.11	0.50
1:A:35:ARG:NH2	2:B:54:MET:O	2.45	0.50
1:G:63:GLU:OE2	1:G:66:LYS:NZ	2.45	0.50
2:K:39:MET:CE	2:K:49:VAL:HG13	2.41	0.50
1:A:256:ASN:HD22	1:A:256:ASN:C	2.15	0.49
1:A:263:HIS:HB3	1:A:266:LEU:HD22	1.94	0.49
3:C:5:ASN:O	2:K:75:THR:HG21	2.11	0.49
2:E:39:MET:HE2	2:E:49:VAL:HG13	1.94	0.49
2:H:39:MET:CE	2:H:49:VAL:HG13	2.43	0.48
2:K:91:LYS:NZ	4:K:120:HOH:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ARG:HG2	1:D:204:TRP:NE1	2.27	0.48
1:D:260:ARG:HA	1:D:270:LEU:O	2.14	0.48
2:B:29:GLN:NE2	2:B:59:ASP:OD2	2.46	0.48
1:A:31:LYS:HD3	1:A:179:LEU:HD21	1.94	0.48
1:A:223:GLU:HA	4:A:386:HOH:O	2.14	0.48
1:D:6:ARG:NH2	1:D:113:TYR:CE1	2.81	0.48
1:G:62:ARG:HG3	4:G:395:HOH:O	2.13	0.48
1:A:62:ARG:HG3	2:K:94:TYR:CE1	2.48	0.47
2:E:32:PRO:HB2	2:E:33:PRO:HD2	1.97	0.47
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.48	0.47
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.49	0.47
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.49	0.47
1:G:234:ARG:HD2	1:G:242:GLN:HB2	1.97	0.47
1:J:251:LEU:HD23	1:J:252:GLY:H	1.80	0.47
1:A:194:ARG:O	1:A:195:SER:C	2.53	0.47
1:A:226:GLN:HG2	1:A:226:GLN:O	2.16	0.46
1:G:23:ILE:HD12	2:H:54:MET:SD	2.56	0.46
1:J:201:LEU:CD1	1:J:249:VAL:HG21	2.45	0.46
1:G:75:ARG:HG3	4:G:399:HOH:O	2.16	0.46
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.51	0.46
1:G:42:ASN:ND2	1:G:44:ARG:HD2	2.31	0.46
2:K:99:MET:CG	4:K:114:HOH:O	2.63	0.46
2:H:75:THR:HG22	4:H:105:HOH:O	2.15	0.45
2:E:50:GLU:HB2	2:E:67:HIS:CE1	2.51	0.45
2:K:39:MET:HE1	2:K:67:HIS:C	2.36	0.45
1:J:223:GLU:O	1:J:224:LEU:HB2	2.17	0.45
2:K:32:PRO:HB2	2:K:33:PRO:HD2	1.99	0.45
1:G:12:VAL:HG13	4:G:381:HOH:O	2.17	0.45
1:G:219:LEU:O	1:G:219:LEU:HG	2.17	0.45
2:B:19:LYS:HE3	2:B:19:LYS:HB3	1.82	0.45
1:D:219:LEU:HB2	1:D:257:TYR:CD1	2.49	0.45
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.51	0.45
1:A:194:ARG:HG2	1:A:195:SER:N	2.32	0.44
1:A:156:TYR:O	1:A:160:LEU:HG	2.18	0.44
1:D:17:LEU:N	4:D:383:HOH:O	2.51	0.44
1:D:66:LYS:NZ	3:F:1:LYS:HE2	2.32	0.44
2:H:32:PRO:HB2	2:H:33:PRO:HD2	1.99	0.44
2:B:50:GLU:HB2	2:B:67:HIS:CE1	2.53	0.44
2:B:39:MET:HE1	2:B:67:HIS:HA	1.98	0.44
2:K:39:MET:HE1	2:K:67:HIS:CA	2.48	0.44
1:D:32:GLU:OE2	1:D:48:ARG:CD	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:MET:HE1	2:B:67:HIS:CA	2.48	0.43
1:A:159:TYR:CG	3:C:3:LEU:HD13	2.53	0.43
1:A:234:ARG:HD2	1:A:242:GLN:HB2	2.00	0.43
1:D:189:VAL:HG23	1:D:272:LEU:HD13	2.00	0.43
1:J:131:LYS:NZ	1:J:157:LYS:HE3	2.32	0.43
1:G:226:GLN:O	1:G:227:ASP:C	2.57	0.43
2:B:9:VAL:HG23	2:B:93:VAL:HG22	2.01	0.43
1:A:99[A]:SER:CA	4:A:413:HOH:O	2.56	0.43
1:A:7:TYR:N	1:A:99[A]:SER:HB2	2.33	0.42
1:A:99[B]:SER:CA	4:A:413:HOH:O	2.56	0.42
1:D:230:LEU:C	1:D:230:LEU:HD12	2.39	0.42
1:J:144:ARG:CD	4:J:404:HOH:O	2.42	0.42
1:A:230:LEU:HD12	1:A:230:LEU:C	2.39	0.42
1:J:32:GLU:OE2	1:J:48:ARG:HD3	2.19	0.42
2:E:39:MET:HE2	2:E:49:VAL:CG1	2.49	0.42
1:A:45:TYR:CE2	1:A:67:ALA:HB2	2.55	0.42
1:D:219:LEU:HG	1:D:220:ASN:HB2	2.02	0.42
1:D:202:ARG:HD3	1:D:244:TRP:CE3	2.54	0.41
1:G:193:PRO:HA	1:G:199:VAL:HG12	2.02	0.41
2:E:4:THR:HA	2:E:5:PRO:HD3	1.91	0.41
1:D:106:ASP:O	1:D:107:TRP:HB2	2.20	0.41
1:D:144:ARG:NH2	4:D:404:HOH:O	2.53	0.41
1:D:209:TYR:CD1	1:D:210:PRO:HA	2.55	0.41
2:H:71:THR:HA	2:H:72:PRO:HD2	1.95	0.41
1:G:167:TRP:CE2	3:I:1:LYS:HD3	2.55	0.41
1:A:11:ALA:HA	1:A:21:ARG:O	2.20	0.41
1:A:219:LEU:C	1:A:221:GLY:H	2.24	0.41
1:D:51:TRP:O	1:D:54:GLN:NE2	2.44	0.41
2:K:10:TYR:CD1	2:K:10:TYR:N	2.88	0.41
1:J:81:LEU:HD13	1:J:118:TYR:CD1	2.55	0.41
1:A:234:ARG:HD3	2:B:10:TYR:CD2	2.56	0.41
2:B:2:GLN:H	2:B:2:GLN:HG2	1.69	0.41
1:J:75:ARG:NH1	4:J:353:HOH:O	2.54	0.41
1:G:66:LYS:HG2	3:I:4:TYR:CE1	2.56	0.40
1:G:146:LYS:NZ	4:G:355:HOH:O	2.53	0.40
1:G:234:ARG:HD3	2:H:10:TYR:CE2	2.56	0.40
2:B:32:PRO:HB2	2:B:33:PRO:HD2	2.03	0.40
1:A:32:GLU:OE2	1:A:48:ARG:HD2	2.21	0.40
1:D:219:LEU:HB2	1:D:257:TYR:CZ	2.53	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	275/338 (81%)	259 (94%)	9 (3%)	7 (2%)	5	6
1	D	274/338 (81%)	258 (94%)	12 (4%)	4 (2%)	10	14
1	G	274/338 (81%)	259 (94%)	10 (4%)	5 (2%)	8	10
1	J	274/338 (81%)	250 (91%)	18 (7%)	6 (2%)	6	7
2	B	96/99 (97%)	94 (98%)	2 (2%)	0	100	100
2	E	97/99 (98%)	93 (96%)	3 (3%)	1 (1%)	15	23
2	H	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	K	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	I	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	L	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1512/1784 (85%)	1426 (94%)	63 (4%)	23 (2%)	10	14

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99[A]	SER
1	A	99[B]	SER
1	G	227	ASP
1	J	196	LYS
1	J	253	LYS
1	A	100	GLY
1	G	196	LYS
1	J	223	GLU
1	D	195	SER
1	D	223	GLU
2	E	98	ASP
1	G	177	ALA

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Mol	Chain	Res	Type
1	G	223	GLU
1	J	174	ASN
1	J	226	GLN
1	A	195	SER
1	A	223	GLU
1	D	220	ASN
1	G	226	GLN
1	J	224	LEU
1	A	220	ASN
1	A	222	GLU
1	D	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	235/280 (84%)	201 (86%)	34 (14%)	3	3
1	D	234/280 (84%)	204 (87%)	30 (13%)	4	5
1	G	234/280 (84%)	210 (90%)	24 (10%)	7	10
1	J	234/280 (84%)	203 (87%)	31 (13%)	4	4
2	B	93/94 (99%)	81 (87%)	12 (13%)	4	5
2	E	93/94 (99%)	83 (89%)	10 (11%)	6	9
2	H	93/94 (99%)	84 (90%)	9 (10%)	8	12
2	K	93/94 (99%)	84 (90%)	9 (10%)	8	12
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	6 (86%)	1 (14%)	3	4
3	I	7/7 (100%)	6 (86%)	1 (14%)	3	4
3	L	7/7 (100%)	6 (86%)	1 (14%)	3	4
All	All	1337/1524 (88%)	1175 (88%)	162 (12%)	5	6

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	17	LEU
1	A	19	GLU
1	A	39	ASP
1	A	44	ARG
1	A	48	ARG
1	A	53	GLU
1	A	72	GLN
1	A	78	LEU
1	A	79	ARG
1	A	110	LEU
1	A	114	LEU
1	A	154	GLU
1	A	166	GLU
1	A	176	ASN
1	A	181	ARG
1	A	194	ARG
1	A	219	LEU
1	A	220	ASN
1	A	223	GLU
1	A	224	LEU
1	A	225	THR
1	A	226	GLN
1	A	227	ASP
1	A	228	MET
1	A	229	GLU
1	A	234	ARG
1	A	251	LEU
1	A	254	GLU
1	A	255	GLN
1	A	256	ASN
1	A	260	ARG
1	A	266	LEU
1	A	270	LEU
2	B	1	ILE
2	B	2	GLN
2	B	4	THR
2	B	19	LYS
2	B	45	LYS
2	B	54	MET
2	B	58	LYS
2	B	64	ILE
2	B	70	PHE

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Mol	Chain	Res	Type
2	B	75	THR
2	B	77	THR
2	B	91	LYS
1	D	14	ARG
1	D	19	GLU
1	D	44	ARG
1	D	48	ARG
1	D	54	GLN
1	D	62	ARG
1	D	78	LEU
1	D	79	ARG
1	D	99	SER
1	D	114	LEU
1	D	149	GLN
1	D	194	ARG
1	D	202	ARG
1	D	215	LEU
1	D	219	LEU
1	D	220	ASN
1	D	223	GLU
1	D	224	LEU
1	D	226	GLN
1	D	227	ASP
1	D	229	GLU
1	D	230	LEU
1	D	234	ARG
1	D	247	VAL
1	D	251	LEU
1	D	254	GLU
1	D	256	ASN
1	D	266	LEU
1	D	268	GLU
1	D	272	LEU
2	E	1	ILE
2	E	4	THR
2	E	44	LYS
2	E	64	ILE
2	E	70	PHE
2	E	74	GLU
2	E	75	THR
2	E	77	THR
2	E	91	LYS

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Mol	Chain	Res	Type
2	E	93	VAL
3	F	1	LYS
1	G	17	LEU
1	G	45	TYR
1	G	48	ARG
1	G	75	ARG
1	G	78	LEU
1	G	79	ARG
1	G	82	LEU
1	G	114	LEU
1	G	155	HIS
1	G	181	ARG
1	G	186	LYS
1	G	212	ASP
1	G	218	GLN
1	G	219	LEU
1	G	223	GLU
1	G	224	LEU
1	G	226	GLN
1	G	230	LEU
1	G	234	ARG
1	G	249	VAL
1	G	254	GLU
1	G	266	LEU
1	G	272	LEU
1	G	273	ARG
2	H	1	ILE
2	H	4	THR
2	H	40	LEU
2	H	48	LYS
2	H	54	MET
2	H	58	LYS
2	H	64	ILE
2	H	70	PHE
2	H	93	VAL
3	I	3	LEU
1	J	17	LEU
1	J	19	GLU
1	J	31	LYS
1	J	48	ARG
1	J	57	PRO
1	J	61	GLU

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Mol	Chain	Res	Type
1	J	75	ARG
1	J	78	LEU
1	J	79	ARG
1	J	105	SER
1	J	111	ARG
1	J	114	LEU
1	J	115	GLN
1	J	149	GLN
1	J	196	LYS
1	J	200	THR
1	J	202	ARG
1	J	218	GLN
1	J	220	ASN
1	J	222	GLU
1	J	223	GLU
1	J	224	LEU
1	J	234	ARG
1	J	249	VAL
1	J	251	LEU
1	J	253	LYS
1	J	254	GLU
1	J	256	ASN
1	J	266	LEU
1	J	273	ARG
1	J	275	GLU
2	K	1	ILE
2	K	4	THR
2	K	22	ILE
2	K	29	GLN
2	K	45	LYS
2	K	48	LYS
2	K	64	ILE
2	K	70	PHE
2	K	93	VAL
3	L	3	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	97	GLN
1	A	176	ASN

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Mol	Chain	Res	Type
1	A	191	HIS
1	A	192	HIS
1	A	256	ASN
2	B	38	GLN
3	C	5	ASN
1	D	97	GLN
1	D	191	HIS
1	D	192	HIS
1	D	256	ASN
2	E	38	GLN
3	F	5	ASN
1	G	97	GLN
1	G	149	GLN
1	G	192	HIS
1	G	218	GLN
2	H	31	HIS
2	H	38	GLN
3	I	5	ASN
1	J	54	GLN
1	J	97	GLN
1	J	191	HIS
1	J	220	ASN
3	L	5	ASN

### 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 ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

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	276/338 (81%)	0.64	35 (12%) 3 3	8, 20, 46, 56	0
1	D	276/338 (81%)	0.69	32 (11%) 4 4	8, 23, 54, 64	0
1	G	276/338 (81%)	0.76	39 (14%) 2 2	6, 23, 48, 59	0
1	J	276/338 (81%)	0.89	49 (17%) 1 1	11, 28, 60, 66	0
2	B	98/99 (98%)	0.07	1 (1%) 82 80	9, 16, 23, 28	0
2	E	99/99 (100%)	0.22	2 (2%) 65 63	8, 18, 26, 29	0
2	H	99/99 (100%)	0.07	1 (1%) 82 80	10, 18, 27, 32	0
2	K	99/99 (100%)	0.13	4 (4%) 38 37	12, 25, 34, 40	0
3	C	9/9 (100%)	0.24	0 100 100	11, 13, 17, 17	0
3	F	9/9 (100%)	0.20	0 100 100	13, 18, 25, 30	0
3	I	9/9 (100%)	0.45	1 (11%) 5 4	13, 18, 24, 28	0
3	L	9/9 (100%)	0.05	0 100 100	35, 37, 45, 46	0
All	All	1535/1784 (86%)	0.57	164 (10%) 6 5	6, 22, 53, 66	0

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	178	THR	11.7
1	D	177	ALA	11.3
1	D	178	THR	10.6
1	A	178	THR	10.5
1	A	177	ALA	10.2
1	J	177	ALA	9.1
1	A	227	ASP	8.9
1	G	177	ALA	8.3
1	J	248	VAL	8.2
1	J	249	VAL	8.1
1	G	178	THR	8.1

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Mol	Chain	Res	Type	RSRZ
1	A	180	LEU	7.5
1	J	196	LYS	7.3
1	G	250	PRO	7.3
1	G	251	LEU	6.5
1	G	179	LEU	6.5
1	G	225	THR	6.5
1	J	226	GLN	6.3
1	J	251	LEU	6.2
1	J	252	GLY	6.1
1	G	252	GLY	6.0
1	G	222	GLU	6.0
1	J	222	GLU	5.8
1	D	180	LEU	5.6
1	G	220	ASN	5.6
1	J	227	ASP	5.5
1	J	250	PRO	5.5
1	A	226	GLN	5.4
1	J	276	PRO	5.4
1	J	199	VAL	5.4
1	D	220	ASN	5.3
1	D	227	ASP	5.2
1	G	249	VAL	5.2
1	J	253	LYS	5.1
1	J	179	LEU	5.1
1	D	179	LEU	5.1
1	G	226	GLN	5.0
1	J	256	ASN	5.0
1	G	200	THR	5.0
1	A	179	LEU	4.8
1	J	197	GLY	4.8
1	A	219	LEU	4.8
1	J	180	LEU	4.7
1	J	224	LEU	4.6
1	A	220	ASN	4.6
1	G	248	VAL	4.6
1	G	219	LEU	4.5
1	G	257	TYR	4.5
1	A	176	ASN	4.5
1	D	249	VAL	4.5
1	D	181	ARG	4.4
1	A	257	TYR	4.3
1	A	222	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	252	GLY	4.3
1	D	257	TYR	4.3
1	G	199	VAL	4.3
1	A	276	PRO	4.2
1	G	180	LEU	4.2
1	D	223	GLU	4.1
1	D	226	GLN	4.1
1	A	18	GLU	4.1
1	D	225	THR	4.0
1	D	256	ASN	4.0
1	D	221	GLY	4.0
1	J	195	SER	4.0
1	J	223	GLU	3.9
1	J	221	GLY	3.9
1	D	176	ASN	3.9
1	J	220	ASN	3.8
1	J	17	LEU	3.8
1	J	217	TRP	3.7
1	J	219	LEU	3.6
1	G	253	LYS	3.6
1	G	247	VAL	3.6
1	G	274	TRP	3.6
1	D	219	LEU	3.6
1	D	16	GLY	3.6
1	J	257	TYR	3.5
1	G	58	GLU	3.5
1	J	200	THR	3.5
1	A	253	LYS	3.5
1	G	227	ASP	3.4
1	A	17	LEU	3.4
1	J	271	THR	3.4
1	J	201	LEU	3.3
1	A	249	VAL	3.3
1	A	252	GLY	3.3
1	D	250	PRO	3.3
1	G	176	ASN	3.2
1	G	194	ARG	3.2
1	J	198	GLU	3.2
1	G	256	ASN	3.2
1	D	248	VAL	3.2
1	A	251	LEU	3.2
1	D	253	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	256	ASN	3.1
1	J	193	PRO	3.1
1	J	274	TRP	3.0
1	G	223	GLU	3.0
2	E	47	PRO	3.0
1	A	225	THR	3.0
1	A	197	GLY	3.0
1	J	225	THR	3.0
1	D	17	LEU	2.9
1	D	251	LEU	2.9
1	A	248	VAL	2.9
2	K	99	MET	2.9
1	A	181	ARG	2.9
1	J	192	HIS	2.8
1	D	276	PRO	2.8
1	A	99[A]	SER	2.8
1	D	18	GLU	2.8
1	G	228	MET	2.8
1	J	190	THR	2.7
1	G	230	LEU	2.7
1	J	228	MET	2.7
1	D	54	GLN	2.7
2	E	99	MET	2.7
1	D	222	GLU	2.7
1	A	224	LEU	2.7
1	G	193	PRO	2.7
1	J	254	GLU	2.7
1	G	254	GLU	2.7
1	A	255	GLN	2.7
1	A	196	LYS	2.6
1	G	182	THR	2.6
1	G	197	GLY	2.6
1	A	100	GLY	2.5
1	J	189	VAL	2.5
1	D	175	GLY	2.5
1	J	176	ASN	2.5
3	I	6	PHE	2.5
1	G	196	LYS	2.5
1	D	41	GLU	2.5
1	A	15	PRO	2.5
2	B	48	LYS	2.5
1	J	272	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	K	1	ILE	2.5
1	J	273	ARG	2.4
1	D	197	GLY	2.4
1	G	198	GLU	2.4
2	H	1	ILE	2.4
1	G	224	LEU	2.4
2	K	48	LYS	2.4
1	J	41	GLU	2.4
1	J	247	VAL	2.3
1	J	194	ARG	2.3
1	A	274	TRP	2.3
1	J	246	SER	2.2
1	J	229	GLU	2.2
1	A	250	PRO	2.2
1	A	221	GLY	2.2
1	G	44	ARG	2.2
1	J	42	ASN	2.2
1	A	14	ARG	2.2
1	J	186	LYS	2.2
1	A	201	LEU	2.1
1	G	255	GLN	2.1
2	K	47	PRO	2.1
1	G	189	VAL	2.1
1	D	199	VAL	2.1
1	G	41	GLU	2.0
1	D	217	TRP	2.0
1	A	54	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.