



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:39 AM UTC

PDB ID : 1S7X / pdb_00001s7x
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 : 2.41 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

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>.

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

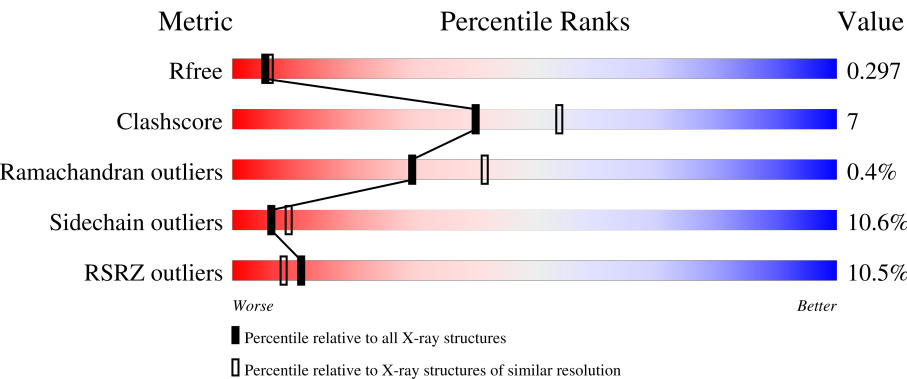
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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 ≥ 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	8% 64% 15% • 18%
1	D	338	7% 69% 10% • 18%
1	G	338	12% 64% 16% • 18%
1	J	338	15% 67% 13% • 18%
2	B	99	80% 15% • •

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Mol	Chain	Length	Quality of chain
2	E	99	2%76%21%.
2	H	99	%83%16%.
2	K	99	7%76%22%.
3	C	9	89%11%
3	F	9	89%11%
3	I	9	22%67%22%11%
3	L	9	44%89%11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13420 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	0	0
			2264	1430	400	425	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	99	Total	C	N	O	S	0	0	0
			818	523	138	151	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
			72	48	11	12	1			
3	F	9	Total	C	N	O	S	0	0	0
			72	48	11	12	1			
3	I	9	Total	C	N	O	S	0	0	0
			72	48	11	12	1			
3	L	9	Total	C	N	O	S	0	0	0
			72	48	11	12	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	PHE	TYR	engineered mutation	UNP P07399
C	9	MET	CYS	SEE REMARK 999	UNP P07399
F	4	PHE	TYR	engineered mutation	UNP P07399
F	9	MET	CYS	SEE REMARK 999	UNP P07399
I	4	PHE	TYR	engineered mutation	UNP P07399
I	9	MET	CYS	SEE REMARK 999	UNP P07399
L	4	PHE	TYR	engineered mutation	UNP P07399
L	9	MET	CYS	SEE REMARK 999	UNP P07399

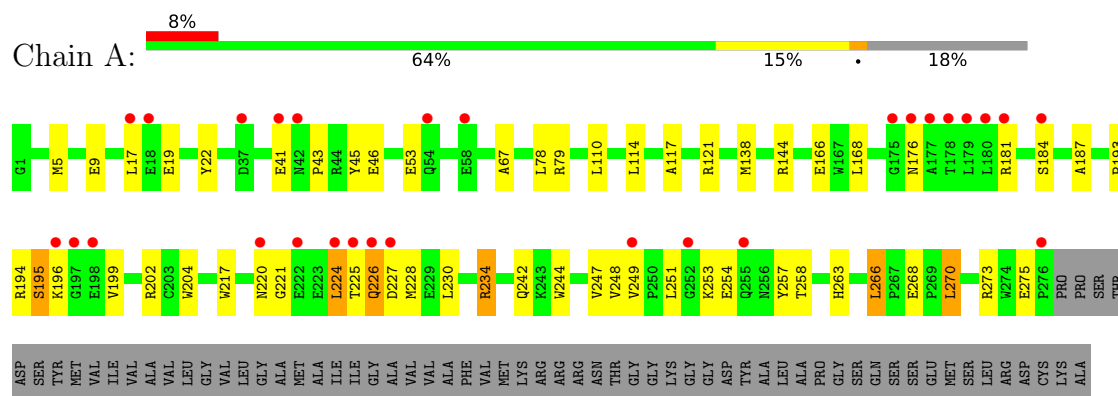
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	107	Total O 107 107	0	0
4	B	91	Total O 91 91	0	0
4	C	2	Total O 2 2	0	0
4	D	126	Total O 126 126	0	0
4	E	74	Total O 74 74	0	0
4	F	5	Total O 5 5	0	0
4	G	145	Total O 145 145	0	0
4	H	78	Total O 78 78	0	0
4	I	4	Total O 4 4	0	0
4	J	112	Total O 112 112	0	0
4	K	53	Total O 53 53	0	0
4	L	7	Total O 7 7	0	0

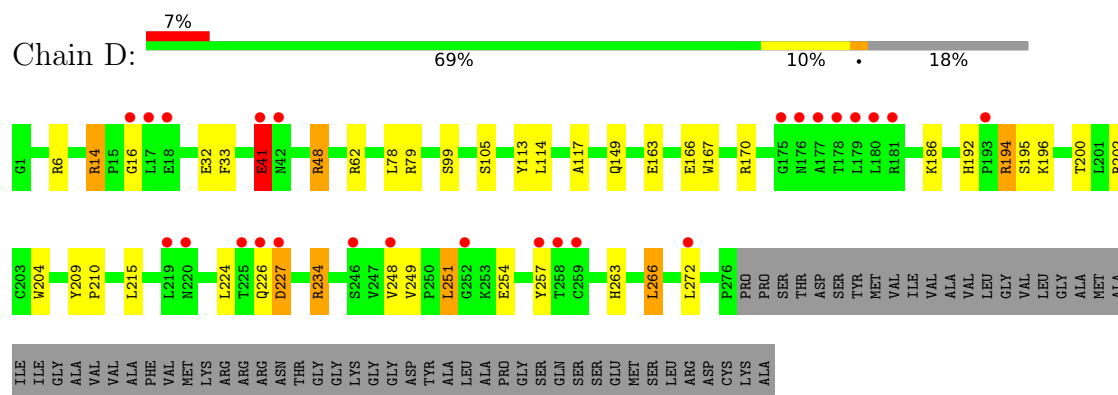
3 Residue-property plots

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.

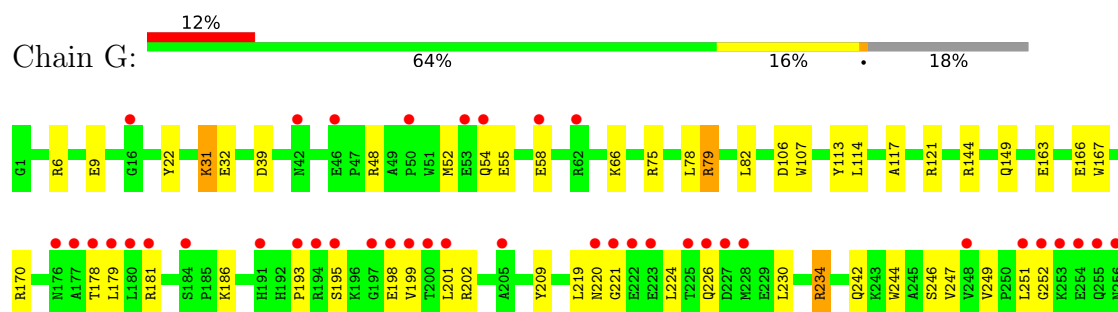
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

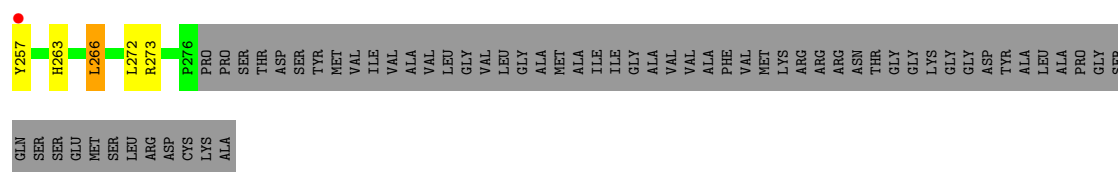


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

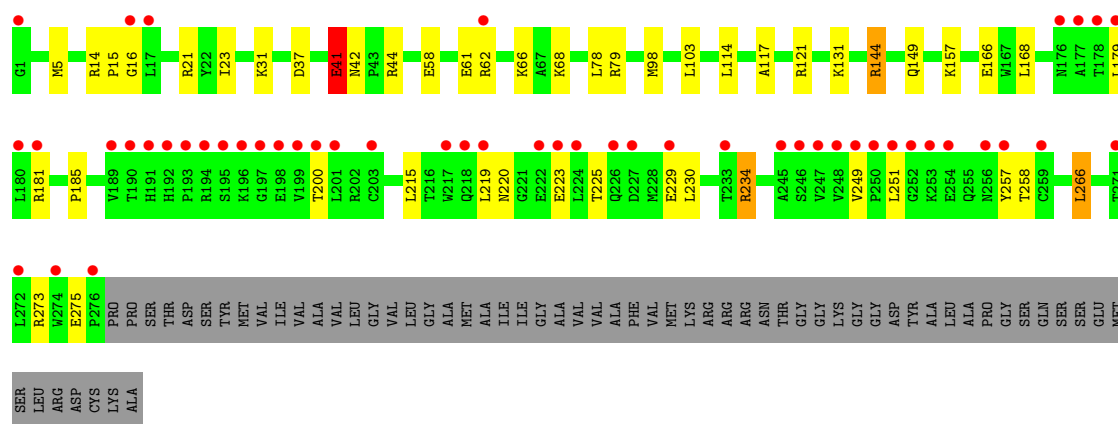


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

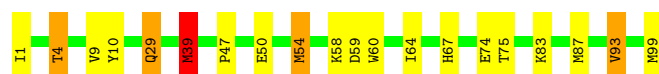
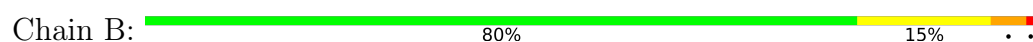




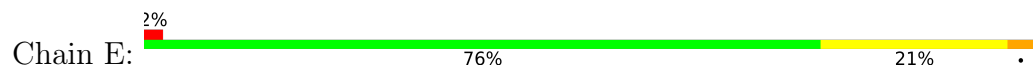
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



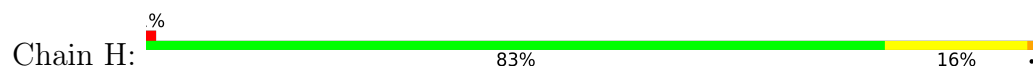
- Molecule 2: Beta-2-microglobulin



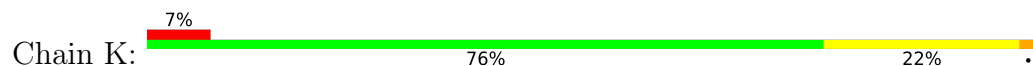
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin





- Molecule 3: Glycoprotein 9-residue peptide

Chain C: 89% 11%



- Molecule 3: Glycoprotein 9-residue peptide

Chain F: 89% 11%



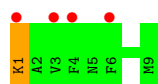
- Molecule 3: Glycoprotein 9-residue peptide

Chain I: 22% 67% 22% 11%



- Molecule 3: Glycoprotein 9-residue peptide

Chain L: 44% 89% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	91.90Å 123.32Å 100.20Å 90.00° 102.82° 90.00°	Depositor
Resolution (Å)	19.80 – 2.41 19.80 – 2.41	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.80-2.41) 98.7 (19.80-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.203 , 0.254 (Not available) , 0.297	Depositor DCC
R_{free} test set	2037 reflections (2.45%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13420	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.62	1/2331 (0.0%)	0.78	0/3166
1	D	0.64	1/2331 (0.0%)	0.82	1/3166 (0.0%)
1	G	0.67	0/2331	0.81	0/3166
1	J	0.88	1/2331 (0.0%)	0.81	1/3166 (0.0%)
2	B	0.83	2/844 (0.2%)	0.85	1/1146 (0.1%)
2	E	0.78	1/844 (0.1%)	0.84	0/1146
2	H	0.77	1/844 (0.1%)	0.84	0/1146
2	K	0.65	0/844	0.80	0/1146
3	C	0.68	0/73	0.83	0/95
3	F	0.78	0/73	0.90	0/95
3	I	0.97	1/73 (1.4%)	1.02	0/95
3	L	0.70	0/73	0.78	0/95
All	All	0.73	8/12992 (0.1%)	0.81	3/17628 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	41	GLU	C-N	30.67	1.74	1.33
2	B	39	MET	SD-CE	-11.36	1.51	1.79
2	E	39	MET	SD-CE	-9.32	1.56	1.79
2	H	39	MET	SD-CE	-9.03	1.56	1.79
1	D	41	GLU	C-N	8.39	1.45	1.33
1	A	138	MET	SD-CE	-7.10	1.61	1.79
2	B	87	MET	SD-CE	-6.69	1.62	1.79
3	I	9	MET	CG-SD	-5.09	1.68	1.80

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	41	GLU	O-C-N	9.28	134.94	122.59
1	D	41	GLU	O-C-N	7.24	129.85	122.03
2	B	47	PRO	N-CA-C	5.71	121.00	113.86

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	2264	0	2136	25	0
1	D	2264	0	2136	33	0
1	G	2264	0	2136	28	0
1	J	2264	0	2135	24	0
2	B	818	0	791	14	0
2	E	818	0	791	23	0
2	H	818	0	791	16	0
2	K	818	0	791	16	0
3	C	72	0	74	0	0
3	F	72	0	74	1	0
3	I	72	0	74	1	0
3	L	72	0	74	2	0
4	A	107	0	0	2	0
4	B	91	0	0	6	0
4	C	2	0	0	0	0
4	D	126	0	0	3	0
4	E	74	0	0	4	0
4	F	5	0	0	0	0
4	G	145	0	0	6	0
4	H	78	0	0	2	0
4	I	4	0	0	0	0
4	J	112	0	0	4	0
4	K	53	0	0	1	0
4	L	7	0	0	1	0
All	All	13420	0	12003	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)
1:J:41:GLU:C	1:J:42:ASN:N	1.74	1.45
2:H:99:MET:C	4:H:102:HOH:O	1.88	1.16
1:J:41:GLU:OE2	1:J:42:ASN:N	1.80	1.14
2:B:99:MET:CG	4:B:180:HOH:O	2.01	1.07
1:D:14:ARG:HG2	1:D:14:ARG:HH11	0.92	1.05
2:E:99:MET:CG	4:E:105:HOH:O	2.09	1.00
2:B:99:MET:C	4:B:101:HOH:O	2.07	0.97
1:D:14:ARG:HH11	1:D:14:ARG:CG	1.80	0.94
1:D:14:ARG:HG2	1:D:14:ARG:NH1	1.73	0.89
2:E:99:MET:O	4:E:100:HOH:O	1.91	0.86
1:D:41:GLU:CD	1:D:41:GLU:H	1.83	0.84
4:J:414:HOH:O	2:K:99:MET:CG	2.24	0.84
1:J:41:GLU:CA	1:J:42:ASN:N	2.46	0.78
2:H:39:MET:HE2	2:H:49:VAL:HG13	1.70	0.71
4:G:420:HOH:O	2:H:99:MET:CG	2.38	0.71
2:K:39:MET:HE3	2:K:49:VAL:HG13	1.73	0.71
2:E:99:MET:C	4:E:100:HOH:O	2.36	0.67
4:D:461:HOH:O	2:E:3:LYS:HE3	1.96	0.65
4:G:478:HOH:O	2:H:3:LYS:HE3	1.94	0.65
2:H:39:MET:HE1	2:H:67:HIS:C	2.24	0.63
4:G:478:HOH:O	2:H:3:LYS:CE	2.47	0.63
1:D:249:VAL:HG22	1:D:257:TYR:CZ	2.33	0.63
1:D:249:VAL:HG22	1:D:257:TYR:CE2	2.34	0.63
1:D:249:VAL:HG13	1:D:257:TYR:CE2	2.34	0.63
4:D:461:HOH:O	2:E:3:LYS:CE	2.48	0.61
1:D:248:VAL:O	1:D:248:VAL:HG23	1.98	0.61
2:K:39:MET:CE	2:K:49:VAL:HG13	2.31	0.60
1:A:144:ARG:HD2	4:A:342:HOH:O	2.01	0.60
1:G:52:MET:HE3	1:G:55:GLU:HG3	1.84	0.60
1:A:194:ARG:O	1:A:195:SER:C	2.45	0.60
1:G:32:GLU:OE2	1:G:48:ARG:HD2	2.02	0.60
1:J:21:ARG:HE	1:J:23:ILE:HD11	1.67	0.59
2:B:99:MET:O	4:B:101:HOH:O	2.14	0.59
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.38	0.59
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.37	0.59
1:D:32:GLU:OE2	1:D:48:ARG:HD2	2.03	0.59
1:G:201:LEU:HD12	1:G:249:VAL:HG21	1.84	0.58
1:A:217:TRP:HD1	1:A:228:MET:HE2	1.69	0.56
1:J:185:PRO:HD2	1:J:266:LEU:HD13	1.88	0.56
1:J:144:ARG:HD2	4:J:429:HOH:O	2.06	0.55
1:J:234:ARG:HD3	2:K:10:TYR:CE2	2.41	0.55
2:K:96:ASP:O	2:K:98:ASP:O	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:98:ASP:C	2:K:99:MET:CG	2.79	0.55
1:G:219:LEU:HG	1:G:220:ASN:HD22	1.72	0.55
4:G:420:HOH:O	2:H:99:MET:CB	2.54	0.54
1:J:41:GLU:C	1:J:42:ASN:CA	2.75	0.54
1:G:224:LEU:HD23	1:G:247:VAL:HG21	1.90	0.54
1:J:41:GLU:CB	1:J:42:ASN:N	2.70	0.54
2:E:39:MET:HE2	2:E:49:VAL:HG13	1.91	0.53
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.46	0.51
1:G:193:PRO:HA	1:G:199:VAL:HG12	1.92	0.51
1:J:14:ARG:HG2	1:J:15:PRO:HD2	1.93	0.51
2:H:54:MET:HB2	4:H:101:HOH:O	2.09	0.51
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.45	0.51
1:D:194:ARG:HG2	4:D:353:HOH:O	2.11	0.51
1:A:234:ARG:HD2	1:A:242:GLN:HB2	1.94	0.50
2:H:39:MET:CE	2:H:49:VAL:HG13	2.38	0.50
2:K:98:ASP:O	2:K:99:MET:CG	2.60	0.50
1:A:263:HIS:HB3	1:A:266:LEU:HD22	1.94	0.49
1:D:234:ARG:HD3	2:E:10:TYR:CE2	2.47	0.49
1:A:224:LEU:HD23	1:A:247:VAL:HG21	1.95	0.49
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.47	0.48
2:H:7:ILE:HD12	2:H:91:LYS:HE2	1.95	0.48
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.49	0.48
3:L:1:LYS:NZ	4:L:731:HOH:O	2.46	0.48
1:A:217:TRP:H	1:A:228:MET:HE1	1.78	0.48
1:J:21:ARG:NE	1:J:23:ILE:HD11	2.27	0.48
1:A:217:TRP:HB2	1:A:228:MET:CE	2.43	0.48
1:G:234:ARG:HD3	2:H:10:TYR:CE2	2.48	0.48
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.49	0.48
1:J:103:LEU:HD11	1:J:168:LEU:HD23	1.95	0.48
2:K:31:HIS:CD2	2:K:32:PRO:HA	2.49	0.48
2:B:29:GLN:NE2	2:B:59:ASP:OD2	2.47	0.47
1:A:217:TRP:N	1:A:228:MET:HE1	2.29	0.47
2:E:39:MET:HE1	2:E:67:HIS:C	2.39	0.47
1:D:263:HIS:HB3	1:D:266:LEU:HD22	1.96	0.47
2:B:9:VAL:HG23	2:B:93:VAL:HG22	1.96	0.47
1:D:234:ARG:HD3	2:E:10:TYR:CZ	2.49	0.47
1:G:144:ARG:NH2	4:G:398:HOH:O	2.47	0.47
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.49	0.47
2:K:39:MET:HE2	2:K:66:ALA:HB1	1.97	0.47
2:E:39:MET:HE1	2:E:67:HIS:CA	2.44	0.47
1:A:217:TRP:CD1	1:A:228:MET:HE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:VAL:HG22	1:G:257:TYR:CE1	2.50	0.47
1:D:14:ARG:NH2	2:E:34:HIS:HB2	2.30	0.46
2:E:39:MET:CE	2:E:49:VAL:HG13	2.45	0.46
1:D:14:ARG:CG	1:D:14:ARG:NH1	2.49	0.46
1:A:187:ALA:HA	1:A:204:TRP:O	2.15	0.46
1:G:251:LEU:HD23	1:G:252:GLY:N	2.31	0.46
2:B:39:MET:HE1	2:B:67:HIS:HA	1.97	0.46
1:D:226:GLN:O	1:D:227:ASP:C	2.58	0.46
2:H:39:MET:HE1	2:H:67:HIS:CA	2.46	0.46
1:G:201:LEU:O	1:G:246:SER:HA	2.16	0.46
1:J:5:MET:HB2	1:J:168:LEU:HD13	1.98	0.46
1:A:226:GLN:HA	1:A:227:ASP:HA	1.72	0.46
2:E:32:PRO:HB2	2:E:33:PRO:HD2	1.98	0.46
1:G:249:VAL:HG22	1:G:257:TYR:CZ	2.50	0.46
1:D:14:ARG:HH21	2:E:34:HIS:HB2	1.80	0.45
1:G:230:LEU:C	1:G:230:LEU:HD12	2.41	0.45
1:D:192:HIS:HE2	2:E:98:ASP:CG	2.25	0.45
1:D:202:ARG:HG2	1:D:204:TRP:NE1	2.32	0.45
1:G:249:VAL:HG13	1:G:257:TYR:CE2	2.52	0.45
1:D:14:ARG:HH21	2:E:34:HIS:CG	2.34	0.45
2:E:9:VAL:HG23	2:E:93:VAL:HG22	1.98	0.45
1:J:131:LYS:NZ	1:J:157:LYS:HE3	2.32	0.45
1:G:178:THR:HG22	1:G:178:THR:O	2.18	0.44
1:A:5:MET:HB2	1:A:168:LEU:HD13	2.00	0.44
1:G:79:ARG:NE	4:G:388:HOH:O	2.51	0.43
1:D:14:ARG:NH2	2:E:34:HIS:CB	2.81	0.43
1:G:9:GLU:OE1	1:G:22:TYR:OH	2.34	0.43
1:J:66:LYS:HZ1	3:L:1:LYS:HE2	1.82	0.43
1:G:263:HIS:HB3	1:G:266:LEU:HD22	2.00	0.43
2:B:4:THR:HG22	4:B:104:HOH:O	2.19	0.43
1:J:41:GLU:HB2	1:J:42:ASN:N	2.33	0.43
1:G:234:ARG:HD2	1:G:242:GLN:HB2	2.01	0.43
1:G:224:LEU:CD2	1:G:247:VAL:HG21	2.49	0.43
2:E:4:THR:HG22	4:E:112:HOH:O	2.18	0.43
1:G:31:LYS:HG3	1:G:209:TYR:OH	2.18	0.43
1:J:98:MET:HE2	2:K:60:TRP:CH2	2.54	0.43
1:J:249:VAL:HG22	1:J:257:TYR:CE1	2.54	0.43
2:B:54:MET:HB2	4:B:110:HOH:O	2.19	0.42
1:D:41:GLU:CD	1:D:41:GLU:N	2.62	0.42
2:E:39:MET:HE1	2:E:67:HIS:HA	2.01	0.42
1:A:230:LEU:HD12	1:A:230:LEU:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:14:ARG:HH11	1:J:16:GLY:H	1.68	0.42
2:K:50:GLU:HB2	2:K:67:HIS:CE1	2.54	0.42
1:A:45:TYR:CE2	1:A:67:ALA:HB2	2.55	0.42
1:D:99:SER:HA	1:D:113:TYR:O	2.19	0.42
2:B:50:GLU:HB2	2:B:67:HIS:CE1	2.55	0.41
1:D:192:HIS:HB2	1:D:200:THR:HB	2.02	0.41
1:G:6:ARG:NH2	1:G:113:TYR:CE1	2.88	0.41
1:J:21:ARG:NH2	1:J:37:ASP:OD2	2.53	0.41
1:A:9:GLU:OE1	1:A:22:TYR:OH	2.36	0.41
1:A:234:ARG:HD3	2:B:10:TYR:CD2	2.56	0.41
1:D:14:ARG:HH21	2:E:34:HIS:CB	2.33	0.41
1:G:167:TRP:HZ3	1:G:170:ARG:HE	1.68	0.41
2:H:7:ILE:HD12	2:H:91:LYS:CE	2.50	0.41
2:K:1:ILE:N	4:K:121:HOH:O	2.34	0.41
1:D:209:TYR:CD1	1:D:210:PRO:HA	2.56	0.41
1:G:106:ASP:O	1:G:107:TRP:HB2	2.20	0.41
1:A:270:LEU:HD12	4:A:377:HOH:O	2.20	0.41
1:D:251:LEU:HD23	1:D:254:GLU:OE1	2.21	0.41
2:H:54:MET:O	2:H:54:MET:HG3	2.20	0.41
1:D:163:GLU:OE1	3:F:1:LYS:NZ	2.53	0.41
1:G:201:LEU:CD1	1:G:249:VAL:HG21	2.50	0.41
1:A:193:PRO:HA	1:A:199:VAL:HG12	2.02	0.41
2:B:9:VAL:CG2	2:B:93:VAL:HG22	2.51	0.41
2:B:99:MET:CB	4:B:180:HOH:O	2.54	0.41
1:D:33:PHE:C	1:D:48:ARG:HB2	2.46	0.41
1:J:41:GLU:HB2	4:J:450:HOH:O	2.20	0.41
1:J:62:ARG:HG3	4:J:384:HOH:O	2.20	0.41
2:K:19:LYS:HB3	2:K:19:LYS:NZ	2.36	0.41
1:D:6:ARG:NH2	1:D:113:TYR:CE1	2.89	0.40
1:D:32:GLU:OE2	1:D:48:ARG:CD	2.68	0.40
1:G:163:GLU:OE1	3:I:1:LYS:NZ	2.53	0.40
2:E:48:LYS:HB3	2:E:48:LYS:NZ	2.35	0.40
2:K:87:MET:HE2	2:K:91:LYS:HD2	2.03	0.40
1:J:41:GLU:OE2	1:J:42:ASN:CA	2.64	0.40
1:A:41:GLU:O	1:A:43:PRO:HD3	2.22	0.40
1:A:249:VAL:HG22	1:A:257:TYR:CE1	2.57	0.40
1:D:167:TRP:CE3	1:D:170:ARG:HD3	2.56	0.40
2:H:32:PRO:HB2	2:H:33:PRO:HD2	2.02	0.40
2:K:32:PRO:HB2	2:K:33:PRO:HD2	2.04	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	274/338 (81%)	258 (94%)	14 (5%)	2 (1%)	18	27
1	D	274/338 (81%)	263 (96%)	9 (3%)	2 (1%)	18	27
1	G	274/338 (81%)	253 (92%)	20 (7%)	1 (0%)	30	42
1	J	274/338 (81%)	260 (95%)	13 (5%)	1 (0%)	30	42
2	B	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	E	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
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%)	1436 (95%)	70 (5%)	6 (0%)	30	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	227	ASP
1	G	221	GLY
1	D	16	GLY
1	A	195	SER
1	J	41	GLU
1	A	221	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	234/280 (84%)	205 (88%)	29 (12%)	4	6
1	D	234/280 (84%)	214 (92%)	20 (8%)	10	15
1	G	234/280 (84%)	211 (90%)	23 (10%)	7	11
1	J	234/280 (84%)	205 (88%)	29 (12%)	4	6
2	B	93/94 (99%)	82 (88%)	11 (12%)	5	7
2	E	93/94 (99%)	82 (88%)	11 (12%)	5	7
2	H	93/94 (99%)	88 (95%)	5 (5%)	20	33
2	K	93/94 (99%)	84 (90%)	9 (10%)	8	11
3	C	7/7 (100%)	6 (86%)	1 (14%)	3	4
3	F	7/7 (100%)	6 (86%)	1 (14%)	3	4
3	I	7/7 (100%)	5 (71%)	2 (29%)	0	0
3	L	7/7 (100%)	6 (86%)	1 (14%)	3	4
All	All	1336/1524 (88%)	1194 (89%)	142 (11%)	6	9

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	19	GLU
1	A	46	GLU
1	A	53	GLU
1	A	78	LEU
1	A	79	ARG
1	A	110	LEU
1	A	114	LEU
1	A	121	ARG
1	A	166	GLU
1	A	176	ASN
1	A	181	ARG
1	A	184	SER
1	A	196	LYS
1	A	220	ASN
1	A	224	LEU
1	A	225	THR
1	A	226	GLN

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Mol	Chain	Res	Type
1	A	234	ARG
1	A	248	VAL
1	A	251	LEU
1	A	253	LYS
1	A	254	GLU
1	A	258	THR
1	A	266	LEU
1	A	268	GLU
1	A	270	LEU
1	A	273	ARG
1	A	275	GLU
2	B	1	ILE
2	B	4	THR
2	B	29	GLN
2	B	39	MET
2	B	54	MET
2	B	58	LYS
2	B	64	ILE
2	B	74	GLU
2	B	75	THR
2	B	83	LYS
2	B	93	VAL
3	C	1	LYS
1	D	14	ARG
1	D	41	GLU
1	D	48	ARG
1	D	62	ARG
1	D	78	LEU
1	D	79	ARG
1	D	105	SER
1	D	114	LEU
1	D	149	GLN
1	D	166	GLU
1	D	186	LYS
1	D	194	ARG
1	D	195	SER
1	D	196	LYS
1	D	215	LEU
1	D	224	LEU
1	D	234	ARG
1	D	251	LEU
1	D	266	LEU

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Mol	Chain	Res	Type
1	D	272	LEU
2	E	1	ILE
2	E	2	GLN
2	E	4	THR
2	E	29	GLN
2	E	40	LEU
2	E	44	LYS
2	E	64	ILE
2	E	70	PHE
2	E	75	THR
2	E	77	THR
2	E	93	VAL
3	F	1	LYS
1	G	31	LYS
1	G	39	ASP
1	G	54	GLN
1	G	58	GLU
1	G	66	LYS
1	G	75	ARG
1	G	78	LEU
1	G	79	ARG
1	G	82	LEU
1	G	114	LEU
1	G	121	ARG
1	G	149	GLN
1	G	166	GLU
1	G	179	LEU
1	G	181	ARG
1	G	186	LYS
1	G	195	SER
1	G	198	GLU
1	G	226	GLN
1	G	234	ARG
1	G	266	LEU
1	G	272	LEU
1	G	273	ARG
2	H	2	GLN
2	H	4	THR
2	H	29	GLN
2	H	75	THR
2	H	93	VAL
3	I	4	PHE

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Mol	Chain	Res	Type
3	I	9	MET
1	J	31	LYS
1	J	41	GLU
1	J	44	ARG
1	J	58	GLU
1	J	61	GLU
1	J	68	LYS
1	J	78	LEU
1	J	79	ARG
1	J	114	LEU
1	J	121	ARG
1	J	144	ARG
1	J	149	GLN
1	J	166	GLU
1	J	179	LEU
1	J	181	ARG
1	J	200	THR
1	J	215	LEU
1	J	219	LEU
1	J	220	ASN
1	J	223	GLU
1	J	225	THR
1	J	229	GLU
1	J	230	LEU
1	J	234	ARG
1	J	251	LEU
1	J	258	THR
1	J	266	LEU
1	J	273	ARG
1	J	275	GLU
2	K	1	ILE
2	K	2	GLN
2	K	19	LYS
2	K	22	ILE
2	K	29	GLN
2	K	54	MET
2	K	64	ILE
2	K	83	LYS
2	K	93	VAL
3	L	1	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	127	ASN
1	A	192	HIS
1	A	220	ASN
1	A	226	GLN
2	B	29	GLN
2	B	38	GLN
3	C	5	ASN
1	D	54	GLN
1	D	97	GLN
2	E	13	HIS
2	E	29	GLN
2	E	67	HIS
3	F	5	ASN
1	G	54	GLN
1	G	97	GLN
1	G	115	GLN
1	G	218	GLN
1	G	220	ASN
1	G	226	GLN
2	H	13	HIS
2	H	34	HIS
3	I	5	ASN
1	J	30	ASN
1	J	72	GLN
1	J	97	GLN
1	J	192	HIS
1	J	220	ASN
2	K	13	HIS
2	K	38	GLN
2	K	67	HIS
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 [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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	41:GLU	C	42:ASN	N	1.74

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, 95th 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 ²)	Q<0.9
1	A	276/338 (81%)	0.75	28 (10%) 12 9	13, 30, 53, 61	0
1	D	276/338 (81%)	0.50	25 (9%) 15 12	10, 25, 51, 60	0
1	G	276/338 (81%)	0.71	41 (14%) 5 4	8, 26, 53, 61	0
1	J	276/338 (81%)	0.95	51 (18%) 3 3	10, 29, 62, 65	0
2	B	99/99 (100%)	0.16	0 100 100	13, 21, 29, 32	0
2	E	99/99 (100%)	0.15	2 (2%) 65 61	11, 21, 28, 32	0
2	H	99/99 (100%)	0.08	1 (1%) 79 77	11, 21, 29, 34	0
2	K	99/99 (100%)	0.94	7 (7%) 22 18	14, 32, 41, 44	0
3	C	9/9 (100%)	0.39	0 100 100	23, 26, 32, 34	0
3	F	9/9 (100%)	0.12	0 100 100	18, 21, 25, 28	0
3	I	9/9 (100%)	0.57	2 (22%) 2 2	13, 20, 28, 31	0
3	L	9/9 (100%)	1.81	4 (44%) 0 0	34, 37, 45, 51	0
All	All	1536/1784 (86%)	0.62	161 (10%) 11 8	8, 26, 56, 65	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	177	ALA	7.5
1	A	177	ALA	6.3
1	J	179	LEU	6.1
1	J	197	GLY	5.3
1	J	199	VAL	5.2
1	G	222	GLU	5.2
1	J	177	ALA	5.2
1	G	177	ALA	5.2
1	J	256	ASN	4.9
1	J	200	THR	4.9
1	G	180	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	J	195	SER	4.6
1	J	178	THR	4.5
1	J	249	VAL	4.4
1	D	175	GLY	4.2
1	G	179	LEU	4.2
1	G	252	GLY	4.1
1	J	219	LEU	4.0
1	J	217	TRP	4.0
1	G	256	ASN	3.9
1	G	197	GLY	3.9
1	G	178	THR	3.8
1	J	180	LEU	3.8
1	D	257	TYR	3.7
1	J	17	LEU	3.7
1	J	198	GLU	3.7
1	A	178	THR	3.6
1	G	199	VAL	3.6
1	D	178	THR	3.5
1	J	251	LEU	3.5
1	J	272	LEU	3.5
1	G	220	ASN	3.4
1	J	201	LEU	3.4
1	A	227	ASP	3.4
1	A	42	ASN	3.4
1	D	179	LEU	3.4
1	D	258	THR	3.4
1	G	191	HIS	3.4
1	G	227	ASP	3.3
1	A	17	LEU	3.3
1	D	259	CYS	3.3
1	J	259	CYS	3.3
1	D	180	LEU	3.2
1	G	53	GLU	3.2
1	A	196	LYS	3.2
1	J	250	PRO	3.2
1	A	249	VAL	3.2
1	J	248	VAL	3.2
1	J	227	ASP	3.2
1	A	41	GLU	3.2
1	A	198	GLU	3.1
1	G	198	GLU	3.1
1	A	179	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	18	GLU	3.1
1	J	257	TYR	3.1
1	G	223	GLU	3.1
3	L	4	PHE	3.0
1	A	175	GLY	2.9
1	D	220	ASN	2.9
1	J	192	HIS	2.9
1	A	180	LEU	2.9
1	D	18	GLU	2.9
1	G	46	GLU	2.9
1	A	176	ASN	2.9
1	G	257	TYR	2.9
1	G	221	GLY	2.9
2	K	19	LYS	2.8
1	J	189	VAL	2.8
1	G	226	GLN	2.8
1	A	197	GLY	2.8
1	J	196	LYS	2.8
1	J	191	HIS	2.8
1	J	223	GLU	2.8
2	K	1	ILE	2.8
2	K	99	MET	2.8
1	D	181	ARG	2.8
1	J	253	LYS	2.8
2	K	81	ARG	2.8
1	D	16	GLY	2.7
1	A	276	PRO	2.7
1	D	176	ASN	2.7
1	D	248	VAL	2.7
1	J	190	THR	2.7
1	G	248	VAL	2.7
1	D	225	THR	2.7
1	G	200	THR	2.7
1	D	246	SER	2.6
1	J	254	GLU	2.6
1	J	245	ALA	2.6
1	A	252	GLY	2.6
1	J	247	VAL	2.6
1	G	251	LEU	2.6
1	G	42	ASN	2.6
1	D	227	ASP	2.6
1	A	226	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	253	LYS	2.6
3	L	1	LYS	2.6
1	D	41	GLU	2.5
1	J	62	ARG	2.5
1	J	193	PRO	2.5
1	D	17	LEU	2.5
1	J	176	ASN	2.5
1	G	195	SER	2.5
1	D	272	LEU	2.5
2	K	82	VAL	2.5
1	J	218	GLN	2.5
1	D	42	ASN	2.5
1	G	181	ARG	2.5
1	G	194	ARG	2.4
1	G	176	ASN	2.4
1	G	228	MET	2.4
1	D	193	PRO	2.4
1	D	252	GLY	2.4
1	J	224	LEU	2.4
3	I	4	PHE	2.4
2	K	71	THR	2.4
1	A	58	GLU	2.4
1	G	193	PRO	2.4
1	D	226	GLN	2.4
1	J	1	GLY	2.4
1	G	62	ARG	2.4
1	J	274	TRP	2.4
1	A	224	LEU	2.3
3	I	6	PHE	2.3
2	E	48	LYS	2.3
1	J	222	GLU	2.3
1	G	184	SER	2.3
1	J	16	GLY	2.3
1	A	255	GLN	2.3
1	A	220	ASN	2.3
1	G	225	THR	2.3
1	J	252	GLY	2.3
1	J	229	GLU	2.3
1	J	181	ARG	2.3
1	G	201	LEU	2.3
1	G	205	ALA	2.2
1	J	271	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	181	ARG	2.2
1	G	54	GLN	2.2
1	A	225	THR	2.2
1	J	233	THR	2.2
1	G	50	PRO	2.2
2	E	47	PRO	2.2
1	G	255	GLN	2.1
1	J	246	SER	2.1
2	K	34	HIS	2.1
3	L	6	PHE	2.1
1	G	254	GLU	2.1
3	L	3	VAL	2.1
1	D	219	LEU	2.1
2	H	89	GLU	2.1
1	A	37	ASP	2.1
1	A	184	SER	2.1
1	A	54	GLN	2.0
1	J	226	GLN	2.0
1	J	194	ARG	2.0
1	A	222	GLU	2.0
1	G	16	GLY	2.0
1	J	203	CYS	2.0
1	G	58	GLU	2.0
1	J	276	PRO	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 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.