



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:45 PM UTC

PDB ID : 3QUL / pdb_00003qul
Title : Crystal structures of the murine class I major histocompatibility complex H-2Db in complex with LCMV-derived gp33 altered peptide ligand (Y4S)
Authors : Allerbring, E.; Duru, A.D.; Uchtenhagen, H.; Madhurantakam, C.; Grimm, S.; Tomek, M.B.; Mazumdar, P.A.; Spetz, A.; Friemann, R.; Sandalova, T.; Uhlin, M.; Nygren, P.; Achour, A.
Deposited on : 2011-02-24
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

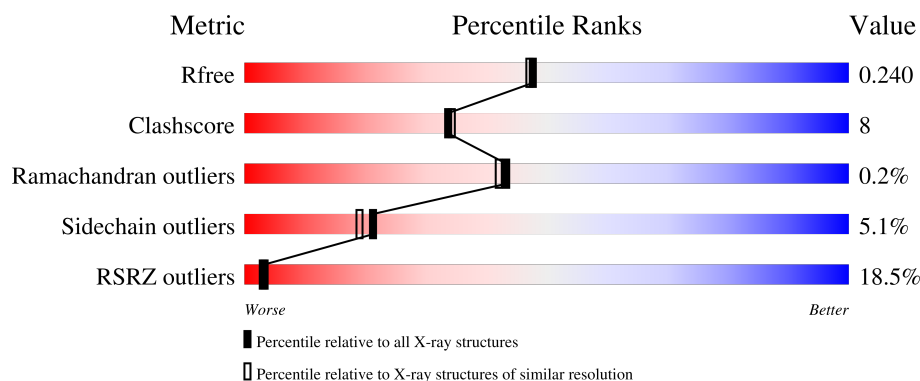
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



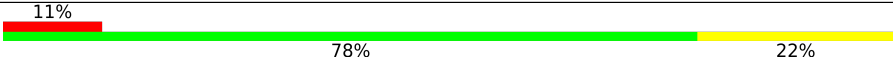
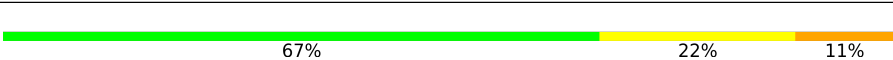
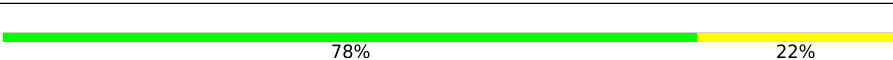
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	276	21% 85% 9% • •
1	D	276	25% 78% 16% • 5%
1	G	276	21% 83% 12% • •
1	J	276	19% 79% 16% • •
2	B	99	11% 82% 17% •

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Mol	Chain	Length	Quality of chain
2	E	99	
2	H	99	
2	K	99	
3	C	9	
3	F	9	
3	I	9	
3	L	9	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13506 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	264	Total	C	N	O	S	0	8	0
			2246	1413	405	419	9			
1	D	262	Total	C	N	O	S	0	4	0
			2193	1386	390	407	10			
1	G	270	Total	C	N	O	S	0	2	0
			2251	1419	402	421	9			
1	J	267	Total	C	N	O	S	0	3	0
			2225	1404	398	414	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	5	0
			859	548	144	159	8			
2	E	99	Total	C	N	O	S	0	5	0
			859	549	143	158	9			
2	H	99	Total	C	N	O	S	0	4	0
			854	544	145	157	8			
2	K	99	Total	C	N	O	S	0	2	0
			836	533	140	155	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ASP	ALA	variant	UNP P01887
E	85	ASP	ALA	variant	UNP P01887
H	85	ASP	ALA	variant	UNP P01887
K	85	ASP	ALA	variant	UNP P01887

- Molecule 3 is a protein called Pre-glycoprotein polyprotein GP complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			67	42	11	13	1			
3	F	9	Total	C	N	O	S	0	0	0
			67	42	11	13	1			
3	I	9	Total	C	N	O	S	0	0	0
			67	42	11	13	1			
3	L	9	Total	C	N	O	S	0	0	0
			67	42	11	13	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	SER	TYR	engineered mutation	UNP P07399
C	9	MET	CYS	engineered mutation	UNP P07399
F	4	SER	TYR	engineered mutation	UNP P07399
F	9	MET	CYS	engineered mutation	UNP P07399
I	4	SER	TYR	engineered mutation	UNP P07399
I	9	MET	CYS	engineered mutation	UNP P07399
L	4	SER	TYR	engineered mutation	UNP P07399
L	9	MET	CYS	engineered mutation	UNP P07399

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	154	Total	O	0	0
			154	154		
4	B	94	Total	O	0	0
			94	94		
4	C	7	Total	O	0	0
			7	7		
4	D	130	Total	O	0	0
			130	130		
4	E	82	Total	O	0	0
			82	82		
4	F	4	Total	O	0	0
			4	4		
4	G	130	Total	O	0	0
			130	130		
4	H	86	Total	O	0	0
			86	86		
4	I	5	Total	O	0	0
			5	5		
4	J	133	Total	O	0	0
			133	133		

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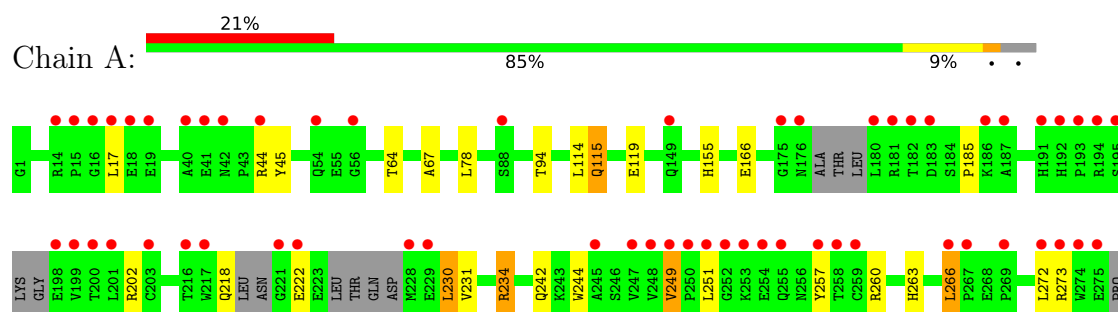
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	83	Total 83	O 83	0	0
4	L	7	Total 7	O 7	0	0

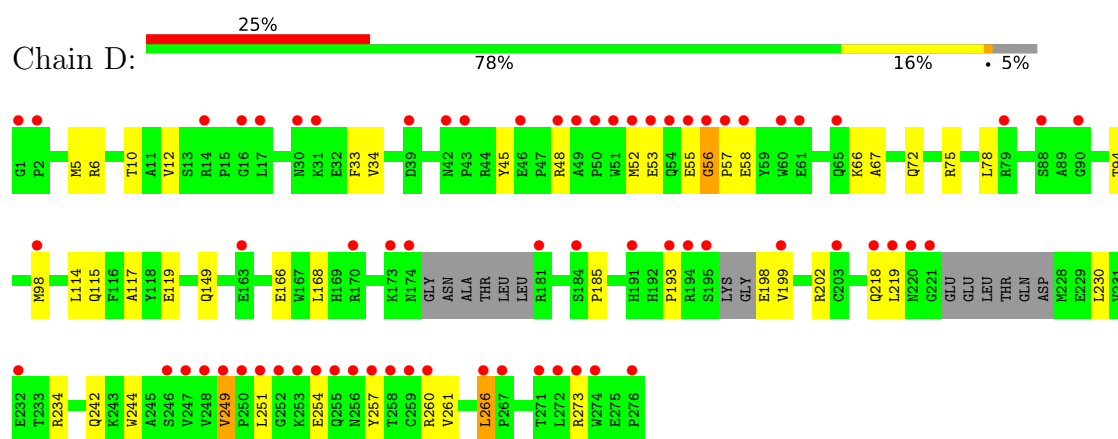
3 Residue-property plots [i](#)

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.

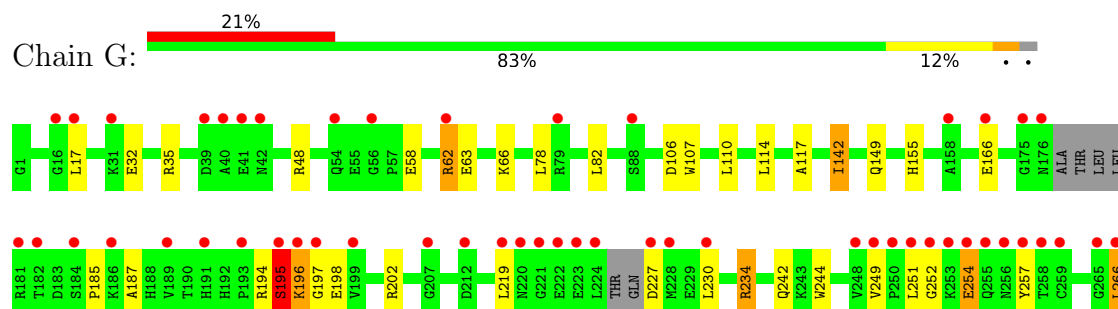
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

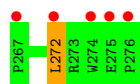


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

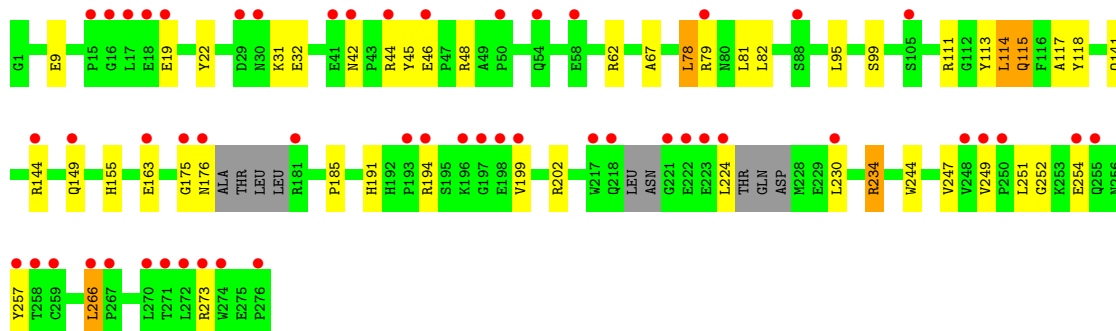
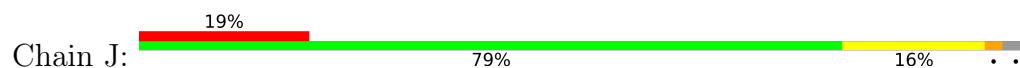


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

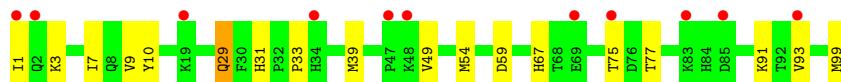
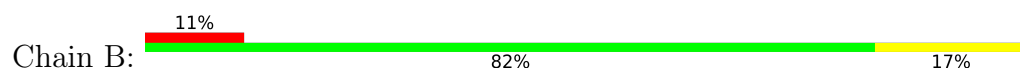




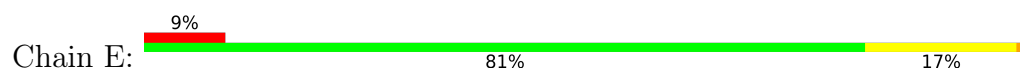
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



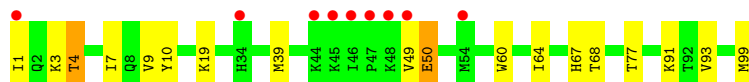
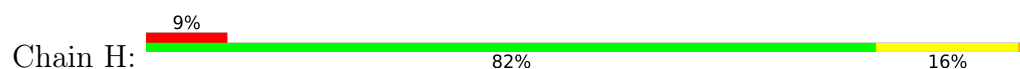
- Molecule 2: Beta-2-microglobulin



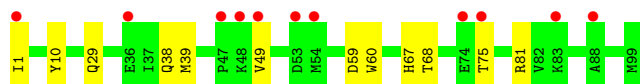
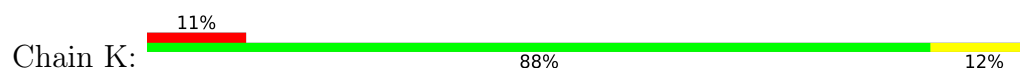
- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



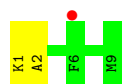
- Molecule 3: Pre-glycoprotein polypeptide GP complex

Chain C:  89% 11%



- Molecule 3: Pre-glycoprotein polyprotein GP complex

Chain F:  11% 78% 22%



- Molecule 3: Pre-glycoprotein polyprotein GP complex

Chain I:  67% 22% 11%



- Molecule 3: Pre-glycoprotein polyprotein GP complex

Chain L:  78% 22%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.04Å 122.70Å 99.12Å 90.00° 103.33° 90.00°	Depositor
Resolution (Å)	51.78 – 2.00 51.78 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (51.78-2.00) 98.9 (51.78-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.208 , 0.234 0.214 , 0.240	Depositor DCC
R_{free} test set	7177 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13506	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.06% 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	0.57	0/2308	0.70	0/3124
1	D	0.58	0/2257	0.73	2/3060 (0.1%)
1	G	0.57	0/2316	0.69	0/3139
1	J	0.57	0/2289	0.69	0/3101
2	B	0.56	0/885	0.71	0/1200
2	E	0.62	0/885	0.73	0/1200
2	H	0.59	0/880	0.72	0/1192
2	K	0.61	0/862	0.74	0/1169
3	C	0.67	0/67	0.84	0/87
3	F	0.62	0/67	0.70	0/87
3	I	0.75	0/67	1.01	0/87
3	L	0.64	0/67	0.83	0/87
All	All	0.58	0/12950	0.71	2/17533 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	56	GLY	CA-C-N	5.04	126.15	119.84
1	D	56	GLY	C-N-CA	5.04	126.15	119.84

There are no chirality outliers.

There are no planarity outliers.

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	2246	0	2107	31	0
1	D	2193	0	2063	38	0
1	G	2251	0	2115	32	0
1	J	2225	0	2093	29	0
2	B	859	0	837	23	0
2	E	859	0	837	21	0
2	H	854	0	830	21	0
2	K	836	0	811	10	0
3	C	67	0	70	1	0
3	F	67	0	70	4	0
3	I	67	0	70	2	0
3	L	67	0	70	1	0
4	A	154	0	0	2	0
4	B	94	0	0	3	0
4	C	7	0	0	0	0
4	D	130	0	0	3	0
4	E	82	0	0	1	0
4	F	4	0	0	0	0
4	G	130	0	0	1	0
4	H	86	0	0	3	0
4	I	5	0	0	0	0
4	J	133	0	0	4	0
4	K	83	0	0	0	0
4	L	7	0	0	0	0
All	All	13506	0	11973	190	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 8.

All (190) 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:A:44[B]:ARG:CG	1:A:44[B]:ARG:HH11	1.62	1.10
2:H:39:MET:HE2	2:H:49:VAL:HG13	1.18	1.09
1:A:44[B]:ARG:HH11	1:A:44[B]:ARG:HG2	1.07	1.08
2:K:39[A]:MET:HE2	2:K:49:VAL:HG13	1.32	1.08
2:H:39:MET:HE2	2:H:49:VAL:CG1	1.94	0.98
1:A:94[B]:THR:HG21	2:B:31:HIS:HE1	1.29	0.95
1:G:187:ALA:HB1	1:G:272:LEU:HD11	1.52	0.91
2:B:77[A]:THR:HG22	4:B:313:HOH:O	1.73	0.87
1:A:44[B]:ARG:HG2	1:A:44[B]:ARG:NH1	1.85	0.85
1:A:94[B]:THR:HG21	2:B:31:HIS:CE1	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:MET:CE	2:H:49:VAL:HG13	2.07	0.82
2:K:39[A]:MET:HE2	2:K:49:VAL:CG1	2.09	0.81
2:H:7:ILE:HG21	2:H:93[A]:VAL:HG11	1.63	0.81
1:A:44[B]:ARG:CG	1:A:44[B]:ARG:NH1	2.34	0.79
2:E:7:ILE:CG2	2:E:93[A]:VAL:HG11	2.13	0.79
2:B:39[A]:MET:HE2	2:B:49:VAL:HG13	1.65	0.77
2:H:7:ILE:CG2	2:H:93[A]:VAL:HG11	2.16	0.76
2:B:9:VAL:HG21	2:B:93[A]:VAL:HG13	1.69	0.74
1:D:72:GLN:OE1	1:D:75:ARG:NH1	2.21	0.73
1:J:44:ARG:NH1	1:J:46:GLU:OE2	2.22	0.72
2:B:9:VAL:CG2	2:B:93[A]:VAL:HG13	2.19	0.71
1:G:142:ILE:H	1:G:142:ILE:HD12	1.56	0.71
2:E:7:ILE:HG21	2:E:93[A]:VAL:HG11	1.73	0.69
2:K:29:GLN:NE2	2:K:59:ASP:OD2	2.26	0.69
1:J:230:LEU:C	1:J:230:LEU:HD12	2.18	0.68
1:G:187:ALA:CB	1:G:272:LEU:HD11	2.23	0.68
1:D:193:PRO:HA	1:D:199:VAL:HG12	1.76	0.67
1:D:98[A]:MET:HE1	4:D:462:HOH:O	1.96	0.66
1:G:195:SER:O	1:G:196:LYS:C	2.38	0.66
1:D:6:ARG:HE	1:D:98[A]:MET:HE3	1.58	0.66
1:G:194:ARG:O	1:G:195:SER:C	2.38	0.65
2:B:9:VAL:HG23	2:B:93[A]:VAL:CG1	2.27	0.65
2:B:7:ILE:HG22	2:B:93[A]:VAL:HG11	1.78	0.64
2:E:33:PRO:HB2	2:E:54[A]:MET:HE1	1.79	0.64
1:D:230:LEU:C	1:D:230:LEU:HD12	2.22	0.64
1:D:199:VAL:HG13	1:D:251:LEU:HG	1.79	0.63
2:E:7:ILE:HG22	2:E:93[A]:VAL:HG11	1.80	0.63
1:A:44[B]:ARG:HH11	1:A:44[B]:ARG:HG3	1.62	0.62
2:B:39[A]:MET:CE	2:B:49:VAL:HG13	2.29	0.62
2:B:39[A]:MET:HE2	2:B:49:VAL:CG1	2.29	0.62
1:D:185:PRO:HD2	1:D:266:LEU:HD13	1.81	0.61
1:G:234:ARG:HD3	2:H:10:TYR:CE2	2.36	0.61
1:G:58:GLU:O	1:G:62:ARG:HG2	2.02	0.60
2:B:9:VAL:HG23	2:B:93[A]:VAL:HG11	1.83	0.60
1:G:155:HIS:HB3	3:I:6:PHE:CZ	2.36	0.60
1:J:42:ASN:HD22	1:J:44:ARG:HH21	1.48	0.60
1:A:230:LEU:HD12	1:A:230:LEU:C	2.27	0.60
1:G:230:LEU:C	1:G:230:LEU:HD12	2.27	0.59
1:G:32:GLU:OE2	1:G:48:ARG:HD2	2.01	0.59
2:H:77[A]:THR:HG23	4:H:298:HOH:O	2.03	0.59
2:B:7:ILE:CG2	2:B:93[A]:VAL:HG11	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:TRP:CZ2	2:B:99:MET:HE2	2.36	0.59
1:J:224:LEU:HD23	1:J:247:VAL:HG21	1.85	0.59
2:B:9:VAL:CG2	2:B:93[A]:VAL:CG1	2.81	0.58
1:D:230:LEU:HD12	1:D:230:LEU:O	2.04	0.58
2:H:39:MET:HE3	2:H:49:VAL:HG22	1.85	0.58
1:J:202:ARG:HD2	1:J:244:TRP:CD2	2.39	0.58
2:K:39[A]:MET:CE	2:K:68:THR:HB	2.34	0.57
1:G:142:ILE:H	1:G:142:ILE:CD1	2.17	0.57
1:G:142:ILE:HD12	1:G:142:ILE:N	2.19	0.56
2:E:38:GLN:HE21	2:E:40:LEU:HD21	1.70	0.56
1:D:234:ARG:HD3	2:E:10:TYR:CE2	2.40	0.56
1:G:142:ILE:HD13	4:G:589:HOH:O	2.05	0.56
1:J:249:VAL:HG22	1:J:257:TYR:CZ	2.41	0.55
2:B:7:ILE:HD12	2:B:91:LYS:HD3	1.87	0.55
2:E:4[A]:THR:HG22	2:E:86:SER:HB2	1.89	0.55
1:G:63:GLU:OE2	3:I:1:LYS:HG3	2.06	0.55
2:E:99:MET:HA	2:E:99:MET:HE2	1.89	0.54
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.43	0.54
2:H:39:MET:HE1	2:H:68:THR:HB	1.90	0.54
1:D:52:MET:CE	1:D:55:GLU:HG3	2.38	0.54
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.43	0.54
2:E:7:ILE:HG21	2:E:93[A]:VAL:CG1	2.38	0.53
2:H:39:MET:CE	2:H:49:VAL:HG22	2.39	0.53
1:J:111:ARG:HD3	1:J:113:TYR:CZ	2.42	0.53
1:J:115:GLN:NE2	4:J:629:HOH:O	2.40	0.53
1:J:202:ARG:NH2	4:J:558:HOH:O	2.42	0.53
2:K:39[A]:MET:HE1	2:K:67:HIS:C	2.34	0.53
1:A:244:TRP:CH2	2:B:99:MET:HE2	2.44	0.53
1:D:5:MET:HB2	1:D:168:LEU:HD13	1.91	0.52
1:D:198:GLU:N	1:D:251:LEU:HD12	2.25	0.52
1:A:115:GLN:NE2	4:B:659:HOH:O	2.41	0.52
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.44	0.52
2:H:39:MET:CE	2:H:68:THR:HB	2.40	0.52
1:J:234:ARG:HD3	2:K:10:TYR:CE2	2.44	0.52
2:E:4[A]:THR:HG21	4:E:757:HOH:O	2.10	0.52
2:H:39:MET:HE1	2:H:67:HIS:C	2.35	0.52
1:G:202:ARG:HD3	1:G:244:TRP:CE3	2.46	0.51
1:D:6:ARG:NE	1:D:98[A]:MET:HE3	2.26	0.51
1:D:119:GLU:HB3	2:E:1:ILE:HD11	1.92	0.51
1:G:219:LEU:HD13	1:G:257:TYR:CE1	2.45	0.51
1:D:249:VAL:HG22	1:D:257:TYR:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:GLU:O	1:G:62:ARG:CG	2.60	0.50
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.47	0.50
2:E:50:GLU:HB2	2:E:67:HIS:CE1	2.46	0.50
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.47	0.50
2:B:39[A]:MET:HE1	2:B:67:HIS:C	2.37	0.50
2:B:93[A]:VAL:HG13	2:B:93[A]:VAL:O	2.11	0.50
1:G:195:SER:O	1:G:196:LYS:O	2.30	0.49
1:D:48:ARG:NH1	2:E:53:ASP:OD2	2.44	0.49
1:D:66:LYS:HZ2	3:F:1:LYS:HZ2	1.61	0.49
2:E:1:ILE:HG23	2:E:2:GLN:N	2.27	0.49
1:G:197:GLY:O	1:G:198:GLU:HG3	2.12	0.49
1:D:234:ARG:HD2	1:D:242:GLN:HB2	1.95	0.49
1:J:78:LEU:HD13	1:J:95:LEU:HB2	1.93	0.49
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.48	0.49
1:D:52:MET:HE1	1:D:55:GLU:HG3	1.95	0.48
2:H:9:VAL:HG21	2:H:93[A]:VAL:HG13	1.94	0.48
1:J:175:GLY:O	1:J:176:ASN:C	2.55	0.48
2:B:33:PRO:O	2:B:54:MET:HE1	2.13	0.48
2:K:39[A]:MET:HE1	2:K:68:THR:HB	1.95	0.48
1:A:249:VAL:HG13	1:A:257:TYR:CE2	2.48	0.48
1:D:219:LEU:HD13	1:D:257:TYR:CZ	2.49	0.48
1:A:44[B]:ARG:NH1	1:A:44[B]:ARG:HG3	2.24	0.48
1:A:263:HIS:HB3	1:A:266:LEU:HD22	1.96	0.48
1:G:249:VAL:HG22	1:G:257:TYR:CZ	2.49	0.48
2:E:29:GLN:HA	2:E:61:SER:HB2	1.96	0.48
2:H:4:THR:HG21	4:H:371:HOH:O	2.14	0.48
1:A:230:LEU:C	1:A:230:LEU:CD1	2.87	0.47
1:J:45:TYR:CE2	1:J:67:ALA:HB2	2.50	0.47
1:G:197:GLY:O	1:G:198:GLU:CG	2.62	0.47
1:A:234:ARG:HD2	1:A:242:GLN:HB2	1.96	0.47
1:G:249:VAL:HG13	1:G:257:TYR:CE2	2.49	0.47
1:D:251:LEU:HD11	4:D:928:HOH:O	2.16	0.46
2:H:7:ILE:HG22	2:H:93[A]:VAL:HG11	1.95	0.46
1:J:32:GLU:OE2	1:J:48:ARG:HD2	2.15	0.46
1:G:251:LEU:HD23	1:G:252:GLY:N	2.31	0.46
1:J:251:LEU:HD23	1:J:252:GLY:N	2.30	0.46
1:G:234:ARG:HD2	1:G:242:GLN:HB2	1.98	0.46
1:G:249:VAL:HG11	1:G:254:GLU:HA	1.98	0.46
1:D:33:PHE:CD2	1:D:34:VAL:HG13	2.51	0.45
2:K:38:GLN:HE22	2:K:81:ARG:NH2	2.13	0.45
1:J:249:VAL:HG13	1:J:257:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7:ILE:HD12	2:H:91:LYS:HD3	1.98	0.45
1:D:66:LYS:NZ	3:F:1:LYS:NZ	2.65	0.45
2:H:93[A]:VAL:HG13	2:H:93[A]:VAL:O	2.15	0.45
1:D:198:GLU:N	1:D:251:LEU:CD1	2.80	0.45
1:J:141:GLN:OE1	1:J:144[A]:ARG:NH1	2.50	0.45
2:B:3:LYS:HE3	4:B:120:HOH:O	2.16	0.45
1:D:98[A]:MET:HE2	1:D:115:GLN:HE21	1.82	0.45
2:E:54[A]:MET:HE2	2:E:54[A]:MET:HB3	1.73	0.45
2:H:3:LYS:HE3	4:H:161:HOH:O	2.17	0.44
1:J:230:LEU:C	1:J:230:LEU:CD1	2.90	0.44
1:G:185:PRO:HD2	1:G:266:LEU:HD13	2.00	0.44
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.52	0.44
1:G:63:GLU:OE2	1:G:66:LYS:HE2	2.17	0.44
1:J:9:GLU:OE1	1:J:22:TYR:OH	2.33	0.44
1:A:218:GLN:NE2	1:A:260:ARG:HE	2.15	0.44
1:D:230:LEU:C	1:D:230:LEU:CD1	2.90	0.44
1:G:32:GLU:OE2	1:G:35:ARG:HD2	2.18	0.43
1:G:106:ASP:O	1:G:107:TRP:HB2	2.17	0.43
1:D:10:THR:HG22	1:D:12:VAL:HG23	2.00	0.43
1:D:56:GLY:O	1:D:58:GLU:N	2.51	0.43
1:D:119:GLU:CB	2:E:1:ILE:HD11	2.48	0.43
1:J:185:PRO:HD2	1:J:266:LEU:HD13	2.00	0.43
1:G:230:LEU:C	1:G:230:LEU:CD1	2.91	0.43
1:A:234:ARG:HD3	2:B:10:TYR:CD2	2.54	0.43
2:E:1:ILE:CG2	2:E:2:GLN:N	2.82	0.43
1:A:94[B]:THR:HG22	1:A:119:GLU:HA	2.00	0.43
1:A:45:TYR:CE2	1:A:67:ALA:HB2	2.54	0.42
1:A:155:HIS:HB3	3:C:6:PHE:CZ	2.54	0.42
1:J:155:HIS:HB3	3:L:6:PHE:CZ	2.55	0.42
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.54	0.42
1:D:12:VAL:HG22	1:D:94[A]:THR:HG23	2.01	0.42
1:D:66:LYS:HZ2	3:F:1:LYS:NZ	2.17	0.42
1:J:99:SER:HB3	1:J:114:LEU:HD23	2.02	0.42
1:D:249:VAL:HG22	1:D:257:TYR:CE2	2.54	0.42
1:J:163:GLU:HG3	4:J:465:HOH:O	2.19	0.42
1:A:185:PRO:HD2	1:A:266:LEU:HD13	2.01	0.42
1:D:219:LEU:HD13	1:D:257:TYR:CE1	2.54	0.42
1:J:79:ARG:NH2	4:J:737:HOH:O	2.53	0.42
1:A:231:VAL:HG13	1:A:244:TRP:CZ2	2.54	0.41
1:A:94[B]:THR:HG23	4:A:339:HOH:O	2.20	0.41
1:D:202:ARG:HD3	1:D:244:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:40:LEU:HD23	2:E:45:LYS:HA	2.02	0.41
1:A:218:GLN:HE22	1:A:260:ARG:HE	1.66	0.41
4:D:360:HOH:O	3:F:2:ALA:HB1	2.20	0.41
1:J:81:LEU:HD13	1:J:118:TYR:CD1	2.56	0.41
1:J:234:ARG:HD3	2:K:10:TYR:CZ	2.55	0.41
1:D:45:TYR:CE2	1:D:67:ALA:HB2	2.55	0.41
2:B:29:GLN:NE2	2:B:59:ASP:OD2	2.54	0.41
1:J:42:ASN:HD22	1:J:44:ARG:NH2	2.18	0.41
1:A:44[B]:ARG:NH1	1:A:64:THR:HG21	2.35	0.41
1:D:234:ARG:HD2	1:D:242:GLN:OE1	2.21	0.41
1:J:191:HIS:CE1	1:J:199:VAL:HG21	2.56	0.41
2:H:7:ILE:HG21	2:H:93[A]:VAL:CG1	2.40	0.40
2:E:54[B]:MET:O	2:E:54[B]:MET:HG3	2.20	0.40
1:A:44[B]:ARG:NH1	4:A:443:HOH:O	2.55	0.40
1:D:218:GLN:OE1	1:D:260:ARG:NE	2.55	0.40
2:H:50:GLU:HB2	2:H:67:HIS:CE1	2.56	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	262/276 (95%)	258 (98%)	4 (2%)	0	100	100
1	D	258/276 (94%)	254 (98%)	3 (1%)	1 (0%)	30	27
1	G	267/276 (97%)	262 (98%)	3 (1%)	2 (1%)	18	14
1	J	262/276 (95%)	258 (98%)	4 (2%)	0	100	100
2	B	102/99 (103%)	101 (99%)	1 (1%)	0	100	100
2	E	102/99 (103%)	100 (98%)	2 (2%)	0	100	100
2	H	101/99 (102%)	101 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	99/99 (100%)	98 (99%)	1 (1%)	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	1481/1536 (96%)	1456 (98%)	22 (2%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	195	SER
1	G	196	LYS
1	D	57	PRO

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	232/234 (99%)	219 (94%)	13 (6%)	19	16
1	D	227/234 (97%)	217 (96%)	10 (4%)	25	24
1	G	232/234 (99%)	217 (94%)	15 (6%)	15	12
1	J	229/234 (98%)	216 (94%)	13 (6%)	18	15
2	B	99/94 (105%)	96 (97%)	3 (3%)	36	38
2	E	99/94 (105%)	97 (98%)	2 (2%)	48	54
2	H	98/94 (104%)	92 (94%)	6 (6%)	17	14
2	K	96/94 (102%)	94 (98%)	2 (2%)	47	52
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
3	I	7/7 (100%)	5 (71%)	2 (29%)	0	0
3	L	7/7 (100%)	6 (86%)	1 (14%)	3	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1340/1340 (100%)	1273 (95%)	67 (5%)	21	20

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	78	LEU
1	A	114	LEU
1	A	115	GLN
1	A	166	GLU
1	A	222	GLU
1	A	230	LEU
1	A	234	ARG
1	A	249	VAL
1	A	251	LEU
1	A	266	LEU
1	A	272	LEU
1	A	273	ARG
2	B	1	ILE
2	B	29	GLN
2	B	75	THR
1	D	53	GLU
1	D	78	LEU
1	D	114	LEU
1	D	149	GLN
1	D	166	GLU
1	D	249	VAL
1	D	254	GLU
1	D	261	VAL
1	D	266	LEU
1	D	273	ARG
2	E	1	ILE
2	E	50	GLU
1	G	17	LEU
1	G	62	ARG
1	G	78	LEU
1	G	82	LEU
1	G	110	LEU
1	G	114	LEU
1	G	142	ILE
1	G	149	GLN
1	G	166	GLU

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Mol	Chain	Res	Type
1	G	195	SER
1	G	227	ASP
1	G	234	ARG
1	G	254	GLU
1	G	266	LEU
1	G	272	LEU
2	H	1	ILE
2	H	4	THR
2	H	19	LYS
2	H	50	GLU
2	H	64	ILE
2	H	99	MET
3	I	1	LYS
3	I	4	SER
1	J	19	GLU
1	J	31	LYS
1	J	62	ARG
1	J	78	LEU
1	J	82	LEU
1	J	114	LEU
1	J	115	GLN
1	J	149	GLN
1	J	194	ARG
1	J	234	ARG
1	J	254	GLU
1	J	266	LEU
1	J	273	ARG
2	K	1	ILE
2	K	75	THR
3	L	1	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	97	GLN
1	A	176	ASN
1	A	191	HIS
1	A	192	HIS
1	A	218	GLN
1	A	255	GLN
2	B	2	GLN

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Mol	Chain	Res	Type
2	B	13	HIS
2	B	29	GLN
2	B	34	HIS
2	B	38	GLN
3	C	5	ASN
1	D	42	ASN
1	D	54	GLN
1	D	97	GLN
1	D	115	GLN
1	D	149	GLN
1	D	191	HIS
1	D	255	GLN
1	D	256	ASN
2	E	13	HIS
2	E	29	GLN
2	E	34	HIS
2	E	38	GLN
2	E	67	HIS
3	F	5	ASN
1	G	54	GLN
1	G	97	GLN
1	G	149	GLN
1	G	176	ASN
1	G	191	HIS
1	G	255	GLN
1	G	256	ASN
2	H	13	HIS
2	H	29	GLN
2	H	38	GLN
3	I	5	ASN
1	J	42	ASN
1	J	54	GLN
1	J	97	GLN
1	J	149	GLN
1	J	191	HIS
1	J	192	HIS
1	J	255	GLN
1	J	256	ASN
2	K	13	HIS
2	K	38	GLN
2	K	67	HIS
3	L	5	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

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	264/276 (95%)	1.05	58 (21%) 2 2	12, 37, 66, 83	8 (3%)
1	D	262/276 (94%)	1.21	68 (25%) 1 1	12, 39, 66, 78	4 (1%)
1	G	270/276 (97%)	1.16	57 (21%) 2 2	9, 38, 70, 85	3 (1%)
1	J	267/276 (96%)	1.03	52 (19%) 3 3	11, 38, 68, 84	3 (1%)
2	B	99/99 (100%)	0.74	11 (11%) 10 9	15, 33, 44, 50	5 (5%)
2	E	99/99 (100%)	0.53	9 (9%) 15 13	13, 32, 43, 48	5 (5%)
2	H	99/99 (100%)	0.70	9 (9%) 15 13	14, 33, 45, 50	4 (4%)
2	K	99/99 (100%)	0.88	11 (11%) 10 9	17, 36, 47, 50	2 (2%)
3	C	9/9 (100%)	-0.11	0 100 100	23, 26, 30, 33	0
3	F	9/9 (100%)	0.62	1 (11%) 10 9	28, 31, 36, 42	0
3	I	9/9 (100%)	0.57	0 100 100	28, 31, 35, 39	0
3	L	9/9 (100%)	0.26	0 100 100	26, 28, 35, 40	0
All	All	1495/1536 (97%)	0.99	276 (18%) 3 3	9, 36, 65, 85	34 (2%)

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	17	LEU	6.7
1	J	224	LEU	6.2
1	D	221	GLY	6.0
1	G	195	SER	5.9
1	G	197	GLY	5.7
1	A	195	SER	5.6
1	G	62	ARG	5.2
1	A	199	VAL	5.0
1	D	272	LEU	5.0
1	J	221	GLY	4.9
1	G	227	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	221	GLY	4.8
1	J	193	PRO	4.7
1	A	251	LEU	4.5
1	D	249	VAL	4.4
1	D	56	GLY	4.4
1	G	16	GLY	4.4
1	G	193	PRO	4.4
1	D	250	PRO	4.3
1	G	258	THR	4.3
1	A	249	VAL	4.3
1	G	224	LEU	4.3
1	D	258	THR	4.3
1	A	19	GLU	4.2
1	A	252	GLY	4.1
1	G	196	LYS	4.0
1	A	274	TRP	4.0
1	G	274	TRP	4.0
2	E	48	LYS	4.0
1	D	219	LEU	4.0
1	J	16	GLY	4.0
1	J	272	LEU	4.0
1	G	248	VAL	4.0
1	D	252	GLY	4.0
1	A	201	LEU	3.9
1	G	251	LEU	3.9
1	G	199	VAL	3.9
1	D	199	VAL	3.9
1	D	181	ARG	3.9
1	D	276	PRO	3.9
1	A	258	THR	3.8
1	A	248	VAL	3.8
1	J	276	PRO	3.8
1	G	220	ASN	3.8
1	G	222	GLU	3.8
1	D	170[A]	ARG	3.8
1	G	42	ASN	3.7
1	A	176	ASN	3.7
2	H	1	ILE	3.7
2	K	1	ILE	3.7
1	D	274	TRP	3.7
1	G	272	LEU	3.7
1	A	16	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	175	GLY	3.7
1	G	221	GLY	3.7
1	D	251	LEU	3.6
1	D	61	GLU	3.6
1	A	17	LEU	3.6
1	D	16	GLY	3.6
1	D	90	GLY	3.6
2	B	48	LYS	3.6
1	G	276	PRO	3.6
1	J	222	GLU	3.5
1	A	42	ASN	3.5
1	G	250	PRO	3.5
1	J	230	LEU	3.5
1	D	57	PRO	3.5
1	J	176	ASN	3.5
1	D	50	PRO	3.4
1	A	250	PRO	3.4
1	D	195	SER	3.4
1	J	273	ARG	3.4
1	G	223	GLU	3.4
2	K	48	LYS	3.4
2	H	48	LYS	3.3
1	G	88	SER	3.3
1	D	254	GLU	3.3
1	G	176	ASN	3.3
1	J	42	ASN	3.3
2	K	54	MET	3.3
2	E	1	ILE	3.2
1	D	98[A]	MET	3.2
1	A	228	MET	3.2
1	G	256	ASN	3.2
1	J	257	TYR	3.2
1	D	88	SER	3.2
2	K	88	ALA	3.2
2	K	53	ASP	3.2
1	J	181	ARG	3.2
1	D	1	GLY	3.2
1	D	220	ASN	3.2
1	A	217	TRP	3.1
1	A	180	LEU	3.1
1	A	273	ARG	3.1
1	J	18	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	K	75	THR	3.1
1	D	30	ASN	3.1
1	A	194	ARG	3.1
1	J	196	LYS	3.1
1	A	181	ARG	3.1
1	D	17	LEU	3.1
1	A	193	PRO	3.0
1	D	259	CYS	3.0
1	A	200	THR	3.0
1	A	245	ALA	3.0
1	A	14	ARG	3.0
1	D	60	TRP	3.0
1	A	255	GLN	3.0
1	J	197	GLY	2.9
1	A	267	PRO	2.9
1	D	53	GLU	2.9
1	G	249	VAL	2.9
1	A	18	GLU	2.9
1	A	41	GLU	2.9
1	D	257	TYR	2.9
1	D	49	ALA	2.9
1	G	219	LEU	2.9
1	A	44[A]	ARG	2.9
2	B	75	THR	2.9
1	J	41	GLU	2.9
1	G	253	LYS	2.9
1	A	56	GLY	2.9
1	D	2	PRO	2.8
1	G	17	LEU	2.8
1	A	254	GLU	2.8
2	B	47	PRO	2.8
1	D	174	ASN	2.8
1	D	218	GLN	2.8
1	D	194	ARG	2.8
2	B	34	HIS	2.8
1	A	257	TYR	2.8
1	A	272	LEU	2.8
1	J	217	TRP	2.7
1	D	79	ARG	2.7
1	A	182	THR	2.7
2	B	83[A]	LYS	2.7
1	G	182	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	275	GLU	2.7
2	E	54[A]	MET	2.7
2	K	36	GLU	2.7
1	G	191	HIS	2.7
1	D	248	VAL	2.7
1	J	271	THR	2.6
1	G	252	GLY	2.6
2	K	74	GLU	2.6
2	H	54[A]	MET	2.6
1	J	79	ARG	2.6
1	A	175	GLY	2.6
1	D	42	ASN	2.6
1	A	266	LEU	2.6
1	G	255	GLN	2.6
1	J	248	VAL	2.6
1	J	249	VAL	2.6
1	G	186	LYS	2.6
1	D	48	ARG	2.6
1	J	274	TRP	2.6
1	G	54	GLN	2.5
2	E	50	GLU	2.5
1	G	79[A]	ARG	2.5
1	J	105	SER	2.5
1	D	54	GLN	2.5
1	D	52	MET	2.5
2	B	93[A]	VAL	2.5
1	A	186	LYS	2.5
1	A	40	ALA	2.5
1	D	46	GLU	2.5
1	J	144[A]	ARG	2.5
1	G	257	TYR	2.5
1	J	29	ASP	2.5
1	J	19	GLU	2.5
1	J	258	THR	2.5
1	J	270	LEU	2.5
1	J	254	GLU	2.4
2	H	47	PRO	2.4
1	J	44	ARG	2.4
1	J	218	GLN	2.4
1	A	247	VAL	2.4
1	D	51	TRP	2.4
1	D	184	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	246	SER	2.4
1	G	184	SER	2.4
1	A	192	HIS	2.4
1	J	58	GLU	2.4
2	H	49	VAL	2.4
1	A	15	PRO	2.4
1	A	269	PRO	2.4
1	J	50	PRO	2.4
1	J	30	ASN	2.4
1	D	273	ARG	2.4
1	J	199	VAL	2.4
1	A	203	CYS	2.4
1	D	193	PRO	2.4
1	J	250	PRO	2.4
2	K	47	PRO	2.4
1	A	198	GLU	2.3
1	A	54	GLN	2.3
1	G	207	GLY	2.3
1	D	31	LYS	2.3
2	H	46	ILE	2.3
1	A	216	THR	2.3
1	D	58	GLU	2.3
1	D	267	PRO	2.3
1	A	259	CYS	2.3
2	H	44	LYS	2.3
2	B	1	ILE	2.3
1	G	41	GLU	2.3
1	G	39	ASP	2.3
1	G	31	LYS	2.3
1	G	267	PRO	2.3
1	J	194	ARG	2.3
1	D	39	ASP	2.3
1	G	166	GLU	2.2
1	J	198	GLU	2.2
1	D	65	GLN	2.2
1	G	259	CYS	2.2
1	J	259	CYS	2.2
2	B	2	GLN	2.2
1	D	253	LYS	2.2
1	J	15	PRO	2.2
2	B	85	ASP	2.2
1	J	175	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	232	GLU	2.2
1	A	191	HIS	2.2
1	J	149	GLN	2.2
1	J	255	GLN	2.2
1	J	223	GLU	2.2
1	A	187	ALA	2.2
1	D	203	CYS	2.2
1	A	88	SER	2.2
1	A	183	ASP	2.2
1	D	43	PRO	2.1
1	D	55	GLU	2.1
1	J	163	GLU	2.1
2	K	49	VAL	2.1
1	J	54	GLN	2.1
2	E	3	LYS	2.1
2	E	87[A]	MET	2.1
1	A	229	GLU	2.1
1	G	254	GLU	2.1
2	E	47	PRO	2.1
1	A	149	GLN	2.1
1	D	247	VAL	2.1
1	D	260	ARG	2.1
1	G	230	LEU	2.1
1	G	266	LEU	2.1
1	J	266	LEU	2.1
2	B	19	LYS	2.1
2	K	83	LYS	2.1
2	E	85	ASP	2.1
1	D	271	THR	2.1
2	H	34	HIS	2.1
1	G	56	GLY	2.1
1	G	189	VAL	2.1
1	G	158	ALA	2.1
1	G	228	MET	2.1
1	G	212	ASP	2.1
1	D	14	ARG	2.1
1	D	191	HIS	2.1
1	J	267	PRO	2.1
2	H	45	LYS	2.1
3	F	6	PHE	2.1
1	A	222	GLU	2.0
2	B	69	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	266	LEU	2.0
1	D	256	ASN	2.0
1	G	181	ARG	2.0
2	E	81	ARG	2.0
1	A	253	LYS	2.0
1	D	173	LYS	2.0
1	G	265	GLY	2.0
1	D	163	GLU	2.0
1	G	275	GLU	2.0
1	J	46	GLU	2.0
1	J	88	SER	2.0
1	G	40	ALA	2.0
1	D	255	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 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.