Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:21 PM GMT

PDB ID	:	3QUL
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

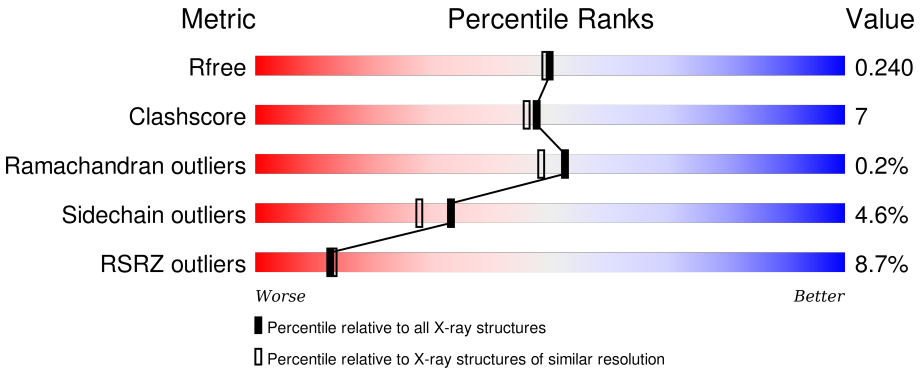
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	9% 69% 7% • 22%
1	D	338	10% 64% 13% 22%
1	G	338	12% 68% 9% • • 20%
1	J	338	6% 65% 12% • 21%
2	B	99	2% 83% 16% •

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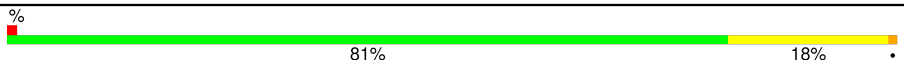
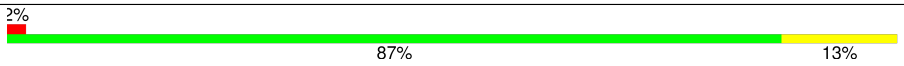
Mol	Chain	Length	Quality of chain
2	E	99	
2	H	99	
2	K	99	
3	C	9	
3	F	9	
3	I	9	
3	L	9	

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			

- Molecule 3 is a protein called Glycoprotein G1.

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.

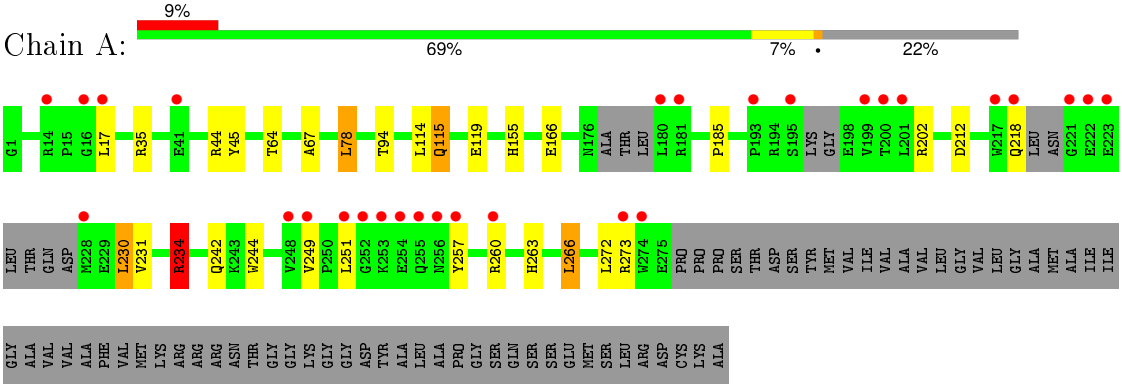
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	154	Total O 154 154	0	0
4	B	94	Total O 94 94	0	0
4	C	7	Total O 7 7	0	0
4	D	130	Total O 130 130	0	0
4	E	82	Total O 82 82	0	0
4	F	4	Total O 4 4	0	0
4	G	130	Total O 130 130	0	0
4	H	86	Total O 86 86	0	0
4	I	5	Total O 5 5	0	0
4	J	133	Total O 133 133	0	0
4	K	83	Total O 83 83	0	0
4	L	7	Total O 7 7	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

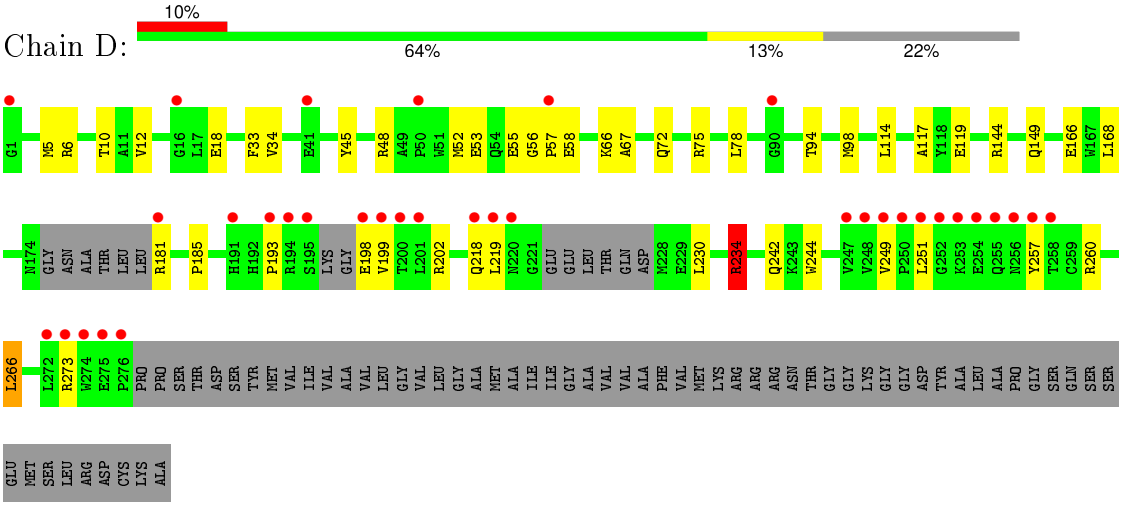
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

Chain A:



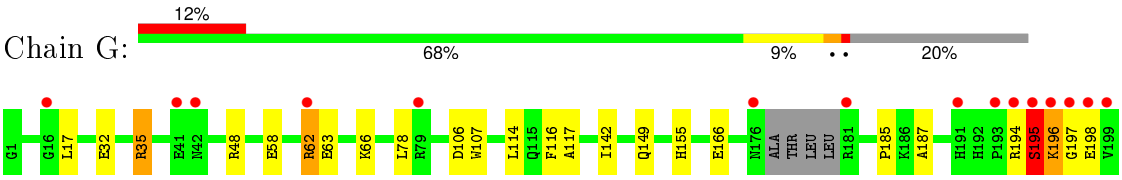
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

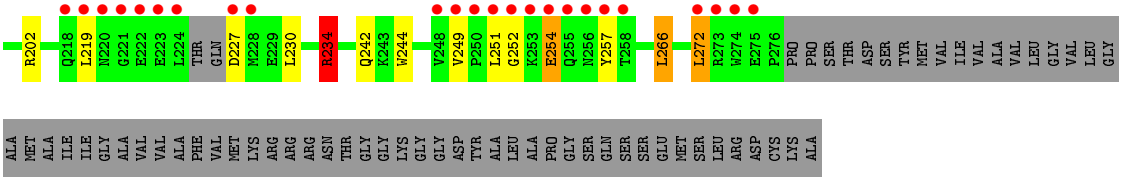
Chain D:



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

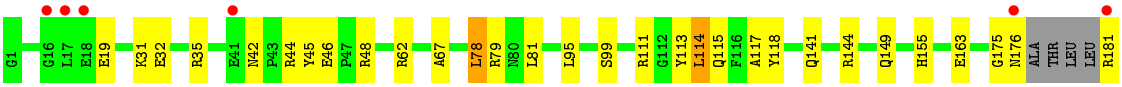
Chain G:

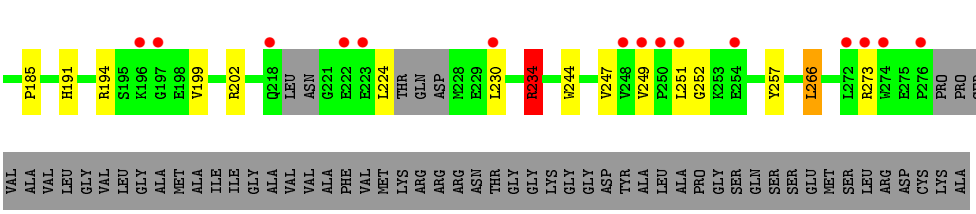




• Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

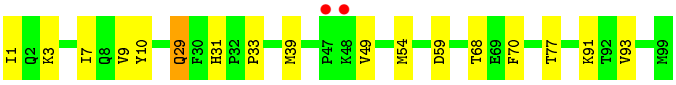
Chain J:





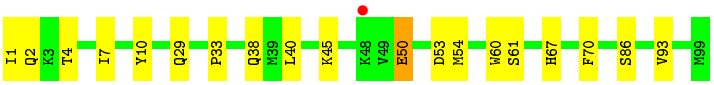
• Molecule 2: Beta-2-microglobulin

Chain B:



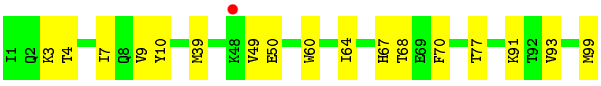
• Molecule 2: Beta-2-microglobulin

Chain E:



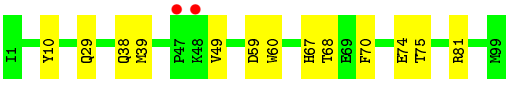
• Molecule 2: Beta-2-microglobulin

Chain H:



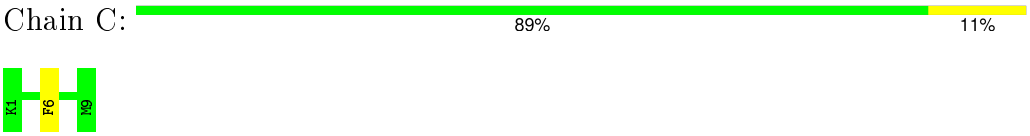
• Molecule 2: Beta-2-microglobulin

Chain K:



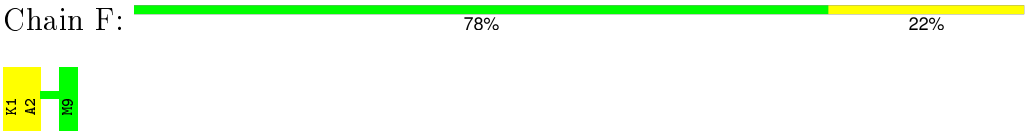
• Molecule 3: Glycoprotein G1

Chain C:



- Molecule 3: Glycoprotein G1

Chain F:

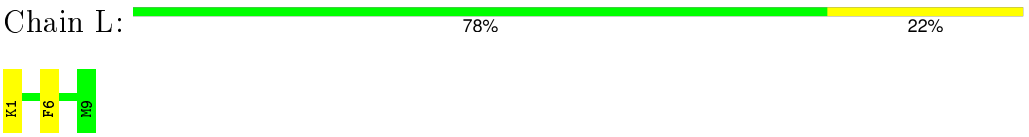


- Molecule 3: Glycoprotein G1

Chain I:

- Molecule 3: Glycoprotein G1

Chain L:



4 Data and refinement statistics (i)

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 51.76 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (51.78-2.00) 98.9 (51.76-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [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 (5.29%)	DCC
Wilson B-factor (Å^2)	28.1	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 58.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 142795 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.46	0/2308	0.67	5/3124 (0.2%)
1	D	0.46	0/2257	0.67	2/3060 (0.1%)
1	G	0.47	0/2316	0.66	4/3139 (0.1%)
1	J	0.47	0/2289	0.66	4/3101 (0.1%)
2	B	0.48	0/885	0.63	0/1200
2	E	0.50	0/885	0.65	0/1200
2	H	0.51	0/880	0.65	0/1192
2	K	0.49	0/862	0.63	0/1169
3	C	0.63	0/67	0.74	0/87
3	F	0.62	0/67	0.59	0/87
3	I	0.74	0/67	0.79	0/87
3	L	0.63	0/67	0.72	0/87
All	All	0.48	0/12950	0.66	15/17533 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	G	234	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	D	234	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	A	234	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	D	234	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	G	234	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	J	234	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	J	234	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	J	35	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	G	35	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	35	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	35	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	G	35	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	78	LEU	CA-CB-CG	5.22	127.30	115.30
1	J	35	ARG	NE-CZ-NH1	5.14	122.87	120.30

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	29	0
1	D	2193	0	2063	35	0
1	G	2251	0	2115	33	0
1	J	2225	0	2093	27	0
2	B	859	0	837	22	0
2	E	859	0	837	19	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	4	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	2	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	183	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 (183) 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	1.21	1.10
2:K:39[A]:MET:HE2	2:K:49:VAL:HG13	1.29	1.09
1:A:44[B]:ARG:HH11	1:A:44[B]:ARG:HG2	1.07	1.08
2:H:39:MET:HE2	2:H:49:VAL:CG1	1.94	0.97
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:NH1	1:A:44[B]:ARG:HG2	1.85	0.85
1:A:94[B]:THR:HG21	2:B:31:HIS:CE1	2.12	0.84
2:H:39:MET:CE	2:H:49:VAL:HG13	2.07	0.82
2:H:7:ILE:HG21	2:H:93[A]:VAL:HG11	1.63	0.81
1:D:6:ARG:HE	1:D:98[A]:MET:HE3	1.47	0.79
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:K:39[A]:MET:HE2	2:K:49:VAL:CG1	2.10	0.78
2:H:7:ILE:CG2	2:H:93[A]:VAL:HG11	2.16	0.76
2:E:33:PRO:HB2	2:E:54[A]:MET:HE1	1.67	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: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
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
1:J:230:LEU:HD12	1:J:230:LEU:C	2.18	0.63
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
1:G:195:SER:O	1:G:196:LYS:C	2.38	0.61
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:194:ARG:O	1:G:195:SER:C	2.38	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:J:42:ASN:HD22	1:J:44:ARG:HH21	1.48	0.60
1:G:155:HIS:HB3	3:I:6:PHE:CZ	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:77[A]:THR:HG23	4:H:298:HOH:O	2.03	0.59
1:G:32:GLU:OE2	1:G:48:ARG:HD2	2.01	0.59
2:B:7:ILE:CG2	2:B:93[A]:VAL:HG11	2.33	0.59
1:D:230:LEU:HD12	1:D:230:LEU:C	2.22	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:O	1:D:230:LEU:HD12	2.04	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:CD1	1:G:142:ILE:H	2.17	0.57
1:G:142:ILE:N	1:G:142:ILE:HD12	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:A:230:LEU:HD12	1:A:230:LEU:C	2.27	0.55
1:G:63:GLU:OE2	3:I:1:LYS:HG3	2.06	0.55
1:G:230:LEU:C	1:G:230:LEU:HD12	2.27	0.55
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.43	0.54
1:D:52:MET:CE	1:D:55:GLU:HG3	2.38	0.54
2:B:39[A]:MET:HE3	2:B:68:THR:HB	1.89	0.54
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.43	0.54
2:H:39:MET:CE	2:H:49:VAL:HG22	2.39	0.53
2:E:7:ILE:HG21	2:E:93[A]:VAL:CG1	2.38	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:H:39:MET:HE3	2:H:49:VAL:HG22	1.90	0.53
1:D:198:GLU:N	1:D:251:LEU:HD12	2.25	0.52
1:D:5:MET:HB2	1:D:168:LEU:HD13	1.91	0.52
2:H:39:MET:CE	2:H:68:THR:HB	2.40	0.52
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.44	0.52
1:J:234:ARG:HD3	2:K:10:TYR:CE2	2.44	0.52
1:A:115:GLN:NE2	4:B:659:HOH:O	2.41	0.52
2:E:4[A]:THR:HG21	4:E:757:HOH:O	2.10	0.52
1:G:202:ARG:HD3	1:G:244:TRP:CE3	2.46	0.51
1:D:119:GLU:HB3	2:E:1:ILE:HD11	1.92	0.51
2:K:39[A]:MET:HE1	2:K:68:THR:HB	1.91	0.51
1:G:219:LEU:HD13	1:G:257:TYR:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:VAL:HG22	1:D:257:TYR:CZ	2.46	0.51
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:93[A]:VAL:O	2:B:93[A]:VAL:HG13	2.11	0.50
2:B:39[A]:MET:HE2	2:B:49:VAL:HG13	1.93	0.49
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
2:B:33:PRO:O	2:B:54:MET:HE1	2.13	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:117:ALA:HB2	2:K:60:TRP:CE2	2.48	0.49
1:J:78:LEU:HD13	1:J:95:LEU:HB2	1.93	0.49
2:H:39:MET:HE1	2:H:67:HIS:C	2.34	0.48
2:H:9:VAL:HG21	2:H:93[A]:VAL:HG13	1.94	0.48
2:H:39:MET:HE1	2:H: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:G:249:VAL:HG22	1:G:257:TYR:CZ	2.49	0.48
1:A:263:HIS:HB3	1:A:266:LEU:HD22	1.96	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: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
2:H:93[A]:VAL:HG13	2:H:93[A]:VAL:O	2.15	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
2:B:39[A]:MET:HE2	2:B:49:VAL:CG1	2.45	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
2:B:39[A]:MET:HE1	2:B:49:VAL:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:249:VAL:HG13	1:J:257:TYR:CE2	2.51	0.45
1:D:66:LYS:HZ2	3:F:1:LYS:NZ	2.14	0.45
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
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:J:175:GLY:O	1:J:176:ASN:C	2.55	0.45
2:H:3:LYS:HE3	4:H:161:HOH:O	2.17	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:D:66:LYS:HZ2	3:F:1:LYS:HZ2	1.66	0.44
1:A:218:GLN:NE2	1:A:260:ARG:HE	2.15	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
2:K:39[A]:MET:HE1	2:K:67:HIS:C	2.39	0.43
1:D:119:GLU:CB	2:E:1:ILE:HD11	2.48	0.43
1:D:56:GLY:O	1:D:58:GLU:N	2.51	0.43
1:D:10:THR:HG22	1:D:12:VAL:HG23	2.00	0.43
1:J:185:PRO:HD2	1:J:266:LEU:HD13	2.00	0.43
1:A:230:LEU:C	1:A:230:LEU:CD1	2.87	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:G:66:LYS:HZ3	3:I:1:LYS:HG2	1.84	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: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:D:219:LEU:HD13	1:D:257:TYR:CE1	2.54	0.42
1:A:185:PRO:HD2	1:A:266:LEU:HD13	2.01	0.42
1:J:79:ARG:NH2	4:J:737:HOH:O	2.53	0.42
1:G:116:PHE:CD2	3:I:9:MET:HE1	2.54	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
2:E:40:LEU:HD23	2:E:45:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ARG:HD3	1:D:244:TRP:CE3	2.55	0.41
1:D:52:MET:HE3	1:D:55:GLU:HG3	2.01	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:234:ARG:HD3	2:K:10:TYR:CZ	2.55	0.41
1:J:81:LEU:HD13	1:J:118:TYR:CD1	2.56	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:D:230:LEU:CD1	1:D:230:LEU:C	2.90	0.40
1:A:44[B]:ARG:NH1	4:A:443:HOH:O	2.55	0.40
2:H:50:GLU:HB2	2:H:67:HIS:CE1	2.56	0.40
1:D:218:GLN:OE1	1:D:260:ARG:NE	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/338 (78%)	258 (98%)	4 (2%)	0	100	100
1	D	258/338 (76%)	254 (98%)	3 (1%)	1 (0%)	39	33
1	G	267/338 (79%)	262 (98%)	3 (1%)	2 (1%)	26	19
1	J	262/338 (78%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	101/99 (102%)	101 (100%)	0	0	100	100
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	1481/1784 (83%)	1456 (98%)	22 (2%)	3 (0%)	52	48

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/280 (83%)	220 (95%)	12 (5%)	29	23
1	D	227/280 (81%)	216 (95%)	11 (5%)	31	26
1	G	232/280 (83%)	220 (95%)	12 (5%)	29	23
1	J	229/280 (82%)	218 (95%)	11 (5%)	31	26
2	B	99/94 (105%)	96 (97%)	3 (3%)	48	47
2	E	99/94 (105%)	97 (98%)	2 (2%)	63	65
2	H	98/94 (104%)	95 (97%)	3 (3%)	47	46
2	K	96/94 (102%)	93 (97%)	3 (3%)	47	46
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	L	7/7 (100%)	6 (86%)	1 (14%)	4 2
All	All	1340/1524 (88%)	1280 (96%)	60 (4%)	33 29

All (60) 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	212	ASP
1	A	230	LEU
1	A	234	ARG
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	70	PHE
1	D	18	GLU
1	D	53	GLU
1	D	78	LEU
1	D	114	LEU
1	D	144	ARG
1	D	149	GLN
1	D	166	GLU
1	D	181	ARG
1	D	234	ARG
1	D	266	LEU
1	D	273	ARG
2	E	50	GLU
2	E	70	PHE
1	G	17	LEU
1	G	62	ARG
1	G	78	LEU
1	G	114	LEU
1	G	149	GLN
1	G	166	GLU
1	G	195	SER
1	G	227	ASP

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Mol	Chain	Res	Type
1	G	234	ARG
1	G	254	GLU
1	G	266	LEU
1	G	272	LEU
2	H	64	ILE
2	H	70	PHE
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	114	LEU
1	J	149	GLN
1	J	181	ARG
1	J	194	ARG
1	J	234	ARG
1	J	266	LEU
1	J	273	ARG
2	K	70	PHE
2	K	74	GLU
2	K	75	THR
3	L	1	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	97	GLN
1	A	191	HIS
1	A	218	GLN
2	B	38	GLN
2	B	67	HIS
3	C	5	ASN
1	D	97	GLN
1	D	149	GLN
1	D	191	HIS
1	D	192	HIS
1	D	256	ASN
2	E	29	GLN
2	E	38	GLN

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Mol	Chain	Res	Type
3	F	5	ASN
1	G	30	ASN
1	G	97	GLN
1	G	149	GLN
1	G	191	HIS
1	G	192	HIS
1	G	256	ASN
2	H	38	GLN
3	I	5	ASN
1	J	42	ASN
1	J	97	GLN
1	J	149	GLN
1	J	191	HIS
1	J	192	HIS
1	J	256	ASN
2	K	38	GLN
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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	264/338 (78%)	0.49	29 (10%) 7 8	21, 38, 66, 83	0
1	D	262/338 (77%)	0.58	35 (13%) 4 5	22, 39, 66, 78	0
1	G	270/338 (79%)	0.64	39 (14%) 3 4	21, 39, 70, 85	1 (0%)
1	J	267/338 (78%)	0.35	21 (7%) 15 16	21, 38, 68, 84	0
2	B	99/99 (100%)	0.02	2 (2%) 68 69	23, 34, 44, 50	0
2	E	99/99 (100%)	0.09	1 (1%) 84 84	24, 32, 43, 48	0
2	H	99/99 (100%)	0.16	1 (1%) 84 84	23, 33, 45, 50	0
2	K	99/99 (100%)	0.01	2 (2%) 68 69	24, 36, 47, 50	0
3	C	9/9 (100%)	-0.05	0 100 100	23, 26, 30, 33	0
3	F	9/9 (100%)	0.08	0 100 100	28, 31, 36, 42	0
3	I	9/9 (100%)	0.05	0 100 100	28, 31, 35, 39	0
3	L	9/9 (100%)	-0.07	0 100 100	26, 28, 35, 40	0
All	All	1495/1784 (83%)	0.39	130 (8%) 13 13	21, 37, 65, 85	1 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	197	GLY	8.6
1	J	17	LEU	7.8
1	D	219	LEU	6.6
1	G	251	LEU	6.4
1	G	220	ASN	6.2
1	A	17	LEU	6.2
1	G	196	LYS	5.8
1	G	227	ASP	5.6
1	G	195	SER	5.6
1	G	222	GLU	5.5
1	G	249	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
1	G	250	PRO	5.2
1	G	224	LEU	5.1
1	J	223	GLU	5.1
1	G	223	GLU	5.1
1	D	249	VAL	5.0
1	D	220	ASN	4.9
1	D	251	LEU	4.9
1	G	253	LYS	4.8
1	D	252	GLY	4.7
1	D	181	ARG	4.5
1	A	251	LEU	4.5
1	G	199	VAL	4.4
1	G	219	LEU	4.4
1	G	274	TRP	4.3
1	A	249	VAL	4.2
1	A	195	SER	4.2
1	D	276	PRO	4.1
1	G	258	THR	4.0
1	A	222	GLU	4.0
1	J	176	ASN	3.9
1	A	252	GLY	3.9
1	A	253	LYS	3.9
1	G	198	GLU	3.9
1	J	222	GLU	3.9
1	D	16	GLY	3.9
1	G	248	VAL	3.9
1	A	274	TRP	3.8
1	G	16	GLY	3.8
1	G	221	GLY	3.8
1	D	274	TRP	3.8
1	J	276	PRO	3.8
1	D	195	SER	3.7
1	G	256	ASN	3.6
1	G	252	GLY	3.5
1	A	248	VAL	3.5
1	D	272	LEU	3.5
1	G	176	ASN	3.4
1	D	57	PRO	3.4
1	J	16	GLY	3.4
1	D	199	VAL	3.3
1	D	250	PRO	3.3
1	A	221	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	198	GLU	3.3
1	G	257	TYR	3.3
1	A	199	VAL	3.3
1	J	273	ARG	3.2
1	J	18	GLU	3.2
1	J	274	TRP	3.2
1	G	255	GLN	3.2
1	D	218	GLN	3.1
1	D	257	TYR	3.1
1	A	223	GLU	3.1
1	A	257	TYR	3.1
1	G	194	ARG	3.1
1	J	272	LEU	3.0
1	J	230	LEU	3.0
1	D	253	LYS	3.0
1	D	254	GLU	3.0
1	G	254	GLU	3.0
1	G	181	ARG	3.0
1	A	41	GLU	3.0
1	J	251	LEU	3.0
2	H	48	LYS	2.8
1	G	193	PRO	2.8
2	B	48	LYS	2.8
1	G	272	LEU	2.8
1	D	255	GLN	2.8
1	D	273	ARG	2.8
1	D	248	VAL	2.8
1	J	196	LYS	2.8
1	G	41	GLU	2.7
1	A	181	ARG	2.7
1	J	197	GLY	2.7
1	A	254	GLU	2.7
1	A	228	MET	2.7
1	G	228	MET	2.7
1	A	201	LEU	2.7
1	A	193	PRO	2.7
1	J	181	ARG	2.6
1	J	249	VAL	2.6
1	A	218	GLN	2.6
1	A	14	ARG	2.6
1	A	260	ARG	2.6
2	K	48	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	248	VAL	2.6
1	A	217	TRP	2.5
2	E	48	LYS	2.5
1	A	180	LEU	2.5
1	G	275	GLU	2.4
1	J	41	GLU	2.4
1	G	42	ASN	2.4
1	A	200	THR	2.4
1	D	200	THR	2.4
1	G	218	GLN	2.4
1	D	258	THR	2.4
1	D	90	GLY	2.4
1	A	256	ASN	2.4
1	D	41	GLU	2.4
1	A	273	ARG	2.3
1	D	194	ARG	2.3
1	A	255	GLN	2.3
1	G	62	ARG	2.3
1	D	1	GLY	2.3
1	G	79[A]	ARG	2.2
1	D	201	LEU	2.2
1	D	50	PRO	2.2
1	D	256	ASN	2.2
1	J	254	GLU	2.2
1	D	247	VAL	2.1
2	K	47	PRO	2.1
1	A	16	GLY	2.1
1	D	275	GLU	2.1
1	G	191	HIS	2.1
1	J	250	PRO	2.1
2	B	47	PRO	2.1
1	G	273	ARG	2.0
1	J	218	GLN	2.0
1	D	193	PRO	2.0
1	D	191	HIS	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.