



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:57 AM UTC

PDB ID : 3TBT / pdb_00003tbt
Title : CRYSTAL STRUCTURE OF THE MURINE CLASS I MAJOR HISTO-COMPATIBILITY COMPLEX H-2DB IN COMPLEX WITH THE LCMV-DERIVED GP33 ALTERED PEPTIDE ligand (V3P, Y4S)
Authors : Duru, A.D.; Allerbring, E.B.; Uchtenhagen, H.; Mazumdar, P.A.; Badia-Martinez, D.; Madhurantakam, C.; Sandalova, T.; Nygren, P.; Achour, A.
Deposited on : 2011-08-08
Resolution : 2.30 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

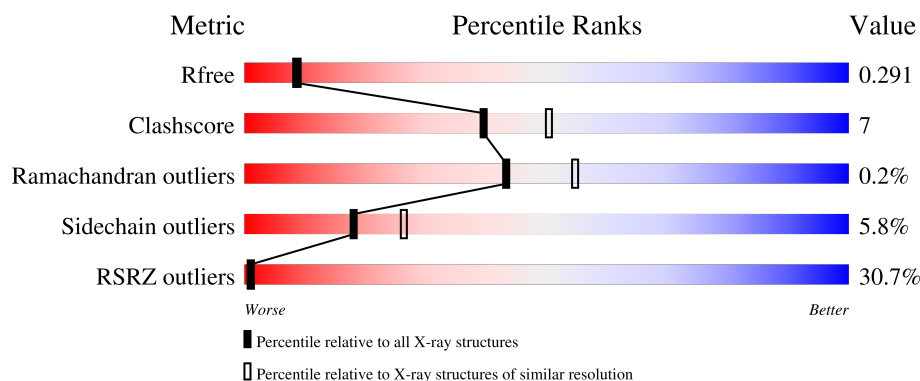
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



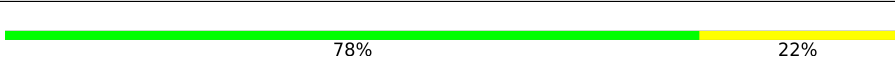
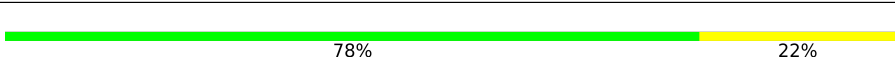
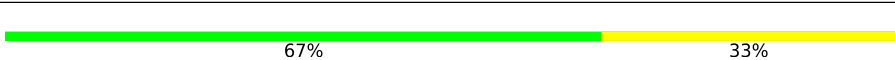
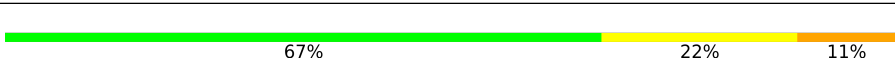
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	33% 81% 13% • 5%
1	D	276	35% 76% 16% • 5%
1	G	276	35% 78% 18% • •
1	J	276	36% 84% 11% • •
2	B	99	21% 88% 12%

Continued on next page...

Continued from previous page...

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 [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13045 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	263	Total	C	N	O	S	0	0	0
			2168	1369	384	406	9			
1	D	263	Total	C	N	O	S	0	0	0
			2170	1373	384	404	9			
1	G	269	Total	C	N	O	S	0	0	0
			2214	1399	392	414	9			
1	J	268	Total	C	N	O	S	0	0	0
			2204	1394	390	411	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
			821	524	138	152	7			
2	E	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	H	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	K	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- 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
			66	42	11	12	1			
3	F	9	Total	C	N	O	S	0	0	0
			63	39	10	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 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	PRO	VAL	engineered mutation	UNP P07399
C	4	SER	TYR	engineered mutation	UNP P07399
C	9	MET	CYS	engineered mutation	UNP P07399
F	3	PRO	VAL	engineered mutation	UNP P07399
F	4	SER	TYR	engineered mutation	UNP P07399
F	9	MET	CYS	engineered mutation	UNP P07399
I	3	PRO	VAL	engineered mutation	UNP P07399
I	4	SER	TYR	engineered mutation	UNP P07399
I	9	MET	CYS	engineered mutation	UNP P07399
L	3	PRO	VAL	engineered mutation	UNP P07399
L	4	SER	TYR	engineered mutation	UNP P07399
L	9	MET	CYS	engineered mutation	UNP P07399

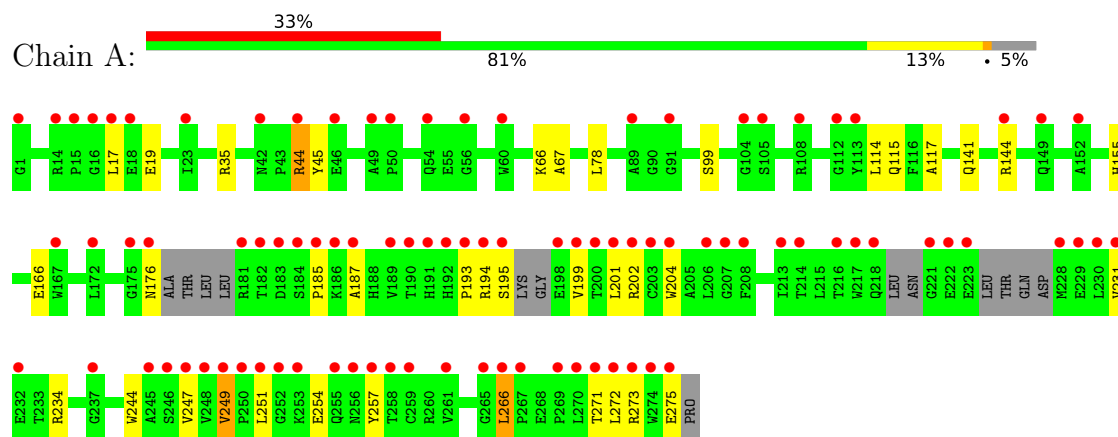
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	115	Total O 115 115	0	0
4	B	60	Total O 60 60	0	0
4	C	7	Total O 7 7	0	0
4	D	93	Total O 93 93	0	0
4	E	65	Total O 65 65	0	0
4	F	2	Total O 2 2	0	0
4	G	131	Total O 131 131	0	0
4	H	65	Total O 65 65	0	0
4	I	3	Total O 3 3	0	0
4	J	130	Total O 130 130	0	0
4	K	66	Total O 66 66	0	0
4	L	5	Total O 5 5	0	0

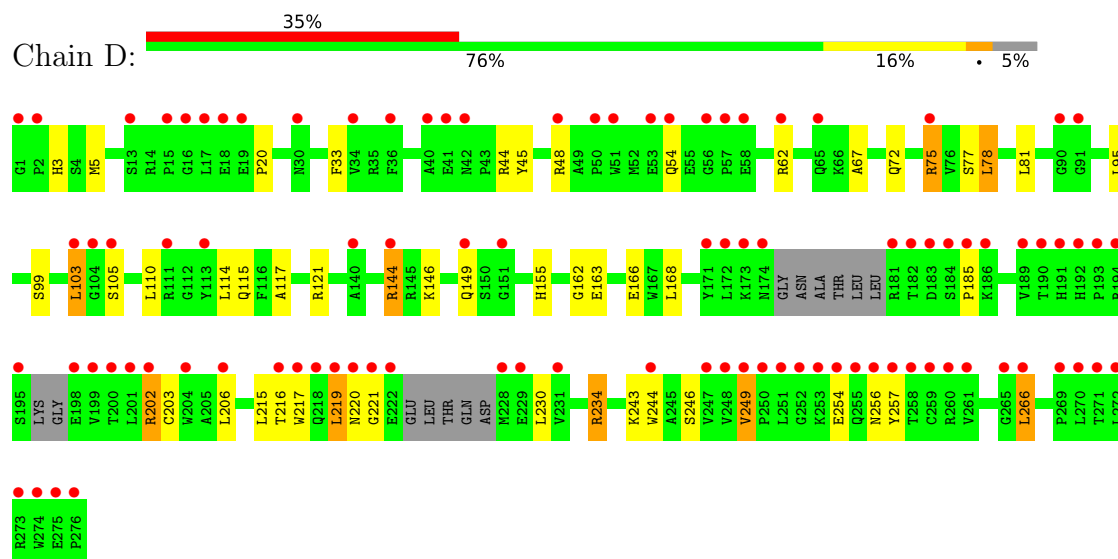
3 Residue-property plots

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.

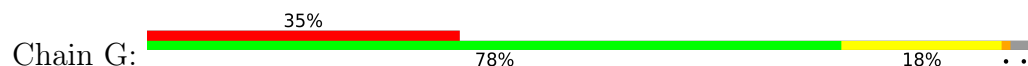
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

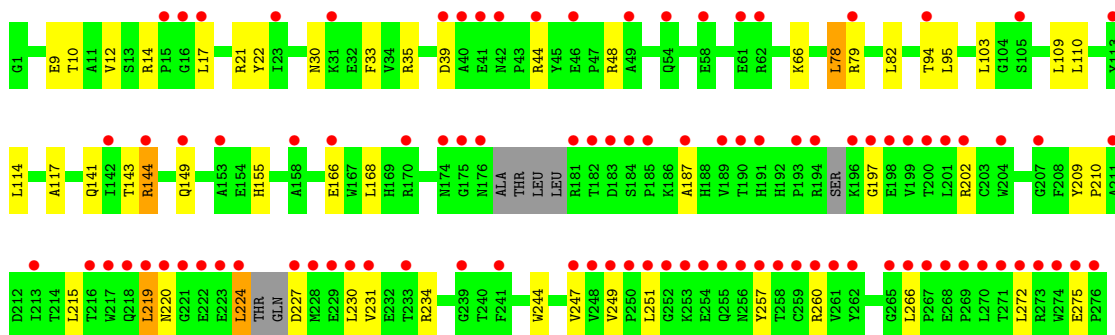


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

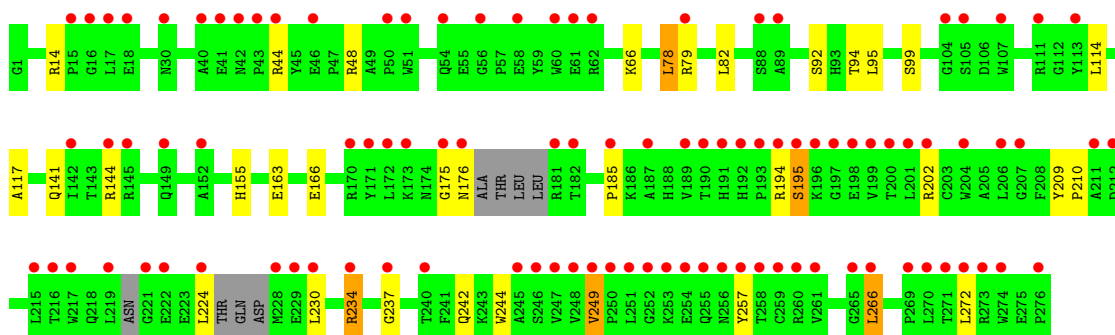
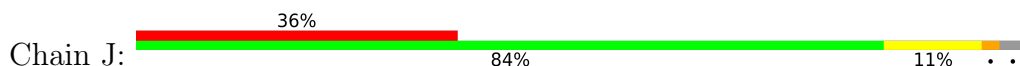


- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain

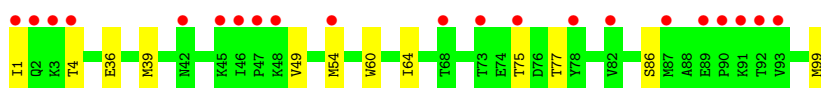
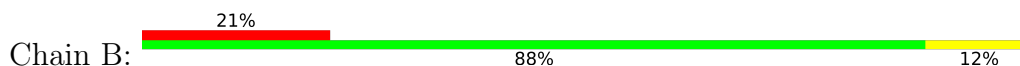




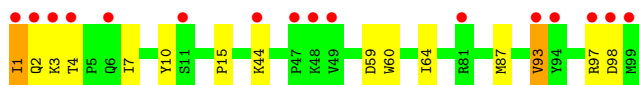
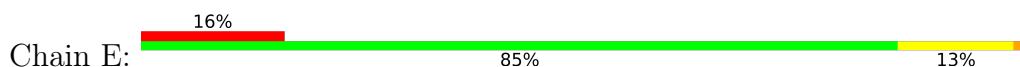
- Molecule 1: H-2 class I histocompatibility antigen, D-B alpha chain



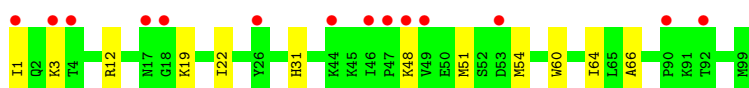
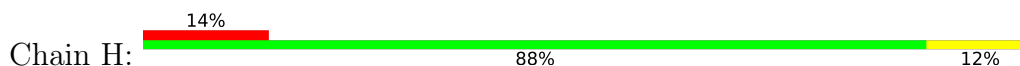
- Molecule 2: Beta-2-microglobulin



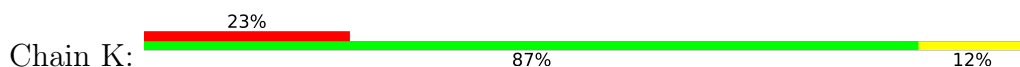
- Molecule 2: Beta-2-microglobulin

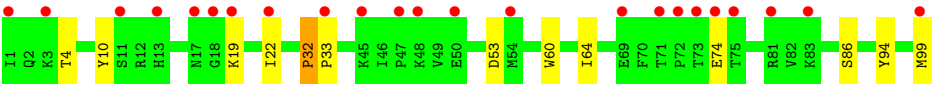


- Molecule 2: Beta-2-microglobulin

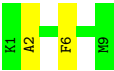
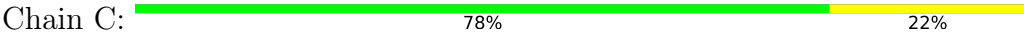


- Molecule 2: Beta-2-microglobulin

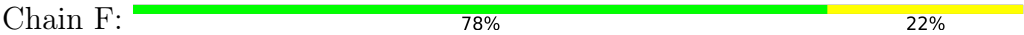




● Molecule 3: GLYCOPROTEIN G1



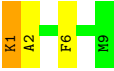
● Molecule 3: GLYCOPROTEIN G1



● Molecule 3: GLYCOPROTEIN G1



● Molecule 3: GLYCOPROTEIN G1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.67Å 123.80Å 99.59Å 90.00° 103.34° 90.00°	Depositor
Resolution (Å)	42.37 – 2.30 42.37 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.37-2.30) 99.5 (42.37-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.242 , 0.295 (Not available) , 0.291	Depositor DCC
R_{free} test set	4821 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.9	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	0.88	EDS
Total number of atoms	13045	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.89% 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	0.71	0/2230	0.80	0/3021
1	D	0.69	0/2234	0.87	3/3030 (0.1%)
1	G	0.70	0/2278	0.89	5/3088 (0.2%)
1	J	0.68	0/2268	0.76	0/3074
2	B	0.73	0/847	0.80	0/1148
2	E	0.76	0/847	0.83	0/1148
2	H	0.79	0/847	0.90	0/1148
2	K	0.74	0/847	0.87	2/1148 (0.2%)
3	C	0.98	0/67	0.99	0/89
3	F	0.85	0/64	0.83	0/85
3	I	0.99	0/68	0.98	0/89
3	L	0.78	0/68	0.85	0/89
All	All	0.72	0/12665	0.84	10/17157 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	219	LEU	N-CA-C	17.79	130.67	111.28
1	D	219	LEU	N-CA-C	14.94	129.25	111.02
1	G	220	ASN	N-CA-CB	-7.82	97.27	110.49
1	G	220	ASN	N-CA-C	-7.58	94.64	110.80
1	D	220	ASN	N-CA-C	-7.13	95.61	110.80
1	D	220	ASN	N-CA-CB	-6.74	99.10	110.49
2	K	32	PRO	CA-C-N	6.17	126.06	119.28
2	K	32	PRO	C-N-CA	6.17	126.06	119.28
1	G	14	ARG	CA-C-N	5.40	126.59	119.84
1	G	14	ARG	C-N-CA	5.40	126.59	119.84

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	2168	0	2028	29	0
1	D	2170	0	2038	37	0
1	G	2214	0	2079	34	0
1	J	2204	0	2074	26	0
2	B	821	0	796	13	0
2	E	821	0	796	16	0
2	H	821	0	796	7	0
2	K	821	0	796	13	0
3	C	66	0	68	2	0
3	F	63	0	57	4	0
3	I	67	0	68	3	0
3	L	67	0	68	4	0
4	A	115	0	0	3	0
4	B	60	0	0	2	0
4	C	7	0	0	1	0
4	D	93	0	0	4	0
4	E	65	0	0	2	0
4	F	2	0	0	0	0
4	G	131	0	0	3	0
4	H	65	0	0	1	0
4	I	3	0	0	0	0
4	J	130	0	0	6	0
4	K	66	0	0	4	0
4	L	5	0	0	0	0
All	All	13045	0	11664	160	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 (160) 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:G:219:LEU:HD12	1:G:219:LEU:O	1.30	1.27
1:D:219:LEU:HD12	1:D:219:LEU:O	1.61	0.99
1:G:219:LEU:O	1:G:219:LEU:CD1	2.22	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:MET:CE	2:B:49:VAL:HG13	2.08	0.83
1:J:144:ARG:NH2	4:J:1467:HOH:O	2.13	0.81
1:D:115:GLN:NE2	4:D:1186:HOH:O	2.18	0.75
2:K:4:THR:HB	4:K:1433:HOH:O	1.85	0.75
1:G:187:ALA:HB3	1:G:272:LEU:HD11	1.70	0.73
1:J:244:TRP:HZ2	2:K:99:MET:HE3	1.53	0.73
2:E:7:ILE:HG21	2:E:93:VAL:HG11	1.70	0.71
2:E:7:ILE:CG2	2:E:93:VAL:HG11	2.20	0.71
2:E:4:THR:HG23	2:E:87:MET:HE3	1.73	0.70
1:A:193:PRO:HA	1:A:199:VAL:HG12	1.73	0.69
1:J:66:LYS:NZ	3:L:2:ALA:O	2.25	0.69
1:G:219:LEU:HD12	1:G:219:LEU:C	2.15	0.69
1:A:144:ARG:HG2	1:A:144:ARG:HH11	1.56	0.68
2:K:4:THR:CB	4:K:1433:HOH:O	2.40	0.68
2:B:60:TRP:O	4:B:1211:HOH:O	2.12	0.68
1:D:155:HIS:HB3	3:F:6:PHE:CZ	2.29	0.68
1:D:103:LEU:HD11	1:D:168:LEU:HD23	1.76	0.67
1:J:234:ARG:HD3	2:K:10:TYR:CE2	2.30	0.67
1:A:244:TRP:CZ2	2:B:99:MET:HE2	2.30	0.67
1:G:249:VAL:HG13	1:G:257:TYR:CE2	2.32	0.65
1:G:230:LEU:C	1:G:230:LEU:HD12	2.21	0.65
1:J:94:THR:HG22	4:J:339:HOH:O	1.95	0.65
1:A:66:LYS:HD3	4:C:1382:HOH:O	1.97	0.64
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.32	0.63
1:D:219:LEU:HD12	1:D:219:LEU:C	2.22	0.63
1:D:206:LEU:HD12	4:D:660:HOH:O	1.99	0.63
1:A:199:VAL:HG13	1:A:251:LEU:HD21	1.81	0.62
2:B:39:MET:HE2	2:B:49:VAL:CG1	2.29	0.62
2:B:4:THR:HB	4:B:1309:HOH:O	2.00	0.61
1:A:115:GLN:NE2	4:A:1152:HOH:O	2.34	0.60
1:G:94:THR:HG22	4:G:1207:HOH:O	2.00	0.60
1:A:19:GLU:CD	4:A:1475:HOH:O	2.43	0.60
1:G:103:LEU:HD11	1:G:168:LEU:HD23	1.84	0.60
1:J:44:ARG:NE	4:J:1056:HOH:O	2.29	0.60
1:A:231:VAL:HG13	1:A:244:TRP:CZ2	2.36	0.59
2:B:39:MET:CE	2:B:49:VAL:CG1	2.78	0.59
1:D:215:LEU:HD13	1:D:243:LYS:HD3	1.84	0.59
2:B:39:MET:HE2	2:B:49:VAL:HG13	1.84	0.59
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.38	0.59
1:J:244:TRP:CZ2	2:K:99:MET:HE3	2.36	0.58
1:J:14:ARG:NH1	4:J:1654:HOH:O	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:VAL:CG1	1:A:251:LEU:HD21	2.34	0.58
1:D:219:LEU:HD13	1:D:257:TYR:CE2	2.39	0.58
1:D:185:PRO:HD2	1:D:266:LEU:HD13	1.85	0.57
1:A:44:ARG:NH1	4:A:1508:HOH:O	2.27	0.57
1:G:35:ARG:NH2	2:H:54:MET:O	2.33	0.57
1:A:249:VAL:HG22	1:A:257:TYR:CE2	2.41	0.56
1:D:81:LEU:HD11	3:F:9:MET:HG3	1.88	0.56
1:D:103:LEU:HD11	1:D:168:LEU:CD2	2.35	0.56
1:D:216:THR:HG22	4:D:996:HOH:O	2.06	0.56
1:J:155:HIS:HB3	3:L:6:PHE:CZ	2.41	0.56
2:K:4:THR:HG22	2:K:86:SER:OG	2.07	0.55
1:G:187:ALA:CB	1:G:272:LEU:HD11	2.35	0.55
1:J:141:GLN:OE1	1:J:144:ARG:NH1	2.40	0.55
1:J:249:VAL:HG22	1:J:257:TYR:CE2	2.42	0.54
1:D:121:ARG:CZ	2:E:1:ILE:HD12	2.37	0.54
1:A:35:ARG:NH2	2:B:54:MET:O	2.38	0.54
1:J:185:PRO:HD2	1:J:266:LEU:HD13	1.89	0.54
1:J:78:LEU:HD13	1:J:95:LEU:HB2	1.89	0.53
1:G:155:HIS:HB3	3:I:6:PHE:CZ	2.44	0.53
1:A:141:GLN:OE1	1:A:144:ARG:NH2	2.42	0.53
2:K:4:THR:HG22	2:K:86:SER:HB2	1.91	0.53
1:J:79:ARG:NH1	4:J:1361:HOH:O	2.40	0.53
1:D:234:ARG:HD3	2:E:10:TYR:CE2	2.43	0.53
1:D:33:PHE:C	1:D:48:ARG:HB2	2.33	0.52
2:K:4:THR:HG22	2:K:86:SER:CB	2.38	0.52
2:E:7:ILE:HG21	2:E:93:VAL:CG1	2.38	0.52
1:D:219:LEU:HD13	1:D:257:TYR:CZ	2.45	0.52
1:D:77:SER:HB3	3:F:9:MET:HG2	1.92	0.52
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.45	0.52
1:A:185:PRO:HD2	1:A:266:LEU:HD13	1.92	0.51
1:D:144:ARG:NH2	4:D:1117:HOH:O	2.43	0.51
1:J:249:VAL:HG22	1:J:257:TYR:CZ	2.45	0.51
1:D:219:LEU:O	1:D:256:ASN:O	2.28	0.51
1:G:141:GLN:OE1	1:G:144:ARG:NH1	2.44	0.50
1:A:194:ARG:NE	1:A:195:SER:OG	2.44	0.50
1:G:10:THR:HG22	1:G:12:VAL:HG23	1.93	0.50
1:G:230:LEU:C	1:G:230:LEU:CD1	2.84	0.50
1:D:20:PRO:HD2	1:D:75:ARG:HD3	1.94	0.49
1:G:30:ASN:ND2	4:G:1402:HOH:O	2.37	0.49
1:G:78:LEU:HD13	1:G:95:LEU:HB2	1.95	0.49
1:A:244:TRP:CH2	2:B:99:MET:HE2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:THR:O	1:A:272:LEU:HD12	2.13	0.49
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.47	0.48
2:E:1:ILE:CG2	2:E:2:GLN:N	2.75	0.48
1:D:72:GLN:HE22	1:D:75:ARG:NH2	2.11	0.48
1:G:103:LEU:CD1	1:G:168:LEU:HD23	2.44	0.48
2:E:59:ASP:O	2:E:60:TRP:HB2	2.13	0.48
1:G:224:LEU:HD23	1:G:247:VAL:HG21	1.94	0.48
1:J:163:GLU:OE1	3:L:1:LYS:NZ	2.43	0.48
1:A:201:LEU:HD11	1:A:254:GLU:HB2	1.95	0.48
1:G:219:LEU:HD13	1:G:257:TYR:CZ	2.49	0.48
2:K:94:TYR:O	4:K:1592:HOH:O	2.20	0.47
1:D:121:ARG:NH2	2:E:1:ILE:HD12	2.28	0.47
1:G:197:GLY:CA	1:G:251:LEU:HD12	2.44	0.47
1:J:175:GLY:O	1:J:176:ASN:C	2.57	0.47
1:J:234:ARG:HD2	1:J:242:GLN:HB2	1.95	0.47
1:G:95:LEU:HD12	1:G:117:ALA:O	2.14	0.47
1:A:144:ARG:HG2	1:A:144:ARG:NH1	2.28	0.46
2:B:39:MET:HE2	2:B:49:VAL:HG11	1.97	0.46
1:G:231:VAL:HG13	1:G:244:TRP:CZ2	2.50	0.46
2:H:3:LYS:NZ	4:H:1250:HOH:O	2.48	0.46
1:D:230:LEU:C	1:D:230:LEU:HD12	2.41	0.46
1:A:199:VAL:HG13	1:A:251:LEU:CD2	2.44	0.46
2:H:12:ARG:CZ	2:H:22:ILE:HD13	2.46	0.46
1:D:45:TYR:CE2	1:D:67:ALA:HB2	2.51	0.45
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.51	0.45
2:E:1:ILE:CG2	2:E:2:GLN:H	2.28	0.45
1:J:202:ARG:HD3	1:J:244:TRP:CE3	2.50	0.45
1:J:209:TYR:CD1	1:J:210:PRO:HA	2.51	0.45
2:K:32:PRO:HB2	2:K:33:PRO:HD2	1.99	0.45
1:D:202:ARG:HD3	1:D:246:SER:HB3	1.97	0.45
1:A:45:TYR:CE2	1:A:67:ALA:HB2	2.52	0.45
2:E:1:ILE:HG23	2:E:2:GLN:N	2.33	0.44
2:E:3:LYS:CE	4:E:1329:HOH:O	2.65	0.44
1:A:194:ARG:O	1:A:195:SER:C	2.61	0.44
2:E:59:ASP:O	2:E:60:TRP:CB	2.65	0.44
1:A:271:THR:C	1:A:272:LEU:HD12	2.43	0.44
2:E:3:LYS:HE2	4:E:1329:HOH:O	2.18	0.44
2:H:51:MET:SD	2:H:66:ALA:HB2	2.58	0.43
1:D:72:GLN:HE22	1:D:75:ARG:HH22	1.64	0.43
2:H:12:ARG:NH1	2:H:22:ILE:HD13	2.32	0.43
1:J:237:GLY:HA3	4:K:1179:HOH:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:GLU:OE1	1:G:22:TYR:OH	2.36	0.43
1:G:21:ARG:HD2	1:G:39:ASP:OD2	2.18	0.43
1:A:155:HIS:HB3	3:C:6:PHE:CZ	2.54	0.43
1:D:249:VAL:HG22	1:D:257:TYR:CZ	2.53	0.43
2:H:3:LYS:HE3	2:H:31:HIS:HB2	2.01	0.43
1:G:103:LEU:HD23	1:G:109:LEU:HA	2.01	0.43
1:G:143:THR:HG21	3:I:9:MET:HG2	2.01	0.42
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.54	0.42
2:K:10:TYR:N	2:K:10:TYR:CD1	2.86	0.42
1:G:260:ARG:NH1	4:G:1483:HOH:O	2.41	0.42
1:G:33:PHE:C	1:G:48:ARG:HB2	2.44	0.42
1:J:66:LYS:HZ1	3:L:1:LYS:HG2	1.83	0.42
1:A:187:ALA:HA	1:A:204:TRP:O	2.20	0.42
1:J:194:ARG:O	1:J:195:SER:O	2.38	0.42
1:D:5:MET:HB2	1:D:168:LEU:HD13	2.01	0.41
1:D:202:ARG:HD2	1:D:244:TRP:CE3	2.56	0.41
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.55	0.41
1:A:66:LYS:HE3	3:C:2:ALA:HB3	2.02	0.41
1:D:78:LEU:HD13	1:D:95:LEU:HB2	2.03	0.41
2:B:54:MET:CE	2:B:64:ILE:HD12	2.51	0.41
2:E:15:PRO:HG3	2:E:97:ARG:HB2	2.01	0.41
1:D:103:LEU:CD1	1:D:168:LEU:HD23	2.46	0.41
1:D:203:CYS:HB2	1:D:217:TRP:CZ2	2.55	0.41
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.56	0.41
1:D:3:HIS:HB2	1:D:103:LEU:HD12	2.03	0.41
1:G:21:ARG:CZ	1:G:39:ASP:OD2	2.69	0.41
1:D:146:LYS:NZ	3:F:9:MET:OXT	2.50	0.41
1:G:66:LYS:HG2	3:I:4:SER:HB3	2.03	0.41
1:D:162:GLY:O	1:D:163:GLU:C	2.63	0.40
1:G:209:TYR:CD1	1:G:210:PRO:HA	2.56	0.40
1:J:48:ARG:NH2	2:K:53:ASP:OD2	2.54	0.40
1:J:202:ARG:NH2	4:J:1345:HOH:O	2.55	0.40
2:B:4:THR:HG22	2:B:86:SER:OG	2.21	0.40
1:G:219:LEU:HD22	1:G:257:TYR:OH	2.22	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	253/276 (92%)	247 (98%)	6 (2%)	0	100	100
1	D	255/276 (92%)	244 (96%)	9 (4%)	2 (1%)	16	20
1	G	261/276 (95%)	255 (98%)	6 (2%)	0	100	100
1	J	260/276 (94%)	254 (98%)	5 (2%)	1 (0%)	30	38
2	B	82/99 (83%)	80 (98%)	2 (2%)	0	100	100
2	E	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	H	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	K	97/99 (98%)	96 (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	1430/1536 (93%)	1389 (97%)	38 (3%)	3 (0%)	43	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	195	SER
1	D	54	GLN
1	D	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	223/234 (95%)	210 (94%)	13 (6%)	18	26
1	D	224/234 (96%)	207 (92%)	17 (8%)	12	16
1	G	228/234 (97%)	212 (93%)	16 (7%)	14	19
1	J	227/234 (97%)	215 (95%)	12 (5%)	20	30
2	B	94/94 (100%)	90 (96%)	4 (4%)	26	39
2	E	94/94 (100%)	89 (95%)	5 (5%)	20	30
2	H	94/94 (100%)	90 (96%)	4 (4%)	26	39
2	K	94/94 (100%)	90 (96%)	4 (4%)	26	39
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	6/7 (86%)	6 (100%)	0	100	100
3	I	7/7 (100%)	7 (100%)	0	100	100
3	L	7/7 (100%)	6 (86%)	1 (14%)	3	3
All	All	1305/1340 (97%)	1229 (94%)	76 (6%)	18	26

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	44	ARG
1	A	78	LEU
1	A	99	SER
1	A	114	LEU
1	A	166	GLU
1	A	176	ASN
1	A	234	ARG
1	A	247	VAL
1	A	249	VAL
1	A	266	LEU
1	A	273	ARG
1	A	275	GLU
2	B	1	ILE
2	B	36	GLU
2	B	75	THR
2	B	77	THR
1	D	44	ARG
1	D	62	ARG
1	D	75	ARG
1	D	78	LEU
1	D	99	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	103	LEU
1	D	105	SER
1	D	110	LEU
1	D	114	LEU
1	D	144	ARG
1	D	149	GLN
1	D	166	GLU
1	D	202	ARG
1	D	234	ARG
1	D	249	VAL
1	D	254	GLU
1	D	266	LEU
2	E	1	ILE
2	E	44	LYS
2	E	64	ILE
2	E	93	VAL
2	E	98	ASP
1	G	17	LEU
1	G	44	ARG
1	G	78	LEU
1	G	79	ARG
1	G	82	LEU
1	G	110	LEU
1	G	114	LEU
1	G	144	ARG
1	G	149	GLN
1	G	166	GLU
1	G	215	LEU
1	G	224	LEU
1	G	227	ASP
1	G	234	ARG
1	G	266	LEU
1	G	275	GLU
2	H	1	ILE
2	H	19	LYS
2	H	48	LYS
2	H	64	ILE
1	J	78	LEU
1	J	82	LEU
1	J	92	SER
1	J	99	SER
1	J	114	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	166	GLU
1	J	224	LEU
1	J	230	LEU
1	J	234	ARG
1	J	249	VAL
1	J	266	LEU
1	J	272	LEU
2	K	19	LYS
2	K	22	ILE
2	K	64	ILE
2	K	74	GLU
3	L	1	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	97	GLN
1	A	176	ASN
1	A	256	ASN
2	B	13	HIS
2	B	31	HIS
2	B	67	HIS
3	C	5	ASN
1	D	54	GLN
1	D	72	GLN
1	D	97	GLN
1	D	256	ASN
2	E	13	HIS
2	E	29	GLN
2	E	31	HIS
3	F	5	ASN
1	G	97	GLN
1	G	218	GLN
1	G	220	ASN
2	H	2	GLN
2	H	13	HIS
2	H	31	HIS
2	H	38	GLN
3	I	5	ASN
1	J	97	GLN
1	J	191	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	256	ASN
2	K	2	GLN
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	263/276 (95%)	1.78	92 (34%)  	40, 56, 88, 98	0
1	D	263/276 (95%)	1.82	96 (36%)  	40, 57, 88, 97	0
1	G	269/276 (97%)	1.82	97 (36%)  	40, 57, 89, 97	0
1	J	268/276 (97%)	1.79	100 (37%)  	40, 57, 86, 96	0
2	B	99/99 (100%)	1.43	21 (21%)  	43, 55, 64, 67	0
2	E	99/99 (100%)	1.40	16 (16%)  	43, 51, 64, 73	0
2	H	99/99 (100%)	1.30	14 (14%)  	39, 51, 63, 67	0
2	K	99/99 (100%)	1.43	23 (23%)  	41, 53, 64, 70	0
3	C	9/9 (100%)	0.57	0  	38, 40, 45, 49	0
3	F	9/9 (100%)	1.02	0  	44, 48, 52, 53	0
3	I	9/9 (100%)	1.01	0  	42, 43, 48, 51	0
3	L	9/9 (100%)	0.90	0  	44, 46, 49, 52	0
All	All	1495/1536 (97%)	1.67	459 (30%)  	38, 55, 86, 98	0

All (459) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	17	LEU	7.9
1	A	17	LEU	7.8
1	J	272	LEU	7.8
1	J	221	GLY	7.1
1	J	224	LEU	6.5
1	J	176	ASN	6.4
1	D	219	LEU	6.2
1	A	272	LEU	6.1
1	A	195	SER	6.0
1	D	222	GLU	5.9
1	A	248	VAL	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	199	VAL	5.8
2	E	99	MET	5.7
1	G	256	ASN	5.5
1	D	193	PRO	5.4
1	G	199	VAL	5.4
1	G	189	VAL	5.4
1	J	16	GLY	5.3
1	J	255	GLN	5.3
1	J	181	ARG	5.3
1	D	17	LEU	5.3
1	D	251	LEU	5.2
1	J	258	THR	5.1
1	G	274	TRP	5.1
1	G	252	GLY	5.1
1	A	257	TYR	5.1
1	G	15	PRO	5.0
1	G	223	GLU	5.0
1	A	249	VAL	5.0
1	A	247	VAL	4.9
1	G	191	HIS	4.9
1	A	251	LEU	4.9
1	D	195	SER	4.8
1	A	258	THR	4.8
2	B	1	ILE	4.8
1	J	276	PRO	4.8
1	D	1	GLY	4.8
1	A	274	TRP	4.8
2	K	1	ILE	4.7
1	G	196	LYS	4.7
1	G	258	THR	4.7
1	D	276	PRO	4.7
2	H	48	LYS	4.7
1	D	248	VAL	4.6
1	D	189	VAL	4.6
1	G	227	ASP	4.6
1	G	219	LEU	4.6
1	A	201	LEU	4.5
1	J	18	GLU	4.5
1	A	228	MET	4.5
1	G	276	PRO	4.4
1	G	41	GLU	4.4
1	A	245	ALA	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	250	PRO	4.4
1	D	190	THR	4.4
1	G	198	GLU	4.4
1	D	249	VAL	4.4
1	G	193	PRO	4.3
1	J	199	VAL	4.3
1	G	250	PRO	4.3
1	J	58	GLU	4.2
1	J	194	ARG	4.2
1	J	189	VAL	4.2
1	A	256	ASN	4.2
1	G	224	LEU	4.2
1	A	191	HIS	4.2
1	D	90	GLY	4.1
1	G	267	PRO	4.1
1	A	187	ALA	4.1
1	D	113	TYR	4.1
1	A	18	GLU	4.1
1	G	222	GLU	4.1
1	G	249	VAL	4.1
1	G	251	LEU	4.1
1	D	257	TYR	4.0
1	G	257	TYR	4.0
1	G	275	GLU	4.0
1	D	272	LEU	4.0
1	D	274	TRP	4.0
2	B	75	THR	4.0
1	A	221	GLY	3.9
1	J	113	TYR	3.9
1	J	193	PRO	3.9
1	J	251	LEU	3.9
1	D	250	PRO	3.9
1	D	200	THR	3.9
1	G	16	GLY	3.9
2	H	1	ILE	3.8
1	J	257	TYR	3.8
1	A	199	VAL	3.8
1	G	248	VAL	3.8
1	G	197	GLY	3.8
1	D	2	PRO	3.8
1	G	149	GLN	3.7
1	J	211	ALA	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	56	GLY	3.7
1	G	266	LEU	3.7
1	D	228	MET	3.7
1	D	266	LEU	3.7
1	D	265	GLY	3.6
1	G	272	LEU	3.6
1	A	181	ARG	3.6
1	G	200	THR	3.6
1	G	213	ILE	3.6
1	J	217	TRP	3.6
2	E	1	ILE	3.6
1	G	17	LEU	3.6
1	G	201	LEU	3.6
1	J	88	SER	3.5
2	H	18	GLY	3.5
1	D	172	LEU	3.5
1	A	218	GLN	3.5
1	A	16	GLY	3.5
1	J	46	GLU	3.5
2	E	11	SER	3.5
1	G	221	GLY	3.5
1	D	19	GLU	3.5
1	G	176	ASN	3.5
1	A	216	THR	3.4
1	J	269	PRO	3.4
2	H	47	PRO	3.4
1	J	249	VAL	3.4
1	J	219	LEU	3.4
1	A	50	PRO	3.4
1	A	193	PRO	3.4
1	G	190	THR	3.4
1	G	259	CYS	3.4
1	G	253	LYS	3.4
1	D	50	PRO	3.4
1	D	56	GLY	3.3
1	G	42	ASN	3.3
1	J	256	ASN	3.3
1	J	172	LEU	3.3
1	J	190	THR	3.3
1	D	191	HIS	3.3
1	G	113	TYR	3.3
1	D	247	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	228	MET	3.3
1	D	201	LEU	3.3
1	A	202	ARG	3.3
1	D	258	THR	3.3
2	E	3	LYS	3.3
1	J	274	TRP	3.3
1	J	89	ALA	3.3
1	A	194	ARG	3.3
1	G	273	ARG	3.3
1	G	218	GLN	3.3
2	E	98	ASP	3.2
1	D	254	GLU	3.2
1	D	105	SER	3.2
1	D	256	ASN	3.2
1	J	247	VAL	3.2
1	A	176	ASN	3.2
1	A	232	GLU	3.2
2	K	47	PRO	3.2
2	K	74	GLU	3.2
1	D	192	HIS	3.2
1	A	217	TRP	3.2
1	A	267	PRO	3.2
1	D	40	ALA	3.1
1	G	39	ASP	3.1
1	A	190	THR	3.1
1	A	271	THR	3.1
1	D	271	THR	3.1
1	G	182	THR	3.1
1	A	246	SER	3.1
1	G	265	GLY	3.1
1	J	175	GLY	3.1
1	D	140	ALA	3.1
1	J	212	ASP	3.1
1	G	247	VAL	3.1
2	H	49	VAL	3.1
1	G	194	ARG	3.1
1	J	192	HIS	3.1
1	D	252	GLY	3.1
1	G	49	ALA	3.1
1	A	189	VAL	3.1
1	A	275	GLU	3.1
1	G	217	TRP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	255	GLN	3.1
1	D	104	GLY	3.1
2	E	47	PRO	3.1
1	G	254	GLU	3.0
1	G	271	THR	3.0
1	D	273	ARG	3.0
1	G	181	ARG	3.0
1	J	44	ARG	3.0
2	B	3	LYS	3.0
1	A	49	ALA	3.0
1	G	228	MET	3.0
1	A	198	GLU	3.0
1	D	18	GLU	3.0
1	A	237	GLY	3.0
1	D	91	GLY	3.0
1	D	270	LEU	3.0
1	A	192	HIS	3.0
1	J	271	THR	3.0
1	D	198	GLU	3.0
1	J	144	ARG	2.9
1	J	260	ARG	2.9
1	A	200	THR	2.9
1	D	174	ASN	2.9
1	G	207	GLY	2.9
1	J	41	GLU	2.9
1	A	253	LYS	2.9
1	A	14	ARG	2.9
1	J	248	VAL	2.9
1	D	58	GLU	2.9
1	J	104	GLY	2.9
1	A	269	PRO	2.9
1	J	250	PRO	2.9
1	D	204	TRP	2.9
2	E	81	ARG	2.9
1	A	231	VAL	2.9
1	D	53	GLU	2.9
2	K	75	THR	2.9
2	E	48	LYS	2.9
1	J	202	ARG	2.9
1	J	149	GLN	2.9
1	J	201	LEU	2.9
1	A	259	CYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	229	GLU	2.9
1	G	220	ASN	2.9
1	J	252	GLY	2.8
2	K	19	LYS	2.8
1	A	185	PRO	2.8
1	G	58	GLU	2.8
1	J	259	CYS	2.8
1	J	30	ASN	2.8
1	D	62	ARG	2.8
1	J	195	SER	2.8
1	A	113	TYR	2.8
1	J	79	ARG	2.8
1	D	54	GLN	2.8
1	A	230	LEU	2.8
2	K	3	LYS	2.8
2	K	48	LYS	2.8
1	A	214	THR	2.8
1	D	42	ASN	2.8
1	A	1	GLY	2.8
1	D	15	PRO	2.8
2	B	47	PRO	2.8
1	J	245	ALA	2.8
1	G	44	ARG	2.8
1	A	23	ILE	2.7
1	J	42	ASN	2.7
1	A	223	GLU	2.7
2	E	44	LYS	2.7
1	J	230	LEU	2.7
2	B	73	THR	2.7
1	G	142	ILE	2.7
1	D	217	TRP	2.7
1	G	79	ARG	2.7
1	J	273	ARG	2.7
2	B	78	TYR	2.7
1	J	265	GLY	2.7
1	J	253	LYS	2.7
2	B	2	GLN	2.7
1	D	261	VAL	2.7
2	K	71	THR	2.7
1	A	206	LEU	2.7
1	J	215	LEU	2.7
1	G	40	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	237	GLY	2.6
1	A	172	LEU	2.6
1	D	149	GLN	2.6
1	D	255	GLN	2.6
1	G	270	LEU	2.6
1	D	253	LYS	2.6
1	A	60	TRP	2.6
1	G	204	TRP	2.6
1	D	181	ARG	2.6
1	A	46	GLU	2.6
1	J	229	GLU	2.6
1	J	254	GLU	2.6
1	D	48	ARG	2.6
1	D	144	ARG	2.6
1	G	62	ARG	2.6
1	G	202	ARG	2.6
1	A	152	ALA	2.6
1	A	104	GLY	2.6
1	D	221	GLY	2.6
2	H	4	THR	2.6
2	H	46	ILE	2.6
2	H	3	LYS	2.6
1	J	198	GLU	2.5
1	D	51	TRP	2.5
1	A	91	GLY	2.5
1	A	112	GLY	2.5
1	D	269	PRO	2.5
1	G	269	PRO	2.5
1	J	50	PRO	2.5
1	A	184	SER	2.5
1	D	184	SER	2.5
1	D	260	ARG	2.5
1	J	62	ARG	2.5
1	G	174	ASN	2.5
2	H	53	ASP	2.5
1	D	218	GLN	2.5
1	G	184	SER	2.5
1	A	229	GLU	2.5
1	J	222	GLU	2.5
1	D	183	ASP	2.5
1	J	40	ALA	2.5
1	J	56	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	K	33	PRO	2.5
1	G	23	ILE	2.5
1	J	60	TRP	2.5
2	B	45	LYS	2.5
2	H	17	ASN	2.5
2	K	17	ASN	2.5
1	J	152	ALA	2.5
1	G	255	GLN	2.5
1	D	41	GLU	2.4
1	D	259	CYS	2.4
1	D	34	VAL	2.4
1	J	261	VAL	2.4
2	K	22	ILE	2.4
1	D	173	LYS	2.4
1	G	54	GLN	2.4
1	J	145	ARG	2.4
1	J	170	ARG	2.4
1	G	216	THR	2.4
1	J	182	THR	2.4
2	K	18	GLY	2.4
1	G	94	THR	2.4
1	A	203	CYS	2.4
1	A	266	LEU	2.4
1	A	149	GLN	2.4
2	B	42	ASN	2.4
1	D	16	GLY	2.4
1	J	187	ALA	2.4
2	E	4	THR	2.4
2	B	93	VAL	2.4
2	E	93	VAL	2.4
1	G	170	ARG	2.4
1	J	191	HIS	2.4
1	D	185	PRO	2.3
1	A	252	GLY	2.3
2	B	48	LYS	2.3
2	K	73	THR	2.3
1	J	270	LEU	2.3
1	G	46	GLU	2.3
1	G	31	LYS	2.3
1	J	171	TYR	2.3
1	J	204	TRP	2.3
1	G	185	PRO	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	44	ARG	2.3
1	D	65	GLN	2.3
2	B	89	GLU	2.3
1	D	57	PRO	2.3
1	J	185	PRO	2.3
1	G	153	ALA	2.3
1	G	187	ALA	2.3
1	A	108	ARG	2.3
1	A	54	GLN	2.3
1	J	54	GLN	2.3
1	A	213	ILE	2.3
2	E	49	VAL	2.3
1	J	196	LYS	2.3
2	K	45	LYS	2.3
2	K	72	PRO	2.3
2	B	54	MET	2.3
1	A	204	TRP	2.3
1	D	111	ARG	2.3
1	D	13	SER	2.3
1	G	105	SER	2.3
1	J	105	SER	2.3
1	A	222	GLU	2.3
1	D	103	LEU	2.2
1	D	220	ASN	2.2
1	A	15	PRO	2.2
2	H	90	PRO	2.2
1	J	111	ARG	2.2
1	J	197	GLY	2.2
1	G	61	GLU	2.2
1	J	200	THR	2.2
2	B	4	THR	2.2
2	E	2	GLN	2.2
1	A	186	LYS	2.2
2	B	46	ILE	2.2
1	A	208	PHE	2.2
1	G	175	GLY	2.2
1	D	275	GLU	2.2
1	G	158	ALA	2.2
1	J	216	THR	2.2
1	J	240	THR	2.2
2	H	92	THR	2.2
1	J	107	TRP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	270	LEU	2.2
1	J	206	LEU	2.2
1	D	194	ARG	2.2
1	J	234	ARG	2.2
2	E	97	ARG	2.2
1	G	166	GLU	2.2
1	A	89	ALA	2.2
1	A	182	THR	2.2
1	G	230	LEU	2.2
1	A	42	ASN	2.2
1	D	36	PHE	2.2
1	G	183	ASP	2.2
1	G	241	PHE	2.2
2	B	87	MET	2.2
2	K	50	GLU	2.2
1	D	151	GLY	2.2
1	G	239	GLY	2.2
1	J	207	GLY	2.2
1	D	182	THR	2.2
1	G	144	ARG	2.1
1	J	15	PRO	2.1
1	J	61	GLU	2.1
2	B	90	PRO	2.1
1	A	273	ARG	2.1
1	D	171	TYR	2.1
1	G	262	TYR	2.1
1	A	183	ASP	2.1
1	D	30	ASN	2.1
1	D	231	VAL	2.1
1	D	244	TRP	2.1
1	G	261	VAL	2.1
1	J	51	TRP	2.1
2	K	13	HIS	2.1
1	D	202	ARG	2.1
2	K	11	SER	2.1
2	K	54	MET	2.1
1	J	142	ILE	2.1
1	J	266	LEU	2.1
2	E	6	GLN	2.1
2	B	82	VAL	2.1
1	A	167	TRP	2.1
1	A	175	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	265	GLY	2.1
1	A	105	SER	2.1
1	G	233	THR	2.1
1	D	186	LYS	2.1
2	H	44	LYS	2.1
1	G	229	GLU	2.1
1	G	268	GLU	2.1
1	J	43	PRO	2.1
2	E	94	TYR	2.1
2	H	26	TYR	2.1
1	G	231	VAL	2.1
1	A	144	ARG	2.1
1	D	75	ARG	2.1
2	B	91	LYS	2.0
2	K	83	LYS	2.0
1	D	216	THR	2.0
2	B	68	THR	2.0
1	G	211	ALA	2.0
2	K	69	GLU	2.0
1	A	261	VAL	2.0
2	K	81	ARG	2.0
1	A	207	GLY	2.0
2	K	99	MET	2.0
1	J	246	SER	2.0
2	B	92	THR	2.0
1	D	206	LEU	2.0
1	G	260	ARG	2.0
1	J	173	LYS	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.