



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:49 AM UTC

PDB ID : 3CII / pdb_00003cii
Title : Structure of NKG2A/CD94 bound to HLA-E
Authors : Strong, R.K.; Kaiser, B.K.; Pizarro, J.C.
Deposited on : 2008-03-11
Resolution : 4.41 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

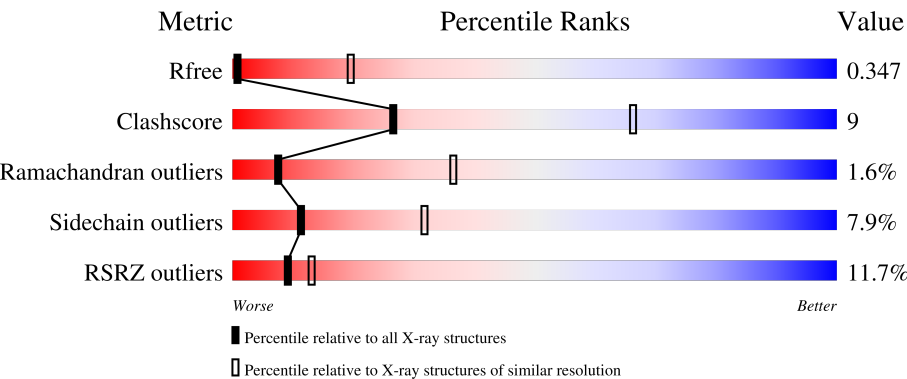
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.41 Å.

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



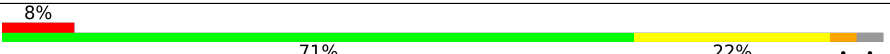
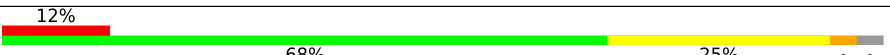
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1092 (4.92-3.90)
Clashscore	190562	1139 (4.92-3.90)
Ramachandran outliers	187476	1028 (4.92-3.90)
Sidechain outliers	187428	1012 (4.92-3.90)
RSRZ outliers	180081	1088 (4.92-3.90)

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	273	10% 75% 21% .
1	D	273	13% 75% 21% .
2	B	100	15% 83% 15% .
2	E	100	23% 85% 13% .
3	C	9	67% 22% 11%

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Mol	Chain	Length	Quality of chain
3	F	9	 56% 33% 11%
4	G	121	 7% 61% 32% 7%
4	I	121	 7% 62% 35% .
5	H	120	 8% 71% 22% . .
5	J	120	 12% 68% 25% . .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10146 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 HLA class I histocompatibility antigen, alpha chain E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2234	1396	401	430	7			
1	D	273	Total	C	N	O	S	0	0	0
			2234	1396	401	430	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called HLA class I histocompatibility antigen peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			73	49	12	11	1			
3	F	9	Total	C	N	O	S	0	0	0
			73	49	12	11	1			

- Molecule 4 is a protein called Natural killer cells antigen CD94.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	121	Total	C	N	O	S	0	0	0
			997	625	165	198	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	121	Total	C	N	O	S	0	0	0
			997	625	165	198	9			

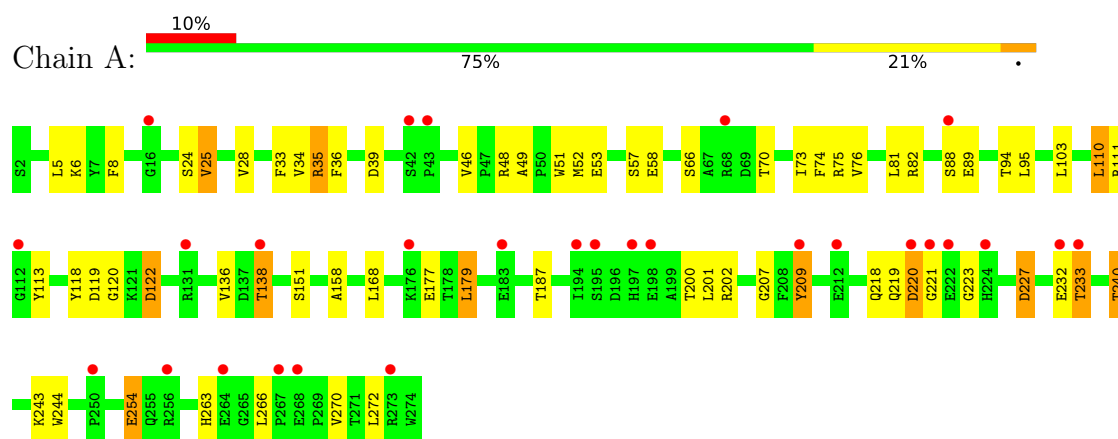
- Molecule 5 is a protein called NKG2-A/NKG2-B type II integral membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	116	Total	C	N	O	S	0	0	0
			932	585	166	172	9			
5	J	116	Total	C	N	O	S	0	0	0
			932	585	166	172	9			

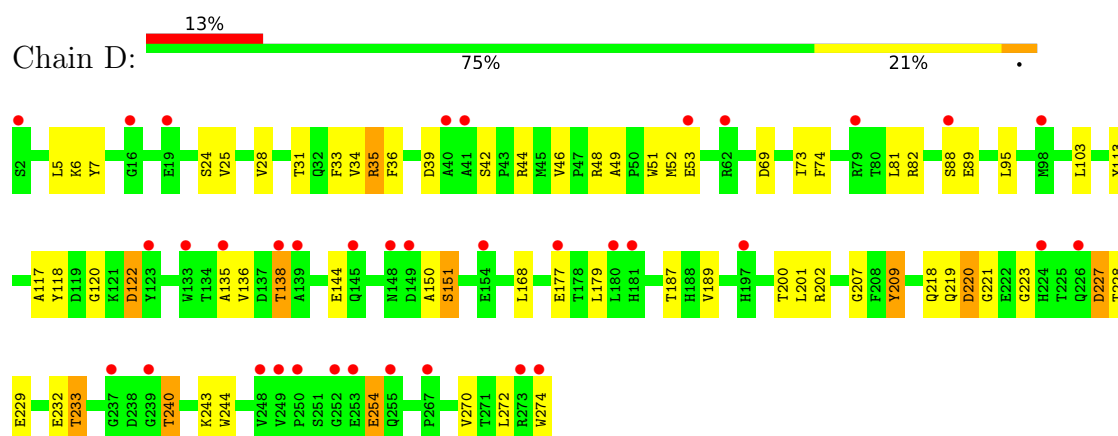
3 Residue-property plots [i](#)

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.

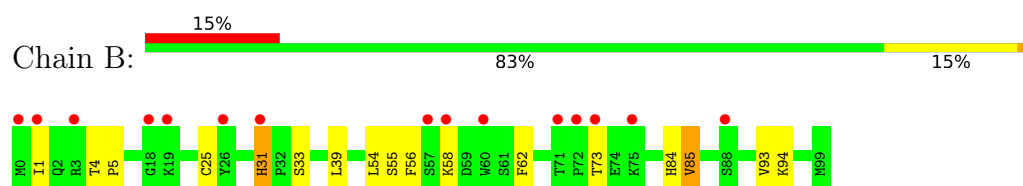
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E



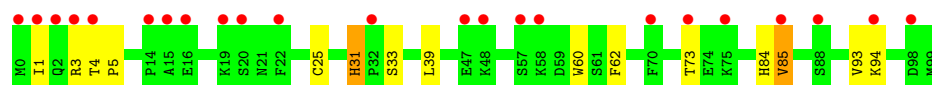
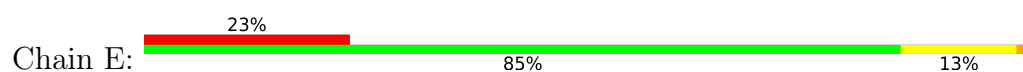
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: HLA class I histocompatibility antigen peptide



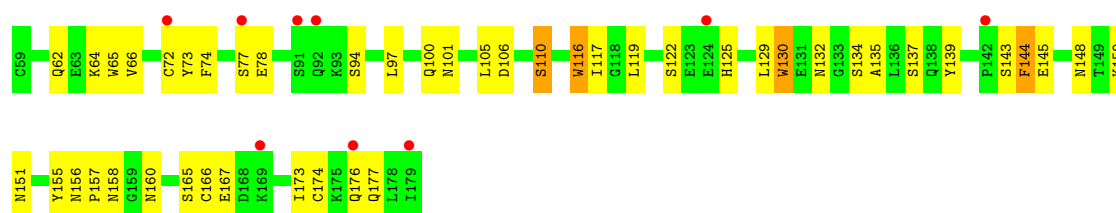
- Molecule 3: HLA class I histocompatibility antigen peptide



- Molecule 4: Natural killer cells antigen CD94

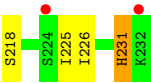


- Molecule 4: Natural killer cells antigen CD94

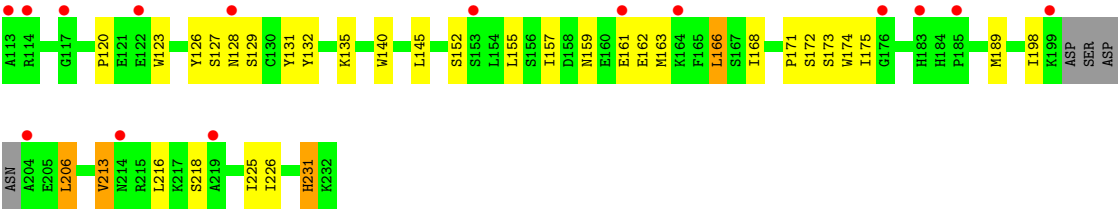


- Molecule 5: NKG2-A/NKG2-B type II integral membrane protein





● Molecule 5: NKG2-A/NKG2-B type II integral membrane protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	345.98Å 345.98Å 345.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.88 – 4.41 67.88 – 4.41	Depositor EDS
% Data completeness (in resolution range)	100.0 (67.88-4.41) 99.9 (67.88-4.41)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.74 (at 4.46Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.321 , 0.355 0.311 , 0.347	Depositor DCC
R_{free} test set	1155 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	101.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 179.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	10146	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.39% 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

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	0.58	0/2300	0.79	2/3127 (0.1%)
1	D	0.55	0/2300	0.78	2/3127 (0.1%)
2	B	0.59	0/860	0.83	2/1162 (0.2%)
2	E	0.56	0/860	0.79	2/1162 (0.2%)
3	C	0.55	0/74	0.78	0/98
3	F	0.50	0/74	0.78	0/98
4	G	0.67	0/1023	0.87	2/1383 (0.1%)
4	I	0.62	0/1023	0.81	2/1383 (0.1%)
5	H	0.60	0/955	0.76	0/1286
5	J	0.58	0/955	0.75	0/1286
All	All	0.59	0/10424	0.80	12/14112 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	H	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	31	HIS	CA-C-N	-8.15	110.53	119.98
2	B	31	HIS	C-N-CA	-8.15	110.53	119.98
2	E	31	HIS	CA-C-N	-6.55	112.38	119.98
2	E	31	HIS	C-N-CA	-6.55	112.38	119.98
4	I	156	ASN	CA-C-N	6.17	127.56	119.84
4	I	156	ASN	C-N-CA	6.17	127.56	119.84
1	D	209	TYR	CA-C-N	-5.67	113.71	119.83
1	D	209	TYR	C-N-CA	-5.67	113.71	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	124	GLU	N-CA-C	-5.25	105.20	111.03
4	G	111	SER	N-CA-C	5.13	117.54	110.35
1	A	209	TYR	CA-C-N	-5.11	114.54	119.90
1	A	209	TYR	C-N-CA	-5.11	114.54	119.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	H	170	SER	Peptide

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	2234	0	2072	44	0
1	D	2234	0	2072	40	0
2	B	837	0	803	10	0
2	E	837	0	803	8	0
3	C	73	0	83	5	0
3	F	73	0	83	5	0
4	G	997	0	905	31	0
4	I	997	0	905	22	0
5	H	932	0	896	19	0
5	J	932	0	896	22	0
All	All	10146	0	9518	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 9.

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)
4:I:119:LEU:HD13	4:I:130:TRP:CE3	2.11	0.85
4:G:62:GLN:HB2	4:G:65:TRP:CD1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:6:THR:HG22	3:F:7:LEU:H	1.48	0.78
5:H:157:ILE:HG21	5:H:163:MET:HE2	1.65	0.78
4:I:117:ILE:HD13	4:I:155:TYR:HB2	1.65	0.77
5:J:157:ILE:HG21	5:J:163:MET:HE2	1.67	0.76
4:G:108:MET:HE2	4:G:157:PRO:HG3	1.70	0.74
4:I:129:LEU:HD13	4:I:135:ALA:HA	1.69	0.74
4:I:62:GLN:HB2	4:I:65:TRP:CD1	2.21	0.74
5:H:225:ILE:HG22	5:H:226:ILE:H	1.53	0.73
3:C:6:THR:HG22	3:C:7:LEU:H	1.55	0.71
5:J:225:ILE:HG22	5:J:226:ILE:H	1.54	0.71
4:G:119:LEU:HD13	4:G:130:TRP:CD2	2.26	0.70
4:G:65:TRP:CZ3	4:G:74:PHE:HB2	2.26	0.70
1:A:73:ILE:HD11	4:G:112:GLN:O	1.92	0.69
4:I:122:SER:HB3	4:I:125:HIS:HB2	1.76	0.68
4:I:65:TRP:CZ3	4:I:74:PHE:HB2	2.30	0.65
5:J:152:SER:HB3	5:J:231:HIS:CE1	2.33	0.63
4:G:97:LEU:HD23	4:G:173:ILE:HD12	1.79	0.63
5:H:152:SER:HB3	5:H:231:HIS:CE1	2.33	0.63
1:A:75:ARG:HD3	4:G:162:LEU:HD22	1.81	0.63
1:A:138:THR:HG21	1:D:232:GLU:HA	1.80	0.63
1:A:158:ALA:HA	5:H:217:LYS:NZ	2.14	0.63
5:H:225:ILE:HG22	5:H:226:ILE:N	2.14	0.62
2:E:25:CYS:HB2	2:E:39:LEU:HD21	1.82	0.62
5:H:131:TYR:OH	5:H:162:GLU:OE1	2.16	0.62
1:D:187:THR:HB	1:D:272:LEU:HD11	1.81	0.61
5:J:225:ILE:HG22	5:J:226:ILE:N	2.14	0.61
1:A:187:THR:HB	1:A:272:LEU:HD11	1.83	0.61
5:J:189:MET:HA	5:J:189:MET:HE3	1.82	0.60
5:H:175:ILE:HD13	5:H:216:LEU:HD22	1.84	0.60
1:A:158:ALA:HA	5:H:217:LYS:HZ1	1.65	0.59
4:G:72:CYS:HB2	4:G:176:GLN:HB2	1.82	0.59
1:A:120:GLY:O	2:B:1:ILE:HD12	2.02	0.59
4:I:119:LEU:HD22	4:I:130:TRP:CZ3	2.37	0.59
2:E:33:SER:HB3	2:E:62:PHE:CE2	2.38	0.59
4:I:72:CYS:HB2	4:I:176:GLN:HB2	1.84	0.59
5:H:189:MET:HE3	5:H:189:MET:HA	1.84	0.58
1:A:122:ASP:HB2	1:A:136:VAL:HG11	1.84	0.58
4:I:66:VAL:HG13	4:I:73:TYR:HB2	1.86	0.58
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.86	0.58
4:G:97:LEU:CD2	4:G:173:ILE:HD12	2.34	0.58
4:G:119:LEU:HD13	4:G:130:TRP:CE3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:155:LEU:HD11	5:J:166:LEU:HD21	1.85	0.57
2:B:33:SER:HB3	2:B:62:PHE:CE2	2.40	0.56
1:A:219:GLN:H	1:A:223:GLY:HA2	1.70	0.56
5:H:155:LEU:HD11	5:H:166:LEU:HD21	1.88	0.56
1:A:138:THR:HG21	1:D:232:GLU:HG3	1.87	0.55
1:D:219:GLN:H	1:D:223:GLY:HA2	1.72	0.55
5:J:131:TYR:OH	5:J:162:GLU:OE1	2.21	0.55
4:G:66:VAL:HG13	4:G:73:TYR:HB2	1.89	0.55
4:I:97:LEU:HD22	4:I:173:ILE:HG21	1.89	0.54
1:D:122:ASP:HB2	1:D:136:VAL:HG11	1.90	0.54
5:J:206:LEU:HB2	5:J:218:SER:OG	2.07	0.54
1:A:138:THR:CG2	1:D:232:GLU:HA	2.38	0.54
4:I:148:ASN:HB3	4:I:151:ASN:HD22	1.72	0.53
4:G:115:TYR:O	4:G:155:TYR:N	2.41	0.53
1:A:5:LEU:HB2	1:A:168:LEU:HD13	1.90	0.52
4:I:97:LEU:HD21	4:I:105:LEU:HD11	1.91	0.52
5:J:225:ILE:CG2	5:J:226:ILE:H	2.22	0.52
1:A:74:PHE:CE1	3:C:6:THR:HG21	2.44	0.52
4:G:144:PHE:HA	4:G:147:PHE:CE2	2.44	0.52
2:E:84:HIS:CG	2:E:85:VAL:H	2.29	0.51
4:G:97:LEU:HD21	4:G:105:LEU:HD11	1.90	0.51
1:A:24:SER:HB2	1:A:36:PHE:HB3	1.91	0.51
1:A:74:PHE:CD2	1:A:95:LEU:HD23	2.46	0.51
1:A:74:PHE:HE1	3:C:6:THR:HG21	1.76	0.51
5:H:225:ILE:CG2	5:H:226:ILE:H	2.22	0.51
4:G:156:ASN:O	4:G:158:ASN:N	2.44	0.51
1:D:24:SER:HB2	1:D:36:PHE:HB3	1.92	0.51
2:E:84:HIS:CG	2:E:85:VAL:N	2.79	0.51
5:J:175:ILE:HD13	5:J:216:LEU:HD22	1.93	0.50
4:I:106:ASP:HB3	5:J:135:LYS:NZ	2.26	0.50
4:I:110:SER:HB2	5:J:171:PRO:HD3	1.93	0.50
2:B:84:HIS:CG	2:B:85:VAL:H	2.30	0.50
1:D:202:ARG:HD3	1:D:244:TRP:CD2	2.47	0.50
1:A:218:GLN:HB2	1:A:223:GLY:HA3	1.94	0.50
4:G:76:SER:HB3	4:G:172:TYR:O	2.12	0.50
5:H:206:LEU:HB2	5:H:218:SER:OG	2.12	0.49
1:A:219:GLN:O	1:A:221:GLY:N	2.46	0.49
4:I:165:SER:C	4:I:167:GLU:H	2.21	0.49
1:A:113:TYR:CD1	1:A:113:TYR:C	2.91	0.49
4:I:143:SER:O	4:I:145:GLU:N	2.39	0.49
4:G:65:TRP:CH2	4:G:74:PHE:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:94:SER:OG	4:G:174:CYS:HB3	2.14	0.48
1:D:5:LEU:HB2	1:D:168:LEU:HD13	1.94	0.48
2:B:84:HIS:CG	2:B:85:VAL:N	2.81	0.48
1:D:120:GLY:O	2:E:1:ILE:HD12	2.13	0.48
4:G:121:TYR:CD2	4:G:121:TYR:C	2.91	0.48
5:J:173:SER:HA	5:J:226:ILE:O	2.14	0.48
4:G:65:TRP:CE3	4:G:74:PHE:HB2	2.49	0.48
4:G:125:HIS:ND1	4:G:129:LEU:HD11	2.28	0.48
1:D:81:LEU:HD13	1:D:118:TYR:CD1	2.49	0.48
1:A:207:GLY:HA2	1:A:240:THR:HB	1.95	0.48
4:G:143:SER:O	4:G:146:THR:HG22	2.13	0.48
1:A:8:PHE:HB2	1:A:25:VAL:HG23	1.96	0.47
4:I:94:SER:OG	4:I:174:CYS:HB3	2.15	0.47
1:A:110:LEU:HD23	1:A:111:ARG:HG2	1.95	0.47
1:D:28:VAL:HG23	1:D:33:PHE:CE1	2.48	0.47
1:D:218:GLN:HB2	1:D:223:GLY:HA3	1.96	0.47
4:I:65:TRP:CE3	4:I:74:PHE:HB2	2.48	0.47
1:D:74:PHE:HE1	3:F:6:THR:HG21	1.79	0.47
1:D:74:PHE:CD2	1:D:95:LEU:HD23	2.50	0.46
1:D:207:GLY:HA2	1:D:240:THR:HB	1.95	0.46
2:B:1:ILE:HD11	2:E:3:ARG:NH1	2.30	0.46
5:H:168:ILE:O	5:H:168:ILE:HG22	2.16	0.46
1:A:103:LEU:HG	1:A:168:LEU:HD23	1.98	0.46
1:D:49:ALA:HB1	1:D:51:TRP:NE1	2.31	0.46
1:D:74:PHE:CE1	3:F:6:THR:HG21	2.51	0.46
5:J:127:SER:C	5:J:129:SER:H	2.23	0.46
1:D:202:ARG:HD3	1:D:244:TRP:CE3	2.51	0.45
1:A:76:VAL:HG21	4:G:114:PHE:HZ	1.81	0.45
5:H:173:SER:HA	5:H:226:ILE:O	2.16	0.45
1:A:232:GLU:HA	1:D:138:THR:HG21	1.98	0.45
1:D:33:PHE:O	1:D:48:ARG:N	2.40	0.45
2:B:54:LEU:HD12	2:B:55:SER:N	2.33	0.44
1:D:113:TYR:CD1	1:D:113:TYR:C	2.95	0.44
1:D:219:GLN:O	1:D:221:GLY:N	2.50	0.44
5:J:159:ASN:C	5:J:161:GLU:H	2.24	0.44
5:H:127:SER:C	5:H:129:SER:H	2.25	0.44
5:H:159:ASN:C	5:H:161:GLU:H	2.26	0.44
1:A:49:ALA:HB1	1:A:51:TRP:NE1	2.33	0.44
1:A:34:VAL:CG1	1:A:52:MET:HE2	2.48	0.44
1:D:150:ALA:O	1:D:151:SER:C	2.60	0.44
2:E:4:THR:HG23	2:E:5:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:225:ILE:CG2	5:H:226:ILE:N	2.81	0.44
4:G:121:TYR:C	4:G:121:TYR:HD2	2.25	0.44
1:D:31:THR:OG1	1:D:209:TYR:OH	2.22	0.44
1:D:35:ARG:HG2	1:D:48:ARG:HD3	1.99	0.44
4:G:97:LEU:HD22	4:G:173:ILE:HG21	2.00	0.44
4:I:116:TRP:CE3	4:I:116:TRP:HA	2.53	0.44
1:A:51:TRP:CZ2	1:A:179:LEU:HD21	2.53	0.43
5:H:140:TRP:HD1	5:H:174:TRP:CE3	2.36	0.43
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.53	0.43
1:D:201:LEU:HD11	1:D:254:GLU:HB3	2.01	0.43
5:J:225:ILE:CG2	5:J:226:ILE:N	2.81	0.43
1:D:135:ALA:HB2	1:D:144:GLU:HB2	2.00	0.43
4:G:153:ILE:HG22	4:G:154:ALA:N	2.33	0.43
2:B:4:THR:HG23	2:B:5:PRO:HD2	2.01	0.43
1:D:82:ARG:NE	1:D:89:GLU:HA	2.34	0.43
4:G:140:LEU:C	4:G:140:LEU:HD12	2.44	0.43
5:J:120:PRO:HB2	5:J:123:TRP:CD1	2.54	0.43
1:A:28:VAL:HG23	1:A:33:PHE:CE1	2.54	0.43
4:G:119:LEU:HD13	4:G:130:TRP:CE2	2.54	0.43
4:I:65:TRP:CH2	4:I:74:PHE:HB2	2.53	0.43
1:D:103:LEU:HG	1:D:168:LEU:HD23	2.00	0.42
1:D:233:THR:OG1	1:D:243:LYS:NZ	2.51	0.42
5:J:168:ILE:O	5:J:168:ILE:HG22	2.19	0.42
1:A:263:HIS:HB3	1:A:266:LEU:HD12	2.01	0.42
1:D:34:VAL:CG1	1:D:52:MET:HE2	2.49	0.42
1:D:42:SER:C	1:D:44:ARG:H	2.27	0.42
1:A:201:LEU:HD11	1:A:254:GLU:HB3	2.01	0.42
1:A:81:LEU:HD11	3:C:9:LEU:CD1	2.50	0.42
1:A:219:GLN:O	1:A:220:ASP:C	2.61	0.42
1:A:35:ARG:HG2	1:A:48:ARG:HD3	2.01	0.42
1:A:66:SER:O	1:A:70:THR:OG1	2.38	0.42
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.55	0.42
1:A:219:GLN:N	1:A:223:GLY:HA2	2.34	0.42
1:A:82:ARG:NE	1:A:89:GLU:HA	2.34	0.41
1:A:57:SER:O	1:A:58:GLU:C	2.63	0.41
1:A:94:THR:N	1:A:119:ASP:OD1	2.45	0.41
1:D:69:ASP:O	1:D:73:ILE:HG12	2.21	0.41
1:D:189:VAL:HB	1:D:274:TRP:HB2	2.02	0.41
5:H:126:TYR:HB3	5:H:131:TYR:HE1	1.85	0.41
5:J:123:TRP:CZ2	5:J:132:TYR:HB2	2.56	0.41
1:A:209:TYR:CD1	1:A:209:TYR:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:GLN:O	1:D:220:ASP:C	2.63	0.41
1:A:202:ARG:HD3	1:A:244:TRP:CD2	2.56	0.41
2:B:54:LEU:HD12	2:B:55:SER:H	1.86	0.41
2:B:56:PHE:HB3	2:B:62:PHE:CD1	2.56	0.41
4:G:147:PHE:CD1	4:G:163:ASP:HB3	2.56	0.41
1:A:233:THR:OG1	1:A:243:LYS:NZ	2.53	0.41
1:D:228:THR:HG22	1:D:229:GLU:N	2.35	0.41
5:J:126:TYR:HB3	5:J:131:TYR:HE1	1.85	0.41
5:J:140:TRP:HD1	5:J:174:TRP:CE3	2.38	0.41
1:D:73:ILE:HD12	3:F:8:PHE:CZ	2.56	0.41
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.56	0.40
4:I:110:SER:CB	5:J:171:PRO:HD3	2.51	0.40
4:G:117:ILE:HD11	4:G:153:ILE:HG21	2.03	0.40
3:C:7:LEU:HD23	3:C:7:LEU:HA	1.94	0.40
4:G:156:ASN:HA	4:G:157:PRO:HD2	1.92	0.40
4:I:119:LEU:HD12	4:I:129:LEU:O	2.20	0.40
1:D:7:TYR:CE2	3:F:2:MET:HB3	2.57	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	271/273 (99%)	238 (88%)	30 (11%)	3 (1%)	11	45
1	D	271/273 (99%)	235 (87%)	33 (12%)	3 (1%)	11	45
2	B	98/100 (98%)	93 (95%)	3 (3%)	2 (2%)	6	31
2	E	98/100 (98%)	93 (95%)	4 (4%)	1 (1%)	12	47
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	G	119/121 (98%)	101 (85%)	16 (13%)	2 (2%)	7	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	I	119/121 (98%)	92 (77%)	22 (18%)	5 (4%)	2	17
5	H	112/120 (93%)	93 (83%)	17 (15%)	2 (2%)	6	33
5	J	112/120 (93%)	94 (84%)	16 (14%)	2 (2%)	6	33
All	All	1214/1246 (97%)	1051 (87%)	143 (12%)	20 (2%)	7	36

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ASP
1	D	220	ASP
4	G	157	PRO
4	I	130	TRP
5	J	128	ASN
1	D	227	ASP
4	G	177	GLN
5	H	128	ASN
4	I	100	GLN
4	I	144	PHE
4	I	157	PRO
1	A	151	SER
1	A	227	ASP
1	D	151	SER
2	B	58	LYS
4	I	166	CYS
2	B	31	HIS
2	E	31	HIS
5	H	213	VAL
5	J	213	VAL

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	236/236 (100%)	218 (92%)	18 (8%)	12	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	236/236 (100%)	219 (93%)	17 (7%)	13	35
2	B	95/95 (100%)	91 (96%)	4 (4%)	26	48
2	E	95/95 (100%)	91 (96%)	4 (4%)	26	48
3	C	8/8 (100%)	7 (88%)	1 (12%)	4	17
3	F	8/8 (100%)	7 (88%)	1 (12%)	4	17
4	G	112/112 (100%)	98 (88%)	14 (12%)	4	17
4	I	112/112 (100%)	97 (87%)	15 (13%)	4	16
5	H	105/109 (96%)	98 (93%)	7 (7%)	15	36
5	J	105/109 (96%)	98 (93%)	7 (7%)	15	36
All	All	1112/1120 (99%)	1024 (92%)	88 (8%)	11	32

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	25	VAL
1	A	35	ARG
1	A	39	ASP
1	A	46	VAL
1	A	53	GLU
1	A	88	SER
1	A	110	LEU
1	A	122	ASP
1	A	138	THR
1	A	177	GLU
1	A	179	LEU
1	A	200	THR
1	A	227	ASP
1	A	233	THR
1	A	240	THR
1	A	254	GLU
1	A	270	VAL
2	B	73	THR
2	B	85	VAL
2	B	93	VAL
2	B	94	LYS
3	C	6	THR
1	D	6	LYS
1	D	25	VAL

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Mol	Chain	Res	Type
1	D	35	ARG
1	D	39	ASP
1	D	46	VAL
1	D	53	GLU
1	D	88	SER
1	D	122	ASP
1	D	138	THR
1	D	177	GLU
1	D	179	LEU
1	D	200	THR
1	D	227	ASP
1	D	233	THR
1	D	240	THR
1	D	254	GLU
1	D	270	VAL
2	E	73	THR
2	E	85	VAL
2	E	93	VAL
2	E	94	LYS
3	F	6	THR
4	G	64	LYS
4	G	76	SER
4	G	77	SER
4	G	78	GLU
4	G	106	ASP
4	G	109	SER
4	G	112	GLN
4	G	121	TYR
4	G	129	LEU
4	G	140	LEU
4	G	144	PHE
4	G	149	THR
4	G	177	GLN
4	G	178	LEU
5	H	145	LEU
5	H	166	LEU
5	H	172	SER
5	H	198	ILE
5	H	206	LEU
5	H	213	VAL
5	H	231	HIS
4	I	64	LYS

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Mol	Chain	Res	Type
4	I	77	SER
4	I	78	GLU
4	I	101	ASN
4	I	110	SER
4	I	116	TRP
4	I	132	ASN
4	I	134	SER
4	I	137	SER
4	I	139	TYR
4	I	144	PHE
4	I	150	LYS
4	I	158	ASN
4	I	160	ASN
4	I	177	GLN
5	J	145	LEU
5	J	166	LEU
5	J	172	SER
5	J	198	ILE
5	J	206	LEU
5	J	213	VAL
5	J	231	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	86	ASN
1	D	86	ASN
1	D	145	GLN
2	E	13	HIS
4	G	98	GLN
4	G	170	ASN
5	H	159	ASN
5	H	180	ASN
5	H	212	GLN
4	I	151	ASN
4	I	177	GLN
5	J	159	ASN
5	J	180	ASN
5	J	231	HIS

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	273/273 (100%)	0.79	28 (10%)	12 15	111, 111, 111, 111	0
1	D	273/273 (100%)	0.99	36 (13%)	7 11	111, 111, 111, 111	0
2	B	100/100 (100%)	1.21	15 (15%)	5 10	111, 111, 111, 111	0
2	E	100/100 (100%)	1.43	23 (23%)	2 5	111, 111, 111, 111	0
3	C	9/9 (100%)	0.66	0	100 100	111, 111, 111, 111	0
3	F	9/9 (100%)	0.43	0	100 100	111, 111, 111, 111	0
4	G	121/121 (100%)	0.77	9 (7%)	20 23	109, 111, 112, 114	0
4	I	121/121 (100%)	0.76	9 (7%)	20 23	109, 111, 112, 113	0
5	H	116/120 (96%)	0.80	10 (8%)	16 19	111, 111, 111, 114	0
5	J	116/120 (96%)	0.97	15 (12%)	7 12	111, 111, 111, 113	0
All	All	1238/1246 (99%)	0.93	145 (11%)	9 13	109, 111, 111, 114	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	58	LYS	6.0
5	J	204	ALA	5.7
4	I	179	ILE	5.3
4	G	179	ILE	5.2
1	D	253	GLU	4.7
5	J	199	LYS	4.7
1	D	252	GLY	4.5
5	H	204	ALA	4.4
4	I	77	SER	4.3
5	H	199	LYS	4.1
2	B	3	ARG	4.1
2	B	31	HIS	4.0
1	A	222	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
2	E	58	LYS	4.0
1	D	138	THR	4.0
1	D	53	GLU	4.0
2	E	1	ILE	3.9
2	B	19	LYS	3.8
1	A	224	HIS	3.7
5	J	128	ASN	3.7
2	E	98	ASP	3.7
5	J	183	HIS	3.6
1	D	197	HIS	3.5
5	J	117	GLY	3.5
2	E	75	LYS	3.4
2	B	88	SER	3.4
5	H	224	SER	3.4
2	B	71	THR	3.4
2	B	26	TYR	3.4
1	D	2	SER	3.4
1	D	250	PRO	3.4
2	E	20	SER	3.3
1	A	267	PRO	3.3
5	H	135	LYS	3.2
2	E	15	ALA	3.2
2	E	19	LYS	3.2
5	J	164	LYS	3.1
5	J	214	ASN	3.1
5	H	114	ARG	3.1
1	A	209	TYR	3.1
2	B	60	TRP	3.1
4	G	77	SER	3.1
2	E	2	GLN	3.1
5	J	153	SER	3.0
2	E	48	LYS	3.0
1	A	43	PRO	3.0
1	D	181	HIS	2.9
1	D	248	VAL	2.9
2	B	1	ILE	2.9
2	E	88	SER	2.9
1	D	16	GLY	2.9
1	D	249	VAL	2.8
5	J	185	PRO	2.8
2	E	47	GLU	2.8
1	D	98	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	250	PRO	2.8
5	H	115	HIS	2.7
4	G	63	GLU	2.7
5	J	122	GLU	2.7
2	E	94	LYS	2.7
1	D	139	ALA	2.7
1	D	274	TRP	2.7
2	E	85	VAL	2.7
1	D	135	ALA	2.6
1	D	177	GLU	2.6
4	G	178	LEU	2.6
5	J	113	ALA	2.6
1	A	138	THR	2.6
1	A	112	GLY	2.5
1	D	41	ALA	2.5
1	D	226	GLN	2.5
5	J	161	GLU	2.5
1	A	176	LYS	2.5
2	B	0	MET	2.5
1	D	273	ARG	2.5
1	D	224	HIS	2.5
2	B	57	SER	2.5
1	A	212	GLU	2.5
4	I	92	GLN	2.5
2	E	16	GLU	2.4
2	B	18	GLY	2.4
1	D	133	TRP	2.4
2	E	70	PHE	2.4
1	A	183	GLU	2.4
2	E	32	PRO	2.4
2	E	57	SER	2.4
1	A	220	ASP	2.4
2	E	22	PHE	2.4
1	D	149	ASP	2.4
4	I	169	LYS	2.4
1	A	264	GLU	2.4
2	E	4	THR	2.4
4	I	124	GLU	2.4
2	E	3	ARG	2.4
4	G	158	ASN	2.4
1	D	19	GLU	2.3
4	G	79	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
5	H	113	ALA	2.3
1	A	194	ILE	2.3
1	A	268	GLU	2.3
1	A	195	SER	2.3
5	H	122	GLU	2.3
1	D	148	ASN	2.3
1	A	232	GLU	2.3
4	I	176	GLN	2.3
1	A	221	GLY	2.2
1	D	237	GLY	2.2
1	A	131	ARG	2.2
1	D	255	GLN	2.2
2	B	73	THR	2.2
5	J	176	GLY	2.2
2	E	14	PRO	2.2
1	D	145	GLN	2.2
1	D	123	TYR	2.2
1	D	79	ARG	2.2
4	G	126	THR	2.2
1	A	256	ARG	2.2
2	E	0	MET	2.2
4	I	142	PRO	2.2
1	D	62	ARG	2.2
1	A	233	THR	2.2
1	A	16	GLY	2.1
1	D	40	ALA	2.1
1	D	180	LEU	2.1
2	B	75	LYS	2.1
1	A	273	ARG	2.1
1	A	68	ARG	2.1
4	G	174	CYS	2.1
5	J	114	ARG	2.1
1	A	88	SER	2.1
1	D	154	GLU	2.1
4	I	91	SER	2.1
4	I	72	CYS	2.1
5	H	180	ASN	2.1
1	D	239	GLY	2.1
1	A	198	GLU	2.1
1	A	197	HIS	2.0
1	A	42	SER	2.0
1	D	88	SER	2.0

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Mol	Chain	Res	Type	RSRZ
5	H	232	LYS	2.0
5	J	219	ALA	2.0
2	E	73	THR	2.0
1	D	267	PRO	2.0
2	B	72	PRO	2.0
4	G	59	CYS	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.