



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:51 pm GMT

PDB ID : 3CII  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

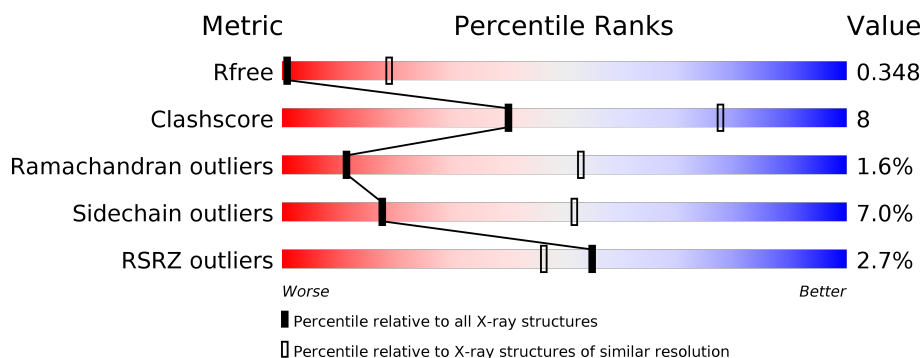
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	1003 (5.20-3.64)
Clashscore	112137	1021 (5.08-3.70)
Ramachandran outliers	110173	1018 (5.08-3.66)
Sidechain outliers	110143	1000 (5.08-3.66)
RSRZ outliers	101464	1011 (5.20-3.64)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>78%</div> <div>18%</div> <div>•</div> </div>
1	D	273	<div> <div>3%</div> <div>79%</div> <div>19%</div> <div>•</div> </div>
2	B	100	<div> <div>8%</div> <div>83%</div> <div>16%</div> <div>•</div> </div>
2	E	100	<div> <div>4%</div> <div>85%</div> <div>14%</div> <div>•</div> </div>
3	C	9	<div> <div>67%</div> <div>22%</div> <div>11%</div> </div>
3	F	9	<div> <div>56%</div> <div>33%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	121	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>65%</div><div>29%</div><div>6%</div></div></div>
4	I	121	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>64%</div><div>32%</div><div></div></div></div>
5	H	120	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>77%</div><div>18%</div><div></div></div></div>
5	J	120	<div><div><div></div><div></div><div></div></div><div><div>7%</div><div>69%</div><div>25%</div><div></div></div></div>

## 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			

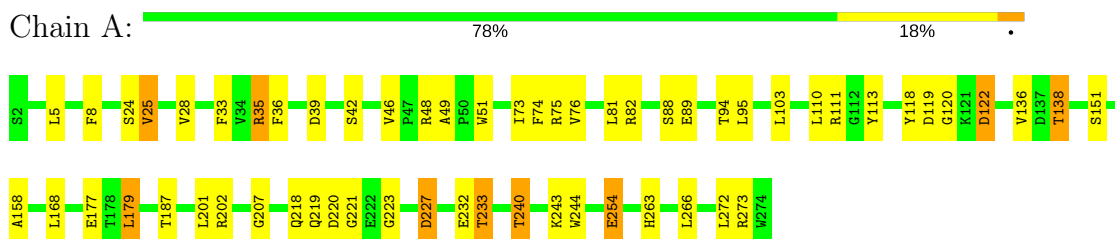
- Molecule 5 is a protein called NKG2-A/NKG2-B type II integral membrane protein.

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			

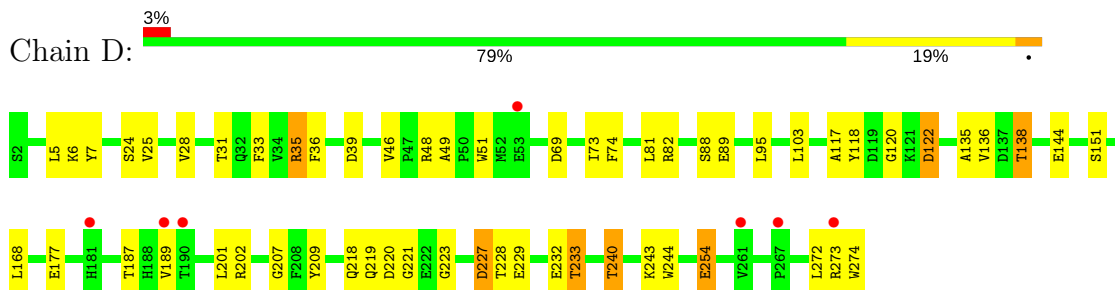
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

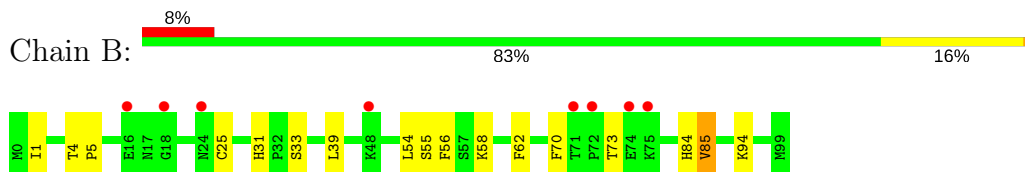
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E



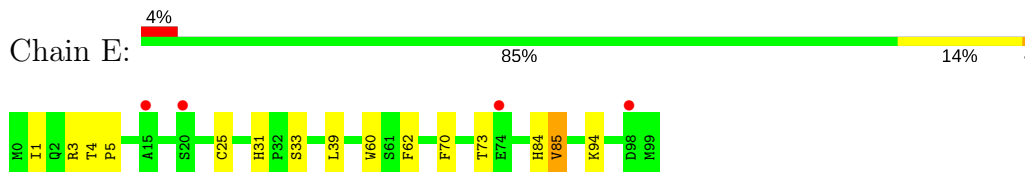
- Molecule 1: HLA class I histocompatibility antigen, alpha chain E



- Molecule 2: Beta-2-microglobulin

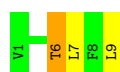


- Molecule 2: Beta-2-microglobulin

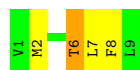


- Molecule 3: HLA class I histocompatibility antigen peptide

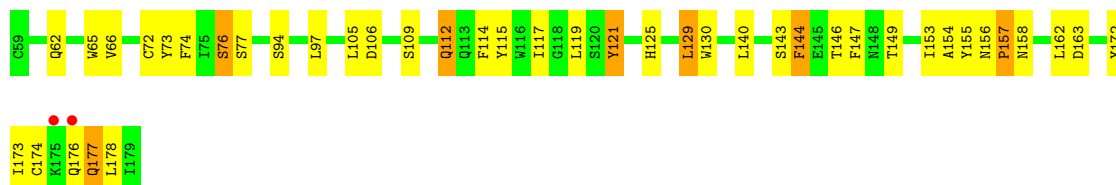




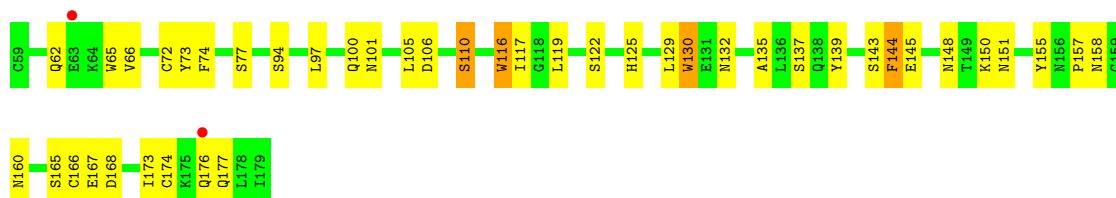
- Molecule 3: HLA class I histocompatibility antigen peptide



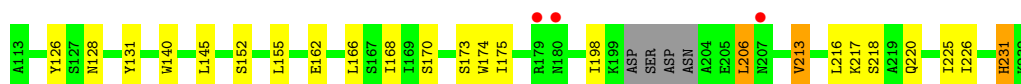
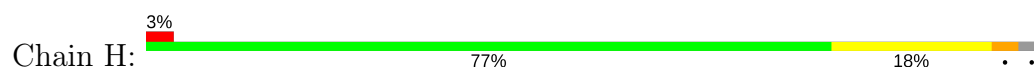
- Molecule 4: Natural killer cells antigen CD94



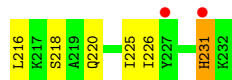
- Molecule 4: Natural killer cells antigen CD94



- 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, $\alpha$ , $\beta$ , $\gamma$	345.98Å 345.98Å 345.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.88 – 4.41 67.85 – 4.41	Depositor EDS
% Data completeness (in resolution range)	100.0 (67.88-4.41) 100.0 (67.85-4.41)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	10.74 (at 4.46Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.321 , 0.355 0.311 , 0.348	Depositor DCC
$R_{free}$ test set	1150 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	101.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 179.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.77	EDS
Total number of atoms	10146	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.47	0/2300	0.58	0/3127
1	D	0.46	0/2300	0.56	0/3127
2	B	0.50	0/860	0.58	0/1162
2	E	0.46	0/860	0.57	0/1162
3	C	0.40	0/74	0.70	0/98
3	F	0.39	0/74	0.67	0/98
4	G	0.59	0/1023	0.65	0/1383
4	I	0.53	0/1023	0.58	0/1383
5	H	0.49	0/955	0.58	0/1286
5	J	0.47	0/955	0.56	0/1286
All	All	0.49	0/10424	0.58	0/14112

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.

There are no bond angle outliers.

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	39	0
1	D	2234	0	2072	35	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	28	0
4	I	997	0	905	22	0
5	H	932	0	896	15	0
5	J	932	0	896	20	0
All	All	10146	0	9518	164	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (164) 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
3:F:6:THR:HG22	3:F:7:LEU:H	1.48	0.78
4:I:117:ILE:HD13	4:I:155:TYR:HB2	1.65	0.77
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:175:ILE:HD13	5:H:216:LEU:HD22	1.84	0.60
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
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
1:D:31:THR:OG1	1:D:209:TYR:OH	2.22	0.57
4:G:119:LEU:HD13	4:G:130:TRP:CE3	2.39	0.57
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
1:A:158:ALA:HA	5:H:217:LYS:HZ1	1.71	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
5:J:173:SER:HA	5:J:226:ILE:O	2.14	0.48
4:G:125:HIS:ND1	4:G:129:LEU:HD11	2.28	0.48
4:G:65:TRP:CE3	4:G:74:PHE:HB2	2.49	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
5:H:168:ILE:HG22	5:H:168:ILE:O	2.16	0.46
2:B:1:ILE:HD11	2:E:3:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:219:GLN:O	1:D:221:GLY:N	2.50	0.44
1:A:49:ALA:HB1	1:A:51:TRP:NE1	2.33	0.44
1:A:113:TYR:C	1:A:113:TYR:CD1	2.91	0.44
4:I:165:SER:C	4:I:167:GLU:H	2.21	0.44
2:E:4:THR:HG23	2:E:5:PRO:HD2	2.00	0.44
5:H:225:ILE:CG2	5:H:226:ILE:N	2.81	0.44
4:G:121:TYR:CD2	4:G:121:TYR:C	2.91	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
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: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:35:ARG:HG2	1:A:48:ARG:HD3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:NE	1:A:89:GLU:HA	2.34	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: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
5:J:127:SER:C	5:J:129:SER:H	2.23	0.41
5:J:159:ASN:C	5:J:161:GLU:H	2.24	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:HA	3:C:7:LEU:HD23	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 [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	271/273 (99%)	238 (88%)	30 (11%)	3 (1%)	17 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	271/273 (99%)	235 (87%)	33 (12%)	3 (1%)	17	60
2	B	98/100 (98%)	93 (95%)	3 (3%)	2 (2%)	9	48
2	E	98/100 (98%)	93 (95%)	4 (4%)	1 (1%)	18	61
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%)	11	52
4	I	119/121 (98%)	92 (77%)	22 (18%)	5 (4%)	3	32
5	H	112/120 (93%)	93 (83%)	17 (15%)	2 (2%)	10	50
5	J	112/120 (93%)	94 (84%)	16 (14%)	2 (2%)	10	50
All	All	1214/1246 (97%)	1051 (87%)	143 (12%)	20 (2%)	11	53

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%)	221 (94%)	15 (6%)	20	54
1	D	236/236 (100%)	222 (94%)	14 (6%)	23	57
2	B	95/95 (100%)	91 (96%)	4 (4%)	34	66
2	E	95/95 (100%)	91 (96%)	4 (4%)	34	66
3	C	8/8 (100%)	7 (88%)	1 (12%)	5	28
3	F	8/8 (100%)	7 (88%)	1 (12%)	5	28
4	G	112/112 (100%)	100 (89%)	12 (11%)	8	34
4	I	112/112 (100%)	99 (88%)	13 (12%)	6	31
5	H	105/109 (96%)	99 (94%)	6 (6%)	24	58
5	J	105/109 (96%)	97 (92%)	8 (8%)	15	49
All	All	1112/1120 (99%)	1034 (93%)	78 (7%)	18	52

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	35	ARG
1	A	39	ASP
1	A	42	SER
1	A	46	VAL
1	A	88	SER
1	A	122	ASP
1	A	138	THR
1	A	177	GLU
1	A	179	LEU
1	A	227	ASP
1	A	233	THR
1	A	240	THR
1	A	254	GLU
1	A	273	ARG
2	B	70	PHE

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Mol	Chain	Res	Type
2	B	73	THR
2	B	85	VAL
2	B	94	LYS
3	C	6	THR
1	D	6	LYS
1	D	25	VAL
1	D	35	ARG
1	D	39	ASP
1	D	46	VAL
1	D	88	SER
1	D	122	ASP
1	D	138	THR
1	D	177	GLU
1	D	227	ASP
1	D	233	THR
1	D	240	THR
1	D	254	GLU
1	D	273	ARG
2	E	70	PHE
2	E	73	THR
2	E	85	VAL
2	E	94	LYS
3	F	6	THR
4	G	76	SER
4	G	77	SER
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	198	ILE
5	H	206	LEU
5	H	213	VAL
5	H	220	GLN
5	H	231	HIS
4	I	77	SER

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Mol	Chain	Res	Type
4	I	101	ASN
4	I	110	SER
4	I	116	TRP
4	I	132	ASN
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	168	ASP
4	I	177	GLN
5	J	114	ARG
5	J	145	LEU
5	J	172	SER
5	J	198	ILE
5	J	206	LEU
5	J	213	VAL
5	J	220	GLN
5	J	231	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
4	G	98	GLN
5	H	212	GLN
4	I	101	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	273/273 (100%)	0.07	0 <span>100</span> <span>100</span>	111, 111, 111, 111	0
1	D	273/273 (100%)	0.29	7 (2%) 56 47	111, 111, 111, 111	0
2	B	100/100 (100%)	0.45	8 (8%) <span>13</span> <span>12</span>	111, 111, 111, 111	0
2	E	100/100 (100%)	0.41	4 (4%) <span>39</span> <span>31</span>	111, 111, 111, 111	0
3	C	9/9 (100%)	-0.26	0 <span>100</span> <span>100</span>	111, 111, 111, 111	0
3	F	9/9 (100%)	-0.29	0 <span>100</span> <span>100</span>	111, 111, 111, 111	0
4	G	121/121 (100%)	0.04	2 (1%) <span>70</span> <span>63</span>	109, 111, 112, 114	0
4	I	121/121 (100%)	0.21	2 (1%) <span>70</span> <span>63</span>	109, 111, 112, 113	0
5	H	116/120 (96%)	0.60	3 (2%) <span>56</span> <span>47</span>	111, 111, 111, 114	0
5	J	116/120 (96%)	0.67	8 (6%) <span>18</span> <span>15</span>	111, 111, 111, 113	0
All	All	1238/1246 (99%)	0.29	34 (2%) <span>55</span> <span>46</span>	109, 111, 111, 114	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	H	180	ASN	4.0
4	I	176	GLN	3.4
2	B	74	GLU	3.1
5	J	128	ASN	3.0
5	H	207	ASN	2.8
2	B	72	PRO	2.7
2	E	15	ALA	2.6
5	J	186	TRP	2.6
2	E	20	SER	2.6
1	D	53	GLU	2.5
1	D	273	ARG	2.5
2	B	71	THR	2.5
1	D	181	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	16	GLU	2.4
2	B	75	LYS	2.4
1	D	267	PRO	2.4
5	J	179	ARG	2.4
1	D	189	VAL	2.4
2	B	48	LYS	2.4
2	E	98	ASP	2.3
5	J	180	ASN	2.3
2	B	18	GLY	2.2
1	D	261	VAL	2.2
1	D	190	THR	2.2
4	G	176	GLN	2.2
2	E	74	GLU	2.2
2	B	24	ASN	2.1
5	J	227	TYR	2.1
5	J	231	HIS	2.1
5	J	182	SER	2.0
5	J	214	ASN	2.0
5	H	179	ARG	2.0
4	G	175	LYS	2.0
4	I	63	GLU	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 carbohydrates 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.