



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 09:03 pm GMT

PDB ID : 3CDG
Title : Human CD94/NKG2A in complex with HLA-E
Authors : Petrie, E.J.; Clements, C.S.; Lin, J.; Sullivan, L.C.; Johnson, D.; Huyton, T.; Heroux, A.; Hoare, H.L.; Beddoe, T.; Reid, H.H.; Wilce, M.C.J.; Brooks, A.G.; Rossjohn, J.
Deposited on : 2008-02-26
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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

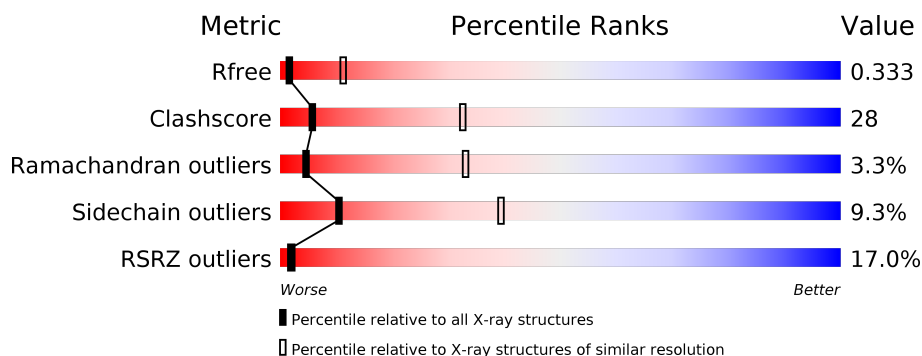
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (3.50-3.30)

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 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 $\leq 5\%$. 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>14%</div> <div>56%</div> <div>38%</div> <div>6%</div> </div>
1	C	273	<div> <div>18%</div> <div>58%</div> <div>36%</div> <div>5%</div> </div>
2	B	100	<div> <div>15%</div> <div>59%</div> <div>36%</div> <div>5%</div> </div>
2	D	100	<div> <div>23%</div> <div>62%</div> <div>33%</div> <div>5%</div> </div>
3	E	123	<div> <div>20%</div> <div>52%</div> <div>39%</div> <div>8%</div> <div>.</div> </div>
3	J	123	<div> <div>15%</div> <div>52%</div> <div>38%</div> <div>9%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	120	<div><div></div><div>16%</div><div>38%</div><div>53%</div><div>8%</div></div>
4	K	120	<div><div></div><div>18%</div><div>40%</div><div>53%</div><div></div></div>
5	P	9	<div><div></div><div>44%</div><div>22%</div><div>56%</div><div>22%</div></div>
5	Q	9	<div><div></div><div>33%</div><div>22%</div><div>67%</div><div>11%</div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10200 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	C	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	D	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	-	EXPRESSION TAG	UNP P61769
D	0	MET	-	EXPRESSION TAG	UNP P61769

- Molecule 3 is a protein called Natural killer cells antigen CD94.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	123	Total	C	N	O	S	0	0	0
			1010	632	167	201	10			
3	E	123	Total	C	N	O	S	0	0	0
			1010	632	167	201	10			

- Molecule 4 is a protein called NKG2-A/NKG2-B type II integral membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	116	Total	C	N	O	S	0	0	0
			931	585	166	171	9			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	120	Total	C	N	O	S	0	0	0
			961	600	171	181	9			

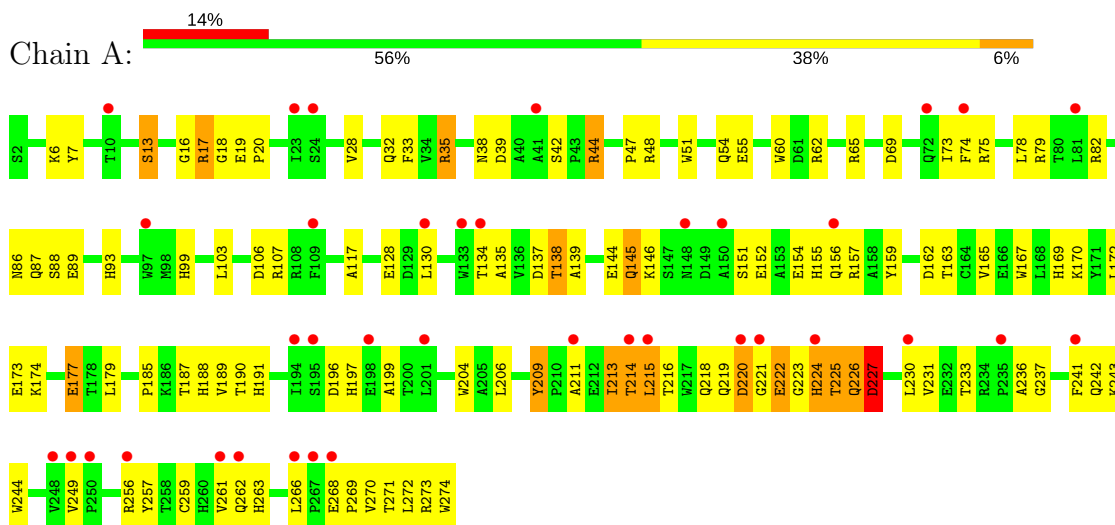
- Molecule 5 is a protein called leader peptide of HLA class I histocompatibility antigen, alpha chain G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	9	Total	C	N	O	S	0	0	0
			73	49	12	11	1			
5	Q	9	Total	C	N	O	S	0	0	0
			73	49	12	11	1			

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

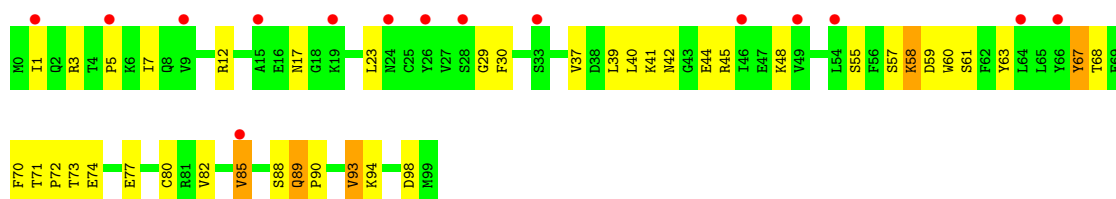


- Molecule 1: HLA class I histocompatibility antigen, alpha chain E

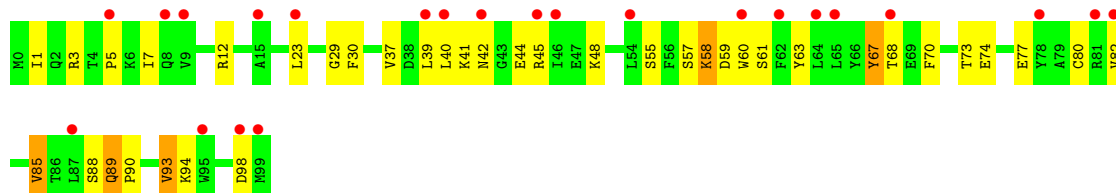


- Molecule 2: Beta-2-microglobulin

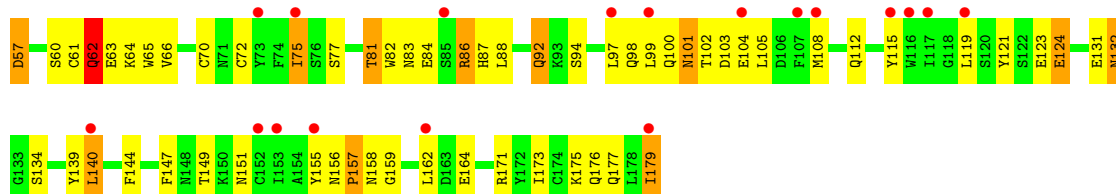




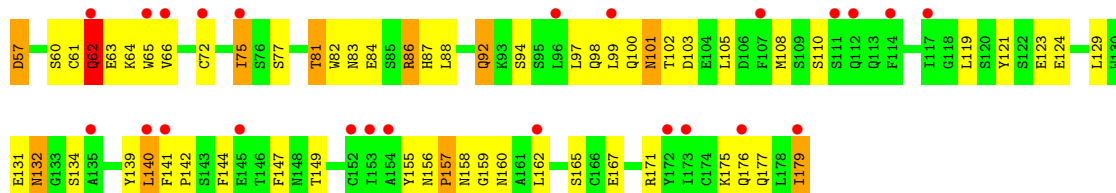
• Molecule 2: Beta-2-microglobulin



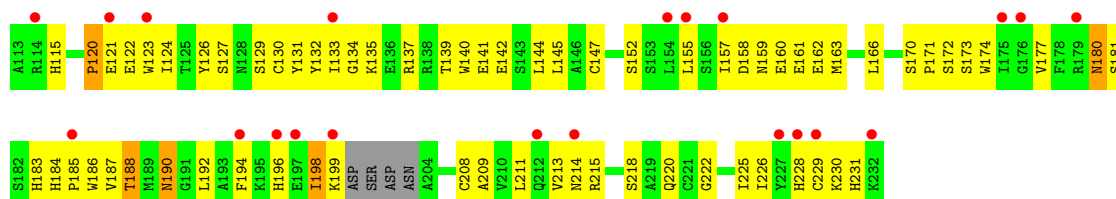
• Molecule 3: Natural killer cells antigen CD94



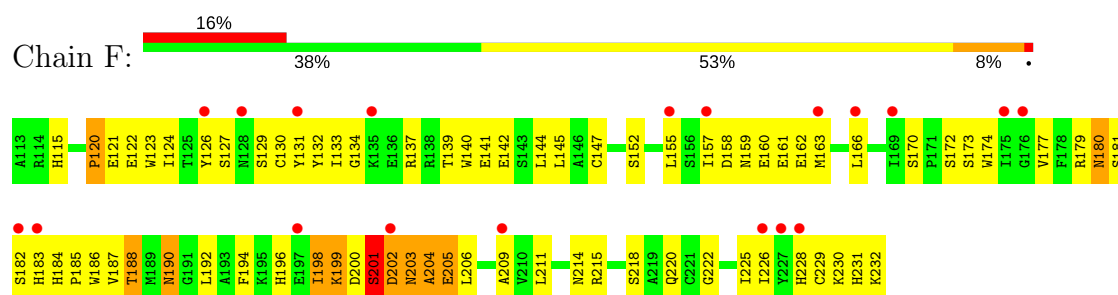
• Molecule 3: Natural killer cells antigen CD94



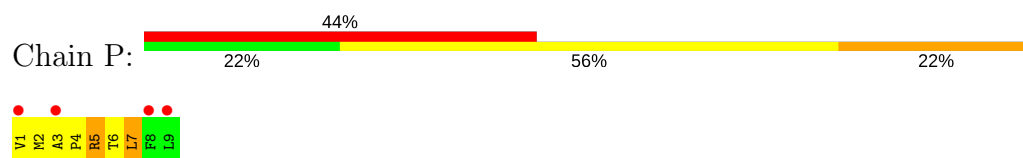
• Molecule 4: NKG2-A/NKG2-B type II integral membrane protein



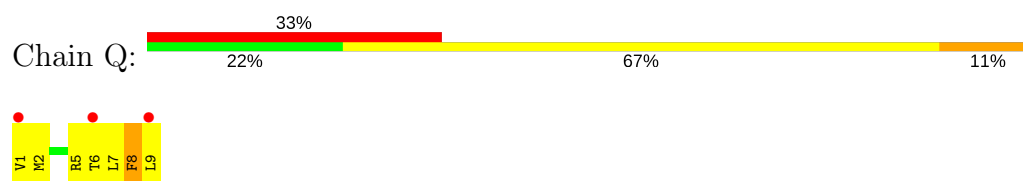
• Molecule 4: NKG2-A/NKG2-B type II integral membrane protein



- Molecule 5: leader peptide of HLA class I histocompatibility antigen, alpha chain G



- Molecule 5: leader peptide of HLA class I histocompatibility antigen, alpha chain G



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	345.20Å 345.20Å 345.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 140.93 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.40) 99.9 (140.93-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.249 , 0.279 0.307 , 0.333	Depositor DCC
R_{free} test set	2434 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	100.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 107.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	10200	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.34% 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	0.36	0/2300	0.52	1/3127 (0.0%)
1	C	0.36	0/2300	0.53	1/3127 (0.0%)
2	B	0.36	0/860	0.47	0/1162
2	D	0.35	0/860	0.46	0/1162
3	E	0.36	0/1036	0.51	1/1402 (0.1%)
3	J	0.37	0/1036	0.51	1/1402 (0.1%)
4	F	0.30	0/985	0.48	0/1330
4	K	0.30	0/954	0.47	0/1286
5	P	0.30	0/74	0.62	0/98
5	Q	0.31	0/74	0.59	0/98
All	All	0.35	0/10479	0.51	4/14194 (0.0%)

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
4	F	3	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	227	ASP	CB-CG-OD2	5.22	123.00	118.30
3	J	57	ASP	CB-CG-OD2	5.20	122.98	118.30
3	E	57	ASP	CB-CG-OD2	5.20	122.97	118.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	199	LYS	CA
4	F	200	ASP	CA
4	F	203	ASN	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	205	GLU	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	148	0
1	C	2234	0	2072	135	0
2	B	837	0	803	36	0
2	D	837	0	803	36	0
3	E	1010	0	913	54	0
3	J	1010	0	913	63	0
4	F	961	0	915	81	0
4	K	931	0	895	58	0
5	P	73	0	83	11	0
5	Q	73	0	83	8	0
All	All	10200	0	9552	554	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 28.

The worst 5 of 554 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:221:GLY:O	1:A:222:GLU:HG3	1.07	1.23
1:C:221:GLY:O	1:C:222:GLU:HG3	1.08	1.22
1:A:219:GLN:HE21	1:A:225:THR:CG2	1.58	1.16
1:A:219:GLN:HE21	1:A:225:THR:HG22	1.14	1.13
1:C:219:GLN:HE21	1:C:225:THR:CG2	1.61	1.13

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%)	225 (83%)	35 (13%)	11 (4%)	3	27
1	C	271/273 (99%)	226 (83%)	35 (13%)	10 (4%)	4	30
2	B	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	18	59
2	D	98/100 (98%)	89 (91%)	9 (9%)	0	100	100
3	E	121/123 (98%)	101 (84%)	16 (13%)	4 (3%)	4	33
3	J	121/123 (98%)	101 (84%)	16 (13%)	4 (3%)	4	33
4	F	118/120 (98%)	91 (77%)	21 (18%)	6 (5%)	2	21
4	K	112/120 (93%)	91 (81%)	17 (15%)	4 (4%)	4	31
5	P	7/9 (78%)	4 (57%)	3 (43%)	0	100	100
5	Q	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
All	All	1224/1250 (98%)	1023 (84%)	161 (13%)	40 (3%)	4	33

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	ILE
1	A	215	LEU
1	A	222	GLU
1	A	224	HIS
3	J	62	GLN

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	236/236 (100%)	214 (91%)	22 (9%)	10	39
1	C	236/236 (100%)	216 (92%)	20 (8%)	12	45
2	B	95/95 (100%)	87 (92%)	8 (8%)	13	45
2	D	95/95 (100%)	87 (92%)	8 (8%)	13	45
3	E	114/114 (100%)	102 (90%)	12 (10%)	8	34
3	J	114/114 (100%)	101 (89%)	13 (11%)	7	29
4	F	109/109 (100%)	99 (91%)	10 (9%)	11	40
4	K	105/109 (96%)	98 (93%)	7 (7%)	19	57
5	P	8/8 (100%)	6 (75%)	2 (25%)	1	3
5	Q	8/8 (100%)	6 (75%)	2 (25%)	1	3
All	All	1120/1124 (100%)	1016 (91%)	104 (9%)	10	39

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	K	190	ASN
1	C	128	GLU
4	F	199	LYS
4	K	198	ILE
1	C	17	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
4	K	214	ASN
1	C	115	GLN
4	F	190	ASN
4	K	228	HIS
1	C	32	GLN

5.3.3 RNA ⓘ

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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	1.12	37 (13%) 3 4	34, 115, 173, 251	0
1	C	273/273 (100%)	1.16	48 (17%) 2 2	34, 115, 172, 251	0
2	B	100/100 (100%)	1.25	15 (15%) 3 3	74, 102, 161, 184	0
2	D	100/100 (100%)	1.28	23 (23%) 1 1	75, 104, 161, 184	0
3	E	123/123 (100%)	1.25	24 (19%) 1 1	38, 109, 150, 203	0
3	J	123/123 (100%)	1.27	18 (14%) 3 3	37, 107, 150, 203	0
4	F	120/120 (100%)	1.15	19 (15%) 2 2	41, 128, 167, 221	0
4	K	116/120 (96%)	1.21	21 (18%) 1 2	93, 128, 165, 178	0
5	P	9/9 (100%)	1.90	4 (44%) 0 0	95, 102, 117, 126	0
5	Q	9/9 (100%)	1.52	3 (33%) 0 0	92, 99, 120, 130	0
All	All	1246/1250 (99%)	1.20	212 (17%) 2 2	34, 115, 165, 251	0

The worst 5 of 212 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	179	ILE	10.0
3	E	179	ILE	6.6
4	F	182	SER	6.5
1	A	249	VAL	4.3
4	F	135	LYS	3.7

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.