



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 08:48 AM GMT

PDB ID : 2ZSW  
Title : Crystal structure of H-2Kb in complex with the Q600Y variant of JH1V epitope S598  
Authors : Theodossis, A.; Dunstone, M.A.; Rossjohn, J.  
Deposited on : 2008-09-18  
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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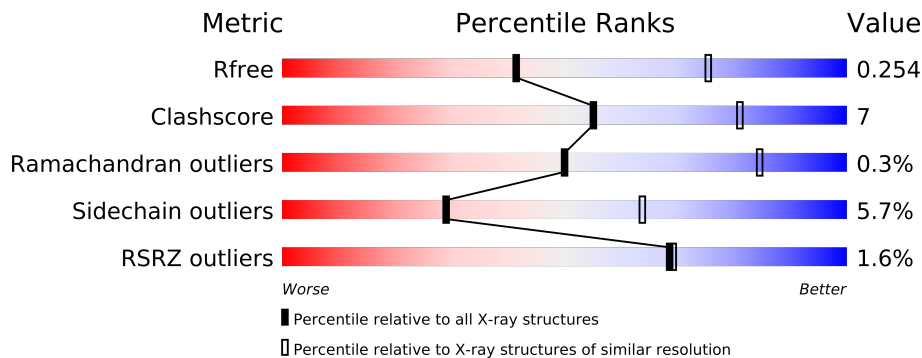
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	278	
1	C	278	
1	E	278	
1	G	278	
2	B	99	
2	D	99	
2	F	99	
2	H	99	
3	M	8	
3	N	8	
3	O	8	
3	P	8	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12321 atoms, of which 0 are hydrogen and 0 are deuterium.

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, K-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2192	1389	379	415	9			
1	E	277	Total	C	N	O	S	0	2	0
			2216	1409	383	415	9			
1	C	277	Total	C	N	O	S	0	0	0
			2166	1375	370	413	8			
1	G	277	Total	C	N	O	S	0	0	0
			2151	1367	362	414	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	98	Total	C	N	O	S	0	0	0
			791	506	131	147	7			
2	F	98	Total	C	N	O	S	0	0	0
			799	511	134	147	7			
2	B	98	Total	C	N	O	S	0	0	0
			795	507	132	149	7			
2	D	98	Total	C	N	O	S	0	0	0
			794	508	132	147	7			

- Molecule 3 is a protein called 8-mer peptide from spike glycoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	8	Total	C	N	O	0	0	0
			67	46	10	11			
3	N	8	Total	C	N	O	0	0	0
			68	47	10	11			
3	O	8	Total	C	N	O	0	0	0
			66	46	9	11			
3	P	8	Total	C	N	O	0	0	0
			67	46	10	11			

- Molecule 4 is water.

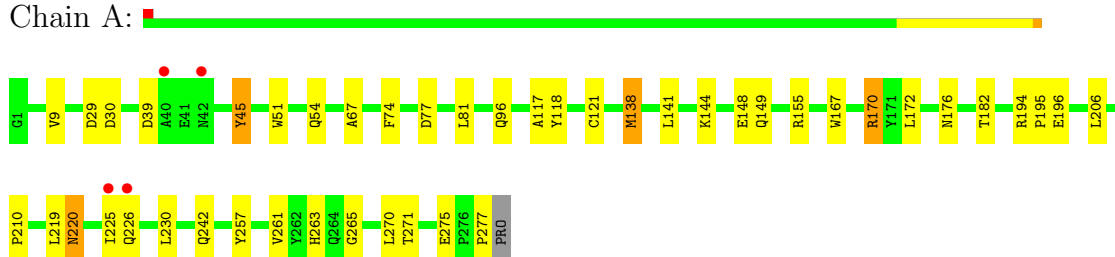
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total 23	O 23	0	0
4	E	33	Total 33	O 33	0	0
4	C	13	Total 13	O 13	0	0
4	G	14	Total 14	O 14	0	0
4	H	14	Total 14	O 14	0	0
4	F	20	Total 20	O 20	0	0
4	B	13	Total 13	O 13	0	0
4	D	13	Total 13	O 13	0	0
4	M	1	Total 1	O 1	0	0
4	N	3	Total 3	O 3	0	0
4	O	2	Total 2	O 2	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

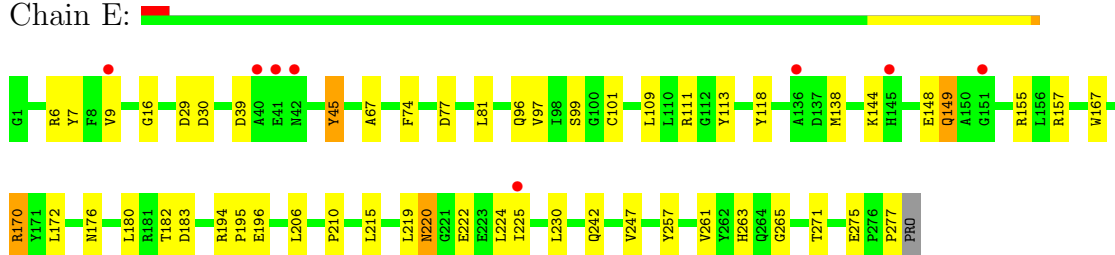
- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain

Chain A:



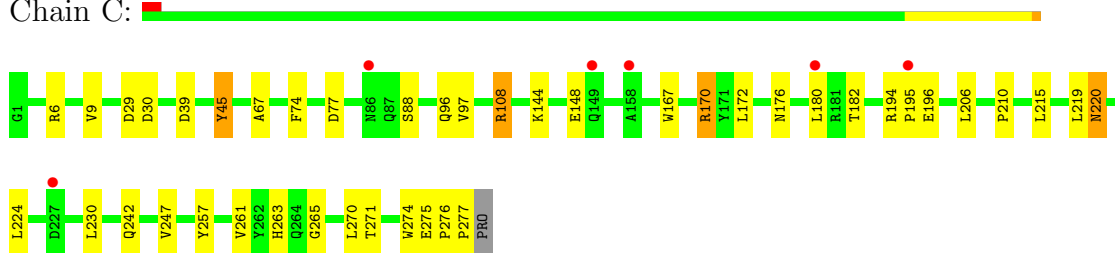
- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain

Chain E:



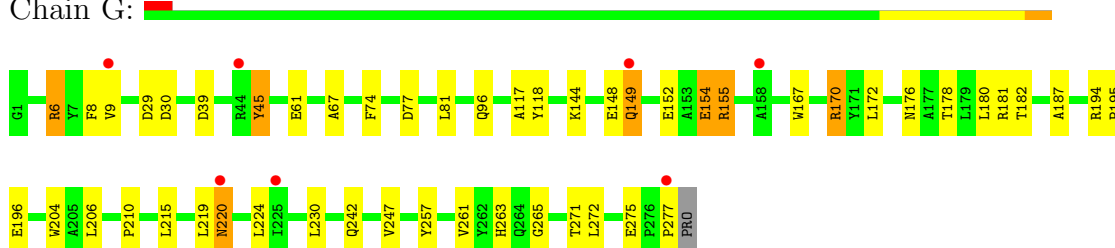
- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain

Chain C:



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

Chain G:



- Molecule 2: Beta-2-microglobulin

Chain H: 



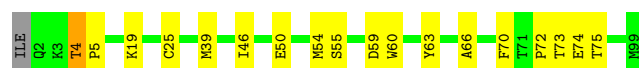
- Molecule 2: Beta-2-microglobulin

Chain F: 



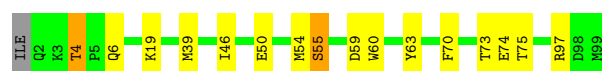
- Molecule 2: Beta-2-microglobulin

Chain B: 



- Molecule 2: Beta-2-microglobulin

Chain D: 



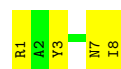
- Molecule 3: 8-mer peptide from spike glycoprotein

Chain M: 



- Molecule 3: 8-mer peptide from spike glycoprotein

Chain N: 



- Molecule 3: 8-mer peptide from spike glycoprotein

Chain O: 



- Molecule 3: 8-mer peptide from spike glycoprotein

Chain P: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.71Å 90.15Å 91.97Å 81.11° 70.58° 68.25°	Depositor
Resolution (Å)	27.00 – 2.80 26.86 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (27.00-2.80) 95.9 (26.86-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.212 , 0.253 0.212 , 0.254	Depositor DCC
$R_{free}$ test set	2240 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 10.8	EDS
Estimated twinning fraction	0.011 for h,h-l,k 0.011 for h,l,h-k 0.078 for h,h-k,h-l 0.089 for -h,-h+k,-l 0.058 for -h,-k,-h+l 0.020 for -h,-h+l,-h+k 0.014 for -h,-l,-k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 44262 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	12321	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ABA

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	0.67	1/2254 (0.0%)	0.68	1/3075 (0.0%)
1	C	0.63	0/2228	0.69	0/3042
1	E	0.65	0/2285	0.69	0/3112
1	G	0.62	0/2213	0.78	3/3024 (0.1%)
2	B	0.66	0/821	0.70	0/1118
2	D	0.65	0/820	0.70	0/1116
2	F	0.76	0/825	0.72	0/1121
2	H	0.71	0/817	0.72	0/1113
3	M	0.59	0/61	0.58	0/78
3	N	0.68	0/62	0.62	0/79
3	O	0.55	0/60	0.59	0/77
3	P	0.58	0/61	0.60	0/78
All	All	0.66	1/12507 (0.0%)	0.71	4/17033 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	CYS	CB-SG	-5.74	1.72	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	155	ARG	NE-CZ-NH1	-16.60	112.00	120.30
1	G	155	ARG	NE-CZ-NH2	15.92	128.26	120.30
1	G	155	ARG	CD-NE-CZ	7.32	133.85	123.60
1	A	155	ARG	NE-CZ-NH2	-5.30	117.65	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2192	0	2034	25	0
1	C	2166	0	1985	27	0
1	E	2216	0	2079	31	0
1	G	2151	0	1948	33	0
2	B	795	0	735	12	0
2	D	794	0	737	10	0
2	F	799	0	753	8	0
2	H	791	0	728	14	0
3	M	67	0	67	0	0
3	N	68	0	68	2	0
3	O	66	0	65	0	0
3	P	67	0	67	1	0
4	A	23	0	0	0	0
4	B	13	0	0	0	0
4	C	13	0	0	0	0
4	D	13	0	0	2	0
4	E	33	0	0	3	0
4	F	20	0	0	0	0
4	G	14	0	0	0	0
4	H	14	0	0	0	0
4	M	1	0	0	0	0
4	N	3	0	0	1	0
4	O	2	0	0	0	0
All	All	12321	0	11266	157	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

The worst 5 of 157 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:108:ARG:HH21	1:C:108:ARG:HG2	1.30	0.95
2:D:73:THR:HG22	2:D:74:GLU:N	1.96	0.80
2:F:73:THR:HG22	2:F:74:GLU:N	1.97	0.79
1:C:167:TRP:CZ3	1:C:170:ARG:HD3	2.23	0.74
1:E:167:TRP:CZ3	1:E:170:ARG:HD3	2.24	0.73

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	275/278 (99%)	263 (96%)	11 (4%)	1 (0%)	43	80
1	C	275/278 (99%)	265 (96%)	9 (3%)	1 (0%)	43	80
1	E	277/278 (100%)	264 (95%)	12 (4%)	1 (0%)	43	80
1	G	275/278 (99%)	263 (96%)	11 (4%)	1 (0%)	43	80
2	B	96/99 (97%)	92 (96%)	4 (4%)	0	100	100
2	D	96/99 (97%)	93 (97%)	3 (3%)	0	100	100
2	F	96/99 (97%)	93 (97%)	3 (3%)	0	100	100
2	H	96/99 (97%)	92 (96%)	4 (4%)	0	100	100
3	M	5/8 (62%)	5 (100%)	0	0	100	100
3	N	5/8 (62%)	5 (100%)	0	0	100	100
3	O	5/8 (62%)	5 (100%)	0	0	100	100
3	P	5/8 (62%)	5 (100%)	0	0	100	100
All	All	1506/1540 (98%)	1445 (96%)	57 (4%)	4 (0%)	50	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	E	220	ASN
1	C	220	ASN
1	G	220	ASN

### 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	220/236 (93%)	212 (96%)	8 (4%)	47	82
1	C	213/236 (90%)	202 (95%)	11 (5%)	32	68
1	E	223/236 (94%)	210 (94%)	13 (6%)	28	63
1	G	209/236 (89%)	197 (94%)	12 (6%)	29	64
2	B	87/94 (93%)	83 (95%)	4 (5%)	37	73
2	D	86/94 (92%)	79 (92%)	7 (8%)	17	43
2	F	88/94 (94%)	83 (94%)	5 (6%)	29	64
2	H	85/94 (90%)	80 (94%)	5 (6%)	28	62
3	M	5/6 (83%)	4 (80%)	1 (20%)	2	6
3	N	6/6 (100%)	4 (67%)	2 (33%)	0	1
3	O	5/6 (83%)	4 (80%)	1 (20%)	2	6
3	P	5/6 (83%)	4 (80%)	1 (20%)	2	6
All	All	1232/1344 (92%)	1162 (94%)	70 (6%)	29	64

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	271	THR
1	G	182	THR
2	D	97	ARG
1	G	6	ARG
1	G	149	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	220	ASN
3	N	7	ASN
1	C	263	HIS
1	A	263	HIS
1	G	263	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ABA	M	2	3	5,5,6	8.00	2 (40%)	3,5,7	1.59	1 (33%)
3	ABA	N	2	3	5,5,6	7.28	1 (20%)	3,5,7	1.19	1 (33%)
3	ABA	O	2	3	5,5,6	7.40	2 (40%)	3,5,7	1.29	1 (33%)
3	ABA	P	2	3	5,5,6	7.74	2 (40%)	3,5,7	1.81	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ABA	M	2	3	-	0/2/4/6	0/0/0/0
3	ABA	N	2	3	-	0/2/4/6	0/0/0/0
3	ABA	O	2	3	-	0/2/4/6	0/0/0/0
3	ABA	P	2	3	-	0/2/4/6	0/0/0/0

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	2	ABA	O-C	17.66	1.23	1.11
3	P	2	ABA	O-C	17.12	1.23	1.11
3	O	2	ABA	O-C	16.26	1.22	1.11
3	N	2	ABA	O-C	16.05	1.22	1.11
3	O	2	ABA	CA-C	2.98	1.53	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	2	ABA	C-CA-N	-3.11	110.72	113.83
3	M	2	ABA	C-CA-N	-2.75	111.08	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	2	ABA	C-CA-N	-2.19	111.64	113.83
3	N	2	ABA	C-CA-N	-2.04	111.79	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	277/278 (99%)	0.03	4 (1%) 72 72	38, 42, 45, 49	0
1	C	277/278 (99%)	-0.03	6 (2%) 59 60	37, 42, 45, 48	0
1	E	277/278 (99%)	0.13	8 (2%) 49 50	37, 42, 45, 46	0
1	G	277/278 (99%)	0.15	7 (2%) 54 55	40, 42, 45, 49	0
2	B	98/99 (98%)	-0.33	0 100 100	40, 42, 44, 45	0
2	D	98/99 (98%)	-0.30	0 100 100	40, 42, 44, 45	0
2	F	98/99 (98%)	-0.28	0 100 100	40, 42, 44, 46	0
2	H	98/99 (98%)	-0.26	0 100 100	40, 42, 44, 45	0
3	M	8/8 (100%)	-0.01	0 100 100	41, 42, 43, 43	0
3	N	8/8 (100%)	-0.12	0 100 100	41, 42, 43, 43	0
3	O	8/8 (100%)	-0.34	0 100 100	41, 42, 43, 43	0
3	P	8/8 (100%)	-0.03	0 100 100	41, 42, 43, 43	0
All	All	1532/1540 (99%)	-0.03	25 (1%) 68 69	37, 42, 45, 49	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	42	ASN	4.6
1	G	149	GLN	4.6
1	E	40	ALA	3.4
1	G	277	PRO	3.2
1	A	225	ILE	3.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ABA	M	2	6/7	0.23	0.81	41,42,42,42	0
3	ABA	N	2	6/7	0.21	0.10	41,42,42,42	0
3	ABA	P	2	6/7	0.19	-0.14	41,42,42,42	0
3	ABA	O	2	6/7	0.17	-0.56	41,42,42,42	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.