



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 05:18 PM GMT

PDB ID : 4E3C  
Title : X-ray crystal structure of human IKK2 in an active conformation  
Authors : Polley, S.; Huang, D.B.; Hauenstein, A.V.; Ghosh, G.; Huxford, T.  
Deposited on : 2012-03-09  
Resolution : 3.98 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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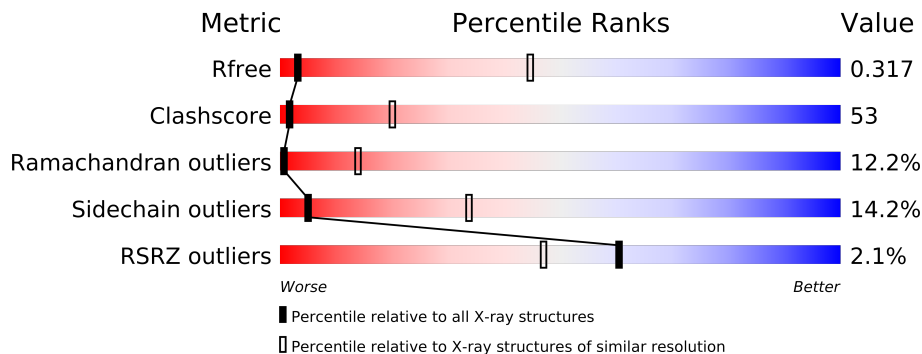
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.98 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	1031 (4.50-3.46)
Clashscore	79885	1202 (4.46-3.50)
Ramachandran outliers	78287	1143 (4.46-3.50)
Sidechain outliers	78261	1130 (4.46-3.50)
RSRZ outliers	66119	1031 (4.50-3.46)

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	669	
1	B	669	
1	C	669	
1	D	669	
1	E	669	
1	F	669	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30416 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 Inhibitor of nuclear factor kappa-B kinase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	B	632	Total	C	N	O	S	0	0	0
			5116	3219	904	959	34			
1	C	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	D	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	E	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			
1	F	624	Total	C	N	O	S	0	0	0
			5060	3186	891	950	33			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASN	-	EXPRESSION TAG	UNP O14920
A	2	LEU	-	EXPRESSION TAG	UNP O14920
A	3	TYR	-	EXPRESSION TAG	UNP O14920
A	4	PHE	-	EXPRESSION TAG	UNP O14920
A	5	GLN	-	EXPRESSION TAG	UNP O14920
A	6	GLY	-	EXPRESSION TAG	UNP O14920
A	7	ALA	-	EXPRESSION TAG	UNP O14920
A	8	MET	-	EXPRESSION TAG	UNP O14920
A	9	GLY	-	EXPRESSION TAG	UNP O14920
A	10	SER	-	EXPRESSION TAG	UNP O14920
A	177	GLU	SER	ENGINEERED MUTATION	UNP O14920
A	181	GLU	SER	ENGINEERED MUTATION	UNP O14920
B	1	ASN	-	EXPRESSION TAG	UNP O14920
B	2	LEU	-	EXPRESSION TAG	UNP O14920
B	3	TYR	-	EXPRESSION TAG	UNP O14920
B	4	PHE	-	EXPRESSION TAG	UNP O14920
B	5	GLN	-	EXPRESSION TAG	UNP O14920

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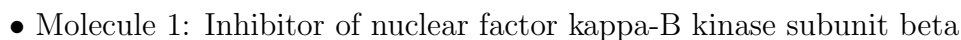
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B	6	GLY	-	EXPRESSION TAG	UNP O14920
B	7	ALA	-	EXPRESSION TAG	UNP O14920
B	8	MET	-	EXPRESSION TAG	UNP O14920
B	9	GLY	-	EXPRESSION TAG	UNP O14920
B	10	SER	-	EXPRESSION TAG	UNP O14920
B	177	GLU	SER	ENGINEERED MUTATION	UNP O14920
B	181	GLU	SER	ENGINEERED MUTATION	UNP O14920
C	1	ASN	-	EXPRESSION TAG	UNP O14920
C	2	LEU	-	EXPRESSION TAG	UNP O14920
C	3	TYR	-	EXPRESSION TAG	UNP O14920
C	4	PHE	-	EXPRESSION TAG	UNP O14920
C	5	GLN	-	EXPRESSION TAG	UNP O14920
C	6	GLY	-	EXPRESSION TAG	UNP O14920
C	7	ALA	-	EXPRESSION TAG	UNP O14920
C	8	MET	-	EXPRESSION TAG	UNP O14920
C	9	GLY	-	EXPRESSION TAG	UNP O14920
C	10	SER	-	EXPRESSION TAG	UNP O14920
C	177	GLU	SER	ENGINEERED MUTATION	UNP O14920
C	181	GLU	SER	ENGINEERED MUTATION	UNP O14920
D	1	ASN	-	EXPRESSION TAG	UNP O14920
D	2	LEU	-	EXPRESSION TAG	UNP O14920
D	3	TYR	-	EXPRESSION TAG	UNP O14920
D	4	PHE	-	EXPRESSION TAG	UNP O14920
D	5	GLN	-	EXPRESSION TAG	UNP O14920
D	6	GLY	-	EXPRESSION TAG	UNP O14920
D	7	ALA	-	EXPRESSION TAG	UNP O14920
D	8	MET	-	EXPRESSION TAG	UNP O14920
D	9	GLY	-	EXPRESSION TAG	UNP O14920
D	10	SER	-	EXPRESSION TAG	UNP O14920
D	177	GLU	SER	ENGINEERED MUTATION	UNP O14920
D	181	GLU	SER	ENGINEERED MUTATION	UNP O14920
E	1	ASN	-	EXPRESSION TAG	UNP O14920
E	2	LEU	-	EXPRESSION TAG	UNP O14920
E	3	TYR	-	EXPRESSION TAG	UNP O14920
E	4	PHE	-	EXPRESSION TAG	UNP O14920
E	5	GLN	-	EXPRESSION TAG	UNP O14920
E	6	GLY	-	EXPRESSION TAG	UNP O14920
E	7	ALA	-	EXPRESSION TAG	UNP O14920
E	8	MET	-	EXPRESSION TAG	UNP O14920
E	9	GLY	-	EXPRESSION TAG	UNP O14920
E	10	SER	-	EXPRESSION TAG	UNP O14920
E	177	GLU	SER	ENGINEERED MUTATION	UNP O14920

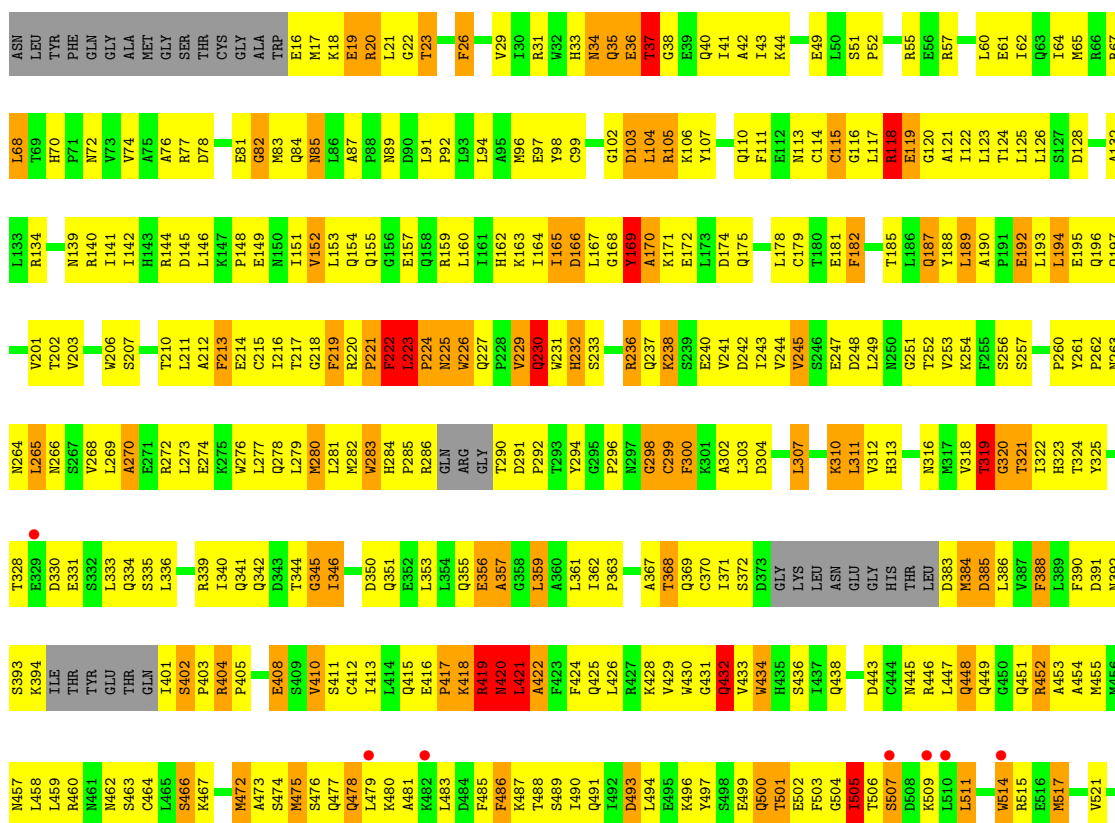
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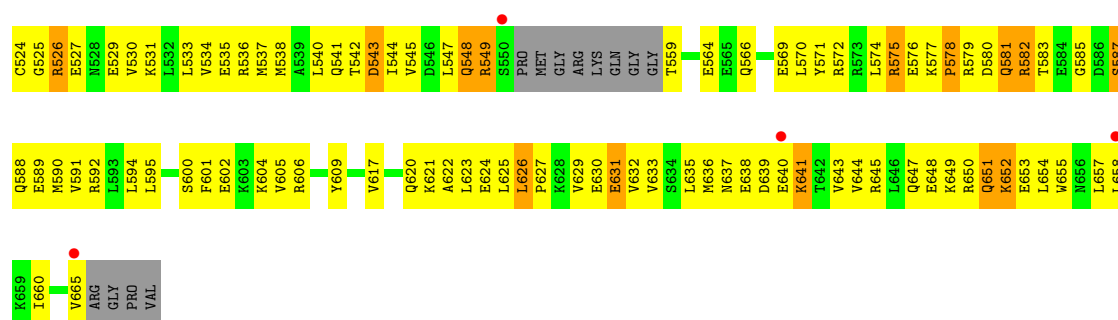
Chain	Residue	Modelled	Actual	Comment	Reference
E	181	GLU	SER	ENGINEERED MUTATION	UNP O14920
F	1	ASN	-	EXPRESSION TAG	UNP O14920
F	2	LEU	-	EXPRESSION TAG	UNP O14920
F	3	TYR	-	EXPRESSION TAG	UNP O14920
F	4	PHE	-	EXPRESSION TAG	UNP O14920
F	5	GLN	-	EXPRESSION TAG	UNP O14920
F	6	GLY	-	EXPRESSION TAG	UNP O14920
F	7	ALA	-	EXPRESSION TAG	UNP O14920
F	8	MET	-	EXPRESSION TAG	UNP O14920
F	9	GLY	-	EXPRESSION TAG	UNP O14920
F	10	SER	-	EXPRESSION TAG	UNP O14920
F	177	GLU	SER	ENGINEERED MUTATION	UNP O14920
F	181	GLU	SER	ENGINEERED MUTATION	UNP O14920





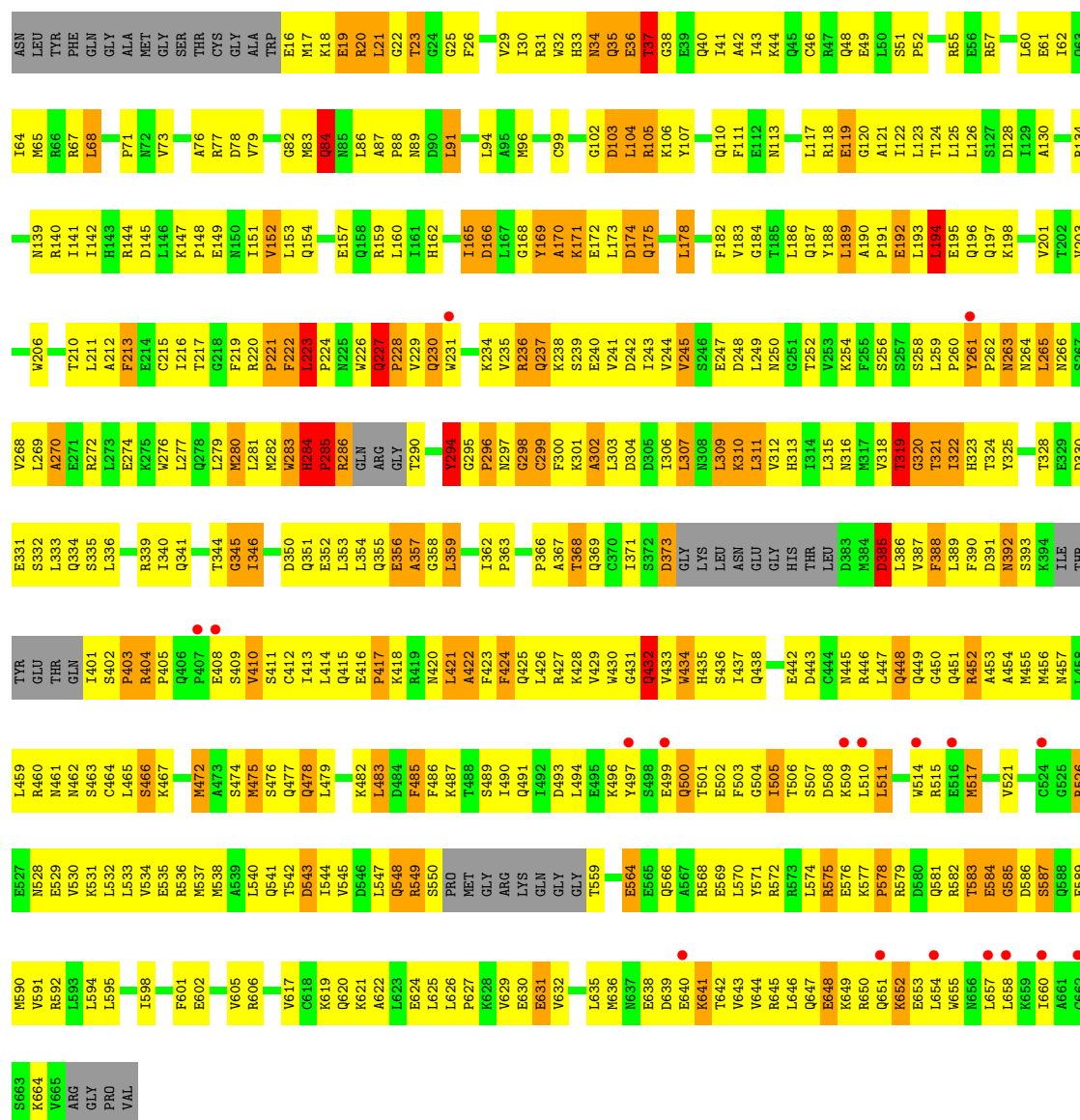






• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

Chain E:



• Molecule 1: Inhibitor of nuclear factor kappa-B kinase subunit beta

Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.81 Å   170.81 Å   509.56 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.84 – 3.98 49.73 – 3.97	Depositor EDS
% Data completeness (in resolution range)	81.0 (29.84-3.98) 88.5 (49.73-3.97)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 4.00 Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.267   ,   0.299 0.285   ,   0.317	Depositor DCC
$R_{free}$ test set	2221 reflections (3.82%)	DCC
Wilson B-factor (Å <sup>2</sup> )	113.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 110.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	3 of 63509 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	30416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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

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	0/5142	0.61	3/6937 (0.0%)
1	B	0.47	0/5200	0.69	3/7014 (0.0%)
1	C	0.44	0/5142	0.58	0/6937
1	D	0.45	0/5142	0.69	3/6937 (0.0%)
1	E	0.44	0/5142	0.57	0/6937
1	F	0.42	0/5142	0.57	0/6937
All	All	0.45	0/30910	0.62	9/41699 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	118	ARG	NE-CZ-NH1	-21.84	109.38	120.30
1	D	118	ARG	NE-CZ-NH2	21.77	131.18	120.30
1	B	144	ARG	NE-CZ-NH1	-20.91	109.84	120.30
1	B	144	ARG	NE-CZ-NH2	19.92	130.26	120.30
1	D	118	ARG	CD-NE-CZ	9.85	137.39	123.60

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	5060	0	5109	581	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5116	0	5169	569	0
1	C	5060	0	5109	522	0
1	D	5060	0	5109	557	0
1	E	5060	0	5107	554	0
1	F	5060	0	5107	584	0
All	All	30416	0	30710	3237	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 53.

The worst 5 of 3237 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:419:ARG:HB2	1:B:419:ARG:NH1	1.55	1.18
1:B:366:PRO:HB2	1:B:368:THR:HG23	1.29	1.14
1:C:496:LYS:HE2	1:C:654:LEU:HD21	1.20	1.14
1:F:626:LEU:H	1:F:627:PRO:HD2	1.13	1.13
1:D:479:LEU:HD11	1:D:641:LYS:HG2	1.28	1.11

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	614/669 (92%)	427 (70%)	112 (18%)	75 (12%)	1	14
1	B	624/669 (93%)	411 (66%)	133 (21%)	80 (13%)	0	13
1	C	614/669 (92%)	423 (69%)	117 (19%)	74 (12%)	1	14
1	D	614/669 (92%)	421 (69%)	119 (19%)	74 (12%)	1	14
1	E	614/669 (92%)	417 (68%)	121 (20%)	76 (12%)	1	14
1	F	614/669 (92%)	421 (69%)	120 (20%)	73 (12%)	1	14
All	All	3694/4014 (92%)	2520 (68%)	722 (20%)	452 (12%)	1	14

5 of 452 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	MET
1	A	35	GLN
1	A	92	PRO
1	A	166	ASP
1	A	182	PHE

### 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	567/601 (94%)	491 (87%)	76 (13%)	6	36
1	B	572/601 (95%)	485 (85%)	87 (15%)	4	30
1	C	567/601 (94%)	490 (86%)	77 (14%)	5	36
1	D	567/601 (94%)	488 (86%)	79 (14%)	5	35
1	E	567/601 (94%)	492 (87%)	75 (13%)	6	37
1	F	567/601 (94%)	478 (84%)	89 (16%)	4	28
All	All	3407/3606 (94%)	2924 (86%)	483 (14%)	5	34

5 of 483 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	493	ASP
1	D	283	TRP
1	F	419	ARG
1	C	514	TRP
1	D	103	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	230	GLN
1	C	500	GLN
1	F	297	ASN
1	C	250	ASN
1	C	355	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	624/669 (93%)	0.38	14 (2%) 59 45	56, 129, 201, 287	0
1	B	632/669 (94%)	0.29	5 (0%) 83 70	56, 130, 204, 256	0
1	C	624/669 (93%)	0.25	9 (1%) 72 57	64, 133, 201, 267	0
1	D	624/669 (93%)	0.23	11 (1%) 65 52	62, 132, 201, 286	0
1	E	624/669 (93%)	0.36	18 (2%) 49 39	63, 134, 205, 264	0
1	F	624/669 (93%)	0.35	21 (3%) 43 35	64, 144, 206, 256	0
All	All	3752/4014 (93%)	0.31	78 (2%) 60 47	56, 133, 204, 287	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	510	LEU	8.9
1	A	505	ILE	6.3
1	A	497	TYR	5.6
1	B	510	LEU	4.9
1	A	494	LEU	4.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 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.