



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 12:59 PM EDT

PDB ID : 4KKT  
Title : Crystal Structure of BesA (P21 form)  
Authors : Greene, N.P.; Hinchliffe, P.; Crow, A.; Ababou, A.; Hughes, C.; Koronakis, V.  
Deposited on : 2013-05-06  
Resolution : 2.53 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

<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>.

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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) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

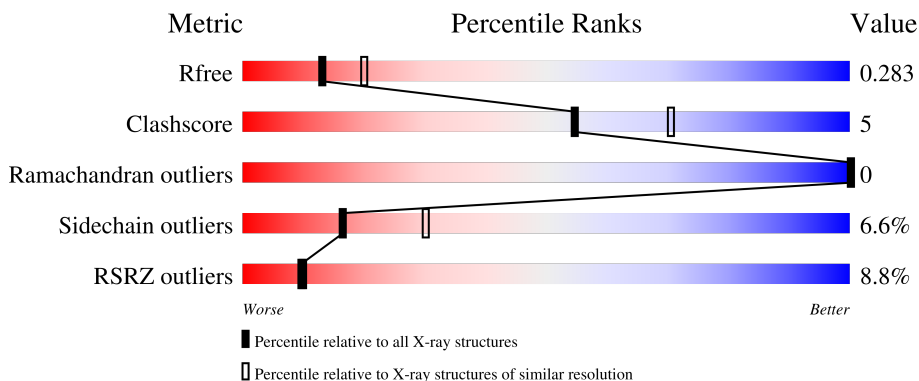
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.53 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))
$R_{free}$	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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  $\geq 3$ , 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	296	 6% 77% 10% • 10%
1	B	296	 6% 77% 11% • 11%
1	C	296	 6% 77% 10% • 11%
1	D	296	 13% 76% 11% • 11%

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 8267 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 Membrane fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	265	Total 2048	C 1314	N 337	O 393	S 4	0	1	0
1	B	262	Total 2043	C 1311	N 335	O 393	S 4	0	3	0
1	C	262	Total 2019	C 1296	N 332	O 387	S 4	0	0	0
1	D	263	Total 2046	C 1313	N 335	O 394	S 4	0	2	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP O51166
A	23	SER	-	expression tag	UNP O51166
A	24	HIS	-	expression tag	UNP O51166
A	25	MET	-	expression tag	UNP O51166
B	22	GLY	-	expression tag	UNP O51166
B	23	SER	-	expression tag	UNP O51166
B	24	HIS	-	expression tag	UNP O51166
B	25	MET	-	expression tag	UNP O51166
C	22	GLY	-	expression tag	UNP O51166
C	23	SER	-	expression tag	UNP O51166
C	24	HIS	-	expression tag	UNP O51166
C	25	MET	-	expression tag	UNP O51166
D	22	GLY	-	expression tag	UNP O51166
D	23	SER	-	expression tag	UNP O51166
D	24	HIS	-	expression tag	UNP O51166
D	25	MET	-	expression tag	UNP O51166

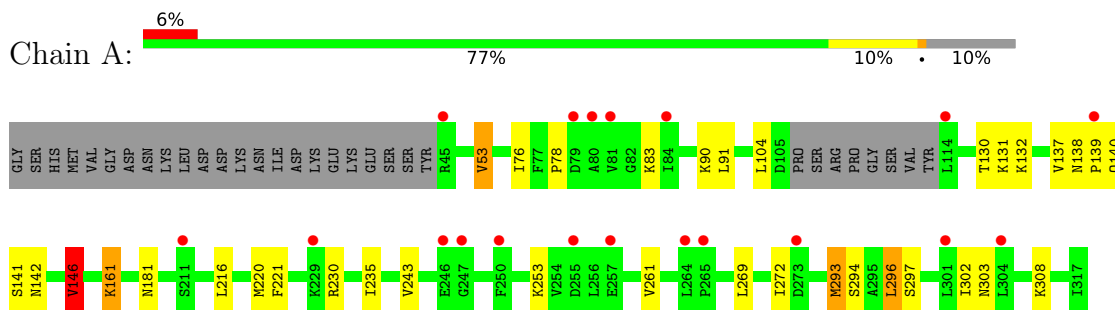
- Molecule 2 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	A	29	Total 29	O 29	0	0
2	B	30	Total 30	O 30	0	0
2	C	23	Total 23	O 23	0	0
2	D	29	Total 29	O 29	0	0

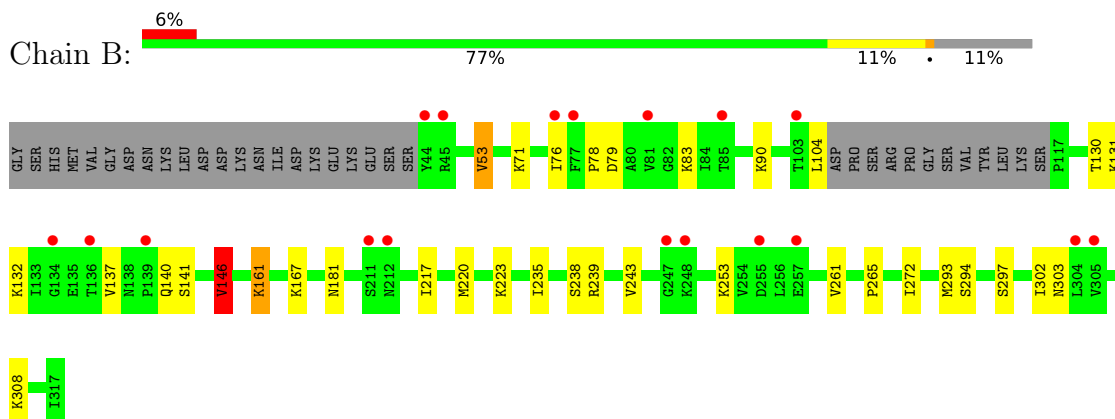
### 3 Residue-property plots [i](#)

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.

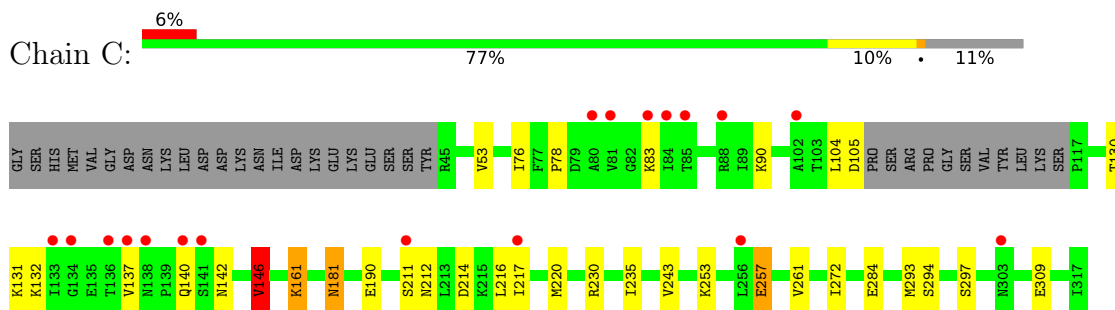
- Molecule 1: Membrane fusion protein



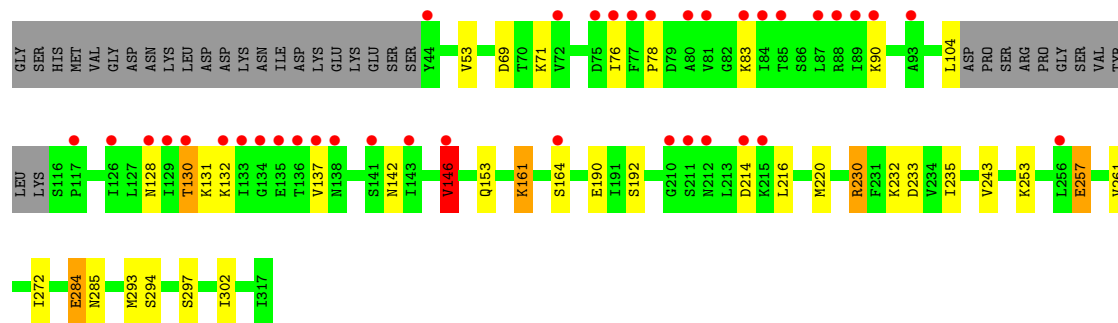
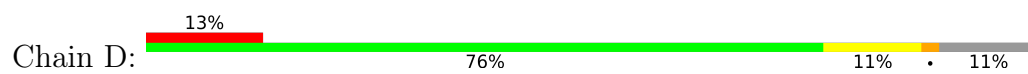
- Molecule 1: Membrane fusion protein



- Molecule 1: Membrane fusion protein



- Molecule 1: Membrane fusion protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.20Å 73.74Å 152.23Å 90.00° 98.06° 90.00°	Depositor
Resolution (Å)	73.27 – 2.53 73.17 – 2.53	Depositor EDS
% Data completeness (in resolution range)	95.2 (73.27-2.53) 95.2 (73.17-2.53)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.52 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.257 , 0.285 0.261 , 0.283	Depositor DCC
$R_{free}$ test set	2784 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtrriage
Anisotropy	0.158	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 31.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8267	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1511e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.75	0/2069	0.86	4/2786 (0.1%)
1	B	0.76	0/2065	0.84	1/2781 (0.0%)
1	C	0.72	0/2040	0.83	2/2747 (0.1%)
1	D	0.71	0/2068	0.82	2/2786 (0.1%)
All	All	0.73	0/8242	0.84	9/11100 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	MET	CG-SD-CE	6.64	110.83	100.20
1	B	146	VAL	CB-CA-C	-6.57	98.92	111.40
1	A	230	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	146	VAL	CB-CA-C	-6.08	99.85	111.40
1	C	146	VAL	CB-CA-C	-6.01	99.97	111.40
1	A	230	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	C	230	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	D	146	VAL	CB-CA-C	-5.77	100.44	111.40
1	D	230	ARG	NE-CZ-NH2	-5.40	117.60	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2048	0	2183	25	0
1	B	2043	0	2167	22	0
1	C	2019	0	2151	23	0
1	D	2046	0	2168	23	0
2	A	29	0	0	2	0
2	B	30	0	0	5	0
2	C	23	0	0	1	0
2	D	29	0	0	9	0
All	All	8267	0	8669	87	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 5.

All (87) 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:D:69:ASP:OD2	2:D:403:HOH:O	1.69	1.08
1:A:78:PRO:HG3	1:A:137:VAL:HG11	1.56	0.88
1:D:190:GLU:OE2	2:D:409:HOH:O	2.01	0.78
1:A:78:PRO:HG3	1:A:137:VAL:CG1	2.12	0.78
1:D:230:ARG:HG3	2:D:428:HOH:O	1.83	0.77
1:C:257:GLU:HA	1:C:257:GLU:OE2	1.85	0.75
1:A:293:MET:HA	1:A:296:LEU:HD22	1.70	0.73
1:A:78:PRO:CG	1:A:137:VAL:CG1	2.69	0.70
1:D:232:LYS:O	1:D:233[B]:ASP:OD1	2.10	0.69
1:A:303:ASN:HA	2:A:425:HOH:O	1.93	0.67
1:D:233[B]:ASP:O	1:D:233[B]:ASP:CG	2.36	0.63
1:A:137:VAL:HG13	1:A:141[B]:SER:HB3	1.80	0.63
1:B:303:ASN:HA	2:B:425:HOH:O	1.97	0.63
1:A:137:VAL:HG13	1:A:141[A]:SER:HB2	1.81	0.62
1:C:53:VAL:CG1	1:C:235:ILE:HD12	2.33	0.59
1:A:131:LYS:HE3	1:A:137:VAL:HG22	1.85	0.58
1:C:211:SER:O	1:C:212:ASN:HB3	2.02	0.58
1:D:53:VAL:CG1	1:D:235:ILE:HD12	2.35	0.57
1:B:53:VAL:CG1	1:B:235:ILE:HD12	2.35	0.56
1:B:79[B]:ASP:O	1:B:79[B]:ASP:OD1	2.23	0.56
1:B:217:ILE:HD12	1:B:220:MET:HE1	1.87	0.56
1:B:272:ILE:HD12	1:C:161:LYS:HB3	1.88	0.56
1:A:53:VAL:CG1	1:A:235:ILE:HD12	2.36	0.56
1:D:153:GLN:NE2	2:D:403:HOH:O	2.38	0.56
1:A:272:ILE:HD12	1:D:161:LYS:HB3	1.88	0.55
1:A:161:LYS:HB3	1:D:272:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:LYS:O	1:D:104:LEU:HA	2.07	0.55
2:A:405:HOH:O	1:D:161:LYS:HD3	2.08	0.54
1:B:83:LYS:O	1:B:104:LEU:HA	2.08	0.54
1:A:91:LEU:HD12	1:B:181:ASN:HB3	1.90	0.53
1:A:76:ILE:HD11	1:A:146:VAL:HG22	1.89	0.53
1:C:220:MET:CE	2:D:412:HOH:O	2.58	0.52
1:B:76:ILE:HD11	1:B:146:VAL:HG22	1.91	0.52
1:C:76:ILE:HD11	1:C:146:VAL:HG22	1.93	0.51
1:D:76:ILE:HD11	1:D:146:VAL:HG22	1.91	0.50
1:D:192:SER:HA	2:D:409:HOH:O	2.11	0.50
1:A:78:PRO:HG2	1:A:137:VAL:CG1	2.42	0.49
1:B:161:LYS:HB3	1:C:272:ILE:HD12	1.94	0.49
1:A:137:VAL:CG1	1:A:138:ASN:N	2.76	0.49
1:C:83:LYS:O	1:C:104:LEU:HA	2.12	0.49
1:A:221:PHE:CE2	1:B:223:LYS:HD2	2.47	0.48
1:B:141[A]:SER:OG	2:B:410:HOH:O	1.99	0.48
2:B:405:HOH:O	1:C:161:LYS:HD3	2.14	0.48
1:A:83:LYS:O	1:A:104:LEU:HA	2.13	0.48
1:C:217:ILE:HD12	1:C:220:MET:HE1	1.96	0.48
1:A:78:PRO:HB3	1:A:104:LEU:HD11	1.98	0.46
1:B:78:PRO:HG3	1:B:137:VAL:HG21	1.97	0.46
1:C:211:SER:O	1:C:212:ASN:CB	2.64	0.46
1:C:190:GLU:HA	2:C:412:HOH:O	2.15	0.46
1:B:131:LYS:HE3	1:B:137:VAL:HG12	1.98	0.45
1:D:164:SER:HB2	2:D:406:HOH:O	2.15	0.45
1:D:253:LYS:O	1:D:261:VAL:HA	2.17	0.45
1:B:217:ILE:HD12	1:B:220:MET:CE	2.47	0.45
1:D:257[B]:GLU:H	1:D:257[B]:GLU:HG2	1.44	0.44
1:B:239:ARG:NH2	2:B:420:HOH:O	2.50	0.44
1:B:302:ILE:C	1:B:302:ILE:HD12	2.38	0.44
1:A:78:PRO:CG	1:A:137:VAL:HG12	2.45	0.44
1:A:302:ILE:HD12	1:A:302:ILE:C	2.38	0.44
1:C:257:GLU:OE2	1:C:257:GLU:CA	2.62	0.44
1:D:128:ASN:OD1	1:D:130:THR:HG23	2.17	0.44
1:C:78:PRO:HG3	1:C:137:VAL:HG21	1.99	0.44
1:C:217:ILE:HB	1:C:220:MET:HE3	1.99	0.43
1:D:131:LYS:HE3	1:D:137:VAL:HG12	2.00	0.43
1:C:78:PRO:HB3	1:C:104:LEU:HD11	2.00	0.43
1:B:217:ILE:HB	1:B:220:MET:HE3	2.01	0.43
1:C:220:MET:HE2	2:D:412:HOH:O	2.18	0.43
1:B:78:PRO:HG3	1:B:137:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:LYS:HE3	1:C:137:VAL:HG12	2.01	0.43
1:C:253:LYS:O	1:C:261:VAL:HA	2.19	0.43
1:B:78:PRO:HB3	1:B:104:LEU:HD11	2.00	0.42
1:C:220:MET:HE1	2:D:412:HOH:O	2.19	0.42
1:A:253:LYS:O	1:A:261:VAL:HA	2.19	0.42
1:B:253:LYS:O	1:B:261:VAL:HA	2.19	0.42
1:A:78:PRO:CG	1:A:137:VAL:HG11	2.34	0.42
1:D:78:PRO:HB3	1:D:104:LEU:HD11	2.01	0.42
1:D:216:LEU:HD12	1:D:216:LEU:HA	1.89	0.42
1:D:78:PRO:HG3	1:D:137:VAL:HG21	2.00	0.42
1:B:265:PRO:O	2:B:424:HOH:O	2.22	0.42
1:A:216:LEU:HD12	1:A:216:LEU:HA	1.86	0.41
1:D:284:GLU:O	1:D:285:ASN:HB2	2.20	0.41
1:C:78:PRO:HG3	1:C:137:VAL:CG2	2.50	0.41
1:B:308:LYS:HB3	1:B:308:LYS:HE3	1.88	0.41
1:C:181:ASN:H	1:C:181:ASN:HD22	1.69	0.41
1:A:308:LYS:HE3	1:A:308:LYS:HB3	1.89	0.41
1:C:216:LEU:HD12	1:C:216:LEU:HA	1.90	0.41
1:A:138:ASN:HB2	1:A:139:PRO:HD2	2.03	0.41
1:D:302:ILE:HD12	1:D:302:ILE:C	2.41	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	262/296 (88%)	256 (98%)	6 (2%)	0	100	100
1	B	261/296 (88%)	258 (99%)	3 (1%)	0	100	100
1	C	258/296 (87%)	253 (98%)	5 (2%)	0	100	100
1	D	261/296 (88%)	256 (98%)	5 (2%)	0	100	100
All	All	1042/1184 (88%)	1023 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	235/262 (90%)	220 (94%)	15 (6%)	17	31
1	B	234/262 (89%)	219 (94%)	15 (6%)	17	31
1	C	231/262 (88%)	214 (93%)	17 (7%)	13	25
1	D	234/262 (89%)	218 (93%)	16 (7%)	16	29
All	All	934/1048 (89%)	871 (93%)	63 (7%)	16	29

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
1	A	90	LYS
1	A	130	THR
1	A	132	LYS
1	A	140	GLN
1	A	142	ASN
1	A	146	VAL
1	A	161	LYS
1	A	181	ASN
1	A	243	VAL
1	A	269	LEU
1	A	293	MET
1	A	294	SER
1	A	296	LEU
1	A	297	SER
1	B	53	VAL
1	B	71	LYS
1	B	90	LYS
1	B	130	THR
1	B	132	LYS
1	B	140	GLN
1	B	146	VAL

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Mol	Chain	Res	Type
1	B	161	LYS
1	B	167	LYS
1	B	238[A]	SER
1	B	238[B]	SER
1	B	243	VAL
1	B	293	MET
1	B	294	SER
1	B	297	SER
1	C	90	LYS
1	C	105	ASP
1	C	130	THR
1	C	132	LYS
1	C	140	GLN
1	C	142	ASN
1	C	146	VAL
1	C	161	LYS
1	C	181	ASN
1	C	214	ASP
1	C	243	VAL
1	C	257	GLU
1	C	284	GLU
1	C	293	MET
1	C	294	SER
1	C	297	SER
1	C	309	GLU
1	D	71	LYS
1	D	90	LYS
1	D	130	THR
1	D	132	LYS
1	D	142	ASN
1	D	146	VAL
1	D	161	LYS
1	D	214	ASP
1	D	220	MET
1	D	243	VAL
1	D	257[A]	GLU
1	D	257[B]	GLU
1	D	284	GLU
1	D	293	MET
1	D	294	SER
1	D	297	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	B	96	GLN
1	B	165	ASN
1	B	170	ASN
1	C	153	GLN
1	C	165	ASN
1	C	181	ASN
1	C	274	ASN
1	D	153	GLN

### 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 monosaccharides 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, 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	265/296 (89%)	0.72	19 (7%) 15 16	15, 30, 57, 96	0
1	B	262/296 (88%)	0.75	18 (6%) 16 17	13, 29, 60, 77	0
1	C	262/296 (88%)	0.65	18 (6%) 16 17	16, 32, 83, 101	0
1	D	263/296 (88%)	0.93	38 (14%) 2 2	15, 33, 99, 134	0
All	All	1052/1184 (88%)	0.76	93 (8%) 10 10	13, 31, 77, 134	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	136	THR	6.1
1	D	132	LYS	5.5
1	D	81	VAL	5.5
1	D	133	ILE	5.5
1	D	212	ASN	5.5
1	D	83	LYS	5.3
1	D	141	SER	4.9
1	A	247	GLY	4.7
1	D	137	VAL	4.7
1	D	129	ILE	4.3
1	A	80	ALA	4.3
1	D	84	ILE	4.2
1	C	136	THR	4.0
1	A	257	GLU	4.0
1	A	45	ARG	3.9
1	D	80	ALA	3.9
1	C	134	GLY	3.7
1	D	138	ASN	3.7
1	D	130	THR	3.6
1	C	138	ASN	3.6
1	A	304	LEU	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	134	GLY	3.5
1	C	81	VAL	3.5
1	D	117	PRO	3.5
1	A	211	SER	3.4
1	B	247	GLY	3.4
1	A	114	LEU	3.4
1	D	214	ASP	3.2
1	D	211	SER	3.2
1	B	212	ASN	3.2
1	C	85	THR	3.1
1	A	255	ASP	3.1
1	D	76	ILE	3.1
1	B	45	ARG	3.1
1	A	229	LYS	3.1
1	D	128	ASN	2.9
1	B	44	TYR	2.9
1	C	84	ILE	2.8
1	D	126	ILE	2.8
1	B	85	THR	2.8
1	B	255	ASP	2.8
1	D	210	GLY	2.7
1	D	143	ILE	2.7
1	D	215	LYS	2.7
1	D	87	LEU	2.7
1	A	246	GLU	2.6
1	D	93	ALA	2.6
1	B	305	VAL	2.6
1	C	256	LEU	2.6
1	D	85	THR	2.6
1	D	78	PRO	2.6
1	D	75	ASP	2.6
1	C	80	ALA	2.5
1	D	89	ILE	2.5
1	B	134	GLY	2.5
1	D	88	ARG	2.5
1	A	81	VAL	2.5
1	D	90	LYS	2.5
1	D	164	SER	2.5
1	C	137	VAL	2.4
1	C	83	LYS	2.4
1	D	135	GLU	2.4
1	C	133	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	211	SER	2.4
1	B	136	THR	2.4
1	B	103	THR	2.3
1	D	256	LEU	2.3
1	C	217	ILE	2.3
1	C	140	GLN	2.2
1	A	84	ILE	2.2
1	B	81	VAL	2.2
1	B	248	LYS	2.2
1	A	264	LEU	2.2
1	B	76	ILE	2.2
1	B	304	LEU	2.2
1	C	211	SER	2.2
1	D	44	TYR	2.2
1	A	139	PRO	2.1
1	C	141	SER	2.1
1	A	79	ASP	2.1
1	A	250	PHE	2.1
1	B	77	PHE	2.1
1	A	265	PRO	2.1
1	A	301	LEU	2.1
1	D	77	PHE	2.1
1	B	139	PRO	2.1
1	C	303	ASN	2.1
1	C	88	ARG	2.1
1	C	102	ALA	2.1
1	B	257	GLU	2.1
1	A	273	ASP	2.0
1	D	146	VAL	2.0
1	D	72	VAL	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 monosaccharides 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.