



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 09:14 pm BST

PDB ID : 3A8Y  
Title : Crystal structure of the complex between the BAG5 BD5 and Hsp70 NBD  
Authors : Arakawa, A.; Handa, N.; Ohsawa, N.; Shirouzu, M.; Yokoyama, S.; RIKEN  
Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2009-10-13  
Resolution : 2.30 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](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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

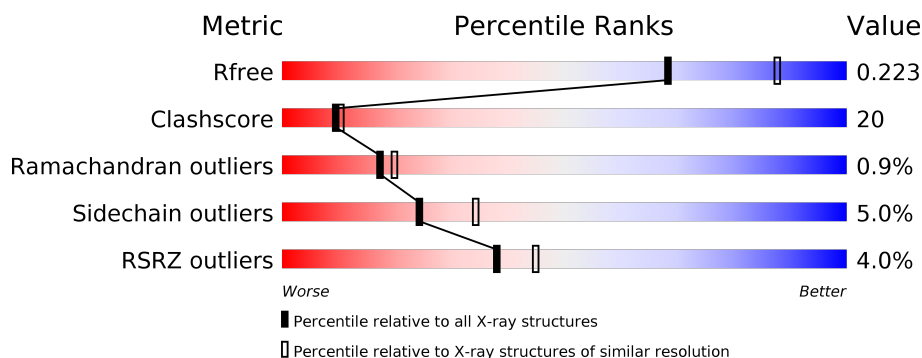
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	392	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>
1	B	392	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>34%</div> <div>• •</div> </div> </div>
2	C	142	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>24%</div> <div>•</div> <div>30%</div> </div> </div>
2	D	142	<div> <div>4%</div> <div> <div></div> <div>38%</div> <div>30%</div> <div>•</div> <div>30%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8057 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 Heat shock 70 kDa protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			2986	1881	523	574	8			
1	B	376	Total	C	N	O	S	0	0	0
			2921	1840	512	562	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P08107
A	-2	SER	-	EXPRESSION TAG	UNP P08107
A	-1	PHE	-	EXPRESSION TAG	UNP P08107
A	0	THR	-	EXPRESSION TAG	UNP P08107
B	-3	GLY	-	EXPRESSION TAG	UNP P08107
B	-2	SER	-	EXPRESSION TAG	UNP P08107
B	-1	PHE	-	EXPRESSION TAG	UNP P08107
B	0	THR	-	EXPRESSION TAG	UNP P08107

- Molecule 2 is a protein called BAG family molecular chaperone regulator 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	99	Total	C	N	O	S	0	0	0
			802	505	140	155	2			
2	D	100	Total	C	N	O	S	0	0	0
			810	511	141	156	2			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	334	GLY	-	EXPRESSION TAG	UNP Q9UL15
C	335	SER	-	EXPRESSION TAG	UNP Q9UL15
C	336	SER	-	EXPRESSION TAG	UNP Q9UL15
C	337	GLY	-	EXPRESSION TAG	UNP Q9UL15

*Continued on next page...*

*Continued from previous page...*

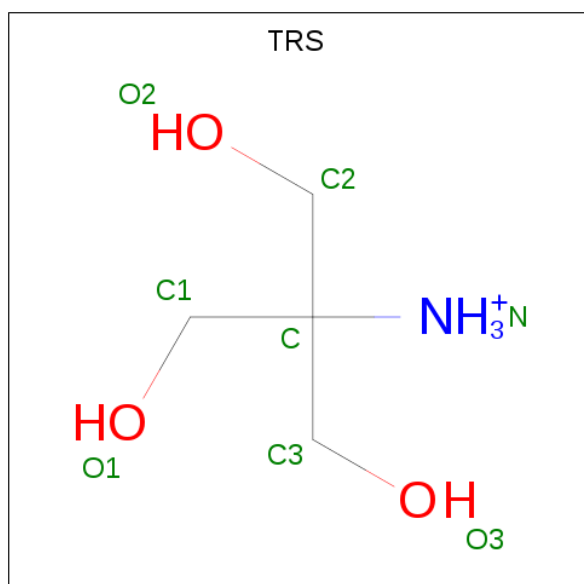
Chain	Residue	Modelled	Actual	Comment	Reference
C	338	SER	-	EXPRESSION TAG	UNP Q9UL15
C	339	SER	-	EXPRESSION TAG	UNP Q9UL15
C	340	GLY	-	EXPRESSION TAG	UNP Q9UL15
C	448	CYS	-	EXPRESSION TAG	UNP Q9UL15
C	449	LYS	-	EXPRESSION TAG	UNP Q9UL15
C	450	ALA	-	EXPRESSION TAG	UNP Q9UL15
C	451	ALA	-	EXPRESSION TAG	UNP Q9UL15
C	452	ARG	-	EXPRESSION TAG	UNP Q9UL15
C	453	LYS	-	EXPRESSION TAG	UNP Q9UL15
C	454	GLN	-	EXPRESSION TAG	UNP Q9UL15
C	455	ALA	-	EXPRESSION TAG	UNP Q9UL15
C	456	VAL	-	EXPRESSION TAG	UNP Q9UL15
C	457	ARG	-	EXPRESSION TAG	UNP Q9UL15
C	458	LEU	-	EXPRESSION TAG	UNP Q9UL15
C	459	ALA	-	EXPRESSION TAG	UNP Q9UL15
C	460	GLN	-	EXPRESSION TAG	UNP Q9UL15
C	461	ASN	-	EXPRESSION TAG	UNP Q9UL15
C	462	ILE	-	EXPRESSION TAG	UNP Q9UL15
C	463	LEU	-	EXPRESSION TAG	UNP Q9UL15
C	464	SER	-	EXPRESSION TAG	UNP Q9UL15
C	465	TYR	-	EXPRESSION TAG	UNP Q9UL15
C	466	LEU	-	EXPRESSION TAG	UNP Q9UL15
C	467	ASP	-	EXPRESSION TAG	UNP Q9UL15
C	468	LEU	-	EXPRESSION TAG	UNP Q9UL15
C	469	LYS	-	EXPRESSION TAG	UNP Q9UL15
C	470	SER	-	EXPRESSION TAG	UNP Q9UL15
C	471	ASP	-	EXPRESSION TAG	UNP Q9UL15
C	472	GLU	-	EXPRESSION TAG	UNP Q9UL15
C	473	TRP	-	EXPRESSION TAG	UNP Q9UL15
C	474	GLU	-	EXPRESSION TAG	UNP Q9UL15
C	475	TYR	-	EXPRESSION TAG	UNP Q9UL15
D	334	GLY	-	EXPRESSION TAG	UNP Q9UL15
D	335	SER	-	EXPRESSION TAG	UNP Q9UL15
D	336	SER	-	EXPRESSION TAG	UNP Q9UL15
D	337	GLY	-	EXPRESSION TAG	UNP Q9UL15
D	338	SER	-	EXPRESSION TAG	UNP Q9UL15
D	339	SER	-	EXPRESSION TAG	UNP Q9UL15
D	340	GLY	-	EXPRESSION TAG	UNP Q9UL15
D	448	CYS	-	EXPRESSION TAG	UNP Q9UL15
D	449	LYS	-	EXPRESSION TAG	UNP Q9UL15
D	450	ALA	-	EXPRESSION TAG	UNP Q9UL15
D	451	ALA	-	EXPRESSION TAG	UNP Q9UL15

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	452	ARG	-	EXPRESSION TAG	UNP Q9UL15
D	453	LYS	-	EXPRESSION TAG	UNP Q9UL15
D	454	GLN	-	EXPRESSION TAG	UNP Q9UL15
D	455	ALA	-	EXPRESSION TAG	UNP Q9UL15
D	456	VAL	-	EXPRESSION TAG	UNP Q9UL15
D	457	ARG	-	EXPRESSION TAG	UNP Q9UL15
D	458	LEU	-	EXPRESSION TAG	UNP Q9UL15
D	459	ALA	-	EXPRESSION TAG	UNP Q9UL15
D	460	GLN	-	EXPRESSION TAG	UNP Q9UL15
D	461	ASN	-	EXPRESSION TAG	UNP Q9UL15
D	462	ILE	-	EXPRESSION TAG	UNP Q9UL15
D	463	LEU	-	EXPRESSION TAG	UNP Q9UL15
D	464	SER	-	EXPRESSION TAG	UNP Q9UL15
D	465	TYR	-	EXPRESSION TAG	UNP Q9UL15
D	466	LEU	-	EXPRESSION TAG	UNP Q9UL15
D	467	ASP	-	EXPRESSION TAG	UNP Q9UL15
D	468	LEU	-	EXPRESSION TAG	UNP Q9UL15
D	469	LYS	-	EXPRESSION TAG	UNP Q9UL15
D	470	SER	-	EXPRESSION TAG	UNP Q9UL15
D	471	ASP	-	EXPRESSION TAG	UNP Q9UL15
D	472	GLU	-	EXPRESSION TAG	UNP Q9UL15
D	473	TRP	-	EXPRESSION TAG	UNP Q9UL15
D	474	GLU	-	EXPRESSION TAG	UNP Q9UL15
D	475	TYR	-	EXPRESSION TAG	UNP Q9UL15

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

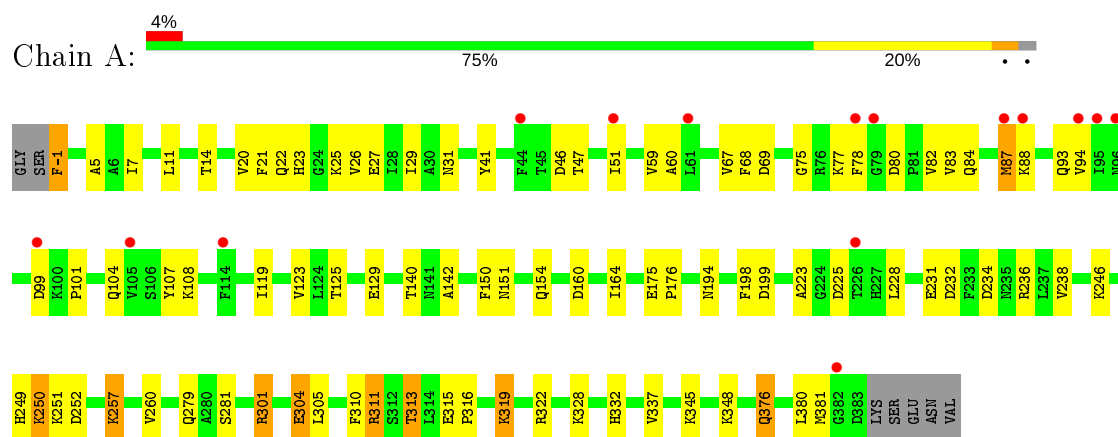
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	234	Total	O	0	0
			234	234		
4	B	207	Total	O	0	0
			207	207		
4	C	57	Total	O	0	0
			57	57		
4	D	24	Total	O	0	0
			24	24		

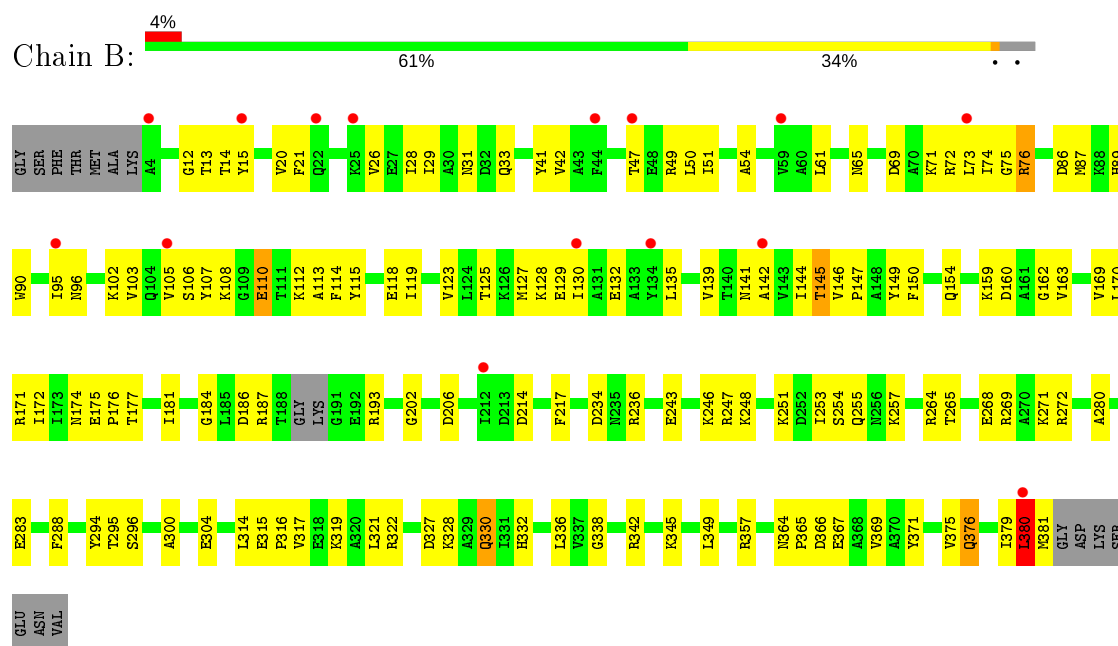
### 3 Residue-property plots [i](#)

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.

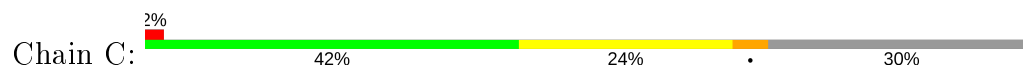
#### • Molecule 1: Heat shock 70 kDa protein 1

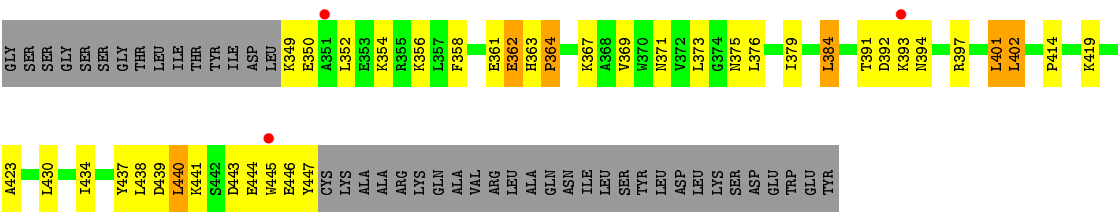


#### • Molecule 1: Heat shock 70 kDa protein 1

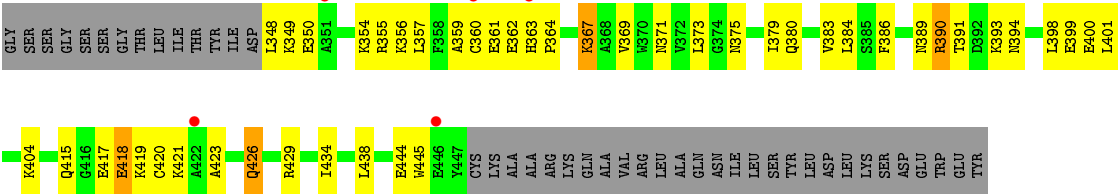


#### • Molecule 2: BAG family molecular chaperone regulator 5





● Molecule 2: BAG family molecular chaperone regulator 5





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.11Å 84.27Å 96.63Å 90.00° 100.73° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30 47.59 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.5 (19.98-2.30) 94.4 (47.59-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.39 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.218 , 0.281 0.219 , 0.223	Depositor DCC
$R_{free}$ test set	2150 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 63.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8057	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.88% 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 [i](#)

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

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

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	0.34	0/3035	0.58	0/4100
1	B	0.34	0/2968	0.58	0/4011
2	C	0.31	0/814	0.55	0/1095
2	D	0.30	0/822	0.52	0/1106
All	All	0.33	0/7639	0.57	0/10312

There are no bond length outliers.

There are no bond angle outliers.

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	2986	0	2993	75	0
1	B	2921	0	2923	145	0
2	C	802	0	800	45	0
2	D	810	0	811	43	0
3	A	8	0	12	0	0
3	B	8	0	12	1	0
4	A	234	0	0	11	0
4	B	207	0	0	14	0
4	C	57	0	0	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	24	0	0	0	0
All	All	8057	0	7551	295	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 20.

The worst 5 of 295 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:B:364:ASN:HD22	1:B:367:GLU:HG2	1.21	1.03
1:B:159:LYS:HG3	1:B:169:VAL:HG21	1.46	0.98
1:B:145:THR:HG23	1:B:175:GLU:HG2	1.42	0.97
1:B:141:ASN:HB3	1:B:170:LEU:HD11	1.48	0.95
2:C:379:ILE:HG21	2:C:402:LEU:HD13	1.48	0.94

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	383/392 (98%)	356 (93%)	24 (6%)	3 (1%)	19	23
1	B	372/392 (95%)	344 (92%)	25 (7%)	3 (1%)	19	23
2	C	97/142 (68%)	89 (92%)	6 (6%)	2 (2%)	7	5
2	D	98/142 (69%)	91 (93%)	6 (6%)	1 (1%)	15	17
All	All	950/1068 (89%)	880 (93%)	61 (6%)	9 (1%)	17	20

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	362	GLU
1	B	254	SER
1	B	380	LEU
2	D	418	GLU

### 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	318/324 (98%)	305 (96%)	13 (4%)	30	43
1	B	312/324 (96%)	301 (96%)	11 (4%)	36	50
2	C	86/122 (70%)	79 (92%)	7 (8%)	11	15
2	D	87/122 (71%)	78 (90%)	9 (10%)	7	8
All	All	803/892 (90%)	763 (95%)	40 (5%)	24	34

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	135	LEU
1	B	376	GLN
2	D	401	LEU
1	B	330	GLN
1	B	380	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	194	ASN
1	B	347	GLN
2	D	415	GLN
1	B	279	GLN
1	B	330	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands 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	TRS	A	7359	-	7,7,7	0.56	0	9,9,9	0.43	0
3	TRS	B	7360	-	7,7,7	0.40	0	9,9,9	0.42	0

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	TRS	A	7359	-	-	0/9/9/9	-
3	TRS	B	7360	-	-	0/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	7360	TRS	1	0

## 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, 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	385/392 (98%)	0.15	15 (3%)	39 46	16, 33, 67, 80	0
1	B	376/392 (95%)	0.32	15 (3%)	38 45	23, 40, 58, 71	0
2	C	99/142 (69%)	0.18	3 (3%)	50 57	24, 42, 67, 79	0
2	D	100/142 (70%)	0.13	5 (5%)	28 35	25, 40, 70, 76	0
All	All	960/1068 (89%)	0.22	38 (3%)	38 45	16, 38, 64, 80	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	PHE	3.7
1	A	95	ILE	3.5
1	A	51	ILE	3.5
1	A	61	LEU	3.3
1	B	142	ALA	3.2

### 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](#)

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. 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TRS	B	7360	8/8	0.76	0.30	58,60,61,65	0
3	TRS	A	7359	8/8	0.93	0.16	25,31,32,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.