



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 05:29 AM GMT

PDB ID : 3A8Y  
Title : Crystal structure of the complex between the BAG5 BD5 and Hsp70 NBD  
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Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2009-10-13  
Resolution : 2.30 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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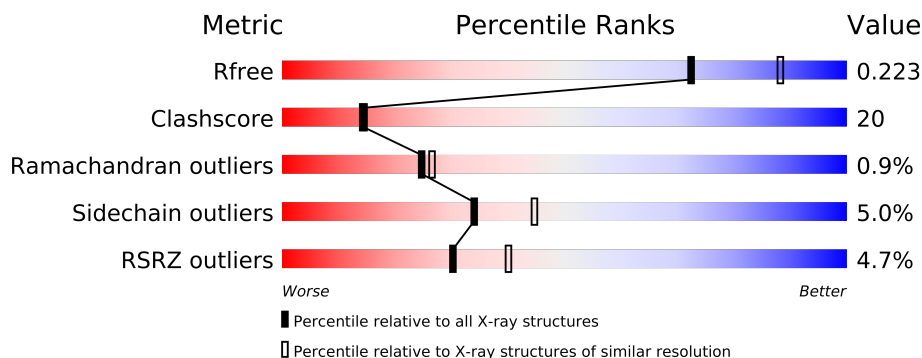
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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. 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	392	
1	B	392	
2	C	142	
2	D	142	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	TRS	B	7360	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8057 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 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

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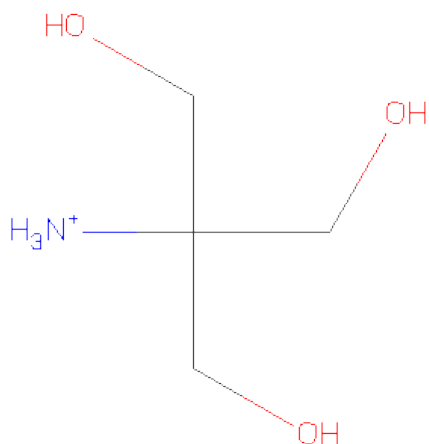
Chain	Residue	Modelled	Actual	Comment	Reference
C	338	SER	-	EXPRESSION TAG	UNP Q9UL15
C	339	SER	-	EXPRESSION TAG	UNP Q9UL15
C	340	GLY	-	EXPRESSION TAG	UNP Q9UL15
C	448	CYS	-	EXPRESSION TAG	UNP Q9UL15
C	449	LYS	-	EXPRESSION TAG	UNP Q9UL15
C	450	ALA	-	EXPRESSION TAG	UNP Q9UL15
C	451	ALA	-	EXPRESSION TAG	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

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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.

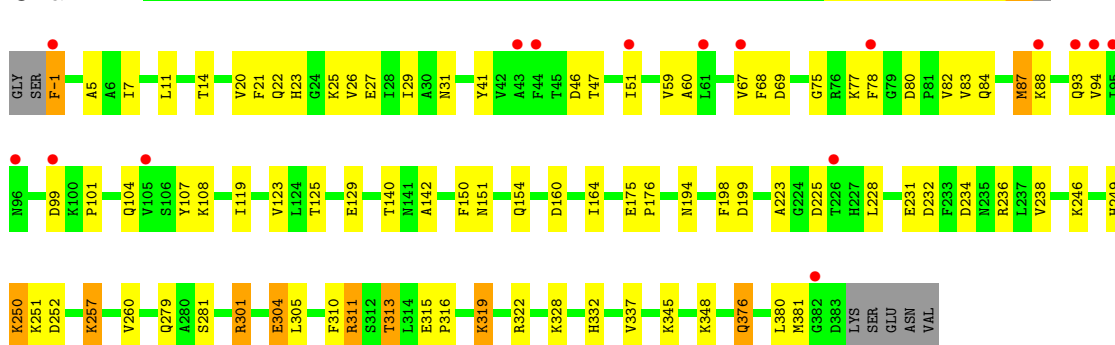
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	234	Total	O	0	0
			234	234		
4	B	207	Total	O	0	0
			207	207		
4	C	57	Total	O	0	0
			57	57		
4	D	24	Total	O	0	0
			24	24		

### 3 Residue-property plots

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.

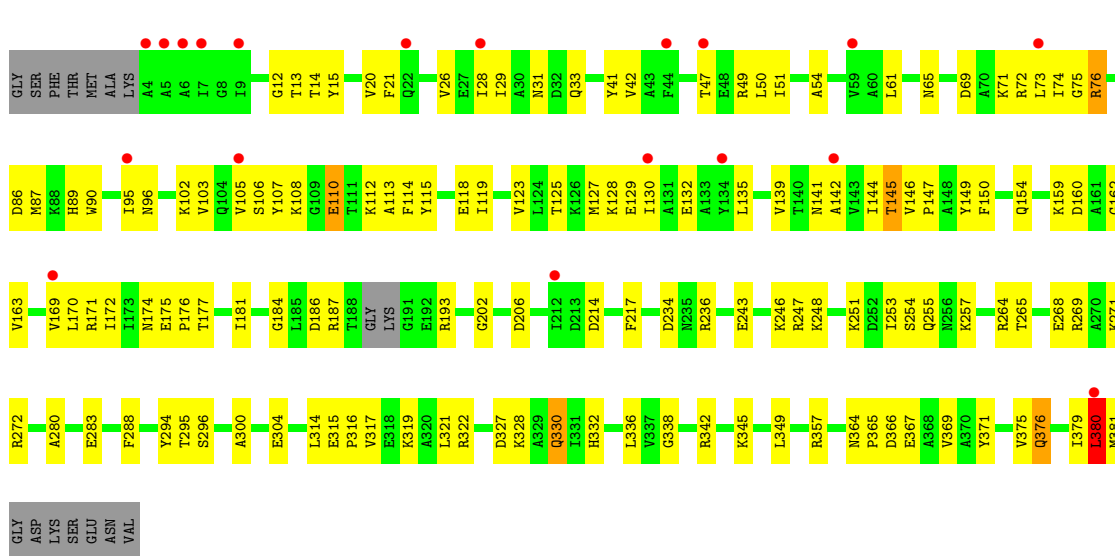
#### • Molecule 1: Heat shock 70 kDa protein 1

Chain A:



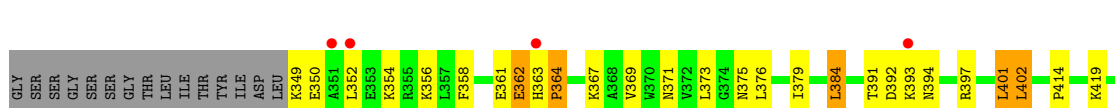
#### • Molecule 1: Heat shock 70 kDa protein 1

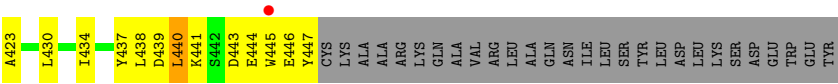
Chain B:



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

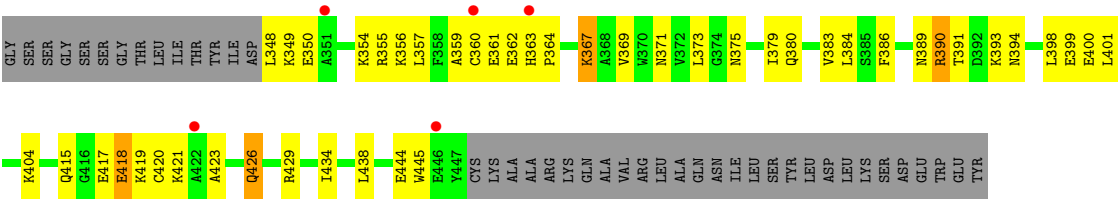
Chain C:





● Molecule 2: BAG family molecular chaperone regulator 5

Chain D:





## 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 0.222 , 0.223	Depositor DCC
$R_{free}$ test set	2148 reflections (5.05%)	DCC
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 , 43.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 42580 reflections (0.002%)	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.

## 5 Model quality

### 5.1 Standard geometry

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 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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	57	0	0	2	0
4	D	24	0	0	0	0
All	All	8057	0	7551	295	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 20.

The worst 5 of 295 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

### 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	383/392 (98%)	356 (93%)	24 (6%)	3 (1%)	27	30
1	B	372/392 (95%)	344 (92%)	25 (7%)	3 (1%)	27	30
2	C	97/142 (68%)	89 (92%)	6 (6%)	2 (2%)	11	8
2	D	98/142 (69%)	91 (93%)	6 (6%)	1 (1%)	22	23
All	All	950/1068 (89%)	880 (93%)	61 (6%)	9 (1%)	25	26

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	MET
2	C	362	GLU
1	B	254	SER

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Mol	Chain	Res	Type
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%)	41	55
1	B	312/324 (96%)	301 (96%)	11 (4%)	48	63
2	C	86/122 (70%)	79 (92%)	7 (8%)	17	20
2	D	87/122 (71%)	78 (90%)	9 (10%)	10	11
All	All	803/892 (90%)	763 (95%)	40 (5%)	34	45

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 ⓘ

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 ⓘ

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	1.14	1 (14%)	9,9,9	0.68	0
3	TRS	B	7360	-	7,7,7	0.99	1 (14%)	9,9,9	0.65	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	0/0/0/0
3	TRS	B	7360	-	-	0/9/9/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	7360	TRS	C-N	-2.30	1.47	1.50
3	A	7359	TRS	C-N	-2.28	1.47	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	385/392 (98%)	0.19	16 (4%) 35 45	16, 33, 67, 80	0
1	B	376/392 (95%)	0.39	19 (5%) 27 37	23, 40, 58, 71	0
2	C	99/142 (69%)	0.27	5 (5%) 27 37	24, 42, 67, 79	0
2	D	100/142 (70%)	0.19	5 (5%) 28 38	25, 40, 70, 76	0
All	All	960/1068 (89%)	0.28	45 (4%) 30 40	16, 38, 64, 80	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	95	ILE	4.3
1	A	44	PHE	4.0
1	B	142	ALA	3.7
1	A	51	ILE	3.4
1	B	22	GLN	3.4

### 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

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( $\text{\AA}^2$ )	Q<0.9
3	TRS	B	7360	8/8	0.28	4.14	58,60,61,65	0
3	TRS	A	7359	8/8	0.15	0.91	25,31,32,35	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.