



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2025 – 02:15 pm BST

PDB ID : 6GVW / pdb\_00006gvw  
Title : Crystal structure of the BRCA1-A complex  
Authors : Bunker, R.D.; Rabl, J.; Thoma, N.H.  
Deposited on : 2018-06-21  
Resolution : 3.75 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)

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<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	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

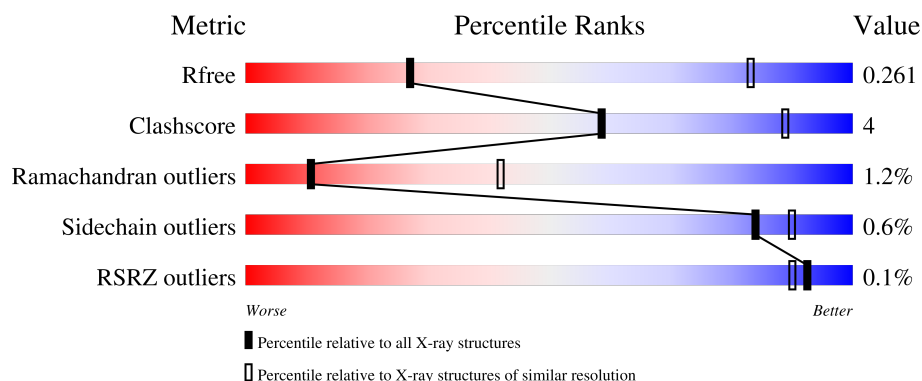
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.75 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))
$R_{free}$	164625	1256 (3.92-3.60)
Clashscore	180529	1321 (3.92-3.60)
Ramachandran outliers	177936	1293 (3.92-3.60)
Sidechain outliers	177891	1288 (3.92-3.60)
RSRZ outliers	164620	1256 (3.92-3.60)

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	411	 65% 10% 24%
1	F	411	 70% 8% 22%
2	B	295	 79% 9% 11%
2	G	295	 83% 6% 11%
3	C	387	 89% 10% ..

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Mol	Chain	Length	Quality of chain
3	H	387	 89% 10%
4	D	337	 59% 11% 29%
4	I	337	 62% 8% 29%
5	E	64	 88% 5% 8%
5	J	64	 78% 14% 8%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 40106 atoms, of which 19968 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 BRCA1-A complex subunit Abraxas 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	312	Total	C	H	N	O	S	160	0	0
			4992	1566	2500	440	472	14			
1	F	320	Total	C	H	N	O	S	162	0	0
			5122	1611	2561	448	486	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q8BPZ8
A	-2	GLY	-	expression tag	UNP Q8BPZ8
A	-1	GLY	-	expression tag	UNP Q8BPZ8
A	0	ARG	-	expression tag	UNP Q8BPZ8
F	-3	GLY	-	expression tag	UNP Q8BPZ8
F	-2	GLY	-	expression tag	UNP Q8BPZ8
F	-1	GLY	-	expression tag	UNP Q8BPZ8
F	0	ARG	-	expression tag	UNP Q8BPZ8

- Molecule 2 is a protein called Lys-63-specific deubiquitinase BRCC36.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	262	Total	C	H	N	O	S	120	0	0
			4202	1316	2101	370	401	14			
2	G	262	Total	C	H	N	O	S	120	0	0
			4202	1316	2101	370	401	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P46737
B	-2	GLY	-	expression tag	UNP P46737
B	-1	GLY	-	expression tag	UNP P46737
B	0	ARG	-	expression tag	UNP P46737

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	GLY	-	expression tag	UNP P46737
G	-2	GLY	-	expression tag	UNP P46737
G	-1	GLY	-	expression tag	UNP P46737
G	0	ARG	-	expression tag	UNP P46737

- Molecule 3 is a protein called BRISC and BRCA1-A complex member 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	383	Total	C	H	N	O	S	161	0	0
			6085	1994	3008	505	564	14			
3	H	383	Total	C	H	N	O	S	161	0	0
			6085	1994	3008	505	564	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q8K3W0
C	-2	GLY	-	expression tag	UNP Q8K3W0
C	-1	GLY	-	expression tag	UNP Q8K3W0
C	0	ARG	-	expression tag	UNP Q8K3W0
H	-3	GLY	-	expression tag	UNP Q8K3W0
H	-2	GLY	-	expression tag	UNP Q8K3W0
H	-1	GLY	-	expression tag	UNP Q8K3W0
H	0	ARG	-	expression tag	UNP Q8K3W0

- Molecule 4 is a protein called BRISC and BRCA1-A complex member 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	239	Total	C	H	N	O	S	103	0	0
			3765	1206	1873	307	361	18			
4	I	238	Total	C	H	N	O	S	103	0	0
			3755	1203	1868	306	360	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-3	GLY	-	expression tag	UNP Q3UI43
D	-2	GLY	-	expression tag	UNP Q3UI43
D	-1	GLY	-	expression tag	UNP Q3UI43
D	0	ARG	-	expression tag	UNP Q3UI43
I	-3	GLY	-	expression tag	UNP Q3UI43
I	-2	GLY	-	expression tag	UNP Q3UI43

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	GLY	-	expression tag	UNP Q3UI43
I	0	ARG	-	expression tag	UNP Q3UI43

- Molecule 5 is a protein called BRCA1-A complex subunit RAP80.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	59	Total	C	H	N	O	S	25	0	0
			947	310	474	82	78	3			
5	J	59	Total	C	H	N	O	S	25	0	0
			947	310	474	82	78	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	271	GLY	-	expression tag	UNP Q5U5Q9
E	272	GLY	-	expression tag	UNP Q5U5Q9
E	273	GLY	-	expression tag	UNP Q5U5Q9
E	274	ARG	-	expression tag	UNP Q5U5Q9
J	271	GLY	-	expression tag	UNP Q5U5Q9
J	272	GLY	-	expression tag	UNP Q5U5Q9
J	273	GLY	-	expression tag	UNP Q5U5Q9
J	274	ARG	-	expression tag	UNP Q5U5Q9

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Zn	0	0
			1	1		
6	G	1	Total	Zn	0	0
			1	1		

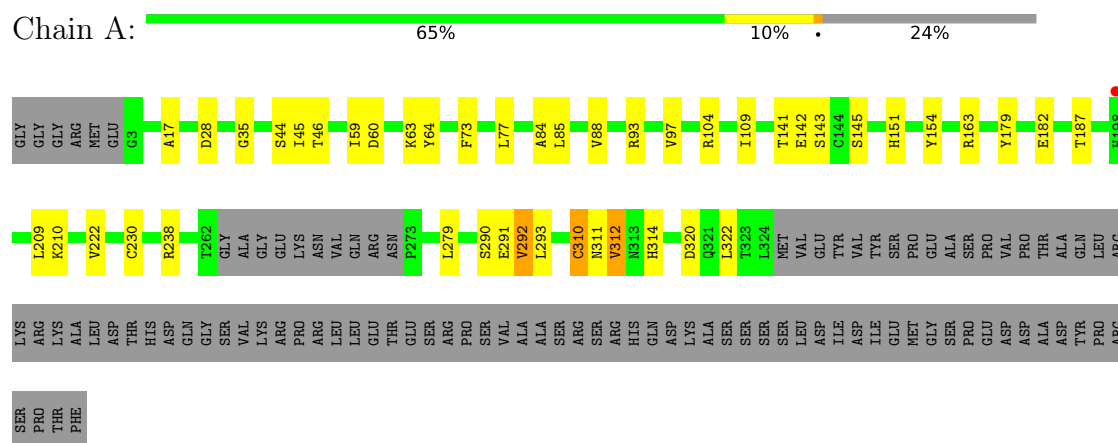
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	O	0	0
			1	1		
7	G	1	Total	O	0	0
			1	1		

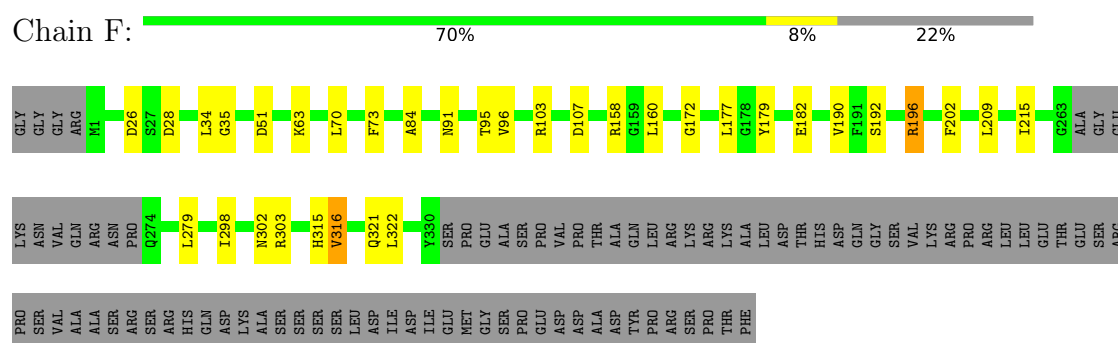
### 3 Residue-property plots [i](#)

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.

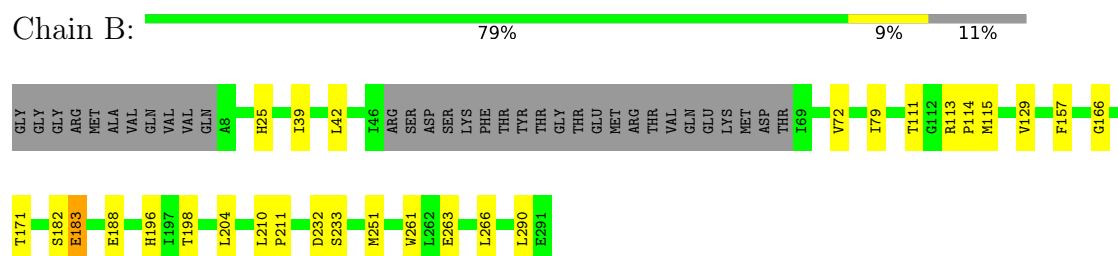
- Molecule 1: BRCA1-A complex subunit Abraxas 1



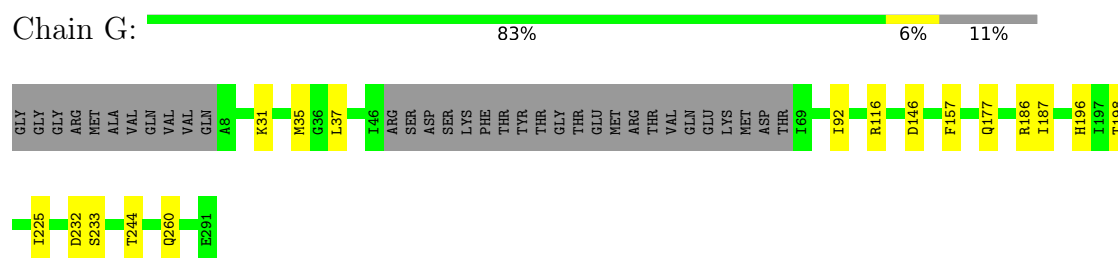
- Molecule 1: BRCA1-A complex subunit Abraxas 1



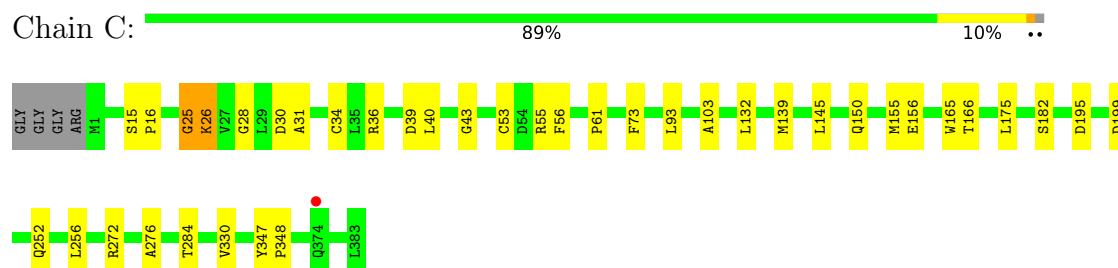
- Molecule 2: Lys-63-specific deubiquitinase BRCC36



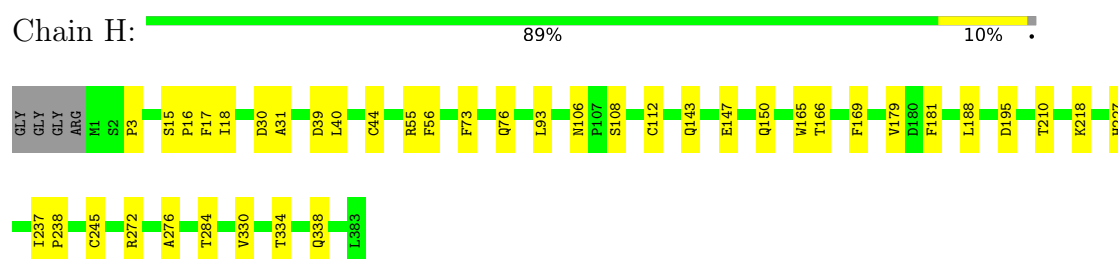
- Molecule 2: Lys-63-specific deubiquitinase BRCC36



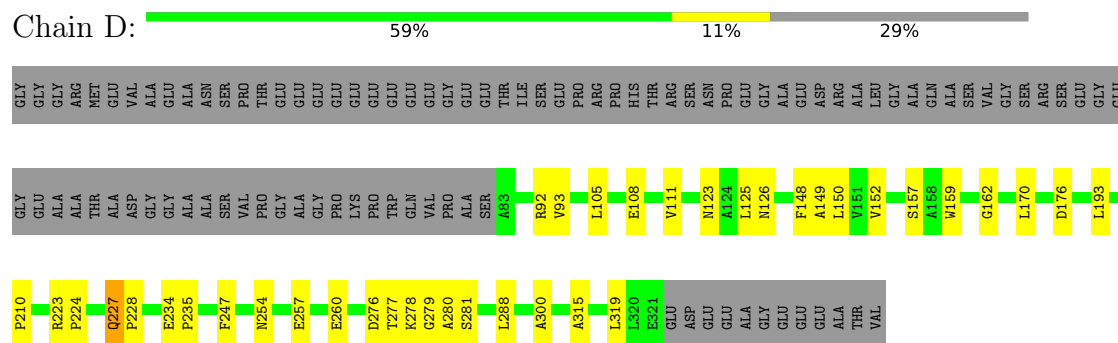
- Molecule 3: BRISC and BRCA1-A complex member 2



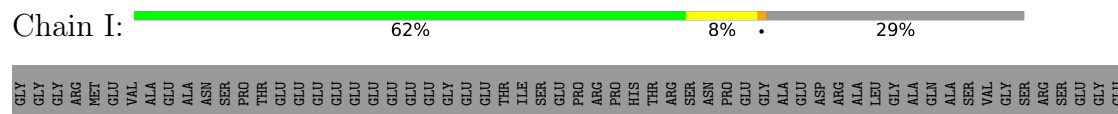
- Molecule 3: BRISC and BRCA1-A complex member 2



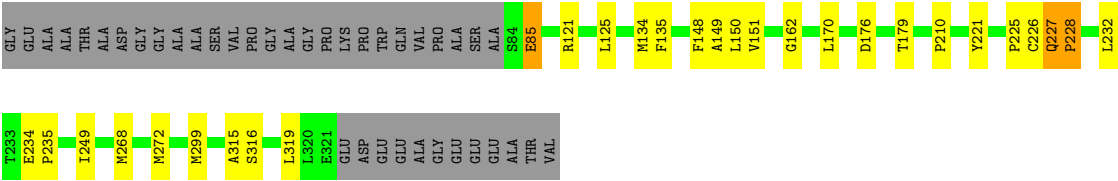
- Molecule 4: BRISC and BRCA1-A complex member 1



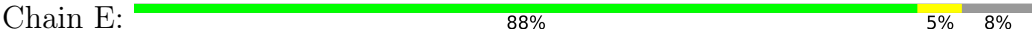
- Molecule 4: BRISC and BRCA1-A complex member 1



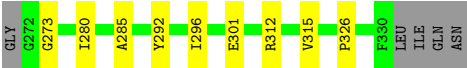




● Molecule 5: BRCA1-A complex subunit RAP80



● Molecule 5: BRCA1-A complex subunit RAP80



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.10Å 122.64Å 431.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 3.75 29.99 – 3.75	Depositor EDS
% Data completeness (in resolution range)	82.3 (29.99-3.75) 82.3 (29.99-3.75)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 3.75Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.227 , 0.259 0.228 , 0.261	Depositor DCC
$R_{free}$ test set	2214 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	187.4	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 165.8	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	0.96	EDS
Total number of atoms	40106	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	223.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: ZN

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	0.91	0/2538	1.09	0/3429
1	F	0.91	0/2608	1.08	0/3523
2	B	0.91	0/2138	1.07	0/2890
2	G	0.91	0/2138	1.08	0/2890
3	C	0.88	0/3169	1.02	0/4311
3	H	0.87	0/3169	0.99	0/4311
4	D	0.90	0/1937	1.04	0/2629
4	I	0.90	0/1932	1.02	0/2622
5	E	0.86	0/489	1.03	0/664
5	J	0.87	0/489	1.01	0/664
All	All	0.89	0/20607	1.05	0/27933

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	2492	2500	2483	27	0
1	F	2561	2561	2547	26	0
2	B	2101	2101	2087	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	2101	2101	2087	12	0
3	C	3077	3008	3000	30	0
3	H	3077	3008	3000	30	0
4	D	1892	1873	1864	27	0
4	I	1887	1868	1859	25	0
5	E	473	474	470	4	0
5	J	473	474	470	12	0
6	B	1	0	0	0	0
6	G	1	0	0	0	0
7	B	1	0	0	0	0
7	G	1	0	0	0	0
All	All	20138	19968	19867	170	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 4.

The worst 5 of 170 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:A:187:THR:HG22	2:G:260:GLN:OE1	1.82	0.78
4:I:148:PHE:HB2	4:I:170:LEU:HD11	1.65	0.77
4:D:276:ASP:O	4:D:277:THR:OG1	2.04	0.76
4:I:249:ILE:HD12	4:I:272:MET:HE2	1.72	0.72
1:A:145:SER:OG	2:B:188:GLU:OE1	2.09	0.70

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	308/411 (75%)	270 (88%)	31 (10%)	7 (2%)	<b>5</b> 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	316/411 (77%)	281 (89%)	30 (10%)	5 (2%)	8	37
2	B	258/295 (88%)	245 (95%)	10 (4%)	3 (1%)	11	42
2	G	258/295 (88%)	243 (94%)	14 (5%)	1 (0%)	30	63
3	C	381/387 (98%)	359 (94%)	20 (5%)	2 (0%)	25	58
3	H	381/387 (98%)	362 (95%)	18 (5%)	1 (0%)	37	68
4	D	237/337 (70%)	212 (90%)	20 (8%)	5 (2%)	5	33
4	I	236/337 (70%)	220 (93%)	11 (5%)	5 (2%)	5	33
5	E	57/64 (89%)	55 (96%)	2 (4%)	0	100	100
5	J	57/64 (89%)	55 (96%)	2 (4%)	0	100	100
All	All	2489/2988 (83%)	2302 (92%)	158 (6%)	29 (1%)	11	42

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	VAL
2	B	290	LEU
1	F	177	LEU
1	F	316	VAL
4	I	227	GLN

### 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	287/371 (77%)	284 (99%)	3 (1%)	73	82
1	F	294/371 (79%)	291 (99%)	3 (1%)	73	82
2	B	239/267 (90%)	238 (100%)	1 (0%)	89	93
2	G	239/267 (90%)	239 (100%)	0	100	100
3	C	336/337 (100%)	335 (100%)	1 (0%)	91	94
3	H	336/337 (100%)	332 (99%)	4 (1%)	67	79
4	D	218/288 (76%)	216 (99%)	2 (1%)	75	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	I	218/288 (76%)	218 (100%)	0	100	100
5	E	50/55 (91%)	50 (100%)	0	100	100
5	J	50/55 (91%)	50 (100%)	0	100	100
All	All	2267/2636 (86%)	2253 (99%)	14 (1%)	84	90

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	51	ASP
1	F	196	ARG
3	H	227	HIS
3	H	93	LEU
3	H	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	126	HIS
3	H	252	GLN
4	I	186	ASN
3	H	266	GLN
2	B	226	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 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 [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	312/411 (75%)	-0.69	1 (0%) 90 80	148, 216, 286, 333	0
1	F	320/411 (77%)	-0.73	0 100 100	152, 230, 304, 338	0
2	B	262/295 (88%)	-0.73	0 100 100	162, 212, 268, 300	0
2	G	262/295 (88%)	-0.86	0 100 100	162, 217, 282, 355	0
3	C	383/387 (98%)	-0.66	1 (0%) 90 80	147, 190, 250, 288	0
3	H	383/387 (98%)	-0.80	0 100 100	160, 226, 295, 358	0
4	D	239/337 (70%)	-0.66	0 100 100	135, 214, 310, 388	0
4	I	238/337 (70%)	-0.66	0 100 100	169, 246, 345, 395	0
5	E	59/64 (92%)	-0.87	0 100 100	154, 197, 248, 264	0
5	J	59/64 (92%)	-0.87	0 100 100	163, 214, 298, 313	0
All	All	2517/2988 (84%)	-0.73	2 (0%) 92 90	135, 217, 294, 395	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	374	GLN	2.3
1	A	198	HIS	2.1

### 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 oligosaccharides 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(Å <sup>2</sup> )	Q<0.9
6	ZN	B	301	1/1	0.99	0.03	192,192,192,192	0
6	ZN	G	301	1/1	1.00	0.02	192,192,192,192	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.