



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2017 – 04:06 PM EDT

PDB ID : 4OQB  
Title : Structure of Human PARP-1 bound to a DNA double strand break in complex with (2Z)-2-{4-[2-(morpholin-4-yl)ethoxy]benzylidene}-3-oxo-2,3-dihydro-1-benzofuran-7-carboxamide  
Authors : Pascal, J.M.; Steffen, J.D.  
Deposited on : unknown  
Resolution : 3.36 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

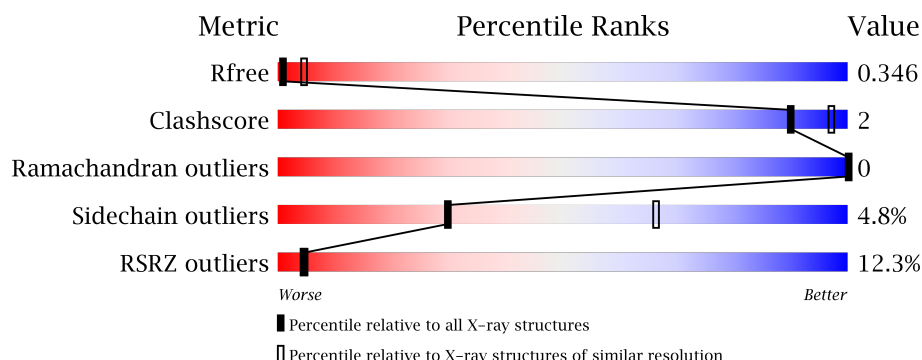
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.36 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))
$R_{free}$	100719	1156 (3.42-3.30)
Clashscore	112137	1231 (3.42-3.30)
Ramachandran outliers	110173	1212 (3.42-3.30)
Sidechain outliers	110143	1211 (3.42-3.30)
RSRZ outliers	101464	1165 (3.42-3.30)

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. 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	267	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>5%</div> <div>17%</div> </div> </div>
1	D	267	<div> <div>12%</div> <div> <div></div> <div>78%</div> <div>5%</div> <div>17%</div> </div> </div>
2	C	505	<div> <div>10%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>10%</div> </div> </div>
2	F	505	<div> <div>16%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>10%</div> </div> </div>
3	M	26	<div> <div></div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	N	26	 92%8%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11775 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 Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	1	0
			1755	1110	305	327	13			
1	D	222	Total	C	N	O	S	0	1	0
			1755	1110	305	327	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	ASP	-	LINKER	UNP P09874
A	206	ILE	-	LINKER	UNP P09874
A	367	LEU	-	EXPRESSION TAG	UNP P09874
A	368	GLU	-	EXPRESSION TAG	UNP P09874
A	369	HIS	-	EXPRESSION TAG	UNP P09874
A	370	HIS	-	EXPRESSION TAG	UNP P09874
A	371	HIS	-	EXPRESSION TAG	UNP P09874
A	372	HIS	-	EXPRESSION TAG	UNP P09874
A	373	HIS	-	EXPRESSION TAG	UNP P09874
A	374	HIS	-	EXPRESSION TAG	UNP P09874
D	205	ASP	-	LINKER	UNP P09874
D	206	ILE	-	LINKER	UNP P09874
D	367	LEU	-	EXPRESSION TAG	UNP P09874
D	368	GLU	-	EXPRESSION TAG	UNP P09874
D	369	HIS	-	EXPRESSION TAG	UNP P09874
D	370	HIS	-	EXPRESSION TAG	UNP P09874
D	371	HIS	-	EXPRESSION TAG	UNP P09874
D	372	HIS	-	EXPRESSION TAG	UNP P09874
D	373	HIS	-	EXPRESSION TAG	UNP P09874
D	374	HIS	-	EXPRESSION TAG	UNP P09874

- Molecule 2 is a protein called Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	456	Total	C	N	O	S	0	0	0
			3586	2296	605	672	13			
2	F	456	Total	C	N	O	S	0	0	0
			3586	2296	605	672	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1015	LEU	-	EXPRESSION TAG	UNP P09874
C	1016	GLU	-	EXPRESSION TAG	UNP P09874
C	1017	HIS	-	EXPRESSION TAG	UNP P09874
C	1018	HIS	-	EXPRESSION TAG	UNP P09874
C	1019	HIS	-	EXPRESSION TAG	UNP P09874
C	1020	HIS	-	EXPRESSION TAG	UNP P09874
C	1021	HIS	-	EXPRESSION TAG	UNP P09874
C	1022	HIS	-	EXPRESSION TAG	UNP P09874
F	1015	LEU	-	EXPRESSION TAG	UNP P09874
F	1016	GLU	-	EXPRESSION TAG	UNP P09874
F	1017	HIS	-	EXPRESSION TAG	UNP P09874
F	1018	HIS	-	EXPRESSION TAG	UNP P09874
F	1019	HIS	-	EXPRESSION TAG	UNP P09874
F	1020	HIS	-	EXPRESSION TAG	UNP P09874
F	1021	HIS	-	EXPRESSION TAG	UNP P09874
F	1022	HIS	-	EXPRESSION TAG	UNP P09874

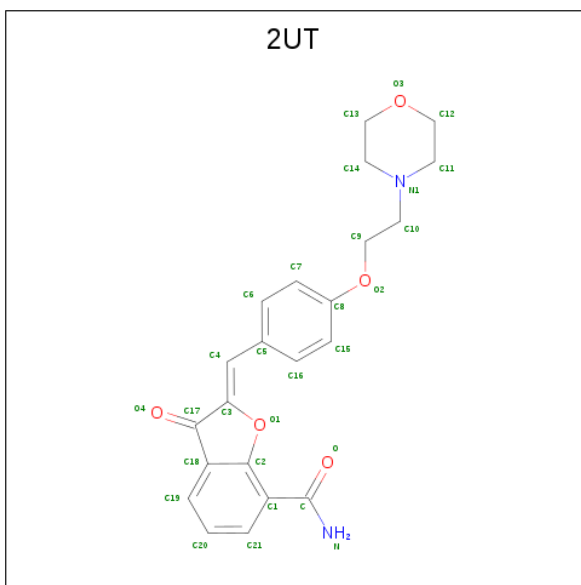
- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	26	Total	C	N	O	P	0	0	0
			530	251	100	154	25			
3	N	26	Total	C	N	O	P	0	0	0
			530	251	100	154	25			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		

- Molecule 5 is (2Z)-2-{4-[2-(morpholin-4-yl)ethoxy]benzylidene}-3-oxo-2,3-dihydro-1-benzofuran-7-carboxamide (three-letter code: 2UT) (formula: C<sub>22</sub>H<sub>22</sub>N<sub>2</sub>O<sub>5</sub>).

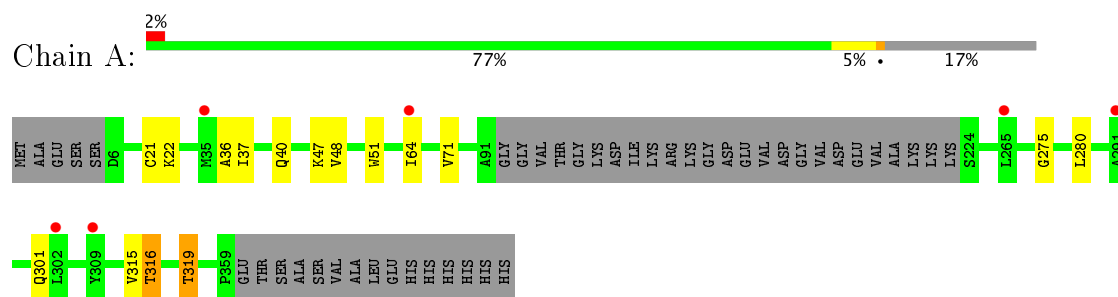


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			29	22	2	5		

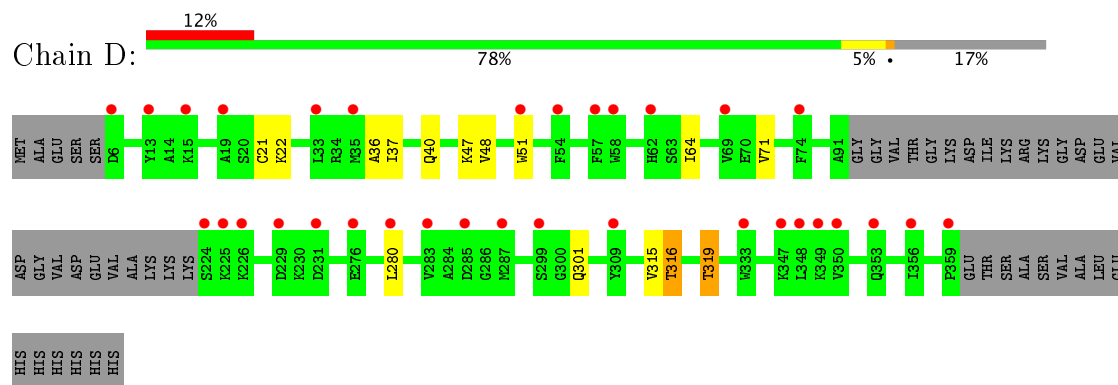
### 3 Residue-property plots [i](#)

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.

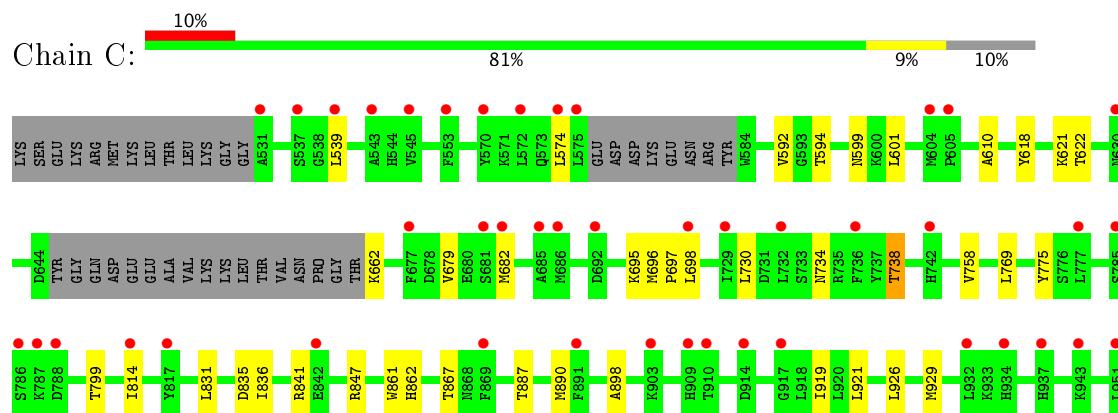
- Molecule 1: Poly [ADP-ribose] polymerase 1

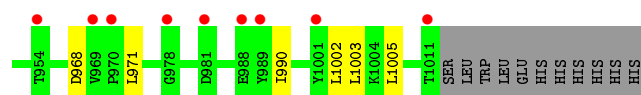


- Molecule 1: Poly [ADP-ribose] polymerase 1

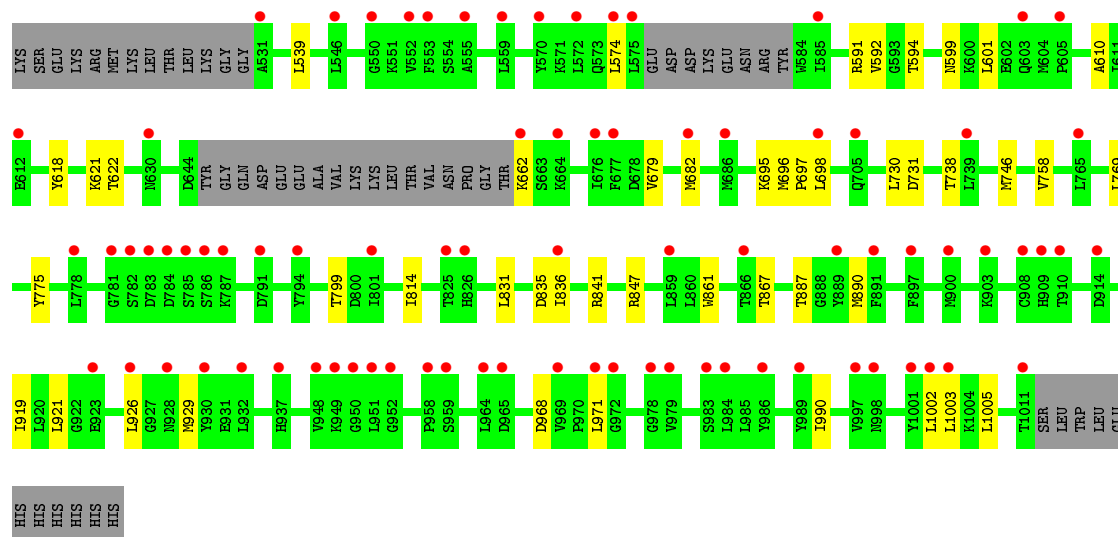
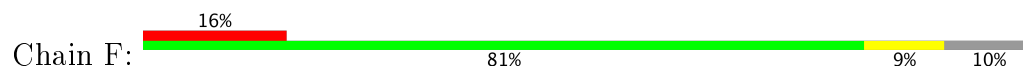


- Molecule 2: Poly [ADP-ribose] polymerase 1





- Molecule 2: Poly [ADP-ribose] polymerase 1



- Molecule 3: DNA (26-MER)



- Molecule 3: DNA (26-MER)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.10Å 113.08Å 296.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.36 49.37 – 3.36	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-3.36) 98.9 (49.37-3.36)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.99 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.322 , 0.349 0.317 , 0.346	Depositor DCC
$R_{free}$ test set	1621 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	136.5	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 108.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11775	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	213.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.91% 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, 2UT

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	0.26	0/1795	0.40	0/2416
1	D	0.26	0/1795	0.40	0/2416
2	C	0.26	0/3660	0.42	0/4940
2	F	0.26	0/3660	0.43	0/4940
3	M	0.27	0/594	0.80	0/915
3	N	0.24	0/594	0.78	2/915 (0.2%)
All	All	0.26	0/12098	0.47	2/16542 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1	DG	C5'-C4'-O4'	5.23	119.23	109.30
3	N	1	DG	C5'-C4'-C3'	5.08	123.25	114.10

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	1755	0	1712	6	0
1	D	1755	0	1712	6	0
2	C	3586	0	3604	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	3586	0	3604	18	0
3	M	530	0	292	1	0
3	N	530	0	292	1	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	C	29	0	22	2	0
All	All	11775	0	11238	48	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 2.

All (48) 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)
2:F:574:LEU:HD11	2:F:610:ALA:HB1	1.69	0.73
2:C:574:LEU:HD11	2:C:610:ALA:HB1	1.70	0.72
1:A:36:ALA:HB2	1:A:51:TRP:CE3	2.39	0.57
1:D:36:ALA:HB2	1:D:51:TRP:CE3	2.39	0.57
2:C:831:LEU:HD12	2:C:1005:LEU:HD23	1.88	0.54
2:F:831:LEU:HD12	2:F:1005:LEU:HD23	1.88	0.54
2:C:898:ALA:HB2	5:C:1101:2UT:H2	1.91	0.53
2:F:814:ILE:HG21	2:F:836:ILE:HD12	1.92	0.52
2:C:814:ILE:HG21	2:C:836:ILE:HD12	1.92	0.51
2:F:679:VAL:HG11	2:F:775:TYR:CZ	2.46	0.50
2:C:679:VAL:HG11	2:C:775:TYR:CZ	2.47	0.50
2:F:919:ILE:HG22	2:F:1005:LEU:HD11	1.94	0.49
2:C:919:ILE:HG22	2:C:1005:LEU:HD11	1.94	0.49
2:F:696:MET:N	2:F:697:PRO:HD2	2.28	0.49
2:C:696:MET:N	2:C:697:PRO:HD2	2.28	0.48
1:D:315:VAL:HG13	1:D:316:THR:HG22	1.95	0.48
1:A:315:VAL:HG13	1:A:316:THR:HG22	1.96	0.47
2:C:861:TRP:CD2	2:C:921:LEU:HD21	2.49	0.47
3:M:22:DT:H2''	3:M:23:DA:C8	2.50	0.47
1:D:319:THR:HG21	2:F:731:ASP:HA	1.96	0.47
2:C:862:HIS:ND1	5:C:1101:2UT:O	2.48	0.46
2:F:861:TRP:CD2	2:F:921:LEU:HD21	2.49	0.46
2:F:926:LEU:HD13	2:F:929:MET:HE3	1.98	0.44
2:C:926:LEU:HD13	2:C:929:MET:HE3	1.99	0.44
1:A:275:GLY:HA2	3:N:23:DA:H3'	1.99	0.44
2:F:799:THR:HG22	2:F:841:ARG:HA	2.00	0.43
2:C:539:LEU:HD11	2:C:601:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:THR:CG2	2:F:731:ASP:HA	2.48	0.42
1:D:64:ILE:HD13	1:D:71:VAL:CG2	2.50	0.42
2:C:814:ILE:CG2	2:C:1003:LEU:HD21	2.50	0.42
1:A:64:ILE:HD13	1:A:71:VAL:CG2	2.50	0.42
2:C:799:THR:HG22	2:C:841:ARG:HA	2.00	0.42
2:F:539:LEU:HD11	2:F:601:LEU:HD21	2.00	0.41
2:C:734:ASN:O	2:C:738:THR:OG1	2.38	0.41
2:C:682:MET:HG2	2:C:867:THR:HG22	2.02	0.41
2:F:682:MET:HG2	2:F:867:THR:HG22	2.03	0.41
2:F:696:MET:N	2:F:697:PRO:CD	2.83	0.41
2:C:990:ILE:HD12	2:C:990:ILE:N	2.36	0.41
1:A:319:THR:HG22	2:C:734:ASN:HD22	1.86	0.41
2:C:618:TYR:CE2	2:C:622:THR:HG21	2.56	0.41
2:C:696:MET:N	2:C:697:PRO:CD	2.83	0.41
2:F:591:ARG:HD3	2:F:746:MET:HE1	2.03	0.41
2:F:814:ILE:CG2	2:F:1003:LEU:HD21	2.50	0.41
1:D:36:ALA:HB2	1:D:51:TRP:CZ3	2.56	0.41
2:F:990:ILE:HD12	2:F:990:ILE:N	2.36	0.41
2:C:618:TYR:O	2:C:622:THR:HG22	2.21	0.40
1:A:36:ALA:HB2	1:A:51:TRP:CZ3	2.56	0.40
2:F:618:TYR:O	2:F:622:THR:HG22	2.21	0.40

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	219/267 (82%)	212 (97%)	7 (3%)	0	100	100
1	D	219/267 (82%)	212 (97%)	7 (3%)	0	100	100
2	C	450/505 (89%)	423 (94%)	27 (6%)	0	100	100
2	F	450/505 (89%)	422 (94%)	28 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1338/1544 (87%)	1269 (95%)	69 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	189/237 (80%)	179 (95%)	10 (5%)	26	63
1	D	189/237 (80%)	179 (95%)	10 (5%)	26	63
2	C	391/443 (88%)	373 (95%)	18 (5%)	31	68
2	F	391/443 (88%)	373 (95%)	18 (5%)	31	68
All	All	1160/1360 (85%)	1104 (95%)	56 (5%)	30	66

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	CYS
1	A	22	LYS
1	A	37	ILE
1	A	40	GLN
1	A	47	LYS
1	A	48	VAL
1	A	280	LEU
1	A	301	GLN
1	A	316	THR
1	A	319	THR
2	C	592	VAL
2	C	594	THR
2	C	599	ASN
2	C	621	LYS
2	C	662	LYS
2	C	695	LYS
2	C	698	LEU

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Mol	Chain	Res	Type
2	C	730	LEU
2	C	738	THR
2	C	758	VAL
2	C	769	LEU
2	C	835	ASP
2	C	847	ARG
2	C	887	THR
2	C	890	MET
2	C	968	ASP
2	C	971	LEU
2	C	1002	LEU
1	D	21	CYS
1	D	22	LYS
1	D	37	ILE
1	D	40	GLN
1	D	47	LYS
1	D	48	VAL
1	D	280	LEU
1	D	301	GLN
1	D	316	THR
1	D	319	THR
2	F	592	VAL
2	F	594	THR
2	F	599	ASN
2	F	621	LYS
2	F	662	LYS
2	F	695	LYS
2	F	698	LEU
2	F	730	LEU
2	F	738	THR
2	F	758	VAL
2	F	769	LEU
2	F	835	ASP
2	F	847	ARG
2	F	887	THR
2	F	890	MET
2	F	968	ASP
2	F	971	LEU
2	F	1002	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	573	GLN
2	C	599	ASN
2	C	613	HIS
2	C	820	ASN
2	C	856	ASN
2	C	906	ASN
2	C	961	ASN
2	F	573	GLN
2	F	599	ASN
2	F	613	HIS
2	F	820	ASN
2	F	856	ASN
2	F	906	ASN
2	F	961	ASN

### 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](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
5	2UT	C	1101	-	32,32,32	0.24	0	42,44,44	1.98	7 (16%)

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
5	2UT	C	1101	-	-	0/12/34/34	0/4/4/4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1101	2UT	C18-C17-C3	-6.46	100.75	104.09
5	C	1101	2UT	C18-C2-C1	-2.89	121.65	124.84
5	C	1101	2UT	C2-C1-C	-2.49	121.86	125.82
5	C	1101	2UT	C2-O1-C3	2.32	107.18	105.46
5	C	1101	2UT	O1-C3-C17	3.22	111.79	109.47
5	C	1101	2UT	O4-C17-C3	6.19	132.27	126.23
5	C	1101	2UT	C2-C18-C17	6.95	109.63	107.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1101	2UT	2	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

### 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	222/267 (83%)	0.15	6 (2%) 55 56	136, 174, 261, 285	0
1	D	222/267 (83%)	0.66	33 (14%) 3 3	176, 243, 321, 342	0
2	C	456/505 (90%)	0.81	53 (11%) 5 5	135, 195, 248, 286	0
2	F	456/505 (90%)	1.01	81 (17%) 2 2	169, 241, 300, 331	0
3	M	26/26 (100%)	-0.59	0 100 100	161, 187, 226, 228	0
3	N	26/26 (100%)	-0.62	0 100 100	157, 203, 226, 230	0
All	All	1408/1596 (88%)	0.70	173 (12%) 5 4	135, 214, 293, 342	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	349	LYS	10.6
1	D	348	LEU	8.5
2	F	951	LEU	6.9
2	C	786	SER	6.7
2	F	930	TYR	6.1
2	F	989	TYR	6.1
2	F	786	SER	5.7
1	D	225	LYS	5.6
2	C	785	SER	5.4
2	C	575	LEU	5.3
2	C	934	HIS	5.2
2	F	928	ASN	4.9
1	D	58	TRP	4.9
2	C	989	TYR	4.9
2	F	958	PRO	4.8
2	C	574	LEU	4.8
2	F	1001	TYR	4.8
2	F	1011	THR	4.7
2	F	605	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	309	TYR	4.6
1	D	359	PRO	4.6
1	D	35	MET	4.4
2	F	783	ASP	4.4
2	F	785	SER	4.3
2	F	923	GLU	4.2
2	F	998	ASN	4.2
2	C	539	LEU	4.1
2	F	781	GLY	4.1
2	F	932	LEU	4.1
2	F	782	SER	4.0
2	F	937	HIS	3.9
2	F	572	LEU	3.9
2	F	612	GLU	3.8
2	F	531	ALA	3.8
2	F	794	TYR	3.8
2	C	951	LEU	3.7
2	F	603	GLN	3.7
2	F	900	MET	3.7
2	C	553	PHE	3.7
2	C	1011	THR	3.6
2	F	836	ILE	3.6
2	F	1003	LEU	3.6
2	F	997	VAL	3.5
2	F	984	LEU	3.5
2	F	959	SER	3.5
1	D	33	LEU	3.5
1	D	229	ASP	3.5
2	F	948	VAL	3.5
2	F	574	LEU	3.5
2	F	801	ILE	3.5
2	F	662	LYS	3.4
2	F	986	TYR	3.4
2	C	543	ALA	3.3
2	F	978	GLY	3.3
1	D	224	SER	3.2
2	C	787	LYS	3.2
2	C	970	PRO	3.2
2	F	555	ALA	3.2
2	F	705	GLN	3.2
2	F	891	PHE	3.2
2	F	553	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	788	ASP	3.1
2	F	575	LEU	3.1
1	A	309	TYR	3.1
2	C	903	LYS	3.0
1	D	283	VAL	3.0
2	F	559	LEU	3.0
1	D	13	TYR	3.0
2	F	971	LEU	2.9
1	D	280	LEU	2.9
1	D	62	HIS	2.9
2	F	889	TYR	2.9
2	F	550	GLY	2.9
2	F	826	HIS	2.9
2	C	686	MET	2.9
2	F	949	LYS	2.9
2	F	1002	LEU	2.9
2	C	969	VAL	2.8
1	D	226	LYS	2.8
2	F	546	LEU	2.8
2	C	914	ASP	2.8
2	C	943	LYS	2.8
2	C	677	PHE	2.8
2	C	572	LEU	2.8
2	F	950	GLY	2.8
2	F	677	PHE	2.8
1	A	302	LEU	2.7
1	D	15	LYS	2.7
2	F	825	THR	2.7
2	F	739	LEU	2.7
2	C	937	HIS	2.7
1	D	6	ASP	2.7
2	C	605	PRO	2.7
2	C	777	LEU	2.7
2	C	954	THR	2.7
1	D	353	GLN	2.7
2	C	537	SER	2.7
2	C	817	TYR	2.7
2	F	585	ILE	2.7
1	D	51	TRP	2.7
1	A	35	MET	2.7
2	F	910	THR	2.6
2	F	682	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	57	PHE	2.6
2	F	791	ASP	2.6
1	D	74	PHE	2.6
2	C	698	LEU	2.6
2	C	681	SER	2.5
2	F	909	HIS	2.5
2	F	979	VAL	2.5
2	C	842	GLU	2.5
2	F	686	MET	2.5
1	D	19	ALA	2.5
2	F	698	LEU	2.5
2	C	869	PHE	2.5
1	D	356	ILE	2.5
2	F	866	THR	2.4
2	C	988	GLU	2.4
2	C	682	MET	2.4
2	C	932	LEU	2.4
2	F	778	LEU	2.4
2	F	914	ASP	2.4
2	F	664	LYS	2.4
2	F	787	LYS	2.4
2	F	972	GLY	2.4
2	C	685	ALA	2.4
2	C	732	LEU	2.4
2	F	765	LEU	2.4
1	D	350	VAL	2.3
2	C	978	GLY	2.3
1	D	287	MET	2.3
2	F	952	GLY	2.3
2	F	964	LEU	2.3
2	F	903	LYS	2.3
2	F	908	CYS	2.3
2	C	729	ILE	2.3
2	C	570	TYR	2.3
2	F	784	ASP	2.3
2	F	897	PHE	2.3
2	C	917	GLY	2.3
1	D	69	VAL	2.3
2	C	736	PHE	2.3
1	A	64	ILE	2.3
1	A	265	LEU	2.2
1	D	54	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	347	LYS	2.2
2	C	909	HIS	2.2
2	F	969	VAL	2.2
1	A	291	ALA	2.2
2	C	531	ALA	2.2
2	F	630	ASN	2.2
1	D	276	GLU	2.2
2	F	859	LEU	2.2
2	F	965	ASP	2.2
2	C	630	ASN	2.2
2	C	814	ILE	2.2
2	C	910	THR	2.2
2	F	926	LEU	2.1
1	D	299	SER	2.1
2	F	570	TYR	2.1
2	C	891	PHE	2.1
1	D	333	TRP	2.1
2	C	545	VAL	2.1
2	C	981	ASP	2.1
2	C	742	HIS	2.1
2	F	983	SER	2.1
2	F	552	VAL	2.1
2	C	692	ASP	2.1
2	C	604	MET	2.1
1	D	285	ASP	2.1
2	F	676	ILE	2.1
2	C	1001	TYR	2.0
1	D	231	ASP	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 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	2UT	C	1101	29/29	0.80	0.28	-0.47	121,127,140,140	0
4	ZN	D	402	1/1	0.88	0.04	-1.44	132,132,132,132	0
4	ZN	A	402	1/1	0.95	0.04	-2.76	62,62,62,62	0
4	ZN	A	401	1/1	0.96	0.04	-	78,78,78,78	0
4	ZN	D	401	1/1	0.91	0.07	-	118,118,118,118	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.