



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:45 AM GMT

PDB ID : 2O3T  
Title : Structural Basis for Formation and Hydrolysis of Calcium Messenger Cyclic ADP-ribose by Human CD38  
Authors : Liu, Q.; Kriksunov, I.A.; Graeff, R.; Lee, H.C.; Hao, Q.  
Deposited on : 2006-12-01  
Resolution : 1.68 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

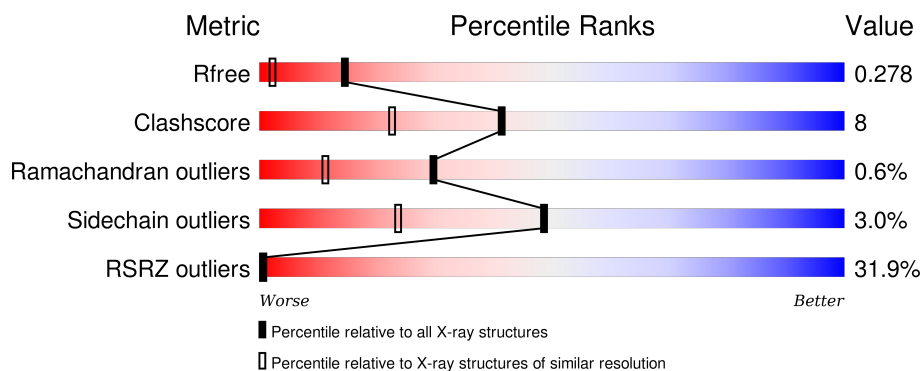
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.68 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))
$R_{free}$	91344	4802 (1.70-1.66)
Clashscore	102246	5317 (1.70-1.66)
Ramachandran outliers	100387	5225 (1.70-1.66)
Sidechain outliers	100360	5224 (1.70-1.66)
RSRZ outliers	91569	4813 (1.70-1.66)

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	262	<div> <div>26%</div> <div>80%</div> <div>15%</div> <div>• •</div> </div>
1	B	262	<div> <div>35%</div> <div>79%</div> <div>15%</div> <div>• •</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4614 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.

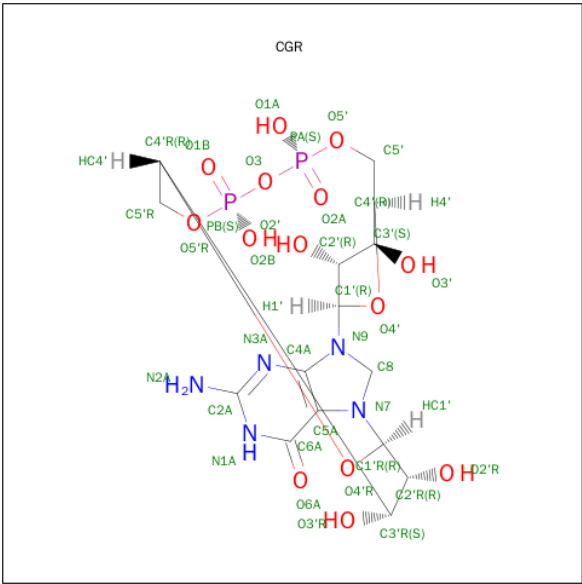
- Molecule 1 is a protein called ADP-ribosyl cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2050	1290	359	385	16			
1	B	252	Total	C	N	O	S	0	0	0
			2050	1290	359	385	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LYS	-	CLONING ARTIFACT	UNP P28907
A	40	ARG	-	CLONING ARTIFACT	UNP P28907
A	41	GLU	-	CLONING ARTIFACT	UNP P28907
A	42	ALA	-	CLONING ARTIFACT	UNP P28907
A	43	GLU	-	CLONING ARTIFACT	UNP P28907
A	44	ALA	-	CLONING ARTIFACT	UNP P28907
A	49	THR	GLN	ENGINEERED	UNP P28907
A	100	ASP	ASN	ENGINEERED	UNP P28907
A	164	ASP	ASN	ENGINEERED	UNP P28907
A	209	ASP	ASN	ENGINEERED	UNP P28907
A	219	ASP	ASN	ENGINEERED	UNP P28907
A	226	GLN	GLU	ENGINEERED	UNP P28907
B	39	LYS	-	CLONING ARTIFACT	UNP P28907
B	40	ARG	-	CLONING ARTIFACT	UNP P28907
B	41	GLU	-	CLONING ARTIFACT	UNP P28907
B	42	ALA	-	CLONING ARTIFACT	UNP P28907
B	43	GLU	-	CLONING ARTIFACT	UNP P28907
B	44	ALA	-	CLONING ARTIFACT	UNP P28907
B	49	THR	GLN	ENGINEERED	UNP P28907
B	100	ASP	ASN	ENGINEERED	UNP P28907
B	164	ASP	ASN	ENGINEERED	UNP P28907
B	209	ASP	ASN	ENGINEERED	UNP P28907
B	219	ASP	ASN	ENGINEERED	UNP P28907
B	226	GLN	GLU	ENGINEERED	UNP P28907

- Molecule 2 is CYCLIC GUANOSINE DIPHOSPHATE-RIBOSE (three-letter code: CGR) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>5</sub>O<sub>14</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

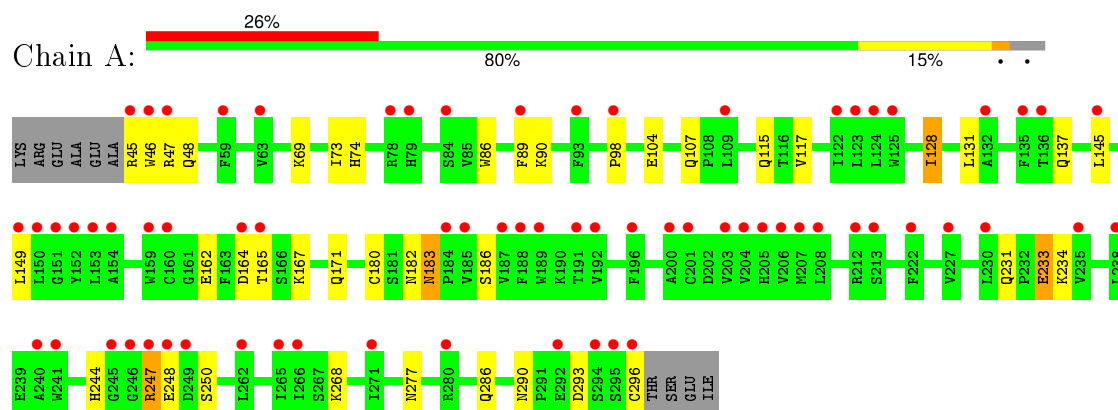
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	280	Total	O	0	0
			280	280		
3	B	198	Total	O	0	0
			198	198		

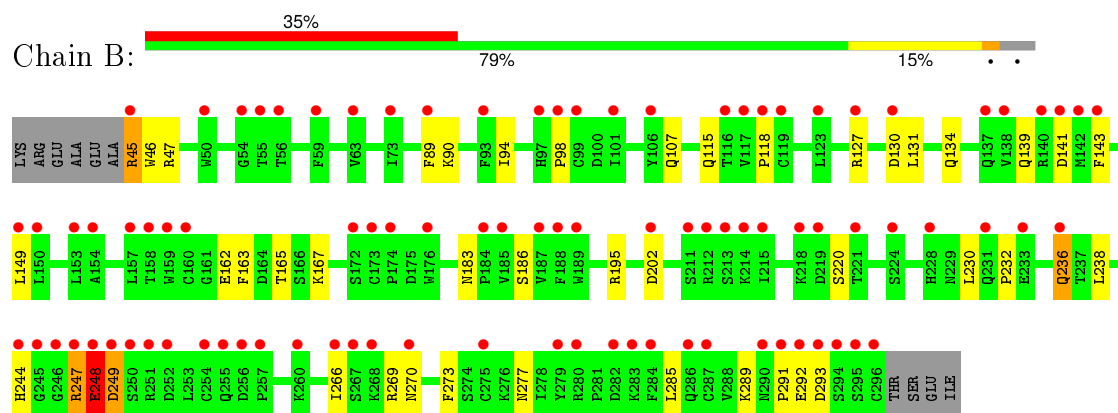
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: ADP-ribosyl cyclase 1



#### • Molecule 1: ADP-ribosyl cyclase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.99 Å 53.29 Å 65.73 Å 105.90° 91.76° 95.16°	Depositor
Resolution (Å)	20.00 – 1.68 19.49 – 1.68	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.68) 88.4 (19.49-1.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 1.68 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.172 , 0.208 0.251 , 0.278	Depositor DCC
$R_{free}$ test set	3002 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.6	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 55.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 59469 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4614	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.40% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.63	0/2101	0.67	0/2846
1	B	0.56	0/2101	0.76	7/2846 (0.2%)
All	All	0.59	0/4202	0.71	7/5692 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	292	GLU	N-CA-C	10.64	139.72	111.00
1	B	292	GLU	CB-CA-C	-10.25	89.90	110.40
1	B	248	GLU	N-CA-C	8.19	133.11	111.00
1	B	248	GLU	CB-CA-C	-8.16	94.09	110.40
1	B	247	ARG	C-N-CA	7.58	140.65	121.70
1	B	247	ARG	O-C-N	-6.79	111.83	122.70
1	B	291	PRO	C-N-CA	5.63	135.78	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	ASP	Peptide

## 5.2 Too-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 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	2050	0	1978	34	0
1	B	2050	0	1978	33	0
2	A	36	0	21	3	0
3	A	280	0	0	6	0
3	B	198	0	0	1	0
All	All	4614	0	3977	69	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 8.

All (69) 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:231:GLN:HG3	3:A:558:HOH:O	1.61	1.00
1:A:69:LYS:HE2	1:A:73:ILE:HD11	1.46	0.96
1:A:69:LYS:CE	1:A:73:ILE:HD11	1.99	0.93
1:B:115:GLN:HE22	1:B:149:LEU:H	1.23	0.87
1:A:115:GLN:HE22	1:A:149:LEU:H	1.24	0.85
1:A:165:THR:HG23	1:A:167:LYS:H	1.38	0.85
1:B:165:THR:HG23	1:B:167:LYS:H	1.47	0.79
1:A:47:ARG:O	1:A:47:ARG:HG3	1.89	0.72
1:A:247:ARG:O	1:A:248:GLU:HG3	1.91	0.71
1:B:127:ARG:NH1	1:B:220:SER:HB3	2.06	0.70
1:B:107:GLN:HE22	1:B:195:ARG:NH2	1.91	0.68
1:B:127:ARG:HH12	1:B:220:SER:HB3	1.58	0.68
1:B:47:ARG:HD2	3:B:460:HOH:O	1.95	0.67
1:B:266:ILE:HD11	1:B:273:PHE:HB2	1.78	0.66
1:B:162:GLU:HB2	1:B:165:THR:HG22	1.80	0.64
1:B:238:LEU:HB3	1:B:266:ILE:HD13	1.80	0.62
1:A:86:TRP:CE2	1:A:90:LYS:HG3	2.35	0.61
2:A:301:CGR:H81	2:A:301:CGR:O5'R	2.01	0.61
1:B:107:GLN:HE22	1:B:195:ARG:HH21	1.50	0.58
1:B:139:GLN:C	1:B:141:ASP:H	2.05	0.57
1:B:183:ASN:ND2	1:B:186:SER:H	2.03	0.57
1:A:183:ASN:ND2	1:A:186:SER:H	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLN:NE2	1:A:149:LEU:H	2.01	0.55
1:A:74:HIS:HE1	3:A:484:HOH:O	1.89	0.55
1:A:268:LYS:HD3	1:B:163:PHE:CE1	2.42	0.55
1:B:115:GLN:NE2	1:B:149:LEU:H	1.99	0.54
1:A:286:GLN:HG3	3:A:457:HOH:O	2.11	0.51
1:B:266:ILE:HD11	1:B:273:PHE:CB	2.40	0.50
1:A:104:GLU:HA	1:A:107:GLN:HG2	1.94	0.50
1:B:130:ASP:OD1	1:B:134:GLN:NE2	2.45	0.50
1:A:47:ARG:O	1:A:47:ARG:CG	2.59	0.49
1:B:232:PRO:HG3	1:B:269:ARG:O	2.12	0.49
1:A:180:CYS:HB2	3:A:439:HOH:O	2.12	0.49
1:A:162:GLU:HB2	1:A:165:THR:HG22	1.95	0.49
1:A:293:ASP:HB3	1:A:296:CYS:SG	2.53	0.48
1:A:137:GLN:NE2	3:A:489:HOH:O	2.44	0.48
1:A:286:GLN:NE2	1:A:290:ASN:OD1	2.46	0.48
1:A:183:ASN:HD21	1:A:186:SER:H	1.61	0.48
1:B:127:ARG:NH1	1:B:220:SER:CB	2.76	0.47
1:A:86:TRP:CZ2	1:A:90:LYS:HG3	2.48	0.47
2:A:301:CGR:O6A	2:A:301:CGR:HC2'	2.14	0.47
2:A:301:CGR:H81	2:A:301:CGR:C5'R	2.45	0.47
1:B:139:GLN:C	1:B:141:ASP:N	2.67	0.47
1:B:248:GLU:O	1:B:249:ASP:HB3	2.15	0.46
1:B:98:PRO:O	1:B:183:ASN:HA	2.15	0.46
1:A:244:HIS:HE1	1:A:277:ASN:OD1	1.99	0.46
1:A:233:GLU:HG2	1:A:234:LYS:HG3	1.98	0.46
1:B:45:ARG:HG2	1:B:46:TRP:CE3	2.51	0.45
1:B:90:LYS:CG	1:B:94:ILE:HG13	2.47	0.45
1:A:48:GLN:NE2	1:A:171:GLN:HB3	2.32	0.45
1:A:182:ASN:OD1	3:A:573:HOH:O	2.21	0.45
1:A:86:TRP:CZ2	1:A:90:LYS:CG	2.99	0.45
1:A:46:TRP:HE1	1:A:47:ARG:NH2	2.15	0.45
1:A:45:ARG:HD3	1:A:47:ARG:O	2.17	0.45
1:B:107:GLN:NE2	1:B:195:ARG:HH21	2.15	0.44
1:A:69:LYS:HE2	1:A:73:ILE:CD1	2.31	0.44
1:B:202:ASP:HA	1:B:236:GLN:HG2	2.00	0.44
1:A:247:ARG:C	1:A:248:GLU:HG3	2.39	0.43
1:A:98:PRO:O	1:A:183:ASN:HA	2.18	0.43
1:A:244:HIS:HD2	1:A:250:SER:OG	2.00	0.43
1:B:285:LEU:HB3	1:B:289:LYS:HE3	2.00	0.43
1:B:247:ARG:C	1:B:248:GLU:HG3	2.36	0.42
1:A:69:LYS:HE3	1:A:73:ILE:HD11	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ARG:HH12	1:B:220:SER:CB	2.29	0.41
1:B:285:LEU:O	1:B:289:LYS:HG3	2.21	0.40
1:B:118:PRO:HD2	1:B:143:PHE:CE2	2.56	0.40
1:B:183:ASN:HD21	1:B:186:SER:H	1.69	0.40
1:B:230:LEU:O	1:B:269:ARG:NH1	2.48	0.40
1:B:244:HIS:HE1	1:B:277:ASN:OD1	2.05	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	250/262 (95%)	244 (98%)	4 (2%)	2 (1%)	24	7
1	B	250/262 (95%)	239 (96%)	10 (4%)	1 (0%)	39	19
All	All	500/524 (95%)	483 (97%)	14 (3%)	3 (1%)	30	11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	249	ASP
1	A	247	ARG
1	A	128	ILE

### 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	233/241 (97%)	226 (97%)	7 (3%)	48	24
1	B	233/241 (97%)	226 (97%)	7 (3%)	48	24
All	All	466/482 (97%)	452 (97%)	14 (3%)	48	24

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	PHE
1	A	117	VAL
1	A	128	ILE
1	A	131	LEU
1	A	145	LEU
1	A	183	ASN
1	A	233	GLU
1	B	45	ARG
1	B	89	PHE
1	B	131	LEU
1	B	236	GLN
1	B	248	GLU
1	B	270	ASN
1	B	293	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	115	GLN
1	A	134	GLN
1	A	137	GLN
1	A	139	GLN
1	A	183	ASN
1	A	244	HIS
1	A	286	GLN
1	A	290	ASN
1	B	107	GLN
1	B	115	GLN
1	B	183	ASN
1	B	229	ASN
1	B	244	HIS
1	B	255	GLN
1	B	270	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is 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$
2	CGR	A	301	-	35,40,40	1.83	4 (11%)	47,64,64	1.77	9 (19%)

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
2	CGR	A	301	-	-	0/26/70/70	0/1/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CGR	C8-N9	-6.85	1.35	1.45
2	A	301	CGR	C8-N7	-6.48	1.36	1.45
2	A	301	CGR	C6A-N1A	2.43	1.37	1.33
2	A	301	CGR	C1'R-N7	2.86	1.50	1.44

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	CGR	C5A-C4A-N3A	-5.32	121.63	126.82
2	A	301	CGR	C5A-C6A-N1A	-3.15	118.62	123.46
2	A	301	CGR	PA-O3-PB	-3.02	124.25	132.73
2	A	301	CGR	N1A-C2A-N3A	-2.14	122.03	125.53
2	A	301	CGR	C3'R-C2'R-C1'R	2.72	106.87	101.40
2	A	301	CGR	C6A-N1A-C2A	2.86	119.91	115.94
2	A	301	CGR	N3A-C4A-N9	2.97	131.21	126.75
2	A	301	CGR	C5A-N7-C1'R	3.44	132.72	125.39
2	A	301	CGR	N9-C8-N7	5.17	110.37	103.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	CGR	3	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	252/262 (96%)	1.52	69 (27%)  	25, 31, 37, 46	0
1	B	252/262 (96%)	1.98	92 (36%)  	26, 31, 37, 43	0
All	All	504/524 (96%)	1.75	161 (31%)  	25, 31, 37, 46	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	ASP	13.0
1	B	295	SER	11.3
1	B	249	ASP	10.9
1	B	248	GLU	9.7
1	B	294	SER	9.5
1	B	247	ARG	9.2
1	B	213	SER	8.2
1	B	245	GLY	8.1
1	B	246	GLY	8.1
1	B	293	ASP	8.0
1	B	292	GLU	7.9
1	A	247	ARG	7.9
1	A	248	GLU	7.7
1	A	246	GLY	7.6
1	B	296	CYS	7.1
1	B	176	TRP	6.5
1	B	291	PRO	5.5
1	B	159	TRP	5.4
1	B	211	SER	5.1
1	B	212	ARG	5.1
1	B	282	ASP	5.1
1	A	294	SER	5.1
1	B	140	ARG	4.9
1	A	245	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	287	CYS	4.8
1	B	141	ASP	4.8
1	A	124	LEU	4.8
1	A	204	VAL	4.8
1	A	222	PHE	4.5
1	B	280	ARG	4.5
1	A	206	VAL	4.5
1	B	116	THR	4.4
1	A	123	LEU	4.4
1	B	224	SER	4.4
1	A	230	LEU	4.3
1	A	93	PHE	4.3
1	B	55	THR	4.3
1	B	254	CYS	4.3
1	A	208	LEU	4.2
1	B	138	VAL	4.2
1	A	47	ARG	4.2
1	B	270	ASN	4.1
1	A	150	LEU	4.1
1	B	252	ASP	4.1
1	B	127	ARG	4.1
1	A	235	VAL	4.1
1	B	279	TYR	4.0
1	B	290	ASN	4.0
1	A	187	VAL	4.0
1	B	93	PHE	4.0
1	B	143	PHE	3.9
1	B	228	HIS	3.9
1	B	153	LEU	3.8
1	B	268	LYS	3.8
1	B	244	HIS	3.7
1	A	189	TRP	3.7
1	B	160	CYS	3.6
1	A	159	TRP	3.6
1	B	123	LEU	3.6
1	B	214	LYS	3.6
1	B	266	ILE	3.6
1	B	89	PHE	3.5
1	A	185	VAL	3.5
1	A	188	PHE	3.5
1	A	227	VAL	3.4
1	B	184	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	238	LEU	3.3
1	A	78	ARG	3.3
1	B	250	SER	3.2
1	A	296	CYS	3.2
1	A	266	ILE	3.2
1	A	125	TRP	3.2
1	A	122	ILE	3.2
1	A	46	TRP	3.1
1	A	192	VAL	3.1
1	B	130	ASP	3.1
1	B	185	VAL	3.1
1	B	188	PHE	3.1
1	A	154	ALA	3.0
1	B	173	CYS	3.0
1	A	262	LEU	3.0
1	B	101	ILE	3.0
1	A	84	SER	3.0
1	B	286	GLN	3.0
1	A	292	GLU	2.9
1	B	137	GLN	2.9
1	B	157	LEU	2.9
1	A	196	PHE	2.9
1	B	187	VAL	2.9
1	A	45	ARG	2.9
1	A	79	HIS	2.9
1	A	200	ALA	2.9
1	A	164	ASP	2.9
1	B	119	CYS	2.9
1	B	73	ILE	2.8
1	B	54	GLY	2.8
1	B	231	GLN	2.8
1	A	213	SER	2.8
1	B	219	ASP	2.8
1	A	165	THR	2.7
1	B	260	LYS	2.7
1	B	215	ILE	2.7
1	A	184	PRO	2.7
1	B	174	PRO	2.7
1	B	158	THR	2.7
1	B	236	GLN	2.7
1	B	63	VAL	2.7
1	B	106	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	295	SER	2.6
1	A	153	LEU	2.6
1	B	50	TRP	2.6
1	B	255	GLN	2.6
1	A	207	MET	2.6
1	A	149	LEU	2.6
1	A	203	VAL	2.5
1	B	283	LYS	2.5
1	B	256	ASP	2.5
1	B	149	LEU	2.5
1	A	160	CYS	2.5
1	B	99	CYS	2.5
1	A	136	THR	2.5
1	A	109	LEU	2.5
1	B	275	CYS	2.5
1	A	280	ARG	2.5
1	A	63	VAL	2.4
1	B	284	PHE	2.4
1	B	98	PRO	2.4
1	B	233	GLU	2.4
1	A	201	CYS	2.4
1	B	150	LEU	2.4
1	A	59	PHE	2.4
1	B	59	PHE	2.4
1	A	89	PHE	2.4
1	A	205	HIS	2.4
1	B	45	ARG	2.3
1	B	267	SER	2.3
1	A	240	ALA	2.3
1	A	271	ILE	2.3
1	A	135	PHE	2.3
1	A	241	TRP	2.2
1	B	202	ASP	2.2
1	A	132	ALA	2.2
1	B	142	MET	2.2
1	A	212	ARG	2.2
1	B	218	LYS	2.2
1	A	145	LEU	2.2
1	B	189	TRP	2.1
1	B	172	SER	2.1
1	A	191	THR	2.1
1	A	98	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	221	THR	2.1
1	B	118	PRO	2.1
1	B	257	PRO	2.1
1	A	265	ILE	2.1
1	B	117	VAL	2.1
1	B	251	ARG	2.1
1	B	56	THR	2.1
1	B	154	ALA	2.1
1	A	152	TYR	2.0
1	B	97	HIS	2.0
1	A	151	GLY	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
2	CGR	A	301	36/36	0.95	0.10	-1.57	15,19,23,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.