



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:45 AM GMT

PDB ID : 2O3Q  
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 : 1.98 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

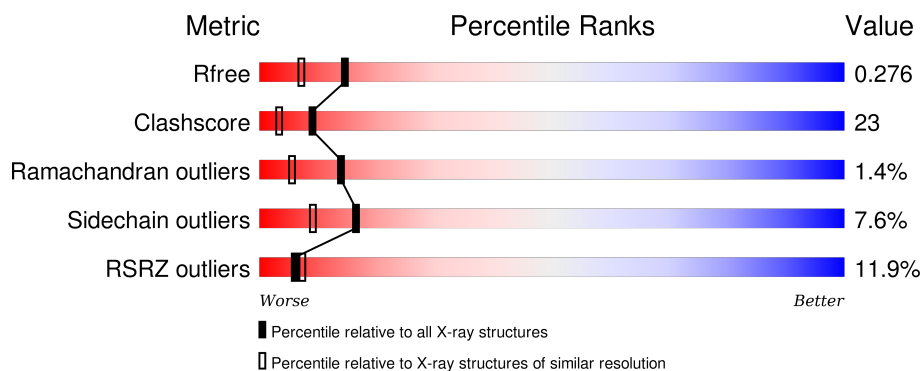
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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>8%</div> <div>65%</div> <div>28%</div> <div>• •</div> </div>
1	B	262	<div> <div>15%</div> <div>47%</div> <div>39%</div> <div>8% • •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CXR	A	301	X	-	-	-
2	CXR	B	301	X	-	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4377 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.

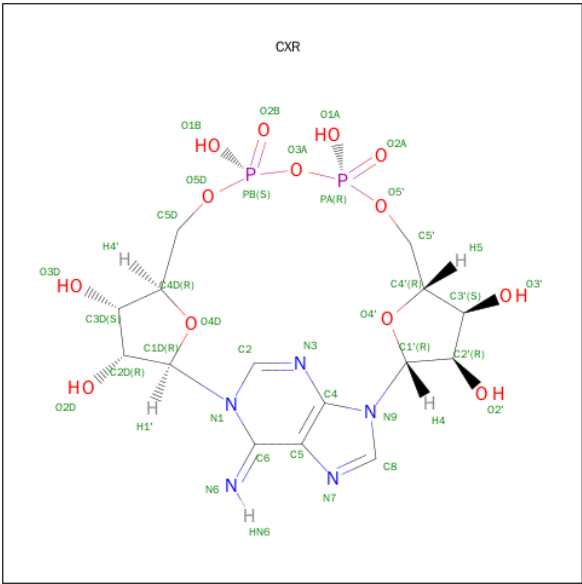
- Molecule 1 is a protein called ADP-ribosyl cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2008	1266	352	374	16			
1	B	252	Total	C	N	O	S	0	0	0
			2008	1266	352	374	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 ADENOSINE DIPHOSPHATE-RIBOSE (three-letter code: CXR) (formula: C<sub>15</sub>H<sub>21</sub>N<sub>5</sub>O<sub>13</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			35	15	5	13	2		
2	B	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

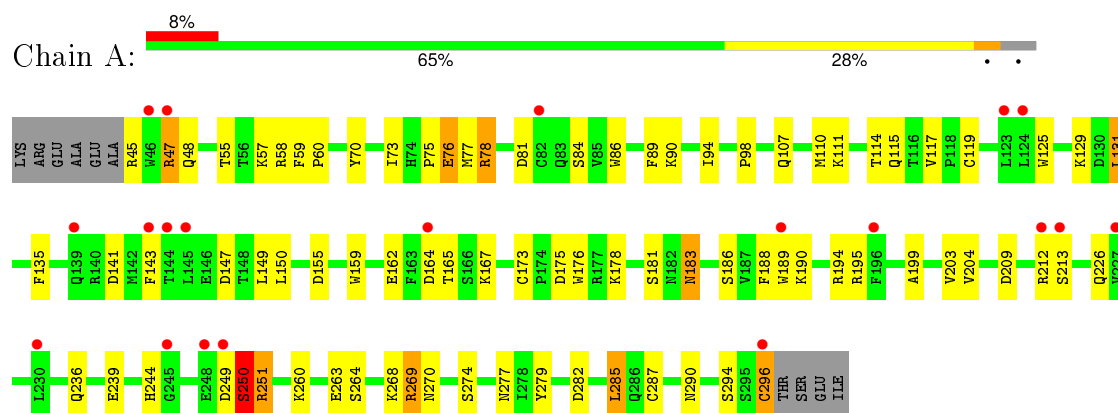
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	157	Total	O	0	0
			157	157		
3	B	134	Total	O	0	0
			134	134		

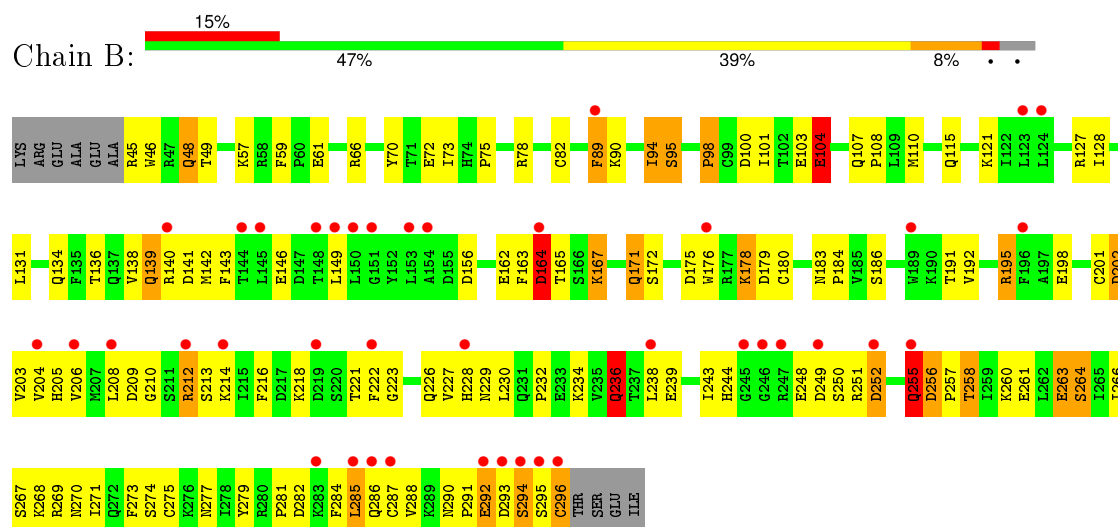
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	41.94Å 53.28Å 65.92Å 105.89° 92.10° 94.81°	Depositor
Resolution (Å)	20.00 – 1.98 28.37 – 1.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.98) 81.8 (28.37-1.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.207 , 0.278 0.211 , 0.276	Depositor DCC
$R_{free}$ test set	1713 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.8	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 33824 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4377	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% 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: CXR

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	1.43	16/2058 (0.8%)	1.25	17/2785 (0.6%)
1	B	1.59	36/2058 (1.7%)	1.21	13/2785 (0.5%)
All	All	1.51	52/4116 (1.3%)	1.23	30/5570 (0.5%)

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	B	0	1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	GLU	C-O	11.62	1.45	1.23
1	B	296	CYS	C-O	11.43	1.45	1.23
1	B	263	GLU	CD-OE1	10.22	1.36	1.25
1	A	173	CYS	CB-SG	-10.14	1.65	1.82
1	B	263	GLU	CD-OE2	8.94	1.35	1.25
1	B	260	LYS	CD-CE	8.84	1.73	1.51
1	B	104	GLU	CG-CD	8.55	1.64	1.51
1	B	255	GLN	C-N	7.98	1.52	1.34
1	B	274	SER	CB-OG	7.76	1.52	1.42
1	B	252	ASP	CG-OD1	7.27	1.42	1.25
1	B	59	PHE	CE2-CZ	7.13	1.50	1.37
1	A	141	ASP	C-N	-7.04	1.17	1.34
1	B	78	ARG	CZ-NH1	6.84	1.42	1.33
1	B	72	GLU	CB-CG	6.71	1.65	1.52
1	A	195	ARG	CG-CD	6.57	1.68	1.51
1	B	292	GLU	C-N	6.48	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	284	PHE	C-O	6.47	1.35	1.23
1	B	292	GLU	C-O	6.42	1.35	1.23
1	A	203	VAL	CB-CG2	6.41	1.66	1.52
1	A	296	CYS	C-O	6.29	1.35	1.23
1	B	72	GLU	CG-CD	6.18	1.61	1.51
1	B	279	TYR	C-N	6.14	1.48	1.34
1	B	270	ASN	CG-ND2	6.05	1.48	1.32
1	B	257	PRO	N-CD	6.03	1.56	1.47
1	B	104	GLU	CB-CG	5.99	1.63	1.52
1	A	70	TYR	CD1-CE1	5.99	1.48	1.39
1	B	252	ASP	CG-OD2	5.86	1.38	1.25
1	B	178	LYS	CE-NZ	5.82	1.63	1.49
1	A	188	PHE	CE2-CZ	5.79	1.48	1.37
1	B	294	SER	C-O	5.78	1.34	1.23
1	A	199	ALA	CA-CB	5.65	1.64	1.52
1	A	263	GLU	CB-CG	-5.59	1.41	1.52
1	A	117	VAL	CB-CG1	-5.50	1.41	1.52
1	A	251	ARG	CZ-NH1	5.42	1.40	1.33
1	B	171	GLN	CG-CD	5.41	1.63	1.51
1	B	61	GLU	CB-CG	5.33	1.62	1.52
1	A	125	TRP	CE3-CZ3	5.31	1.47	1.38
1	B	261	GLU	CG-CD	5.31	1.59	1.51
1	A	226	GLN	CB-CG	5.30	1.66	1.52
1	B	204	VAL	CB-CG2	-5.29	1.41	1.52
1	B	143	PHE	CE1-CZ	5.27	1.47	1.37
1	B	256	ASP	C-N	5.26	1.44	1.34
1	B	236	GLN	CG-CD	5.24	1.63	1.51
1	A	189	TRP	CE3-CZ3	5.21	1.47	1.38
1	B	167	LYS	CB-CG	5.19	1.66	1.52
1	B	294	SER	C-N	5.17	1.46	1.34
1	B	70	TYR	CE2-CZ	-5.14	1.31	1.38
1	B	89	PHE	CE2-CZ	5.12	1.47	1.37
1	A	290	ASN	C-N	5.06	1.43	1.34
1	B	78	ARG	CZ-NH2	5.06	1.39	1.33
1	A	135	PHE	CD1-CE1	5.05	1.49	1.39
1	B	263	GLU	C-N	5.02	1.45	1.34

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH1	10.63	125.61	120.30
1	A	195	ARG	NE-CZ-NH1	8.96	124.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	A	251	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	B	263	GLU	OE1-CD-OE2	7.29	132.05	123.30
1	A	47	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	251	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	178	LYS	CD-CE-NZ	-6.47	96.81	111.70
1	A	141	ASP	C-N-CA	6.43	137.78	121.70
1	A	204	VAL	CG1-CB-CG2	-6.39	100.68	110.90
1	A	131	LEU	CB-CG-CD2	6.30	121.72	111.00
1	B	89	PHE	CB-CG-CD2	-6.00	116.60	120.80
1	B	78	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	117	VAL	N-CA-C	-5.73	95.53	111.00
1	A	195	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	66	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	175	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	282	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	147	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	179	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	209	ASP	CB-CG-OD2	-5.29	113.53	118.30
1	B	260	LYS	O-C-N	5.29	131.16	122.70
1	B	279	TYR	C-N-CA	-5.28	108.49	121.70
1	B	94	ILE	CG1-CB-CG2	-5.26	99.82	111.40
1	B	292	GLU	O-C-N	5.24	131.08	122.70
1	A	47	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	B	204	VAL	CB-CA-C	-5.19	101.55	111.40
1	A	209	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	291	PRO	O-C-N	5.10	130.86	122.70
1	A	285	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	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	2008	0	1918	77	0
1	B	2008	0	1919	108	0
2	A	35	0	18	1	0
2	B	35	0	19	5	0
3	A	157	0	0	25	0
3	B	134	0	0	11	0
All	All	4377	0	3874	184	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 23.

All (184) 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:104:GLU:HG3	3:B:423:HOH:O	1.38	1.20
1:A:78:ARG:HH11	1:A:78:ARG:HG3	1.06	1.16
1:A:176:TRP:HB3	3:A:351:HOH:O	1.53	1.08
1:B:266:ILE:HD11	1:B:273:PHE:HB2	1.20	1.08
1:A:162:GLU:HB2	1:A:165:THR:HG22	1.36	1.05
1:A:45:ARG:HA	3:A:330:HOH:O	1.61	0.99
1:B:180:CYS:HB2	3:B:313:HOH:O	1.67	0.94
1:A:73:ILE:HD13	3:A:346:HOH:O	1.67	0.94
1:B:107:GLN:HE22	1:B:195:ARG:HH21	1.04	0.92
1:A:165:THR:HG23	1:A:167:LYS:H	1.33	0.90
1:A:162:GLU:HB2	1:A:165:THR:CG2	2.02	0.89
1:B:222:PHE:HA	1:B:226:GLN:HG3	1.54	0.88
1:A:165:THR:HB	3:A:422:HOH:O	1.74	0.88
1:A:78:ARG:NH1	1:A:78:ARG:HG3	1.88	0.87
1:A:269:ARG:HD3	1:B:100:ASP:CG	1.96	0.86
1:B:165:THR:HG23	1:B:167:LYS:H	1.40	0.84
1:B:266:ILE:HD11	1:B:273:PHE:CB	2.07	0.83
1:A:78:ARG:HH11	1:A:78:ARG:CG	1.90	0.83
1:B:115:GLN:HE22	1:B:149:LEU:H	1.24	0.83
1:B:264:SER:HA	3:B:413:HOH:O	1.79	0.82
1:B:162:GLU:HB2	1:B:165:THR:HG22	1.62	0.81
1:A:270:ASN:HB2	3:A:452:HOH:O	1.81	0.79
1:B:266:ILE:CD1	1:B:273:PHE:HB2	2.10	0.78
1:A:57:LYS:O	1:A:58:ARG:HG2	1.82	0.78
1:B:290:ASN:CB	3:B:338:HOH:O	2.31	0.78
1:A:260:LYS:HE2	1:A:260:LYS:N	1.98	0.78
1:B:252:ASP:HA	1:B:277:ASN:HD21	1.48	0.77
1:A:270:ASN:CB	3:A:452:HOH:O	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ARG:O	1:A:213:SER:OG	2.02	0.76
1:A:268:LYS:CE	3:A:354:HOH:O	2.33	0.76
1:B:107:GLN:NE2	1:B:195:ARG:HH21	1.82	0.76
1:A:190:LYS:HE2	3:B:359:HOH:O	1.85	0.76
1:B:221:THR:CB	2:B:301:CXR:H11	2.16	0.74
1:B:121:LYS:HD3	3:B:393:HOH:O	1.86	0.74
1:B:107:GLN:HE22	1:B:195:ARG:NH2	1.84	0.74
1:A:77:MET:SD	1:A:115:GLN:HG3	2.28	0.73
1:B:216:PHE:O	1:B:258:THR:HG21	1.87	0.73
1:A:115:GLN:HE22	1:A:149:LEU:H	1.34	0.73
1:A:194:ARG:HD3	3:A:357:HOH:O	1.90	0.71
1:A:270:ASN:CG	3:A:452:HOH:O	2.29	0.70
1:B:48:GLN:NE2	1:B:49:THR:H	1.89	0.70
1:A:268:LYS:HE3	3:A:354:HOH:O	1.89	0.70
1:A:86:TRP:CZ2	1:A:90:LYS:HG3	2.29	0.68
1:B:206:VAL:HG12	1:B:238:LEU:HD11	1.74	0.68
2:B:301:CXR:O5D	2:B:301:CXR:H3	1.94	0.68
1:B:252:ASP:HA	1:B:277:ASN:ND2	2.09	0.67
1:B:45:ARG:HG2	1:B:46:TRP:N	2.10	0.67
1:A:268:LYS:HE2	3:A:354:HOH:O	1.95	0.66
1:B:48:GLN:OE1	1:B:171:GLN:NE2	2.24	0.66
1:B:287:CYS:HB2	1:B:296:CYS:C	2.16	0.66
1:B:212:ARG:C	1:B:214:LYS:H	1.99	0.66
1:B:90:LYS:HG2	1:B:94:ILE:HG13	1.78	0.66
1:A:244:HIS:HE1	1:A:277:ASN:OD1	1.79	0.65
1:B:221:THR:HB	2:B:301:CXR:H11	1.78	0.65
1:A:162:GLU:CB	1:A:165:THR:HG22	2.20	0.65
1:B:140:ARG:HB2	3:B:363:HOH:O	1.99	0.62
1:B:139:GLN:HE21	1:B:139:GLN:HA	1.65	0.61
1:B:162:GLU:OE2	1:B:165:THR:HG21	2.01	0.61
1:A:264:SER:O	1:A:268:LYS:HG3	2.01	0.61
1:B:263:GLU:O	1:B:267:SER:HB2	2.00	0.61
1:A:110:MET:HE1	1:A:150:LEU:HD13	1.82	0.60
1:B:183:ASN:ND2	1:B:186:SER:H	1.99	0.60
1:B:156:ASP:HA	2:B:301:CXR:H8	1.82	0.60
1:B:230:LEU:O	1:B:269:ARG:NH2	2.34	0.60
1:A:81:ASP:CG	3:A:440:HOH:O	2.40	0.59
1:B:232:PRO:HG3	1:B:269:ARG:O	2.03	0.58
1:B:138:VAL:HG11	1:B:288:VAL:HG12	1.85	0.58
1:B:206:VAL:CG1	1:B:238:LEU:HD11	2.33	0.58
1:A:107:GLN:HB3	1:A:111:LYS:NZ	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:HD3	1:B:100:ASP:OD2	2.02	0.57
1:A:175:ASP:OD1	1:A:178:LYS:HG3	2.04	0.57
1:B:223:GLY:O	1:B:227:VAL:HG12	2.04	0.56
1:B:232:PRO:HD3	1:B:269:ARG:HH21	1.70	0.56
1:B:222:PHE:HA	1:B:226:GLN:CG	2.33	0.55
1:B:201:CYS:O	1:B:202:ASP:HB2	2.06	0.55
1:A:75:PRO:HA	1:A:78:ARG:HD3	1.88	0.55
1:A:183:ASN:HD21	1:A:186:SER:H	1.55	0.55
1:A:260:LYS:NZ	3:A:438:HOH:O	2.37	0.55
1:A:183:ASN:ND2	1:A:186:SER:H	2.05	0.55
1:B:136:THR:HG22	1:B:142:MET:HB2	1.88	0.55
1:B:293:ASP:CA	3:B:419:HOH:O	2.55	0.55
1:A:165:THR:CB	3:A:422:HOH:O	2.44	0.54
1:A:165:THR:HG23	1:A:167:LYS:N	2.12	0.54
1:B:216:PHE:O	1:B:258:THR:CG2	2.55	0.54
1:B:243:ILE:CG2	1:B:281:PRO:HG3	2.38	0.54
1:A:270:ASN:ND2	3:A:452:HOH:O	2.39	0.53
1:A:115:GLN:NE2	1:A:149:LEU:H	2.06	0.53
1:B:45:ARG:HD2	3:B:367:HOH:O	2.08	0.53
1:B:255:GLN:O	1:B:256:ASP:C	2.46	0.53
1:B:57:LYS:HE3	3:B:333:HOH:O	2.06	0.53
1:A:212:ARG:O	1:A:213:SER:CB	2.55	0.53
1:A:86:TRP:CE2	1:A:90:LYS:HG3	2.44	0.53
1:B:266:ILE:HD13	1:B:271:ILE:HG22	1.91	0.53
1:A:270:ASN:HB2	3:A:376:HOH:O	2.08	0.53
1:B:266:ILE:HD12	1:B:267:SER:N	2.24	0.52
1:B:295:SER:O	1:B:296:CYS:HB3	2.09	0.52
1:A:98:PRO:O	1:A:183:ASN:HA	2.10	0.52
1:B:165:THR:HG23	1:B:167:LYS:N	2.18	0.52
1:B:209:ASP:CG	1:B:212:ARG:HD3	2.31	0.51
2:A:301:CXR:O5D	2:A:301:CXR:H3	2.10	0.51
1:A:165:THR:O	1:A:165:THR:CG2	2.59	0.50
1:A:73:ILE:CD1	3:A:346:HOH:O	2.40	0.50
1:A:176:TRP:CZ3	1:A:181:SER:CB	2.93	0.50
1:B:191:THR:O	1:B:195:ARG:HD3	2.11	0.50
1:B:222:PHE:CA	1:B:226:GLN:HG3	2.33	0.50
1:B:107:GLN:NE2	1:B:195:ARG:NH2	2.53	0.50
1:A:167:LYS:CE	3:A:387:HOH:O	2.60	0.50
1:B:115:GLN:NE2	1:B:149:LEU:H	2.01	0.50
1:B:212:ARG:C	1:B:214:LYS:N	2.64	0.49
1:B:48:GLN:HE21	1:B:49:THR:H	1.57	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ILE:C	1:B:266:ILE:HD12	2.33	0.49
1:B:45:ARG:CG	1:B:46:TRP:N	2.76	0.49
1:B:45:ARG:HG2	1:B:46:TRP:H	1.78	0.49
1:A:250:SER:HA	3:A:400:HOH:O	2.12	0.49
1:B:128:ILE:HG13	1:B:128:ILE:O	2.12	0.48
1:B:183:ASN:HD21	1:B:186:SER:H	1.62	0.48
1:B:82:CYS:HB2	3:B:416:HOH:O	2.12	0.48
1:A:249:ASP:CA	1:A:279:TYR:CD1	2.97	0.48
1:A:58:ARG:HB3	1:A:58:ARG:HH11	1.79	0.48
1:B:209:ASP:HB3	1:B:212:ARG:HG2	1.96	0.48
1:A:48:GLN:HA	1:A:48:GLN:OE1	2.13	0.48
1:A:239:GLU:OE2	1:A:274:SER:OG	2.27	0.47
1:A:114:THR:HG23	3:A:414:HOH:O	2.13	0.47
1:A:167:LYS:NZ	3:A:387:HOH:O	2.48	0.47
1:B:98:PRO:O	1:B:183:ASN:HA	2.14	0.47
1:B:101:ILE:HG13	1:B:184:PRO:HG3	1.97	0.47
1:B:248:GLU:O	1:B:250:SER:N	2.48	0.47
1:B:212:ARG:O	1:B:214:LYS:N	2.48	0.47
1:B:223:GLY:O	1:B:227:VAL:CG1	2.63	0.46
1:A:260:LYS:HG3	3:A:455:HOH:O	2.15	0.46
1:B:230:LEU:O	1:B:232:PRO:HD3	2.16	0.46
1:B:48:GLN:NE2	1:B:172:SER:OG	2.46	0.46
1:B:94:ILE:HD12	1:B:94:ILE:HG23	1.58	0.45
1:B:221:THR:O	1:B:222:PHE:C	2.55	0.45
1:B:286:GLN:HA	1:B:286:GLN:NE2	2.32	0.45
1:B:48:GLN:HG3	1:B:172:SER:HB3	1.98	0.45
1:B:73:ILE:O	1:B:75:PRO:HD3	2.17	0.45
1:B:273:PHE:CE2	1:B:275:CYS:HB2	2.52	0.45
1:A:107:GLN:HB3	1:A:111:LYS:HZ1	1.80	0.45
1:B:273:PHE:CZ	1:B:275:CYS:HB2	2.51	0.45
1:B:202:ASP:HB3	1:B:203:VAL:H	1.23	0.45
1:B:127:ARG:HE	1:B:212:ARG:HG3	1.82	0.45
1:A:59:PHE:HB3	1:A:60:PRO:HD3	1.98	0.45
1:A:287:CYS:HB3	1:A:296:CYS:HB3	1.93	0.44
1:B:163:PHE:O	1:B:164:ASP:C	2.55	0.44
1:B:90:LYS:HG2	1:B:94:ILE:CG1	2.46	0.44
1:B:90:LYS:HB3	1:B:90:LYS:HE2	1.60	0.44
1:A:176:TRP:CZ3	1:A:181:SER:HB3	2.53	0.44
1:B:94:ILE:O	1:B:95:SER:HB2	2.17	0.44
1:A:47:ARG:O	1:A:48:GLN:HB2	2.17	0.44
1:B:195:ARG:HH11	1:B:195:ARG:HG3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:TRP:CZ3	1:A:181:SER:HB2	2.53	0.43
1:B:232:PRO:CD	1:B:269:ARG:HH21	2.31	0.43
1:B:205:HIS:CD2	1:B:239:GLU:HB3	2.54	0.43
1:A:81:ASP:O	1:A:84:SER:HB2	2.19	0.43
1:A:269:ARG:HD2	3:A:321:HOH:O	2.18	0.43
1:B:295:SER:O	1:B:296:CYS:CB	2.67	0.43
1:B:230:LEU:O	1:B:269:ARG:NE	2.52	0.43
1:A:236:GLN:NE2	3:A:453:HOH:O	2.48	0.43
1:A:129:LYS:NZ	1:A:155:ASP:OD2	2.23	0.43
1:B:202:ASP:HA	1:B:236:GLN:HG3	2.01	0.43
1:A:165:THR:CG2	1:A:167:LYS:H	2.17	0.42
1:B:198:GLU:HG3	1:B:229:ASN:HB3	2.01	0.42
1:A:76:GLU:H	1:A:76:GLU:CD	2.21	0.42
1:A:119:CYS:HB3	3:A:359:HOH:O	2.17	0.42
1:A:57:LYS:C	1:A:58:ARG:HG2	2.39	0.42
1:B:121:LYS:HZ3	1:B:121:LYS:HG3	1.58	0.42
1:B:45:ARG:CG	1:B:46:TRP:H	2.32	0.42
1:B:139:GLN:C	1:B:141:ASP:N	2.71	0.42
1:A:94:ILE:HG23	1:A:94:ILE:HD12	1.81	0.42
1:B:134:GLN:HB3	1:B:285:LEU:HD11	2.01	0.42
1:B:110:MET:SD	1:B:192:VAL:HG12	2.60	0.42
1:A:165:THR:O	1:A:165:THR:HG23	2.17	0.42
1:B:162:GLU:HB2	1:B:165:THR:CG2	2.43	0.41
1:B:248:GLU:O	1:B:250:SER:OG	2.23	0.41
1:B:107:GLN:O	1:B:108:PRO:C	2.58	0.41
1:B:244:HIS:CD2	1:B:250:SER:HB2	2.56	0.41
1:A:107:GLN:HB3	1:A:111:LYS:HZ3	1.85	0.41
1:B:127:ARG:NE	1:B:212:ARG:NE	2.70	0.40
1:A:55:THR:HG23	1:A:159:TRP:HA	2.03	0.40
1:B:146:GLU:OE2	2:B:301:CXR:O2D	2.35	0.40
1:A:143:PHE:CD2	1:A:143:PHE:N	2.89	0.40
1:A:268:LYS:HD2	1:B:163:PHE:HE1	1.86	0.40
1:B:210:GLY:N	1:B:243:ILE:O	2.53	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%)	226 (90%)	22 (9%)	2 (1%)	24	14
1	B	250/262 (95%)	216 (86%)	29 (12%)	5 (2%)	9	3
All	All	500/524 (95%)	442 (88%)	51 (10%)	7 (1%)	14	5

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	SER
1	B	213	SER
1	B	249	ASP
1	A	294	SER
1	B	164	ASP
1	B	294	SER
1	B	292	GLU

### 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	223/241 (92%)	214 (96%)	9 (4%)	38	31
1	B	223/241 (92%)	198 (89%)	25 (11%)	7	3
All	All	446/482 (92%)	412 (92%)	34 (8%)	16	9

All (34) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	76	GLU
1	A	78	ARG
1	A	89	PHE
1	A	131	LEU
1	A	164	ASP
1	A	183	ASN
1	A	250	SER
1	A	251	ARG
1	A	285	LEU
1	B	48	GLN
1	B	89	PHE
1	B	95	SER
1	B	98	PRO
1	B	103	GLU
1	B	104	GLU
1	B	131	LEU
1	B	139	GLN
1	B	176	TRP
1	B	178	LYS
1	B	195	ARG
1	B	202	ASP
1	B	208	LEU
1	B	212	ARG
1	B	218	LYS
1	B	228	HIS
1	B	234	LYS
1	B	236	GLN
1	B	251	ARG
1	B	255	GLN
1	B	258	THR
1	B	264	SER
1	B	268	LYS
1	B	282	ASP
1	B	285	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	134	GLN
1	A	171	GLN
1	A	183	ASN
1	A	244	HIS

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Mol	Chain	Res	Type
1	A	286	GLN
1	B	83	GLN
1	B	107	GLN
1	B	115	GLN
1	B	139	GLN
1	B	183	ASN
1	B	205	HIS
1	B	236	GLN
1	B	255	GLN
1	B	286	GLN

### 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 ⓘ

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	$\# Z  > 2$
2	CXR	A	301	-	28,39,39	4.07	14 (50%)	37,62,62	2.11	9 (24%)
2	CXR	B	301	-	28,39,39	3.36	11 (39%)	37,62,62	1.62	8 (21%)

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	CXR	A	301	-	1/1/10/10	0/18/58/58	0/0/5/5
2	CXR	B	301	-	1/1/10/10	0/18/58/58	0/0/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	CXR	O3D-C3D	-4.62	1.31	1.43
2	A	301	CXR	C5'-C4'	-4.30	1.37	1.51
2	A	301	CXR	C5D-C4D	-3.01	1.41	1.51
2	A	301	CXR	PB-O1B	-2.72	1.43	1.54
2	B	301	CXR	C2D-C3D	-2.23	1.47	1.53
2	A	301	CXR	PA-O5'	2.03	1.68	1.59
2	B	301	CXR	O3D-C3D	2.06	1.47	1.43
2	A	301	CXR	O2'-C2'	2.12	1.48	1.43
2	A	301	CXR	O4'-C4'	2.18	1.50	1.45
2	B	301	CXR	C2-N3	2.19	1.34	1.30
2	B	301	CXR	PA-O5'	2.34	1.69	1.59
2	B	301	CXR	C8-N7	2.64	1.39	1.34
2	A	301	CXR	C6-N6	3.75	1.35	1.29
2	B	301	CXR	PA-O2A	3.83	1.65	1.51
2	B	301	CXR	C5-C4	3.89	1.49	1.40
2	B	301	CXR	O2D-C2D	4.22	1.53	1.43
2	A	301	CXR	O2D-C2D	4.26	1.53	1.43
2	A	301	CXR	C6-C5	4.28	1.49	1.41
2	A	301	CXR	PA-O2A	4.93	1.69	1.51
2	A	301	CXR	PB-O2B	5.25	1.70	1.51
2	A	301	CXR	O4D-C1D	5.80	1.48	1.41
2	B	301	CXR	C6-C5	6.22	1.52	1.41
2	B	301	CXR	C6-N6	8.06	1.43	1.29
2	B	301	CXR	O4'-C1'	10.87	1.54	1.41
2	A	301	CXR	O4'-C1'	15.59	1.60	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	CXR	PA-O3A-PB	-5.54	117.18	132.73
2	A	301	CXR	C4-C5-N7	-5.16	104.74	109.48
2	A	301	CXR	C4'-O4'-C1'	-3.99	105.33	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	CXR	O4'-C1'-N9	-3.41	100.96	108.10
2	B	301	CXR	O2'-C2'-C3'	-3.28	101.16	111.83
2	A	301	CXR	O3'-C3'-C2'	-2.72	102.98	111.83
2	B	301	CXR	PA-O3A-PB	-2.32	126.21	132.73
2	B	301	CXR	C4-C5-N7	-2.13	107.52	109.48
2	B	301	CXR	O5'-C5'-C4'	2.03	116.61	109.12
2	A	301	CXR	O4D-C1D-N1	2.06	112.43	108.08
2	B	301	CXR	C6-C5-C4	2.18	118.50	116.78
2	A	301	CXR	O4'-C1'-N9	2.33	112.97	108.10
2	A	301	CXR	O1B-PB-O3A	2.49	116.37	105.09
2	B	301	CXR	C2-N3-C4	2.54	120.34	116.40
2	A	301	CXR	C2'-C3'-C4'	3.66	110.14	102.61
2	A	301	CXR	C2-N3-C4	4.91	124.01	116.40
2	B	301	CXR	C2'-C1'-N9	4.98	121.91	114.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	301	CXR	C3'
2	B	301	CXR	C3'

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	CXR	1	0
2	B	301	CXR	5	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%)	0.62	20 (7%) 15 18	23, 33, 45, 53	0
1	B	252/262 (96%)	0.88	40 (15%) 3 3	21, 33, 46, 57	0
All	All	504/524 (96%)	0.75	60 (11%) 6 7	21, 33, 46, 57	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	ASP	7.4
1	B	294	SER	6.8
1	B	246	GLY	6.6
1	B	249	ASP	6.3
1	A	296	CYS	5.6
1	B	296	CYS	4.5
1	B	293	ASP	4.1
1	A	145	LEU	4.0
1	A	248	GLU	3.5
1	A	124	LEU	3.5
1	B	123	LEU	3.4
1	A	196	PHE	3.3
1	B	145	LEU	3.3
1	B	245	GLY	3.3
1	A	213	SER	3.2
1	B	164	ASP	2.9
1	B	255	GLN	2.9
1	B	124	LEU	2.9
1	B	238	LEU	2.9
1	A	46	TRP	2.9
1	B	247	ARG	2.8
1	A	123	LEU	2.7
1	A	144	THR	2.7
1	B	151	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	189	TRP	2.7
1	B	206	VAL	2.6
1	B	150	LEU	2.6
1	B	212	ARG	2.6
1	B	204	VAL	2.6
1	A	164	ASP	2.6
1	B	295	SER	2.6
1	B	176	TRP	2.5
1	B	149	LEU	2.5
1	B	285	LEU	2.5
1	B	283	LYS	2.5
1	B	148	THR	2.5
1	B	144	THR	2.4
1	B	153	LEU	2.4
1	B	286	GLN	2.4
1	B	222	PHE	2.4
1	B	228	HIS	2.3
1	B	189	TRP	2.3
1	A	47	ARG	2.3
1	B	219	ASP	2.2
1	B	214	LYS	2.2
1	A	143	PHE	2.2
1	B	89	PHE	2.2
1	B	140	ARG	2.2
1	B	196	PHE	2.1
1	B	287	CYS	2.1
1	A	230	LEU	2.1
1	B	154	ALA	2.1
1	B	292	GLU	2.1
1	A	82	CYS	2.1
1	B	252	ASP	2.1
1	A	227	VAL	2.1
1	A	212	ARG	2.0
1	B	208	LEU	2.0
1	A	139	GLN	2.0
1	A	245	GLY	2.0

## 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 [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( $\text{\AA}^2$ )	Q<0.9
2	CXR	B	301	35/35	0.85	0.18	0.43	23,44,59,62	0
2	CXR	A	301	35/35	0.93	0.12	-1.00	21,29,43,46	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.