



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:39 pm GMT

PDB ID : 2PGJ
Title : Catalysis associated conformational changes revealed by human cd38 complexed with a non-hydrolyzable substrate analog
Authors : Liu, Q.; Kriksunov, I.A.; Moreau, C.; Graeff, R.; Potter, B.V.L.; Lee, H.C.; Hao, Q.
Deposited on : 2007-04-09
Resolution : 1.71 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : trunk28620
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) : recalc28949

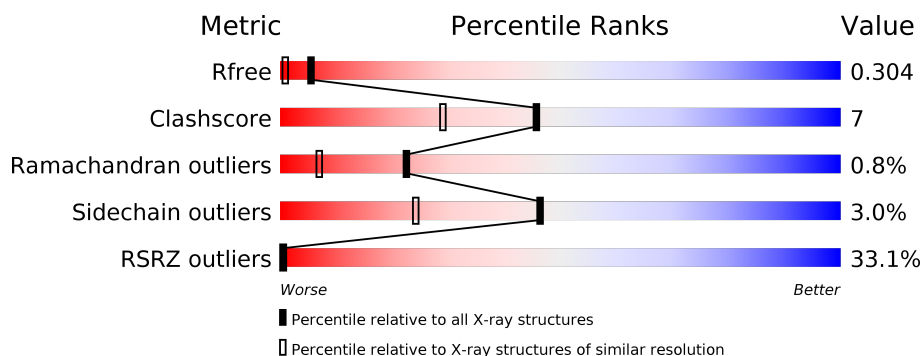
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	4385 (1.74-1.70)
Clashscore	112137	4841 (1.74-1.70)
Ramachandran outliers	110173	4771 (1.74-1.70)
Sidechain outliers	110143	4771 (1.74-1.70)
RSRZ outliers	101464	4426 (1.74-1.70)

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 ≥ 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>27%</div> <div>78%</div> <div>16%</div> <div>• •</div> </div>
1	B	262	<div> <div>37%</div> <div>79%</div> <div>17%</div> <div>•</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	N1C	A	301	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4535 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.

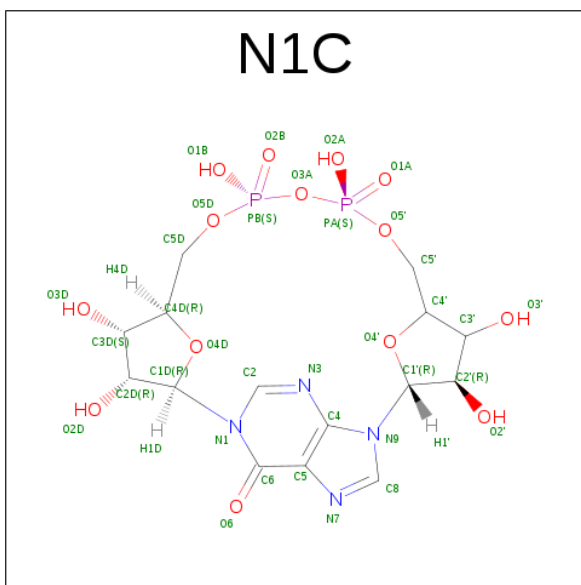
- Molecule 1 is a protein called ADP-ribosyl cyclase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			
1	B	252	Total	C	N	O	S	0	0	0
			2050	1290	358	386	16			

There are 22 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
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

- Molecule 2 is N1-CYCLIC INOSINE 5'-DIPHOSPHORIBOSE (three-letter code: N1C) (formula: $C_{15}H_{20}N_4O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 35	C 15	N 4	O 14	P 2	0	0

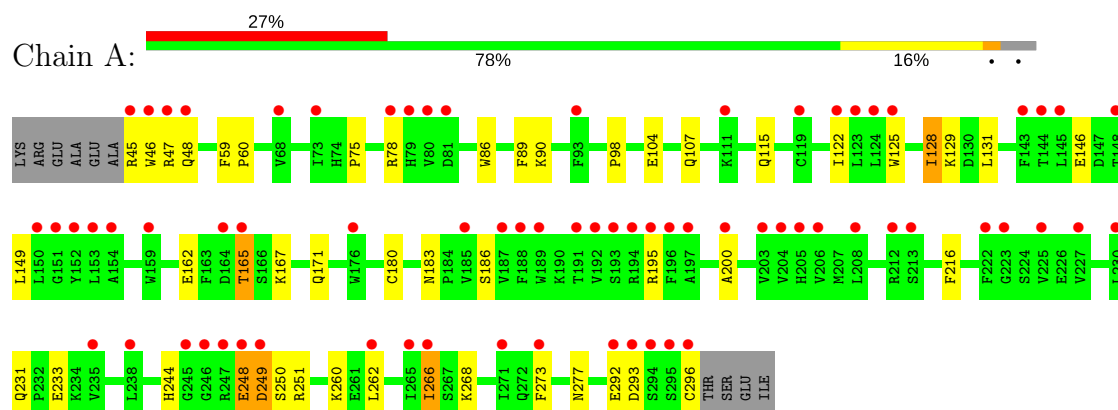
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	210	Total O 210 210	0	0
3	B	190	Total O 190 190	0	0

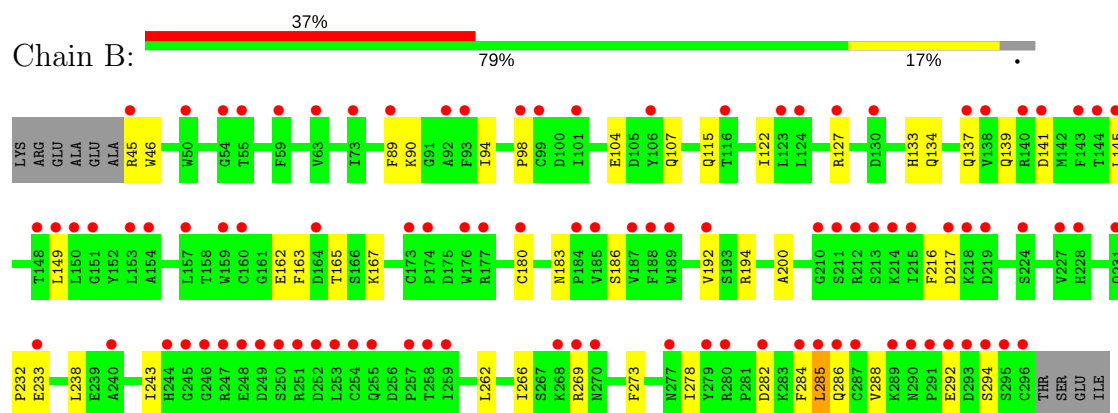
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 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, α , β , γ	41.89Å 53.20Å 65.64Å 105.34° 91.96° 94.94°	Depositor
Resolution (Å)	28.41 – 1.71 28.41 – 1.71	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.41-1.71) 83.8 (28.41-1.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.3.0021	Depositor
R, R_{free}	0.191 , 0.224 0.280 , 0.304	Depositor DCC
R_{free} test set	2761 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 62.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4535	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: N1C

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	0.44	0/2101	0.57	0/2846
1	B	0.46	0/2101	0.55	0/2846
All	All	0.45	0/4202	0.56	0/5692

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

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	1976	34	0
1	B	2050	0	1976	26	0
2	A	35	0	15	3	0
3	A	210	0	0	5	0
3	B	190	0	0	1	0
All	All	4535	0	3967	59	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 7.

All (59) 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:115:GLN:HE22	1:B:149:LEU:H	1.20	0.88
1:A:115:GLN:HE22	1:A:149:LEU:H	1.23	0.86
1:B:165:THR:HG23	1:B:167:LYS:H	1.46	0.80
1:A:268:LYS:HD3	1:B:163:PHE:CE1	2.17	0.79
1:A:165:THR:HG23	1:A:167:LYS:H	1.47	0.78
1:A:268:LYS:HD3	1:B:163:PHE:HE1	1.49	0.77
2:A:301:N1C:H2D	2:A:301:N1C:O6	1.94	0.67
1:B:162:GLU:HB2	1:B:165:THR:HG22	1.79	0.64
1:A:180:CYS:HB2	3:A:432:HOH:O	2.00	0.61
1:A:183:ASN:ND2	1:A:186:SER:H	2.00	0.60
1:A:162:GLU:HB2	1:A:165:THR:HG22	1.84	0.59
1:A:266:ILE:HD11	1:A:273:PHE:HB2	1.86	0.57
1:A:75:PRO:O	1:A:78:ARG:HB2	2.03	0.57
1:B:266:ILE:HD11	1:B:273:PHE:HB2	1.86	0.57
1:B:127:ARG:HH12	1:B:217:ASP:HB3	1.68	0.57
1:A:104:GLU:HA	1:A:107:GLN:HG2	1.87	0.57
1:B:104:GLU:HA	1:B:107:GLN:HG2	1.86	0.56
1:B:133:HIS:O	1:B:137:GLN:HG3	2.06	0.56
1:A:231:GLN:HG3	3:A:510:HOH:O	2.05	0.56
1:A:115:GLN:NE2	1:A:149:LEU:H	2.01	0.56
1:A:146:GLU:OE2	2:A:301:N1C:O6	2.24	0.55
1:B:238:LEU:HB3	1:B:266:ILE:HD13	1.89	0.54
1:A:183:ASN:HD21	1:A:186:SER:H	1.54	0.54
1:B:115:GLN:NE2	1:B:149:LEU:H	1.98	0.53
1:B:284:PHE:O	1:B:288:VAL:HG23	2.08	0.53
1:A:293:ASP:HB3	1:A:296:CYS:SG	2.50	0.52
1:B:139:GLN:C	1:B:141:ASP:H	2.13	0.51
1:A:195:ARG:HG3	3:A:326:HOH:O	2.11	0.50
1:B:183:ASN:ND2	1:B:186:SER:H	2.10	0.49
1:A:216:PHE:CE1	1:A:262:LEU:HD13	2.48	0.49
1:B:145:LEU:HD21	1:B:192:VAL:HG23	1.95	0.49
1:A:48:GLN:NE2	1:A:171:GLN:HB3	2.28	0.48
1:B:45:ARG:HG2	1:B:46:TRP:H	1.79	0.48
1:B:134:GLN:HB3	1:B:285:LEU:HD11	1.96	0.47
1:A:86:TRP:CE2	1:A:90:LYS:HG3	2.49	0.47
1:B:90:LYS:HG3	1:B:94:ILE:HG13	1.96	0.45
1:A:125:TRP:CH2	1:A:129:LYS:HB3	2.51	0.45
1:A:125:TRP:CZ3	1:A:129:LYS:HB3	2.52	0.44
1:A:260:LYS:NZ	3:A:446:HOH:O	2.49	0.44
1:A:125:TRP:O	2:A:301:N1C:H5D1	2.16	0.44
1:A:59:PHE:HB3	1:A:60:PRO:HD3	2.00	0.44
1:B:122:ILE:HD12	1:B:200:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ARG:NH1	3:A:382:HOH:O	2.51	0.43
1:B:216:PHE:CE1	1:B:262:LEU:HD13	2.53	0.43
1:B:232:PRO:HG3	1:B:269:ARG:O	2.18	0.43
1:B:180:CYS:HB2	3:B:324:HOH:O	2.18	0.43
1:A:46:TRP:HE1	1:A:47:ARG:NH1	2.17	0.42
1:A:162:GLU:OE2	1:A:165:THR:HG21	2.19	0.42
1:B:233:GLU:CD	1:B:233:GLU:H	2.22	0.42
1:A:98:PRO:O	1:A:183:ASN:HA	2.20	0.42
1:A:248:GLU:O	1:A:249:ASP:CB	2.67	0.42
1:B:98:PRO:O	1:B:183:ASN:HA	2.18	0.42
1:B:243:ILE:CD1	1:B:278:ILE:HD12	2.50	0.42
1:A:233:GLU:H	1:A:233:GLU:CD	2.22	0.42
1:A:244:HIS:HD2	1:A:250:SER:HB3	1.85	0.41
1:A:122:ILE:HD12	1:A:200:ALA:HA	2.03	0.41
1:A:248:GLU:O	1:A:249:ASP:HB2	2.20	0.41
1:A:244:HIS:HE1	1:A:277:ASN:OD1	2.04	0.40
1:B:139:GLN:C	1:B:141:ASP:N	2.74	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	250/262 (95%)	239 (96%)	8 (3%)	3 (1%)	15	3
1	B	250/262 (95%)	237 (95%)	12 (5%)	1 (0%)	38	20
All	All	500/524 (95%)	476 (95%)	20 (4%)	4 (1%)	22	7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	ASP

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Mol	Chain	Res	Type
1	A	248	GLU
1	B	292	GLU
1	A	128	ILE

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	233/241 (97%)	225 (97%)	8 (3%)	42	19
1	B	233/241 (97%)	227 (97%)	6 (3%)	51	30
All	All	466/482 (97%)	452 (97%)	14 (3%)	46	24

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

Mol	Chain	Res	Type
1	A	45	ARG
1	A	89	PHE
1	A	128	ILE
1	A	131	LEU
1	A	165	THR
1	A	251	ARG
1	A	266	ILE
1	A	292	GLU
1	B	89	PHE
1	B	194	ARG
1	B	282	ASP
1	B	285	LEU
1	B	286	GLN
1	B	294	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN

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Mol	Chain	Res	Type
1	A	115	GLN
1	A	134	GLN
1	A	139	GLN
1	A	183	ASN
1	A	244	HIS
1	A	290	ASN
1	B	115	GLN
1	B	137	GLN
1	B	171	GLN
1	B	183	ASN
1	B	244	HIS

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](#)

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	N1C	A	301	-	32,39,39	1.98	5 (15%)	32,62,62	2.20	11 (34%)

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	N1C	A	301	-	3/3/10/10	0/18/58/58	0/0/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	N1C	C3'-C4'	-7.91	1.32	1.53
2	A	301	N1C	O3'-C3'	-4.11	1.33	1.43
2	A	301	N1C	C2-N3	2.61	1.34	1.30
2	A	301	N1C	C6-N1	2.81	1.42	1.38
2	A	301	N1C	C6-C5	4.17	1.48	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	N1C	C5-C6-N1	-3.77	117.84	120.52
2	A	301	N1C	C4'-O4'-C1'	-3.06	106.51	109.77
2	A	301	N1C	C6-C5-C4	-2.00	118.54	119.92
2	A	301	N1C	C4D-O4D-C1D	2.64	112.58	109.77
2	A	301	N1C	C5'-C4'-C3'	2.72	125.65	115.29
2	A	301	N1C	O4'-C4'-C3'	2.94	111.00	105.17
2	A	301	N1C	C2-N3-C4	3.61	121.95	116.41
2	A	301	N1C	O3'-C3'-C2'	3.77	123.91	111.83
2	A	301	N1C	O4'-C4'-C5'	4.13	123.35	109.40
2	A	301	N1C	C2'-C3'-C4'	4.25	110.89	102.62
2	A	301	N1C	O3'-C3'-C4'	4.82	125.17	111.09

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	301	N1C	C4'
2	A	301	N1C	N1
2	A	301	N1C	C3'

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	N1C	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, 95th 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 ²)	Q<0.9
1	A	252/262 (96%)	1.68	71 (28%)  	23, 29, 36, 43	0
1	B	252/262 (96%)	2.07	96 (38%)  	23, 29, 35, 40	0
All	All	504/524 (96%)	1.88	167 (33%)  	23, 29, 36, 43	0

All (167) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	CYS	11.7
1	A	246	GLY	10.1
1	B	246	GLY	9.8
1	B	245	GLY	9.4
1	B	295	SER	9.3
1	A	249	ASP	9.1
1	B	248	GLU	9.0
1	B	249	ASP	9.0
1	B	213	SER	8.8
1	B	291	PRO	8.7
1	B	247	ARG	7.3
1	B	287	CYS	7.3
1	B	292	GLU	7.1
1	A	296	CYS	6.6
1	B	290	ASN	6.4
1	A	247	ARG	6.3
1	A	295	SER	6.2
1	A	294	SER	6.1
1	A	47	ARG	6.0
1	B	294	SER	5.6
1	A	292	GLU	5.6
1	A	124	LEU	5.5
1	B	212	ARG	5.4
1	A	189	TRP	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	293	ASP	5.2
1	A	145	LEU	5.2
1	A	222	PHE	5.1
1	B	254	CYS	5.1
1	B	159	TRP	5.0
1	A	143	PHE	5.0
1	A	248	GLU	4.9
1	A	188	PHE	4.9
1	B	153	LEU	4.8
1	A	230	LEU	4.7
1	B	188	PHE	4.6
1	B	211	SER	4.5
1	A	46	TRP	4.5
1	B	215	ILE	4.5
1	B	141	ASP	4.5
1	B	270	ASN	4.5
1	A	238	LEU	4.4
1	B	286	GLN	4.4
1	B	219	ASP	4.4
1	A	187	VAL	4.3
1	A	192	VAL	4.2
1	A	204	VAL	4.2
1	A	206	VAL	4.1
1	B	214	LYS	4.1
1	A	123	LEU	4.1
1	B	185	VAL	4.0
1	B	116	THR	4.0
1	A	266	ILE	3.9
1	A	227	VAL	3.9
1	A	154	ALA	3.8
1	A	196	PHE	3.8
1	B	145	LEU	3.8
1	B	279	TYR	3.8
1	B	140	ARG	3.7
1	B	176	TRP	3.7
1	A	150	LEU	3.7
1	B	252	ASP	3.7
1	B	160	CYS	3.7
1	A	213	SER	3.7
1	B	138	VAL	3.7
1	B	189	TRP	3.7
1	A	125	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	157	LEU	3.6
1	B	154	ALA	3.6
1	A	165	THR	3.6
1	A	212	ARG	3.6
1	B	89	PHE	3.5
1	B	285	LEU	3.5
1	B	282	ASP	3.5
1	A	79	HIS	3.5
1	B	268	LYS	3.5
1	B	218	LYS	3.5
1	A	122	ILE	3.4
1	B	150	LEU	3.4
1	B	257	PRO	3.4
1	A	197	ALA	3.3
1	A	185	VAL	3.3
1	A	271	ILE	3.3
1	B	259	ILE	3.3
1	A	235	VAL	3.2
1	A	159	TRP	3.2
1	B	127	ARG	3.2
1	B	149	LEU	3.2
1	B	184	PRO	3.2
1	A	144	THR	3.2
1	A	245	GLY	3.2
1	A	203	VAL	3.1
1	A	164	ASP	3.1
1	A	262	LEU	3.1
1	A	93	PHE	3.1
1	B	93	PHE	3.1
1	B	180	CYS	3.0
1	B	224	SER	3.0
1	A	225	VAL	3.0
1	A	293	ASP	3.0
1	A	73	ILE	3.0
1	B	231	GLN	3.0
1	B	255	GLN	3.0
1	B	289	LYS	2.9
1	A	194	ARG	2.9
1	A	265	ILE	2.9
1	B	233	GLU	2.9
1	A	148	THR	2.9
1	B	63	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	144	THR	2.9
1	B	250	SER	2.8
1	B	251	ARG	2.8
1	A	80	VAL	2.8
1	B	123	LEU	2.8
1	A	152	TYR	2.7
1	B	217	ASP	2.7
1	B	143	PHE	2.7
1	B	55	THR	2.7
1	B	284	PHE	2.7
1	B	73	ILE	2.7
1	A	223	GLY	2.7
1	B	130	ASP	2.7
1	B	244	HIS	2.6
1	B	151	GLY	2.6
1	A	48	GLN	2.6
1	B	124	LEU	2.6
1	A	176	TRP	2.6
1	B	269	ARG	2.6
1	B	187	VAL	2.6
1	A	111	LYS	2.5
1	B	280	ARG	2.5
1	A	191	THR	2.5
1	B	50	TRP	2.5
1	A	78	ARG	2.5
1	B	227	VAL	2.5
1	A	151	GLY	2.5
1	B	59	PHE	2.5
1	B	106	TYR	2.4
1	B	253	LEU	2.4
1	A	205	HIS	2.4
1	B	228	HIS	2.4
1	B	148	THR	2.4
1	B	192	VAL	2.4
1	B	137	GLN	2.4
1	A	68	VAL	2.4
1	A	273	PHE	2.4
1	A	193	SER	2.4
1	A	200	ALA	2.4
1	A	208	LEU	2.3
1	A	195	ARG	2.3
1	A	81	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	101	ILE	2.3
1	B	174	PRO	2.3
1	B	173	CYS	2.3
1	A	45	ARG	2.2
1	B	177	ARG	2.2
1	B	277	ASN	2.2
1	B	99	CYS	2.2
1	B	45	ARG	2.2
1	A	153	LEU	2.2
1	B	54	GLY	2.2
1	B	258	THR	2.1
1	B	164	ASP	2.1
1	A	119	CYS	2.1
1	B	98	PRO	2.1
1	B	92	ALA	2.0
1	B	210	GLY	2.0
1	B	240	ALA	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, 95th 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 ²)	Q<0.9
2	N1C	A	301	35/35	0.89	0.13	-1.29	25,33,38,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.