



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2020 – 10:53 pm BST

PDB ID : 1R15  
Title : Aplysia ADP ribosyl cyclase with bound nicotinamide and R5P  
Authors : Love, M.L.; Szebenyi, D.M.E.; Kriksunov, I.A.; Thiel, D.J.; Munshi, C.; Graeff, R.; Lee, H.C.; Hao, Q.  
Deposited on : 2003-09-23  
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

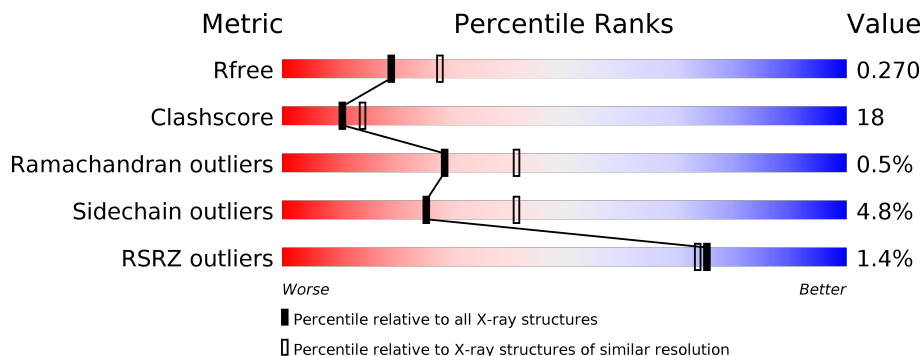
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	258	
1	B	258	
1	C	258	
1	D	258	
1	E	258	
1	F	258	

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Mol	Chain	Length	Quality of chain
1	G	258	
1	H	258	

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	N	A	1179	X	-	-	-
2	N	B	1179	X	-	-	-
2	N	C	1179	X	-	-	-
2	N	D	1179	X	-	-	-
2	N	E	1179	X	-	-	-
2	N	F	1179	X	-	-	-
2	N	G	1179	X	-	-	-
2	N	H	1179	X	-	-	-
3	NCA	B	429	-	X	-	-
3	NCA	E	459	-	-	X	-
3	NCA	F	469	-	X	-	-
3	NCA	G	379	-	-	X	-
3	NCA	G	479	-	X	-	-
3	NCA	H	389	-	X	-	-
3	NCA	H	489	-	-	X	-

## 2 Entry composition

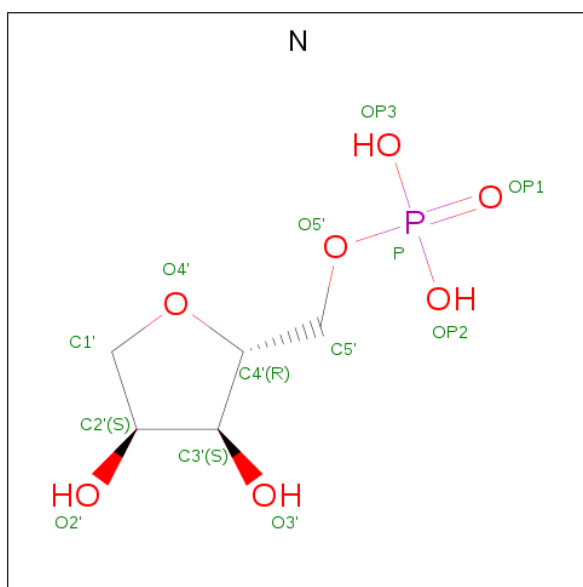
There are 3 unique types of molecules in this entry. The entry contains 16344 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

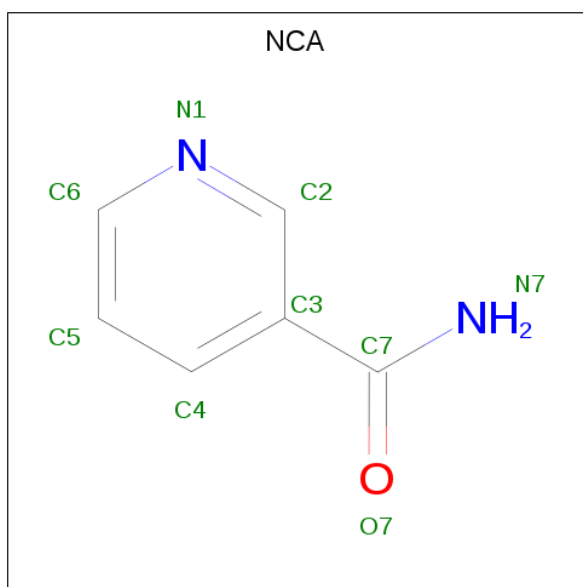
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	251	2012	1288	342	368	14	0	0	0
1	B	251	2012	1288	342	368	14	0	0	0
1	C	251	2012	1288	342	368	14	0	0	0
1	D	251	2012	1288	342	368	14	0	0	0
1	E	251	2012	1288	342	368	14	0	0	0
1	F	251	2012	1288	342	368	14	0	0	0
1	G	251	2012	1288	342	368	14	0	0	0
1	H	251	2012	1288	342	368	14	0	0	0

- Molecule 2 is ANY 5'-MONOPHOSPHATE NUCLEOTIDE (three-letter code: N) (formula: C<sub>5</sub>H<sub>11</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			13	5	7	1		
2	B	1	Total	C	O	P	0	0
			13	5	7	1		
2	C	1	Total	C	O	P	0	0
			13	5	7	1		
2	D	1	Total	C	O	P	0	0
			13	5	7	1		
2	E	1	Total	C	O	P	0	0
			13	5	7	1		
2	F	1	Total	C	O	P	0	0
			13	5	7	1		
2	G	1	Total	C	O	P	0	0
			13	5	7	1		
2	H	1	Total	C	O	P	0	0
			13	5	7	1		

- Molecule 3 is NICOTINAMIDE (three-letter code: NCA) (formula: C<sub>6</sub>H<sub>6</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total 9	C 6	N 2	O 1	0	0
3	A	1	Total 9	C 6	N 2	O 1	0	0
3	B	1	Total 9	C 6	N 2	O 1	0	0
3	B	1	Total 9	C 6	N 2	O 1	0	0
3	C	1	Total 9	C 6	N 2	O 1	0	0
3	C	1	Total 9	C 6	N 2	O 1	0	0
3	D	1	Total 9	C 6	N 2	O 1	0	0
3	D	1	Total 9	C 6	N 2	O 1	0	0
3	E	1	Total 9	C 6	N 2	O 1	0	0
3	E	1	Total 9	C 6	N 2	O 1	0	0
3	F	1	Total 9	C 6	N 2	O 1	0	0
3	F	1	Total 9	C 6	N 2	O 1	0	0
3	G	1	Total 9	C 6	N 2	O 1	0	0
3	G	1	Total 9	C 6	N 2	O 1	0	0

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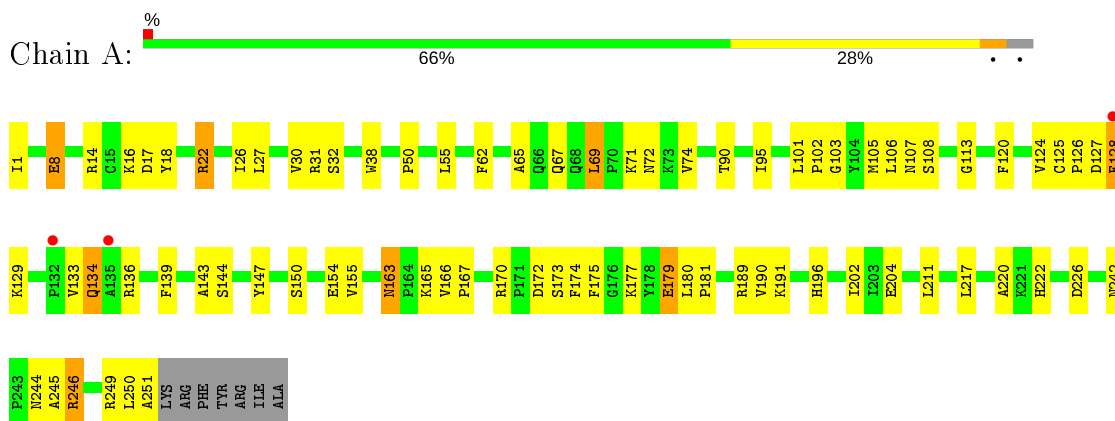
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>				<b>ZeroOcc</b>	<b>AltConf</b>
3	H	1	Total	C	N	O	0	0
			9	6	2	1		
3	H	1	Total	C	N	O	0	0
			9	6	2	1		

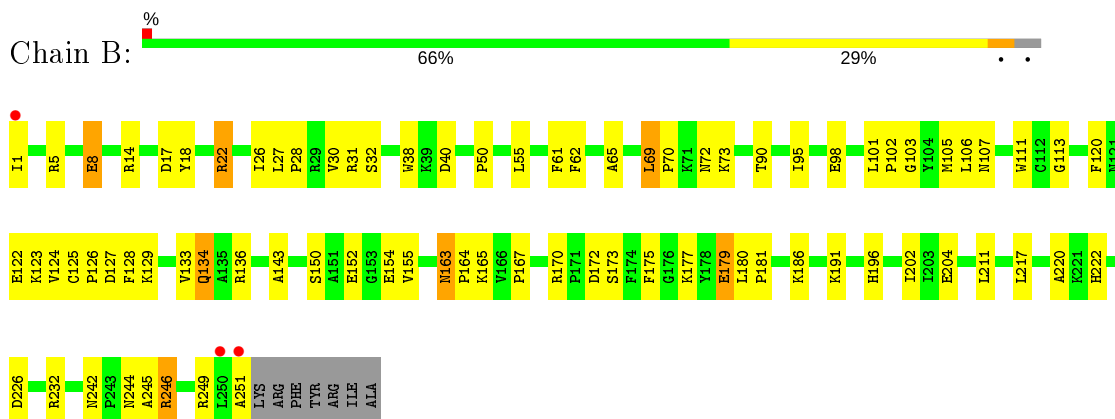
### 3 Residue-property plots

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.

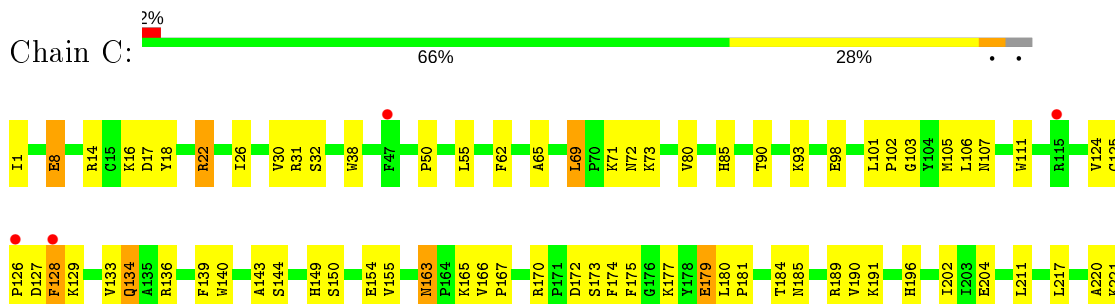
- Molecule 1: ADP-ribosyl cyclase



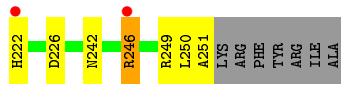
- Molecule 1: ADP-ribosyl cyclase



- Molecule 1: ADP-ribosyl cyclase



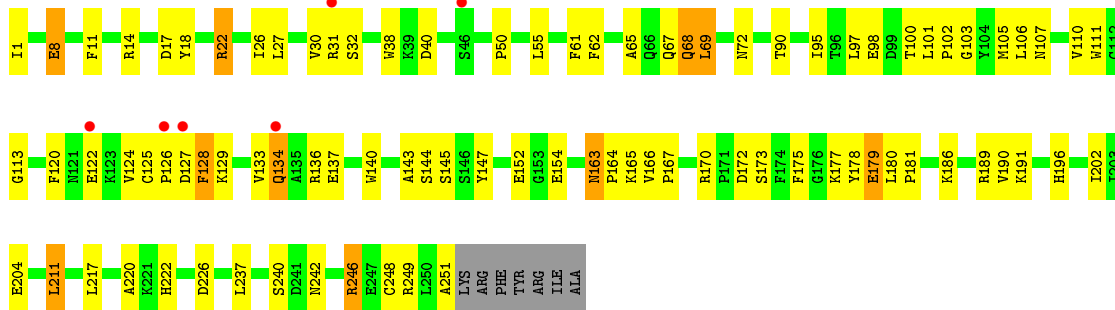




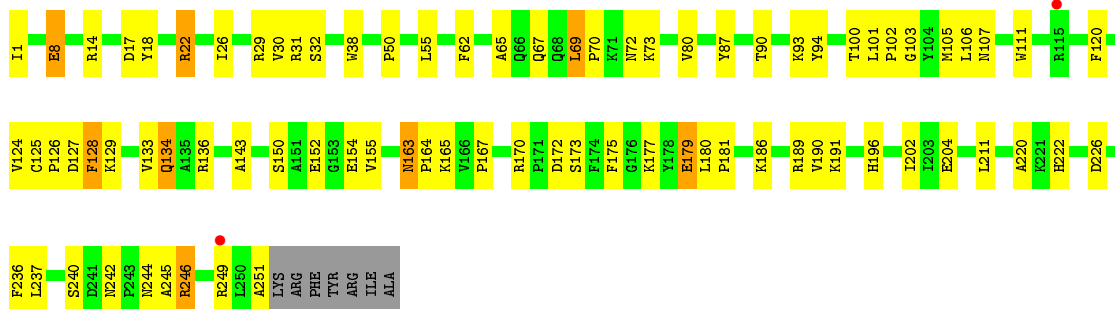
• Molecule 1: ADP-ribosyl cyclase



• Molecule 1: ADP-ribosyl cyclase

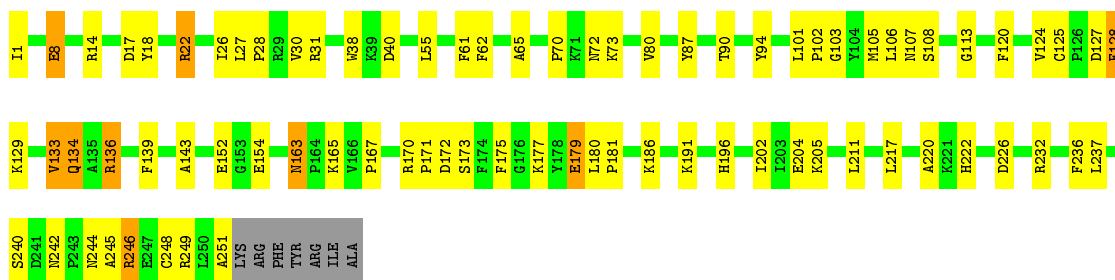


• Molecule 1: ADP-ribosyl cyclase

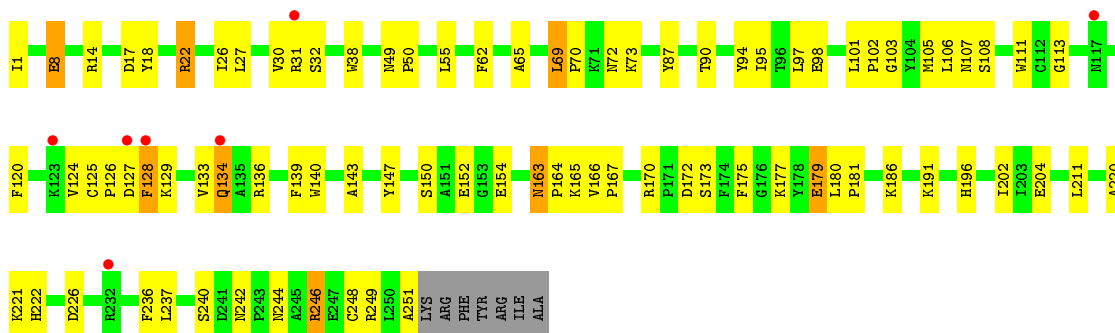


• Molecule 1: ADP-ribosyl cyclase





- Molecule 1: ADP-ribosyl cyclase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.40Å 75.32Å 138.13Å 88.16° 89.22° 89.09°	Depositor
Resolution (Å)	33.00 – 2.40 32.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (33.00-2.40) 60.1 (32.95-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.244 , 0.269 0.244 , 0.270	Depositor DCC
$R_{free}$ test set	2873 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 33.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-l 0.022 for -h,k,-l 0.008 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	16344	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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:  
NCA

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	0.84	1/2064 (0.0%)	0.77	2/2793 (0.1%)
1	B	0.85	2/2064 (0.1%)	0.79	2/2793 (0.1%)
1	C	0.84	1/2064 (0.0%)	0.77	2/2793 (0.1%)
1	D	0.84	1/2064 (0.0%)	0.80	2/2793 (0.1%)
1	E	0.82	1/2064 (0.0%)	0.78	2/2793 (0.1%)
1	F	0.86	2/2064 (0.1%)	0.79	2/2793 (0.1%)
1	G	0.87	2/2064 (0.1%)	1.15	6/2793 (0.2%)
1	H	0.80	1/2064 (0.0%)	0.77	2/2793 (0.1%)
All	All	0.84	11/16512 (0.1%)	0.84	20/22344 (0.1%)

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	GLU	CD-OE2	23.53	1.51	1.25
1	E	179	GLU	CD-OE2	23.07	1.51	1.25
1	C	179	GLU	CD-OE2	23.00	1.50	1.25
1	H	179	GLU	CD-OE2	22.84	1.50	1.25
1	G	179	GLU	CD-OE2	22.59	1.50	1.25

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	136	ARG	NE-CZ-NH1	-29.87	105.36	120.30
1	G	136	ARG	NE-CZ-NH2	29.33	134.96	120.30
1	G	136	ARG	CD-NE-CZ	13.46	142.44	123.60
1	G	136	ARG	CG-CD-NE	8.30	129.23	111.80
1	B	22	ARG	N-CA-C	6.93	129.72	111.00

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	2012	0	1968	80	0
1	B	2012	0	1968	82	0
1	C	2012	0	1968	86	0
1	D	2012	0	1968	79	0
1	E	2012	0	1968	82	1
1	F	2012	0	1968	68	0
1	G	2012	0	1968	83	0
1	H	2012	0	1968	84	1
2	A	13	0	8	2	0
2	B	13	0	8	0	0
2	C	13	0	8	2	0
2	D	13	0	8	0	0
2	E	13	0	8	1	0
2	F	13	0	8	1	0
2	G	13	0	8	3	0
2	H	13	0	8	0	0
3	A	18	0	12	3	0
3	B	18	0	12	3	0
3	C	18	0	12	4	0
3	D	18	0	12	2	0
3	E	18	0	12	7	0
3	F	18	0	12	3	0
3	G	18	0	12	5	0
3	H	18	0	12	7	0
All	All	16344	0	15904	592	1

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 18.

The worst 5 of 592 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:123:LYS:HD2	1:C:149:HIS:CE1	1.86	1.10
1:B:123:LYS:HD2	1:C:149:HIS:ND1	1.76	0.99
1:D:152:GLU:HG2	1:D:186:LYS:HB3	1.40	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PHE:HB3	3:A:419:NCA:H6	1.42	0.97
1:G:152:GLU:HG2	1:G:186:LYS:HB3	1.46	0.96

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:GLU:OE1	1:H:31:ARG:NH2[1_545]	1.99	0.21

## 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	249/258 (96%)	233 (94%)	15 (6%)	1 (0%)	34	48
1	B	249/258 (96%)	235 (94%)	14 (6%)	0	100	100
1	C	249/258 (96%)	232 (93%)	15 (6%)	2 (1%)	19	29
1	D	249/258 (96%)	230 (92%)	18 (7%)	1 (0%)	34	48
1	E	249/258 (96%)	234 (94%)	14 (6%)	1 (0%)	34	48
1	F	249/258 (96%)	234 (94%)	13 (5%)	2 (1%)	19	29
1	G	249/258 (96%)	234 (94%)	13 (5%)	2 (1%)	19	29
1	H	249/258 (96%)	232 (93%)	16 (6%)	1 (0%)	34	48
All	All	1992/2064 (96%)	1864 (94%)	118 (6%)	10 (0%)	29	41

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	128	PHE
1	E	128	PHE
1	F	128	PHE

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Mol	Chain	Res	Type
1	G	128	PHE
1	H	128	PHE

### 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	220/226 (97%)	208 (94%)	12 (6%)	21	35
1	B	220/226 (97%)	209 (95%)	11 (5%)	24	40
1	C	220/226 (97%)	208 (94%)	12 (6%)	21	35
1	D	220/226 (97%)	210 (96%)	10 (4%)	27	44
1	E	220/226 (97%)	209 (95%)	11 (5%)	24	40
1	F	220/226 (97%)	209 (95%)	11 (5%)	24	40
1	G	220/226 (97%)	212 (96%)	8 (4%)	35	54
1	H	220/226 (97%)	210 (96%)	10 (4%)	27	44
All	All	1760/1808 (97%)	1675 (95%)	85 (5%)	25	41

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	69	LEU
1	E	32	SER
1	H	69	LEU
1	D	133	VAL
1	D	242	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	163	ASN
1	E	134	GLN
1	H	134	GLN

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Mol	Chain	Res	Type
1	D	196	HIS
1	E	66	GLN

### 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](#)

24 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
3	NCA	H	389	-	9,9,9	3.48	5 (55%)	11,11,11	2.02	5 (45%)
3	NCA	H	489	-	9,9,9	2.26	4 (44%)	11,11,11	1.49	2 (18%)
3	NCA	C	439	-	9,9,9	2.83	4 (44%)	11,11,11	2.02	4 (36%)
3	NCA	D	349	-	9,9,9	2.78	5 (55%)	11,11,11	1.83	4 (36%)
3	NCA	B	429	-	9,9,9	2.94	5 (55%)	11,11,11	1.89	5 (45%)
3	NCA	C	339	-	9,9,9	2.86	3 (33%)	11,11,11	1.91	4 (36%)
3	NCA	E	459	-	9,9,9	2.51	4 (44%)	11,11,11	1.88	3 (27%)
3	NCA	D	449	-	9,9,9	2.92	5 (55%)	11,11,11	1.78	3 (27%)
3	NCA	A	419	-	9,9,9	2.34	3 (33%)	11,11,11	1.84	3 (27%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NCA	F	369	-	9,9,9	3.00	5 (55%)	11,11,11	1.83	4 (36%)
3	NCA	A	319	-	9,9,9	3.12	5 (55%)	11,11,11	1.93	4 (36%)
3	NCA	B	329	-	9,9,9	2.66	5 (55%)	11,11,11	1.81	4 (36%)
3	NCA	F	469	-	9,9,9	3.31	7 (77%)	11,11,11	1.89	4 (36%)
3	NCA	G	379	-	9,9,9	3.01	5 (55%)	11,11,11	2.06	4 (36%)
3	NCA	E	359	-	9,9,9	2.56	5 (55%)	11,11,11	1.66	3 (27%)
3	NCA	G	479	-	9,9,9	3.60	7 (77%)	11,11,11	2.07	4 (36%)

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
3	NCA	H	489	-	-	0/4/4/4	0/1/1/1
3	NCA	D	349	-	-	0/4/4/4	0/1/1/1
3	NCA	B	429	-	-	0/4/4/4	0/1/1/1
3	NCA	A	419	-	-	0/4/4/4	0/1/1/1
2	N	D	1179	1	1/1/4/4	-	-
2	N	E	1179	1	1/1/4/4	-	-
2	N	B	1179	1	1/1/4/4	-	-
2	N	C	1179	1	1/1/4/4	-	-
3	NCA	F	369	-	-	0/4/4/4	0/1/1/1
3	NCA	A	319	-	-	0/4/4/4	0/1/1/1
3	NCA	B	329	-	-	0/4/4/4	0/1/1/1
3	NCA	G	379	-	-	0/4/4/4	0/1/1/1
3	NCA	G	479	-	-	0/4/4/4	0/1/1/1
2	N	H	1179	1	1/1/4/4	-	-
2	N	F	1179	1	1/1/4/4	-	-
3	NCA	F	469	-	-	0/4/4/4	0/1/1/1
3	NCA	H	389	-	-	0/4/4/4	0/1/1/1
3	NCA	C	439	-	-	0/4/4/4	0/1/1/1
3	NCA	C	339	-	-	0/4/4/4	0/1/1/1
3	NCA	E	459	-	-	0/4/4/4	0/1/1/1
3	NCA	D	449	-	-	0/4/4/4	0/1/1/1
2	N	A	1179	1	1/1/4/4	-	-
2	N	G	1179	1	1/1/4/4	-	-
3	NCA	E	359	-	-	0/4/4/4	0/1/1/1

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	389	NCA	C3-C7	6.97	1.61	1.50
3	G	479	NCA	C2-N1	6.59	1.48	1.34
3	F	469	NCA	C2-N1	6.13	1.47	1.34
3	F	369	NCA	C3-C7	5.95	1.59	1.50
3	C	339	NCA	C3-C7	5.83	1.59	1.50

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	479	NCA	C3-C7-N7	3.52	121.97	117.75
3	G	379	NCA	C5-C4-C3	3.49	124.47	120.34
3	G	479	NCA	C5-C4-C3	3.47	124.44	120.34
3	G	379	NCA	C3-C7-N7	3.46	121.90	117.75
3	F	469	NCA	C3-C7-N7	3.40	121.83	117.75

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	1179	N	C3'
2	E	1179	N	C3'
2	B	1179	N	C3'
2	C	1179	N	C3'
2	H	1179	N	C3'

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	489	NCA	4	0
3	B	429	NCA	3	0
3	A	419	NCA	1	0
2	E	1179	N	1	0
2	C	1179	N	2	0
3	F	369	NCA	1	0
3	A	319	NCA	2	0
3	G	379	NCA	4	0
3	G	479	NCA	1	0
2	F	1179	N	1	0
3	F	469	NCA	2	0
3	H	389	NCA	3	0
3	C	439	NCA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	339	NCA	1	0
3	E	459	NCA	5	0
3	D	449	NCA	2	0
2	A	1179	N	2	0
2	G	1179	N	3	0
3	E	359	NCA	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	251/258 (97%)	0.01	3 (1%) 79 77	21, 41, 63, 72	0
1	B	251/258 (97%)	-0.09	3 (1%) 79 77	15, 35, 55, 68	0
1	C	251/258 (97%)	-0.02	6 (2%) 59 57	19, 39, 60, 73	0
1	D	251/258 (97%)	-0.17	2 (0%) 86 84	14, 34, 53, 75	0
1	E	251/258 (97%)	0.10	6 (2%) 59 57	23, 46, 63, 71	0
1	F	251/258 (97%)	-0.13	2 (0%) 86 84	14, 34, 54, 75	0
1	G	251/258 (97%)	-0.17	0 100 100	12, 35, 55, 78	0
1	H	251/258 (97%)	0.17	7 (2%) 53 51	26, 49, 63, 74	0
All	All	2008/2064 (97%)	-0.04	29 (1%) 75 73	12, 39, 61, 78	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	128	PHE	6.4
1	D	251	ALA	5.4
1	B	251	ALA	5.3
1	A	128	PHE	5.3
1	E	134	GLN	3.0

### 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NCA	A	419	9/9	0.70	0.40	58,59,60,61	0
3	NCA	D	349	9/9	0.71	0.36	67,67,68,68	0
2	N	A	1179	13/13	0.72	0.33	69,71,85,86	0
3	NCA	G	379	9/9	0.74	0.26	61,62,62,63	0
2	N	C	1179	13/13	0.74	0.26	71,74,82,84	0
3	NCA	H	489	9/9	0.76	0.31	48,49,54,54	0
3	NCA	A	319	9/9	0.76	0.28	59,61,62,62	0
3	NCA	F	369	9/9	0.77	0.26	49,52,52,53	0
3	NCA	H	389	9/9	0.79	0.28	57,58,60,62	0
3	NCA	B	329	9/9	0.79	0.27	35,39,40,41	0
2	N	H	1179	13/13	0.81	0.23	69,71,74,74	0
2	N	G	1179	13/13	0.81	0.22	59,60,66,66	0
3	NCA	E	359	9/9	0.81	0.23	54,54,55,55	0
2	N	B	1179	13/13	0.82	0.25	58,61,66,67	0
2	N	F	1179	13/13	0.82	0.24	59,61,68,68	0
2	N	E	1179	13/13	0.83	0.20	69,72,79,80	0
3	NCA	F	469	9/9	0.84	0.29	48,49,53,55	0
3	NCA	B	429	9/9	0.84	0.28	43,45,49,49	0
3	NCA	C	339	9/9	0.84	0.23	53,54,54,55	0
3	NCA	D	449	9/9	0.85	0.24	41,44,46,47	0
2	N	D	1179	13/13	0.85	0.20	53,54,68,68	0
3	NCA	C	439	9/9	0.86	0.22	52,54,55,56	0
3	NCA	G	479	9/9	0.90	0.26	38,40,44,44	0
3	NCA	E	459	9/9	0.90	0.29	52,53,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.