



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 08:12 PM EDT

PDB ID : 2O3U  
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 : 2.11 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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 : 2.35  
buster-report : 1.1.7 (2018)  
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) : 2.35

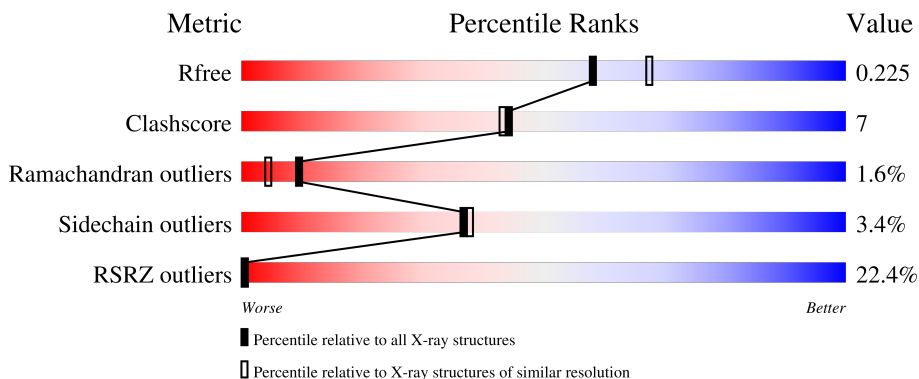
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 of 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	262	
1	B	262	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4374 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.

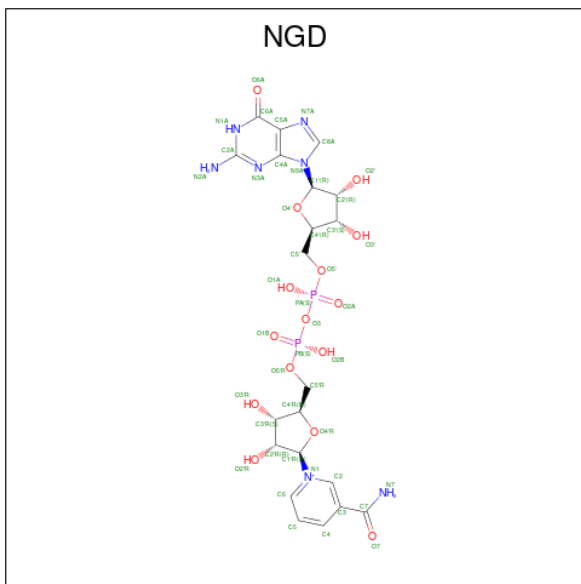
- Molecule 1 is a protein called ADP-ribosyl cyclase 1.

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

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 mutation	UNP P28907
A	100	ASP	ASN	engineered mutation	UNP P28907
A	164	ASP	ASN	engineered mutation	UNP P28907
A	209	ASP	ASN	engineered mutation	UNP P28907
A	219	ASP	ASN	engineered mutation	UNP P28907
A	226	GLN	GLU	engineered mutation	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 mutation	UNP P28907
B	100	ASP	ASN	engineered mutation	UNP P28907
B	164	ASP	ASN	engineered mutation	UNP P28907
B	209	ASP	ASN	engineered mutation	UNP P28907
B	219	ASP	ASN	engineered mutation	UNP P28907
B	226	GLN	GLU	engineered mutation	UNP P28907

- Molecule 2 is 3-(AMINOCARBONYL)-1-[(2R,3R,4S,5R)-5-({[(S)-{(S)-{(2R,3S,4R,5R)-5-(2-AMINO-6-OXO-1,6-DIHYDRO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHOXY}(HYDROXY)PHOSPHORYL]OXY}(HYDROXY)PHOSPHORYL]OXY}METHYL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]PYRIDINIUM (three-letter code: NGD) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total	C	N	O	P	0	0
			45	21	7	15	2		
2	B	1	Total	C	N	O	P	0	0
			45	21	7	15	2		

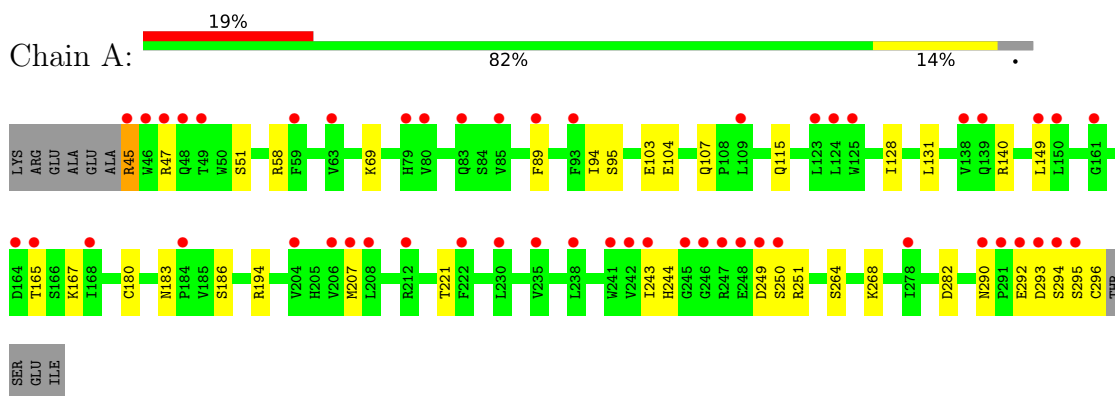
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	93	Total	O	0	0
			93	93		
3	B	91	Total	O	0	0
			91	91		

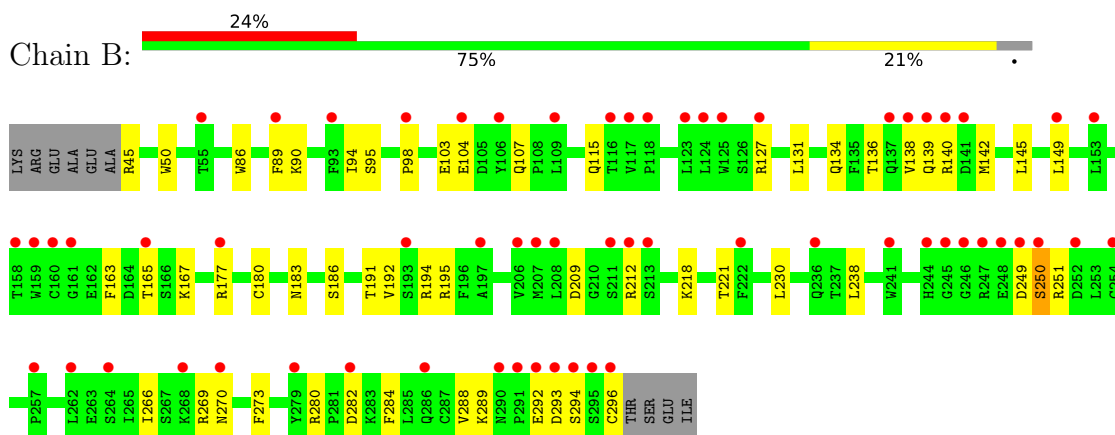
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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, $\alpha$ , $\beta$ , $\gamma$	41.98Å 53.09Å 65.68Å 106.08° 91.92° 95.18°	Depositor
Resolution (Å)	20.00 – 2.11 19.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.9 (20.00-2.11) 95.1 (19.94-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.09Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.178 , 0.223 0.180 , 0.225	Depositor DCC
$R_{free}$ test set	1509 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtrriage
Anisotropy	0.157	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 57.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4374	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.14% 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: NGD

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	0.60	1/2101 (0.0%)	0.63	1/2846 (0.0%)
1	B	0.56	1/2101 (0.0%)	0.63	0/2846
All	All	0.58	2/4202 (0.0%)	0.63	1/5692 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	ARG	N-CA	8.60	1.63	1.46
1	B	296	CYS	C-O	6.13	1.35	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ARG	N-CA-CB	5.31	120.16	110.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2050	0	1978	21	0
1	B	2050	0	1978	36	0
2	A	45	0	26	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	45	0	26	2	0
3	A	93	0	0	3	0
3	B	91	0	0	1	0
All	All	4374	0	4008	54	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 (54) 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:165:THR:HG22	1:B:167:LYS:H	1.33	0.94
1:A:115:GLN:HE22	1:A:149:LEU:H	1.19	0.91
1:B:115:GLN:HE22	1:B:149:LEU:H	1.21	0.87
1:A:268:LYS:HD2	1:B:163:PHE:HE1	1.50	0.77
1:B:103:GLU:HG2	1:B:191:THR:OG1	1.90	0.72
1:B:90:LYS:HG2	1:B:94:ILE:HG13	1.72	0.72
1:B:209:ASP:HB3	1:B:212:ARG:HD3	1.73	0.71
1:A:264:SER:HG	1:B:163:PHE:HZ	1.43	0.66
1:A:268:LYS:HD2	1:B:163:PHE:CE1	2.34	0.63
1:B:266:ILE:HD11	1:B:273:PHE:HB2	1.82	0.61
1:B:230:LEU:O	1:B:269:ARG:NH1	2.36	0.59
1:B:136:THR:HG22	1:B:142:MET:HB2	1.85	0.58
1:A:180:CYS:HB2	3:A:312:HOH:O	2.02	0.58
1:B:127:ARG:HB3	1:B:212:ARG:HE	1.70	0.57
1:A:165:THR:HG22	1:A:167:LYS:H	1.68	0.57
1:B:94:ILE:O	1:B:95:SER:HB2	2.06	0.55
1:A:183:ASN:ND2	1:A:186:SER:H	2.05	0.55
1:B:86:TRP:NE1	1:B:90:LYS:HE2	2.23	0.54
1:B:238:LEU:HB3	1:B:266:ILE:HD13	1.90	0.54
1:B:221:THR:HG21	2:B:301:NGD:H6	1.90	0.53
1:B:50:TRP:CZ2	1:B:98:PRO:HG2	2.44	0.53
1:B:138:VAL:HG11	1:B:288:VAL:HG12	1.91	0.52
1:B:191:THR:O	1:B:195:ARG:HG3	2.11	0.51
1:A:115:GLN:NE2	1:A:149:LEU:H	1.99	0.49
1:B:98:PRO:O	1:B:183:ASN:HA	2.13	0.49
1:A:69:LYS:HD3	3:A:353:HOH:O	2.13	0.49
1:B:145:LEU:HD21	1:B:192:VAL:HG23	1.95	0.49
1:B:284:PHE:O	1:B:288:VAL:HG23	2.12	0.48
1:A:264:SER:OG	1:B:163:PHE:HZ	1.95	0.48
1:A:292:GLU:O	1:A:294:SER:N	2.45	0.48

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ASN:ND2	1:B:186:SER:H	2.12	0.48
1:B:104:GLU:HA	1:B:107:GLN:HG2	1.95	0.48
1:A:103:GLU:OE1	1:A:194:ARG:NH1	2.47	0.47
1:B:266:ILE:HD11	1:B:273:PHE:CB	2.44	0.47
1:B:134:GLN:O	1:B:138:VAL:HG23	2.15	0.46
1:B:165:THR:HG22	1:B:167:LYS:N	2.15	0.46
1:A:94:ILE:O	1:A:95:SER:HB2	2.16	0.46
1:A:290:ASN:HB3	3:A:382:HOH:O	2.16	0.45
1:A:294:SER:O	1:A:296:CYS:N	2.49	0.45
1:B:103:GLU:OE1	1:B:194:ARG:NH1	2.50	0.44
1:B:249:ASP:O	1:B:250:SER:HB2	2.18	0.44
1:B:180:CYS:HB2	3:B:320:HOH:O	2.17	0.43
1:B:249:ASP:HB3	1:B:250:SER:H	1.54	0.43
2:B:301:NGD:H2	2:B:301:NGD:HC2'	1.86	0.42
1:A:282:ASP:OD1	1:A:282:ASP:N	2.53	0.42
1:B:90:LYS:HG2	1:B:94:ILE:CG1	2.47	0.42
1:A:244:HIS:HD2	1:A:250:SER:HB3	1.86	0.41
1:A:221:THR:HG21	2:A:301:NGD:H6	2.02	0.41
1:B:138:VAL:CG1	1:B:288:VAL:HG12	2.50	0.41
1:B:282:ASP:OD1	1:B:282:ASP:N	2.54	0.41
1:A:207:MET:HG2	1:A:243:ILE:HD11	2.02	0.41
1:A:45:ARG:HD3	1:A:47:ARG:O	2.20	0.40
1:A:104:GLU:HA	1:A:107:GLN:HG2	2.04	0.40
1:B:289:LYS:HB2	1:B:289:LYS:HE3	1.76	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%)	237 (95%)	9 (4%)	4 (2%)	<b>9</b> <b>4</b>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	250/262 (95%)	235 (94%)	11 (4%)	4 (2%)	9	4
All	All	500/524 (95%)	472 (94%)	20 (4%)	8 (2%)	9	4

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	ASP
1	A	295	SER
1	A	249	ASP
1	B	250	SER
1	B	292	GLU
1	B	293	ASP
1	B	294	SER
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%)	227 (97%)	6 (3%)	46	49
1	B	233/241 (97%)	223 (96%)	10 (4%)	29	28
All	All	466/482 (97%)	450 (97%)	16 (3%)	37	38

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	58	ARG
1	A	89	PHE
1	A	131	LEU
1	A	140	ARG
1	A	251	ARG
1	B	45	ARG
1	B	89	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	131	LEU
1	B	139	GLN
1	B	140	ARG
1	B	177	ARG
1	B	218	LYS
1	B	251	ARG
1	B	270	ASN
1	B	280	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	115	GLN
1	A	134	GLN
1	A	182	ASN
1	A	183	ASN
1	A	244	HIS
1	A	286	GLN
1	B	115	GLN
1	B	183	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	NGD	A	301	-	42,49,49	1.32	5 (11%)	51,75,75	1.66	9 (17%)
2	NGD	B	301	-	42,49,49	1.24	5 (11%)	51,75,75	1.68	11 (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	NGD	A	301	-	-	8/26/62/62	0/5/5/5
2	NGD	B	301	-	-	9/26/62/62	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	NGD	C5A-C6A	-4.07	1.39	1.47
2	A	301	NGD	O7-C7	4.05	1.31	1.24
2	B	301	NGD	O7-C7	3.84	1.31	1.24
2	A	301	NGD	C5A-C6A	-3.70	1.39	1.47
2	A	301	NGD	C7-N7	-3.12	1.27	1.33
2	B	301	NGD	C7-N7	-2.91	1.27	1.33
2	A	301	NGD	O4'-C1'	2.35	1.44	1.41
2	A	301	NGD	O4'R-C1'R	2.15	1.44	1.41
2	B	301	NGD	O4'-C1'	2.10	1.44	1.41
2	B	301	NGD	O4'R-C1'R	2.10	1.44	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NGD	C3-C7-N7	5.14	123.92	117.75
2	A	301	NGD	C3-C7-N7	4.92	123.65	117.75
2	B	301	NGD	C3'R-C2'R-C1'R	4.05	107.07	100.98
2	A	301	NGD	C3'R-C2'R-C1'R	3.15	105.72	100.98

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NGD	C5A-C6A-N1A	2.99	119.23	113.95
2	B	301	NGD	PB-O3-PA	-2.96	122.66	132.83
2	A	301	NGD	O4'-C1'-C2'	-2.94	102.63	106.93
2	A	301	NGD	C5A-C6A-N1A	2.78	118.87	113.95
2	A	301	NGD	C8A-N7A-C5A	2.72	108.17	102.99
2	A	301	NGD	O5'-C5'-C4'	2.58	117.89	108.99
2	A	301	NGD	O4'-C4'-C5'	2.53	117.69	109.37
2	A	301	NGD	O7-C7-N7	-2.52	118.99	122.58
2	B	301	NGD	O4'R-C1'R-C2'R	-2.46	103.34	106.93
2	B	301	NGD	C6-N1-C2	-2.43	119.76	121.97
2	B	301	NGD	O7-C7-C3	-2.42	116.73	119.63
2	A	301	NGD	PB-O3-PA	-2.42	124.53	132.83
2	B	301	NGD	O3'-C3'-C4'	-2.38	104.17	111.05
2	B	301	NGD	O7-C7-N7	-2.28	119.33	122.58
2	B	301	NGD	O6A-C6A-C5A	-2.24	120.00	124.37
2	B	301	NGD	C8A-N7A-C5A	2.16	107.11	102.99

There are no chirality outliers.

All (17) torsion outliers are listed below:

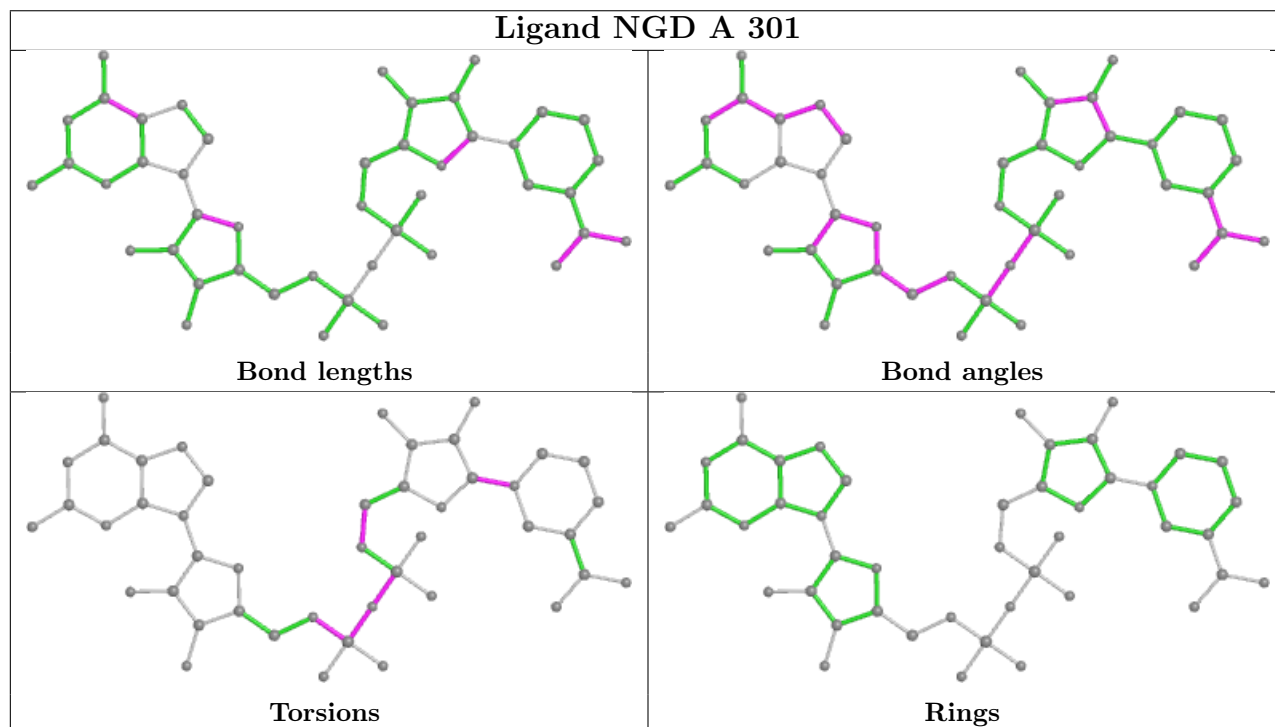
Mol	Chain	Res	Type	Atoms
2	A	301	NGD	C5'-O5'-PA-O1A
2	A	301	NGD	C5'-O5'-PA-O2A
2	A	301	NGD	PB-O3-PA-O5'
2	A	301	NGD	C2'R-C1'R-N1-C6
2	A	301	NGD	C2'R-C1'R-N1-C2
2	B	301	NGD	C5'-O5'-PA-O1A
2	B	301	NGD	PB-O3-PA-O5'
2	B	301	NGD	C2'R-C1'R-N1-C6
2	B	301	NGD	C2'R-C1'R-N1-C2
2	B	301	NGD	C5'-O5'-PA-O3
2	B	301	NGD	PA-O3-PB-O1B
2	B	301	NGD	C5'-O5'-PA-O2A
2	A	301	NGD	C4'R-C5'R-O5'R-PB
2	A	301	NGD	C5'-O5'-PA-O3
2	B	301	NGD	C4'R-C5'R-O5'R-PB
2	A	301	NGD	PA-O3-PB-O2B
2	B	301	NGD	PA-O3-PB-O2B

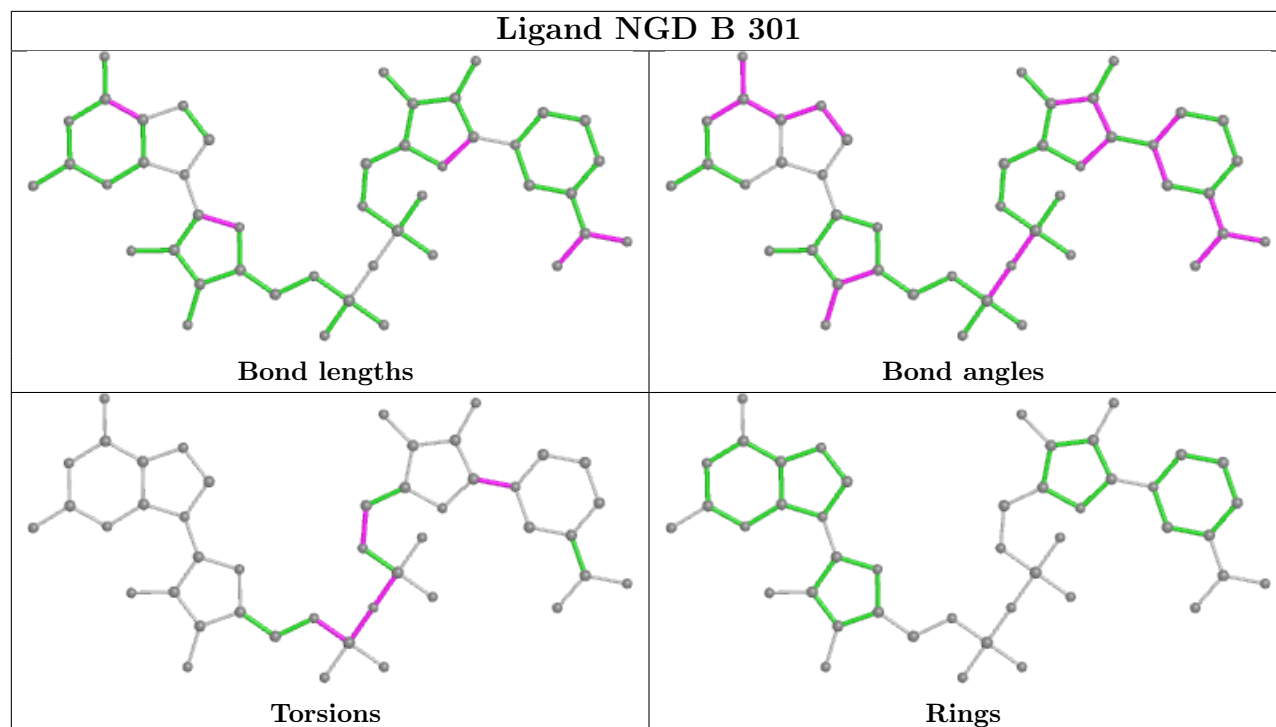
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NGD	1	0
2	B	301	NGD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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%)	1.25	51 (20%) <b>1</b> <b>1</b>	35, 40, 46, 50	0
1	B	252/262 (96%)	1.43	62 (24%) <b>0</b> <b>0</b>	35, 40, 45, 51	0
All	All	504/524 (96%)	1.34	113 (22%) <b>0</b> <b>0</b>	35, 40, 46, 51	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	ASP	13.3
1	A	293	ASP	12.2
1	B	294	SER	11.9
1	B	247	ARG	8.8
1	B	208	LEU	6.9
1	B	292	GLU	6.5
1	B	293	ASP	5.9
1	B	295	SER	5.9
1	A	294	SER	5.8
1	A	247	ARG	5.8
1	B	139	GLN	5.6
1	A	124	LEU	5.4
1	A	248	GLU	5.1
1	B	138	VAL	5.0
1	B	296	CYS	5.0
1	A	246	GLY	4.9
1	B	213	SER	4.7
1	A	208	LEU	4.6
1	A	46	TRP	4.6
1	B	124	LEU	4.6
1	B	246	GLY	4.4
1	B	123	LEU	4.3
1	A	292	GLU	4.3
1	B	206	VAL	4.2

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	248	GLU	4.2
1	A	49	THR	4.2
1	B	249	ASP	4.1
1	A	123	LEU	4.1
1	B	140	ARG	4.0
1	B	222	PHE	3.9
1	B	290	ASN	3.9
1	A	206	VAL	3.9
1	A	79	HIS	3.8
1	B	245	GLY	3.8
1	A	295	SER	3.7
1	A	138	VAL	3.7
1	A	48	GLN	3.6
1	B	116	THR	3.6
1	B	250	SER	3.5
1	A	165	THR	3.5
1	A	150	LEU	3.5
1	B	159	TRP	3.5
1	A	109	LEU	3.4
1	B	268	LYS	3.2
1	B	118	PRO	3.1
1	B	291	PRO	3.1
1	A	47	ARG	3.0
1	A	241	TRP	3.0
1	B	236	GLN	3.0
1	B	282	ASP	2.9
1	A	242	VAL	2.9
1	A	222	PHE	2.9
1	A	168	ILE	2.8
1	A	164	ASP	2.8
1	A	93	PHE	2.8
1	A	139	GLN	2.8
1	A	85	VAL	2.8
1	B	89	PHE	2.8
1	A	290	ASN	2.7
1	B	270	ASN	2.7
1	A	89	PHE	2.7
1	B	279	TYR	2.7
1	B	177	ARG	2.7
1	B	197	ALA	2.7
1	A	204	VAL	2.6
1	B	127	ARG	2.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	149	LEU	2.6
1	B	252	ASP	2.5
1	B	211	SER	2.5
1	A	245	GLY	2.5
1	B	207	MET	2.5
1	A	125	TRP	2.5
1	A	291	PRO	2.5
1	A	207	MET	2.4
1	A	184	PRO	2.4
1	A	212	ARG	2.4
1	B	160	CYS	2.4
1	B	117	VAL	2.4
1	B	55	THR	2.4
1	B	212	ARG	2.4
1	B	109	LEU	2.4
1	B	149	LEU	2.4
1	B	264	SER	2.4
1	B	165	THR	2.3
1	A	63	VAL	2.3
1	A	230	LEU	2.3
1	B	98	PRO	2.3
1	B	141	ASP	2.3
1	B	161	GLY	2.3
1	B	137	GLN	2.3
1	A	161	GLY	2.3
1	B	244	HIS	2.2
1	B	153	LEU	2.2
1	A	45	ARG	2.2
1	B	93	PHE	2.2
1	A	243	ILE	2.2
1	A	59	PHE	2.2
1	B	104	GLU	2.2
1	A	80	VAL	2.2
1	A	83	GLN	2.1
1	B	241	TRP	2.1
1	B	254	CYS	2.1
1	B	257	PRO	2.1
1	A	278	ILE	2.1
1	B	262	LEU	2.1
1	B	125	TRP	2.1
1	B	193	SER	2.1
1	B	158	THR	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	106	TYR	2.1
1	A	238	LEU	2.0
1	A	235	VAL	2.0
1	A	250	SER	2.0
1	B	286	GLN	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

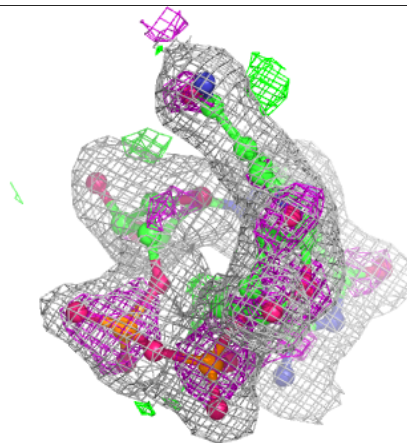
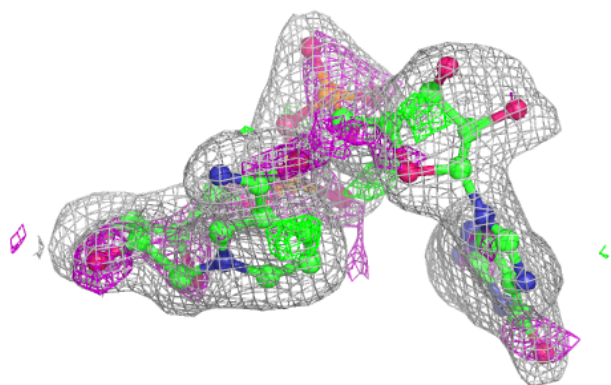
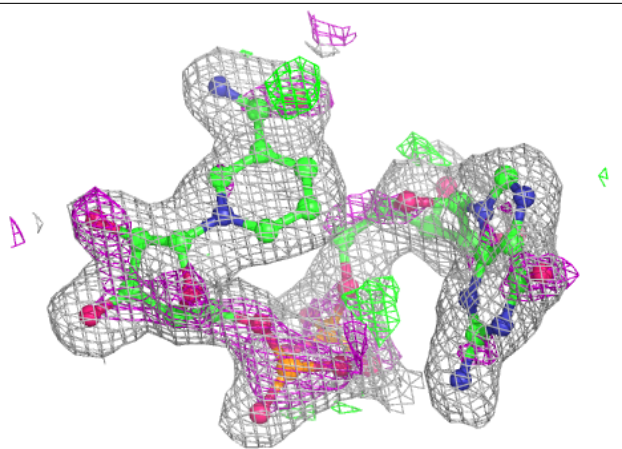
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

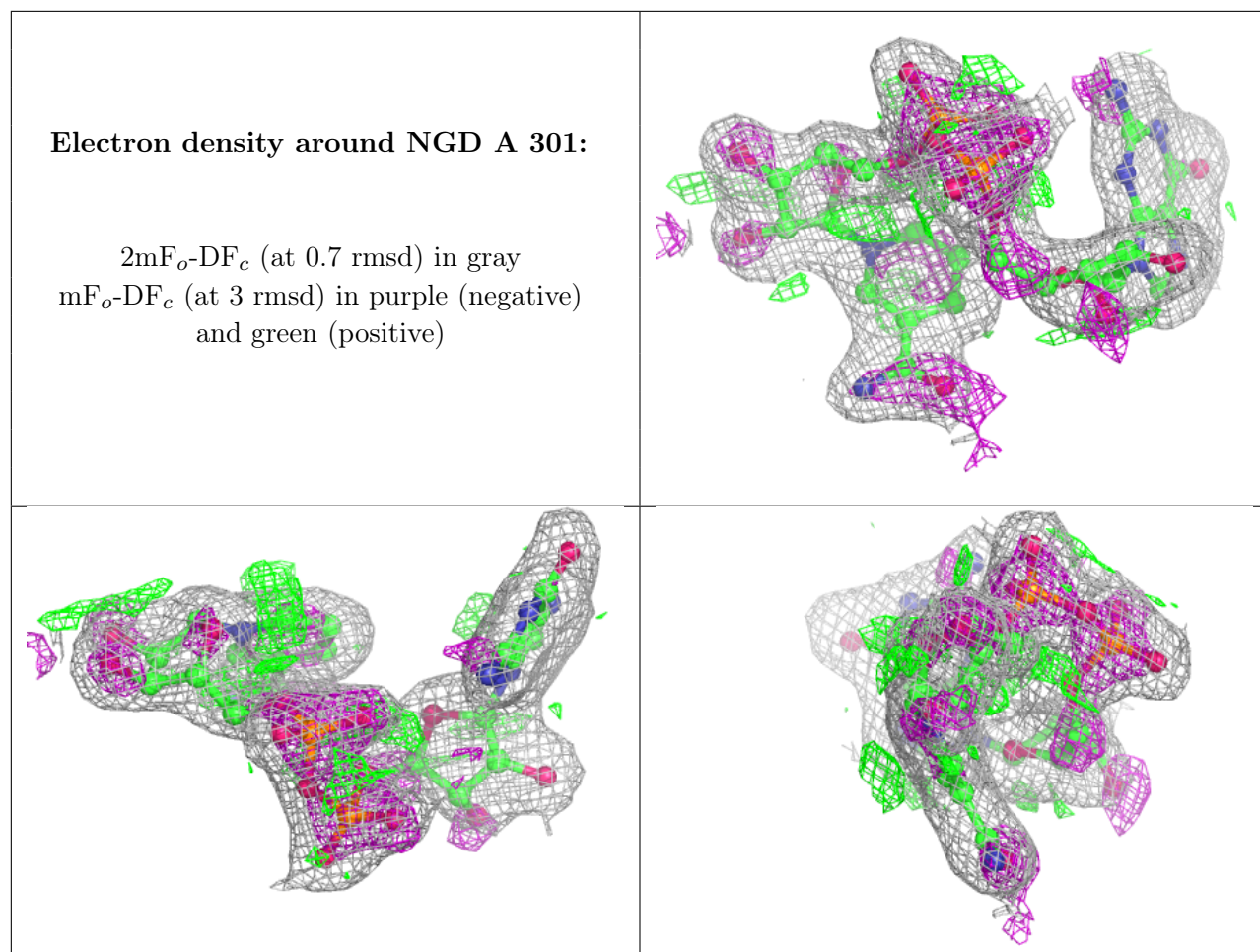
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NGD	B	301	45/45	0.93	0.20	32,40,50,53	0
2	NGD	A	301	45/45	0.94	0.17	26,34,49,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around NGD B 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.