



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 09:21 PM UTC

PDB ID : 4CZM / pdb_00004czm
Title : C. crescentus MreB, monomeric, AMPPNP
Authors : Lowe, J.; van den Ent, F.
Deposited on : 2014-04-19
Resolution : 2.20 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

<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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

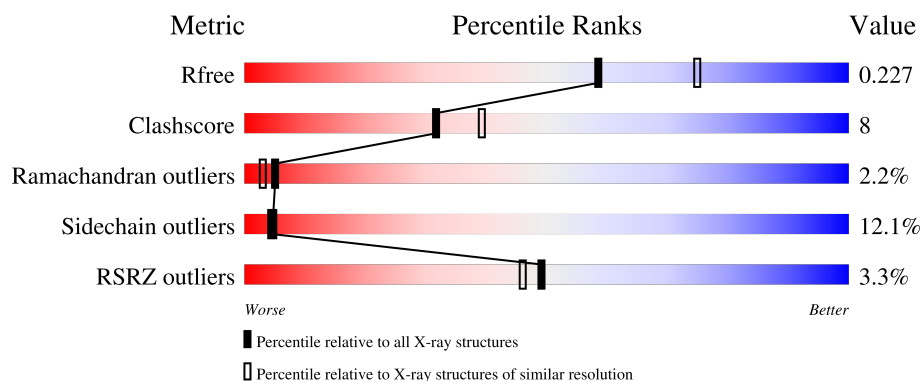
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

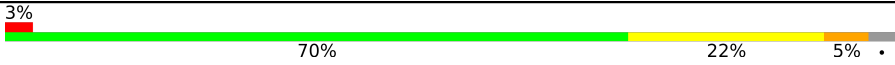
The reported resolution of this entry is 2.20 Å.

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 ≥ 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	348	 3% 70% 22% 5% .
1	B	348	 4% 67% 25% . . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10221 atoms, of which 5156 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 ROD SHAPE-DETERMINING PROTEIN MREB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	336	Total	C	H	N	O	S	0	0	0
			5045	1542	2566	451	471	15			
1	B	336	Total	C	H	N	O	S	0	0	0
			5045	1542	2566	451	471	15			

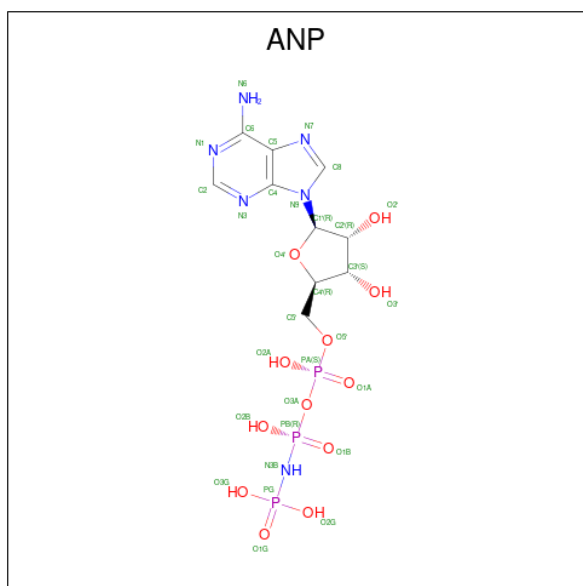
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	expression tag	UNP B8H609
A	348	GLY	-	expression tag	UNP B8H609
A	349	SER	-	expression tag	UNP B8H609
A	350	HIS	-	expression tag	UNP B8H609
A	351	HIS	-	expression tag	UNP B8H609
A	352	HIS	-	expression tag	UNP B8H609
A	353	HIS	-	expression tag	UNP B8H609
A	354	HIS	-	expression tag	UNP B8H609
A	355	HIS	-	expression tag	UNP B8H609
A	102	SER	PHE	engineered mutation	UNP B8H609
A	103	GLY	VAL	engineered mutation	UNP B8H609
A	283	ASP	SER	engineered mutation	UNP B8H609
B	8	MET	-	expression tag	UNP B8H609
B	348	GLY	-	expression tag	UNP B8H609
B	349	SER	-	expression tag	UNP B8H609
B	350	HIS	-	expression tag	UNP B8H609
B	351	HIS	-	expression tag	UNP B8H609
B	352	HIS	-	expression tag	UNP B8H609
B	353	HIS	-	expression tag	UNP B8H609
B	354	HIS	-	expression tag	UNP B8H609
B	355	HIS	-	expression tag	UNP B8H609
B	102	SER	PHE	engineered mutation	UNP B8H609
B	103	GLY	VAL	engineered mutation	UNP B8H609
B	283	ASP	SER	engineered mutation	UNP B8H609

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			43	10	12	6	12	3		
3	B	1	Total	C	H	N	O	P	0	0
			43	10	12	6	12	3		

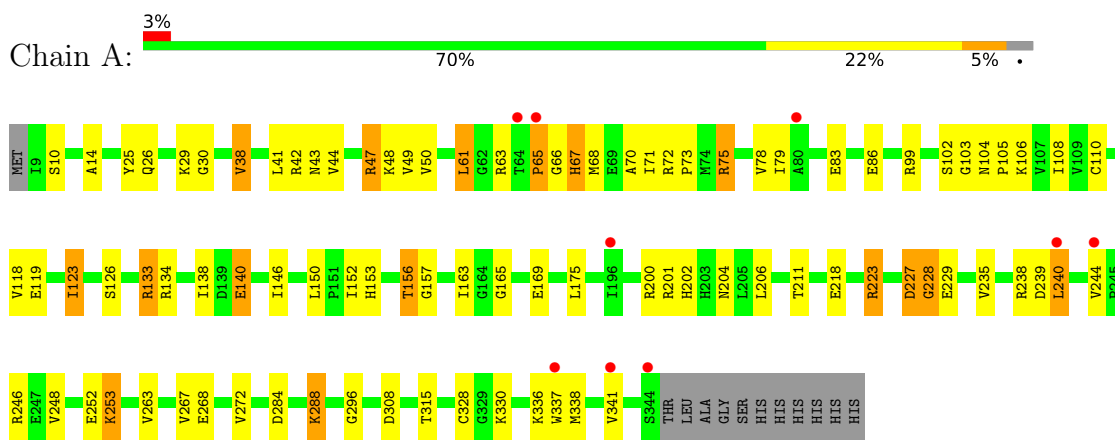
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total	O	0	0
			27	27		
4	B	16	Total	O	0	0
			16	16		

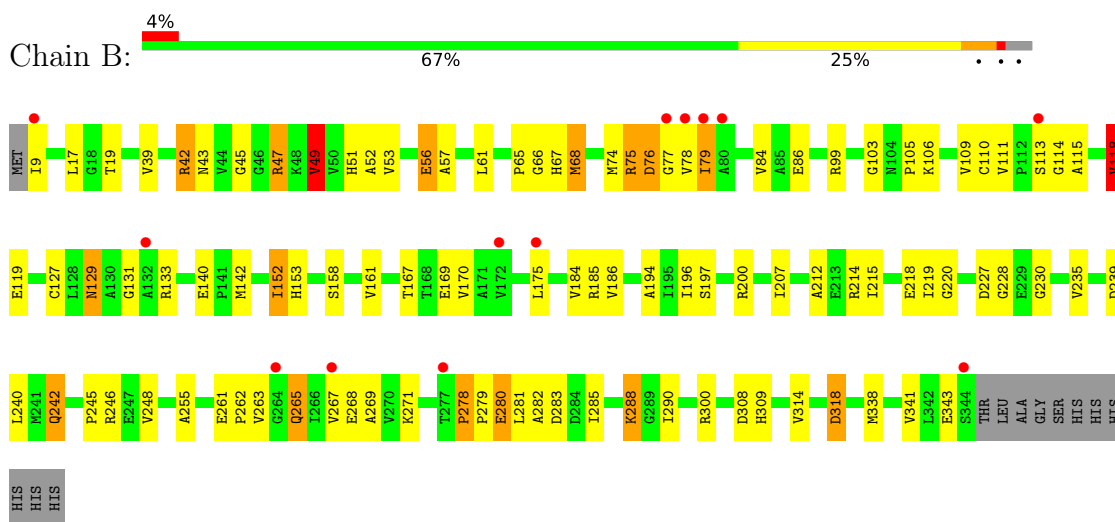
3 Residue-property plots

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: ROD SHAPE-DETERMINING PROTEIN MREB



• Molecule 1: ROD SHAPE-DETERMINING PROTEIN MREB



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	67.79Å 67.79Å 320.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.14 – 2.20 41.14 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (41.14-2.20) 99.9 (41.14-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.209 , 0.277 0.227 , 0.227	Depositor DCC
R_{free} test set	1973 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	61.9	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10221	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.10	4/2510 (0.2%)	1.18	10/3392 (0.3%)
1	B	1.17	4/2510 (0.2%)	1.24	12/3392 (0.4%)
All	All	1.14	8/5020 (0.2%)	1.21	22/6784 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	278	PRO	CA-C	9.71	1.57	1.51
1	A	267	VAL	CA-CB	-5.51	1.48	1.54
1	A	263	VAL	CA-CB	-5.50	1.48	1.54
1	B	212	ALA	CA-C	5.29	1.59	1.52
1	A	146	ILE	C-O	-5.22	1.18	1.24
1	B	263	VAL	CA-CB	-5.17	1.48	1.54
1	B	194	ALA	CA-CB	-5.15	1.45	1.53
1	A	140	GLU	C-O	-5.02	1.19	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	VAL	CB-CA-C	-8.57	97.62	110.82
1	B	318	ASP	N-CA-C	8.20	120.00	111.14
1	B	278	PRO	N-CA-C	7.43	117.60	110.47
1	A	140	GLU	CA-C-N	-6.62	111.63	118.85
1	A	140	GLU	C-N-CA	-6.62	111.63	118.85
1	B	111	VAL	CA-C-N	-6.49	113.26	120.14
1	B	111	VAL	C-N-CA	-6.49	113.26	120.14
1	B	341	VAL	N-CA-C	-6.00	106.41	113.42
1	B	78	VAL	N-CA-C	5.91	117.68	109.29
1	A	146	ILE	N-CA-C	-5.87	105.02	110.53
1	A	105	PRO	N-CA-C	5.81	119.78	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	GLY	N-CA-C	-5.74	103.78	112.84
1	B	133	ARG	N-CA-C	-5.60	106.49	113.55
1	A	123	ILE	CB-CA-C	-5.48	104.84	112.02
1	B	194	ALA	N-CA-C	-5.36	105.44	111.28
1	A	211	THR	N-CA-C	-5.28	105.52	111.28
1	B	118	VAL	N-CA-C	-5.24	105.39	110.42
1	A	202	HIS	N-CA-C	5.21	117.75	111.40
1	A	118	VAL	CB-CA-C	-5.20	105.32	111.97
1	A	150	LEU	N-CA-C	5.18	115.56	109.60
1	B	131	GLY	CA-C-O	5.16	123.62	118.77
1	B	49	VAL	N-CA-C	5.09	115.37	107.78

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	2479	2566	2558	43	1
1	B	2479	2566	2558	42	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	12	13	1	0
3	B	31	12	13	0	0
4	A	27	0	0	1	0
4	B	16	0	0	1	0
All	All	5065	5156	5142	82	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ARG:NH1	1:B:119:GLU:OE2	2.03	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:HIS:ND1	4:A:2010:HOH:O	2.27	0.68
1:A:65:PRO:O	1:A:67:HIS:N	2.34	0.60
1:A:239:ASP:OD1	1:A:246:ARG:NH2	2.34	0.60
1:B:227:ASP:OD1	1:B:228:GLY:N	2.36	0.58
1:B:269:ALA:O	4:B:2012:HOH:O	2.17	0.58
1:B:219:ILE:HD13	1:B:255:ALA:HB2	1.85	0.57
1:B:86:GLU:OE1	1:B:129:ASN:ND2	2.38	0.56
1:A:201:ARG:NH2	1:B:114:GLY:O	2.35	0.56
1:B:184:VAL:HG12	1:B:186:VAL:HG12	1.88	0.56
1:B:52:ALA:HB1	1:B:56:GLU:HG2	1.87	0.55
1:B:110:CYS:SG	1:B:140:GLU:HG2	2.45	0.55
1:B:113:SER:C	1:B:115:ALA:H	2.14	0.55
1:A:119:GLU:O	1:A:123:ILE:HG12	2.06	0.55
1:A:43:ASN:HB3	1:A:48:LYS:HD3	1.92	0.52
1:A:200:ARG:HG3	1:A:240:LEU:CD1	2.40	0.52
1:A:108:ILE:HG13	1:A:338:MET:HE3	1.93	0.50
1:A:14:ALA:HB1	1:A:328:CYS:HB3	1.93	0.50
1:A:104:ASN:O	1:A:133:ARG:CZ	2.59	0.50
1:A:47:ARG:HH11	1:A:47:ARG:HG3	1.76	0.49
1:A:163:ILE:HG22	1:A:296:GLY:HA3	1.94	0.49
1:B:19:THR:HA	1:B:74:MET:HB2	1.95	0.49
1:B:215:ILE:HG23	1:B:219:ILE:HD11	1.96	0.48
1:A:104:ASN:O	1:A:133:ARG:HG2	2.13	0.48
1:B:109:VAL:HG21	1:B:127:CYS:SG	2.54	0.48
1:B:308:ASP:OD1	1:B:308:ASP:N	2.44	0.48
1:B:281:LEU:O	1:B:285:ILE:N	2.41	0.47
1:A:47:ARG:HH11	1:A:47:ARG:CG	2.27	0.47
1:B:279:PRO:O	1:B:283:ASP:N	2.42	0.47
1:A:223:ARG:NH2	1:A:308:ASP:OD2	2.48	0.47
1:A:79:ILE:HD12	1:A:79:ILE:N	2.30	0.47
1:B:262:PRO:HA	1:B:265:GLN:HG3	1.97	0.47
1:A:204:ASN:OD1	1:A:240:LEU:HB3	2.16	0.46
1:A:41:LEU:HD23	1:A:50:VAL:HA	1.96	0.46
1:B:75:ARG:O	1:B:77:GLY:N	2.49	0.46
1:A:61:LEU:HD12	1:A:70:ALA:HB2	1.98	0.46
1:B:279:PRO:HA	1:B:282:ALA:HB3	1.98	0.45
1:A:133:ARG:HD2	1:A:134:ARG:HH21	1.80	0.45
1:A:103:GLY:O	1:A:104:ASN:C	2.58	0.45
1:A:204:ASN:HB2	1:B:118:VAL:CG1	2.47	0.45
1:B:42:ARG:HD2	1:B:51:HIS:CE1	2.52	0.45
1:A:110:CYS:SG	1:A:140:GLU:HG2	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ASP:CG	1:A:228:GLY:N	2.72	0.45
1:A:26:GLN:HB3	1:A:29:LYS:HB2	1.99	0.44
1:B:220:GLY:O	1:B:300:ARG:HD2	2.17	0.44
1:A:25:TYR:CE2	1:A:30:GLY:HA2	2.53	0.44
1:B:39:VAL:HG11	1:B:84:VAL:CG1	2.48	0.44
1:A:106:LYS:HB3	1:A:338:MET:HE1	1.99	0.44
1:B:39:VAL:HG11	1:B:84:VAL:HG11	2.00	0.44
1:B:158:SER:OG	1:B:288:LYS:NZ	2.50	0.43
1:B:278:PRO:HB2	1:B:280:GLU:HG3	2.00	0.43
1:B:219:ILE:CD1	1:B:255:ALA:HB2	2.46	0.43
1:A:268:GLU:O	1:A:272:VAL:HG23	2.17	0.43
1:B:142:MET:SD	1:B:152:ILE:HD13	2.58	0.43
1:B:290:ILE:HD12	1:B:314:VAL:HG22	2.00	0.43
1:A:104:ASN:O	1:A:133:ARG:NE	2.53	0.42
1:A:157:GLY:O	1:A:288:LYS:NZ	2.52	0.42
1:B:39:VAL:HG23	1:B:53:VAL:HG22	1.99	0.42
1:B:75:ARG:O	1:B:76:ASP:C	2.61	0.42
1:B:239:ASP:OD1	1:B:246:ARG:NE	2.52	0.42
1:A:228:GLY:O	1:A:253:LYS:HG3	2.19	0.42
1:B:103:GLY:C	1:B:105:PRO:HD3	2.45	0.42
1:A:156:THR:HG23	1:A:284:ASP:HB3	2.01	0.42
1:B:267:VAL:CG1	1:B:309:HIS:HB2	2.49	0.42
1:A:163:ILE:CG2	1:A:296:GLY:HA3	2.49	0.42
1:B:110:CYS:SG	1:B:140:GLU:HA	2.60	0.41
1:A:71:ILE:O	1:A:73:PRO:HD3	2.20	0.41
1:B:79:ILE:HG12	1:B:79:ILE:O	2.20	0.41
1:B:153:HIS:HB3	1:B:338:MET:CE	2.51	0.41
1:B:47:ARG:NH2	1:B:49:VAL:HG11	2.35	0.41
1:A:41:LEU:HD13	1:A:48:LYS:HB3	2.03	0.41
1:A:75:ARG:HG2	1:A:75:ARG:HH11	1.86	0.41
1:A:229:GLU:HA	1:A:253:LYS:HB2	2.02	0.41
1:B:68:MET:HE3	1:B:68:MET:HA	2.02	0.41
1:A:108:ILE:HD11	1:A:338:MET:HG3	2.02	0.41
1:A:152:ILE:HD11	1:A:153:HIS:CE1	2.56	0.41
1:A:165:GLY:H	3:A:1346:ANP:HNB1	1.69	0.40
1:B:196:ILE:HA	1:B:207:ILE:HD11	2.02	0.40
1:A:86:GLU:HG2	1:A:126:SER:OG	2.21	0.40
1:B:161:VAL:HG13	1:B:170:VAL:HG22	2.03	0.40
1:A:75:ARG:HH11	1:A:75:ARG:CG	2.35	0.40
1:B:57:ALA:O	1:B:61:LEU:HD12	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLU:O	1:B:300:ARG:NH2[7_375]	2.05	0.15
1:A:42:ARG:NH1	1:A:252:GLU:OE2[6_485]	2.18	0.02
1:B:214:ARG:NH2	1:B:318:ASP:O[7_375]	2.19	0.01

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	334/348 (96%)	312 (93%)	17 (5%)	5 (2%)	8	6
1	B	334/348 (96%)	296 (89%)	28 (8%)	10 (3%)	3	1
All	All	668/696 (96%)	608 (91%)	45 (7%)	15 (2%)	5	3

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	GLY
1	A	227	ASP
1	B	65	PRO
1	B	76	ASP
1	A	65	PRO
1	A	102	SER
1	B	66	GLY
1	B	185	ARG
1	B	242	GLN
1	B	45	GLY
1	B	47	ARG
1	B	67	HIS
1	B	268	GLU
1	A	228	GLY
1	B	245	PRO

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	261/271 (96%)	227 (87%)	34 (13%)	4	3
1	B	261/271 (96%)	232 (89%)	29 (11%)	6	6
All	All	522/542 (96%)	459 (88%)	63 (12%)	5	4

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	38	VAL
1	A	44	VAL
1	A	47	ARG
1	A	49	VAL
1	A	61	LEU
1	A	63	ARG
1	A	67	HIS
1	A	68	MET
1	A	72	ARG
1	A	75	ARG
1	A	78	VAL
1	A	83	GLU
1	A	99	ARG
1	A	133	ARG
1	A	138	ILE
1	A	156	THR
1	A	169	GLU
1	A	175	LEU
1	A	206	LEU
1	A	218	GLU
1	A	223	ARG
1	A	235	VAL
1	A	238	ARG
1	A	240	LEU
1	A	244	VAL
1	A	248	VAL

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Mol	Chain	Res	Type
1	A	253	LYS
1	A	288	LYS
1	A	315	THR
1	A	330	LYS
1	A	336	LYS
1	A	337	TRP
1	A	341	VAL
1	B	9	ILE
1	B	17	LEU
1	B	42	ARG
1	B	43	ASN
1	B	49	VAL
1	B	56	GLU
1	B	68	MET
1	B	75	ARG
1	B	79	ILE
1	B	99	ARG
1	B	106	LYS
1	B	118	VAL
1	B	129	ASN
1	B	152	ILE
1	B	167	THR
1	B	169	GLU
1	B	175	LEU
1	B	197	SER
1	B	200	ARG
1	B	235	VAL
1	B	240	LEU
1	B	242	GLN
1	B	248	VAL
1	B	261	GLU
1	B	265	GLN
1	B	271	LYS
1	B	280	GLU
1	B	288	LYS
1	B	343	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	51	HIS

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Mol	Chain	Res	Type
1	A	97	HIS
1	A	124	ASN
1	A	203	HIS
1	A	254	GLN
1	A	334	HIS
1	B	51	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	ANP	B	1346	2	33,33,33	1.45	4 (12%)	45,52,52	1.55	7 (15%)
3	ANP	A	1346	2	33,33,33	0.87	2 (6%)	45,52,52	1.30	8 (17%)

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	ANP	B	1346	2	-	2/18/38/38	0/3/3/3
3	ANP	A	1346	2	-	2/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1346	ANP	PB-O3A	-6.08	1.51	1.59
3	B	1346	ANP	PA-O5'	-2.64	1.49	1.59
3	B	1346	ANP	PG-O3G	-2.31	1.50	1.56
3	B	1346	ANP	PB-O1B	2.30	1.49	1.46
3	A	1346	ANP	PB-N3B	2.24	1.69	1.63
3	A	1346	ANP	PG-N3B	2.09	1.68	1.63

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1346	ANP	O1B-PB-N3B	-5.90	103.08	111.77
3	B	1346	ANP	O2B-PB-O3A	3.82	117.38	104.64
3	A	1346	ANP	O1B-PB-N3B	-3.78	106.20	111.77
3	B	1346	ANP	O1G-PG-N3B	3.75	117.29	111.77
3	A	1346	ANP	O3G-PG-O1G	-2.98	105.98	113.45
3	A	1346	ANP	O2A-PA-O1A	2.96	126.20	112.44
3	A	1346	ANP	O2G-PG-O1G	-2.70	106.69	113.45
3	B	1346	ANP	O2G-PG-O1G	-2.46	107.28	113.45
3	B	1346	ANP	O3A-PA-O1A	2.38	117.85	110.70
3	B	1346	ANP	O5'-PA-O1A	-2.28	99.91	108.94
3	B	1346	ANP	O3'-C3'-C2'	-2.21	104.73	111.82
3	A	1346	ANP	O2B-PB-O1B	2.12	114.42	109.87
3	A	1346	ANP	O2B-PB-O3A	2.11	111.69	104.64
3	A	1346	ANP	O1G-PG-N3B	2.09	114.85	111.77
3	A	1346	ANP	O3A-PA-O1A	2.08	116.97	110.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

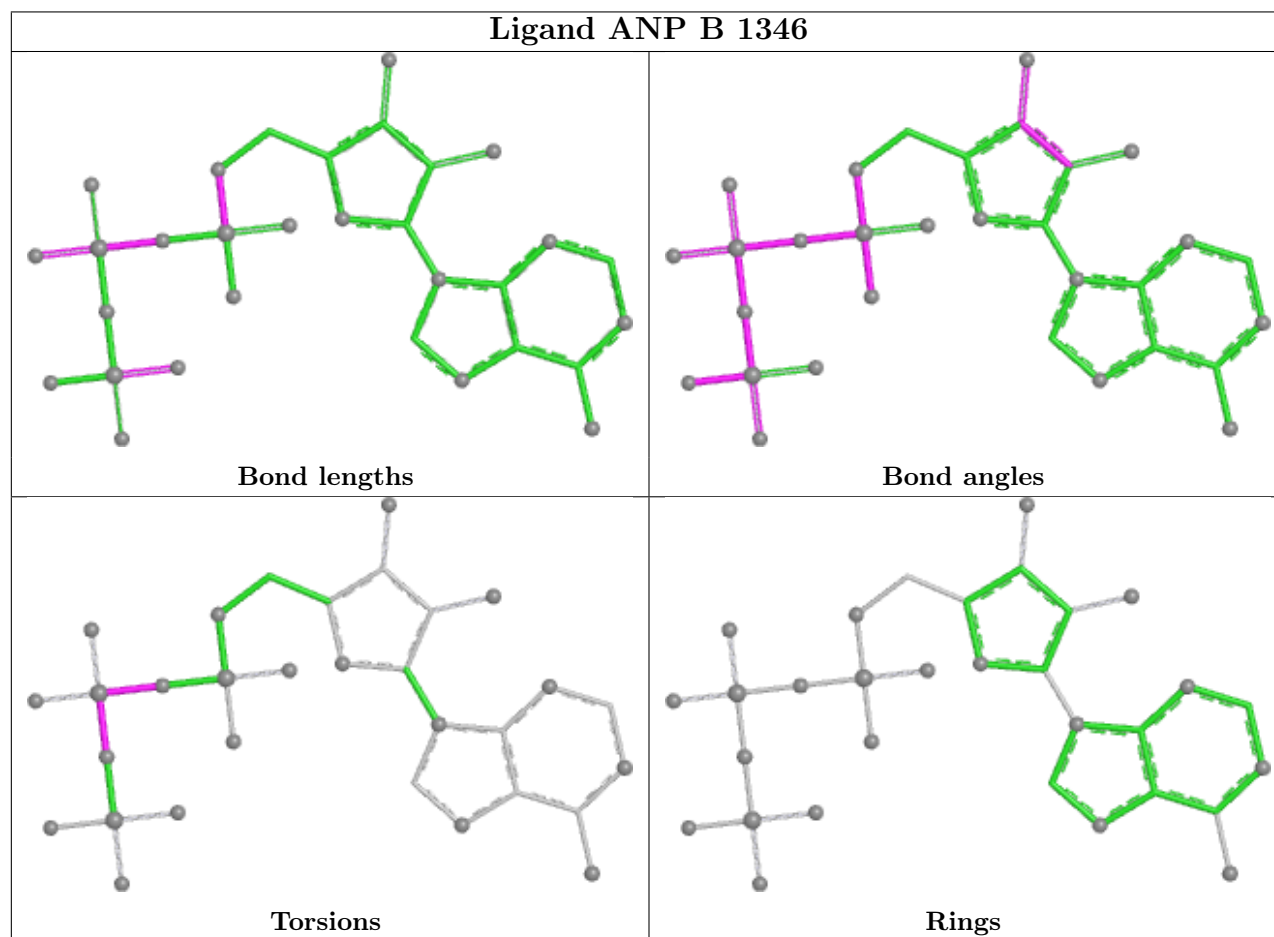
Mol	Chain	Res	Type	Atoms
3	A	1346	ANP	PB-N3B-PG-O1G
3	A	1346	ANP	PG-N3B-PB-O1B
3	B	1346	ANP	PG-N3B-PB-O1B
3	B	1346	ANP	PA-O3A-PB-O1B

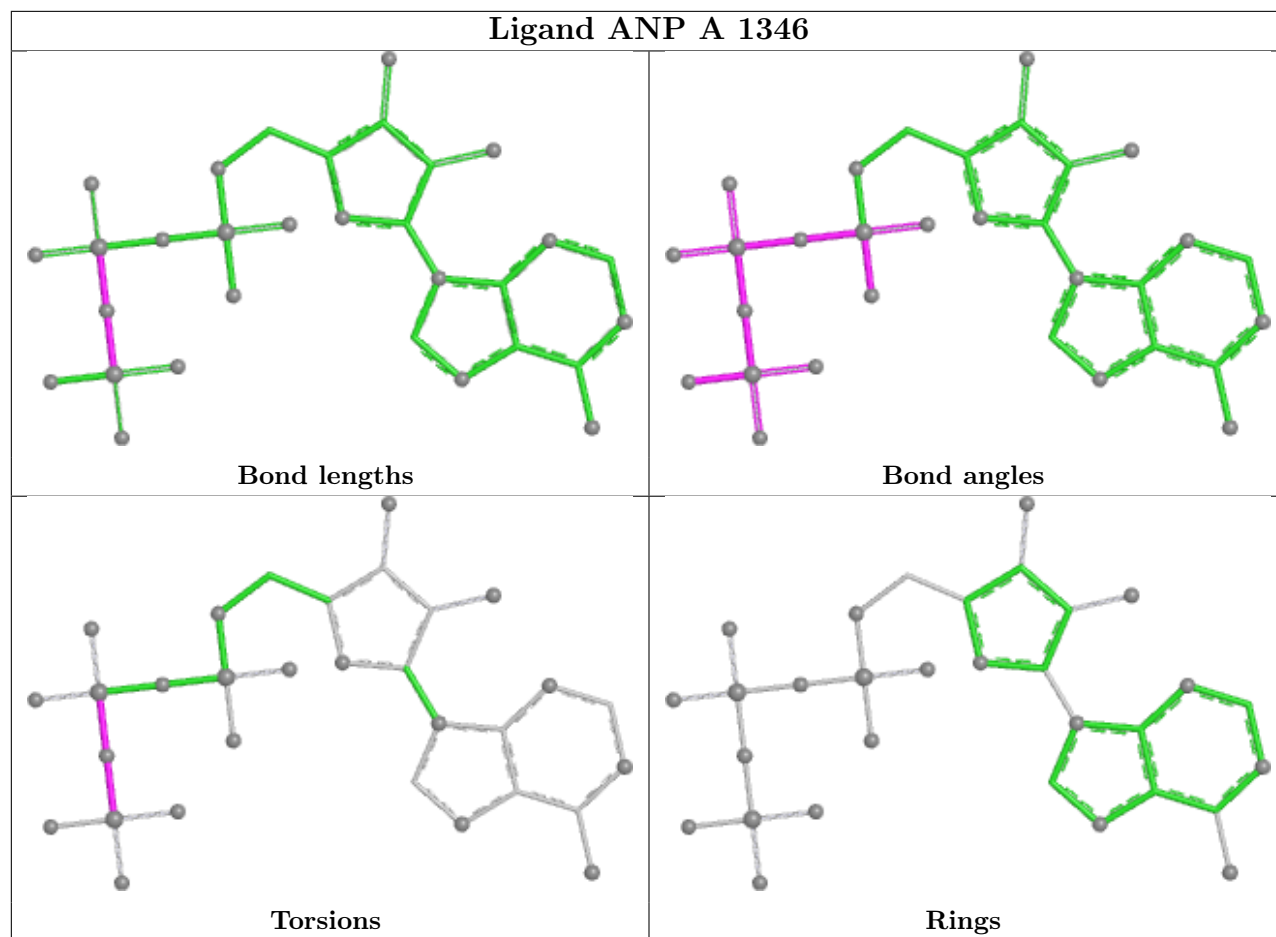
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1346	ANP	1	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, 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	336/348 (96%)	0.20	9 (2%) 56 53	49, 76, 124, 160	0
1	B	336/348 (96%)	0.45	13 (3%) 43 40	50, 83, 122, 166	0
All	All	672/696 (96%)	0.33	22 (3%) 49 46	49, 79, 124, 166	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	PRO	3.6
1	A	337	TRP	3.4
1	B	77	GLY	2.9
1	B	78	VAL	2.8
1	A	341	VAL	2.8
1	B	267	VAL	2.7
1	B	172	VAL	2.6
1	A	240	LEU	2.5
1	A	244	VAL	2.4
1	A	196	ILE	2.3
1	B	79	ILE	2.3
1	B	132	ALA	2.3
1	A	344	SER	2.3
1	B	264	GLY	2.2
1	B	277	THR	2.2
1	B	113	SER	2.2
1	B	344	SER	2.2
1	B	80	ALA	2.2
1	B	9	ILE	2.1
1	A	80	ALA	2.1
1	A	64	THR	2.1
1	B	175	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

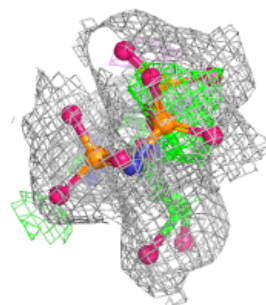
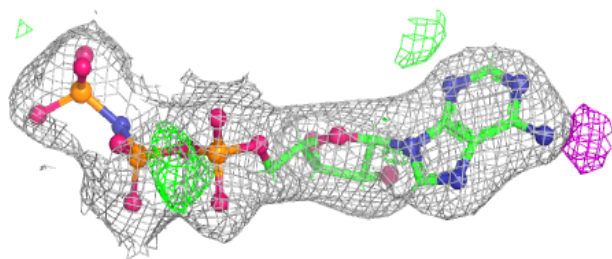
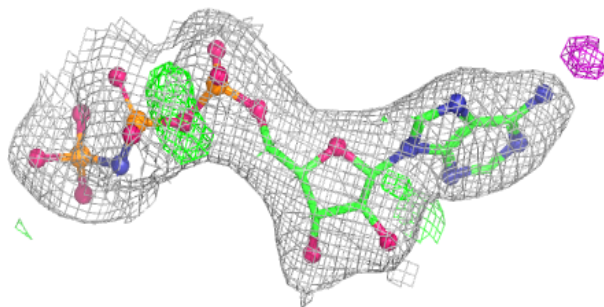
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ANP	A	1346	31/31	0.97	0.07	42,57,73,78	0
3	ANP	B	1346	31/31	0.97	0.07	40,50,59,71	0
2	MG	A	1345	1/1	0.99	0.03	49,49,49,49	0
2	MG	B	1345	1/1	0.99	0.02	46,46,46,46	0

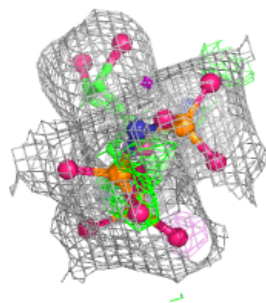
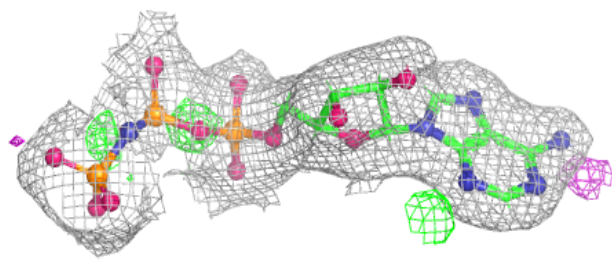
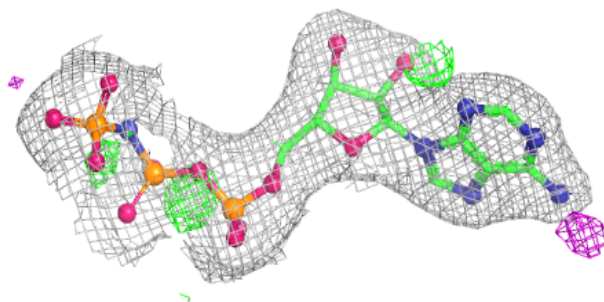
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 1346:

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

**Electron density around ANP B 1346:**

$2mF_o-DF_c$ (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.