



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:50 pm BST

PDB ID : 1ND2
Title : The structure of Rhinovirus 16
Authors : Zhang, Y.; Simpson, A.A.; Bator, C.M.; Chakravarty, S.; Pevear, D.C.;
Skochko, G.A.; Tull, T.M.; Diana, G.; Rossmann, M.G.
Deposited on : 2002-12-06
Resolution : 2.50 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 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

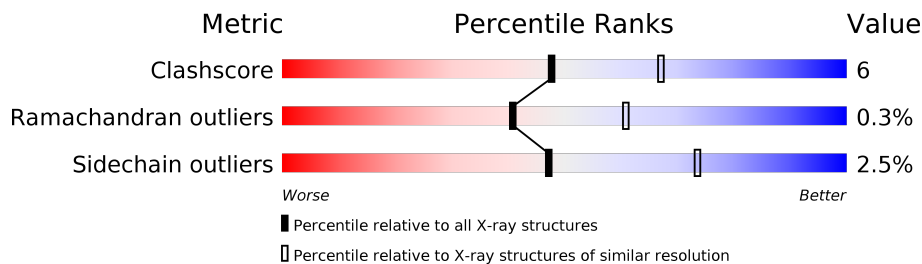
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	285	
2	B	261	
3	C	238	
4	D	68	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6858 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 coat protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	285	2287	1442	397	437	11	0	0	0

- Molecule 2 is a protein called coat protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	252	1977	1252	343	372	10	0	0	0

- Molecule 3 is a protein called coat protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	238	1845	1186	298	346	15	0	0	0

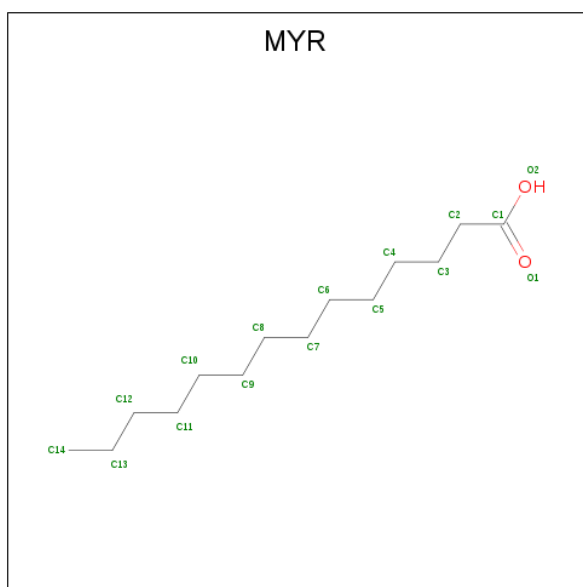
- Molecule 4 is a protein called coat protein VP4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	29	224	138	41	45	0	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
5	A	1	1	1	0	0

- Molecule 6 is MYRISTIC ACID (three-letter code: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 16 14 2	0	0
6	D	1	Total C O 15 14 1	0	0

- Molecule 7 is water.

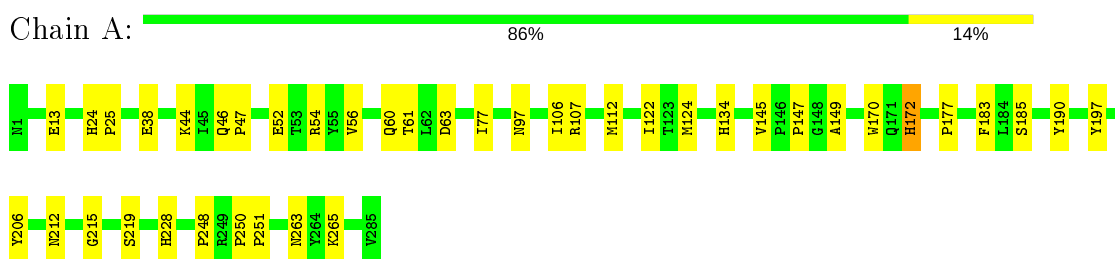
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	169	Total O 169 169	0	0
7	B	174	Total O 174 174	0	0
7	C	142	Total O 142 142	0	0
7	D	8	Total O 8 8	0	0

3 Residue-property plots [i](#)

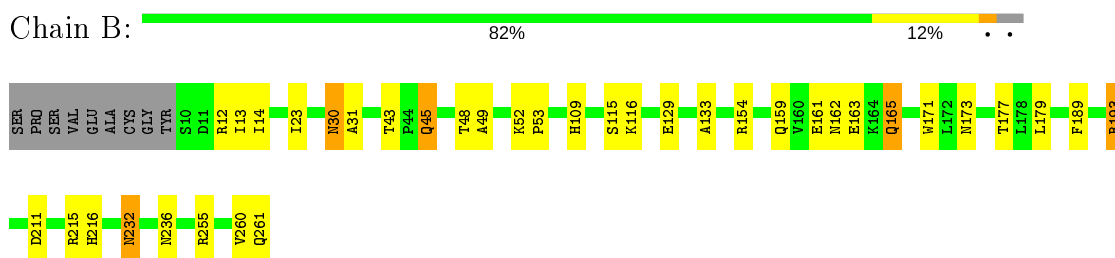
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

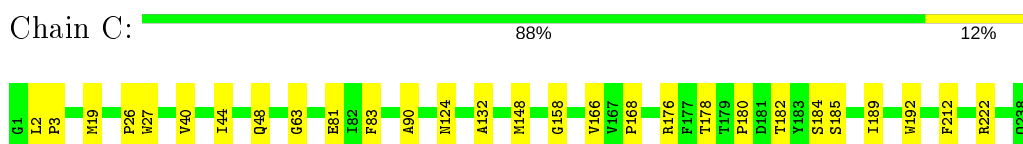
- Molecule 1: coat protein VP1



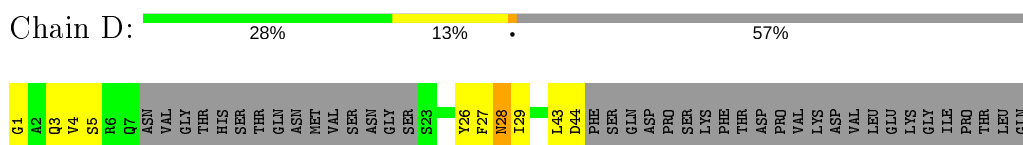
- Molecule 2: coat protein VP2



- Molecule 3: coat protein VP3



- Molecule 4: coat protein VP4



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	360.37Å 343.63Å 332.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.202 , 0.206	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6858	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

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: ZN, MYR

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	0.32	0/2349	0.59	0/3204
2	B	0.33	0/2029	0.64	0/2770
3	C	0.36	0/1897	0.64	0/2596
4	D	0.35	0/226	0.55	0/301
All	All	0.34	0/6501	0.62	0/8871

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 [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	2287	0	2201	29	0
2	B	1977	0	1920	28	0
3	C	1845	0	1826	17	0
4	D	224	0	211	9	0
5	A	1	0	0	0	0
6	A	16	0	27	4	0
6	D	15	0	27	2	0
7	A	169	0	0	1	0
7	B	174	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	142	0	0	2	0
7	D	8	0	0	0	0
All	All	6858	0	6212	77	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 6.

All (77) 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)
2:B:173:ASN:HD21	2:B:179:LEU:HA	1.42	0.84
1:A:122:ILE:HG12	6:A:6001:MYR:H112	1.59	0.84
1:A:124:MET:HB2	1:A:177:PRO:HG2	1.67	0.77
2:B:255:ARG:HG3	2:B:255:ARG:HH11	1.51	0.73
3:C:176:ARG:HG2	3:C:184:SER:HB2	1.71	0.72
1:A:122:ILE:CG1	6:A:6001:MYR:H112	2.20	0.71
2:B:260:VAL:O	2:B:261:GLN:HB2	1.91	0.71
1:A:24:HIS:HB3	1:A:25:PRO:HD2	1.82	0.61
4:D:1:GLY:O	4:D:29:ILE:HA	2.01	0.60
3:C:185:SER:HB2	7:C:5170:HOH:O	2.02	0.59
2:B:173:ASN:ND2	2:B:179:LEU:HA	2.18	0.57
1:A:38:GLU:HA	2:B:189:PHE:HB2	1.85	0.57
1:A:13:GLU:HA	1:A:61:THR:HG21	1.86	0.56
1:A:263:ASN:HA	2:B:133:ALA:HB1	1.87	0.55
3:C:2:LEU:HD12	3:C:3:PRO:HD2	1.88	0.55
1:A:170:TRP:CD1	1:A:177:PRO:HD3	2.42	0.54
4:D:4:VAL:HG22	4:D:27:PHE:CD1	2.43	0.54
2:B:255:ARG:HG3	2:B:255:ARG:NH1	2.22	0.54
2:B:211:ASP:OD2	2:B:216:HIS:HD2	1.91	0.53
2:B:12:ARG:HH11	2:B:12:ARG:HG3	1.74	0.53
1:A:112:MET:CE	1:A:251:PRO:HG3	2.40	0.52
1:A:60:GLN:H	1:A:60:GLN:CD	2.13	0.51
3:C:90:ALA:HB3	3:C:178:THR:O	2.10	0.51
2:B:193:ARG:HD3	7:B:5510:HOH:O	2.10	0.51
1:A:106:ILE:HG13	1:A:107:ARG:N	2.25	0.51
2:B:159:GLN:NE2	7:B:5313:HOH:O	2.42	0.50
4:D:43:LEU:O	4:D:44:ASP:HB3	2.12	0.50
1:A:250:PRO:HB2	2:B:177:THR:HB	1.93	0.50
1:A:46:GLN:HB3	1:A:47:PRO:HD2	1.94	0.50
1:A:145:VAL:HG13	1:A:149:ALA:HB3	1.94	0.49
2:B:215:ARG:NH1	7:B:5439:HOH:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ILE:HG22	1:A:106:ILE:CD1	2.43	0.49
2:B:129:GLU:OE1	2:B:216:HIS:HE1	1.95	0.48
3:C:19:MET:HE3	3:C:19:MET:HA	1.95	0.48
2:B:162:ASN:OD1	2:B:163:GLU:N	2.46	0.48
2:B:162:ASN:HB3	2:B:165:GLN:HE21	1.77	0.48
3:C:81:GLU:HB2	3:C:192:TRP:CZ3	2.49	0.48
2:B:171:TRP:CD2	3:C:63:GLY:HA2	2.48	0.48
4:D:43:LEU:O	4:D:44:ASP:CB	2.62	0.47
4:D:26:TYR:CE2	4:D:28:ASN:HB2	2.49	0.47
2:B:154:ARG:NE	2:B:159:GLN:HG3	2.30	0.47
3:C:26:PRO:O	3:C:27:TRP:HB2	2.14	0.47
2:B:171:TRP:CE2	3:C:63:GLY:HA2	2.49	0.47
1:A:112:MET:HE1	1:A:251:PRO:HG3	1.97	0.46
1:A:170:TRP:CH2	1:A:172:HIS:HA	2.51	0.46
2:B:232:ASN:N	2:B:232:ASN:HD22	2.13	0.46
3:C:83:PHE:C	3:C:83:PHE:CD1	2.88	0.46
7:A:5019:HOH:O	3:C:222:ARG:HG3	2.16	0.46
4:D:1:GLY:HA2	6:D:4000:MYR:O2	2.16	0.45
3:C:212:PHE:N	3:C:212:PHE:CD1	2.85	0.45
2:B:30:ASN:ND2	2:B:31:ALA:H	2.14	0.45
2:B:43:THR:OG1	2:B:45:GLN:HG2	2.17	0.44
3:C:44:ILE:O	3:C:48:GLN:HG3	2.17	0.44
1:A:248:PRO:HD3	3:C:40:VAL:CG2	2.47	0.44
4:D:1:GLY:N	6:D:4000:MYR:O2	2.48	0.44
1:A:54:ARG:HG3	1:A:56:VAL:HG23	2.00	0.43
1:A:183:PHE:CZ	1:A:185:SER:HB3	2.54	0.43
3:C:166:VAL:O	3:C:168:PRO:HD3	2.17	0.43
4:D:5:SER:HB2	4:D:26:TYR:HB3	2.00	0.43
1:A:44:LYS:HA	1:A:44:LYS:HD3	1.60	0.43
4:D:4:VAL:HG22	4:D:27:PHE:CE1	2.54	0.43
1:A:250:PRO:HA	1:A:251:PRO:HD3	1.90	0.43
1:A:25:PRO:HD3	1:A:52:GLU:OE1	2.19	0.43
3:C:132:ALA:O	3:C:189:ILE:HA	2.19	0.43
3:C:158:GLY:HA2	7:C:5548:HOH:O	2.19	0.42
1:A:147:PRO:HD3	1:A:215:GLY:CA	2.49	0.42
1:A:197:TYR:CE2	1:A:206:TYR:HB2	2.54	0.42
2:B:165:GLN:HB2	2:B:165:GLN:HE21	1.54	0.42
2:B:48:THR:HG23	2:B:49:ALA:N	2.36	0.41
2:B:13:ILE:HG22	2:B:14:ILE:N	2.35	0.41
2:B:23:ILE:HG21	2:B:109:HIS:CD2	2.56	0.41
1:A:134:HIS:ND1	1:A:228:HIS:CE1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:LYS:HA	2:B:53:PRO:HD3	1.89	0.41
1:A:190:TYR:CG	6:A:6001:MYR:H41	2.55	0.41
1:A:212:ASN:HD22	6:A:6001:MYR:C2	2.34	0.41
2:B:13:ILE:HD11	7:B:5464:HOH:O	2.21	0.40
1:A:77:ILE:HG22	1:A:106:ILE:HD11	2.02	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	283/285 (99%)	275 (97%)	8 (3%)	0	100	100
2	B	250/261 (96%)	232 (93%)	17 (7%)	1 (0%)	34	54
3	C	236/238 (99%)	225 (95%)	10 (4%)	1 (0%)	34	54
4	D	25/68 (37%)	24 (96%)	1 (4%)	0	100	100
All	All	794/852 (93%)	756 (95%)	36 (4%)	2 (0%)	41	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	161	GLU
3	C	180	PRO

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	256/256 (100%)	251 (98%)	5 (2%)	55	79
2	B	221/228 (97%)	213 (96%)	8 (4%)	35	61
3	C	210/210 (100%)	207 (99%)	3 (1%)	67	86
4	D	23/59 (39%)	21 (91%)	2 (9%)	10	20
All	All	710/753 (94%)	692 (98%)	18 (2%)	47	73

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ASP
1	A	97	ASN
1	A	172	HIS
1	A	219	SER
1	A	265	LYS
2	B	30	ASN
2	B	45	GLN
2	B	115	SER
2	B	116	LYS
2	B	165	GLN
2	B	193	ARG
2	B	232	ASN
2	B	236	ASN
3	C	124	ASN
3	C	148	MET
3	C	182	THR
4	D	3	GLN
4	D	28	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	ASN
1	A	12	ASN
1	A	57	GLN
1	A	89	ASN
1	A	97	ASN
1	A	171	GLN
2	B	30	ASN
2	B	45	GLN

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Mol	Chain	Res	Type
2	B	55	GLN
2	B	159	GLN
2	B	165	GLN
2	B	173	ASN
2	B	216	HIS
2	B	230	GLN
2	B	232	ASN
2	B	236	ASN
3	C	59	GLN
3	C	174	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](#)

Of 3 ligands modelled in this entry, 1 is 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	$\# Z > 2$
6	MYR	D	4000	-	14,14,15	1.13	1 (7%)	13,13,15	0.90	0
6	MYR	A	6001	-	12,15,15	0.79	0	11,15,15	1.00	1 (9%)

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
6	MYR	D	4000	-	-	7/12/12/13	-
6	MYR	A	6001	-	-	7/11/13/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	4000	MYR	O2-C1	-3.57	1.23	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	6001	MYR	C13-C12-C11	-2.99	87.51	115.30

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	6001	MYR	C1-C2-C3-C4
6	D	4000	MYR	C9-C10-C11-C12
6	A	6001	MYR	C10-C11-C12-C13
6	D	4000	MYR	C11-C10-C9-C8
6	A	6001	MYR	C5-C6-C7-C8
6	A	6001	MYR	C6-C7-C8-C9
6	D	4000	MYR	O2-C1-C2-C3
6	A	6001	MYR	C3-C4-C5-C6
6	D	4000	MYR	C11-C12-C13-C14
6	D	4000	MYR	C6-C7-C8-C9
6	A	6001	MYR	C11-C12-C13-C14
6	D	4000	MYR	C4-C5-C6-C7
6	D	4000	MYR	C1-C2-C3-C4
6	A	6001	MYR	C2-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	4000	MYR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	6001	MYR	4	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.