



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 08:53 pm BST

PDB ID : 2HWE  
Title : A COMPARISON OF THE ANTI-RHINOVIRAL DRUG BINDING  
POCKET IN HRV14 AND HRV1A  
Authors : Kim, K.H.; Rossmann, M.G.  
Deposited on : 1994-01-25  
Resolution : 3.80 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
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

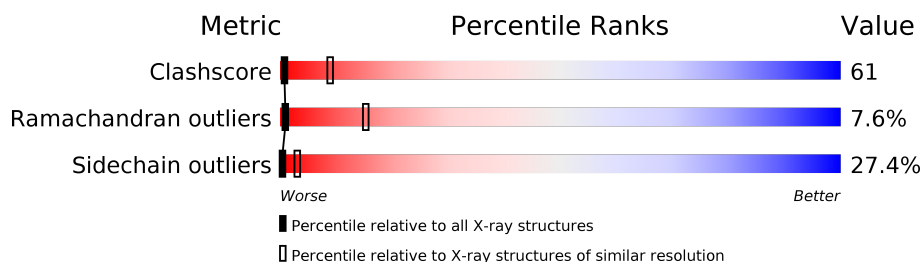
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	287	
2	2	263	
3	3	238	
4	4	44	

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
5	W54	1	500	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6248 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 HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	283	Total	C	N	O	S	0	0	0
			2262	1431	389	430	12			

- Molecule 2 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	253	Total	C	N	O	S	0	0	0
			1979	1249	349	371	10			

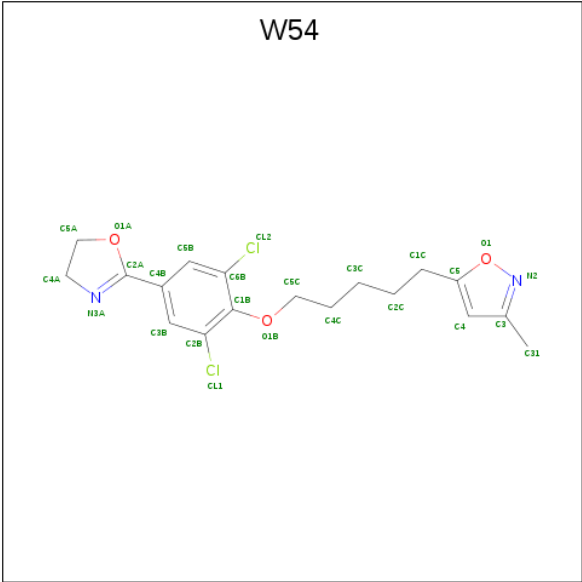
- Molecule 3 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	238	Total	C	N	O	S	0	0	0
			1831	1169	297	348	17			

- Molecule 4 is a protein called HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP4).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	4	19	Total	C	N	O	0	0	0
			151	96	25	30			

- Molecule 5 is 5-(5-(2,6-DICHLORO-4-(4,5-DIHYDRO-2-OXAZOLY)PHENOXY)PENTYL)-3-METHYL ISOXAZOLE (three-letter code: W54) (formula: C<sub>18</sub>H<sub>20</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>3</sub>).



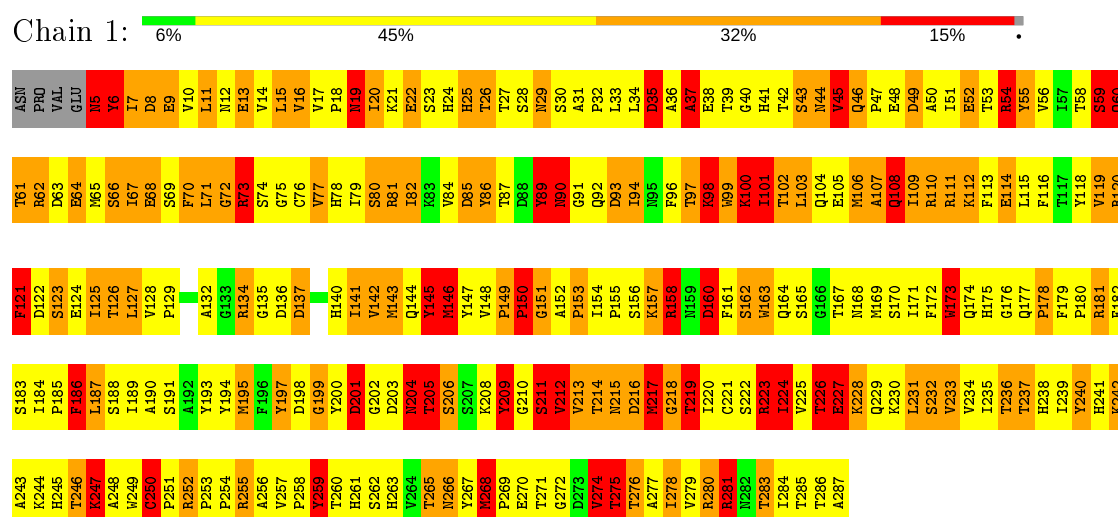
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
5	1	1	25	18	2	2	3	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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: HUMAN RHINOVIRUS 1A COAT PROTEIN (SUBUNIT VP1)



S184	G121	M61	G1
M185	T122	V62	L2
A186	A123	G63	P3
I187	M124	M64	V4
G188	T125	V65	V5
I189	T126	S66	I6
T190	L127	M67	T7
C191	K128	V68	P8
W192	L129	T69	G9
A193	L130	V70	S10
Q194	L131	Q71	G11
T195	A132	L72	Q12
M196	Y133	G73	F13
L197	T134	M74	M14
	P135	Q75	T15
	P136	T76	T16
		G77	D17
		M78	D18
	D139	A79	M19
	E140	Q80	Q20
	P141	K81	S21
	T142	V82	P22
	T143	F83	C23
	R144	S84	A24
	K145		
	D146	I85	L25
	A147	K86	P26
	M148	V87	W27
	L149	D88	Y28
	G150	I89	H29
	T151	T90	P30
	H152	S91	T31
	V153	T92	R32
	M154	P93	E33
	W155	L94	I34
	D156	A95	S35
	V157	T96	I36
	G158	T97	P37
	L159	L98	G38
	Q160	I99	E39
	S161	G100	V40
	T162	E101	K41
	I163	I102	M42
	S164	A103	L43
	V166	S104	I44
	V167	Y105	E45
	P168	V106	M46
	W169	T107	C47
		H108	Q48
		W109	V49
	A172	T110	D50
	S173	G111	T51
	H174	S112	L52
	T175	L113	I53
	R176	R114	P54
	T177	F115	V55
	L178	S116	S56
		F117	M57
		M118	V58
	M161	F119	G59
	K182	Y120	M60
	Y183		

GLY	ALA	GLY	VAL	SER	ARG	GLN	ASN	VAL	GLY	THR	HIS	SER	THR	GLN	ASN	SER	VAL	SER	ASN	GLY	SER	SER	LEU	ASN	Y26	F27	N28	I29	N30	Y31	F32	K33	D34	A35	A36	S37	S38	G39	A40	S41	R42	L43	D44
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	341.30Å 341.30Å 465.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	unknown	Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6248	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: W54

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	1	1.19	8/2322 (0.3%)	2.59	145/3162 (4.6%)
2	2	0.95	0/2033	2.59	151/2770 (5.5%)
3	3	0.93	0/1878	2.46	110/2570 (4.3%)
4	4	1.25	0/154	3.16	21/206 (10.2%)
All	All	1.05	8/6387 (0.1%)	2.57	427/8708 (4.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	7

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	146	MET	C-N	-15.38	0.98	1.34
1	1	213	VAL	C-N	11.92	1.61	1.34
1	1	98	LYS	C-N	-8.12	1.15	1.34
1	1	218	GLY	CA-C	-6.87	1.40	1.51
1	1	223	ARG	C-N	6.80	1.49	1.34

The worst 5 of 427 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	98	LYS	O-C-N	-28.02	77.86	122.70
2	2	62	ARG	CD-NE-CZ	24.81	158.33	123.60
1	1	134	ARG	NE-CZ-NH1	24.02	132.31	120.30
2	2	216	ARG	NE-CZ-NH2	-22.09	109.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	280	ARG	NE-CZ-NH2	-20.40	110.10	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	110	ARG	Mainchain
1	1	150	PRO	Peptide
1	1	186	PHE	Mainchain
1	1	211	SER	Mainchain
1	1	98	LYS	Mainchain,Peptide

## 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	1	2262	0	2191	387	1486
2	2	1979	0	1920	211	738
3	3	1831	0	1809	234	1610
4	4	151	0	136	16	345
5	1	25	0	20	3	49
All	All	6248	0	6076	756	2841

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 61.

The worst 5 of 756 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)
1:1:154:ILE:HG23	1:1:221:CYS:SG	1.55	1.47
1:1:101:ILE:H	1:1:101:ILE:CD1	1.07	1.44
1:1:108:GLN:NE2	3:3:226:ASP:OD2	1.69	1.24
1:1:23:SER:OG	1:1:53:THR:HG22	1.36	1.23
1:1:218:GLY:O	1:1:219:THR:CG2	1.89	1.21

The worst 5 of 2841 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)
1:1:39:THR:N	3:3:30:PRO:CD[12_555]	0.04	2.16
1:1:25:HIS:C	1:1:223:ARG:N[12_555]	0.17	2.03
1:1:243:ALA:N	3:3:215:ALA:N[12_555]	0.21	1.99
2:2:38:TRP:CE3	2:2:210:PRO:CG[12_555]	0.26	1.94
3:3:10:SER:CB	3:3:140:GLU:CA[12_555]	0.32	1.88

## 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	1	281/287 (98%)	206 (73%)	51 (18%)	24 (8%)	1	12
2	2	251/263 (95%)	201 (80%)	35 (14%)	15 (6%)	1	20
3	3	236/238 (99%)	179 (76%)	37 (16%)	20 (8%)	1	12
4	4	17/44 (39%)	9 (53%)	7 (41%)	1 (6%)	1	21
All	All	785/832 (94%)	595 (76%)	130 (17%)	60 (8%)	1	15

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	59	SER
1	1	72	GLY
1	1	107	ALA
1	1	108	GLN
1	1	114	GLU

### 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	1	254/258 (98%)	182 (72%)	72 (28%)	0	2
2	2	219/227 (96%)	159 (73%)	60 (27%)	0	3
3	3	209/209 (100%)	156 (75%)	53 (25%)	0	4
4	4	15/35 (43%)	9 (60%)	6 (40%)	0	0
All	All	697/729 (96%)	506 (73%)	191 (27%)	0	3

5 of 191 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	63	PHE
2	2	159	GLU
3	3	211	CYS
2	2	68	SER
2	2	103	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	2	111	GLN
2	2	197	ASN
3	3	124	ASN
2	2	192	ASN
2	2	207	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 carbohydrates in this entry.

## 5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	W54	1	500	-	24,27,27	3.13	5 (20%)	31,36,36	2.84	9 (29%)

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
5	W54	1	500	-	-	4/12/20/20	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	500	W54	C2A-N3A	12.19	1.43	1.27
5	1	500	W54	C4A-N3A	-6.37	1.36	1.47
5	1	500	W54	O1A-C2A	-4.05	1.29	1.36
5	1	500	W54	C4-C5	-3.66	1.34	1.39
5	1	500	W54	O1A-C5A	-3.13	1.38	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	500	W54	O1A-C2A-N3A	-9.64	109.94	118.23
5	1	500	W54	C4A-N3A-C2A	6.76	112.81	106.77
5	1	500	W54	O1A-C2A-C4B	6.18	124.04	115.85
5	1	500	W54	O1B-C1B-C6B	-4.62	115.18	121.17
5	1	500	W54	O1A-C5A-C4A	3.65	111.72	104.28

There are no chirality outliers.

All (4) torsion outliers are listed below:

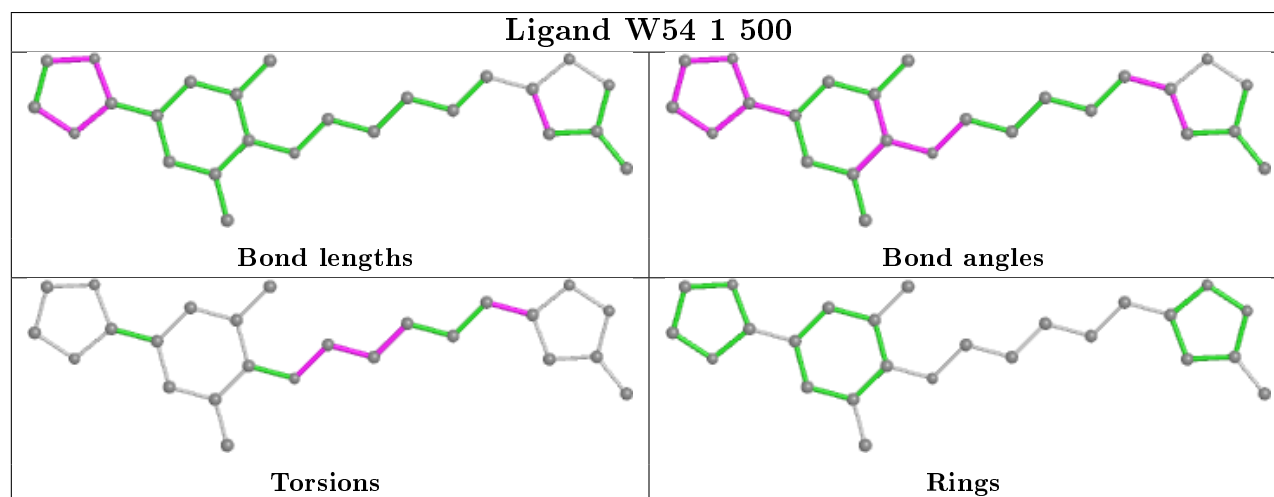
Mol	Chain	Res	Type	Atoms
5	1	500	W54	C2C-C1C-C5-C4
5	1	500	W54	C3C-C4C-C5C-O1B
5	1	500	W54	C2C-C3C-C4C-C5C
5	1	500	W54	C4C-C5C-O1B-C1B

There are no ring outliers.

1 monomer is involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	500	W54	3	49

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	213:VAL	C	214:THR	N	1.61
1	1	118:TYR	C	119:VAL	N	1.19
1	1	98:LYS	C	99:TRP	N	1.15
1	1	146:MET	C	147:TYR	N	0.98

## 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.