



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:12 pm BST

PDB ID : 1G7V  
Title : CRYSTAL STRUCTURES OF KDO8P SYNTHASE IN ITS BINARY COMPLEXES WITH THE MECHANISM-BASED INHIBITOR  
Authors : Asojo, O.A.; Friedman, J.M.; Belakhov, V.; Shoham, Y.; Adir, N.; Baasov, T.  
Deposited on : 2000-11-14  
Resolution : 2.40 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.

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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)  
Xtrriage (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

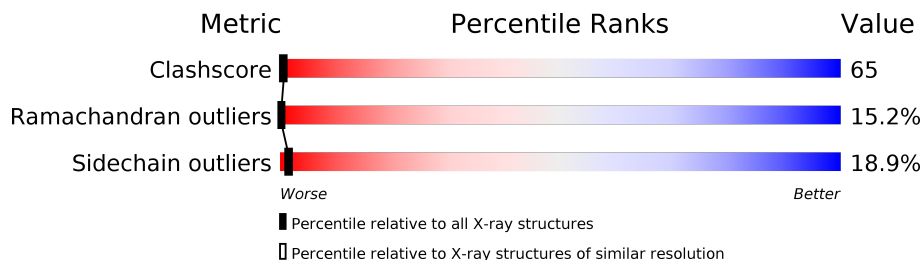
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	284	

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	PAI	A	300	-	X	-	-

## 2 Entry composition [i](#)

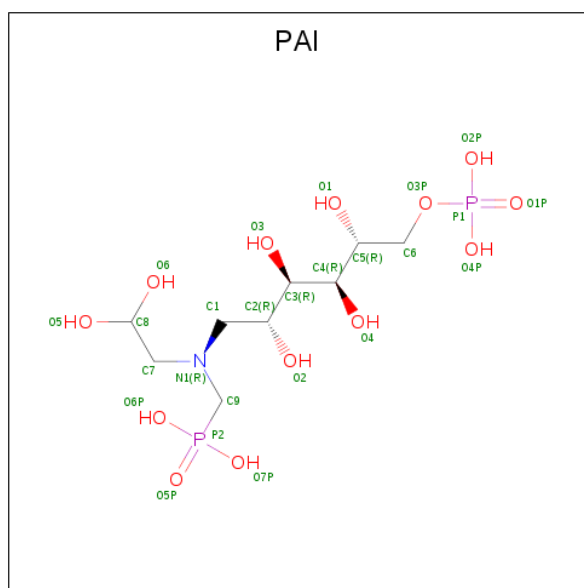
There are 3 unique types of molecules in this entry. The entry contains 2210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2-DEHYDRO-3-DEOXYPHOSPHOCTONATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	284	2164	1377	371	402	14	65	0	0

- Molecule 2 is {[ (2,2-DIHYDROXY-ETHYL)-(2,3,4,5-TETRAHYDROXY-6-PHOSPHONOXY-HEXYL)-AMINO]-METHYL}-PHOSPHONIC ACID (three-letter code: PAI) (formula: C<sub>9</sub>H<sub>23</sub>NO<sub>13</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	25	9	1	13	2	0	0

- Molecule 3 is water.

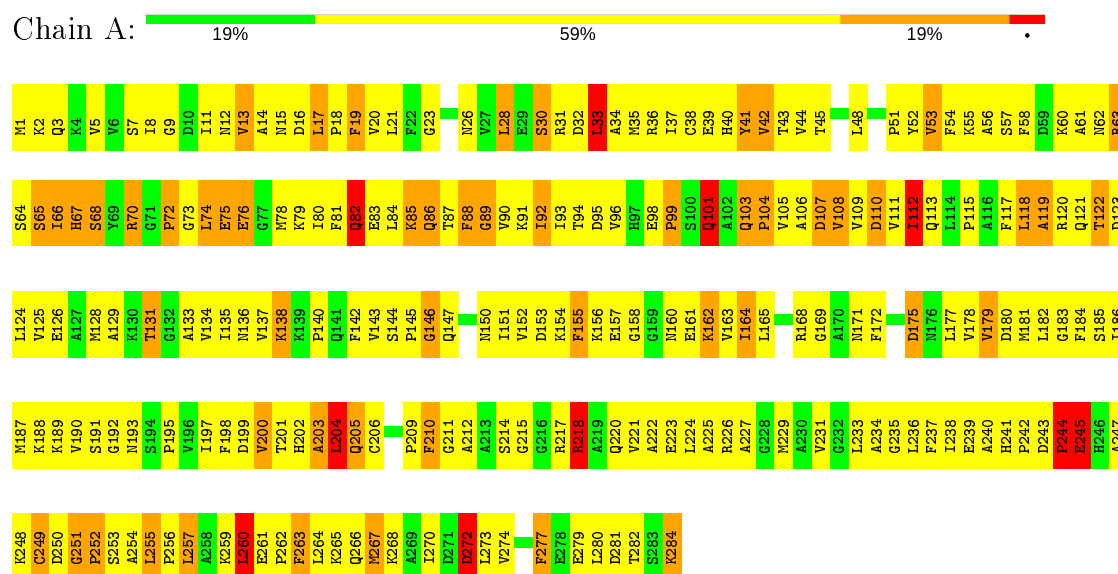
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		

### 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: 2-DEHYDRO-3-DEOXYPHOSHOCTONATE ALDOLASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.60Å 117.60Å 117.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.40)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.221 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	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: PAI

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	0.79	2/2204 (0.1%)	1.16	11/2972 (0.4%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	PRO	N-CD	-18.11	1.22	1.47
1	A	204	LEU	C-N	-10.85	1.09	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	LEU	O-C-N	-25.62	81.70	122.70
1	A	204	LEU	CA-C-N	14.05	148.12	117.20
1	A	204	LEU	C-N-CA	10.86	148.84	121.70
1	A	210	PHE	N-CA-C	-7.22	91.51	111.00
1	A	65	SER	N-CA-C	6.29	127.99	111.00
1	A	33	LEU	CA-CB-CG	6.07	129.27	115.30
1	A	260	LEU	CA-CB-CG	5.70	128.40	115.30
1	A	209	PRO	N-CD-CG	5.52	111.48	103.20
1	A	53	VAL	N-CA-C	-5.37	96.50	111.00
1	A	28	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	249	CYS	CA-CB-SG	5.21	123.37	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	LEU	Mainchain

## 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	2164	0	2196	278	0
2	A	25	0	16	3	0
3	A	21	0	0	4	0
All	All	2210	0	2212	279	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 65.

All (279) 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:241:HIS:ND1	1:A:245:GLU:HG2	1.84	0.90
1:A:14:ALA:HB3	1:A:17:LEU:HB2	1.56	0.88
1:A:92:ILE:HG13	1:A:109:VAL:HG12	1.56	0.87
1:A:169:GLY:HA3	3:A:303:HOH:O	1.72	0.87
1:A:78:MET:SD	1:A:108:VAL:HG22	2.15	0.86
1:A:81:PHE:HD1	1:A:92:ILE:HD12	1.40	0.84
1:A:199:ASP:HA	1:A:237:PHE:HB3	1.60	0.83
1:A:217:ARG:HG3	1:A:218:ARG:H	1.42	0.82
1:A:128:MET:O	1:A:131:THR:HB	1.80	0.82
1:A:241:HIS:CG	1:A:245:GLU:HA	2.17	0.80
1:A:113:GLN:HG2	1:A:136:ASN:HB3	1.63	0.80
1:A:19:PHE:HB2	1:A:235:GLY:HA2	1.62	0.80
1:A:19:PHE:HA	1:A:234:ALA:O	1.81	0.79
1:A:54:PHE:HB3	1:A:92:ILE:HG22	1.65	0.78
1:A:2:LYS:HD3	1:A:3:GLN:N	1.99	0.77
1:A:140:PRO:HB2	1:A:143:VAL:HG23	1.66	0.77
1:A:19:PHE:HZ	1:A:264:LEU:HD23	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:HB3	1:A:224:LEU:HD22	1.67	0.77
1:A:241:HIS:CD2	1:A:245:GLU:HA	2.21	0.75
1:A:125:VAL:HG21	1:A:154:LYS:HE2	1.68	0.75
1:A:161:GLU:O	1:A:163:VAL:HG23	1.85	0.75
1:A:8:ILE:HG22	1:A:91:LYS:HG2	1.69	0.75
1:A:78:MET:SD	1:A:108:VAL:CG2	2.75	0.74
1:A:38:CYS:SG	1:A:84:LEU:HB3	2.28	0.73
1:A:241:HIS:CG	1:A:245:GLU:HG2	2.22	0.73
1:A:154:LYS:HA	1:A:157:GLU:HB3	1.70	0.72
1:A:181:MET:HA	1:A:184:PHE:CE2	2.24	0.72
1:A:26:ASN:HB2	1:A:248:LYS:HZ2	1.54	0.72
1:A:156:LYS:HA	1:A:160:ASN:O	1.90	0.72
1:A:229:MET:SD	1:A:236:LEU:HD11	2.30	0.71
1:A:93:ILE:HG13	1:A:111:VAL:O	1.90	0.71
1:A:81:PHE:CD1	1:A:92:ILE:HD12	2.26	0.71
1:A:226:ARG:HG2	1:A:267:MET:SD	2.31	0.71
1:A:76:GLU:HA	1:A:79:LYS:HG2	1.73	0.70
1:A:135:ILE:O	1:A:164:ILE:HG13	1.91	0.70
1:A:55:LYS:HA	1:A:93:ILE:HG23	1.72	0.70
1:A:204:LEU:O	1:A:204:LEU:HD22	1.92	0.70
1:A:248:LYS:HB3	1:A:254:ALA:HB2	1.72	0.70
1:A:75:GLU:O	1:A:79:LYS:HE3	1.92	0.69
1:A:85:LYS:HE2	1:A:108:VAL:O	1.92	0.69
1:A:28:LEU:HD22	1:A:72:PRO:HG3	1.73	0.69
1:A:93:ILE:HB	1:A:111:VAL:HB	1.75	0.69
1:A:135:ILE:HG21	1:A:155:PHE:HE1	1.58	0.69
1:A:256:PRO:HB2	1:A:259:LYS:HB2	1.74	0.69
1:A:181:MET:HB3	1:A:231:VAL:HG21	1.74	0.68
1:A:38:CYS:SG	1:A:84:LEU:HD22	2.33	0.68
1:A:222:ALA:O	1:A:226:ARG:HG3	1.93	0.68
1:A:135:ILE:HG21	1:A:155:PHE:CE1	2.29	0.67
1:A:117:PHE:C	1:A:118:LEU:HD13	2.14	0.67
1:A:118:LEU:HD13	1:A:118:LEU:N	2.10	0.66
1:A:181:MET:SD	1:A:227:ALA:HB1	2.36	0.66
1:A:48:LEU:HD21	1:A:265:LYS:HZ2	1.60	0.66
1:A:138:LYS:O	1:A:140:PRO:HD3	1.95	0.66
1:A:217:ARG:O	1:A:218:ARG:HB2	1.95	0.66
1:A:217:ARG:HG3	1:A:218:ARG:N	2.11	0.66
1:A:125:VAL:HG11	1:A:154:LYS:HG2	1.78	0.66
1:A:189:LYS:HG2	1:A:190:VAL:N	2.09	0.66
1:A:31:ARG:HA	1:A:80:ILE:HG21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LYS:HE2	1:A:16:ASP:OD2	1.97	0.65
1:A:273:LEU:HD12	1:A:274:VAL:N	2.12	0.65
1:A:5:VAL:HG13	1:A:13:VAL:O	1.98	0.64
1:A:168:ARG:HH21	1:A:202:HIS:HB3	1.62	0.64
1:A:31:ARG:HA	1:A:80:ILE:CG2	2.27	0.64
1:A:44:VAL:HG13	1:A:261:GLU:HG3	1.79	0.64
1:A:32:ASP:HA	1:A:35:MET:HG2	1.80	0.64
1:A:20:VAL:HA	1:A:51:PRO:CG	2.28	0.64
1:A:229:MET:HG3	1:A:267:MET:HG3	1.80	0.64
1:A:20:VAL:HA	1:A:51:PRO:HG2	1.80	0.63
1:A:261:GLU:HB3	1:A:262:PRO:HD3	1.80	0.63
1:A:9:GLY:HA3	1:A:91:LYS:HE2	1.79	0.63
1:A:133:ALA:O	1:A:162:LYS:HB2	1.99	0.63
1:A:8:ILE:O	1:A:11:ILE:HB	1.99	0.62
1:A:93:ILE:HD11	1:A:113:GLN:HE21	1.64	0.62
1:A:140:PRO:HB2	1:A:143:VAL:CG2	2.30	0.62
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.64	0.62
1:A:9:GLY:HA3	1:A:91:LYS:CE	2.29	0.61
1:A:95:ASP:HA	1:A:113:GLN:HB2	1.81	0.61
1:A:205:GLN:HG3	1:A:206:CYS:H	1.66	0.61
1:A:35:MET:SD	1:A:84:LEU:HD23	2.41	0.61
1:A:244:PRO:O	1:A:245:GLU:HB2	2.00	0.61
1:A:200:VAL:HG11	1:A:236:LEU:HD23	1.83	0.61
1:A:3:GLN:HG3	1:A:15:ASN:HB2	1.83	0.60
1:A:41:TYR:HD1	1:A:260:LEU:HD11	1.66	0.60
1:A:48:LEU:HD21	1:A:265:LYS:NZ	2.15	0.60
1:A:134:VAL:CG1	1:A:164:ILE:HD11	2.32	0.60
1:A:115:PRO:HB2	1:A:118:LEU:CD2	2.32	0.60
1:A:245:GLU:HB2	1:A:248:LYS:HB2	1.82	0.60
1:A:115:PRO:HB2	1:A:118:LEU:HD21	1.85	0.58
1:A:1:MET:SD	1:A:193:ASN:OD1	2.61	0.58
1:A:125:VAL:HG13	1:A:155:PHE:CD2	2.39	0.58
1:A:35:MET:HE2	1:A:83:GLU:OE2	2.03	0.58
1:A:205:GLN:HG3	1:A:206:CYS:N	2.19	0.58
1:A:248:LYS:HA	1:A:252:PRO:HD2	1.87	0.57
1:A:45:THR:HG21	1:A:52:TYR:HB2	1.86	0.57
1:A:229:MET:SD	1:A:236:LEU:CD1	2.92	0.57
1:A:82:GLN:HA	1:A:85:LYS:HB2	1.86	0.57
1:A:221:VAL:HG21	1:A:255:LEU:HD12	1.85	0.57
1:A:248:LYS:CB	1:A:254:ALA:HB2	2.34	0.57
1:A:178:VAL:HG12	1:A:179:VAL:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:HIS:HB3	1:A:244:PRO:C	2.26	0.56
1:A:245:GLU:OE1	1:A:247:ALA:HB3	2.05	0.56
1:A:23:GLY:O	1:A:55:LYS:HB3	2.05	0.56
1:A:60:LYS:HD2	1:A:64:SER:O	2.06	0.56
1:A:151:ILE:HG23	3:A:320:HOH:O	2.05	0.56
1:A:220:GLN:OE1	1:A:223:GLU:HB2	2.06	0.56
1:A:185:SER:O	1:A:188:LYS:N	2.39	0.55
1:A:140:PRO:HB3	1:A:142:PHE:CE1	2.40	0.55
1:A:26:ASN:HB2	1:A:248:LYS:NZ	2.22	0.55
1:A:205:GLN:OE1	1:A:206:CYS:SG	2.61	0.55
1:A:23:GLY:HA3	1:A:52:TYR:HE1	1.72	0.55
1:A:96:VAL:HG21	1:A:124:LEU:HD11	1.90	0.54
1:A:225:ALA:HB1	1:A:236:LEU:HD21	1.87	0.54
1:A:81:PHE:HD1	1:A:92:ILE:CD1	2.16	0.54
1:A:28:LEU:HD21	1:A:80:ILE:HD12	1.90	0.53
1:A:19:PHE:CB	1:A:235:GLY:HA2	2.34	0.53
1:A:40:HIS:HB3	1:A:257:LEU:HD21	1.90	0.53
1:A:48:LEU:HD21	1:A:265:LYS:HG2	1.91	0.53
1:A:115:PRO:O	1:A:118:LEU:HD22	2.09	0.53
1:A:53:VAL:HG13	1:A:91:LYS:HB3	1.90	0.53
1:A:85:LYS:O	1:A:89:GLY:N	2.41	0.52
1:A:101:GLN:HA	1:A:104:PRO:HD2	1.90	0.52
1:A:150:ASN:C	1:A:151:ILE:HD12	2.29	0.52
1:A:125:VAL:HG11	1:A:154:LYS:HE2	1.90	0.52
1:A:64:SER:HB3	1:A:68:SER:CB	2.39	0.52
1:A:56:ALA:HB3	1:A:81:PHE:CZ	2.44	0.52
1:A:143:VAL:CG1	1:A:147:GLN:HB2	2.40	0.52
1:A:186:ILE:O	1:A:190:VAL:HG13	2.08	0.52
1:A:2:LYS:HD3	1:A:3:GLN:H	1.74	0.52
1:A:245:GLU:CB	1:A:248:LYS:HB2	2.39	0.52
1:A:65:SER:C	1:A:67:HIS:H	2.12	0.52
1:A:126:GLU:O	1:A:129:ALA:N	2.43	0.52
1:A:145:PRO:O	1:A:147:GLN:N	2.42	0.52
1:A:226:ARG:HD2	1:A:270:ILE:CD1	2.40	0.52
1:A:177:LEU:HD12	1:A:203:ALA:O	2.10	0.52
1:A:105:VAL:O	1:A:107:ASP:N	2.43	0.51
1:A:241:HIS:HB3	1:A:244:PRO:O	2.11	0.51
1:A:41:TYR:O	1:A:45:THR:HG23	2.10	0.51
1:A:60:LYS:O	1:A:61:ALA:HB3	2.10	0.51
1:A:204:LEU:HB3	1:A:224:LEU:CD2	2.38	0.51
1:A:91:LYS:HG3	1:A:110:ASP:OD1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLU:HB2	1:A:248:LYS:HE3	1.91	0.51
1:A:248:LYS:HD2	1:A:253:SER:O	2.11	0.51
1:A:181:MET:SD	1:A:227:ALA:CB	2.99	0.51
1:A:41:TYR:CD1	1:A:260:LEU:HD11	2.45	0.51
1:A:20:VAL:HG22	1:A:51:PRO:HG3	1.92	0.51
1:A:241:HIS:HB2	1:A:245:GLU:CG	2.41	0.50
1:A:273:LEU:HD13	1:A:277:PHE:CZ	2.47	0.50
1:A:34:ALA:O	1:A:37:ILE:N	2.43	0.50
1:A:14:ALA:HB3	1:A:17:LEU:HD22	1.94	0.50
1:A:85:LYS:HE2	1:A:92:ILE:HD11	1.93	0.50
1:A:240:ALA:O	1:A:241:HIS:HB2	2.11	0.49
1:A:122:THR:O	1:A:125:VAL:N	2.45	0.49
1:A:183:GLY:O	1:A:187:MET:HG3	2.13	0.49
1:A:268:LYS:O	1:A:272:ASP:HB2	2.12	0.49
1:A:65:SER:OG	1:A:66:ILE:N	2.44	0.49
1:A:14:ALA:CB	1:A:17:LEU:HD22	2.43	0.49
1:A:129:ALA:HA	1:A:160:ASN:HB2	1.94	0.49
1:A:172:PHE:CB	1:A:178:VAL:HG23	2.42	0.49
1:A:200:VAL:HG21	1:A:225:ALA:HB2	1.94	0.49
1:A:98:GLU:O	1:A:101:GLN:HG3	2.11	0.49
1:A:284:LYS:NZ	1:A:284:LYS:HB3	2.28	0.49
1:A:8:ILE:HD11	1:A:134:VAL:HG11	1.95	0.49
1:A:78:MET:SD	1:A:108:VAL:HG21	2.52	0.48
1:A:58:PHE:CD2	1:A:94:THR:HG21	2.48	0.48
1:A:280:LEU:HG	1:A:281:ASP:H	1.77	0.48
1:A:264:LEU:O	1:A:268:LYS:N	2.47	0.48
1:A:217:ARG:HH11	1:A:217:ARG:CG	2.25	0.48
1:A:263:PHE:O	1:A:266:GLN:HB2	2.14	0.48
1:A:129:ALA:HB1	1:A:158:GLY:O	2.13	0.48
1:A:41:TYR:CE1	1:A:260:LEU:HG	2.49	0.48
1:A:126:GLU:O	1:A:129:ALA:HB3	2.14	0.48
1:A:169:GLY:HA2	1:A:179:VAL:CG1	2.44	0.48
1:A:33:LEU:HD13	1:A:33:LEU:C	2.34	0.48
1:A:265:LYS:NZ	3:A:312:HOH:O	2.46	0.47
1:A:122:THR:HG22	1:A:154:LYS:HE3	1.96	0.47
1:A:263:PHE:CE2	1:A:267:MET:HE3	2.50	0.47
1:A:112:ILE:HD11	1:A:128:MET:HG2	1.97	0.47
1:A:144:SER:HB3	1:A:147:GLN:HG2	1.96	0.47
2:A:300:PAI:O7P	2:A:300:PAI:HC12	2.15	0.47
1:A:226:ARG:HD3	1:A:266:GLN:OE1	2.14	0.47
1:A:115:PRO:HD2	1:A:118:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:PRO:HB3	1:A:142:PHE:CZ	2.50	0.47
1:A:41:TYR:HE1	1:A:260:LEU:HG	1.79	0.47
1:A:38:CYS:O	1:A:42:VAL:HG23	2.15	0.47
1:A:15:ASN:OD1	1:A:195:PRO:HA	2.16	0.46
1:A:248:LYS:HD2	1:A:254:ALA:HB2	1.97	0.46
1:A:88:PHE:O	1:A:89:GLY:C	2.54	0.46
1:A:202:HIS:O	1:A:203:ALA:C	2.54	0.46
1:A:129:ALA:HB1	1:A:158:GLY:HA3	1.98	0.46
1:A:238:ILE:HD11	1:A:255:LEU:HD13	1.98	0.46
1:A:252:PRO:HG2	1:A:253:SER:H	1.81	0.46
1:A:113:GLN:HG2	1:A:136:ASN:CB	2.41	0.45
1:A:152:VAL:HG21	1:A:191:SER:OG	2.16	0.45
1:A:28:LEU:HB2	1:A:57:SER:O	2.16	0.45
1:A:124:LEU:O	1:A:128:MET:HG3	2.15	0.45
1:A:122:THR:O	1:A:125:VAL:HB	2.17	0.45
1:A:178:VAL:HG12	1:A:179:VAL:H	1.78	0.45
1:A:151:ILE:O	1:A:155:PHE:CD2	2.70	0.45
1:A:239:GLU:CB	1:A:248:LYS:HE3	2.47	0.45
1:A:220:GLN:HG3	1:A:223:GLU:OE2	2.16	0.45
1:A:19:PHE:O	1:A:19:PHE:CG	2.69	0.45
1:A:145:PRO:HB3	1:A:187:MET:HG3	1.99	0.44
1:A:60:LYS:HB2	1:A:70:ARG:HA	1.99	0.44
1:A:93:ILE:HD11	1:A:113:GLN:HG3	1.99	0.44
1:A:17:LEU:HD12	1:A:17:LEU:HA	1.82	0.44
1:A:168:ARG:NH2	1:A:202:HIS:HB3	2.28	0.44
1:A:220:GLN:NE2	1:A:220:GLN:HA	2.32	0.44
1:A:197:ILE:HG23	1:A:234:ALA:HB3	1.99	0.44
1:A:274:VAL:HA	1:A:277:PHE:CD2	2.53	0.44
1:A:66:ILE:O	1:A:67:HIS:HB2	2.17	0.44
1:A:169:GLY:HA2	1:A:179:VAL:HG13	2.00	0.44
1:A:19:PHE:O	1:A:19:PHE:CD2	2.70	0.44
1:A:20:VAL:HG13	1:A:51:PRO:HG2	2.00	0.44
1:A:96:VAL:HG22	1:A:128:MET:HE2	2.00	0.44
1:A:125:VAL:HG11	1:A:154:LYS:CG	2.46	0.44
1:A:248:LYS:HG2	1:A:252:PRO:HD2	1.99	0.43
1:A:31:ARG:HA	1:A:80:ILE:HG23	2.00	0.43
1:A:248:LYS:CD	1:A:254:ALA:HB2	2.48	0.43
1:A:260:LEU:O	1:A:263:PHE:HB3	2.18	0.43
1:A:137:VAL:HB	1:A:165:LEU:HD23	1.99	0.43
1:A:7:SER:OG	1:A:12:ASN:ND2	2.51	0.43
1:A:95:ASP:HB2	1:A:115:PRO:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:VAL:HG22	1:A:261:GLU:OE1	2.19	0.43
1:A:152:VAL:O	1:A:153:ASP:C	2.57	0.43
1:A:146:GLY:HA2	1:A:190:VAL:HG11	2.00	0.43
1:A:19:PHE:HZ	1:A:264:LEU:CD2	2.22	0.43
1:A:205:GLN:CG	1:A:206:CYS:N	2.81	0.43
1:A:284:LYS:HZ3	1:A:284:LYS:HB3	1.83	0.43
1:A:40:HIS:CB	1:A:257:LEU:HD21	2.49	0.43
1:A:28:LEU:O	1:A:72:PRO:HG3	2.19	0.43
1:A:87:THR:HB	1:A:88:PHE:CE2	2.53	0.43
1:A:95:ASP:CA	1:A:113:GLN:HB2	2.49	0.42
1:A:205:GLN:NE2	2:A:300:PAI:O6	2.52	0.42
1:A:26:ASN:H	1:A:248:LYS:NZ	2.17	0.42
1:A:251:GLY:CA	2:A:300:PAI:O4	2.67	0.42
1:A:26:ASN:N	1:A:248:LYS:NZ	2.67	0.42
1:A:82:GLN:CA	1:A:85:LYS:HB2	2.48	0.42
1:A:74:LEU:O	1:A:75:GLU:C	2.57	0.42
1:A:93:ILE:HD11	1:A:113:GLN:NE2	2.32	0.42
1:A:201:THR:HG22	1:A:202:HIS:N	2.33	0.42
1:A:103:GLN:H	1:A:104:PRO:CD	2.32	0.42
1:A:111:VAL:HG13	1:A:134:VAL:HG12	2.01	0.42
1:A:80:ILE:O	1:A:80:ILE:HG22	2.19	0.42
1:A:70:ARG:HB2	1:A:70:ARG:HE	1.63	0.42
1:A:73:GLY:CA	3:A:315:HOH:O	2.67	0.42
1:A:119:ALA:O	1:A:121:GLN:N	2.52	0.42
1:A:96:VAL:CG2	1:A:124:LEU:HD21	2.50	0.42
1:A:205:GLN:CD	1:A:206:CYS:HG	2.18	0.42
1:A:101:GLN:C	1:A:104:PRO:HD2	2.40	0.42
1:A:156:LYS:HG3	1:A:161:GLU:HG2	2.01	0.42
1:A:180:ASP:C	1:A:182:LEU:H	2.23	0.42
1:A:3:GLN:CG	1:A:15:ASN:HB2	2.49	0.42
1:A:21:LEU:HD13	1:A:264:LEU:HD21	2.02	0.42
1:A:62:ASN:O	1:A:63:ARG:HB2	2.20	0.41
1:A:60:LYS:HB2	1:A:70:ARG:CA	2.50	0.41
1:A:30:SER:O	1:A:33:LEU:HB3	2.20	0.41
1:A:118:LEU:CD1	1:A:118:LEU:N	2.81	0.41
1:A:135:ILE:CG2	1:A:155:PHE:HE1	2.28	0.41
1:A:273:LEU:HD12	1:A:274:VAL:H	1.85	0.41
1:A:226:ARG:HD2	1:A:270:ILE:HD11	2.01	0.41
1:A:34:ALA:O	1:A:37:ILE:HB	2.21	0.41
1:A:245:GLU:O	1:A:249:CYS:SG	2.78	0.41
1:A:198:PHE:HB2	1:A:233:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LEU:HD22	1:A:118:LEU:H	1.86	0.41
1:A:150:ASN:OD1	1:A:150:ASN:N	2.53	0.41
1:A:185:SER:O	1:A:188:LYS:HB2	2.19	0.41
1:A:104:PRO:O	1:A:105:VAL:C	2.59	0.41
1:A:255:LEU:HA	1:A:256:PRO:HD3	1.94	0.41
1:A:105:VAL:O	1:A:109:VAL:HG22	2.21	0.40
1:A:217:ARG:CG	1:A:218:ARG:N	2.82	0.40
1:A:54:PHE:O	1:A:92:ILE:HA	2.21	0.40
1:A:96:VAL:HG22	1:A:128:MET:CE	2.50	0.40
1:A:143:VAL:HG12	1:A:147:GLN:HB2	2.03	0.40
1:A:86:GLN:C	1:A:88:PHE:N	2.75	0.40
1:A:91:LYS:HA	1:A:110:ASP:CG	2.42	0.40
1:A:125:VAL:CG2	1:A:154:LYS:HE2	2.45	0.40
1:A:180:ASP:C	1:A:182:LEU:N	2.75	0.40
1:A:243:ASP:HA	1:A:244:PRO:HD2	1.73	0.40
1:A:103:GLN:HB3	1:A:104:PRO:HD3	2.04	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	282/284 (99%)	182 (64%)	57 (20%)	43 (15%)	<b>0</b> <b>0</b>

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	68	SER
1	A	85	LYS
1	A	99	PRO
1	A	119	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	203	ALA
1	A	211	GLY
1	A	212	ALA
1	A	214	SER
1	A	242	PRO
1	A	244	PRO
1	A	245	GLU
1	A	252	PRO
1	A	18	PRO
1	A	63	ARG
1	A	66	ILE
1	A	89	GLY
1	A	146	GLY
1	A	162	LYS
1	A	175	ASP
1	A	277	PHE
1	A	106	ALA
1	A	122	THR
1	A	123	ASP
1	A	204	LEU
1	A	279	GLU
1	A	43	THR
1	A	72	PRO
1	A	75	GLU
1	A	107	ASP
1	A	215	GLY
1	A	218	ARG
1	A	74	LEU
1	A	101	GLN
1	A	104	PRO
1	A	131	THR
1	A	82	GLN
1	A	103	GLN
1	A	272	ASP
1	A	112	ILE
1	A	251	GLY
1	A	42	VAL
1	A	192	GLY

### 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	233/233 (100%)	189 (81%)	44 (19%)	<b>1</b> <b>1</b>

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	VAL
1	A	17	LEU
1	A	19	PHE
1	A	30	SER
1	A	33	LEU
1	A	36	ARG
1	A	39	GLU
1	A	41	TYR
1	A	70	ARG
1	A	76	GLU
1	A	82	GLN
1	A	86	GLN
1	A	88	PHE
1	A	90	VAL
1	A	92	ILE
1	A	99	PRO
1	A	101	GLN
1	A	108	VAL
1	A	110	ASP
1	A	112	ILE
1	A	118	LEU
1	A	120	ARG
1	A	138	LYS
1	A	155	PHE
1	A	164	ILE
1	A	171	ASN
1	A	175	ASP
1	A	179	VAL
1	A	200	VAL
1	A	204	LEU

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Mol	Chain	Res	Type
1	A	205	GLN
1	A	210	PHE
1	A	218	ARG
1	A	244	PRO
1	A	245	GLU
1	A	250	ASP
1	A	255	LEU
1	A	257	LEU
1	A	260	LEU
1	A	263	PHE
1	A	267	MET
1	A	272	ASP
1	A	282	THR
1	A	284	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	86	GLN
1	A	97	HIS
1	A	113	GLN
1	A	121	GLN
1	A	141	GLN
1	A	147	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

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
2	PAI	A	300	-	24,24,24	3.93	17 (70%)	34,35,35	2.50	15 (44%)

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	PAI	A	300	-	-	7/31/31/31	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	PAI	C6-C5	7.70	1.62	1.51
2	A	300	PAI	C3-C4	7.14	1.67	1.53
2	A	300	PAI	O6-C8	-6.85	1.24	1.40
2	A	300	PAI	P2-O5P	5.74	1.62	1.50
2	A	300	PAI	O5-C8	-4.86	1.29	1.40
2	A	300	PAI	C1-C2	4.77	1.59	1.52
2	A	300	PAI	C2-C3	4.73	1.62	1.53
2	A	300	PAI	P1-O1P	4.43	1.64	1.50
2	A	300	PAI	C5-C4	4.39	1.61	1.53
2	A	300	PAI	P1-O3P	3.80	1.72	1.60
2	A	300	PAI	P2-O6P	3.37	1.62	1.54
2	A	300	PAI	C7-N1	3.35	1.53	1.47
2	A	300	PAI	C7-C8	2.49	1.56	1.51
2	A	300	PAI	P2-O7P	2.21	1.60	1.54
2	A	300	PAI	C1-N1	2.09	1.51	1.47
2	A	300	PAI	C9-N1	2.06	1.52	1.48
2	A	300	PAI	P1-O4P	2.05	1.62	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	PAI	O6-C8-O5	5.71	121.85	111.36
2	A	300	PAI	C5-C4-C3	5.08	120.42	112.47
2	A	300	PAI	O5-C8-C7	4.43	120.46	109.76
2	A	300	PAI	C2-C1-N1	4.32	120.07	112.21
2	A	300	PAI	O6P-P2-C9	3.76	114.71	106.66
2	A	300	PAI	O3P-C6-C5	3.57	118.90	109.36
2	A	300	PAI	C2-C3-C4	3.54	118.00	112.47
2	A	300	PAI	O6-C8-C7	3.26	117.64	109.76
2	A	300	PAI	C1-C2-C3	3.16	118.62	109.79
2	A	300	PAI	O3-C3-C4	-2.70	103.19	109.47
2	A	300	PAI	O2-C2-C1	-2.53	103.68	109.80
2	A	300	PAI	P1-O3P-C6	2.48	125.14	118.30
2	A	300	PAI	C6-C5-C4	2.28	116.60	112.20
2	A	300	PAI	O3-C3-C2	-2.25	103.37	108.81
2	A	300	PAI	C7-N1-C1	2.01	116.86	111.52

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	300	PAI	C2-C3-C4-C5
2	A	300	PAI	C2-C3-C4-O4
2	A	300	PAI	N1-C7-C8-O6
2	A	300	PAI	N1-C9-P2-O6P
2	A	300	PAI	N1-C9-P2-O7P
2	A	300	PAI	O3-C3-C4-C5
2	A	300	PAI	N1-C9-P2-O5P

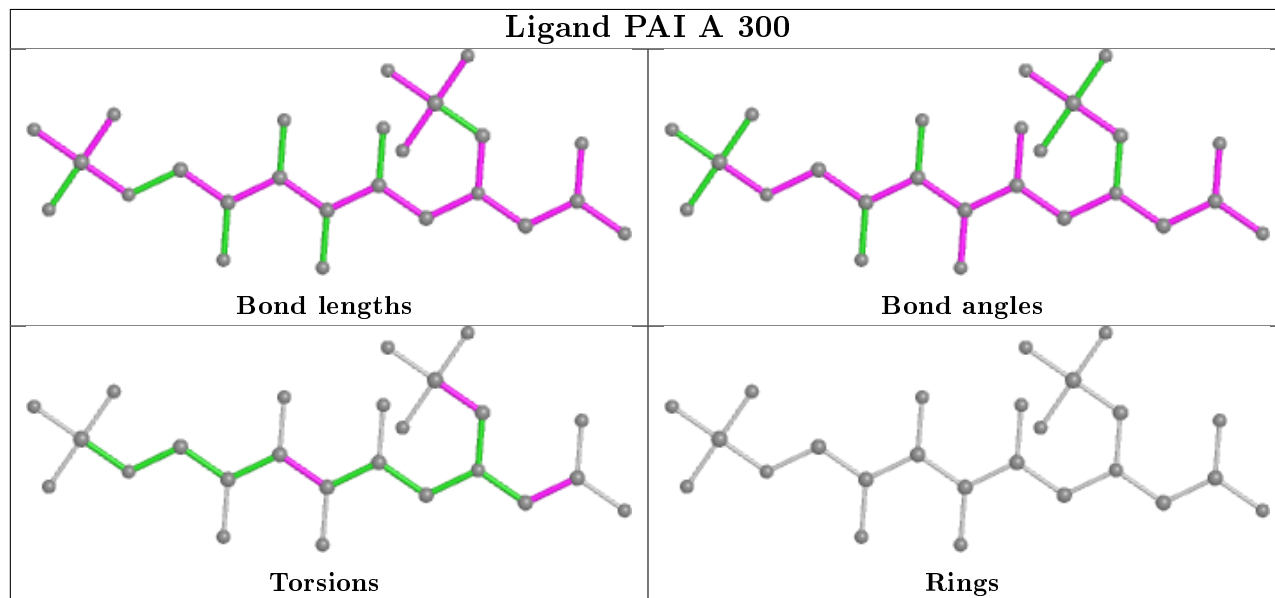
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	PAI	3	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	204:LEU	C	205:GLN	N	1.09

## 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.