



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 06:10 pm GMT

PDB ID : 1GGR  
Title : COMPLEX OF ENZYME IIAGLC AND THE HISTIDINE-CONTAINING PHOSPHOCARRIER PROTEIN HPR FROM ESCHERICHIA COLI NMR, RESTRAINED REGULARIZED MEAN STRUCTURE  
Authors : Clore, G.M.; Wang, G.  
Deposited on : 2000-09-18

This is a Full wwPDB NMR 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

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

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:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

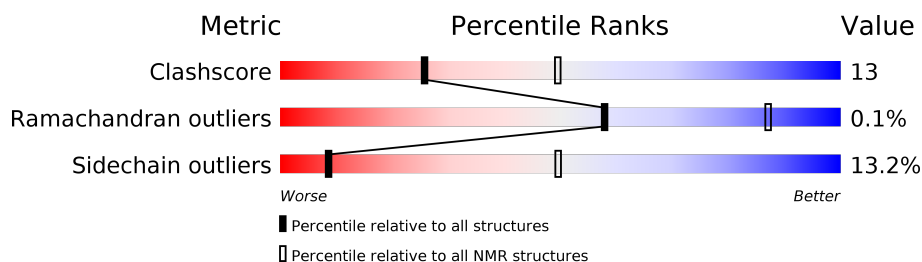
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	168	
2	B	85	

## 2 Ensemble composition and analysis

This entry contains 3 models. Model 2 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:19-A:168, B:301-B:385 (235)	0.04	2

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3

### 3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3595 atoms, of which 1817 are hydrogens and 0 are deuteriums.

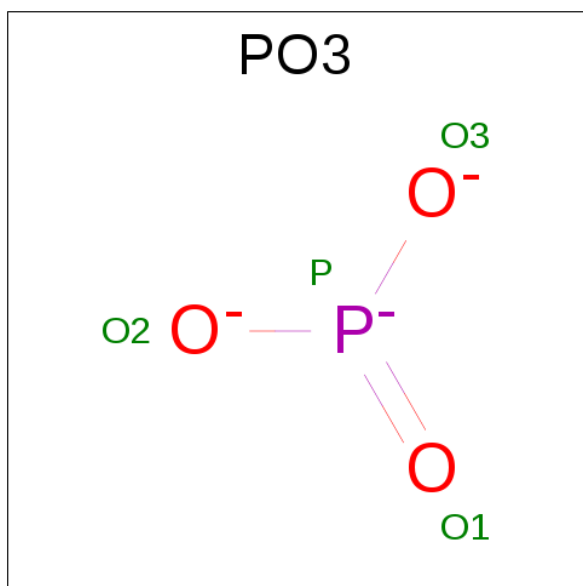
- Molecule 1 is a protein called PTS SYSTEM, GLUCOSE-SPECIFIC IIA COMPONENT.

Mol	Chain	Residues	Atoms						Trace
1	A	150	Total	C	H	N	O	S	0
			2305	729	1169	181	224	2	

- Molecule 2 is a protein called PHOSPHOCARRIER PROTEIN HPR.

Mol	Chain	Residues	Atoms						Trace
2	B	85	Total	C	H	N	O	S	0
			1286	401	648	107	128	2	

- Molecule 3 is PHOSPHITE ION (three-letter code: PO3) (formula: O<sub>3</sub>P).



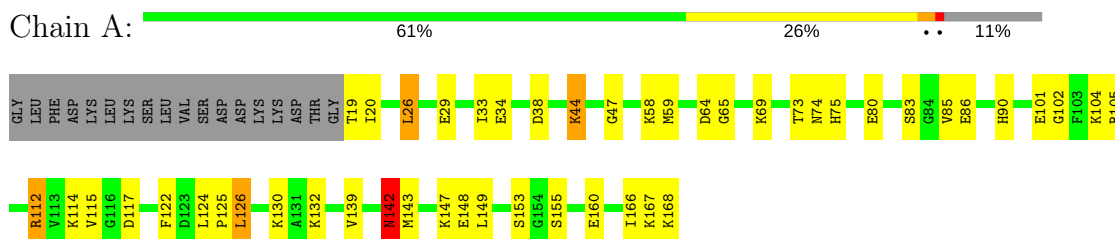
Mol	Chain	Residues	Atoms		
3	B	1	Total	O	P
			4	3	1

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

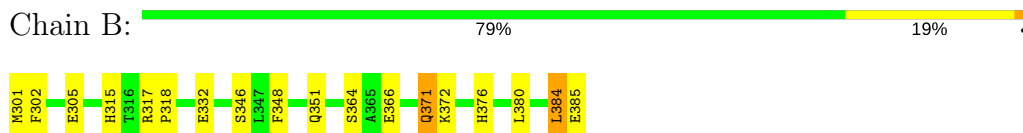
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: PTS SYSTEM, GLUCOSE-SPECIFIC IIA COMPONENT



- Molecule 2: PHOSPHOCARRIER PROTEIN HPR

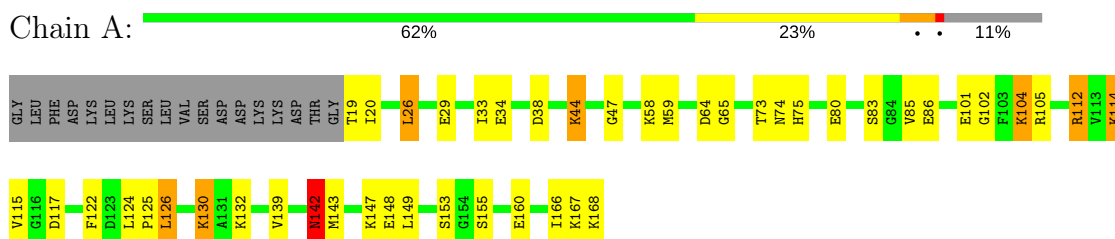


### 4.2 Scores per residue for each member of the ensemble


Colouring as in section 4.1 above.

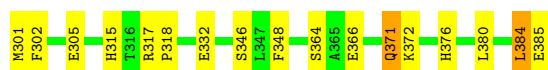
#### 4.2.1 Score per residue for model 1

- Molecule 1: PTS SYSTEM, GLUCOSE-SPECIFIC IIA COMPONENT



- Molecule 2: PHOSPHOCARRIER PROTEIN HPR

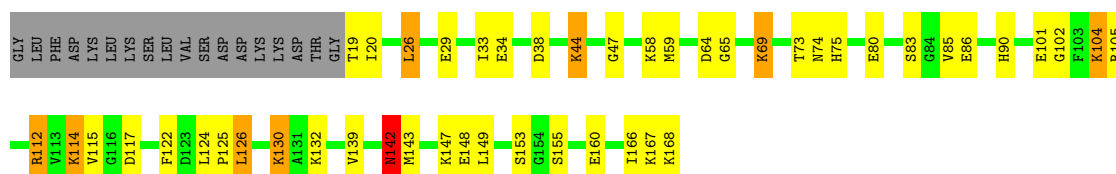
Chain B:  80% 18% .




#### 4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: PTS SYSTEM, GLUCOSE-SPECIFIC IIA COMPONENT

Chain A:  61% 23% 5% . 11%



- Molecule 2: PHOSPHOCARRIER PROTEIN HPR

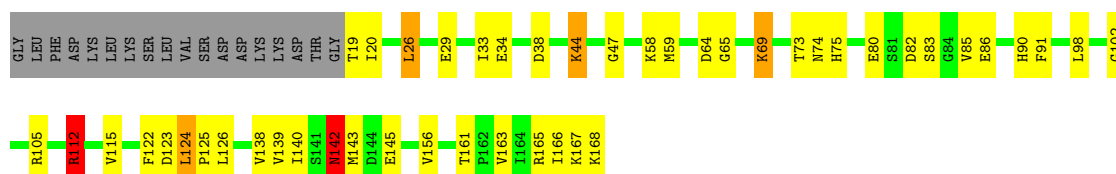
Chain B:  79% 19% .




#### 4.2.3 Score per residue for model 3

- Molecule 1: PTS SYSTEM, GLUCOSE-SPECIFIC IIA COMPONENT

Chain A:  61% 24% . . 11%



- Molecule 2: PHOSPHOCARRIER PROTEIN HPR

Chain B:  76% 20% .



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *RIGID BODY MINIMIZATION AND CONSTRAINED/RESTRAINED SIMULATED ANNEALING*.

Of the 30 calculated structures, 3 were deposited, based on the following criterion: *REGULARIZED MEAN STRUCTURES*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	NIH

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO3

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 (average) 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	1.11±0.01	0±0/1151 (0.0±0.0%)	1.08±0.01	2±0/1557 (0.1±0.0%)
2	B	1.09±0.00	0±0/645 (0.0±0.0%)	1.19±0.00	0±0/870 (0.0±0.0%)
All	All	1.10	1/5388 (0.0%)	1.12	7/7281 (0.1%)

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	Planarity
1	A	0.0±0.0	0.7±0.9
All	All	0	2

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	124	LEU	C-N	-5.12	1.24	1.34	3	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	142	ASN	N-CA-CB	-5.44	100.80	110.60	1	3
1	A	26	LEU	N-CA-CB	5.17	120.74	110.40	2	3
1	A	142	ASN	CB-CA-C	-5.13	100.13	110.40	3	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the



ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	165	ARG	Sidechain	1
1	A	112	ARG	Sidechain	1

## 6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1136	1169	1178	34±2
2	B	638	648	649	16±4
3	B	4	0	0	1±2
All	All	5334	5451	5482	140

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 13.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:HIS:NE2	3:B:200:PO3:P	1.24	2.11	3	1
2:B:315:HIS:ND1	3:B:200:PO3:P	1.22	2.13	3	1
1:A:64:ASP:OD1	1:A:115:VAL:HG23	0.74	1.82	3	3
1:A:20:ILE:HB	1:A:166:ILE:CG1	0.70	2.16	1	3
1:A:126:LEU:CD1	1:A:130:LYS:HG3	0.70	2.17	2	2
1:A:20:ILE:HB	1:A:166:ILE:HG13	0.69	1.62	3	3
1:A:74:ASN:ND2	1:A:105:ARG:HH21	0.66	1.88	1	3
2:B:315:HIS:CG	2:B:316:THR:N	0.65	2.63	3	1
1:A:75:HIS:NE2	1:A:90:HIS:CE1	0.63	2.67	2	2
1:A:85:VAL:HG21	1:A:166:ILE:CD1	0.62	2.25	1	3
1:A:85:VAL:HG21	1:A:166:ILE:HD11	0.62	1.71	1	3
2:B:315:HIS:CE1	3:B:200:PO3:P	0.62	2.92	3	1
1:A:75:HIS:CD2	1:A:90:HIS:CE1	0.60	2.89	2	1
2:B:315:HIS:CG	2:B:316:THR:H	0.60	2.15	3	1
1:A:98:LEU:HD12	1:A:98:LEU:N	0.60	2.12	3	1
1:A:74:ASN:HD21	1:A:105:ARG:NH2	0.59	1.94	3	1
1:A:126:LEU:HD12	1:A:126:LEU:O	0.58	1.97	1	2
1:A:74:ASN:ND2	1:A:105:ARG:HE	0.58	1.96	1	3
1:A:75:HIS:HE2	1:A:90:HIS:CE1	0.58	2.16	2	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:372:LYS:NZ	2:B:376:HIS:CE1	0.57	2.72	3	3
1:A:147:LYS:HB2	1:A:168:LYS:HB3	0.56	1.76	2	2
1:A:98:LEU:N	1:A:98:LEU:CD1	0.56	2.69	3	1
1:A:126:LEU:HD12	1:A:130:LYS:HG3	0.55	1.78	2	2
1:A:142:ASN:HD21	1:A:145:GLU:CD	0.54	2.06	3	1
1:A:69:LYS:CD	2:B:351:GLN:O	0.54	2.56	3	2
1:A:73:THR:OG1	1:A:75:HIS:ND1	0.54	2.39	3	3
1:A:140:ILE:HD12	1:A:140:ILE:N	0.53	2.19	3	1
1:A:74:ASN:ND2	1:A:105:ARG:NH2	0.52	2.55	3	3
1:A:102:GLY:O	1:A:104:LYS:NZ	0.52	2.36	1	2
2:B:315:HIS:CE1	2:B:317:ARG:H	0.52	2.22	3	1
2:B:315:HIS:CE1	3:B:200:PO3:O3	0.51	2.64	3	1
1:A:64:ASP:OD1	1:A:115:VAL:N	0.51	2.39	1	3
1:A:123:ASP:OD1	1:A:126:LEU:N	0.51	2.39	3	1
1:A:126:LEU:C	1:A:126:LEU:HD12	0.51	2.26	1	2
2:B:315:HIS:ND1	2:B:316:THR:N	0.50	2.60	3	1
1:A:33:ILE:CD1	1:A:139:VAL:CG1	0.49	2.90	3	3
1:A:124:LEU:HB3	1:A:125:PRO:HD3	0.48	1.84	2	2
1:A:156:VAL:HG12	1:A:161:THR:CG2	0.48	2.37	3	1
1:A:112:ARG:NH1	1:A:112:ARG:CG	0.47	2.77	1	1
2:B:372:LYS:HZ1	2:B:376:HIS:CE1	0.47	2.28	3	3
2:B:380:LEU:HG	2:B:384:LEU:CD2	0.47	2.40	1	3
1:A:112:ARG:CG	1:A:112:ARG:NH1	0.46	2.77	2	1
1:A:123:ASP:OD1	1:A:126:LEU:CB	0.46	2.63	3	1
1:A:44:LYS:HB3	1:A:47:GLY:O	0.45	2.11	1	3
2:B:317:ARG:N	2:B:318:PRO:CD	0.45	2.80	3	3
1:A:167:LYS:O	1:A:168:LYS:C	0.45	2.54	3	3
1:A:112:ARG:CG	1:A:112:ARG:HH11	0.44	2.24	2	1
1:A:112:ARG:HH11	1:A:112:ARG:CG	0.44	2.24	1	1
2:B:315:HIS:CD2	2:B:318:PRO:CD	0.44	3.01	3	1
2:B:315:HIS:CD2	2:B:318:PRO:CG	0.44	3.01	2	1
1:A:124:LEU:N	1:A:125:PRO:CD	0.43	2.81	1	3
1:A:86:GLU:OE1	2:B:348:PHE:CB	0.43	2.66	3	3
1:A:142:ASN:O	1:A:143:MET:C	0.43	2.55	2	3
1:A:102:GLY:O	1:A:122:PHE:HA	0.43	2.13	2	3
1:A:38:ASP:OD1	2:B:317:ARG:NH2	0.43	2.49	2	2
1:A:140:ILE:CD1	1:A:140:ILE:N	0.43	2.81	3	1
1:A:74:ASN:HD22	1:A:105:ARG:HE	0.42	1.57	3	1
2:B:301:MET:CG	2:B:302:PHE:N	0.42	2.83	3	3
2:B:314:LEU:O	2:B:315:HIS:O	0.42	2.37	3	1
2:B:302:PHE:CD2	2:B:371:GLN:HA	0.42	2.50	3	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:ASN:ND2	1:A:105:ARG:NE	0.42	2.67	3	3
2:B:376:HIS:CD2	2:B:376:HIS:N	0.42	2.85	1	2
2:B:376:HIS:N	2:B:376:HIS:CD2	0.41	2.85	2	1
1:A:90:HIS:O	1:A:91:PHE:C	0.41	2.58	3	1
1:A:114:LYS:HE3	1:A:117:ASP:OD2	0.41	2.16	1	2
1:A:38:ASP:CG	2:B:317:ARG:HH21	0.41	2.19	1	3
2:B:380:LEU:O	2:B:384:LEU:HD22	0.41	2.16	1	3
1:A:65:GLY:HA3	1:A:80:GLU:O	0.41	2.16	1	3
1:A:82:ASP:OD1	1:A:112:ARG:NH1	0.41	2.53	3	1
2:B:317:ARG:N	2:B:318:PRO:HD2	0.40	2.32	1	2
1:A:156:VAL:HG11	1:A:163:VAL:HG12	0.40	1.93	3	1
2:B:315:HIS:CD2	2:B:315:HIS:H	0.40	2.34	1	1
1:A:69:LYS:CG	2:B:351:GLN:O	0.40	2.70	3	1

## 6.3 Torsion angles [i](#)

### 6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	148/168 (88%)	140±1 (95±1%)	8±1 (5±1%)	0±0 (0±0%)	100	100
2	B	83/85 (98%)	81±0 (97±1%)	2±0 (2±0%)	0±0 (0±1%)	42	80
All	All	693/759 (91%)	662 (96%)	30 (4%)	1 (0%)	58	87

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
2	B	315	HIS	1

### 6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	129/145 (89%)	111±4 (86±3%)	18±4 (14±3%)	8	47
2	B	70/70 (100%)	62±0 (89±0%)	8±0 (11±0%)	11	54
All	All	597/645 (93%)	518 (87%)	79 (13%)	8	49

All 31 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	29	GLU	3
2	B	385	GLU	3
1	A	112	ARG	3
1	A	58	LYS	3
1	A	19	THR	3
1	A	142	ASN	3
1	A	44	LYS	3
1	A	59	MET	3
1	A	34	GLU	3
2	B	371	GLN	3
2	B	346	SER	3
1	A	26	LEU	3
2	B	366	GLU	3
1	A	83	SER	3
2	B	332	GLU	3
2	B	384	LEU	3
2	B	305	GLU	3
2	B	364	SER	3
1	A	101	GLU	2
1	A	126	LEU	2
1	A	114	LYS	2
1	A	153	SER	2
1	A	149	LEU	2
1	A	132	LYS	2
1	A	155	SER	2
1	A	69	LYS	2
1	A	160	GLU	2
1	A	148	GLU	2
1	A	130	LYS	2
1	A	104	LYS	2
1	A	138	VAL	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PO3	B	200	-	0,3,3	0.00±0.00	-

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PO3	B	200	-	0,3,3	0.00±0.00	-

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	PO3	B	200	-	-	0±0,0,0,0	0±0,0,0,0

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided