



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2022 – 04:09 pm BST

PDB ID : 6RKY
Title : STRUCTURE OF ESTER-HYDROLASE EH1AB1 FROM THE
METAGENOME OF LAKE ARREO COMPLEXED WITH A DERIVATIVE
OF BIPYRIDINE PHOSPHONATE
Authors : Cea-Rama, I.; Sanz-Aparicio, J.
Deposited on : 2019-04-30
Resolution : 2.79 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

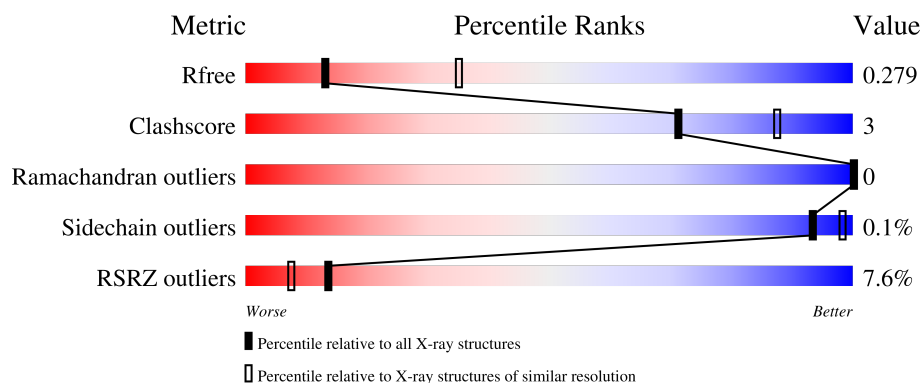
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	329	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>.</div> </div> </div>
1	B	329	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>.</div> </div> </div>
1	C	329	<div> <div>13%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>.</div> </div> </div>
1	D	329	<div> <div>7%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

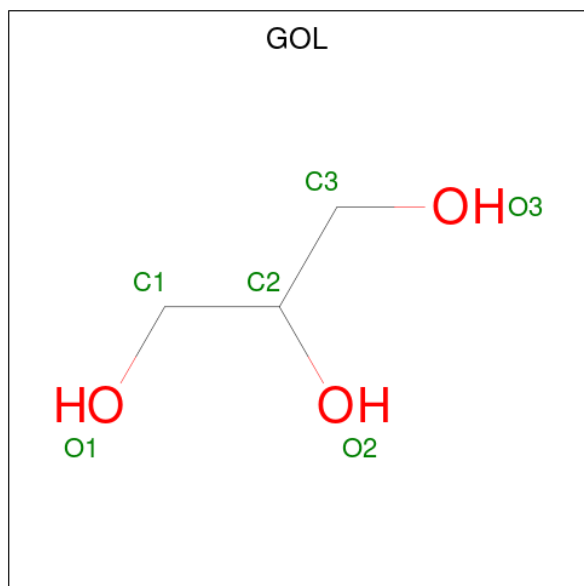
There are 4 unique types of molecules in this entry. The entry contains 9764 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EH1AB1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	P	S	0	0	0
			2407	1516	421	458	1	11			
1	B	315	Total	C	N	O	P	S	0	0	0
			2407	1516	421	458	1	11			
1	C	315	Total	C	N	O	P	S	0	0	0
			2407	1516	421	458	1	11			
1	D	315	Total	C	N	O	P	S	0	0	0
			2407	1516	421	458	1	11			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



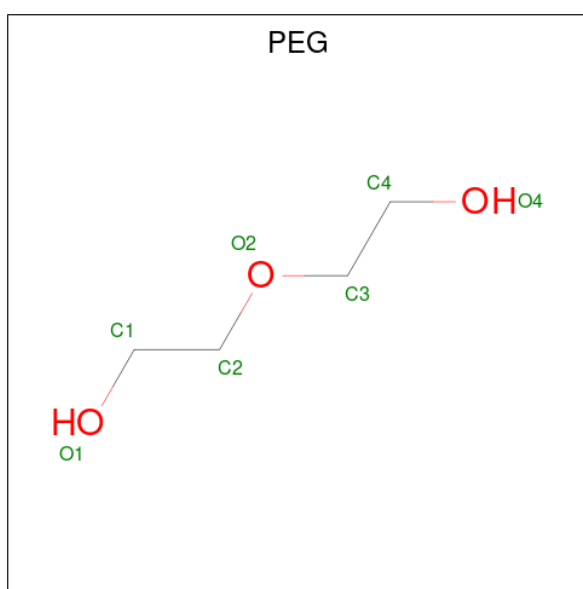
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is water.

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

Continued on next page...


Continued from previous page...

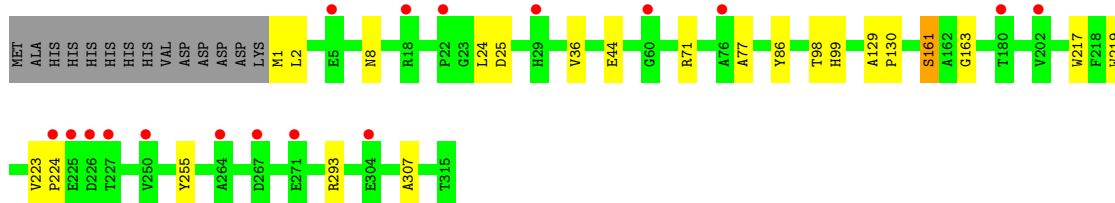
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	14	Total 14	O 14	0	0
4	C	19	Total 19	O 19	0	0
4	D	23	Total 23	O 23	0	0

3 Residue-property plots [i](#)

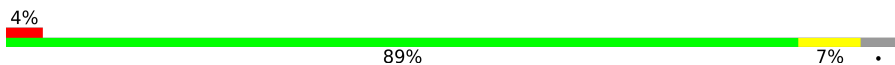
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

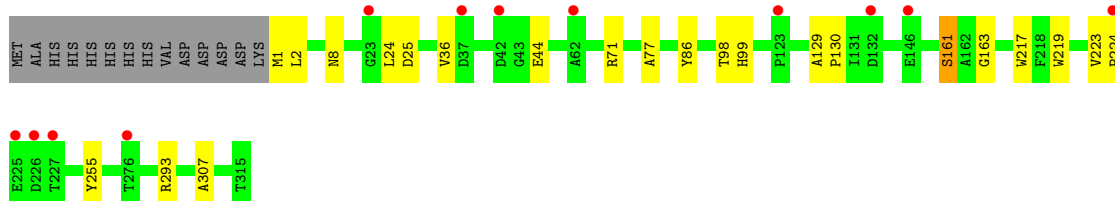
• Molecule 1: EH1AB1

Chain A: 




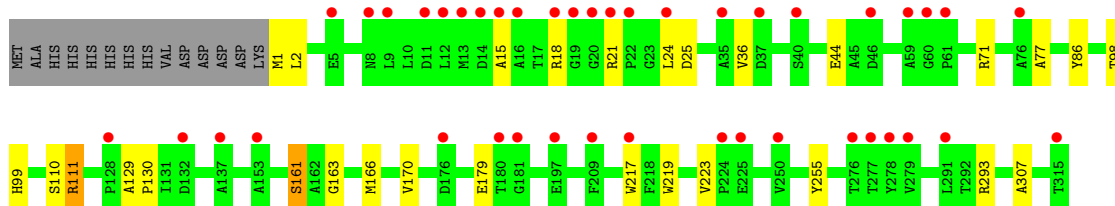
• Molecule 1: EH1AB1

Chain B: 




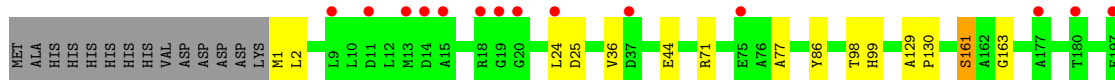
• Molecule 1: EH1AB1

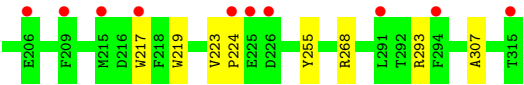
Chain C: 



• Molecule 1: EH1AB1

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.77Å 201.92Å 90.64Å 90.00° 112.19° 90.00°	Depositor
Resolution (Å)	49.08 – 2.79 49.08 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.08-2.79) 99.1 (49.08-2.79)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.239 , 0.276 0.241 , 0.279	Depositor DCC
R_{free} test set	1823 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9764	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3736e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PEG, GOL, K7K

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	0.68	0/2436	0.78	0/3307
1	B	0.68	0/2436	0.78	0/3307
1	C	0.69	0/2436	0.78	0/3307
1	D	0.69	0/2436	0.78	0/3307
All	All	0.69	0/9744	0.78	0/13228

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	2407	0	2293	18	0
1	B	2407	0	2293	18	0
1	C	2407	0	2293	19	0
1	D	2407	0	2293	16	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	12	0	16	0	0
2	D	12	0	16	0	0
3	C	21	0	30	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	7	0	10	0	0
4	A	16	0	0	0	0
4	B	14	0	0	0	0
4	C	19	0	0	1	0
4	D	23	0	0	1	0
All	All	9764	0	9260	66	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 3.

All (66) 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:B:307:ALA:HB1	1:D:307:ALA:HB1	1.38	1.02
1:A:307:ALA:HB1	1:C:307:ALA:HB1	1.45	0.99
1:C:161:K7K:O02	1:C:161:K7K:O03	2.16	0.64
1:B:161:K7K:O03	1:B:161:K7K:O02	2.16	0.63
1:A:161:K7K:O03	1:A:161:K7K:O02	2.16	0.63
1:D:161:K7K:O03	1:D:161:K7K:O02	2.16	0.63
1:D:268:ARG:HG2	4:D:507:HOH:O	2.01	0.58
1:A:98:THR:OG1	1:A:99:HIS:HD2	1.87	0.58
1:D:44:GLU:O	1:D:293:ARG:NH1	2.37	0.57
1:B:24:LEU:HD13	1:B:36:VAL:HG21	1.86	0.57
1:B:98:THR:OG1	1:B:99:HIS:HD2	1.87	0.57
1:D:98:THR:OG1	1:D:99:HIS:HD2	1.87	0.57
1:A:24:LEU:HD13	1:A:36:VAL:HG21	1.86	0.57
1:A:1:MET:HB2	1:A:255:TYR:OH	2.05	0.56
1:C:44:GLU:O	1:C:293:ARG:NH1	2.38	0.56
1:A:44:GLU:O	1:A:293:ARG:NH1	2.39	0.56
1:C:98:THR:OG1	1:C:99:HIS:HD2	1.87	0.56
1:B:44:GLU:O	1:B:293:ARG:NH1	2.39	0.56
1:A:8:ASN:HD22	1:B:8:ASN:ND2	2.05	0.55
1:A:219:TRP:CZ2	1:A:223:VAL:HG21	2.42	0.55
1:C:219:TRP:CZ2	1:C:223:VAL:HG21	2.43	0.54
1:C:1:MET:HB2	1:C:255:TYR:OH	2.07	0.54
1:D:219:TRP:CZ2	1:D:223:VAL:HG21	2.42	0.54
1:D:1:MET:HB2	1:D:255:TYR:OH	2.09	0.53
1:A:8:ASN:ND2	1:B:8:ASN:HD22	2.07	0.53
1:B:219:TRP:CZ2	1:B:223:VAL:HG21	2.44	0.53
1:B:1:MET:HB2	1:B:255:TYR:OH	2.09	0.52
1:C:110:SER:O	1:C:111:ARG:HB2	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HD13	1:A:36:VAL:CG2	2.40	0.51
1:A:71:ARG:NH2	1:A:77:ALA:O	2.44	0.51
1:C:25:ASP:HA	1:C:217:TRP:CD1	2.46	0.50
1:B:71:ARG:NH2	1:B:77:ALA:O	2.43	0.50
1:D:25:ASP:HA	1:D:217:TRP:CD1	2.47	0.49
1:A:25:ASP:HA	1:A:217:TRP:CD1	2.47	0.49
1:B:24:LEU:HD13	1:B:36:VAL:CG2	2.42	0.49
1:B:25:ASP:HA	1:B:217:TRP:CD1	2.48	0.49
1:C:24:LEU:HD13	1:C:36:VAL:HG21	1.95	0.49
1:A:8:ASN:HD22	1:B:8:ASN:HD22	1.59	0.48
1:D:86:TYR:O	1:D:163:GLY:HA3	2.14	0.48
1:D:71:ARG:NH2	1:D:77:ALA:O	2.44	0.48
1:A:86:TYR:O	1:A:163:GLY:HA3	2.13	0.48
1:B:86:TYR:O	1:B:163:GLY:HA3	2.14	0.47
1:C:1:MET:HG3	1:C:2:LEU:H	1.79	0.47
1:A:219:TRP:CE2	1:A:223:VAL:HG21	2.50	0.47
1:C:86:TYR:O	1:C:163:GLY:HA3	2.14	0.47
1:D:219:TRP:CE2	1:D:223:VAL:HG21	2.50	0.47
1:C:71:ARG:NH2	1:C:77:ALA:O	2.47	0.47
1:C:179:GLU:OE2	3:C:405:PEG:C2	2.63	0.47
1:A:1:MET:HG3	1:A:2:LEU:H	1.80	0.46
1:D:24:LEU:HD13	1:D:36:VAL:HG21	1.96	0.46
1:B:219:TRP:CE2	1:B:223:VAL:HG21	2.51	0.46
1:C:219:TRP:CE2	1:C:223:VAL:HG21	2.50	0.46
1:D:24:LEU:HD13	1:D:36:VAL:CG2	2.46	0.46
1:C:129:ALA:HB3	1:C:130:PRO:HD3	1.98	0.46
1:A:129:ALA:HB3	1:A:130:PRO:HD3	1.98	0.46
1:D:129:ALA:HB3	1:D:130:PRO:HD3	1.97	0.46
1:B:1:MET:HG3	1:B:2:LEU:H	1.82	0.45
1:B:129:ALA:HB3	1:B:130:PRO:HD3	1.98	0.45
1:C:24:LEU:HD13	1:C:36:VAL:CG2	2.46	0.45
1:C:21:ARG:HD3	4:C:508:HOH:O	2.16	0.45
1:D:1:MET:HG3	1:D:2:LEU:H	1.83	0.43
1:D:223:VAL:HA	1:D:224:PRO:HD2	1.91	0.43
1:A:223:VAL:HA	1:A:224:PRO:HD2	1.92	0.43
1:C:15:ALA:HA	1:C:18:ARG:NH1	2.33	0.43
1:B:223:VAL:HA	1:B:224:PRO:HD2	1.92	0.41
1:C:166:MET:O	1:C:170:VAL:HG23	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	312/329 (95%)	296 (95%)	16 (5%)	0	100	100
1	B	312/329 (95%)	299 (96%)	13 (4%)	0	100	100
1	C	312/329 (95%)	298 (96%)	14 (4%)	0	100	100
1	D	312/329 (95%)	299 (96%)	13 (4%)	0	100	100
All	All	1248/1316 (95%)	1192 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	237/250 (95%)	237 (100%)	0	100	100
1	B	237/250 (95%)	237 (100%)	0	100	100
1	C	237/250 (95%)	236 (100%)	1 (0%)	91	97
1	D	237/250 (95%)	237 (100%)	0	100	100
All	All	948/1000 (95%)	947 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	111	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	B	8	ASN
1	B	99	HIS
1	C	99	HIS
1	D	99	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
1	K7K	B	161	1	27,29,30	2.25	6 (22%)	30,38,40	4.90	14 (46%)
1	K7K	A	161	1	27,29,30	2.22	6 (22%)	30,38,40	4.90	14 (46%)
1	K7K	D	161	1	27,29,30	2.43	5 (18%)	30,38,40	4.93	14 (46%)
1	K7K	C	161	1	27,29,30	2.44	6 (22%)	30,38,40	4.93	14 (46%)

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
1	K7K	B	161	1	-	17/21/24/26	0/2/2/2
1	K7K	A	161	1	-	17/21/24/26	0/2/2/2
1	K7K	D	161	1	-	17/21/24/26	0/2/2/2
1	K7K	C	161	1	-	17/21/24/26	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	161	K7K	C08-C13	-8.17	1.36	1.49
1	A	161	K7K	C08-C13	-8.09	1.36	1.49
1	D	161	K7K	C08-C13	-8.09	1.36	1.49
1	B	161	K7K	C08-C13	-8.09	1.36	1.49
1	D	161	K7K	P01-O03	7.05	1.65	1.59
1	C	161	K7K	P01-O03	6.85	1.65	1.59
1	B	161	K7K	P01-O03	5.39	1.64	1.59
1	A	161	K7K	P01-O03	4.86	1.63	1.59
1	C	161	K7K	O02-C14	3.63	1.43	1.36
1	D	161	K7K	O03-C07	3.44	1.46	1.40
1	C	161	K7K	O03-C07	3.39	1.46	1.40
1	D	161	K7K	O02-C14	3.34	1.43	1.36
1	A	161	K7K	O03-C07	3.26	1.46	1.40
1	B	161	K7K	O03-C07	3.11	1.45	1.40
1	B	161	K7K	O02-C14	3.11	1.42	1.36
1	A	161	K7K	O02-C14	3.01	1.42	1.36
1	C	161	K7K	C07-C08	2.75	1.44	1.40
1	A	161	K7K	C07-C08	2.68	1.44	1.40
1	B	161	K7K	C07-C08	2.60	1.44	1.40
1	D	161	K7K	C07-C08	2.54	1.44	1.40
1	A	161	K7K	P01-OG	2.48	1.63	1.57
1	B	161	K7K	P01-OG	2.40	1.63	1.57
1	C	161	K7K	P01-OG	2.07	1.62	1.57

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	161	K7K	OG-CB-CA	14.71	122.46	108.14
1	D	161	K7K	OG-CB-CA	14.64	122.39	108.14
1	A	161	K7K	OG-CB-CA	14.51	122.27	108.14
1	B	161	K7K	OG-CB-CA	14.49	122.24	108.14
1	C	161	K7K	C07-C08-N01	-11.40	112.63	121.68
1	D	161	K7K	C07-C08-N01	-11.26	112.74	121.68
1	B	161	K7K	C07-C08-N01	-11.22	112.77	121.68
1	A	161	K7K	C07-C08-N01	-11.22	112.78	121.68
1	D	161	K7K	C10-N01-C08	9.17	134.76	116.81
1	B	161	K7K	C10-N01-C08	9.15	134.72	116.81
1	C	161	K7K	C10-N01-C08	9.15	134.72	116.81
1	D	161	K7K	C17-N02-C13	9.14	134.71	116.81
1	A	161	K7K	C10-N01-C08	9.12	134.67	116.81
1	C	161	K7K	C17-N02-C13	9.09	134.61	116.81
1	B	161	K7K	C17-N02-C13	9.06	134.55	116.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	K7K	C17-N02-C13	9.01	134.44	116.81
1	D	161	K7K	C14-C13-N02	-7.18	111.34	121.20
1	B	161	K7K	C14-C13-N02	-7.18	111.35	121.20
1	A	161	K7K	C14-C13-N02	-7.13	111.41	121.20
1	C	161	K7K	C14-C13-N02	-7.11	111.44	121.20
1	B	161	K7K	C11-C10-N01	-6.58	112.68	123.43
1	D	161	K7K	C11-C10-N01	-6.57	112.69	123.43
1	A	161	K7K	C11-C10-N01	-6.49	112.83	123.43
1	C	161	K7K	C11-C10-N01	-6.49	112.83	123.43
1	D	161	K7K	C16-C17-N02	-6.27	113.19	123.43
1	C	161	K7K	C16-C17-N02	-6.16	113.37	123.43
1	A	161	K7K	C16-C17-N02	-6.15	113.39	123.43
1	B	161	K7K	C16-C17-N02	-6.05	113.54	123.43
1	A	161	K7K	C14-C13-C08	5.19	127.61	121.53
1	B	161	K7K	C14-C13-C08	5.14	127.56	121.53
1	C	161	K7K	C14-C13-C08	5.09	127.50	121.53
1	D	161	K7K	C14-C13-C08	5.05	127.45	121.53
1	A	161	K7K	O03-P01-OG	4.16	111.77	102.99
1	B	161	K7K	O03-P01-OG	4.12	111.68	102.99
1	D	161	K7K	O03-P01-OG	4.09	111.62	102.99
1	C	161	K7K	O03-P01-OG	3.92	111.25	102.99
1	D	161	K7K	C08-C13-N02	3.23	121.20	114.84
1	B	161	K7K	C08-C13-N02	3.16	121.08	114.84
1	C	161	K7K	C08-C13-N02	3.14	121.04	114.84
1	A	161	K7K	C08-C13-N02	3.11	120.97	114.84
1	A	161	K7K	C15-C14-C13	2.70	120.54	118.30
1	B	161	K7K	O03-C07-C08	2.65	122.53	117.38
1	A	161	K7K	O03-C07-C08	2.62	122.48	117.38
1	D	161	K7K	C15-C14-C13	2.61	120.47	118.30
1	C	161	K7K	O03-C07-C08	2.57	122.38	117.38
1	D	161	K7K	OG-P01-O01	-2.55	106.85	114.21
1	B	161	K7K	C15-C14-C13	2.54	120.41	118.30
1	D	161	K7K	O03-C07-C08	2.48	122.21	117.38
1	A	161	K7K	C13-C08-N01	2.37	119.50	114.84
1	C	161	K7K	OG-P01-O01	-2.36	107.40	114.21
1	A	161	K7K	OG-P01-O01	-2.36	107.41	114.21
1	C	161	K7K	C15-C14-C13	2.36	120.25	118.30
1	B	161	K7K	C13-C08-N01	2.35	119.47	114.84
1	B	161	K7K	OG-P01-O01	-2.32	107.52	114.21
1	C	161	K7K	C13-C08-N01	2.30	119.38	114.84
1	D	161	K7K	C13-C08-N01	2.25	119.28	114.84

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	161	K7K	C07-C08-C13-C14
1	A	161	K7K	N01-C08-C13-N02
1	A	161	K7K	CB-OG-P01-C01
1	A	161	K7K	C02-C01-P01-OG
1	A	161	K7K	C02-C01-P01-O01
1	A	161	K7K	C02-C01-P01-O03
1	A	161	K7K	C07-O03-P01-O01
1	A	161	K7K	P01-C01-C02-C03
1	B	161	K7K	C07-C08-C13-C14
1	B	161	K7K	N01-C08-C13-N02
1	B	161	K7K	CB-OG-P01-C01
1	B	161	K7K	C02-C01-P01-OG
1	B	161	K7K	C02-C01-P01-O01
1	B	161	K7K	C02-C01-P01-O03
1	B	161	K7K	C07-O03-P01-O01
1	B	161	K7K	P01-C01-C02-C03
1	C	161	K7K	C07-C08-C13-C14
1	C	161	K7K	N01-C08-C13-N02
1	C	161	K7K	CB-OG-P01-C01
1	C	161	K7K	C02-C01-P01-OG
1	C	161	K7K	C02-C01-P01-O01
1	C	161	K7K	C02-C01-P01-O03
1	C	161	K7K	C07-O03-P01-O01
1	C	161	K7K	P01-C01-C02-C03
1	C	161	K7K	C08-C07-O03-P01
1	D	161	K7K	C07-C08-C13-C14
1	D	161	K7K	N01-C08-C13-N02
1	D	161	K7K	CB-OG-P01-C01
1	D	161	K7K	C02-C01-P01-OG
1	D	161	K7K	C02-C01-P01-O01
1	D	161	K7K	C02-C01-P01-O03
1	D	161	K7K	C07-O03-P01-O01
1	D	161	K7K	P01-C01-C02-C03
1	D	161	K7K	C08-C07-O03-P01
1	A	161	K7K	C07-O03-P01-OG
1	B	161	K7K	C07-O03-P01-OG
1	C	161	K7K	C07-O03-P01-OG
1	D	161	K7K	C07-O03-P01-OG
1	D	161	K7K	C02-C03-C04-C05
1	B	161	K7K	C02-C03-C04-C05
1	C	161	K7K	C02-C03-C04-C05
1	A	161	K7K	C02-C03-C04-C05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	161	K7K	CB-OG-P01-O01
1	B	161	K7K	CB-OG-P01-O01
1	C	161	K7K	CB-OG-P01-O01
1	D	161	K7K	CB-OG-P01-O01
1	C	161	K7K	C12-C07-O03-P01
1	D	161	K7K	C12-C07-O03-P01
1	A	161	K7K	C08-C07-O03-P01
1	B	161	K7K	C08-C07-O03-P01
1	A	161	K7K	C12-C07-O03-P01
1	B	161	K7K	C12-C07-O03-P01
1	C	161	K7K	C03-C04-C05-C06
1	B	161	K7K	C03-C04-C05-C06
1	D	161	K7K	C03-C04-C05-C06
1	A	161	K7K	N01-C08-C13-C14
1	A	161	K7K	C07-C08-C13-N02
1	B	161	K7K	N01-C08-C13-C14
1	B	161	K7K	C07-C08-C13-N02
1	C	161	K7K	N01-C08-C13-C14
1	C	161	K7K	C07-C08-C13-N02
1	D	161	K7K	N01-C08-C13-C14
1	D	161	K7K	C07-C08-C13-N02
1	A	161	K7K	C03-C04-C05-C06
1	A	161	K7K	C07-O03-P01-C01
1	B	161	K7K	C07-O03-P01-C01
1	D	161	K7K	C07-O03-P01-C01
1	C	161	K7K	C07-O03-P01-C01

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	161	K7K	1	0
1	A	161	K7K	1	0
1	D	161	K7K	1	0
1	C	161	K7K	1	0

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

10 ligands are 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	GOL	A	401	-	5,5,5	0.15	0	5,5,5	0.41	0
2	GOL	C	401	-	5,5,5	0.11	0	5,5,5	0.36	0
2	GOL	D	402	-	5,5,5	0.18	0	5,5,5	0.51	0
3	PEG	D	403	-	6,6,6	0.31	0	5,5,5	0.21	0
2	GOL	B	401	-	5,5,5	0.11	0	5,5,5	0.23	0
2	GOL	D	401	-	5,5,5	0.13	0	5,5,5	0.34	0
3	PEG	C	403	-	6,6,6	0.20	0	5,5,5	0.11	0
2	GOL	C	402	-	5,5,5	0.15	0	5,5,5	0.31	0
3	PEG	C	405	-	6,6,6	0.32	0	5,5,5	0.23	0
3	PEG	C	404	-	6,6,6	0.34	0	5,5,5	0.29	0

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	GOL	A	401	-	-	2/4/4/4	-
2	GOL	C	401	-	-	2/4/4/4	-
2	GOL	D	402	-	-	3/4/4/4	-
3	PEG	D	403	-	-	2/4/4/4	-
2	GOL	B	401	-	-	2/4/4/4	-
2	GOL	D	401	-	-	1/4/4/4	-
3	PEG	C	403	-	-	3/4/4/4	-
2	GOL	C	402	-	-	4/4/4/4	-
3	PEG	C	405	-	-	1/4/4/4	-
3	PEG	C	404	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GOL	O1-C1-C2-C3
2	B	401	GOL	O1-C1-C2-C3
2	C	401	GOL	C1-C2-C3-O3
2	D	402	GOL	C1-C2-C3-O3
2	B	401	GOL	O1-C1-C2-O2
3	C	403	PEG	O2-C3-C4-O4
3	C	405	PEG	O1-C1-C2-O2
3	D	403	PEG	O2-C3-C4-O4
2	C	402	GOL	C1-C2-C3-O3
2	C	401	GOL	O2-C2-C3-O3
3	D	403	PEG	O1-C1-C2-O2
2	A	401	GOL	O1-C1-C2-O2
3	C	403	PEG	O1-C1-C2-O2
2	D	402	GOL	O1-C1-C2-C3
3	C	404	PEG	O1-C1-C2-O2
3	C	403	PEG	C4-C3-O2-C2
2	C	402	GOL	O1-C1-C2-C3
2	C	402	GOL	O2-C2-C3-O3
3	C	404	PEG	C4-C3-O2-C2
2	D	402	GOL	O2-C2-C3-O3
2	C	402	GOL	O1-C1-C2-O2
2	D	401	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	405	PEG	1	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 ⓘ

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	314/329 (95%)	0.45	17 (5%)	25 17	25, 46, 74, 103	0
1	B	314/329 (95%)	0.39	12 (3%)	40 30	25, 47, 77, 111	0
1	C	314/329 (95%)	0.82	42 (13%)	3 1	32, 52, 90, 110	0
1	D	314/329 (95%)	0.61	24 (7%)	13 7	25, 48, 77, 116	0
All	All	1256/1316 (95%)	0.57	95 (7%)	13 7	25, 48, 80, 116	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	19	GLY	5.9
1	C	20	GLY	5.1
1	D	11	ASP	4.9
1	C	224	PRO	4.8
1	D	226	ASP	4.7
1	D	209	PHE	4.7
1	C	209	PHE	4.5
1	C	18	ARG	4.3
1	C	9	LEU	4.2
1	D	18	ARG	4.2
1	D	177	ALA	4.1
1	C	8	ASN	4.0
1	B	224	PRO	3.7
1	A	224	PRO	3.6
1	C	14	ASP	3.6
1	C	15	ALA	3.5
1	D	206	GLU	3.4
1	A	18	ARG	3.4
1	C	137	ALA	3.4
1	C	24	LEU	3.4
1	D	294	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	225	GLU	3.3
1	D	19	GLY	3.2
1	D	14	ASP	3.2
1	B	227	THR	3.2
1	C	37	ASP	3.1
1	C	59	ALA	3.0
1	C	291	LEU	3.0
1	D	225	GLU	3.0
1	C	277	THR	3.0
1	D	224	PRO	3.0
1	C	276	THR	3.0
1	D	24	LEU	2.9
1	C	225	GLU	2.8
1	C	278	TYR	2.8
1	C	176	ASP	2.8
1	A	225	GLU	2.8
1	A	250	VAL	2.8
1	D	315	THR	2.8
1	D	37	ASP	2.8
1	C	180	THR	2.8
1	C	128	PRO	2.8
1	C	11	ASP	2.7
1	B	23	GLY	2.7
1	C	46	ASP	2.7
1	C	279	VAL	2.6
1	D	197	GLU	2.6
1	D	217	TRP	2.6
1	C	16	ALA	2.6
1	C	315	THR	2.6
1	A	271	GLU	2.6
1	A	304	GLU	2.6
1	C	22	PRO	2.6
1	C	153	ALA	2.5
1	C	61	PRO	2.5
1	A	267	ASP	2.5
1	C	12	LEU	2.5
1	B	37	ASP	2.5
1	D	180	THR	2.5
1	D	13	MET	2.5
1	A	226	ASP	2.4
1	A	227	THR	2.4
1	C	250	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	264	ALA	2.4
1	C	217	TRP	2.4
1	A	180	THR	2.4
1	C	60	GLY	2.4
1	C	13	MET	2.3
1	C	40	SER	2.3
1	B	226	ASP	2.3
1	D	9	LEU	2.3
1	D	215	MET	2.3
1	D	20	GLY	2.2
1	B	146	GLU	2.2
1	C	5	GLU	2.2
1	D	15	ALA	2.2
1	B	276	THR	2.2
1	D	291	LEU	2.2
1	A	76	ALA	2.2
1	A	202	VAL	2.1
1	B	42	ASP	2.1
1	A	29	HIS	2.1
1	B	123	PRO	2.1
1	B	132	ASP	2.1
1	C	132	ASP	2.1
1	C	181	GLY	2.1
1	C	76	ALA	2.1
1	A	22	PRO	2.1
1	B	62	ALA	2.1
1	A	5	GLU	2.1
1	C	21	ARG	2.0
1	D	75	GLU	2.0
1	A	60	GLY	2.0
1	C	35	ALA	2.0
1	C	197	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	K7K	C	161	28/29	0.75	0.37	48,88,135,139	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	K7K	D	161	28/29	0.76	0.39	41,89,129,134	0
1	K7K	A	161	28/29	0.80	0.36	46,83,150,157	0
1	K7K	B	161	28/29	0.82	0.33	47,86,129,140	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
2	GOL	D	402	6/6	0.66	0.30	56,61,66,67	0
3	PEG	C	404	7/7	0.69	0.25	65,75,81,82	0
2	GOL	C	401	6/6	0.71	0.26	82,86,90,92	0
3	PEG	C	403	7/7	0.78	0.26	69,76,81,83	0
3	PEG	C	405	7/7	0.80	0.25	47,52,58,59	0
2	GOL	A	401	6/6	0.86	0.40	64,80,83,83	0
3	PEG	D	403	7/7	0.86	0.26	56,63,67,69	0
2	GOL	C	402	6/6	0.88	0.21	51,61,65,65	0
2	GOL	B	401	6/6	0.89	0.30	72,73,77,86	0
2	GOL	D	401	6/6	0.93	0.12	68,74,75,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.