



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2021 – 08:22 AM GMT

PDB ID : 6YQH
Title : GH146 beta-L-arabinofuranosidase bound to covalent inhibitor
Authors : McGregor, N.G.S.; Davies, G.J.
Deposited on : 2020-04-17
Resolution : 1.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.17.1.dev1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.17.1.dev1

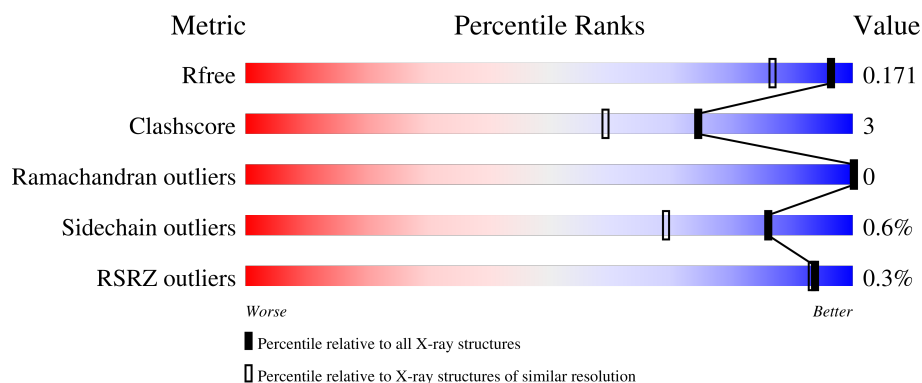
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.41 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	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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 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	AAA	802	

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	PEG	AAA	1201	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	FMT	AAA	1207	-	-	X	-
6	FMT	AAA	1215	-	-	X	-

2 Entry composition [i](#)

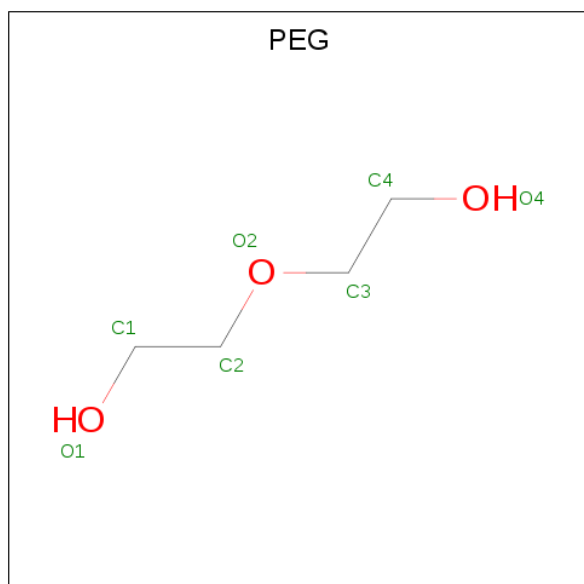
There are 8 unique types of molecules in this entry. The entry contains 13030 atoms, of which 6157 are hydrogens and 0 are deuteriums.

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 Acetyl-CoA carboxylase, biotin carboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	774	Total	C	H	N	O	S	390	20	1
			12285	3954	6074	1077	1153	27			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



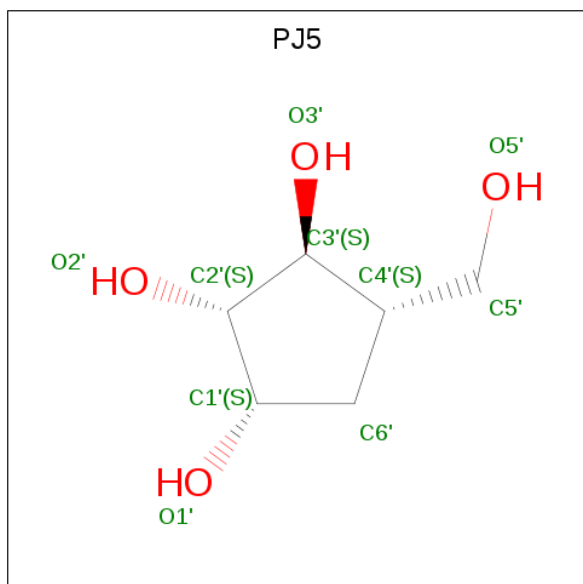
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	0	0
			11	3	6	2		
2	AAA	1	Total	C	H	O	1	0
			17	4	10	3		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	H	O	1	0
			24	6	14	4		

- Molecule 4 is (1 {S},2 {S},3 {S},4 {S})-4-(hydroxymethyl)cyclopentane-1,2,3-triol (three-letter code: PJ5) (formula: C₆H₁₂O₄) (labeled as "Ligand of Interest" by depositor).



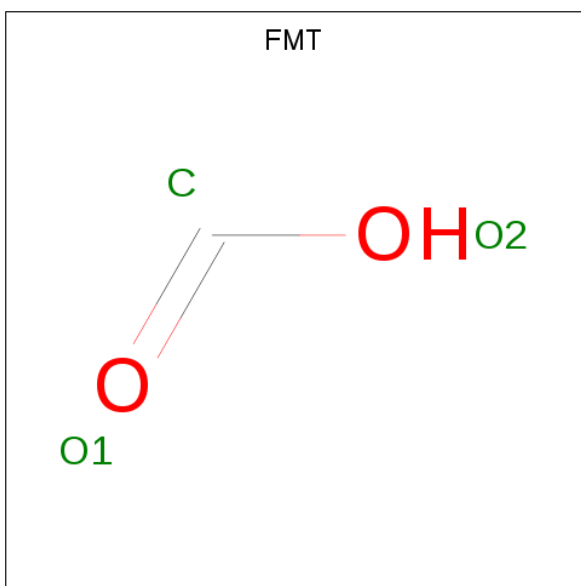
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	H	O	3	0
			22	6	12	4		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	AAA	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
6	AAA	1	Total	C	H	O	1	0
			5	1	2	2		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	1	Total	Zn	0	0
			1	1		

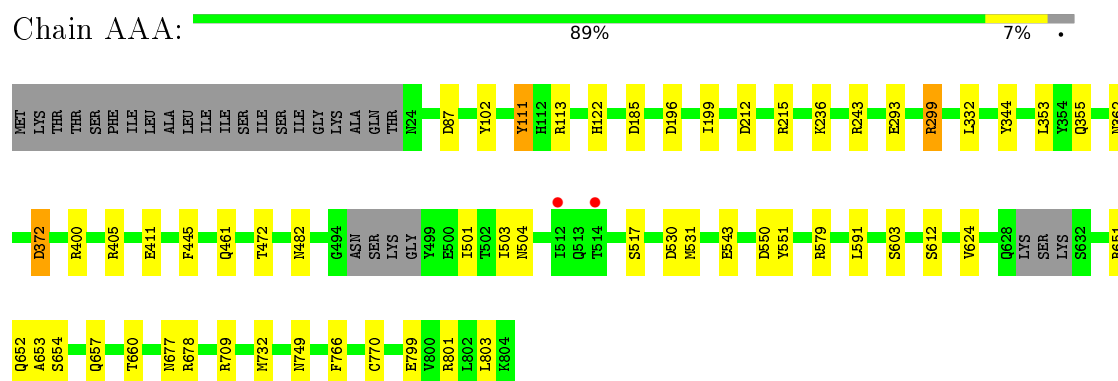
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	573	Total	O	0	2
			575	575		

3 Residue-property plots

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: Acetyl-CoA carboxylase, biotin carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.42Å 95.42Å 189.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.33 – 1.41 85.18 – 1.40	Depositor EDS
% Data completeness (in resolution range)	97.0 (85.33-1.41) 99.9 (85.18-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 1.39Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.129 , 0.170 0.130 , 0.171	Depositor DCC
R_{free} test set	8656 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	13030	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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: FMT, PEG, PJ5, MES, ZN, PGE

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	AAA	0.82	7/6422 (0.1%)	0.98	14/8718 (0.2%)

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	AAA	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	543	GLU	CD-OE2	-7.93	1.17	1.25
1	AAA	411	GLU	CD-OE2	7.90	1.34	1.25
1	AAA	799	GLU	CD-OE1	-6.66	1.18	1.25
1	AAA	550	ASP	CG-OD1	5.64	1.38	1.25
1	AAA	612	SER	CA-CB	-5.30	1.45	1.52
1	AAA	293	GLU	CD-OE1	5.15	1.31	1.25
1	AAA	372	ASP	CG-OD2	-5.11	1.13	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	400	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	AAA	405	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	AAA	405	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	AAA	243	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	AAA	299[A]	ARG	CG-CD-NE	-6.93	97.24	111.80
1	AAA	299[B]	ARG	CG-CD-NE	-6.93	97.24	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	243	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	AAA	579	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	AAA	299[A]	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	AAA	299[B]	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	AAA	624	VAL	CA-CB-CG1	5.70	119.44	110.90
1	AAA	678	ARG	CG-CD-NE	5.49	123.33	111.80
1	AAA	550	ASP	CB-CA-C	5.45	121.30	110.40
1	AAA	801	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	111	TYR	Sidechain

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	AAA	6211	6074	5971	36	1
2	AAA	12	16	15	6	0
3	AAA	10	14	14	0	0
4	AAA	10	12	0	0	0
5	AAA	12	13	13	0	0
6	AAA	42	28	16	10	0
7	AAA	1	0	0	0	0
8	AAA	575	0	0	7	0
All	All	6873	6157	6029	39	1

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 (39) 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:AAA:591[B]:LEU:HD21	8:AAA:1338:HOH:O	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:591[A]:LEU:HD11	8:AAA:1338:HOH:O	1.77	0.83
1:AAA:732:MET:HE3	1:AAA:803:LEU:HD11	1.72	0.72
1:AAA:653:ALA:HA	6:AAA:1215:FMT:H	1.74	0.70
1:AAA:651:ARG:NH1	1:AAA:652:GLN:O	2.25	0.69
1:AAA:122:HIS:HD2	8:AAA:1347:HOH:O	1.75	0.68
1:AAA:299[A]:ARG:HG2	1:AAA:353:LEU:HD22	1.78	0.66
1:AAA:504:ASN:HD21	1:AAA:530:ASP:HA	1.61	0.65
1:AAA:196:ASP:HB3	2:AAA:1201:PEG:H42	1.78	0.63
1:AAA:657:GLN:NE2	6:AAA:1215:FMT:O2	2.32	0.62
1:AAA:654:SER:H	6:AAA:1215:FMT:H	1.66	0.60
1:AAA:472:THR:CG2	1:AAA:531[A]:MET:HE3	2.35	0.56
1:AAA:654:SER:H	6:AAA:1215:FMT:C	2.18	0.55
2:AAA:1201:PEG:C2	8:AAA:1701:HOH:O	2.55	0.55
1:AAA:355:GLN:NE2	6:AAA:1217:FMT:O2	2.40	0.54
1:AAA:472:THR:HG21	1:AAA:531[A]:MET:CE	2.37	0.54
6:AAA:1214:FMT:C	8:AAA:1729:HOH:O	2.56	0.54
1:AAA:501:ILE:HD12	1:AAA:503:ILE:HG13	1.90	0.52
1:AAA:472:THR:HG21	1:AAA:531[A]:MET:HE3	1.93	0.51
1:AAA:770[A]:CYS:SG	8:AAA:1750:HOH:O	2.59	0.50
1:AAA:212:ASP:HA	6:AAA:1207:FMT:H	1.94	0.48
1:AAA:199:ILE:HB	2:AAA:1201:PEG:H41	1.95	0.48
1:AAA:372:ASP:OD2	1:AAA:517[B]:SER:OG	2.19	0.48
1:AAA:102:TYR:CE1	1:AAA:111:TYR:HB2	2.50	0.47
1:AAA:196:ASP:CB	2:AAA:1201:PEG:H42	2.45	0.46
1:AAA:732:MET:HE3	1:AAA:803:LEU:CD1	2.43	0.46
1:AAA:236:LYS:NZ	2:AAA:1201:PEG:C2	2.78	0.46
1:AAA:215:ARG:HE	6:AAA:1207:FMT:H	1.81	0.46
1:AAA:501:ILE:CD1	1:AAA:503:ILE:HG13	2.46	0.46
1:AAA:660:THR:HG23	8:AAA:1748:HOH:O	2.18	0.43
1:AAA:445:PHE:HA	1:AAA:461:GLN:OE1	2.18	0.43
1:AAA:677:ASN:HD22	6:AAA:1208:FMT:C	2.32	0.43
1:AAA:709:ARG:HD3	1:AAA:766:PHE:CE2	2.55	0.42
6:AAA:1211:FMT:O1	6:AAA:1218:FMT:C	2.67	0.41
1:AAA:531[A]:MET:HE3	1:AAA:531[A]:MET:HB3	1.98	0.41
1:AAA:113:ARG:HE	2:AAA:1202:PEG:H31	1.86	0.41
1:AAA:504:ASN:ND2	1:AAA:531[B]:MET:H	2.18	0.41
1:AAA:332:LEU:HD13	1:AAA:551:TYR:CD1	2.56	0.40

All (1) 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:AAA:185:ASP:OD2	1:AAA:603:SER:HG[3_444]	1.46	0.14

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	AAA	788/802 (98%)	770 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	651/697 (93%)	647 (99%)	4 (1%)	86	69

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	87	ASP
1	AAA	344	TYR
1	AAA	482	ASN
1	AAA	749	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	FMT	AAA	1207	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	1209	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	1213	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	1217	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	1212	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	1211	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	1210	-	0,2,2	0.00	-	0,1,1	0.00	-
5	MES	AAA	1205	-	12,12,12	0.67	0	14,16,16	0.61	0
6	FMT	AAA	1218	-	0,2,2	0.00	-	0,1,1	0.00	-
2	PEG	AAA	1202	-	6,6,6	0.50	0	5,5,5	0.46	0
2	PEG	AAA	1201	-	4,4,6	0.43	0	3,3,5	0.77	0
6	FMT	AAA	1219	-	0,2,2	0.00	-	0,1,1	0.00	-
3	PGE	AAA	1203	-	9,9,9	0.44	0	8,8,8	0.41	0
4	PJ5	AAA	1204	1	10,10,10	1.12	2 (20%)	10,14,14	1.47	2 (20%)
6	FMT	AAA	1216	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	1208	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	1215	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FMT	AAA	1206	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	AAA	1214	-	0,2,2	0.00	-	0,1,1	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	PGE	AAA	1203	-	-	3/7/7/7	-
4	PJ5	AAA	1204	1	-	2/2/18/18	0/1/1/1
2	PEG	AAA	1202	-	-	2/4/4/4	-
2	PEG	AAA	1201	-	-	1/2/2/4	-
5	MES	AAA	1205	-	-	3/6/14/14	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	1204	PJ5	C6'-C4'	2.31	1.59	1.53
4	AAA	1204	PJ5	O3'-C3'	2.16	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AAA	1204	PJ5	O5'-C5'-C4'	2.98	118.19	111.36
4	AAA	1204	PJ5	O1'-C1'-C2'	-2.16	107.17	111.27

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	1204	PJ5	C6'-C4'-C5'-O5'
4	AAA	1204	PJ5	C3'-C4'-C5'-O5'
5	AAA	1205	MES	C7-C8-S-O1S
5	AAA	1205	MES	C7-C8-S-O2S
5	AAA	1205	MES	C7-C8-S-O3S
3	AAA	1203	PGE	C4-C3-O2-C2
2	AAA	1202	PEG	O2-C3-C4-O4
2	AAA	1202	PEG	O1-C1-C2-O2
2	AAA	1201	PEG	O2-C3-C4-O4

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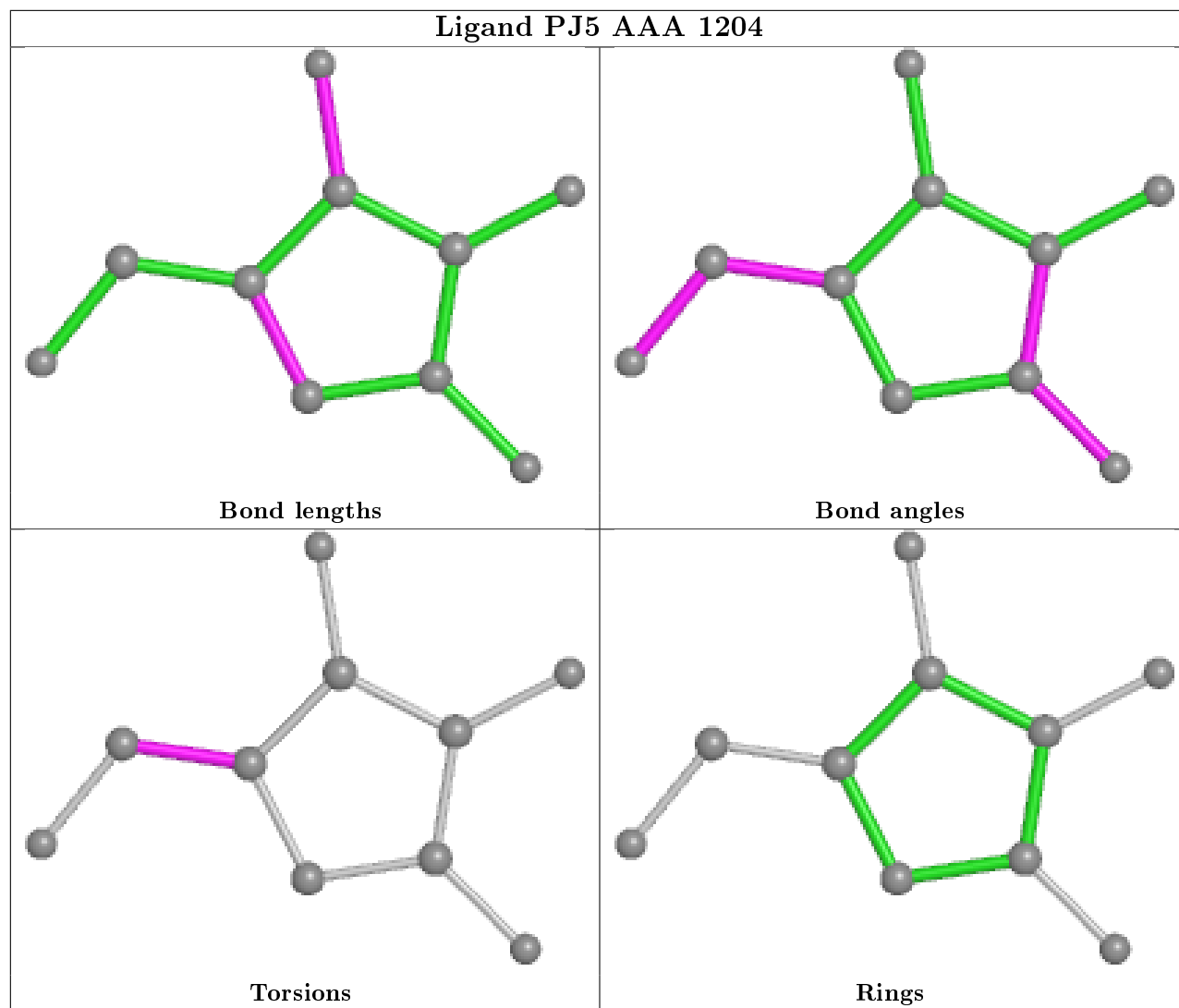
Mol	Chain	Res	Type	Atoms
3	AAA	1203	PGE	O2-C3-C4-O3
3	AAA	1203	PGE	C6-C5-O3-C4

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	AAA	1207	FMT	2	0
6	AAA	1217	FMT	1	0
6	AAA	1211	FMT	1	0
6	AAA	1218	FMT	1	0
2	AAA	1202	PEG	1	0
2	AAA	1201	PEG	5	0
6	AAA	1208	FMT	1	0
6	AAA	1215	FMT	4	0
6	AAA	1214	FMT	1	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](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	AAA	774/802 (96%)	-0.66	2 (0%) 94 93	13, 20, 34, 67	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	514	THR	3.8
1	AAA	512	ILE	3.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

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(Å ²)	Q<0.9
6	FMT	AAA	1217	3/3	0.76	0.17	25,27,31,33	5
6	FMT	AAA	1219	3/3	0.78	0.22	44,45,47,51	1
6	FMT	AAA	1211	3/3	0.80	0.17	41,43,50,54	1
6	FMT	AAA	1218	3/3	0.81	0.09	48,50,56,57	1
6	FMT	AAA	1207	3/3	0.82	0.33	38,38,45,52	1

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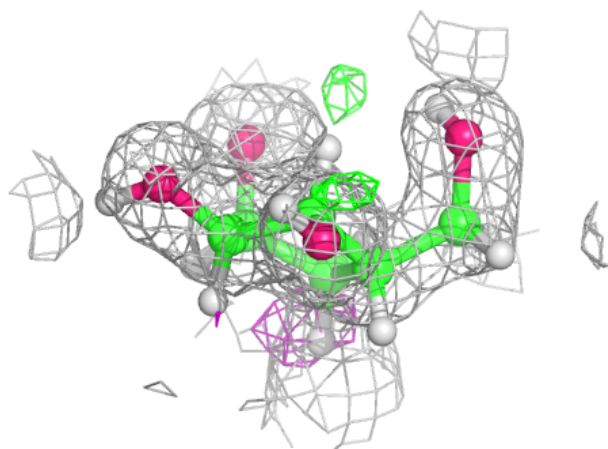
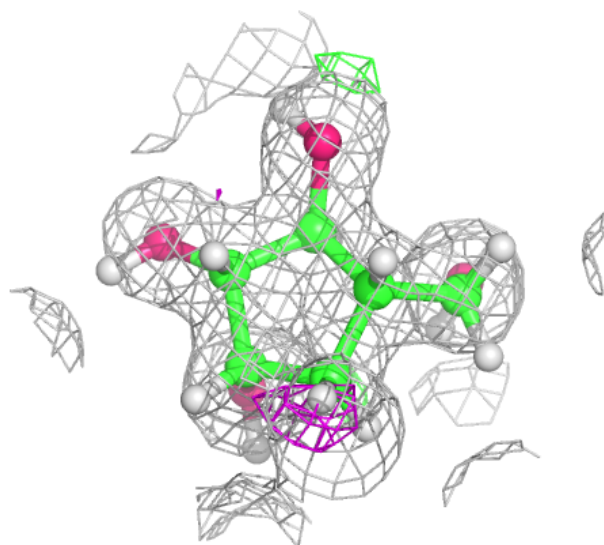
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PGE	AAA	1203	10/10	0.86	0.11	28,35,52,58	1
6	FMT	AAA	1210	3/3	0.88	0.08	43,46,52,55	1
6	FMT	AAA	1216	3/3	0.89	0.11	33,36,48,60	1
5	MES	AAA	1205	12/12	0.90	0.11	38,44,50,51	25
2	PEG	AAA	1202	7/7	0.91	0.10	33,42,46,51	1
6	FMT	AAA	1206	3/3	0.91	0.16	34,37,62,68	1
2	PEG	AAA	1201	5/7	0.91	0.13	19,22,23,25	11
6	FMT	AAA	1208	3/3	0.92	0.21	32,34,47,53	1
6	FMT	AAA	1212	3/3	0.92	0.14	33,35,50,58	1
6	FMT	AAA	1209	3/3	0.93	0.12	25,33,43,51	1
6	FMT	AAA	1213	3/3	0.94	0.20	30,33,43,54	1
6	FMT	AAA	1214	3/3	0.95	0.17	34,37,40,47	1
4	PJ5	AAA	1204	10/10	0.98	0.07	16,18,19,19	3
6	FMT	AAA	1215	3/3	0.98	0.21	26,30,47,52	1
7	ZN	AAA	1220	1/1	1.00	0.08	14,14,14,14	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PJ5 AAA 1204:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.