Full wwPDB X-ray Structure Validation Report (i)

Feb 27, 2024 – 06:15 pm GMT

PDB ID	:	6Q4Q
Title	:	The Crystal structure of CK2a bound to P2-C4
Authors	:	Brear, P.; Iegre, J.; Baker, D.; Tan, Y.; Sore, H.; Donovan, D.; Spring, D.; Chandra, V.; Hyvonen, M.
Deposited on	:	2018-12-06
Resolution	:	1.45 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 (i) 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 (i)) were used in the production of this report:

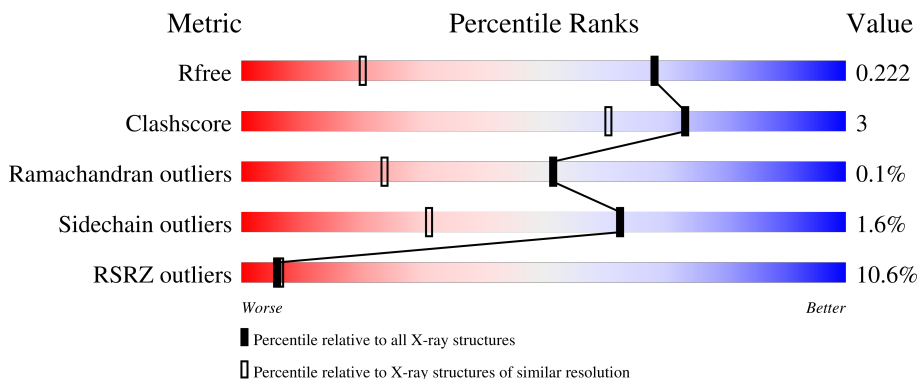|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
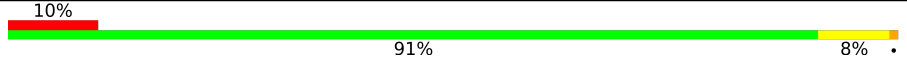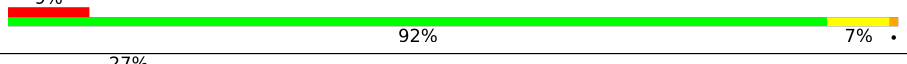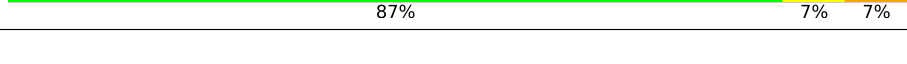*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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	Percentile Ranks	Value
Rfree		0.222
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		1.6%
RSRZ outliers		10.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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 <=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	327	10% / 91% 8% ·
1	B	327	9% / 92% 7% ·
2	C	15	27% / 87% 7% 7%
2	D	15	20% / 87% 7% 7%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 6406 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 Casein kinase II subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	9	0
			2830	1810	497	510	13			
1	B	327	Total	C	N	O	S	0	11	0
			2849	1821	499	516	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	SER	ARG	engineered mutation	UNP P68400
B	21	SER	ARG	engineered mutation	UNP P68400

- Molecule 2 is a protein called Stapled peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	0	0	1
			103	67	21	15			
2	D	15	Total	C	N	O	0	0	1
			103	67	21	15			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

- Molecule 4 is BENZOIC ACID (three-letter code: BEZ) (formula: $C_7H_6O_2$).

BEZ
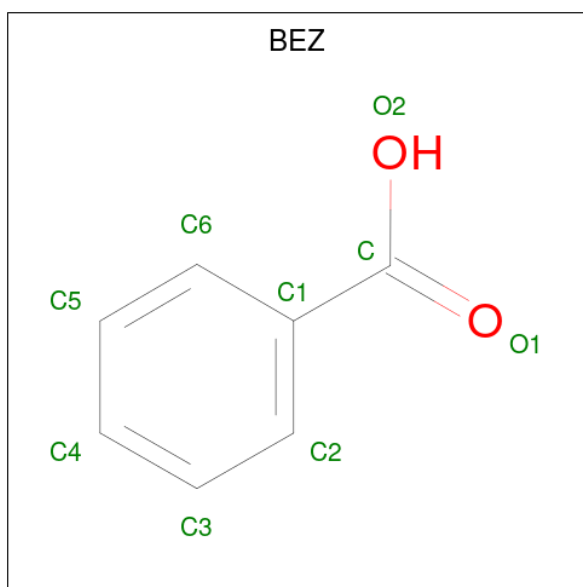
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 9	C 7	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 9	C 7	O 2	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0

- Molecule 6 is 3,5-bis(1-methyl-1,2,3-triazol-4-yl)benzoic acid (three-letter code: A1H27) (formula: $C_{13}H_{12}N_6O_2$) (labeled as "Ligand of Interest" by depositor).

A1H27

O5
O6 HO O
C23
C10 C9
C11 N3
C8 C7 N4
C15 C12 N2
N5 C14 C13 C6
C16 N1 N2 C5
N10 N11
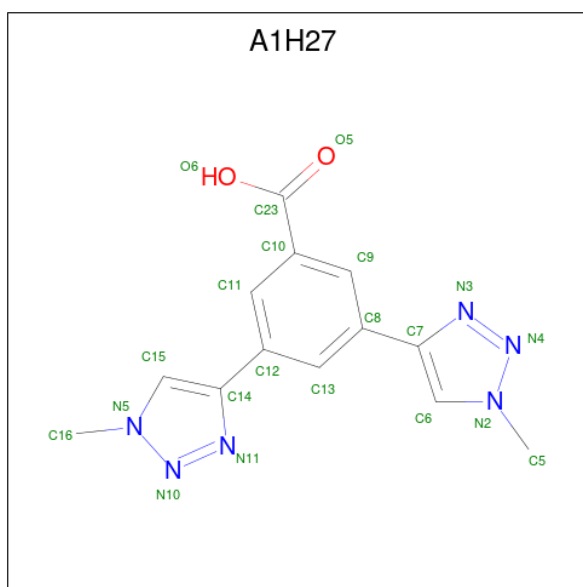
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			21	13	6	2		
6	D	1	Total	C	N	O	0	0
			21	13	6	2		

• Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	218	Total	O	0	0
			218	218		
7	B	200	Total	O	0	0
			200	200		
7	C	7	Total	O	0	0
			7	7		
7	D	10	Total	O	0	0
			10	10		

W O R L D W I D E
PDB
PROTEIN DATA BANK

3 Residue-property plots ⓘ

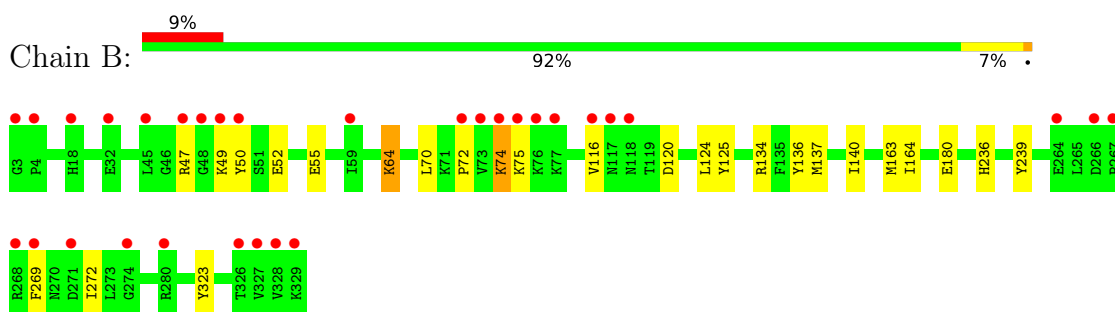These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.
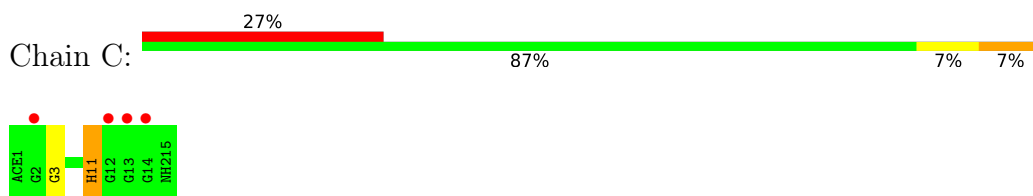
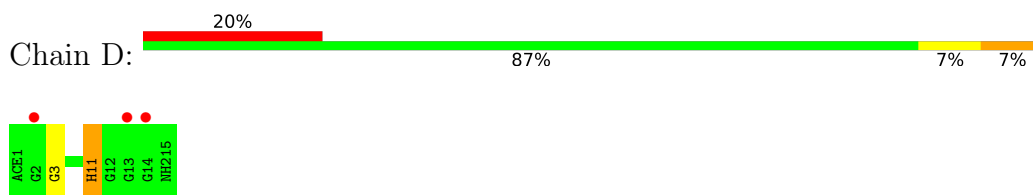• Molecule 1: Casein kinase II subunit alpha
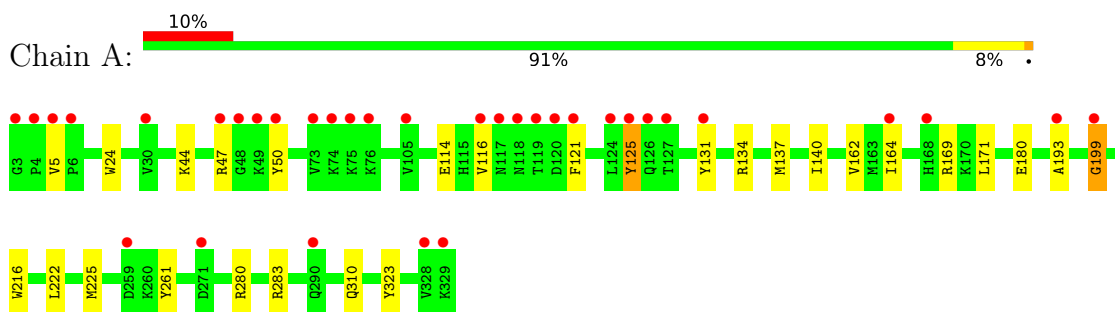
Chain A:

• Molecule 1: Casein kinase II subunit alpha

Chain B:

• Molecule 2: Stapled peptide

Chain C:

• Molecule 2: Stapled peptide

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.27Å 125.22Å 66.46Å 90.00° 92.60° 90.00°	Depositor
Resolution (Å)	66.39 – 1.45 66.39 – 1.44	Depositor EDS
% Data completeness (in resolution range)	98.4 (66.39-1.45) 98.5 (66.39-1.44)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 1.45Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.205 , 0.215 0.207 , 0.222	Depositor DCC
R_{free} test set	6995 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6406	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, NH2, BEZ, ACE, GOL, A1H27

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	0.57	1/2905 (0.0%)	0.63	0/3927
1	B	0.55	0/2924	0.62	0/3953
2	C	1.44	2/104 (1.9%)	1.26	4/137 (2.9%)
2	D	1.82	1/104 (1.0%)	1.17	1/137 (0.7%)
All	All	0.63	4/6037 (0.1%)	0.65	5/8154 (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 outliers	#Planarity outliers
2	C	0	1
2	D	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	11	HIS	C-N	17.01	1.63	1.33
2	C	11	HIS	C-N	10.36	1.51	1.33
1	A	199	GLY	C-N	8.41	1.50	1.34
2	C	3	GLY	C-N	7.47	1.51	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	GLY	O-C-N	7.51	134.72	122.70
2	C	11	HIS	O-C-N	-6.38	112.36	123.20
2	D	11	HIS	O-C-N	-5.67	113.56	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	GLY	C-N-CA	-5.23	108.62	121.70
2	C	3	GLY	CA-C-N	-5.07	106.05	117.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	11	HIS	Mainchain
2	D	11	HIS	Mainchain
2	D	3	GLY	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	2830	0	2767	21	0
1	B	2849	0	2781	20	0
2	C	103	0	93	0	0
2	D	103	0	93	0	0
3	A	6	0	8	0	0
3	B	12	0	16	2	0
4	A	9	0	5	0	0
4	B	9	0	5	0	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	C	21	0	0	0	0
6	D	21	0	0	0	0
7	A	218	0	0	0	0
7	B	200	0	0	0	0
7	C	7	0	0	0	0
7	D	10	0	0	0	0
All	All	6406	0	5774	39	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 (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:B:116:VAL:HG22	3:B:402:GOL:H32	1.76	0.67
1:A:131:TYR:HE1	1:A:169:ARG:HH22	1.43	0.66
1:B:116:VAL:HA	3:B:402:GOL:H11	1.77	0.66
1:B:124:LEU:HD23	1:B:164[B]:ILE:HD13	1.79	0.64
1:A:162:VAL:HG12	1:A:164:ILE:HD11	1.78	0.64
1:A:199:GLY:HA2	1:A:216:TRP:CD1	2.34	0.63
1:A:222:LEU:HA	1:A:225[B]:MET:HE2	1.82	0.62
1:A:261:TYR:OH	1:A:310[A]:GLN:HG3	2.02	0.60
1:A:114:GLU:O	1:A:114:GLU:HG3	2.01	0.59
1:B:137[B]:MET:HE2	1:B:140:ILE:HD12	1.88	0.56
1:B:72:PRO:HA	1:B:75:LYS:HG2	1.87	0.55
1:B:50:TYR:HB2	1:B:74:LYS:HB2	1.88	0.55
1:A:137[B]:MET:HE1	1:A:140:ILE:HD12	1.90	0.53
1:B:134:ARG:HG2	1:B:323:TYR:CZ	2.44	0.52
1:A:5:VAL:HG22	1:B:47:ARG:HB3	1.91	0.52
1:A:121:PHE:CE2	1:A:225[B]:MET:SD	3.05	0.49
1:A:44:LYS:NZ	1:A:47:ARG:HB2	2.29	0.48
1:B:124:LEU:CD2	1:B:164[B]:ILE:HD13	2.44	0.48
1:B:70:LEU:HB3	1:B:74:LYS:HG3	1.96	0.48
1:B:55:GLU:CG	1:B:64:LYS:HZ3	2.27	0.47
1:B:136:TYR:CZ	1:B:164[B]:ILE:HD11	2.49	0.47
1:A:44:LYS:HZ1	1:A:47:ARG:HB2	1.81	0.46
1:A:225[B]:MET:HB2	1:A:225[B]:MET:HE3	1.53	0.46
1:B:47:ARG:HG3	1:B:52:GLU:HG2	1.96	0.46
1:B:50:TYR:HB2	1:B:74:LYS:CB	2.45	0.46
1:A:199:GLY:CA	1:A:216:TRP:CD1	2.98	0.45
1:A:131:TYR:HE1	1:A:169:ARG:NH2	2.12	0.45
1:B:120:ASP:CB	1:B:163:MET:HE1	2.45	0.45
1:B:120:ASP:HB3	1:B:163:MET:HE1	1.98	0.45
1:B:64:LYS:HD2	1:B:64:LYS:HA	1.46	0.44
1:A:125:TYR:CD2	1:A:225[B]:MET:CG	3.01	0.44
1:B:239:TYR:HB3	1:B:272:ILE:HD11	2.00	0.44
1:A:24:TRP:CZ3	1:B:236:HIS:HD2	2.36	0.44
1:A:121:PHE:HA	1:A:164:ILE:HD13	2.01	0.43
1:B:55:GLU:CG	1:B:64:LYS:NZ	2.82	0.42
1:A:121:PHE:HB2	1:A:162:VAL:HB	2.02	0.42
1:A:134:ARG:HG2	1:A:323:TYR:CZ	2.55	0.41
1:A:280:ARG:H	1:A:283[B]:ARG:NH2	2.19	0.41
1:A:171:LEU:C	1:A:171:LEU:HD23	2.41	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	334/327 (102%)	324 (97%)	9 (3%)	1 (0%)	41	18
1	B	337/327 (103%)	326 (97%)	11 (3%)	0	100	100
2	C	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
2	D	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
All	All	697/684 (102%)	672 (96%)	24 (3%)	1 (0%)	51	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ALA

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	310/301 (103%)	306 (99%)	4 (1%)	69	40
1	B	313/301 (104%)	307 (98%)	6 (2%)	57	23
2	C	7/7 (100%)	7 (100%)	0	100	100
2	D	7/7 (100%)	7 (100%)	0	100	100
All	All	637/616 (103%)	627 (98%)	10 (2%)	62	31

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	TYR
1	A	116	VAL
1	A	125	TYR
1	A	180	GLU
1	B	49	LYS
1	B	64	LYS
1	B	74	LYS
1	B	125	TYR
1	B	180	GLU
1	B	269	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	36	GLN
1	A	117	ASN
1	A	118	ASN
1	A	270	ASN
1	B	36	GLN
1	B	117	ASN
1	B	118	ASN
1	B	186	GLN
1	B	236	HIS

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 ⓘ

9 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	$\#|Z| > 2$
3	GOL	A	501	-	5,5,5	0.22	0	5,5,5	0.27	0
3	GOL	B	403	-	5,5,5	0.07	0	5,5,5	0.41	0
6	A1H27	C	16	2	19,23,23	1.20	2 (10%)	21,33,33	1.25	2 (9%)
4	BEZ	B	404	-	9,9,9	1.21	2 (22%)	11,11,11	0.95	2 (18%)
3	GOL	B	402	-	5,5,5	0.19	0	5,5,5	0.31	0
5	ACT	A	503	-	3,3,3	1.33	0	3,3,3	1.16	0
4	BEZ	A	502	-	9,9,9	0.27	0	11,11,11	0.11	0
6	A1H27	D	16	2	19,23,23	1.11	2 (10%)	21,33,33	1.15	2 (9%)
5	ACT	B	401	-	3,3,3	1.49	0	3,3,3	1.20	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
3	GOL	A	501	-	-	0/4/4/4	-
3	GOL	B	403	-	-	1/4/4/4	-
6	A1H27	C	16	2	-	0/12/12/12	0/3/3/3
4	BEZ	B	404	-	-	0/4/4/4	0/1/1/1
3	GOL	B	402	-	-	1/4/4/4	-
4	BEZ	A	502	-	-	0/4/4/4	0/1/1/1
6	A1H27	D	16	2	-	0/12/12/12	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	16	A1H27	O6-C23	-2.96	1.21	1.30
6	D	16	A1H27	O5-C23	2.79	1.31	1.22
6	D	16	A1H27	O6-C23	-2.56	1.22	1.30
4	B	404	BEZ	O2-C	-2.56	1.22	1.30
4	B	404	BEZ	O1-C	2.48	1.30	1.22
6	C	16	A1H27	N11-N10	-2.07	1.30	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	16	A1H27	O6-C23-C10	2.96	122.52	114.85
6	C	16	A1H27	O5-C23-C10	-2.94	113.62	121.45
6	D	16	A1H27	O6-C23-C10	2.78	122.06	114.85
6	D	16	A1H27	O5-C23-C10	-2.55	114.66	121.45
4	B	404	BEZ	O2-C-C1	2.24	120.65	114.85
4	B	404	BEZ	O1-C-C1	-2.18	115.65	121.45

There are no chirality outliers.

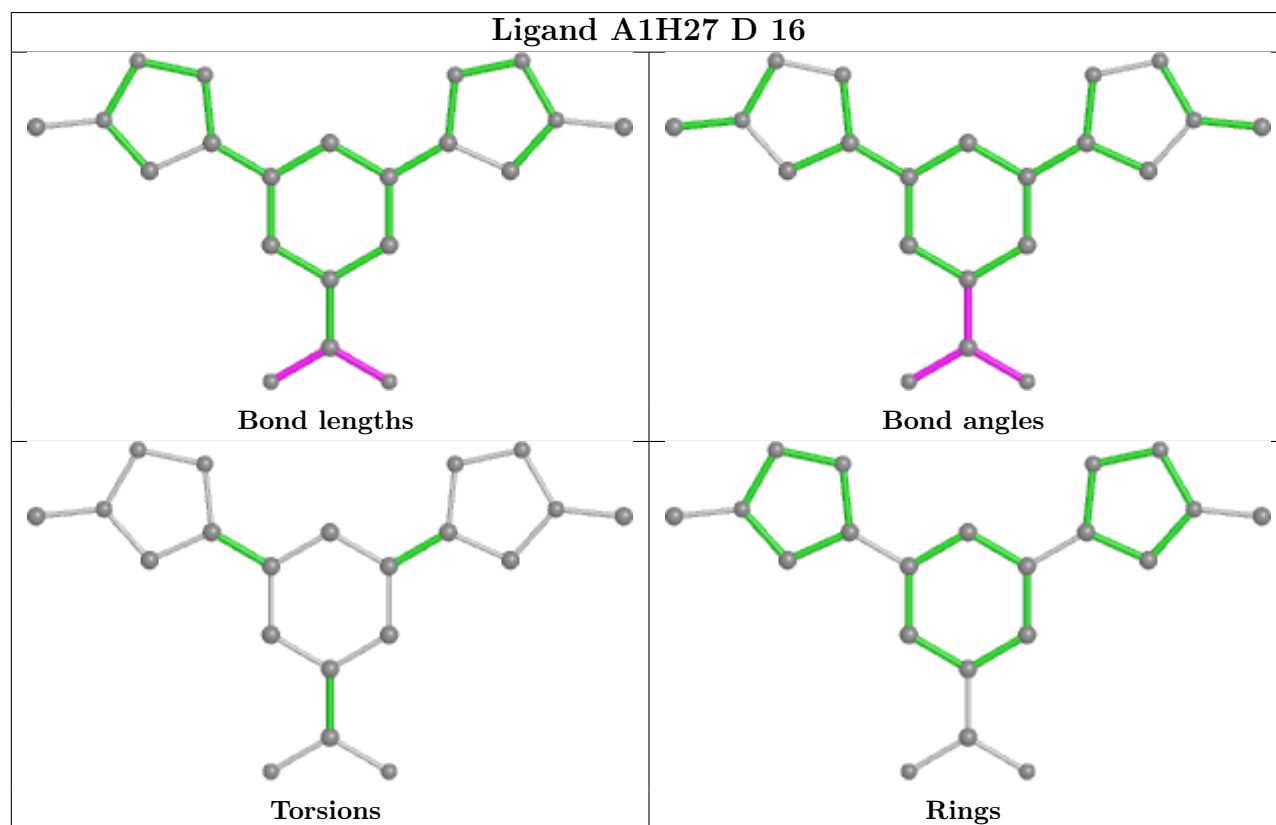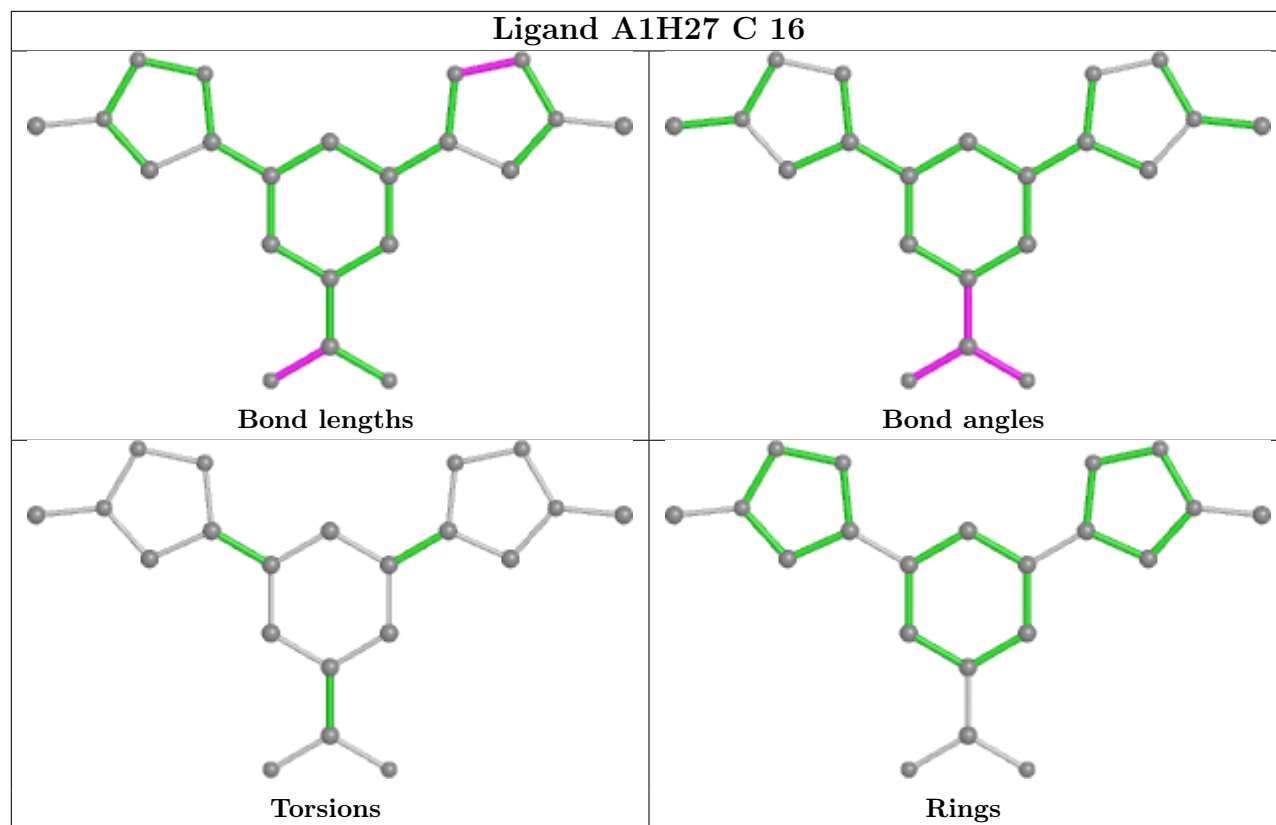All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	403	GOL	O1-C1-C2-C3
3	B	402	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	GOL	2	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 then 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.

Ligand A1H27 C 16

Bond lengths

Bond angles

Torsions

Rings

Ligand A1H27 D 16

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	11:HIS	C	12:GLY	N	1.63

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	327/327 (100%)	0.91	34 (10%)	6	7	9, 22, 55, 76	0
1	B	327/327 (100%)	0.76	31 (9%)	8	9	11, 23, 53, 97	0
2	C	13/15 (86%)	2.49	4 (30%)	0	0	21, 36, 68, 74	0
2	D	13/15 (86%)	2.29	3 (23%)	0	1	24, 33, 47, 49	0
All	All	680/684 (99%)	0.90	72 (10%)	6	6	9, 23, 54, 97	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	TYR	20.5
1	B	73	VAL	15.6
2	C	14	GLY	13.5
2	D	14	GLY	11.2
1	B	50	TYR	9.3
1	A	73	VAL	8.6
1	A	125	TYR	7.9
1	A	3	GLY	7.1
1	A	5	VAL	7.0
2	D	2	GLY	7.0
1	A	118	ASN	6.5
1	B	49	LYS	6.4
1	A	4	PRO	6.2
1	A	124	LEU	5.8
1	B	47	ARG	5.6
2	C	13	GLY	5.4
1	A	48	GLY	5.3
1	B	329	LYS	4.9
1	A	121	PHE	4.8
1	B	327	VAL	4.8
1	B	269	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
2	D	13	GLY	4.7
2	C	2	GLY	4.7
1	B	74	LYS	4.7
1	A	49	LYS	4.3
1	B	328	VAL	4.2
1	B	266	ASP	4.2
1	A	117	ASN	4.1
1	B	271	ASP	3.7
1	A	127	THR	3.7
1	A	6	PRO	3.6
1	B	48	GLY	3.5
1	A	74	LYS	3.4
1	A	47	ARG	3.3
1	A	328	VAL	3.3
1	A	75	LYS	3.2
1	B	75	LYS	3.2
1	B	77	LYS	3.1
1	A	168	HIS	3.1
1	A	116	VAL	3.1
1	A	199	GLY	3.1
1	A	329	LYS	3.0
1	B	268	ARG	2.9
1	B	118	ASN	2.7
1	B	72	PRO	2.7
1	A	193	ALA	2.7
1	A	119	THR	2.6
1	B	267	PRO	2.6
1	B	326[A]	THR	2.5
1	B	4	PRO	2.5
1	B	274	GLY	2.5
1	B	18	HIS	2.4
1	B	264	GLU	2.4
1	B	59	ILE	2.4
1	B	76	LYS	2.4
1	A	76	LYS	2.4
1	A	120	ASP	2.3
1	B	3	GLY	2.3
2	C	12	GLY	2.3
1	A	164	ILE	2.2
1	A	131	TYR	2.2
1	B	116	VAL	2.2
1	A	259	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	30	VAL	2.2
1	A	290[A]	GLN	2.2
1	B	117	ASN	2.2
1	B	32	GLU	2.2
1	B	280	ARG	2.1
1	A	271	ASP	2.1
1	A	126	GLN	2.1
1	B	45	LEU	2.0
1	A	105	VAL	2.0

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

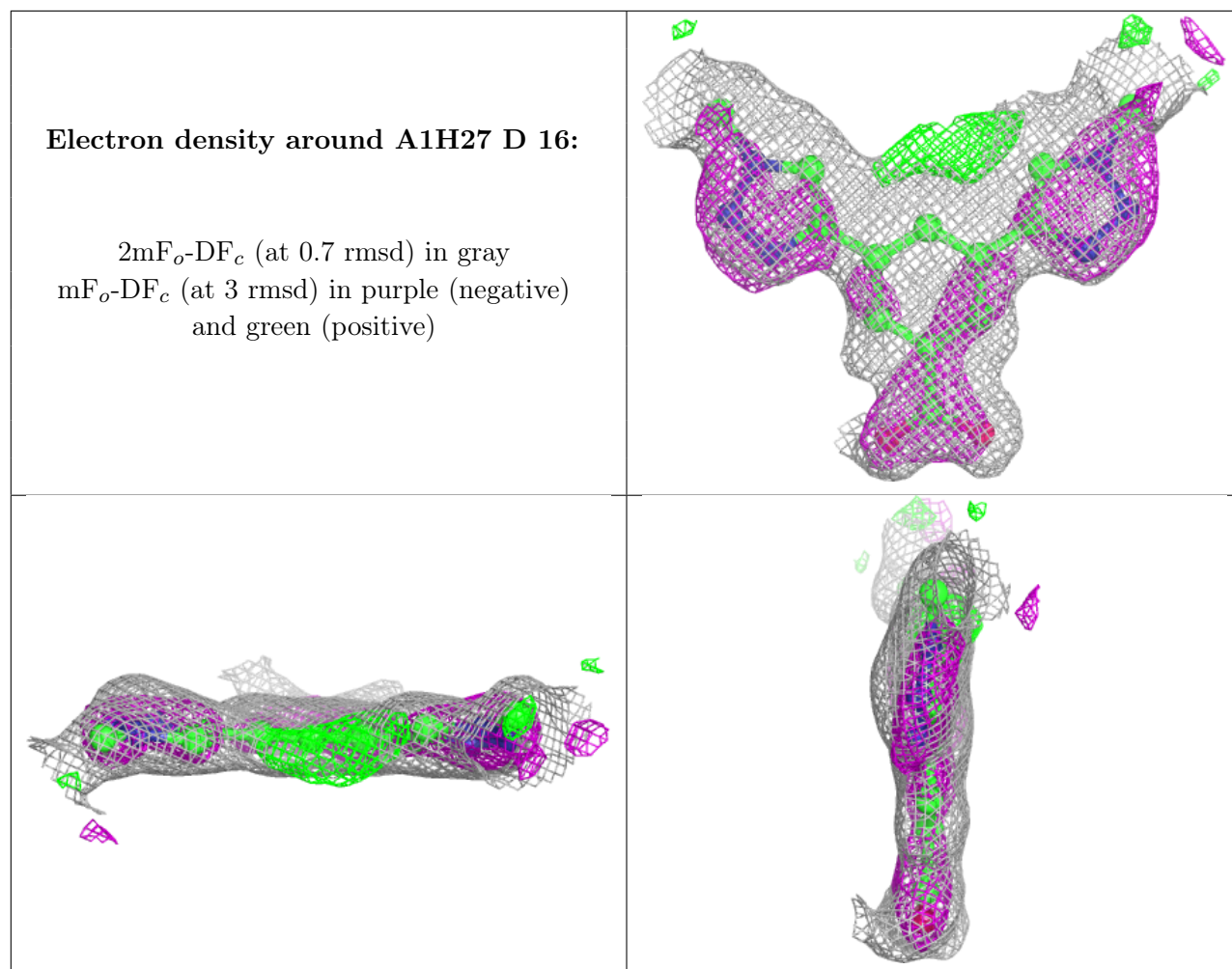There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

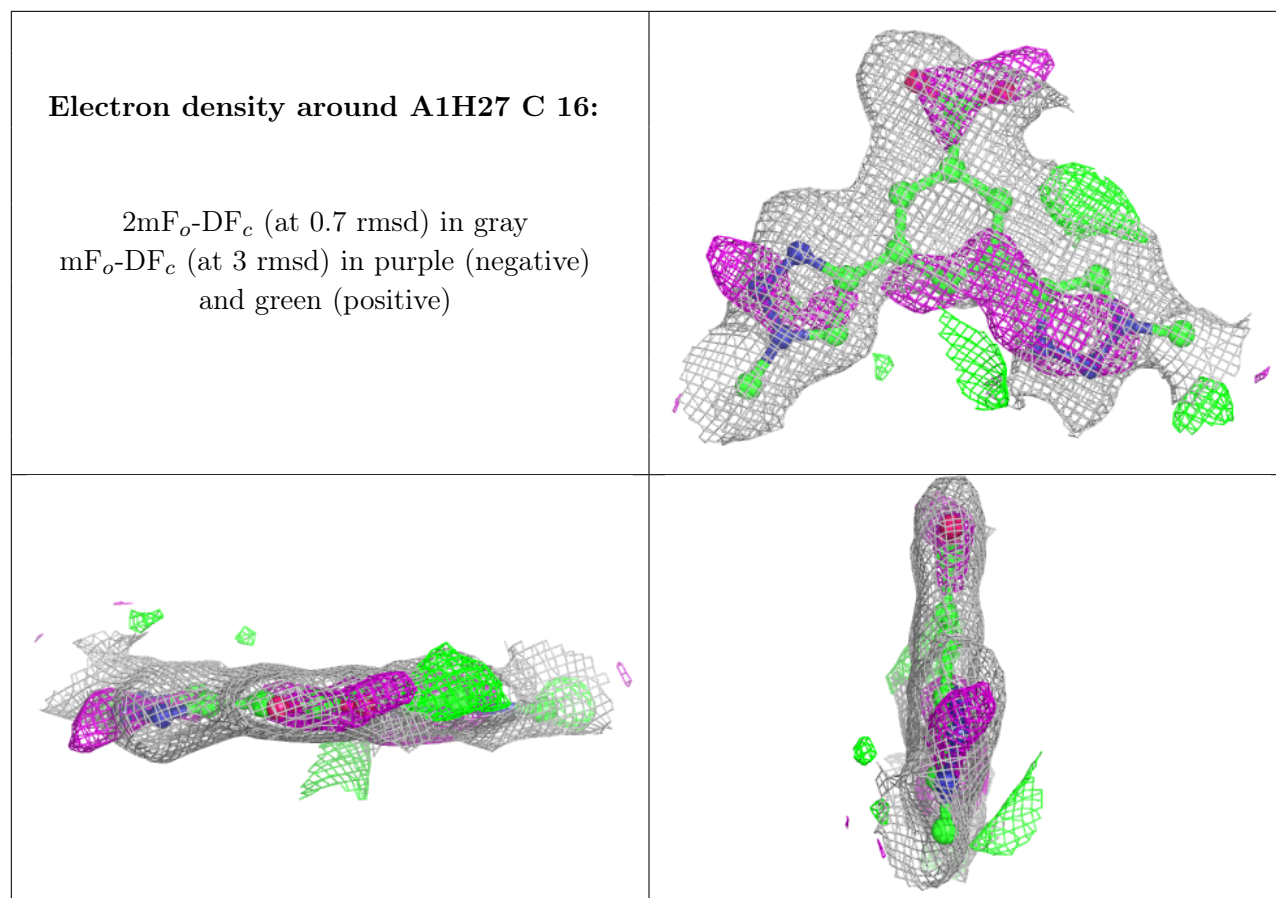## 6.4 Ligands ⓘ

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	A1H27	D	16	21/21	0.74	0.20	22,27,34,36	0
3	GOL	B	402	6/6	0.82	0.30	37,50,54,57	0
6	A1H27	C	16	21/21	0.83	0.14	25,28,34,44	0
5	ACT	B	401	4/4	0.84	0.17	22,32,36,36	0
5	ACT	A	503	4/4	0.86	0.15	24,34,37,38	0
3	GOL	A	501	6/6	0.86	0.11	26,30,36,39	0
3	GOL	B	403	6/6	0.87	0.13	31,39,45,47	0
4	BEZ	A	502	9/9	0.95	0.08	19,22,24,26	0
4	BEZ	B	404	9/9	0.96	0.08	17,19,21,21	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 A1H27 D 16:

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

Electron density around A1H27 C 16:

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 ⓘ

There are no such residues in this entry.