



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 12:01 am BST

PDB ID : 3ZG6
Title : The novel de-long chain fatty acid function of human sirt6
Authors : Wang, Y.; Hao, Q.
Deposited on : 2012-12-15
Resolution : 2.20 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 : 2.11
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) : 2.11

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2589 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 NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	294	2276	1434	418	412	12	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	VAL	conflict	UNP Q8N6T7

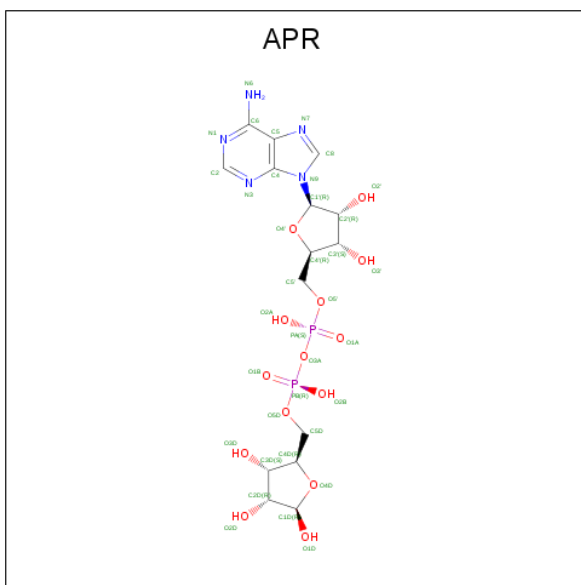
- Molecule 2 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	F	12	114	77	20	17	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

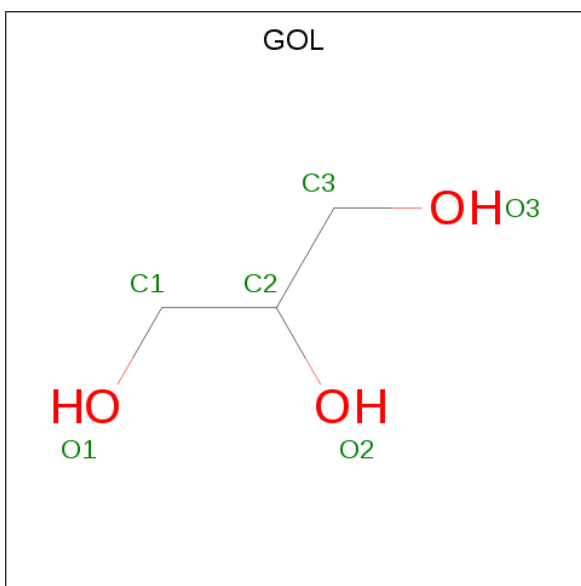
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: C₁₅H₂₃N₅O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	36	15	5	14	2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

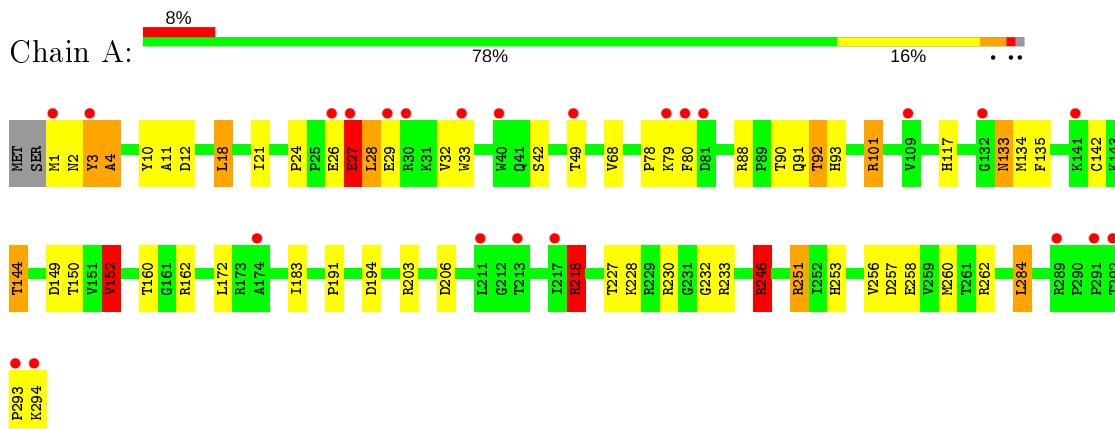
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	146	Total 146	O 146	0	0
6	F	4	Total 4	O 4	0	0

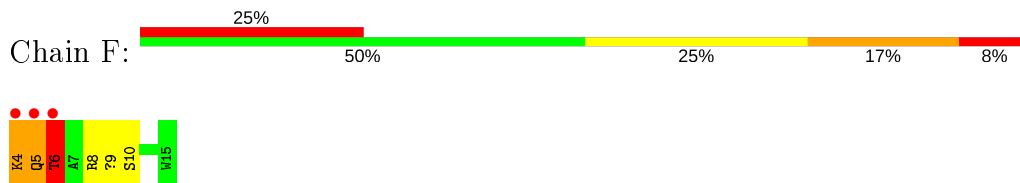
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-6



- Molecule 2: PEPTIDE



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	104.89Å 104.89Å 231.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.73 – 2.20 35.73 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (35.73-2.20) 99.0 (35.73-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.71 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.191 , 0.236 0.231 , 0.267	Depositor DCC
R_{free} test set	1268 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtrriage
Anisotropy	0.003	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2589	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: APR, GOL, ZN, MYK

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	1.10	3/2327 (0.1%)	1.15	14/3155 (0.4%)
2	F	1.35	0/92	0.98	0/122
All	All	1.11	3/2419 (0.1%)	1.14	14/3277 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	TYR	CE2-CZ	-7.34	1.29	1.38
1	A	10	TYR	CD1-CE1	-5.95	1.30	1.39
1	A	11	ALA	CA-CB	5.33	1.63	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ARG	NE-CZ-NH2	-16.48	112.06	120.30
1	A	246	ARG	NE-CZ-NH1	14.81	127.70	120.30
1	A	162	ARG	NE-CZ-NH2	-12.45	114.08	120.30
1	A	251	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	A	162	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	218	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	251	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	A	152	VAL	CG1-CB-CG2	6.40	121.14	110.90
1	A	18	LEU	CB-CG-CD1	5.98	121.16	111.00
1	A	218	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	27	GLU	N-CA-C	-5.40	96.42	111.00
1	A	12	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	246	ARG	CD-NE-CZ	5.13	130.78	123.60
1	A	203	ARG	NE-CZ-NH1	5.06	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

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	A	2276	0	2286	50	0
2	F	114	0	119	18	0
3	A	1	0	0	0	0
4	A	36	0	21	0	0
5	A	12	0	16	0	0
6	A	146	0	0	12	0
6	F	4	0	0	1	0
All	All	2589	0	2442	65	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 13.

All (65) 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)
2:F:10:SER:HB2	6:F:2003:HOH:O	1.23	1.36
1:A:142:CYS:SG	1:A:144:THR:HG23	2.00	1.01
6:A:2146:HOH:O	2:F:9:MYK:CE	2.15	0.94
6:A:2146:HOH:O	2:F:9:MYK:NZ	2.04	0.89
1:A:27:GLU:O	1:A:28:LEU:HB2	1.71	0.88
6:A:2146:HOH:O	2:F:9:MYK:CD	2.22	0.87
1:A:246:ARG:HD2	6:A:2127:HOH:O	1.77	0.85
1:A:88:ARG:NE	6:A:2048:HOH:O	2.09	0.85
1:A:27:GLU:O	1:A:28:LEU:CB	2.29	0.79
1:A:32:VAL:HG11	1:A:262:ARG:HB2	1.66	0.78
1:A:80:PHE:HZ	2:F:9:MYK:HQ	1.49	0.77
1:A:3:TYR:N	1:A:4:ALA:HB3	2.01	0.76
1:A:24:PRO:O	1:A:27:GLU:O	2.05	0.75
6:A:2146:HOH:O	2:F:9:MYK:HD	1.83	0.75
2:F:4:LYS:HG3	2:F:5:GLN:H	1.51	0.74
1:A:246:ARG:CD	6:A:2127:HOH:O	2.33	0.74
1:A:133:ASN:HD22	1:A:135:PHE:H	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4:LYS:CG	2:F:5:GLN:H	2.05	0.70
2:F:6:THR:HG23	2:F:8:ARG:H	1.56	0.70
1:A:92:THR:HB	1:A:260:MET:HG3	1.75	0.69
1:A:133:ASN:ND2	1:A:135:PHE:H	1.91	0.67
1:A:80:PHE:CZ	2:F:9:MYK:HQ	2.33	0.64
1:A:152:VAL:HG13	1:A:160:THR:HG21	1.82	0.61
1:A:133:ASN:C	1:A:133:ASN:HD22	2.06	0.59
1:A:142:CYS:SG	1:A:144:THR:CG2	2.87	0.59
2:F:9:MYK:HS	2:F:9:MYK:HPA	1.84	0.59
1:A:93:HIS:HE1	6:A:2037:HOH:O	1.84	0.58
1:A:33:TRP:CH2	1:A:294:LYS:HG3	2.39	0.57
1:A:218:ARG:NH2	6:A:2122:HOH:O	2.37	0.57
6:A:2146:HOH:O	2:F:9:MYK:CX	2.49	0.56
1:A:206:ASP:HB3	1:A:230:ARG:HH12	1.71	0.55
2:F:9:MYK:CP	2:F:9:MYK:HS	2.37	0.55
1:A:284:LEU:H	1:A:284:LEU:HD22	1.71	0.54
1:A:26:GLU:HG2	1:A:27:GLU:N	2.24	0.53
1:A:33:TRP:HH2	1:A:294:LYS:CD	2.20	0.53
1:A:80:PHE:HZ	2:F:9:MYK:CQ	2.20	0.53
1:A:90:THR:H	1:A:93:HIS:CD2	2.26	0.52
1:A:90:THR:H	1:A:93:HIS:HD2	1.57	0.52
1:A:152:VAL:HG13	1:A:160:THR:CG2	2.40	0.51
1:A:33:TRP:HH2	1:A:294:LYS:HD2	1.76	0.51
2:F:4:LYS:HG3	2:F:5:GLN:N	2.22	0.51
1:A:92:THR:HG23	1:A:257:ASP:OD1	2.12	0.50
2:F:4:LYS:CG	2:F:5:GLN:N	2.74	0.50
1:A:42:SER:HB3	1:A:206:ASP:OD1	2.13	0.49
1:A:29:GLU:HG3	1:A:262:ARG:HH12	1.76	0.49
1:A:68:VAL:HG13	1:A:78:PRO:HG3	1.96	0.48
1:A:92:THR:HG22	1:A:257:ASP:HA	1.95	0.47
1:A:92:THR:HG21	1:A:256:VAL:HB	1.97	0.47
1:A:92:THR:CG2	1:A:257:ASP:OD1	2.63	0.47
1:A:258:GLU:O	1:A:262:ARG:HG2	2.14	0.46
1:A:91:GLN:NE2	1:A:91:GLN:HA	2.30	0.46
1:A:2:ASN:C	1:A:4:ALA:HB3	2.36	0.46
2:F:4:LYS:CD	2:F:5:GLN:H	2.31	0.44
1:A:191:PRO:HG2	1:A:194:ASP:HB2	1.99	0.44
1:A:134:MET:HA	1:A:183:ILE:HD11	2.00	0.43
1:A:133:ASN:HD22	1:A:134:MET:N	2.16	0.43
2:F:4:LYS:HD2	2:F:5:GLN:H	1.83	0.43
1:A:246:ARG:HD3	6:A:2127:HOH:O	2.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ILE:O	1:A:253:HIS:HB3	2.19	0.43
1:A:117:HIS:HD2	6:A:2054:HOH:O	2.01	0.42
1:A:101:ARG:HE	1:A:101:ARG:HA	1.85	0.42
1:A:227:THR:HG22	1:A:232:GLY:HA3	2.02	0.42
1:A:49:THR:OG1	1:A:117:HIS:HE1	2.04	0.41
1:A:21:ILE:HB	1:A:253:HIS:CD2	2.56	0.41
1:A:293:PRO:O	1:A:294:LYS:CE	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	292/296 (99%)	282 (97%)	8 (3%)	2 (1%)	22	22
2	F	9/12 (75%)	7 (78%)	1 (11%)	1 (11%)	0	0
All	All	301/308 (98%)	289 (96%)	9 (3%)	3 (1%)	15	14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	4	ALA
2	F	6	THR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	241/248 (97%)	222 (92%)	19 (8%)	12	12
2	F	8/8 (100%)	5 (62%)	3 (38%)	0	0
All	All	249/256 (97%)	227 (91%)	22 (9%)	10	10

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	TYR
1	A	18	LEU
1	A	27	GLU
1	A	79	LYS
1	A	92	THR
1	A	101	ARG
1	A	133	ASN
1	A	144	THR
1	A	149	ASP
1	A	150	THR
1	A	152	VAL
1	A	172	LEU
1	A	218	ARG
1	A	228	LYS
1	A	233	ARG
1	A	246	ARG
1	A	251	ARG
1	A	284	LEU
2	F	4	LYS
2	F	5	GLN
2	F	6	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	93	HIS
1	A	117	HIS
1	A	133	ASN
1	A	222	ASN
1	A	240	GLN

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Mol	Chain	Res	Type
1	A	253	HIS
2	F	5	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MYK	F	9	2	22,23,24	0.93	1 (4%)	19,24,26	3.59	5 (26%)

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	MYK	F	9	2	-	13/22/23/25	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	9	MYK	CY-CX	-3.00	1.45	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	9	MYK	CE-NZ-CX	12.74	146.48	122.84
2	F	9	MYK	CY-CX-NZ	5.43	125.56	116.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	9	MYK	OX-CX-NZ	-4.15	115.17	123.01
2	F	9	MYK	CD-CE-NZ	-3.55	102.06	112.21
2	F	9	MYK	CT-CY-CX	-2.71	105.66	113.26

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	9	MYK	CI-CT-CY-CX
2	F	9	MYK	CY-CX-NZ-CE
2	F	9	MYK	OX-CX-NZ-CE
2	F	9	MYK	CG-CD-CE-NZ
2	F	9	MYK	CU-CQ-CS-CW
2	F	9	MYK	CI-CK-CL-CM
2	F	9	MYK	CK-CI-CT-CY
2	F	9	MYK	CQ-CS-CW-CV
2	F	9	MYK	CK-CL-CM-CP
2	F	9	MYK	CP-CR-CU-CQ
2	F	9	MYK	CL-CM-CP-CR
2	F	9	MYK	CM-CP-CR-CU
2	F	9	MYK	CS-CQ-CU-CR

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	9	MYK	10	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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
5	GOL	A	1299	-	5,5,5	0.37	0	5,5,5	1.29	0
5	GOL	A	1298	-	5,5,5	0.68	0	5,5,5	0.54	0
4	APR	A	1296	-	34,39,39	1.18	2 (5%)	40,60,60	2.82	13 (32%)

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
5	GOL	A	1299	-	-	2/4/4/4	-
5	GOL	A	1298	-	-	2/4/4/4	-
4	APR	A	1296	-	-	1/18/54/54	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1296	APR	O4'-C1'	3.62	1.46	1.41
4	A	1296	APR	C2-N1	2.22	1.38	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1296	APR	O1D-C1D-O4D	10.55	124.65	111.13
4	A	1296	APR	N3-C2-N1	-6.19	119.00	128.68
4	A	1296	APR	O4D-C1D-C2D	5.91	111.73	104.46
4	A	1296	APR	O2D-C2D-C1D	-5.72	96.04	111.82
4	A	1296	APR	C2-N1-C6	4.36	126.22	118.75
4	A	1296	APR	O2'-C2'-C1'	-3.05	99.60	110.85
4	A	1296	APR	PB-O3A-PA	-2.93	122.77	132.83
4	A	1296	APR	O3'-C3'-C4'	-2.85	102.80	111.05
4	A	1296	APR	O2D-C2D-C3D	-2.57	103.52	111.82
4	A	1296	APR	O4'-C1'-C2'	-2.54	103.21	106.93
4	A	1296	APR	C5'-C4'-C3'	-2.44	106.02	115.18
4	A	1296	APR	C2'-C3'-C4'	2.40	107.31	102.64
4	A	1296	APR	O2A-PA-O1A	2.28	123.49	112.24

There are no chirality outliers.

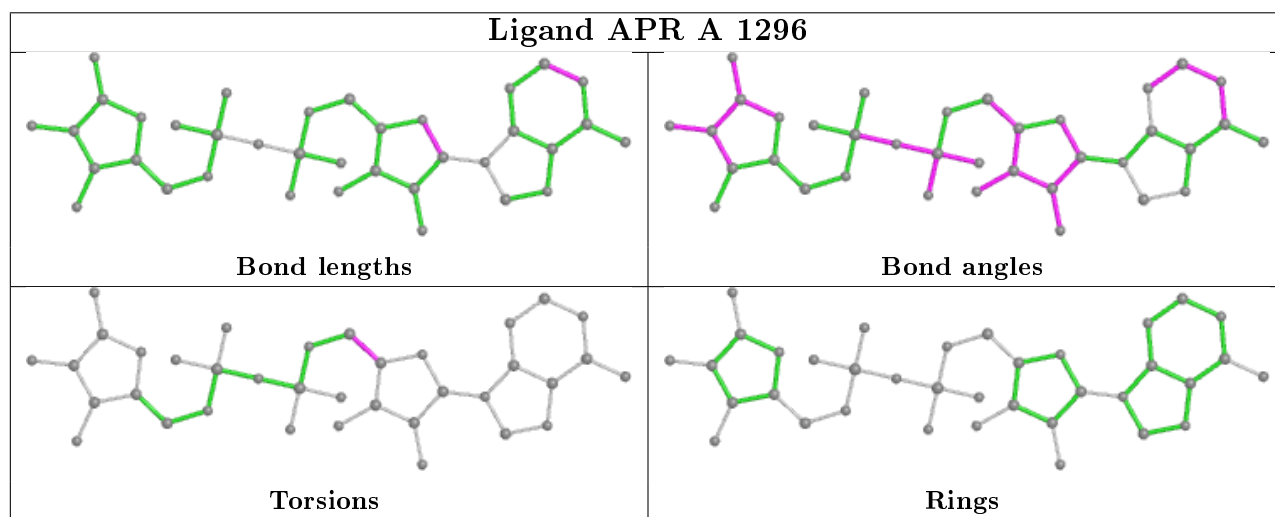
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1299	GOL	O1-C1-C2-C3
5	A	1298	GOL	O1-C1-C2-C3
5	A	1299	GOL	O1-C1-C2-O2
5	A	1298	GOL	O1-C1-C2-O2
4	A	1296	APR	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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

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	294/296 (99%)	0.41	24 (8%) 11 10	16, 38, 67, 106	0
2	F	11/12 (91%)	1.50	3 (27%) 0 0	39, 57, 89, 94	0
All	All	305/308 (99%)	0.45	27 (8%) 9 8	16, 39, 69, 106	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	4	LYS	6.7
1	A	80	PHE	5.7
1	A	293	PRO	5.0
1	A	294	LYS	4.8
1	A	33	TRP	4.4
1	A	40	TRP	4.2
1	A	291	PRO	4.0
1	A	174	ALA	3.9
1	A	1	MET	3.9
2	F	6	THR	3.5
1	A	81	ASP	3.3
1	A	292	THR	3.2
1	A	26	GLU	3.1
2	F	5	GLN	2.9
1	A	79	LYS	2.9
1	A	141	LYS	2.6
1	A	29	GLU	2.3
1	A	217	ILE	2.3
1	A	27	GLU	2.2
1	A	211	LEU	2.2
1	A	3	TYR	2.2
1	A	109	VAL	2.1
1	A	289	ARG	2.1
1	A	49	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	30	ARG	2.0
1	A	213	THR	2.0
1	A	132	GLY	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
2	MYK	F	9	24/25	0.95	0.23	35,47,67,69	0

6.3 Carbohydrates [i](#)

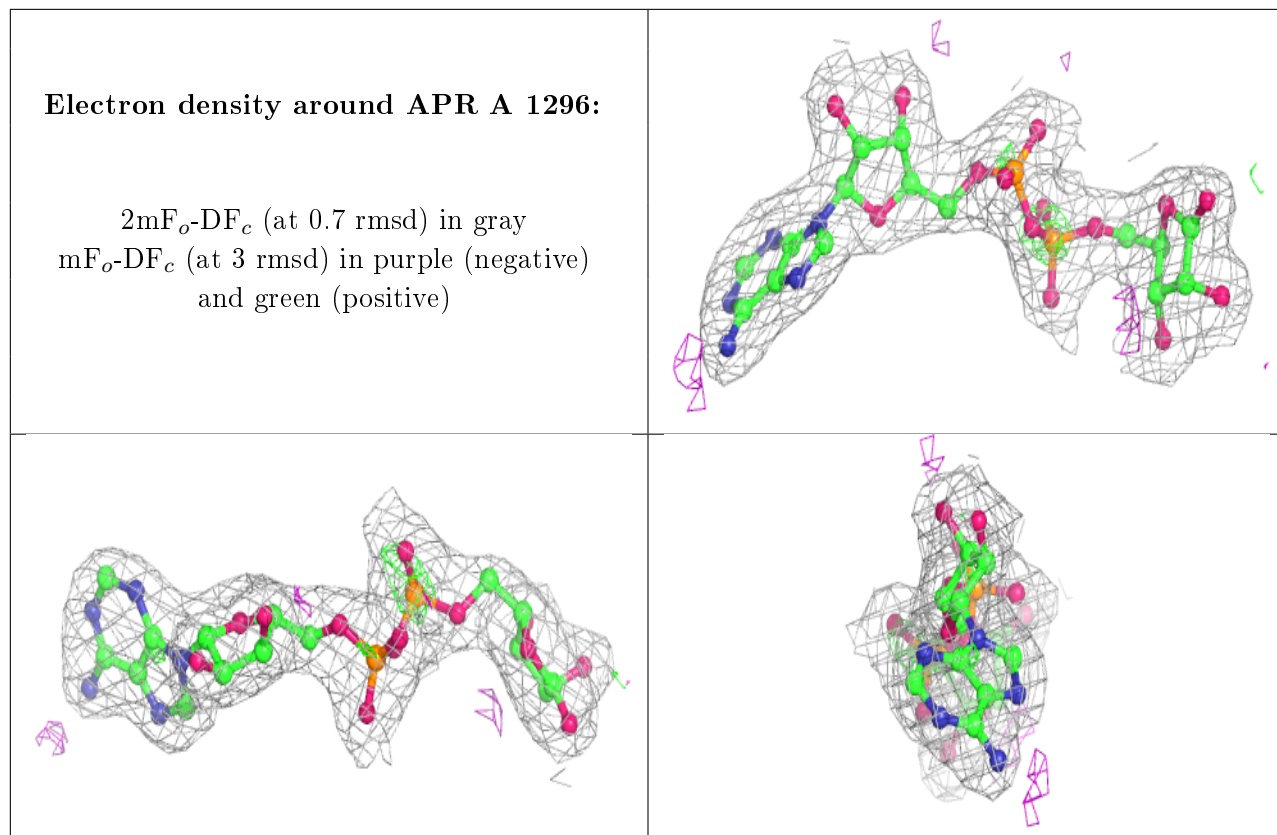
There are no carbohydrates in this entry.

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
5	GOL	A	1299	6/6	0.87	0.16	50,66,70,73	0
5	GOL	A	1298	6/6	0.98	0.17	46,50,52,54	0
4	APR	A	1296	36/36	0.98	0.17	29,34,38,41	0
3	ZN	A	1295	1/1	0.99	0.06	49,49,49,49	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.