



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:58 PM UTC

PDB ID : 6EV6 / pdb_00006ev6
Title : Structure of E282Q A. niger Fdc1 with prFMN in the hydroxylated and ketimine forms
Authors : Bailey, S.S.; David, L.; Payne, K.A.P.
Deposited on : 2017-11-01
Resolution : 1.10 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

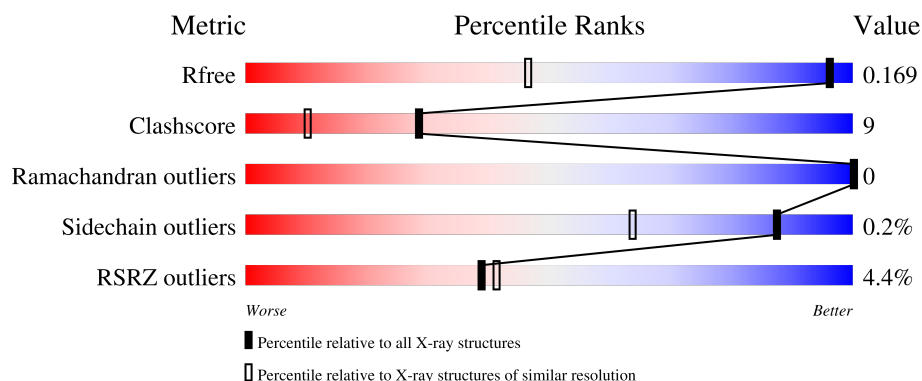
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.10 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}	180053	1625 (1.12-1.08)
Clashscore	190562	1656 (1.12-1.08)
Ramachandran outliers	187476	1616 (1.12-1.08)
Sidechain outliers	187428	1612 (1.12-1.08)
RSRZ outliers	180081	1625 (1.12-1.08)

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	508	4% 78% 19% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5021 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 Ferulic acid decarboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	500	Total	C	N	O	S	0	35	1
			4122	2610	711	771	30			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	GLN	GLU	conflict	UNP A2QHE5
A	499B	LEU	-	expression tag	UNP A2QHE5
A	499C	GLU	-	expression tag	UNP A2QHE5
A	502	HIS	-	expression tag	UNP A2QHE5
A	503	HIS	-	expression tag	UNP A2QHE5
A	504	HIS	-	expression tag	UNP A2QHE5
A	505	HIS	-	expression tag	UNP A2QHE5
A	506	HIS	-	expression tag	UNP A2QHE5
A	507	HIS	-	expression tag	UNP A2QHE5

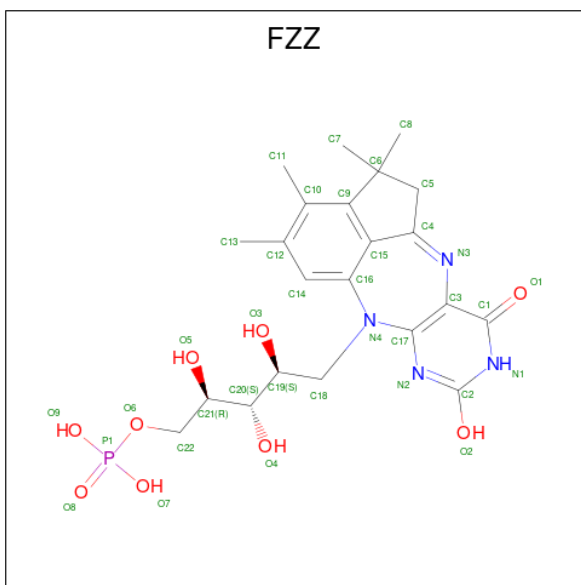
- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

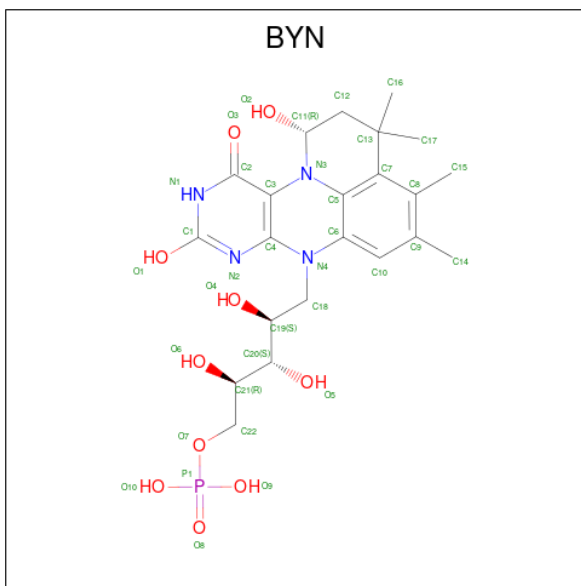
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	K	0	0
			2	2		

- Molecule 4 is 1-deoxy-5-O-phosphono-1-[(10aR)-2,2,3,4-tetramethyl-8,10-dioxo-1,2,8,9,10,10a-hexahydro-6H-indeno[1,7-ef]pyrimido[4,5-b][1,4]diazepin-6-yl]-D-ribitol (CCD ID: FZZ) (formula: C₂₂H₂₉N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			36	22	4	9	1		

- Molecule 5 is hydroxylated prenyl-FMN (CCD ID: BYN) (formula: $C_{22}H_{31}N_4O_{10}P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	1
			37	22	4	10	1		

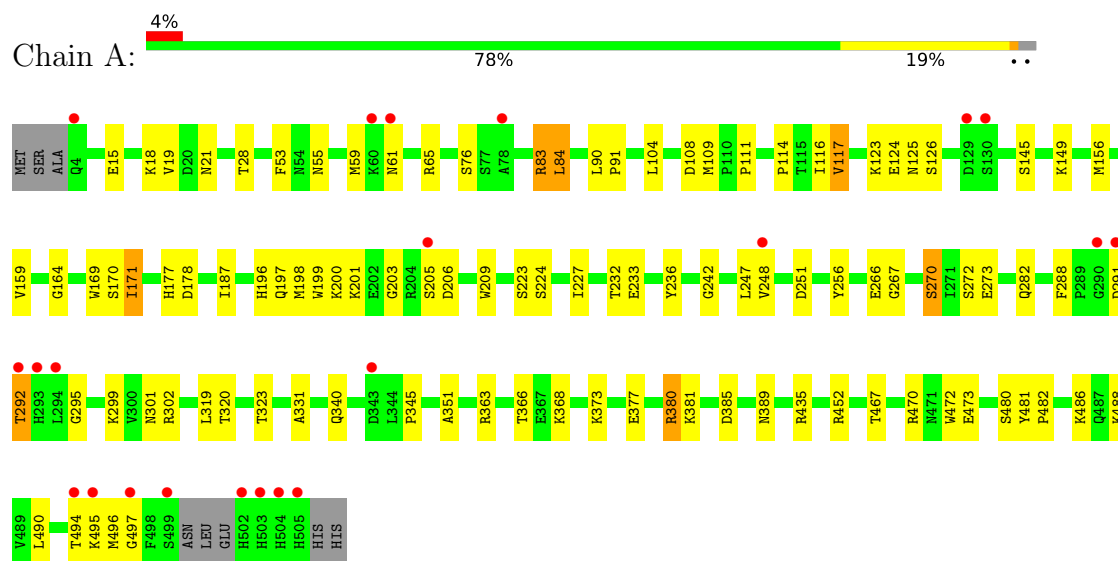
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	823	Total 823	O 823	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: Ferulic acid decarboxylase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.05Å 63.68Å 87.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.07 – 1.10 53.07 – 1.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (53.07-1.10) 99.6 (53.07-1.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.10Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.148 , 0.169 0.148 , 0.169	Depositor DCC
R_{free} test set	10911 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	12.5	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.1	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	5021	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FZZ, K, MN, BYN

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	1.82	60/4224 (1.4%)	1.37	25/5738 (0.4%)

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	A	0	3

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	ARG	CZ-NH1	-12.66	1.15	1.32
1	A	380	ARG	CA-CB	9.86	1.68	1.53
1	A	472	TRP	CA-C	-7.98	1.42	1.52
1	A	116	ILE	C-O	7.94	1.33	1.24
1	A	156	MET	CA-CB	7.88	1.64	1.53
1	A	111	PRO	C-O	7.84	1.33	1.23
1	A	198	MET	C-O	7.80	1.33	1.24
1	A	272	SER	CB-OG	-7.30	1.27	1.42
1	A	380	ARG	CA-C	-7.20	1.43	1.52
1	A	323	THR	C-O	7.08	1.33	1.24
1	A	178	ASP	CA-C	-6.93	1.44	1.53
1	A	178	ASP	C-O	6.80	1.30	1.24
1	A	116	ILE	CA-C	-6.54	1.44	1.52
1	A	124	GLU	CA-C	-6.50	1.43	1.52
1	A	209	TRP	CA-C	-6.29	1.44	1.52
1	A	270	SER	CA-C	-6.24	1.44	1.52
1	A	114	PRO	N-CA	-6.24	1.39	1.47
1	A	203	GLY	CA-C	-6.23	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84[A]	LEU	N-CA	6.10	1.53	1.46
1	A	84[B]	LEU	N-CA	6.10	1.53	1.46
1	A	126	SER	N-CA	-6.09	1.38	1.45
1	A	201	LYS	C-O	6.06	1.31	1.24
1	A	467	THR	N-CA	6.03	1.53	1.46
1	A	340	GLN	C-O	6.03	1.31	1.24
1	A	273	GLU	CA-CB	-5.91	1.44	1.53
1	A	83	ARG	CA-C	-5.87	1.45	1.52
1	A	292	THR	N-CA	5.83	1.53	1.46
1	A	351	ALA	N-CA	5.76	1.52	1.45
1	A	91	PRO	CA-C	-5.76	1.48	1.51
1	A	473	GLU	CA-CB	5.72	1.67	1.53
1	A	345	PRO	CA-C	5.68	1.58	1.53
1	A	435	ARG	N-CA	-5.65	1.38	1.46
1	A	206	ASP	CA-CB	-5.62	1.44	1.53
1	A	124	GLU	C-O	5.59	1.31	1.24
1	A	28	THR	C-O	5.58	1.31	1.23
1	A	114	PRO	C-N	-5.57	1.26	1.33
1	A	389	ASN	CG-ND2	-5.57	1.21	1.33
1	A	177	HIS	C-O	5.55	1.30	1.23
1	A	116	ILE	C-N	-5.50	1.27	1.33
1	A	256	TYR	C-N	-5.49	1.27	1.33
1	A	301	ASN	CA-C	-5.48	1.45	1.52
1	A	177	HIS	ND1-CE1	5.45	1.38	1.32
1	A	389	ASN	CA-C	-5.43	1.45	1.52
1	A	117	VAL	C-N	5.39	1.40	1.34
1	A	473	GLU	CD-OE1	5.36	1.35	1.25
1	A	242	GLY	CA-C	-5.33	1.44	1.51
1	A	366	THR	CA-C	5.30	1.60	1.52
1	A	61	ASN	C-O	5.30	1.30	1.23
1	A	164	GLY	C-N	-5.28	1.25	1.33
1	A	270	SER	C-N	5.24	1.39	1.34
1	A	251	ASP	C-O	5.23	1.30	1.24
1	A	199	TRP	C-O	5.22	1.30	1.24
1	A	90	LEU	C-N	5.19	1.38	1.33
1	A	247	LEU	C-O	5.18	1.30	1.23
1	A	302	ARG	C-N	-5.13	1.26	1.33
1	A	21	ASN	C-O	-5.12	1.17	1.23
1	A	482	PRO	CA-C	-5.10	1.46	1.52
1	A	366	THR	CB-OG1	-5.06	1.35	1.43
1	A	486	LYS	CA-C	5.05	1.59	1.52
1	A	123	LYS	C-O	5.01	1.30	1.24

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	MET	CA-C-O	-7.53	111.59	120.10
1	A	435	ARG	NE-CZ-NH2	-7.16	112.76	119.20
1	A	380	ARG	CG-CD-NE	6.94	127.27	112.00
1	A	452	ARG	NE-CZ-NH2	-6.44	113.40	119.20
1	A	496	MET	CA-C-N	6.26	133.67	121.41
1	A	496	MET	C-N-CA	6.26	133.67	121.41
1	A	495	LYS	N-CA-CB	6.13	118.89	110.01
1	A	295	GLY	O-C-N	-6.07	118.31	123.59
1	A	494	THR	CA-C-N	6.02	128.26	120.44
1	A	494	THR	C-N-CA	6.02	128.26	120.44
1	A	473	GLU	CA-C-O	-5.77	114.59	121.11
1	A	266	GLU	CA-C-O	-5.65	114.72	120.71
1	A	178	ASP	O-C-N	-5.63	116.25	122.72
1	A	125	ASN	OD1-CG-ND2	-5.53	117.08	122.60
1	A	497	GLY	N-CA-C	5.35	125.85	113.18
1	A	116	ILE	CA-C-N	5.33	130.08	122.24
1	A	116	ILE	C-N-CA	5.33	130.08	122.24
1	A	156	MET	N-CA-CB	-5.30	102.23	110.55
1	A	19[A]	VAL	CA-C-O	5.24	126.13	120.47
1	A	19[B]	VAL	CA-C-O	5.24	126.13	120.47
1	A	91	PRO	O-C-N	-5.10	118.96	121.31
1	A	373	LYS	CA-C-O	5.09	128.46	122.14
1	A	488	LYS	CA-C-O	5.09	126.16	120.82
1	A	288	PHE	CB-CA-C	5.07	115.50	110.33
1	A	490	LEU	O-C-N	5.04	127.46	122.12

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	171[B]	ILE	Mainchain
1	A	380	ARG	Sidechain
1	A	83	ARG	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	A	4122	0	4010	69	0
2	A	1	0	0	0	0
3	A	2	0	0	1	0
4	A	36	0	25	6	0
5	A	37	0	0	1	0
6	A	823	0	0	47	10
All	All	5021	0	4035	73	10

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 9.

All (73) 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:A:292:THR:HA	6:A:701:HOH:O	1.33	1.27
1:A:381[A]:LYS:CD	6:A:703:HOH:O	1.90	1.19
1:A:381[A]:LYS:HG3	6:A:742:HOH:O	1.60	1.02
1:A:381[A]:LYS:HD2	6:A:703:HOH:O	1.56	0.96
1:A:291:ASP:O	6:A:701:HOH:O	1.84	0.94
1:A:381[B]:LYS:HD3	6:A:711:HOH:O	1.69	0.92
1:A:18[B]:LYS:NZ	6:A:702:HOH:O	1.94	0.91
1:A:480[B]:SER:HB2	1:A:481:TYR:CE2	2.13	0.83
1:A:109:MET:SD	6:A:1238:HOH:O	2.38	0.81
1:A:381[B]:LYS:HE2	1:A:385:ASP:OD2	1.80	0.80
1:A:236:TYR:OH	6:A:704:HOH:O	2.00	0.80
1:A:197:GLN:HB2	6:A:732:HOH:O	1.81	0.80
1:A:59[A]:MET:CE	6:A:1100:HOH:O	2.31	0.78
1:A:381[B]:LYS:CE	1:A:385:ASP:OD1	2.33	0.76
1:A:170:SER:HB2	4:A:604[A]:FZZ:H27	1.69	0.75
3:A:602:K:K	6:A:708:HOH:O	1.98	0.73
1:A:59[A]:MET:SD	6:A:1100:HOH:O	2.46	0.73
1:A:381[B]:LYS:CE	1:A:385:ASP:CG	2.65	0.70
1:A:196[B]:HIS:HE1	1:A:270:SER:O	1.76	0.68
1:A:381[B]:LYS:HE3	1:A:385:ASP:OD1	1.93	0.67
1:A:232:THR:O	6:A:705:HOH:O	2.14	0.65
1:A:381[B]:LYS:HE2	1:A:385:ASP:CG	2.21	0.65
1:A:248[B]:VAL:HG13	6:A:804:HOH:O	2.00	0.62
1:A:381[A]:LYS:HE3	6:A:742:HOH:O	2.01	0.60
1:A:291:ASP:OD2	6:A:706:HOH:O	2.16	0.59
1:A:381[A]:LYS:HD3	6:A:703:HOH:O	1.78	0.58
4:A:604[A]:FZZ:H20	4:A:604[A]:FZZ:N2	2.17	0.58
1:A:292:THR:CA	6:A:701:HOH:O	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381[B]:LYS:HE3	1:A:385:ASP:CG	2.30	0.57
1:A:377[B]:GLU:HG3	6:A:742:HOH:O	2.04	0.57
1:A:381[B]:LYS:CD	6:A:711:HOH:O	2.37	0.56
1:A:76[B]:SER:HB3	6:A:926:HOH:O	2.04	0.55
1:A:223:SER:O	4:A:604[A]:FZZ:O4	2.23	0.55
1:A:200[B]:LYS:NZ	6:A:720:HOH:O	2.40	0.54
1:A:381[A]:LYS:HE2	6:A:1357:HOH:O	2.07	0.54
1:A:381[A]:LYS:CG	6:A:742:HOH:O	2.35	0.54
1:A:363:ARG:NH1	6:A:722:HOH:O	2.41	0.54
1:A:171[B]:ILE:HG22	1:A:171[B]:ILE:O	2.08	0.54
1:A:149[A]:LYS:CE	6:A:1239:HOH:O	2.55	0.53
1:A:59[A]:MET:HE3	6:A:1100:HOH:O	2.03	0.53
1:A:196[B]:HIS:CE1	1:A:270:SER:O	2.60	0.53
1:A:84[B]:LEU:HD12	1:A:84[B]:LEU:H	1.74	0.52
5:A:605[B]:BYN:C17	5:A:605[B]:BYN:C15	2.88	0.52
1:A:108[A]:ASP:OD1	1:A:108[A]:ASP:C	2.46	0.51
1:A:205[A]:SER:HB2	6:A:1277:HOH:O	2.09	0.51
1:A:104:LEU:HD23	6:A:704:HOH:O	2.11	0.51
1:A:55:ASN:C	6:A:779:HOH:O	2.54	0.50
1:A:170:SER:HB2	4:A:604[A]:FZZ:C22	2.39	0.50
1:A:169:TRP:NE1	6:A:725:HOH:O	2.44	0.50
1:A:470:ARG:NE	6:A:726:HOH:O	2.44	0.50
1:A:480[B]:SER:HB2	1:A:481:TYR:CD2	2.46	0.50
1:A:227:ILE:HG12	6:A:708:HOH:O	2.11	0.50
1:A:368:LYS:HE3	6:A:727:HOH:O	2.10	0.50
1:A:149[A]:LYS:HD3	6:A:1133:HOH:O	2.12	0.49
1:A:149[A]:LYS:CD	6:A:1133:HOH:O	2.63	0.47
1:A:170:SER:CB	4:A:604[A]:FZZ:H27	2.39	0.47
1:A:117:VAL:HG23	1:A:248[B]:VAL:HG22	1.97	0.46
1:A:149[A]:LYS:HE2	6:A:1239:HOH:O	2.16	0.46
1:A:171[A]:ILE:HD12	1:A:224[A]:SER:OG	2.16	0.46
1:A:84[B]:LEU:HD12	1:A:84[B]:LEU:N	2.30	0.45
1:A:53:PHE:HB3	6:A:779:HOH:O	2.16	0.45
1:A:331:ALA:HB2	6:A:1157:HOH:O	2.16	0.45
4:A:604[A]:FZZ:H14	4:A:604[A]:FZZ:H13	1.79	0.44
1:A:381[B]:LYS:HE2	6:A:1098:HOH:O	2.17	0.44
1:A:145:SER:HB3	6:A:954:HOH:O	2.17	0.43
1:A:59[A]:MET:HG2	6:A:800:HOH:O	2.17	0.43
1:A:187:ILE:HD12	6:A:1440:HOH:O	2.19	0.42
1:A:159:VAL:HB	6:A:712:HOH:O	2.18	0.42
1:A:267:GLY:HA3	1:A:299:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLU:HB2	6:A:718:HOH:O	2.19	0.41
1:A:381[B]:LYS:CG	6:A:1098:HOH:O	2.68	0.41
1:A:15[B]:GLU:OE1	1:A:18[B]:LYS:HD2	2.22	0.40
1:A:319:LEU:HA	1:A:320:THR:HA	1.91	0.40

All (10) 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)
6:A:1432:HOH:O	6:A:1436:HOH:O[3_555]	0.84	1.36
6:A:872:HOH:O	6:A:872:HOH:O[2_655]	1.05	1.15
6:A:889:HOH:O	6:A:940:HOH:O[2_555]	1.53	0.67
6:A:764:HOH:O	6:A:823:HOH:O[2_555]	1.62	0.58
6:A:812:HOH:O	6:A:1016:HOH:O[2_655]	1.63	0.57
6:A:1514:HOH:O	6:A:1514:HOH:O[2_555]	2.00	0.20
6:A:1066:HOH:O	6:A:1268:HOH:O[2_655]	2.03	0.17
6:A:846:HOH:O	6:A:1291:HOH:O[2_555]	2.05	0.15
6:A:785:HOH:O	6:A:1304:HOH:O[2_555]	2.06	0.14
6:A:1247:HOH:O	6:A:1286:HOH:O[3_545]	2.18	0.02

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	531/508 (104%)	514 (97%)	17 (3%)	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	A	445/430 (104%)	444 (100%)	1 (0%)	87	64

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

Mol	Chain	Res	Type
1	A	282	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	33	ASN
1	A	160	GLN
1	A	504	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	BYN	A	605[B]	3,2	36,40,40	1.92	10 (27%)	47,64,64	1.87	11 (23%)
4	FZZ	A	604[A]	3,2	36,39,39	2.42	11 (30%)	38,62,62	3.24	14 (36%)

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	BYN	A	605[B]	3,2	-	5/18/33/33	0/4/4/4
4	FZZ	A	604[A]	3,2	-	10/18/29/29	0/3/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604[A]	FZZ	C18-C19	-8.09	1.41	1.52
5	A	605[B]	BYN	C12-C11	-6.19	1.47	1.52
4	A	604[A]	FZZ	C5-C4	-5.05	1.45	1.50
4	A	604[A]	FZZ	O6-C22	-4.50	1.27	1.44
4	A	604[A]	FZZ	C17-N2	3.94	1.43	1.34
4	A	604[A]	FZZ	C3-C17	3.80	1.49	1.40
4	A	604[A]	FZZ	C4-N3	3.70	1.33	1.28
5	A	605[B]	BYN	C19-C20	-3.54	1.47	1.53
5	A	605[B]	BYN	C3-C2	-3.38	1.34	1.43
5	A	605[B]	BYN	O4-C19	-3.27	1.36	1.43
5	A	605[B]	BYN	C18-C19	-3.23	1.48	1.52
4	A	604[A]	FZZ	C21-C20	-3.06	1.48	1.53
5	A	605[B]	BYN	C21-C20	-2.74	1.48	1.53
5	A	605[B]	BYN	C22-C21	2.67	1.55	1.51
5	A	605[B]	BYN	C3-N3	2.65	1.41	1.37
4	A	604[A]	FZZ	C3-N3	2.64	1.47	1.39
4	A	604[A]	FZZ	C14-C16	-2.46	1.35	1.39
5	A	605[B]	BYN	C5-C6	-2.24	1.37	1.40
4	A	604[A]	FZZ	P1-O8	2.20	1.57	1.50
4	A	604[A]	FZZ	C2-N1	2.12	1.41	1.37
5	A	605[B]	BYN	O5-C20	-2.01	1.38	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	604[A]	FZZ	C22-C21-C20	-14.64	84.59	112.22
5	A	605[B]	BYN	C13-C7-C5	-5.74	115.21	121.48
4	A	604[A]	FZZ	O3-C19-C20	-5.08	97.37	109.25
4	A	604[A]	FZZ	O7-P1-O6	-4.94	93.78	106.67
4	A	604[A]	FZZ	C8-C6-C7	4.33	114.75	109.17
5	A	605[B]	BYN	O4-C19-C20	4.30	119.31	109.25
5	A	605[B]	BYN	O3-C2-N1	-4.18	112.25	120.11
5	A	605[B]	BYN	O5-C20-C19	4.03	118.09	108.93
4	A	604[A]	FZZ	C5-C6-C9	3.90	103.78	102.22
4	A	604[A]	FZZ	O1-C1-C3	-3.58	117.08	126.53
5	A	605[B]	BYN	C3-C2-N1	3.55	117.18	110.94
4	A	604[A]	FZZ	O5-C21-C20	3.49	117.42	109.25
4	A	604[A]	FZZ	O6-P1-O8	3.27	115.27	106.44
5	A	605[B]	BYN	C18-C19-C20	3.13	118.16	109.66
4	A	604[A]	FZZ	C21-C20-C19	3.08	118.69	113.57
4	A	604[A]	FZZ	O9-P1-O6	-2.88	99.15	106.67
5	A	605[B]	BYN	C21-C20-C19	2.68	118.03	113.57
4	A	604[A]	FZZ	O1-C1-N1	2.41	124.65	120.11
5	A	605[B]	BYN	O4-C19-C18	2.20	119.26	110.20
4	A	604[A]	FZZ	O9-P1-O8	2.20	119.40	110.83
4	A	604[A]	FZZ	C12-C10-C9	-2.15	117.58	119.50
4	A	604[A]	FZZ	C14-C12-C10	2.12	121.24	119.10
5	A	605[B]	BYN	C17-C13-C7	2.10	118.27	112.06
5	A	605[B]	BYN	C10-C9-C8	2.06	121.18	119.10
5	A	605[B]	BYN	O5-C20-C21	2.03	113.54	108.93

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604[A]	FZZ	C18-C19-C20-O4
4	A	604[A]	FZZ	C18-C19-C20-C21
4	A	604[A]	FZZ	O5-C21-C22-O6
4	A	604[A]	FZZ	C22-O6-P1-O7
4	A	604[A]	FZZ	C22-O6-P1-O8
4	A	604[A]	FZZ	C22-O6-P1-O9
5	A	605[B]	BYN	O4-C19-C20-C21
4	A	604[A]	FZZ	C20-C21-C22-O6
4	A	604[A]	FZZ	O3-C19-C20-C21
4	A	604[A]	FZZ	C21-C22-O6-P1
5	A	605[B]	BYN	C18-C19-C20-O5
5	A	605[B]	BYN	C22-O7-P1-O9
4	A	604[A]	FZZ	O3-C19-C20-O4

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Mol	Chain	Res	Type	Atoms
5	A	605[B]	BYN	N4-C18-C19-O4
5	A	605[B]	BYN	C21-C22-O7-P1

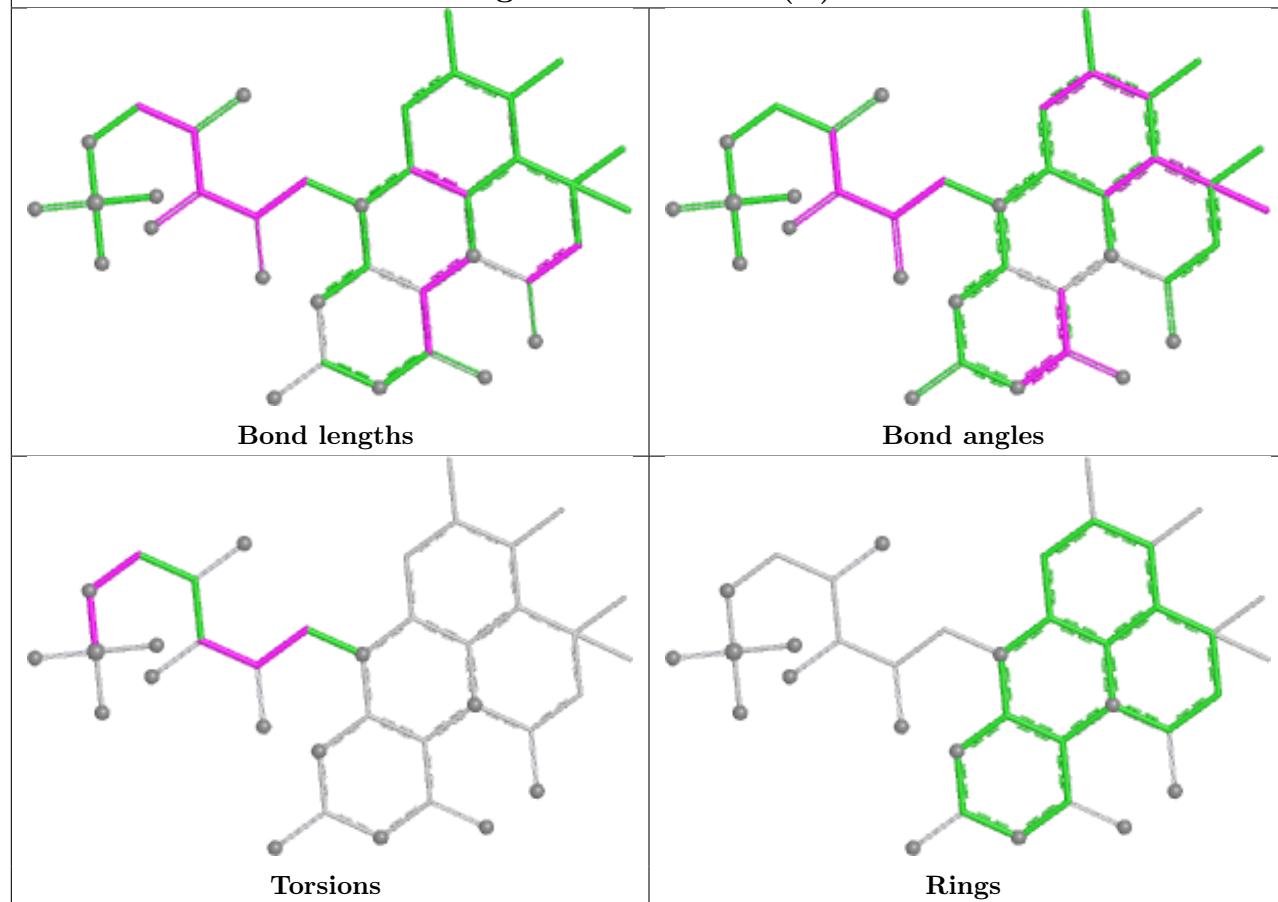
There are no ring outliers.

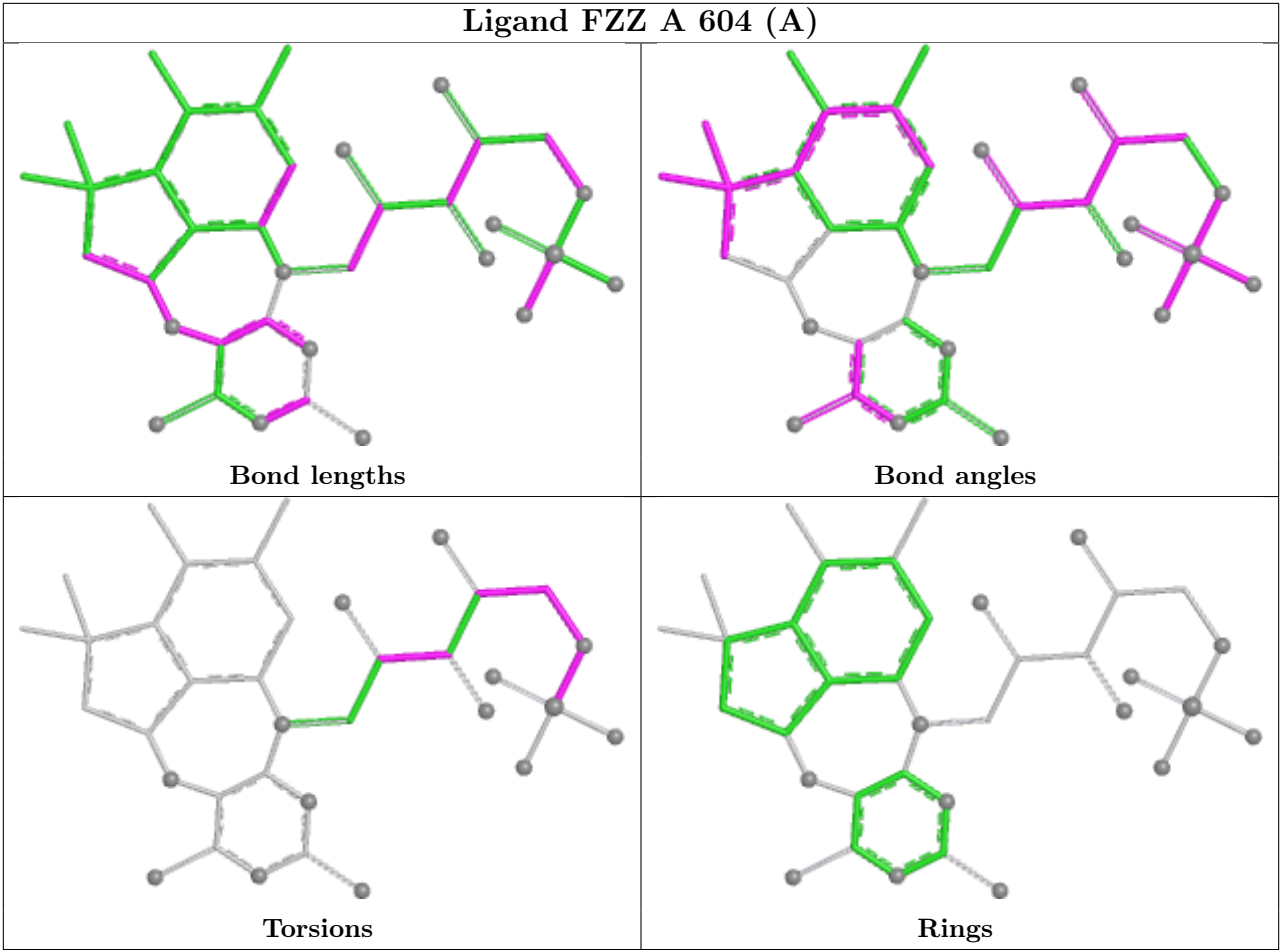
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605[B]	BYN	1	0
4	A	604[A]	FZZ	6	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.

Ligand BYN A 605 (B)





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
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	171[B]:ILE	C	172:ALA	N	1.17

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	500/508 (98%)	0.33	22 (4%)	39 41	5, 13, 22, 64	35 (7%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	HIS	5.6
1	A	505	HIS	4.9
1	A	504	HIS	4.6
1	A	502	HIS	4.1
1	A	61	ASN	3.7
1	A	129[A]	ASP	3.3
1	A	495	LYS	3.2
1	A	292	THR	3.0
1	A	78	ALA	2.9
1	A	497	GLY	2.9
1	A	499	SER	2.8
1	A	291	ASP	2.6
1	A	290[A]	GLY	2.5
1	A	494	THR	2.4
1	A	205[A]	SER	2.4
1	A	343	ASP	2.3
1	A	293	HIS	2.3
1	A	248[A]	VAL	2.3
1	A	4	GLN	2.2
1	A	294	LEU	2.2
1	A	60	LYS	2.2
1	A	130	SER	2.1

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

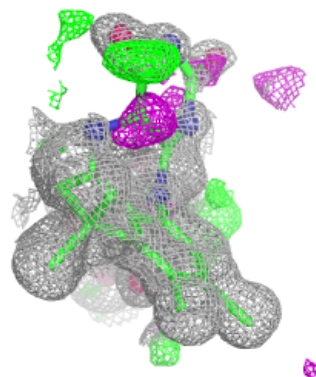
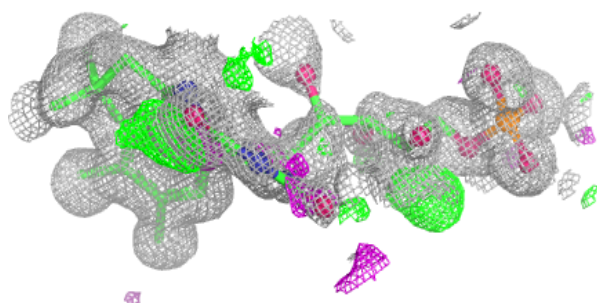
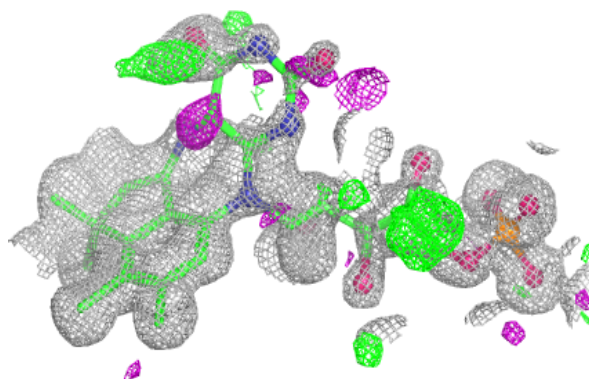
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

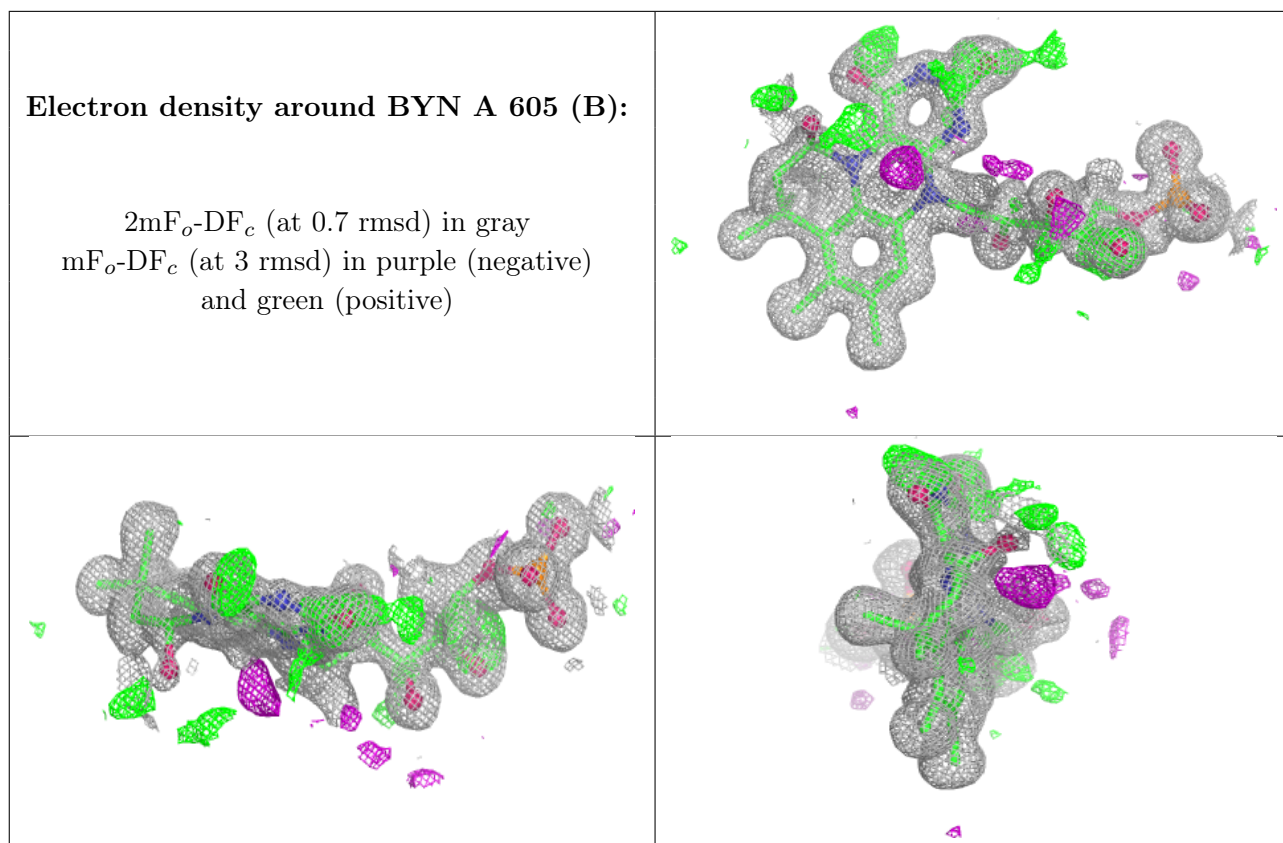
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FZZ	A	604[A]	36/36	0.91	0.12	10,16,19,22	36
5	BYN	A	605[B]	37/37	0.97	0.07	5,7,13,14	37
3	K	A	603	1/1	1.00	0.02	10,10,10,10	0
2	MN	A	601	1/1	1.00	0.01	9,9,9,9	0
3	K	A	602	1/1	1.00	0.02	10,10,10,10	0

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 FZZ A 604 (A):

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.