



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 10:54 pm BST

PDB ID : 3EU5
Title : Crystal structure of FTase(ALPHA-subunit; BETA-subunit DELTA C10) in complex with BiotinGPP
Authors : Guo, Z.; Nguyen, U.T.T.; Delon, C.; Bon, R.S.; Blankenfeldt, W.; Goody, R.S.; Waldmann, H.; Wolters, D.; Alexandrov, K.
Deposited on : 2008-10-09
Resolution : 2.80 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

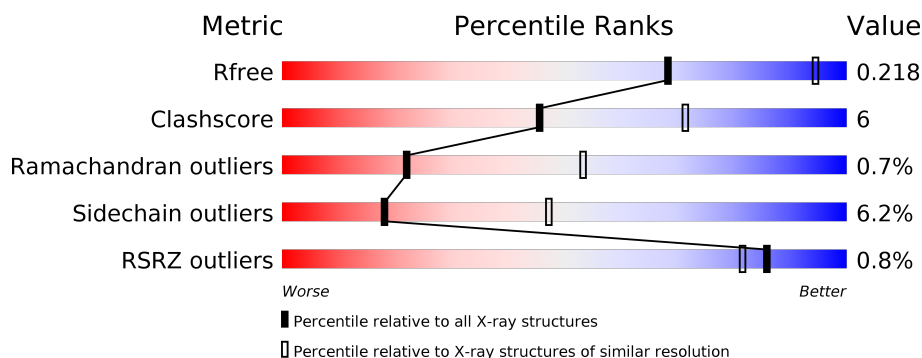
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	377	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>15%</div> <div>•</div> <div>16%</div> </div> </div>
2	B	427	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>•</div> <div>6%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6010 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 Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	1	0
			2696	1717	476	498	5			

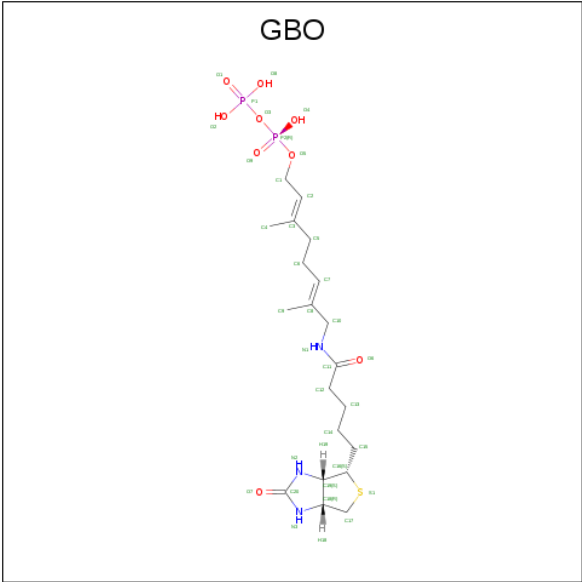
- Molecule 2 is a protein called Protein farnesyltransferase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	1	0
			3146	2008	540	575	23			

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

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

- Molecule 4 is (2E,6E)-3,7-dimethyl-8-({5-[(3aS,4S,6aR)-2-oxohexahydro-1H-thieno[3,4-d]imidazol-4-yl]pentanoyl}amino)octa-2,6-dien-1-yl trihydrogen diphosphate (three-letter code: GBO) (formula: C₂₀H₃₅N₃O₉P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	S	0	0
			35	20	3	9	2	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	132	Total	O	0	0
			132	132		

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	175.06 Å 175.06 Å 70.62 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.96 – 2.80 29.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.96-2.80) 99.8 (29.96-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.36 (at 2.80 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.153 , 0.207 0.164 , 0.218	Depositor DCC
R_{free} test set	1544 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6010	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: GBO, ZN

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	0.93	1/2765 (0.0%)	0.89	3/3752 (0.1%)
2	B	0.91	2/3232 (0.1%)	0.93	10/4387 (0.2%)
All	All	0.91	3/5997 (0.1%)	0.91	13/8139 (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	A	0	1
2	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	345	CYS	CB-SG	-7.07	1.70	1.82
2	B	120	GLN	CG-CD	5.67	1.64	1.51
1	A	342	GLU	CG-CD	5.50	1.60	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	ARG	NE-CZ-NH2	-7.82	116.39	120.30
2	B	308	LEU	CA-CB-CG	-7.45	98.17	115.30
2	B	280	ARG	NE-CZ-NH1	7.41	124.00	120.30
2	B	277	VAL	CB-CA-C	-7.11	97.89	111.40
2	B	245	MET	CG-SD-CE	6.62	110.78	100.20
2	B	280	ARG	NE-CZ-NH2	-6.54	117.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	393	VAL	CB-CA-C	-6.49	99.07	111.40
2	B	313	ARG	NE-CZ-NH2	-6.07	117.27	120.30
2	B	313	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	A	352	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	B	280	ARG	CG-CD-NE	-5.18	100.91	111.80
2	B	325	MET	CG-SD-CE	5.09	108.35	100.20
1	A	352	ARG	CG-CD-NE	-5.05	101.19	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	368	SER	Peptide
2	B	421	PRO	Peptide

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	2696	0	2627	39	0
2	B	3146	0	3061	40	0
3	B	1	0	0	0	0
4	B	35	0	32	1	0
5	B	132	0	0	3	2
All	All	6010	0	5720	74	2

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 6.

All (74) 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:B:280:ARG:HH11	2:B:289:GLN:NE2	1.75	0.83
2:B:280:ARG:HH11	2:B:289:GLN:HE21	1.34	0.73
1:A:207:GLN:HE21	1:A:239:GLN:NE2	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLN:HA	1:A:239:GLN:HE21	1.62	0.65
1:A:152:MET:O	1:A:156:ILE:HG13	1.97	0.64
1:A:170:HIS:HE1	2:B:196:GLY:O	1.81	0.63
1:A:159:ILE:HG12	1:A:168:VAL:HG13	1.80	0.63
1:A:207:GLN:HE21	1:A:239:GLN:HE22	1.47	0.62
2:B:227:GLU:O	2:B:231:ARG:HG3	2.00	0.61
1:A:160:GLU:OE2	1:A:191:ASP:OD1	2.19	0.59
2:B:134:GLN:HE22	2:B:173:ASN:H	1.51	0.58
1:A:170:HIS:HD2	2:B:198[B]:GLU:OE2	1.87	0.57
1:A:112:ARG:O	1:A:144:LEU:HD21	2.06	0.56
1:A:170:HIS:CE1	2:B:196:GLY:O	2.59	0.55
2:B:386:VAL:HG21	2:B:393:VAL:HG13	1.87	0.55
2:B:173:ASN:ND2	2:B:176:LYS:HB2	2.23	0.54
2:B:78:HIS:HD1	2:B:349:GLY:H	1.56	0.54
2:B:149:HIS:CE1	2:B:193:MET:HG3	2.43	0.53
1:A:287:ARG:HA	5:B:494:HOH:O	2.08	0.53
2:B:338:TYR:CE2	2:B:343:CYS:SG	3.02	0.52
1:A:286:ASP:OD1	1:A:286:ASP:N	2.43	0.52
1:A:303:GLN:HB3	1:A:304:PRO:CD	2.39	0.52
1:A:159:ILE:CG1	1:A:168:VAL:HG13	2.40	0.51
2:B:74:GLN:H	2:B:344:GLN:HE22	1.57	0.51
2:B:227:GLU:HG3	5:B:471:HOH:O	2.11	0.51
2:B:78:HIS:HD1	2:B:349:GLY:N	2.09	0.51
2:B:353:LYS:O	2:B:356:LYS:HB2	2.11	0.51
1:A:58:LEU:HD23	1:A:63:TYR:CE1	2.46	0.50
2:B:424:GLU:O	2:B:425:GLU:C	2.49	0.50
1:A:353:LYS:O	1:A:357:ARG:HG3	2.11	0.50
1:A:349:ASP:OD2	1:A:352:ARG:HD2	2.12	0.50
2:B:296:VAL:O	2:B:353:LYS:HE2	2.12	0.49
2:B:231:ARG:HD3	5:B:445:HOH:O	2.13	0.48
1:A:312:ILE:HG23	1:A:340:LEU:HD22	1.95	0.48
2:B:406:ASP:N	2:B:406:ASP:OD1	2.47	0.48
2:B:386:VAL:CG2	2:B:393:VAL:HG13	2.43	0.47
1:A:159:ILE:HG12	1:A:168:VAL:CG1	2.44	0.47
1:A:106:VAL:HG11	1:A:116:ALA:HB1	1.96	0.47
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.96	0.47
2:B:259:LEU:HD12	2:B:268:LEU:HD11	1.97	0.47
2:B:302:PHE:CZ	2:B:402:ASN:HB2	2.50	0.47
2:B:335:LEU:HD23	2:B:373:ALA:HB2	1.97	0.47
2:B:78:HIS:NE2	2:B:344:GLN:NE2	2.60	0.46
1:A:256:LEU:HD22	1:A:287:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LEU:O	1:A:180:LYS:C	2.54	0.46
1:A:251:SER:O	1:A:252:ASP:C	2.53	0.46
1:A:219:GLU:OE1	1:A:219:GLU:HA	2.15	0.46
2:B:423:PHE:HA	2:B:424:GLU:CB	2.46	0.45
1:A:224:ASP:OD1	1:A:240:ARG:NH2	2.49	0.45
1:A:170:HIS:CD2	2:B:198[B]:GLU:OE2	2.69	0.45
2:B:177:LEU:HD21	2:B:210:VAL:HG13	1.96	0.45
2:B:239:ILE:HB	2:B:252:THR:HA	2.00	0.44
1:A:204:GLN:HA	2:B:245:MET:SD	2.58	0.44
1:A:320:GLU:O	1:A:324:GLU:HG2	2.18	0.43
1:A:303:GLN:HB3	1:A:304:PRO:HD2	1.99	0.43
2:B:350:LEU:HB2	2:B:363:THR:HA	1.99	0.43
2:B:173:ASN:ND2	2:B:176:LYS:CG	2.82	0.43
2:B:375:HIS:HE1	2:B:394:LEU:O	2.03	0.42
1:A:213:PHE:O	1:A:215:LEU:HG	2.19	0.42
1:A:329:ASN:O	1:A:330:LYS:C	2.58	0.42
1:A:213:PHE:O	1:A:214:ARG:C	2.58	0.41
2:B:25:SER:OG	2:B:337:GLU:OE1	2.32	0.41
2:B:280:ARG:HD3	2:B:289:GLN:HE21	1.84	0.41
2:B:93:TYR:HD2	2:B:96:LEU:HD12	1.84	0.41
1:A:265:GLU:OE2	1:A:268:LYS:NZ	2.53	0.41
1:A:223:VAL:HG11	1:A:240:ARG:HB2	2.02	0.41
2:B:250:GLY:HA3	4:B:429:GBO:C8	2.52	0.41
2:B:332:GLN:O	2:B:336:GLN:HG3	2.20	0.41
1:A:266:MET:CE	1:A:266:MET:HA	2.51	0.40
1:A:66:TYR:CE2	1:A:119:LEU:HD13	2.56	0.40
1:A:101:ASP:HA	1:A:104:ARG:HH11	1.86	0.40
2:B:174:ARG:HD2	2:B:415:PHE:CD1	2.56	0.40
1:A:78:VAL:O	1:A:104:ARG:HD2	2.21	0.40
2:B:352:ASP:C	2:B:352:ASP:OD1	2.59	0.40

All (2) 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)
5:B:540:HOH:O	5:B:551:HOH:O[4_544]	1.72	0.48
5:B:524:HOH:O	5:B:541:HOH:O[3_655]	1.80	0.40

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	314/377 (83%)	293 (93%)	20 (6%)	1 (0%)	41	72
2	B	398/427 (93%)	383 (96%)	11 (3%)	4 (1%)	15	44
All	All	712/804 (89%)	676 (95%)	31 (4%)	5 (1%)	22	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	LYS
2	B	424	GLU
2	B	74	GLN
2	B	413	THR
2	B	379	GLY

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	295/338 (87%)	274 (93%)	21 (7%)	14	39
2	B	336/363 (93%)	316 (94%)	20 (6%)	19	48
All	All	631/701 (90%)	590 (94%)	41 (6%)	18	44

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU

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Mol	Chain	Res	Type
1	A	97[A]	ARG
1	A	97[B]	ARG
1	A	121	ARG
1	A	143	SER
1	A	145	GLN
1	A	156	ILE
1	A	160	GLU
1	A	168	VAL
1	A	180	LYS
1	A	187	GLU
1	A	239	GLN
1	A	261	GLN
1	A	266	MET
1	A	269	LEU
1	A	287	ARG
1	A	291	ARG
1	A	305	SER
1	A	307	SER
1	A	331	GLU
1	A	369	ARG
2	B	25	SER
2	B	29	GLU
2	B	64	PHE
2	B	71	LEU
2	B	77	LYS
2	B	121	ILE
2	B	124	THR
2	B	185	LYS
2	B	198[A]	GLU
2	B	198[B]	GLU
2	B	201	VAL
2	B	264	LYS
2	B	266	ARG
2	B	271	LYS
2	B	277	VAL
2	B	280	ARG
2	B	283	ARG
2	B	308	LEU
2	B	325	MET
2	B	393	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	162	GLN
1	A	170	HIS
1	A	184	GLN
1	A	239	GLN
1	A	246	ASN
1	A	285	GLN
1	A	294	ASN
1	A	367	HIS
2	B	128	GLN
2	B	134	GLN
2	B	173	ASN
2	B	186	GLN
2	B	289	GLN
2	B	344	GLN
2	B	375	HIS
2	B	410	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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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
4	GBO	B	429	-	33,36,36	1.59	7 (21%)	44,50,50	2.00	14 (31%)

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
4	GBO	B	429	-	-	10/31/52/52	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	429	GBO	C1-C2	-3.37	1.39	1.49
4	B	429	GBO	C6-C7	-3.35	1.39	1.50
4	B	429	GBO	C12-C11	2.86	1.56	1.51
4	B	429	GBO	C16-S1	2.43	1.86	1.82
4	B	429	GBO	O5-C1	-2.34	1.40	1.43
4	B	429	GBO	C7-C8	2.15	1.38	1.33
4	B	429	GBO	C19-N2	2.12	1.49	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	429	GBO	C17-C18-N3	-5.75	105.72	113.03
4	B	429	GBO	C16-C19-N2	-3.64	109.86	113.13
4	B	429	GBO	N3-C20-N2	3.44	111.99	108.76
4	B	429	GBO	C19-C16-S1	-3.41	101.95	105.20
4	B	429	GBO	C18-C17-S1	-3.38	103.41	106.31
4	B	429	GBO	C17-C18-C19	3.26	111.49	108.66
4	B	429	GBO	C10-N1-C11	3.20	130.53	121.53
4	B	429	GBO	C1-C2-C3	-2.92	121.00	126.04
4	B	429	GBO	C19-N2-C20	-2.30	110.48	112.62
4	B	429	GBO	C12-C11-N1	-2.29	112.56	116.42
4	B	429	GBO	C9-C8-C10	2.24	120.39	114.81
4	B	429	GBO	C9-C8-C7	-2.19	118.05	123.68
4	B	429	GBO	O6-C11-N1	2.19	127.15	123.01
4	B	429	GBO	P2-O3-P1	-2.02	125.90	132.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

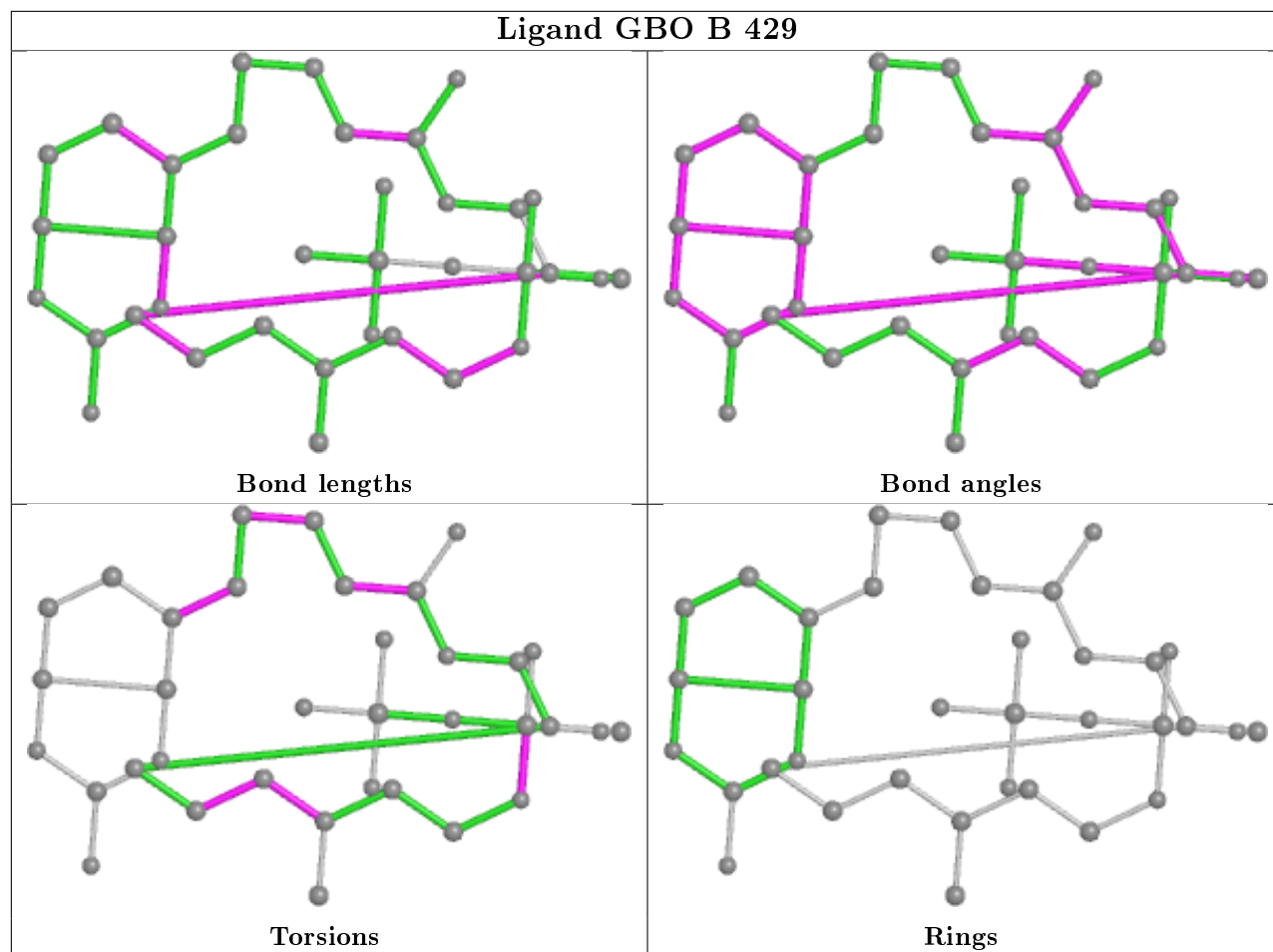
Mol	Chain	Res	Type	Atoms
4	B	429	GB0	C1-O5-P2-O4
4	B	429	GB0	C14-C15-C16-S1
4	B	429	GB0	C14-C15-C16-C19
4	B	429	GB0	C4-C3-C5-C6
4	B	429	GB0	C2-C3-C5-C6
4	B	429	GB0	C12-C13-C14-C15
4	B	429	GB0	O6-C11-C12-C13
4	B	429	GB0	N1-C11-C12-C13
4	B	429	GB0	C1-O5-P2-O3
4	B	429	GB0	C3-C5-C6-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	429	GB0	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	A	315/377 (83%)	-0.56	2 (0%) 89 86	32, 57, 78, 103	0
2	B	401/427 (93%)	-0.46	4 (0%) 82 77	31, 50, 82, 122	0
All	All	716/804 (89%)	-0.50	6 (0%) 86 81	31, 54, 80, 122	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	417	GLN	3.5
2	B	66	HIS	2.3
1	A	55	PHE	2.3
2	B	64	PHE	2.1
2	B	379	GLY	2.1
1	A	326	GLN	2.0

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](#)

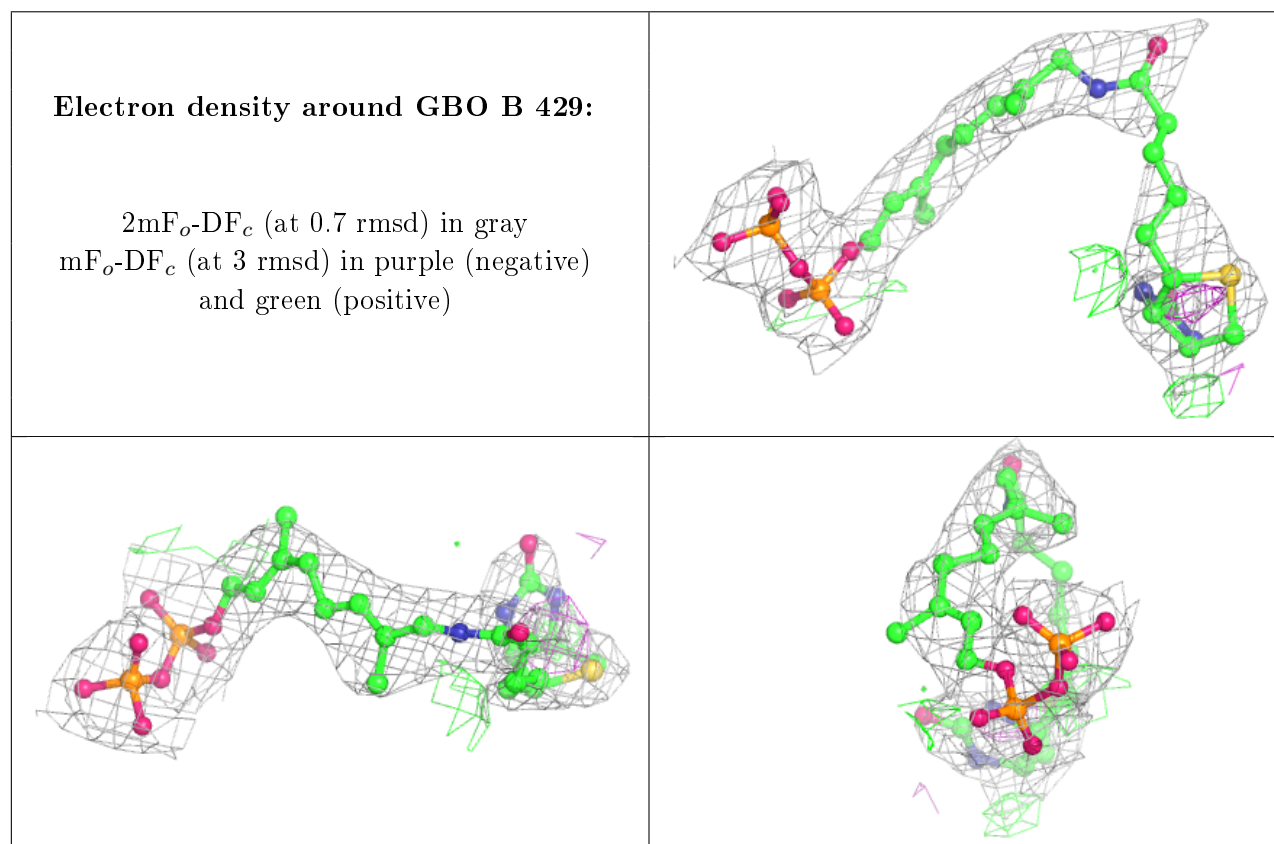
There are no carbohydrates in this entry.

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(\AA^2)	Q<0.9
3	ZN	B	428	1/1	0.96	0.13	34,34,34,34	0
4	GBO	B	429	35/35	0.97	0.17	28,45,91,94	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.