



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 11, 2021 – 04:45 PM EDT

PDB ID : 2ONG
Title : Crystal Structure of of limonene synthase with 2-fluorogeranyl diphosphate (FGPP).
Authors : Hyatt, D.C.; Youn, B.; Croteau, R.; Kang, C.
Deposited on : 2007-01-23
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	2.23.2
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)	:	2.23.2

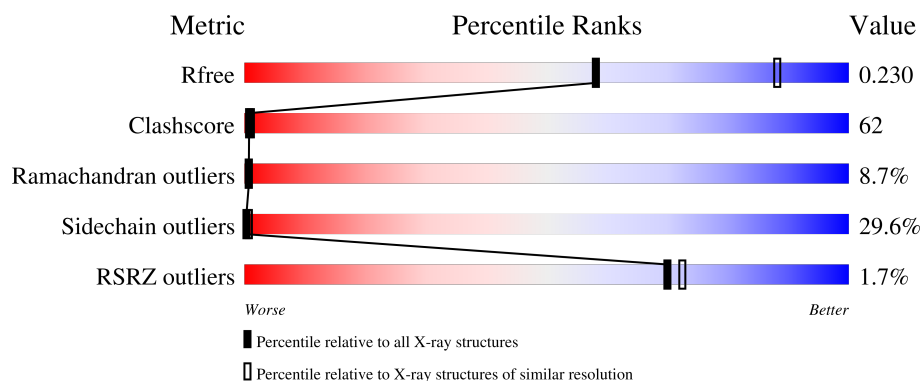
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	543	<div> <div>2%</div> <div>19%</div> <div>47%</div> <div>29%</div> <div>6%</div> </div>
1	B	543	<div> <div>%</div> <div>20%</div> <div>45%</div> <div>30%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FPG	A	600	-	-	X	-
3	FPG	B	1600	-	-	X	-
4	BTB	A	605	-	-	X	-
4	BTB	B	1604	-	-	X	-
4	BTB	B	1605	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9181 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 4S-limonene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	0	0
			4495	2871	761	843	20			
1	B	543	Total	C	N	O	S	0	0	0
			4491	2870	758	843	20			

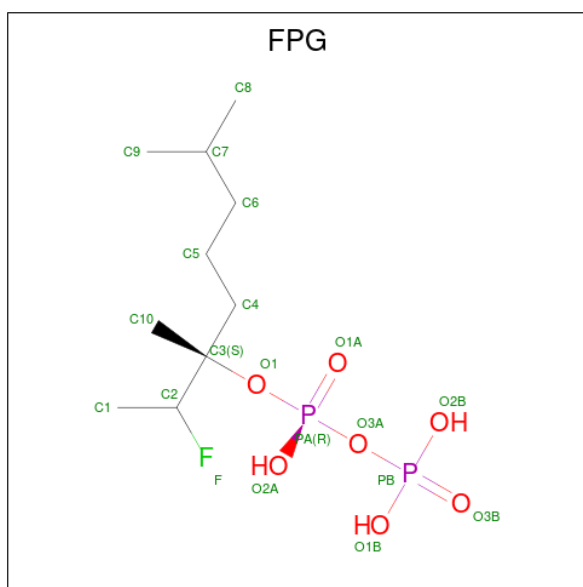
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	MET	GLU	engineered mutation	UNP Q40322
B	57	MET	GLU	engineered mutation	UNP Q40322

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

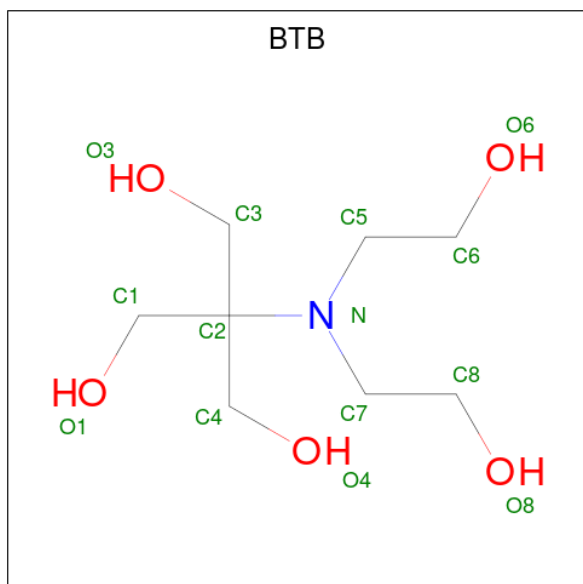
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mn	0	0
			3	3		
2	B	3	Total	Mn	0	0
			3	3		

- Molecule 3 is (1S)-1-[(1R)-1-FLUOROETHYL]-1,5-DIMETHYLHEXYL TRIHYDROGEN DIPHOSPHATE (three-letter code: FPG) (formula: C₁₀H₂₃FO₇P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	O	P	0	0
			20	10	1	7	2		
3	B	1	Total	C	F	O	P	0	0
			20	10	1	7	2		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

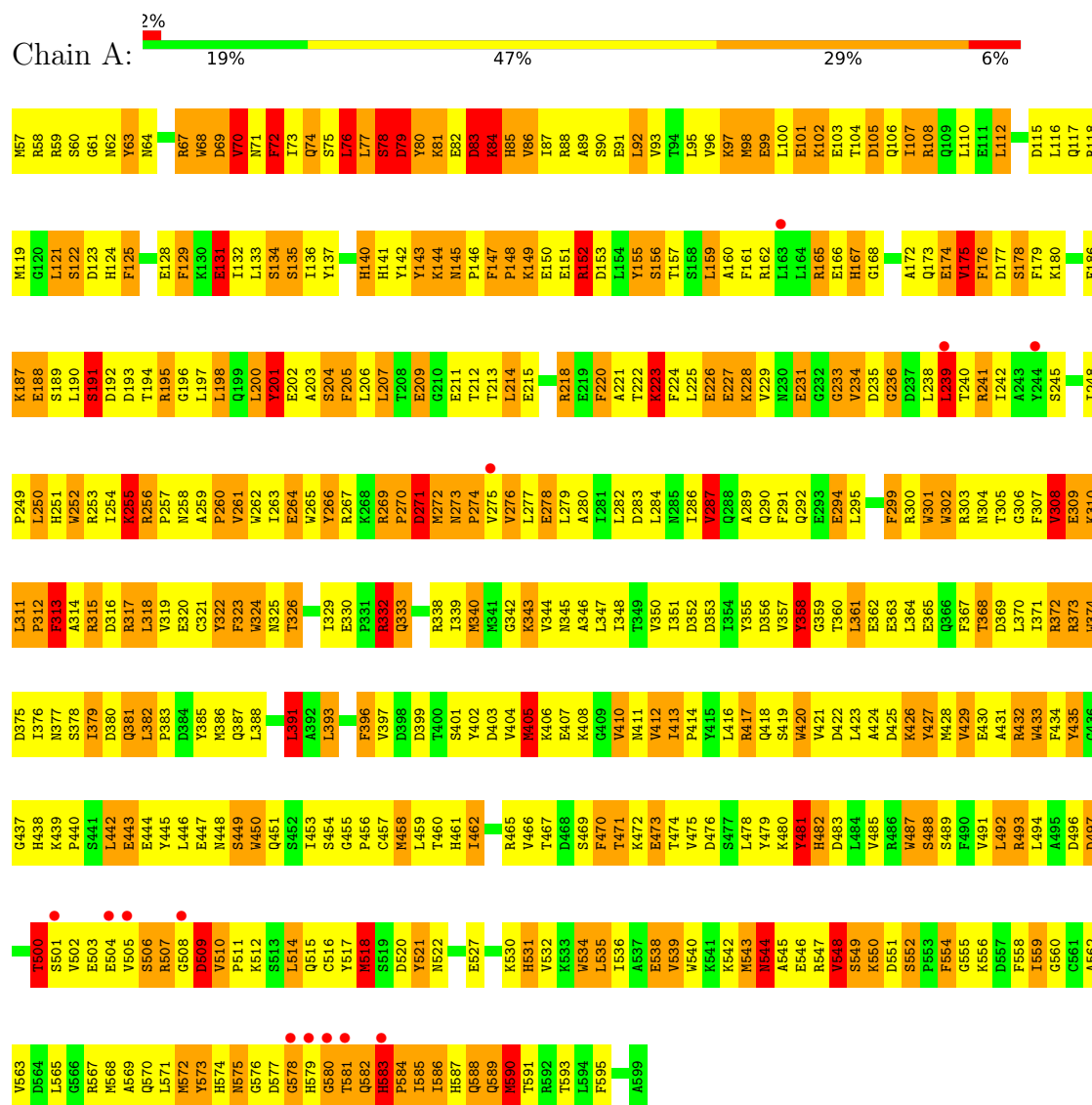
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total	O	0	0
			39	39		
5	B	54	Total	O	0	0
			54	54		

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: 4S-limonene synthase



G560	L494	A495	D496	D497	L498	G499	T500	S501	V502	E503	E504	L505	S506	R507	G508	D509	V510	P511	K512	L513	L514	Q515	C516	Y517	M518	S519	D520	A526	E527	A528	R529	K530	H531	W534	L535	I536	A537	W540	K541	M542	M543	N544	A545	E546	R547	V548	S549	K550	D551	S552	P553	F554	G555	K556	D557	L492	I559			
F434	F435	G436	G437	H438	H439	K440	P441	S441	L442	E443	E444	Y445	L446	E447	M448	S449	G450	Y451	L452	S453	S454	G455	P456	C457	M458	L459	T460	H461	L462	F463	F464	R465	V466	D467	D468	S469	F470	T471	K472	E473	T474	V475	D476	S477	L478	Y479	K480	Y481	H482	D483	L484	V485	R486	Y487	S488	S489	F490	V491	L492	R493
I371	R372	K373	W374	D375	L376	K377	S378	L379	D380	Q381	L382	P383	D384	Y385	K386	Q387	L388	L391	A392	L393	G394	N395	F396	V397	D398	D399	T400	S401	L402	F403	A404	K406	E407	K408	G409	V410	N411	I412	P413	Y414	V415	L416	R417	Q418	S419	V420	Y421	D422	L423	A424	D425	K426	Y427	M428	V429	E430	A431	R432	W433	
V308	E309	K310	L311	P312	F313	A314	R315	D316	R317	L318	V319	E320	C321	T322	F323	W324	N325	T326	T329	K332	Q333	Q334	A335	S336	P337	R338	T339	L340	K341	G342	K343	V344	A345	L346	L347	I348	T349	V350	I351	D352	Q353	L354	V357	E362	L363	L364	R365	K366	F367	T368	D369	L370								
D247	I248	P249	L250	P251	W252	R253	L254	K255	R256	P257	W258	F259	P260	W261	W262	I263	W264	W265	W266	R267	K268	R269	P270	D271	W272	R273	P274	W275	V276	L277	E278	L279	A280	I281	L282	D283	L284	W285	L286	V287	Q288	A289	Q290	F291	Q292	E293	E294	L295	K296	F299	K300	W301	K302	R303	I304	T305	G306	F307		
E185	E188	E189	L190	S191	D192	D193	D194	R195	G196	Q199	L200	W201	E202	A203	S204	F205	L206	L207	T208	E209	G210	E211	T212	T213	L214	E215	S216	A217	R218	E219	F220	D221	T222	K223	F224	L225	E226	E227	K228	V229	W230	E231	G232	G233	V234	D235	G236	D237	L238	L239	T240	R241	L242	A243	Y244	S245	L246			
Q117	R118	M119	G120	S121	L121	D123	H124	F125	Q126	N127	E128	F129	K130	E131	I132	Y137	L138	D139	H140	H141	Y142	Y143	K144	N145	P146	F147	P148	K149	V150	E151	R152	D153	L154	Y155	S156	T157	S158	L159	A160	F161	R162	L163	L164	R165	F169	E174	V176	D177	S178	F179	K180	N181	E182	S183	G184					
M57	R58	R59	S60	G61	M62	Y63	M64	P65	S66	R67	W68	F69	D70	W71	F72	I73	Q74	S75	L76	L77	S78	D79	Y80	K81	E82	K83	P84	H85	V86	I87	R88	A89	S90	E91	L92	V93	T94	L95	V96	K97	M98	E99	L100	E101	A102	E103	T104	D105	Q106	I107	R108	Q109	L110	E111	L112	I113	D114	L115	L116	

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	200.48Å 200.48Å 123.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 27.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 93.0 (27.90-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.61Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.208 , 0.241 0.221 , 0.230	Depositor DCC
R_{free} test set	3503 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 120.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.478 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9181	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: BTB, FPG, MN

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	0.91	9/4607 (0.2%)	1.67	129/6234 (2.1%)
1	B	0.89	4/4603 (0.1%)	1.62	108/6230 (1.7%)
All	All	0.90	13/9210 (0.1%)	1.65	237/12464 (1.9%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	THR	C-O	8.06	1.38	1.23
1	A	131	GLU	CG-CD	7.48	1.63	1.51
1	B	368	THR	C-O	6.90	1.36	1.23
1	A	487	TRP	CG-CD2	-6.30	1.32	1.43
1	A	433	TRP	CG-CD2	-6.29	1.32	1.43

The worst 5 of 237 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	TYR	N-CA-C	-11.62	79.63	111.00
1	B	266	TYR	CB-CG-CD1	-11.53	114.08	121.00
1	A	266	TYR	CB-CG-CD1	-10.92	114.45	121.00
1	A	433	TRP	CD1-CG-CD2	10.65	114.82	106.30
1	A	143	TYR	CB-CG-CD1	-10.62	114.62	121.00

There are no chirality outliers.

There are no planarity outliers.

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	4495	0	4346	544	0
1	B	4491	0	4342	495	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	20	0	18	9	0
3	B	20	0	18	13	0
4	A	28	0	38	22	0
4	B	28	0	38	40	0
5	A	39	0	0	1	0
5	B	54	0	0	2	0
All	All	9181	0	8800	1101	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 62.

The worst 5 of 1101 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)
4:B:1604:BTB:N	4:B:1604:BTB:C2	1.68	1.56
4:B:1605:BTB:N	4:B:1605:BTB:C2	1.69	1.51
4:A:605:BTB:N	4:A:605:BTB:C2	1.71	1.49
1:B:579:HIS:CD2	3:B:1600:FPG:H92	1.67	1.28
4:B:1605:BTB:C7	4:B:1605:BTB:H32	1.72	1.19

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	541/543 (100%)	400 (74%)	93 (17%)	48 (9%)	1 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	541/543 (100%)	409 (76%)	86 (16%)	46 (8%)	1	1
All	All	1082/1086 (100%)	809 (75%)	179 (16%)	94 (9%)	1	1

5 of 94 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	78	SER
1	A	83	ASP
1	A	125	PHE
1	A	152	ARG

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	490/492 (100%)	352 (72%)	138 (28%)	0	1
1	B	490/492 (100%)	338 (69%)	152 (31%)	0	0
All	All	980/984 (100%)	690 (70%)	290 (30%)	0	1

5 of 290 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	362	GLU
1	B	588	GLN
1	B	394	ASN
1	B	474	THR
1	A	426	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	574	HIS
1	B	575	ASN

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Mol	Chain	Res	Type
1	A	461	HIS
1	A	438	HIS
1	B	579	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 ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	BTB	B	1604	-	13,13,13	4.34	6 (46%)	7,16,16	1.07	1 (14%)
3	FPG	B	1600	2	16,19,19	1.82	3 (18%)	20,29,29	2.54	4 (20%)
4	BTB	B	1605	-	13,13,13	4.11	6 (46%)	7,16,16	1.04	1 (14%)
4	BTB	A	604	-	13,13,13	1.89	4 (30%)	7,16,16	0.57	0
3	FPG	A	600	2	16,19,19	1.88	4 (25%)	20,29,29	2.13	4 (20%)
4	BTB	A	605	-	13,13,13	4.35	5 (38%)	7,16,16	1.13	1 (14%)

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	BTB	B	1604	-	-	10/21/21/21	-
3	FPG	B	1600	2	-	7/19/25/25	-
4	BTB	B	1605	-	-	8/21/21/21	-
4	BTB	A	604	-	-	2/21/21/21	-
3	FPG	A	600	2	-	8/19/25/25	-
4	BTB	A	605	-	-	9/21/21/21	-

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	BTB	C2-N	11.49	1.71	1.48
4	B	1605	BTB	C2-N	10.46	1.69	1.48
4	B	1604	BTB	C2-N	10.25	1.68	1.48
4	B	1604	BTB	C5-N	7.72	1.59	1.48
4	A	605	BTB	C5-N	7.58	1.59	1.48

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1600	FPG	F-C2-C1	8.32	121.86	108.18
3	A	600	FPG	F-C2-C1	7.14	119.92	108.18
3	B	1600	FPG	O1-C3-C10	-4.70	86.95	107.58
3	B	1600	FPG	PA-O3A-PB	-3.89	119.46	132.83
3	A	600	FPG	PA-O3A-PB	-3.38	121.22	132.83

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

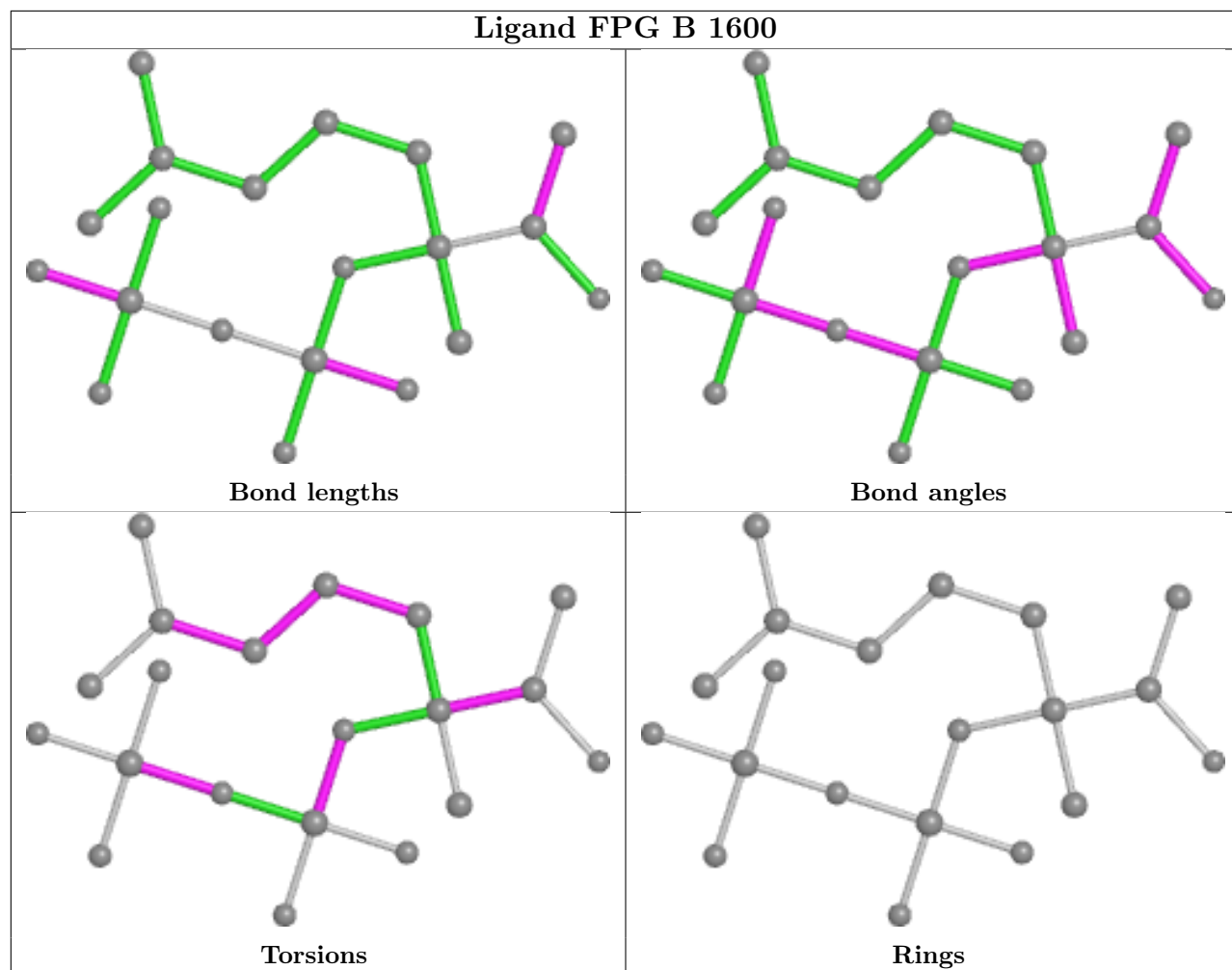
Mol	Chain	Res	Type	Atoms
3	A	600	FPG	C1-C2-C3-C10
3	A	600	FPG	C1-C2-C3-C4
3	A	600	FPG	C2-C3-C4-C5
3	B	1600	FPG	C1-C2-C3-C10
3	B	1600	FPG	C1-C2-C3-C4

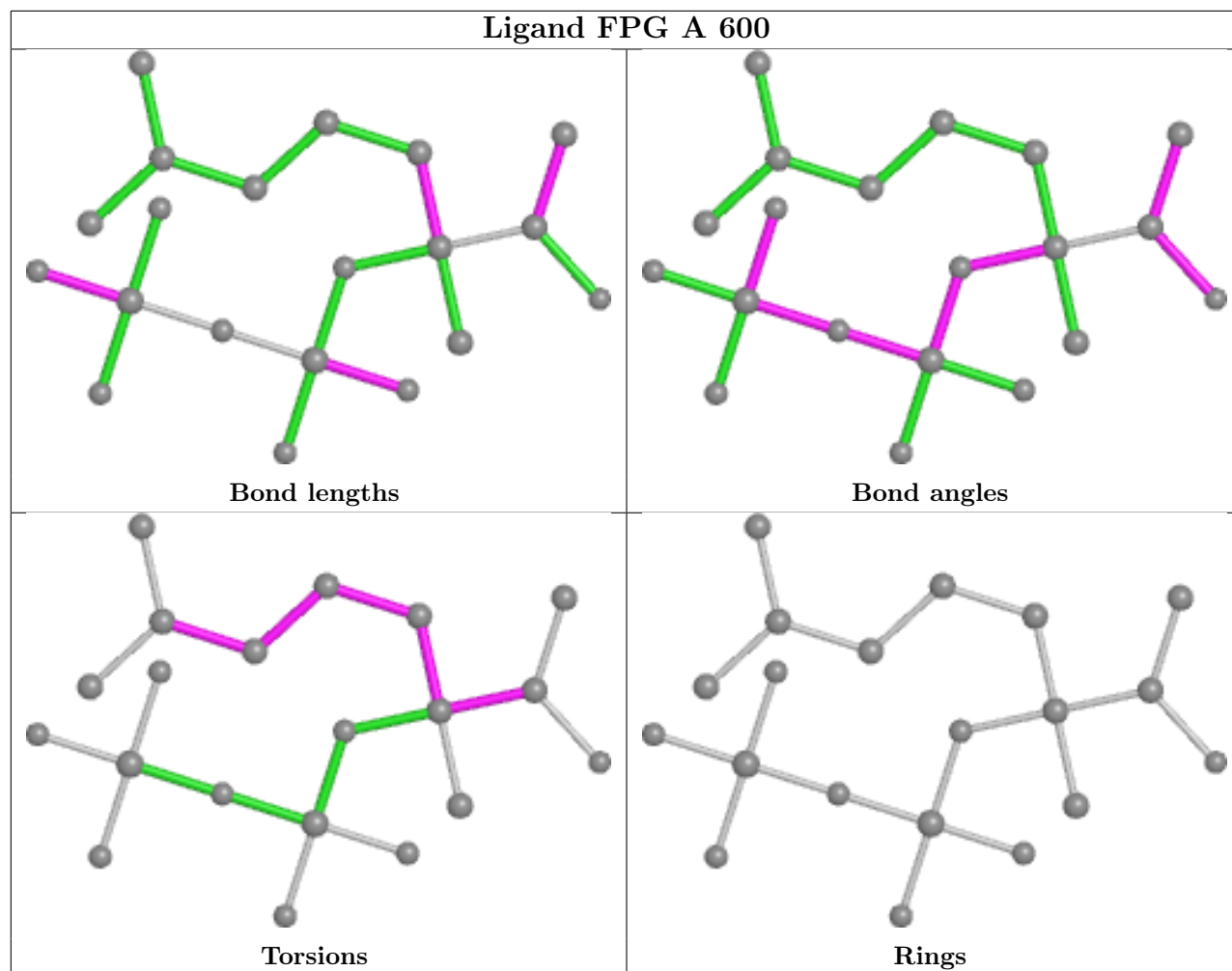
There are no ring outliers.

6 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1604	BTB	19	0
3	B	1600	FPG	13	0
4	B	1605	BTB	21	0
4	A	604	BTB	3	0
3	A	600	FPG	9	0
4	A	605	BTB	19	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	543/543 (100%)	0.07	13 (2%) 59 60	18, 46, 94, 100	0
1	B	543/543 (100%)	0.04	6 (1%) 80 82	16, 46, 96, 100	0
All	All	1086/1086 (100%)	0.05	19 (1%) 70 72	16, 46, 95, 100	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	579	HIS	6.5
1	B	579	HIS	6.3
1	B	505	VAL	4.9
1	B	580	GLY	4.3
1	B	504	GLU	4.1

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

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

6.3 Carbohydrates [i](#)

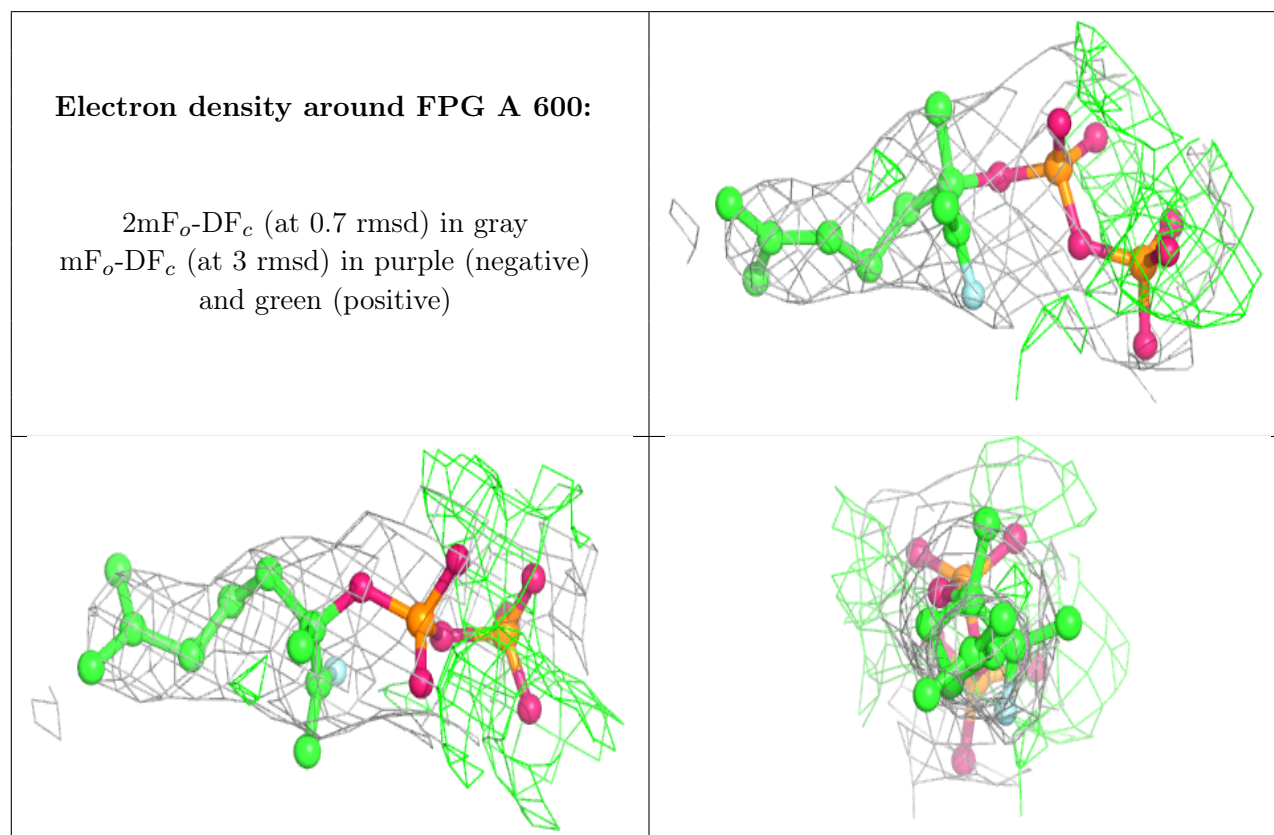
There are no monosaccharides in this entry.

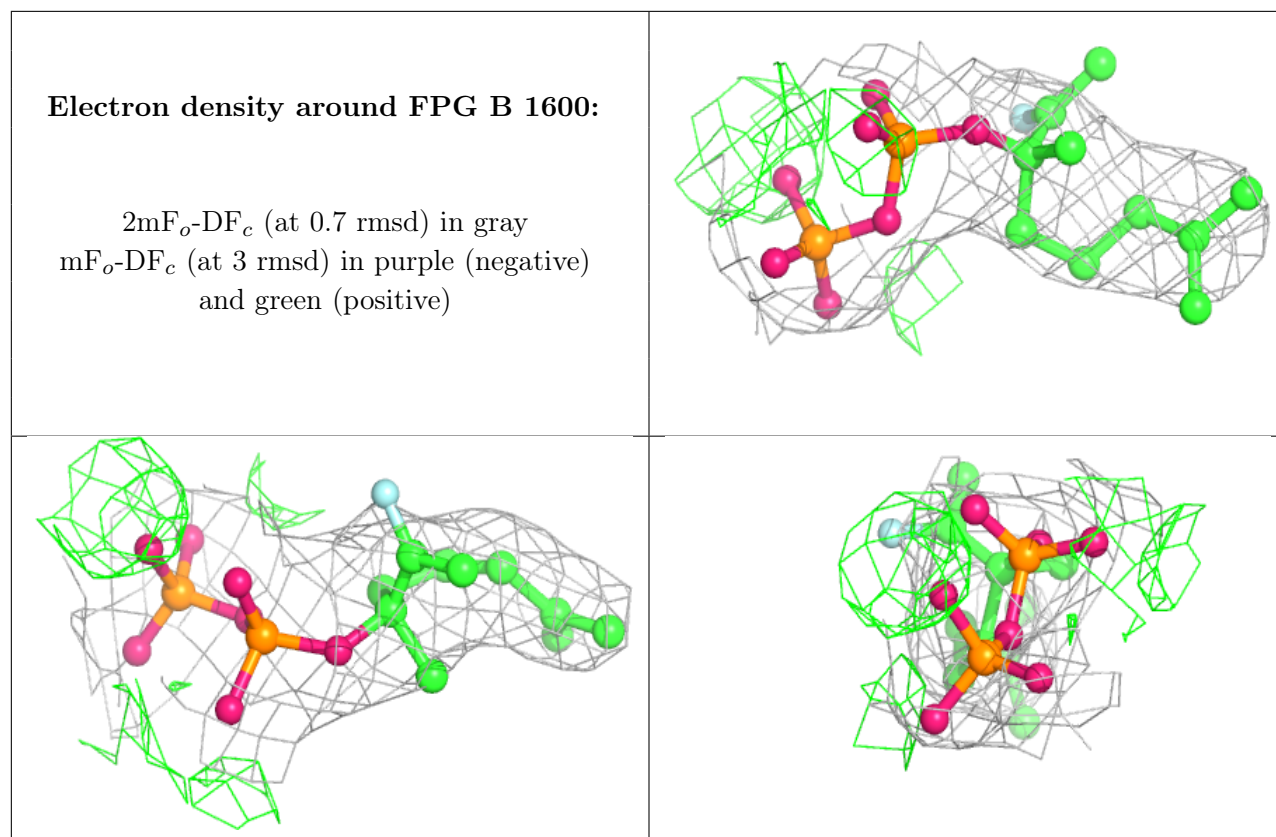
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	BTB	B	1604	14/14	0.66	0.33	67,89,100,100	0
4	BTB	A	604	14/14	0.82	0.50	83,90,96,100	0
4	BTB	A	605	14/14	0.83	0.23	98,100,100,100	0
4	BTB	B	1605	14/14	0.87	0.20	93,100,100,100	0
3	FPG	A	600	20/20	0.97	0.26	54,69,76,82	0
3	FPG	B	1600	20/20	0.97	0.27	44,71,100,100	0
2	MN	A	602	1/1	0.97	0.27	41,41,41,41	0
2	MN	A	601	1/1	0.98	0.26	52,52,52,52	0
2	MN	B	1602	1/1	0.98	0.24	49,49,49,49	0
2	MN	B	1601	1/1	0.99	0.25	52,52,52,52	0
2	MN	B	1603	1/1	0.99	0.25	44,44,44,44	0
2	MN	A	603	1/1	1.00	0.26	43,43,43,43	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.