



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:57 AM UTC

PDB ID : 2ONG / pdb_00002ong
Title : Crystal Structure of of limonene synthase with 2-fluorogeranyl diphosphate (FGPP) enzymatically converted to 2-fluorolinalyl diphosphate (FLPP)
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 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

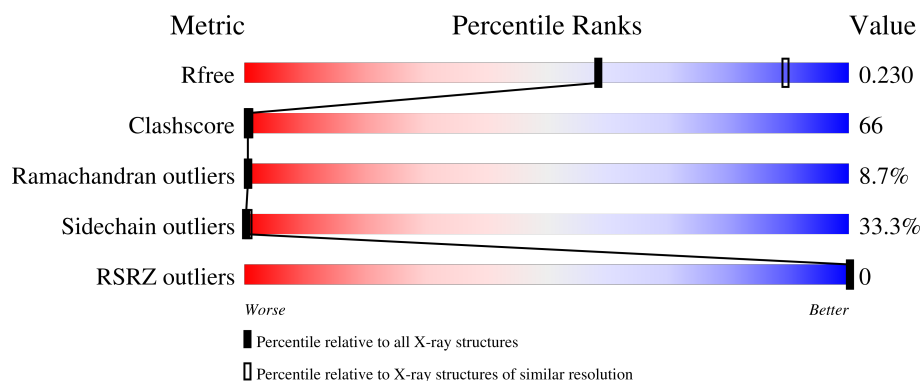
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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	
1	B	543	

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	F3P	A	600	-	-	X	-
3	F3P	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			

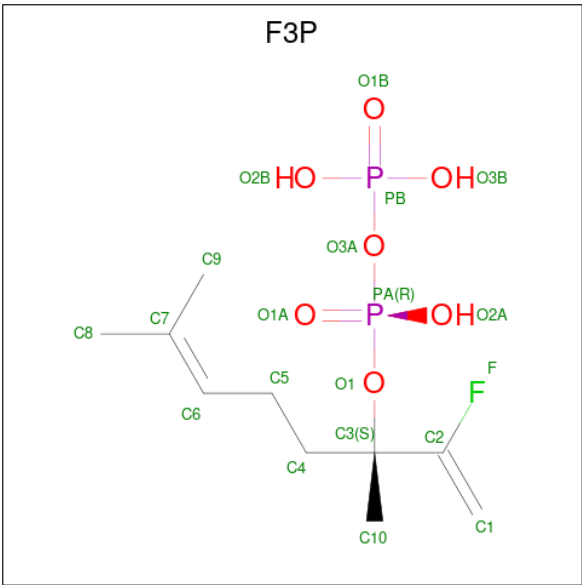
There are 2 discrepancies between the modelled and reference sequences:

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 (CCD ID: MN) (formula: Mn).

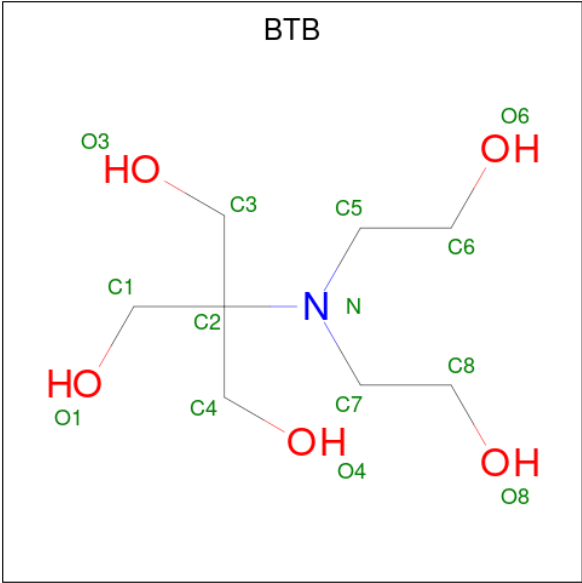
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mn	0	0
			3	3		
2	B	3	Total	Mn	0	0
			3	3		

- Molecule 3 is (3S)-2-fluoro-3,7-dimethylocta-1,6-dien-3-yl trihydrogen diphosphate (CCD ID: F3P) (formula: C₁₀H₁₉FO₇P₂).



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 (CCD ID: BTB) (formula: C₈H₁₉NO₅).



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		

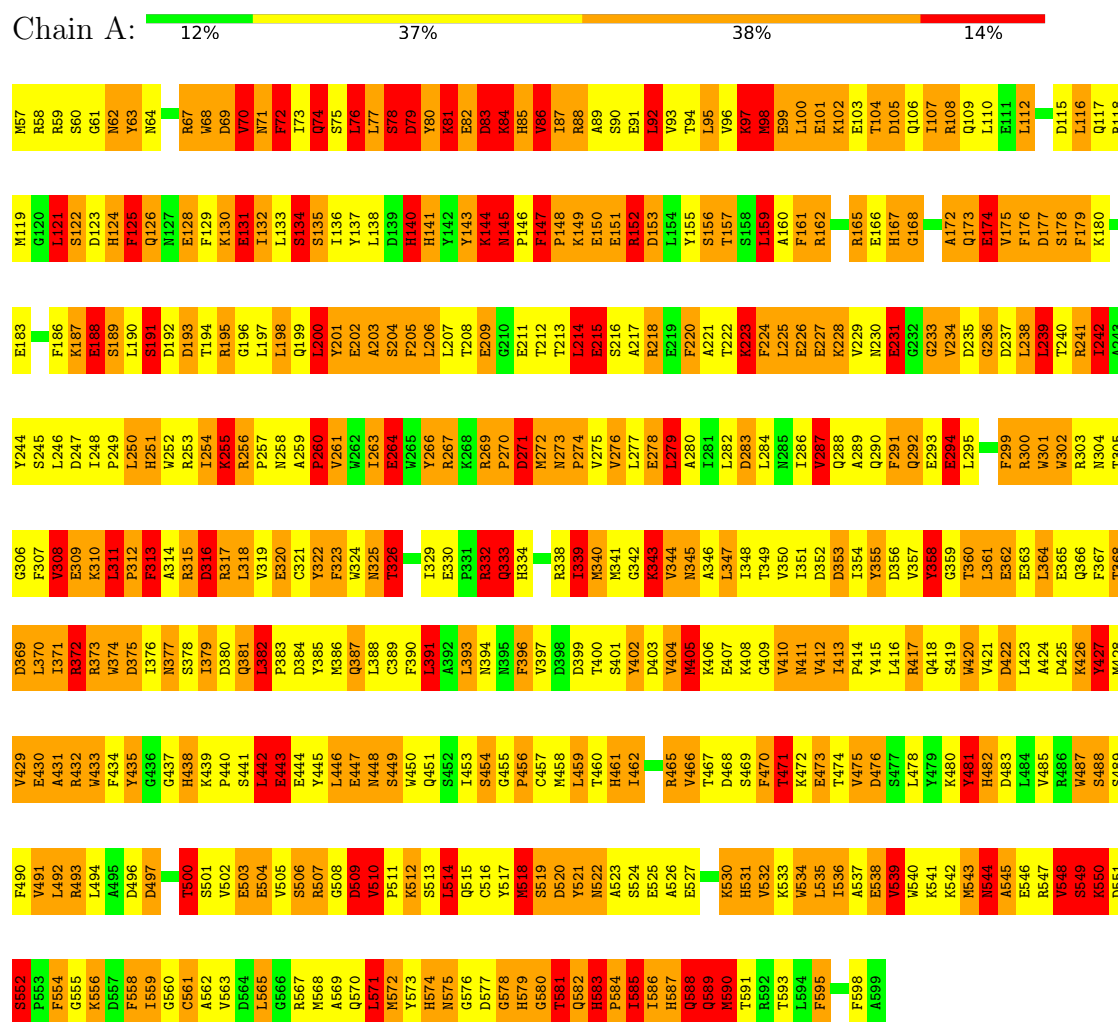
- Molecule 5 is water.

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

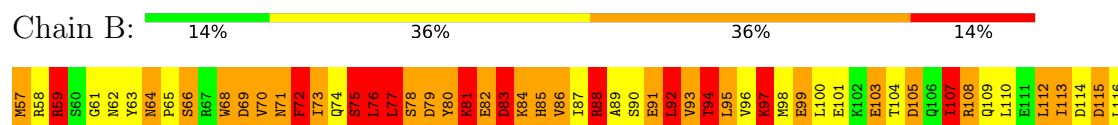
3 Residue-property plots

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



• Molecule 1: 4S-limonene synthase



K550	D551	S552	F553	F554	G555	K556	D557	F558	T559	G560	C561	A562	V563	D564	L565	G566	R567	M568	A569	Q570	L571	M572	Y573	H574	M575	G576	D577	G578	H579	G580	T581	Q582	H583	P584	I585	I586	H587	Q588	Q589	M590	T591	R592	T593	L594	F595	E596	P597	F598	A599										
K426	Y427	M428	F429	E430	A431	R432	W433	G436	G437	H438	K439	P440	S441	L442	E443	E444	Y445	L446	E447	N448	S449	W450	Q451	S452	L453	S454	P455	P456	C457	M458	L459	T460	H461	I462	F463	F464	R465	V466	T467	D468	S469	F470	T471	K472	E473	T474	Y475	D476	S477	L478	Y479	K480	Y481	H482	D483	L484	V485	R486	
W487	S488	S489	F490	V491	L492	R493	L494	A495	D496	D497	L498	G499	T500	S501	V502	E503	E504	V505	S506	R507	G508	D509	Y510	P511	K512	S513	L514	Q515	C516	Y517	H518	S519	D520	P521	N522	A526	E527	A528	R529	K530	H531	W534	L535	T536	A537	E538	V539	W540	K541	M542	M543	N544	A545	E546	R547	V548	S549		
Q366	F367	T368	D369	L370	L371	R372	R373	W374	D375	L376	N377	S378	I379	D380	Q381	L382	P383	D384	Y385	N386	Q387	L388	C389	F390	L391	A392	L393	N394	N395	F396	V397	D398	D399	T400	S401	Y402	D403	Y404	M405	K406	E407	K408	G409	V410	M411	V412	I413	P414	Y415	L416	R417	Q418	S419	W420	V421	D422	L423	A424	D425
W302	R303	N304	G305	L306	F307	V308	E309	K310	L311	P312	F313	A314	R315	D316	R317	L318	V319	E320	C321	Y322	F323	W324	N325	T326	I329	R332	Q333	H334	A335	S336	A337	R338	I339	M340	M341	G342	K343	V344	N345	A346	L347	I348	T349	V350	I351	D352	D353	I354	V357	T360	L361	E362	E363	L364	E365				
Q117	R118	M119	G120	L121	L122	D123	H124	F125	Q126	N127	E128	T129	K130	E131	I132	L133	S134	Y137	L138	D139	H140	H141	Y142	Y143	K144	M145	P146	F147	P148	K149	E150	E151	R152	D153	L154	Y155	S158	L159	A160	F161	R162	L163	L164	R165	E166	V167	G168	F169	E174	V175	F176	D177	S178	F179	K180	N181			

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 10.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.70) 93.1 (10.00-2.70)	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 0.220 , 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)	0.32 , 97.6	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	0.97	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, MN, F3P

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	1.18	39/4607 (0.8%)	2.37	351/6234 (5.6%)
1	B	1.15	42/4603 (0.9%)	2.27	324/6230 (5.2%)
All	All	1.17	81/9210 (0.9%)	2.32	675/12464 (5.4%)

The worst 5 of 81 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	THR	C-O	12.06	1.38	1.24
1	B	368	THR	C-O	9.90	1.36	1.24
1	B	413	ILE	CA-CB	8.17	1.59	1.53
1	B	255	LYS	N-CA	-6.65	1.38	1.46
1	A	482	HIS	N-CA	-6.45	1.38	1.46

The worst 5 of 675 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	LYS	N-CA-C	-18.45	91.25	111.36
1	A	313	PHE	N-CA-C	-16.93	92.29	113.97
1	A	551	ASP	N-CA-C	-16.47	88.00	111.56
1	A	410	VAL	N-CA-C	15.58	129.93	108.11
1	A	313	PHE	CA-C-N	15.53	142.72	120.82

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	592	0
1	B	4491	0	4342	536	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	21	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	1186	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 66.

The worst 5 of 1186 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:F3P: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%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	541/543 (100%)	409 (76%)	86 (16%)	46 (8%)	0	1
All	All	1082/1086 (100%)	809 (75%)	179 (16%)	94 (9%)	0	0

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%)	331 (68%)	159 (32%)	0	1
1	B	490/492 (100%)	323 (66%)	167 (34%)	0	0
All	All	980/984 (100%)	654 (67%)	326 (33%)	0	1

5 of 326 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	242	ILE
1	B	459	LEU
1	B	263	ILE
1	B	362	GLU
1	B	510	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	145	ASN
1	B	579	HIS

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Mol	Chain	Res	Type
1	B	395	ASN
1	B	589	GLN
1	B	544	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	4.55	6 (46%)	7,16,16	1.13	1 (14%)
3	F3P	B	1600	2	14,19,19	2.49	4 (28%)	20,29,29	2.05	2 (10%)
3	F3P	A	600	2	14,19,19	2.54	5 (35%)	20,29,29	1.67	3 (15%)
4	BTB	A	604	-	13,13,13	2.01	4 (30%)	7,16,16	0.57	0
4	BTB	B	1605	-	13,13,13	4.32	6 (46%)	7,16,16	1.08	1 (14%)
4	BTB	A	605	-	13,13,13	4.54	6 (46%)	7,16,16	1.18	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	-	-	11/21/21/21	-
3	F3P	B	1600	2	-	3/17/25/25	-
3	F3P	A	600	2	-	4/17/25/25	-
4	BTB	A	604	-	-	2/21/21/21	-
4	BTB	B	1605	-	-	8/21/21/21	-
4	BTB	A	605	-	-	12/21/21/21	-

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	BTB	C2-N	11.69	1.71	1.48
4	B	1605	BTB	C2-N	10.65	1.69	1.48
4	B	1604	BTB	C2-N	10.43	1.68	1.48
4	B	1604	BTB	C5-N	7.93	1.59	1.48
4	A	605	BTB	C5-N	7.78	1.59	1.48

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1600	F3P	O1-C3-C10	-6.21	86.95	108.11
3	B	1600	F3P	C5-C6-C7	-4.78	111.69	127.64
3	A	600	F3P	C5-C6-C7	-4.57	112.42	127.64
3	A	600	F3P	C10-C3-C2	3.09	116.41	110.69
4	A	605	BTB	C6-C5-N	2.61	121.79	111.59

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

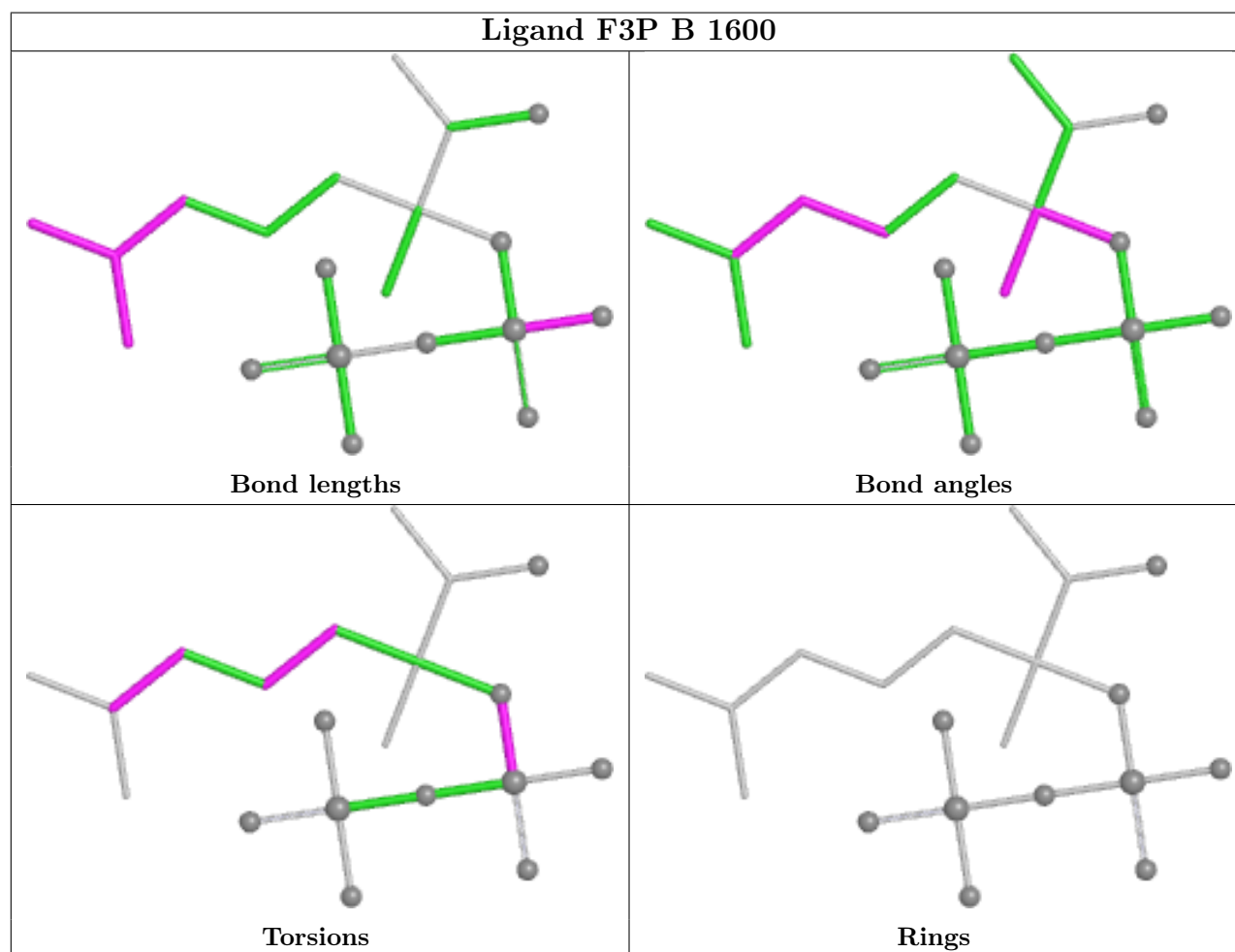
Mol	Chain	Res	Type	Atoms
3	A	600	F3P	C2-C3-C4-C5
3	A	600	F3P	C10-C3-C4-C5
3	B	1600	F3P	C3-C4-C5-C6
4	A	605	BTB	O1-C1-C2-C4
4	A	605	BTB	O1-C1-C2-N

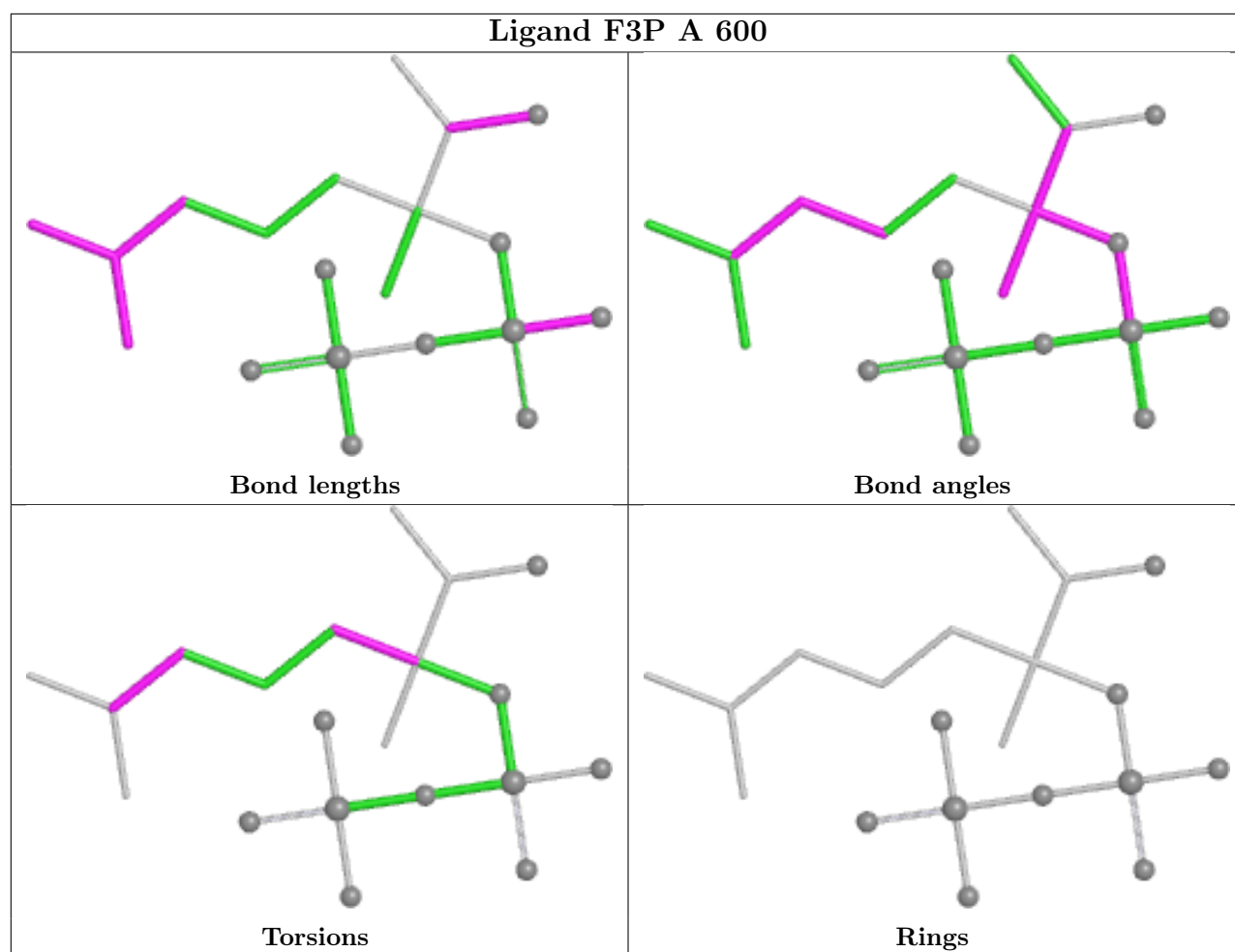
There are no ring outliers.

6 monomers are involved in 83 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1604	BTB	19	0
3	B	1600	F3P	13	0
3	A	600	F3P	9	0
4	A	604	BTB	3	0
4	B	1605	BTB	21	0
4	A	605	BTB	18	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%)	-1.59	0 100 100	18, 46, 94, 100	0
1	B	543/543 (100%)	-1.59	0 100 100	16, 46, 96, 100	0
All	All	1086/1086 (100%)	-1.59	0 100 100	16, 46, 95, 100	0

There are no RSRZ outliers to report.

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 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	BTB	A	605	14/14	0.98	0.05	98,100,100,100	0
4	BTB	A	604	14/14	0.99	0.07	83,90,96,100	0
4	BTB	B	1604	14/14	0.99	0.05	67,89,100,100	0
4	BTB	B	1605	14/14	0.99	0.04	93,100,100,100	0
2	MN	B	1602	1/1	1.00	0.02	49,49,49,49	0
2	MN	B	1603	1/1	1.00	0.01	44,44,44,44	0
3	F3P	A	600	20/20	1.00	0.05	54,69,76,82	0

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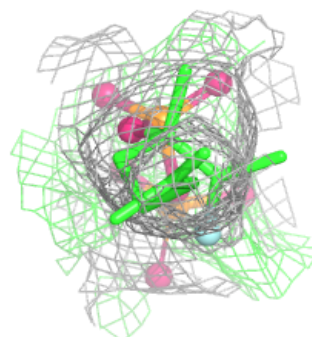
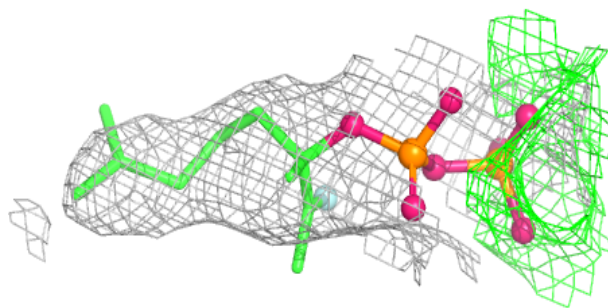
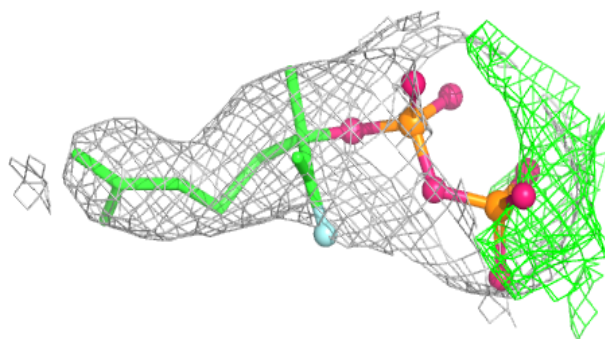
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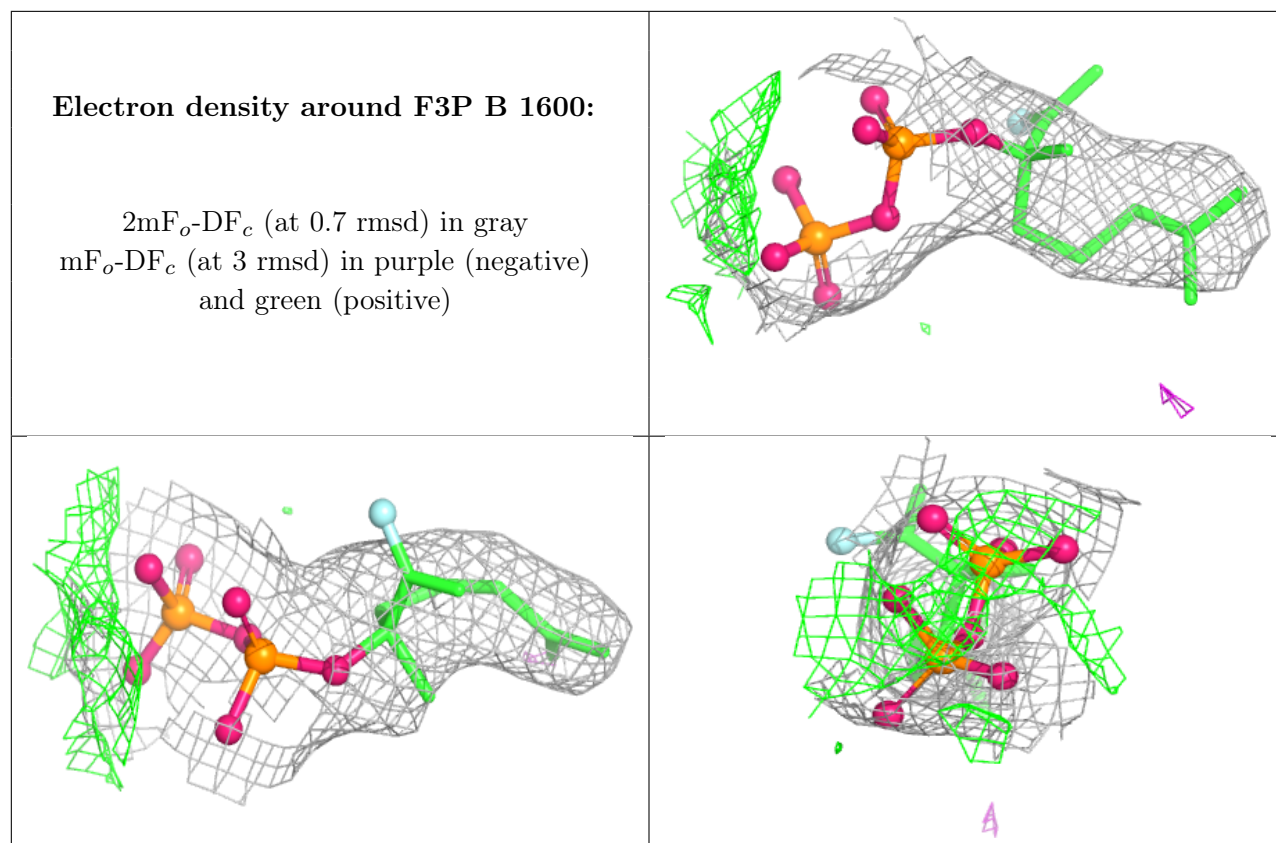
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	F3P	B	1600	20/20	1.00	0.04	44,71,100,100	0
2	MN	A	601	1/1	1.00	0.04	52,52,52,52	0
2	MN	A	602	1/1	1.00	0.03	41,41,41,41	0
2	MN	A	603	1/1	1.00	0.03	43,43,43,43	0
2	MN	B	1601	1/1	1.00	0.04	52,52,52,52	0

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 F3P A 600:

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.