



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:53 AM UTC

PDB ID : 2ONH / pdb_00002onh
Title : Crystal Structure of of limonene synthase with 2-fluorolinalyl diphosphate(FLPP)
Authors : Hyatt, D.C.; Youn, B.; Croteau, R.; Kang, C.
Deposited on : 2007-01-24
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

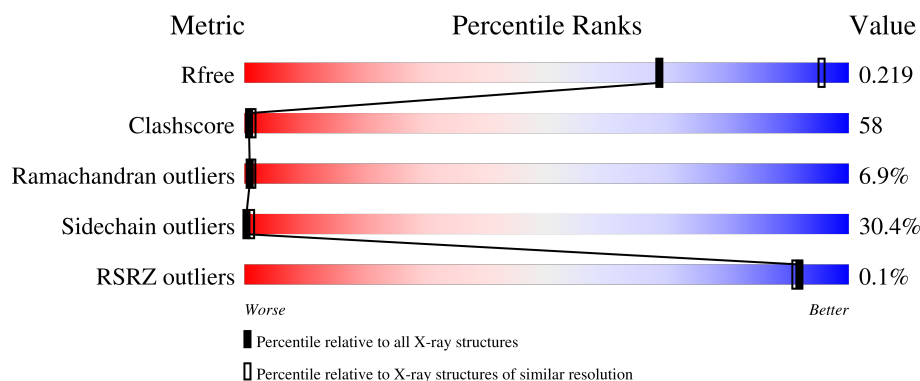
1 Overall quality at a glance

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	 20% 41% 32% 7%
1	B	543	 23% 42% 27% 8%

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	604	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9165 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
			4497	2873	761	843	20			
1	B	543	Total	C	N	O	S	0	0	0
			4497	2873	761	843	20			

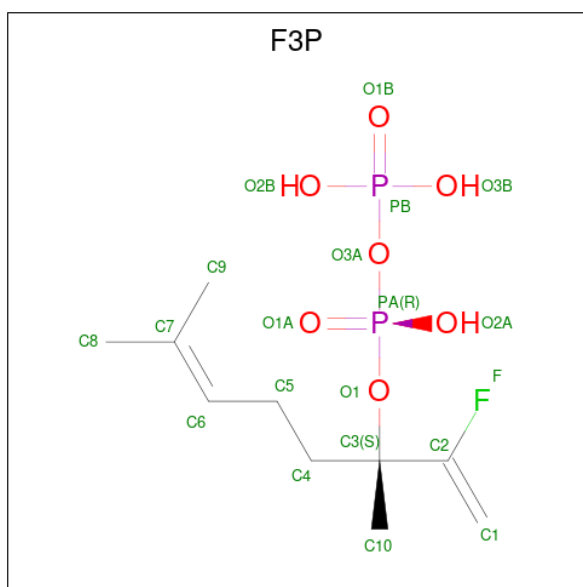
There are 2 discrepancies between the modelled and reference sequences:

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).

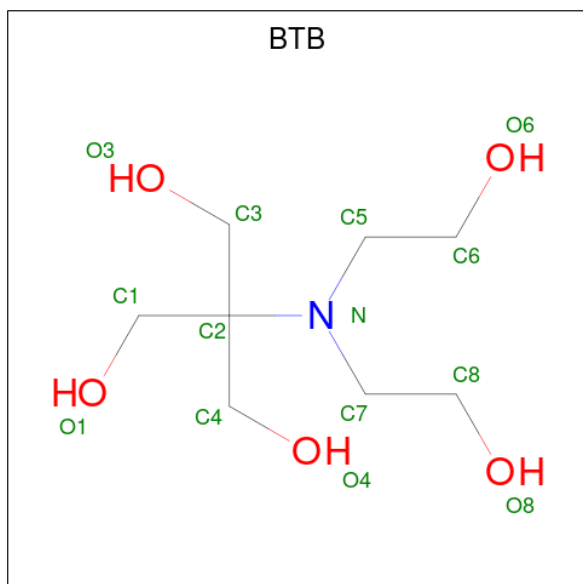
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mn	0	0
			3	3		
2	B	3	Total	Mn	0	0
			3	3		

- 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: $C_8H_{19}NO_5$).



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

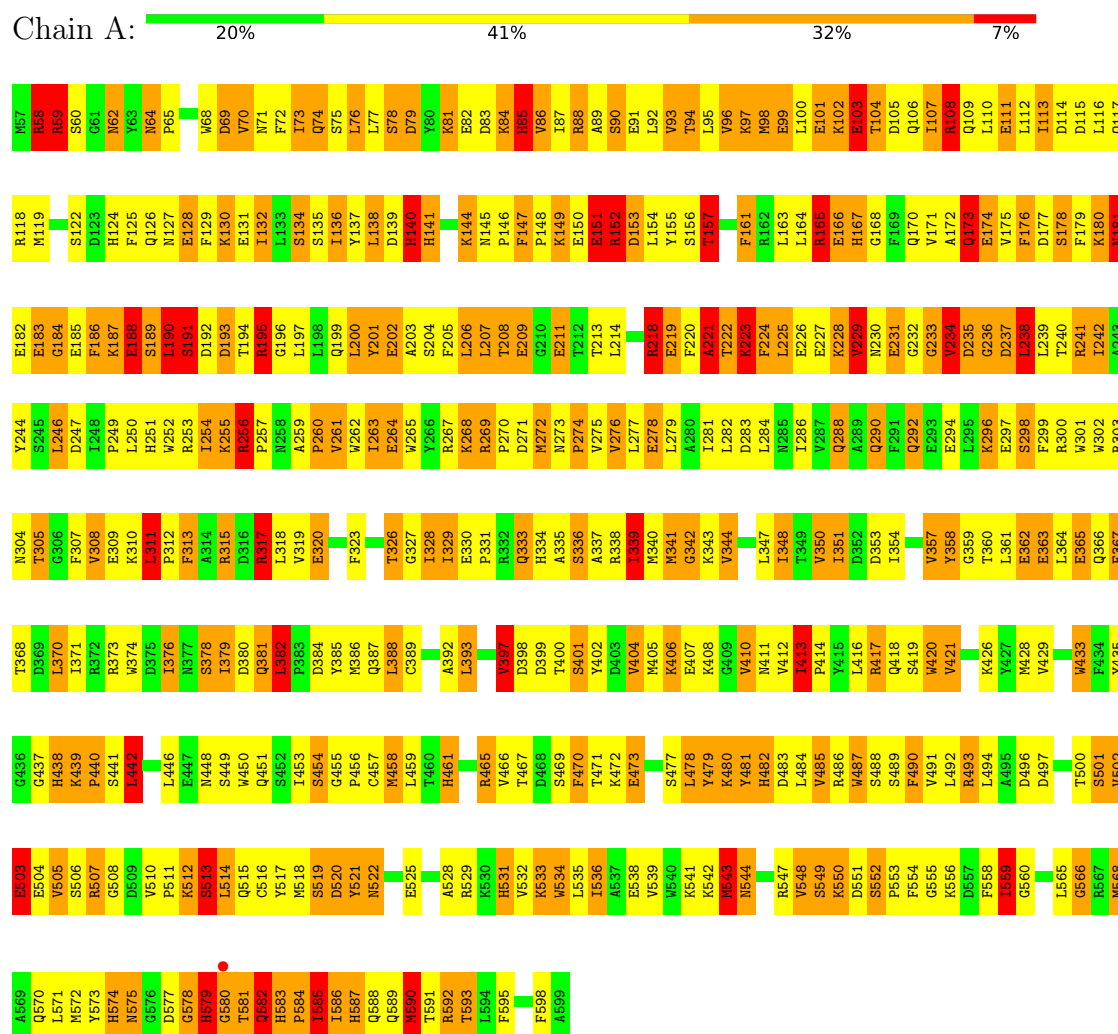
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total 58	O 58	0	0
5	B	53	Total 53	O 53	0	0

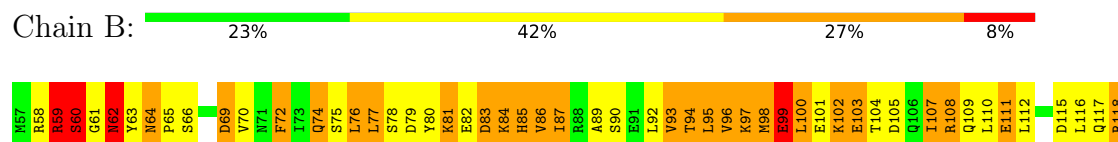
3 Residue-property plots

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



G578	G580	T581	Q582	R583	P584	I585	I586	H587	Q588	Q589	R590	T591	R592	F595	R596	P597	A598	A599
B509	V510	P511	K512	S513	L514	Q515	M518	S519	D520	P456	Y521	M522	A523	S524	E525	A526	R529	K530
K531	S532	K533	V534	L535	V539	M540	M541	V542	F543	V544	M545	M546	M547	M548	M549	M550	M551	M552
M553	M554	M555	M556	M557	M558	M559	M560	M561	M562	M563	M564	M565	M566	M567	M568	M569	M570	M571
M572	M573	M574	M575	M576	M577	M578	M579	M580	M581	M582	M583	M584	M585	M586	M587	M588	M589	M590
M591	M592	M593	M594	M595	M596	M597	M598	M599	M600	M601	M602	M603	M604	M605	M606	M607	M608	M609
M610	M611	M612	M613	M614	M615	M616	M617	M618	M619	M620	M621	M622	M623	M624	M625	M626	M627	M628
M629	M630	M631	M632	M633	M634	M635	M636	M637	M638	M639	M640	M641	M642	M643	M644	M645	M646	M647
M648	M649	M650	M651	M652	M653	M654	M655	M656	M657	M658	M659	M660	M661	M662	M663	M664	M665	M666
M667	M668	M669	M670	M671	M672	M673	M674	M675	M676	M677	M678	M679	M680	M681	M682	M683	M684	M685
M686	M687	M688	M689	M690	M691	M692	M693	M694	M695	M696	M697	M698	M699	M700	M701	M702	M703	M704
M705	M706	M707	M708	M709	M710	M711	M712	M713	M714	M715	M716	M717	M718	M719	M720	M721	M722	M723
M724	M725	M726	M727	M728	M729	M730	M731	M732	M733	M734	M735	M736	M737	M738	M739	M740	M741	M742
M743	M744	M745	M746	M747	M748	M749	M750	M751	M752	M753	M754	M755	M756	M757	M758	M759	M760	M761
M762	M763	M764	M765	M766	M767	M768	M769	M770	M771	M772	M773	M774	M775	M776	M777	M778	M779	M780
M781	M782	M783	M784	M785	M786	M787	M788	M789	M790	M791	M792	M793	M794	M795	M796	M797	M798	M799
M800	M801	M802	M803	M804	M805	M806	M807	M808	M809	M810	M811	M812	M813	M814	M815	M816	M817	M818
M819	M820	M821	M822	M823	M824	M825	M826	M827	M828	M829	M830	M831	M832	M833	M834	M835	M836	M837
M838	M839	M840	M841	M842	M843	M844	M845	M846	M847	M848	M849	M850	M851	M852	M853	M854	M855	M856
M857	M858	M859	M860	M861	M862	M863	M864	M865	M866	M867	M868	M869	M870	M871	M872	M873	M874	M875
M876	M877	M878	M879	M880	M881	M882	M883	M884	M885	M886	M887	M888	M889	M890	M891	M892	M893	M894
M895	M896	M897	M898	M899	M900	M901	M902	M903	M904	M905	M906	M907	M908	M909	M910	M911	M912	M913
M914	M915	M916	M917	M918	M919	M920	M921	M922	M923	M924	M925	M926	M927	M928	M929	M930	M931	M932
M933	M934	M935	M936	M937	M938	M939	M940	M941	M942	M943	M944	M945	M946	M947	M948	M949	M950	M951
M952	M953	M954	M955	M956	M957	M958	M959	M960	M961	M962	M963	M964	M965	M966	M967	M968	M969	M970
M971	M972	M973	M974	M975	M976	M977	M978	M979	M980	M981	M982	M983	M984	M985	M986	M987	M988	M989
M990	M991	M992	M993	M994	M995	M996	M997	M998	M999									

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	198.66Å 198.66Å 122.67Å 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) 91.0 (10.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.61Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.206 , 0.234 0.217 , 0.219	Depositor DCC
R_{free} test set	3309 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	63.2	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.487 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9165	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: F3P, BTB, 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	1.47	80/4609 (1.7%)	1.65	124/6237 (2.0%)
1	B	1.44	66/4609 (1.4%)	1.62	100/6237 (1.6%)
All	All	1.46	146/9218 (1.6%)	1.63	224/12474 (1.8%)

The worst 5 of 146 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	539	VAL	CA-CB	-10.83	1.42	1.54
1	A	413	ILE	CA-CB	10.55	1.61	1.53
1	A	368	THR	C-N	9.92	1.47	1.33
1	B	404	VAL	CA-CB	-9.77	1.43	1.54
1	A	368	THR	C-O	9.32	1.35	1.24

The worst 5 of 224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	GLU	CB-CG-CD	15.43	138.82	112.60
1	A	482	HIS	ND1-CG-CD2	14.23	120.33	106.10
1	B	426	LYS	CA-CB-CG	-12.87	88.35	114.10
1	A	209	GLU	CB-CG-CD	11.20	131.64	112.60
1	A	480	LYS	N-CA-C	-11.10	99.75	113.18

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	4497	0	4353	498	0
1	B	4497	0	4353	493	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	20	0	18	7	0
3	B	20	0	18	12	0
4	A	14	0	19	29	0
5	A	58	0	0	5	1
5	B	53	0	0	3	1
All	All	9165	0	8761	1028	1

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 58.

The worst 5 of 1028 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:A:604:BTB:N	4:A:604:BTB:C2	1.68	1.55
3:B:1600:F3P:H13	3:B:1600:F3P:C6	1.62	1.29
3:B:1600:F3P:H61	3:B:1600:F3P:C1	1.62	1.29
4:A:604:BTB:C7	4:A:604:BTB:H32	1.74	1.16
4:A:604:BTB:N	4:A:604:BTB:C3	2.12	1.12

All (1) 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:A:737:HOH:O	5:B:707:HOH:O[7_554]	2.12	0.08

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	541/543 (100%)	428 (79%)	78 (14%)	35 (6%)	1	1
1	B	541/543 (100%)	407 (75%)	94 (17%)	40 (7%)	1	1
All	All	1082/1086 (100%)	835 (77%)	172 (16%)	75 (7%)	1	1

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	76	LEU
1	A	181	ASN
1	A	193	ASP
1	A	235	ASP

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	491/492 (100%)	337 (69%)	154 (31%)	0	1
1	B	491/492 (100%)	346 (70%)	145 (30%)	0	1
All	All	982/984 (100%)	683 (70%)	299 (30%)	0	1

5 of 299 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	290	GLN
1	B	550	LYS
1	B	332	ARG
1	B	453	ILE
1	A	370	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	461	HIS
1	B	515	GLN
1	B	587	HIS
1	A	451	GLN
1	A	411	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 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	BTB	A	604	-	13,13,13	3.77	5 (38%)	7,16,16	0.72	0
3	F3P	B	1600	2	14,19,19	2.02	5 (35%)	20,29,29	1.34	2 (10%)
3	F3P	A	600	2	14,19,19	2.03	6 (42%)	20,29,29	1.29	2 (10%)

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	A	604	-	-	8/21/21/21	-
3	F3P	B	1600	2	-	2/17/25/25	-
3	F3P	A	600	2	-	2/17/25/25	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	604	BTB	C2-N	10.39	1.68	1.48
4	A	604	BTB	C5-N	5.05	1.55	1.48
4	A	604	BTB	C7-N	4.69	1.54	1.48
3	A	600	F3P	C10-C3	-3.98	1.42	1.52
3	B	1600	F3P	C10-C3	-3.94	1.42	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1600	F3P	C3-C2-C1	-3.71	111.36	122.08
3	A	600	F3P	C3-C2-C1	-3.01	113.40	122.08
3	B	1600	F3P	C9-C7-C8	2.34	119.97	114.59
3	A	600	F3P	C9-C7-C8	2.26	119.78	114.59

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	F3P	PA-O3A-PB-O2B
4	A	604	BTB	O1-C1-C2-C4
4	A	604	BTB	O1-C1-C2-N
4	A	604	BTB	C4-C2-C3-O3
4	A	604	BTB	N-C2-C3-O3

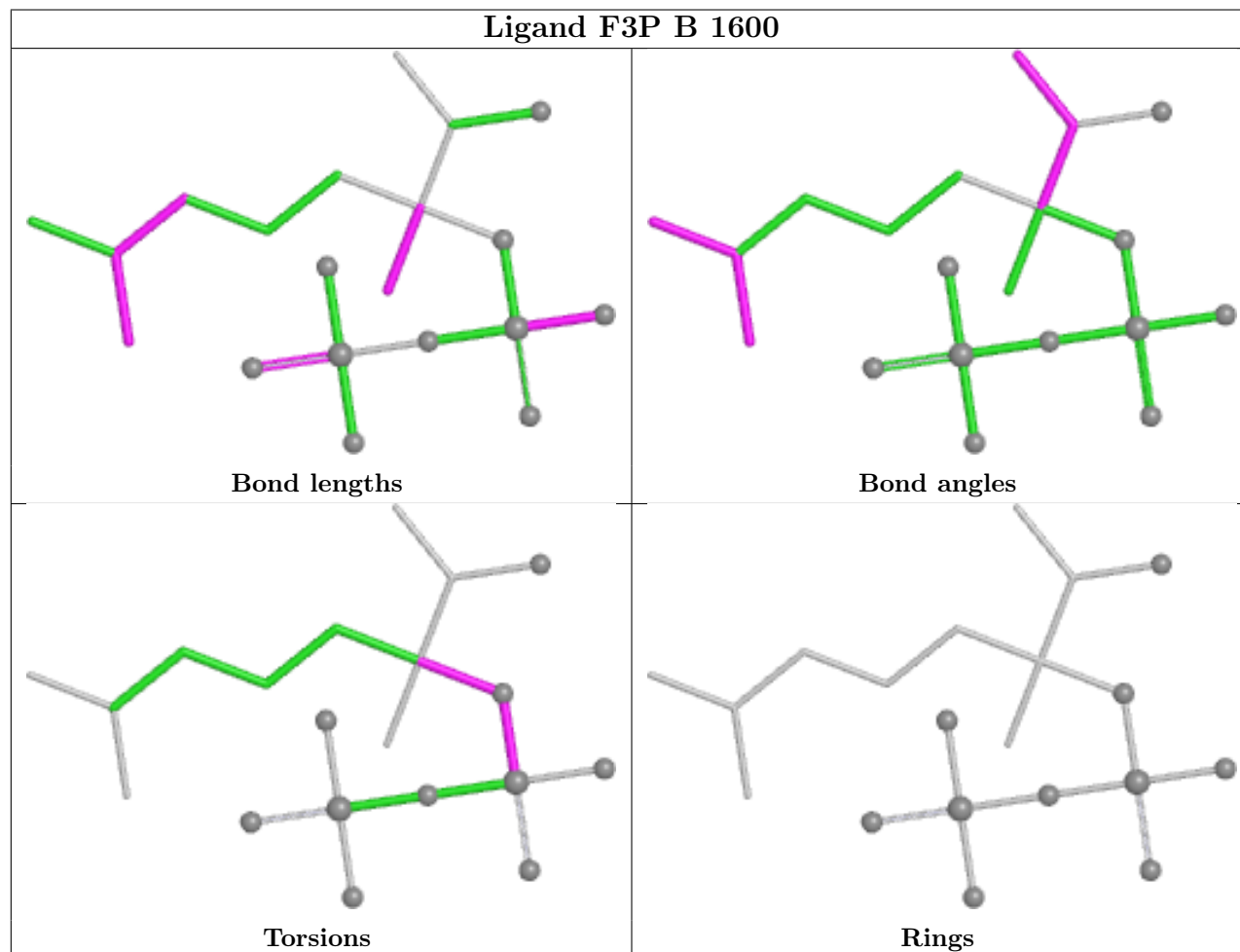
There are no ring outliers.

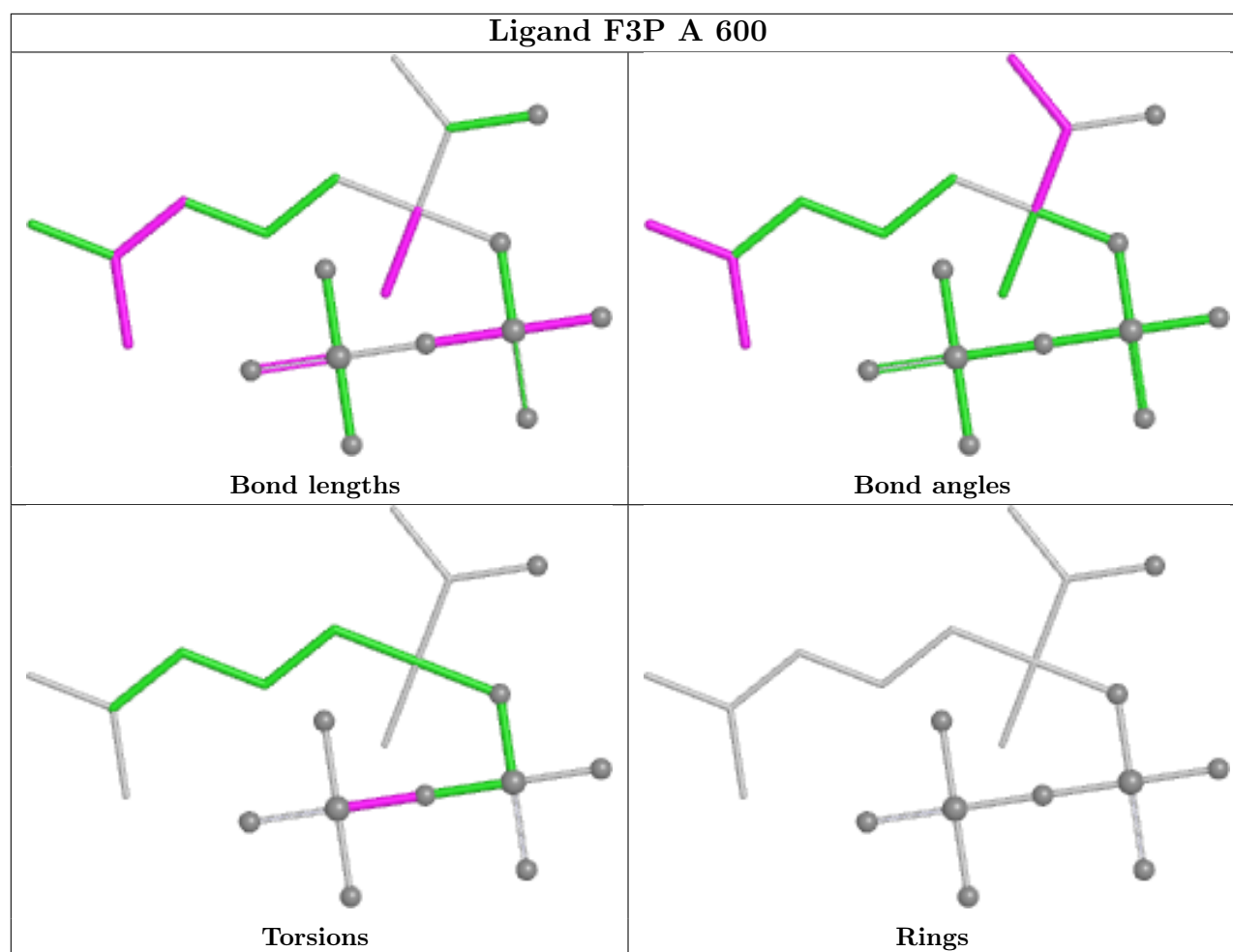
3 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	604	BTB	29	0
3	B	1600	F3P	12	0
3	A	600	F3P	7	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%)	-1.33	1 (0%) 91 90	24, 52, 97, 100	0
1	B	543/543 (100%)	-1.37	0 100 100	23, 52, 98, 100	0
All	All	1086/1086 (100%)	-1.35	1 (0%) 92 91	23, 52, 98, 100	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	580	GLY	2.1

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 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	604	14/14	0.99	0.05	84,91,100,100	0
2	MN	A	602	1/1	1.00	0.02	52,52,52,52	0
2	MN	A	603	1/1	1.00	0.01	54,54,54,54	0
2	MN	B	1601	1/1	1.00	0.04	49,49,49,49	0

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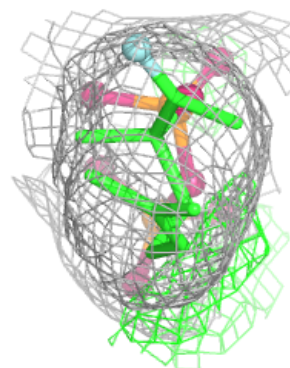
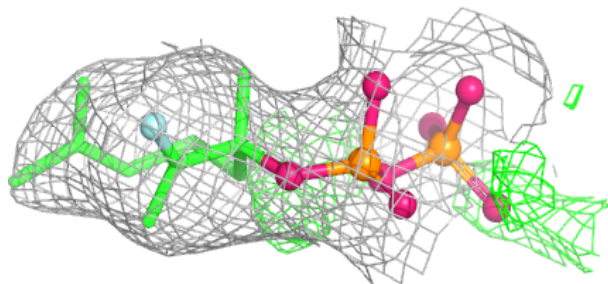
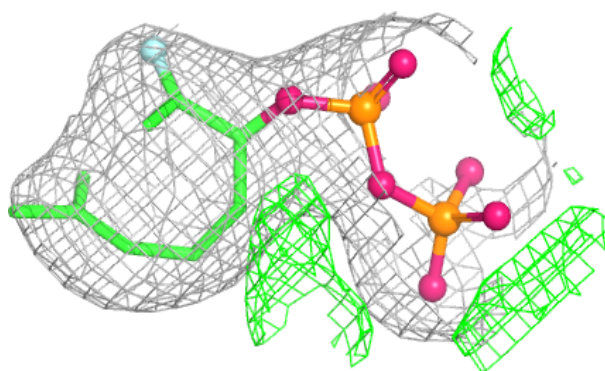
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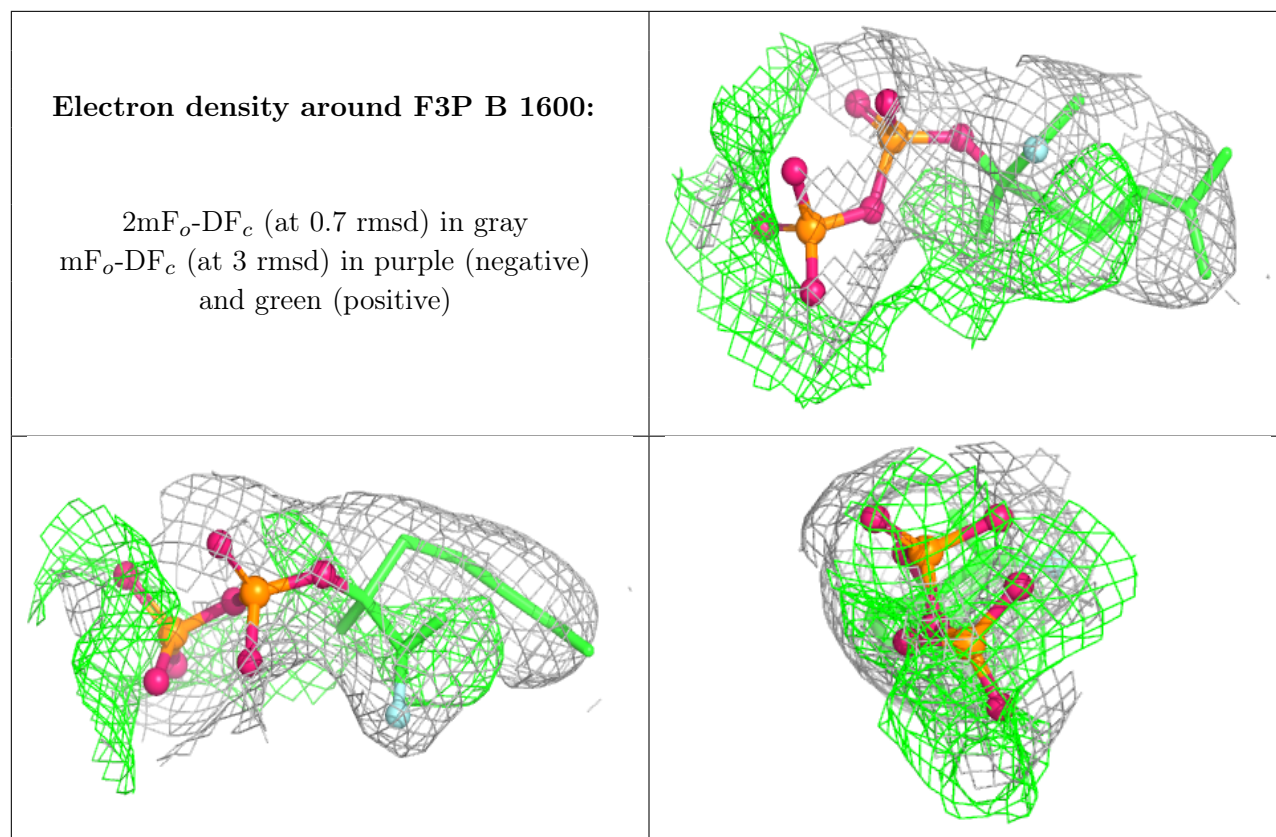
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	B	1602	1/1	1.00	0.04	70,70,70,70	0
2	MN	B	1603	1/1	1.00	0.04	55,55,55,55	0
3	F3P	A	600	20/20	1.00	0.03	45,55,64,67	0
3	F3P	B	1600	20/20	1.00	0.03	45,53,63,66	0
2	MN	A	601	1/1	1.00	0.04	61,61,61,61	0

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.