



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:11 AM UTC

PDB ID : 8BM3 / pdb_00008bm3
Title : H207A mutant of E. coli PgpB, a PAP2 type phosphatidyl glycerol phosphate and C55-PP phosphatase, in complex with farnesyl pyrophosphate
Authors : Delbrassine, F.; El Ghachi, M.; Lambion, A.; Herman, R.; Kerff, F.
Deposited on : 2022-11-10
Resolution : 3.50 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

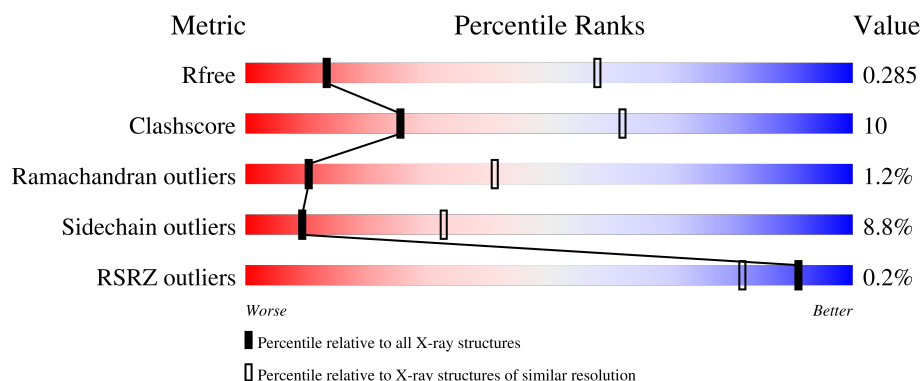
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	264	 60% 26% 5% 9%
1	B	264	 60% 27% 5% 9%
1	C	264	 62% 24% 5% 9%
1	D	264	 60% 26% 5% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7808 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 Phosphatidylglycerophosphatase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1928	1284	335	302	7			
1	B	239	Total	C	N	O	S	0	0	0
			1928	1284	335	302	7			
1	C	239	Total	C	N	O	S	0	0	0
			1928	1284	335	302	7			
1	D	239	Total	C	N	O	S	0	0	0
			1928	1284	335	302	7			

There are 44 discrepancies between the modelled and reference sequences:

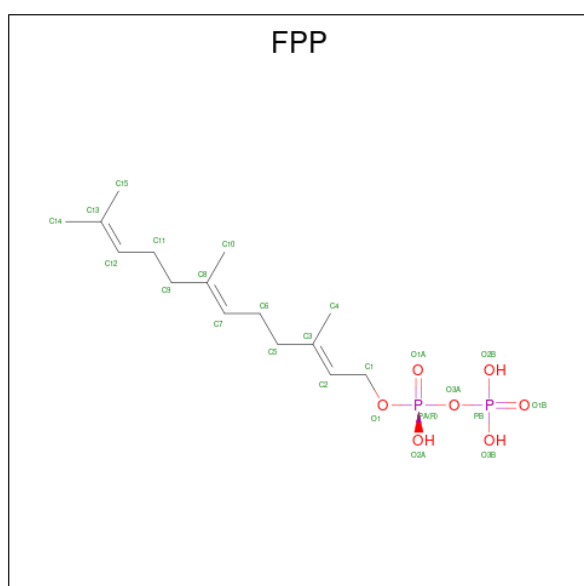
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P0A924
A	0	ALA	-	expression tag	UNP P0A924
A	207	ALA	HIS	engineered mutation	UNP P0A924
A	255	ARG	-	expression tag	UNP P0A924
A	256	SER	-	expression tag	UNP P0A924
A	257	HIS	-	expression tag	UNP P0A924
A	258	HIS	-	expression tag	UNP P0A924
A	259	HIS	-	expression tag	UNP P0A924
A	260	HIS	-	expression tag	UNP P0A924
A	261	HIS	-	expression tag	UNP P0A924
A	262	HIS	-	expression tag	UNP P0A924
B	-1	MET	-	initiating methionine	UNP P0A924
B	0	ALA	-	expression tag	UNP P0A924
B	207	ALA	HIS	engineered mutation	UNP P0A924
B	255	ARG	-	expression tag	UNP P0A924
B	256	SER	-	expression tag	UNP P0A924
B	257	HIS	-	expression tag	UNP P0A924
B	258	HIS	-	expression tag	UNP P0A924
B	259	HIS	-	expression tag	UNP P0A924
B	260	HIS	-	expression tag	UNP P0A924
B	261	HIS	-	expression tag	UNP P0A924

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Chain	Residue	Modelled	Actual	Comment	Reference
B	262	HIS	-	expression tag	UNP P0A924
C	-1	MET	-	initiating methionine	UNP P0A924
C	0	ALA	-	expression tag	UNP P0A924
C	207	ALA	HIS	engineered mutation	UNP P0A924
C	255	ARG	-	expression tag	UNP P0A924
C	256	SER	-	expression tag	UNP P0A924
C	257	HIS	-	expression tag	UNP P0A924
C	258	HIS	-	expression tag	UNP P0A924
C	259	HIS	-	expression tag	UNP P0A924
C	260	HIS	-	expression tag	UNP P0A924
C	261	HIS	-	expression tag	UNP P0A924
C	262	HIS	-	expression tag	UNP P0A924
D	-1	MET	-	initiating methionine	UNP P0A924
D	0	ALA	-	expression tag	UNP P0A924
D	207	ALA	HIS	engineered mutation	UNP P0A924
D	255	ARG	-	expression tag	UNP P0A924
D	256	SER	-	expression tag	UNP P0A924
D	257	HIS	-	expression tag	UNP P0A924
D	258	HIS	-	expression tag	UNP P0A924
D	259	HIS	-	expression tag	UNP P0A924
D	260	HIS	-	expression tag	UNP P0A924
D	261	HIS	-	expression tag	UNP P0A924
D	262	HIS	-	expression tag	UNP P0A924

- Molecule 2 is FARNESYL DIPHOSPHATE (CCD ID: FPP) (formula: $C_{15}H_{28}O_7P_2$) (labeled as "Ligand of Interest" by depositor).

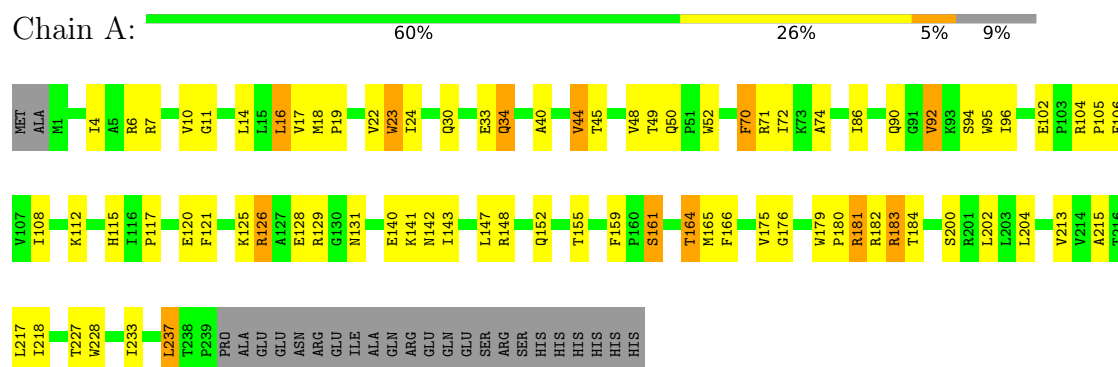


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 24	C 15	O 7	P 2	0	0
2	B	1	Total 24	C 15	O 7	P 2	0	0
2	C	1	Total 24	C 15	O 7	P 2	0	0
2	D	1	Total 24	C 15	O 7	P 2	0	0

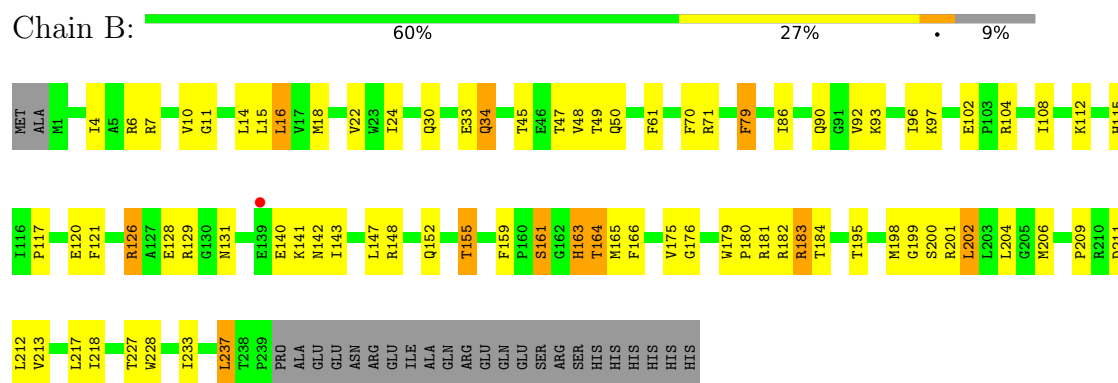
3 Residue-property plots [i](#)

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.

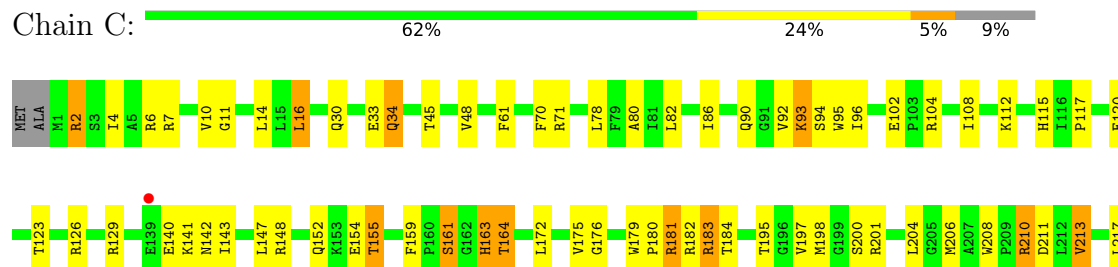
• Molecule 1: Phosphatidylglycerophosphatase B

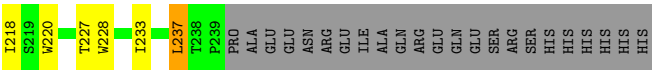


• Molecule 1: Phosphatidylglycerophosphatase B

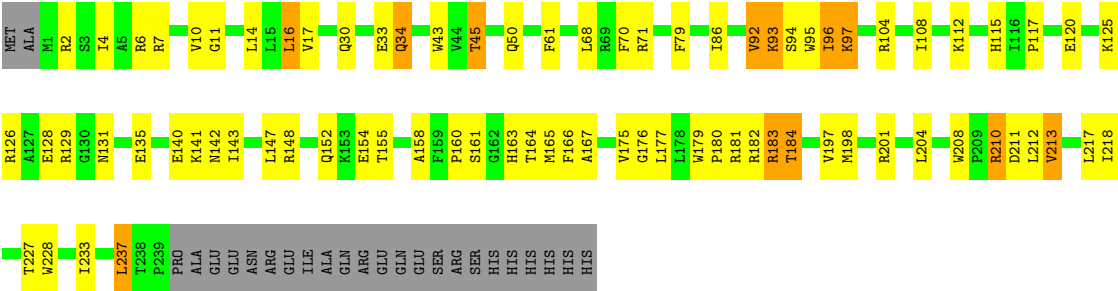


• Molecule 1: Phosphatidylglycerophosphatase B





● Molecule 1: Phosphatidylglycerophosphatase B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.72Å 61.62Å 144.24Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	47.77 – 3.50 47.77 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.77-3.50) 97.6 (47.77-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.48Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.237 , 0.273 0.271 , 0.285	Depositor DCC
R_{free} test set	981 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	103.4	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 93.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.329 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7808	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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: FPP

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	1/1991 (0.1%)	1.53	23/2722 (0.8%)
1	B	0.88	0/1991	1.57	23/2722 (0.8%)
1	C	0.86	0/1991	1.55	20/2722 (0.7%)
1	D	0.85	0/1991	1.57	23/2722 (0.8%)
All	All	0.88	1/7964 (0.0%)	1.56	89/10888 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	HIS	C-N	5.11	1.37	1.32

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211	ASP	CA-CB-CG	7.92	120.52	112.60
1	B	211	ASP	CA-C-N	6.98	129.96	120.54
1	B	211	ASP	C-N-CA	6.98	129.96	120.54
1	D	211	ASP	CA-CB-CG	6.79	119.39	112.60
1	B	183	ARG	CA-C-N	6.77	129.24	120.44
1	B	183	ARG	C-N-CA	6.77	129.24	120.44
1	A	183	ARG	CA-C-N	6.71	129.17	120.44
1	A	183	ARG	C-N-CA	6.71	129.17	120.44
1	B	96	ILE	N-CA-C	-6.58	106.42	111.62
1	C	152	GLN	CA-C-N	6.43	128.79	120.44
1	C	152	GLN	C-N-CA	6.43	128.79	120.44
1	B	152	GLN	CA-C-N	6.42	128.79	120.44
1	B	152	GLN	C-N-CA	6.42	128.79	120.44
1	D	96	ILE	N-CA-CB	6.42	116.90	111.64
1	A	152	GLN	CA-C-N	6.38	128.73	120.44
1	A	152	GLN	C-N-CA	6.38	128.73	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	183	ARG	CA-C-N	6.36	128.70	120.44
1	D	183	ARG	C-N-CA	6.36	128.70	120.44
1	C	183	ARG	CA-C-N	6.32	128.66	120.44
1	C	183	ARG	C-N-CA	6.32	128.66	120.44
1	D	70	PHE	CA-CB-CG	6.23	120.03	113.80
1	D	135	GLU	CB-CG-CD	6.22	123.17	112.60
1	B	209	PRO	CA-C-N	6.17	128.45	120.44
1	B	209	PRO	C-N-CA	6.17	128.45	120.44
1	D	152	GLN	CA-C-N	6.16	128.45	120.44
1	D	152	GLN	C-N-CA	6.16	128.45	120.44
1	D	92	VAL	CA-C-N	6.06	129.91	120.82
1	D	92	VAL	C-N-CA	6.06	129.91	120.82
1	B	96	ILE	N-CA-CB	6.06	116.61	111.64
1	B	79	PHE	CA-CB-CG	-5.88	107.92	113.80
1	A	159	PHE	N-CA-C	5.83	117.35	109.24
1	A	92	VAL	CA-C-N	5.82	128.35	120.38
1	A	92	VAL	C-N-CA	5.82	128.35	120.38
1	A	181	ARG	CA-C-N	5.75	130.31	122.19
1	A	181	ARG	C-N-CA	5.75	130.31	122.19
1	C	80	ALA	CA-C-N	5.61	127.74	120.56
1	C	80	ALA	C-N-CA	5.61	127.74	120.56
1	B	70	PHE	CA-CB-CG	5.59	119.39	113.80
1	B	165	MET	N-CA-C	-5.52	106.48	113.43
1	D	115	HIS	CA-C-N	5.50	129.48	123.43
1	D	115	HIS	C-N-CA	5.50	129.48	123.43
1	B	115	HIS	CA-C-N	5.50	129.48	123.43
1	B	115	HIS	C-N-CA	5.50	129.48	123.43
1	D	16	LEU	CA-C-N	5.49	127.96	120.77
1	D	16	LEU	C-N-CA	5.49	127.96	120.77
1	A	70	PHE	CA-CB-CG	5.49	119.29	113.80
1	C	210	ARG	CA-C-N	5.48	127.94	120.54
1	C	210	ARG	C-N-CA	5.48	127.94	120.54
1	B	202	LEU	N-CA-C	-5.47	105.23	111.14
1	C	70	PHE	CA-CB-CG	5.40	119.20	113.80
1	A	115	HIS	CA-C-N	5.40	129.37	123.43
1	A	115	HIS	C-N-CA	5.40	129.37	123.43
1	D	212	LEU	CA-C-N	5.35	127.41	120.56
1	D	212	LEU	C-N-CA	5.35	127.41	120.56
1	C	16	LEU	CA-C-N	5.35	127.78	120.77
1	C	16	LEU	C-N-CA	5.35	127.78	120.77
1	A	16	LEU	CA-C-N	5.33	127.76	120.77
1	A	16	LEU	C-N-CA	5.33	127.76	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	HIS	CA-C-N	5.29	129.25	123.43
1	C	115	HIS	C-N-CA	5.29	129.25	123.43
1	B	47	THR	N-CA-C	-5.28	106.97	113.41
1	B	16	LEU	CA-C-N	5.27	127.68	120.77
1	B	16	LEU	C-N-CA	5.27	127.68	120.77
1	D	211	ASP	CA-C-N	5.25	127.32	120.28
1	D	211	ASP	C-N-CA	5.25	127.32	120.28
1	A	34	GLN	CA-C-N	5.24	128.68	120.82
1	A	34	GLN	C-N-CA	5.24	128.68	120.82
1	B	34	GLN	CA-C-N	5.21	128.63	120.82
1	B	34	GLN	C-N-CA	5.21	128.63	120.82
1	C	34	GLN	CA-C-N	5.19	128.61	120.82
1	C	34	GLN	C-N-CA	5.19	128.61	120.82
1	A	44	VAL	N-CA-C	-5.18	105.45	110.42
1	C	181	ARG	CA-C-N	5.16	129.47	122.19
1	C	181	ARG	C-N-CA	5.16	129.47	122.19
1	A	202	LEU	CA-C-N	5.14	127.43	120.38
1	A	202	LEU	C-N-CA	5.14	127.43	120.38
1	A	52	TRP	CA-C-N	5.10	125.61	120.00
1	A	52	TRP	C-N-CA	5.10	125.61	120.00
1	D	210	ARG	CA-C-N	5.09	127.42	120.54
1	D	210	ARG	C-N-CA	5.09	127.42	120.54
1	C	195	THR	CA-C-N	5.07	125.57	120.00
1	C	195	THR	C-N-CA	5.07	125.57	120.00
1	B	212	LEU	CA-C-N	5.04	126.91	120.56
1	B	212	LEU	C-N-CA	5.04	126.91	120.56
1	D	34	GLN	CA-C-N	5.03	128.37	120.82
1	D	34	GLN	C-N-CA	5.03	128.37	120.82
1	A	23	TRP	CA-C-N	5.03	127.62	120.53
1	A	23	TRP	C-N-CA	5.03	127.62	120.53
1	D	166	PHE	N-CA-C	-5.02	104.88	111.96

There are no chirality outliers.

There are no planarity outliers.

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	1928	0	1998	45	0
1	B	1928	0	1998	34	0
1	C	1928	0	1998	34	0
1	D	1928	0	1998	48	0
2	A	24	0	25	3	0
2	B	24	0	25	3	0
2	C	24	0	25	2	0
2	D	24	0	25	1	0
All	All	7808	0	8092	152	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 10.

All (152) 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:B:180:PRO:HG2	1:B:237:LEU:HD13	1.66	0.77
1:A:180:PRO:HG2	1:A:237:LEU:HD13	1.68	0.76
1:C:180:PRO:HG2	1:C:237:LEU:HD13	1.67	0.74
1:D:180:PRO:HG2	1:D:237:LEU:HD13	1.68	0.73
1:C:104:ARG:HH12	1:C:154:GLU:HB3	1.55	0.68
1:D:104:ARG:HH12	1:D:154:GLU:HB3	1.59	0.66
1:D:161:SER:HB3	1:D:164:THR:OG1	1.95	0.66
1:C:164:THR:HB	1:C:198:MET:HG2	1.80	0.63
1:C:104:ARG:HD3	1:C:206:MET:O	1.99	0.62
1:A:104:ARG:HD2	1:A:106:PHE:HE2	1.65	0.61
1:B:90:GLN:HG3	2:B:301:FPP:H103	1.81	0.61
1:B:161:SER:HA	2:B:301:FPP:O3B	2.00	0.61
1:B:6:ARG:O	1:B:10:VAL:HG23	2.03	0.59
1:C:6:ARG:O	1:C:10:VAL:HG23	2.03	0.59
1:B:16:LEU:HD11	1:B:217:LEU:HD21	1.85	0.58
1:B:161:SER:HB3	1:B:164:THR:OG1	2.04	0.58
1:A:6:ARG:O	1:A:10:VAL:HG23	2.04	0.58
1:A:24:ILE:HG22	1:D:10:VAL:HG22	1.86	0.58
1:A:104:ARG:HD2	1:A:106:PHE:CE2	2.39	0.58
1:D:6:ARG:O	1:D:10:VAL:HG23	2.04	0.58
1:D:50:GLN:HG3	2:D:301:FPP:H52	1.88	0.56
1:B:50:GLN:HG3	2:B:301:FPP:H52	1.86	0.56
1:A:11:GLY:HA2	1:A:14:LEU:HD12	1.89	0.54
1:B:195:THR:HA	1:B:198:MET:HE2	1.90	0.54
1:A:50:GLN:HG3	2:A:301:FPP:H52	1.89	0.53
1:B:11:GLY:HA2	1:B:14:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:THR:HG22	1:D:198:MET:HA	1.90	0.53
1:C:11:GLY:HA2	1:C:14:LEU:HD12	1.91	0.53
1:A:200:SER:O	1:A:204:LEU:HG	2.09	0.53
1:B:200:SER:O	1:B:204:LEU:HG	2.10	0.52
1:A:48:VAL:HG13	1:A:166:PHE:CD2	2.45	0.52
1:D:11:GLY:HA2	1:D:14:LEU:HD12	1.92	0.52
1:D:126:ARG:HE	1:D:129:ARG:HH22	1.57	0.52
1:D:7:ARG:HD3	1:D:179:TRP:HD1	1.74	0.52
1:A:17:VAL:CG1	1:D:17:VAL:HG21	2.40	0.51
1:D:167:ALA:HB2	1:D:197:VAL:HG11	1.93	0.51
1:D:94:SER:C	1:D:96:ILE:H	2.18	0.51
1:C:143:ILE:HG23	1:C:147:LEU:HD23	1.93	0.50
1:C:7:ARG:HD3	1:C:179:TRP:HD1	1.76	0.50
1:D:16:LEU:HD11	1:D:217:LEU:HD21	1.93	0.50
1:D:104:ARG:NH1	1:D:154:GLU:HB3	2.27	0.50
1:A:90:GLN:HG3	2:A:301:FPP:H103	1.92	0.50
1:A:161:SER:HB3	1:A:164:THR:OG1	2.12	0.49
1:A:117:PRO:HG2	1:A:120:GLU:HB3	1.95	0.49
1:D:143:ILE:HG23	1:D:147:LEU:HD23	1.93	0.49
1:C:48:VAL:HG21	1:C:197:VAL:HG11	1.94	0.49
1:B:117:PRO:HG2	1:B:120:GLU:HB3	1.95	0.49
1:D:68:LEU:HD21	1:D:177:LEU:HB3	1.95	0.49
1:A:17:VAL:HG21	1:D:17:VAL:CG1	2.43	0.49
1:A:7:ARG:HD3	1:A:179:TRP:HD1	1.78	0.48
1:B:176:GLY:HA3	1:B:227:THR:HG21	1.95	0.48
1:A:16:LEU:HD11	1:A:217:LEU:HD11	1.95	0.48
1:A:17:VAL:HG21	1:D:17:VAL:HG13	1.96	0.48
1:B:92:VAL:HG11	1:B:218:ILE:HG21	1.96	0.47
1:B:7:ARG:HD3	1:B:179:TRP:HD1	1.78	0.47
1:B:143:ILE:HG23	1:B:147:LEU:HD23	1.94	0.47
1:D:104:ARG:HG2	1:D:158:ALA:HB2	1.96	0.47
1:D:163:HIS:HB2	1:D:201:ARG:HD2	1.96	0.47
1:D:176:GLY:HA3	1:D:227:THR:HG21	1.97	0.47
1:A:128:GLU:HA	1:A:131:ASN:HD22	1.80	0.47
1:A:143:ILE:HG23	1:A:147:LEU:HD23	1.94	0.47
1:C:90:GLN:HG3	2:C:301:FPP:H103	1.96	0.47
1:C:92:VAL:HG11	1:C:218:ILE:HG21	1.97	0.47
1:D:92:VAL:HG11	1:D:218:ILE:HG21	1.97	0.47
1:A:19:PRO:HB2	1:A:213:VAL:HG23	1.97	0.47
1:B:181:ARG:HD3	1:B:237:LEU:O	2.15	0.47
1:C:161:SER:HB3	1:C:164:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:GLY:HA3	1:C:227:THR:HG21	1.97	0.47
1:C:126:ARG:HE	1:C:129:ARG:HH22	1.62	0.47
1:A:72:ILE:HG21	1:C:2:ARG:HA	1.98	0.46
1:A:181:ARG:HD3	1:A:237:LEU:O	2.15	0.46
1:B:128:GLU:HA	1:B:131:ASN:HD22	1.80	0.46
1:B:97:LYS:HA	1:B:159:PHE:O	2.16	0.46
1:C:213:VAL:O	1:C:217:LEU:HG	2.15	0.46
1:A:176:GLY:HA3	1:A:227:THR:HG21	1.96	0.46
1:B:140:GLU:C	1:B:142:ASN:H	2.24	0.46
1:D:117:PRO:HG2	1:D:120:GLU:HB3	1.97	0.46
1:A:140:GLU:C	1:A:142:ASN:H	2.24	0.46
1:B:22:VAL:HG11	1:B:202:LEU:HD13	1.97	0.46
1:C:140:GLU:C	1:C:142:ASN:H	2.23	0.46
1:B:18:MET:CE	1:B:199:GLY:HA2	2.46	0.46
1:C:181:ARG:HD3	1:C:237:LEU:O	2.16	0.46
1:D:181:ARG:HD3	1:D:237:LEU:O	2.16	0.46
1:D:108:ILE:HD12	1:D:208:TRP:CZ2	2.52	0.45
1:C:61:PHE:HD1	1:C:82:LEU:HD12	1.81	0.45
1:D:140:GLU:C	1:D:142:ASN:H	2.23	0.45
1:A:125:LYS:HD3	1:C:123:THR:HG21	1.99	0.45
1:C:102:GLU:HB3	1:C:159:PHE:H	1.82	0.45
1:D:128:GLU:HA	1:D:131:ASN:HD22	1.82	0.45
1:D:125:LYS:HB2	1:D:128:GLU:HG2	1.99	0.44
1:B:163:HIS:HB3	1:B:201:ARG:HD2	1.98	0.44
1:C:200:SER:O	1:C:204:LEU:HG	2.18	0.44
1:B:163:HIS:CB	1:B:201:ARG:HD2	2.47	0.44
1:B:15:LEU:O	1:B:198:MET:HE1	2.18	0.44
1:A:92:VAL:HG11	1:A:218:ILE:HG21	2.00	0.44
1:A:105:PRO:HA	1:A:108:ILE:HG12	1.99	0.43
1:A:17:VAL:HG13	1:D:17:VAL:CG2	2.47	0.43
1:A:126:ARG:HE	1:A:129:ARG:HH22	1.66	0.43
1:C:163:HIS:HB2	1:C:201:ARG:HD2	2.00	0.43
2:C:301:FPP:H111	2:C:301:FPP:H101	1.64	0.43
1:B:141:LYS:HA	1:B:148:ARG:NH2	2.33	0.43
1:A:141:LYS:HA	1:A:148:ARG:NH2	2.33	0.43
1:C:16:LEU:HD11	1:C:217:LEU:HD21	2.00	0.43
1:C:117:PRO:HG2	1:C:120:GLU:HB3	2.00	0.43
1:D:61:PHE:CZ	1:D:79:PHE:HB2	2.54	0.43
1:A:4:ILE:HD13	1:A:228:TRP:HA	2.01	0.43
1:A:18:MET:O	1:A:22:VAL:HG23	2.18	0.43
1:B:201:ARG:HH22	1:B:206:MET:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:ILE:HD13	1:D:228:TRP:HA	2.01	0.43
1:B:108:ILE:O	1:B:112:LYS:HB2	2.19	0.43
1:D:213:VAL:O	1:D:217:LEU:HG	2.19	0.43
1:C:4:ILE:HD13	1:C:228:TRP:HA	2.01	0.43
1:A:16:LEU:HD11	1:A:217:LEU:CD1	2.49	0.43
1:A:108:ILE:O	1:A:112:LYS:HB2	2.19	0.43
1:C:95:TRP:HA	1:C:95:TRP:CE3	2.54	0.43
1:D:167:ALA:CB	1:D:197:VAL:HG11	2.49	0.43
1:A:17:VAL:HG11	1:D:17:VAL:HG21	2.00	0.43
1:A:19:PRO:O	1:A:23:TRP:HB2	2.18	0.43
1:D:93:LYS:HD3	1:D:97:LYS:HE2	2.00	0.42
1:D:93:LYS:HE2	1:D:160:PRO:C	2.44	0.42
1:D:165:MET:HE2	1:D:165:MET:HB3	1.96	0.42
1:C:108:ILE:HD12	1:C:208:TRP:CZ2	2.55	0.42
1:C:141:LYS:HA	1:C:148:ARG:NH2	2.35	0.42
1:B:24:ILE:HG22	1:C:10:VAL:HG22	2.01	0.42
1:B:104:ARG:HD3	1:B:206:MET:O	2.20	0.42
1:A:94:SER:C	1:A:96:ILE:H	2.27	0.42
1:C:90:GLN:O	1:C:93:LYS:HD3	2.19	0.42
1:A:121:PHE:O	1:A:129:ARG:HD3	2.19	0.42
2:A:301:FPP:H111	2:A:301:FPP:H101	1.86	0.42
1:B:4:ILE:HD13	1:B:228:TRP:HA	2.02	0.41
1:D:95:TRP:HA	1:D:95:TRP:CE3	2.55	0.41
1:D:141:LYS:HA	1:D:148:ARG:NH2	2.35	0.41
1:A:70:PHE:HB3	1:A:74:ALA:HB3	2.03	0.41
1:A:40:ALA:O	1:A:44:VAL:HG23	2.21	0.41
1:C:108:ILE:O	1:C:112:LYS:HB2	2.20	0.41
1:D:108:ILE:O	1:D:112:LYS:HB2	2.20	0.41
1:A:165:MET:HG3	1:A:215:ALA:HB1	2.03	0.41
1:B:126:ARG:HE	1:B:129:ARG:HH22	1.69	0.41
1:D:45:THR:HG21	1:D:204:LEU:HD11	2.02	0.41
1:A:17:VAL:HG13	1:D:17:VAL:HG21	2.03	0.41
1:C:94:SER:C	1:C:96:ILE:H	2.28	0.41
1:D:164:THR:HG22	1:D:198:MET:HG2	2.03	0.41
1:A:17:VAL:CG2	1:D:17:VAL:HG13	2.50	0.41
1:B:48:VAL:HG13	1:B:166:PHE:CD2	2.56	0.41
1:D:93:LYS:HB2	1:D:93:LYS:NZ	2.36	0.41
1:B:61:PHE:CZ	1:B:79:PHE:HB2	2.56	0.40
1:D:43:TRP:CD1	1:D:43:TRP:C	2.99	0.40
1:A:179:TRP:N	1:A:180:PRO:CD	2.84	0.40
1:D:179:TRP:HZ3	1:D:184:THR:HG23	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:PHE:O	1:B:129:ARG:HD3	2.21	0.40
1:A:95:TRP:HA	1:A:95:TRP:CE3	2.56	0.40
1:C:172:LEU:HD13	1:C:220:TRP:HA	2.03	0.40

There are no symmetry-related clashes.

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	237/264 (90%)	227 (96%)	7 (3%)	3 (1%)	9	39
1	B	237/264 (90%)	229 (97%)	5 (2%)	3 (1%)	9	39
1	C	237/264 (90%)	229 (97%)	5 (2%)	3 (1%)	9	39
1	D	237/264 (90%)	227 (96%)	8 (3%)	2 (1%)	16	49
All	All	948/1056 (90%)	912 (96%)	25 (3%)	11 (1%)	10	41

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	GLU
1	B	33	GLU
1	B	155	THR
1	C	33	GLU
1	D	33	GLU
1	A	34	GLN
1	A	155	THR
1	B	34	GLN
1	C	34	GLN
1	C	155	THR
1	D	34	GLN

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	196/218 (90%)	181 (92%)	15 (8%)	12	37
1	B	196/218 (90%)	177 (90%)	19 (10%)	8	30
1	C	196/218 (90%)	177 (90%)	19 (10%)	8	30
1	D	196/218 (90%)	180 (92%)	16 (8%)	10	34
All	All	784/872 (90%)	715 (91%)	69 (9%)	9	32

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	45	THR
1	A	49	THR
1	A	71	ARG
1	A	86	ILE
1	A	102	GLU
1	A	126	ARG
1	A	161	SER
1	A	164	THR
1	A	175	VAL
1	A	182	ARG
1	A	183	ARG
1	A	184	THR
1	A	233	ILE
1	A	237	LEU
1	B	30	GLN
1	B	45	THR
1	B	49	THR
1	B	71	ARG
1	B	86	ILE
1	B	93	LYS
1	B	102	GLU
1	B	126	ARG
1	B	155	THR

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Mol	Chain	Res	Type
1	B	161	SER
1	B	163	HIS
1	B	164	THR
1	B	175	VAL
1	B	182	ARG
1	B	183	ARG
1	B	184	THR
1	B	213	VAL
1	B	233	ILE
1	B	237	LEU
1	C	2	ARG
1	C	30	GLN
1	C	45	THR
1	C	71	ARG
1	C	78	LEU
1	C	86	ILE
1	C	93	LYS
1	C	155	THR
1	C	161	SER
1	C	163	HIS
1	C	164	THR
1	C	175	VAL
1	C	182	ARG
1	C	183	ARG
1	C	184	THR
1	C	210	ARG
1	C	213	VAL
1	C	233	ILE
1	C	237	LEU
1	D	2	ARG
1	D	30	GLN
1	D	45	THR
1	D	71	ARG
1	D	86	ILE
1	D	93	LYS
1	D	97	LYS
1	D	155	THR
1	D	175	VAL
1	D	182	ARG
1	D	183	ARG
1	D	184	THR
1	D	210	ARG

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Mol	Chain	Res	Type
1	D	213	VAL
1	D	233	ILE
1	D	237	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	57	HIS
1	A	90	GLN
1	A	131	ASN
1	A	142	ASN
1	A	152	GLN
1	B	30	GLN
1	B	57	HIS
1	B	90	GLN
1	B	131	ASN
1	B	142	ASN
1	B	152	GLN
1	C	30	GLN
1	C	57	HIS
1	C	142	ASN
1	C	150	HIS
1	C	152	GLN
1	D	30	GLN
1	D	57	HIS
1	D	131	ASN
1	D	142	ASN
1	D	152	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	$\# Z > 2$
2	FPP	B	301	-	22,23,23	0.99	1 (4%)	27,31,31	0.78	1 (3%)
2	FPP	D	301	-	22,23,23	1.07	2 (9%)	27,31,31	0.68	0
2	FPP	A	301	-	22,23,23	1.13	1 (4%)	27,31,31	0.88	0
2	FPP	C	301	-	22,23,23	1.44	2 (9%)	27,31,31	0.76	0

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
2	FPP	B	301	-	-	6/25/25/25	-
2	FPP	D	301	-	-	8/25/25/25	-
2	FPP	A	301	-	-	8/25/25/25	-
2	FPP	C	301	-	-	9/25/25/25	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	FPP	PA-O3A	4.66	1.64	1.59
2	A	301	FPP	C7-C8	2.67	1.39	1.33
2	C	301	FPP	C7-C8	2.65	1.39	1.33
2	B	301	FPP	C7-C8	2.56	1.39	1.33
2	D	301	FPP	C9-C8	2.18	1.55	1.51
2	D	301	FPP	C7-C8	2.17	1.38	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	FPP	C1-C2-C3	2.08	129.61	126.20

There are no chirality outliers.

All (31) torsion outliers are listed below:

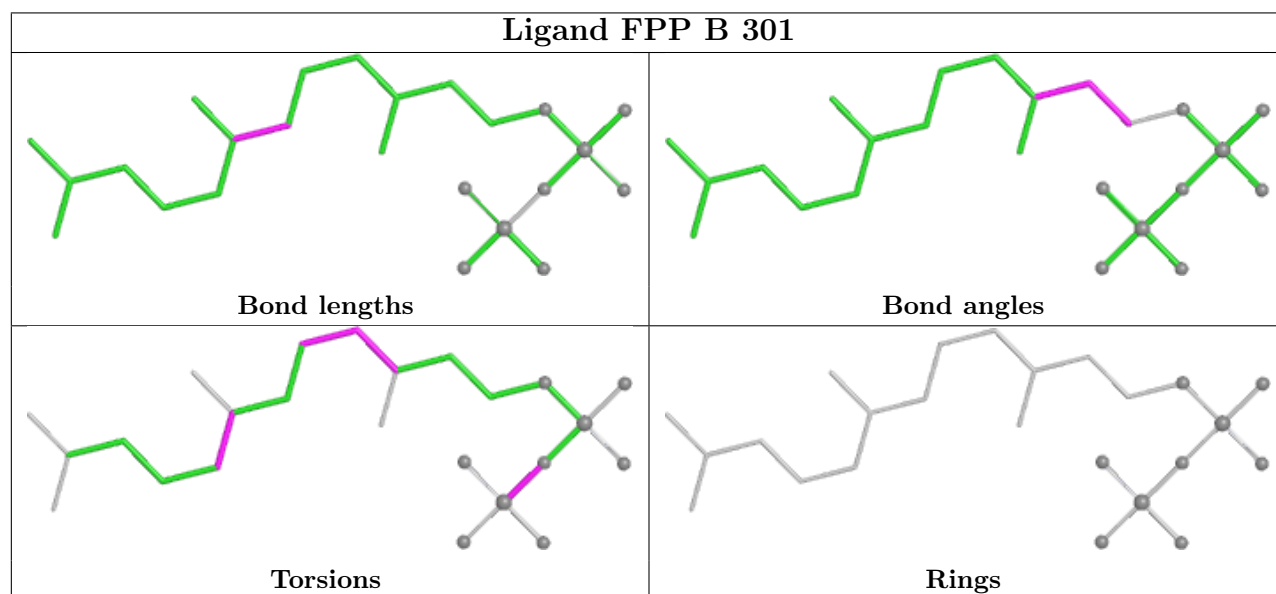
Mol	Chain	Res	Type	Atoms
2	A	301	FPP	C7-C8-C9-C11
2	A	301	FPP	PA-O3A-PB-O2B
2	C	301	FPP	PA-O3A-PB-O2B
2	D	301	FPP	C7-C8-C9-C11
2	D	301	FPP	PA-O3A-PB-O2B
2	A	301	FPP	C10-C8-C9-C11
2	C	301	FPP	C10-C8-C9-C11
2	D	301	FPP	C10-C8-C9-C11
2	C	301	FPP	C7-C8-C9-C11
2	B	301	FPP	C3-C5-C6-C7
2	C	301	FPP	C12-C11-C9-C8
2	A	301	FPP	C4-C3-C5-C6
2	B	301	FPP	C4-C3-C5-C6
2	B	301	FPP	C2-C3-C5-C6
2	A	301	FPP	C2-C3-C5-C6
2	B	301	FPP	PA-O3A-PB-O2B
2	B	301	FPP	PA-O3A-PB-O3B
2	D	301	FPP	PA-O3A-PB-O3B
2	C	301	FPP	C3-C5-C6-C7
2	C	301	FPP	C1-O1-PA-O1A
2	D	301	FPP	C4-C3-C5-C6
2	D	301	FPP	C2-C3-C5-C6
2	B	301	FPP	C10-C8-C9-C11
2	C	301	FPP	PA-O3A-PB-O1B
2	D	301	FPP	PA-O3A-PB-O1B
2	A	301	FPP	PA-O3A-PB-O3B
2	C	301	FPP	PA-O3A-PB-O3B
2	A	301	FPP	PA-O3A-PB-O1B
2	A	301	FPP	PB-O3A-PA-O2A
2	C	301	FPP	PB-O3A-PA-O2A
2	D	301	FPP	PB-O3A-PA-O2A

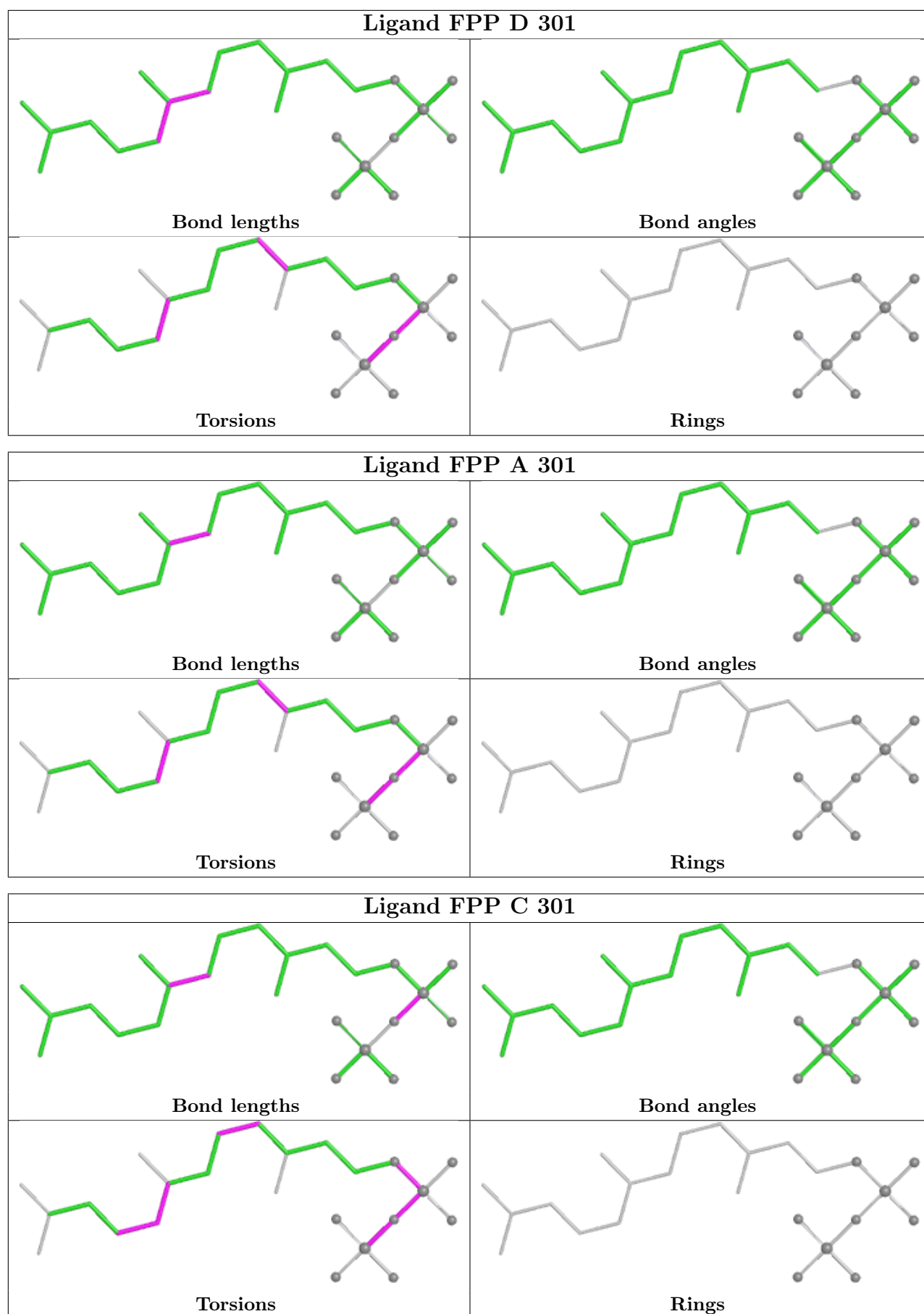
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	FPP	3	0
2	D	301	FPP	1	0
2	A	301	FPP	3	0
2	C	301	FPP	2	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	239/264 (90%)	-0.75	0 100 100	67, 99, 148, 182	0
1	B	239/264 (90%)	-0.77	1 (0%) 88 72	64, 102, 150, 177	0
1	C	239/264 (90%)	-0.75	1 (0%) 88 72	77, 117, 159, 186	0
1	D	239/264 (90%)	-0.83	0 100 100	65, 114, 155, 175	0
All	All	956/1056 (90%)	-0.78	2 (0%) 91 82	64, 107, 154, 186	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	GLU	2.7
1	C	139	GLU	2.2

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](#)

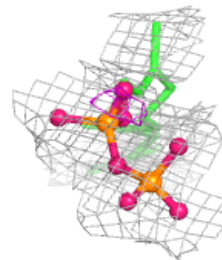
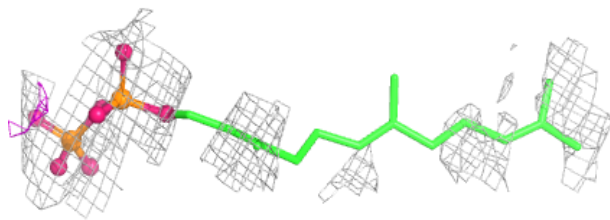
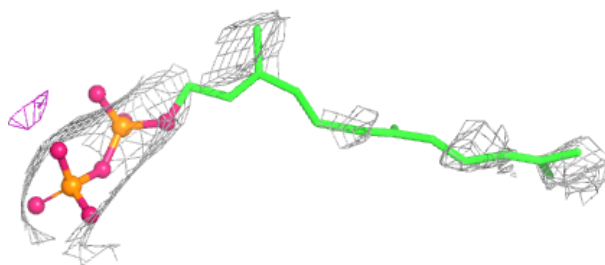
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FPP	A	301	24/24	0.98	0.09	75,126,146,152	0
2	FPP	B	301	24/24	0.98	0.08	73,130,149,153	0
2	FPP	C	301	24/24	0.98	0.07	110,132,135,136	0
2	FPP	D	301	24/24	0.98	0.09	111,140,143,145	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.

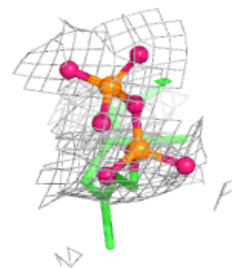
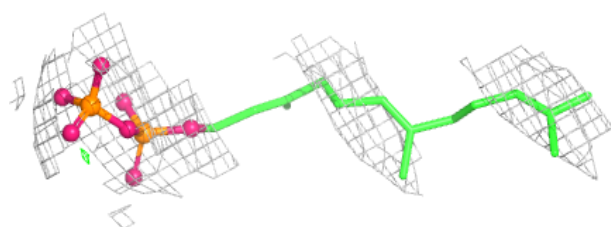
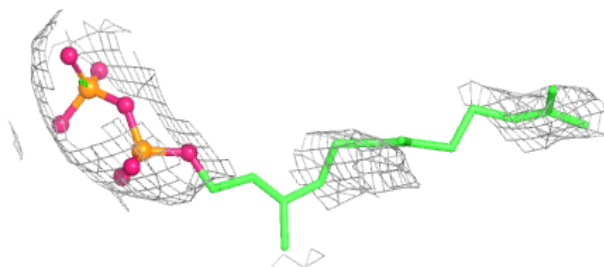
Electron density around FPP A 301:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

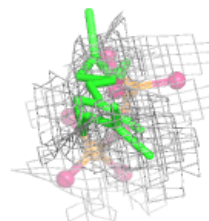
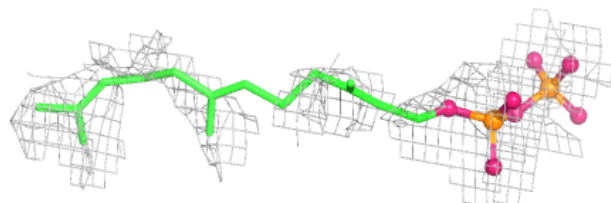
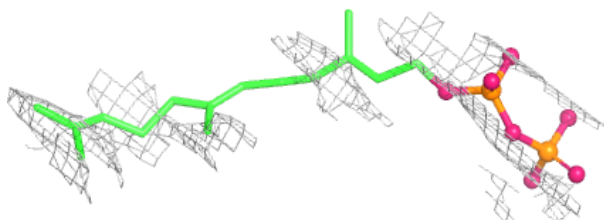


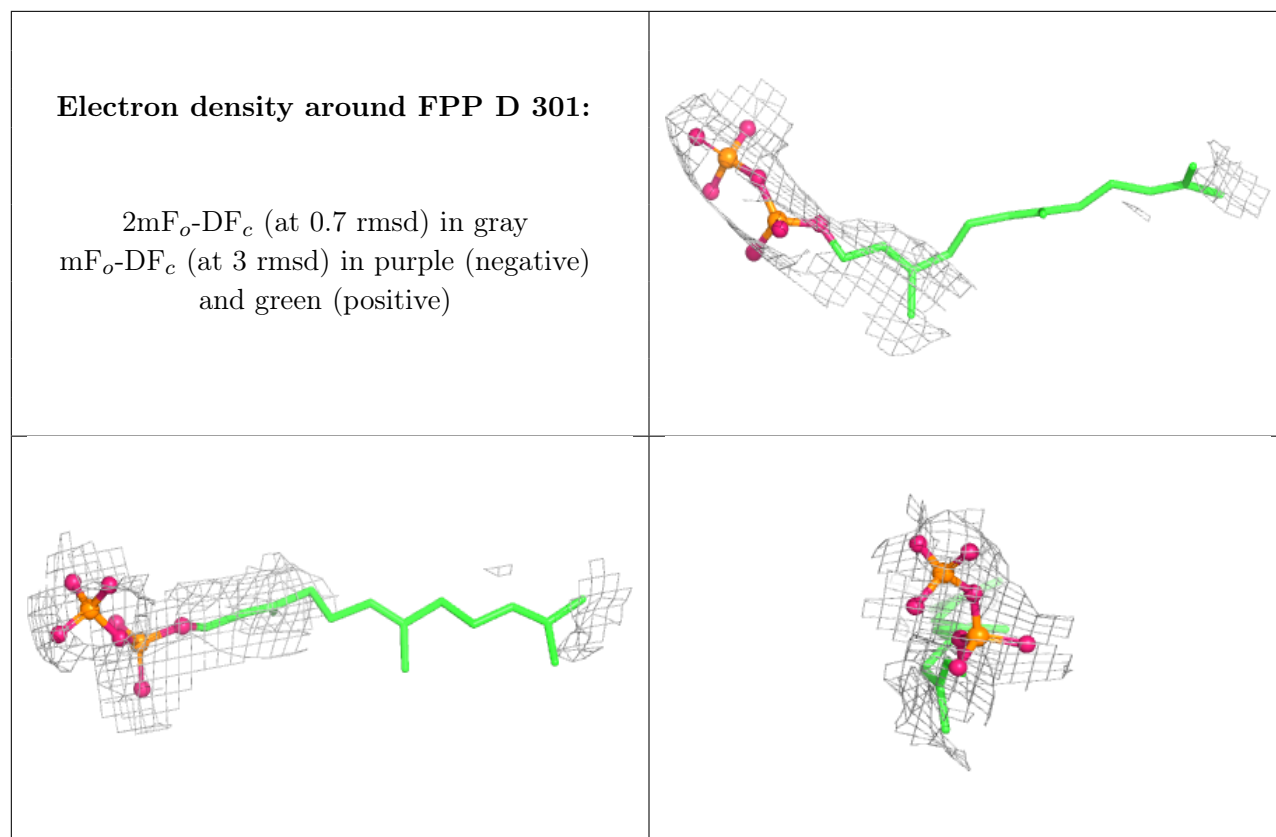
Electron density around FPP B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FPP C 301:**

$2mF_o-DF_c$ (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.