



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 04:59 PM BST

PDB ID : 5IVG  
Title : Crystal structure of Aspergillus terreus aristolochene synthase N299A complexed with farnesyl thiolodiphosphate  
Authors : Chen, M.; Christianson, D.W.  
Deposited on : 2016-03-20  
Resolution : 1.95 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](mailto: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.

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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	:	2.13.1
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)	:	2.13.1

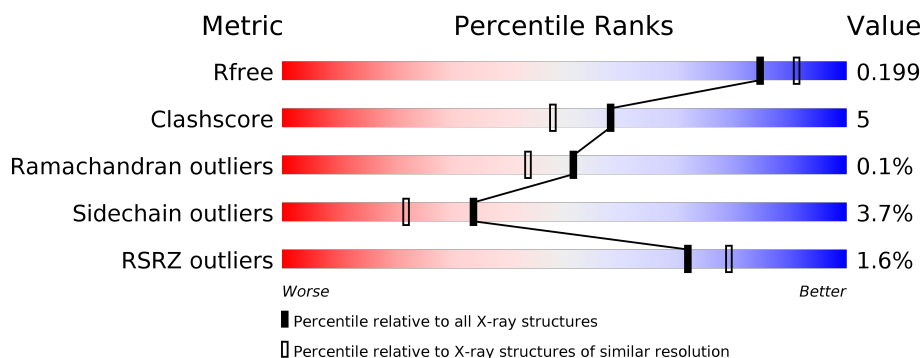
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	314	<div> <div>88%</div> <div>8%</div> <div>• •</div> </div>
1	B	314	<div> <div>90%</div> <div>6%</div> <div>• •</div> </div>
1	C	314	<div> <div>87%</div> <div>8%</div> <div>• •</div> </div>
1	D	314	<div> <div>6%</div> <div>84%</div> <div>12%</div> <div>•</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11372 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 Aristolochene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	2	0
			2469	1578	415	460	16			
1	B	304	Total	C	N	O	S	0	4	0
			2470	1580	414	460	16			
1	C	304	Total	C	N	O	S	0	3	0
			2472	1579	420	457	16			
1	D	305	Total	C	N	O	S	0	1	0
			2463	1574	415	458	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9UR08
A	2	HIS	-	expression tag	UNP Q9UR08
A	3	HIS	-	expression tag	UNP Q9UR08
A	4	HIS	-	expression tag	UNP Q9UR08
A	5	HIS	-	expression tag	UNP Q9UR08
A	6	HIS	-	expression tag	UNP Q9UR08
A	7	HIS	-	expression tag	UNP Q9UR08
A	299	ALA	ASN	engineered mutation	UNP Q9UR08
B	1	MET	-	initiating methionine	UNP Q9UR08
B	2	HIS	-	expression tag	UNP Q9UR08
B	3	HIS	-	expression tag	UNP Q9UR08
B	4	HIS	-	expression tag	UNP Q9UR08
B	5	HIS	-	expression tag	UNP Q9UR08
B	6	HIS	-	expression tag	UNP Q9UR08
B	7	HIS	-	expression tag	UNP Q9UR08
B	299	ALA	ASN	engineered mutation	UNP Q9UR08
C	1	MET	-	initiating methionine	UNP Q9UR08
C	2	HIS	-	expression tag	UNP Q9UR08
C	3	HIS	-	expression tag	UNP Q9UR08
C	4	HIS	-	expression tag	UNP Q9UR08
C	5	HIS	-	expression tag	UNP Q9UR08

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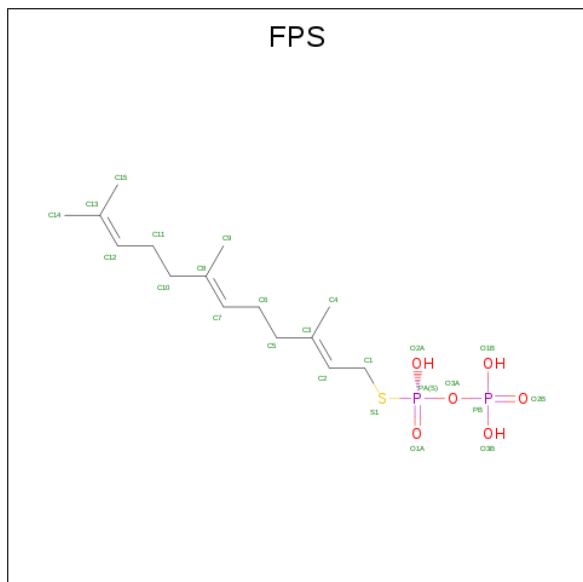
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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	HIS	-	expression tag	UNP Q9UR08
C	7	HIS	-	expression tag	UNP Q9UR08
C	299	ALA	ASN	engineered mutation	UNP Q9UR08
D	1	MET	-	initiating methionine	UNP Q9UR08
D	2	HIS	-	expression tag	UNP Q9UR08
D	3	HIS	-	expression tag	UNP Q9UR08
D	4	HIS	-	expression tag	UNP Q9UR08
D	5	HIS	-	expression tag	UNP Q9UR08
D	6	HIS	-	expression tag	UNP Q9UR08
D	7	HIS	-	expression tag	UNP Q9UR08
D	299	ALA	ASN	engineered mutation	UNP Q9UR08

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0
2	A	3	Total Mg 3 3	0	0
2	D	3	Total Mg 3 3	0	0
2	C	3	Total Mg 3 3	0	0

- Molecule 3 is S-[(2E,6E)-3,7,11-TRIMETHYLDODECA-2,6,10-TRIENYL] TRIHYDROGEN THIODIPHOSPHATE (three-letter code: FPS) (formula: C<sub>15</sub>H<sub>28</sub>O<sub>6</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	O	P	S	0	0
			24	15	6	2	1		
3	B	1	Total	C	O	P	S	0	0
			24	15	6	2	1		
3	C	1	Total	C	O	P	S	0	0
			24	15	6	2	1		
3	D	1	Total	C	O	P	S	0	0
			24	15	6	2	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	395	Total	O	0	0
			395	395		
5	B	454	Total	O	0	0
			454	454		
5	C	313	Total	O	0	0
			313	313		

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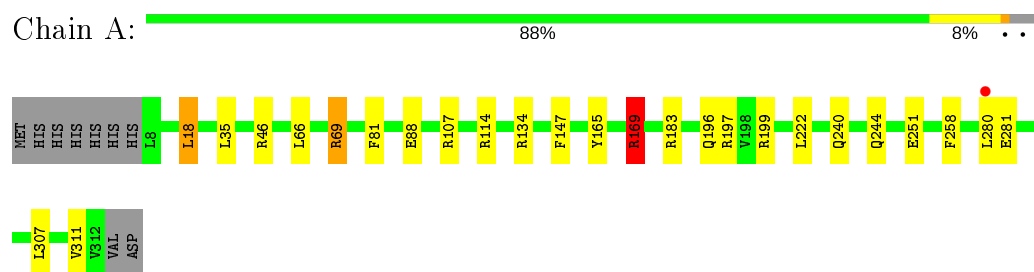
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	210	Total	O	0	0
			210	210		

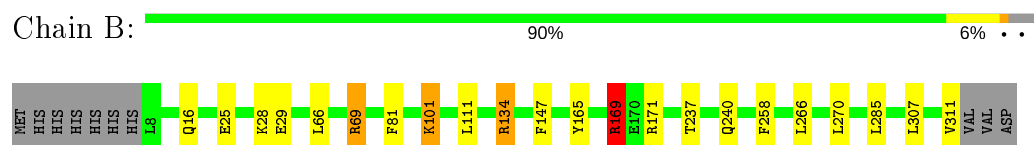
### 3 Residue-property plots

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.

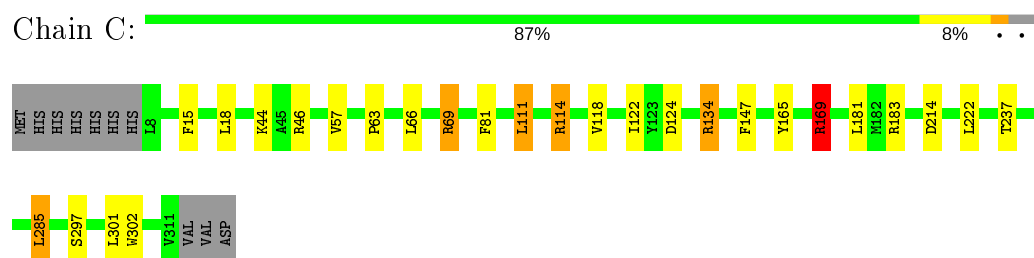
- Molecule 1: Aristolochene synthase



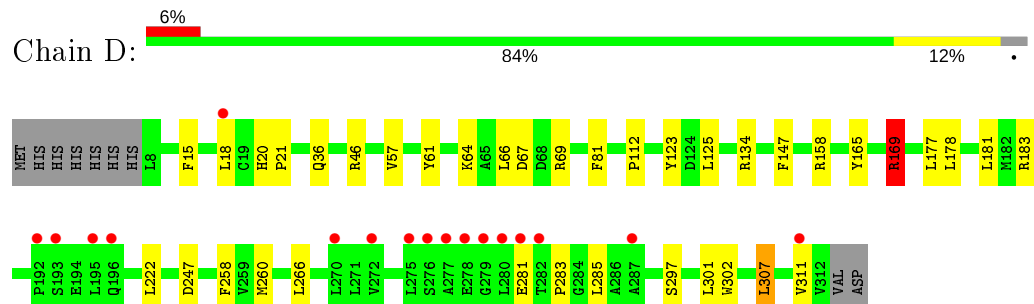
- Molecule 1: Aristolochene synthase



- Molecule 1: Aristolochene synthase



- Molecule 1: Aristolochene synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.41Å 123.41Å 203.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.31 – 1.95 47.31 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.31-1.95) 96.2 (47.31-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 1.95Å)	Xtriage
Refinement program	PHENIX dev_1839	Depositor
R, $R_{free}$	0.162 , 0.199 0.162 , 0.199	Depositor DCC
$R_{free}$ test set	2001 reflections (1.53%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11372	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, MG, FPS

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	0.78	0/2530	0.87	7/3424 (0.2%)
1	B	0.81	3/2537 (0.1%)	0.96	6/3433 (0.2%)
1	C	0.67	0/2536	0.85	9/3430 (0.3%)
1	D	0.56	0/2521	0.65	2/3412 (0.1%)
All	All	0.71	3/10124 (0.0%)	0.84	24/13699 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	240	GLN	CB-CG	-5.82	1.36	1.52
1	B	29	GLU	CG-CD	5.64	1.60	1.51
1	B	101	LYS	CE-NZ	5.12	1.61	1.49

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	ARG	NE-CZ-NH2	-22.60	109.00	120.30
1	B	169	ARG	NE-CZ-NH1	17.47	129.03	120.30
1	A	169	ARG	NE-CZ-NH2	-15.61	112.50	120.30
1	A	169	ARG	NE-CZ-NH1	12.90	126.75	120.30
1	B	69	ARG	NE-CZ-NH1	12.55	126.58	120.30
1	A	114	ARG	NE-CZ-NH2	-11.93	114.33	120.30
1	A	69	ARG	NE-CZ-NH1	11.63	126.11	120.30
1	C	169	ARG	NE-CZ-NH2	-11.30	114.65	120.30
1	C	169	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	B	69	ARG	NE-CZ-NH2	-10.59	115.01	120.30
1	C	114[A]	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	C	114[B]	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	A	69	ARG	NE-CZ-NH2	-9.69	115.46	120.30
1	C	69	ARG	NE-CZ-NH1	9.56	125.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	114[A]	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	C	114[B]	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	D	169	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	D	169	ARG	NE-CZ-NH2	-8.39	116.10	120.30
1	C	69	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	A	114	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	B	169	ARG	CD-NE-CZ	6.10	132.14	123.60
1	B	101	LYS	CD-CE-NZ	5.90	125.28	111.70
1	C	111	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	114	ARG	CG-CD-NE	-5.04	101.21	111.80

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	2469	0	2448	25	0
1	B	2470	0	2454	14	0
1	C	2472	0	2458	20	0
1	D	2463	0	2442	27	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	24	0	25	7	0
3	B	24	0	25	6	0
3	C	24	0	25	3	0
3	D	24	0	25	6	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
5	A	395	0	0	11	0
5	B	454	0	0	8	0
5	C	313	0	0	8	0
5	D	210	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11372	0	9926	95	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 5.

All (95) 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:A:107:ARG:NH1	5:A:802:HOH:O	2.07	0.88
1:C:114[B]:ARG:NH2	5:C:801:HOH:O	2.06	0.85
1:C:165:TYR:CZ	1:C:169:ARG:HG3	2.11	0.84
1:A:88:GLU:OE1	5:A:801:HOH:O	2.03	0.77
1:A:81:PHE:CE1	3:A:704:FPS:H91	2.20	0.76
1:C:183:ARG:NH1	5:C:803:HOH:O	2.20	0.73
1:A:69:ARG:HD2	5:A:981:HOH:O	1.86	0.73
1:D:165:TYR:CZ	1:D:169:ARG:HG3	2.24	0.72
3:A:704:FPS:H151	5:A:953:HOH:O	1.88	0.72
1:B:165:TYR:OH	1:B:169:ARG:HD2	1.90	0.71
1:A:240:GLN:NE2	5:A:807:HOH:O	2.26	0.68
1:D:307:LEU:O	1:D:311:VAL:HG12	1.93	0.68
1:A:46:ARG:NH1	5:A:806:HOH:O	2.26	0.68
1:A:165:TYR:CZ	1:A:169:ARG:HG3	2.29	0.67
1:D:69:ARG:NH1	5:D:802:HOH:O	2.20	0.67
1:D:81:PHE:CE1	3:D:704:FPS:H91	2.31	0.65
1:B:171:ARG:NH1	5:B:801:HOH:O	2.15	0.65
1:A:300:GLU:OE2	5:A:803:HOH:O	2.15	0.64
1:A:165:TYR:OH	1:A:169:ARG:HD2	1.96	0.64
3:C:704:FPS:H151	5:C:839:HOH:O	1.97	0.63
1:B:165:TYR:CZ	1:B:169:ARG:HG3	2.34	0.62
3:B:704:FPS:H151	5:B:857:HOH:O	2.00	0.62
1:D:283:PRO:O	5:D:801:HOH:O	2.16	0.62
1:B:69:ARG:HD2	5:B:1002:HOH:O	1.99	0.62
1:D:66:LEU:HD12	1:D:69:ARG:HD2	1.82	0.61
1:C:134:ARG:NH1	5:C:802:HOH:O	2.18	0.61
1:A:281:GLU:OE2	5:A:804:HOH:O	2.16	0.60
3:A:704:FPS:H92	3:A:704:FPS:H42	1.84	0.60
3:B:704:FPS:H42	3:B:704:FPS:H92	1.84	0.60
1:D:147:PHE:CE1	3:D:704:FPS:H51	2.37	0.59
1:A:197:ARG:HD3	1:A:280:LEU:HB3	1.83	0.59
1:D:311:VAL:HG13	5:D:857:HOH:O	2.02	0.58
1:A:307:LEU:O	1:A:311:VAL:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:LEU:O	1:D:311:VAL:CG1	2.52	0.56
1:B:66:LEU:HD12	1:B:69:ARG:HD3	1.87	0.56
3:D:704:FPS:H92	3:D:704:FPS:H42	1.87	0.55
1:C:248:VAL:HG21	1:D:260[A]:MET:HE1	1.89	0.55
1:B:25:GLU:OE1	5:B:802:HOH:O	2.18	0.55
1:B:81:PHE:CE1	3:B:704:FPS:H91	2.42	0.54
1:C:69:ARG:HD2	5:C:1010:HOH:O	2.07	0.53
1:A:35:LEU:O	1:A:46:ARG:NH2	2.42	0.52
1:A:66:LEU:HD12	1:A:69:ARG:HD3	1.92	0.51
1:B:165:TYR:HH	1:B:169:ARG:HD2	1.75	0.51
3:D:704:FPS:H92	3:D:704:FPS:C4	2.42	0.50
1:A:251:GLU:HG2	5:A:1056:HOH:O	2.10	0.50
1:C:46[B]:ARG:NH1	5:C:808:HOH:O	2.42	0.50
1:C:66:LEU:HD12	1:C:69:ARG:HD3	1.93	0.50
1:D:311:VAL:HG13	1:D:311:VAL:O	2.12	0.50
1:A:183:ARG:HD2	5:A:829:HOH:O	2.12	0.49
3:A:704:FPS:H92	3:A:704:FPS:C4	2.42	0.49
3:B:704:FPS:H92	3:B:704:FPS:C4	2.42	0.49
1:C:15:PHE:HB3	1:C:297:SER:HB3	1.95	0.49
1:A:244:GLN:NE2	5:A:815:HOH:O	2.45	0.49
1:C:165:TYR:OH	1:C:169:ARG:HD2	2.13	0.48
1:D:67:ASP:OD1	5:D:803:HOH:O	2.20	0.48
1:A:147:PHE:CZ	3:A:704:FPS:H51	2.48	0.48
1:D:112:PRO:HD3	1:D:123:TYR:CD1	2.49	0.48
1:D:36:GLN:HG2	5:D:846:HOH:O	2.14	0.47
1:B:147:PHE:CE1	3:B:704:FPS:H51	2.49	0.47
1:C:114[A]:ARG:NH2	1:C:124:ASP:OD1	2.39	0.47
1:B:16:GLN:HG3	5:B:1134:HOH:O	2.15	0.46
1:C:44:LYS:NZ	5:C:815:HOH:O	2.47	0.46
1:A:147:PHE:CE1	3:A:704:FPS:H51	2.50	0.46
1:C:81:PHE:CE1	3:C:704:FPS:H91	2.50	0.45
1:C:147:PHE:CZ	3:C:704:FPS:H51	2.51	0.45
1:D:189:LYS:NZ	5:D:821:HOH:O	2.49	0.45
1:A:311:VAL:O	1:A:311:VAL:HG23	2.16	0.45
3:D:704:FPS:H151	5:D:805:HOH:O	2.17	0.45
1:A:285:LEU:HA	1:A:285:LEU:HD12	1.87	0.44
1:D:266:LEU:HD13	1:D:266:LEU:HA	1.86	0.44
1:D:112:PRO:HD3	1:D:123:TYR:CG	2.52	0.44
1:B:147:PHE:CZ	3:B:704:FPS:H51	2.53	0.44
1:D:158:ARG:NH1	5:D:822:HOH:O	2.50	0.44
1:C:118:VAL:O	1:C:122:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:LYS:O	1:D:186:MET:HG2	2.17	0.43
1:D:46:ARG:HD2	5:D:967:HOH:O	2.18	0.43
1:D:15:PHE:HB3	1:D:297:SER:HB3	1.99	0.43
1:C:165:TYR:OH	1:C:214:ASP:OD2	2.32	0.43
1:A:18:LEU:HD22	1:A:294:TYR:CE2	2.54	0.43
1:A:196:GLN:HG2	1:A:199:ARG:CZ	2.49	0.43
1:D:20:HIS:HA	1:D:21:PRO:HD3	1.94	0.42
1:B:101:LYS:HE3	5:B:941:HOH:O	2.19	0.42
1:C:285:LEU:HD12	1:C:285:LEU:HA	1.94	0.42
1:B:28:LYS:NZ	5:B:815:HOH:O	2.48	0.42
1:C:46[A]:ARG:HD3	5:C:808:HOH:O	2.19	0.42
1:A:81:PHE:CD1	3:A:704:FPS:H91	2.54	0.42
1:C:57:VAL:HB	1:C:302:TRP:CE2	2.55	0.41
1:C:18:LEU:HD22	1:C:63:PRO:HB2	2.01	0.41
1:D:183:ARG:HD2	5:D:902:HOH:O	2.19	0.41
1:D:61:TYR:HE1	1:D:178:LEU:HD13	1.86	0.41
1:A:165:TYR:CE2	1:A:169:ARG:HG3	2.55	0.41
1:D:57:VAL:HB	1:D:302:TRP:CE2	2.56	0.41
1:D:165:TYR:OH	1:D:169:ARG:HD2	2.21	0.41
1:D:147:PHE:CZ	3:D:704:FPS:H51	2.56	0.40
1:B:134:ARG:HG3	5:B:1082:HOH:O	2.21	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	305/314 (97%)	302 (99%)	3 (1%)	0	100	100
1	B	306/314 (98%)	303 (99%)	3 (1%)	0	100	100
1	C	305/314 (97%)	303 (99%)	2 (1%)	0	100	100
1	D	304/314 (97%)	298 (98%)	5 (2%)	1 (0%)	41	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1220/1256 (97%)	1206 (99%)	13 (1%)	1 (0%)	51 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	281	GLU

### 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	268/275 (98%)	262 (98%)	6 (2%)	52 44
1	B	269/275 (98%)	258 (96%)	11 (4%)	30 18
1	C	268/275 (98%)	258 (96%)	10 (4%)	34 22
1	D	267/275 (97%)	254 (95%)	13 (5%)	25 12
All	All	1072/1100 (98%)	1032 (96%)	40 (4%)	34 22

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	134	ARG
1	A	169	ARG
1	A	222	LEU
1	A	258	PHE
1	A	285	LEU
1	B	111	LEU
1	B	134	ARG
1	B	169	ARG
1	B	237	THR
1	B	258	PHE
1	B	266	LEU
1	B	270	LEU
1	B	285	LEU

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Mol	Chain	Res	Type
1	B	307[A]	LEU
1	B	307[B]	LEU
1	B	311	VAL
1	C	111	LEU
1	C	134	ARG
1	C	169	ARG
1	C	181	LEU
1	C	222	LEU
1	C	237	THR
1	C	251	GLU
1	C	258	PHE
1	C	285	LEU
1	C	301	LEU
1	D	18	LEU
1	D	125	LEU
1	D	134	ARG
1	D	169	ARG
1	D	177	LEU
1	D	181	LEU
1	D	188	LEU
1	D	222	LEU
1	D	247	ASP
1	D	258	PHE
1	D	285	LEU
1	D	301	LEU
1	D	307	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 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	GOL	A	705	-	5,5,5	0.32	0	5,5,5	0.56	0
3	FPS	D	704	2	19,23,23	1.25	1 (5%)	23,31,31	2.29	7 (30%)
4	GOL	B	705	-	5,5,5	0.32	0	5,5,5	0.72	0
4	GOL	C	705	-	5,5,5	0.36	0	5,5,5	0.60	0
3	FPS	B	704	2	19,23,23	1.58	2 (10%)	23,31,31	2.44	9 (39%)
3	FPS	A	704	2	19,23,23	1.56	2 (10%)	23,31,31	2.44	9 (39%)
3	FPS	C	704	2	19,23,23	1.56	2 (10%)	23,31,31	2.42	10 (43%)

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	GOL	A	705	-	-	2/4/4/4	-
3	FPS	D	704	2	-	3/19/25/25	-
4	GOL	B	705	-	-	0/4/4/4	-
4	GOL	C	705	-	-	0/4/4/4	-
3	FPS	B	704	2	-	3/19/25/25	-
3	FPS	A	704	2	-	3/19/25/25	-
3	FPS	C	704	2	-	3/19/25/25	-

All (7) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	704	FPS	C1-S1	-5.92	1.77	1.84
3	B	704	FPS	C1-S1	-5.17	1.78	1.84
3	A	704	FPS	C1-S1	-5.06	1.78	1.84
3	D	704	FPS	C1-S1	-4.85	1.78	1.84
3	B	704	FPS	PA-O2A	-3.90	1.46	1.56
3	A	704	FPS	PA-O2A	-3.89	1.46	1.56
3	C	704	FPS	PA-O2A	-2.09	1.51	1.56

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	704	FPS	C9-C8-C10	5.02	123.71	115.27
3	B	704	FPS	C9-C8-C10	4.99	123.66	115.27
3	C	704	FPS	C6-C7-C8	-4.98	115.66	127.66
3	D	704	FPS	C6-C7-C8	-4.72	116.30	127.66
3	A	704	FPS	C10-C11-C12	-4.52	97.01	111.88
3	B	704	FPS	C10-C11-C12	-4.52	97.02	111.88
3	B	704	FPS	C6-C7-C8	-4.31	117.28	127.66
3	C	704	FPS	C10-C11-C12	-4.31	97.71	111.88
3	A	704	FPS	C6-C7-C8	-4.30	117.31	127.66
3	C	704	FPS	C15-C13-C14	4.04	123.53	114.60
3	D	704	FPS	C10-C11-C12	-4.02	98.68	111.88
3	C	704	FPS	C4-C3-C5	3.99	121.98	115.27
3	D	704	FPS	O2A-PA-O1A	3.91	119.30	109.82
3	C	704	FPS	C9-C8-C10	3.88	121.80	115.27
3	D	704	FPS	C15-C13-C14	3.69	122.76	114.60
3	A	704	FPS	C15-C13-C14	3.69	122.75	114.60
3	B	704	FPS	C15-C13-C14	3.69	122.75	114.60
3	C	704	FPS	O3B-PB-O1B	3.33	120.37	107.64
3	A	704	FPS	C4-C3-C5	3.29	120.80	115.27
3	B	704	FPS	C4-C3-C5	3.26	120.76	115.27
3	D	704	FPS	C4-C3-C5	3.23	120.70	115.27
3	D	704	FPS	C9-C8-C10	3.10	120.49	115.27
3	A	704	FPS	O2A-PA-O1A	2.78	116.55	109.82
3	B	704	FPS	O2A-PA-O1A	2.77	116.53	109.82
3	B	704	FPS	C5-C6-C7	-2.68	103.07	111.88
3	A	704	FPS	C5-C6-C7	-2.67	103.12	111.88
3	D	704	FPS	O3B-PB-O1B	2.38	116.74	107.64
3	C	704	FPS	C15-C13-C12	-2.26	116.13	122.65
3	C	704	FPS	O2A-PA-O1A	2.23	115.23	109.82
3	B	704	FPS	C10-C8-C7	-2.20	116.66	121.12
3	A	704	FPS	C10-C8-C7	-2.20	116.67	121.12
3	A	704	FPS	C6-C5-C3	-2.18	105.81	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	704	FPS	C6-C5-C3	-2.17	105.83	112.98
3	C	704	FPS	C5-C3-C2	-2.07	116.92	121.12
3	C	704	FPS	C11-C10-C8	-2.03	106.29	112.98

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	705	GOL	O1-C1-C2-C3
3	D	704	FPS	C8-C10-C11-C12
3	C	704	FPS	C8-C10-C11-C12
3	A	704	FPS	C8-C10-C11-C12
3	B	704	FPS	C8-C10-C11-C12
4	A	705	GOL	O1-C1-C2-O2
3	D	704	FPS	C11-C10-C8-C9
3	C	704	FPS	C11-C10-C8-C9
3	D	704	FPS	C11-C10-C8-C7
3	C	704	FPS	C11-C10-C8-C7
3	A	704	FPS	C11-C10-C8-C9
3	B	704	FPS	C11-C10-C8-C9
3	A	704	FPS	C11-C10-C8-C7
3	B	704	FPS	C11-C10-C8-C7

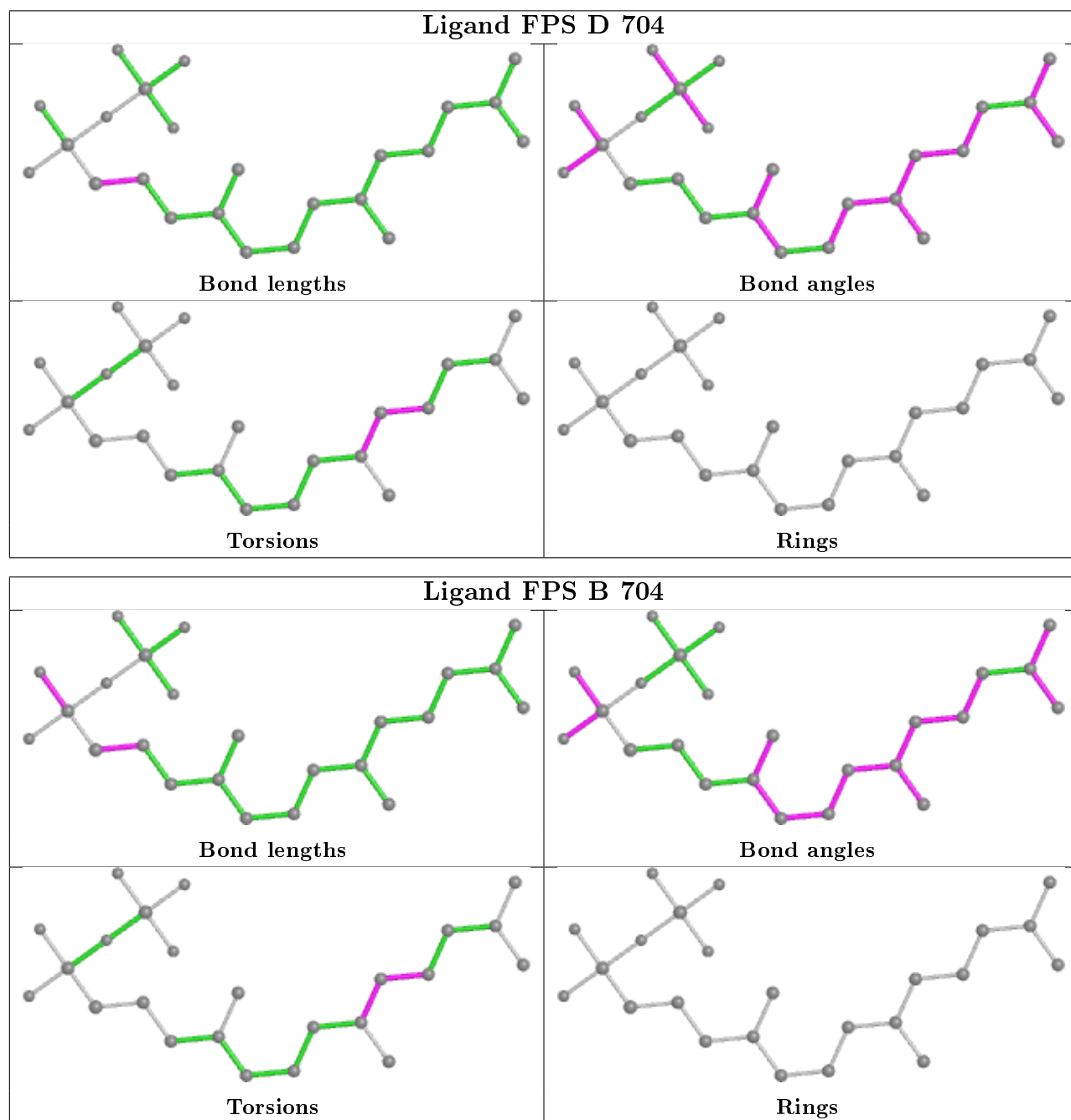
There are no ring outliers.

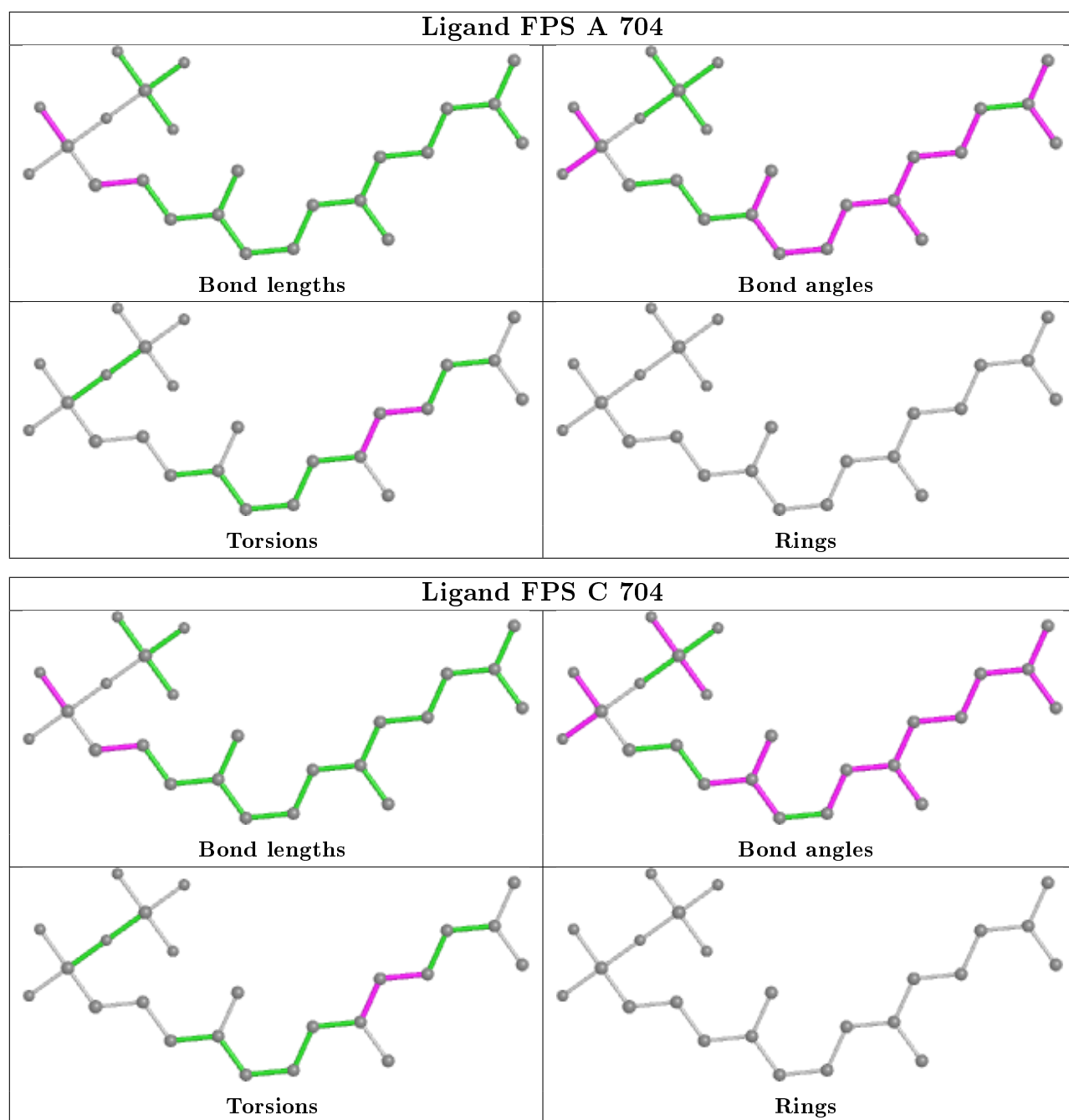
4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	704	FPS	6	0
3	B	704	FPS	6	0
3	A	704	FPS	7	0
3	C	704	FPS	3	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

### 6.1 Protein, DNA and RNA chains

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	305/314 (97%)	-0.51	1 (0%) 94 96	19, 28, 47, 67	0
1	B	304/314 (96%)	-0.52	0 100 100	18, 25, 42, 70	0
1	C	304/314 (96%)	-0.41	0 100 100	23, 34, 54, 88	0
1	D	305/314 (97%)	0.18	18 (5%) 22 30	29, 45, 71, 98	0
All	All	1218/1256 (96%)	-0.31	19 (1%) 72 79	18, 33, 59, 98	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	280	LEU	5.5
1	D	279	GLY	4.8
1	D	18	LEU	4.1
1	D	275	LEU	3.9
1	D	192	PRO	3.3
1	D	277	ALA	2.9
1	D	272	VAL	2.8
1	D	270	LEU	2.8
1	D	188	LEU	2.7
1	D	278	GLU	2.5
1	D	196	GLN	2.4
1	A	280	LEU	2.3
1	D	287	ALA	2.3
1	D	193	SER	2.2
1	D	281	GLU	2.2
1	D	282	THR	2.1
1	D	276	SER	2.1
1	D	195	LEU	2.0
1	D	311	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

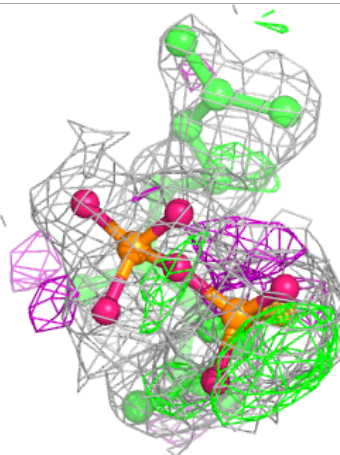
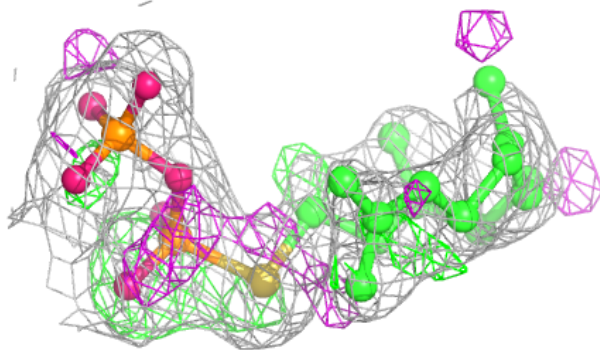
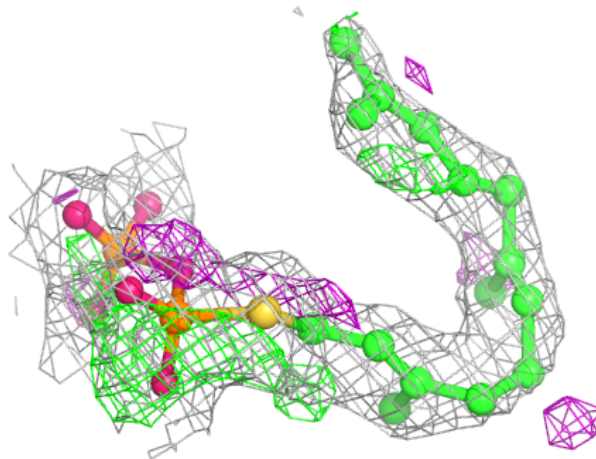
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	GOL	A	705	6/6	0.85	0.23	42,65,67,70	0
4	GOL	B	705	6/6	0.95	0.13	33,38,46,46	0
2	MG	D	702	1/1	0.96	0.05	37,37,37,37	0
2	MG	D	701	1/1	0.97	0.07	29,29,29,29	0
2	MG	A	703	1/1	0.97	0.08	22,22,22,22	0
3	FPS	A	704	24/24	0.97	0.13	20,38,52,60	0
4	GOL	C	705	6/6	0.97	0.09	32,36,45,49	0
2	MG	C	702	1/1	0.97	0.05	36,36,36,36	0
2	MG	A	702	1/1	0.97	0.07	26,26,26,26	0
2	MG	D	703	1/1	0.98	0.07	32,32,32,32	0
3	FPS	D	704	24/24	0.98	0.13	27,54,67,70	0
2	MG	C	703	1/1	0.98	0.05	26,26,26,26	0
2	MG	B	701	1/1	0.99	0.08	20,20,20,20	0
2	MG	A	701	1/1	0.99	0.11	22,22,22,22	0
3	FPS	C	704	24/24	0.99	0.10	23,45,61,65	0
2	MG	B	702	1/1	0.99	0.07	22,22,22,22	0
3	FPS	B	704	24/24	0.99	0.10	16,33,49,58	0
2	MG	C	701	1/1	0.99	0.05	29,29,29,29	0
2	MG	B	703	1/1	0.99	0.09	19,19,19,19	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.

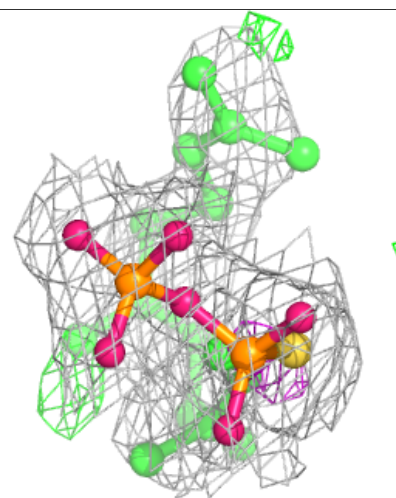
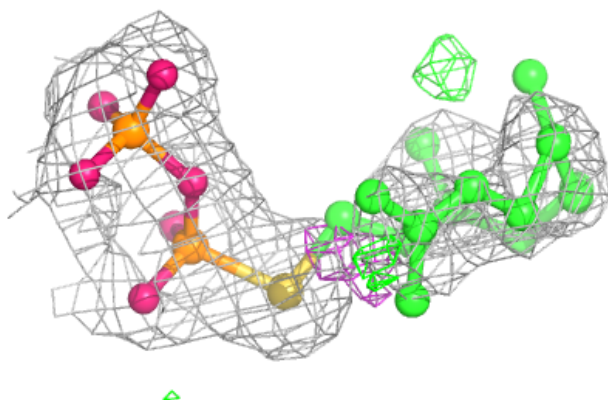
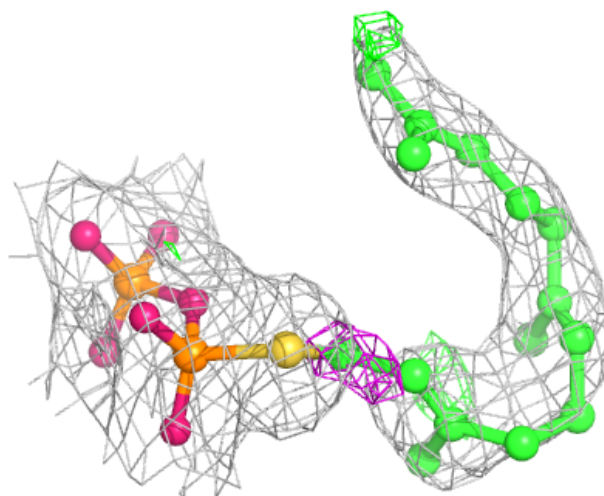
**Electron density around FPS A 704:**

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



**Electron density around FPS D 704:**

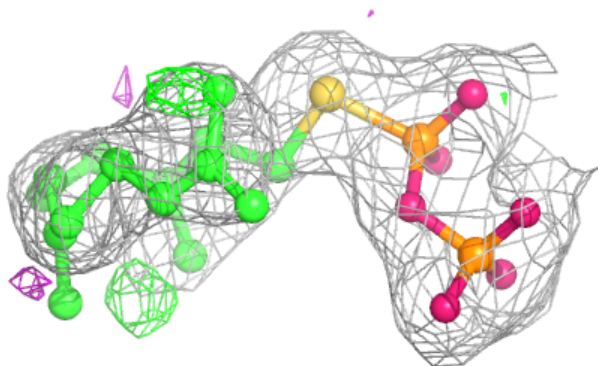
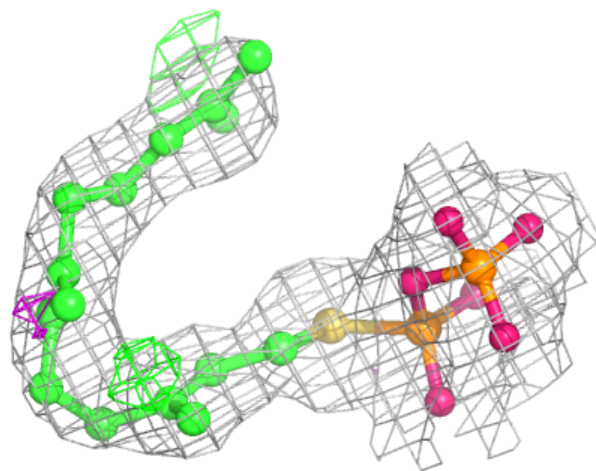
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





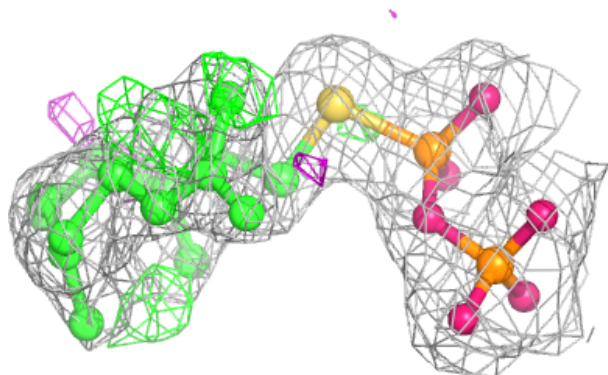
**Electron density around FPS C 704:**

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



**Electron density around FPS B 704:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.