



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:42 AM UTC

PDB ID : 6I3Y / pdb_00006i3y
Title : Crystal structure of the human mitochondrial PRELID1K58V-TRIAP1 complex with PS
Authors : Miliara, X.; Berry, J.-L.; Morgan, R.M.L.; Matthews, S.J.
Deposited on : 2018-11-08
Resolution : 2.98 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

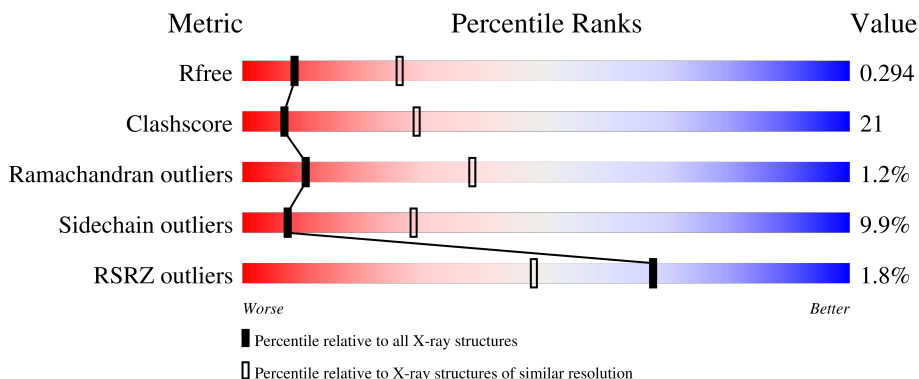
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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 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	C	185	2% 58% 32% 6%
1	F	185	% 61% 33% 5%
2	A	90	3% 54% 26% 18%
2	H	90	% 63% 10% 24%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3899 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 PRELI domain-containing protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	173	Total	C	N	O	S	0	0	0
			1352	870	238	239	5			
1	F	182	Total	C	N	O	S	0	0	0
			1459	934	263	258	4			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP Q9Y255
C	1	SER	-	expression tag	UNP Q9Y255
C	2	SER	-	expression tag	UNP Q9Y255
C	3	HIS	-	expression tag	UNP Q9Y255
C	4	HIS	-	expression tag	UNP Q9Y255
C	5	HIS	-	expression tag	UNP Q9Y255
C	6	HIS	-	expression tag	UNP Q9Y255
C	7	HIS	-	expression tag	UNP Q9Y255
C	8	HIS	-	expression tag	UNP Q9Y255
C	9	SER	-	expression tag	UNP Q9Y255
C	10	ASP	-	expression tag	UNP Q9Y255
C	11	GLN	-	expression tag	UNP Q9Y255
C	69	VAL	LYS	engineered mutation	UNP Q9Y255
C	123	SER	CYS	conflict	UNP Q9Y255
C	126	SER	CYS	conflict	UNP Q9Y255
F	0	GLY	-	expression tag	UNP Q9Y255
F	1	SER	-	expression tag	UNP Q9Y255
F	2	SER	-	expression tag	UNP Q9Y255
F	3	HIS	-	expression tag	UNP Q9Y255
F	4	HIS	-	expression tag	UNP Q9Y255
F	5	HIS	-	expression tag	UNP Q9Y255
F	6	HIS	-	expression tag	UNP Q9Y255
F	7	HIS	-	expression tag	UNP Q9Y255
F	8	HIS	-	expression tag	UNP Q9Y255
F	9	SER	-	expression tag	UNP Q9Y255

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Chain	Residue	Modelled	Actual	Comment	Reference
F	10	ASP	-	expression tag	UNP Q9Y255
F	11	GLN	-	expression tag	UNP Q9Y255
F	69	VAL	LYS	engineered mutation	UNP Q9Y255
F	123	SER	CYS	conflict	UNP Q9Y255
F	126	SER	CYS	conflict	UNP Q9Y255

- Molecule 2 is a protein called TP53-regulated inhibitor of apoptosis 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	74	Total	C	N	O	S	0	0	0
			538	340	89	103	6			
2	H	68	Total	C	N	O	S	0	0	0
			468	300	75	86	7			

There are 28 discrepancies between the modelled and reference sequences:

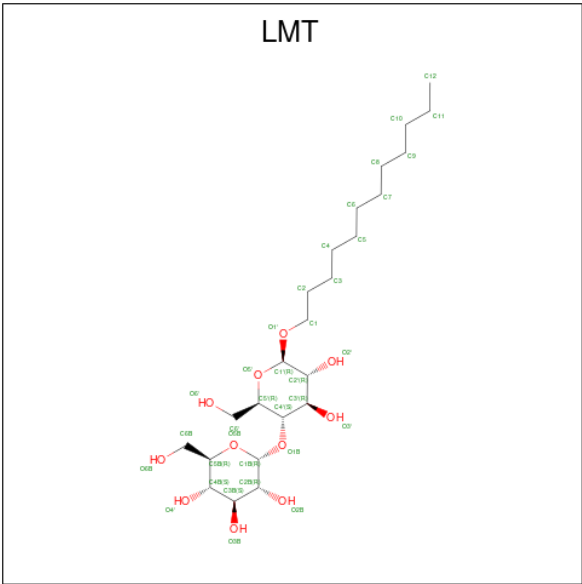
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP O43715
A	1	ALA	-	expression tag	UNP O43715
A	2	HIS	-	expression tag	UNP O43715
A	3	HIS	-	expression tag	UNP O43715
A	4	HIS	-	expression tag	UNP O43715
A	5	HIS	-	expression tag	UNP O43715
A	6	HIS	-	expression tag	UNP O43715
A	7	HIS	-	expression tag	UNP O43715
A	8	VAL	-	expression tag	UNP O43715
A	9	ASP	-	expression tag	UNP O43715
A	10	ASP	-	expression tag	UNP O43715
A	11	ASP	-	expression tag	UNP O43715
A	12	ASP	-	expression tag	UNP O43715
A	13	LYS	-	expression tag	UNP O43715
H	0	MET	-	initiating methionine	UNP O43715
H	1	ALA	-	expression tag	UNP O43715
H	2	HIS	-	expression tag	UNP O43715
H	3	HIS	-	expression tag	UNP O43715
H	4	HIS	-	expression tag	UNP O43715
H	5	HIS	-	expression tag	UNP O43715
H	6	HIS	-	expression tag	UNP O43715
H	7	HIS	-	expression tag	UNP O43715
H	8	VAL	-	expression tag	UNP O43715
H	9	ASP	-	expression tag	UNP O43715
H	10	ASP	-	expression tag	UNP O43715

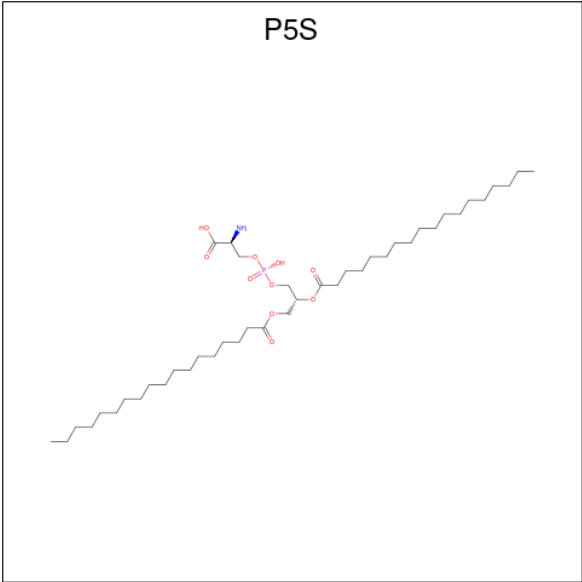
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Chain	Residue	Modelled	Actual	Comment	Reference
H	11	ASP	-	expression tag	UNP O43715
H	12	ASP	-	expression tag	UNP O43715
H	13	LYS	-	expression tag	UNP O43715

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	C	1	Total	C	O				0	0
			14	12	2					
4	F	1	Total	C	N	O	P	0	0	
			35	23	1	10	1			

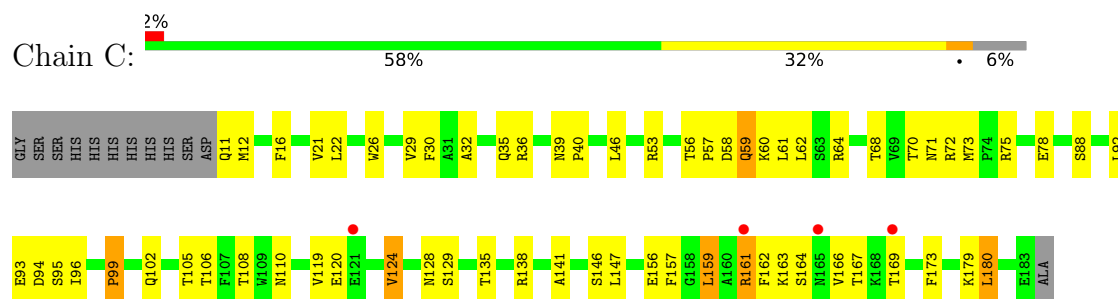
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	4	Total	O	0	0
			4	4		
5	F	16	Total	O	0	0
			16	16		
5	A	1	Total	O	0	0
			1	1		

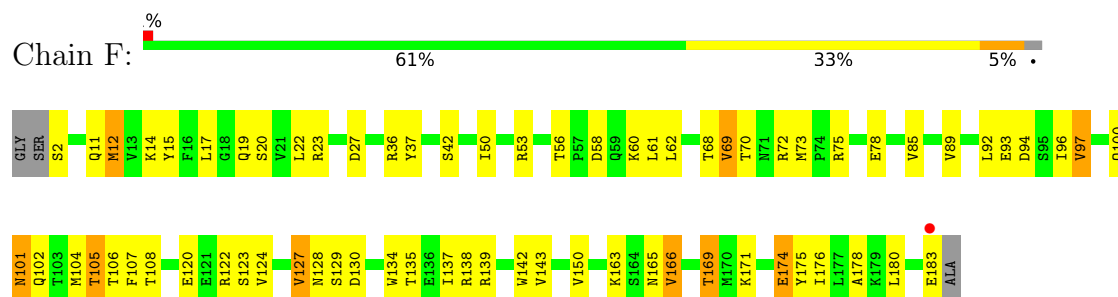
3 Residue-property plots [i](#)

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.

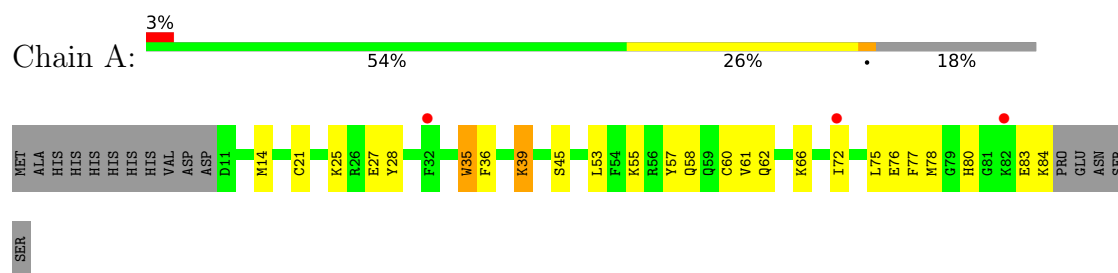
- Molecule 1: PRELI domain-containing protein 1, mitochondrial



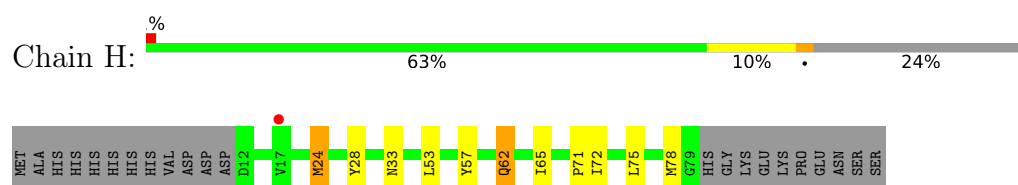
- Molecule 1: PRELI domain-containing protein 1, mitochondrial



- Molecule 2: TP53-regulated inhibitor of apoptosis 1



- Molecule 2: TP53-regulated inhibitor of apoptosis 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	126.00Å 126.00Å 178.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	63.00 – 2.98 63.00 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.8 (63.00-2.98) 99.8 (63.00-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.244 , 0.299 0.247 , 0.294	Depositor DCC
R_{free} test set	874 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	97.1	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 129.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3899	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% 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: LMT, P5S

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	C	0.74	0/1388	0.88	0/1895
1	F	0.79	0/1501	0.92	0/2044
2	A	0.78	0/549	1.02	1/740 (0.1%)
2	H	0.68	0/478	1.03	0/651
All	All	0.76	0/3916	0.94	1/5330 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	55	LYS	N-CA-C	6.65	118.53	111.28

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	C	1352	0	1265	46	0
1	F	1459	0	1382	75	0
2	A	538	0	450	34	0
2	H	468	0	375	13	0
3	C	12	0	11	1	0
4	C	14	0	20	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	35	0	36	1	0
5	A	1	0	0	0	0
5	C	4	0	0	0	0
5	F	16	0	0	1	0
All	All	3899	0	3539	157	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 21.

All (157) 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:C:56:THR:OG1	1:C:57:PRO:HD2	1.27	1.32
1:F:23:ARG:HA	1:F:134:TRP:NE1	1.56	1.17
1:C:166:VAL:O	1:C:169:THR:HG22	1.59	1.03
1:F:128:ASN:HD22	1:F:129:SER:N	1.56	1.02
1:C:56:THR:OG1	1:C:57:PRO:CD	2.09	1.00
1:F:23:ARG:HA	1:F:134:TRP:CD1	1.98	0.98
1:C:16:PHE:HB3	1:C:141:ALA:HB3	1.46	0.95
2:A:35:TRP:CG	2:A:39:LYS:HZ1	1.87	0.93
1:C:119:VAL:HB	4:C:202:P5S:H41A	1.50	0.91
1:C:56:THR:HG1	1:C:57:PRO:HD2	1.12	0.90
1:F:23:ARG:CA	1:F:134:TRP:NE1	2.36	0.89
1:F:11:GLN:HG2	1:F:12:MET:N	1.89	0.88
1:F:11:GLN:HG2	1:F:12:MET:H	1.41	0.85
1:F:105:THR:HG23	1:F:124:VAL:HG23	1.59	0.84
1:F:20:SER:O	1:F:137:ILE:HG22	1.77	0.84
1:F:128:ASN:HD22	1:F:129:SER:H	1.29	0.81
1:F:61:LEU:HB3	1:F:97:VAL:CG2	2.14	0.78
2:A:35:TRP:C	2:A:39:LYS:HZ2	1.94	0.75
1:F:23:ARG:CA	1:F:134:TRP:HE1	1.98	0.75
1:F:128:ASN:ND2	1:F:130:ASP:H	1.85	0.74
1:F:178:ALA:O	1:F:183:GLU:CB	2.35	0.74
1:F:11:GLN:CG	1:F:12:MET:H	2.02	0.73
2:A:78:MET:HA	2:A:78:MET:HE2	1.70	0.72
2:A:35:TRP:C	2:A:39:LYS:NZ	2.49	0.70
2:H:53:LEU:HD23	2:H:53:LEU:O	1.94	0.68
1:C:71:ASN:HD22	1:C:72:ARG:N	1.93	0.67
1:F:94:ASP:HB2	2:A:78:MET:CE	2.24	0.67
1:C:35:GLN:HE21	2:H:33:ASN:HD22	1.43	0.66
2:A:39:LYS:HG2	2:A:45:SER:CB	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:VAL:HG12	1:C:138:ARG:HB3	1.77	0.64
1:F:20:SER:O	1:F:137:ILE:CG2	2.44	0.64
1:F:37:TYR:HB3	2:A:14:MET:HE3	1.80	0.64
1:F:23:ARG:HA	1:F:134:TRP:HE1	1.50	0.63
1:F:128:ASN:ND2	1:F:129:SER:N	2.39	0.63
1:F:15:TYR:HE1	1:F:17:LEU:HB2	1.62	0.63
1:F:50:ILE:HD13	1:F:53:ARG:HH12	1.64	0.63
2:A:78:MET:HE2	2:A:78:MET:CA	2.27	0.62
1:C:21:VAL:HG21	1:C:128:ASN:HD22	1.63	0.61
1:F:123:SER:HB2	1:F:137:ILE:HD11	1.80	0.61
1:C:93:GLU:HG3	1:C:108:THR:HG22	1.81	0.61
1:F:61:LEU:HB3	1:F:97:VAL:HG21	1.81	0.61
1:F:70:THR:O	4:F:201:P5S:H42A	2.00	0.61
1:C:163:LYS:O	1:C:166:VAL:HG12	1.99	0.61
1:F:122:ARG:NE	5:F:301:HOH:O	2.33	0.61
1:C:156:GLU:O	1:C:159:LEU:HD23	2.01	0.61
2:H:24:MET:HE3	2:H:24:MET:C	2.26	0.61
1:F:75:ARG:HA	1:F:78:GLU:OE2	2.01	0.60
2:H:28:TYR:HB2	2:H:53:LEU:HD22	1.82	0.60
1:C:56:THR:HG23	1:C:58:ASP:H	1.66	0.60
1:F:128:ASN:ND2	1:F:130:ASP:N	2.48	0.60
2:H:24:MET:HE2	2:H:57:TYR:HB2	1.83	0.60
1:F:94:ASP:HB2	2:A:78:MET:HE1	1.83	0.59
1:F:61:LEU:H	1:F:97:VAL:HG23	1.67	0.59
1:F:128:ASN:HD21	1:F:130:ASP:H	1.48	0.59
1:F:78:GLU:OE2	1:F:78:GLU:N	2.35	0.59
1:F:124:VAL:O	1:F:137:ILE:HD12	2.03	0.58
2:A:39:LYS:N	2:A:39:LYS:HD3	2.16	0.58
1:C:35:GLN:HE21	2:H:33:ASN:ND2	2.01	0.58
2:A:58:GLN:HA	2:A:61:VAL:HG22	1.86	0.58
1:F:105:THR:HG23	1:F:124:VAL:CG2	2.32	0.58
2:A:35:TRP:CD1	2:A:39:LYS:CE	2.88	0.57
2:H:24:MET:CE	2:H:57:TYR:HB2	2.34	0.57
1:F:120:GLU:OE1	2:A:84:LYS:HA	2.05	0.56
1:C:75:ARG:HA	1:C:78:GLU:OE1	2.05	0.56
1:C:59:GLN:N	1:C:59:GLN:OE1	2.38	0.56
2:A:35:TRP:CD1	2:A:39:LYS:HE3	2.41	0.56
2:H:24:MET:HE1	2:H:53:LEU:HD21	1.87	0.55
1:C:169:THR:O	1:C:173:PHE:HB2	2.06	0.55
1:F:93:GLU:CB	1:F:108:THR:HG23	2.37	0.55
1:C:120:GLU:OE2	3:C:201:LMT:H3B	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:62:GLN:O	2:H:65:ILE:HG13	2.08	0.54
2:H:53:LEU:HD23	2:H:53:LEU:C	2.33	0.54
1:F:61:LEU:O	1:F:97:VAL:HG22	2.08	0.54
1:F:176:ILE:O	1:F:180:LEU:HD12	2.07	0.53
1:C:62:LEU:HD12	1:C:96:ILE:HG22	1.89	0.53
2:A:83:GLU:O	2:A:84:LYS:NZ	2.25	0.53
1:C:110:ASN:OD1	4:C:202:P5S:H41	2.09	0.53
1:C:96:ILE:HG23	2:H:78:MET:HE3	1.90	0.52
2:A:72:ILE:O	2:A:75:LEU:HD12	2.09	0.52
1:F:93:GLU:HA	1:F:107:PHE:O	2.10	0.52
2:A:39:LYS:HD3	2:A:39:LYS:H	1.75	0.52
1:F:27:ASP:N	1:F:27:ASP:OD1	2.43	0.51
1:F:123:SER:HB3	1:F:139:ARG:HB2	1.92	0.51
2:A:78:MET:HE2	2:A:78:MET:N	2.25	0.51
1:F:56:THR:CG2	1:F:60:LYS:H	2.24	0.51
1:F:14:LYS:HB2	1:F:143:VAL:HG22	1.93	0.51
1:F:69:VAL:HG22	1:F:89:VAL:HB	1.93	0.51
1:F:23:ARG:CA	1:F:134:TRP:CD1	2.85	0.50
1:C:53:ARG:HG3	1:C:61:LEU:HD11	1.92	0.50
2:A:35:TRP:CG	2:A:39:LYS:NZ	2.71	0.50
2:A:77:PHE:CD2	2:A:78:MET:HE3	2.46	0.50
1:C:21:VAL:HG23	1:C:135:THR:C	2.37	0.49
1:C:110:ASN:CG	4:C:202:P5S:H41	2.37	0.49
1:F:165:ASN:O	1:F:169:THR:HG23	2.13	0.49
2:A:27:GLU:HG2	2:A:53:LEU:HD21	1.93	0.49
1:F:163:LYS:O	1:F:166:VAL:HG12	2.13	0.49
1:C:166:VAL:O	1:C:169:THR:CG2	2.47	0.49
2:A:27:GLU:OE1	2:A:27:GLU:N	2.28	0.49
2:A:83:GLU:OE1	2:A:84:LYS:HG2	2.13	0.49
1:F:17:LEU:C	1:F:17:LEU:HD23	2.38	0.48
1:F:128:ASN:HD22	1:F:128:ASN:C	2.13	0.47
1:F:56:THR:HG22	1:F:60:LYS:O	2.15	0.47
2:A:28:TYR:HB2	2:A:53:LEU:HG	1.97	0.47
1:F:102:GLN:OE1	1:F:127:VAL:HG11	2.15	0.47
1:F:96:ILE:C	1:F:96:ILE:HD12	2.39	0.47
1:F:23:ARG:CB	1:F:134:TRP:HE1	2.27	0.46
2:A:78:MET:HE2	2:A:78:MET:H	1.80	0.46
1:F:53:ARG:CG	1:F:61:LEU:HD11	2.44	0.46
1:C:29:VAL:HG23	1:C:30:PHE:HD1	1.80	0.46
1:F:175:TYR:CD2	1:F:176:ILE:HD12	2.51	0.46
1:F:94:ASP:CB	2:A:78:MET:CE	2.93	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:GLN:HA	1:F:100:GLN:OE1	2.17	0.45
1:F:101:ASN:HD22	1:F:101:ASN:N	2.14	0.45
1:C:71:ASN:HD22	1:C:71:ASN:C	2.23	0.45
1:F:50:ILE:HD13	1:F:53:ARG:NH1	2.29	0.45
1:F:62:LEU:HD22	1:F:96:ILE:HG22	1.99	0.45
2:A:35:TRP:O	2:A:36:PHE:C	2.60	0.44
1:F:142:TRP:CD2	2:A:84:LYS:HE3	2.53	0.44
1:C:56:THR:HG22	1:C:60:LYS:H	1.83	0.44
1:F:93:GLU:CB	1:F:108:THR:OG1	2.66	0.44
2:A:62:GLN:O	2:A:66:LYS:HG3	2.17	0.44
1:F:23:ARG:CB	1:F:134:TRP:NE1	2.80	0.44
1:C:71:ASN:HD21	1:C:73:MET:HG3	1.83	0.44
1:C:56:THR:HG23	1:C:58:ASP:N	2.32	0.43
1:C:99:PRO:O	1:C:102:GLN:N	2.50	0.43
1:F:106:THR:CG2	1:F:123:SER:OG	2.65	0.43
2:A:35:TRP:CD2	2:A:39:LYS:NZ	2.79	0.43
2:H:24:MET:HE1	2:H:53:LEU:CD2	2.48	0.43
1:F:56:THR:HG21	1:F:58:ASP:OD1	2.17	0.43
1:F:135:THR:HG23	1:F:135:THR:O	2.18	0.43
1:C:21:VAL:HG23	1:C:135:THR:O	2.18	0.43
1:C:71:ASN:HD22	1:C:72:ARG:H	1.66	0.43
1:F:123:SER:HB3	1:F:139:ARG:CB	2.48	0.43
1:F:120:GLU:OE1	2:A:84:LYS:HD3	2.18	0.43
1:F:124:VAL:HG12	1:F:138:ARG:HB3	2.01	0.43
1:F:171:LYS:O	1:F:174:GLU:OE2	2.37	0.43
1:C:32:ALA:O	1:C:36:ARG:HG3	2.19	0.43
1:C:26:TRP:CZ2	1:C:102:GLN:HG2	2.54	0.42
1:F:96:ILE:HD12	1:F:96:ILE:O	2.20	0.42
2:A:57:TYR:O	2:A:60:CYS:HB3	2.19	0.42
1:C:162:PHE:CD1	1:C:162:PHE:C	2.98	0.42
1:C:180:LEU:HA	1:C:180:LEU:HD13	1.72	0.42
1:F:106:THR:HG22	1:F:123:SER:O	2.19	0.42
1:C:11:GLN:HB2	1:F:12:MET:CE	2.50	0.41
1:C:164:SER:O	1:C:167:THR:OG1	2.31	0.41
1:F:73:MET:HE2	1:F:85:VAL:HG12	2.01	0.41
1:F:93:GLU:HA	1:F:108:THR:HA	2.01	0.41
1:C:39:ASN:HB2	1:C:40:PRO:HD2	2.02	0.41
1:C:94:ASP:O	1:C:106:THR:HA	2.21	0.41
1:F:22:LEU:HB2	1:F:135:THR:CG2	2.50	0.41
2:H:53:LEU:C	2:H:53:LEU:CD2	2.94	0.41
1:C:64:ARG:HD3	1:C:92:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:21:CYS:O	2:A:25:LYS:N	2.54	0.41
1:C:71:ASN:C	1:C:71:ASN:ND2	2.79	0.40
1:C:46:LEU:HD11	1:C:70:THR:HG22	2.03	0.40
2:A:58:GLN:O	2:A:62:GLN:HG2	2.22	0.40
1:C:157:PHE:CE1	1:C:161:ARG:HG3	2.56	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	C	171/185 (92%)	158 (92%)	11 (6%)	2 (1%)	10	38
1	F	180/185 (97%)	174 (97%)	5 (3%)	1 (1%)	21	53
2	A	72/90 (80%)	62 (86%)	9 (12%)	1 (1%)	9	34
2	H	66/90 (73%)	56 (85%)	8 (12%)	2 (3%)	3	17
All	All	489/550 (89%)	450 (92%)	33 (7%)	6 (1%)	10	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	12	MET
1	F	36	ARG
2	A	35	TRP
1	C	99	PRO
2	H	71	PRO
2	H	72	ILE

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	C	135/167 (81%)	121 (90%)	14 (10%)	7	26
1	F	152/167 (91%)	135 (89%)	17 (11%)	6	23
2	A	47/80 (59%)	44 (94%)	3 (6%)	16	45
2	H	38/80 (48%)	35 (92%)	3 (8%)	11	37
All	All	372/494 (75%)	335 (90%)	37 (10%)	7	28

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	22	LEU
1	C	59	GLN
1	C	68	THR
1	C	88	SER
1	C	95	SER
1	C	105	THR
1	C	124	VAL
1	C	129	SER
1	C	146	SER
1	C	147	LEU
1	C	159	LEU
1	C	161	ARG
1	C	179	LYS
1	C	180	LEU
1	F	2	SER
1	F	12	MET
1	F	19	GLN
1	F	42	SER
1	F	68	THR
1	F	69	VAL
1	F	72	ARG
1	F	92	LEU
1	F	97	VAL
1	F	101	ASN

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Mol	Chain	Res	Type
1	F	104	MET
1	F	105	THR
1	F	127	VAL
1	F	150	VAL
1	F	166	VAL
1	F	169	THR
1	F	174	GLU
2	A	39	LYS
2	A	76	GLU
2	A	80	HIS
2	H	24	MET
2	H	62	GLN
2	H	75	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	35	GLN
1	C	71	ASN
1	F	19	GLN
1	F	35	GLN
1	F	101	ASN
1	F	128	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](#)

3 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	$\# Z > 2$
4	P5S	C	202	-	13,13,53	2.14	2 (15%)	13,13,60	1.37	2 (15%)
3	LMT	C	201	-	12,12,36	0.99	0	17,17,47	1.42	3 (17%)
4	P5S	F	201	-	33,34,53	1.28	2 (6%)	35,41,60	1.61	7 (20%)

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	P5S	C	202	-	-	6/11/11/59	-
3	LMT	C	201	-	-	2/2/22/61	0/1/1/2
4	P5S	F	201	-	-	20/40/40/59	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	202	P5S	O47-C38	6.79	1.44	1.22
4	F	201	P5S	O19-C17	4.53	1.46	1.33
4	F	201	P5S	O37-C38	4.47	1.46	1.34
4	C	202	P5S	O37-C38	-3.38	1.19	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	201	P5S	OG-CB-CA	4.42	111.92	108.06
4	C	202	P5S	C40-C39-C38	-3.70	104.85	114.51
3	C	201	LMT	O5B-C1B-C2B	3.15	115.83	110.30
4	F	201	P5S	O37-C38-C39	3.08	118.14	111.48
4	F	201	P5S	O19-C17-C20	3.00	121.00	111.83
4	F	201	P5S	OXT-C-O	-2.96	117.36	124.08
4	F	201	P5S	C2-O37-C38	-2.85	110.98	117.80
4	F	201	P5S	O19-C1-C2	2.80	116.48	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	201	P5S	C23-C22-C21	-2.67	100.86	114.37
4	C	202	P5S	O37-C38-O47	-2.43	117.08	123.33
3	C	201	LMT	C1B-C2B-C3B	2.14	114.72	110.36
3	C	201	LMT	O5B-C5B-C4B	-2.02	106.06	109.70

There are no chirality outliers.

All (28) torsion outliers are listed below:

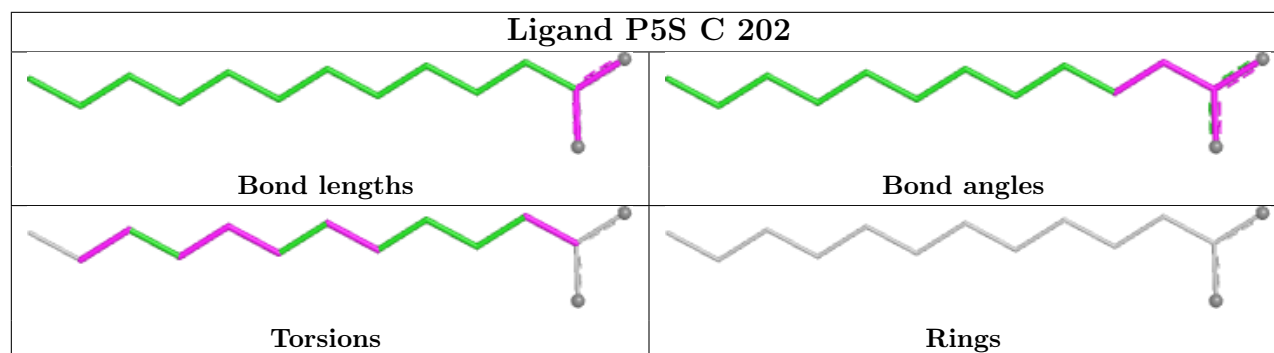
Mol	Chain	Res	Type	Atoms
4	F	201	P5S	C2-C3-O16-P12
4	F	201	P5S	C-CA-CB-OG
4	F	201	P5S	N-CA-CB-OG
4	F	201	P5S	CB-OG-P12-O13
4	F	201	P5S	CB-OG-P12-O16
4	F	201	P5S	O18-C17-O19-C1
4	F	201	P5S	C20-C17-O19-C1
4	F	201	P5S	C2-C1-O19-C17
3	C	201	LMT	O5B-C5B-C6B-O6B
3	C	201	LMT	C4B-C5B-C6B-O6B
4	F	201	P5S	C25-C26-C27-C28
4	F	201	P5S	C24-C25-C26-C27
4	C	202	P5S	C44-C45-C46-C48
4	C	202	P5S	C46-C48-C49-C50
4	F	201	P5S	C17-C20-C21-C22
4	F	201	P5S	C23-C24-C25-C26
4	F	201	P5S	C21-C22-C23-C24
4	F	201	P5S	C22-C23-C24-C25
4	F	201	P5S	O19-C1-C2-O37
4	F	201	P5S	O19-C1-C2-C3
4	C	202	P5S	C41-C42-C43-C44
4	F	201	P5S	CB-OG-P12-O15
4	F	201	P5S	C26-C27-C28-C29
4	C	202	P5S	C43-C44-C45-C46
4	C	202	P5S	O47-C38-C39-C40
4	C	202	P5S	O37-C38-C39-C40
4	F	201	P5S	C20-C21-C22-C23
4	F	201	P5S	C39-C38-O37-C2

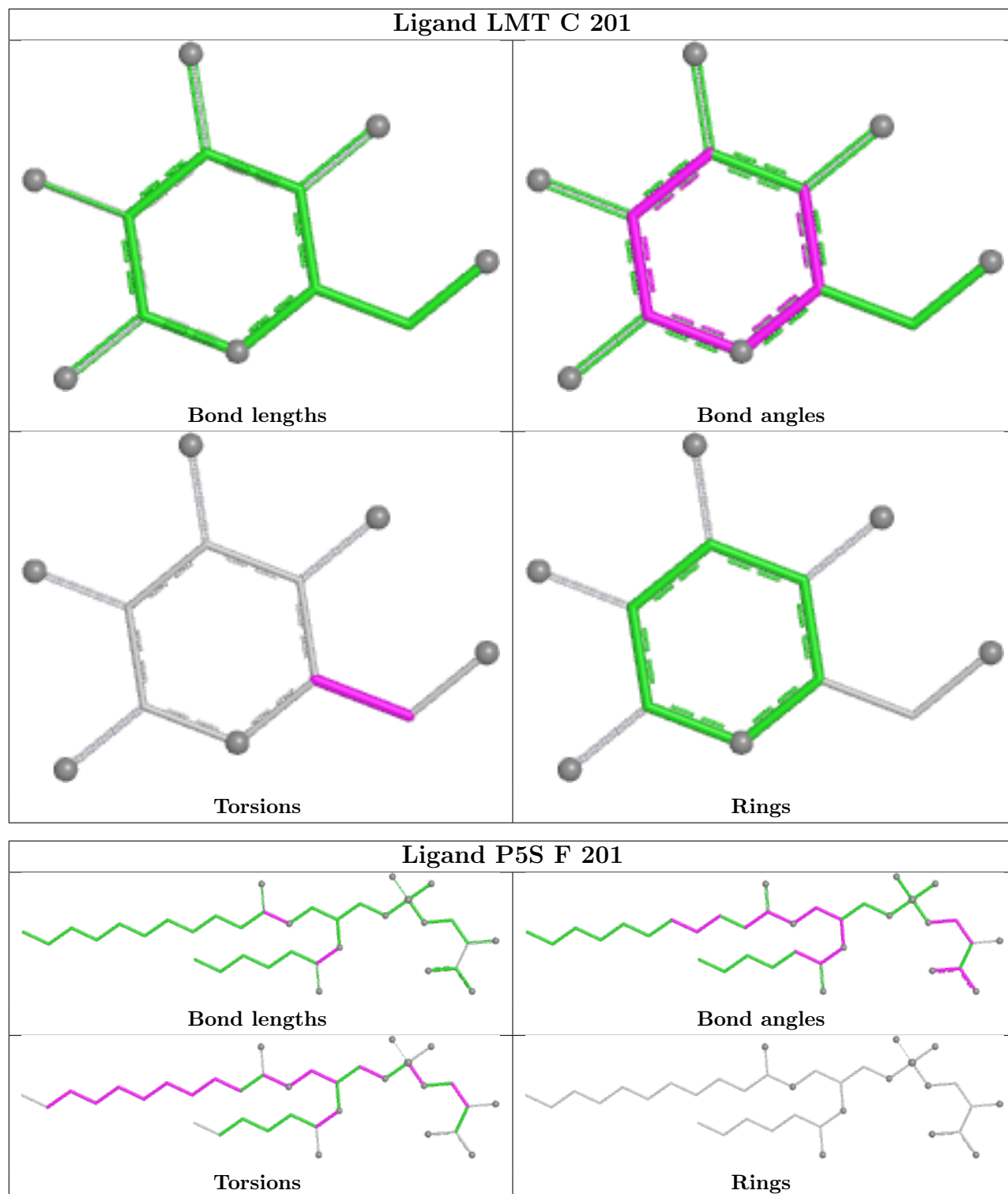
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	202	P5S	3	0
3	C	201	LMT	1	0
4	F	201	P5S	1	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	C	173/185 (93%)	0.10	4 (2%) 61 42	73, 106, 141, 177	0
1	F	182/185 (98%)	0.10	1 (0%) 87 75	71, 99, 144, 175	0
2	A	74/90 (82%)	0.21	3 (4%) 41 25	101, 128, 179, 198	0
2	H	68/90 (75%)	0.25	1 (1%) 72 53	105, 140, 171, 184	0
All	All	497/550 (90%)	0.14	9 (1%) 67 48	71, 112, 164, 198	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	82	LYS	3.2
1	F	183	GLU	3.0
1	C	161	ARG	2.6
1	C	165	ASN	2.6
2	A	72	ILE	2.5
2	H	17	VAL	2.3
2	A	32	PHE	2.1
1	C	169	THR	2.0
1	C	121	GLU	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](#)

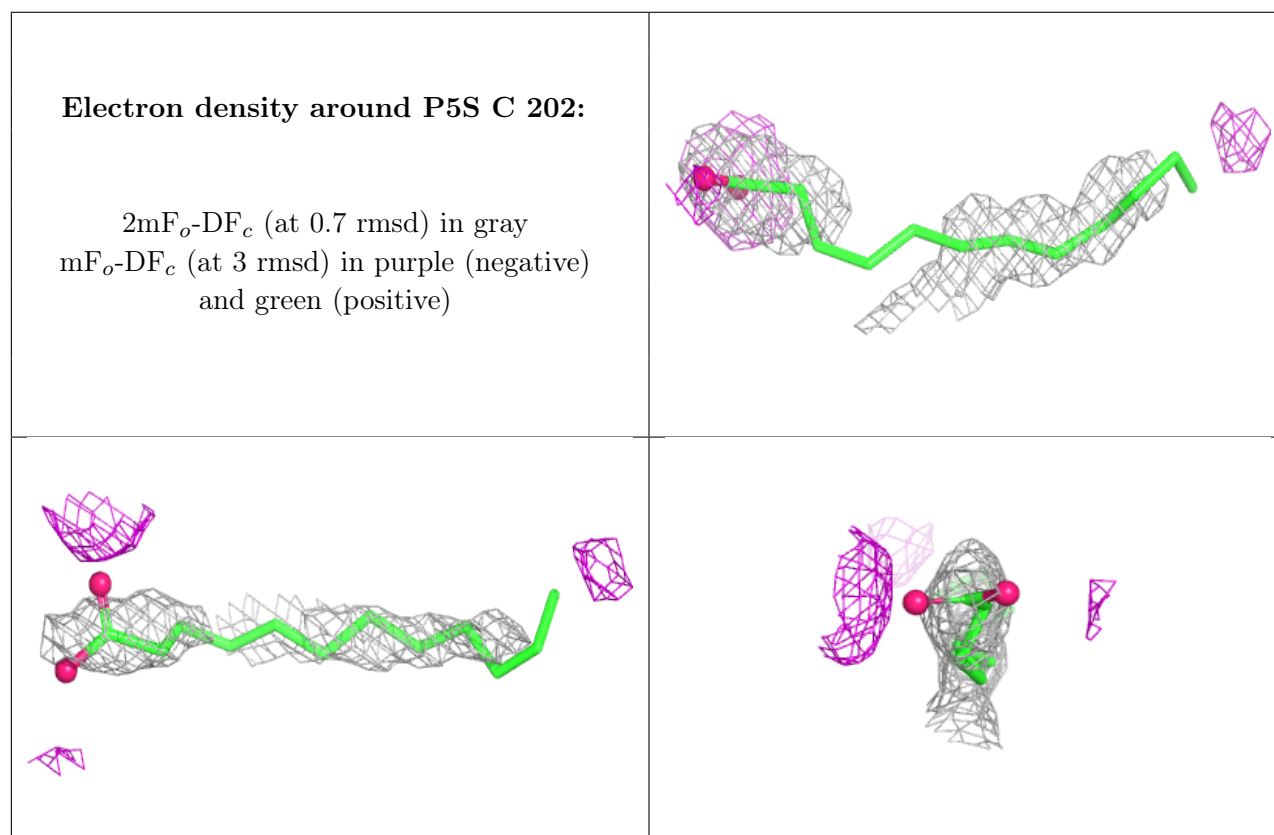
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

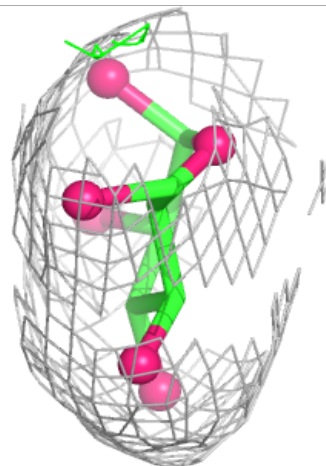
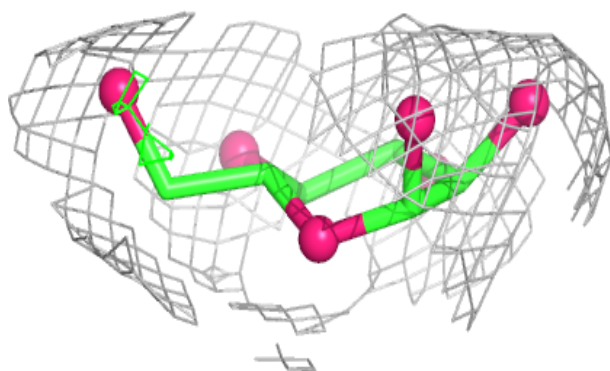
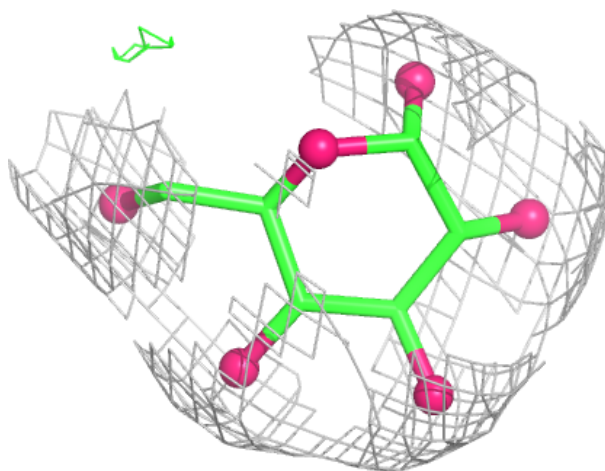
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	P5S	C	202	14/54	0.87	0.23	99,115,128,152	0
3	LMT	C	201	12/35	0.89	0.07	88,106,109,115	0
4	P5S	F	201	35/54	0.92	0.33	20,55,68,71	35

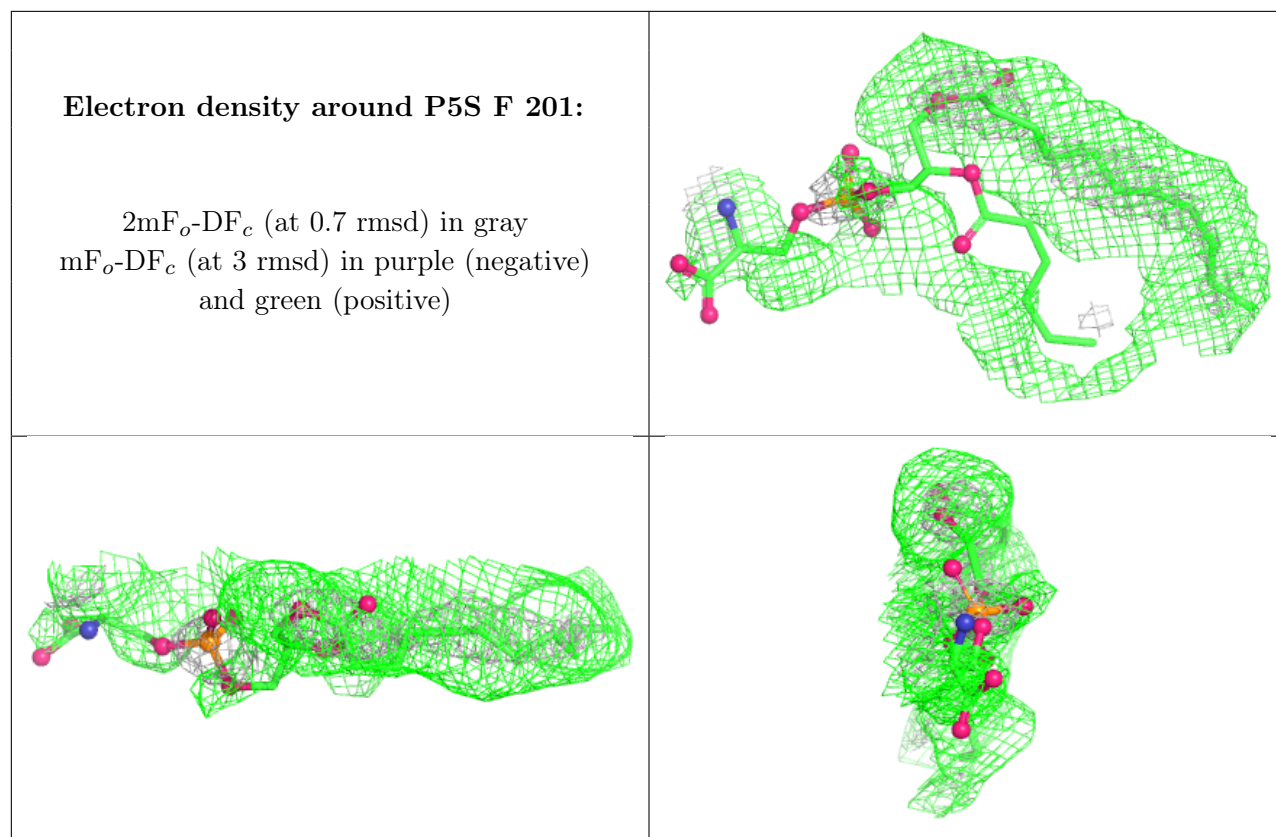
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around LMT C 201:

$2mF_o-DF_c$ (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.