wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 05:41 PM JST

PDB ID	:	6LKN / pdb_00006lkn
Title	:	Crystal structure of ATP11C-CDC50A in PtdSer-bound E2P state
Authors	:	Abe, K.; Irie, K.; Nakanishi, H.; Hasegawa, K.
Deposited on	:	2019-12-19
Resolution	:	3.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

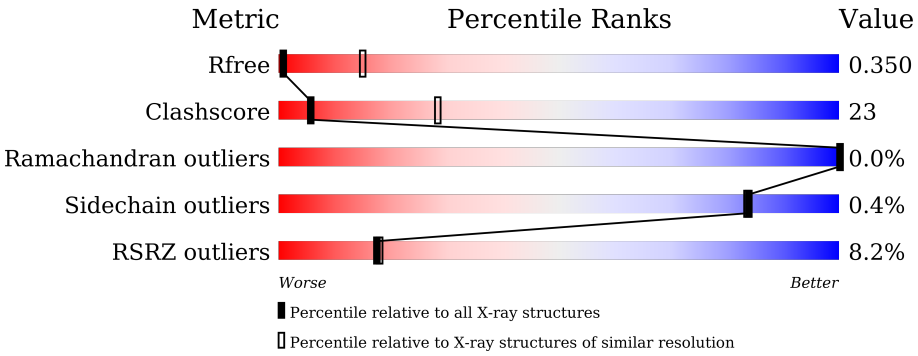
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1129	6% 58% 35% • 6%
1	E	1129	9% 59% 35% • 6%
1	I	1129	7% 66% 27% • 6%
1	M	1129	12% 66% 28% 6%
2	C	361	5% 60% 30% 10%
2	F	361	% 58% 31% 10%

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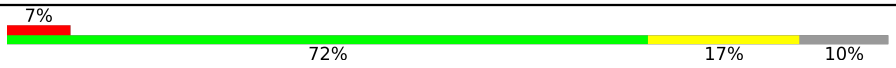
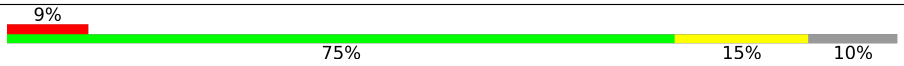
Mol	Chain	Length	Quality of chain
2	J	361	
2	N	361	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BEF	E	1204	-	-	X	-
5	BEF	M	1203	-	-	X	-
6	NAG	F	405	-	-	X	-
6	NAG	J	404	-	-	X	-
6	NAG	J	405	-	-	X	-
6	NAG	N	405	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 45252 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 Phospholipid-transporting ATPase IG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1064	Total	C	N	O	S	0	0	0
			8597	5556	1401	1594	46			
1	E	1064	Total	C	N	O	S	0	0	0
			8597	5556	1401	1594	46			
1	I	1064	Total	C	N	O	S	0	0	0
			8597	5556	1401	1594	46			
1	M	1064	Total	C	N	O	S	0	0	0
			8597	5556	1401	1594	46			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8NB49
A	2	PHE	-	expression tag	UNP Q8NB49
A	3	ARG	-	expression tag	UNP Q8NB49
A	4	ARG	-	expression tag	UNP Q8NB49
A	5	SER	-	expression tag	UNP Q8NB49
A	6	LEU	-	expression tag	UNP Q8NB49
A	7	ASN	-	expression tag	UNP Q8NB49
A	8	ARG	-	expression tag	UNP Q8NB49
A	9	PHE	-	expression tag	UNP Q8NB49
A	111	TRP	CYS	engineered mutation	UNP Q8NB49
E	1	MET	-	initiating methionine	UNP Q8NB49
E	2	PHE	-	expression tag	UNP Q8NB49
E	3	ARG	-	expression tag	UNP Q8NB49
E	4	ARG	-	expression tag	UNP Q8NB49
E	5	SER	-	expression tag	UNP Q8NB49
E	6	LEU	-	expression tag	UNP Q8NB49
E	7	ASN	-	expression tag	UNP Q8NB49
E	8	ARG	-	expression tag	UNP Q8NB49
E	9	PHE	-	expression tag	UNP Q8NB49
E	111	TRP	CYS	engineered mutation	UNP Q8NB49
I	1	MET	-	initiating methionine	UNP Q8NB49

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Chain	Residue	Modelled	Actual	Comment	Reference
I	2	PHE	-	expression tag	UNP Q8NB49
I	3	ARG	-	expression tag	UNP Q8NB49
I	4	ARG	-	expression tag	UNP Q8NB49
I	5	SER	-	expression tag	UNP Q8NB49
I	6	LEU	-	expression tag	UNP Q8NB49
I	7	ASN	-	expression tag	UNP Q8NB49
I	8	ARG	-	expression tag	UNP Q8NB49
I	9	PHE	-	expression tag	UNP Q8NB49
I	111	TRP	CYS	engineered mutation	UNP Q8NB49
M	1	MET	-	initiating methionine	UNP Q8NB49
M	2	PHE	-	expression tag	UNP Q8NB49
M	3	ARG	-	expression tag	UNP Q8NB49
M	4	ARG	-	expression tag	UNP Q8NB49
M	5	SER	-	expression tag	UNP Q8NB49
M	6	LEU	-	expression tag	UNP Q8NB49
M	7	ASN	-	expression tag	UNP Q8NB49
M	8	ARG	-	expression tag	UNP Q8NB49
M	9	PHE	-	expression tag	UNP Q8NB49
M	111	TRP	CYS	engineered mutation	UNP Q8NB49

- Molecule 2 is a protein called Cell cycle control protein 50A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	324	Total	C	N	O	S	0	0	0
			2613	1696	439	466	12			
2	F	324	Total	C	N	O	S	0	0	0
			2613	1696	439	466	12			
2	J	324	Total	C	N	O	S	0	0	0
			2613	1696	439	466	12			
2	N	324	Total	C	N	O	S	0	0	0
			2613	1696	439	466	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	190	GLN	ASN	engineered mutation	UNP Q9NV96
C	292	TRP	SER	engineered mutation	UNP Q9NV96
F	190	GLN	ASN	engineered mutation	UNP Q9NV96
F	292	TRP	SER	engineered mutation	UNP Q9NV96
J	190	GLN	ASN	engineered mutation	UNP Q9NV96
J	292	TRP	SER	engineered mutation	UNP Q9NV96
N	190	GLN	ASN	engineered mutation	UNP Q9NV96

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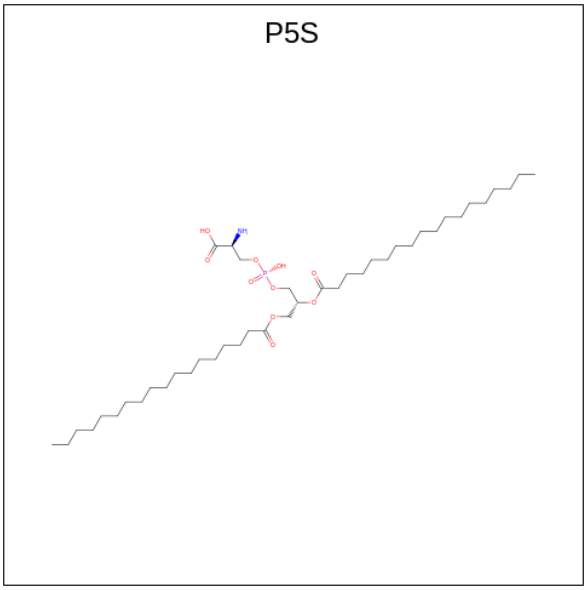
Chain	Residue	Modelled	Actual	Comment	Reference
N	292	TRP	SER	engineered mutation	UNP Q9NV96

- Molecule 3 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: $C_{42}H_{82}NO_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			11	3	1	6	1		
3	C	1	Total	C	N	O	P	0	0
			54	42	1	10	1		
3	E	1	Total	C	N	O	P	0	0
			11	3	1	6	1		
3	E	1	Total	C	N	O	P	0	0
			11	3	1	6	1		
3	I	1	Total	C	N	O	P	0	0
			11	3	1	6	1		
3	I	1	Total	C	N	O	P	0	0
			11	3	1	6	1		
3	M	1	Total	C	N	O	P	0	0
			11	3	1	6	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

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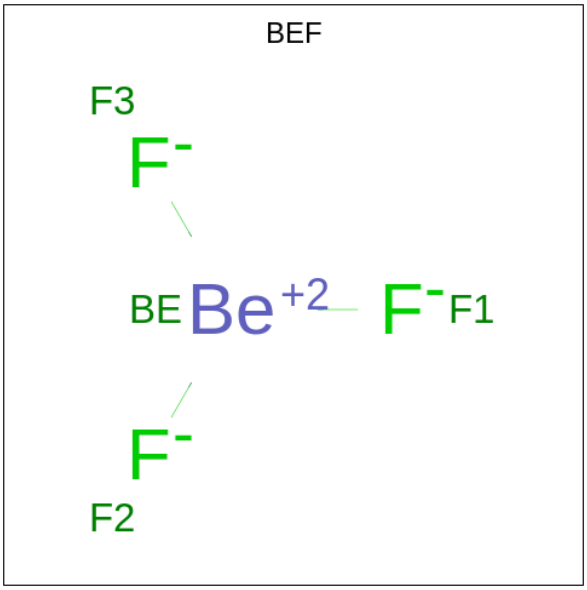
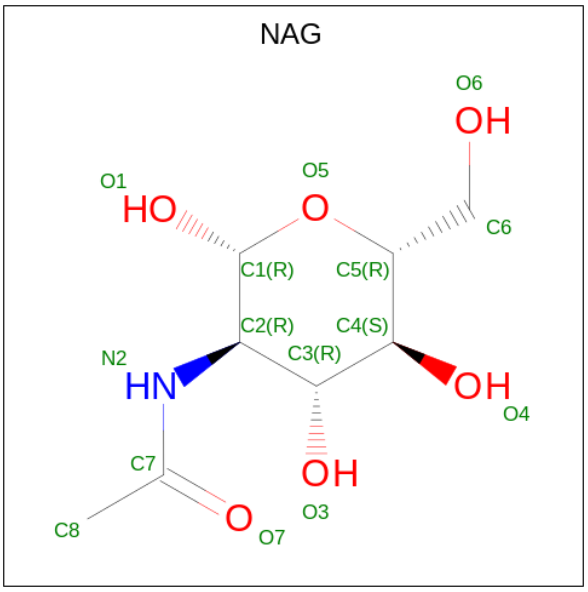
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total Mg 1 1	0	0
4	I	1	Total Mg 1 1	0	0
4	M	1	Total Mg 1 1	0	0

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Be F 4 1 3	0	0
5	E	1	Total Be F 4 1 3	0	0
5	I	1	Total Be F 4 1 3	0	0
5	M	1	Total Be F 4 1 3	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 14 8 1 5	0	0
6	C	1	Total C N O 13 8 1 4	0	0
6	F	1	Total C N O 14 8 1 5	0	0
6	F	1	Total C N O 14 8 1 5	0	0
6	F	1	Total C N O 14 8 1 5	0	0
6	F	1	Total C N O 13 8 1 4	0	0
6	J	1	Total C N O 14 8 1 5	0	0
6	J	1	Total C N O 14 8 1 5	0	0
6	J	1	Total C N O 14 8 1 5	0	0
6	J	1	Total C N O 13 8 1 4	0	0
6	N	1	Total C N O 14 8 1 5	0	0
6	N	1	Total C N O 14 8 1 5	0	0

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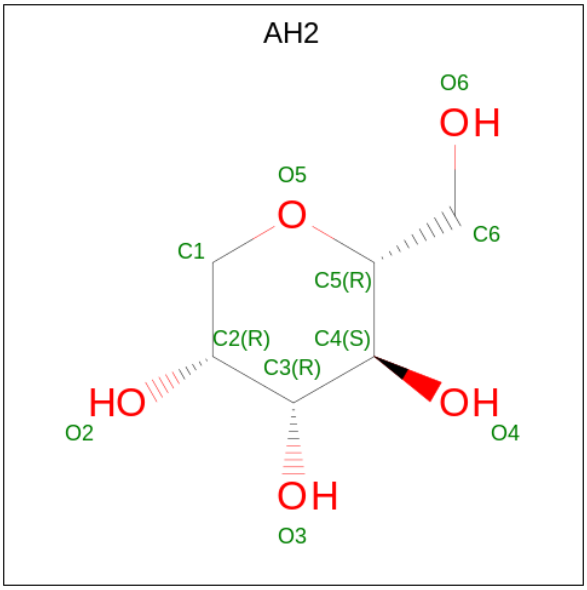
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	N	1	Total C N O 14 8 1 5	0	0
6	N	1	Total C N O 13 8 1 4	0	0

- Molecule 7 is 1-deoxy-alpha-D-mannopyranose (CCD ID: AH2) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 11 6 5	0	0
7	F	1	Total C O 11 6 5	0	0
7	J	1	Total C O 11 6 5	0	0
7	N	1	Total C O 11 6 5	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total O 2 2	0	0
8	E	2	Total O 2 2	0	0
8	I	2	Total O 2 2	0	0

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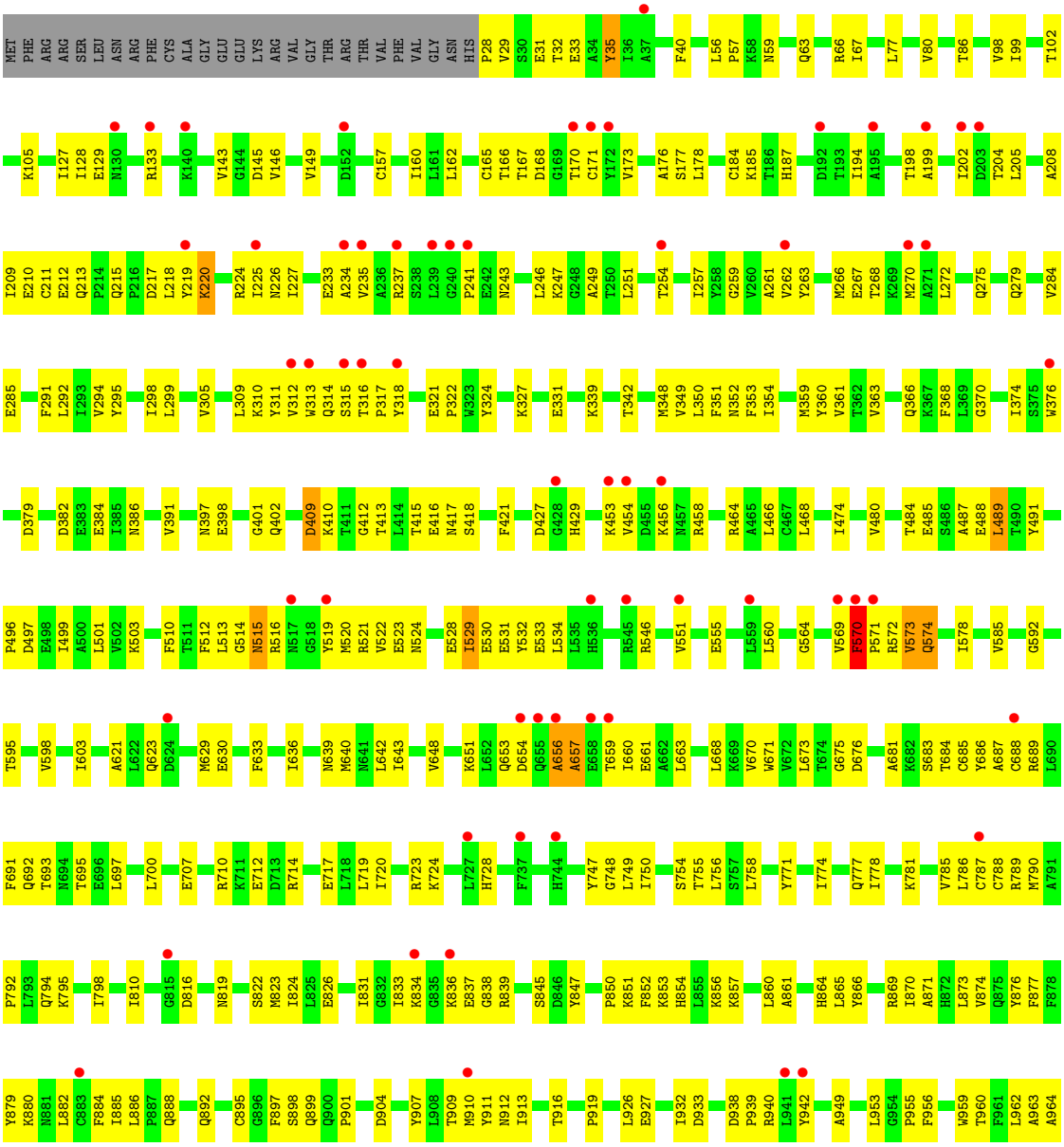
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	2	Total O 2 2	0	0

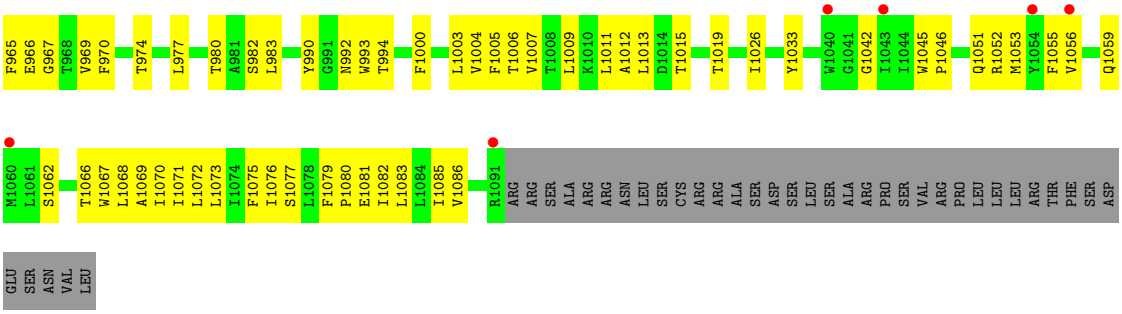
3 Residue-property plots (i)

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: Phospholipid-transporting ATPase IG

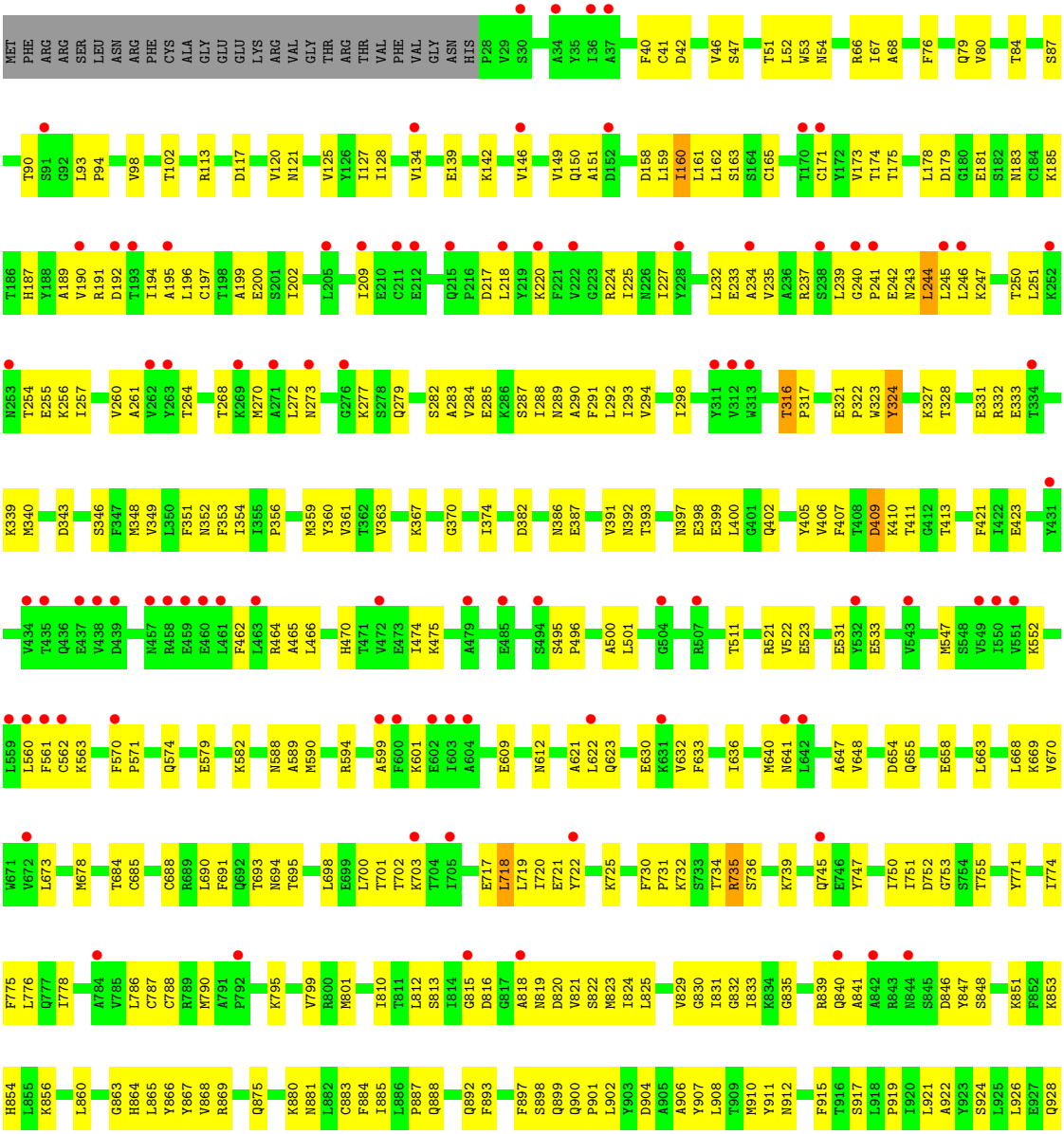
Chain A:

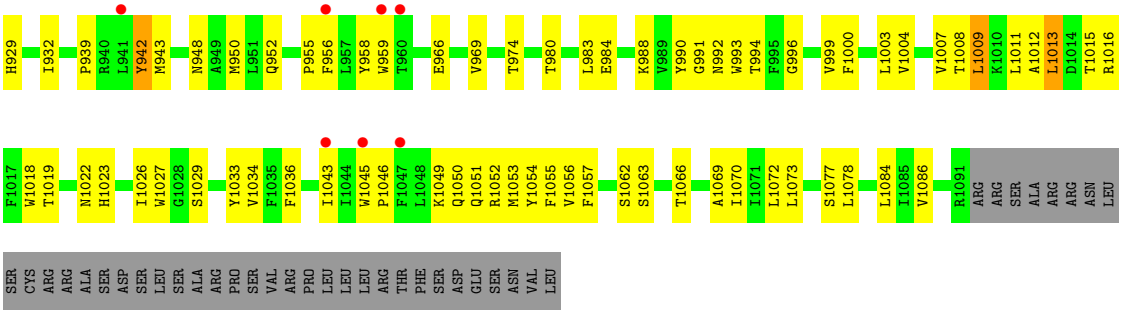




• Molecule 1: Phospholipid-transporting ATPase IG

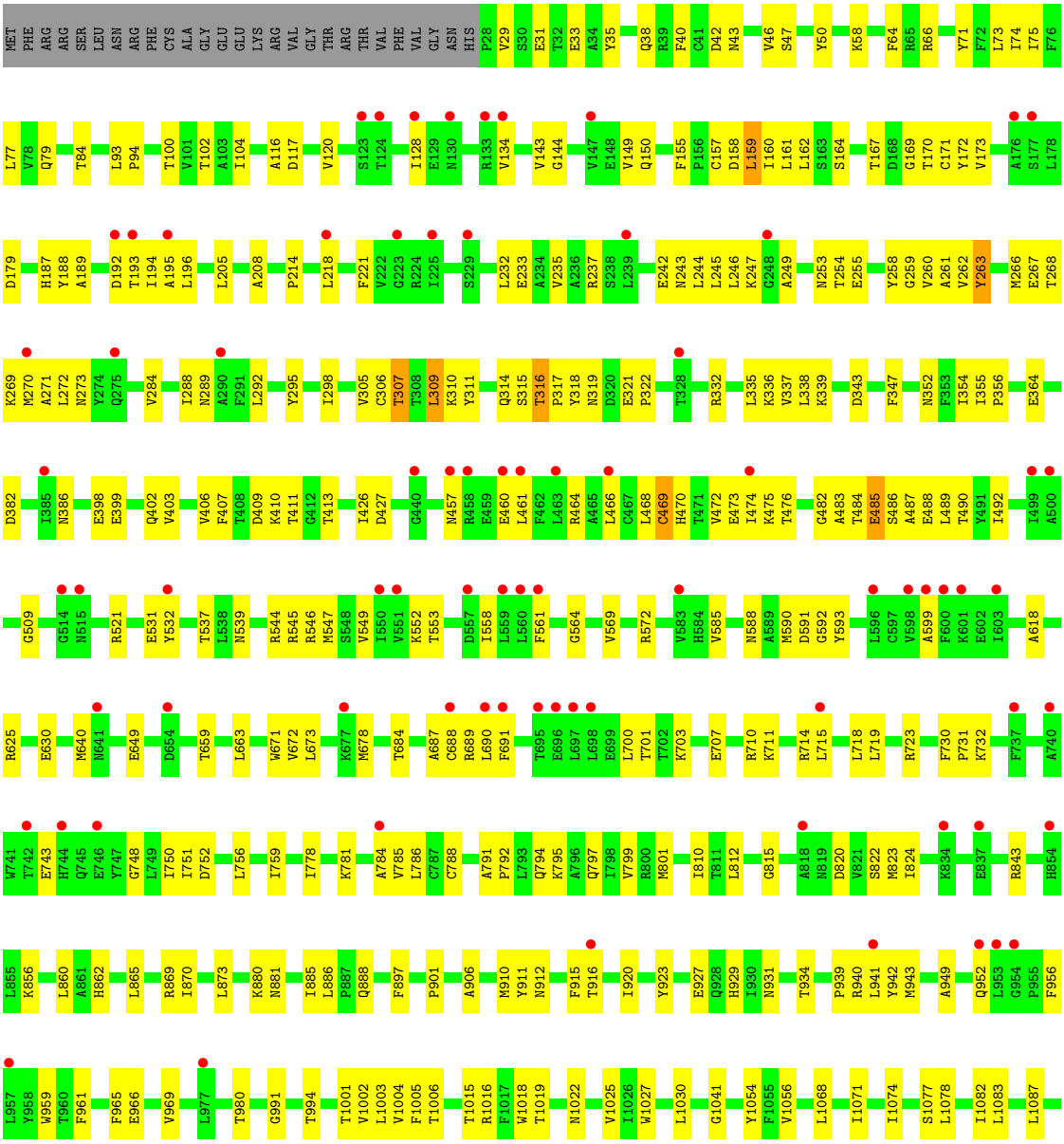
Chain E:



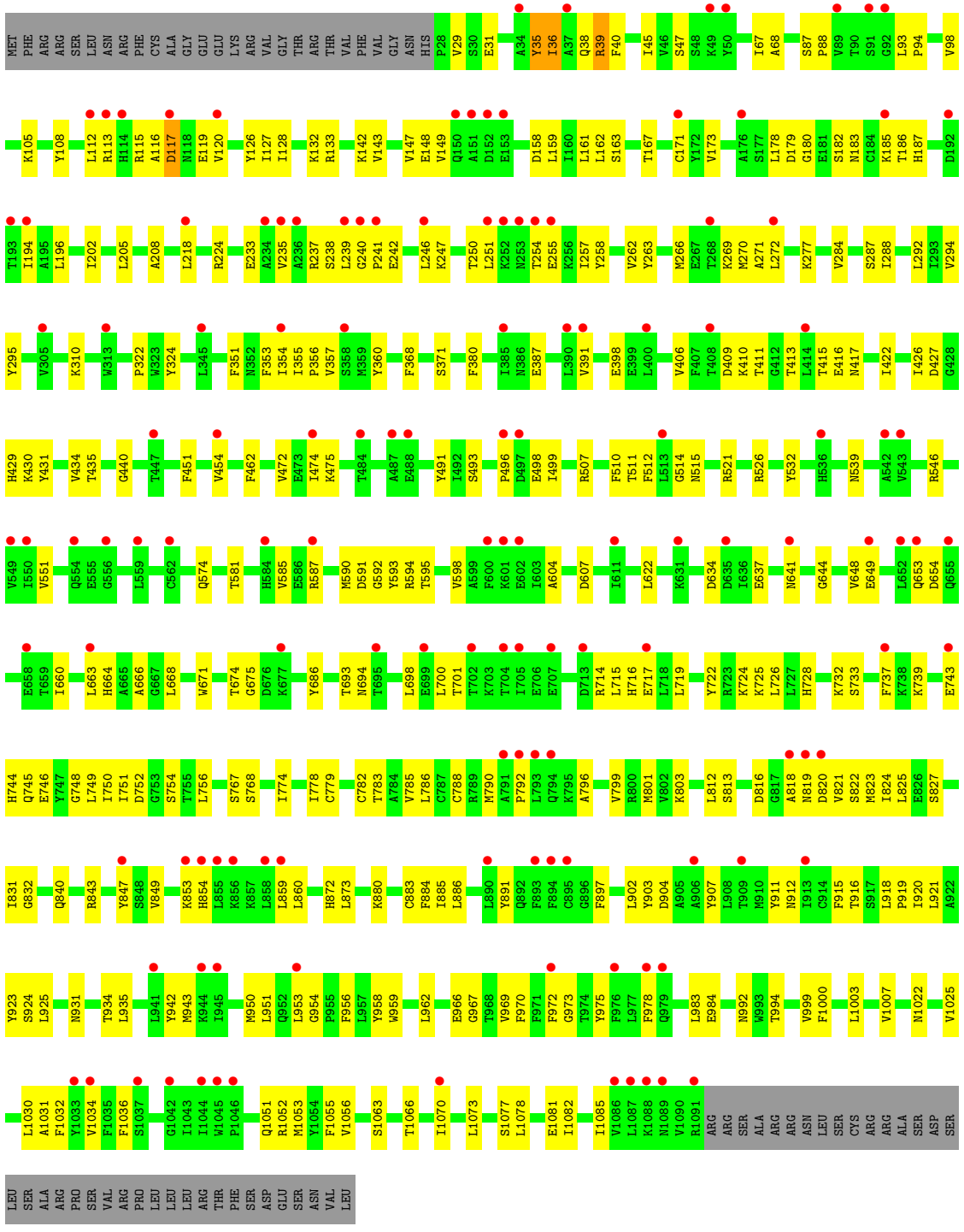


• Molecule 1: Phospholipid-transporting ATPase IG

Chain I:

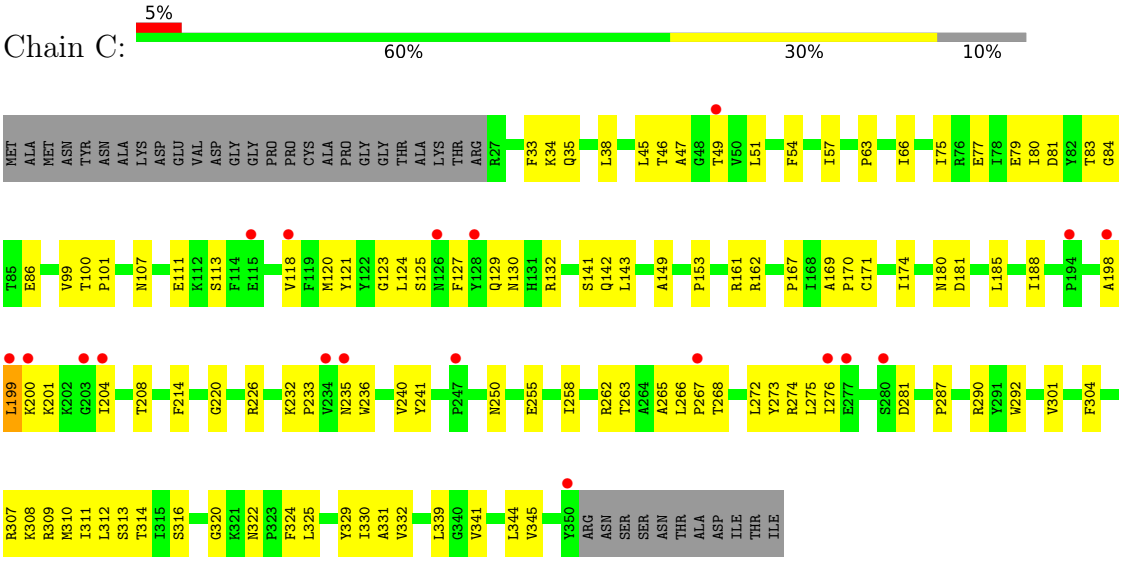


• Molecule 1: Phospholipid-transporting ATPase IG



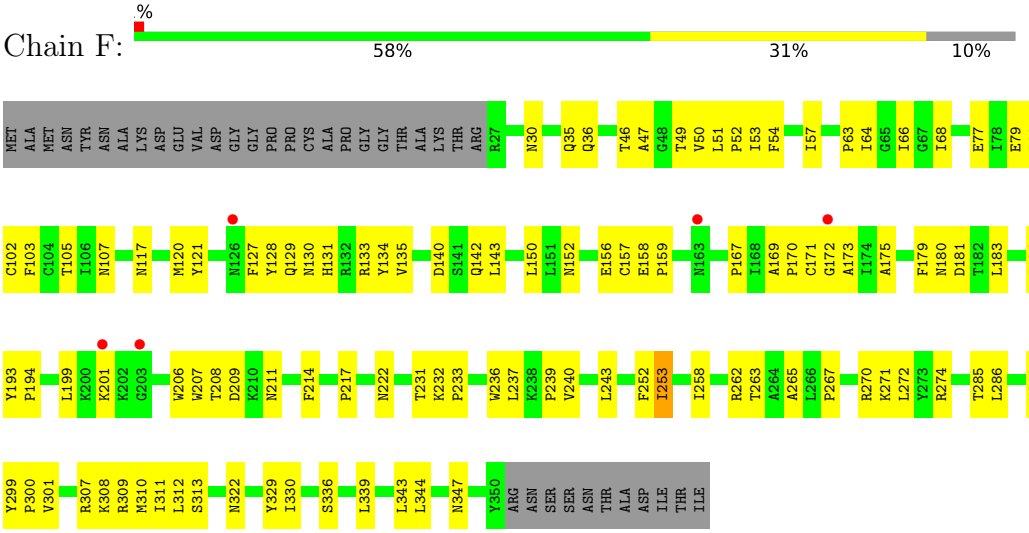
• Molecule 2: Cell cycle control protein 50A

Chain C:



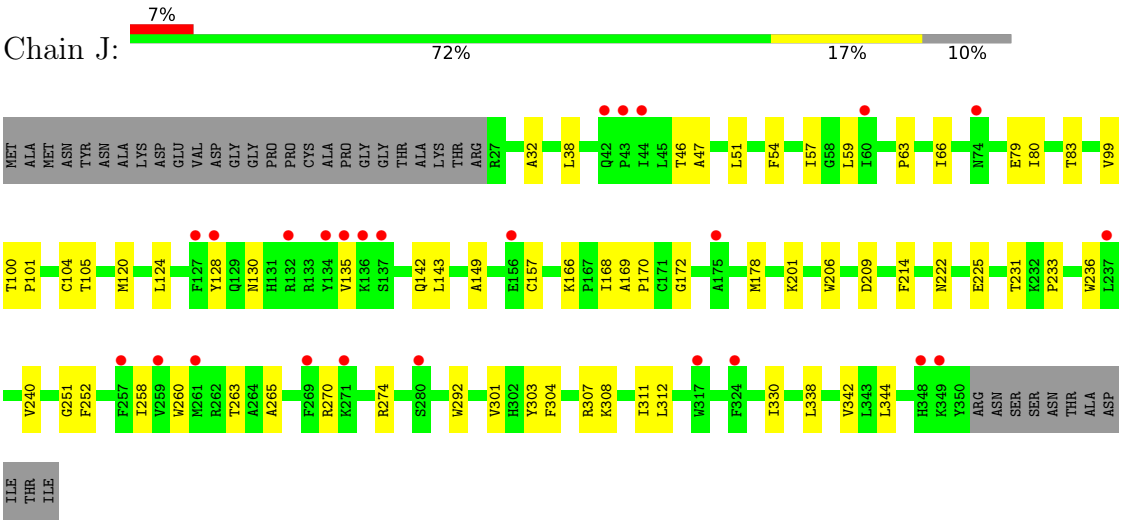
• Molecule 2: Cell cycle control protein 50A

Chain F:



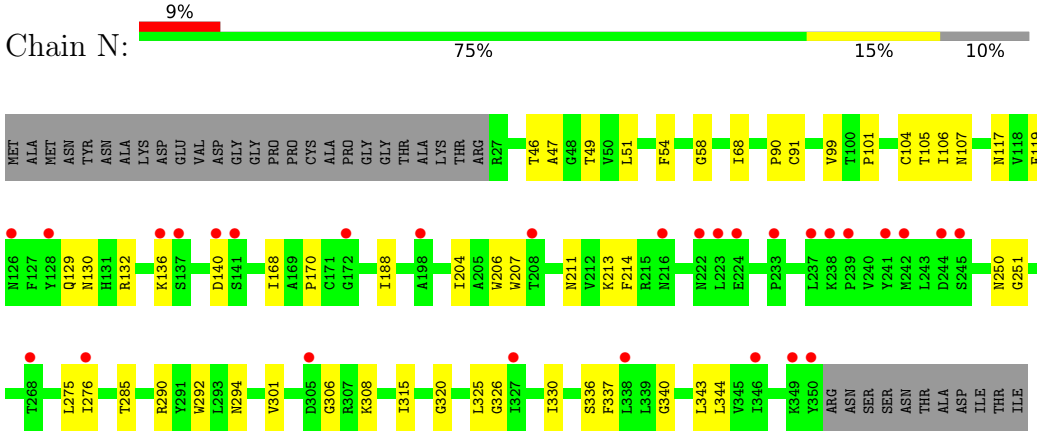
• Molecule 2: Cell cycle control protein 50A

Chain J:



• Molecule 2: Cell cycle control protein 50A

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.46Å 232.83Å 492.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 3.90 49.97 – 3.90	Depositor EDS
% Data completeness (in resolution range)	71.4 (49.97-3.90) 71.3 (49.97-3.90)	Depositor EDS
R_{merge}	1.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.281 , 0.350 0.283 , 0.350	Depositor DCC
R_{free} test set	3779 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å^2)	98.3	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 105.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	45252	wwPDB-VP
Average B, all atoms (Å^2)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG, MG, AH2, P5S, BEF

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	0.32	1/8786 (0.0%)	0.77	14/11897 (0.1%)
1	E	0.31	1/8786 (0.0%)	0.77	6/11897 (0.1%)
1	I	0.27	1/8786 (0.0%)	0.70	5/11897 (0.0%)
1	M	0.25	1/8786 (0.0%)	0.67	4/11897 (0.0%)
2	C	0.27	0/2690	0.71	0/3659
2	F	0.28	0/2690	0.75	3/3659 (0.1%)
2	J	0.20	0/2690	0.57	0/3659
2	N	0.21	0/2690	0.55	0/3659
All	All	0.28	4/45904 (0.0%)	0.71	32/62224 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	409	ASP	CG-OD2	10.69	1.45	1.25
1	I	409	ASP	CG-OD2	10.68	1.45	1.25
1	M	409	ASP	CG-OD2	10.60	1.45	1.25
1	A	409	ASP	CG-OD2	10.38	1.45	1.25

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	512	PHE	N-CA-C	11.28	124.11	110.91
1	I	307	THR	N-CA-C	10.61	122.42	111.07
1	M	454	VAL	N-CA-C	-10.25	102.66	112.29
1	E	195	ALA	N-CA-C	9.89	122.06	111.28
1	A	573	VAL	N-CA-C	7.75	117.86	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8597	0	8588	608	0
1	E	8597	0	8589	441	0
1	I	8597	0	8588	460	0
1	M	8597	0	8589	277	0
2	C	2613	0	2592	108	0
2	F	2613	0	2594	112	0
2	J	2613	0	2592	70	0
2	N	2613	0	2592	88	0
3	A	11	0	5	0	0
3	C	54	0	80	2	0
3	E	22	0	10	1	0
3	I	22	0	10	9	0
3	M	11	0	5	1	0
4	A	1	0	0	0	0
4	E	1	0	0	0	0
4	I	1	0	0	0	0
4	M	1	0	0	0	0
5	A	4	0	0	1	0
5	E	4	0	0	4	0
5	I	4	0	0	0	0
5	M	4	0	0	2	0
6	C	55	0	50	3	0
6	F	55	0	50	24	0
6	J	55	0	50	20	0
6	N	55	0	49	15	0
7	C	11	0	0	0	0
7	F	11	0	0	0	0
7	J	11	0	0	0	0
7	N	11	0	0	0	0
8	A	2	0	0	0	0
8	E	2	0	0	4	0
8	I	2	0	0	1	0
8	M	2	0	0	1	0
All	All	45252	0	45033	2106	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 23.

The worst 5 of 2106 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:I:678:MET:HE1	1:I:700:LEU:CD1	1.21	1.65
1:I:214:PRO:HB3	1:I:268:THR:CG2	1.23	1.60
1:I:678:MET:CE	1:I:700:LEU:HD13	1.27	1.60
1:A:28:PRO:CD	1:A:212:GLU:HA	1.15	1.58
1:A:519:TYR:HD2	1:A:532:TYR:CB	0.97	1.58

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	1062/1129 (94%)	918 (86%)	143 (14%)	1 (0%)	48 80
1	E	1062/1129 (94%)	876 (82%)	186 (18%)	0	100 100
1	I	1062/1129 (94%)	879 (83%)	182 (17%)	1 (0%)	48 80
1	M	1062/1129 (94%)	886 (83%)	176 (17%)	0	100 100
2	C	322/361 (89%)	266 (83%)	56 (17%)	0	100 100
2	F	322/361 (89%)	275 (85%)	47 (15%)	0	100 100
2	J	322/361 (89%)	281 (87%)	41 (13%)	0	100 100
2	N	322/361 (89%)	297 (92%)	25 (8%)	0	100 100
All	All	5536/5960 (93%)	4678 (84%)	856 (16%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	316	THR
1	A	570	PHE

5.3.2 Protein sidechains (i)

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	947/1005 (94%)	940 (99%)	7 (1%)	76 78
1	E	947/1005 (94%)	940 (99%)	7 (1%)	76 78
1	I	947/1005 (94%)	944 (100%)	3 (0%)	86 85
1	M	947/1005 (94%)	943 (100%)	4 (0%)	84 83
2	C	288/316 (91%)	287 (100%)	1 (0%)	86 85
2	F	288/316 (91%)	288 (100%)	0	100 100
2	J	288/316 (91%)	288 (100%)	0	100 100
2	N	288/316 (91%)	288 (100%)	0	100 100
All	All	4940/5284 (94%)	4918 (100%)	22 (0%)	84 83

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1013	LEU
1	I	485	GLU
1	I	469	CYS
1	M	35	TYR
1	A	574	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	254	ASN
2	N	235	ASN
1	I	429	HIS
2	N	216	ASN
1	M	694	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 35 ligands modelled in this entry, 4 are monoatomic - leaving 31 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	$\#\|Z\| > 2$
6	NAG	J	404	-	14,14,15	0.38	0	17,19,21	0.72	1 (5%)
6	NAG	N	405	-	13,13,15	0.35	0	14,17,21	0.53	0
3	P5S	E	1201	-	9,10,53	0.92	0	12,14,60	1.09	1 (8%)
3	P5S	M	1201	-	9,10,53	0.91	0	12,14,60	1.28	3 (25%)
3	P5S	A	1201	-	9,10,53	0.93	0	12,14,60	1.18	1 (8%)
6	NAG	C	405	-	14,14,15	0.63	1 (7%)	17,19,21	0.82	1 (5%)
5	BEF	A	1203	1	0,3,3	-	-	-		
6	NAG	C	406	-	13,13,15	0.49	0	14,17,21	0.52	0
6	NAG	N	402	-	14,14,15	0.22	0	17,19,21	0.42	0
3	P5S	I	1201	-	9,10,53	0.91	0	12,14,60	1.44	3 (25%)
7	AH2	J	403	-	11,11,11	0.83	0	15,15,15	1.28	1 (6%)
7	AH2	N	403	-	11,11,11	0.81	0	15,15,15	1.39	3 (20%)
3	P5S	I	1202	-	9,10,53	0.92	0	12,14,60	1.12	0
6	NAG	N	404	-	14,14,15	0.29	0	17,19,21	0.65	1 (5%)
3	P5S	C	401	-	52,53,53	0.98	2 (3%)	56,60,60	1.09	2 (3%)
5	BEF	E	1204	1	0,3,3	-	-	-		
6	NAG	C	402	-	14,14,15	1.24	1 (7%)	17,19,21	0.63	0
6	NAG	F	405	-	13,13,15	0.34	0	14,17,21	0.59	0
6	NAG	F	401	-	14,14,15	1.12	1 (7%)	17,19,21	1.00	2 (11%)
6	NAG	F	402	-	14,14,15	0.51	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	J	402	-	14,14,15	0.21	0	17,19,21	0.37	0
7	AH2	F	403	-	11,11,11	0.99	0	15,15,15	1.14	1 (6%)
6	NAG	N	401	-	14,14,15	0.40	0	17,19,21	0.38	0
5	BEF	M	1203	1	0,3,3	-	-	-		
7	AH2	C	404	-	11,11,11	0.72	0	15,15,15	1.16	1 (6%)
6	NAG	F	404	-	14,14,15	0.25	0	17,19,21	0.61	1 (5%)
6	NAG	J	401	-	14,14,15	0.18	0	17,19,21	0.49	0
6	NAG	C	403	-	14,14,15	0.56	0	17,19,21	0.97	2 (11%)
3	P5S	E	1202	-	9,10,53	0.92	0	12,14,60	1.35	2 (16%)
6	NAG	J	405	-	13,13,15	0.56	0	14,17,21	0.71	0
5	BEF	I	1204	1	0,3,3	-	-	-		

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
6	NAG	J	404	-	-	2/6/23/26	0/1/1/1
6	NAG	N	405	-	-	1/6/19/26	0/1/1/1
3	P5S	E	1201	-	-	9/10/10/59	-
3	P5S	M	1201	-	-	4/10/10/59	-
3	P5S	A	1201	-	-	3/10/10/59	-
6	NAG	C	405	-	-	1/6/23/26	0/1/1/1
6	NAG	C	406	-	-	2/6/19/26	0/1/1/1
6	NAG	N	402	-	-	0/6/23/26	0/1/1/1
3	P5S	I	1201	-	-	5/10/10/59	-
7	AH2	J	403	-	-	2/2/19/19	1/1/1/1
7	AH2	N	403	-	-	1/2/19/19	1/1/1/1
3	P5S	I	1202	-	-	2/10/10/59	-
6	NAG	N	404	-	-	2/6/23/26	0/1/1/1
3	P5S	C	401	-	-	19/59/59/59	-
6	NAG	C	402	-	-	4/6/23/26	0/1/1/1
6	NAG	F	405	-	-	3/6/19/26	1/1/1/1
6	NAG	F	401	-	-	4/6/23/26	0/1/1/1
6	NAG	F	402	-	-	1/6/23/26	0/1/1/1
6	NAG	J	402	-	-	1/6/23/26	0/1/1/1
7	AH2	F	403	-	-	1/2/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	N	401	-	-	2/6/23/26	0/1/1/1
7	AH2	C	404	-	-	1/2/19/19	1/1/1/1
6	NAG	F	404	-	-	1/6/23/26	0/1/1/1
6	NAG	J	401	-	-	3/6/23/26	0/1/1/1
6	NAG	C	403	-	-	2/6/23/26	0/1/1/1
3	P5S	E	1202	-	-	3/10/10/59	-
6	NAG	J	405	-	-	3/6/19/26	1/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	P5S	O37-C38	4.53	1.47	1.34
3	C	401	P5S	O19-C17	4.43	1.46	1.33
6	C	402	NAG	O5-C1	-4.43	1.36	1.43
6	F	401	NAG	O5-C1	-3.72	1.37	1.43
6	C	405	NAG	O5-C1	2.07	1.47	1.43

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	P5S	O37-C38-C39	4.42	121.02	111.50
7	J	403	AH2	C1-O5-C5	3.87	117.44	112.19
7	N	403	AH2	C1-O5-C5	3.75	117.27	112.19
7	C	404	AH2	C1-O5-C5	3.38	116.78	112.19
3	I	1201	P5S	OG-CB-CA	3.25	110.89	108.06

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1201	P5S	C-CA-CB-OG
3	A	1201	P5S	N-CA-CB-OG
3	C	401	P5S	O-C-CA-N
3	C	401	P5S	N-CA-CB-OG
3	C	401	P5S	C39-C38-O37-C2

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	405	NAG	C1-C2-C3-C4-C5-O5

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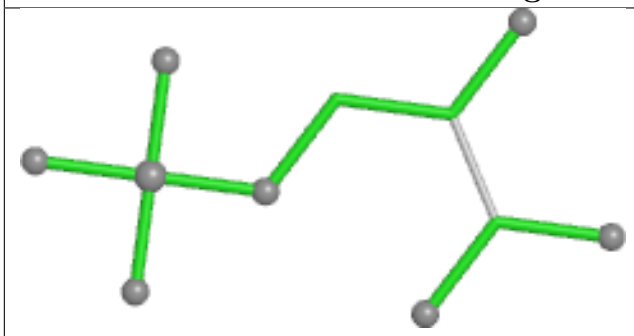
Mol	Chain	Res	Type	Atoms
7	N	403	AH2	C1-C2-C3-C4-C5-O5
7	J	403	AH2	C1-C2-C3-C4-C5-O5
7	C	404	AH2	C1-C2-C3-C4-C5-O5
6	J	405	NAG	C1-C2-C3-C4-C5-O5

15 monomers are involved in 82 short contacts:

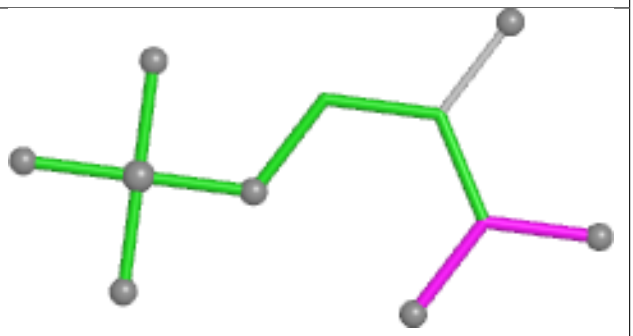
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	404	NAG	13	0
6	N	405	NAG	15	0
3	M	1201	P5S	1	0
5	A	1203	BEF	1	0
6	C	406	NAG	1	0
3	I	1201	P5S	9	0
3	C	401	P5S	2	0
5	E	1204	BEF	4	0
6	C	402	NAG	2	0
6	F	405	NAG	19	0
6	F	401	NAG	1	0
5	M	1203	BEF	2	0
6	F	404	NAG	4	0
3	E	1202	P5S	1	0
6	J	405	NAG	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

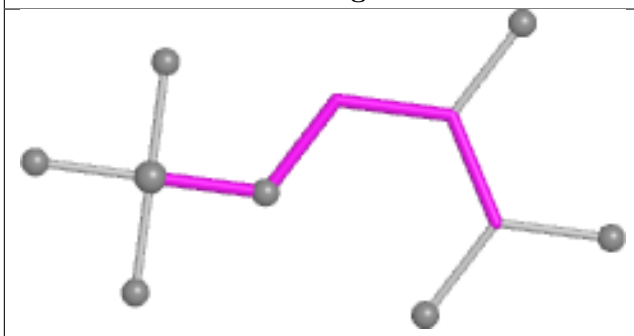
Ligand P5S E 1201



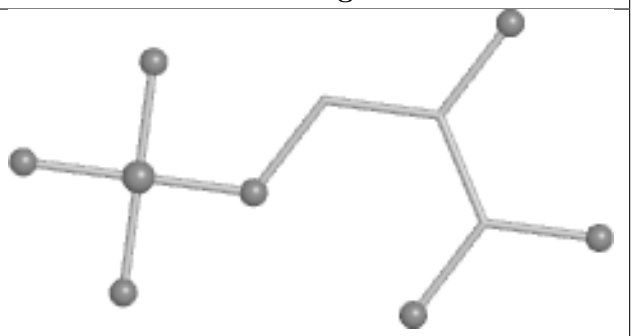
Bond lengths



Bond angles

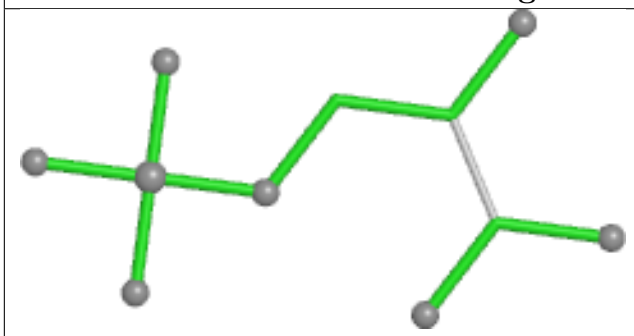


Torsions



Rings

Ligand P5S M 1201



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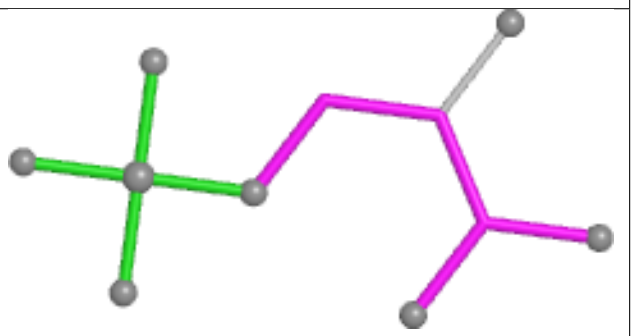

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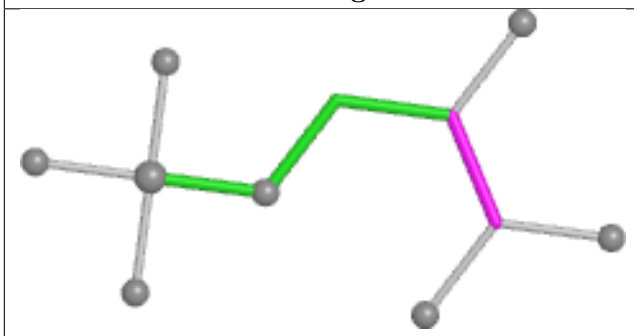

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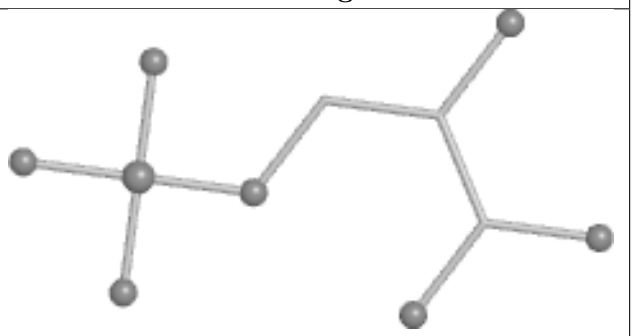

Rings

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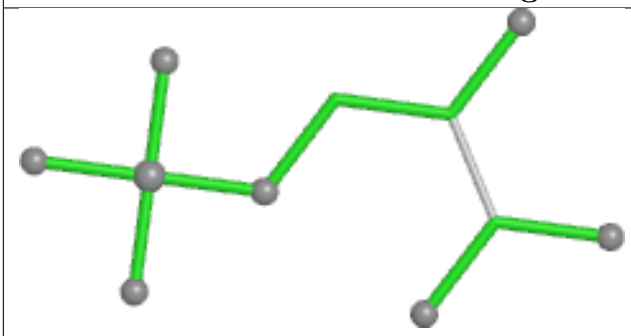

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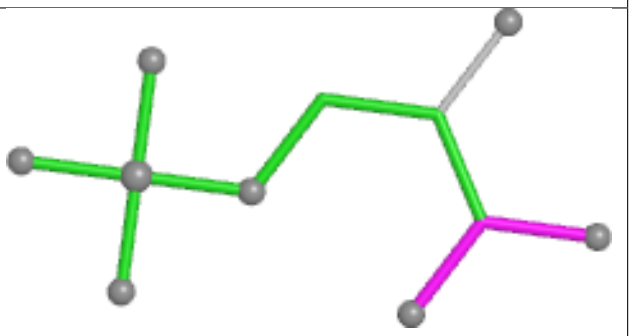

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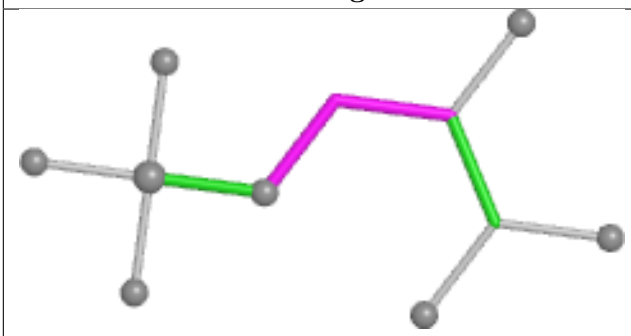

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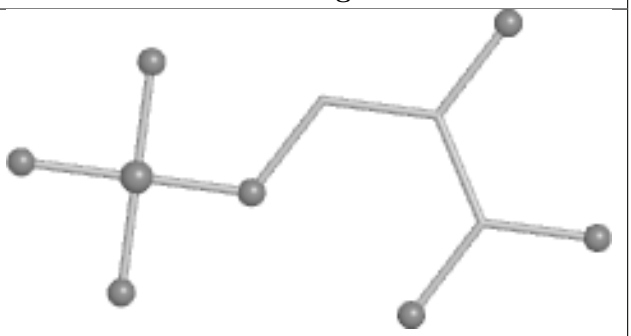

Rings

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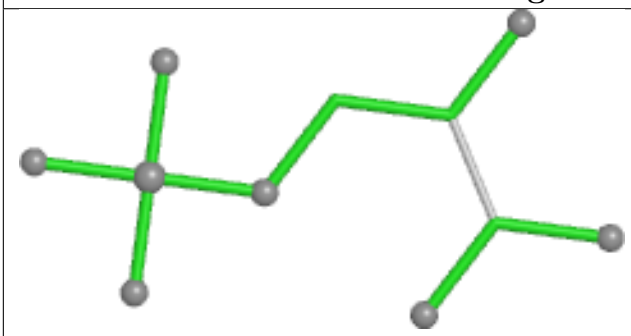

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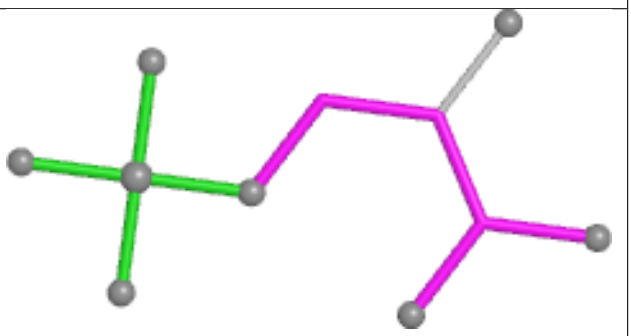
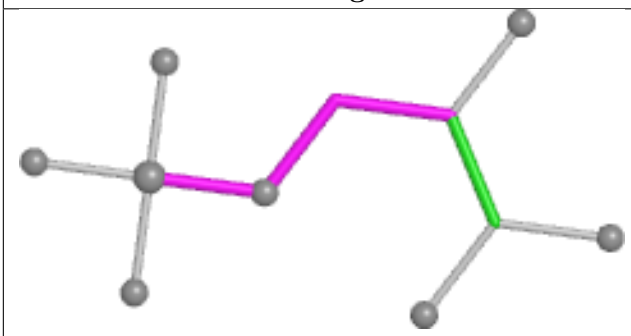


Bond angles



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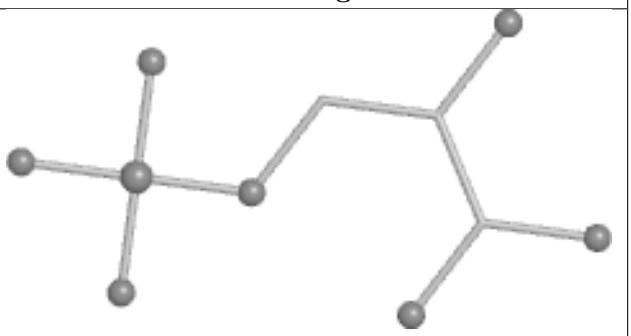
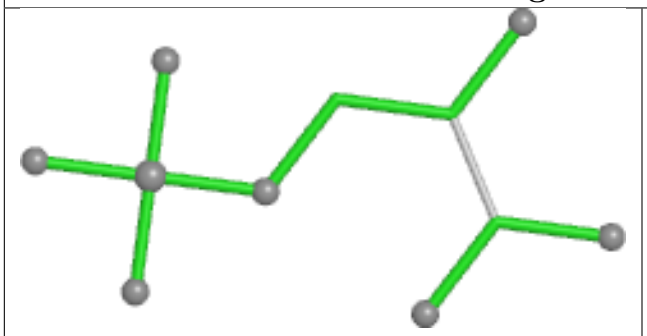
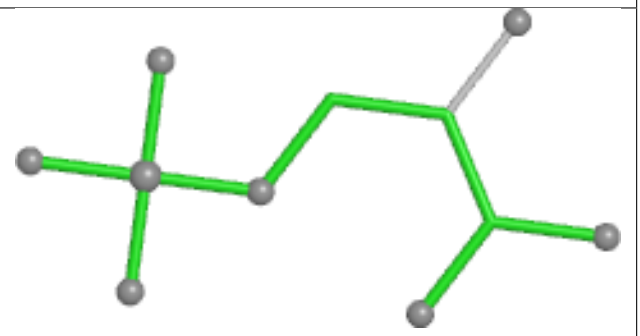


Rings

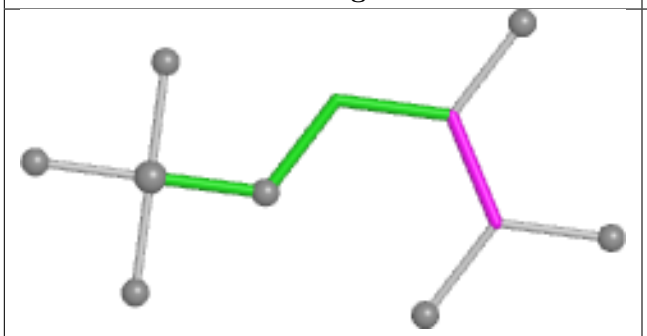
Ligand P5S I 1202



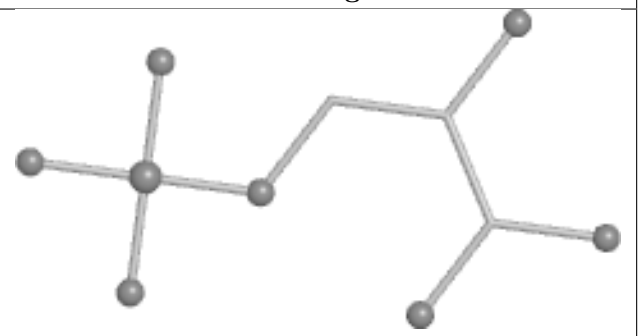
Bond lengths



Bond angles

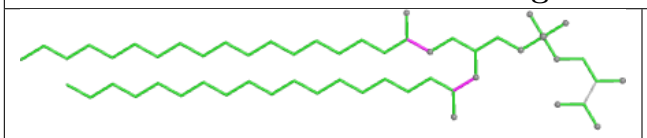


Torsions

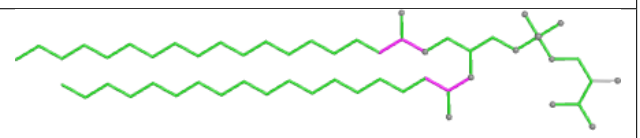


Rings

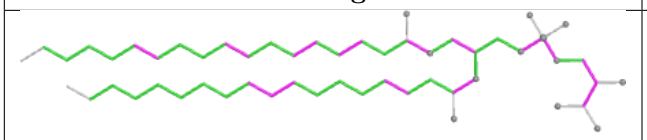
Ligand P5S C 401



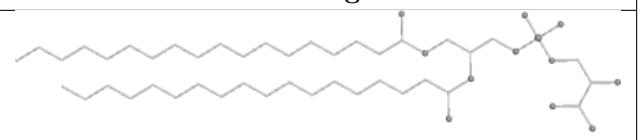
Bond lengths



Bond angles

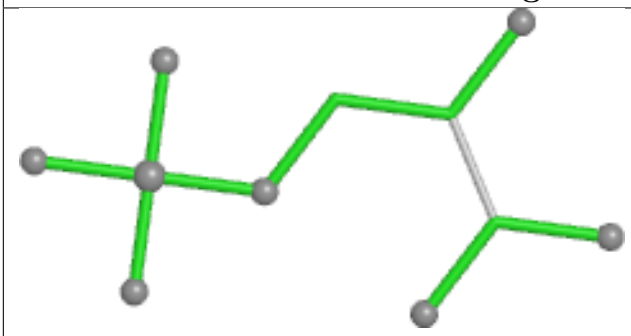


Torsions

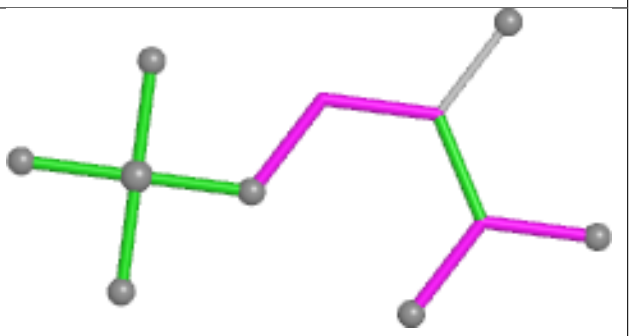


Rings

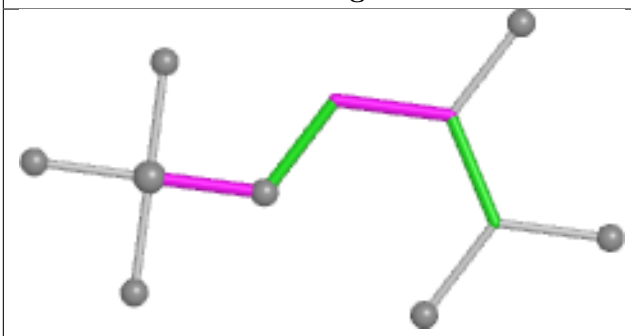
Ligand P5S E 1202



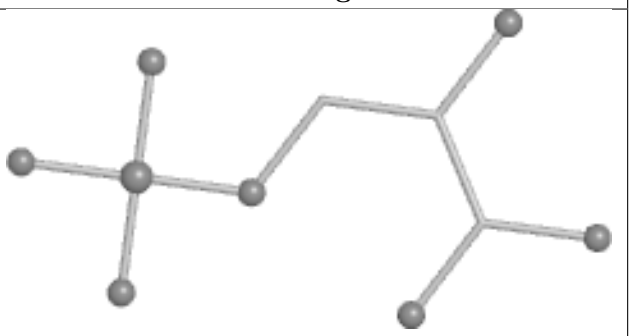
Bond lengths



Bond angles



Torsions



Rings

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^{th} 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	1064/1129 (94%)	0.49	68 (6%)	25	22	24, 120, 194, 235	0
1	E	1064/1129 (94%)	0.61	97 (9%)	15	16	31, 115, 211, 246	0
1	I	1064/1129 (94%)	0.63	77 (7%)	21	20	96, 173, 226, 261	0
1	M	1064/1129 (94%)	0.90	134 (12%)	8	11	124, 214, 315, 367	0
2	C	324/361 (89%)	0.27	19 (5%)	28	24	21, 79, 153, 183	0
2	F	324/361 (89%)	0.05	5 (1%)	72	50	25, 71, 136, 166	0
2	J	324/361 (89%)	0.67	25 (7%)	19	18	118, 189, 255, 281	0
2	N	324/361 (89%)	0.81	31 (9%)	13	16	204, 340, 392, 416	0
All	All	5552/5960 (93%)	0.61	456 (8%)	17	18	21, 164, 320, 416	0

The worst 5 of 456 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	560	LEU	13.6
1	E	551	VAL	11.6
1	E	550	ILE	10.6
1	A	192	ASP	9.4
1	E	460	GLU	8.9

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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, 95^{th} 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.

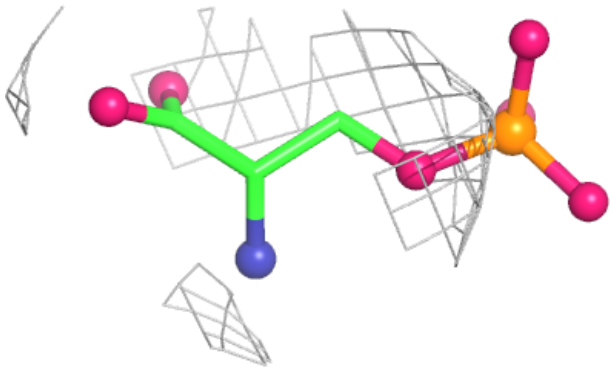
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	AH2	N	403	11/11	-0.10	0.21	347,350,356,359	0
7	AH2	J	403	11/11	0.38	0.10	155,161,168,172	0
3	P5S	M	1201	11/54	0.45	0.12	293,299,310,312	0
6	NAG	N	404	14/15	0.46	0.14	398,409,413,415	0
6	NAG	J	405	13/15	0.47	0.16	255,269,274,276	0
7	AH2	F	403	11/11	0.50	0.14	143,165,168,170	0
7	AH2	C	404	11/11	0.57	0.13	117,126,144,145	0
6	NAG	N	405	13/15	0.61	0.12	356,362,366,367	0
6	NAG	N	402	14/15	0.62	0.11	309,312,317,319	0
6	NAG	N	401	14/15	0.66	0.12	335,342,344,344	0
6	NAG	J	404	14/15	0.67	0.12	238,242,246,249	0
3	P5S	I	1202	11/54	0.75	0.18	151,162,189,189	0
3	P5S	I	1201	11/54	0.75	0.09	220,231,238,239	0
5	BEF	I	1204	4/4	0.76	0.12	148,152,155,162	0
3	P5S	C	401	54/54	0.77	0.21	92,120,135,141	0
6	NAG	J	401	14/15	0.79	0.13	145,176,183,185	0
6	NAG	J	402	14/15	0.79	0.10	156,172,186,190	0
6	NAG	F	405	13/15	0.80	0.15	125,133,149,153	0
3	P5S	E	1202	11/54	0.81	0.18	78,97,159,160	0
5	BEF	M	1203	4/4	0.82	0.13	232,233,238,250	0
4	MG	E	1203	1/1	0.82	0.17	91,91,91,91	0
6	NAG	C	405	14/15	0.89	0.11	99,111,127,137	0
3	P5S	A	1201	11/54	0.89	0.13	107,117,167,172	0
6	NAG	F	401	14/15	0.90	0.14	66,80,102,109	0
6	NAG	F	404	14/15	0.90	0.11	61,100,139,145	0
6	NAG	C	406	13/15	0.90	0.10	70,93,122,127	0
6	NAG	C	402	14/15	0.91	0.14	41,71,97,98	0
5	BEF	A	1203	4/4	0.92	0.11	78,83,84,109	0
6	NAG	F	402	14/15	0.92	0.09	45,82,110,113	0
4	MG	A	1202	1/1	0.93	0.11	172,172,172,172	0
6	NAG	C	403	14/15	0.93	0.10	75,107,121,124	0
3	P5S	E	1201	11/54	0.97	0.07	70,85,102,110	0
5	BEF	E	1204	4/4	0.97	0.08	74,78,80,87	0
4	MG	I	1203	1/1	0.97	0.06	139,139,139,139	0
4	MG	M	1202	1/1	0.98	0.17	185,185,185,185	0

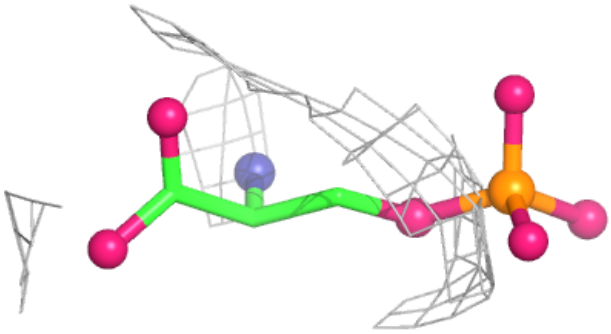
The following is a graphical depiction of the model fit to experimental electron density of all

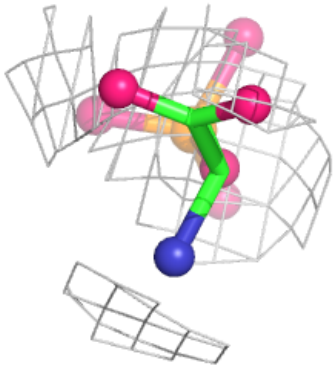
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around P5S M 1201:

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

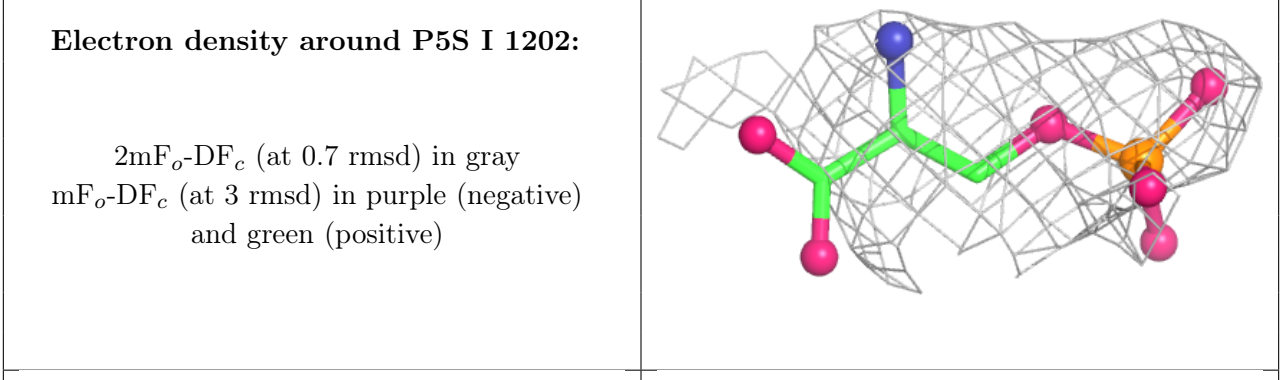






Electron density around P5S I 1202:

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



Electron density around P5S I 1201:

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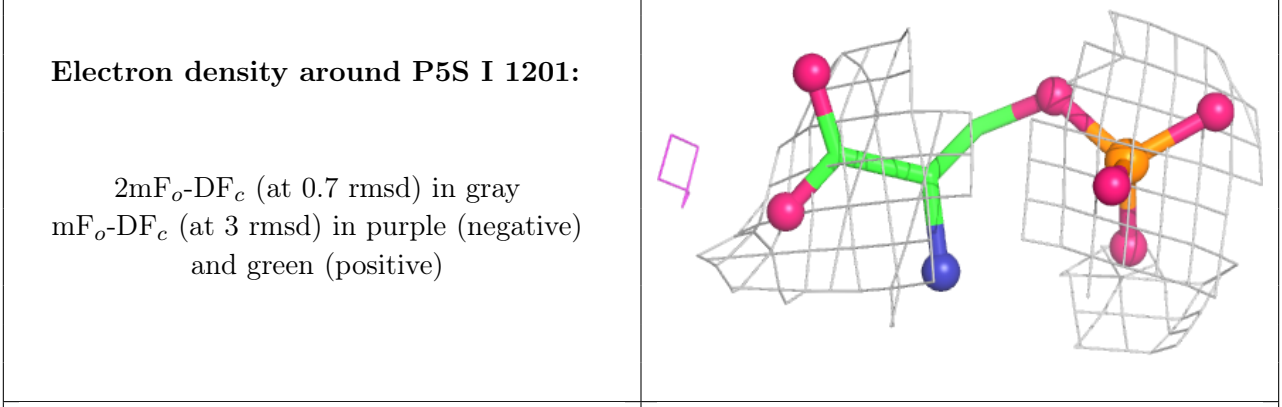
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around P5S C 401:

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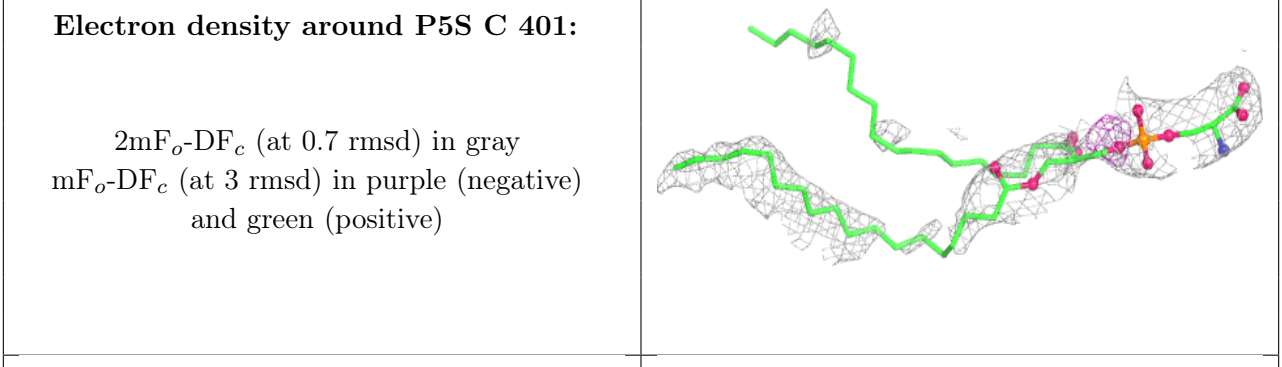
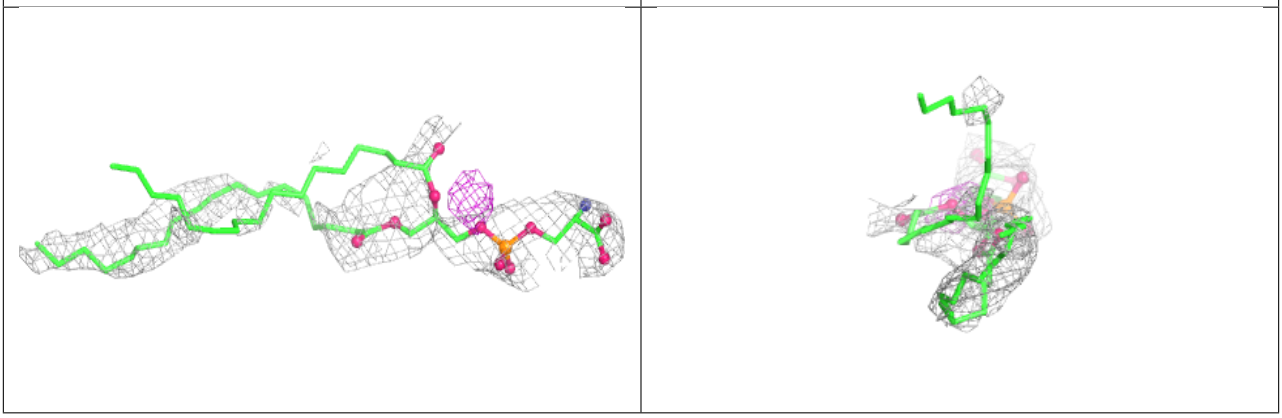
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around P5S E 1202:

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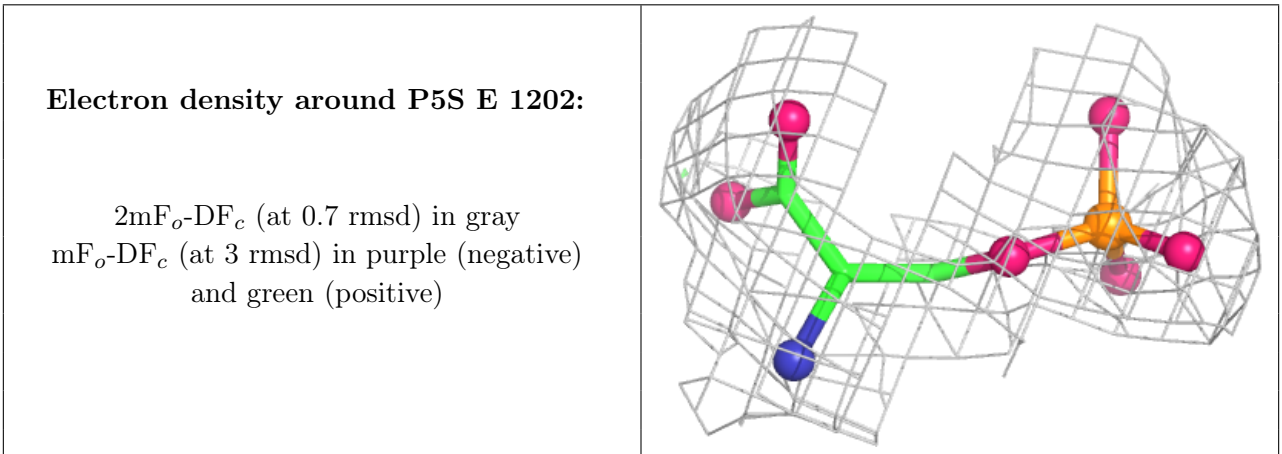
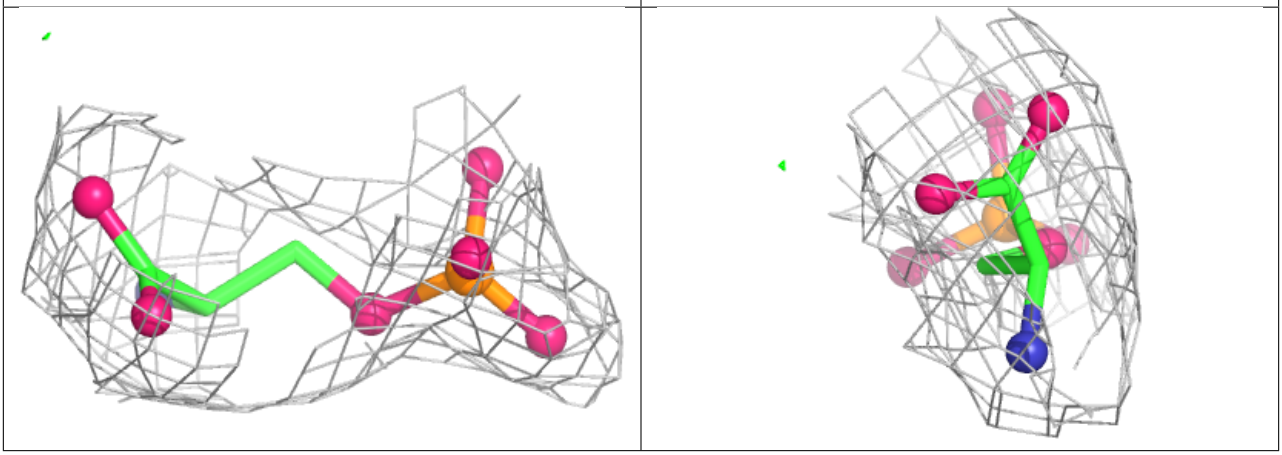
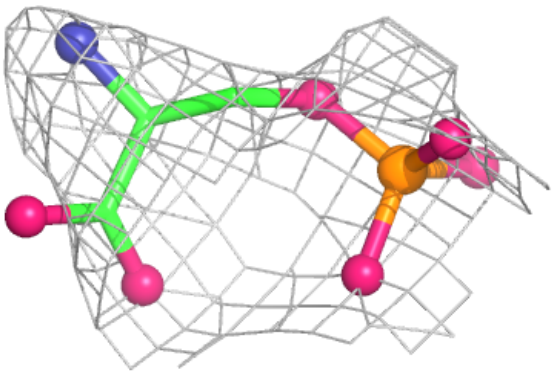
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

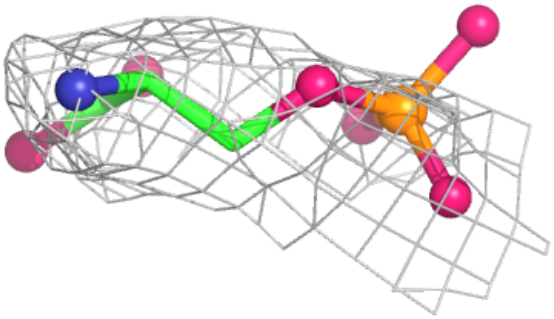


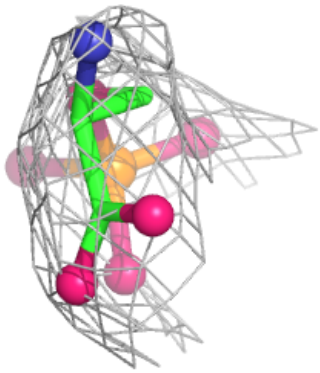


Electron density around P5S A 1201:

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







Electron density around P5S E 1201:

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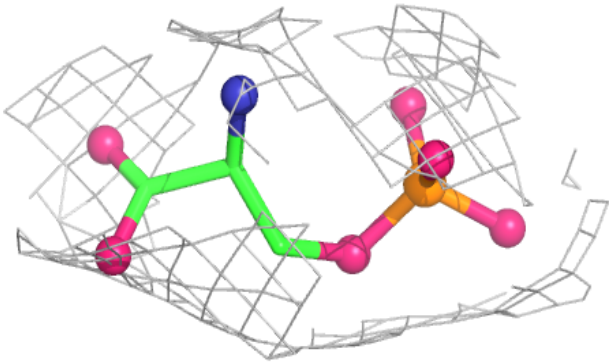
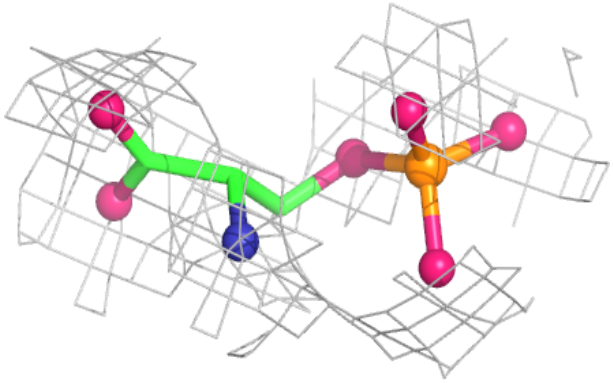
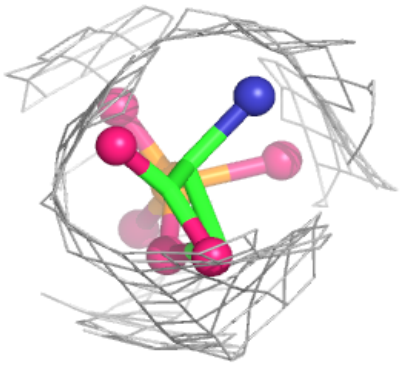
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.