



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 04:34 PM BST

PDB ID : 5G1N  
Title : Aspartate transcarbamoylase domain of human CAD bound to PALA  
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Deposited on : 2016-03-29  
Resolution : 2.10 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
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

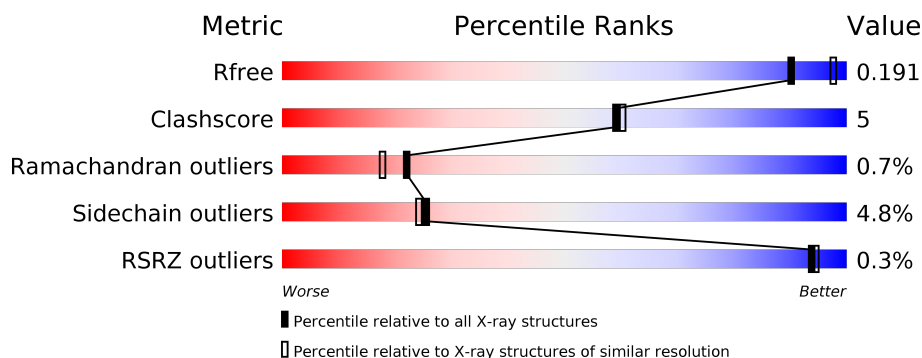
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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>82%</div> <div>13%</div> <div>• •</div> </div>
1	B	314	<div> <div>%</div> <div>85%</div> <div>12%</div> <div>• •</div> </div>
1	C	314	<div> <div>81%</div> <div>16%</div> <div>• •</div> </div>
1	D	314	<div> <div>83%</div> <div>14%</div> <div>• •</div> </div>
1	E	314	<div> <div>81%</div> <div>15%</div> <div>• •</div> </div>
1	F	314	<div> <div>84%</div> <div>12%</div> <div>• •</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14721 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 CAD PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2366	1488	419	438	21			
1	B	306	Total	C	N	O	S	0	0	0
			2365	1487	420	437	21			
1	C	306	Total	C	N	O	S	0	0	0
			2359	1485	420	433	21			
1	D	306	Total	C	N	O	S	0	0	0
			2365	1487	420	437	21			
1	E	307	Total	C	N	O	S	0	0	0
			2329	1468	411	429	21			
1	F	306	Total	C	N	O	S	0	0	0
			2350	1479	415	435	21			

There are 18 discrepancies between the modelled and reference sequences:

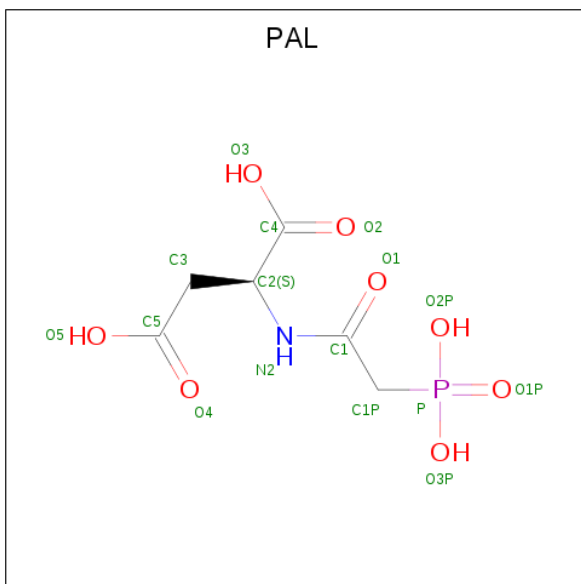
Chain	Residue	Modelled	Actual	Comment	Reference
A	1912	GLY	-	expression tag	UNP P27708
A	1913	PRO	-	expression tag	UNP P27708
A	1914	MET	-	expression tag	UNP P27708
B	1912	GLY	-	expression tag	UNP P27708
B	1913	PRO	-	expression tag	UNP P27708
B	1914	MET	-	expression tag	UNP P27708
C	1912	GLY	-	expression tag	UNP P27708
C	1913	PRO	-	expression tag	UNP P27708
C	1914	MET	-	expression tag	UNP P27708
D	1912	GLY	-	expression tag	UNP P27708
D	1913	PRO	-	expression tag	UNP P27708
D	1914	MET	-	expression tag	UNP P27708
E	1912	GLY	-	expression tag	UNP P27708
E	1913	PRO	-	expression tag	UNP P27708
E	1914	MET	-	expression tag	UNP P27708
F	1912	GLY	-	expression tag	UNP P27708
F	1913	PRO	-	expression tag	UNP P27708

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1914	MET	-	expression tag	UNP P27708

- Molecule 2 is N-(PHOSPHONACETYL)-L-ASPARTIC ACID (three-letter code: PAL) (formula:  $C_6H_{10}NO_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
2	B	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
2	C	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
2	D	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
2	E	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
2	F	1	Total	C	N	O	P	0	0
			16	6	1	8	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

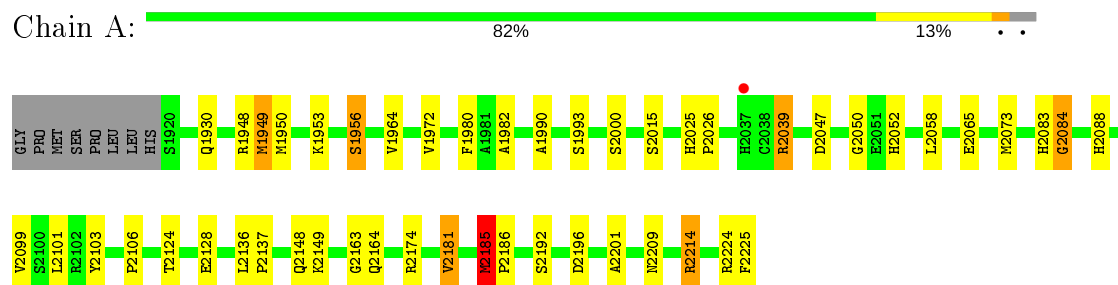
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		
4	B	86	Total	O	0	0
			86	86		
4	C	68	Total	O	0	0
			68	68		
4	D	98	Total	O	0	0
			98	98		
4	E	92	Total	O	0	0
			92	92		
4	F	67	Total	O	0	0
			67	67		

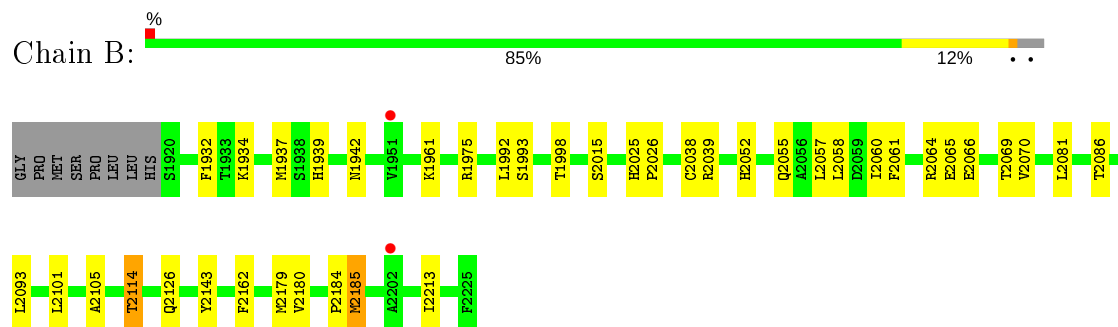
### 3 Residue-property plots

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.

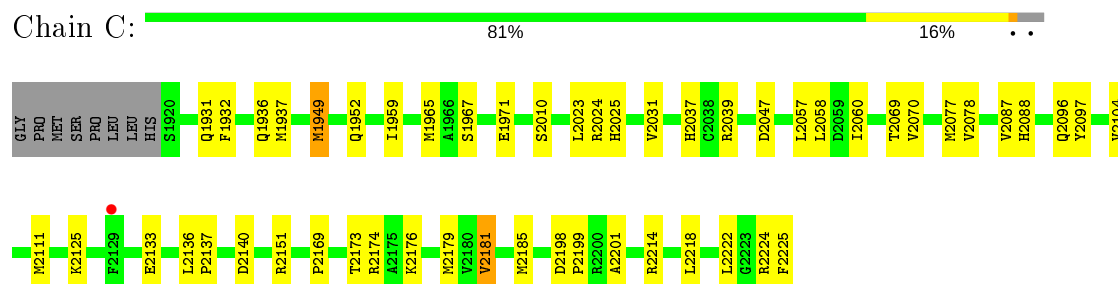
#### • Molecule 1: CAD PROTEIN



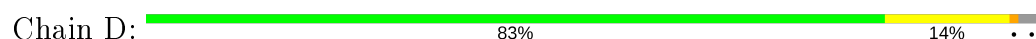
#### • Molecule 1: CAD PROTEIN

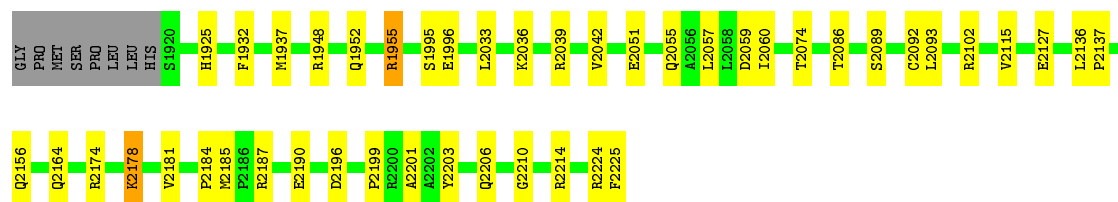


#### • Molecule 1: CAD PROTEIN



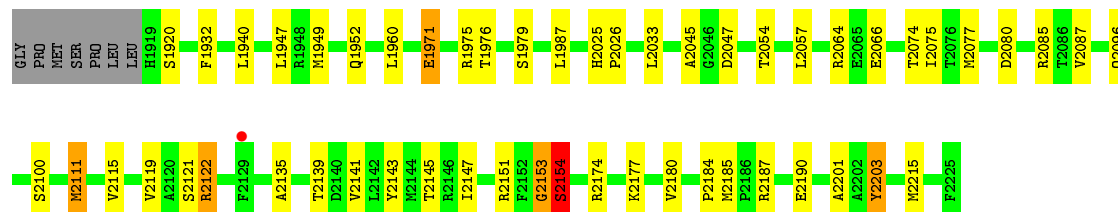
#### • Molecule 1: CAD PROTEIN





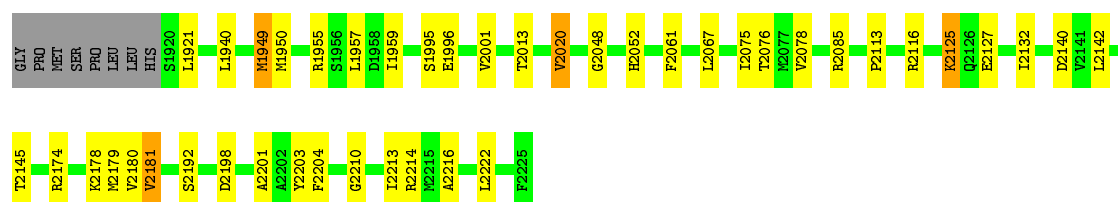
• Molecule 1: CAD PROTEIN

Chain E: 81% 15% ..



• Molecule 1: CAD PROTEIN

Chain F: 84% 12% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.03Å 145.12Å 83.16Å 90.00° 120.03° 90.00°	Depositor
Resolution (Å)	41.58 – 2.10 41.58 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (41.58-2.10) 97.9 (41.58-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.152 , 0.208 0.157 , 0.191	Depositor DCC
$R_{free}$ test set	4878 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 25.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.460 for l,k,-h-l 0.460 for -h-l,k,h 0.457 for h,-k,-h-l 0.467 for l,-k,h 0.467 for -h-l,-k,l	Xtriage
Reported twinning fraction	0.220 for H, K, L 0.174 for H+L, -K, -L 0.100 for H, -K, -H-L 0.144 for -H-L, K, H 0.162 for L, K, -H-L 0.200 for L, -K, H	Depositor
Outliers	2 of 97555 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14721	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 8.53% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PAL, EDO

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	0.40	0/2408	0.63	0/3252
1	B	0.42	0/2408	0.65	0/3254
1	C	0.40	0/2402	0.63	0/3246
1	D	0.40	0/2408	0.65	0/3254
1	E	0.40	0/2371	0.66	0/3210
1	F	0.40	0/2392	0.66	1/3234 (0.0%)
All	All	0.40	0/14389	0.65	1/19450 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	2198	ASP	CB-CG-OD1	5.88	123.59	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	1995	SER	Peptide

## 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	2366	0	2386	21	0
1	B	2365	0	2381	19	0
1	C	2359	0	2371	24	0
1	D	2365	0	2381	23	0
1	E	2329	0	2323	29	0
1	F	2350	0	2361	22	0
2	A	16	0	6	0	0
2	B	16	0	6	0	0
2	C	16	0	6	0	0
2	D	16	0	6	0	0
2	E	16	0	6	1	0
2	F	16	0	6	0	0
3	D	4	0	6	0	0
3	F	4	0	6	0	0
4	A	72	0	0	1	0
4	B	86	0	0	4	0
4	C	68	0	0	0	0
4	D	98	0	0	1	0
4	E	92	0	0	1	0
4	F	67	0	0	2	0
All	All	14721	0	14251	135	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 (135) 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:2077:MET:SD	1:C:2087:VAL:HG13	2.20	0.82
1:B:2064:ARG:NH2	4:B:3006:HOH:O	2.14	0.78
1:B:2162:PHE:O	4:B:3069:HOH:O	2.04	0.74
1:A:2163:GLY:HA3	4:A:3057:HOH:O	1.87	0.73
1:E:2153:GLY:HA3	1:E:2154:SER:CB	2.25	0.66
1:A:2025:HIS:O	1:A:2047:ASP:HA	1.97	0.63
1:B:2114:THR:OG1	4:B:3054:HOH:O	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:3082:HOH:O	1:D:1955:ARG:HD3	2.00	0.60
1:C:1937:MET:HE1	1:C:2060:ILE:HG21	1.84	0.59
1:E:2054:THR:HA	1:E:2057:LEU:HD12	1.84	0.59
1:A:2099:VAL:O	1:A:2124:THR:HG23	2.02	0.59
1:D:2102:ARG:HA	1:D:2127:GLU:O	2.02	0.59
1:C:2077:MET:SD	1:C:2087:VAL:CG1	2.91	0.58
1:E:1976:THR:HG21	1:E:2045:ALA:HB1	1.86	0.58
1:D:1948:ARG:O	1:D:1952:GLN:HG3	2.04	0.58
1:D:2051:GLU:HG2	1:D:2089:SER:OG	2.03	0.58
1:C:1971:GLU:HB2	1:C:2024:ARG:HD3	1.87	0.56
1:E:2025:HIS:CG	1:E:2026:PRO:HD2	2.40	0.56
1:F:2048:GLY:O	1:F:2085:ARG:HD3	2.05	0.56
1:C:1949:MET:HA	1:C:1952:GLN:HB2	1.87	0.56
1:D:1925:HIS:HD2	1:D:2042:VAL:H	1.52	0.56
1:A:2083:HIS:HB2	1:A:2148:GLN:HG3	1.87	0.56
1:D:1932:PHE:CZ	1:D:2057:LEU:HD11	2.40	0.56
1:E:2143:TYR:CZ	1:E:2184:PRO:HD3	2.41	0.55
1:B:2066:GLU:HB3	1:B:2180:VAL:HG11	1.89	0.55
1:B:2101:LEU:O	1:B:2126:GLN:HA	2.07	0.55
1:A:2101:LEU:HD22	1:A:2103:TYR:HE1	1.72	0.54
1:A:1948:ARG:NH1	1:A:2209:ASN:OD1	2.40	0.53
1:C:2133:GLU:HB2	1:C:2174:ARG:NH1	2.23	0.53
1:E:2153:GLY:HA3	1:E:2154:SER:OG	2.09	0.53
1:F:2020:VAL:HG22	1:F:2222:LEU:HD21	1.89	0.53
1:E:1960:LEU:CD1	1:E:1987:LEU:HD13	2.38	0.52
1:A:2015:SER:O	1:A:2039:ARG:NH1	2.42	0.52
1:F:2181:VAL:HG22	1:F:2201:ALA:HA	1.91	0.52
1:C:1965:MET:CE	1:C:1967:SER:HB2	2.40	0.52
1:F:2210:GLY:O	1:F:2214:ARG:HD2	2.11	0.51
1:D:2033:LEU:HD12	1:D:2036:LYS:HD2	1.93	0.51
1:E:2111:MET:SD	1:E:2115:VAL:HG11	2.51	0.51
1:E:2135:ALA:O	1:E:2139:THR:OG1	2.28	0.51
1:C:2218:LEU:O	1:C:2222:LEU:HB2	2.11	0.50
1:D:2178:LYS:HG3	1:D:2178:LYS:O	2.11	0.50
1:A:2084:GLY:O	1:A:2088:HIS:CD2	2.64	0.50
1:E:1960:LEU:HD12	1:E:1987:LEU:HD13	1.92	0.50
1:A:1972:VAL:HG12	1:B:1998:THR:HA	1.94	0.50
1:A:2185:MET:HB3	1:A:2186:PRO:HA	1.94	0.50
1:E:2066:GLU:HB3	1:E:2180:VAL:HG11	1.92	0.50
1:F:1957:LEU:HD22	1:F:1959:ILE:HD12	1.95	0.49
1:E:1971:GLU:OE1	1:E:2151:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1996:GLU:HG2	1:F:2001:VAL:HG11	1.95	0.49
1:C:2025:HIS:O	1:C:2047:ASP:HA	2.13	0.49
1:C:2078:VAL:HG22	1:C:2104:VAL:HB	1.95	0.48
1:F:2078:VAL:HG11	1:F:2132:ILE:HD11	1.95	0.48
1:A:2025:HIS:CG	1:A:2026:PRO:HD2	2.48	0.48
1:F:2116:ARG:NH1	4:F:3047:HOH:O	2.46	0.48
1:C:1932:PHE:CZ	1:C:2057:LEU:HD11	2.49	0.48
1:A:1964:VAL:HG22	1:A:1990:ALA:HB3	1.95	0.48
1:D:2060:ILE:HD12	1:D:2093:LEU:HD23	1.94	0.48
1:E:2077:MET:SD	1:E:2087:VAL:HG13	2.54	0.47
1:D:2055:GLN:HG2	1:D:2086:THR:HG22	1.96	0.47
1:F:2174:ARG:HB2	1:F:2174:ARG:CZ	2.44	0.47
1:B:2015:SER:OG	1:B:2038:CYS:SG	2.55	0.47
1:A:1949:MET:HE2	1:A:1950:MET:SD	2.55	0.47
1:F:1940:LEU:HD22	1:F:2216:ALA:HB1	1.96	0.47
1:E:2025:HIS:O	1:E:2047:ASP:HA	2.16	0.46
1:E:2153:GLY:HA3	1:E:2154:SER:HB3	1.96	0.46
1:C:1959:ILE:O	1:C:2224:ARG:CZ	2.63	0.46
1:E:1975:ARG:HG3	1:F:2013:THR:HG21	1.97	0.46
1:D:2187:ARG:HA	1:D:2190:GLU:OE2	2.16	0.45
1:B:1975:ARG:NE	1:B:2185:MET:HB2	2.31	0.45
1:E:1947:LEU:HD13	1:E:2215:MET:HB3	1.99	0.45
1:B:2143:TYR:CZ	1:B:2184:PRO:HD3	2.51	0.45
1:A:2181:VAL:HG13	1:A:2201:ALA:HA	1.99	0.45
1:B:1939:HIS:O	1:B:1942:ASN:HB2	2.17	0.45
1:F:2078:VAL:O	1:F:2145:THR:HG23	2.17	0.45
1:F:1940:LEU:HD11	1:F:2213:ILE:HG23	1.99	0.45
1:A:1980:PHE:CE1	1:A:2214:ARG:HG3	2.52	0.45
1:E:1932:PHE:O	1:E:2096:GLN:NE2	2.47	0.45
1:C:1965:MET:HE2	1:C:1967:SER:HB2	1.99	0.44
1:C:2023:LEU:HD23	1:C:2031:VAL:HG13	2.00	0.44
1:A:1982:ALA:HB2	1:B:1992:LEU:HD11	1.99	0.44
1:F:2204:PHE:N	4:F:3065:HOH:O	2.50	0.44
1:E:2187:ARG:HA	1:E:2190:GLU:OE2	2.18	0.44
1:D:1937:MET:CE	1:D:2060:ILE:HG21	2.47	0.44
1:E:1975:ARG:CD	1:E:2185:MET:HB2	2.48	0.44
1:E:2096:GLN:NE2	4:E:3003:HOH:O	2.49	0.44
1:F:2067:LEU:HD21	1:F:2180:VAL:HG23	2.00	0.44
1:A:2103:TYR:O	1:A:2128:GLU:HA	2.18	0.43
1:B:2061:PHE:CE2	1:B:2065:GLU:HG3	2.53	0.43
1:C:1959:ILE:O	1:C:2224:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1925:HIS:HD2	1:D:2042:VAL:N	2.15	0.43
1:D:2092:CYS:SG	1:D:2115:VAL:HG13	2.58	0.43
1:D:2174:ARG:HD3	4:D:3070:HOH:O	2.18	0.43
1:F:2061:PHE:CD1	1:F:2213:ILE:HD11	2.53	0.43
1:C:2088:HIS:HD2	1:C:2111:MET:CE	2.31	0.43
1:C:2136:LEU:N	1:C:2137:PRO:CD	2.82	0.43
1:C:2169:PRO:O	1:C:2173:THR:HG23	2.19	0.43
1:C:2181:VAL:HG13	1:C:2201:ALA:HA	2.01	0.43
1:D:2184:PRO:O	1:D:2185:MET:HB2	2.19	0.43
1:D:2210:GLY:O	1:D:2214:ARG:HD2	2.18	0.43
1:E:2111:MET:HA	1:E:2111:MET:HE2	1.99	0.43
1:D:2059:ASP:OD1	1:D:2206:GLN:NE2	2.46	0.43
1:F:2075:ILE:HD12	1:F:2075:ILE:N	2.34	0.43
1:B:2081:LEU:HG	1:B:2105:ALA:HB2	2.01	0.42
1:D:2181:VAL:HG13	1:D:2201:ALA:HA	2.00	0.42
1:E:2115:VAL:O	1:E:2119:VAL:HG23	2.19	0.42
1:F:2125:LYS:HZ1	1:F:2127:GLU:HB2	1.84	0.42
1:F:2076:THR:HB	1:F:2142:LEU:HD12	2.02	0.42
1:A:2083:HIS:CB	1:A:2148:GLN:HG3	2.50	0.42
1:E:2121:SER:OG	1:E:2122:ARG:NH2	2.53	0.42
1:B:2069:THR:HG22	1:B:2070:VAL:N	2.34	0.42
1:D:2196:ASP:OD1	1:D:2203:TYR:OH	2.30	0.42
1:F:1949:MET:HG3	1:F:1950:MET:N	2.35	0.42
1:C:1932:PHE:HA	1:C:1936:GLN:OE1	2.20	0.42
1:C:1932:PHE:O	1:C:2096:GLN:NE2	2.53	0.42
1:B:2025:HIS:CG	1:B:2026:PRO:HD2	2.54	0.41
1:E:2080:ASP:HB2	1:E:2147:ILE:HA	2.01	0.41
1:C:2070:VAL:HB	1:C:2097:TYR:CD2	2.55	0.41
1:E:2085:ARG:HE	2:E:3226:PAL:C4	2.31	0.41
1:F:2052:HIS:HB2	1:F:2085:ARG:HG3	2.02	0.41
1:A:2136:LEU:N	1:A:2137:PRO:CD	2.83	0.41
1:B:1932:PHE:CZ	1:B:2057:LEU:HD11	2.56	0.41
1:E:2075:ILE:HD12	1:E:2075:ILE:N	2.35	0.41
1:E:2075:ILE:HG13	1:E:2141:VAL:HB	2.02	0.41
1:B:1937:MET:HE3	1:B:2093:LEU:HD21	2.02	0.41
1:B:2060:ILE:HD12	1:B:2093:LEU:HD23	2.02	0.41
1:C:2198:ASP:OD1	1:C:2199:PRO:HD2	2.21	0.41
1:F:2178:LYS:O	1:F:2179:MET:HB2	2.20	0.41
1:D:2178:LYS:CG	1:D:2178:LYS:O	2.69	0.41
1:A:2073:MET:O	1:A:2099:VAL:CG1	2.69	0.40
1:B:2055:GLN:HG2	1:B:2086:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2201:ALA:HB1	1:E:2203:TYR:CZ	2.57	0.40
1:A:2106:PRO:HB3	1:A:2164:GLN:OE1	2.21	0.40
1:D:2136:LEU:N	1:D:2137:PRO:CD	2.85	0.40
1:C:2140:ASP:OD1	1:C:2176:LYS:NZ	2.49	0.40
1:D:2060:ILE:HD12	1:D:2093:LEU:CD2	2.52	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	304/314 (97%)	290 (95%)	8 (3%)	6 (2%)	7	3
1	B	304/314 (97%)	283 (93%)	21 (7%)	0	100	100
1	C	304/314 (97%)	294 (97%)	9 (3%)	1 (0%)	41	41
1	D	304/314 (97%)	287 (94%)	15 (5%)	2 (1%)	22	18
1	E	305/314 (97%)	284 (93%)	18 (6%)	3 (1%)	15	11
1	F	304/314 (97%)	287 (94%)	16 (5%)	1 (0%)	41	41
All	All	1825/1884 (97%)	1725 (94%)	87 (5%)	13 (1%)	22	18

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1996	GLU
1	A	1956	SER
1	E	1920	SER
1	E	2153	GLY
1	E	2154	SER
1	A	2149	LYS
1	A	2050	GLY

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Mol	Chain	Res	Type
1	A	2196	ASP
1	A	2185	MET
1	A	2084	GLY
1	C	2185	MET
1	D	2199	PRO
1	F	2113	PRO

### 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	258/268 (96%)	241 (93%)	17 (7%)	16	14
1	B	258/268 (96%)	248 (96%)	10 (4%)	32	33
1	C	255/268 (95%)	242 (95%)	13 (5%)	24	22
1	D	258/268 (96%)	250 (97%)	8 (3%)	40	43
1	E	249/268 (93%)	233 (94%)	16 (6%)	17	14
1	F	255/268 (95%)	245 (96%)	10 (4%)	32	33
All	All	1533/1608 (95%)	1459 (95%)	74 (5%)	25	24

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1930	GLN
1	A	1949	MET
1	A	1953	LYS
1	A	1956	SER
1	A	1993	SER
1	A	2000	SER
1	A	2039	ARG
1	A	2052	HIS
1	A	2058	LEU
1	A	2065	GLU
1	A	2174	ARG
1	A	2181	VAL

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Mol	Chain	Res	Type
1	A	2185	MET
1	A	2192	SER
1	A	2214	ARG
1	A	2224	ARG
1	A	2225	PHE
1	B	1934	LYS
1	B	1961	LYS
1	B	1993	SER
1	B	2039	ARG
1	B	2052	HIS
1	B	2058	LEU
1	B	2114	THR
1	B	2179	MET
1	B	2185	MET
1	B	2213	ILE
1	C	1931	GLN
1	C	1949	MET
1	C	2010	SER
1	C	2037	HIS
1	C	2039	ARG
1	C	2058	LEU
1	C	2069	THR
1	C	2125	LYS
1	C	2151	ARG
1	C	2179	MET
1	C	2181	VAL
1	C	2214	ARG
1	C	2225	PHE
1	D	1955	ARG
1	D	2039	ARG
1	D	2074	THR
1	D	2156	GLN
1	D	2164	GLN
1	D	2178	LYS
1	D	2224	ARG
1	D	2225	PHE
1	E	1940	LEU
1	E	1949	MET
1	E	1952	GLN
1	E	1971	GLU
1	E	1979	SER
1	E	2033	LEU

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Mol	Chain	Res	Type
1	E	2064	ARG
1	E	2074	THR
1	E	2100	SER
1	E	2111	MET
1	E	2122	ARG
1	E	2145	THR
1	E	2154	SER
1	E	2174	ARG
1	E	2177	LYS
1	E	2203	TYR
1	F	1921	LEU
1	F	1949	MET
1	F	1955	ARG
1	F	1995	SER
1	F	2020	VAL
1	F	2125	LYS
1	F	2140	ASP
1	F	2181	VAL
1	F	2192	SER
1	F	2203	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1930	GLN
1	C	2088	HIS
1	C	2164	GLN
1	D	1925	HIS
1	D	2164	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](#)

8 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	$\# Z  > 2$
3	EDO	F	3227	-	3,3,3	0.46	0	2,2,2	0.25	0
2	PAL	A	3226	-	9,15,15	1.51	2 (22%)	11,21,21	1.59	2 (18%)
2	PAL	E	3226	-	9,15,15	1.43	2 (22%)	11,21,21	0.94	0
2	PAL	B	3226	-	9,15,15	1.40	2 (22%)	11,21,21	1.61	3 (27%)
2	PAL	C	3226	-	9,15,15	1.37	2 (22%)	11,21,21	1.23	0
2	PAL	F	3226	-	9,15,15	1.27	2 (22%)	11,21,21	1.36	1 (9%)
2	PAL	D	3226	-	9,15,15	1.20	1 (11%)	11,21,21	1.42	2 (18%)
3	EDO	D	3227	-	3,3,3	0.44	0	2,2,2	0.40	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	F	3227	-	-	1/1/1/1	-
2	PAL	A	3226	-	-	0/11/17/17	-
2	PAL	E	3226	-	-	0/11/17/17	-
2	PAL	B	3226	-	-	0/11/17/17	-
2	PAL	C	3226	-	-	1/11/17/17	-
2	PAL	F	3226	-	-	5/11/17/17	-
2	PAL	D	3226	-	-	2/11/17/17	-
3	EDO	D	3227	-	-	0/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3226	PAL	P-O2P	2.98	1.61	1.54
2	E	3226	PAL	P-O2P	2.91	1.61	1.54
2	A	3226	PAL	P-O3P	2.82	1.61	1.54
2	C	3226	PAL	P-O3P	2.76	1.61	1.54
2	E	3226	PAL	P-O3P	2.70	1.61	1.54
2	A	3226	PAL	P-O2P	2.66	1.61	1.54
2	C	3226	PAL	P-O2P	2.52	1.60	1.54
2	B	3226	PAL	P-O3P	2.51	1.60	1.54
2	F	3226	PAL	P-O2P	2.45	1.60	1.54
2	F	3226	PAL	P-O3P	2.34	1.60	1.54
2	D	3226	PAL	P-O3P	2.26	1.60	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3226	PAL	O3P-P-C1P	3.25	113.66	106.84
2	F	3226	PAL	O2P-P-O1P	-3.22	103.88	112.39
2	D	3226	PAL	C1P-C1-N2	-2.79	112.54	115.19
2	A	3226	PAL	O2P-P-O1P	-2.44	105.94	112.39
2	A	3226	PAL	O3P-P-O2P	2.33	114.90	108.08
2	D	3226	PAL	O3P-P-O2P	2.19	114.49	108.08
2	B	3226	PAL	O1P-P-C1P	-2.11	106.13	110.94
2	B	3226	PAL	C1P-C1-N2	2.01	117.11	115.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

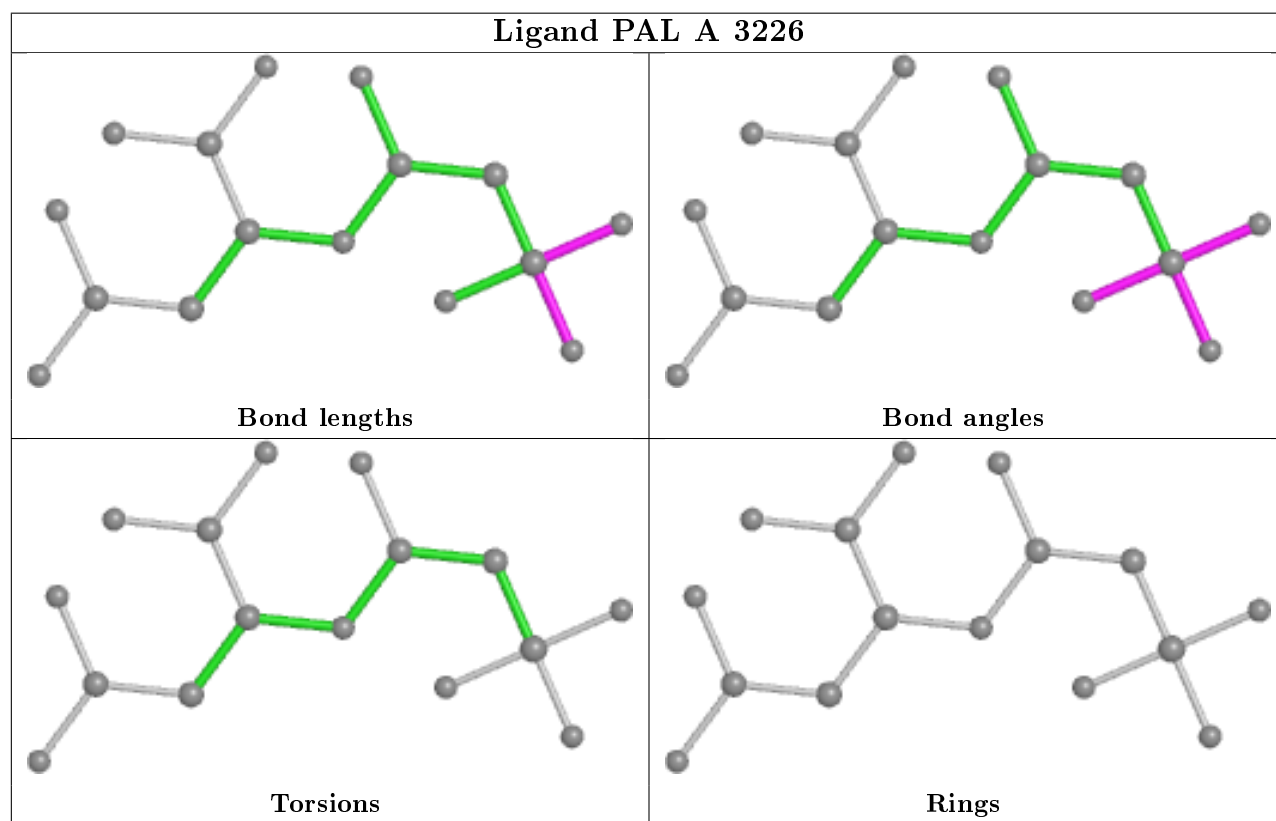
Mol	Chain	Res	Type	Atoms
2	F	3226	PAL	C1-C1P-P-O3P
2	F	3226	PAL	C3-C2-N2-C1
3	F	3227	EDO	O1-C1-C2-O2
2	D	3226	PAL	C3-C2-N2-C1
2	F	3226	PAL	C4-C2-N2-C1
2	F	3226	PAL	C1-C1P-P-O1P
2	D	3226	PAL	C4-C2-N2-C1
2	C	3226	PAL	C1-C1P-P-O2P
2	F	3226	PAL	C1-C1P-P-O2P

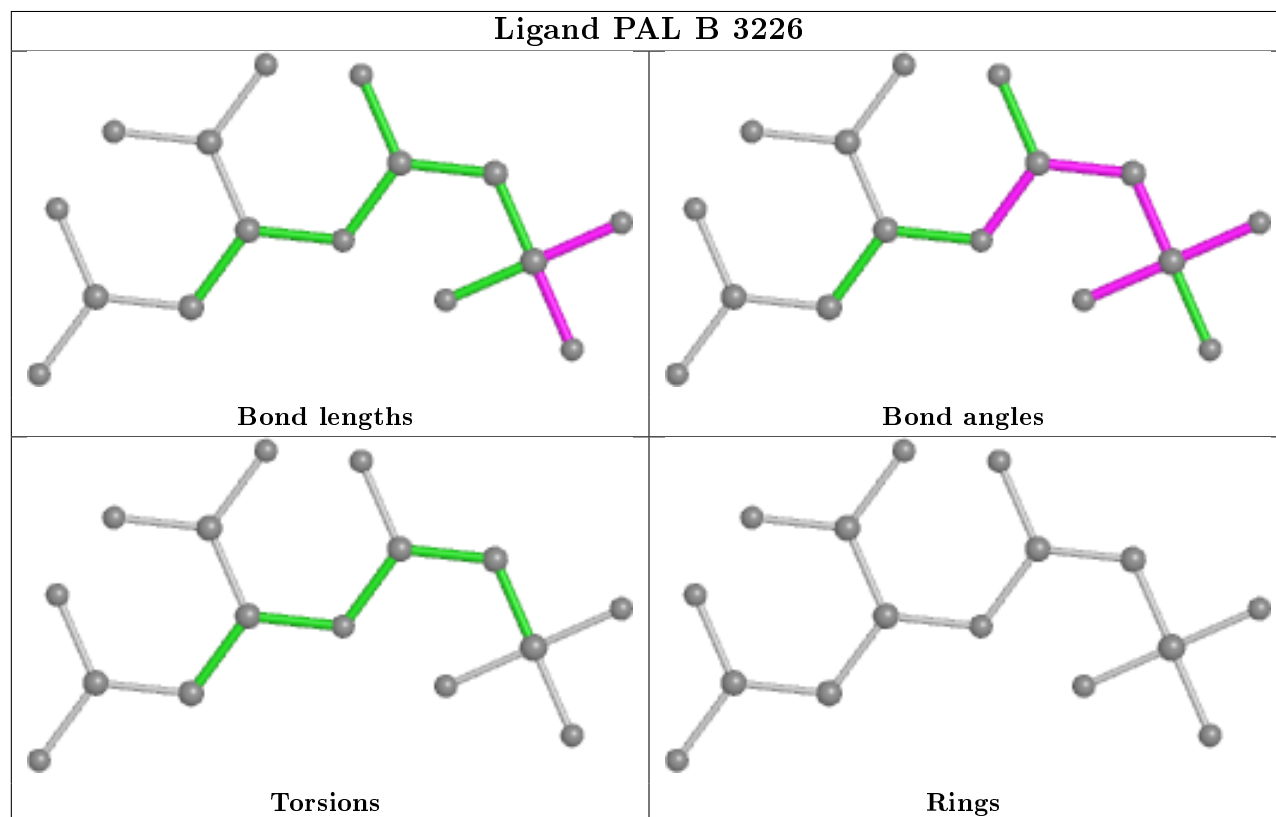
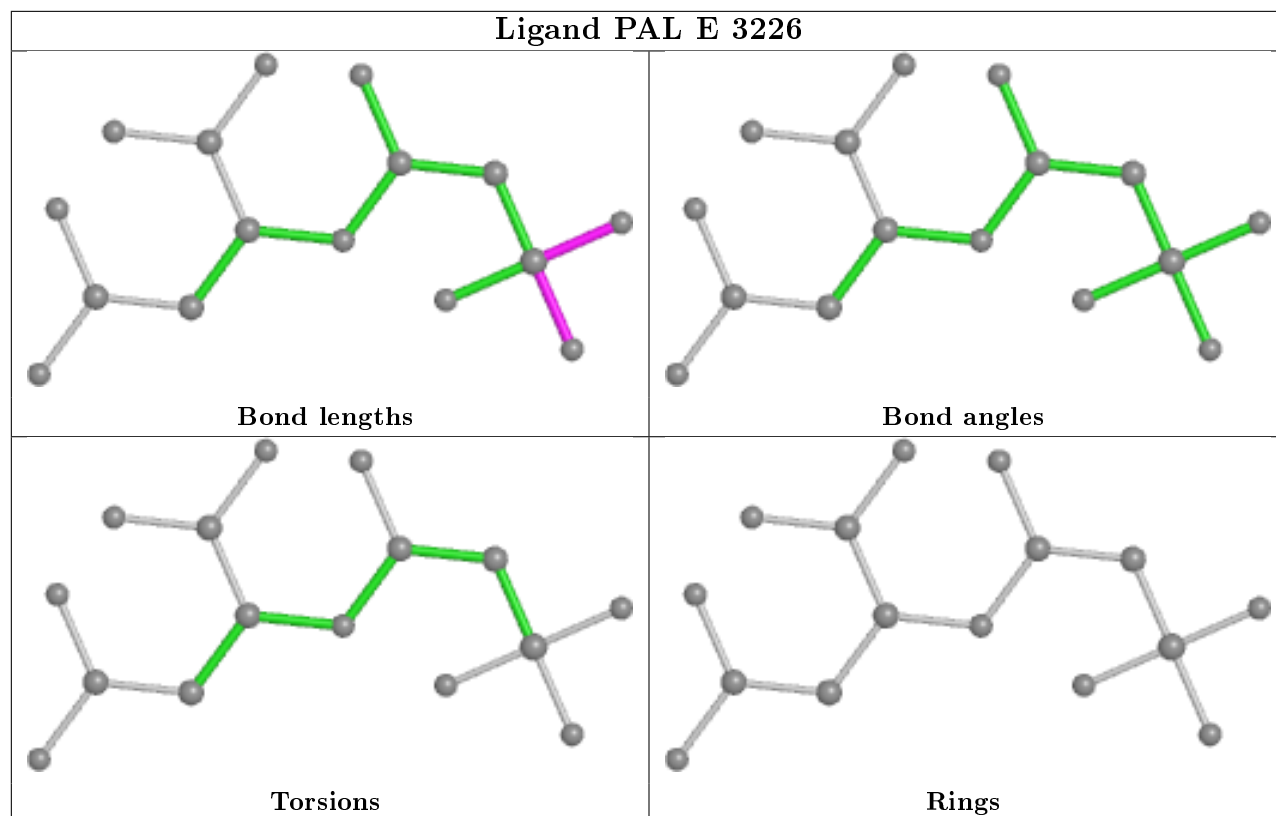
There are no ring outliers.

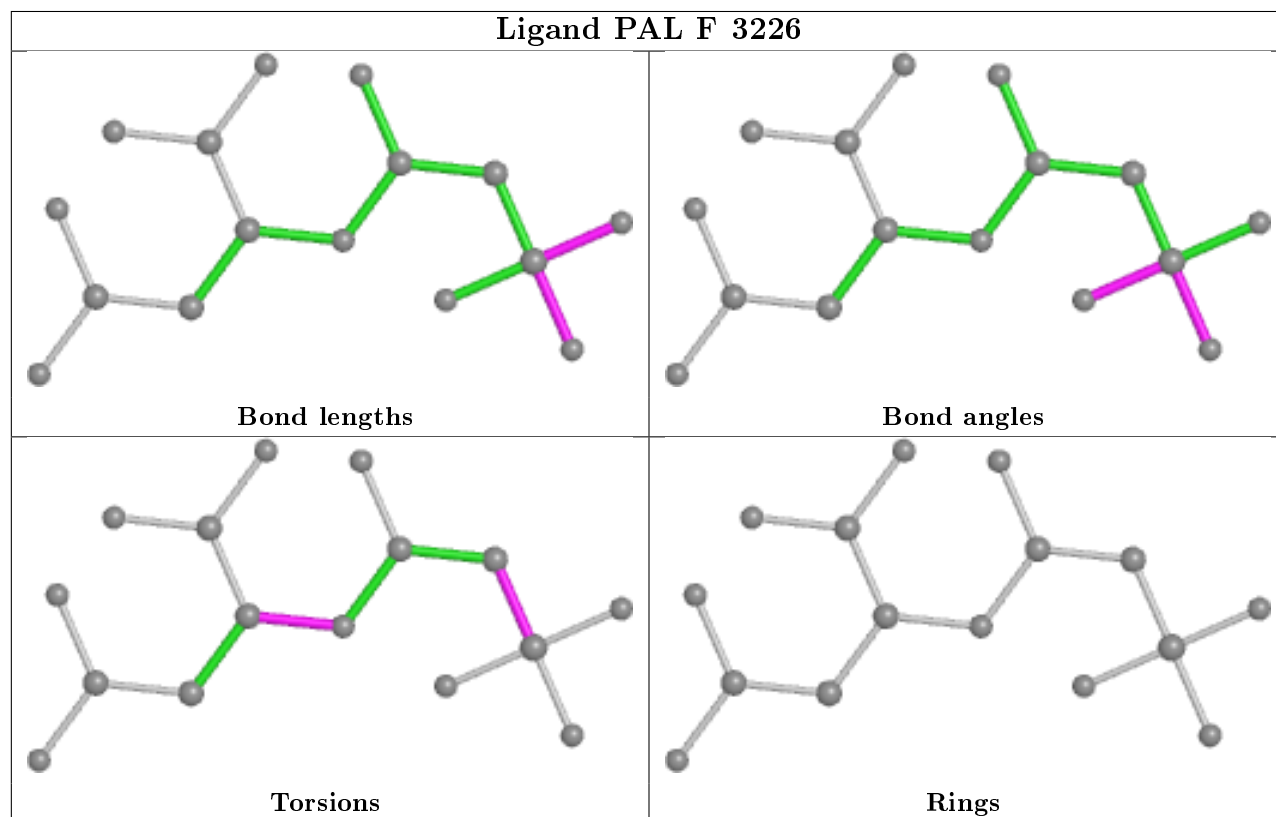
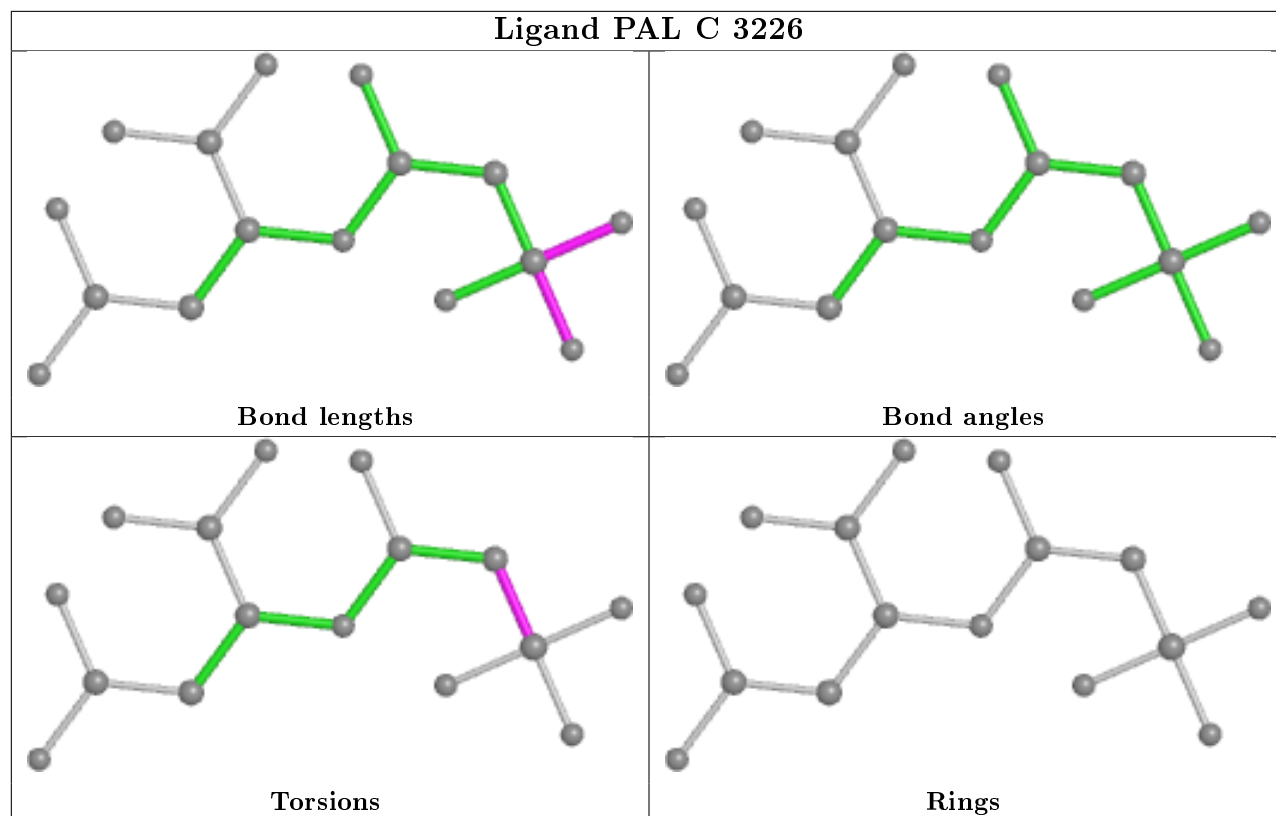
1 monomer is involved in 1 short contact:

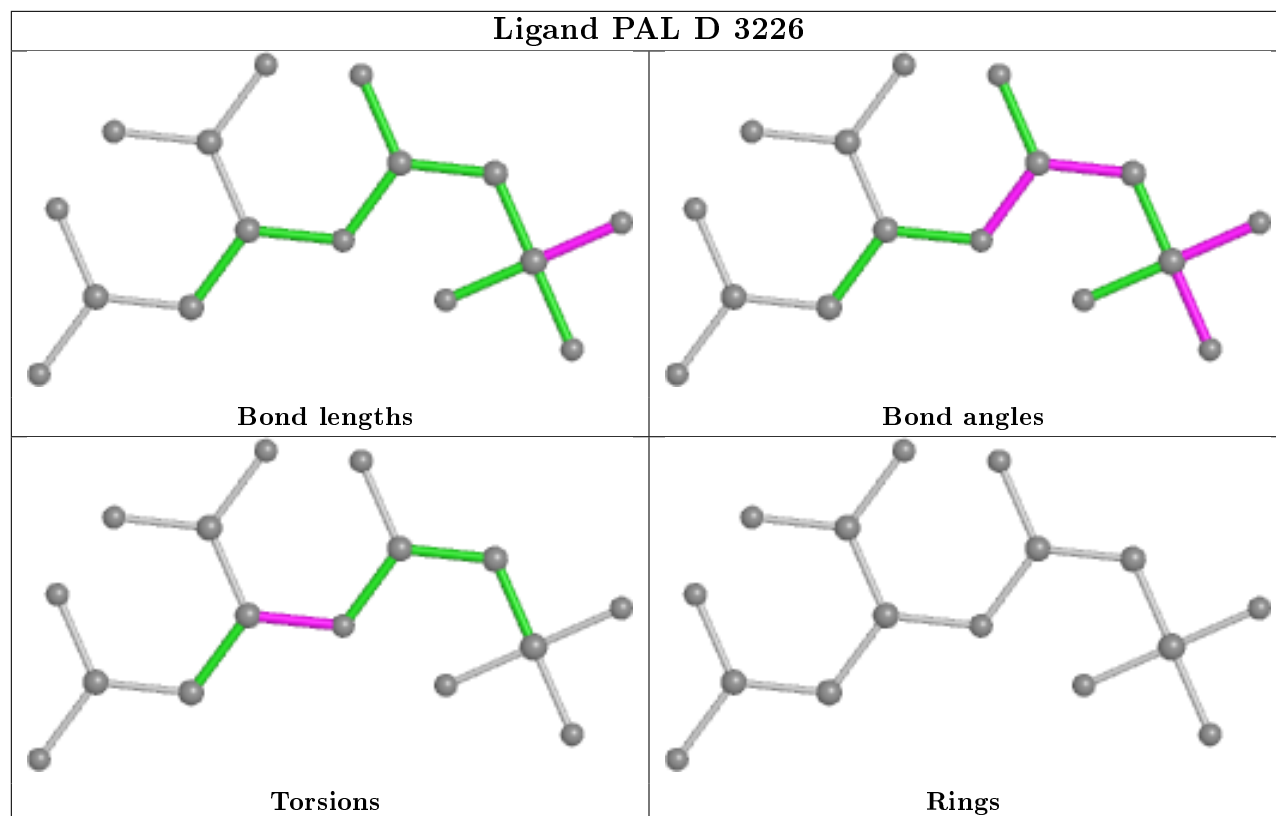
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3226	PAL	1	0

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 [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	306/314 (97%)	-0.06	1 (0%) 94 94	23, 36, 50, 67	0
1	B	306/314 (97%)	-0.08	2 (0%) 87 89	24, 35, 50, 59	0
1	C	306/314 (97%)	-0.12	1 (0%) 94 94	24, 35, 48, 61	0
1	D	306/314 (97%)	-0.11	0 100 100	21, 36, 49, 57	0
1	E	307/314 (97%)	-0.09	1 (0%) 94 94	23, 37, 50, 58	0
1	F	306/314 (97%)	-0.03	0 100 100	21, 37, 50, 59	0
All	All	1837/1884 (97%)	-0.08	5 (0%) 94 94	21, 36, 50, 67	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2129	PHE	3.0
1	C	2129	PHE	2.4
1	A	2037	HIS	2.2
1	B	1951	VAL	2.1
1	B	2202	ALA	2.0

### 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 monosaccharides in this entry.

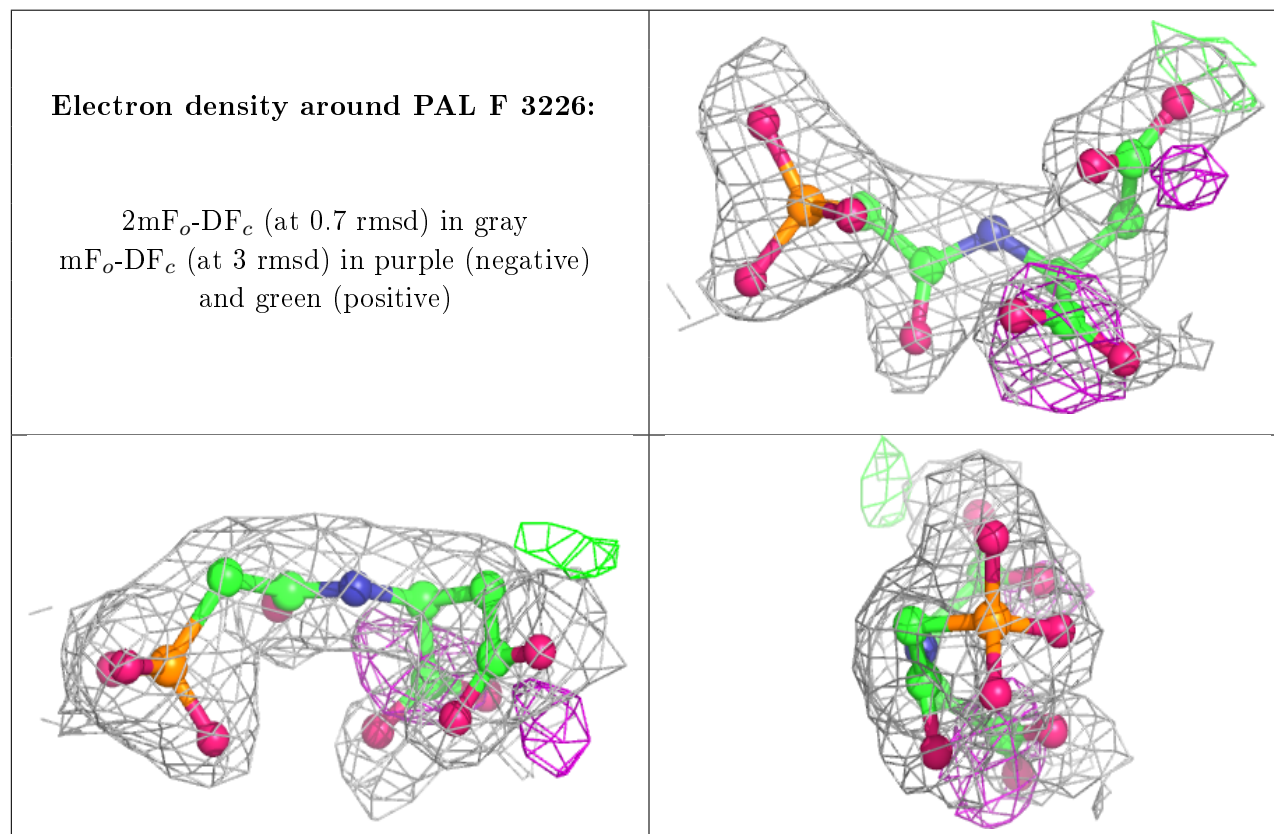


## 6.4 Ligands ⓘ

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, 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.

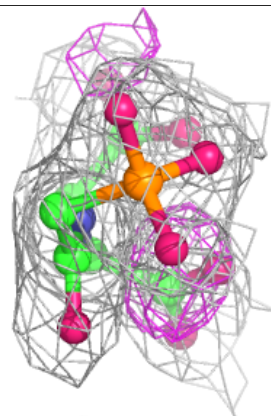
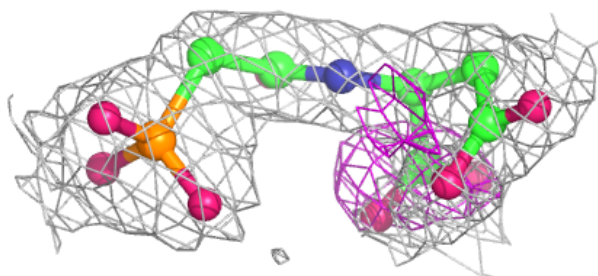
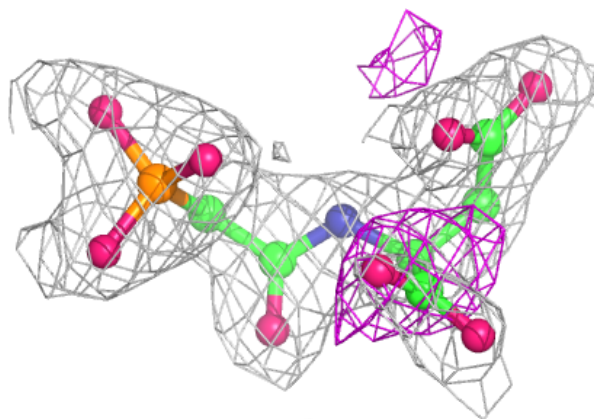
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	PAL	F	3226	16/16	0.92	0.15	27,32,41,42	0
2	PAL	C	3226	16/16	0.93	0.17	29,35,41,44	0
2	PAL	E	3226	16/16	0.94	0.16	31,38,45,49	0
2	PAL	A	3226	16/16	0.95	0.18	30,40,48,49	0
3	EDO	F	3227	4/4	0.96	0.07	30,31,31,34	0
2	PAL	B	3226	16/16	0.97	0.17	25,35,43,44	0
2	PAL	D	3226	16/16	0.97	0.15	26,34,46,50	0
3	EDO	D	3227	4/4	0.97	0.08	37,38,38,38	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.



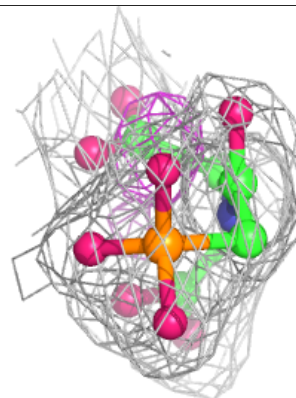
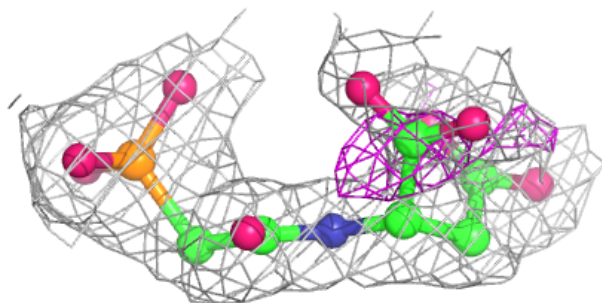
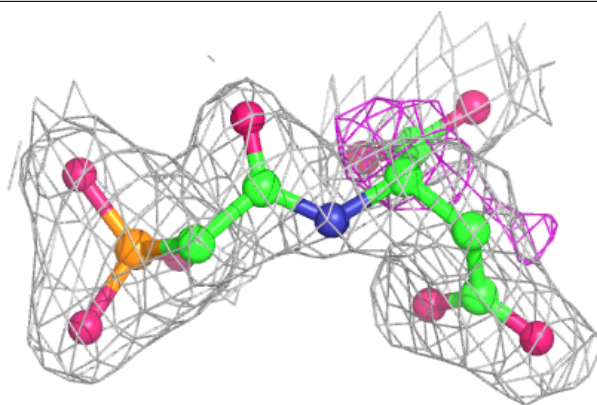
**Electron density around PAL C 3226:**

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



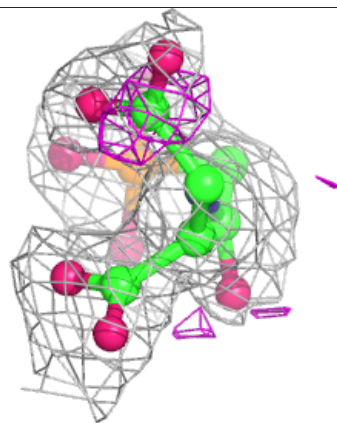
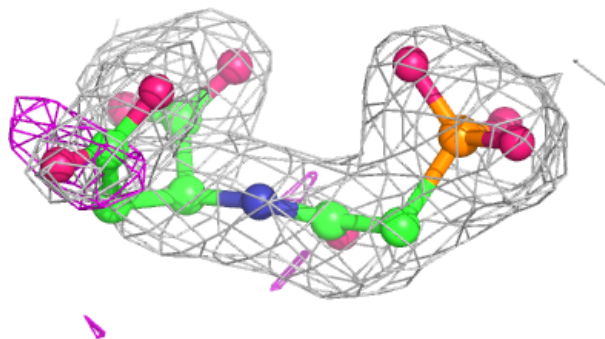
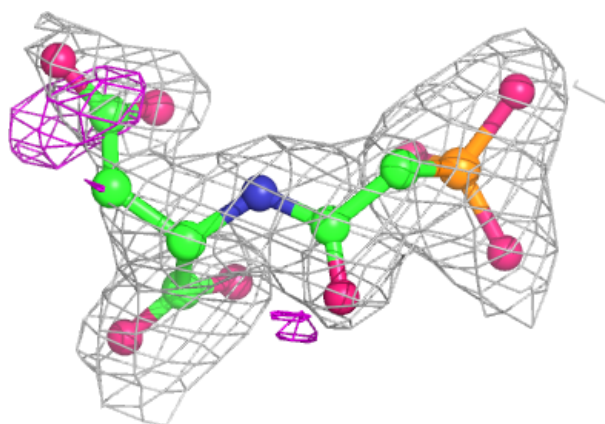
**Electron density around PAL E 3226:**

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

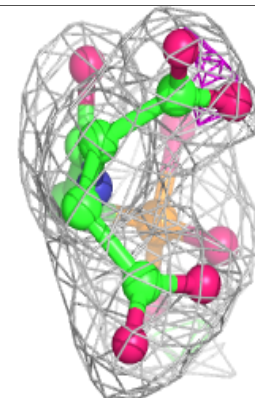
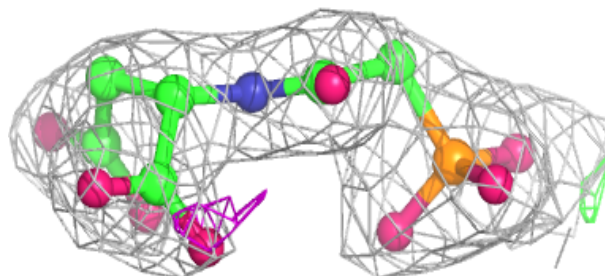
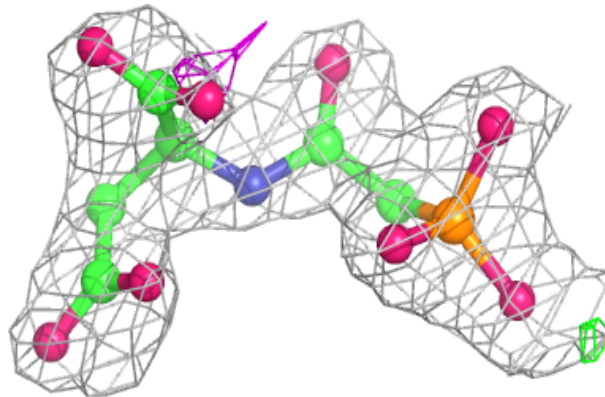


**Electron density around PAL A 3226:**

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

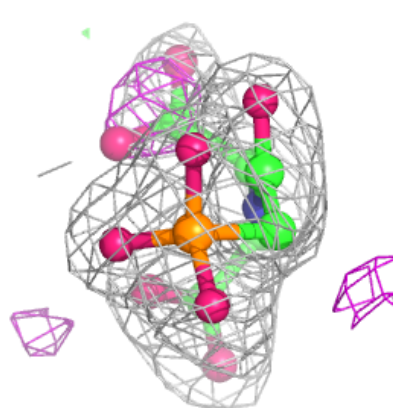
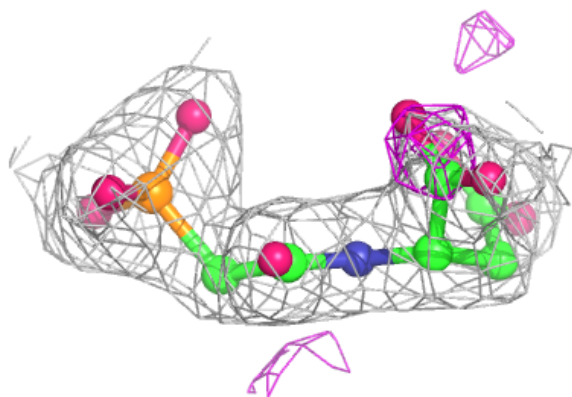
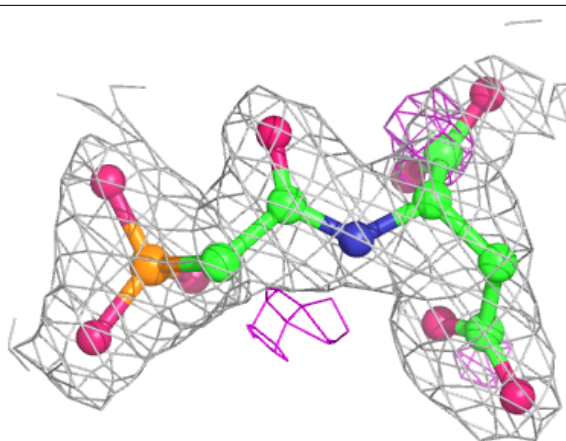
**Electron density around PAL B 3226:**

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



**Electron density around PAL D 3226:**

$2mF_o-DF_c$  (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.