



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:43 PM UTC

PDB ID : 2I14 / pdb_00002i14
Title : Crystal structure of nicotinate-nucleotide pyrophosphorylase from *Pyrococcus furiosus*
Authors : Shin, D.H.; Kim, R.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)
Deposited on : 2006-08-12
Resolution : 2.90 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 ⓘ 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:

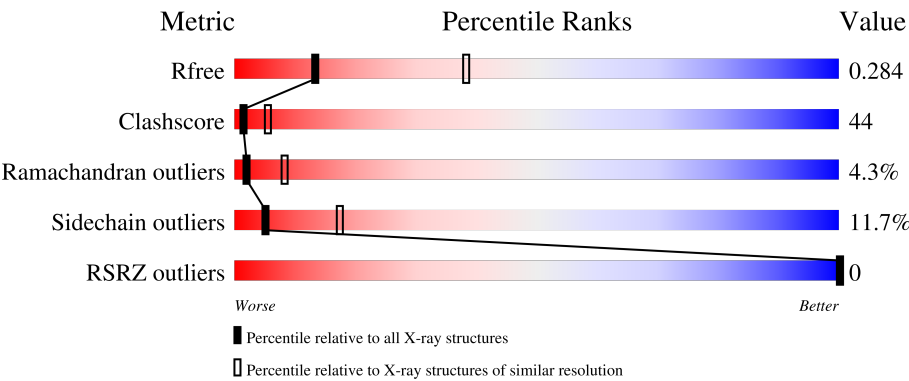
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	395	38%49%10%..
1	B	395	36%50%10%..
1	C	395	38%49%11%..
1	D	395	36%50%10%..

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Mol	Chain	Length	Quality of chain
1	E	395	37% 50% 10% ••
1	F	395	36% 50% 11% ••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18539 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 Nicotinate-nucleotide pyrophosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			
1	B	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			
1	C	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			
1	D	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			
1	E	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			
1	F	389	Total	C	N	O	S	0	0	0
			3055	1974	517	551	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	cloning artifact	UNP Q8TZS9
A	-4	GLY	-	cloning artifact	UNP Q8TZS9
A	-3	GLY	-	cloning artifact	UNP Q8TZS9
A	-2	GLY	-	cloning artifact	UNP Q8TZS9
A	-1	GLY	-	cloning artifact	UNP Q8TZS9
A	0	GLY	-	cloning artifact	UNP Q8TZS9
B	395	GLY	-	cloning artifact	UNP Q8TZS9
B	396	GLY	-	cloning artifact	UNP Q8TZS9
B	397	GLY	-	cloning artifact	UNP Q8TZS9
B	398	GLY	-	cloning artifact	UNP Q8TZS9
B	399	GLY	-	cloning artifact	UNP Q8TZS9
B	400	GLY	-	cloning artifact	UNP Q8TZS9
C	995	GLY	-	cloning artifact	UNP Q8TZS9
C	996	GLY	-	cloning artifact	UNP Q8TZS9
C	997	GLY	-	cloning artifact	UNP Q8TZS9
C	998	GLY	-	cloning artifact	UNP Q8TZS9
C	999	GLY	-	cloning artifact	UNP Q8TZS9

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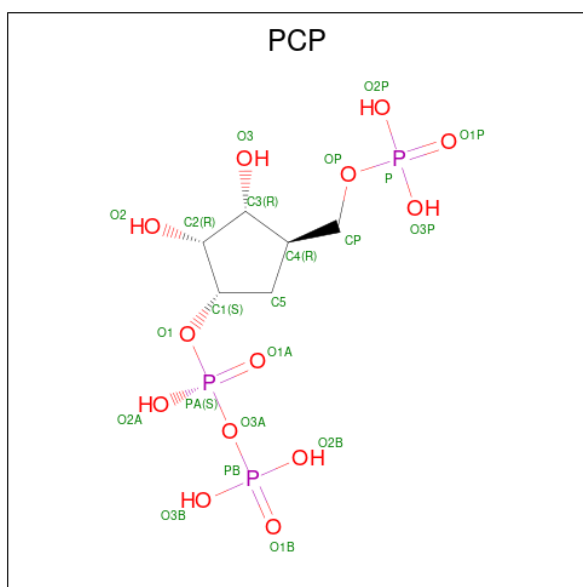
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1000	GLY	-	cloning artifact	UNP Q8TZS9
D	1395	GLY	-	cloning artifact	UNP Q8TZS9
D	1396	GLY	-	cloning artifact	UNP Q8TZS9
D	1397	GLY	-	cloning artifact	UNP Q8TZS9
D	1398	GLY	-	cloning artifact	UNP Q8TZS9
D	1399	GLY	-	cloning artifact	UNP Q8TZS9
D	1400	GLY	-	cloning artifact	UNP Q8TZS9
E	1995	GLY	-	cloning artifact	UNP Q8TZS9
E	1996	GLY	-	cloning artifact	UNP Q8TZS9
E	1997	GLY	-	cloning artifact	UNP Q8TZS9
E	1998	GLY	-	cloning artifact	UNP Q8TZS9
E	1999	GLY	-	cloning artifact	UNP Q8TZS9
E	2000	GLY	-	cloning artifact	UNP Q8TZS9
F	2395	GLY	-	cloning artifact	UNP Q8TZS9
F	2396	GLY	-	cloning artifact	UNP Q8TZS9
F	2397	GLY	-	cloning artifact	UNP Q8TZS9
F	2398	GLY	-	cloning artifact	UNP Q8TZS9
F	2399	GLY	-	cloning artifact	UNP Q8TZS9
F	2400	GLY	-	cloning artifact	UNP Q8TZS9

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0

- Molecule 3 is 1-ALPHA-PYROPHOSPHORYL-2-ALPHA,3-ALPHA-DIHYDROXY-4-BETA-CYCLOPENTANE-METHANOL-5-PHOSPHATE (CCD ID: PCP) (formula: C₆H₁₅O₁₃P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			22	6	13	3		
3	B	1	Total	C	O	P	0	0
			22	6	13	3		
3	C	1	Total	C	O	P	0	0
			22	6	13	3		
3	D	1	Total	C	O	P	0	0
			22	6	13	3		
3	E	1	Total	C	O	P	0	0
			22	6	13	3		
3	F	1	Total	C	O	P	0	0
			22	6	13	3		

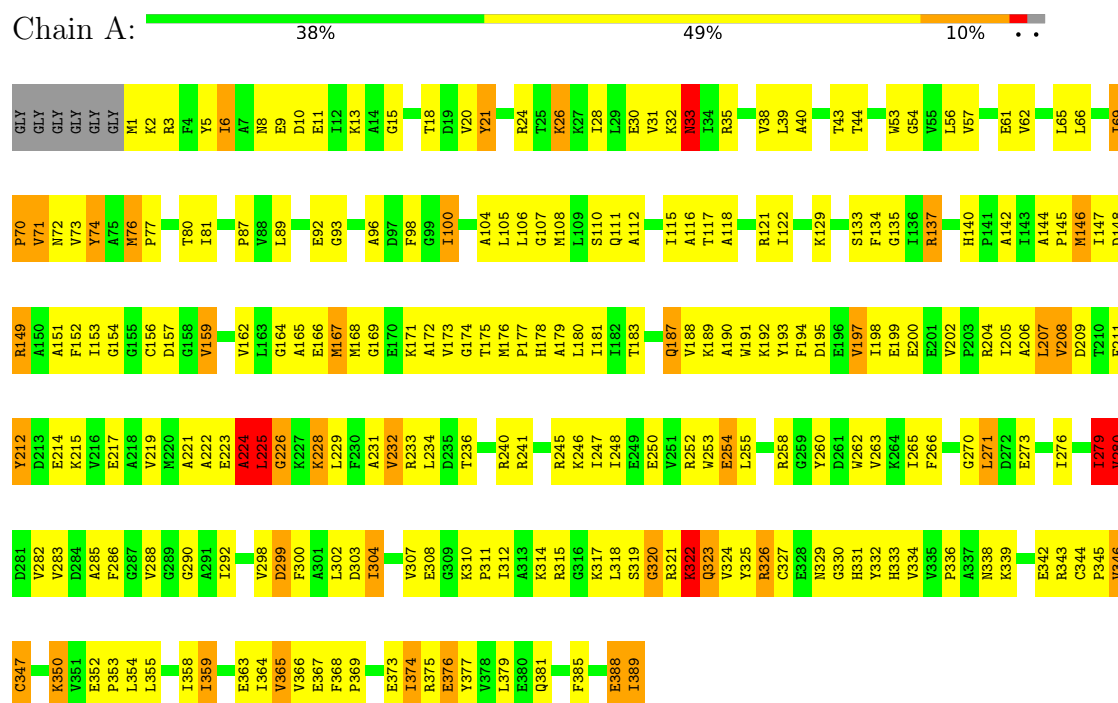
- Molecule 4 is water.

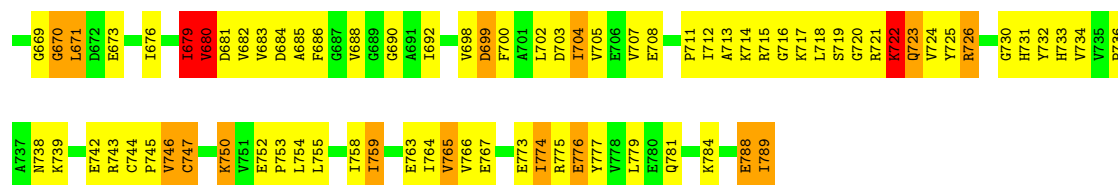
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	10	Total	O	0	0
			10	10		
4	C	9	Total	O	0	0
			9	9		
4	D	10	Total	O	0	0
			10	10		
4	E	16	Total	O	0	0
			16	16		
4	F	12	Total	O	0	0
			12	12		

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.

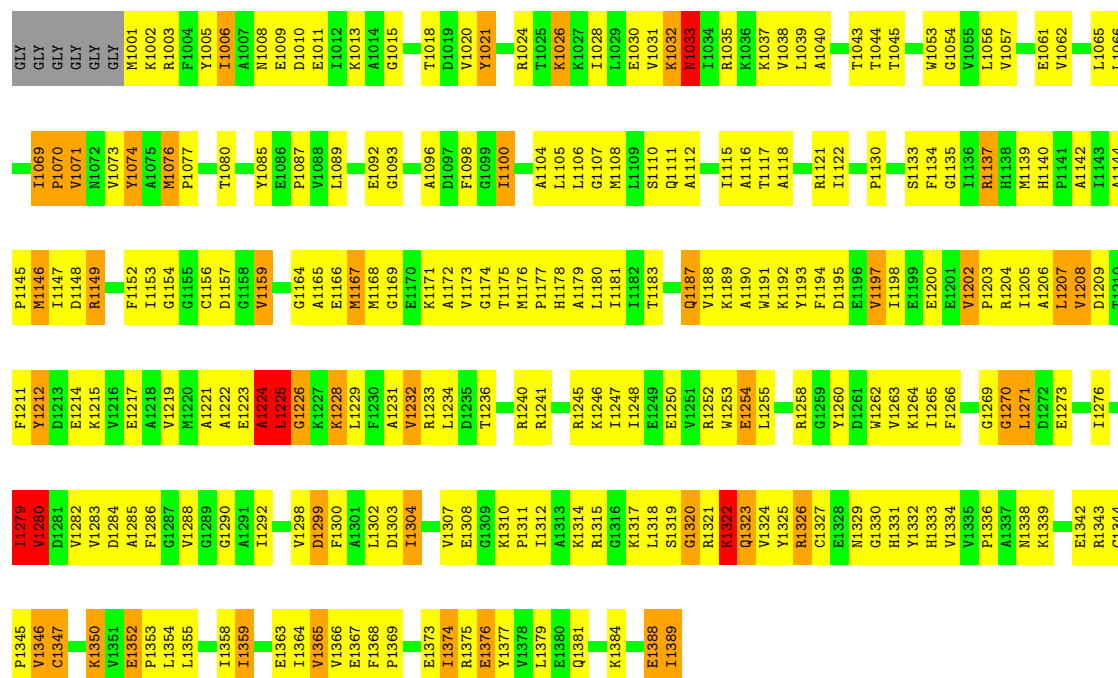
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase





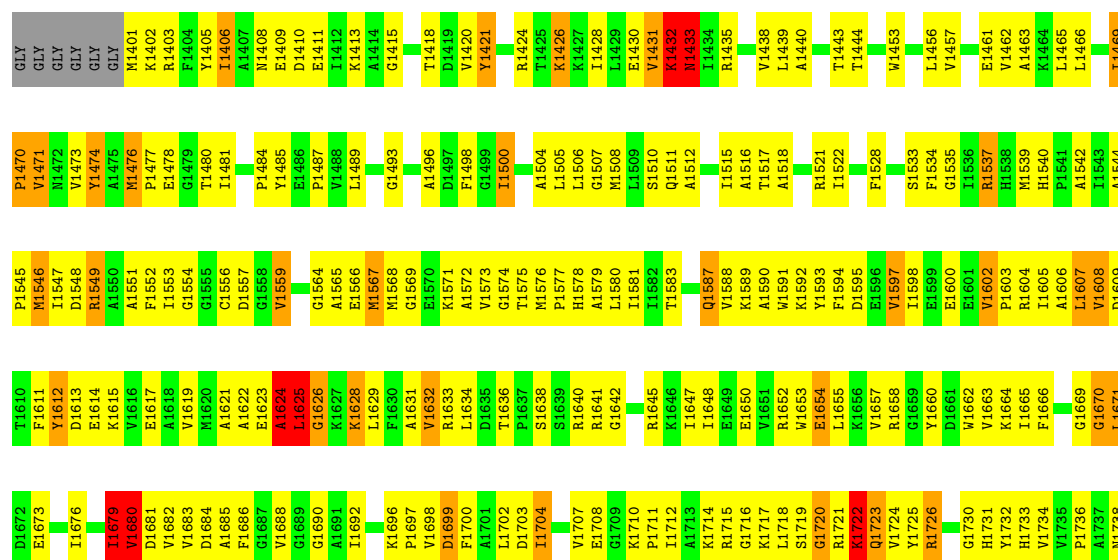
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase

Chain C: 38% 49% 11% ..



• Molecule 1: Nicotinate-nucleotide pyrophosphorylase

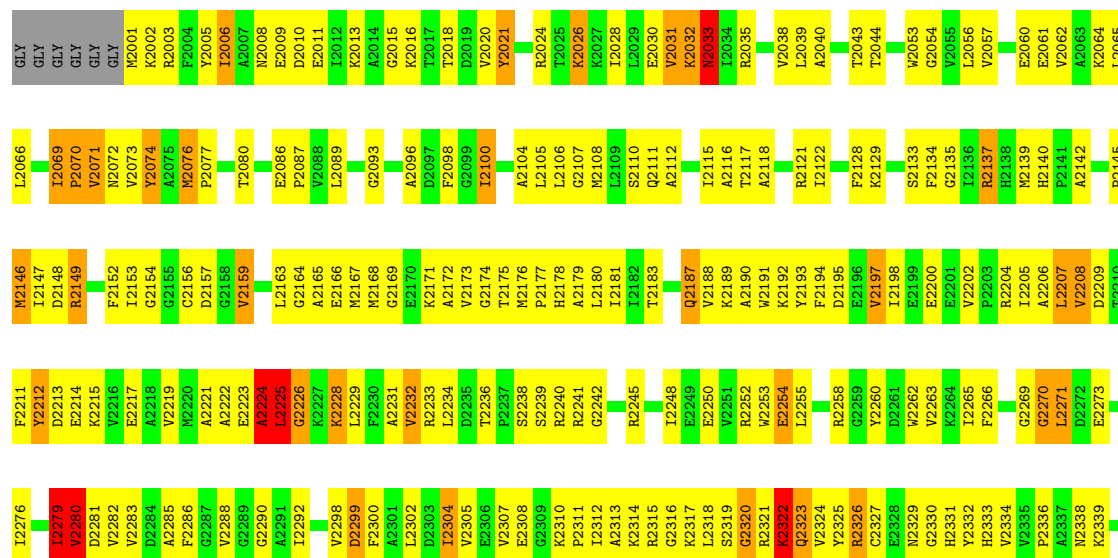
Chain D: 36% 50% 10% ..





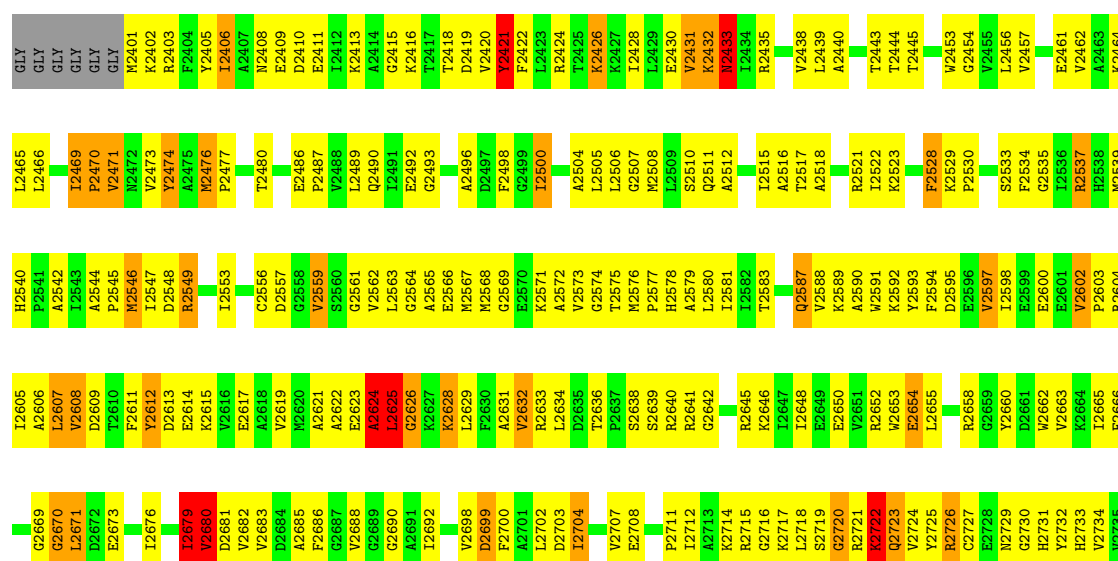
• Molecule 1: Nicotinate-nucleotide pyrophosphorylase

Chain E: 37% 50% 10% . .



• Molecule 1: Nicotinate-nucleotide pyrophosphorylase

Chain F: 36% 50% 11% . .



P2736	A2737	N2738	K2739
E2742	R2743	C2744	P2745
V2746	C2747	K2750	V2751
E2752	P2753	L2754	L2755
12758	12759	E2763	12764
V2765	V2766	E2767	E2773
12774	R2775	E2776	Y2777
V2778	L2779	E2780	Q2781
K2784	E2788	12789	

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	111.48Å 111.48Å 178.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.90 19.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	85.3 (19.99-2.90) 94.9 (19.99-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.282 0.250 , 0.284	Depositor DCC
R_{free} test set	5584 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.478 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18539	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2409e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.51	0/3117	1.02	21/4211 (0.5%)
1	B	0.53	0/3117	1.02	18/4211 (0.4%)
1	C	0.51	0/3117	1.02	20/4211 (0.5%)
1	D	0.52	0/3117	1.02	19/4211 (0.5%)
1	E	0.53	0/3117	1.03	21/4211 (0.5%)
1	F	0.53	0/3117	1.03	21/4211 (0.5%)
All	All	0.52	0/18702	1.02	120/25266 (0.5%)

There are no bond length outliers.

The worst 5 of 120 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1135	GLY	N-CA-C	11.28	127.08	114.67
1	E	2135	GLY	N-CA-C	10.95	126.72	114.67
1	F	2535	GLY	N-CA-C	10.90	126.66	114.67
1	B	535	GLY	N-CA-C	10.47	126.83	114.16
1	D	1535	GLY	N-CA-C	10.34	126.67	114.16

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3055	0	3140	289	0
1	B	3055	0	3138	293	0
1	C	3055	0	3137	295	1
1	D	3055	0	3138	304	1
1	E	3055	0	3138	302	1
1	F	3055	0	3138	310	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	22	0	10	2	0
3	B	22	0	10	1	0
3	C	22	0	10	1	0
3	D	22	0	10	2	0
3	E	22	0	10	1	0
3	F	22	0	10	1	0
4	A	8	0	0	0	0
4	B	10	0	0	0	0
4	C	9	0	0	2	0
4	D	10	0	0	0	0
4	E	16	0	0	1	0
4	F	12	0	0	1	0
All	All	18539	0	18889	1627	2

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 44.

The worst 5 of 1627 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LYS:HG3	1:A:336:PRO:HA	1.23	1.19
1:E:2322:LYS:HG3	1:E:2336:PRO:HA	1.23	1.15
1:B:722:LYS:HG3	1:B:736:PRO:HA	1.21	1.14
1:F:2722:LYS:HG3	1:F:2736:PRO:HA	1.23	1.11
1:A:157:ASP:HA	1:A:375:ARG:HH12	1.16	1.09

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2376:GLU:OE1	1:F:2776:GLU:OE1[3_884]	1.90	0.30
1:C:1373:GLU:OE2	1:D:1780:GLU:OE1[2_865]	2.17	0.03

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	387/395 (98%)	329 (85%)	44 (11%)	14 (4%)	2	11
1	B	387/395 (98%)	328 (85%)	40 (10%)	19 (5%)	1	6
1	C	387/395 (98%)	329 (85%)	45 (12%)	13 (3%)	3	12
1	D	387/395 (98%)	329 (85%)	41 (11%)	17 (4%)	2	8
1	E	387/395 (98%)	330 (85%)	40 (10%)	17 (4%)	2	8
1	F	387/395 (98%)	326 (84%)	42 (11%)	19 (5%)	1	6
All	All	2322/2370 (98%)	1971 (85%)	252 (11%)	99 (4%)	2	8

5 of 99 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	346	VAL
1	B	746	VAL
1	C	1346	VAL
1	D	1746	VAL
1	E	2346	VAL

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	321/321 (100%)	284 (88%)	37 (12%)	5	18
1	B	321/321 (100%)	283 (88%)	38 (12%)	5	17
1	C	321/321 (100%)	283 (88%)	38 (12%)	5	17
1	D	321/321 (100%)	284 (88%)	37 (12%)	5	18
1	E	321/321 (100%)	283 (88%)	38 (12%)	5	17
1	F	321/321 (100%)	283 (88%)	38 (12%)	5	17
All	All	1926/1926 (100%)	1700 (88%)	226 (12%)	5	17

5 of 226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1410	ASP
1	F	2759	ILE
1	D	1726	ARG
1	F	2733	HIS
1	F	2500	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	2381	GLN
1	F	2408	ASN
1	F	2578	HIS
1	C	1033	ASN
1	C	1008	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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
3	PCP	E	2392	-	21,22,22	1.34	3 (14%)	30,35,35	1.49	4 (13%)
3	PCP	B	792	-	21,22,22	1.38	4 (19%)	30,35,35	1.50	4 (13%)
3	PCP	A	392	-	21,22,22	1.40	4 (19%)	30,35,35	1.47	3 (10%)
3	PCP	D	1792	-	21,22,22	1.44	4 (19%)	30,35,35	1.51	4 (13%)
3	PCP	C	1392	-	21,22,22	1.41	4 (19%)	30,35,35	1.45	4 (13%)
3	PCP	F	2792	-	21,22,22	1.32	3 (14%)	30,35,35	1.51	4 (13%)

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	PCP	E	2392	-	-	4/17/33/33	0/1/1/1
3	PCP	B	792	-	-	4/17/33/33	0/1/1/1
3	PCP	A	392	-	-	4/17/33/33	0/1/1/1
3	PCP	D	1792	-	-	4/17/33/33	0/1/1/1
3	PCP	C	1392	-	-	4/17/33/33	0/1/1/1
3	PCP	F	2792	-	-	4/17/33/33	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1792	PCP	O1-C1	2.87	1.53	1.46
3	A	392	PCP	O1-C1	2.80	1.53	1.46
3	B	792	PCP	O1-C1	2.73	1.52	1.46
3	D	1792	PCP	PA-O3A	-2.73	1.56	1.59
3	F	2792	PCP	O1-C1	2.70	1.52	1.46

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2792	PCP	C4-C5-C1	5.90	113.24	103.73
3	D	1792	PCP	C4-C5-C1	5.83	113.11	103.73
3	B	792	PCP	C4-C5-C1	5.82	113.11	103.73
3	E	2392	PCP	C4-C5-C1	5.77	113.02	103.73
3	A	392	PCP	C4-C5-C1	5.75	112.98	103.73

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	392	PCP	CP-OP-P-O1P
3	A	392	PCP	CP-OP-P-O2P
3	A	392	PCP	CP-OP-P-O3P
3	B	792	PCP	CP-OP-P-O1P
3	B	792	PCP	CP-OP-P-O2P

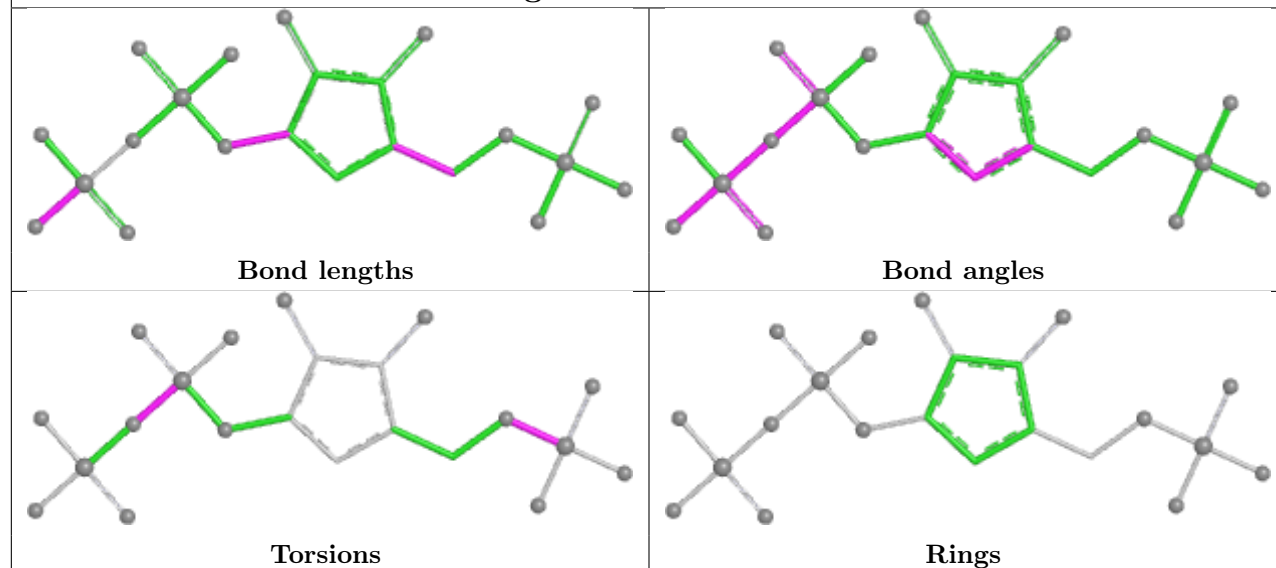
There are no ring outliers.

6 monomers are involved in 8 short contacts:

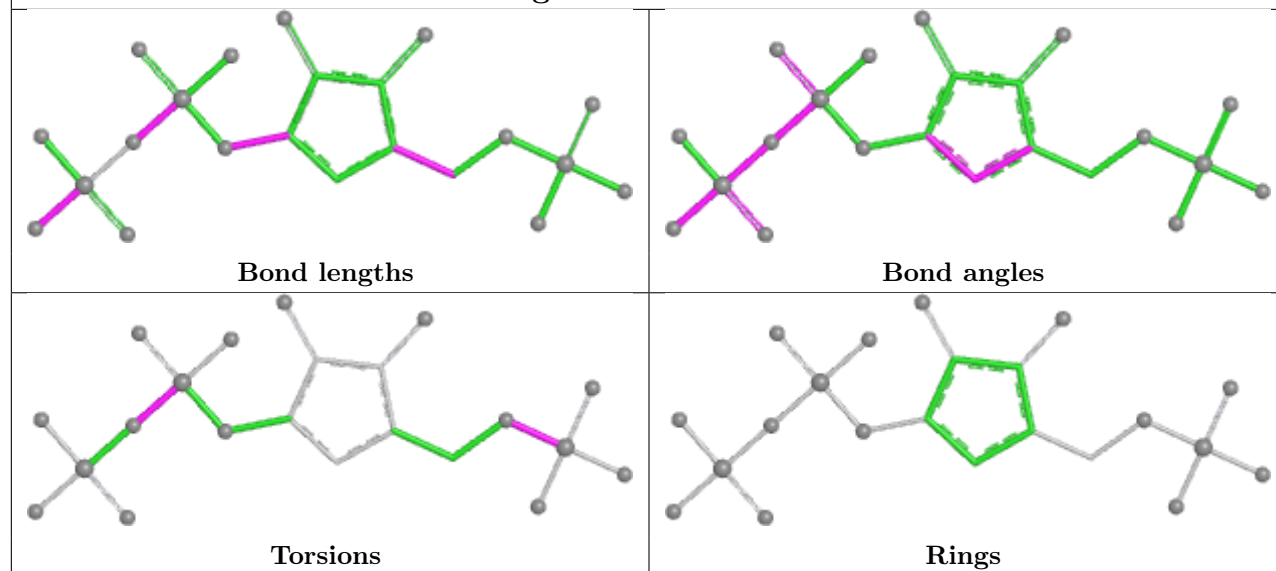
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2392	PCP	1	0
3	B	792	PCP	1	0
3	A	392	PCP	2	0
3	D	1792	PCP	2	0
3	C	1392	PCP	1	0
3	F	2792	PCP	1	0

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.

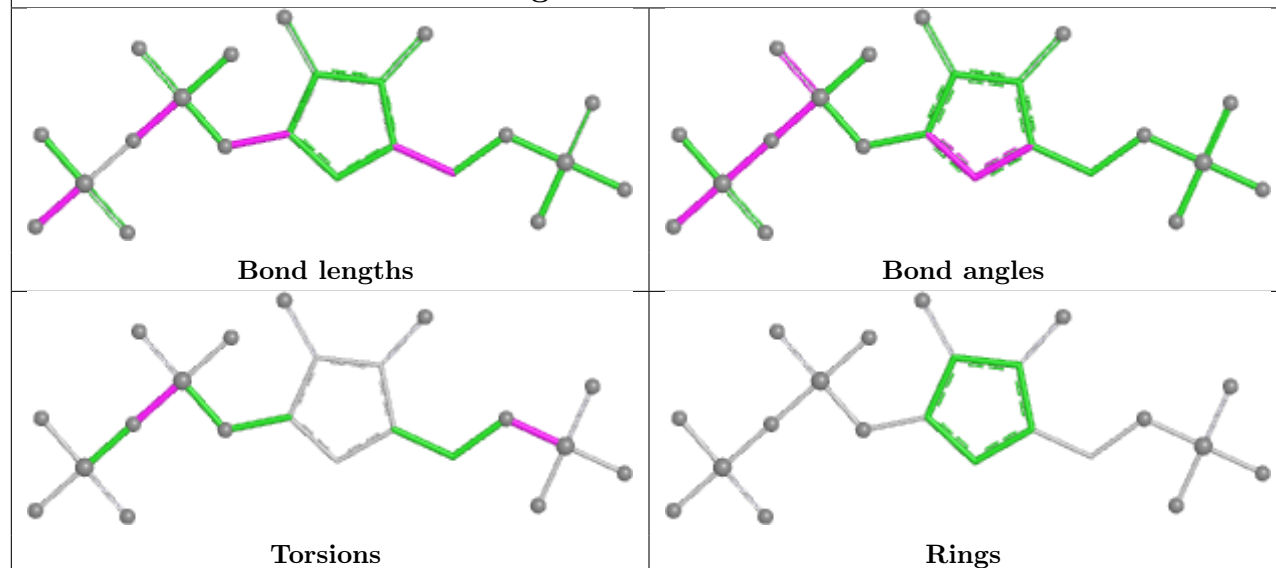
Ligand PCP E 2392



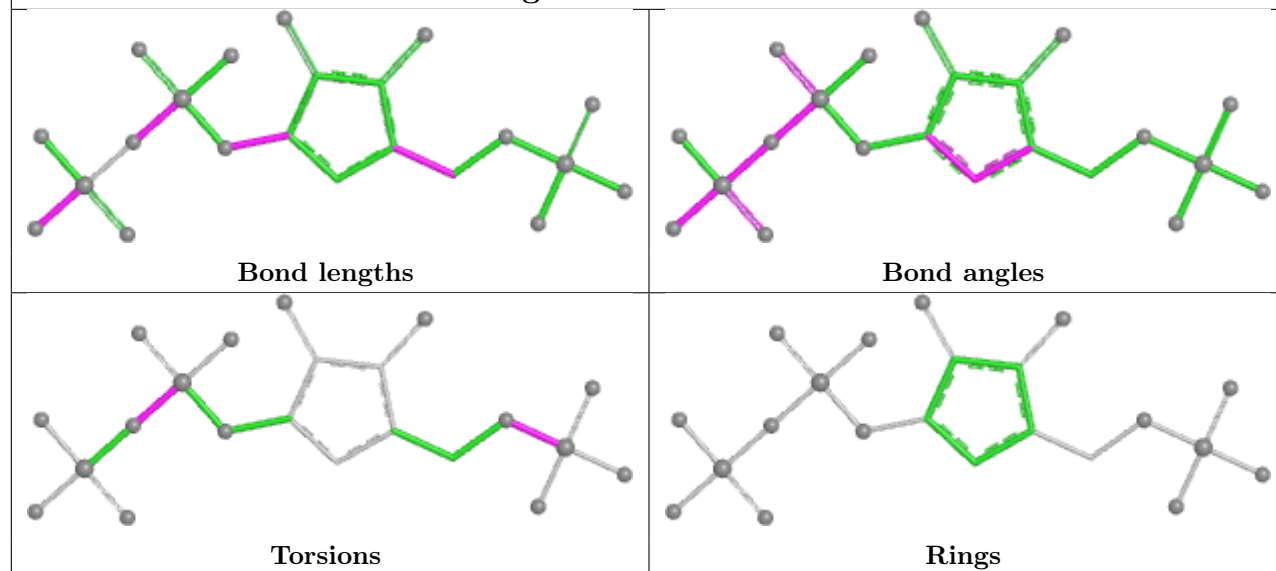
Ligand PCP B 792

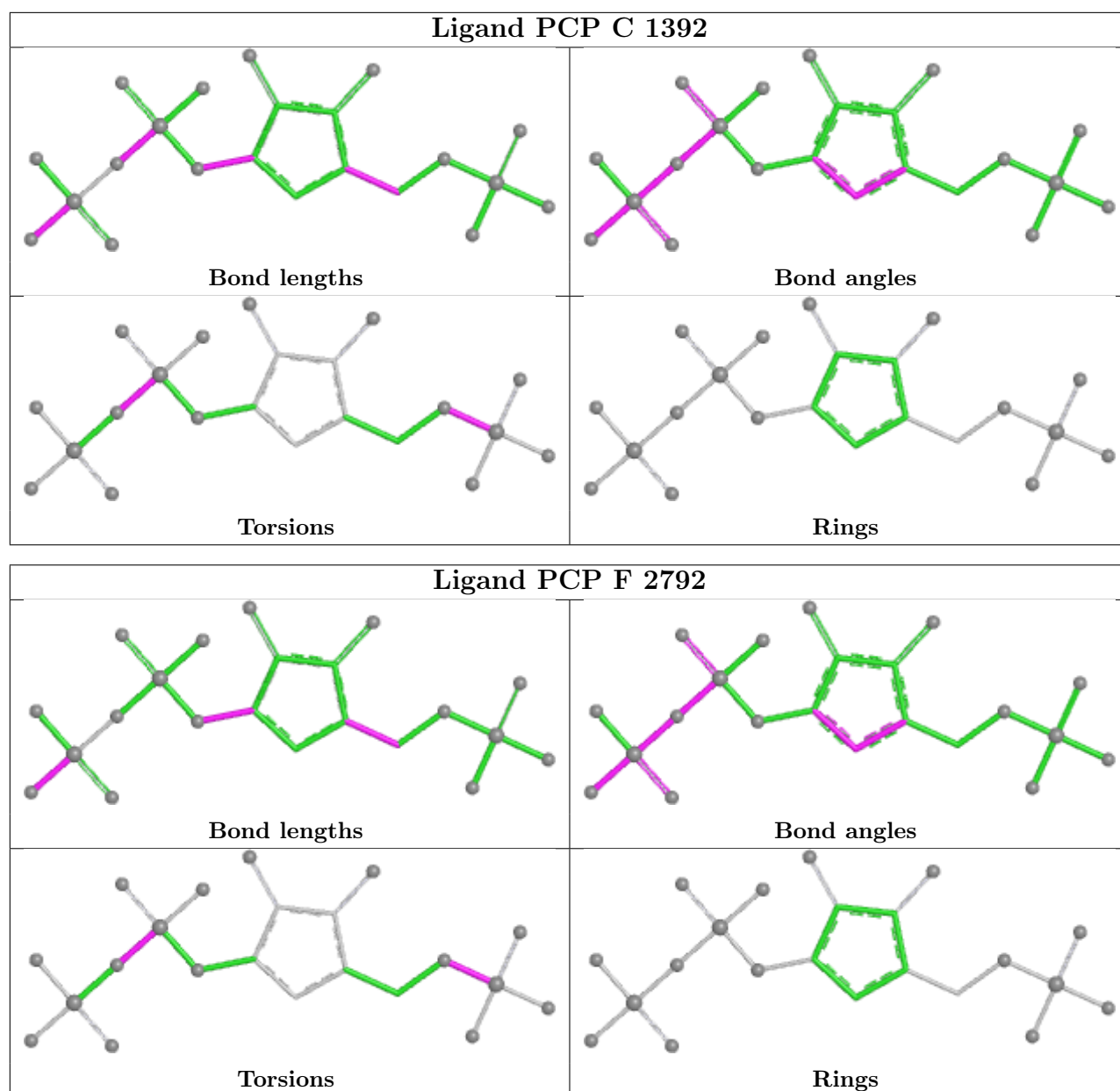


Ligand PCP A 392



Ligand PCP D 1792





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	389/395 (98%)	-0.98	0 100 100	32, 65, 86, 105	0
1	B	389/395 (98%)	-0.94	0 100 100	34, 66, 86, 106	0
1	C	389/395 (98%)	-0.97	0 100 100	31, 65, 85, 105	0
1	D	389/395 (98%)	-0.96	0 100 100	35, 66, 86, 106	0
1	E	389/395 (98%)	-0.96	0 100 100	32, 65, 86, 106	0
1	F	389/395 (98%)	-0.95	0 100 100	32, 65, 86, 106	0
All	All	2334/2370 (98%)	-0.96	0 100 100	31, 65, 87, 106	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PCP	B	792	22/22	0.97	0.07	103,109,112,112	0

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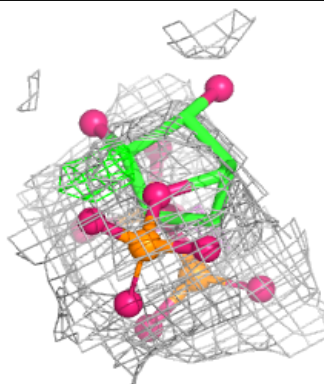
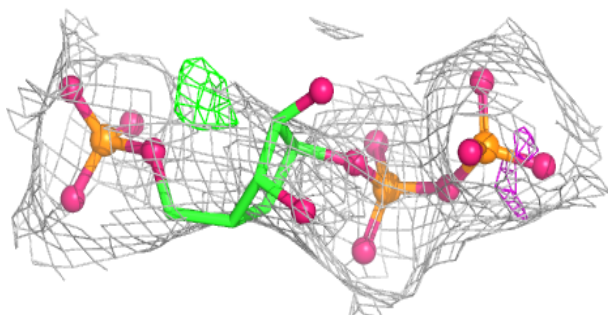
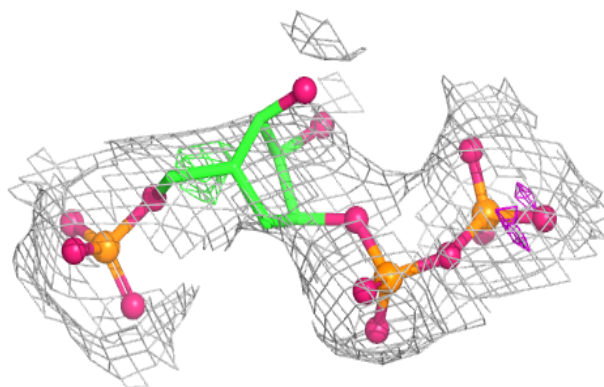
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PCP	A	392	22/22	0.98	0.06	103,109,112,112	0
3	PCP	C	1392	22/22	0.98	0.06	104,110,112,113	0
3	PCP	D	1792	22/22	0.98	0.06	102,109,112,113	0
3	PCP	E	2392	22/22	0.98	0.07	103,109,112,112	0
3	PCP	F	2792	22/22	0.98	0.06	103,109,112,112	0
2	ZN	B	793	1/1	0.99	0.02	85,85,85,85	0
2	ZN	C	1391	1/1	0.99	0.02	62,62,62,62	0
2	ZN	E	2391	1/1	0.99	0.02	82,82,82,82	0
2	ZN	E	2393	1/1	0.99	0.02	77,77,77,77	0
2	ZN	F	2791	1/1	0.99	0.02	83,83,83,83	0
2	ZN	F	2793	1/1	0.99	0.02	77,77,77,77	0
2	ZN	D	1791	1/1	1.00	0.02	77,77,77,77	0
2	ZN	D	1793	1/1	1.00	0.02	84,84,84,84	0
2	ZN	B	791	1/1	1.00	0.01	78,78,78,78	0
2	ZN	A	391	1/1	1.00	0.02	57,57,57,57	0
2	ZN	A	393	1/1	1.00	0.02	76,76,76,76	0
2	ZN	C	1393	1/1	1.00	0.01	85,85,85,85	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.

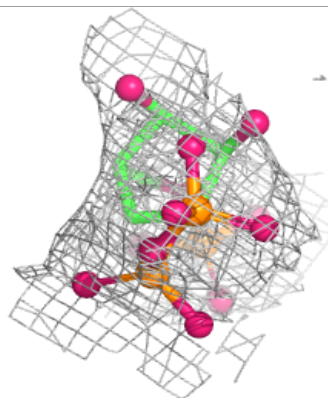
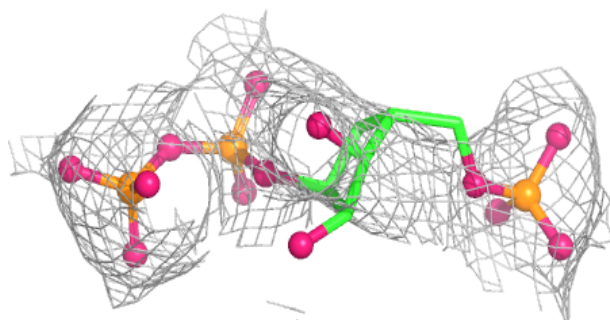
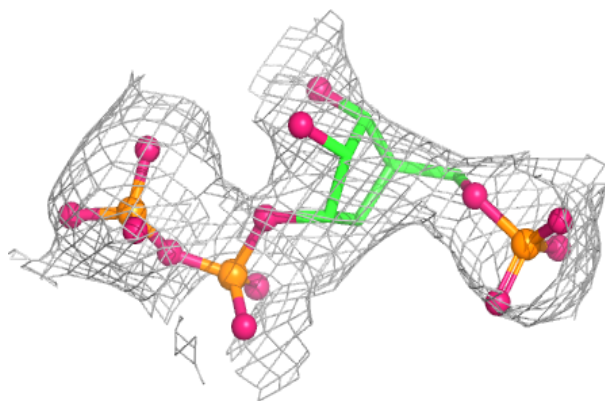
Electron density around PCP B 792:

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

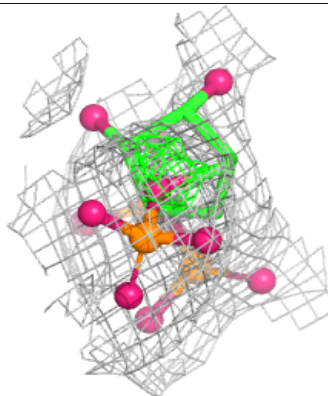
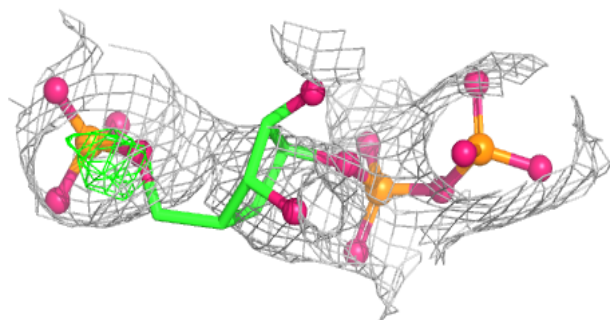
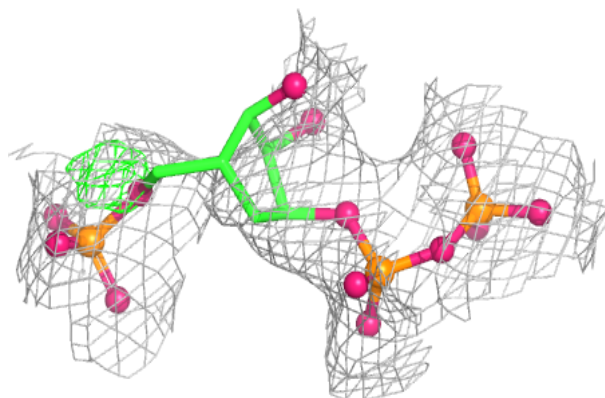


Electron density around PCP A 392:

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

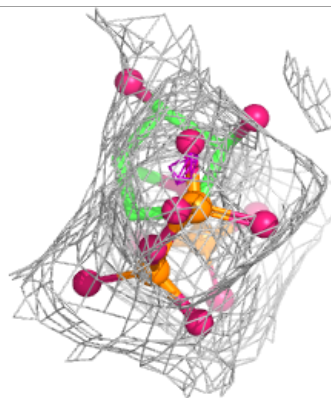
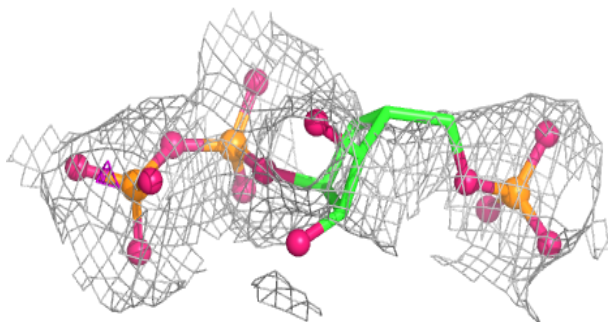
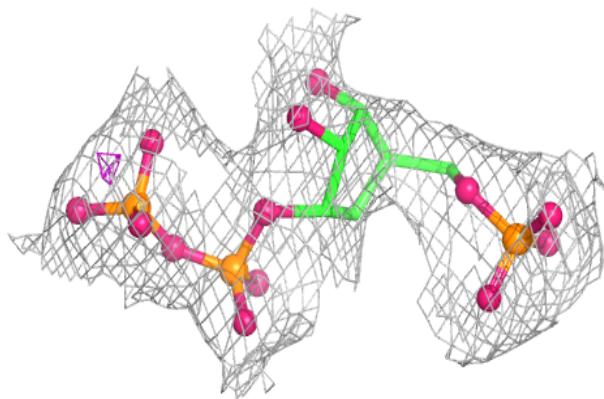
**Electron density around PCP C 1392:**

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

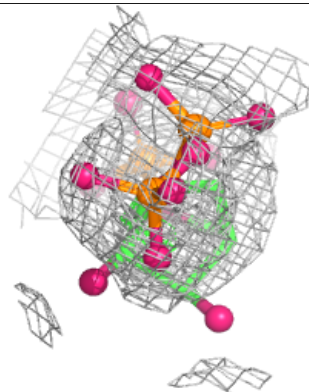
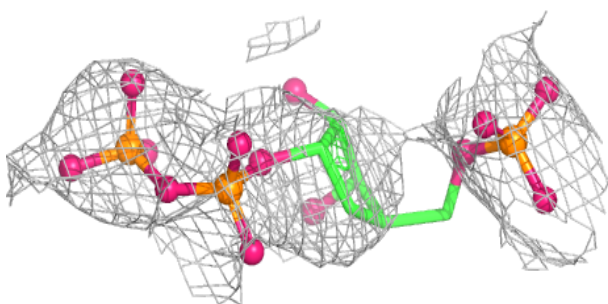
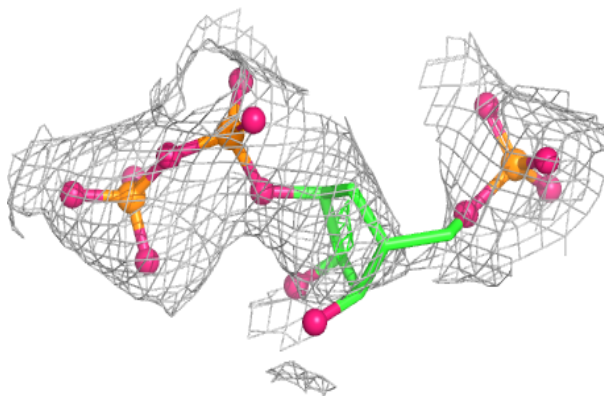


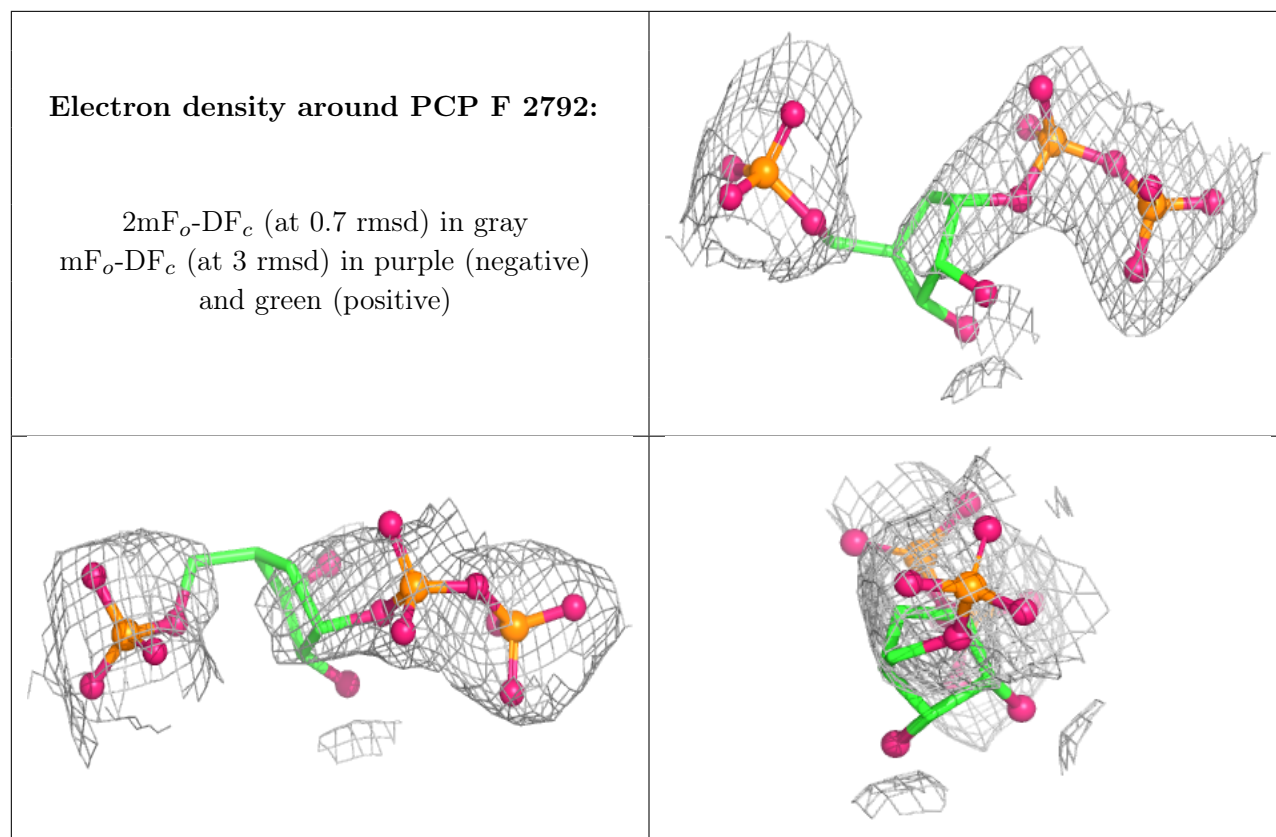
Electron density around PCP D 1792:

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

**Electron density around PCP E 2392:**

$2mF_o-DF_c$ (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.