



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 05:48 PM EDT

PDB ID : 1U80
Title : Phosphopantothienoylcysteine synthetase from E. coli, CMP complex
Authors : Stanitzek, S.; Augustin, M.A.; Huber, R.; Kupke, T.; Steinbacher, S.
Deposited on : 2004-08-04
Resolution : 2.85 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.23.2
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) : 2.23.2

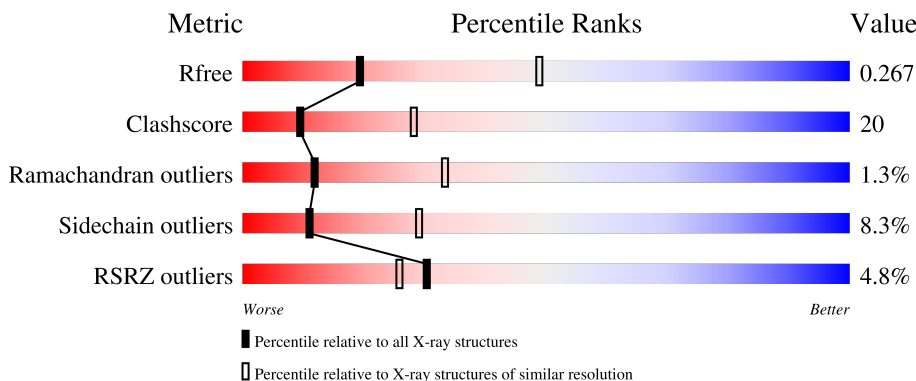
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	226	<div> <div>4%</div> <div>65%</div> <div>27%</div> <div>.</div> <div>.</div> </div>
1	B	226	<div> <div>6%</div> <div>64%</div> <div>28%</div> <div>.</div> <div>.</div> </div>
1	C	226	<div> <div>4%</div> <div>62%</div> <div>31%</div> <div>.</div> <div>.</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5209 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.

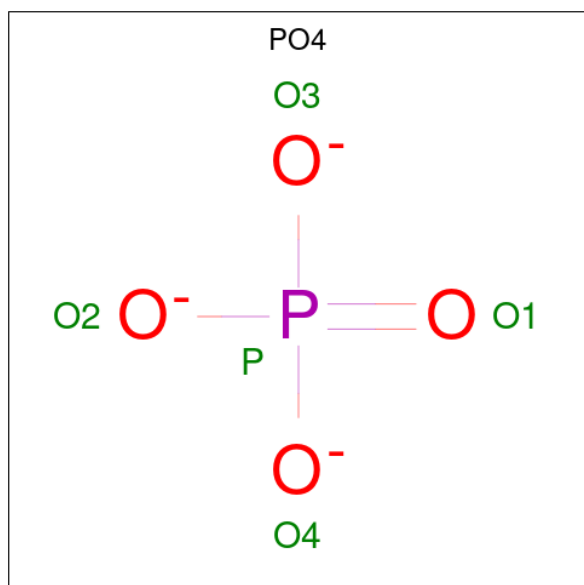
- Molecule 1 is a protein called Coenzyme A biosynthesis bifunctional protein coaBC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1676	1054	301	314	7			
1	B	218	Total	C	N	O	S	0	0	0
			1683	1056	303	317	7			
1	C	216	Total	C	N	O	S	0	0	0
			1666	1046	298	315	7			

There are 3 discrepancies between the modelled and reference sequences:

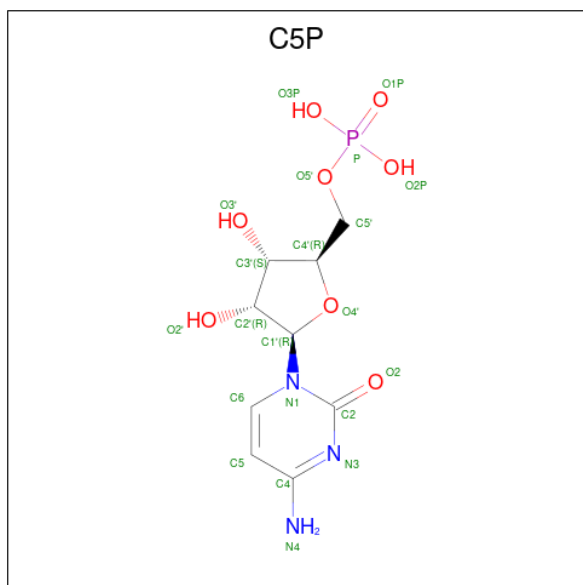
Chain	Residue	Modelled	Actual	Comment	Reference
A	210	ASP	ASN	engineered mutation	UNP P0ABQ0
B	210	ASP	ASN	engineered mutation	UNP P0ABQ0
C	210	ASP	ASN	engineered mutation	UNP P0ABQ0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0

- Molecule 3 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C5P) (formula: $C_9H_{14}N_3O_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 21 9 3 8 1	0	0
3	B	1	Total C N O P 21 9 3 8 1	0	0
3	C	1	Total C N O P 21 9 3 8 1	0	0


- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	30	Total O 30 30	0	0
4	B	46	Total O 46 46	0	0
4	C	30	Total O 30 30	0	0

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.

- Chain A:
-

- Chain B:
-
- 6% 64% 28%
- ASP E299 V314 L317 K318 D319 F327 A328 A329 E330 N331 N332 N333 V334 E335 E336 R339 Q340 K341 R342 R343 R344 K345 N346 L347 T350 N353 D354 V355 S356 Q357 F358 T359 Q360 G361 F362 N363 S364 D365 N366 N367 L371 D375 K378 P381 L382 E383 R384 K385 F386
- S181 P182 V183 N184 D185 L186 K187 H188 L189 N190 T194 P197 T198 R199 E200 D203 P204 V205 Y207 H211 S212 S213 M216 L220 A224 A225 R226 R227 G228 A229 N230 V234 S235 G236 N269 C274 V277 E288 K289 T290 LYS LYS GLN ALA THR GLN CTV

- Chain C: 

P381	L382	E383	R384	K385	E386	L387	L388	G389	Q390	L391	L392	L393	T398	R399	N404	R405	ARG
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	45.80Å 144.29Å 245.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.85 19.97 – 2.84	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.85) 98.2 (19.97-2.84)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.22 (at 2.83Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.275 0.202 , 0.267	Depositor DCC
R_{free} test set	936 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5209	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: C5P, PO4

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	0.59	0/1703	0.77	0/2309
1	B	0.64	0/1711	0.82	0/2321
1	C	0.58	1/1693 (0.1%)	0.79	2/2298 (0.1%)
All	All	0.61	1/5107 (0.0%)	0.79	2/6928 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	274	CYS	CB-SG	-5.86	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	344	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	C	344	ARG	NE-CZ-NH2	5.27	122.94	120.30

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	1676	0	1704	70	0
1	B	1683	0	1703	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1666	0	1682	71	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	21	0	12	2	0
3	B	21	0	12	3	0
3	C	21	0	12	2	0
4	A	30	0	0	4	0
4	B	46	0	0	4	0
4	C	30	0	0	1	0
All	All	5209	0	5125	200	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 20.

All (200) 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:190:ASN:H	1:C:269:ASN:ND2	1.37	1.21
1:B:190:ASN:H	1:B:269:ASN:ND2	1.44	1.14
1:A:190:ASN:H	1:A:269:ASN:ND2	1.44	1.14
1:C:190:ASN:N	1:C:269:ASN:HD22	1.52	1.06
1:B:190:ASN:H	1:B:269:ASN:HD22	1.03	0.97
1:A:190:ASN:N	1:A:269:ASN:HD22	1.66	0.92
1:A:206:ARG:HH11	1:A:290:ILE:HD12	1.41	0.84
1:A:398:THR:HG22	1:A:399:ARG:HH12	1.41	0.83
1:C:340:GLN:O	1:C:344:ARG:HG2	1.78	0.83
1:A:184:ASN:N	1:A:184:ASN:HD22	1.78	0.80
1:A:190:ASN:H	1:A:269:ASN:HD22	0.84	0.79
1:B:384:ARG:HG3	4:B:13:HOH:O	1.82	0.79
1:B:336:GLU:HA	1:B:336:GLU:OE1	1.82	0.79
1:B:190:ASN:N	1:B:269:ASN:HD22	1.80	0.77
1:A:190:ASN:N	1:A:269:ASN:ND2	2.28	0.75
1:B:190:ASN:N	1:B:269:ASN:ND2	2.28	0.75
1:C:336:GLU:OE1	1:C:336:GLU:HA	1.84	0.75
1:B:342:ARG:HH11	1:B:342:ARG:HG2	1.53	0.73
1:C:190:ASN:N	1:C:269:ASN:ND2	2.22	0.72
1:C:203:ASP:HB3	1:C:290:ILE:HD11	1.69	0.72
1:A:292:LYS:HD2	1:A:292:LYS:H	1.53	0.72
1:A:335:GLU:HG3	1:A:372:PHE:CZ	2.25	0.72
1:B:366:ASN:HB3	1:B:382:LEU:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLU:HB2	4:A:51:HOH:O	1.89	0.71
4:B:18:HOH:O	1:C:405:ARG:HD2	1.91	0.70
1:A:198:THR:CG2	1:A:200:GLU:OE2	2.40	0.70
1:C:366:ASN:HB3	1:C:382:LEU:HD11	1.75	0.68
1:B:226:ARG:NH2	1:B:390:GLN:HE21	1.91	0.67
1:C:190:ASN:H	1:C:269:ASN:HD22	0.70	0.67
1:A:184:ASN:N	1:A:184:ASN:ND2	2.43	0.67
1:C:206:ARG:HH11	1:C:290:ILE:HD12	1.60	0.67
1:B:328:ALA:HB2	1:B:350:ILE:HD11	1.79	0.65
1:A:187:LYS:HA	1:A:228:GLY:O	1.97	0.64
1:B:386:GLU:HB3	4:B:15:HOH:O	1.98	0.64
1:A:366:ASN:HB3	1:A:382:LEU:HD11	1.79	0.64
1:B:342:ARG:HG2	1:B:342:ARG:NH1	2.12	0.64
1:B:335:GLU:O	1:B:339:ARG:HG3	1.98	0.63
1:A:289:LYS:HZ3	1:A:292:LYS:HE3	1.64	0.62
1:C:399:ARG:HH11	1:C:399:ARG:HG2	1.61	0.62
1:A:336:GLU:HA	1:A:336:GLU:OE1	1.99	0.62
1:C:211:HIS:HB3	1:C:363:ASN:HD21	1.64	0.62
1:A:289:LYS:HZ3	1:A:292:LYS:CE	2.13	0.61
1:B:277:VAL:HB	3:B:1500:C5P:C4	2.32	0.60
1:C:247:LYS:HE3	4:C:63:HOH:O	2.01	0.60
1:A:206:ARG:NH1	1:A:290:ILE:HD12	2.15	0.59
1:A:206:ARG:HH11	1:A:290:ILE:CD1	2.12	0.58
1:C:224:ALA:HA	1:C:393:LEU:HD21	1.86	0.58
1:B:353:ASN:H	1:B:353:ASN:HD22	1.51	0.58
1:B:277:VAL:HB	3:B:1500:C5P:C5	2.34	0.58
1:C:226:ARG:NH2	1:C:390:GLN:HE21	2.01	0.58
1:C:220:ILE:HD11	1:C:392:LEU:HD23	1.86	0.58
1:A:291:LYS:NZ	1:C:405:ARG:HH12	2.02	0.57
1:C:399:ARG:HH11	1:C:399:ARG:CA	2.16	0.57
1:C:399:ARG:HH11	1:C:399:ARG:CG	2.18	0.57
1:B:198:THR:CG2	1:B:200:GLU:OE2	2.53	0.56
1:B:353:ASN:H	1:B:353:ASN:ND2	2.04	0.56
1:C:314:VAL:O	1:C:317:LEU:HB2	2.05	0.56
1:A:341:LYS:HE3	3:A:500:C5P:O2P	2.06	0.56
1:C:208:ILE:HD12	1:C:304:MET:CE	2.35	0.56
1:A:281:ARG:NH1	1:A:305:VAL:HG21	2.20	0.56
1:A:211:HIS:HB3	1:A:363:ASN:HD21	1.70	0.56
1:A:353:ASN:HB3	1:A:369:LEU:HD23	1.87	0.55
1:C:198:THR:HG21	1:C:254:ALA:N	2.22	0.55
1:A:398:THR:HA	4:A:9:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:THR:CG2	1:A:399:ARG:HH12	2.18	0.55
1:C:202:LEU:HD21	1:C:208:ILE:HG13	1.87	0.54
1:A:309:ASP:HA	3:A:500:C5P:N4	2.22	0.54
1:C:208:ILE:HD12	1:C:304:MET:HE2	1.90	0.54
1:C:398:THR:HG22	1:C:399:ARG:HH12	1.72	0.54
1:A:342:ARG:HH11	1:A:342:ARG:HG2	1.72	0.54
1:C:335:GLU:HG3	1:C:372:PHE:CZ	2.43	0.54
1:A:402:GLU:O	1:A:405:ARG:HB2	2.07	0.53
1:A:398:THR:HG22	1:A:399:ARG:NH1	2.17	0.53
1:A:203:ASP:HB2	1:A:204:PRO:CD	2.38	0.53
1:C:341:LYS:HE3	3:C:2500:C5P:O1P	2.08	0.53
1:A:203:ASP:HB3	1:A:290:ILE:HG13	1.90	0.53
1:A:292:LYS:HD2	1:A:292:LYS:N	2.23	0.53
1:C:203:ASP:HB2	1:C:204:PRO:CD	2.38	0.53
1:A:184:ASN:ND2	1:A:184:ASN:H	2.06	0.53
1:C:399:ARG:HG2	1:C:399:ARG:NH1	2.20	0.52
1:B:345:LYS:O	1:B:346:ASN:HB3	2.08	0.52
1:C:206:ARG:HH11	1:C:290:ILE:CD1	2.22	0.52
1:A:208:ILE:HD12	1:A:304:MET:HE1	1.90	0.52
1:C:330:GLU:HB2	1:C:334:VAL:HG22	1.92	0.52
1:A:401:ASP:O	1:A:405:ARG:HD3	2.10	0.52
1:B:342:ARG:NH1	1:B:347:LEU:O	2.42	0.52
1:C:198:THR:HG21	1:C:254:ALA:CA	2.40	0.51
1:C:335:GLU:O	1:C:339:ARG:HG3	2.10	0.51
1:A:208:ILE:HD12	1:A:304:MET:CE	2.41	0.51
1:C:383:GLU:CG	1:C:387:LEU:HD23	2.41	0.51
1:B:187:LYS:HA	1:B:228:GLY:O	2.11	0.50
1:A:335:GLU:OE1	1:A:339:ARG:HD2	2.12	0.50
1:B:183:VAL:O	1:B:184:ASN:HB3	2.12	0.50
1:A:342:ARG:HD2	1:A:373:TRP:HA	1.94	0.50
1:C:226:ARG:HH21	1:C:390:GLN:HE21	1.60	0.50
1:A:330:GLU:HB2	1:A:334:VAL:HG22	1.95	0.49
1:A:224:ALA:HA	1:A:393:LEU:HD21	1.95	0.49
1:C:199:ARG:HD3	1:C:207:TYR:CE1	2.48	0.48
1:C:342:ARG:HG2	1:C:342:ARG:HH11	1.78	0.48
1:A:290:ILE:HG22	1:A:290:ILE:O	2.12	0.48
1:A:291:LYS:HZ2	1:C:405:ARG:NH1	2.10	0.48
1:C:370:HIS:CD2	1:C:379:VAL:HG22	2.49	0.48
1:C:265:VAL:HG21	1:C:314:VAL:HG13	1.95	0.48
1:C:309:ASP:OD2	1:C:345:LYS:HE2	2.14	0.48
1:A:299:GLU:O	1:A:300:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ASN:HD22	1:A:353:ASN:H	1.62	0.48
1:A:342:ARG:HG2	1:A:342:ARG:NH1	2.29	0.48
1:C:353:ASN:HB3	1:C:369:LEU:HD23	1.96	0.48
1:C:353:ASN:ND2	1:C:353:ASN:H	2.12	0.48
1:A:335:GLU:O	1:A:339:ARG:HG3	2.13	0.48
1:B:405:ARG:HD3	1:B:405:ARG:HA	1.74	0.48
1:C:399:ARG:HH11	1:C:399:ARG:HA	1.79	0.47
1:A:353:ASN:H	1:A:353:ASN:ND2	2.12	0.47
1:C:198:THR:HG21	1:C:254:ALA:HA	1.97	0.47
1:B:216:MET:O	1:B:220:ILE:HG13	2.14	0.47
1:C:353:ASN:H	1:C:353:ASN:HD22	1.61	0.47
1:A:220:ILE:HD11	1:A:392:LEU:HD23	1.97	0.47
1:A:314:VAL:O	1:A:317:LEU:HB2	2.15	0.47
1:B:226:ARG:HH21	1:B:390:GLN:HE21	1.61	0.47
1:C:187:LYS:HA	1:C:228:GLY:O	2.14	0.47
1:C:208:ILE:CD1	1:C:304:MET:HE2	2.45	0.47
1:C:311:VAL:CG1	1:C:312:ALA:N	2.78	0.46
1:B:353:ASN:ND2	1:B:353:ASN:N	2.61	0.46
1:A:319:ASP:O	1:A:320:HIS:HB2	2.15	0.46
1:B:197:PRO:O	1:B:236:GLY:HA3	2.15	0.46
1:C:311:VAL:HG13	1:C:312:ALA:N	2.31	0.46
1:A:299:GLU:HA	1:A:299:GLU:OE1	2.15	0.46
1:B:190:ASN:OD1	1:B:230:ASN:HB3	2.16	0.45
1:B:224:ALA:HA	1:B:393:LEU:HD21	1.97	0.45
1:B:381:PRO:O	1:B:383:GLU:HG2	2.16	0.45
1:B:327:PHE:O	3:B:1500:C5P:H5'2	2.16	0.45
1:A:353:ASN:ND2	1:A:353:ASN:N	2.64	0.45
1:B:382:LEU:O	1:B:383:GLU:HG2	2.17	0.45
1:B:328:ALA:O	1:B:353:ASN:ND2	2.50	0.45
1:B:185:ASP:OD2	1:B:185:ASP:N	2.50	0.45
1:B:318:LYS:CE	1:C:376:GLY:HA2	2.47	0.45
1:B:342:ARG:HH11	1:B:342:ARG:CG	2.25	0.45
1:A:291:LYS:HZ1	1:C:405:ARG:HH12	1.65	0.45
1:B:398:THR:HG22	1:B:399:ARG:HH12	1.79	0.45
1:A:291:LYS:NZ	1:C:405:ARG:NH1	2.64	0.44
1:A:290:ILE:O	1:A:291:LYS:O	2.36	0.44
1:C:309:ASP:HA	3:C:2500:C5P:N4	2.33	0.44
1:B:288:GLU:O	1:B:289:LYS:C	2.55	0.44
1:B:366:ASN:HA	1:B:383:GLU:O	2.18	0.44
1:B:199:ARG:HD3	1:B:207:TYR:CE1	2.54	0.43
1:B:211:HIS:HB3	1:B:363:ASN:HD21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ILE:CD1	1:B:392:LEU:HD23	2.47	0.43
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.77	0.43
1:A:385:LYS:HA	1:A:388:LEU:HB3	1.99	0.43
1:B:213:SER:HB3	1:B:363:ASN:HA	2.01	0.43
1:B:314:VAL:O	1:B:317:LEU:HB2	2.19	0.43
1:C:239:SER:O	1:C:240:LEU:HD23	2.19	0.43
1:B:182:PRO:O	1:B:183:VAL:O	2.36	0.43
1:C:319:ASP:O	1:C:320:HIS:HB2	2.19	0.43
1:B:367:ASN:N	1:B:382:LEU:HD12	2.34	0.43
1:C:341:LYS:HA	1:C:344:ARG:HG3	2.00	0.43
1:C:353:ASN:ND2	1:C:353:ASN:N	2.66	0.43
1:A:289:LYS:O	1:A:291:LYS:N	2.52	0.42
1:A:349:LEU:HD11	1:A:371:LEU:HB3	2.01	0.42
1:B:362:PHE:O	1:B:363:ASN:HB2	2.20	0.42
1:C:281:ARG:HD3	1:C:307:ASN:HD21	1.83	0.42
1:B:199:ARG:HD3	1:B:207:TYR:CD1	2.55	0.42
1:B:336:GLU:OE1	1:B:336:GLU:CA	2.61	0.42
1:B:194:THR:HA	1:B:234:VAL:O	2.20	0.42
1:C:203:ASP:OD2	1:C:203:ASP:C	2.58	0.42
1:C:399:ARG:NH1	1:C:399:ARG:HA	2.35	0.42
1:B:341:LYS:O	1:B:342:ARG:C	2.58	0.42
1:A:267:GLN:HG2	4:A:99:HOH:O	2.20	0.42
1:B:203:ASP:HB2	1:B:204:PRO:CD	2.50	0.42
1:B:381:PRO:O	1:B:382:LEU:C	2.58	0.42
1:B:181:SER:HB2	1:B:182:PRO:HD2	2.02	0.41
1:B:367:ASN:C	1:B:382:LEU:HD12	2.40	0.41
1:B:371:LEU:HD12	1:B:395:GLU:HG2	2.01	0.41
1:C:385:LYS:HA	1:C:388:LEU:HB3	2.02	0.41
1:A:335:GLU:CB	4:A:51:HOH:O	2.57	0.41
1:A:292:LYS:HB2	1:C:405:ARG:HE	1.84	0.41
1:A:289:LYS:NZ	1:A:292:LYS:CE	2.80	0.41
1:B:386:GLU:CB	4:B:15:HOH:O	2.64	0.41
1:C:198:THR:HG22	1:C:253:THR:C	2.41	0.41
1:A:184:ASN:O	1:A:187:LYS:HG2	2.21	0.41
1:B:388:LEU:HD12	1:B:388:LEU:HA	1.85	0.41
1:C:190:ASN:OD1	1:C:230:ASN:HB3	2.21	0.41
1:C:203:ASP:HB2	1:C:204:PRO:HD2	2.03	0.41
1:C:268:GLN:O	1:C:322:PRO:HB3	2.21	0.41
1:B:383:GLU:HA	1:B:383:GLU:OE1	2.20	0.40
1:C:197:PRO:O	1:C:236:GLY:HA3	2.21	0.40
1:C:381:PRO:O	1:C:382:LEU:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ASP:C	1:A:203:ASP:OD2	2.59	0.40
1:A:307:ASN:HD22	1:A:307:ASN:HA	1.66	0.40
1:C:342:ARG:HG2	1:C:342:ARG:NH1	2.36	0.40
1:A:197:PRO:O	1:A:236:GLY:HA3	2.22	0.40
1:A:226:ARG:NH2	1:A:390:GLN:HE21	2.20	0.40
1:B:190:ASN:HB2	1:B:269:ASN:ND2	2.36	0.40
1:B:353:ASN:HD22	1:B:353:ASN:N	2.15	0.40
1:C:367:ASN:O	1:C:388:LEU:HD22	2.20	0.40
1:A:353:ASN:HD22	1:A:353:ASN:C	2.20	0.40
1:B:203:ASP:OD2	1:B:203:ASP:C	2.60	0.40
1:B:220:ILE:HD11	1:B:392:LEU:HD23	2.04	0.40
1:B:329:ALA:HA	1:B:353:ASN:ND2	2.36	0.40
1:B:329:ALA:HB1	1:B:355:VAL:HG21	2.02	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	213/226 (94%)	189 (89%)	20 (9%)	4 (2%)	8	24
1	B	214/226 (95%)	191 (89%)	20 (9%)	3 (1%)	11	31
1	C	212/226 (94%)	195 (92%)	16 (8%)	1 (0%)	29	57
All	All	639/678 (94%)	575 (90%)	56 (9%)	8 (1%)	12	33

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	LYS
1	B	183	VAL
1	B	184	ASN
1	A	184	ASN

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Mol	Chain	Res	Type
1	A	290	ILE
1	B	382	LEU
1	C	289	LYS
1	A	300	LEU

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	180/187 (96%)	165 (92%)	15 (8%)	11	29
1	B	181/187 (97%)	165 (91%)	16 (9%)	10	26
1	C	179/187 (96%)	165 (92%)	14 (8%)	12	32
All	All	540/561 (96%)	495 (92%)	45 (8%)	11	29

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	198	THR
1	A	292	LYS
1	A	301	THR
1	A	317	LEU
1	A	333	ASN
1	A	344	ARG
1	A	353	ASN
1	A	360	GLN
1	A	362	PHE
1	A	375	ASP
1	A	378	LYS
1	A	384	ARG
1	A	399	ARG
1	A	404	ASN
1	B	189	LEU
1	B	198	THR
1	B	205	VAL

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Mol	Chain	Res	Type
1	B	274	CYS
1	B	317	LEU
1	B	319	ASP
1	B	333	ASN
1	B	336	GLU
1	B	344	ARG
1	B	353	ASN
1	B	362	PHE
1	B	375	ASP
1	B	378	LYS
1	B	394	ASP
1	B	399	ARG
1	B	405	ARG
1	C	198	THR
1	C	307	ASN
1	C	317	LEU
1	C	336	GLU
1	C	344	ARG
1	C	353	ASN
1	C	360	GLN
1	C	362	PHE
1	C	375	ASP
1	C	378	LYS
1	C	384	ARG
1	C	399	ARG
1	C	404	ASN
1	C	405	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	230	ASN
1	A	262	ASN
1	A	269	ASN
1	A	307	ASN
1	A	333	ASN
1	A	346	ASN
1	A	353	ASN
1	A	363	ASN
1	A	390	GLN
1	B	230	ASN

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Mol	Chain	Res	Type
1	B	269	ASN
1	B	307	ASN
1	B	333	ASN
1	B	346	ASN
1	B	353	ASN
1	B	360	GLN
1	B	363	ASN
1	B	390	GLN
1	C	230	ASN
1	C	269	ASN
1	C	307	ASN
1	C	333	ASN
1	C	346	ASN
1	C	353	ASN
1	C	363	ASN
1	C	390	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
2	PO4	C	2501	-	4,4,4	1.71	1 (25%)	6,6,6	0.38	0
3	C5P	A	500	-	19,22,22	1.49	3 (15%)	24,33,33	1.49	2 (8%)
2	PO4	A	501	-	4,4,4	1.37	0	6,6,6	0.49	0
2	PO4	B	1501	-	4,4,4	1.59	0	6,6,6	0.45	0
3	C5P	B	1500	-	19,22,22	1.54	4 (21%)	24,33,33	1.47	2 (8%)
3	C5P	C	2500	-	19,22,22	1.52	4 (21%)	24,33,33	1.44	2 (8%)

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	C5P	A	500	-	-	4/8/26/26	0/2/2/2
3	C5P	C	2500	-	-	0/8/26/26	0/2/2/2
3	C5P	B	1500	-	-	2/8/26/26	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1500	C5P	C6-N1	3.94	1.40	1.35
3	C	2500	C5P	C6-N1	3.79	1.40	1.35
3	A	500	C5P	C6-N1	3.78	1.40	1.35
3	A	500	C5P	P-O1P	3.43	1.61	1.50
3	C	2500	C5P	P-O1P	3.41	1.61	1.50
3	B	1500	C5P	P-O1P	3.39	1.61	1.50
3	C	2500	C5P	O4'-C1'	2.36	1.44	1.41
2	C	2501	PO4	P-O3	-2.22	1.47	1.54
3	B	1500	C5P	C2-N3	-2.20	1.33	1.38
3	A	500	C5P	O4'-C1'	2.18	1.44	1.41
3	B	1500	C5P	O4'-C1'	2.16	1.44	1.41
3	C	2500	C5P	C2-N3	-2.01	1.34	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2500	C5P	C2-N3-C4	5.44	121.85	116.34
3	A	500	C5P	C2-N3-C4	5.34	121.75	116.34
3	B	1500	C5P	C2-N3-C4	5.21	121.63	116.34
3	C	2500	C5P	O2P-P-O5'	2.36	113.00	106.73
3	B	1500	C5P	O2P-P-O5'	2.30	112.86	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	C5P	O2P-P-O5'	2.15	112.45	106.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	C5P	C5'-O5'-P-O3P
3	B	1500	C5P	O4'-C1'-N1-C6
3	B	1500	C5P	C2'-C1'-N1-C6
3	A	500	C5P	O4'-C4'-C5'-O5'
3	A	500	C5P	C3'-C4'-C5'-O5'
3	A	500	C5P	C5'-O5'-P-O2P

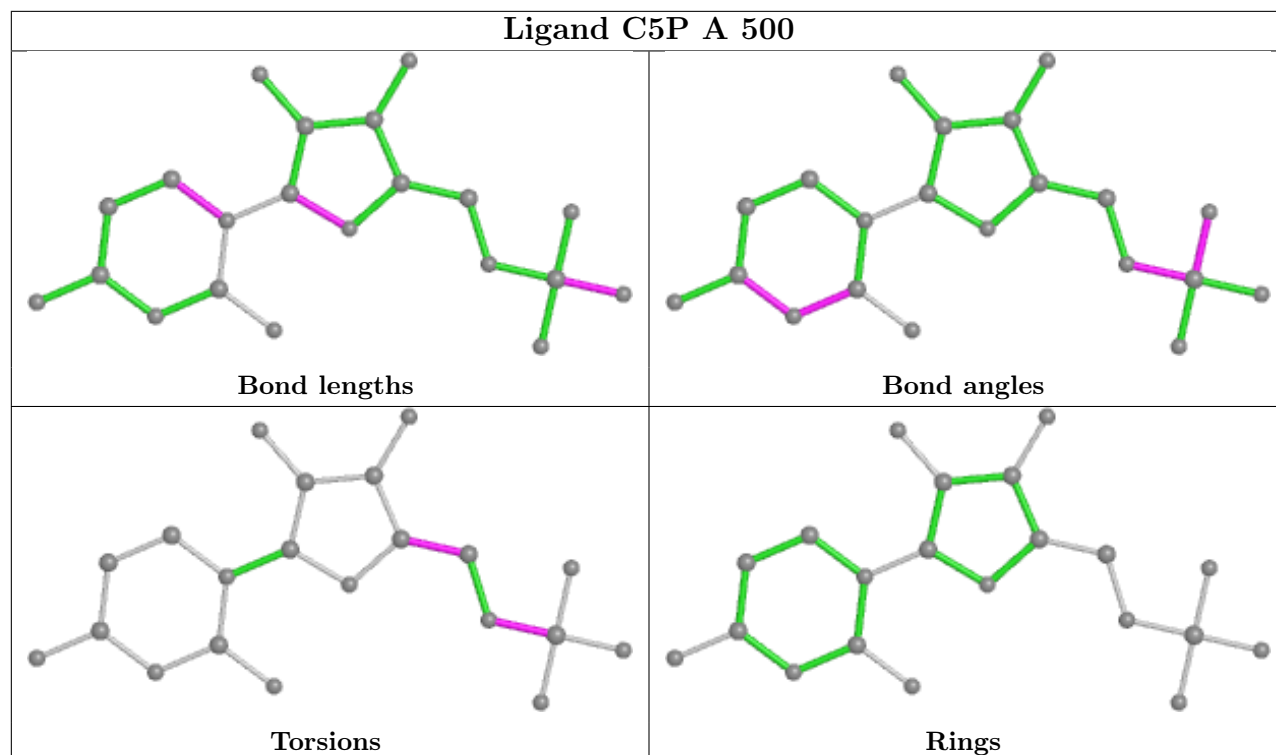
There are no ring outliers.

3 monomers are involved in 7 short contacts:

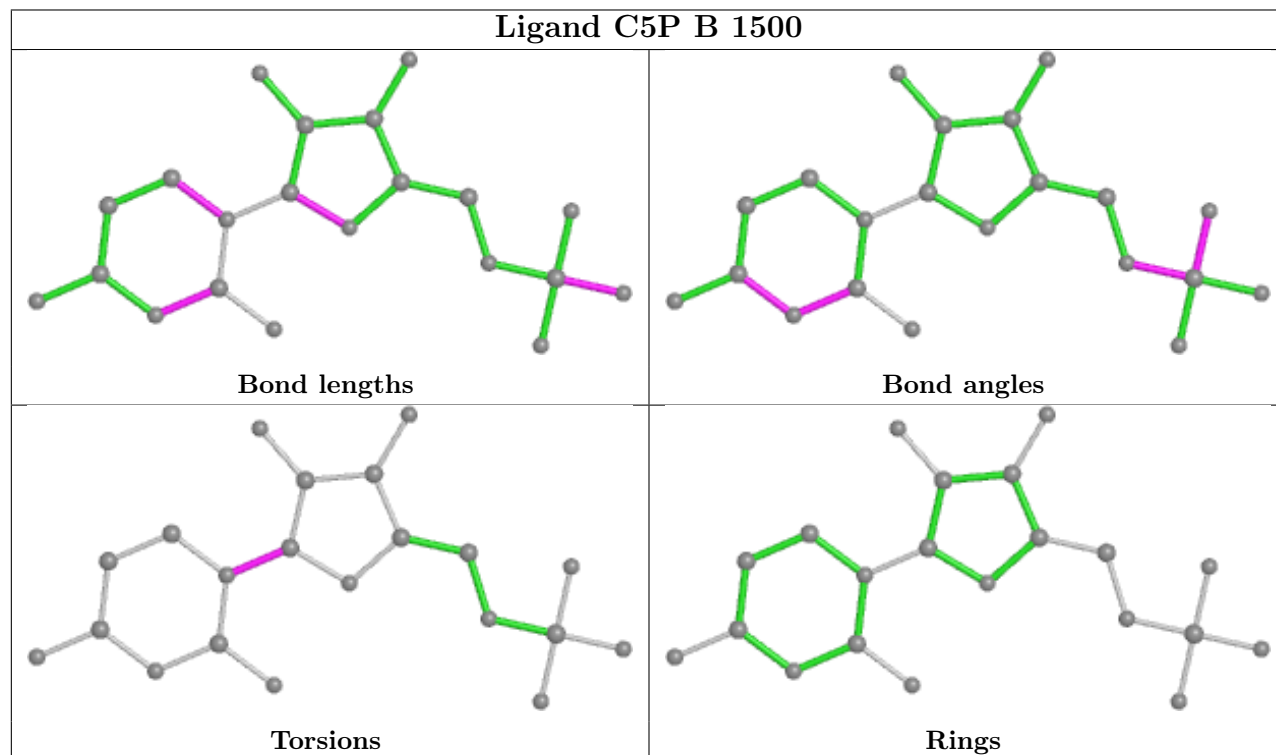
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	C5P	2	0
3	B	1500	C5P	3	0
3	C	2500	C5P	2	0

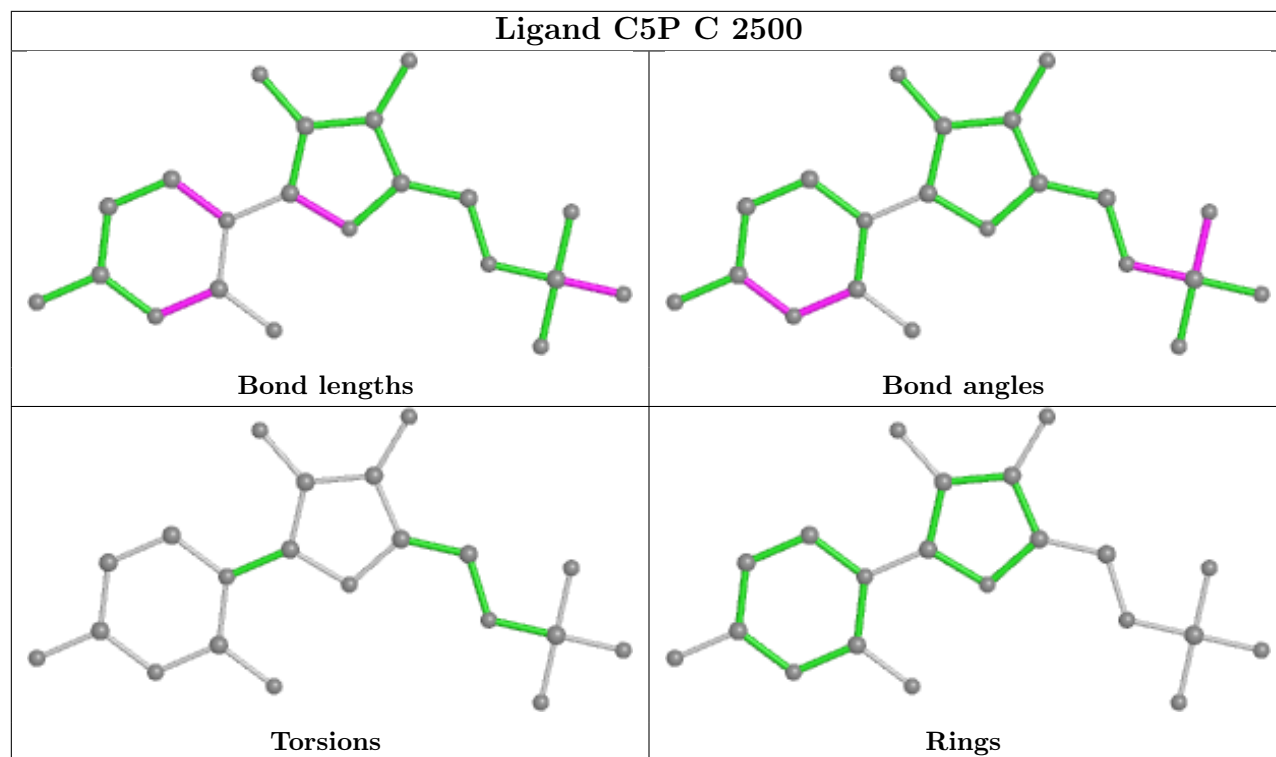
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 C5P A 500



Ligand C5P B 1500





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, 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	217/226 (96%)	-0.11	8 (3%) 41 36	29, 63, 106, 148	0
1	B	218/226 (96%)	-0.18	14 (6%) 19 15	24, 46, 124, 150	0
1	C	216/226 (95%)	-0.17	9 (4%) 36 31	33, 61, 120, 141	0
All	All	651/678 (96%)	-0.15	31 (4%) 30 26	24, 57, 116, 150	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	LYS	9.1
1	B	361	GLY	6.3
1	B	366	ASN	6.1
1	B	360	GLN	5.4
1	B	406	ARG	5.0
1	A	188	HIS	4.7
1	B	358	PRO	4.5
1	C	358	PRO	4.4
1	C	357	GLN	4.2
1	B	363	ASN	4.1
1	A	359	THR	3.9
1	C	359	THR	3.9
1	A	183	VAL	3.8
1	B	362	PHE	3.8
1	B	182	PRO	3.7
1	C	360	GLN	3.5
1	B	181	SER	3.5
1	B	359	THR	3.3
1	C	362	PHE	3.2
1	C	298	ASP	3.0
1	B	357	GLN	2.9
1	A	375	ASP	2.9
1	C	337	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	358	PRO	2.7
1	C	356	SER	2.5
1	A	287	PRO	2.5
1	B	367	ASN	2.3
1	B	331	THR	2.2
1	C	405	ARG	2.1
1	B	364	SER	2.1
1	A	318	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

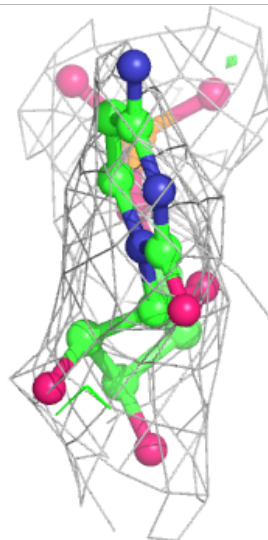
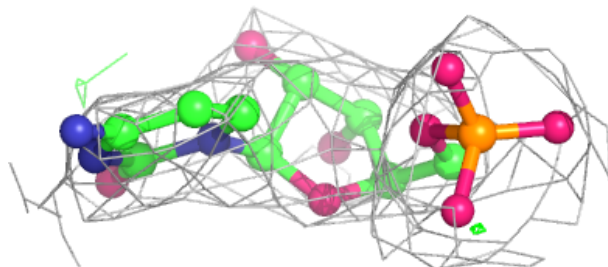
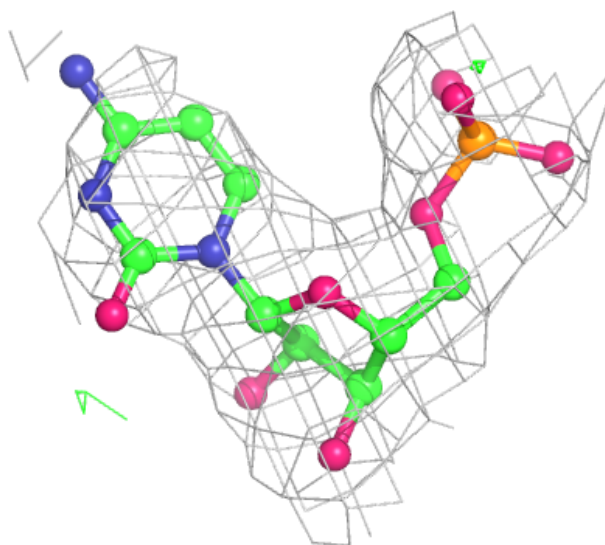
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	C5P	A	500	21/21	0.92	0.18	66,89,111,112	0
2	PO4	B	1501	5/5	0.93	0.15	99,104,106,106	0
2	PO4	C	2501	5/5	0.95	0.15	66,68,74,77	0
3	C5P	C	2500	21/21	0.95	0.15	48,68,82,85	0
3	C5P	B	1500	21/21	0.96	0.12	49,66,81,86	0
2	PO4	A	501	5/5	0.96	0.18	38,55,65,68	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.

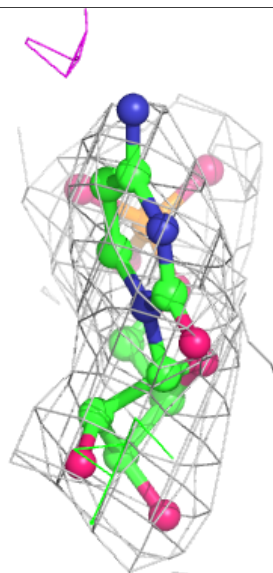
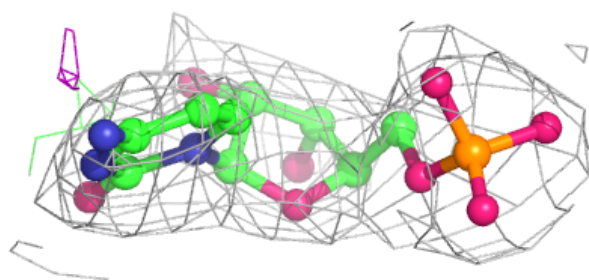
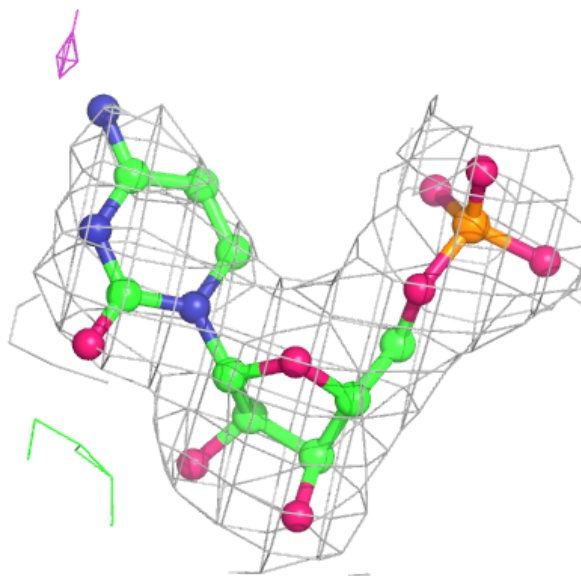
Electron density around C5P A 500:

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



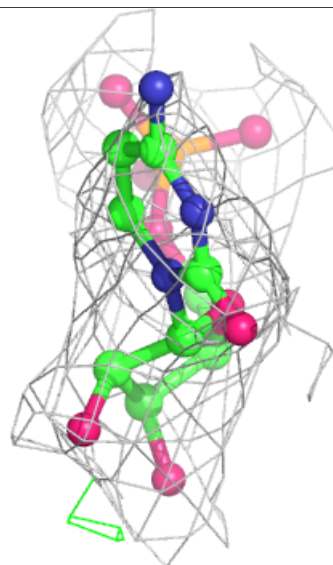
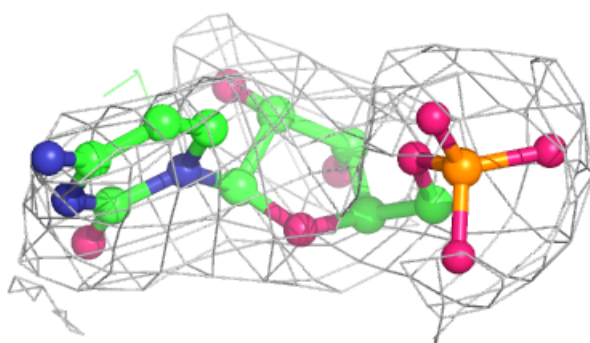
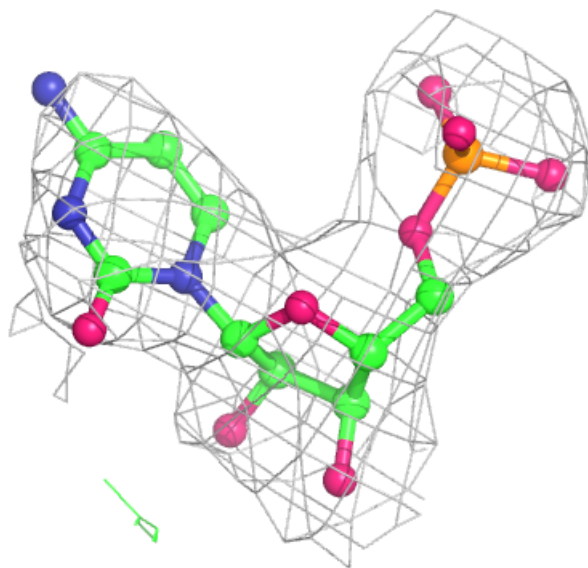
Electron density around C5P C 2500:

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



Electron density around C5P B 1500:

$2mF_o-DF_c$ (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.