Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 10:38 PM JST

PDB ID	:	7XIN
Title	:	Crystal structure of DODC from Pseudomonas
Authors	:	Li, X.; Zhou, Y.L.; Liao, L.J.; Liu, X.K.; Liu, B.; Guo, Y.; Feng, Z.; Sun, D.Y.; Zeng, Z.X.
Deposited on	:	2022-04-13
Resolution	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

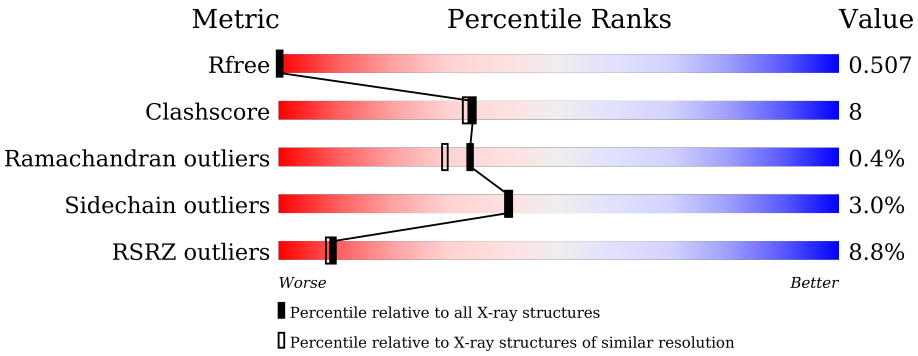
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	476	9% 79% 18% ··
1	C	476	8% 76% 22% ··
1	E	476	9% 77% 21% ··

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10953 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 DOPA decarboxylase.

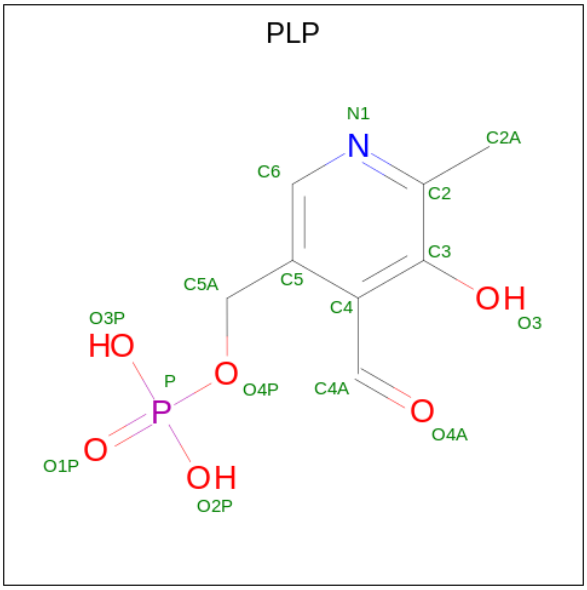
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3636	2302	649	673	12			
1	C	470	Total	C	N	O	S	0	0	0
			3636	2302	649	673	12			
1	E	470	Total	C	N	O	S	0	0	0
			3636	2302	649	673	12			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q88JU5
A	1	ALA	-	expression tag	UNP Q88JU5
A	471	LEU	-	expression tag	UNP Q88JU5
A	472	GLU	-	expression tag	UNP Q88JU5
A	473	HIS	-	expression tag	UNP Q88JU5
A	474	HIS	-	expression tag	UNP Q88JU5
A	475	HIS	-	expression tag	UNP Q88JU5
C	0	MET	-	expression tag	UNP Q88JU5
C	1	ALA	-	expression tag	UNP Q88JU5
C	471	LEU	-	expression tag	UNP Q88JU5
C	472	GLU	-	expression tag	UNP Q88JU5
C	473	HIS	-	expression tag	UNP Q88JU5
C	474	HIS	-	expression tag	UNP Q88JU5
C	475	HIS	-	expression tag	UNP Q88JU5
E	0	MET	-	expression tag	UNP Q88JU5
E	1	ALA	-	expression tag	UNP Q88JU5
E	471	LEU	-	expression tag	UNP Q88JU5
E	472	GLU	-	expression tag	UNP Q88JU5
E	473	HIS	-	expression tag	UNP Q88JU5
E	474	HIS	-	expression tag	UNP Q88JU5
E	475	HIS	-	expression tag	UNP Q88JU5

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$)

(labeled as "Ligand of Interest" by depositor).



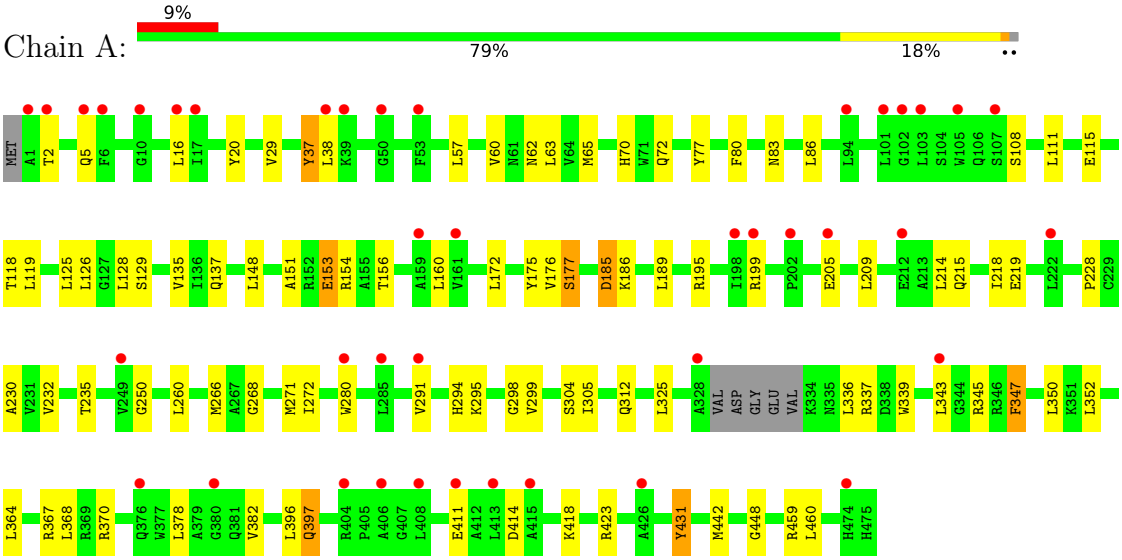
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	15	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	15	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	15	0
			15	8	1	5	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

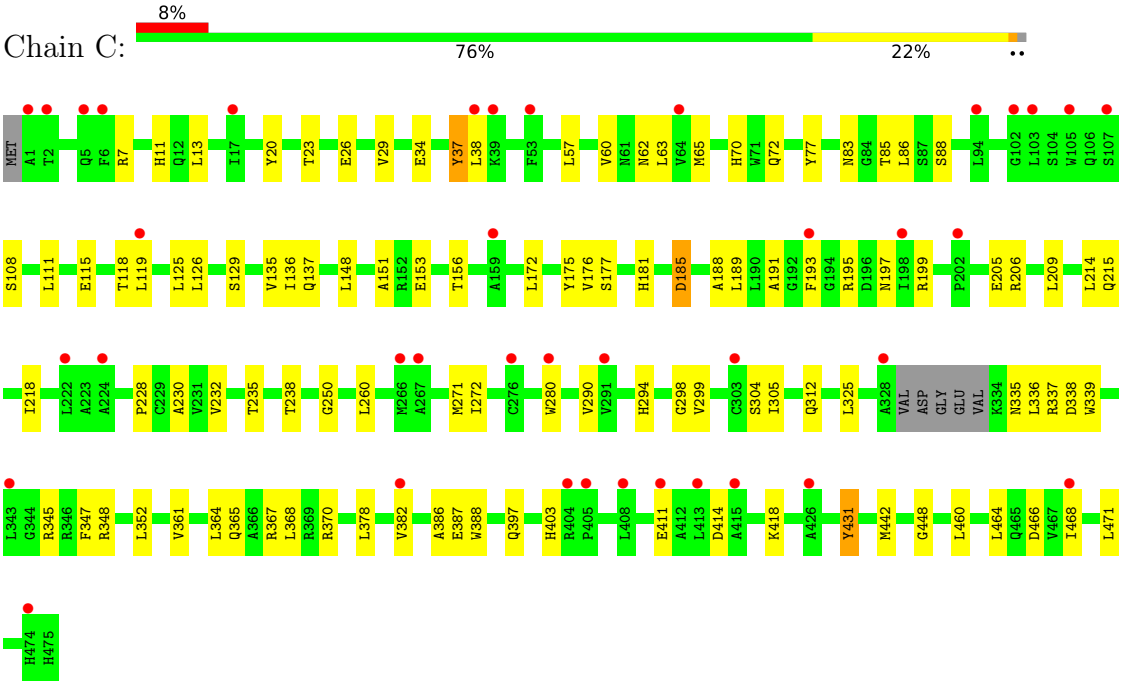
• Molecule 1: DOPA decarboxylase

Chain A:



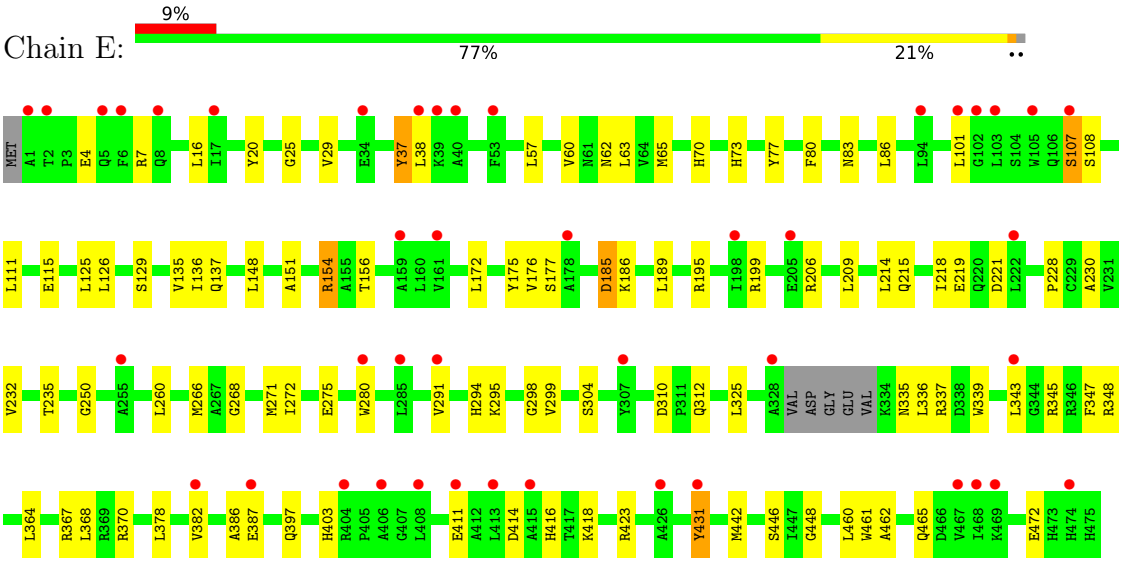
• Molecule 1: DOPA decarboxylase

Chain C:



• Molecule 1: DOPA decarboxylase

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.77Å 67.01Å 168.58Å 90.27° 92.38° 90.36°	Depositor
Resolution (Å)	43.59 – 2.00 43.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	70.0 (43.59-2.00) 70.0 (43.59-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.473 , 0.521 0.467 , 0.507	Depositor DCC
R_{free} test set	5767 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , -10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l 0.000 for -h,k,-l 0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	10953	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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 96.32 % 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 6.0910e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.48	0/3723	0.64	1/5081 (0.0%)
1	C	0.47	0/3723	0.65	1/5081 (0.0%)
1	E	0.47	0/3723	0.65	0/5081
All	All	0.47	0/11169	0.65	2/15243 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	72	GLN	C-N-CA	6.09	136.93	121.70
1	A	72	GLN	C-N-CA	5.62	135.75	121.70

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	3636	0	3586	58	0
1	C	3636	0	3586	63	0
1	E	3636	0	3586	58	0
2	A	15	0	7	0	0
2	C	15	0	7	0	0
2	E	15	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10953	0	10779	179	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 8.

All (179) 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:199:ARG:HG2	1:A:199:ARG:HH11	1.37	0.89
1:A:266:MET:HE2	1:A:295:LYS:HB3	1.57	0.83
1:E:423:ARG:CZ	1:E:472:GLU:OE2	2.29	0.81
1:E:266:MET:HE2	1:E:295:LYS:HB3	1.63	0.80
1:C:388:TRP:CZ2	1:C:468:ILE:HD11	2.19	0.77
1:E:115:GLU:OE2	1:E:345:ARG:NH2	2.22	0.69
1:A:115:GLU:OE2	1:A:345:ARG:NH2	2.23	0.67
1:C:388:TRP:HZ2	1:C:468:ILE:CD1	2.07	0.66
1:E:185:ASP:OD1	1:E:195:ARG:NH1	2.29	0.65
1:A:294:HIS:HA	1:A:299:VAL:O	1.96	0.65
1:C:115:GLU:OE2	1:C:345:ARG:NH2	2.26	0.65
1:C:294:HIS:HA	1:C:299:VAL:O	1.97	0.65
1:C:176:VAL:HG12	1:C:232:VAL:HB	1.78	0.65
1:C:388:TRP:HZ2	1:C:468:ILE:HD11	1.63	0.64
1:A:199:ARG:HH11	1:A:199:ARG:CG	2.10	0.64
1:C:388:TRP:CZ2	1:C:468:ILE:CD1	2.81	0.64
1:E:294:HIS:HA	1:E:299:VAL:O	1.98	0.64
1:A:20:TYR:OH	1:A:70:HIS:HD2	1.82	0.63
1:C:199:ARG:HG3	1:C:199:ARG:HH11	1.64	0.62
1:C:20:TYR:OH	1:C:70:HIS:HD2	1.83	0.62
1:A:176:VAL:HG12	1:A:232:VAL:HB	1.81	0.61
1:E:268:GLY:HA3	1:E:291:VAL:HG22	1.83	0.60
1:E:423:ARG:NH2	1:E:472:GLU:OE2	2.35	0.60
1:E:176:VAL:HG12	1:E:232:VAL:HB	1.82	0.60
1:E:20:TYR:OH	1:E:70:HIS:HD2	1.85	0.59
1:E:136:ILE:O	1:E:348:ARG:NH2	2.36	0.58
1:E:125:LEU:O	1:E:272:ILE:HA	2.03	0.58
1:A:80:PHE:HB3	1:A:266:MET:HE3	1.84	0.58
1:C:271:MET:HG3	1:C:280:TRP:CE2	2.39	0.57
1:A:125:LEU:O	1:A:272:ILE:HA	2.04	0.57
1:E:266:MET:CE	1:E:295:LYS:HB3	2.34	0.57
1:E:135:VAL:HG23	1:E:336:LEU:HD22	1.88	0.56
1:A:80:PHE:HB3	1:A:266:MET:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LEU:O	1:C:272:ILE:HA	2.08	0.54
1:C:185:ASP:O	1:C:189:LEU:HG	2.06	0.53
1:A:199:ARG:CG	1:A:199:ARG:NH1	2.71	0.53
1:A:266:MET:CE	1:A:295:LYS:HB3	2.34	0.53
1:C:361:VAL:O	1:C:365:GLN:HG3	2.08	0.53
1:E:154:ARG:NH2	1:E:310:ASP:OD2	2.27	0.53
1:A:185:ASP:O	1:A:189:LEU:HG	2.09	0.53
1:A:268:GLY:HA3	1:A:291:VAL:HG12	1.90	0.53
1:E:185:ASP:O	1:E:189:LEU:HG	2.09	0.53
1:E:250:GLY:HA2	1:E:260:LEU:HD22	1.91	0.53
1:A:111:LEU:HD21	1:A:345:ARG:HG3	1.91	0.52
1:C:135:VAL:HG23	1:C:336:LEU:HD22	1.92	0.52
1:A:199:ARG:HG2	1:A:199:ARG:NH1	2.15	0.52
1:E:111:LEU:HD21	1:E:345:ARG:HG3	1.90	0.52
1:C:271:MET:HG3	1:C:280:TRP:CZ2	2.44	0.52
1:C:235:THR:HG21	1:C:280:TRP:CD1	2.44	0.52
1:A:414:ASP:O	1:A:418:LYS:HG2	2.10	0.52
1:C:137:GLN:N	1:C:304:SER:O	2.41	0.51
1:A:266:MET:HE3	1:A:295:LYS:HD3	1.92	0.51
1:C:367:ARG:O	1:C:370:ARG:HB3	2.11	0.51
1:C:199:ARG:HG3	1:C:199:ARG:NH1	2.25	0.51
1:C:335:ASN:HB3	1:C:338:ASP:OD1	2.12	0.50
1:A:83:ASN:HB3	1:A:298:GLY:HA2	1.94	0.50
1:C:111:LEU:HD21	1:C:345:ARG:HG3	1.93	0.50
1:E:403:HIS:HD2	1:E:416:HIS:NE2	2.10	0.50
1:C:136:ILE:O	1:C:348:ARG:NH2	2.45	0.50
1:A:205:GLU:H	1:A:205:GLU:CD	2.14	0.50
1:A:118:THR:HB	1:A:352:LEU:HD23	1.94	0.49
1:E:126:LEU:HD22	1:E:271:MET:HB2	1.93	0.49
1:A:135:VAL:HG23	1:A:336:LEU:HD22	1.95	0.49
1:C:135:VAL:HG11	1:C:339:TRP:HB3	1.94	0.49
1:C:386:ALA:O	1:C:387:GLU:HB2	2.10	0.49
1:A:185:ASP:OD1	1:A:195:ARG:NH1	2.45	0.49
1:C:466:ASP:HB3	1:C:471:LEU:HB2	1.95	0.49
1:A:137:GLN:N	1:A:304:SER:O	2.43	0.49
1:C:250:GLY:HA2	1:C:260:LEU:HD22	1.94	0.48
1:C:205:GLU:H	1:C:205:GLU:CD	2.16	0.48
1:A:2:THR:H	1:A:5:GLN:HE21	1.60	0.48
1:C:335:ASN:HD21	1:C:337:ARG:CZ	2.25	0.48
1:A:126:LEU:HD22	1:A:271:MET:HB2	1.96	0.48
1:C:62:ASN:C	1:C:63:LEU:HD23	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ALA:HB1	1:A:230:ALA:HB2	1.96	0.48
1:C:214:LEU:O	1:C:218:ILE:HG13	2.14	0.47
1:E:186:LYS:HA	1:E:189:LEU:HD12	1.96	0.47
1:A:250:GLY:HA2	1:A:260:LEU:HD22	1.97	0.47
1:E:414:ASP:O	1:E:418:LYS:HG2	2.14	0.47
1:A:135:VAL:HG11	1:A:339:TRP:HB3	1.97	0.47
1:A:128:LEU:HD21	1:A:280:TRP:CZ3	2.49	0.47
1:A:266:MET:CE	1:A:295:LYS:HD3	2.44	0.47
1:C:378:LEU:O	1:C:382:VAL:HG23	2.15	0.47
1:E:62:ASN:C	1:E:63:LEU:HD23	2.35	0.47
1:C:118:THR:HB	1:C:352:LEU:HD23	1.97	0.47
1:E:80:PHE:HB3	1:E:266:MET:HE3	1.96	0.47
1:A:364:LEU:O	1:A:368:LEU:HG	2.15	0.47
1:C:215:GLN:O	1:C:215:GLN:HG3	2.15	0.47
1:E:77:TYR:CE2	1:E:460:LEU:HD22	2.50	0.46
1:E:337:ARG:HD3	1:E:343:LEU:HD23	1.97	0.46
1:C:151:ALA:HB1	1:C:230:ALA:HB2	1.98	0.46
1:A:62:ASN:C	1:A:63:LEU:HD23	2.36	0.46
1:C:83:ASN:HB3	1:C:298:GLY:HA2	1.98	0.46
1:E:83:ASN:HB3	1:E:298:GLY:HA2	1.98	0.46
1:C:290:VAL:HG23	1:C:305:ILE:O	2.16	0.46
1:A:378:LEU:O	1:A:382:VAL:HG23	2.16	0.46
1:E:86:LEU:HD23	1:E:86:LEU:HA	1.68	0.46
1:E:364:LEU:O	1:E:368:LEU:HG	2.16	0.46
1:A:214:LEU:O	1:A:218:ILE:HG13	2.16	0.45
1:A:235:THR:HG21	1:A:280:TRP:CD1	2.51	0.45
1:A:367:ARG:O	1:A:370:ARG:HB3	2.16	0.45
1:C:29:VAL:CG1	1:C:431:TYR:HB2	2.47	0.45
1:E:137:GLN:N	1:E:304:SER:O	2.46	0.45
1:E:148:LEU:HD23	1:E:148:LEU:HA	1.78	0.45
1:A:312:GLN:OE1	1:A:325:LEU:HA	2.16	0.45
1:A:186:LYS:HA	1:A:189:LEU:HD12	1.98	0.45
1:C:77:TYR:CE2	1:C:460:LEU:HD22	2.52	0.45
1:E:60:VAL:O	1:E:65:MET:HG2	2.17	0.45
1:E:335:ASN:HD21	1:E:337:ARG:CZ	2.29	0.45
1:A:86:LEU:HD23	1:A:86:LEU:HA	1.71	0.45
1:C:188:ALA:O	1:C:193:PHE:HD1	1.98	0.45
1:E:151:ALA:HB1	1:E:230:ALA:HB2	1.99	0.45
1:E:367:ARG:O	1:E:370:ARG:HB3	2.17	0.45
1:E:235:THR:HG21	1:E:280:TRP:CD1	2.52	0.44
1:C:126:LEU:HD22	1:C:271:MET:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:VAL:HG11	1:E:339:TRP:HB3	1.99	0.44
1:E:177:SER:HB2	1:E:209:LEU:HB3	2.00	0.44
1:C:156:THR:CG2	1:C:172:LEU:HD11	2.47	0.44
1:C:364:LEU:O	1:C:368:LEU:HG	2.17	0.44
1:E:199:ARG:HH11	1:E:199:ARG:HG3	1.81	0.44
1:A:77:TYR:CE2	1:A:460:LEU:HD22	2.53	0.44
1:A:153:GLU:OE1	1:A:160:LEU:HD22	2.16	0.44
1:A:135:VAL:HG11	1:A:339:TRP:O	2.18	0.44
1:E:135:VAL:HG11	1:E:339:TRP:O	2.18	0.44
1:C:460:LEU:O	1:C:464:LEU:HD12	2.17	0.44
1:A:60:VAL:O	1:A:65:MET:HG2	2.18	0.44
1:C:175:TYR:HE2	1:C:228:PRO:HB3	1.82	0.44
1:A:177:SER:HB2	1:A:209:LEU:HB3	2.00	0.44
1:C:7:ARG:HG2	1:C:11:HIS:CE1	2.53	0.43
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.79	0.43
1:A:29:VAL:CG1	1:A:431:TYR:HB2	2.49	0.43
1:A:37:TYR:CG	1:A:38:LEU:N	2.87	0.43
1:A:396:LEU:HD23	1:A:397:GLN:OE1	2.17	0.43
1:A:175:TYR:HE2	1:A:228:PRO:HB3	1.82	0.43
1:A:337:ARG:CG	1:A:343:LEU:HD23	2.49	0.43
1:C:37:TYR:CG	1:C:38:LEU:N	2.87	0.43
1:E:37:TYR:CG	1:E:38:LEU:N	2.87	0.43
1:E:215:GLN:HG3	1:E:219:GLU:OE2	2.18	0.43
1:E:29:VAL:CG1	1:E:431:TYR:HB2	2.49	0.43
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.82	0.43
1:C:414:ASP:O	1:C:418:LYS:HG2	2.19	0.43
1:E:312:GLN:OE1	1:E:325:LEU:HA	2.19	0.43
1:A:156:THR:CG2	1:A:172:LEU:HD11	2.48	0.43
1:C:185:ASP:OD1	1:C:195:ARG:NH2	2.51	0.43
1:E:378:LEU:O	1:E:382:VAL:HG23	2.19	0.43
1:A:215:GLN:O	1:A:215:GLN:HG3	2.18	0.42
1:C:411:GLU:H	1:C:411:GLU:HG2	1.57	0.42
1:E:175:TYR:HE2	1:E:228:PRO:HB3	1.84	0.42
1:A:411:GLU:H	1:A:411:GLU:HG2	1.56	0.42
1:E:80:PHE:HB3	1:E:266:MET:CE	2.49	0.42
1:E:386:ALA:O	1:E:387:GLU:HB2	2.20	0.42
1:A:119:LEU:CD2	1:A:305:ILE:HD12	2.49	0.42
1:C:119:LEU:CD2	1:C:305:ILE:HD12	2.49	0.42
1:C:23:THR:HB	1:C:26:GLU:OE2	2.20	0.42
1:A:215:GLN:HG3	1:A:219:GLU:OE2	2.19	0.41
1:C:135:VAL:HG11	1:C:339:TRP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:PHE:O	1:C:197:ASN:ND2	2.38	0.41
1:E:266:MET:HE3	1:E:295:LYS:HD3	2.00	0.41
1:A:16:LEU:HD13	1:A:57:LEU:HD22	2.02	0.41
1:C:177:SER:HB2	1:C:209:LEU:HB3	2.03	0.41
1:C:387:GLU:HB3	1:C:403:HIS:CD2	2.55	0.41
1:C:60:VAL:O	1:C:65:MET:HG2	2.20	0.41
1:C:312:GLN:OE1	1:C:325:LEU:HA	2.21	0.41
1:E:77:TYR:HA	1:E:446:SER:O	2.21	0.41
1:E:461:TRP:O	1:E:465:GLN:HG3	2.19	0.41
1:E:214:LEU:O	1:E:218:ILE:HG13	2.19	0.41
1:E:16:LEU:HD13	1:E:57:LEU:HD22	2.02	0.41
1:C:85:THR:O	1:C:88:SER:OG	2.35	0.41
1:C:86:LEU:HD23	1:C:86:LEU:HA	1.78	0.41
1:E:4:GLU:OE2	1:E:7:ARG:NE	2.54	0.41
1:E:101:LEU:O	1:E:107:SER:OG	2.39	0.41
1:E:411:GLU:H	1:E:411:GLU:HG2	1.57	0.41
1:E:156:THR:CG2	1:E:172:LEU:HD11	2.51	0.41
1:E:462:ALA:HA	1:E:465:GLN:HE21	1.86	0.40
1:C:181:HIS:CD2	1:C:238:THR:HG21	2.57	0.40
1:C:191:ALA:HB3	1:C:193:PHE:CE1	2.56	0.40
1:A:347:PHE:CD1	1:A:350:LEU:HG	2.56	0.40
1:C:13:LEU:HD13	1:C:57:LEU:HD21	2.04	0.40
1:E:25:GLY:HA2	1:E:73:HIS:NE2	2.37	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	466/476 (98%)	440 (94%)	24 (5%)	2 (0%)	34	30
1	C	466/476 (98%)	438 (94%)	26 (6%)	2 (0%)	34	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	E	466/476 (98%)	441 (95%)	23 (5%)	2 (0%)	34 30
All	All	1398/1428 (98%)	1319 (94%)	73 (5%)	6 (0%)	34 30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	SER
1	C	108	SER
1	E	108	SER
1	E	448	GLY
1	A	448	GLY
1	C	448	GLY

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	375/380 (99%)	363 (97%)	12 (3%)	39 38
1	C	375/380 (99%)	365 (97%)	10 (3%)	44 46
1	E	375/380 (99%)	363 (97%)	12 (3%)	39 38
All	All	1125/1140 (99%)	1091 (97%)	34 (3%)	41 41

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	TYR
1	A	129	SER
1	A	153	GLU
1	A	154	ARG
1	A	177	SER
1	A	185	ASP
1	A	347	PHE
1	A	397	GLN
1	A	423	ARG

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Mol	Chain	Res	Type
1	A	431	TYR
1	A	442	MET
1	A	459	ARG
1	C	34	GLU
1	C	37	TYR
1	C	129	SER
1	C	153	GLU
1	C	185	ASP
1	C	206	ARG
1	C	347	PHE
1	C	397	GLN
1	C	431	TYR
1	C	442	MET
1	E	37	TYR
1	E	107	SER
1	E	129	SER
1	E	154	ARG
1	E	185	ASP
1	E	206	ARG
1	E	221	ASP
1	E	275	GLU
1	E	347	PHE
1	E	397	GLN
1	E	431	TYR
1	E	442	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	70	HIS
1	A	131	GLN
1	A	474	HIS
1	C	49	GLN
1	C	70	HIS
1	C	474	HIS
1	E	70	HIS
1	E	106	GLN
1	E	403	HIS
1	E	458	GLN
1	E	465	GLN
1	E	474	HIS

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)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PLP	A	501	1	15,15,16	1.08	1 (6%)	20,22,23	1.09	2 (10%)
2	PLP	E	501	1	15,15,16	1.03	1 (6%)	20,22,23	1.25	2 (10%)
2	PLP	C	501	1	15,15,16	1.08	1 (6%)	20,22,23	1.04	2 (10%)

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
2	PLP	A	501	1	-	0/6/6/8	0/1/1/1
2	PLP	E	501	1	-	1/6/6/8	0/1/1/1
2	PLP	C	501	1	-	0/6/6/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PLP	C2-N1	2.48	1.38	1.33
2	C	501	PLP	C2-N1	2.44	1.38	1.33
2	E	501	PLP	C6-N1	2.09	1.38	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	PLP	C5-C6-N1	-3.20	118.49	123.82
2	E	501	PLP	C6-C5-C4	2.53	120.15	118.16
2	A	501	PLP	C6-C5-C4	2.47	120.11	118.16
2	A	501	PLP	C5-C6-N1	-2.34	119.92	123.82
2	C	501	PLP	C6-C5-C4	2.33	119.99	118.16
2	C	501	PLP	C5-C6-N1	-2.28	120.02	123.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

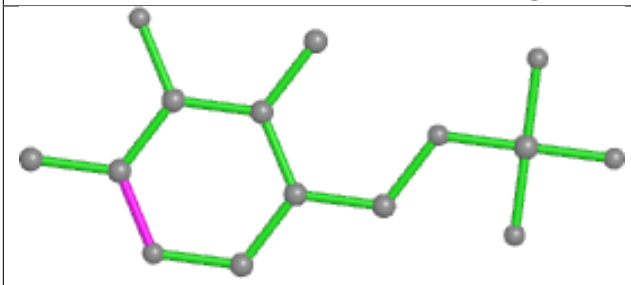
Mol	Chain	Res	Type	Atoms
2	E	501	PLP	C5A-O4P-P-O1P

There are no ring outliers.

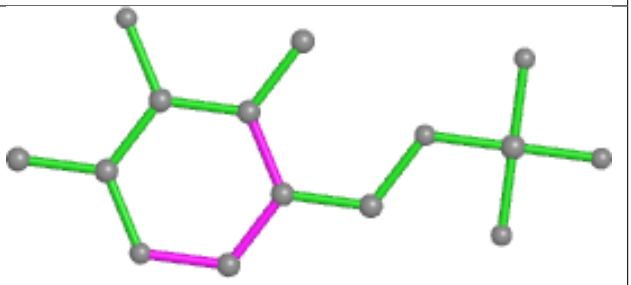
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

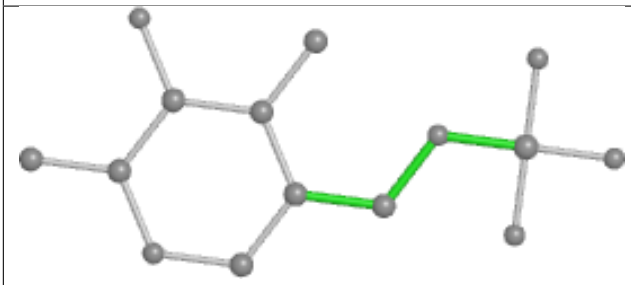
Ligand PLP A 501



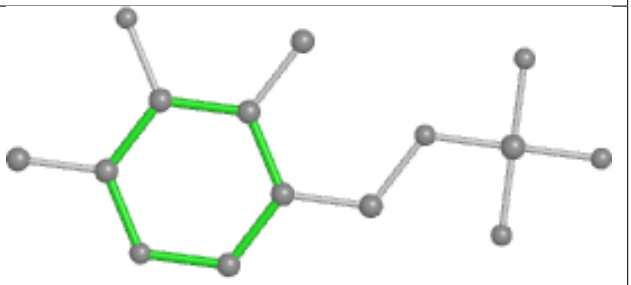
Bond lengths



Bond angles

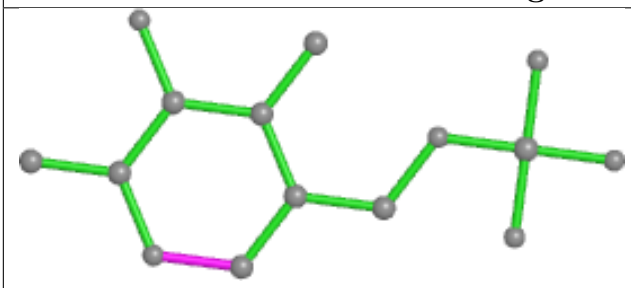


Torsions

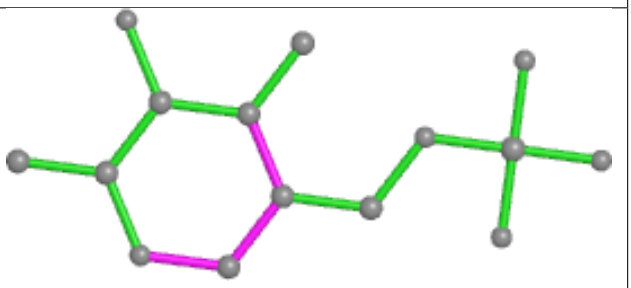


Rings

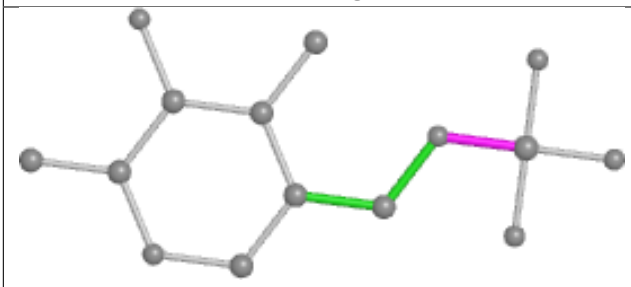
Ligand PLP E 501



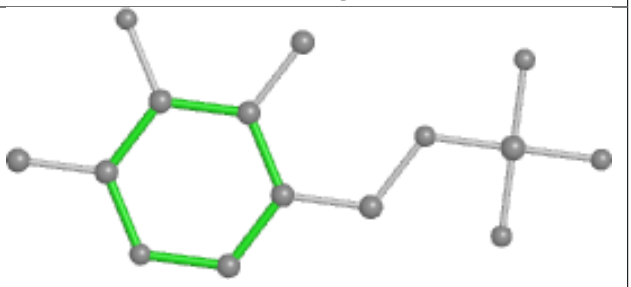
Bond lengths



Bond angles

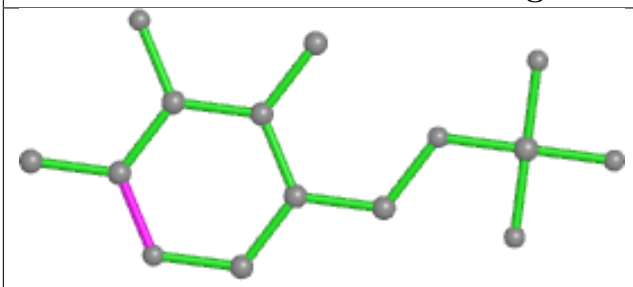


Torsions

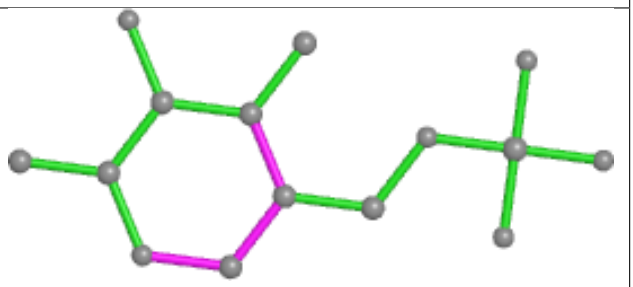


Rings

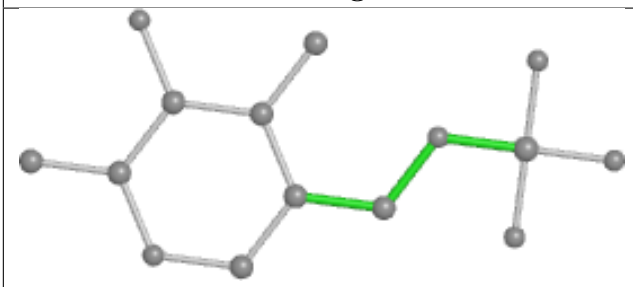
Ligand PLP C 501



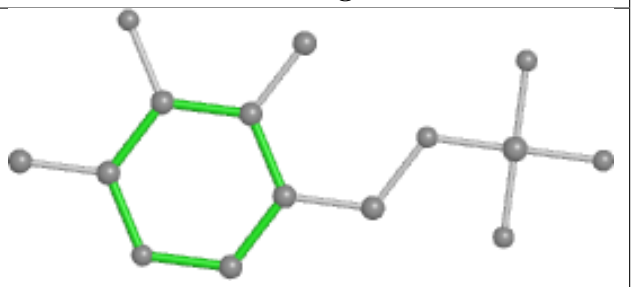
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	470/476 (98%)	1.02	41 (8%) 10 9	17, 30, 41, 51	0
1	C	470/476 (98%)	1.01	39 (8%) 11 10	17, 30, 42, 51	0
1	E	470/476 (98%)	1.04	44 (9%) 8 8	17, 30, 42, 52	0
All	All	1410/1428 (98%)	1.02	124 (8%) 10 9	17, 30, 42, 52	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	THR	5.2
1	C	2	THR	4.8
1	E	328	ALA	4.7
1	E	2	THR	4.4
1	A	328	ALA	4.3
1	E	415	ALA	3.9
1	A	107	SER	3.9
1	A	17	ILE	3.9
1	C	224	ALA	3.7
1	C	343	LEU	3.7
1	C	5	GLN	3.7
1	C	328	ALA	3.7
1	C	107	SER	3.5
1	C	280	TRP	3.5
1	E	34	GLU	3.4
1	A	343	LEU	3.4
1	E	101	LEU	3.4
1	C	266	MET	3.3
1	E	343	LEU	3.3
1	E	107	SER	3.3
1	A	103	LEU	3.2
1	E	426	ALA	3.2
1	C	6	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	1	ALA	3.1
1	A	426	ALA	3.0
1	A	5	GLN	3.0
1	A	39	LYS	3.0
1	E	291	VAL	3.0
1	C	303	CYS	2.9
1	A	198	ILE	2.8
1	E	404	ARG	2.8
1	E	159	ALA	2.8
1	E	105	TRP	2.8
1	C	415	ALA	2.8
1	A	161	VAL	2.8
1	A	202	PRO	2.8
1	E	39	LYS	2.8
1	E	5	GLN	2.8
1	C	38	LEU	2.7
1	A	6	PHE	2.7
1	C	404	ARG	2.7
1	C	426	ALA	2.7
1	C	159	ALA	2.7
1	C	411	GLU	2.7
1	E	198	ILE	2.7
1	C	103	LEU	2.7
1	E	222	LEU	2.7
1	E	6	PHE	2.6
1	C	105	TRP	2.6
1	A	415	ALA	2.6
1	E	406	ALA	2.6
1	E	468	ILE	2.6
1	E	102	GLY	2.6
1	E	103	LEU	2.5
1	C	222	LEU	2.5
1	E	408	LEU	2.5
1	A	380	GLY	2.5
1	C	17	ILE	2.5
1	C	102	GLY	2.5
1	A	101	LEU	2.5
1	A	408	LEU	2.5
1	E	94	LEU	2.5
1	A	474	HIS	2.5
1	E	474	HIS	2.5
1	C	39	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	17	ILE	2.4
1	A	404	ARG	2.4
1	A	411	GLU	2.4
1	C	468	ILE	2.4
1	C	474	HIS	2.4
1	A	38	LEU	2.4
1	E	161	VAL	2.4
1	A	280	TRP	2.4
1	C	198	ILE	2.4
1	E	38	LEU	2.3
1	A	291	VAL	2.3
1	A	406	ALA	2.3
1	E	53	PHE	2.3
1	A	249	VAL	2.3
1	A	1	ALA	2.3
1	C	1	ALA	2.3
1	E	467	VAL	2.3
1	E	387	GLU	2.3
1	C	53	PHE	2.3
1	A	285	LEU	2.2
1	C	291	VAL	2.2
1	E	205	GLU	2.2
1	A	102	GLY	2.2
1	A	199	ARG	2.2
1	A	376	GLN	2.2
1	A	205	GLU	2.2
1	A	105	TRP	2.2
1	C	276	CYS	2.2
1	A	159	ALA	2.2
1	C	405	PRO	2.2
1	C	408	LEU	2.1
1	A	53	PHE	2.1
1	E	382	VAL	2.1
1	E	178	ALA	2.1
1	C	202	PRO	2.1
1	E	413	LEU	2.1
1	C	193	PHE	2.1
1	E	8	GLN	2.1
1	E	411	GLU	2.1
1	A	413	LEU	2.1
1	C	94	LEU	2.1
1	C	119	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	431	TYR	2.1
1	A	94	LEU	2.1
1	E	469	LYS	2.1
1	E	255	ALA	2.1
1	A	222	LEU	2.1
1	E	285	LEU	2.1
1	C	64	VAL	2.1
1	C	382	VAL	2.1
1	E	40	ALA	2.1
1	E	280	TRP	2.1
1	A	50	GLY	2.1
1	A	16	LEU	2.0
1	C	413	LEU	2.0
1	C	267	ALA	2.0
1	A	10	GLY	2.0
1	E	307	TYR	2.0
1	A	212	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers (i)

There are no such residues in this entry.