



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2026 – 11:32 AM EDT

PDB ID : 2VU2 / pdb_00002vu2
Title : Biosynthetic thiolase from *Z. ramigera*. Complex with S-pantetheine-11- pivalate.
Authors : Kursula, P.; Merilainen, G.; Schmitz, W.; Wierenga, R.K.
Deposited on : 2008-05-19
Resolution : 2.65 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

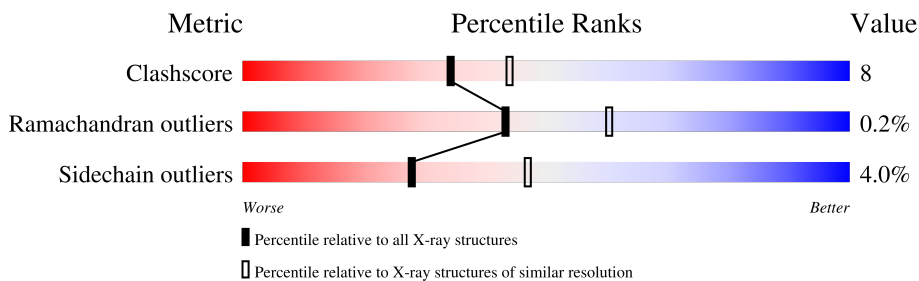
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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))
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	392	81% 16% ..
1	B	392	80% 18% ..
1	C	392	83% 15% ..
1	D	392	85% 14% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11858 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.

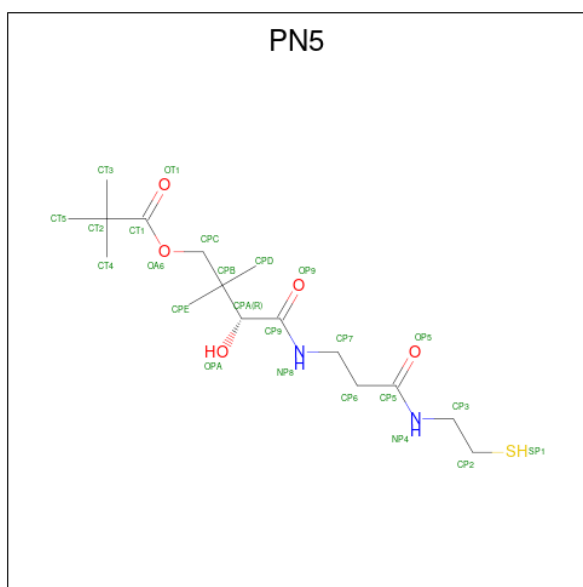
- Molecule 1 is a protein called ACETYL-COA ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	389	2813	1746	509	537	21	0	0	0
1	B	389	2813	1746	509	537	21	0	0	0
1	C	389	2813	1746	509	537	21	0	0	0
1	D	389	2813	1746	509	537	21	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ARG	ALA	conflict	UNP P07097
B	129	ARG	ALA	conflict	UNP P07097
C	129	ARG	ALA	conflict	UNP P07097
D	129	ARG	ALA	conflict	UNP P07097

- Molecule 2 is (3R)-3-hydroxy-2,2-dimethyl-4-oxo-4-({3-oxo-3-[(2-sulfanylethyl)amino]propyl}amino)butyl 2,2-dimethylpropanoate (CCD ID: PN5) (formula: C₁₆H₃₀N₂O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	24	16	2	5	1	0	0
2	B	1	24	16	2	5	1	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
3	A	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

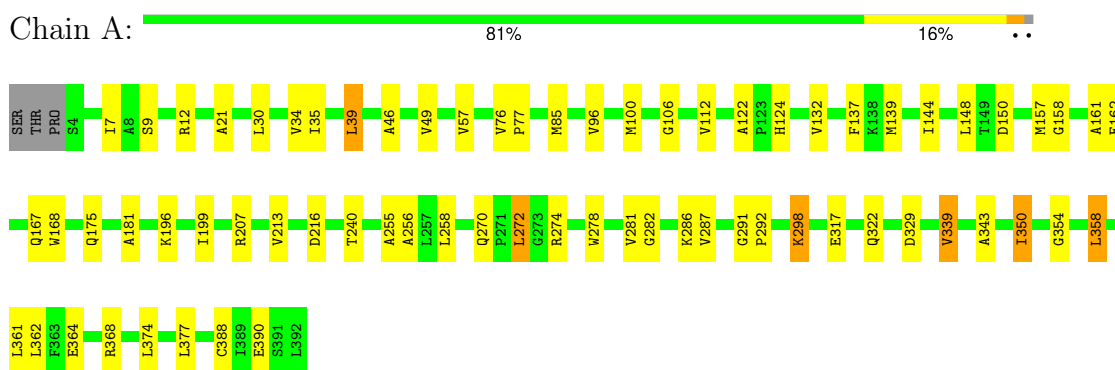
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	240	Total	O	0	0
			240	240		
4	B	228	Total	O	0	0
			228	228		
4	C	36	Total	O	0	0
			36	36		
4	D	24	Total	O	0	0
			24	24		

3 Residue-property plots [i](#)

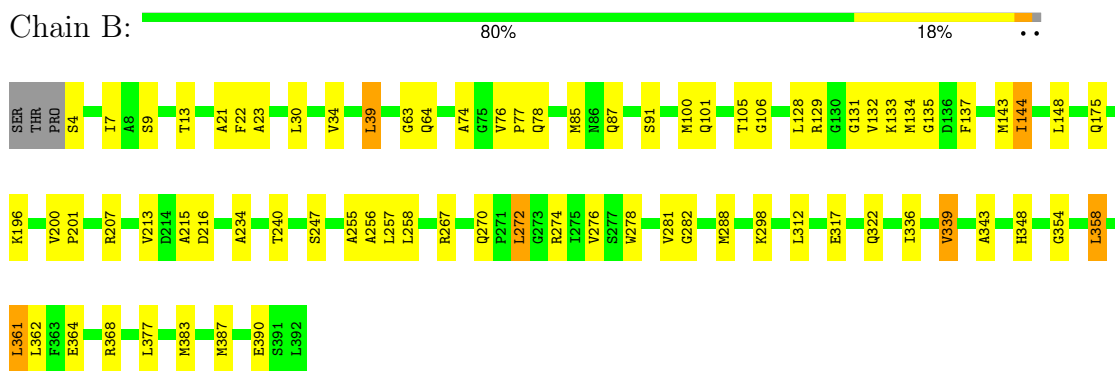
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

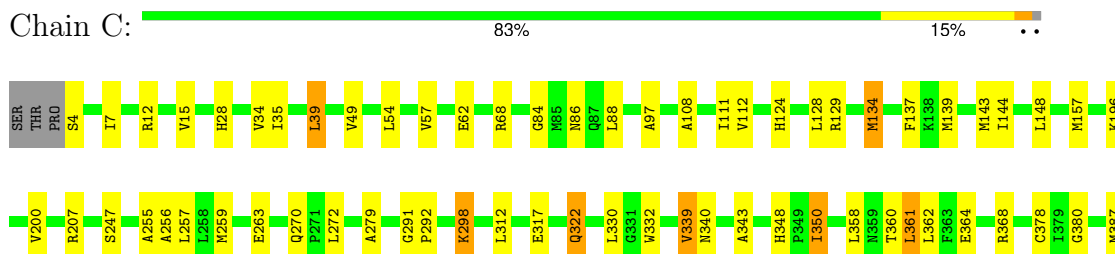
- Molecule 1: ACETYL-COA ACETYLTRANSFERASE



- Molecule 1: ACETYL-COA ACETYLTRANSFERASE




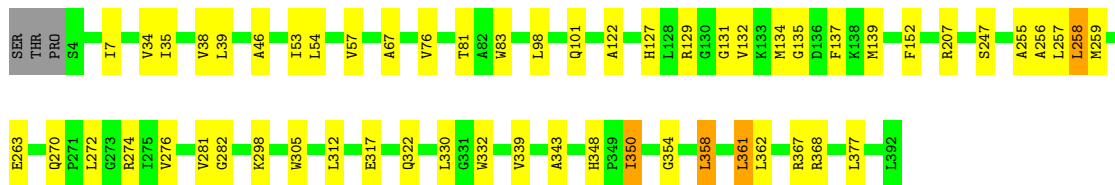
- Molecule 1: ACETYL-COA ACETYLTRANSFERASE



L392

- Molecule 1: ACETYL-COA ACETYLTRANSFERASE

Chain D:  85% 14% ..



4 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.32Å 79.15Å 150.79Å 90.00° 92.92° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65	Depositor
% Data completeness (in resolution range)	95.3 (20.00-2.65)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.67Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.231 , 0.286	Depositor
Wilson B-factor (Å ²)	28.9	Xtrriage
Anisotropy	0.628	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.146 for h,-k,-l	Xtrriage
Total number of atoms	11858	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% 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: PN5, SO4

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	0.87	0/2854	0.97	0/3853
1	B	0.87	0/2854	0.98	1/3853 (0.0%)
1	C	0.53	1/2854 (0.0%)	0.76	0/3853
1	D	0.52	0/2854	0.78	1/3853 (0.0%)
All	All	0.72	1/11416 (0.0%)	0.88	2/15412 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	134	MET	SD-CE	5.80	1.94	1.79

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	ILE	CB-CA-C	-6.20	103.93	112.24
1	D	367	ARG	NE-CZ-NH2	5.13	123.82	119.20

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	2813	0	2819	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2813	0	2819	52	0
1	C	2813	0	2819	42	0
1	D	2813	0	2819	39	0
2	A	24	0	30	3	0
2	B	24	0	30	3	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
4	A	240	0	0	7	0
4	B	228	0	0	9	0
4	C	36	0	0	2	0
4	D	24	0	0	1	0
All	All	11858	0	11336	172	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 (172) 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:258:LEU:HD22	1:A:258:LEU:N	1.87	0.87
1:D:34:VAL:HG12	1:D:255:ALA:HB3	1.66	0.78
1:C:257:LEU:CD2	1:C:259:MET:HE3	2.14	0.78
2:A:1393:PN5:HT53	1:D:134:MET:HE1	1.67	0.76
1:C:7:ILE:HD13	1:C:362:LEU:HD11	1.67	0.76
1:C:128:LEU:HD21	1:C:137:PHE:CE2	2.20	0.75
1:D:57:VAL:HG21	1:D:350:ILE:HG22	1.68	0.74
1:C:257:LEU:HD21	1:C:259:MET:HE3	1.72	0.71
1:B:175:GLN:HE22	1:B:240:THR:CG2	2.03	0.71
1:D:57:VAL:HG21	1:D:350:ILE:CG2	2.21	0.70
1:A:144:ILE:HD13	1:A:148:LEU:HD12	1.73	0.70
1:C:34:VAL:HG12	1:C:255:ALA:HB3	1.74	0.70
1:B:364:GLU:OE2	4:B:2217:HOH:O	2.09	0.69
1:B:128:LEU:HD21	1:B:137:PHE:CE2	2.28	0.68
1:D:339:VAL:HG11	1:D:368:ARG:NH2	2.09	0.67
1:B:274:ARG:NH1	1:B:276:VAL:HG12	2.08	0.67
2:A:1393:PN5:HPE3	4:A:2234:HOH:O	1.96	0.65
1:C:339:VAL:HG11	1:C:368:ARG:NH2	2.12	0.64
1:B:215:ALA:O	4:B:2148:HOH:O	2.15	0.64
1:B:144:ILE:CD1	1:B:148:LEU:HD12	2.27	0.64
1:D:132:VAL:HG21	1:D:137:PHE:CD2	2.32	0.64
2:A:1393:PN5:HT53	1:D:134:MET:CE	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:GLN:HE22	1:B:240:THR:HG23	1.65	0.61
1:B:74:ALA:O	4:B:2058:HOH:O	2.16	0.60
1:C:7:ILE:HG23	1:C:256:ALA:HB1	1.84	0.60
1:B:312:LEU:HD23	1:B:361:LEU:CD2	2.33	0.59
1:A:34:VAL:HG12	1:A:255:ALA:HB3	1.85	0.59
1:A:258:LEU:N	1:A:258:LEU:CD2	2.65	0.58
1:B:144:ILE:HD13	1:B:148:LEU:HD12	1.85	0.58
1:B:288:MET:HE1	2:B:1393:PN5:SP1	2.44	0.58
1:A:148:LEU:O	1:A:157:MET:HG2	2.03	0.57
1:B:339:VAL:HG11	1:B:368:ARG:NH2	2.20	0.57
1:C:257:LEU:HD21	1:C:259:MET:CE	2.34	0.57
1:B:143:MET:HE3	1:B:144:ILE:CD1	2.35	0.57
1:C:330:LEU:HD13	1:C:332:TRP:CH2	2.40	0.57
1:B:34:VAL:HG12	1:B:255:ALA:HB3	1.86	0.57
1:B:234:ALA:HB1	2:B:1393:PN5:HPD2	1.88	0.56
1:C:247:SER:OG	1:C:348:HIS:HB2	2.06	0.56
1:B:132:VAL:O	1:D:129:ARG:HA	2.05	0.56
1:A:144:ILE:CD1	1:A:148:LEU:HD12	2.36	0.55
1:D:247:SER:OG	1:D:348:HIS:HB2	2.07	0.55
1:A:339:VAL:HG11	1:A:368:ARG:NH2	2.22	0.55
1:D:354:GLY:HA2	1:D:377:LEU:HD21	1.89	0.54
1:C:139:MET:HE1	1:D:139:MET:HE1	1.90	0.54
1:B:133:LYS:O	1:D:129:ARG:HD3	2.07	0.54
1:C:57:VAL:HG21	1:C:350:ILE:HG22	1.90	0.54
1:B:312:LEU:HD23	1:B:361:LEU:HD22	1.90	0.54
1:A:57:VAL:HG21	1:A:350:ILE:HG22	1.90	0.54
1:A:175:GLN:HE22	1:A:240:THR:CG2	2.21	0.54
1:B:175:GLN:HE22	1:B:240:THR:HG21	1.71	0.54
1:B:7:ILE:HG23	1:B:256:ALA:HB1	1.90	0.53
1:B:336:ILE:HG13	1:B:336:ILE:O	2.09	0.53
1:D:98:LEU:HD23	1:D:101:GLN:OE1	2.08	0.53
1:D:34:VAL:CG1	1:D:255:ALA:HB3	2.38	0.53
1:A:132:VAL:HG21	1:A:137:PHE:CD2	2.44	0.52
1:A:7:ILE:HG23	1:A:256:ALA:HB1	1.90	0.52
1:C:35:ILE:HG12	1:C:112:VAL:HG11	1.92	0.52
1:D:35:ILE:O	1:D:38:VAL:HG22	2.09	0.52
1:A:258:LEU:HD22	1:A:258:LEU:H	1.73	0.52
1:A:216:ASP:HB3	4:A:2009:HOH:O	2.10	0.52
1:B:143:MET:HE3	1:B:144:ILE:HD11	1.91	0.52
1:A:39:LEU:HD11	1:A:49:VAL:CG2	2.40	0.51
1:C:54:LEU:O	1:C:84:GLY:HA2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:LEU:HD13	1:D:332:TRP:CH2	2.46	0.51
1:B:247:SER:OG	1:B:348:HIS:HB2	2.11	0.51
1:B:196:LYS:NZ	4:B:2133:HOH:O	2.40	0.51
1:C:28:HIS:ND1	1:C:62:GLU:OE2	2.37	0.50
1:D:7:ILE:HD13	1:D:362:LEU:HD11	1.93	0.50
1:A:274:ARG:NH2	1:A:390:GLU:OE1	2.44	0.50
1:B:267:ARG:HB3	4:B:2171:HOH:O	2.12	0.50
1:D:127:HIS:HB3	4:D:2009:HOH:O	2.11	0.50
1:A:317:GLU:O	1:A:343:ALA:HB3	2.12	0.50
1:C:330:LEU:CD1	1:C:332:TRP:CH2	2.95	0.50
1:A:9:SER:HA	1:A:272:LEU:HD22	1.93	0.50
1:A:158:GLY:O	1:A:161:ALA:HB3	2.12	0.49
1:A:100:MET:HE1	1:A:278:TRP:CD1	2.47	0.49
1:B:39:LEU:HD13	1:B:257:LEU:HD12	1.95	0.49
1:A:30:LEU:O	1:A:34:VAL:HG23	2.12	0.49
1:A:85:MET:HA	1:B:85:MET:HA	1.95	0.49
1:A:124:HIS:NE2	1:D:135:GLY:O	2.45	0.49
1:B:21:ALA:HB1	1:B:213:VAL:HG21	1.95	0.49
1:A:122:ALA:HB3	1:B:129:ARG:HH21	1.78	0.48
1:B:131:GLY:HA2	1:D:131:GLY:HA2	1.94	0.48
1:C:157:MET:HG3	4:C:2019:HOH:O	2.12	0.48
1:C:57:VAL:HG21	1:C:350:ILE:CG2	2.44	0.48
1:B:78:GLN:HG2	4:B:2065:HOH:O	2.13	0.48
1:D:7:ILE:HG23	1:D:256:ALA:HB1	1.96	0.47
1:A:291:GLY:N	1:A:292:PRO:CD	2.77	0.47
1:C:129:ARG:HH21	1:D:122:ALA:HB3	1.79	0.47
1:D:54:LEU:HD12	1:D:67:ALA:HA	1.96	0.47
1:C:312:LEU:HD23	1:C:361:LEU:CD2	2.44	0.47
1:C:88:LEU:HD12	1:C:380:GLY:O	2.15	0.47
1:B:9:SER:HA	1:B:272:LEU:HD22	1.95	0.47
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.49	0.47
1:B:106:GLY:HA2	4:B:2075:HOH:O	2.15	0.46
1:C:330:LEU:HD13	1:C:332:TRP:CZ3	2.51	0.46
1:A:181:ALA:HB1	4:A:2064:HOH:O	2.14	0.46
1:D:132:VAL:HG21	1:D:137:PHE:HD2	1.78	0.46
1:A:7:ILE:HG12	1:A:258:LEU:HD11	1.96	0.46
1:A:175:GLN:HE22	1:A:240:THR:HG23	1.81	0.46
1:C:257:LEU:C	1:C:257:LEU:HD23	2.41	0.46
1:A:298:LYS:HE3	1:A:298:LYS:HA	1.97	0.46
1:C:144:ILE:HD13	1:C:148:LEU:HD12	1.98	0.45
1:A:35:ILE:HG12	1:A:112:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:GLN:NE2	1:C:378:CYS:SG	2.89	0.45
1:B:354:GLY:HA2	1:B:377:LEU:HD21	1.98	0.45
1:A:374:LEU:HD12	1:A:388:CYS:SG	2.57	0.45
1:B:135:GLY:O	1:C:124:HIS:NE2	2.43	0.45
1:B:358:LEU:HD22	1:B:362:LEU:HG	1.99	0.45
1:C:97:ALA:HB2	1:C:387:MET:CE	2.46	0.45
1:C:257:LEU:HD22	1:C:259:MET:HE3	1.97	0.44
1:D:57:VAL:HG21	1:D:350:ILE:HG21	1.99	0.44
1:A:46:ALA:HB1	1:A:76:VAL:HA	1.99	0.44
1:D:312:LEU:HD23	1:D:361:LEU:CD2	2.48	0.44
1:A:21:ALA:HB1	1:A:213:VAL:HG21	2.00	0.44
1:D:257:LEU:CD2	1:D:259:MET:HE3	2.48	0.44
1:A:85:MET:HE2	1:A:85:MET:HB2	1.92	0.44
1:C:279:ALA:HB1	1:C:298:LYS:HB3	1.98	0.44
1:A:139:MET:HG3	1:D:137:PHE:CE1	2.53	0.44
1:C:157:MET:HA	1:C:157:MET:HE2	2.00	0.44
1:D:281:VAL:HG12	1:D:282:GLY:N	2.33	0.44
1:D:257:LEU:HD21	1:D:259:MET:HE3	2.00	0.43
1:C:68:ARG:HG3	1:D:152:PHE:HZ	1.83	0.43
1:A:96:VAL:HG21	1:A:358:LEU:HD12	2.00	0.43
1:A:281:VAL:HG12	1:A:282:GLY:N	2.33	0.43
1:B:274:ARG:HH12	1:B:276:VAL:HG12	1.81	0.43
1:D:276:VAL:HG21	1:D:305:TRP:CZ2	2.53	0.43
1:B:76:VAL:HG13	1:B:77:PRO:HD2	2.01	0.43
2:B:1393:PN5:HT33	1:C:134:MET:HE1	2.00	0.43
1:D:274:ARG:NH1	1:D:276:VAL:HG12	2.34	0.43
1:A:377:LEU:HD12	1:A:377:LEU:N	2.35	0.42
1:C:340:ASN:ND2	1:C:364:GLU:OE1	2.47	0.42
1:D:7:ILE:HG12	1:D:258:LEU:CD1	2.49	0.42
1:D:46:ALA:HB1	1:D:76:VAL:HA	2.01	0.42
1:A:162:GLU:OE1	1:A:240:THR:HG22	2.19	0.42
1:C:108:ALA:CB	1:C:111:ILE:HD11	2.49	0.42
1:A:286:LYS:NZ	4:A:2188:HOH:O	2.52	0.42
1:A:7:ILE:HD13	1:A:362:LEU:HD11	2.02	0.42
1:B:143:MET:HE3	1:B:144:ILE:HD13	2.00	0.42
1:B:216:ASP:HB3	4:B:2213:HOH:O	2.18	0.42
1:A:196:LYS:NZ	4:A:2139:HOH:O	2.37	0.42
1:B:281:VAL:HG12	1:B:282:GLY:N	2.35	0.42
1:D:317:GLU:O	1:D:343:ALA:HB3	2.19	0.42
1:B:63:GLY:O	1:B:64:GLN:C	2.62	0.42
1:B:274:ARG:NH2	1:B:390:GLU:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LYS:NZ	4:C:2024:HOH:O	2.52	0.42
1:A:76:VAL:CG1	1:A:77:PRO:HD2	2.50	0.41
1:A:106:GLY:HA2	4:A:2085:HOH:O	2.20	0.41
1:B:101:GLN:O	1:B:105:THR:HG23	2.20	0.41
1:C:317:GLU:O	1:C:343:ALA:HB3	2.20	0.41
1:B:317:GLU:O	1:B:343:ALA:HB3	2.20	0.41
1:C:86:ASN:OD1	1:C:86:ASN:C	2.62	0.41
1:A:354:GLY:HA2	1:A:377:LEU:HD21	2.03	0.41
1:B:278:TRP:HA	1:B:387:MET:HA	2.02	0.41
1:C:39:LEU:HD11	1:C:49:VAL:CG2	2.51	0.41
1:B:22:PHE:O	1:B:23:ALA:C	2.63	0.41
1:B:200:VAL:O	1:B:201:PRO:C	2.62	0.41
1:C:200:VAL:O	1:C:200:VAL:HG13	2.20	0.41
1:A:167:GLN:OE1	1:A:287:VAL:HG11	2.21	0.41
1:B:13:THR:HG21	1:B:30:LEU:HD22	2.03	0.41
1:B:87:GLN:N	1:B:91:SER:OG	2.50	0.41
1:D:34:VAL:O	1:D:38:VAL:HG13	2.21	0.41
1:D:53:ILE:HD13	1:D:83:TRP:CZ2	2.56	0.41
1:A:150:ASP:OD1	4:A:2110:HOH:O	2.22	0.41
1:B:383:MET:HE2	4:B:2221:HOH:O	2.20	0.41
1:A:364:GLU:O	1:A:368:ARG:HG2	2.21	0.40
1:D:358:LEU:HD22	1:D:362:LEU:HG	2.04	0.40
1:A:12:ARG:O	1:A:199:ILE:HA	2.21	0.40
1:C:291:GLY:N	1:C:292:PRO:CD	2.84	0.40
1:A:57:VAL:HG21	1:A:350:ILE:CG2	2.51	0.40
1:B:134:MET:SD	1:C:143:MET:HE1	2.62	0.40
1:C:12:ARG:HH12	1:C:15:VAL:HG23	1.87	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	387/392 (99%)	369 (95%)	17 (4%)	1 (0%)	36	52
1	B	387/392 (99%)	366 (95%)	21 (5%)	0	100	100
1	C	387/392 (99%)	372 (96%)	14 (4%)	1 (0%)	36	52
1	D	387/392 (99%)	374 (97%)	12 (3%)	1 (0%)	36	52
All	All	1548/1568 (99%)	1481 (96%)	64 (4%)	3 (0%)	43	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	350	ILE
1	D	350	ILE
1	A	350	ILE

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	276/279 (99%)	267 (97%)	9 (3%)	33	55
1	B	276/279 (99%)	264 (96%)	12 (4%)	26	44
1	C	276/279 (99%)	264 (96%)	12 (4%)	26	44
1	D	276/279 (99%)	265 (96%)	11 (4%)	28	47
All	All	1104/1116 (99%)	1060 (96%)	44 (4%)	28	47

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	207	ARG
1	A	270	GLN
1	A	272	LEU
1	A	298	LYS
1	A	322	GLN
1	A	339	VAL
1	A	358	LEU

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Mol	Chain	Res	Type
1	A	361	LEU
1	B	4	SER
1	B	39	LEU
1	B	100	MET
1	B	207	ARG
1	B	258	LEU
1	B	270	GLN
1	B	272	LEU
1	B	298	LYS
1	B	322	GLN
1	B	339	VAL
1	B	358	LEU
1	B	361	LEU
1	C	4	SER
1	C	39	LEU
1	C	207	ARG
1	C	263	GLU
1	C	270	GLN
1	C	272	LEU
1	C	298	LYS
1	C	322	GLN
1	C	339	VAL
1	C	358	LEU
1	C	360	THR
1	C	361	LEU
1	D	39	LEU
1	D	81	THR
1	D	207	ARG
1	D	258	LEU
1	D	263	GLU
1	D	270	GLN
1	D	272	LEU
1	D	298	LYS
1	D	322	GLN
1	D	358	LEU
1	D	361	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	156	HIS

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Mol	Chain	Res	Type
1	A	175	GLN
1	A	184	ASN
1	A	221	HIS
1	B	78	GLN
1	B	124	HIS
1	B	156	HIS
1	B	167	GLN
1	B	175	GLN
1	B	184	ASN
1	B	270	GLN
1	B	316	ASN
1	C	78	GLN
1	C	184	ASN
1	C	316	ASN
1	C	322	GLN
1	D	78	GLN
1	D	167	GLN
1	D	175	GLN
1	D	184	ASN
1	D	316	ASN
1	D	322	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 oligosaccharides 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	SO4	B	1394	-	4,4,4	0.23	0	6,6,6	0.15	0
3	SO4	A	1394	-	4,4,4	0.25	0	6,6,6	0.16	0
3	SO4	B	1396	-	4,4,4	0.24	0	6,6,6	0.39	0
2	PN5	B	1393	-	20,23,23	1.41	1 (5%)	29,32,32	1.99	8 (27%)
2	PN5	A	1393	-	20,23,23	1.39	1 (5%)	29,32,32	1.48	6 (20%)
3	SO4	A	1396	-	4,4,4	0.31	0	6,6,6	0.42	0
3	SO4	B	1395	-	4,4,4	0.21	0	6,6,6	0.48	0
3	SO4	A	1395	-	4,4,4	0.26	0	6,6,6	0.21	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
2	PN5	B	1393	-	-	9/32/32/32	-
2	PN5	A	1393	-	-	11/32/32/32	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1393	PN5	OA6-CT1	5.91	1.46	1.33
2	A	1393	PN5	OA6-CT1	5.82	1.46	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1393	PN5	CPC-OA6-CT1	4.97	123.72	116.75
2	B	1393	PN5	OA6-CT1-CT2	4.02	120.44	112.57
2	B	1393	PN5	CP7-NP8-CP9	3.84	129.44	122.55
2	A	1393	PN5	OA6-CT1-CT2	3.63	119.67	112.57
2	B	1393	PN5	OA6-CT1-OT1	-3.41	117.74	124.57
2	B	1393	PN5	CP3-NP4-CP5	3.25	128.88	122.82
2	B	1393	PN5	CP6-CP7-NP8	-3.12	105.36	112.00
2	A	1393	PN5	CPC-OA6-CT1	3.10	121.10	116.75
2	B	1393	PN5	CP2-CP3-NP4	-3.03	105.43	112.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1393	PN5	CP7-NP8-CP9	3.01	127.96	122.55
2	A	1393	PN5	OA6-CT1-OT1	-2.68	119.21	124.57
2	A	1393	PN5	CP2-CP3-NP4	-2.65	106.29	112.31
2	B	1393	PN5	OPA-CPA-CPB	-2.45	104.52	110.18
2	A	1393	PN5	CP3-NP4-CP5	2.06	126.66	122.82

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1393	PN5	SP1-CP2-CP3-NP4
2	A	1393	PN5	CPA-CPB-CPC-OA6
2	A	1393	PN5	CPE-CPB-CPC-OA6
2	A	1393	PN5	CPD-CPB-CPC-OA6
2	B	1393	PN5	SP1-CP2-CP3-NP4
2	B	1393	PN5	CPA-CPB-CPC-OA6
2	B	1393	PN5	CPE-CPB-CPC-OA6
2	B	1393	PN5	CPD-CPB-CPC-OA6
2	B	1393	PN5	OT1-CT1-OA6-CPC
2	B	1393	PN5	CT2-CT1-OA6-CPC
2	A	1393	PN5	CPB-CPC-OA6-CT1
2	A	1393	PN5	CP5-CP6-CP7-NP8
2	B	1393	PN5	CP5-CP6-CP7-NP8
2	A	1393	PN5	NP8-CP9-CPA-CPB
2	A	1393	PN5	NP8-CP9-CPA-OPA
2	A	1393	PN5	OP9-CP9-CPA-CPB
2	B	1393	PN5	OP9-CP9-CPA-CPB
2	B	1393	PN5	NP8-CP9-CPA-CPB
2	A	1393	PN5	OA6-CT1-CT2-CT4
2	A	1393	PN5	OA6-CT1-CT2-CT5

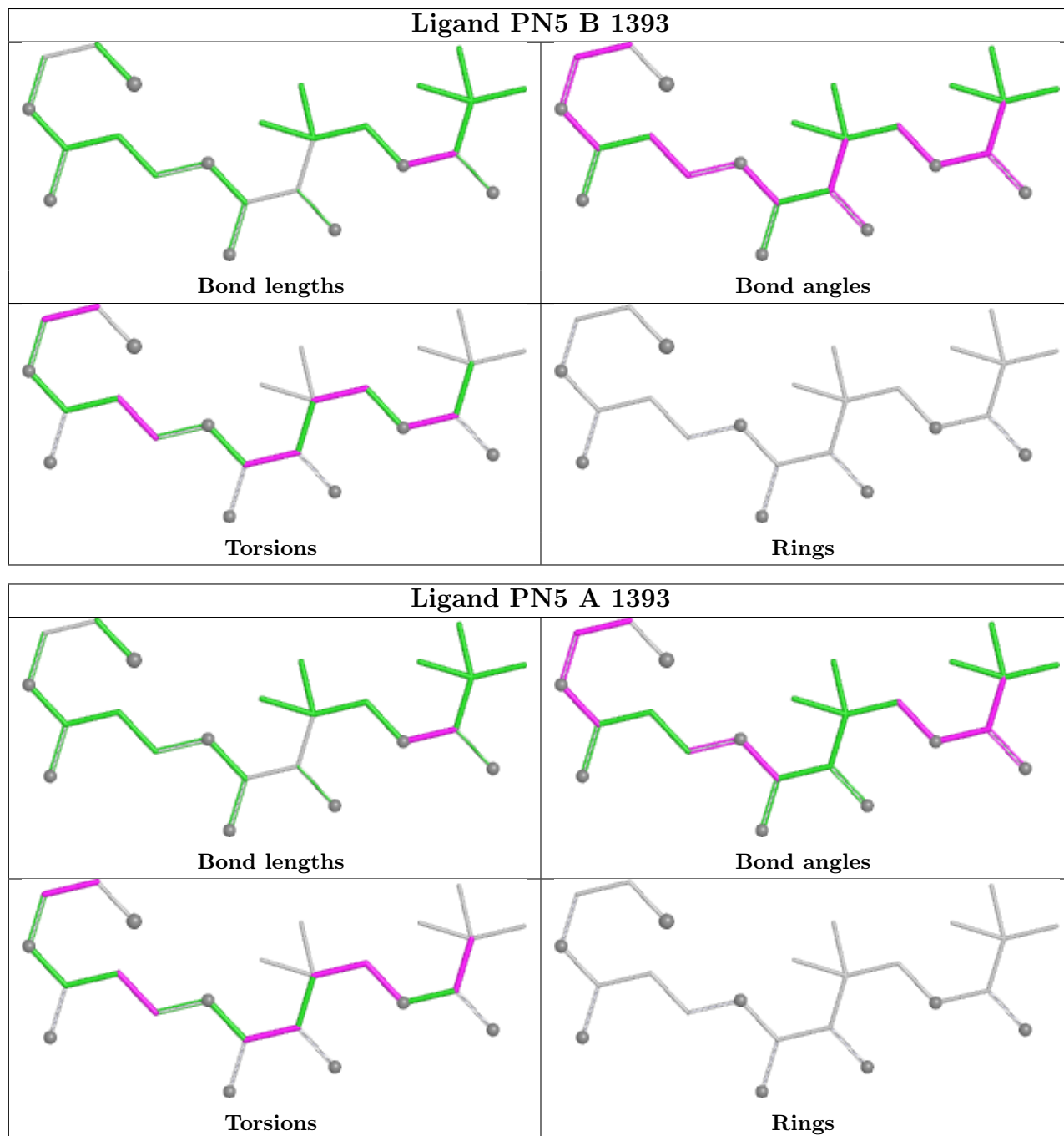
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1393	PN5	3	0
2	A	1393	PN5	3	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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.