



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:05 pm BST

PDB ID : 2VU2
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 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 : 2.11
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) : 2.11

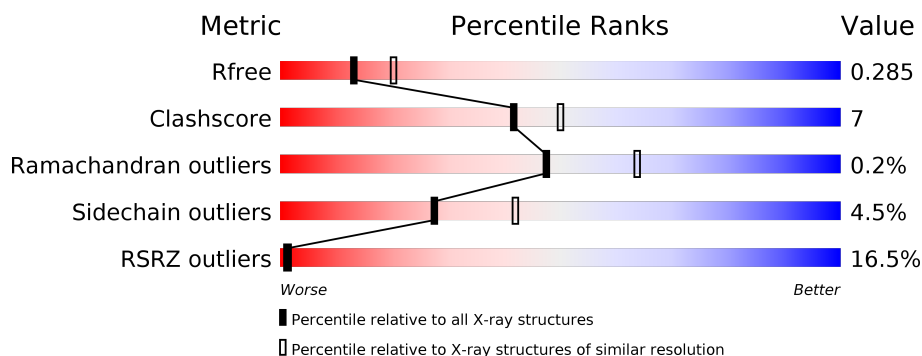
1 Overall quality at a glance

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))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	392	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>..</div> </div> </div>
1	B	392	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>..</div> </div> </div>
1	C	392	<div> <div>23%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>..</div> </div> </div>
1	D	392	<div> <div>39%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>

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.

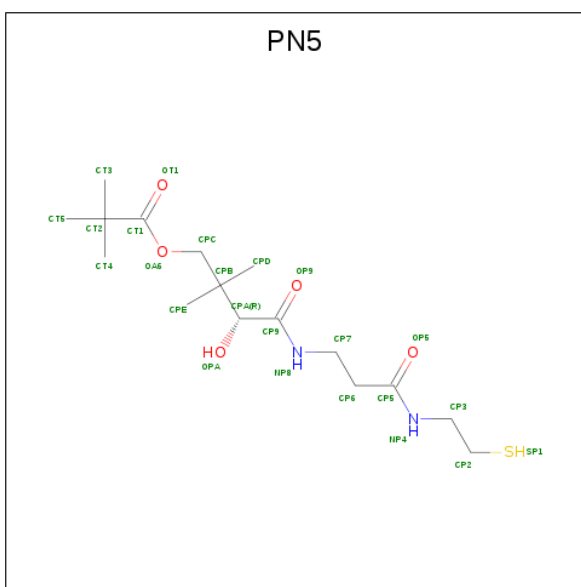
- Molecule 1 is a protein called ACETYL-COA ACETYLTRANSFERASE.

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

There are 4 discrepancies between the modelled and reference sequences:

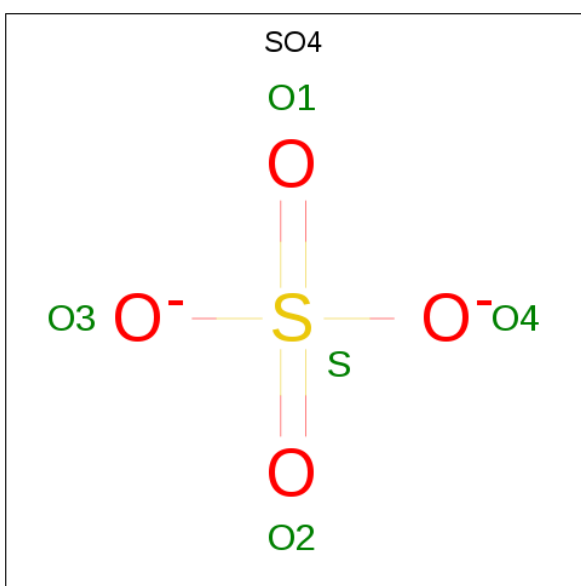
Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ARG	ALA	conflict	UNP P07097
B	129	ARG	ALA	conflict	UNP P07097
C	129	ARG	ALA	conflict	UNP P07097
D	129	ARG	ALA	conflict	UNP P07097

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



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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		

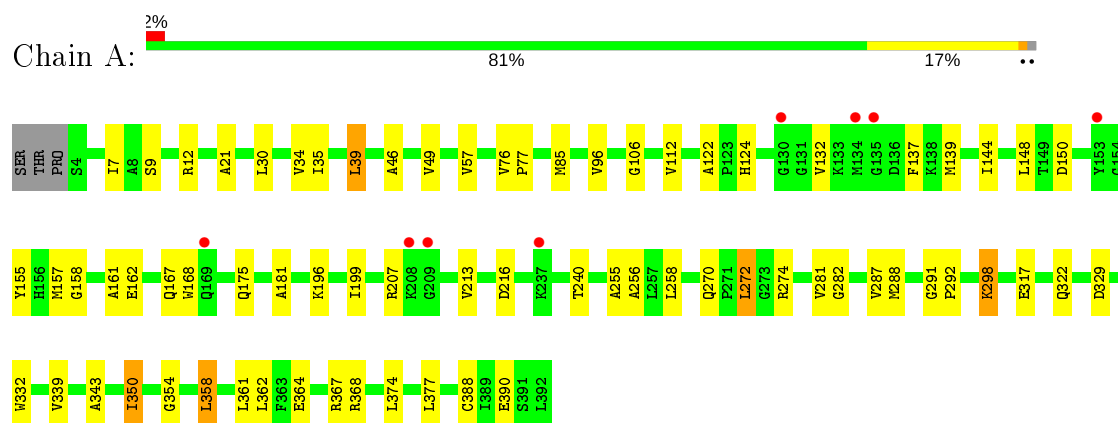
- Molecule 4 is water.

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		

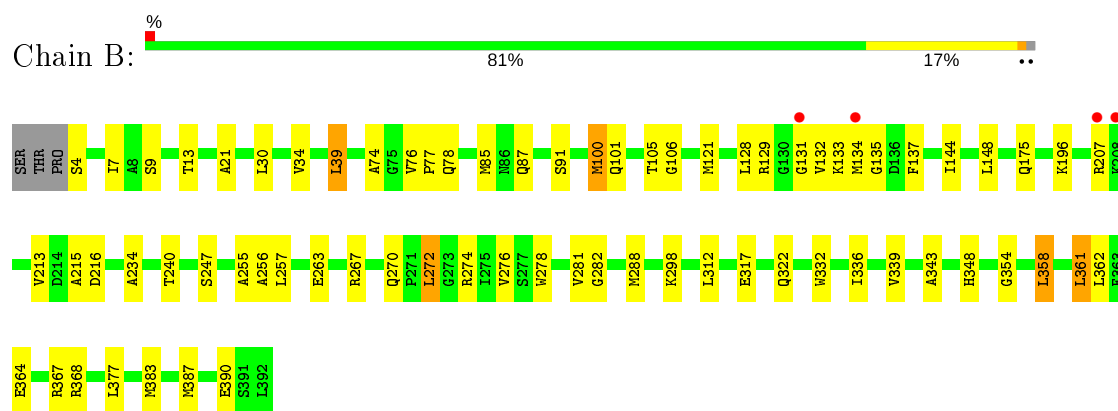
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

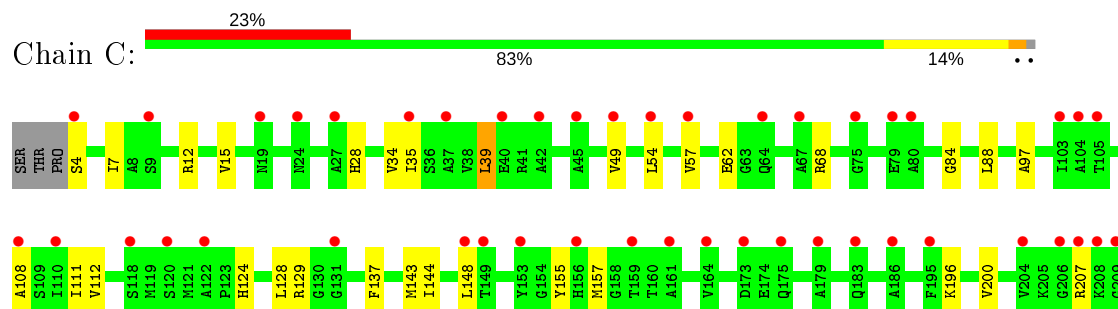
• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

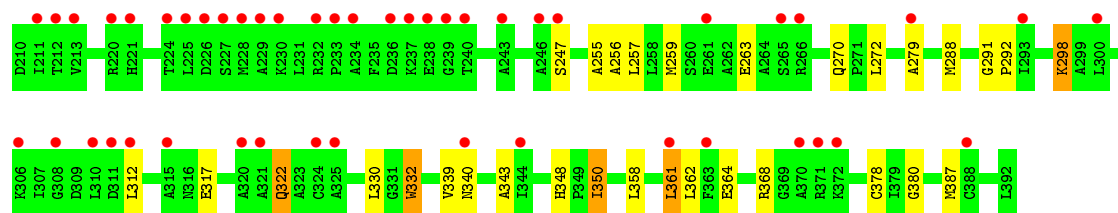


• Molecule 1: ACETYL-COA ACETYLTRANSFERASE

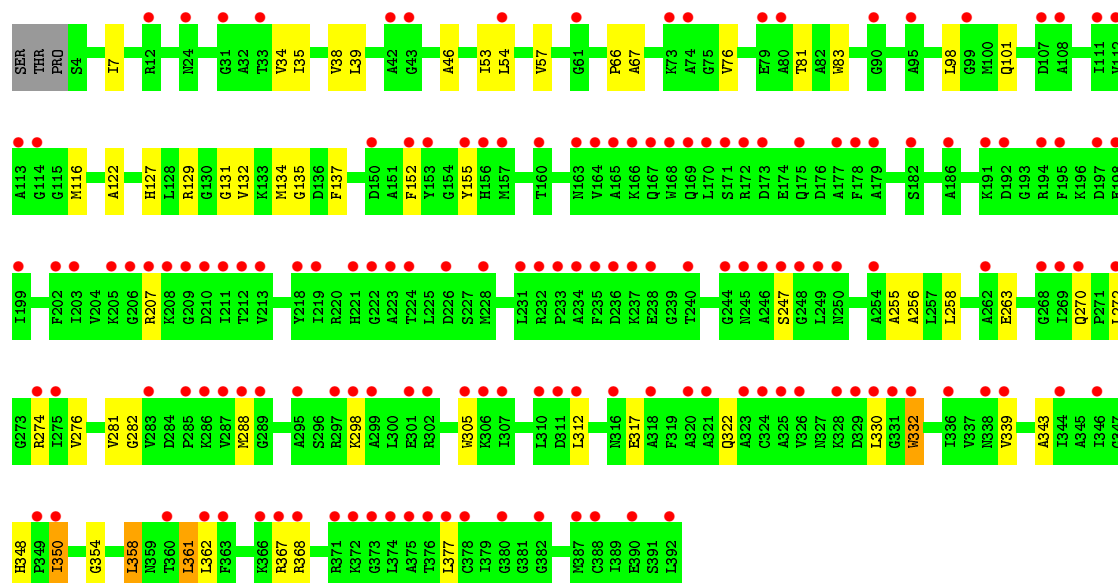
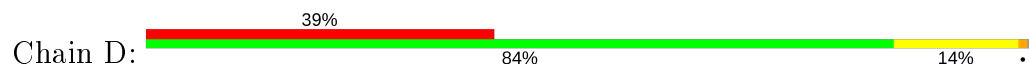


• Molecule 1: ACETYL-COA ACETYLTRANSFERASE





● Molecule 1: ACETYL-COA ACETYLTRANSFERASE



4 Data and refinement statistics

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 19.62 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.3 (20.00-2.65) 82.0 (19.62-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.231 , 0.286 0.236 , 0.285	Depositor DCC
R_{free} test set	2756 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.146 for h,-k,-l	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	11858	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage'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

5.1 Standard geometry

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	0.64	0/2854	0.74	2/3853 (0.1%)
1	B	0.62	0/2854	0.72	3/3853 (0.1%)
1	C	0.36	0/2854	0.52	0/3853
1	D	0.36	0/2854	0.55	2/3853 (0.1%)
All	All	0.51	0/11416	0.64	7/15412 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	367	ARG	NE-CZ-NH2	7.03	123.82	120.30
1	D	367	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	B	367	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	367	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	367	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	100	MET	CG-SD-CE	5.37	108.78	100.20
1	A	367	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	2813	0	2819	47	0
1	B	2813	0	2819	46	0
1	C	2813	0	2819	38	0
1	D	2813	0	2819	37	0
2	A	24	0	30	3	0
2	B	24	0	30	1	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
4	A	240	0	0	6	0
4	B	228	0	0	10	0
4	C	36	0	0	2	0
4	D	24	0	0	1	0
All	All	11858	0	11336	158	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 7.

All (158) 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
2:A:1393:PN5:HT53	1:D:134:MET:HE1	1.64	0.78
1:D:34:VAL:HG12	1:D:255:ALA:HB3	1.66	0.78
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: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
1:C:257:LEU:HD21	1:C:259:MET:HE2	1.83	0.61
1:B:175:GLN:HE22	1:B:240:THR:HG23	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD2	1:A:258:LEU:N	2.65	0.58
1:B:144:ILE:HD13	1:B:148:LEU:HD12	1.85	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: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:B:196:LYS:NZ	4:B:2133:HOH:O	2.40	0.55
1:D:354:GLY:HA2	1:D:377:LEU:HD21	1.89	0.54
1:C:57:VAL:HG21	1:C:350:ILE:HG22	1.90	0.54
1:B:133:LYS:O	1:D:129:ARG:HD3	2.07	0.54
1:B:312:LEU:HD23	1:B:361:LEU:HD22	1.90	0.54
1:A:175:GLN:HE22	1:A:240:THR:CG2	2.21	0.54
1:A:57:VAL:HG21	1:A:350:ILE:HG22	1.90	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:O	1:B:336:ILE:HG13	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:H	1:A:258:LEU:HD22	1.73	0.52
1:A:216:ASP:HB3	4:A:2009:HOH:O	2.10	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:21:ALA:HB1	1:B:213:VAL:HG21	1.95	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: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:D:66:PRO:HB2	1:D:116:MET:HE3	1.95	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:B:121:MET:HE1	4:B:2021:HOH:O	2.15	0.46
1:A:175:GLN:HE22	1:A:240:THR:HG23	1.81	0.46
1:A:298:LYS:HE3	1:A:298:LYS:HA	1.97	0.46
1:C:257:LEU:CD2	1:C:259:MET:HE2	2.46	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:134:MET:HG3	1:C:143:MET:HE1	2.00	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: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:D:281:VAL:HG12	1:D:282:GLY:N	2.33	0.44
1:C:68:ARG:HG3	1:D:152:PHE:HZ	1.83	0.43
1:A:281:VAL:HG12	1:A:282:GLY:N	2.33	0.43
1:A:96:VAL:HG21	1:A:358:LEU:HD12	2.00	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
1:D:274:ARG:NH1	1:D:276:VAL:HG12	2.34	0.43
1:A:377:LEU:N	1:A:377:LEU:HD12	2.35	0.42
1:C:340:ASN:ND2	1:C:364:GLU:OE1	2.47	0.42
1:D:46:ALA:HB1	1:D:76:VAL:HA	2.01	0.42
1:D:7:ILE:HG12	1:D:258:LEU:CD1	2.49	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:7:ILE:HD13	1:A:362:LEU:HD11	2.02	0.42
1:B:216:ASP:HB3	4:B:2213:HOH:O	2.18	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:274:ARG:NH2	1:B:390:GLU:OE1	2.52	0.42
1:C:196:LYS:NZ	4:C:2024:HOH:O	2.52	0.42
1:A:106:GLY:HA2	4:A:2085:HOH:O	2.20	0.41
1:A:76:VAL:CG1	1:A:77:PRO:HD2	2.50	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:257:LEU:CD2	1:C:259:MET:CE	2.98	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:257:LEU:C	1:C:257:LEU:HD23	2.41	0.41
1:C:39:LEU:HD11	1:C:49:VAL:CG2	2.51	0.41
1:B:383:MET:HE2	4:B:2221:HOH:O	2.20	0.41
1:C:200:VAL:HG13	1:C:200:VAL:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLN:OE1	1:A:287:VAL:HG11	2.21	0.41
1:B:87:GLN:N	1:B:91:SER:OG	2.50	0.41
1:D:53:ILE:HD13	1:D:83:TRP:CZ2	2.56	0.41
1:B:13:THR:HG21	1:B:30:LEU:HD22	2.03	0.41
1:D:34:VAL:O	1:D:38:VAL:HG13	2.21	0.41
1:A:150:ASP:OD1	4:A:2110:HOH:O	2.22	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:196:LYS:NZ	4:A:2139:HOH:O	2.37	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: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%)	41	56
1	B	387/392 (99%)	366 (95%)	21 (5%)	0	100	100
1	C	387/392 (99%)	372 (96%)	14 (4%)	1 (0%)	41	56
1	D	387/392 (99%)	374 (97%)	12 (3%)	1 (0%)	41	56
All	All	1548/1568 (99%)	1481 (96%)	64 (4%)	3 (0%)	47	64

All (3) Ramachandran outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	350	ILE

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	276/279 (99%)	265 (96%)	11 (4%)	31	47
1	B	276/279 (99%)	263 (95%)	13 (5%)	26	40
1	C	276/279 (99%)	263 (95%)	13 (5%)	26	40
1	D	276/279 (99%)	263 (95%)	13 (5%)	26	40
All	All	1104/1116 (99%)	1054 (96%)	50 (4%)	27	42

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	155	TYR
1	A	207	ARG
1	A	270	GLN
1	A	272	LEU
1	A	288	MET
1	A	298	LYS
1	A	322	GLN
1	A	332	TRP
1	A	358	LEU
1	A	361	LEU
1	B	4	SER
1	B	39	LEU
1	B	100	MET
1	B	207	ARG
1	B	263	GLU
1	B	270	GLN
1	B	272	LEU
1	B	288	MET
1	B	298	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	322	GLN
1	B	332	TRP
1	B	358	LEU
1	B	361	LEU
1	C	4	SER
1	C	39	LEU
1	C	155	TYR
1	C	207	ARG
1	C	263	GLU
1	C	270	GLN
1	C	272	LEU
1	C	288	MET
1	C	298	LYS
1	C	322	GLN
1	C	332	TRP
1	C	358	LEU
1	C	361	LEU
1	D	39	LEU
1	D	81	THR
1	D	155	TYR
1	D	207	ARG
1	D	263	GLU
1	D	270	GLN
1	D	272	LEU
1	D	288	MET
1	D	298	LYS
1	D	322	GLN
1	D	332	TRP
1	D	358	LEU
1	D	361	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	156	HIS
1	A	175	GLN
1	A	184	ASN
1	B	78	GLN
1	B	156	HIS
1	B	175	GLN
1	B	184	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	78	GLN
1	C	184	ASN
1	C	270	GLN
1	C	316	ASN
1	C	322	GLN
1	D	78	GLN
1	D	175	GLN
1	D	184	ASN
1	D	316	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	1395	-	4,4,4	0.12	0	6,6,6	0.47	0
2	PN5	A	1393	-	19,23,23	1.39	1 (5%)	29,32,32	1.47	7 (24%)
3	SO4	B	1396	-	4,4,4	0.12	0	6,6,6	0.37	0
3	SO4	A	1396	-	4,4,4	0.21	0	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PN5	B	1393	-	19,23,23	1.42	1 (5%)	29,32,32	1.98	8 (27%)
3	SO4	A	1395	-	4,4,4	0.15	0	6,6,6	0.19	0
3	SO4	A	1394	-	4,4,4	0.15	0	6,6,6	0.11	0
3	SO4	B	1394	-	4,4,4	0.13	0	6,6,6	0.13	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	A	1393	-	-	12/32/32/32	-
2	PN5	B	1393	-	-	9/32/32/32	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1393	PN5	OA6-CT1	5.82	1.46	1.33
2	A	1393	PN5	OA6-CT1	5.74	1.46	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1393	PN5	CPC-OA6-CT1	4.89	123.72	116.81
2	B	1393	PN5	OA6-CT1-CT2	3.95	120.44	112.56
2	B	1393	PN5	CP7-NP8-CP9	3.84	129.44	122.59
2	A	1393	PN5	OA6-CT1-CT2	3.56	119.67	112.56
2	B	1393	PN5	OA6-CT1-OT1	-3.31	117.74	124.54
2	B	1393	PN5	CP3-NP4-CP5	3.25	128.88	122.84
2	B	1393	PN5	CP6-CP7-NP8	-3.24	105.36	111.90
2	A	1393	PN5	CPC-OA6-CT1	3.03	121.10	116.81
2	A	1393	PN5	CP7-NP8-CP9	3.01	127.96	122.59
2	B	1393	PN5	CP2-CP3-NP4	-3.01	105.43	112.31
2	A	1393	PN5	CP2-CP3-NP4	-2.63	106.29	112.31
2	A	1393	PN5	OA6-CT1-OT1	-2.59	119.21	124.54
2	B	1393	PN5	OPA-CPA-CPB	-2.44	104.52	110.25
2	A	1393	PN5	CP3-NP4-CP5	2.06	126.66	122.84
2	A	1393	PN5	CP6-CP7-NP8	-2.04	107.78	111.90

There are no chirality outliers.

All (21) torsion outliers are listed below:

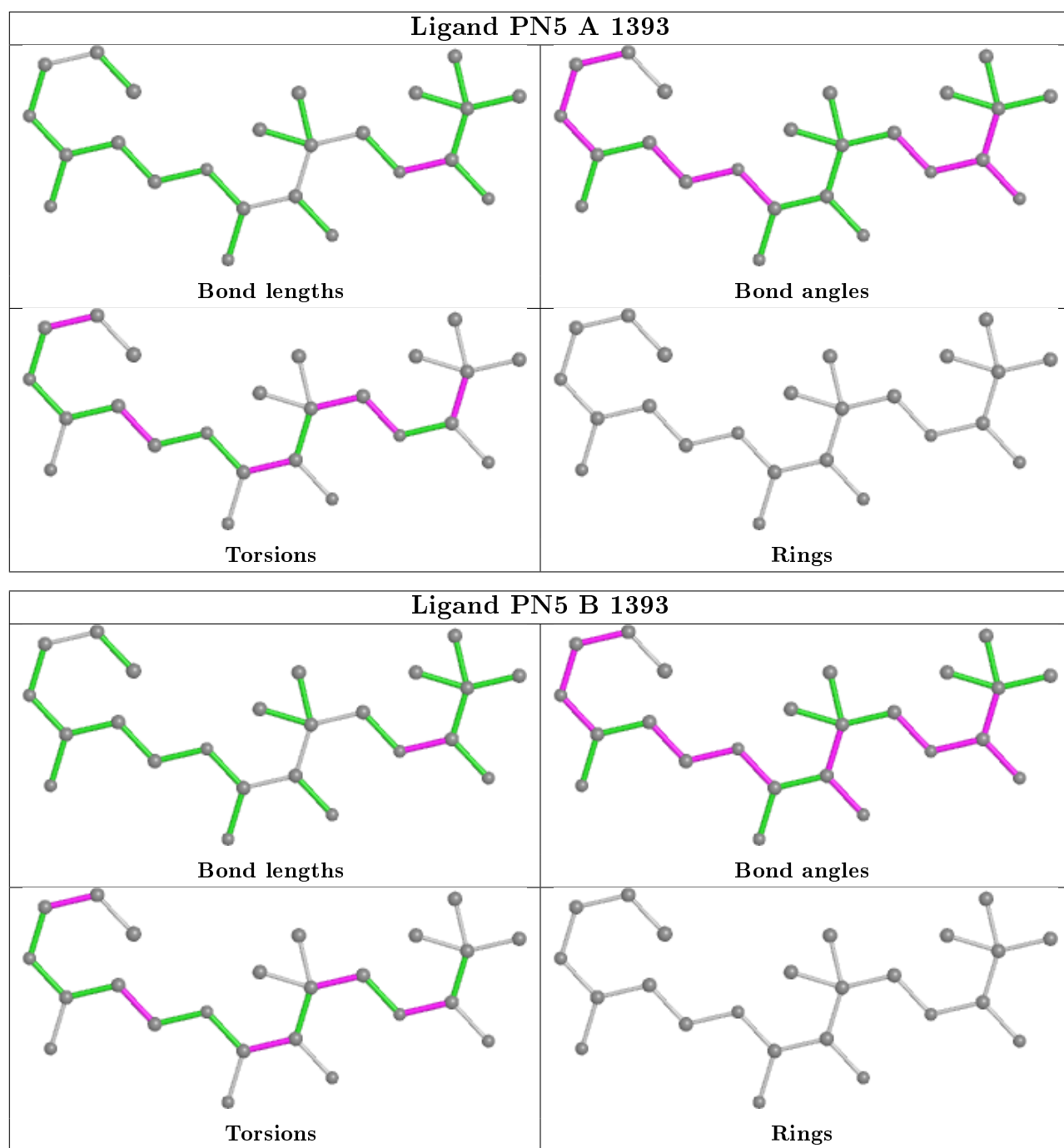
Mol	Chain	Res	Type	Atoms
2	A	1393	PN5	SP1-CP2-CP3-NP4
2	A	1393	PN5	CPA-CPB-CPC-OA6
2	A	1393	PN5	CPE-CPB-CPC-OA6
2	A	1393	PN5	CPD-CPB-CPC-OA6
2	B	1393	PN5	SP1-CP2-CP3-NP4
2	B	1393	PN5	CPA-CPB-CPC-OA6
2	B	1393	PN5	CPE-CPB-CPC-OA6
2	B	1393	PN5	CPD-CPB-CPC-OA6
2	B	1393	PN5	OT1-CT1-OA6-CPC
2	B	1393	PN5	CT2-CT1-OA6-CPC
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	OP9-CP9-CPA-CPB
2	A	1393	PN5	NP8-CP9-CPA-CPB
2	A	1393	PN5	NP8-CP9-CPA-OPA
2	B	1393	PN5	OP9-CP9-CPA-CPB
2	B	1393	PN5	NP8-CP9-CPA-CPB
2	A	1393	PN5	OP9-CP9-CPA-OPA
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 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1393	PN5	3	0
2	B	1393	PN5	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	389/392 (99%)	0.03	8 (2%) 63 59	69, 78, 90, 105	0
1	B	389/392 (99%)	0.06	4 (1%) 82 81	69, 78, 89, 107	0
1	C	389/392 (99%)	1.39	92 (23%) 0 0	65, 80, 92, 98	0
1	D	389/392 (99%)	1.94	153 (39%) 0 0	67, 81, 95, 101	0
All	All	1556/1568 (99%)	0.85	257 (16%) 1 1	65, 79, 92, 107	0

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	331	GLY	12.8
1	D	371	ARG	8.6
1	D	228	MET	8.3
1	D	157	MET	8.1
1	D	231	LEU	7.2
1	C	243	ALA	6.3
1	D	238	GLU	6.3
1	C	80	ALA	6.2
1	D	367	ARG	6.0
1	D	269	ILE	5.9
1	D	219	ILE	5.9
1	D	226	ASP	5.7
1	D	173	ASP	5.6
1	D	170	LEU	5.3
1	C	315	ALA	5.1
1	D	320	ALA	5.0
1	D	368	ARG	5.0
1	D	362	LEU	5.0
1	C	221	HIS	4.9
1	D	232	ARG	4.9
1	D	245	ASN	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	153	TYR	4.9
1	C	204	VAL	4.8
1	C	57	VAL	4.7
1	C	208	LYS	4.6
1	D	240	THR	4.5
1	D	330	LEU	4.5
1	C	370	ALA	4.4
1	C	236	ASP	4.4
1	D	207	ARG	4.3
1	C	232	ARG	4.3
1	D	166	LYS	4.3
1	C	186	ALA	4.2
1	D	222	GLY	4.2
1	D	73	LYS	4.2
1	D	388	CYS	4.2
1	D	167	GLN	4.1
1	D	235	PHE	4.1
1	D	310	LEU	4.1
1	D	268	GLY	4.0
1	C	213	VAL	4.0
1	C	156	HIS	4.0
1	C	246	ALA	4.0
1	D	208	LYS	4.0
1	D	152	PHE	4.0
1	D	246	ALA	4.0
1	C	226	ASP	3.9
1	D	244	GLY	3.9
1	D	191	LYS	3.9
1	D	262	ALA	3.9
1	D	221	HIS	3.9
1	C	320	ALA	3.8
1	C	321	ALA	3.8
1	D	206	GLY	3.8
1	C	164	VAL	3.7
1	C	173	ASP	3.7
1	D	374	LEU	3.7
1	C	110	ILE	3.6
1	D	61	GLY	3.6
1	C	233	PRO	3.6
1	D	349	PRO	3.6
1	D	318	ALA	3.6
1	C	220	ARG	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	208	LYS	3.6
1	C	308	GLY	3.6
1	C	131	GLY	3.6
1	D	328	LYS	3.5
1	D	289	GLY	3.5
1	C	67	ALA	3.5
1	D	42	ALA	3.5
1	D	378	CYS	3.4
1	C	159	THR	3.4
1	C	9	SER	3.4
1	C	227	SER	3.4
1	D	156	HIS	3.4
1	D	165	ALA	3.4
1	D	312	LEU	3.4
1	D	323	ALA	3.4
1	D	218	TYR	3.4
1	D	301	GLU	3.4
1	D	31	GLY	3.4
1	C	207	ARG	3.3
1	C	179	ALA	3.3
1	D	286	LYS	3.3
1	D	285	PRO	3.3
1	D	168	TRP	3.3
1	D	288	MET	3.3
1	D	387	MET	3.3
1	D	373	GLY	3.2
1	D	336	ILE	3.2
1	C	104	ALA	3.2
1	D	150	ASP	3.2
1	D	329	ASP	3.2
1	D	298	LYS	3.2
1	D	182	SER	3.2
1	C	230	LYS	3.2
1	D	99	GLY	3.2
1	C	212	THR	3.2
1	D	233	PRO	3.2
1	D	324	CYS	3.2
1	D	237	LYS	3.2
1	C	224	THR	3.1
1	D	295	ALA	3.1
1	D	326	VAL	3.1
1	C	371	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	208	LYS	3.1
1	C	211	ILE	3.1
1	C	149	THR	3.1
1	D	194	ARG	3.0
1	D	205	LYS	3.0
1	D	249	LEU	3.0
1	D	79	GLU	3.0
1	D	372	LYS	3.0
1	D	107	ASP	3.0
1	C	229	ALA	3.0
1	C	311	ASP	3.0
1	D	175	GLN	2.9
1	D	321	ALA	2.9
1	D	202	PHE	2.9
1	D	43	GLY	2.9
1	D	366	LYS	2.9
1	D	169	GLN	2.9
1	C	266	ARG	2.8
1	D	12	ARG	2.8
1	D	186	ALA	2.8
1	C	161	ALA	2.8
1	C	325	ALA	2.8
1	D	302	ARG	2.8
1	D	164	VAL	2.8
1	D	171	SER	2.8
1	D	177	ALA	2.8
1	C	225	LEU	2.8
1	D	350	ILE	2.8
1	D	377	LEU	2.7
1	C	310	LEU	2.7
1	C	265	SER	2.7
1	D	382	GLY	2.7
1	B	131	GLY	2.7
1	C	79	GLU	2.7
1	D	332	TRP	2.7
1	D	172	ARG	2.6
1	C	183	GLN	2.6
1	D	209	GLY	2.6
1	D	272	LEU	2.6
1	D	155	TYR	2.6
1	C	19	ASN	2.6
1	C	238	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	213	VAL	2.6
1	D	316	ASN	2.6
1	D	95	ALA	2.6
1	C	103	ILE	2.6
1	C	240	THR	2.6
1	D	33	THR	2.6
1	C	42	ALA	2.6
1	D	114	GLY	2.6
1	C	237	LYS	2.6
1	D	248	GLY	2.6
1	A	134	MET	2.6
1	D	236	ASP	2.5
1	C	340	ASN	2.5
1	C	45	ALA	2.5
1	D	179	ALA	2.5
1	D	254	ALA	2.5
1	C	312	LEU	2.5
1	B	207	ARG	2.5
1	C	293	ILE	2.5
1	C	306	LYS	2.5
1	D	198	GLU	2.5
1	C	105	THR	2.5
1	D	212	THR	2.5
1	D	360	THR	2.5
1	C	4	SER	2.5
1	C	209	GLY	2.4
1	C	361	LEU	2.4
1	C	195	PHE	2.4
1	C	40	GLU	2.4
1	C	153	TYR	2.4
1	D	90	GLY	2.4
1	D	234	ALA	2.4
1	C	300	LEU	2.4
1	C	363	PHE	2.4
1	D	111	ILE	2.4
1	B	134	MET	2.4
1	C	388	CYS	2.4
1	A	209	GLY	2.4
1	D	287	VAL	2.4
1	D	108	ALA	2.4
1	D	24	ASN	2.3
1	D	199	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	375	ALA	2.3
1	C	206	GLY	2.3
1	D	197	ASP	2.3
1	D	250	ASN	2.3
1	D	376	THR	2.3
1	D	297	ARG	2.3
1	C	24	ASN	2.3
1	C	279	ALA	2.3
1	D	74	ALA	2.3
1	D	113	ALA	2.3
1	D	163	ASN	2.3
1	D	178	PHE	2.3
1	D	339	VAL	2.3
1	D	211	ILE	2.3
1	D	305	TRP	2.3
1	C	261	GLU	2.3
1	D	363	PHE	2.3
1	D	311	ASP	2.3
1	A	135	GLY	2.2
1	C	247	SER	2.2
1	C	108	ALA	2.2
1	D	299	ALA	2.2
1	D	306	LYS	2.2
1	D	325	ALA	2.2
1	C	324	CYS	2.2
1	D	247	SER	2.2
1	C	372	LYS	2.2
1	D	274	ARG	2.2
1	C	122	ALA	2.2
1	D	160	THR	2.2
1	D	275	ILE	2.2
1	C	120	SER	2.2
1	D	338	ASN	2.2
1	D	270	GLN	2.2
1	D	195	PHE	2.2
1	D	203	ILE	2.2
1	D	344	ILE	2.2
1	A	130	GLY	2.2
1	D	210	ASP	2.2
1	A	169	GLN	2.1
1	C	344	ILE	2.1
1	C	37	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	49	VAL	2.1
1	D	112	VAL	2.1
1	D	283	VAL	2.1
1	C	175	GLN	2.1
1	D	307	ILE	2.1
1	D	346	ILE	2.1
1	D	223	ALA	2.1
1	C	228	MET	2.1
1	D	192	ASP	2.1
1	D	80	ALA	2.1
1	C	239	GLY	2.1
1	C	54	LEU	2.1
1	C	148	LEU	2.1
1	D	392	LEU	2.1
1	D	380	GLY	2.1
1	C	35	ILE	2.0
1	A	153	TYR	2.0
1	A	237	LYS	2.0
1	C	75	GLY	2.0
1	C	118	SER	2.0
1	D	390	GLU	2.0
1	C	27	ALA	2.0
1	C	234	ALA	2.0
1	C	64	GLN	2.0
1	D	224	THR	2.0
1	D	54	LEU	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](#)

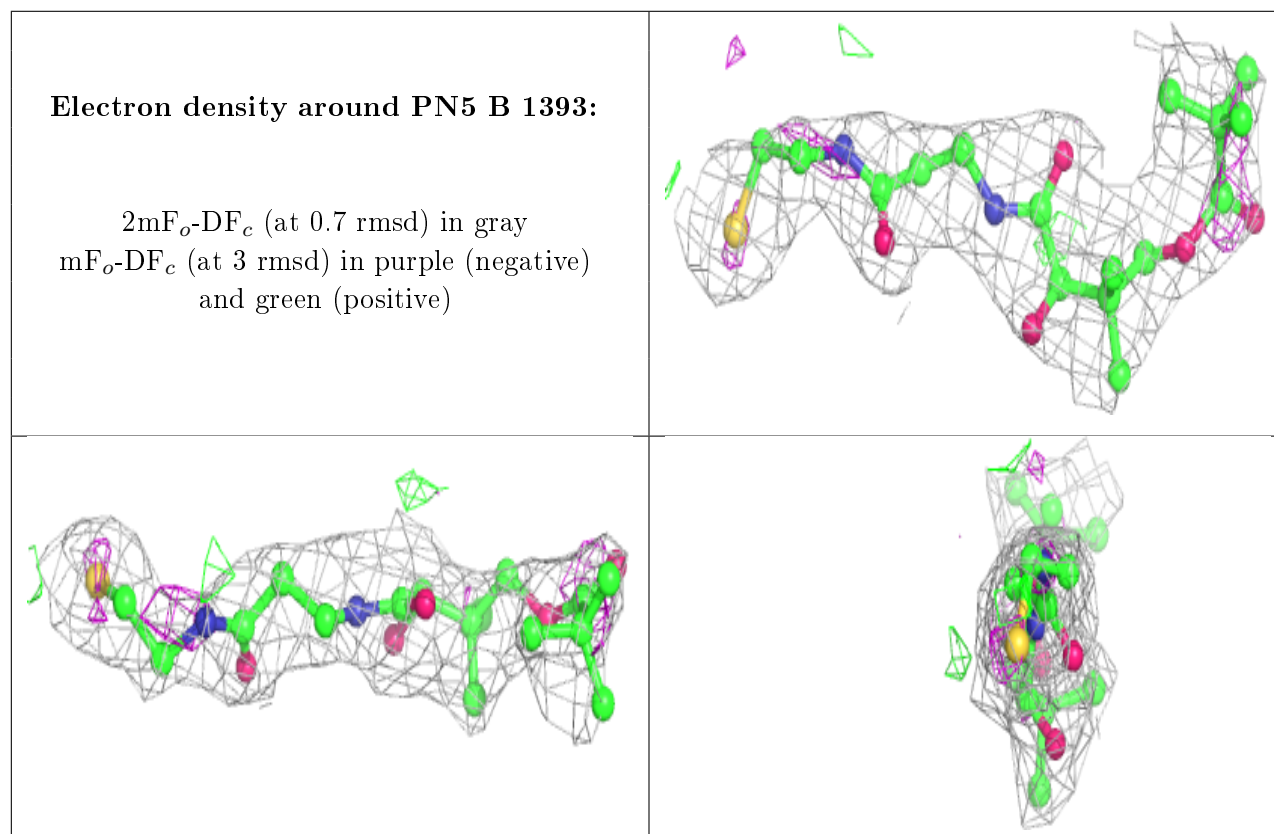
There are no carbohydrates in this entry.

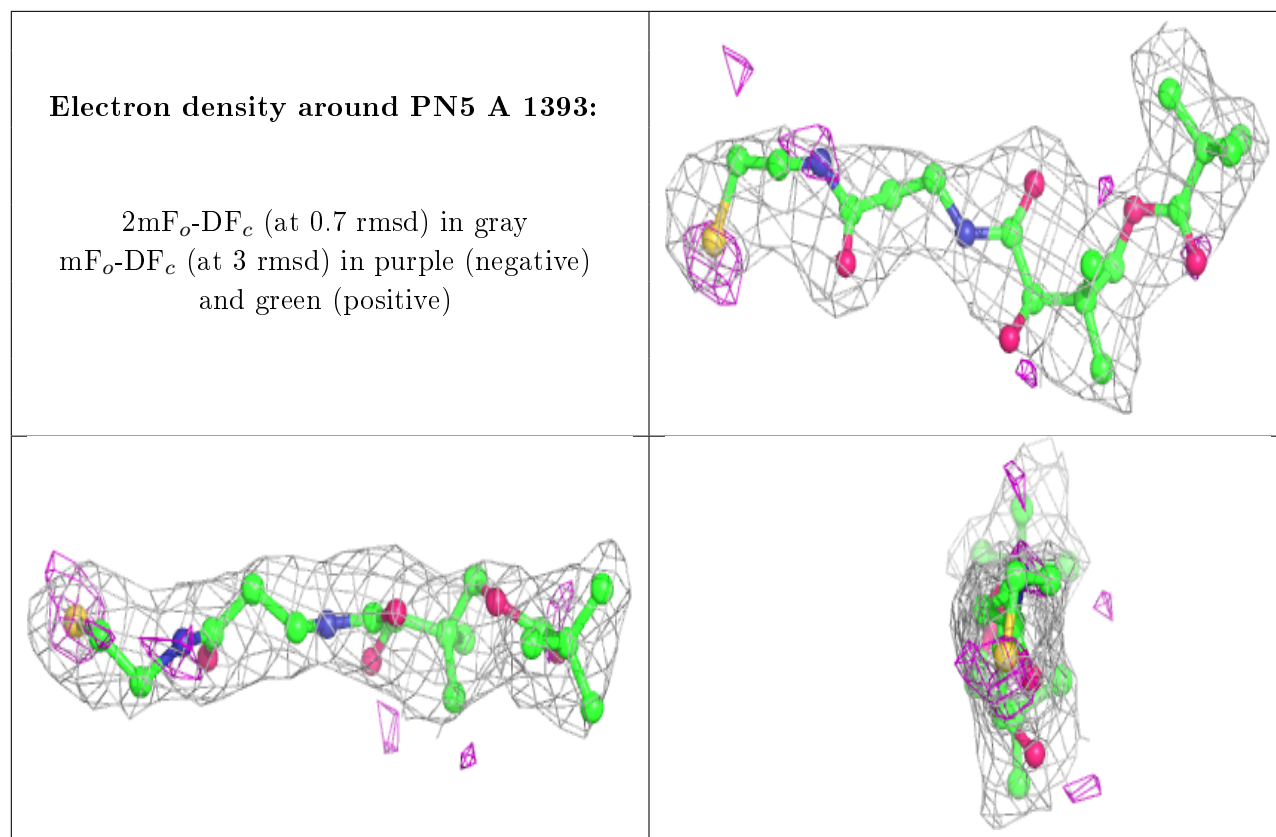
6.4 Ligands [i](#)

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
2	PN5	B	1393	24/24	0.83	0.27	70,86,91,94	0
2	PN5	A	1393	24/24	0.87	0.23	72,75,81,83	0
3	SO4	B	1394	5/5	0.90	0.26	95,96,96,96	0
3	SO4	A	1395	5/5	0.92	0.32	91,91,92,93	0
3	SO4	A	1394	5/5	0.94	0.32	79,81,82,83	0
3	SO4	B	1395	5/5	0.96	0.29	70,73,75,77	0
3	SO4	A	1396	5/5	0.96	0.30	69,72,74,77	0
3	SO4	B	1396	5/5	0.97	0.27	66,66,68,69	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.