



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:44 am BST

PDB ID : 1VFS  
Title : Crystal structure of D-cycloserine-bound form of alanine racemase from D-cycloserine-producing *Streptomyces lavendulae*  
Authors : Noda, M.; Matoba, Y.; Kumagai, T.; Sugiyama, M.  
Deposited on : 2004-04-19  
Resolution : 1.90 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](mailto: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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

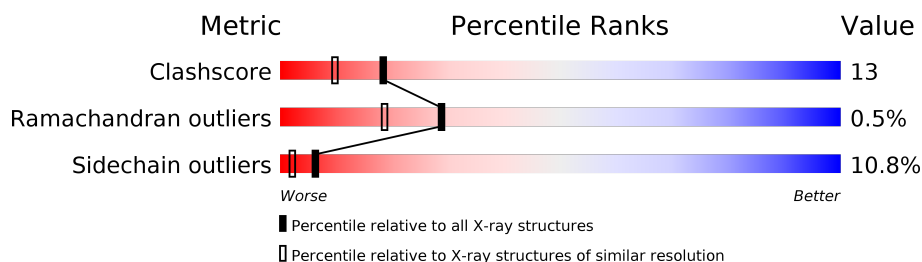
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 was not executed.

Mol	Chain	Length	Quality of chain
1	A	386	
1	B	386	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DCS	A	401	X	-	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5914 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.

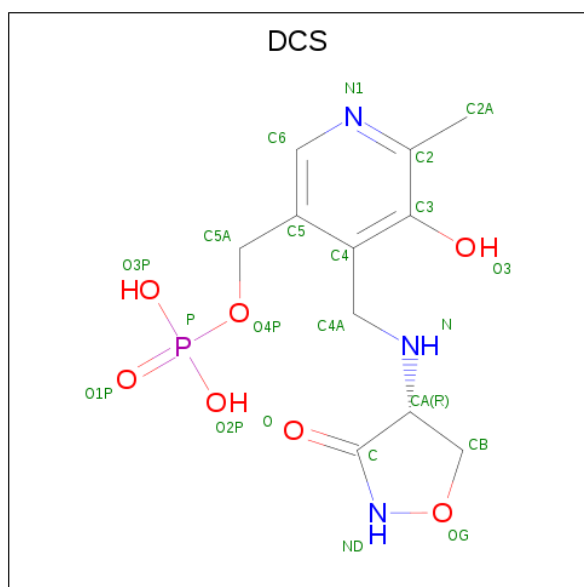
- Molecule 1 is a protein called alanine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			2861	1784	531	536	10			
1	B	382	Total	C	N	O	S	0	0	0
			2851	1778	528	535	10			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is D-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL]-N,O-CYCLOSERYLAMIDE (three-letter code: DCS) (formula:  $C_{11}H_{16}N_3O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
3	B	1	Total	C	N	O	P	0	0
			22	11	3	7	1		

- Molecule 4 is water.

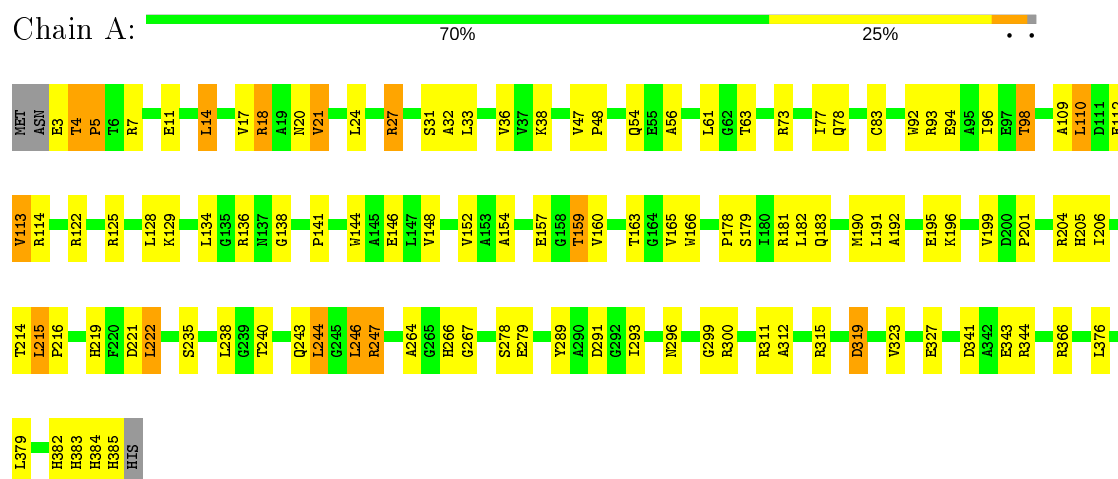
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total	O	0	0
			75	75		
4	B	82	Total	O	0	0
			82	82		

### 3 Residue-property plots

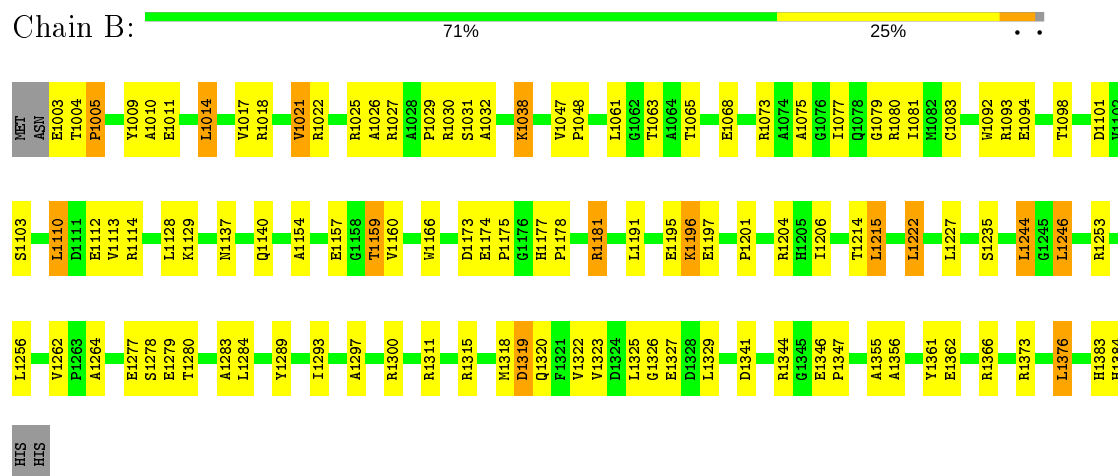
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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 was not executed.

- Molecule 1: alanine racemase



- Molecule 1: alanine racemase



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.96 Å   63.55 Å   84.62 Å 90.00°   118.61°   90.00°	Depositor
Resolution (Å)	30.00 – 1.90	Depositor
% Data completeness (in resolution range)	97.8 (30.00-1.90)	Depositor
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.11	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.209 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5914	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, DCS, KCX

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	0.31	0/2913	0.58	0/3975
1	B	0.31	0/2902	0.57	0/3960
All	All	0.31	0/5815	0.58	0/7935

There are no bond length outliers.

There are no bond angle outliers.

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	2861	0	2800	81	0
1	B	2851	0	2793	76	0
2	A	1	0	0	0	0
3	A	22	0	12	1	0
3	B	22	0	12	2	0
4	A	75	0	0	2	0
4	B	82	0	0	1	0
All	All	5914	0	5617	151	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 13.

All (151) 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:159:THR:HG23	1:A:160:VAL:HG13	1.52	0.92
1:B:1181:ARG:HB3	1:B:1181:ARG:HH21	1.47	0.79
1:A:54:GLN:NE2	1:A:77:ILE:HG23	1.98	0.79
1:A:366:ARG:HD3	1:B:1289:TYR:O	1.84	0.78
1:A:54:GLN:HE22	1:A:77:ILE:HG23	1.48	0.77
1:B:1157:GLU:HG3	1:B:1159:THR:HB	1.66	0.77
1:B:1178:PRO:HA	1:B:1181:ARG:HE	1.51	0.76
1:A:247:ARG:HH21	1:A:247:ARG:HG2	1.53	0.73
1:B:1011:GLU:CG	1:B:1376:LEU:HD21	2.19	0.72
1:A:109:ALA:O	1:A:113:VAL:HG12	1.89	0.71
1:A:32:ALA:O	1:A:222:LEU:HD23	1.92	0.69
1:B:1011:GLU:HG3	1:B:1376:LEU:HD21	1.75	0.69
1:A:18:ARG:HG2	1:A:56:ALA:HB2	1.76	0.68
1:B:1181:ARG:HB3	1:B:1181:ARG:NH2	2.08	0.68
1:B:1159:THR:HG23	1:B:1160:VAL:HG13	1.77	0.67
1:A:114:ARG:HD3	1:A:154:ALA:CB	2.25	0.67
1:A:3:GLU:HG2	1:A:4:THR:H	1.61	0.66
1:B:1038:LYS:HZ1	3:B:1401:DCS:H4A1	1.61	0.66
1:B:1017:VAL:O	1:B:1021:VAL:HG12	1.96	0.64
1:B:1114:ARG:HG2	1:B:1159:THR:HG21	1.80	0.64
1:A:17:VAL:O	1:A:21:VAL:HG12	1.97	0.63
1:B:1110:LEU:O	1:B:1113:VAL:HG12	1.99	0.63
1:B:1159:THR:CG2	1:B:1160:VAL:HG13	2.29	0.62
1:B:1341:ASP:HB3	1:B:1344:ARG:HE	1.65	0.62
1:A:192:ALA:O	1:A:196:LYS:HG2	1.98	0.62
1:A:11:GLU:CD	1:A:376:LEU:HD11	2.20	0.61
1:B:1014:LEU:O	1:B:1018:ARG:HG3	2.00	0.61
1:B:1018:ARG:HB3	1:B:1022:ARG:NH1	2.15	0.61
1:A:114:ARG:HD3	1:A:154:ALA:HB1	1.83	0.60
1:A:38:LYS:HE2	1:B:1319:ASP:OD2	2.02	0.60
1:B:1300:ARG:HG3	1:B:1300:ARG:HH21	1.68	0.59
1:B:1038:LYS:NZ	3:B:1401:DCS:H4A1	2.17	0.59
1:B:1094:GLU:O	1:B:1098:THR:HG23	2.02	0.59
1:A:157:GLU:HG3	1:A:159:THR:HB	1.85	0.58
1:A:110:LEU:O	1:A:114:ARG:HG3	2.02	0.58
1:A:20:ASN:O	1:A:24:LEU:HG	2.04	0.58
1:A:148:VAL:O	1:A:152:VAL:HG13	2.04	0.58
1:A:216:PRO:HA	1:A:219:HIS:CE1	2.38	0.57
1:B:1154:ALA:O	1:B:1157:GLU:HG2	2.04	0.57
1:B:1157:GLU:CG	1:B:1159:THR:HB	2.34	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:OG1	1:A:243:GLN:HG3	2.04	0.57
1:A:299:GLY:HA2	1:A:312:ALA:O	2.05	0.57
1:B:1244:LEU:HB3	1:B:1246:LEU:HD22	1.87	0.57
1:A:92:TRP:O	1:A:96:ILE:HD12	2.05	0.56
1:B:1300:ARG:NH1	1:B:1355:ALA:O	2.39	0.56
1:A:235:SER:OG	1:A:238:LEU:HD13	2.05	0.56
1:A:11:GLU:OE2	1:A:376:LEU:HD11	2.07	0.55
1:A:266:HIS:HD2	1:A:267:GLY:O	1.89	0.55
1:A:247:ARG:HG2	1:A:247:ARG:NH2	2.16	0.55
1:A:215:LEU:HD13	1:A:215:LEU:N	2.22	0.55
1:B:1264:ALA:HB2	1:B:1278:SER:HA	1.89	0.54
1:B:1280:THR:OG1	1:B:1326:GLY:HA2	2.08	0.54
1:A:319:ASP:OD2	1:B:1038:LYS:HE3	2.07	0.54
1:B:1366:ARG:HD2	4:B:622:HOH:O	2.07	0.54
1:A:7:ARG:HH22	1:A:291:ASP:CG	2.11	0.54
1:B:1173:ASP:O	1:B:1175:PRO:HD3	2.07	0.54
1:A:114:ARG:HD2	1:A:159:THR:HG21	1.91	0.53
1:A:47:VAL:HB	1:A:48:PRO:HD3	1.91	0.53
1:A:63:THR:O	1:A:83:CYS:HA	2.08	0.53
1:A:114:ARG:CD	1:A:159:THR:HG21	2.38	0.53
1:B:1129:KCX:HG2	1:B:1166:TRP:CE2	2.44	0.53
1:B:1018:ARG:O	1:B:1021:VAL:HG13	2.09	0.53
1:A:289:TYR:O	1:B:1366:ARG:HD3	2.08	0.52
1:A:3:GLU:HG2	1:A:4:THR:N	2.23	0.52
1:A:154:ALA:O	1:A:157:GLU:HG2	2.09	0.52
1:A:264:ALA:CB	1:A:278:SER:HA	2.40	0.52
1:B:1032:ALA:O	1:B:1222:LEU:HD23	2.10	0.52
1:B:1003:GLU:HG2	1:B:1004:THR:N	2.26	0.51
1:A:47:VAL:HG11	1:A:385:HIS:HB2	1.92	0.51
1:B:1073:ARG:NH1	1:B:1079:GLY:O	2.34	0.51
1:B:1214:THR:O	1:B:1215:LEU:HD13	2.10	0.51
1:B:1005:PRO:HG2	1:B:1009:TYR:HB3	1.93	0.51
1:A:114:ARG:HD3	1:A:154:ALA:HB2	1.91	0.51
1:A:110:LEU:O	1:A:113:VAL:HG13	2.10	0.50
1:B:1018:ARG:HB3	1:B:1022:ARG:HH12	1.74	0.50
1:B:1114:ARG:HG2	1:B:1159:THR:CG2	2.41	0.50
1:B:1011:GLU:CD	1:B:1253:ARG:HH12	2.14	0.50
1:B:1010:ALA:HB3	1:B:1373:ARG:HG3	1.92	0.50
1:A:165:VAL:HG11	1:A:191:LEU:HD13	1.92	0.50
1:B:1289:TYR:HA	1:B:1293:ILE:O	2.11	0.50
1:B:1021:VAL:O	1:B:1025:ARG:HG3	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1196:LYS:HD3	1:B:1196:LYS:N	2.27	0.49
1:B:1284:LEU:HD21	1:B:1320:GLN:HE21	1.78	0.49
1:B:1201:PRO:HG2	1:B:1204:ARG:CZ	2.42	0.49
1:A:94:GLU:O	1:A:98:THR:OG1	2.31	0.49
1:A:7:ARG:NH2	1:A:291:ASP:OD1	2.46	0.49
1:B:1026:ALA:O	1:B:1029:PRO:HD3	2.13	0.49
1:A:296:ASN:HB2	4:A:584:HOH:O	2.12	0.49
1:A:178:PRO:O	1:A:182:LEU:HD23	2.14	0.48
1:A:264:ALA:HB2	1:A:278:SER:HA	1.96	0.48
1:B:1300:ARG:NH2	1:B:1300:ARG:HG3	2.29	0.47
1:A:165:VAL:CG1	1:A:191:LEU:HD13	2.45	0.47
1:A:204:ARG:HD2	1:A:221:ASP:OD2	2.14	0.47
1:B:1005:PRO:HG2	1:B:1009:TYR:CB	2.44	0.47
1:A:244:LEU:HB3	1:A:246:LEU:HD22	1.95	0.47
1:B:1262:VAL:O	1:B:1279:GLU:HA	2.15	0.47
1:A:296:ASN:O	1:A:300:ARG:NH1	2.47	0.46
1:B:1191:LEU:O	1:B:1195:GLU:HG3	2.15	0.46
1:B:1177:HIS:O	1:B:1181:ARG:NH1	2.45	0.46
1:A:166:TRP:HB2	1:A:205:HIS:O	2.16	0.46
1:A:341:ASP:HB2	1:A:344:ARG:NH2	2.30	0.46
1:A:94:GLU:OE2	1:A:94:GLU:N	2.40	0.46
1:A:134:LEU:HG	1:A:136:ARG:HB2	1.96	0.46
1:A:157:GLU:CG	1:A:159:THR:HB	2.44	0.46
1:B:1065:THR:OG1	1:B:1068:GLU:HG3	2.16	0.46
1:B:1003:GLU:CG	1:B:1004:THR:N	2.80	0.45
1:B:1011:GLU:HG2	1:B:1376:LEU:HD21	1.96	0.45
1:A:179:SER:O	1:A:183:GLN:HG3	2.17	0.45
1:A:214:THR:O	1:A:216:PRO:HD3	2.16	0.45
1:A:129:KCX:HD2	1:A:138:GLY:CA	2.47	0.45
1:A:204:ARG:H	1:A:221:ASP:HB2	1.82	0.45
1:A:125:ARG:HB3	1:A:163:THR:HG21	2.00	0.44
1:A:36:VAL:CG1	1:A:38:LYS:HD3	2.48	0.44
1:A:191:LEU:HD21	1:A:204:ARG:HG2	1.97	0.44
1:B:1047:VAL:HB	1:B:1048:PRO:HD3	2.00	0.44
1:B:1063:THR:O	1:B:1083:CYS:HA	2.18	0.44
1:B:1178:PRO:O	1:B:1181:ARG:HG2	2.17	0.44
1:A:192:ALA:O	1:A:196:LYS:HE2	2.17	0.44
1:A:18:ARG:CG	1:A:56:ALA:HB2	2.47	0.44
1:B:1094:GLU:N	1:B:1094:GLU:OE2	2.48	0.44
1:B:1227:LEU:HD22	1:B:1361:TYR:CZ	2.53	0.43
1:A:73:ARG:HD2	1:A:98:THR:O	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:LYS:HD3	1:A:196:LYS:N	2.34	0.43
1:A:266:HIS:CE1	1:B:1140:GLN:HE22	2.36	0.43
1:A:14:LEU:HA	1:A:14:LEU:HD12	1.84	0.43
1:B:1322:VAL:HG23	1:B:1323:VAL:N	2.34	0.43
1:A:27:ARG:CG	1:A:27:ARG:HH11	2.32	0.42
1:B:1157:GLU:OE1	1:B:1159:THR:HG21	2.20	0.42
1:B:1346:GLU:HB3	1:B:1347:PRO:CD	2.48	0.42
1:A:92:TRP:NE1	1:A:112:GLU:OE2	2.49	0.42
1:A:195:GLU:HA	1:A:199:VAL:O	2.19	0.42
1:B:1297:ALA:HB2	1:B:1356:ALA:HB2	2.00	0.42
1:A:199:VAL:HG12	1:A:201:PRO:HD3	2.02	0.42
1:A:315:ARG:NH2	4:A:534:HOH:O	2.50	0.42
1:A:289:TYR:HA	1:A:293:ILE:O	2.20	0.42
1:B:1038:LYS:HG2	1:B:1038:LYS:HZ2	1.68	0.42
1:B:1283:ALA:HB2	1:B:1325:LEU:HD11	2.02	0.42
1:A:379:LEU:O	1:A:382:HIS:HB2	2.20	0.41
1:A:141:PRO:HA	1:A:190:MET:CE	2.50	0.41
3:A:401:DCS:HB1	1:B:1318:MET:HE3	2.03	0.41
1:A:4:THR:HA	1:A:5:PRO:HD2	1.88	0.41
1:B:1092:TRP:NE1	1:B:1112:GLU:OE2	2.48	0.41
1:B:1103:SER:HG	1:B:1166:TRP:HZ2	1.69	0.41
1:B:1075:ALA:HB3	1:B:1077:ILE:HD12	2.02	0.41
1:B:1061:LEU:HB2	1:B:1081:ILE:HG12	2.03	0.40
1:B:1256:LEU:HD22	1:B:1283:ALA:HB1	2.03	0.40
1:A:144:TRP:HB2	1:A:190:MET:HE3	2.02	0.40
1:B:1004:THR:O	1:B:1005:PRO:C	2.60	0.40
1:A:289:TYR:CD1	1:B:1362:GLU:HG3	2.57	0.40
1:B:1383:HIS:N	1:B:1383:HIS:CD2	2.88	0.40
1:A:33:LEU:HD13	1:A:33:LEU:C	2.42	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	380/386 (98%)	365 (96%)	13 (3%)	2 (0%)	29	18
1	B	379/386 (98%)	358 (94%)	19 (5%)	2 (0%)	29	18
All	All	759/772 (98%)	723 (95%)	32 (4%)	4 (0%)	29	18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	PRO
1	B	1005	PRO
1	A	206	ILE
1	B	1206	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	277/280 (99%)	247 (89%)	30 (11%)	6	2
1	B	276/280 (99%)	246 (89%)	30 (11%)	6	2
All	All	553/560 (99%)	493 (89%)	60 (11%)	6	2

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	14	LEU
1	A	18	ARG
1	A	21	VAL
1	A	27	ARG
1	A	31	SER
1	A	61	LEU
1	A	78	GLN
1	A	93	ARG
1	A	98	THR
1	A	110	LEU
1	A	113	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	122	ARG
1	A	128	LEU
1	A	146	GLU
1	A	159	THR
1	A	181	ARG
1	A	215	LEU
1	A	222	LEU
1	A	244	LEU
1	A	246	LEU
1	A	247	ARG
1	A	279	GLU
1	A	311	ARG
1	A	319	ASP
1	A	323	VAL
1	A	327	GLU
1	A	343	GLU
1	A	383	HIS
1	A	384	HIS
1	B	1014	LEU
1	B	1021	VAL
1	B	1027	ARG
1	B	1030	ARG
1	B	1031	SER
1	B	1038	LYS
1	B	1080	ARG
1	B	1093	ARG
1	B	1101	ASP
1	B	1110	LEU
1	B	1128	LEU
1	B	1137	ASN
1	B	1159	THR
1	B	1174	GLU
1	B	1181	ARG
1	B	1196	LYS
1	B	1197	GLU
1	B	1215	LEU
1	B	1222	LEU
1	B	1235	SER
1	B	1244	LEU
1	B	1246	LEU
1	B	1277	GLU
1	B	1311	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	1315	ARG
1	B	1319	ASP
1	B	1327	GLU
1	B	1329	LEU
1	B	1376	LEU
1	B	1384	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	140	GLN
1	A	155	GLN
1	A	243	GLN
1	A	266	HIS
1	A	320	GLN
1	B	1137	ASN
1	B	1320	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	KCX	B	1129	1	7,11,12	0.76	0	4,12,14	0.62	0
1	KCX	A	129	1	7,11,12	0.59	0	4,12,14	0.60	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
1	KCX	B	1129	1	-	3/7/10/12	-
1	KCX	A	129	1	-	3/7/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	1129	KCX	CG-CD-CE-NZ
1	A	129	KCX	CG-CD-CE-NZ
1	B	1129	KCX	N-CA-CB-CG
1	B	1129	KCX	CA-CB-CG-CD
1	A	129	KCX	CD-CE-NZ-CX
1	A	129	KCX	CA-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1129	KCX	1	0
1	A	129	KCX	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	DCS	B	1401	-	22,23,23	4.04	11 (50%)	25,33,33	1.53	6 (24%)
3	DCS	A	401	-	22,23,23	4.04	11 (50%)	25,33,33	1.43	6 (24%)

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	DCS	B	1401	-	-	1/10/21/21	0/2/2/2
3	DCS	A	401	-	1/1/3/5	2/10/21/21	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	DCS	CA-C	-13.29	1.42	1.52
3	B	1401	DCS	CA-C	-13.11	1.42	1.52
3	B	1401	DCS	CB-CA	-7.46	1.37	1.54
3	A	401	DCS	CB-CA	-7.35	1.37	1.54
3	B	1401	DCS	O-C	6.48	1.36	1.23
3	A	401	DCS	O-C	6.38	1.36	1.23
3	B	1401	DCS	OG-CB	-4.38	1.35	1.44
3	A	401	DCS	OG-CB	-4.29	1.35	1.44
3	B	1401	DCS	C2-N1	3.76	1.40	1.33
3	A	401	DCS	C3-C2	-3.57	1.37	1.40
3	A	401	DCS	C2-N1	3.56	1.40	1.33
3	B	1401	DCS	C3-C2	-3.25	1.37	1.40
3	B	1401	DCS	CA-N	-2.96	1.39	1.46
3	A	401	DCS	CA-N	-2.91	1.39	1.46
3	B	1401	DCS	C-ND	-2.63	1.31	1.34
3	B	1401	DCS	C6-C5	-2.47	1.32	1.37
3	A	401	DCS	C-ND	-2.44	1.31	1.34
3	A	401	DCS	C6-C5	-2.37	1.32	1.37
3	A	401	DCS	P-O3P	-2.29	1.46	1.54
3	B	1401	DCS	P-O3P	-2.20	1.46	1.54
3	B	1401	DCS	P-O2P	-2.10	1.46	1.54
3	A	401	DCS	P-O2P	-2.08	1.46	1.54

All (12) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1401	DCS	C6-C5-C4	3.34	120.48	118.12
3	A	401	DCS	C6-C5-C4	2.98	120.23	118.12
3	B	1401	DCS	C4A-N-CA	2.76	119.15	113.92
3	B	1401	DCS	C6-N1-C2	2.75	124.27	119.17
3	A	401	DCS	C6-N1-C2	2.72	124.20	119.17
3	A	401	DCS	C3-C2-N1	-2.67	117.32	120.77
3	B	1401	DCS	C3-C2-N1	-2.61	117.40	120.77
3	B	1401	DCS	C5-C6-N1	-2.54	119.59	123.82
3	A	401	DCS	C5-C6-N1	-2.41	119.80	123.82
3	A	401	DCS	CB-OG-ND	2.18	109.04	105.72
3	A	401	DCS	C2A-C2-N1	2.11	121.79	117.67
3	B	1401	DCS	CB-OG-ND	2.02	108.80	105.72

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	401	DCS	CA

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	DCS	C5-C4-C4A-N
3	B	1401	DCS	C5-C4-C4A-N
3	A	401	DCS	C3-C4-C4A-N

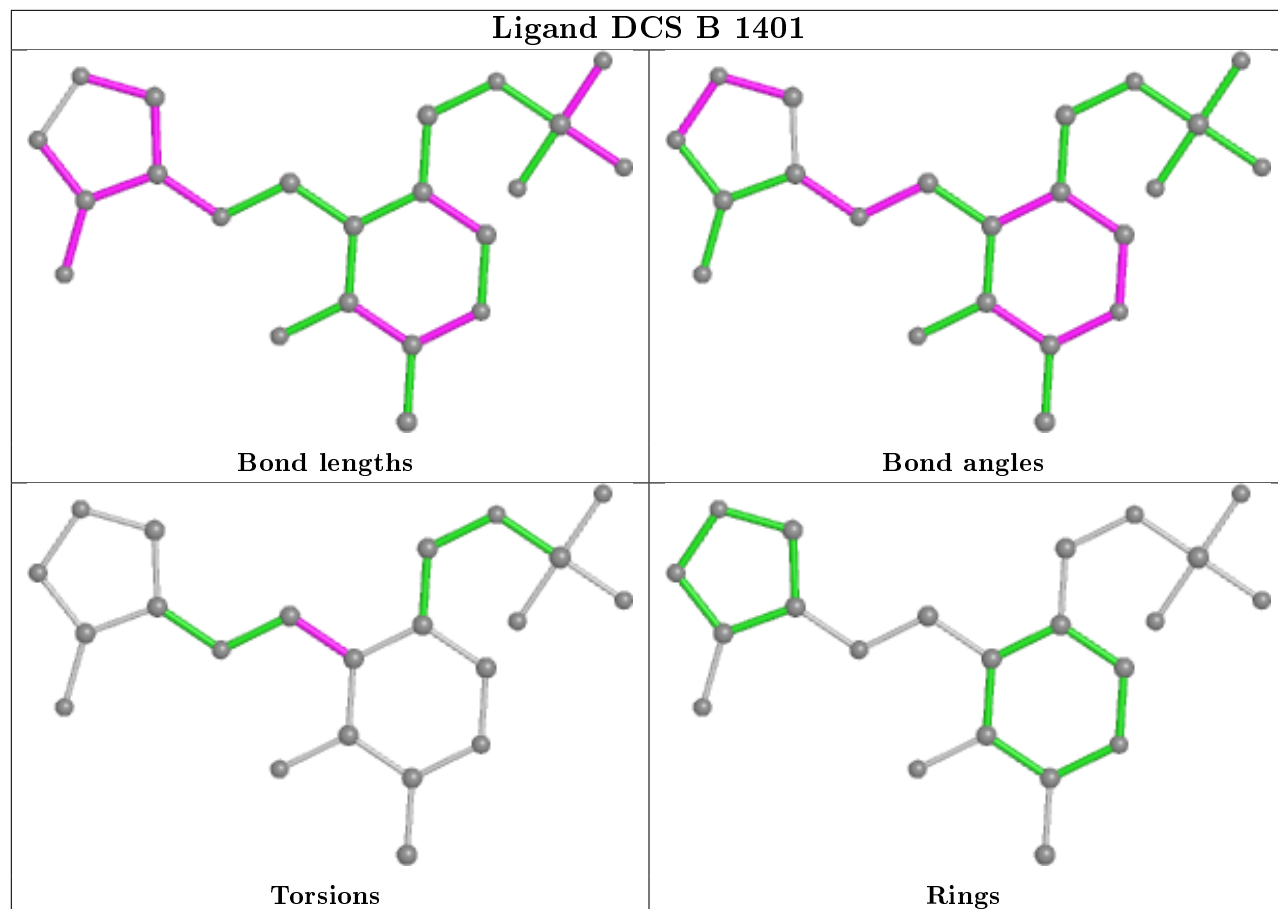
There are no ring outliers.

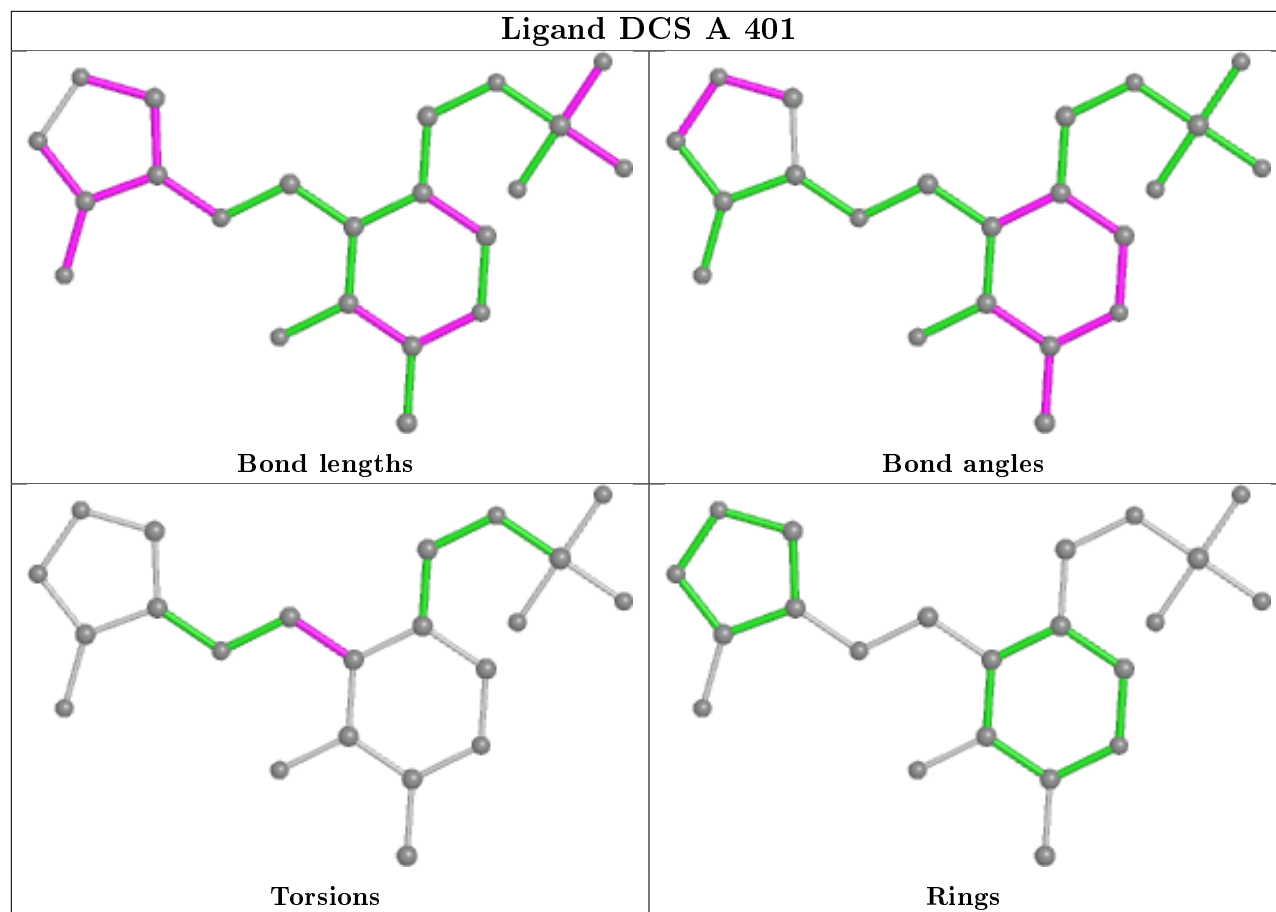
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1401	DCS	2	0
3	A	401	DCS	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.