Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:51 PM GMT

PDB ID	:	1VFT
Title	:	Crystal structure of L-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	:	2.30 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
http://wwpdb.org/validation/2016/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:

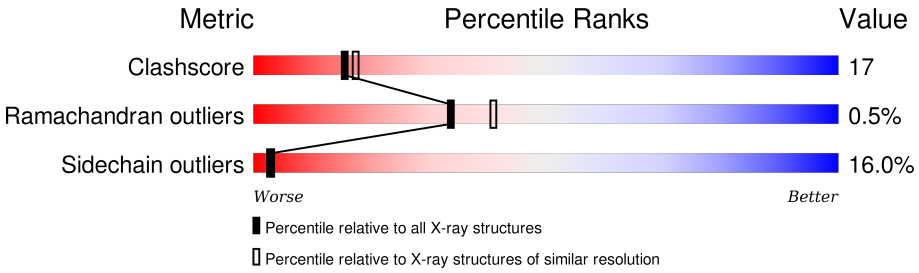
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	386	58% 34% 7% •
1	B	386	63% 31% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5849 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.

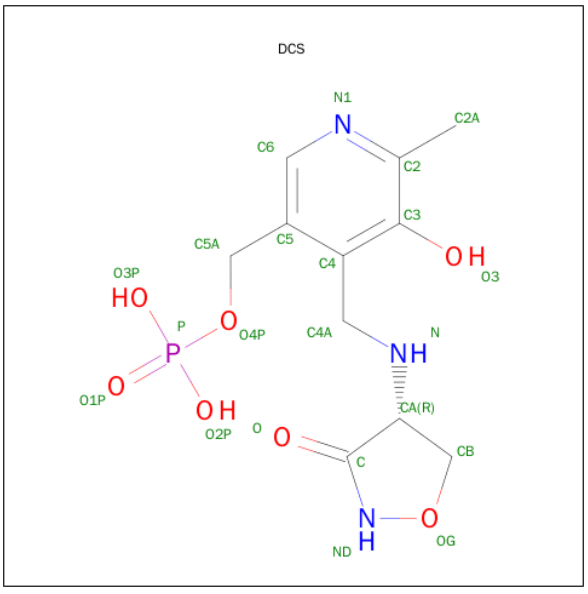
- Molecule 1 is a protein called alanine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2852	1779	530	533	10			
1	B	380	Total	C	N	O	S	0	0	0
			2835	1769	526	530	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	56	Total	O	0	0
			56	56		
4	B	61	Total	O	0	0
			61	61		

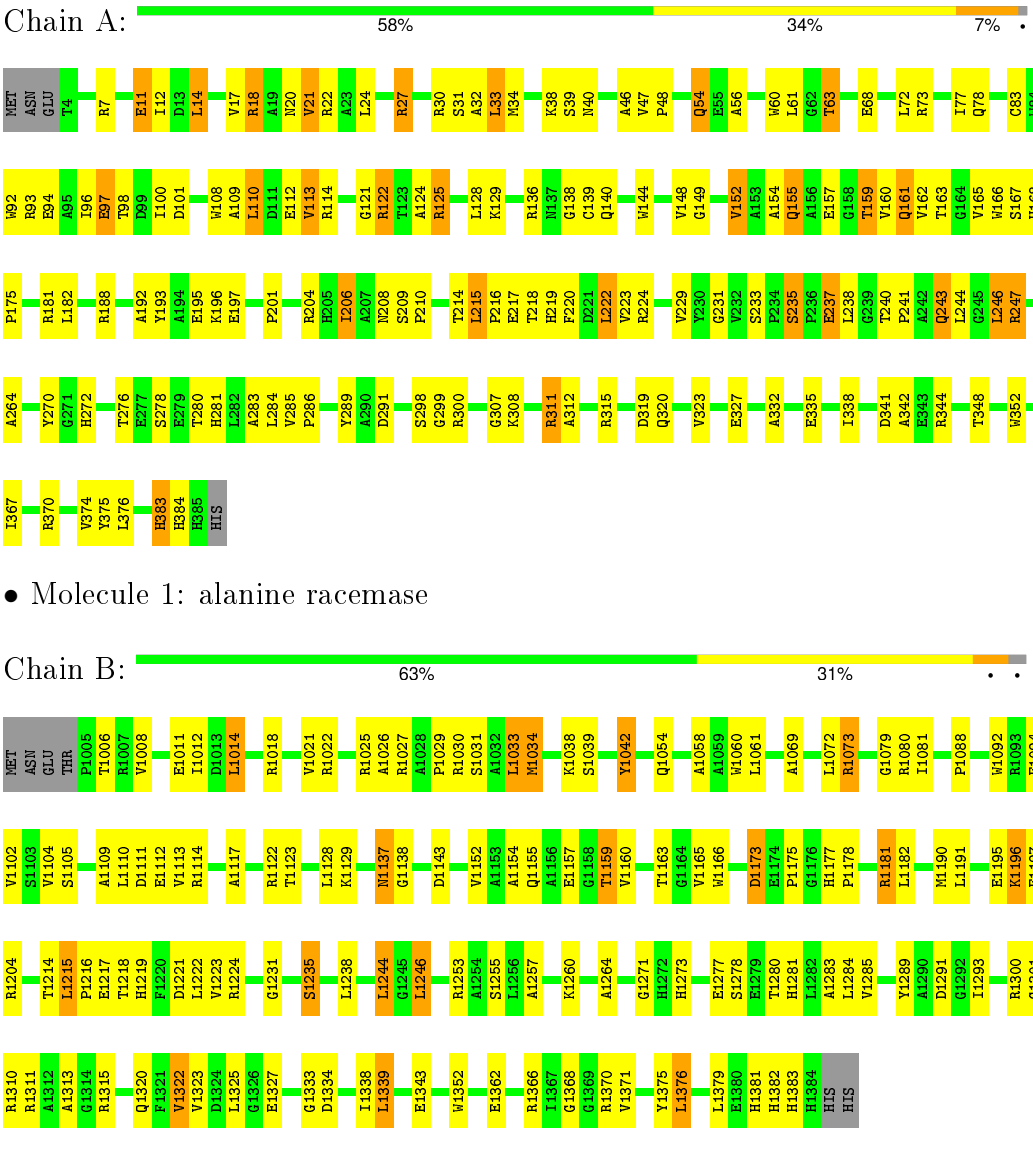
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: alanine racemase

Chain A:



- Molecule 1: alanine racemase

Chain B:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.77Å 63.54Å 85.32Å 90.00° 118.02° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30	Depositor
% Data completeness (in resolution range)	90.6 (30.00-2.30)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.197 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5849	wwPDB-VP
Average B, all atoms (Å^2)	35.0	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	0.32	0/2904	0.58	0/3963
1	B	0.32	0/2886	0.58	0/3937
All	All	0.32	0/5790	0.58	0/7900

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	2852	0	2795	116	0
1	B	2835	0	2781	85	0
2	A	1	0	0	0	0
3	A	22	0	12	3	0
3	B	22	0	12	1	0
4	A	56	0	0	2	0
4	B	61	0	0	1	0
All	All	5849	0	5600	195	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 17.

All (195) 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:HG22	1:A:160:VAL:HG13	1.54	0.87
1:B:1181:ARG:HH21	1:B:1181:ARG:HB3	1.40	0.87
1:A:284:LEU:HD11	1:A:320:GLN:HG3	1.58	0.85
1:B:1034:MET:HB2	1:B:1222:LEU:HD21	1.60	0.83
1:B:1159:THR:HG23	1:B:1160:VAL:HG13	1.61	0.83
1:B:1181:ARG:NH2	1:B:1181:ARG:HB3	1.97	0.79
1:A:247:ARG:HH21	1:A:247:ARG:HG2	1.48	0.79
1:A:284:LEU:HD22	1:B:1137:ASN:ND2	1.98	0.78
1:A:18:ARG:HG2	1:A:56:ALA:HB2	1.66	0.78
1:A:148:VAL:O	1:A:152:VAL:HG22	1.86	0.76
1:A:94:GLU:O	1:A:98:THR:HG23	1.88	0.74
1:B:1011:GLU:HG3	1:B:1376:LEU:HD21	1.69	0.74
1:B:1014:LEU:O	1:B:1018:ARG:HG3	1.91	0.70
1:B:1283:ALA:HB2	1:B:1325:LEU:HD11	1.73	0.70
1:B:1154:ALA:O	1:B:1157:GLU:HG2	1.92	0.69
1:A:32:ALA:O	1:A:223:VAL:HG22	1.96	0.66
1:A:92:TRP:O	1:A:96:ILE:HG13	1.95	0.66
1:A:285:VAL:O	1:A:320:GLN:HB2	1.96	0.65
1:A:38:LYS:CE	3:A:401:DCS:HN	2.08	0.65
1:A:18:ARG:HH11	1:A:22:ARG:HD2	1.60	0.65
1:B:1073:ARG:NH1	1:B:1079:GLY:O	2.30	0.65
1:B:1235:SER:OG	1:B:1238:LEU:HD12	1.96	0.64
1:A:154:ALA:O	1:A:157:GLU:HG2	1.99	0.63
1:B:1034:MET:HB2	1:B:1222:LEU:CD2	2.27	0.63
1:B:1173:ASP:O	1:B:1175:PRO:HD3	1.99	0.63
1:A:256:LEU:HD13	1:A:283:ALA:HB1	1.80	0.63
1:B:1033:LEU:HD13	1:B:1034:MET:N	2.13	0.63
1:A:237:GLU:C	1:A:238:LEU:HD12	2.19	0.62
1:B:1018:ARG:HH11	1:B:1022:ARG:HH22	1.48	0.62
1:A:54:GLN:NE2	1:A:77:ILE:HG23	2.14	0.61
1:A:109:ALA:O	1:A:113:VAL:HG12	2.00	0.61
1:A:93:ARG:HG2	1:A:97:GLU:OE1	2.00	0.61
1:B:1196:LYS:HD3	1:B:1196:LYS:N	2.16	0.61
1:A:291:ASP:CG	1:A:370:ARG:HH21	2.03	0.61
1:A:125:ARG:HB3	1:A:163:THR:HG21	1.83	0.60
1:B:1054:GLN:HA	1:B:1058:ALA:HB3	1.82	0.60
1:B:1178:PRO:HA	1:B:1181:ARG:HE	1.67	0.59
1:A:342:ALA:HB2	1:A:348:THR:HG21	1.85	0.59
1:B:1094:GLU:O	1:B:1098:THR:HG23	2.03	0.58
1:A:54:GLN:HE22	1:A:77:ILE:HG23	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:HB	1:A:48:PRO:HD3	1.84	0.58
1:A:96:ILE:HD13	1:A:124:ALA:HB2	1.84	0.57
1:B:1159:THR:CG2	1:B:1160:VAL:HG13	2.33	0.57
1:B:1092:TRP:NE1	1:B:1112:GLU:OE2	2.38	0.57
1:A:159:THR:HG22	1:A:160:VAL:CG1	2.31	0.56
1:B:1114:ARG:HG2	1:B:1159:THR:CG2	2.35	0.56
1:A:93:ARG:HB3	1:A:94:GLU:OE2	2.05	0.56
1:A:38:LYS:HE2	3:A:401:DCS:HN	1.69	0.56
1:A:238:LEU:O	1:A:244:LEU:HD11	2.04	0.56
1:A:20:ASN:O	1:A:24:LEU:HG	2.05	0.56
1:B:1191:LEU:HD21	1:B:1204:ARG:HG2	1.85	0.56
1:B:1114:ARG:HG2	1:B:1159:THR:HG21	1.86	0.56
1:B:1157:GLU:HG3	1:B:1159:THR:HB	1.88	0.56
1:A:21:VAL:HG12	1:A:229:VAL:HG13	1.88	0.56
1:A:201:PRO:HG2	1:A:204:ARG:CZ	2.35	0.56
1:A:342:ALA:HB2	1:A:348:THR:CG2	2.36	0.56
1:A:247:ARG:NH2	1:A:247:ARG:HG2	2.13	0.55
1:A:341:ASP:HB3	1:A:344:ARG:HE	1.72	0.55
1:A:257:ALA:HB3	1:A:284:LEU:HD23	1.90	0.54
1:A:264:ALA:CB	1:A:278:SER:HA	2.37	0.54
1:A:114:ARG:HG2	1:A:159:THR:HG21	1.89	0.54
1:A:192:ALA:O	1:A:196:LYS:HE2	2.07	0.54
1:B:1104:VAL:HG13	1:B:1109:ALA:HB3	1.89	0.54
1:A:366:ARG:HD3	1:B:1289:TYR:O	2.08	0.54
1:A:18:ARG:NH1	1:A:22:ARG:HD2	2.23	0.54
1:A:192:ALA:O	1:A:196:LYS:HG2	2.08	0.54
1:A:358:THR:HG23	1:A:359:ILE:N	2.22	0.53
1:A:240:THR:H	1:A:243:GLN:HG3	1.74	0.53
1:B:1291:ASP:CG	1:B:1370:ARG:HH21	2.12	0.53
1:B:1201:PRO:HG2	1:B:1204:ARG:CZ	2.39	0.52
1:B:1111:ASP:OD2	1:B:1114:ARG:NH1	2.43	0.52
1:A:149:GLY:O	1:A:152:VAL:HG23	2.10	0.52
1:A:33:LEU:HD22	1:A:223:VAL:HG23	1.92	0.52
1:A:155:GLN:NE2	1:A:162:VAL:H	2.07	0.51
1:A:129:KCX:HG2	1:A:166:TRP:CE2	2.46	0.51
1:A:319:ASP:OD2	1:B:1038:LYS:HE2	2.10	0.51
1:A:209:SER:HB2	1:A:210:PRO:HD3	1.91	0.51
1:A:34:MET:HB2	1:A:60:TRP:HB2	1.92	0.51
1:A:222:LEU:HD22	1:A:223:VAL:H	1.75	0.51
1:A:208:ASN:HA	1:A:224:ARG:O	2.11	0.51
1:A:68:GLU:HG2	4:A:572:HOH:O	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:HIS:N	1:A:383:HIS:CD2	2.80	0.50
1:B:1061:LEU:HB2	1:B:1081:ILE:HG12	1.92	0.50
1:B:1231:GLY:HA2	1:B:1246:LEU:HB3	1.93	0.50
1:A:33:LEU:HD22	1:A:223:VAL:CG2	2.42	0.50
1:B:1031:SER:OG	1:B:1219:HIS:HB3	2.13	0.49
1:A:7:ARG:NH1	4:A:582:HOH:O	2.45	0.49
1:A:217:GLU:N	1:A:217:GLU:OE1	2.46	0.49
1:B:1244:LEU:HB3	1:B:1246:LEU:HD22	1.95	0.49
1:B:1012:ILE:HB	1:B:1375:TYR:CD2	2.48	0.49
1:A:299:GLY:HA2	1:A:312:ALA:O	2.13	0.48
1:B:1255:SER:HA	1:B:1334:ASP:O	2.13	0.48
1:A:284:LEU:HD22	1:B:1137:ASN:HD22	1.77	0.48
1:B:1018:ARG:HH11	1:B:1022:ARG:NH2	2.12	0.48
1:B:1322:VAL:HG23	1:B:1323:VAL:N	2.28	0.48
1:B:1152:VAL:HA	1:B:1155:GLN:HE21	1.77	0.48
1:A:128:LEU:HD22	1:A:128:LEU:N	2.29	0.48
1:A:159:THR:HG22	1:A:160:VAL:N	2.29	0.48
1:A:32:ALA:HB3	1:A:222:LEU:HD23	1.96	0.47
1:A:244:LEU:HB3	1:A:246:LEU:HD22	1.95	0.47
1:B:1038:LYS:NZ	3:B:1401:DCS:H4A1	2.28	0.47
1:B:1271:GLY:HA3	1:B:1273:HIS:CE1	2.49	0.47
1:A:155:GLN:HE22	1:A:162:VAL:H	1.63	0.47
1:A:14:LEU:HB2	1:A:376:LEU:O	2.14	0.47
1:B:1284:LEU:HD11	1:B:1320:GLN:HE21	1.79	0.47
1:A:144:TRP:CE3	1:A:144:TRP:HA	2.49	0.47
1:B:1117:ALA:HB1	1:B:1122:ARG:O	2.15	0.47
1:B:1214:THR:OG1	1:B:1215:LEU:HD22	2.15	0.46
1:A:157:GLU:CG	1:A:159:THR:HB	2.46	0.46
1:A:11:GLU:HA	1:A:374:VAL:O	2.16	0.46
1:B:1222:LEU:HD23	1:B:1223:VAL:N	2.31	0.46
1:A:173:ASP:HA	1:A:210:PRO:HB3	1.98	0.46
1:A:264:ALA:HB2	1:A:278:SER:HA	1.99	0.45
1:B:1379:LEU:O	1:B:1382:HIS:HB2	2.17	0.45
1:A:125:ARG:HB3	1:A:163:THR:CG2	2.46	0.45
1:B:1338:ILE:O	1:B:1352:TRP:NE1	2.48	0.45
1:B:1214:THR:C	1:B:1215:LEU:HD13	2.37	0.45
1:A:63:THR:O	1:A:83:CYS:HA	2.17	0.45
1:A:129:KCX:HD2	1:A:138:GLY:HA3	1.99	0.45
1:B:1129:KCX:HG2	1:B:1166:TRP:CE2	2.52	0.45
1:A:289:TYR:O	1:B:1366:ARG:HD3	2.17	0.45
1:A:7:ARG:HH22	1:A:291:ASP:CG	2.20	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1285:VAL:O	1:B:1320:GLN:HB2	2.17	0.45
1:B:1214:THR:O	1:B:1215:LEU:HD13	2.16	0.45
1:A:40:ASN:HA	1:A:46:ALA:HB2	1.99	0.45
1:B:1177:HIS:O	1:B:1181:ARG:NH1	2.50	0.44
1:B:1034:MET:HB3	1:B:1224:ARG:HA	1.99	0.44
1:A:307:GLY:O	1:A:308:LYS:HG2	2.17	0.44
1:A:114:ARG:HA	1:A:159:THR:HG21	2.00	0.44
1:A:235:SER:OG	1:A:238:LEU:HD13	2.17	0.44
1:B:1038:LYS:O	1:B:1039:SER:HB2	2.16	0.44
1:A:155:GLN:HE21	1:A:161:GLN:HA	1.83	0.44
1:B:1280:THR:OG1	1:B:1281:HIS:N	2.50	0.44
1:A:110:LEU:O	1:A:113:VAL:HG13	2.17	0.44
1:B:1244:LEU:HD12	1:B:1244:LEU:HA	1.80	0.44
1:B:1022:ARG:HG3	1:B:1025:ARG:HH21	1.81	0.44
1:A:181:ARG:CZ	1:A:181:ARG:HB2	2.47	0.44
1:A:140:GLN:NE2	1:A:140:GLN:HA	2.32	0.44
1:B:1264:ALA:HB2	1:B:1278:SER:HA	1.98	0.44
1:A:332:ALA:C	1:B:1088:PRO:HG2	2.38	0.44
1:A:215:LEU:O	1:A:218:THR:OG1	2.34	0.44
1:A:280:THR:OG1	1:A:281:HIS:N	2.51	0.44
1:A:136:ARG:NH1	1:A:168:HIS:HD2	2.16	0.43
1:B:1092:TRP:HZ3	1:B:1102:VAL:HG21	1.83	0.43
1:B:1313:ALA:HB3	1:B:1322:VAL:HG22	2.01	0.43
1:A:231:GLY:O	1:A:241:PRO:HB3	2.18	0.43
1:A:216:PRO:HD2	1:A:217:GLU:OE1	2.18	0.43
1:A:223:VAL:HG23	1:A:223:VAL:O	2.19	0.43
3:A:401:DCS:H4A1	3:A:401:DCS:O4P	2.18	0.43
1:A:193:TYR:CZ	1:A:197:GLU:HG3	2.53	0.43
1:B:1008:VAL:HG13	1:B:1371:VAL:HG22	2.00	0.43
1:A:27:ARG:CG	1:A:27:ARG:HH11	2.32	0.42
1:B:1060:TRP:CZ2	1:B:1080:ARG:HD3	2.54	0.42
1:A:193:TYR:C	1:A:193:TYR:CD1	2.93	0.42
1:A:366:ARG:HD2	4:B:587:HOH:O	2.19	0.42
1:A:300:ARG:O	1:A:311:ARG:NH1	2.53	0.42
1:B:1215:LEU:HA	1:B:1216:PRO:HD2	1.95	0.42
1:A:214:THR:C	1:A:215:LEU:HD13	2.40	0.42
1:A:270:TYR:C	1:A:272:HIS:H	2.22	0.42
1:B:1283:ALA:HB2	1:B:1325:LEU:CD1	2.47	0.42
1:A:136:ARG:NH1	1:A:168:HIS:CD2	2.88	0.42
1:B:1289:TYR:HA	1:B:1293:ILE:O	2.19	0.42
1:A:129:KCX:HG2	1:A:166:TRP:CZ2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ILE:HB	1:A:375:TYR:CD2	2.55	0.41
1:A:17:VAL:O	1:A:21:VAL:HG13	2.21	0.41
1:A:165:VAL:O	1:A:204:ARG:HA	2.21	0.41
1:A:167:SER:O	1:A:206:ILE:HA	2.20	0.41
1:B:1042:TYR:N	1:B:1042:TYR:CD1	2.88	0.41
1:B:1204:ARG:HD2	1:B:1221:ASP:OD2	2.20	0.41
1:B:1109:ALA:O	1:B:1113:VAL:HG12	2.21	0.41
1:B:1069:ALA:O	1:B:1072:LEU:HB2	2.20	0.41
1:A:114:ARG:HA	1:A:159:THR:CG2	2.51	0.41
1:A:114:ARG:CG	1:A:159:THR:HG21	2.49	0.41
1:B:1339:LEU:HD12	1:B:1339:LEU:C	2.40	0.41
1:B:1301:GLY:HA3	1:B:1352:TRP:CZ3	2.55	0.41
1:B:1305:VAL:HB	1:B:1310:ARG:HG3	2.02	0.41
1:A:169:PHE:CE2	1:A:206:ILE:HG12	2.55	0.41
1:A:121:GLY:O	1:A:122:ARG:HG2	2.21	0.41
1:A:98:THR:OG1	1:A:100:ILE:HG13	2.21	0.41
1:A:237:GLU:O	1:A:238:LEU:HD12	2.20	0.41
1:A:72:LEU:HD22	1:A:77:ILE:HD13	2.02	0.41
1:A:88:PRO:HG2	1:B:1333:GLY:HA3	2.02	0.41
1:B:1163:THR:O	1:B:1202:GLU:N	2.51	0.41
1:A:255:SER:O	1:A:286:PRO:HG3	2.20	0.41
1:B:1216:PRO:C	1:B:1218:THR:H	2.24	0.40
1:B:1105:SER:OG	1:B:1138:GLY:HA2	2.21	0.40
1:A:338:ILE:HG23	1:A:352:TRP:CZ2	2.56	0.40
1:B:1191:LEU:O	1:B:1195:GLU:HG3	2.22	0.40
1:B:1204:ARG:HB2	1:B:1221:ASP:OD2	2.21	0.40
1:B:1257:ALA:HB3	1:B:1284:LEU:HD23	2.04	0.40
1:A:367:ILE:HD13	1:A:367:ILE:HA	1.90	0.40
1:A:219:HIS:O	1:A:220:PHE:HB2	2.20	0.40
1:B:1215:LEU:HB3	1:B:1218:THR:HG23	2.02	0.40
1:B:1026:ALA:O	1:B:1029:PRO:HD3	2.20	0.40
1:A:108:TRP:O	1:A:112:GLU:HG3	2.21	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	379/386 (98%)	350 (92%)	27 (7%)	2 (0%)	34 41
1	B	377/386 (98%)	352 (93%)	23 (6%)	2 (0%)	34 41
All	All	756/772 (98%)	702 (93%)	50 (7%)	4 (0%)	34 41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1368	GLY
1	B	1383	HIS
1	A	206	ILE
1	A	175	PRO

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	276/280 (99%)	230 (83%)	46 (17%)	3 2
1	B	274/280 (98%)	232 (85%)	42 (15%)	3 3
All	All	550/560 (98%)	462 (84%)	88 (16%)	3 3

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	14	LEU
1	A	18	ARG
1	A	21	VAL
1	A	27	ARG
1	A	30	ARG
1	A	31	SER
1	A	33	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	39	SER
1	A	54	GLN
1	A	61	LEU
1	A	63	THR
1	A	73	ARG
1	A	78	GLN
1	A	85	LEU
1	A	97	GLU
1	A	101	ASP
1	A	110	LEU
1	A	113	VAL
1	A	122	ARG
1	A	125	ARG
1	A	139	CYS
1	A	152	VAL
1	A	155	GLN
1	A	159	THR
1	A	161	GLN
1	A	182	LEU
1	A	188	ARG
1	A	195	GLU
1	A	215	LEU
1	A	222	LEU
1	A	233	SER
1	A	235	SER
1	A	237	GLU
1	A	243	GLN
1	A	246	LEU
1	A	247	ARG
1	A	276	THR
1	A	298	SER
1	A	311	ARG
1	A	315	ARG
1	A	323	VAL
1	A	327	GLU
1	A	335	GLU
1	A	383	HIS
1	A	384	HIS
1	B	1006	THR
1	B	1014	LEU
1	B	1021	VAL
1	B	1027	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1030	ARG
1	B	1033	LEU
1	B	1034	MET
1	B	1042	TYR
1	B	1073	ARG
1	B	1101	ASP
1	B	1110	LEU
1	B	1123	THR
1	B	1128	LEU
1	B	1137	ASN
1	B	1143	ASP
1	B	1159	THR
1	B	1165	VAL
1	B	1173	ASP
1	B	1181	ARG
1	B	1182	LEU
1	B	1190	MET
1	B	1196	LYS
1	B	1197	GLU
1	B	1215	LEU
1	B	1217	GLU
1	B	1235	SER
1	B	1244	LEU
1	B	1246	LEU
1	B	1253	ARG
1	B	1260	LYS
1	B	1277	GLU
1	B	1300	ARG
1	B	1304	LEU
1	B	1311	ARG
1	B	1315	ARG
1	B	1322	VAL
1	B	1327	GLU
1	B	1339	LEU
1	B	1343	GLU
1	B	1362	GLU
1	B	1376	LEU
1	B	1381	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) 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	A	383	HIS
1	B	1078	GLN
1	B	1137	ASN
1	B	1155	GLN
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	A	129	1	7,11,12	0.73	0	7,12,14	0.84	0
1	KCX	B	1129	1	7,11,12	0.68	0	7,12,14	0.83	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	A	129	1	-	0/6/10/12	0/0/0/0
1	KCX	B	1129	1	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	129	KCX	3	0
1	B	1129	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	A	401	-	23,23,23	4.04	12 (52%)	24,33,33	1.38	6 (25%)
3	DCS	B	1401	-	23,23,23	3.89	12 (52%)	24,33,33	1.64	6 (25%)

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	DCS	CA-C	-12.87	1.42	1.52
3	B	1401	DCS	CA-C	-11.41	1.44	1.52
3	B	1401	DCS	CB-CA	-6.48	1.37	1.54
3	A	401	DCS	CB-CA	-6.46	1.37	1.54
3	B	1401	DCS	C3-C2	-5.75	1.36	1.40
3	A	401	DCS	OG-CB	-4.88	1.35	1.44
3	B	1401	DCS	OG-CB	-4.84	1.35	1.44
3	A	401	DCS	C3-C2	-4.80	1.37	1.40
3	A	401	DCS	CA-N	-4.72	1.39	1.47
3	B	1401	DCS	CA-N	-4.26	1.40	1.47
3	B	1401	DCS	OG-ND	-3.27	1.38	1.45
3	A	401	DCS	OG-ND	-3.13	1.38	1.45
3	B	1401	DCS	C-ND	-2.40	1.31	1.34
3	B	1401	DCS	P-O2P	-2.39	1.46	1.54
3	A	401	DCS	C-ND	-2.37	1.31	1.34
3	B	1401	DCS	P-O3P	-2.30	1.46	1.54
3	B	1401	DCS	C6-C5	-2.30	1.32	1.37
3	A	401	DCS	P-O3P	-2.27	1.46	1.54
3	A	401	DCS	P-O2P	-2.22	1.46	1.54
3	A	401	DCS	C6-C5	-2.17	1.32	1.37
3	B	1401	DCS	C2-N1	3.02	1.40	1.34
3	A	401	DCS	C2-N1	3.10	1.40	1.34
3	A	401	DCS	O-C	6.65	1.36	1.23
3	B	1401	DCS	O-C	6.72	1.36	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1401	DCS	C5-C6-N1	-2.42	119.66	123.86
3	A	401	DCS	C5-C6-N1	-2.39	119.71	123.86
3	A	401	DCS	C3-C2-N1	-2.26	117.49	120.61
3	B	1401	DCS	C3-C2-N1	-2.20	117.58	120.61
3	A	401	DCS	C4A-N-CA	2.04	116.92	113.81
3	A	401	DCS	CA-C-ND	2.28	108.97	107.45
3	B	1401	DCS	C6-N1-C2	2.34	124.05	119.28
3	A	401	DCS	C6-N1-C2	2.35	124.07	119.28
3	B	1401	DCS	CA-C-ND	2.73	109.27	107.45
3	A	401	DCS	C6-C5-C4	3.03	120.35	118.09
3	B	1401	DCS	C6-C5-C4	3.18	120.47	118.09
3	B	1401	DCS	C4A-N-CA	4.48	120.65	113.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	DCS	3	0
3	B	1401	DCS	1	0

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.