Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 08:19 PM EDT

PDB ID	:	1DJO
Title	:	Crystal structure of Pseudomonas 7A Glutaminase-asparaginase with the inhibitor donv covalently bound in the active site
Authors	:	Ortlund, E.; Lacount, M.W.; Lewinski, K.; Lebioda, L.
Deposited on	:	1999-12-03
Resolution	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

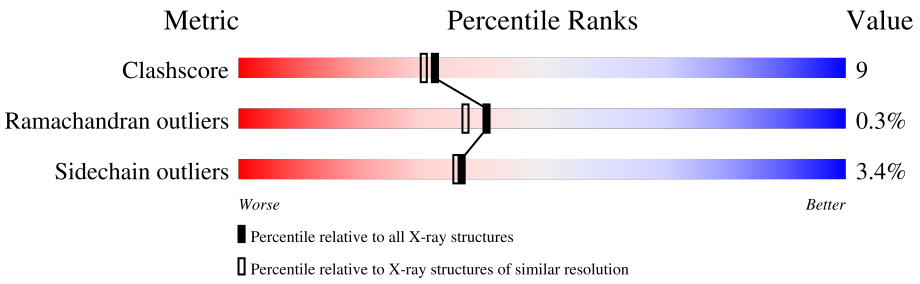
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	330	82% 16% •
1	B	330	82% 17% •

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
2	CAB	A	4001	-	X	-	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4988 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.

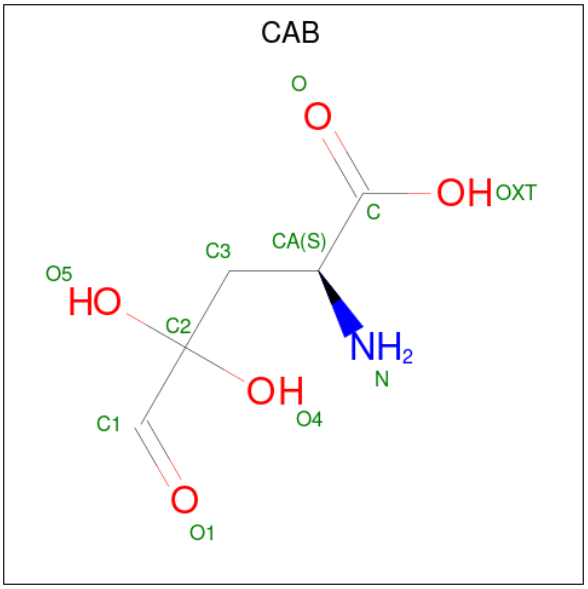
- Molecule 1 is a protein called GLUTAMINASE-ASPARAGINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2485	1550	440	487	8	0	0	0
1	B	330	2485	1550	440	487	8	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1111	ASN	ASP	SEE REMARK 999	UNP P10182
A	1113	VAL	THR	SEE REMARK 999	UNP P10182
A	1114	GLN	LEU	SEE REMARK 999	UNP P10182
A	1115	LYS	ASN	SEE REMARK 999	UNP P10182
A	1263	VAL	LEU	SEE REMARK 999	UNP P10182
A	1264	VAL	THR	SEE REMARK 999	UNP P10182
A	1269	GLN	THR	SEE REMARK 999	UNP P10182
A	1273	ASN	THR	SEE REMARK 999	UNP P10182
A	1317	ALA	VAL	SEE REMARK 999	UNP P10182
A	1318	MET	GLU	SEE REMARK 999	UNP P10182
A	1319	VAL	LEU	SEE REMARK 999	UNP P10182
A	1322	THR	VAL	SEE REMARK 999	UNP P10182
B	3111	ASN	ASP	SEE REMARK 999	UNP P10182
B	3113	VAL	THR	SEE REMARK 999	UNP P10182
B	3114	GLN	LEU	SEE REMARK 999	UNP P10182
B	3115	LYS	ASN	SEE REMARK 999	UNP P10182
B	3263	VAL	LEU	SEE REMARK 999	UNP P10182
B	3264	VAL	THR	SEE REMARK 999	UNP P10182
B	3269	GLN	THR	SEE REMARK 999	UNP P10182
B	3273	ASN	THR	SEE REMARK 999	UNP P10182
B	3317	ALA	VAL	SEE REMARK 999	UNP P10182
B	3318	MET	GLU	SEE REMARK 999	UNP P10182
B	3319	VAL	LEU	SEE REMARK 999	UNP P10182
B	3322	THR	VAL	SEE REMARK 999	UNP P10182

- Molecule 2 is 4,4-dihydroxy-5-oxo-L-norvaline (three-letter code: CAB) (formula: $C_5H_9NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	9	5	1	3	0	0
			Total	C	N	O		
2	B	1	9	5	1	3	0	0

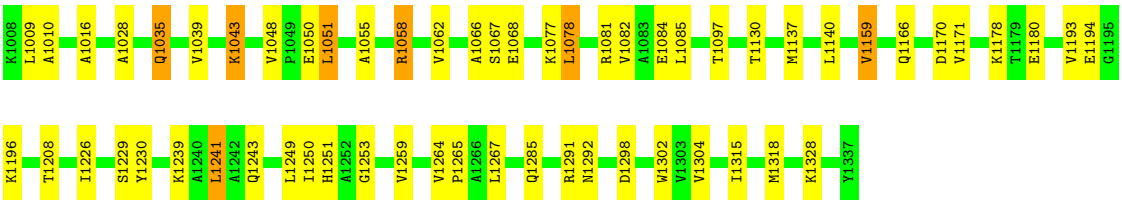
3 Residue-property plots (i)

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 was not executed.

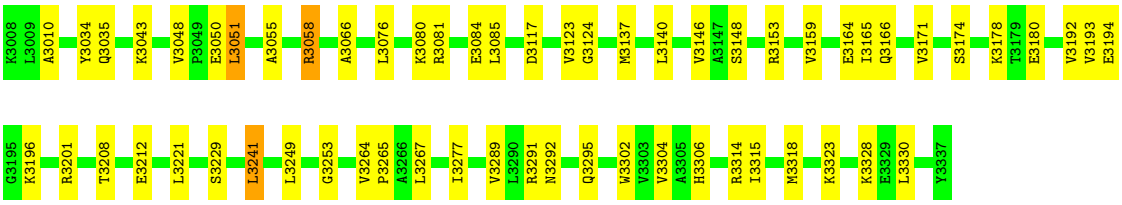
• Molecule 1: GLUTAMINASE-ASPARAGINASE

Chain A: 82% 16%



• Molecule 1: GLUTAMINASE-ASPARAGINASE

Chain B: 82% 17%



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	78.37Å 135.89Å 137.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.92 – 2.00	Depositor
% Data completeness (in resolution range)	74.3 (25.92-2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4988	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

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: CAB

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	0.30	0/2520	0.59	0/3413
1	B	0.30	0/2520	0.60	1/3413 (0.0%)
All	All	0.30	0/5040	0.60	1/6826 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3066	ALA	N-CA-C	-5.21	96.94	111.00

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	2485	0	2503	46	1
1	B	2485	0	2503	43	2
2	A	9	0	5	1	0
2	B	9	0	6	0	0
All	All	4988	0	5017	88	2

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 9.

All (88) 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:1058:ARG:HB2	1:A:1058:ARG:HH21	1.23	1.02
1:B:3058:ARG:HB2	1:B:3058:ARG:HH21	1.24	1.00
1:B:3159:VAL:HG13	1:B:3166:GLN:HB2	1.49	0.92
1:A:1159:VAL:HG11	1:A:1171:VAL:HG11	1.55	0.88
1:B:3328:LYS:HA	1:B:3328:LYS:HE2	1.58	0.85
1:A:1328:LYS:HA	1:A:1328:LYS:HE2	1.60	0.84
1:B:3304:VAL:HG12	1:B:3306:HIS:H	1.45	0.82
1:B:3159:VAL:HG11	1:B:3171:VAL:HG11	1.73	0.70
1:B:3328:LYS:HE2	1:B:3328:LYS:CA	2.27	0.64
1:A:1178:LYS:HE2	1:A:1180:GLU:OE1	1.98	0.63
1:B:3081:ARG:O	1:B:3085:LEU:HD23	1.98	0.62
1:A:1039:VAL:HG11	1:A:1043:LYS:HE3	1.82	0.62
1:B:3178:LYS:HE2	1:B:3180:GLU:OE1	1.99	0.61
1:A:1035:GLN:NE2	1:A:1035:GLN:N	2.48	0.61
1:A:1081:ARG:O	1:A:1085:LEU:HD23	2.01	0.61
1:A:1081:ARG:CZ	1:A:1085:LEU:HD21	2.31	0.59
1:A:1010:ALA:O	1:A:1055:ALA:HB1	2.03	0.59
1:B:3058:ARG:HH21	1:B:3058:ARG:CB	2.09	0.59
1:A:1058:ARG:HH21	1:A:1058:ARG:CB	2.05	0.58
1:A:1058:ARG:HB2	1:A:1058:ARG:NH2	2.07	0.58
1:B:3193:VAL:HG12	1:B:3194:GLU:HG3	1.86	0.57
1:B:3048:VAL:CG1	1:B:3051:LEU:HD13	2.35	0.57
1:B:3146:VAL:CG2	1:B:3192:VAL:HG21	2.35	0.57
1:B:3229:SER:HB3	1:B:3253:GLY:HA2	1.85	0.57
1:B:3291:ARG:NH1	1:B:3328:LYS:NZ	2.53	0.57
1:A:1159:VAL:HG13	1:A:1166:GLN:HB2	1.87	0.57
1:B:3137:MET:SD	1:B:3137:MET:N	2.77	0.56
1:B:3212:GLU:OE2	1:B:3323:LYS:HE3	2.05	0.56
1:B:3117:ASP:OD2	1:B:3153:ARG:NH1	2.39	0.56
1:A:1178:LYS:HE2	1:A:1180:GLU:CD	2.27	0.55
1:B:3159:VAL:CG1	1:B:3166:GLN:HB2	2.29	0.55
1:B:3264:VAL:HB	1:B:3265:PRO:HD3	1.89	0.55
1:A:1048:VAL:HG11	1:A:1051:LEU:HD13	1.87	0.54
1:A:1048:VAL:CG1	1:A:1051:LEU:HD13	2.38	0.54
1:A:1229:SER:HB3	1:A:1253:GLY:HA2	1.90	0.54
1:A:1062:VAL:HG13	1:A:1077:LYS:HE2	1.90	0.54
1:B:3058:ARG:HB2	1:B:3058:ARG:NH2	2.08	0.54
1:A:1137:MET:SD	1:A:1137:MET:N	2.81	0.53
1:A:1035:GLN:N	1:A:1035:GLN:HE21	2.06	0.52
1:B:3055:ALA:HB2	1:B:3148:SER:OG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3010:ALA:O	1:B:3055:ALA:HB1	2.10	0.51
1:A:1039:VAL:CG1	1:A:1043:LYS:HB3	2.41	0.51
1:B:3076:LEU:HD11	1:B:3221:LEU:HD22	1.93	0.51
1:A:1009:LEU:HB3	1:A:1055:ALA:HA	1.93	0.50
1:A:1291:ARG:NH1	1:A:1328:LYS:NZ	2.59	0.50
1:B:3328:LYS:HA	1:B:3328:LYS:CE	2.35	0.50
1:A:1264:VAL:HB	1:A:1265:PRO:HD3	1.93	0.50
1:A:1067:SER:OG	2:A:4001:CAB:OXT	2.28	0.49
1:B:3267:LEU:HB3	1:B:3302:TRP:CZ2	2.48	0.49
1:B:3048:VAL:HG11	1:B:3051:LEU:HD13	1.95	0.49
1:A:1193:VAL:HG12	1:A:1194:GLU:HG3	1.95	0.48
1:A:1267:LEU:HB3	1:A:1302:TRP:CZ2	2.49	0.48
1:B:3050:GLU:H	1:B:3050:GLU:CD	2.17	0.47
1:B:3277:ILE:HB	1:B:3302:TRP:CD1	2.50	0.47
1:B:3123:VAL:HG22	1:B:3124:GLY:N	2.30	0.46
1:B:3289:VAL:O	1:B:3304:VAL:HG11	2.15	0.46
1:B:3314:ARG:O	1:B:3318:MET:HG3	2.15	0.46
1:A:1328:LYS:HE2	1:A:1328:LYS:CA	2.41	0.46
1:B:3315:ILE:HA	1:B:3318:MET:HE2	1.99	0.45
1:A:1241:LEU:HB3	1:A:1249:LEU:HD21	1.99	0.45
1:B:3323:LYS:NZ	1:B:3323:LYS:HB3	2.32	0.44
1:A:1048:VAL:O	1:A:1051:LEU:HB2	2.18	0.44
1:A:1035:GLN:HE21	1:A:1035:GLN:H	1.65	0.44
1:A:1315:ILE:HD13	1:A:1318:MET:CE	2.47	0.44
1:B:3081:ARG:CZ	1:B:3085:LEU:HD21	2.47	0.43
1:B:3291:ARG:NH1	1:B:3328:LYS:HZ1	2.13	0.43
1:A:1066:ALA:HB1	1:A:1068:GLU:OE1	2.17	0.43
1:A:1078:LEU:O	1:A:1082:VAL:HG23	2.18	0.43
1:B:3165:ILE:HG13	1:B:3192:VAL:HG23	2.01	0.43
1:B:3241:LEU:HB3	1:B:3249:LEU:HD21	2.01	0.43
1:B:3292:ASN:HA	1:B:3295:GLN:O	2.18	0.43
1:A:1226:ILE:HG12	1:A:1250:ILE:HB	2.00	0.42
1:A:1081:ARG:NH1	1:A:1084:GLU:OE1	2.52	0.42
1:A:1050:GLU:CD	1:A:1050:GLU:H	2.22	0.42
1:A:1285:GLN:HE21	1:B:3174:SER:HB3	1.85	0.41
1:A:1251:HIS:NE2	1:A:1259:VAL:HG22	2.35	0.41
1:A:1016:ALA:HA	1:A:1097:THR:OG1	2.19	0.41
1:B:3291:ARG:NH1	1:B:3328:LYS:HZ2	2.17	0.41
1:A:1239:LYS:O	1:A:1243:GLN:HG3	2.19	0.41
1:A:1230:TYR:CD1	1:A:1230:TYR:N	2.88	0.41
1:B:3034:TYR:CD2	1:B:3034:TYR:C	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3048:VAL:O	1:B:3051:LEU:HB2	2.21	0.41
1:A:1085:LEU:HD22	1:A:1085:LEU:N	2.37	0.40
1:A:1081:ARG:CZ	1:A:1085:LEU:CD2	2.99	0.40
1:A:1028:ALA:HA	1:A:1130:THR:O	2.22	0.40
1:B:3080:LYS:O	1:B:3084:GLU:HG3	2.21	0.40
1:A:1039:VAL:CG1	1:A:1043:LYS:HE3	2.50	0.40
1:A:1292:ASN:ND2	1:A:1298:ASP:OD2	2.53	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3164:GLU:OE2	1:B:3178:LYS:NZ[3_656]	2.11	0.09
1:A:1170:ASP:OD1	1:B:3201:ARG:NH1[3_656]	2.17	0.03

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	328/330 (99%)	318 (97%)	9 (3%)	1 (0%)	41	37
1	B	328/330 (99%)	319 (97%)	8 (2%)	1 (0%)	41	37
All	All	656/660 (99%)	637 (97%)	17 (3%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1208	THR
1	B	3208	THR

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	265/265 (100%)	255 (96%)	10 (4%)	33	31
1	B	265/265 (100%)	257 (97%)	8 (3%)	41	41
All	All	530/530 (100%)	512 (97%)	18 (3%)	37	36

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1035	GLN
1	A	1043	LYS
1	A	1051	LEU
1	A	1058	ARG
1	A	1078	LEU
1	A	1140	LEU
1	A	1159	VAL
1	A	1196	LYS
1	A	1241	LEU
1	A	1304	VAL
1	B	3035	GLN
1	B	3043	LYS
1	B	3051	LEU
1	B	3058	ARG
1	B	3140	LEU
1	B	3196	LYS
1	B	3241	LEU
1	B	3330	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1035	GLN
1	A	1166	GLN
1	A	1244	ASN
1	A	1273	ASN

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Mol	Chain	Res	Type
1	A	1285	GLN
1	B	3035	GLN
1	B	3166	GLN
1	B	3244	ASN
1	B	3273	ASN
1	B	3285	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CAB	B	4000	1	7,8,10	1.75	2 (28%)	7,9,14	2.82	3 (42%)
2	CAB	A	4001	1	7,8,10	2.44	3 (42%)	7,9,14	4.29	5 (71%)

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	CAB	B	4000	1	-	3/7/8/12	-
2	CAB	A	4001	1	-	3/7/8/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4001	CAB	O1-C1	4.48	1.45	1.19
2	B	4000	CAB	O-C	3.72	1.33	1.22
2	A	4001	CAB	O-C	3.68	1.33	1.22
2	A	4001	CAB	OXT-C	-2.48	1.22	1.30
2	B	4000	CAB	OXT-C	-2.48	1.22	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	4001	CAB	C3-CA-C	8.49	130.51	110.30
2	A	4001	CAB	C3-C2-C1	-6.05	95.06	112.29
2	B	4000	CAB	C3-CA-N	5.39	124.30	110.17
2	B	4000	CAB	C3-CA-C	-4.05	100.66	110.30
2	A	4001	CAB	C3-CA-N	2.46	116.61	110.17
2	B	4000	CAB	OXT-C-CA	2.42	121.63	113.38
2	A	4001	CAB	OXT-C-CA	2.41	121.59	113.38
2	A	4001	CAB	O1-C1-C2	-2.20	112.42	126.89

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4001	CAB	C2-C3-CA-C
2	A	4001	CAB	O-C-CA-N
2	B	4000	CAB	C2-C3-CA-C
2	B	4000	CAB	O-C-CA-N
2	A	4001	CAB	OXT-C-CA-N
2	B	4000	CAB	OXT-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4001	CAB	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.