Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:38 am BST

PDB ID	:	1V7Y
Title	:	Crystal structure of tryptophan synthase alpha-subunit from Escherichia coli at room temperature
Authors	:	Nishio, K.; Morimoto, Y.; Ishizuka, M.; Ogasahara, K.; Yutani, K.; Tsukihara, T.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2003-12-25
Resolution	:	2.50 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:

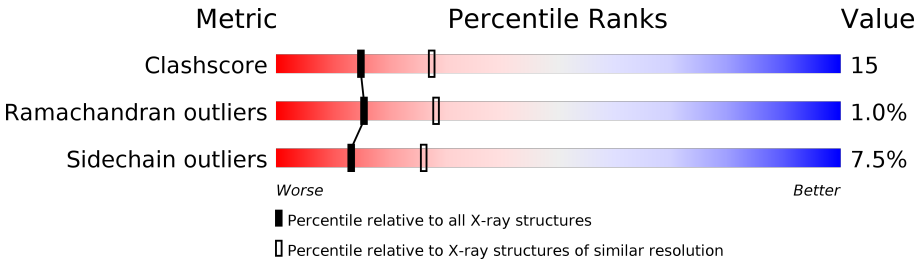
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	268	64% 25% • 7%
1	B	268	63% 25% 5% 7%

2 Entry composition

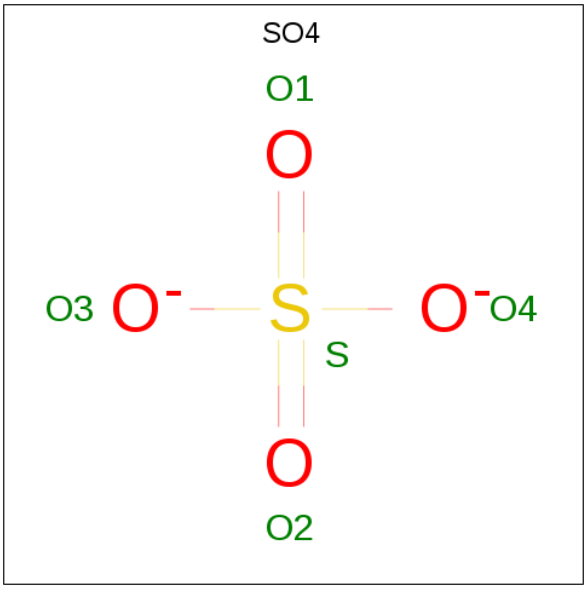
There are 3 unique types of molecules in this entry. The entry contains 3868 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1882	1212	317	345	8			
1	B	249	Total	C	N	O	S	0	0	0
			1889	1216	318	347	8			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	61	Total O 61 61	0	0
3	B	26	Total O 26 26	0	0

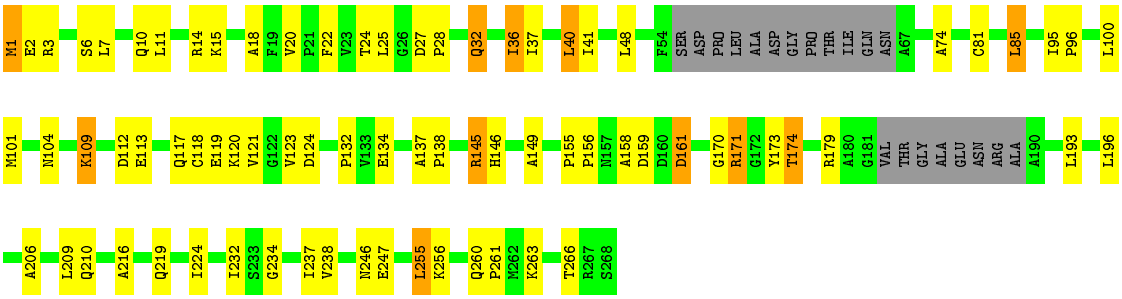
3 Residue-property plots (i)

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

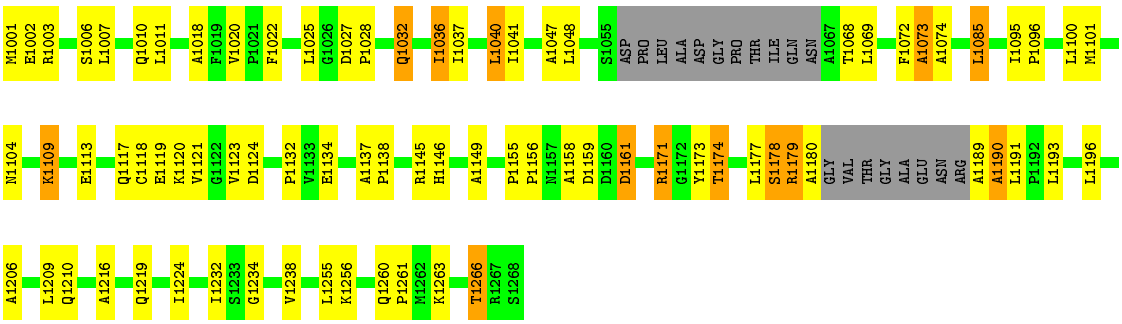
- Molecule 1: Tryptophan synthase alpha chain

Chain A:



- Molecule 1: Tryptophan synthase alpha chain

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	158.42Å 45.10Å 72.06Å 90.00° 96.90° 90.00°	Depositor
Resolution (Å)	19.56 – 2.50	Depositor
% Data completeness (in resolution range)	89.8 (19.56-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3868	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: 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	0.39	0/1919	0.81	6/2601 (0.2%)
1	B	0.40	0/1926	0.82	6/2611 (0.2%)
All	All	0.39	0/3845	0.81	12/5212 (0.2%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1145	ARG	NE-CZ-NH2	-14.49	113.06	120.30
1	A	145	ARG	NE-CZ-NH1	-14.13	113.24	120.30
1	A	145	ARG	NE-CZ-NH2	13.93	127.26	120.30
1	B	1171	ARG	NE-CZ-NH1	-13.75	113.42	120.30
1	B	1145	ARG	NE-CZ-NH1	13.61	127.11	120.30
1	B	1171	ARG	NE-CZ-NH2	13.48	127.04	120.30
1	A	171	ARG	NE-CZ-NH2	-13.41	113.59	120.30
1	A	171	ARG	NE-CZ-NH1	12.95	126.78	120.30
1	B	1171	ARG	CD-NE-CZ	7.11	133.56	123.60
1	A	145	ARG	CD-NE-CZ	7.02	133.43	123.60
1	A	171	ARG	CD-NE-CZ	6.92	133.28	123.60
1	B	1145	ARG	CD-NE-CZ	6.84	133.17	123.60

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	1882	0	1921	57	0
1	B	1889	0	1925	58	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	61	0	0	4	0
3	B	26	0	0	2	0
All	All	3868	0	3846	115	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 15.

All (115) 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:B:1178:SER:HB3	1:B:1179:ARG:HD3	1.56	0.87
1:A:156:PRO:HA	1:A:196:LEU:HD11	1.59	0.84
1:B:1263:LYS:HZ2	1:B:1266:THR:HG21	1.45	0.80
1:A:3:ARG:HD3	1:A:124:ASP:OD1	1.83	0.79
1:B:1003:ARG:HD3	1:B:1124:ASP:OD1	1.83	0.78
1:B:1263:LYS:NZ	1:B:1266:THR:HG21	2.01	0.76
1:B:1260:GLN:HB2	1:B:1261:PRO:HD3	1.70	0.73
1:A:260:GLN:HB2	1:A:261:PRO:HD3	1.70	0.73
1:A:104:ASN:HD22	1:A:104:ASN:H	1.37	0.71
1:A:32:GLN:O	1:A:36:ILE:HG23	1.94	0.68
1:B:1104:ASN:H	1:B:1104:ASN:HD22	1.41	0.66
1:A:118:CYS:HB3	1:A:123:VAL:HG22	1.77	0.66
1:A:134:GLU:CD	1:A:134:GLU:H	2.00	0.65
1:B:1085:LEU:HB3	1:B:1121:VAL:HG11	1.78	0.65
1:B:1134:GLU:H	1:B:1134:GLU:CD	1.99	0.65
1:A:85:LEU:HB3	1:A:121:VAL:HG11	1.78	0.65
1:A:25:LEU:HD21	1:A:85:LEU:HD13	1.79	0.65
1:B:1032:GLN:O	1:B:1036:ILE:HG23	1.98	0.64
1:B:1263:LYS:HE2	3:B:4:HOH:O	1.97	0.64
1:B:1118:CYS:HB3	1:B:1123:VAL:HG22	1.79	0.63
1:A:193:LEU:HD23	3:A:311:HOH:O	1.97	0.63
1:B:1156:PRO:HA	1:B:1196:LEU:HD11	1.81	0.62
1:A:109:LYS:NZ	1:A:109:LYS:HB3	2.14	0.62
1:B:1109:LYS:HB3	1:B:1109:LYS:NZ	2.15	0.61
1:B:1189:ALA:HA	3:B:87:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:THR:HG23	1:A:206:ALA:O	2.01	0.61
1:A:119:GLU:HB2	1:A:146:HIS:HB3	1.86	0.57
1:A:85:LEU:HB3	1:A:121:VAL:CG1	2.33	0.57
1:B:1085:LEU:HB3	1:B:1121:VAL:CG1	2.34	0.57
1:B:1179:ARG:N	1:B:1179:ARG:HD3	2.19	0.57
1:B:1025:LEU:HD21	1:B:1085:LEU:HD13	1.87	0.56
1:B:1119:GLU:HB2	1:B:1146:HIS:HB3	1.88	0.56
1:A:155:PRO:HG2	1:A:158:ALA:HB2	1.87	0.56
1:A:156:PRO:HG3	1:A:179:ARG:HA	1.87	0.56
1:B:1007:LEU:HD22	1:B:1096:PRO:HG2	1.89	0.55
1:A:25:LEU:HD23	1:A:81:CYS:HB3	1.89	0.55
1:A:24:THR:HB	3:A:328:HOH:O	2.07	0.54
1:B:1179:ARG:H	1:B:1179:ARG:HD3	1.72	0.54
1:B:1263:LYS:O	1:B:1266:THR:HG22	2.08	0.54
1:A:216:ALA:HB3	1:A:219:GLN:HG3	1.90	0.54
1:B:1216:ALA:HB3	1:B:1219:GLN:HG3	1.90	0.53
1:B:1155:PRO:HG2	1:B:1158:ALA:HB2	1.89	0.53
1:B:1036:ILE:HD12	1:B:1040:LEU:HD22	1.89	0.53
1:A:104:ASN:H	1:A:104:ASN:ND2	2.06	0.52
1:A:6:SER:O	1:A:10:GLN:HG3	2.10	0.52
1:B:1072:PHE:O	1:B:1073:ALA:C	2.48	0.52
1:B:1068:THR:HB	1:B:1069:LEU:HD12	1.91	0.51
1:A:118:CYS:HB3	1:A:123:VAL:CG2	2.40	0.51
1:B:1068:THR:C	1:B:1069:LEU:HD12	2.31	0.51
1:A:36:ILE:HD12	1:A:40:LEU:HD22	1.93	0.51
1:B:1177:LEU:HD21	1:B:1180:ALA:HB3	1.93	0.50
1:B:1132:PRO:HB3	1:B:1134:GLU:OE1	2.11	0.50
1:A:28:PRO:HD2	1:A:32:GLN:HB3	1.93	0.50
1:A:193:LEU:HG	1:A:210:GLN:NE2	2.26	0.50
1:B:1006:SER:O	1:B:1010:GLN:HG3	2.11	0.50
1:B:1189:ALA:O	1:B:1190:ALA:HB2	2.11	0.50
1:B:1028:PRO:HD2	1:B:1032:GLN:HB3	1.94	0.50
1:B:1173:TYR:CD2	1:B:1209:LEU:HD12	2.46	0.50
1:B:1104:ASN:H	1:B:1104:ASN:ND2	2.09	0.49
1:A:1:MET:CE	1:A:6:SER:HB2	2.42	0.49
1:B:1193:LEU:HG	1:B:1210:GLN:NE2	2.26	0.49
1:A:132:PRO:HB3	1:A:134:GLU:OE1	2.14	0.48
1:A:7:LEU:HD22	1:A:96:PRO:HG2	1.94	0.48
1:A:170:GLY:O	1:A:171:ARG:HD3	2.13	0.48
1:B:1118:CYS:HB3	1:B:1123:VAL:CG2	2.44	0.48
1:A:117:GLN:OE1	1:A:120:LYS:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1224:ILE:CD1	1:B:1266:THR:HA	2.44	0.47
1:B:1011:LEU:CD1	1:B:1018:ALA:HB2	2.43	0.47
1:A:159:ASP:OD2	1:A:161:ASP:HB2	2.15	0.47
1:A:224:ILE:HD11	1:A:266:THR:HG22	1.97	0.47
1:A:149:ALA:HB1	1:A:171:ARG:HB2	1.96	0.47
1:B:1159:ASP:OD2	1:B:1161:ASP:HB2	2.16	0.46
1:B:1174:THR:HG23	1:B:1206:ALA:O	2.16	0.46
1:B:1022:PHE:CD1	1:B:1022:PHE:C	2.89	0.46
1:A:109:LYS:HZ3	1:A:109:LYS:HB3	1.80	0.46
1:A:224:ILE:CD1	1:A:266:THR:HA	2.46	0.46
1:A:95:ILE:HA	1:A:96:PRO:HD3	1.83	0.46
1:A:173:TYR:CD2	1:A:209:LEU:HD12	2.51	0.46
1:B:1095:ILE:HA	1:B:1096:PRO:HD3	1.83	0.45
1:B:1069:LEU:N	1:B:1069:LEU:HD12	2.31	0.45
1:B:1156:PRO:HG3	1:B:1178:SER:O	2.15	0.45
1:B:1036:ILE:HG13	1:B:1037:ILE:N	2.32	0.45
1:B:1117:GLN:OE1	1:B:1120:LYS:HD2	2.15	0.45
1:A:156:PRO:HA	1:A:196:LEU:CD1	2.40	0.45
1:B:1191:LEU:H	1:B:1191:LEU:HD12	1.82	0.45
1:A:11:LEU:CD1	1:A:18:ALA:HB2	2.47	0.45
1:B:1134:GLU:CD	1:B:1134:GLU:N	2.68	0.45
1:A:137:ALA:N	1:A:138:PRO:HD2	2.32	0.45
1:A:20:VAL:O	1:A:232:ILE:HA	2.16	0.45
1:A:256:LYS:NZ	1:A:256:LYS:HB2	2.31	0.45
1:B:1234:GLY:O	1:B:1238:VAL:HG23	2.16	0.45
1:A:36:ILE:HG13	1:A:37:ILE:N	2.31	0.44
1:B:1149:ALA:HB1	1:B:1171:ARG:HB2	1.99	0.44
1:A:174:THR:CG2	1:A:206:ALA:O	2.65	0.44
1:A:22:PHE:C	1:A:22:PHE:CD1	2.91	0.44
1:A:234:GLY:O	1:A:238:VAL:HG23	2.18	0.44
1:B:1007:LEU:CD2	1:B:1096:PRO:HG2	2.48	0.43
1:B:1137:ALA:N	1:B:1138:PRO:HD2	2.33	0.43
1:A:41:ILE:HD11	1:A:48:LEU:HD21	2.00	0.43
1:A:109:LYS:O	1:A:113:GLU:HB3	2.18	0.43
1:A:237:ILE:HG23	1:A:255:LEU:HD11	2.00	0.43
1:A:109:LYS:NZ	1:A:109:LYS:CB	2.82	0.43
1:B:1256:LYS:HB2	1:B:1256:LYS:NZ	2.34	0.42
1:A:14:ARG:O	1:A:15:LYS:C	2.58	0.42
1:B:1109:LYS:HB3	1:B:1109:LYS:HZ3	1.84	0.42
1:B:1020:VAL:O	1:B:1232:ILE:HA	2.18	0.42
1:A:134:GLU:CD	1:A:134:GLU:N	2.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1109:LYS:O	1:B:1113:GLU:HB3	2.20	0.42
1:A:246:ASN:O	1:A:247:GLU:HG3	2.20	0.41
1:B:1041:ILE:HD11	1:B:1048:LEU:HD21	2.01	0.41
1:A:112:ASP:OD2	1:A:146:HIS:HE1	2.04	0.41
1:A:1:MET:HE1	1:A:6:SER:HB2	2.03	0.41
1:A:171:ARG:NH2	3:A:273:HOH:O	2.51	0.40
1:B:1020:VAL:HG22	1:B:1047:ALA:HB3	2.03	0.40
1:A:263:LYS:HE2	3:A:271:HOH:O	2.20	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	242/268 (90%)	229 (95%)	12 (5%)	1 (0%)	34 54
1	B	243/268 (91%)	226 (93%)	13 (5%)	4 (2%)	9 17
All	All	485/536 (90%)	455 (94%)	25 (5%)	5 (1%)	15 28

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1190	ALA
1	B	1073	ALA
1	B	1178	SER
1	A	74	ALA
1	B	1074	ALA

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	194/209 (93%)	180 (93%)	14 (7%)	14 28
1	B	195/209 (93%)	180 (92%)	15 (8%)	13 25
All	All	389/418 (93%)	360 (92%)	29 (8%)	13 26

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	27	ASP
1	A	32	GLN
1	A	36	ILE
1	A	40	LEU
1	A	85	LEU
1	A	100	LEU
1	A	101	MET
1	A	109	LYS
1	A	145	ARG
1	A	161	ASP
1	A	174	THR
1	A	255	LEU
1	B	1001	MET
1	B	1002	GLU
1	B	1027	ASP
1	B	1032	GLN
1	B	1036	ILE
1	B	1040	LEU
1	B	1085	LEU
1	B	1100	LEU
1	B	1101	MET
1	B	1109	LYS
1	B	1161	ASP
1	B	1174	THR
1	B	1179	ARG

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Mol	Chain	Res	Type
1	B	1255	LEU
1	B	1266	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	90	GLN
1	A	104	ASN
1	A	141	GLN
1	A	210	GLN
1	A	243	GLN
1	A	260	GLN
1	B	1080	GLN
1	B	1090	GLN
1	B	1104	ASN
1	B	1141	GLN
1	B	1210	GLN
1	B	1243	GLN
1	B	1260	GLN

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

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	SO4	A	269	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	B	88	-	4,4,4	0.21	0	6,6,6	0.16	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.

No monomer is involved in short contacts.

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 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.