



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:39 AM GMT

PDB ID : 1J0N  
Title : Crystal Structure of Bacillus sp. GL1 Xanthan Lyase that Acts on Side Chains of Xanthan  
Authors : Hashimoto, W.; Nankai, H.; Mikami, B.; Murata, K.  
Deposited on : 2002-11-19  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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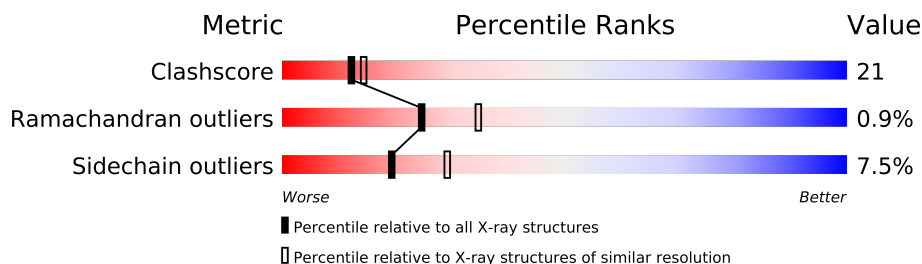
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	752	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5975 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

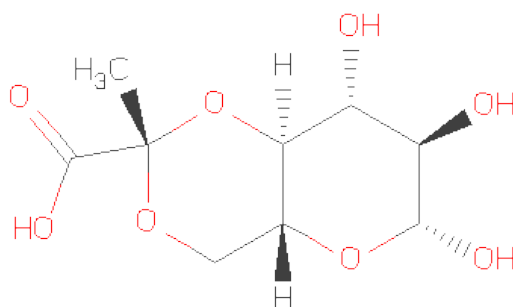
- Molecule 1 is a protein called XANTHAN LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	752	5697	3585	970	1128	14	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	161	THR	ILE	CONFLICT	UNP Q9AQS0

- Molecule 2 is SUGAR (4,6-O-(1-CARBOXYETHYLIDENE)-BETA-D-GLUCOSE) (three-letter code: CEG) (formula: C<sub>9</sub>H<sub>14</sub>O<sub>8</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	17	9	8	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	260	Total 260	O 260	0	0

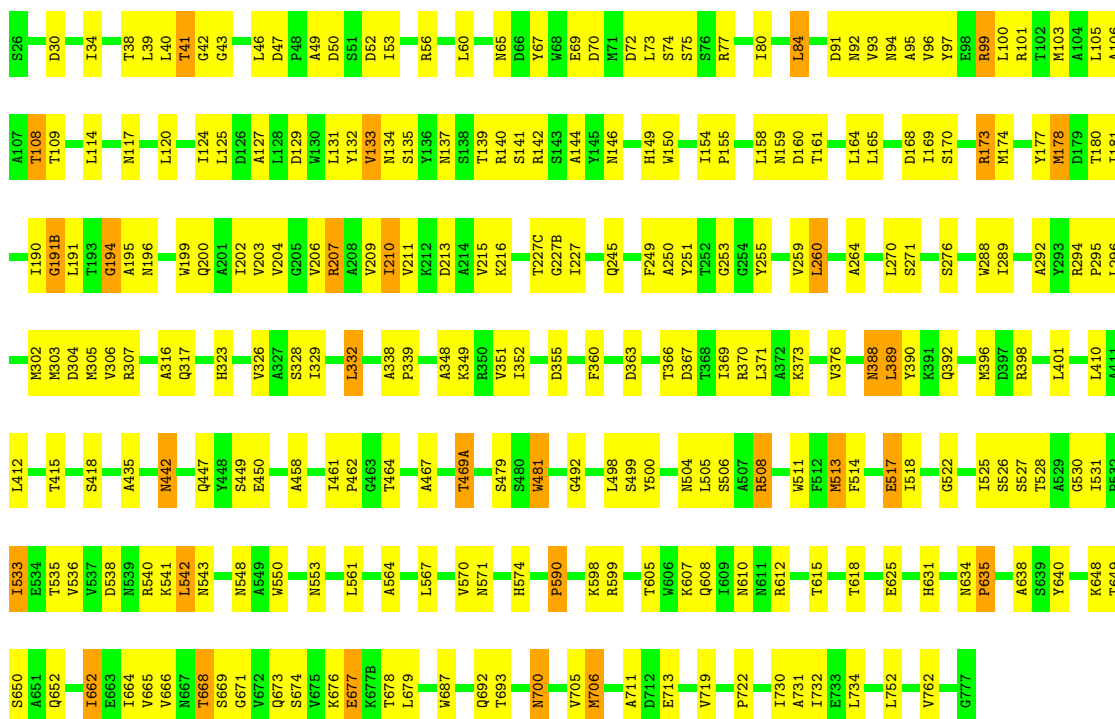
### 3 Residue-property plots

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

Chain A: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.36Å 91.31Å 159.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.48 – 2.40	Depositor
% Data completeness (in resolution range)	82.6 (27.48-2.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.169 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	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: CEG, CA

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	0.34	0/5829	0.62	0/7957

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5697	0	5477	238	0
2	A	17	0	10	0	0
3	A	1	0	0	0	0
4	A	260	0	0	18	0
All	All	5975	0	5487	238	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (238) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:610:ASN:HD21	1:A:612:ARG:HD3	1.23	1.03
1:A:178:MET:HE1	1:A:181:ILE:HD12	1.44	0.97
1:A:553:ASN:HD21	1:A:571:ASN:H	1.09	0.97
1:A:178:MET:HE2	1:A:207:ARG:HB2	1.51	0.92
1:A:610:ASN:O	1:A:615:THR:HG21	1.76	0.86
1:A:504:ASN:HD22	1:A:528:THR:H	1.19	0.86
1:A:108:THR:HG21	1:A:164:LEU:HD22	1.57	0.85
1:A:447:GLN:HE22	1:A:541:LYS:H	1.23	0.84
1:A:610:ASN:ND2	1:A:612:ARG:HD3	1.93	0.82
1:A:612:ARG:O	1:A:615:THR:HG22	1.80	0.81
1:A:41:THR:HG22	1:A:43:GLY:H	1.47	0.80
1:A:207:ARG:HA	1:A:210:ILE:HD11	1.64	0.79
1:A:178:MET:CE	1:A:181:ILE:HD12	2.13	0.79
1:A:169:ILE:HG21	1:A:174:MET:HG2	1.67	0.76
1:A:304:ASP:HA	1:A:307:ARG:HD3	1.65	0.76
1:A:260:LEU:HD22	1:A:328:SER:HB3	1.68	0.75
1:A:504:ASN:HD22	1:A:528:THR:N	1.84	0.74
1:A:665:VAL:HG12	1:A:666:VAL:HG13	1.69	0.73
1:A:700:ASN:H	1:A:700:ASN:HD22	1.36	0.72
1:A:191(B):GLY:H	1:A:200:GLN:HE22	1.38	0.72
1:A:46:LEU:HD22	1:A:53:ILE:HG21	1.72	0.72
1:A:525:ILE:HB	1:A:638:ALA:HB3	1.71	0.72
1:A:46:LEU:HD22	1:A:53:ILE:CG2	2.21	0.71
1:A:135:SER:O	1:A:140:ARG:HD2	1.90	0.71
1:A:535:THR:OG1	1:A:631:HIS:HE1	1.74	0.71
1:A:190:ILE:HD11	1:A:204:VAL:HG11	1.72	0.70
1:A:158:LEU:HD11	1:A:177:TYR:HB3	1.72	0.70
1:A:105:LEU:O	1:A:109:THR:HG22	1.92	0.69
1:A:132:TYR:O	1:A:137:ASN:HB3	1.93	0.69
1:A:574:HIS:HD2	4:A:929:HOH:O	1.75	0.68
1:A:100:LEU:HA	1:A:103:MET:HE3	1.76	0.68
1:A:94:ASN:HA	1:A:154:ILE:HD13	1.75	0.68
1:A:700:ASN:HD21	1:A:731:ALA:H	1.39	0.68
1:A:195:ALA:H	1:A:245:GLN:HE22	1.42	0.67
1:A:100:LEU:HD23	1:A:103:MET:CE	2.24	0.67
1:A:307:ARG:NH2	1:A:316:ALA:O	2.27	0.67
1:A:30:ASP:O	1:A:34:ILE:HG12	1.96	0.66
1:A:100:LEU:HD23	1:A:103:MET:HE3	1.77	0.66
1:A:548:ASN:H	1:A:548:ASN:HD22	1.41	0.66
1:A:93:VAL:O	1:A:96:VAL:HG22	1.96	0.66
1:A:666:VAL:HG22	1:A:674:SER:HB3	1.77	0.66
1:A:498:LEU:HD23	1:A:499:SER:N	2.11	0.66
1:A:180:THR:HG21	4:A:832:HOH:O	1.95	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:294:ARG:HB3	1:A:295:PRO:HD3	1.77	0.65
1:A:338:ALA:HB3	1:A:339:PRO:HD3	1.79	0.64
1:A:133:VAL:HA	4:A:973:HOH:O	1.96	0.64
1:A:317:GLN:HE22	1:A:450:GLU:H	1.45	0.63
1:A:530:GLY:H	1:A:634:ASN:HD21	1.46	0.63
1:A:388:ASN:HD22	1:A:388:ASN:C	2.01	0.63
1:A:67:TYR:CD1	1:A:99:ARG:HD3	2.34	0.63
1:A:348:ALA:O	1:A:352:ILE:HG12	1.98	0.63
1:A:401:LEU:HD22	1:A:513:MET:HB3	1.81	0.63
1:A:605:THR:OG1	1:A:608:GLN:HG3	1.99	0.62
1:A:317:GLN:HE22	1:A:450:GLU:N	1.97	0.62
1:A:506:SER:HB3	4:A:1038:HOH:O	2.00	0.62
1:A:677:GLU:CD	1:A:679:LEU:HD23	2.20	0.62
1:A:191:LEU:HD13	1:A:200:GLN:NE2	2.14	0.61
1:A:508:ARG:HG2	1:A:687:TRP:CD2	2.36	0.61
1:A:69:GLU:O	1:A:69:GLU:HG2	2.00	0.60
1:A:543:ASN:H	1:A:548:ASN:HD21	1.47	0.60
1:A:195:ALA:HA	1:A:259:VAL:HG22	1.84	0.60
1:A:46:LEU:CD2	1:A:53:ILE:HD12	2.31	0.60
1:A:508:ARG:HG2	1:A:687:TRP:CE2	2.36	0.60
1:A:213:ASP:OD1	1:A:215:VAL:HG12	2.01	0.60
1:A:191(B):GLY:H	1:A:200:GLN:NE2	1.99	0.60
1:A:74:SER:HB3	4:A:1061:HOH:O	2.02	0.60
1:A:390:TYR:CE1	1:A:513:MET:HG3	2.38	0.59
1:A:190:ILE:HD11	1:A:204:VAL:CG1	2.31	0.59
1:A:84:LEU:HD21	1:A:95:ALA:HB3	1.84	0.59
1:A:323:HIS:HE1	1:A:355:ASP:OD1	1.85	0.59
1:A:349:LYS:HE3	1:A:376:VAL:HA	1.85	0.59
1:A:245:GLN:HG2	1:A:255:TYR:CG	2.37	0.59
1:A:96:VAL:HG21	1:A:131:LEU:HD21	1.84	0.58
1:A:323:HIS:HD2	1:A:363:ASP:OD2	1.86	0.58
1:A:461:ILE:HD12	1:A:461:ILE:N	2.17	0.58
1:A:94:ASN:HA	1:A:154:ILE:CD1	2.33	0.58
1:A:207:ARG:HA	1:A:210:ILE:CD1	2.34	0.57
1:A:253:GLY:H	1:A:306:VAL:HG13	1.69	0.57
1:A:165:LEU:O	1:A:169:ILE:HG13	2.05	0.57
1:A:67:TYR:CG	1:A:99:ARG:HD3	2.39	0.57
1:A:553:ASN:HD21	1:A:571:ASN:N	1.92	0.57
1:A:169:ILE:CG2	1:A:174:MET:HG2	2.35	0.56
1:A:125:LEU:HD21	1:A:169:ILE:HG12	1.88	0.56
1:A:504:ASN:ND2	1:A:527:SER:HA	2.20	0.56
1:A:649:THR:H	1:A:652:GLN:NE2	2.03	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:195:ALA:H	1:A:245:GLN:NE2	2.03	0.55
1:A:305:MET:O	1:A:398:ARG:NH1	2.39	0.55
1:A:531:ILE:O	1:A:533:ILE:HD13	2.07	0.55
1:A:664:ILE:N	1:A:664:ILE:HD12	2.22	0.55
1:A:215:VAL:HG13	1:A:216:LYS:N	2.21	0.55
1:A:39:LEU:O	1:A:39:LEU:HD23	2.07	0.55
1:A:530:GLY:H	1:A:634:ASN:ND2	2.04	0.55
1:A:462:PRO:HB3	1:A:538:ASP:HA	1.89	0.55
1:A:56:ARG:HG3	1:A:56:ARG:HH11	1.72	0.55
1:A:211:VAL:O	1:A:211:VAL:HG12	2.06	0.54
1:A:412:LEU:N	1:A:412:LEU:HD22	2.23	0.54
1:A:191:LEU:HD13	1:A:200:GLN:CD	2.28	0.54
1:A:390:TYR:CE2	1:A:492:GLY:HA3	2.42	0.54
1:A:84:LEU:CD2	1:A:95:ALA:HB3	2.38	0.54
1:A:352:ILE:HD12	1:A:360:PHE:CG	2.43	0.53
1:A:178:MET:CE	1:A:207:ARG:HB2	2.32	0.53
1:A:101:ARG:NH1	1:A:160:ASP:OD2	2.42	0.53
1:A:149:HIS:O	1:A:154:ILE:HG12	2.09	0.53
1:A:542:LEU:HB3	1:A:548:ASN:ND2	2.24	0.53
1:A:129:ASP:OD2	1:A:173:ARG:NH1	2.42	0.52
1:A:574:HIS:HE1	1:A:648:LYS:O	1.92	0.52
1:A:504:ASN:ND2	1:A:528:THR:N	2.54	0.52
1:A:511:TRP:C	1:A:513:MET:HE2	2.30	0.52
1:A:41:THR:CG2	1:A:43:GLY:H	2.20	0.52
1:A:631:HIS:HD2	4:A:1117:HOH:O	1.92	0.52
1:A:206:VAL:O	1:A:210:ILE:HG12	2.11	0.51
1:A:664:ILE:H	1:A:664:ILE:HD12	1.75	0.51
1:A:668:THR:OG1	1:A:669:SER:N	2.44	0.51
1:A:200:GLN:O	1:A:204:VAL:HG12	2.11	0.51
1:A:730:ILE:HD13	1:A:762:VAL:HG11	1.92	0.51
1:A:498:LEU:HD21	1:A:500:TYR:CZ	2.46	0.51
1:A:92:ASN:O	1:A:96:VAL:HG13	2.11	0.50
1:A:673:GLN:HE21	1:A:687:TRP:HE1	1.58	0.50
1:A:730:ILE:HG22	1:A:732:ILE:HG12	1.92	0.50
1:A:137:ASN:ND2	1:A:139:THR:H	2.10	0.50
1:A:326:VAL:HG21	1:A:351:VAL:HG11	1.92	0.50
1:A:514:PHE:HB2	1:A:517:GLU:OE1	2.11	0.50
1:A:164:LEU:HD21	4:A:1058:HOH:O	2.12	0.49
1:A:39:LEU:C	1:A:39:LEU:HD23	2.32	0.49
1:A:191:LEU:HD13	1:A:200:GLN:OE1	2.12	0.49
1:A:705:VAL:HG22	1:A:719:VAL:HG13	1.93	0.49
1:A:60:LEU:HG	1:A:106:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:481:TRP:CZ2	1:A:722:PRO:HG3	2.48	0.49
1:A:80:ILE:HD12	1:A:127:ALA:HB1	1.94	0.49
1:A:154:ILE:N	1:A:155:PRO:HD2	2.27	0.49
1:A:700:ASN:HD22	1:A:700:ASN:N	2.02	0.48
1:A:700:ASN:ND2	1:A:731:ALA:H	2.10	0.48
1:A:129:ASP:OD1	1:A:173:ARG:HD2	2.12	0.48
1:A:46:LEU:HD21	1:A:53:ILE:HD12	1.94	0.48
1:A:207:ARG:HA	1:A:210:ILE:CG1	2.44	0.48
1:A:548:ASN:H	1:A:548:ASN:ND2	2.11	0.48
1:A:500:TYR:CE2	1:A:505:LEU:HD23	2.49	0.48
1:A:165:LEU:N	1:A:165:LEU:HD22	2.29	0.48
1:A:317:GLN:NE2	1:A:449:SER:HA	2.29	0.48
1:A:598:LYS:NZ	4:A:1001:HOH:O	2.47	0.47
1:A:154:ILE:HB	1:A:155:PRO:CD	2.44	0.47
1:A:207:ARG:HG3	4:A:1078:HOH:O	2.14	0.47
1:A:170:SER:HA	4:A:1076:HOH:O	2.13	0.47
1:A:142:ARG:HD3	4:A:1079:HOH:O	2.14	0.47
1:A:159:ASN:HB3	1:A:206:VAL:HG11	1.97	0.47
1:A:530:GLY:N	1:A:634:ASN:HD21	2.11	0.47
1:A:461:ILE:O	1:A:536:VAL:HG11	2.14	0.47
1:A:288:TRP:O	1:A:292:ALA:HB3	2.14	0.47
1:A:296:LEU:O	1:A:303:MET:HG3	2.15	0.47
1:A:458:ALA:O	1:A:461:ILE:HD11	2.15	0.47
1:A:199:TRP:O	1:A:202:ILE:HG22	2.15	0.47
1:A:40:LEU:HB2	4:A:1058:HOH:O	2.15	0.46
1:A:561:LEU:HD23	1:A:599:ARG:HG2	1.98	0.46
1:A:46:LEU:HD22	1:A:53:ILE:HG23	1.94	0.46
1:A:141:SER:HA	4:A:1070:HOH:O	2.14	0.46
1:A:289:ILE:HD12	1:A:329:ILE:HG12	1.98	0.46
1:A:542:LEU:HD21	1:A:625:GLU:HB2	1.98	0.45
1:A:498:LEU:HD23	1:A:499:SER:H	1.79	0.45
1:A:52:ASP:OD1	1:A:373:LYS:NZ	2.49	0.45
1:A:467:ALA:HA	1:A:533:ILE:HD12	1.98	0.45
1:A:41:THR:HG22	1:A:43:GLY:N	2.23	0.45
1:A:349:LYS:HE2	4:A:1098:HOH:O	2.16	0.45
1:A:649:THR:H	1:A:652:GLN:HE21	1.63	0.45
1:A:178:MET:HG2	1:A:211:VAL:CG2	2.47	0.45
1:A:191:LEU:HD13	1:A:200:GLN:HE22	1.80	0.45
1:A:607:LYS:HD2	1:A:615:THR:HG23	1.99	0.45
1:A:50:ASP:HB3	1:A:53:ILE:CG1	2.47	0.45
1:A:678:THR:OG1	1:A:679:LEU:HD22	2.17	0.45
1:A:249:PHE:CE2	1:A:418:SER:HB2	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:469(A):THR:HG21	1:A:531:ILE:HD13	1.99	0.44
1:A:73:LEU:HD22	1:A:73:LEU:N	2.33	0.44
1:A:649:THR:HB	4:A:1127:HOH:O	2.16	0.44
1:A:264:ALA:HB1	1:A:332:LEU:HD13	1.99	0.44
1:A:304:ASP:HA	1:A:307:ARG:CD	2.42	0.44
1:A:97:TYR:CD1	1:A:154:ILE:HG23	2.52	0.44
1:A:133:VAL:HG22	1:A:134:ASN:HD22	1.83	0.44
1:A:526:SER:HA	1:A:635:PRO:O	2.18	0.44
1:A:47:ASP:OD2	1:A:49:ALA:HB3	2.18	0.44
1:A:160:ASP:O	1:A:164:LEU:HG	2.17	0.44
1:A:648:LYS:HA	1:A:652:GLN:NE2	2.32	0.44
1:A:461:ILE:O	1:A:536:VAL:CG1	2.66	0.44
1:A:302:MET:HE3	1:A:306:VAL:HG11	1.99	0.44
1:A:97:TYR:HE2	1:A:158:LEU:HD23	1.82	0.44
1:A:700:ASN:H	1:A:700:ASN:ND2	2.10	0.44
1:A:178:MET:HE3	1:A:178:MET:HA	1.99	0.43
1:A:442:ASN:HD22	1:A:442:ASN:C	2.20	0.43
1:A:370:ARG:HG2	1:A:370:ARG:HH11	1.82	0.43
1:A:84:LEU:HD22	1:A:92:ASN:O	2.17	0.43
1:A:56:ARG:NH1	1:A:56:ARG:HG3	2.32	0.43
1:A:435:ALA:O	1:A:464:THR:HG22	2.18	0.43
1:A:574:HIS:CD2	1:A:650:SER:HB3	2.54	0.43
1:A:127:ALA:O	1:A:131:LEU:HD12	2.18	0.43
1:A:514:PHE:CE1	1:A:662:ILE:HD11	2.52	0.43
1:A:389:LEU:C	1:A:389:LEU:CD1	2.86	0.43
1:A:100:LEU:HD23	1:A:103:MET:HE1	1.99	0.43
1:A:398:ARG:NH2	4:A:863:HOH:O	2.47	0.43
1:A:38:THR:O	1:A:42:GLY:N	2.47	0.43
1:A:65:ASN:HD22	1:A:114:LEU:HD21	1.82	0.43
1:A:97:TYR:CE2	1:A:158:LEU:HD23	2.54	0.43
1:A:574:HIS:CE1	1:A:648:LYS:O	2.70	0.43
1:A:41:THR:CG2	1:A:43:GLY:N	2.80	0.43
1:A:369:ILE:O	1:A:373:LYS:HB2	2.19	0.43
1:A:42:GLY:HA2	1:A:367:ASP:OD1	2.19	0.43
1:A:158:LEU:HB3	1:A:181:ILE:HD11	2.00	0.43
1:A:564:ALA:HA	1:A:598:LYS:HA	1.99	0.43
1:A:72:ASP:O	1:A:77:ARG:HD3	2.19	0.43
1:A:498:LEU:HD21	1:A:500:TYR:CE1	2.54	0.43
1:A:250:ALA:HB2	1:A:396:MET:HB2	2.01	0.43
1:A:120:LEU:O	1:A:124:ILE:HG13	2.19	0.42
1:A:458:ALA:O	1:A:461:ILE:CD1	2.67	0.42
1:A:264:ALA:CB	1:A:332:LEU:HD13	2.48	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:676:LYS:HG2	1:A:677:GLU:N	2.35	0.42
1:A:481:TRP:CH2	1:A:722:PRO:HG3	2.54	0.42
1:A:567:LEU:HB3	1:A:570:VAL:HG11	2.01	0.42
1:A:161:THR:HG22	1:A:165:LEU:HD23	2.02	0.42
1:A:304:ASP:OD1	1:A:307:ARG:NH1	2.48	0.42
1:A:144:ALA:HB3	1:A:150:TRP:CD1	2.54	0.42
1:A:170:SER:O	1:A:174:MET:HB2	2.19	0.42
1:A:129:ASP:OD2	1:A:173:ARG:HD2	2.19	0.42
1:A:194:GLY:H	1:A:227(B):GLY:HA3	1.84	0.42
1:A:253:GLY:N	1:A:306:VAL:HG13	2.33	0.42
1:A:60:LEU:HD23	1:A:109:THR:HG21	2.02	0.42
1:A:99:ARG:HG2	1:A:99:ARG:HH11	1.85	0.42
1:A:671:GLY:HA3	1:A:692:GLN:HE22	1.83	0.42
1:A:705:VAL:HG12	1:A:706:MET:N	2.36	0.41
1:A:518:ILE:HD12	1:A:518:ILE:N	2.34	0.41
1:A:390:TYR:OH	1:A:392:GLN:NE2	2.53	0.41
1:A:69:GLU:O	1:A:69:GLU:CG	2.66	0.41
1:A:500:TYR:HA	4:A:912:HOH:O	2.21	0.41
1:A:199:TRP:O	1:A:203:VAL:HG23	2.21	0.41
1:A:415:THR:HG23	1:A:479:SER:O	2.21	0.41
1:A:467:ALA:O	1:A:469(A):THR:HG23	2.20	0.41
1:A:270:LEU:O	1:A:276:SER:HA	2.20	0.41
1:A:522:GLY:HA3	1:A:640:TYR:CE2	2.56	0.40
1:A:177:TYR:O	1:A:181:ILE:HG13	2.21	0.40
1:A:46:LEU:HD11	1:A:366:THR:HB	2.04	0.40
1:A:196:ASN:O	1:A:200:GLN:HG3	2.21	0.40
1:A:713:GLU:HG2	4:A:1109:HOH:O	2.21	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	750/752 (100%)	692 (92%)	51 (7%)	7 (1%)	25	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	ASP
1	A	117	ASN
1	A	194	GLY
1	A	590	PRO
1	A	191(B)	GLY
1	A	227	ILE
1	A	711	ALA

### 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	584/584 (100%)	540 (92%)	44 (8%)	19	29

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	75	SER
1	A	84	LEU
1	A	91	ASP
1	A	99	ARG
1	A	108	THR
1	A	133	VAL
1	A	146	ASN
1	A	168	ASP
1	A	173	ARG
1	A	178	MET
1	A	207	ARG
1	A	209	VAL
1	A	210	ILE
1	A	227(C)	THR
1	A	251	TYR
1	A	260	LEU
1	A	271	SER
1	A	332	LEU
1	A	371	LEU

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Mol	Chain	Res	Type
1	A	388	ASN
1	A	389	LEU
1	A	410	LEU
1	A	442	ASN
1	A	469(A)	THR
1	A	481	TRP
1	A	508	ARG
1	A	513	MET
1	A	517	GLU
1	A	533	ILE
1	A	540	ARG
1	A	542	LEU
1	A	550	TRP
1	A	590	PRO
1	A	618	THR
1	A	635	PRO
1	A	662	ILE
1	A	668	THR
1	A	677	GLU
1	A	693	THR
1	A	700	ASN
1	A	706	MET
1	A	734	LEU
1	A	752	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	92	ASN
1	A	134	ASN
1	A	146	ASN
1	A	151	GLN
1	A	200	GLN
1	A	222	ASN
1	A	245	GLN
1	A	284	ASN
1	A	317	GLN
1	A	323	HIS
1	A	353	GLN
1	A	388	ASN
1	A	392	GLN

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Mol	Chain	Res	Type
1	A	424	ASN
1	A	427	ASN
1	A	442	ASN
1	A	447	GLN
1	A	504	ASN
1	A	548	ASN
1	A	553	ASN
1	A	565	GLN
1	A	574	HIS
1	A	608	GLN
1	A	610	ASN
1	A	631	HIS
1	A	634	ASN
1	A	652	GLN
1	A	673	GLN
1	A	685	ASN
1	A	692	GLN
1	A	700	ASN
1	A	724	GLN
1	A	775	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z  > 2$
2	CEG	A	780	-	18,18,18	4.40	3 (16%)	28,28,28	4.45	12 (42%)

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	CEG	A	780	-	2/2/7/7	0/6/37/37	0/0/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	780	CEG	C6-C5	-13.04	1.29	1.51
2	A	780	CEG	O6-C7	9.91	1.52	1.42
2	A	780	CEG	C7-C8	-7.91	1.44	1.55

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	780	CEG	O5-C5-C6	12.72	127.55	108.87
2	A	780	CEG	O6-C7-C9	-11.03	92.86	106.28
2	A	780	CEG	O6-C6-C5	8.65	129.11	110.77
2	A	780	CEG	C6-O6-C7	-8.04	108.84	114.02
2	A	780	CEG	C9-C7-C8	5.30	117.35	107.95
2	A	780	CEG	C6-C5-C4	-5.20	101.42	109.39
2	A	780	CEG	C1-O5-C5	4.23	120.97	113.40
2	A	780	CEG	O4-C7-C9	-4.03	97.98	107.76
2	A	780	CEG	O6-C7-O4	3.52	114.46	110.86
2	A	780	CEG	C7-O4-C4	-2.55	108.06	114.12
2	A	780	CEG	O6-C7-C8	2.52	119.42	108.59
2	A	780	CEG	O5-C1-C2	2.36	113.52	109.86

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	780	CEG	C2
2	A	780	CEG	C1

There are no torsion outliers.

There are no ring outliers.

## 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.