



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 10:19 PM EDT

PDB ID : 1J0M
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 : unknown
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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

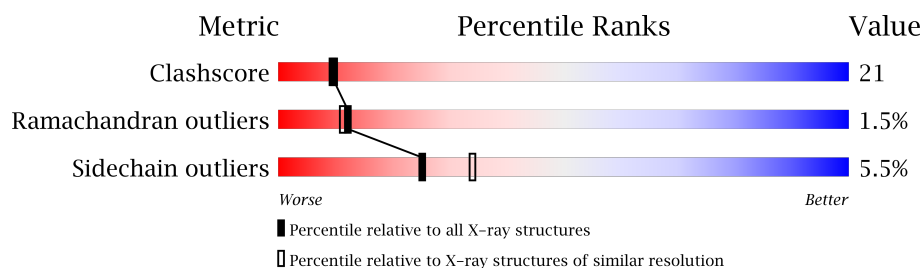
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (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 $\leq 5\%$. 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	752	 66% 30% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5945 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 XANTHAN LYASE.

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

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

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

- Molecule 3 is water.

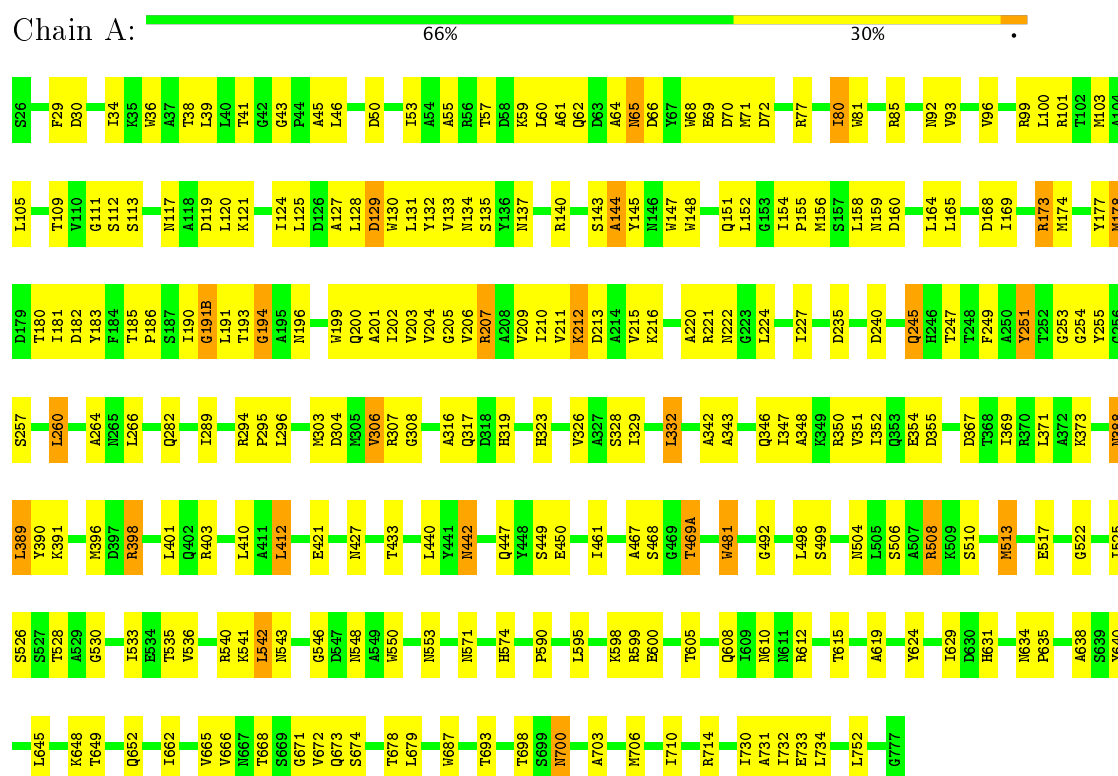
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	247	Total	O	0	0
			247	247		

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 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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.32Å 91.45Å 160.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.31 – 2.30	Depositor
% Data completeness (in resolution range)	83.9 (32.31-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.175 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5945	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: 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 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	5697	0	5477	238	0
2	A	1	0	0	0	0
3	A	247	0	0	12	0
All	All	5945	0	5477	238	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 21.

All (238) 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:700:ASN:HD21	1:A:731:ALA:H	1.07	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:MET:HE3	1:A:181:ILE:HD12	1.47	0.94
1:A:121:LYS:O	1:A:125:LEU:HD12	1.73	0.88
1:A:700:ASN:H	1:A:700:ASN:HD22	1.22	0.87
1:A:610:ASN:O	1:A:615:THR:HG21	1.75	0.85
1:A:553:ASN:HD21	1:A:571:ASN:H	1.21	0.85
1:A:191:LEU:HD13	1:A:200:GLN:HE22	1.42	0.84
1:A:178:MET:CE	1:A:181:ILE:HD12	2.08	0.83
1:A:542:LEU:HB3	1:A:548:ASN:ND2	1.94	0.82
1:A:169:ILE:HG21	1:A:174:MET:HG2	1.62	0.81
1:A:191:LEU:HD13	1:A:200:GLN:NE2	1.95	0.80
1:A:612:ARG:O	1:A:615:THR:HG22	1.83	0.79
1:A:668:THR:HG23	1:A:671:GLY:H	1.46	0.79
1:A:60:LEU:HD23	1:A:109:THR:HG21	1.65	0.79
1:A:304:ASP:HA	1:A:307:ARG:HD3	1.66	0.76
1:A:100:LEU:HA	1:A:103:MET:HE3	1.66	0.76
1:A:213:ASP:OD1	1:A:215:VAL:HG12	1.87	0.75
1:A:289:ILE:HD12	1:A:329:ILE:CD1	2.17	0.74
1:A:41:THR:HG23	1:A:109:THR:HA	1.70	0.74
1:A:180:THR:HG21	3:A:832:HOH:O	1.88	0.74
1:A:307:ARG:NH2	1:A:316:ALA:O	2.22	0.73
1:A:710:ILE:HD12	1:A:714:ARG:NH2	2.04	0.73
1:A:253:GLY:H	1:A:306:VAL:HG13	1.53	0.72
1:A:700:ASN:ND2	1:A:731:ALA:H	1.84	0.72
1:A:447:GLN:HE22	1:A:541:LYS:H	1.39	0.69
1:A:350:ARG:HA	3:A:1122:HOH:O	1.93	0.69
1:A:649:THR:H	1:A:652:GLN:HE21	1.41	0.69
1:A:132:TYR:O	1:A:137:ASN:HB3	1.92	0.68
1:A:535:THR:OG1	1:A:631:HIS:HE1	1.77	0.68
1:A:93:VAL:O	1:A:96:VAL:HG22	1.94	0.67
1:A:498:LEU:HD23	1:A:499:SER:N	2.09	0.67
1:A:504:ASN:HD22	1:A:528:THR:H	1.41	0.67
1:A:543:ASN:H	1:A:548:ASN:HD21	1.42	0.66
1:A:506:SER:HB3	3:A:1038:HOH:O	1.95	0.65
1:A:649:THR:H	1:A:652:GLN:NE2	1.96	0.64
1:A:127:ALA:O	1:A:131:LEU:HD13	1.99	0.63
1:A:390:TYR:CE2	1:A:492:GLY:HA3	2.33	0.63
1:A:193:THR:HG21	1:A:235:ASP:OD2	1.99	0.63
1:A:666:VAL:HG22	1:A:674:SER:HB3	1.80	0.62
1:A:253:GLY:N	1:A:306:VAL:HG13	2.13	0.62
1:A:296:LEU:HA	1:A:303:MET:HE3	1.82	0.62
1:A:668:THR:CG2	1:A:672:VAL:H	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HD23	1:A:103:MET:CE	2.30	0.61
1:A:668:THR:HG23	1:A:672:VAL:H	1.66	0.60
1:A:388:ASN:HD22	1:A:388:ASN:C	2.05	0.60
1:A:294:ARG:HB3	1:A:295:PRO:HD3	1.82	0.60
1:A:135:SER:O	1:A:140:ARG:HD2	2.02	0.60
1:A:245:GLN:HG2	1:A:255:TYR:CG	2.37	0.60
1:A:50:ASP:HB3	1:A:53:ILE:HB	1.83	0.60
1:A:120:LEU:O	1:A:124:ILE:HG12	2.01	0.59
1:A:38:THR:HG22	1:A:43:GLY:HA2	1.83	0.59
1:A:401:LEU:HD22	1:A:513:MET:HB3	1.84	0.59
1:A:72:ASP:O	1:A:77:ARG:HD3	2.02	0.59
1:A:668:THR:HG23	1:A:671:GLY:N	2.15	0.59
1:A:178:MET:HG2	1:A:211:VAL:CG2	2.33	0.59
1:A:30:ASP:OD2	1:A:212:LYS:HE2	2.02	0.59
1:A:204:VAL:HG23	3:A:1085:HOH:O	2.02	0.59
1:A:80:ILE:HG23	3:A:1116:HOH:O	2.03	0.59
1:A:130:TRP:HE3	1:A:131:LEU:HD12	1.68	0.58
1:A:440:LEU:HB3	1:A:540:ARG:NH2	2.18	0.58
1:A:367:ASP:O	1:A:371:LEU:HD13	2.04	0.58
1:A:46:LEU:HD22	1:A:53:ILE:HG21	1.86	0.58
1:A:289:ILE:HD12	1:A:329:ILE:HD13	1.86	0.58
1:A:306:VAL:HG13	1:A:306:VAL:O	2.03	0.58
1:A:468:SER:O	1:A:469(A):THR:HG22	2.04	0.58
1:A:700:ASN:HD21	1:A:731:ALA:N	1.89	0.57
1:A:178:MET:HG2	1:A:210:ILE:HD11	1.86	0.57
1:A:508:ARG:HG2	1:A:687:TRP:CE2	2.39	0.57
1:A:101:ARG:NH1	1:A:160:ASP:OD2	2.37	0.57
1:A:317:GLN:HE22	1:A:450:GLU:N	2.03	0.57
1:A:610:ASN:HD21	1:A:612:ARG:HD3	1.70	0.57
1:A:125:LEU:HD21	1:A:169:ILE:HG12	1.86	0.56
1:A:100:LEU:HD23	1:A:103:MET:HE3	1.87	0.56
1:A:178:MET:HG3	1:A:207:ARG:HD2	1.85	0.56
1:A:548:ASN:H	1:A:548:ASN:HD22	1.53	0.56
1:A:193:THR:HB	3:A:1080:HOH:O	2.05	0.55
1:A:215:VAL:HG13	1:A:216:LYS:N	2.21	0.55
1:A:100:LEU:HA	1:A:103:MET:CE	2.35	0.55
1:A:129:ASP:OD1	1:A:173:ARG:HD2	2.06	0.55
1:A:240:ASP:O	1:A:391:LYS:NZ	2.38	0.55
1:A:533:ILE:HG22	1:A:631:HIS:HB2	1.88	0.55
1:A:530:GLY:H	1:A:634:ASN:HD21	1.56	0.54
1:A:260:LEU:HD22	1:A:328:SER:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ILE:HB	1:A:638:ALA:HB3	1.88	0.54
1:A:80:ILE:O	1:A:80:ILE:HD12	2.07	0.54
1:A:69:GLU:O	1:A:69:GLU:HG2	2.08	0.54
1:A:133:VAL:HG13	1:A:134:ASN:ND2	2.23	0.54
1:A:182:ASP:OD2	1:A:207:ARG:NH2	2.41	0.53
1:A:178:MET:SD	1:A:210:ILE:HD11	2.48	0.53
1:A:211:VAL:O	1:A:211:VAL:HG12	2.08	0.53
1:A:317:GLN:NE2	1:A:449:SER:HA	2.23	0.53
1:A:700:ASN:N	1:A:700:ASN:HD22	1.98	0.53
1:A:412:LEU:N	1:A:412:LEU:HD22	2.24	0.53
1:A:221:ARG:HE	1:A:222:ASN:ND2	2.07	0.53
1:A:178:MET:CG	1:A:210:ILE:HD11	2.38	0.53
1:A:202:ILE:O	1:A:206:VAL:HG23	2.08	0.52
1:A:190:ILE:HD11	1:A:204:VAL:HG11	1.91	0.52
1:A:60:LEU:HD23	1:A:109:THR:CG2	2.39	0.52
1:A:207:ARG:O	1:A:211:VAL:HG23	2.10	0.51
1:A:504:ASN:HD22	1:A:528:THR:N	2.05	0.51
1:A:693:THR:HG22	1:A:698:THR:HG23	1.92	0.51
1:A:55:ALA:O	1:A:59:LYS:HG2	2.10	0.51
1:A:196:ASN:O	1:A:200:GLN:HG3	2.09	0.51
1:A:65:ASN:HA	1:A:68:TRP:HB3	1.92	0.51
1:A:224:LEU:HD21	1:A:266:LEU:HD23	1.93	0.51
1:A:62:GLN:O	1:A:66:ASP:HB2	2.12	0.50
1:A:81:TRP:HH2	1:A:103:MET:CE	2.23	0.50
1:A:605:THR:HG22	1:A:619:ALA:HA	1.92	0.50
1:A:193:THR:CG2	1:A:235:ASP:HB2	2.42	0.50
1:A:326:VAL:HG21	1:A:351:VAL:HG11	1.94	0.49
1:A:710:ILE:CD1	1:A:714:ARG:NH2	2.74	0.49
1:A:81:TRP:HH2	1:A:103:MET:HE1	1.77	0.49
1:A:574:HIS:HD2	3:A:929:HOH:O	1.95	0.49
1:A:498:LEU:HD23	1:A:498:LEU:C	2.33	0.49
1:A:648:LYS:HA	1:A:652:GLN:NE2	2.27	0.49
1:A:180:THR:O	1:A:183:TYR:HB3	2.13	0.49
1:A:46:LEU:CD2	1:A:53:ILE:HD13	2.42	0.49
1:A:433:THR:HG22	3:A:847:HOH:O	2.12	0.49
1:A:678:THR:OG1	1:A:679:LEU:HD22	2.13	0.49
1:A:92:ASN:O	1:A:96:VAL:HG13	2.12	0.49
1:A:703:ALA:HB2	1:A:730:ILE:HD13	1.94	0.48
1:A:508:ARG:HG2	1:A:687:TRP:CD2	2.48	0.48
1:A:317:GLN:HE22	1:A:450:GLU:H	1.60	0.48
1:A:61:ALA:HB1	1:A:113:SER:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ASP:O	1:A:164:LEU:HG	2.14	0.48
1:A:182:ASP:HB2	1:A:207:ARG:NH1	2.28	0.48
1:A:215:VAL:HG13	1:A:216:LYS:H	1.79	0.48
1:A:398:ARG:NH2	1:A:412:LEU:O	2.46	0.48
1:A:530:GLY:H	1:A:634:ASN:ND2	2.11	0.48
1:A:481:TRP:C	1:A:481:TRP:HE3	2.17	0.48
1:A:543:ASN:OD1	1:A:546:GLY:N	2.45	0.47
1:A:714:ARG:HH11	1:A:714:ARG:HB2	1.80	0.47
1:A:39:LEU:O	1:A:39:LEU:HD23	2.15	0.47
1:A:57:THR:HG21	1:A:111:GLY:C	2.35	0.47
1:A:574:HIS:HE1	1:A:648:LYS:O	1.98	0.47
1:A:665:VAL:HG12	1:A:666:VAL:HG13	1.96	0.47
1:A:38:THR:HG22	1:A:43:GLY:CA	2.45	0.47
1:A:158:LEU:HD11	1:A:177:TYR:HB3	1.97	0.47
1:A:159:ASN:OD1	1:A:178:MET:HE1	2.14	0.47
1:A:182:ASP:O	1:A:186:PRO:HB3	2.15	0.46
1:A:190:ILE:CD1	1:A:220:ALA:HA	2.46	0.46
1:A:264:ALA:HB1	1:A:332:LEU:HD13	1.96	0.46
1:A:45:ALA:O	1:A:46:LEU:C	2.54	0.46
1:A:599:ARG:HA	1:A:624:TYR:O	2.15	0.46
1:A:645:LEU:HB3	1:A:648:LYS:HD2	1.97	0.46
1:A:461:ILE:O	1:A:536:VAL:HG11	2.15	0.46
1:A:191:LEU:HB2	1:A:200:GLN:NE2	2.31	0.46
1:A:522:GLY:HA3	1:A:640:TYR:CE2	2.51	0.46
1:A:96:VAL:HG21	1:A:131:LEU:HD21	1.98	0.46
1:A:147:TRP:HB2	1:A:151:GLN:OE1	2.16	0.46
1:A:200:GLN:O	1:A:204:VAL:HG12	2.16	0.46
1:A:388:ASN:ND2	1:A:403:ARG:HH11	2.14	0.46
1:A:105:LEU:O	1:A:109:THR:HG22	2.17	0.45
1:A:147:TRP:O	1:A:151:GLN:HG3	2.16	0.45
1:A:169:ILE:CG2	1:A:174:MET:HG2	2.39	0.45
1:A:649:THR:N	1:A:652:GLN:HE21	2.12	0.45
1:A:152:LEU:O	1:A:156:MET:HG3	2.16	0.45
1:A:199:TRP:O	1:A:203:VAL:HG23	2.17	0.45
1:A:46:LEU:HD22	1:A:53:ILE:HD13	1.96	0.45
1:A:574:HIS:CE1	1:A:648:LYS:O	2.70	0.45
1:A:165:LEU:O	1:A:169:ILE:HG13	2.17	0.45
1:A:178:MET:HA	1:A:178:MET:CE	2.46	0.45
1:A:39:LEU:C	1:A:39:LEU:HD23	2.37	0.45
1:A:143:SER:O	1:A:144:ALA:C	2.54	0.45
1:A:249:PHE:CE2	1:A:421:GLU:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ALA:O	1:A:352:ILE:HG13	2.17	0.45
1:A:530:GLY:N	1:A:634:ASN:HD21	2.14	0.45
1:A:154:ILE:N	1:A:155:PRO:HD2	2.32	0.45
1:A:71:MET:CE	1:A:80:ILE:HD13	2.47	0.45
1:A:390:TYR:CD2	1:A:492:GLY:HA3	2.52	0.45
1:A:45:ALA:HB3	3:A:885:HOH:O	2.16	0.44
1:A:282:GLN:NE2	3:A:869:HOH:O	2.50	0.44
1:A:542:LEU:HB3	1:A:548:ASN:HD21	1.75	0.44
1:A:710:ILE:HD12	1:A:714:ARG:CZ	2.48	0.44
1:A:96:VAL:O	1:A:99:ARG:HB2	2.17	0.44
1:A:461:ILE:O	1:A:536:VAL:CG1	2.66	0.44
1:A:254:GLY:O	1:A:257:SER:HB3	2.18	0.44
1:A:29:PHE:HB3	1:A:212:LYS:HG2	1.98	0.44
1:A:144:ALA:O	1:A:145:TYR:C	2.55	0.44
1:A:204:VAL:HG13	1:A:220:ALA:HB2	1.99	0.44
1:A:700:ASN:H	1:A:700:ASN:ND2	2.03	0.44
1:A:221:ARG:HH21	1:A:222:ASN:HD21	1.66	0.43
1:A:36:TRP:CH2	1:A:202:ILE:HD11	2.52	0.43
1:A:191:LEU:HB3	1:A:193:THR:H	1.68	0.43
1:A:190:ILE:CD1	1:A:201:ALA:HA	2.49	0.43
1:A:46:LEU:HD22	1:A:53:ILE:CG2	2.47	0.43
1:A:193:THR:HG22	1:A:194:GLY:N	2.32	0.43
1:A:81:TRP:CH2	1:A:99:ARG:HB3	2.53	0.43
1:A:732:ILE:HG22	1:A:733:GLU:N	2.34	0.43
1:A:124:ILE:O	1:A:128:LEU:HG	2.18	0.43
1:A:210:ILE:CD1	1:A:211:VAL:HG23	2.48	0.43
1:A:319:HIS:HB2	3:A:906:HOH:O	2.18	0.43
1:A:350:ARG:HD2	1:A:354:GLU:CD	2.39	0.43
1:A:317:GLN:NE2	1:A:449:SER:CA	2.82	0.43
1:A:467:ALA:O	1:A:469(A):THR:HG23	2.19	0.43
1:A:598:LYS:HE3	1:A:600:GLU:OE1	2.19	0.42
1:A:595:LEU:HD23	1:A:629:ILE:HD13	2.00	0.42
1:A:69:GLU:O	1:A:69:GLU:CG	2.66	0.42
1:A:71:MET:HE2	1:A:80:ILE:HD13	2.01	0.42
1:A:245:GLN:CA	1:A:245:GLN:HE21	2.32	0.42
1:A:30:ASP:O	1:A:34:ILE:HG13	2.19	0.42
1:A:536:VAL:O	1:A:536:VAL:HG13	2.19	0.42
1:A:666:VAL:HG21	1:A:672:VAL:HG13	2.02	0.42
1:A:130:TRP:CE3	1:A:131:LEU:HD12	2.52	0.42
1:A:46:LEU:HA	1:A:46:LEU:HD23	1.86	0.42
1:A:109:THR:HG23	1:A:112:SER:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TRP:O	1:A:134:ASN:HB2	2.20	0.42
1:A:323:HIS:HE1	1:A:355:ASP:OD1	2.02	0.42
1:A:191(B):GLY:H	1:A:200:GLN:NE2	2.18	0.42
1:A:245:GLN:HA	1:A:245:GLN:NE2	2.34	0.42
1:A:148:TRP:CD1	1:A:152:LEU:HD12	2.55	0.42
1:A:100:LEU:HD23	1:A:103:MET:HE1	2.00	0.42
1:A:369:ILE:O	1:A:373:LYS:HB2	2.20	0.42
1:A:389:LEU:C	1:A:389:LEU:HD12	2.39	0.42
1:A:396:MET:O	1:A:398:ARG:HG2	2.20	0.42
1:A:526:SER:HA	1:A:635:PRO:O	2.19	0.42
1:A:598:LYS:HE2	3:A:902:HOH:O	2.20	0.42
1:A:251:TYR:CZ	1:A:308:GLY:HA3	2.54	0.42
1:A:510:SER:OG	1:A:673:GLN:NE2	2.53	0.41
1:A:103:MET:HB3	1:A:124:ILE:HD11	2.02	0.41
1:A:206:VAL:O	1:A:209:VAL:HG22	2.20	0.41
1:A:190:ILE:HD11	1:A:220:ALA:HA	2.01	0.41
1:A:245:GLN:HG2	1:A:255:TYR:CD2	2.56	0.41
1:A:81:TRP:CH2	1:A:103:MET:HE1	2.55	0.41
1:A:178:MET:HE2	1:A:207:ARG:HB2	2.02	0.41
1:A:343:ALA:O	1:A:347:ILE:HG13	2.21	0.41
1:A:177:TYR:O	1:A:180:THR:HG22	2.21	0.41
1:A:151:GLN:HB3	1:A:185:THR:OG1	2.20	0.41
1:A:193:THR:O	1:A:194:GLY:C	2.59	0.41
1:A:605:THR:OG1	1:A:608:GLN:HG3	2.21	0.41
1:A:204:VAL:HG13	1:A:205:GLY:N	2.35	0.40
1:A:668:THR:HG22	1:A:672:VAL:O	2.21	0.40
1:A:714:ARG:NH1	1:A:714:ARG:CB	2.84	0.40
1:A:129:ASP:OD1	1:A:129:ASP:N	2.54	0.40
1:A:158:LEU:HB3	1:A:181:ILE:HD11	2.04	0.40
1:A:442:ASN:HD22	1:A:442:ASN:C	2.24	0.40
1:A:178:MET:CE	1:A:207:ARG:HB2	2.52	0.40
1:A:342:ALA:O	1:A:346:GLN:HG3	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%)	686 (92%)	53 (7%)	11 (2%)	12 11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	ASP
1	A	194	GLY
1	A	70	ASP
1	A	117	ASN
1	A	144	ALA
1	A	212	LYS
1	A	227	ILE
1	A	247	THR
1	A	64	ALA
1	A	191(B)	GLY
1	A	590	PRO

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%)	552 (94%)	32 (6%)	25 34

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	80	ILE
1	A	85	ARG
1	A	119	ASP
1	A	129	ASP
1	A	173	ARG

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Mol	Chain	Res	Type
1	A	178	MET
1	A	207	ARG
1	A	245	GLN
1	A	251	TYR
1	A	260	LEU
1	A	306	VAL
1	A	332	LEU
1	A	388	ASN
1	A	389	LEU
1	A	398	ARG
1	A	410	LEU
1	A	412	LEU
1	A	427	ASN
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	542	LEU
1	A	550	TRP
1	A	662	ILE
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 (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	134	ASN
1	A	200	GLN
1	A	222	ASN
1	A	284	ASN
1	A	287	GLN
1	A	317	GLN
1	A	323	HIS
1	A	346	GLN
1	A	388	ASN
1	A	392	GLN
1	A	424	ASN

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Mol	Chain	Res	Type
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	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

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 ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.