Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 12:10 PM JST

PDB ID	:	7XGV
Title	:	Legionella glucosyltransferase
Authors	:	Chen, T.T.; Ouyang, S.Y.
Deposited on	:	2022-04-06
Resolution	:	2.27 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

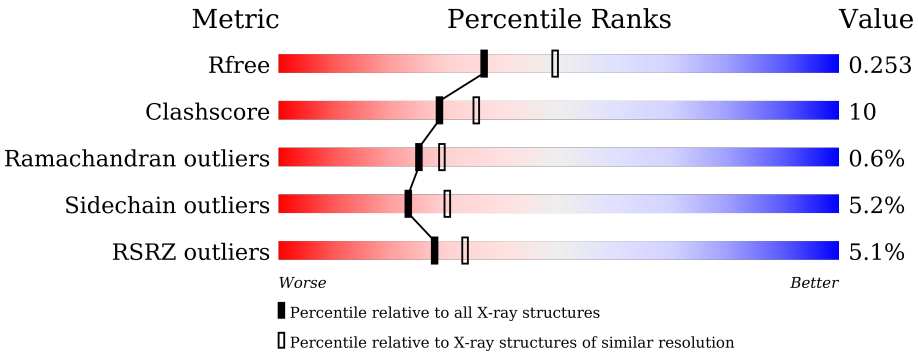
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.27 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))
R_{free}	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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% 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.

Mol	Chain	Length	Quality of chain
1	A	655	4% 74% 16% · 8%
1	B	655	5% 72% 19% · 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10094 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 Lgt2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	605	Total	C	N	O	S	0	0	0
			4779	3024	821	908	26			
1	B	604	Total	C	N	O	S	0	0	0
			4775	3023	823	903	26			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP A0A2S6F0H5
A	-17	GLY	-	expression tag	UNP A0A2S6F0H5
A	-16	SER	-	expression tag	UNP A0A2S6F0H5
A	-15	SER	-	expression tag	UNP A0A2S6F0H5
A	-14	HIS	-	expression tag	UNP A0A2S6F0H5
A	-13	HIS	-	expression tag	UNP A0A2S6F0H5
A	-12	HIS	-	expression tag	UNP A0A2S6F0H5
A	-11	HIS	-	expression tag	UNP A0A2S6F0H5
A	-10	HIS	-	expression tag	UNP A0A2S6F0H5
A	-9	HIS	-	expression tag	UNP A0A2S6F0H5
A	-8	SER	-	expression tag	UNP A0A2S6F0H5
A	-7	SER	-	expression tag	UNP A0A2S6F0H5
A	-6	GLY	-	expression tag	UNP A0A2S6F0H5
A	-5	LEU	-	expression tag	UNP A0A2S6F0H5
A	-4	VAL	-	expression tag	UNP A0A2S6F0H5
A	-3	PRO	-	expression tag	UNP A0A2S6F0H5
A	-2	PRO	-	expression tag	UNP A0A2S6F0H5
A	-1	GLY	-	expression tag	UNP A0A2S6F0H5
A	0	SER	-	expression tag	UNP A0A2S6F0H5
B	-18	MET	-	initiating methionine	UNP A0A2S6F0H5
B	-17	GLY	-	expression tag	UNP A0A2S6F0H5
B	-16	SER	-	expression tag	UNP A0A2S6F0H5
B	-15	SER	-	expression tag	UNP A0A2S6F0H5
B	-14	HIS	-	expression tag	UNP A0A2S6F0H5
B	-13	HIS	-	expression tag	UNP A0A2S6F0H5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP A0A2S6F0H5
B	-11	HIS	-	expression tag	UNP A0A2S6F0H5
B	-10	HIS	-	expression tag	UNP A0A2S6F0H5
B	-9	HIS	-	expression tag	UNP A0A2S6F0H5
B	-8	SER	-	expression tag	UNP A0A2S6F0H5
B	-7	SER	-	expression tag	UNP A0A2S6F0H5
B	-6	GLY	-	expression tag	UNP A0A2S6F0H5
B	-5	LEU	-	expression tag	UNP A0A2S6F0H5
B	-4	VAL	-	expression tag	UNP A0A2S6F0H5
B	-3	PRO	-	expression tag	UNP A0A2S6F0H5
B	-2	PRO	-	expression tag	UNP A0A2S6F0H5
B	-1	GLY	-	expression tag	UNP A0A2S6F0H5
B	0	SER	-	expression tag	UNP A0A2S6F0H5

- Molecule 2 is water.

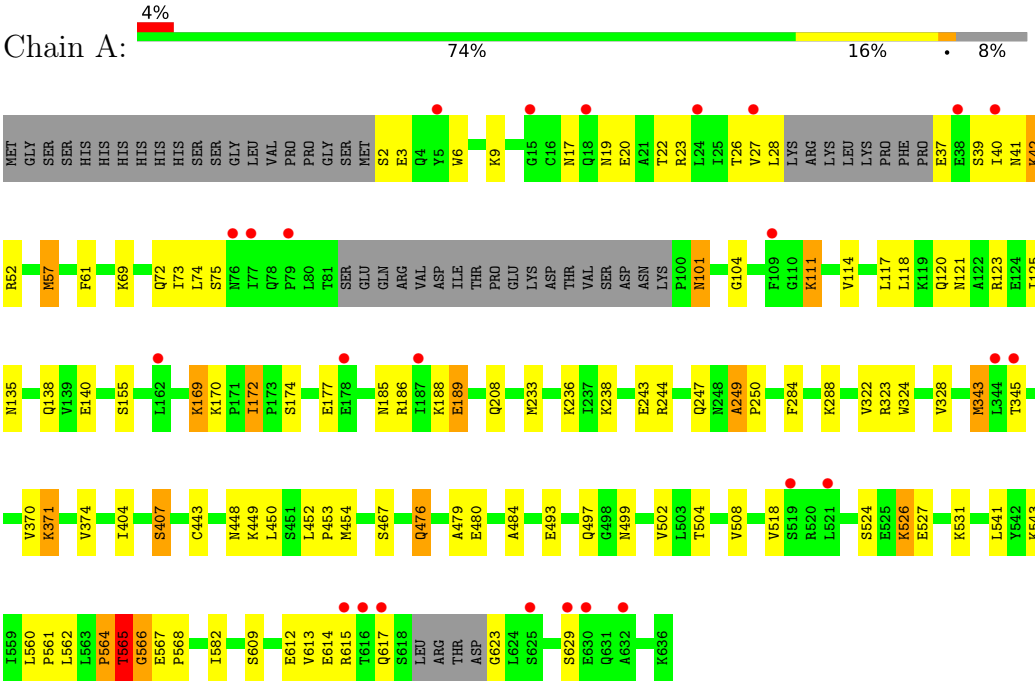
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	265	Total O 265 265	0	0
2	B	275	Total O 275 275	0	0

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 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.

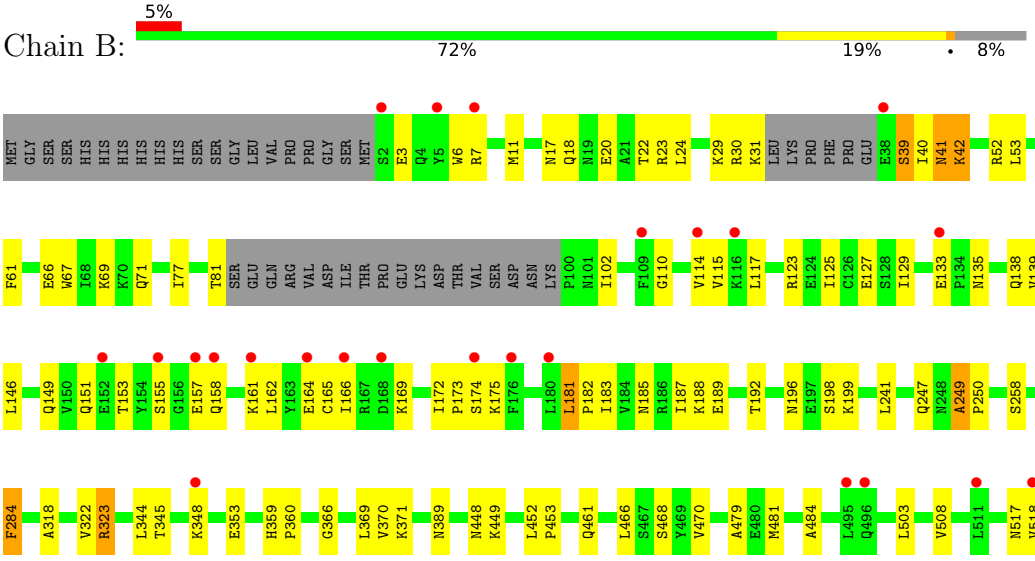
• Molecule 1: Lgt2

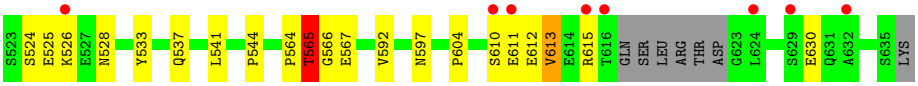
Chain A:



• Molecule 1: Lgt2

Chain B:




S523
S524
E525
K526
E527
N528
Y533
Q537
L541
P544
P564
T565
G566
E567
V592
N597
P604
S610
E611
E612
V613
E614
R615
T616
GLN
SER
LEU
ARG
THR
ASP
G623
L624
S629
E630
Q631
A632
S635
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.18Å 76.01Å 126.58Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	29.22 – 2.27 63.29 – 2.27	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.22-2.27) 95.7 (63.29-2.27)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, R_{free}	0.206 , 0.253 0.208 , 0.253	Depositor DCC
R_{free} test set	2030 reflections (3.05%)	wwPDB-VP
Wilson B-factor (Å^2)	44.2	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l 0.016 for k,h,-l 0.155 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10094	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.55	0/4865	0.61	3/6576 (0.0%)
1	B	0.60	0/4861	0.64	2/6569 (0.0%)
All	All	0.58	0/9726	0.62	5/13145 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	565	THR	CB-CA-C	-7.94	90.17	111.60
1	A	566	GLY	C-N-CA	6.46	137.84	121.70
1	A	623	GLY	N-CA-C	-5.19	100.12	113.10
1	B	461	GLN	CB-CA-C	-5.17	100.05	110.40
1	A	565	THR	CB-CA-C	-5.03	98.03	111.60

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	4779	0	4815	80	0
1	B	4775	0	4822	106	0
2	A	265	0	0	3	0
2	B	275	0	0	4	0
All	All	10094	0	9637	186	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 10.

All (186) 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:249:ALA:HB1	1:A:250:PRO:CD	1.50	1.42
1:A:249:ALA:CB	1:A:250:PRO:CD	1.99	1.39
1:A:249:ALA:CB	1:A:250:PRO:HD2	1.52	1.31
1:B:249:ALA:CB	1:B:250:PRO:CD	2.17	1.23
1:B:249:ALA:HB1	1:B:250:PRO:CD	1.75	1.15
1:A:249:ALA:HB3	1:A:250:PRO:HD2	1.17	1.13
1:B:249:ALA:HB1	1:B:250:PRO:HD3	1.09	1.05
1:B:249:ALA:HB3	1:B:250:PRO:HD2	1.38	1.05
1:A:249:ALA:HB1	1:A:250:PRO:HD3	1.08	1.04
1:A:111:LYS:CD	1:A:169:LYS:HD3	1.89	1.03
1:B:249:ALA:CB	1:B:250:PRO:HD3	1.88	0.98
1:A:111:LYS:HE3	1:A:169:LYS:HD3	1.47	0.97
1:B:249:ALA:CB	1:B:250:PRO:HD2	1.93	0.96
1:A:111:LYS:HD2	1:A:169:LYS:HD3	1.44	0.95
1:A:565:THR:O	1:A:565:THR:HG23	1.67	0.93
1:A:111:LYS:CE	1:A:169:LYS:HD3	1.98	0.92
1:B:42:LYS:H	1:B:42:LYS:HE2	1.36	0.88
1:A:111:LYS:HE3	1:A:169:LYS:CD	2.07	0.84
1:A:6:TRP:CE2	1:A:40:ILE:HD11	2.13	0.84
1:B:17:ASN:OD1	1:B:20:GLU:HG2	1.77	0.83
1:B:162:LEU:O	1:B:166:ILE:HG12	1.82	0.79
1:B:42:LYS:HE2	1:B:42:LYS:N	1.96	0.79
1:A:111:LYS:HE3	1:A:169:LYS:CE	2.16	0.75
1:B:521:LEU:HD23	1:B:521:LEU:N	2.03	0.74
1:B:66:GLU:HA	1:B:69:LYS:HG3	1.72	0.72
1:B:158:GLN:OE1	1:B:161:LYS:HB3	1.91	0.71
1:B:161:LYS:O	1:B:164:GLU:N	2.23	0.70
1:B:611:GLU:N	1:B:611:GLU:OE1	2.24	0.70
1:B:481:MET:HE2	1:B:533:TYR:OH	1.92	0.69
1:B:161:LYS:O	1:B:165:CYS:N	2.23	0.68
1:A:247:GLN:HG3	1:A:345:THR:OG1	1.95	0.66
1:B:452:LEU:HB3	1:B:453:PRO:HD3	1.79	0.65
1:B:517:ASN:O	1:B:521:LEU:HD21	1.96	0.64
1:A:617:GLN:HA	1:A:617:GLN:OE1	1.97	0.64
1:B:66:GLU:HG2	1:B:69:LYS:HE2	1.80	0.64
1:A:612:GLU:O	1:A:615:ARG:HG2	1.99	0.63
1:A:101:ASN:ND2	1:A:104:GLY:H	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:ASN:ND2	1:B:524:SER:H	1.96	0.62
1:B:196:ASN:OD1	1:B:198:SER:N	2.32	0.62
1:B:6:TRP:CE2	1:B:40:ILE:HG21	2.35	0.62
1:B:258:SER:HB2	1:B:284:PHE:HE1	1.66	0.60
1:A:121:ASN:O	1:A:125:ILE:HG13	2.02	0.59
1:B:114:VAL:HG12	1:B:172:ILE:HG22	1.83	0.59
1:B:153:THR:HG21	1:B:183:ILE:HD11	1.84	0.59
1:A:111:LYS:HE3	1:A:169:LYS:HE2	1.85	0.59
1:B:42:LYS:H	1:B:42:LYS:CE	2.12	0.58
1:A:6:TRP:CD2	1:A:40:ILE:HD11	2.37	0.58
1:B:6:TRP:CE2	1:B:40:ILE:CG2	2.87	0.58
1:B:40:ILE:CD1	1:B:40:ILE:H	2.17	0.58
1:A:140:GLU:HG2	1:A:374:VAL:HG23	1.85	0.58
1:A:567:GLU:HG3	1:A:568:PRO:HD2	1.85	0.57
1:B:31:LYS:HG2	1:B:31:LYS:O	2.04	0.57
1:B:449:LYS:N	1:B:449:LYS:HD2	2.19	0.57
1:B:528:ASN:O	1:B:528:ASN:ND2	2.38	0.57
1:B:158:GLN:OE1	1:B:158:GLN:HA	2.04	0.57
1:B:481:MET:HE2	2:B:737:HOH:O	2.05	0.57
1:B:123:ARG:O	1:B:127:GLU:HG3	2.05	0.57
1:B:17:ASN:CG	1:B:20:GLU:HG2	2.24	0.57
1:A:125:ILE:HG23	1:A:188:LYS:HB2	1.87	0.56
1:A:23:ARG:O	1:A:27:VAL:HG12	2.05	0.56
1:B:344:LEU:HD22	1:B:348:LYS:HG2	1.88	0.55
1:B:508:VAL:HG12	1:B:518:VAL:HG22	1.89	0.55
1:A:452:LEU:HB3	1:A:453:PRO:HD3	1.89	0.54
1:B:481:MET:CE	1:B:533:TYR:OH	2.55	0.54
1:A:41:ASN:HD21	1:A:370:VAL:HG13	1.72	0.54
1:A:117:LEU:O	1:A:121:ASN:ND2	2.32	0.54
1:A:443:CYS:HB3	1:A:448:ASN:O	2.08	0.54
1:B:17:ASN:OD1	1:B:20:GLU:CG	2.53	0.54
1:B:102:ILE:HB	1:B:151:GLN:HB2	1.90	0.54
1:B:40:ILE:CD1	1:B:40:ILE:N	2.71	0.53
1:B:348:LYS:O	1:B:348:LYS:HG3	2.07	0.53
1:A:407:SER:OG	1:A:558:GLU:OE2	2.25	0.53
1:B:359:HIS:CG	1:B:360:PRO:HD2	2.43	0.53
1:B:521:LEU:N	1:B:521:LEU:CD2	2.71	0.53
1:A:135:ASN:HB3	1:A:138:GLN:HG3	1.91	0.52
1:A:543:LYS:HB3	1:A:544:PRO:HD3	1.91	0.52
1:B:185:ASN:O	1:B:189:GLU:HG2	2.09	0.52
1:A:42:LYS:N	1:A:42:LYS:CD	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:MET:HE1	1:A:61:PHE:HD1	1.74	0.52
1:A:249:ALA:HB3	1:A:250:PRO:CD	1.98	0.52
1:A:45:GLU:HB2	1:A:371:LYS:HB3	1.91	0.52
1:A:41:ASN:HD21	1:A:370:VAL:CG1	2.23	0.52
1:B:140:GLU:O	1:B:144:ARG:HG3	2.10	0.52
1:B:158:GLN:OE1	1:B:161:LYS:HD2	2.10	0.52
1:B:188:LYS:O	1:B:192:THR:HG23	2.10	0.51
1:A:19:ASN:O	1:A:22:THR:OG1	2.22	0.51
1:B:161:LYS:NZ	1:B:173:PRO:HB3	2.26	0.51
1:B:146:LEU:HD23	1:B:187:ILE:HD12	1.93	0.51
1:A:123:ARG:O	1:A:127:GLU:HG3	2.11	0.50
1:B:318:ALA:O	1:B:322:VAL:HG13	2.10	0.50
1:A:449:LYS:HE3	2:A:792:HOH:O	2.11	0.50
1:B:161:LYS:HZ1	1:B:173:PRO:HB3	1.76	0.50
1:A:37:GLU:C	1:A:39:SER:H	2.15	0.50
1:B:369:LEU:O	1:B:610:SER:HB2	2.11	0.50
1:B:564:PRO:O	1:B:566:GLY:N	2.44	0.50
1:B:57:MET:HE1	1:B:61:PHE:HD2	1.77	0.50
1:A:560:LEU:HB2	1:A:561:PRO:HD3	1.94	0.50
1:A:17:ASN:OD1	1:A:20:GLU:HG2	2.12	0.49
1:B:67:TRP:HE1	1:B:71:GLN:HE21	1.60	0.49
1:B:541:LEU:O	1:B:544:PRO:HD2	2.12	0.49
1:B:110:GLY:HA2	1:B:115:VAL:HG11	1.94	0.49
1:B:522:ASN:OD1	1:B:525:GLU:CD	2.51	0.49
1:A:324:TRP:CE2	1:A:404:ILE:HG21	2.47	0.49
1:A:479:ALA:HB1	1:A:484:ALA:O	2.13	0.49
1:B:162:LEU:HA	1:B:165:CYS:HB3	1.94	0.48
1:B:166:ILE:O	1:B:166:ILE:HG22	2.14	0.48
1:B:52:ARG:HD3	1:B:77:ILE:HG23	1.94	0.48
1:B:613:VAL:HG12	1:B:613:VAL:O	2.14	0.48
1:A:322:VAL:HG13	1:A:328:VAL:HG21	1.94	0.47
1:B:389:ASN:HB2	1:B:592:VAL:HG12	1.95	0.47
1:B:145:LEU:HB3	1:B:187:ILE:HD13	1.95	0.47
1:A:351:LYS:HB3	1:A:351:LYS:HE2	1.63	0.47
1:B:533:TYR:O	1:B:537:GLN:HG2	2.14	0.47
1:A:111:LYS:HD2	1:A:169:LYS:CD	2.31	0.47
1:B:40:ILE:N	1:B:40:ILE:HD12	2.29	0.46
1:B:6:TRP:CD2	1:B:40:ILE:HG21	2.50	0.46
1:A:452:LEU:N	1:A:453:PRO:CD	2.79	0.46
1:B:17:ASN:H	1:B:20:GLU:HG3	1.79	0.46
1:B:196:ASN:HD21	1:B:199:LYS:HG3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:HD12	1:B:117:LEU:O	2.16	0.46
1:B:366:GLY:HA3	1:B:604:PRO:O	2.16	0.46
1:A:541:LEU:O	1:A:545:LEU:HG	2.16	0.46
1:B:149:GLN:O	1:B:153:THR:HG22	2.16	0.46
1:A:57:MET:HE1	1:A:61:PHE:CD1	2.51	0.46
1:A:504:THR:O	1:A:508:VAL:HG23	2.16	0.46
1:B:371:LYS:HE3	1:B:611:GLU:OE2	2.16	0.46
1:B:565:THR:O	1:B:565:THR:OG1	2.23	0.45
1:A:244:ARG:HA	1:A:343:MET:HE1	1.98	0.45
1:B:129:ILE:HG22	1:B:192:THR:CG2	2.46	0.45
1:B:181:LEU:N	1:B:182:PRO:HD2	2.31	0.45
1:B:249:ALA:HB3	1:B:250:PRO:CD	2.02	0.45
1:B:470:VAL:HG21	1:B:503:LEU:HD13	1.98	0.45
1:A:562:LEU:HD11	1:A:582:ILE:HD11	1.99	0.45
1:A:564:PRO:O	1:A:566:GLY:N	2.50	0.45
1:B:612:GLU:O	1:B:615:ARG:HG2	2.18	0.44
1:A:172:ILE:O	1:A:172:ILE:HG13	2.16	0.44
1:A:508:VAL:HG11	1:A:526:LYS:HG2	1.99	0.44
1:B:40:ILE:H	1:B:40:ILE:HD13	1.81	0.44
1:A:233:MET:HG2	1:A:238:LYS:HG3	1.99	0.44
1:B:42:LYS:HE3	1:B:42:LYS:HB2	1.68	0.44
1:A:40:ILE:CD1	1:A:44:PHE:HE2	2.30	0.44
1:A:359:HIS:CG	1:A:360:PRO:HD2	2.53	0.44
1:A:19:ASN:O	1:A:23:ARG:HG3	2.18	0.44
1:A:527:GLU:O	1:A:531:LYS:HG2	2.18	0.44
1:B:135:ASN:HB3	1:B:138:GLN:H	1.83	0.44
1:B:323:ARG:HE	1:B:323:ARG:HB2	1.59	0.44
1:A:476:GLN:O	1:A:480:GLU:HG3	2.18	0.44
1:B:123:ARG:HE	1:B:123:ARG:HB3	1.67	0.44
1:B:353:GLU:OE1	2:B:701:HOH:O	2.20	0.44
1:A:37:GLU:CD	1:A:39:SER:HB2	2.38	0.43
1:A:101:ASN:HD21	1:A:104:GLY:H	1.66	0.43
1:A:120:GLN:OE1	2:A:701:HOH:O	2.21	0.43
1:B:135:ASN:O	1:B:139:VAL:HG13	2.18	0.43
1:B:466:LEU:O	1:B:470:VAL:HG23	2.18	0.43
1:B:39:SER:HA	1:B:42:LYS:NZ	2.34	0.43
1:B:544:PRO:HG3	2:B:906:HOH:O	2.18	0.43
1:B:630:GLU:OE1	1:B:630:GLU:N	2.42	0.43
1:B:247:GLN:OE1	1:B:345:THR:HG23	2.19	0.43
1:B:53:LEU:HD23	1:B:67:TRP:HZ3	1.82	0.43
1:B:174:SER:O	1:B:175:LYS:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:GLU:O	1:A:497:GLN:HG2	2.19	0.42
1:A:3:GLU:HA	1:A:6:TRP:CE3	2.54	0.42
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.83	0.42
1:A:117:LEU:HD21	1:A:177:GLU:HG2	2.01	0.42
1:B:6:TRP:CE2	1:B:40:ILE:HG22	2.55	0.42
1:B:541:LEU:C	1:B:544:PRO:HD2	2.40	0.42
1:B:479:ALA:HB1	1:B:484:ALA:O	2.20	0.42
1:A:567:GLU:N	2:A:734:HOH:O	2.53	0.41
1:B:6:TRP:HZ3	1:B:29:LYS:HZ1	1.68	0.41
1:B:11:MET:SD	1:B:18:GLN:HA	2.59	0.41
1:B:597:ASN:ND2	2:B:702:HOH:O	2.23	0.41
1:A:74:LEU:O	1:A:75:SER:OG	2.27	0.41
1:A:609:SER:O	1:A:613:VAL:HG23	2.20	0.41
1:A:185:ASN:O	1:A:189:GLU:HB3	2.20	0.41
1:A:499:ASN:O	1:A:502:VAL:HG12	2.21	0.41
1:A:288:LYS:HA	1:A:288:LYS:HD3	1.88	0.41
1:A:560:LEU:HD23	1:A:560:LEU:HA	1.89	0.41
1:B:273:TRP:CH2	1:B:279:ILE:HD13	2.56	0.41
1:A:323:ARG:HE	1:A:323:ARG:HB2	1.70	0.41
1:B:41:ASN:OD1	1:B:370:VAL:CG1	2.69	0.41
1:B:125:ILE:HG22	1:B:129:ILE:HD13	2.03	0.40
1:A:450:LEU:HA	1:A:454:MET:HE2	2.02	0.40
1:B:42:LYS:N	1:B:42:LYS:CE	2.73	0.40
1:A:126:CYS:HB3	1:A:134:PRO:HG3	2.04	0.40
1:B:448:ASN:OD1	1:B:448:ASN:N	2.55	0.40
1:A:114:VAL:O	1:A:118:LEU:HG	2.22	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	597/655 (91%)	567 (95%)	27 (4%)	3 (0%)	29	34
1	B	596/655 (91%)	576 (97%)	16 (3%)	4 (1%)	22	25
All	All	1193/1310 (91%)	1143 (96%)	43 (4%)	7 (1%)	25	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	ALA
1	A	565	THR
1	B	249	ALA
1	B	565	THR
1	B	323	ARG
1	A	564	PRO
1	B	613	VAL

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	531/578 (92%)	498 (94%)	33 (6%)	18	23
1	B	530/578 (92%)	508 (96%)	22 (4%)	30	39
All	All	1061/1156 (92%)	1006 (95%)	55 (5%)	23	30

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	9	LYS
1	A	26	THR
1	A	42	LYS
1	A	52	ARG
1	A	57	MET
1	A	69	LYS
1	A	72	GLN
1	A	73	ILE

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Mol	Chain	Res	Type
1	A	101	ASN
1	A	111	LYS
1	A	155	SER
1	A	169	LYS
1	A	170	LYS
1	A	172	ILE
1	A	174	SER
1	A	186	ARG
1	A	189	GLU
1	A	208	GLN
1	A	236	LYS
1	A	243	GLU
1	A	284	PHE
1	A	343	MET
1	A	371	LYS
1	A	407	SER
1	A	467	SER
1	A	476	GLN
1	A	518	VAL
1	A	524	SER
1	A	526	LYS
1	A	565	THR
1	A	614	GLU
1	A	629	SER
1	B	3	GLU
1	B	7	ARG
1	B	22	THR
1	B	23	ARG
1	B	24	LEU
1	B	30	ARG
1	B	39	SER
1	B	41	ASN
1	B	42	LYS
1	B	81	THR
1	B	133	GLU
1	B	155	SER
1	B	157	GLU
1	B	169	LYS
1	B	181	LEU
1	B	241	LEU
1	B	284	PHE
1	B	468	SER

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Mol	Chain	Res	Type
1	B	520	ARG
1	B	521	LEU
1	B	526	LYS
1	B	567	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	41	ASN
1	A	101	ASN
1	A	528	ASN
1	A	631	GLN
1	B	71	GLN
1	B	135	ASN
1	B	522	ASN
1	B	528	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	605/655 (92%)	0.30	26 (4%)	35	40	30, 59, 93, 113	0
1	B	604/655 (92%)	0.33	36 (5%)	21	26	35, 56, 97, 112	0
All	All	1209/1310 (92%)	0.32	62 (5%)	28	33	30, 58, 95, 113	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	PHE	5.4
1	A	632	ALA	4.6
1	B	521	LEU	4.6
1	A	615	ARG	4.2
1	B	157	GLU	4.1
1	B	168	ASP	3.9
1	B	180	LEU	3.8
1	B	496	GLN	3.8
1	B	624	LEU	3.8
1	B	616	THR	3.8
1	B	526	LYS	3.7
1	A	519	SER	3.6
1	B	114	VAL	3.6
1	A	345	THR	3.4
1	A	44	PHE	3.4
1	A	162	LEU	3.3
1	B	5	TYR	3.2
1	B	348	LYS	3.2
1	A	629	SER	3.2
1	A	630	GLU	3.2
1	A	5	TYR	3.1
1	A	76	ASN	3.1
1	B	133	GLU	3.0
1	A	24	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	59	TYR	3.0
1	B	158	GLN	3.0
1	B	164	GLU	3.0
1	A	77	ILE	2.9
1	B	611	GLU	2.7
1	B	155	SER	2.7
1	B	629	SER	2.6
1	B	176	PHE	2.6
1	B	495	LEU	2.6
1	A	79	PRO	2.6
1	B	2	SER	2.5
1	B	519	SER	2.5
1	B	166	ILE	2.5
1	B	632	ALA	2.5
1	A	617	GLN	2.5
1	A	18	GLN	2.4
1	B	615	ARG	2.4
1	B	511	LEU	2.4
1	A	38	GLU	2.4
1	A	27	VAL	2.4
1	B	518	VAL	2.3
1	B	116	LYS	2.3
1	B	174	SER	2.3
1	B	7	ARG	2.3
1	B	520	ARG	2.2
1	B	161	LYS	2.2
1	A	616	THR	2.2
1	A	625	SER	2.2
1	A	187	ILE	2.2
1	B	38	GLU	2.1
1	A	40	ILE	2.1
1	A	178	GLU	2.1
1	A	15	GLY	2.1
1	A	521	LEU	2.1
1	B	610	SER	2.1
1	A	109	PHE	2.1
1	A	344	LEU	2.0
1	B	152	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.