Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:37 PM GMT

PDB ID	:	5CIM
Title	:	Structure of Mycobacterium thermoresistibile GlgE in complex with maltose (cocrystallisation with maltose-1-phosphate) at 3.32A resolution
Authors	:	Mendes, V.; Blaszczyk, M.; Maranha, A.; Empadinhas, N.; Blundell, T.L.
Deposited on	:	2015-07-13
Resolution	:	3.32 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 ①) were used in the production of this report:

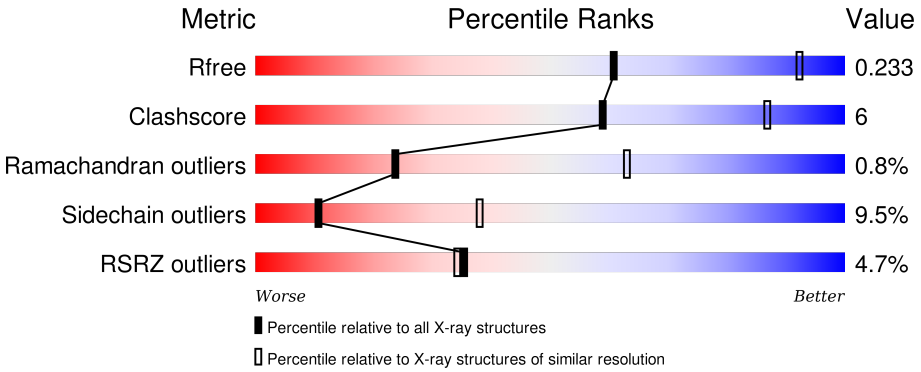
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 3.32 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}	91344	1198 (3.40-3.24)
Clashscore	102246	1280 (3.40-3.24)
Ramachandran outliers	100387	1260 (3.40-3.24)
Sidechain outliers	100360	1259 (3.40-3.24)
RSRZ outliers	91569	1203 (3.40-3.24)

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 <=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	698	5% 72% 18% • 9%
1	B	698	4% 79% 15% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10246 atoms, of which 22 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.

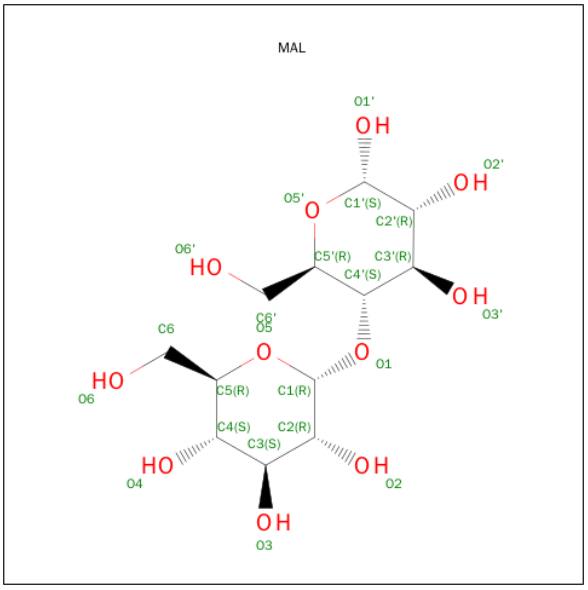
- Molecule 1 is a protein called Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	636	Total	C	N	O	S	0	0	0
			4924	3158	870	887	9			
1	B	675	Total	C	N	O	S	0	0	0
			5211	3347	901	954	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP G7CL00
A	0	SER	-	expression tag	UNP G7CL00
A	1	VAL	-	cloning artifact	UNP G7CL00
B	-1	GLY	-	expression tag	UNP G7CL00
B	0	SER	-	expression tag	UNP G7CL00
B	1	VAL	-	cloning artifact	UNP G7CL00

- Molecule 2 is MALTOSE (three-letter code: MAL) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			45	12	22	11		

- Molecule 3 is water.

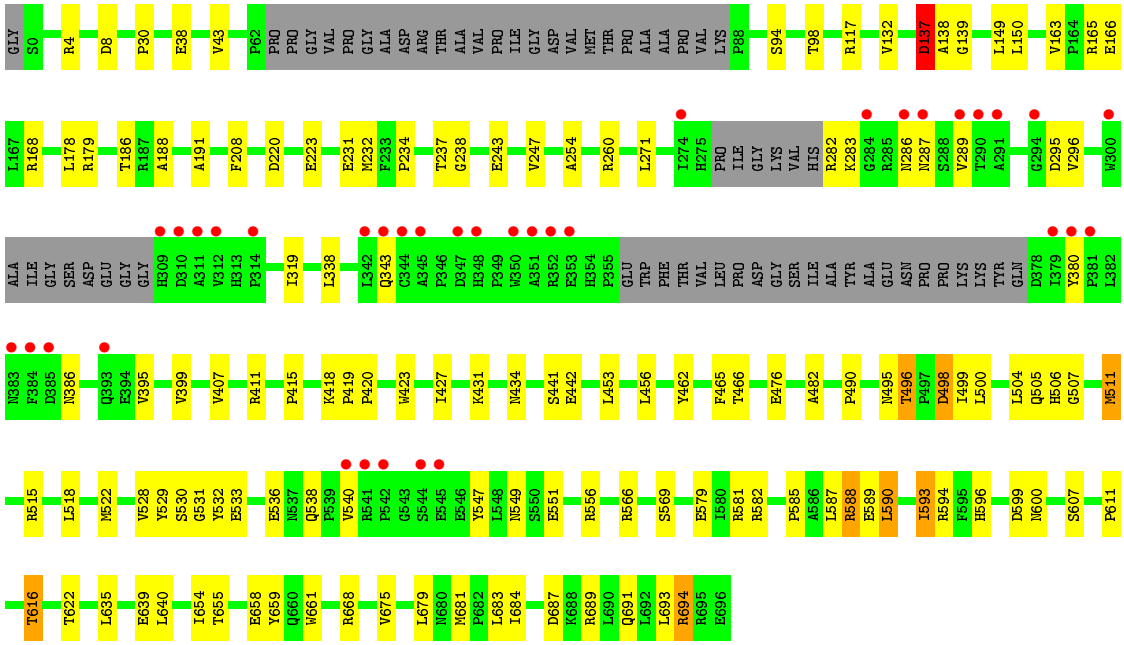
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total	O	0	0
			41	41		
3	B	25	Total	O	0	0
			25	25		

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 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.

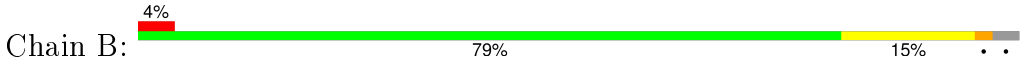
- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase

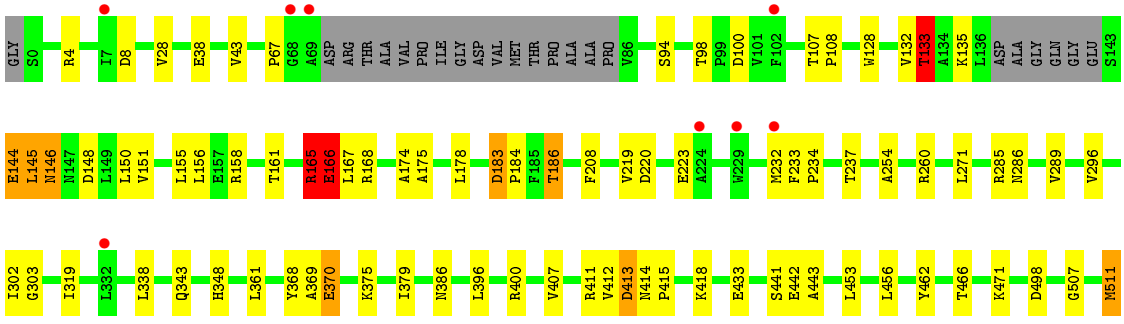
Chain A:

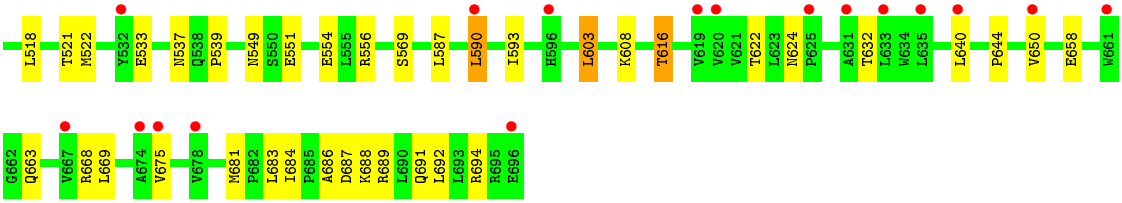


- Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase

Chain B:






L518
T521
N522
Y532
E533
N537
Q538
P539
N549
S550
E551
E554
L555
R556
S569
L587
L590
I593
H596
L603
K608
T616
V619
V620
V621
T622
L623
N624
P625
A631
T632
L633
W634
L635
L640
P644
V650
E658
W661
G662
Q663
V667
R668
L669
A674
V675
V678
M681
P682
L683
I684
P685
A686
D687
K688
R689
L690
Q691
L692
L693
R694
R695
E696

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.54Å 112.97Å 221.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.63 – 3.32 100.63 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.7 (100.63-3.32) 99.7 (100.63-3.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.00 (at 3.33Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, R_{free}	0.178 , 0.214 0.194 , 0.233	Depositor DCC
R_{free} test set	1494 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	94.5	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 94.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 29512 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10246	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAL

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	0.54	0/5071	0.75	1/6940 (0.0%)
1	B	0.52	0/5373	0.77	4/7367 (0.1%)
All	All	0.53	0/10444	0.76	5/14307 (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	A	137	ASP	C-N-CA	6.50	137.95	121.70
1	B	166	GLU	C-N-CA	6.37	137.63	121.70
1	B	133	THR	C-N-CA	6.07	136.86	121.70
1	B	186	THR	C-N-CA	5.92	136.50	121.70
1	B	165	ARG	C-N-CA	5.11	134.48	121.70

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	4924	0	4704	56	0
1	B	5211	0	4953	58	0
2	B	23	22	21	0	0
3	A	41	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	0	1	0
All	All	10224	22	9678	114	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 6.

All (114) 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:133:THR:HA	1:B:135:LYS:H	1.39	0.88
1:A:137:ASP:HB3	1:A:138:ALA:HB3	1.60	0.83
1:A:495:ASN:HD21	1:A:504:LEU:HD13	1.45	0.79
1:B:183:ASP:HB3	1:B:184:PRO:HD2	1.65	0.78
1:B:593:ILE:HG12	1:B:608:LYS:HE2	1.69	0.74
1:A:684:ILE:O	1:A:689:ARG:NH2	2.22	0.72
1:B:174:ALA:O	1:B:178:LEU:HD23	1.90	0.71
1:B:590:LEU:O	1:B:593:ILE:HG13	1.91	0.70
1:B:415:PRO:HG2	1:B:441:SER:HB2	1.76	0.67
1:B:183:ASP:CB	1:B:184:PRO:HD2	2.26	0.66
1:A:684:ILE:HG22	1:A:689:ARG:HB3	1.80	0.64
1:A:163:VAL:O	1:A:168:ARG:HD2	1.98	0.64
1:A:585:PRO:HA	1:A:588:ARG:HE	1.62	0.64
1:A:551:GLU:HG3	1:A:556:ARG:HB2	1.81	0.63
1:B:370:GLU:HG3	1:B:375:LYS:HA	1.82	0.61
1:B:144:GLU:OE2	1:B:145:LEU:HA	2.02	0.60
1:A:581:ARG:HA	1:A:587:LEU:HD12	1.83	0.60
1:B:551:GLU:HG3	1:B:556:ARG:HB2	1.84	0.59
1:A:654:ILE:HG22	1:A:655:THR:HG23	1.85	0.59
1:A:611:PRO:O	1:A:689:ARG:HD2	2.02	0.59
1:B:688:LYS:O	1:B:692:LEU:HG	2.04	0.58
1:A:178:LEU:HD21	1:A:191:ALA:HB2	1.86	0.57
1:B:128:TRP:CE2	1:B:132:VAL:HG21	2.39	0.57
1:B:686:ALA:HA	1:B:689:ARG:HG3	1.87	0.56
1:B:148:ASP:C	1:B:150:LEU:H	2.08	0.56
1:B:640:LEU:HD22	1:B:681:MET:HE2	1.88	0.56
1:B:183:ASP:HB3	1:B:184:PRO:CD	2.35	0.55
1:B:303:GLY:HA3	1:B:348:HIS:CD2	2.42	0.55
1:A:282:ARG:HG2	1:A:283:LYS:H	1.72	0.55
1:B:165:ARG:HA	1:B:168:ARG:HE	1.73	0.53
1:A:234:PRO:HG3	1:A:271:LEU:HD22	1.90	0.53
1:A:415:PRO:HG2	1:A:441:SER:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:GLU:HA	1:A:462:TYR:CD1	2.45	0.51
1:B:234:PRO:HG3	1:B:271:LEU:HD22	1.92	0.50
1:A:616:THR:HB	1:A:681:MET:HB2	1.93	0.50
1:B:400:ARG:HE	1:B:433:GLU:CD	2.15	0.50
1:B:411:ARG:NH1	1:B:413:ASP:OD1	2.45	0.49
1:A:531:GLY:O	1:A:536:GLU:HG2	2.11	0.49
1:B:412:VAL:HG12	1:B:415:PRO:HG3	1.94	0.49
1:B:166:GLU:O	1:B:166:GLU:HG2	2.12	0.49
1:B:132:VAL:O	1:B:132:VAL:HG12	2.13	0.49
1:A:338:LEU:HG	1:A:407:VAL:HG11	1.95	0.49
1:A:482:ALA:HB2	1:A:593:ILE:HG23	1.94	0.48
1:B:442:GLU:HA	1:B:462:TYR:CD1	2.48	0.48
1:B:684:ILE:HG22	1:B:689:ARG:HG2	1.95	0.48
1:B:148:ASP:C	1:B:150:LEU:N	2.67	0.48
1:B:537:ASN:O	1:B:539:PRO:HD3	2.13	0.48
1:B:616:THR:HB	1:B:681:MET:HB2	1.95	0.47
1:A:528:VAL:HG13	1:A:532:TYR:HB3	1.96	0.47
1:A:282:ARG:CG	1:A:283:LYS:H	2.26	0.47
1:B:338:LEU:HG	1:B:407:VAL:HG11	1.96	0.47
1:A:635:LEU:HD22	1:A:640:LEU:HD11	1.96	0.47
1:B:156:LEU:HB2	1:B:175:ALA:HB2	1.96	0.47
1:B:148:ASP:HA	1:B:151:VAL:HG13	1.97	0.47
1:A:237:THR:HG21	1:A:254:ALA:HA	1.97	0.47
1:B:233:PHE:HB2	1:B:551:GLU:OE2	2.15	0.46
1:B:28:VAL:HG22	1:B:107:THR:OG1	2.15	0.46
1:A:165:ARG:HA	1:A:168:ARG:HD3	1.97	0.46
1:A:622:THR:HG22	1:A:675:VAL:O	2.16	0.46
1:B:622:THR:HG22	1:B:675:VAL:O	2.15	0.45
1:B:151:VAL:O	1:B:155:LEU:HG	2.17	0.45
1:B:471:LYS:HE3	1:B:603:LEU:O	2.17	0.45
1:B:237:THR:HG21	1:B:254:ALA:HA	1.99	0.45
1:B:650:VAL:O	1:B:658:GLU:HA	2.16	0.45
1:A:231:GLU:HB3	1:A:529:TYR:HA	1.99	0.45
1:A:500:LEU:HG	1:A:505:GLN:HE21	1.81	0.45
1:B:260:ARG:NH2	1:B:533:GLU:OE2	2.50	0.44
1:B:166:GLU:CG	1:B:166:GLU:O	2.65	0.44
1:B:644:PRO:O	1:B:663:GLN:HB2	2.17	0.44
1:A:507:GLY:HA3	1:A:511:MET:HG2	2.00	0.44
1:B:148:ASP:O	1:B:151:VAL:HG22	2.18	0.44
1:A:590:LEU:O	1:A:593:ILE:HG22	2.18	0.44
1:B:507:GLY:HA3	1:B:511:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:HD21	1:A:191:ALA:CB	2.47	0.43
1:B:396:LEU:HG	1:B:400:ARG:HD2	2.00	0.43
1:B:302:ILE:O	1:B:348:HIS:HD2	2.01	0.43
1:B:286:ASN:HD21	1:B:549:ASN:HA	1.82	0.43
1:A:149:LEU:HD21	1:A:188:ALA:HB2	2.01	0.43
1:B:518:LEU:O	1:B:522:MET:HB2	2.18	0.43
1:A:238:GLY:HA3	1:A:247:VAL:O	2.19	0.43
1:A:593:ILE:O	1:A:594:ARG:NH2	2.52	0.43
1:A:260:ARG:NH1	1:A:533:GLU:OE2	2.52	0.42
1:B:183:ASP:CB	1:B:184:PRO:CD	2.94	0.42
1:A:518:LEU:O	1:A:522:MET:HB2	2.19	0.42
1:B:4:ARG:HG2	1:B:208:PHE:CG	2.54	0.42
1:B:369:ALA:HB3	1:B:379:ILE:HG13	2.00	0.42
1:A:495:ASN:HB3	1:A:499:ILE:O	2.19	0.42
1:A:589:GLU:HG3	1:A:611:PRO:HD2	2.01	0.42
1:A:529:TYR:CZ	1:A:547:TYR:OH	2.67	0.42
1:A:286:ASN:HD21	1:A:549:ASN:HA	1.84	0.42
1:A:453:LEU:HA	1:A:456:LEU:HD12	2.02	0.42
1:A:419:PRO:HA	1:A:420:PRO:HD3	1.87	0.41
1:B:415:PRO:HD2	1:B:443:ALA:HB2	2.02	0.41
1:A:178:LEU:HD22	1:A:188:ALA:HA	2.01	0.41
1:A:490:PRO:CD	1:A:590:LEU:HD11	2.50	0.41
1:A:684:ILE:CG2	1:A:689:ARG:HB3	2.48	0.41
1:A:465:PHE:O	1:A:515:ARG:NH2	2.53	0.41
1:A:30:PRO:HG3	1:A:693:LEU:HG	2.02	0.41
1:A:137:ASP:HB3	1:A:138:ALA:CB	2.42	0.41
1:A:654:ILE:HG22	1:A:655:THR:N	2.35	0.41
1:B:108:PRO:HB2	1:B:219:VAL:HG11	2.03	0.41
1:A:490:PRO:HD3	1:A:590:LEU:HD11	2.01	0.41
1:A:495:ASN:HD21	1:A:504:LEU:CD1	2.25	0.41
1:A:496:THR:C	1:A:498:ASP:H	2.24	0.41
1:B:453:LEU:HA	1:B:456:LEU:HD12	2.02	0.41
1:A:4:ARG:HG2	1:A:208:PHE:CG	2.56	0.41
1:B:603:LEU:HD21	1:B:669:LEU:HD12	2.03	0.41
1:B:144:GLU:HA	1:B:146:ASN:HD22	1.85	0.40
1:A:691:GLN:O	1:A:694:ARG:HB2	2.21	0.40
1:B:624:ASN:HA	3:B:813:HOH:O	2.22	0.40
1:A:395:VAL:O	1:A:399:VAL:HG23	2.21	0.40
1:A:596:HIS:NE2	1:A:607:SER:HB3	2.37	0.40
1:B:521:THR:HA	1:B:587:LEU:HD22	2.03	0.40
1:A:423:TRP:HA	1:A:423:TRP:CE3	2.57	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	626/698 (90%)	589 (94%)	33 (5%)	4 (1%)	30 69
1	B	669/698 (96%)	616 (92%)	47 (7%)	6 (1%)	21 61
All	All	1295/1396 (93%)	1205 (93%)	80 (6%)	10 (1%)	24 63

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	166	GLU
1	B	183	ASP
1	A	694	ARG
1	B	67	PRO
1	B	144	GLU
1	B	165	ARG
1	B	694	ARG
1	A	139	GLY
1	A	600	ASN
1	A	540	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	490/566 (87%)	436 (89%)	54 (11%)	8 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	523/566 (92%)	481 (92%)	42 (8%)	15 49
All	All	1013/1132 (90%)	917 (90%)	96 (10%)	11 38

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	38	GLU
1	A	43	VAL
1	A	94	SER
1	A	98	THR
1	A	117	ARG
1	A	132	VAL
1	A	137	ASP
1	A	150	LEU
1	A	166	GLU
1	A	179	ARG
1	A	186	THR
1	A	220	ASP
1	A	223	GLU
1	A	232	MET
1	A	243	GLU
1	A	287	ASN
1	A	289	VAL
1	A	295	ASP
1	A	296	VAL
1	A	319	ILE
1	A	343	GLN
1	A	380	TYR
1	A	386	ASN
1	A	411	ARG
1	A	418	LYS
1	A	427	ILE
1	A	431	LYS
1	A	434	ASN
1	A	466	THR
1	A	476	GLU
1	A	496	THR
1	A	498	ASP
1	A	506	HIS
1	A	511	MET
1	A	530	SER

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Mol	Chain	Res	Type
1	A	538	GLN
1	A	566	ARG
1	A	569	SER
1	A	579	GLU
1	A	582	ARG
1	A	588	ARG
1	A	590	LEU
1	A	593	ILE
1	A	599	ASP
1	A	616	THR
1	A	639	GLU
1	A	658	GLU
1	A	659	TYR
1	A	661	TRP
1	A	668	ARG
1	A	679	LEU
1	A	683	LEU
1	A	687	ASP
1	B	8	ASP
1	B	38	GLU
1	B	43	VAL
1	B	94	SER
1	B	98	THR
1	B	100	ASP
1	B	133	THR
1	B	145	LEU
1	B	146	ASN
1	B	158	ARG
1	B	161	THR
1	B	166	GLU
1	B	167	LEU
1	B	186	THR
1	B	220	ASP
1	B	223	GLU
1	B	232	MET
1	B	285	ARG
1	B	289	VAL
1	B	296	VAL
1	B	319	ILE
1	B	343	GLN
1	B	361	LEU
1	B	368	TYR

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Mol	Chain	Res	Type
1	B	370	GLU
1	B	386	ASN
1	B	413	ASP
1	B	414	ASN
1	B	418	LYS
1	B	466	THR
1	B	498	ASP
1	B	511	MET
1	B	554	GLU
1	B	569	SER
1	B	590	LEU
1	B	603	LEU
1	B	616	THR
1	B	632	THR
1	B	668	ARG
1	B	683	LEU
1	B	687	ASP
1	B	691	GLN

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

Mol	Chain	Res	Type
1	A	405	HIS
1	A	505	GLN
1	A	538	GLN
1	B	97	HIS
1	B	146	ASN
1	B	343	GLN
1	B	405	HIS
1	B	506	HIS
1	B	680	ASN
1	B	691	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	MAL	B	701	-	24,24,24	1.47	3 (12%)	35,35,35	0.86	1 (2%)

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	MAL	B	701	-	-	0/8/48/48	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	MAL	O5-C5	2.22	1.49	1.44
2	B	701	MAL	O5-C1	2.46	1.48	1.41
2	B	701	MAL	O5'-C1'	4.96	1.52	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	MAL	O1-C4'-C3'	2.07	112.59	107.18

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

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	636/698 (91%)	0.42	36 (5%)	27	26	53, 91, 172, 196	0
1	B	675/698 (96%)	0.35	25 (3%)	45	44	74, 118, 162, 190	0
All	All	1311/1396 (93%)	0.38	61 (4%)	35	34	53, 107, 168, 196	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	380	TYR	6.8
1	A	344	CYS	6.7
1	A	309	HIS	5.7
1	B	68	GLY	5.7
1	A	379	ILE	5.6
1	A	350	TRP	5.4
1	B	633	LEU	4.9
1	A	384	PHE	4.9
1	A	289	VAL	4.7
1	A	300	TRP	4.5
1	B	232	MET	4.2
1	B	590	LEU	4.2
1	A	381	PRO	4.2
1	B	675	VAL	4.1
1	B	667	VAL	4.0
1	A	286	ASN	3.8
1	A	311	ALA	3.7
1	B	631	ALA	3.7
1	A	353	GLU	3.7
1	A	352	ARG	3.7
1	B	635	LEU	3.6
1	A	310	ASP	3.6
1	A	343	GLN	3.5
1	A	291	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	342	LEU	3.4
1	A	348	HIS	3.3
1	B	678	VAL	3.3
1	A	284	GLY	3.3
1	B	102	PHE	3.3
1	B	674	ALA	3.3
1	B	69	ALA	3.2
1	A	540	VAL	3.2
1	B	640	LEU	3.1
1	A	345	ALA	3.0
1	B	224	ALA	3.0
1	A	541	ARG	3.0
1	A	351	ALA	2.9
1	A	347	ASP	2.9
1	B	596	HIS	2.8
1	B	625	PRO	2.8
1	B	532	TYR	2.7
1	A	274	ILE	2.6
1	A	385	ASP	2.6
1	B	661	TRP	2.6
1	B	229	TRP	2.5
1	B	696	GLU	2.4
1	B	619	VAL	2.4
1	A	383	ASN	2.4
1	A	314	PRO	2.3
1	A	393	GLN	2.3
1	A	294	GLY	2.3
1	A	287	ASN	2.3
1	A	544	SER	2.3
1	A	545	GLU	2.2
1	B	620	VAL	2.2
1	B	332	LEU	2.2
1	B	650	VAL	2.1
1	A	312	VAL	2.1
1	A	290	THR	2.1
1	B	7	ILE	2.1
1	A	542	PRO	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MAL	B	701	23/23	0.93	0.18	-0.81	112,116,131,133	0

6.5 Other polymers (i)

There are no such residues in this entry.