



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:47 PM GMT

PDB ID : 1CGW  
Title : SITE DIRECTED MUTATIONS OF THE ACTIVE SITE RESIDUE TYROSINE 195 OF CYCLODEXTRIN GLYCOSYLTRANSFERASE FROM BACILLUS CIRCULANS STRAIN 251 AFFECTING ACTIVITY AND PRODUCT SPECIFICITY  
Authors : Strokopytov, B.V.; Dijkstra, B.W.  
Deposited on : 1994-08-05  
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](mailto: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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

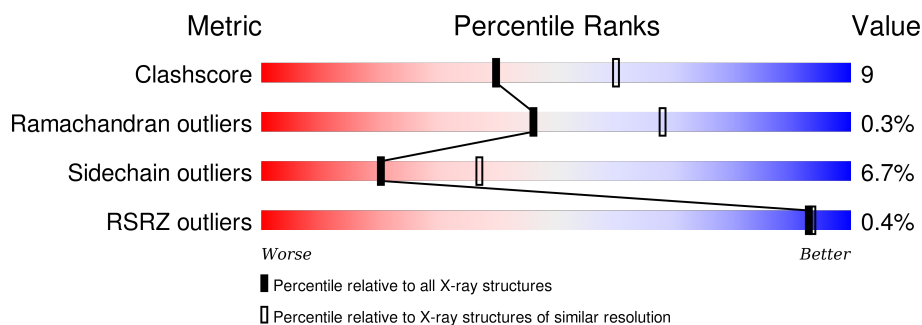
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	686	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAL	A	688	-	-	-	X
2	MAL	A	689	-	-	-	X
2	MAL	A	690	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5506 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.

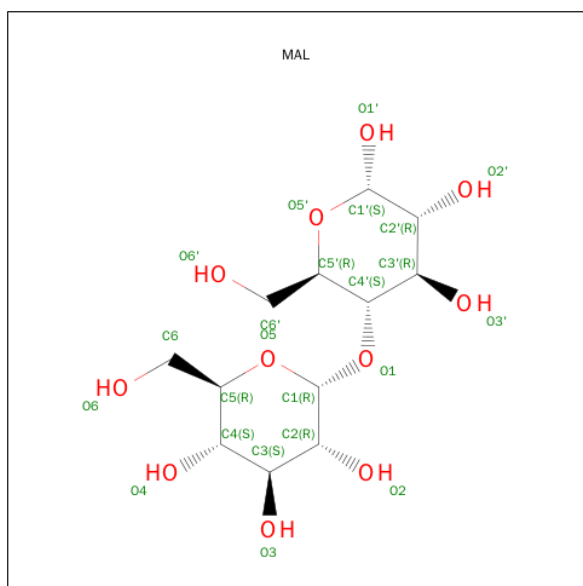
- Molecule 1 is a protein called CYCLOMALTODEXTRIN GLUCANOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	686	5256	3314	900	1026	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	GLY	TYR	ENGINEERED MUTATION	UNP P43379

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		
2	A	1	Total	C	O	0	0
			23	12	11		
2	A	1	Total	C	O	0	0
			23	12	11		

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

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

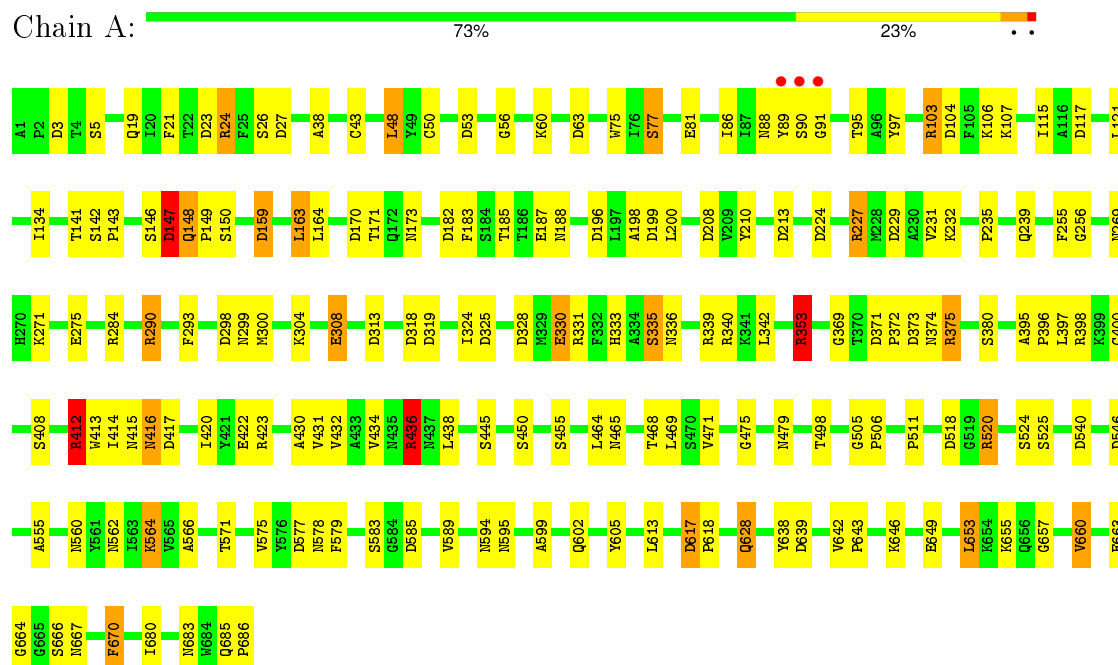
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	179	Total 179	O 179	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.

#### • Molecule 1: CYCLOMALTODEXTRIN GLUCANOTRANSFERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.09 Å   111.18 Å   66.80 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.50 29.34 – 2.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 92.1 (29.34-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.73 (at 2.54 Å)	Xtriage
Refinement program	PROLSQ, TNT	Depositor
R, $R_{free}$	0.160 , (Not available) 0.145 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 74.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 27835 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5506	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: CA, 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	0.74	0/5385	1.41	82/7339 (1.1%)

There are no bond length outliers.

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	ARG	NE-CZ-NH2	-15.19	112.70	120.30
1	A	331	ARG	NE-CZ-NH2	-14.44	113.08	120.30
1	A	196	ASP	CB-CG-OD2	-13.41	106.23	118.30
1	A	290	ARG	NE-CZ-NH1	13.10	126.85	120.30
1	A	196	ASP	CB-CG-OD1	12.24	129.32	118.30
1	A	353	ARG	NE-CZ-NH1	12.15	126.37	120.30
1	A	63	ASP	CB-CG-OD2	-11.77	107.71	118.30
1	A	63	ASP	CB-CG-OD1	11.54	128.69	118.30
1	A	331	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	A	412	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	A	353	ARG	CD-NE-CZ	8.31	135.23	123.60
1	A	375	ARG	NE-CZ-NH1	8.25	124.43	120.30
1	A	104	ASP	CB-CG-OD2	-8.25	110.87	118.30
1	A	147	ASP	CB-CG-OD2	-8.25	110.88	118.30
1	A	328	ASP	CB-CG-OD2	-8.24	110.88	118.30
1	A	585	ASP	CB-CG-OD2	-7.85	111.24	118.30
1	A	617	ASP	CB-CG-OD1	7.79	125.31	118.30
1	A	373	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	A	23	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	A	284	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	A	104	ASP	CB-CG-OD1	7.43	124.98	118.30
1	A	159	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	A	318	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	A	213	ASP	CB-CG-OD1	7.32	124.89	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	213	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	A	436	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	27	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	325	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	290	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	A	540	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	24	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	170	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	A	318	ASP	CB-CG-OD1	6.97	124.57	118.30
1	A	336	ASN	N-CA-CB	-6.90	98.18	110.60
1	A	53	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	27	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	A	208	ASP	CB-CG-OD1	6.65	124.29	118.30
1	A	103	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	A	103	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	A	430	ALA	N-CA-CB	6.53	119.24	110.10
1	A	199	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	A	577	ASP	CB-CG-OD1	6.44	124.10	118.30
1	A	208	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	A	229	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	97	TYR	CB-CG-CD1	-6.21	117.27	121.00
1	A	617	ASP	CB-CG-OD2	-6.21	112.72	118.30
1	A	319	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	A	227	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	23	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	3	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	328	ASP	CB-CG-OD1	5.97	123.68	118.30
1	A	284	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	159	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	398	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	540	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	585	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	319	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	313	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	412	ARG	N-CA-CB	5.74	120.94	110.60
1	A	577	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	199	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	182	ASP	CB-CG-OD2	-5.64	113.23	118.30
1	A	639	ASP	CB-CG-OD1	5.58	123.33	118.30
1	A	373	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	546	ASP	CB-CG-OD2	-5.56	113.30	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	313	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	53	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	117	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	170	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	520	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	224	ASP	CB-CG-OD2	-5.33	113.51	118.30
1	A	518	ASP	CB-CG-OD2	-5.29	113.53	118.30
1	A	182	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	657	GLY	N-CA-C	-5.20	100.09	113.10
1	A	639	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	339	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	298	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	546	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	416	ASN	CB-CA-C	-5.11	100.19	110.40
1	A	564	LYS	CB-CA-C	5.06	120.52	110.40
1	A	638	TYR	CB-CG-CD1	-5.04	117.97	121.00

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	5256	0	5019	91	0
2	A	69	0	66	2	0
3	A	2	0	0	0	0
4	A	179	0	0	3	0
All	All	5506	0	5085	92	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 9.

All (92) 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:88:ASN:HD21	1:A:91:GLY:H	1.01	0.92
1:A:142:SER:HB2	1:A:143:PRO:HD2	1.63	0.81
1:A:88:ASN:HD21	1:A:91:GLY:N	1.80	0.78
1:A:159:ASP:HB2	1:A:164:LEU:HD11	1.68	0.74
1:A:560:ASN:HD21	1:A:578:ASN:HA	1.53	0.74
1:A:643:PRO:HB2	1:A:646:LYS:HG3	1.68	0.74
1:A:594:ASN:HB2	1:A:683:ASN:OD1	1.91	0.70
1:A:163:LEU:HD22	1:A:164:LEU:N	2.07	0.69
1:A:147:ASP:C	1:A:149:PRO:HD3	2.16	0.66
1:A:88:ASN:ND2	1:A:91:GLY:H	1.86	0.66
1:A:333:HIS:HB2	1:A:342:LEU:HD13	1.79	0.64
1:A:304:LYS:O	1:A:308:GLU:HG2	1.98	0.64
1:A:670:PHE:CE2	1:A:680:ILE:HD11	2.33	0.63
1:A:562:ASN:HB3	1:A:575:VAL:HG13	1.82	0.61
1:A:395:ALA:HB3	1:A:396:PRO:HD3	1.82	0.61
1:A:227:ARG:HG2	1:A:255:PHE:CE2	2.36	0.60
1:A:589:VAL:HG11	1:A:680:ILE:HD11	1.83	0.59
1:A:560:ASN:ND2	1:A:578:ASN:HA	2.15	0.59
1:A:81:GLU:OE1	1:A:103:ARG:HD3	2.02	0.59
1:A:471:VAL:CG1	1:A:475:GLY:HA2	2.32	0.59
1:A:653:LEU:HD12	1:A:660:VAL:CG2	2.34	0.58
1:A:142:SER:HB2	1:A:143:PRO:CD	2.33	0.57
1:A:445:SER:HB3	1:A:479:ASN:ND2	2.21	0.55
1:A:141:THR:OG1	1:A:198:ALA:HB3	2.07	0.55
1:A:670:PHE:CZ	1:A:680:ILE:HD11	2.41	0.54
1:A:653:LEU:N	1:A:653:LEU:HD23	2.22	0.54
1:A:422:GLU:HG3	1:A:431:VAL:HG22	1.90	0.54
1:A:121:LEU:HD12	1:A:121:LEU:O	2.07	0.54
1:A:353:ARG:HD2	4:A:1044:HOH:O	2.08	0.53
1:A:185:THR:OG1	1:A:188:ASN:HB2	2.09	0.52
1:A:38:ALA:O	1:A:48:LEU:HB3	2.09	0.52
1:A:148:GLN:N	1:A:149:PRO:HD3	2.23	0.52
1:A:520:ARG:HG2	1:A:520:ARG:HH11	1.75	0.51
1:A:232:LYS:HG2	1:A:232:LYS:O	2.10	0.51
1:A:642:VAL:HB	1:A:643:PRO:HD2	1.93	0.51
1:A:589:VAL:HG11	1:A:680:ILE:CD1	2.41	0.50
1:A:599:ALA:O	1:A:602:GLN:HB3	2.12	0.50
1:A:663:GLU:HG2	1:A:685:GLN:O	2.12	0.50
1:A:566:ALA:HA	1:A:571:THR:O	2.11	0.50
1:A:417:ASP:O	1:A:436:ARG:HG3	2.11	0.50
1:A:414:ILE:HG12	1:A:415:ASN:N	2.26	0.49
1:A:232:LYS:HB3	4:A:1166:HOH:O	2.12	0.49

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:LEU:HA	1:A:400:CYS:SG	2.53	0.48
1:A:649:GLU:OE1	1:A:667:ASN:HB2	2.13	0.48
1:A:271:LYS:O	1:A:275:GLU:HG3	2.14	0.48
1:A:333:HIS:HB2	1:A:342:LEU:CD1	2.44	0.47
1:A:562:ASN:HB3	1:A:575:VAL:CG1	2.44	0.47
1:A:408:SER:O	1:A:423:ARG:HA	2.14	0.47
1:A:468:THR:HG22	1:A:469:LEU:N	2.29	0.47
1:A:445:SER:CB	1:A:479:ASN:ND2	2.78	0.47
1:A:300:MET:HB2	1:A:415:ASN:O	2.14	0.47
1:A:420:ILE:HA	1:A:432:VAL:O	2.14	0.47
1:A:19:GLN:HG3	1:A:75:TRP:CD2	2.49	0.47
1:A:605:TYR:CE1	1:A:655:LYS:HB2	2.50	0.47
1:A:664:GLY:O	1:A:685:GLN:HB2	2.15	0.47
1:A:511:PRO:HB3	1:A:555:ALA:HA	1.98	0.46
1:A:653:LEU:HD12	1:A:660:VAL:HG21	1.97	0.46
1:A:187:GLU:CD	1:A:628:GLN:HG2	2.36	0.46
1:A:293:PHE:HE1	1:A:434:VAL:HG11	1.80	0.46
1:A:235:PRO:O	1:A:239:GLN:HG3	2.16	0.46
1:A:340:ARG:O	1:A:340:ARG:HG3	2.15	0.46
1:A:617:ASP:OD1	1:A:618:PRO:HD2	2.16	0.46
1:A:506:PRO:O	1:A:579:PHE:HE1	2.00	0.45
1:A:227:ARG:CG	1:A:255:PHE:CE2	3.00	0.45
1:A:148:GLN:N	1:A:149:PRO:CD	2.79	0.45
1:A:374:ASN:OD1	1:A:375:ARG:HD3	2.17	0.45
1:A:505:GLY:HA2	1:A:506:PRO:C	2.38	0.44
1:A:24:ARG:HD2	1:A:375:ARG:O	2.17	0.44
1:A:77:SER:HB3	4:A:1021:HOH:O	2.17	0.44
1:A:48:LEU:HD12	1:A:95:THR:HG23	1.99	0.44
1:A:330:GLU:HB3	1:A:369:GLY:HA2	2.00	0.44
1:A:106:LYS:HD2	1:A:210:TYR:HE1	1.83	0.43
2:A:690:MAL:H6'2	2:A:690:MAL:C5	2.48	0.43
1:A:371:ASP:OD1	1:A:372:PRO:HA	2.17	0.43
1:A:685:GLN:HA	1:A:686:PRO:HD3	1.89	0.43
1:A:464:LEU:O	1:A:465:ASN:HB2	2.20	0.42
1:A:395:ALA:N	1:A:396:PRO:CD	2.82	0.42
1:A:290:ARG:NH2	1:A:330:GLU:O	2.53	0.42
1:A:227:ARG:HG2	1:A:255:PHE:CD2	2.54	0.42
1:A:106:LYS:HD2	1:A:210:TYR:CE1	2.55	0.42
1:A:413:TRP:O	1:A:414:ILE:HB	2.19	0.42
1:A:89:TYR:O	1:A:90:SER:HB2	2.18	0.41
1:A:231:VAL:HG11	1:A:256:GLY:HA3	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:CYS:HB2	1:A:50:CYS:HB3	1.86	0.41
1:A:60:LYS:HD2	1:A:60:LYS:HA	1.70	0.41
1:A:299:ASN:HB2	1:A:416:ASN:O	2.21	0.41
1:A:583:SER:HB2	1:A:643:PRO:HG3	2.03	0.41
1:A:417:ASP:OD1	1:A:436:ARG:HD2	2.21	0.41
1:A:134:ILE:O	1:A:134:ILE:HG13	2.20	0.41
1:A:26:SER:O	1:A:56:GLY:HA3	2.21	0.40
1:A:200:LEU:HA	1:A:200:LEU:HD23	1.92	0.40
1:A:412:ARG:O	2:A:688:MAL:H1	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	684/686 (100%)	645 (94%)	37 (5%)	2 (0%)	46 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	SER
1	A	183	PHE

### 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	555/555 (100%)	518 (93%)	37 (7%)	20	37

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	21	PHE
1	A	48	LEU
1	A	77	SER
1	A	86	ILE
1	A	107	LYS
1	A	115	ILE
1	A	146	SER
1	A	147	ASP
1	A	148	GLN
1	A	150	SER
1	A	163	LEU
1	A	171	THR
1	A	173	ASN
1	A	269	ASN
1	A	308	GLU
1	A	324	ILE
1	A	330	GLU
1	A	335	SER
1	A	353	ARG
1	A	380	SER
1	A	412	ARG
1	A	436	ARG
1	A	438	LEU
1	A	450	SER
1	A	455	SER
1	A	498	THR
1	A	524	SER
1	A	525	SER
1	A	564	LYS
1	A	595	ASN
1	A	613	LEU
1	A	628	GLN
1	A	653	LEU
1	A	660	VAL
1	A	666	SER
1	A	670	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	62	ASN
1	A	88	ASN
1	A	94	ASN
1	A	119	GLN
1	A	120	ASN
1	A	269	ASN
1	A	410	GLN
1	A	416	ASN
1	A	479	ASN
1	A	560	ASN
1	A	685	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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	MAL	A	688	-	24,24,24	0.40	0	35,35,35	1.22	2 (5%)
2	MAL	A	689	-	24,24,24	0.40	0	35,35,35	1.37	4 (11%)
2	MAL	A	690	-	24,24,24	0.33	0	35,35,35	1.20	3 (8%)

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	A	688	-	-	0/8/48/48	0/2/2/2
2	MAL	A	689	-	-	0/8/48/48	0/2/2/2
2	MAL	A	690	-	-	0/8/48/48	0/2/2/2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	688	MAL	C1-C2-C3	-3.08	103.91	109.97
2	A	689	MAL	O2-C2-C3	-2.62	104.43	110.34
2	A	688	MAL	O2-C2-C3	-2.22	105.33	110.34
2	A	689	MAL	O1-C1-O5	-2.11	105.33	110.68
2	A	689	MAL	O5-C1-C2	2.37	115.14	110.28
2	A	690	MAL	C1-O5-C5	2.62	118.82	113.75
2	A	690	MAL	O5-C1-C2	2.92	116.27	110.28
2	A	690	MAL	O5'-C1'-C2'	2.93	114.46	109.80
2	A	689	MAL	O5'-C1'-C2'	4.08	116.31	109.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	688	MAL	1	0
2	A	690	MAL	1	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	686/686 (100%)	-0.64	3 (0%) 93 93	9, 22, 43, 81	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	91	GLY	2.9
1	A	90	SER	2.8
1	A	89	TYR	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	MAL	A	690	23/23	0.65	0.59	9.67	91,96,100,100	0
2	MAL	A	689	23/23	0.85	0.21	6.77	48,52,57,63	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAL	A	688	23/23	0.91	0.14	3.45	18,26,30,32	0
3	CA	A	691	1/1	0.98	0.07	-1.36	22,22,22,22	0
3	CA	A	692	1/1	0.99	0.07	-1.69	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.