



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:33 PM GMT

PDB ID : 3ZT5  
Title : GLGE ISOFORM 1 FROM STREPTOMYCES COELICOLOR WITH MALTOSE BOUND  
Authors : Syson, K.; Stevenson, C.E.M.; Rejzek, M.; Fairhurst, S.A.; Nair, A.; Bruton, C.J.; Field, R.A.; Chater, K.F.; Lawson, D.M.; Bornemann, S.  
Deposited on : 2011-07-01  
Resolution : 2.09 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.

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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 : 1.7 (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

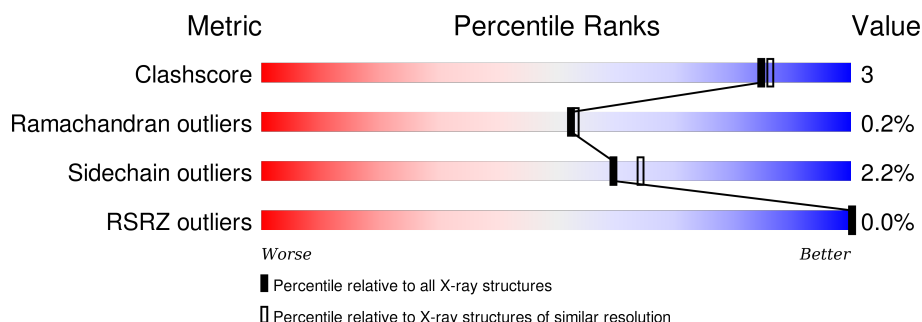
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	695	
1	B	695	
1	C	695	
1	D	695	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20964 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 PUTATIVE GLUCANOHYDROLASE PEP1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	0	0
			5101	3227	919	945	10			
1	B	649	Total	C	N	O	S	0	0	0
			5090	3221	913	946	10			
1	C	649	Total	C	N	O	S	0	0	0
			5098	3227	918	943	10			
1	D	649	Total	C	N	O	S	0	0	0
			5097	3224	918	945	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q9L1K2
A	-18	GLY	-	EXPRESSION TAG	UNP Q9L1K2
A	-17	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	-16	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	-15	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-14	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-13	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-12	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-11	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-10	HIS	-	EXPRESSION TAG	UNP Q9L1K2
A	-9	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	-8	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	-7	GLY	-	EXPRESSION TAG	UNP Q9L1K2
A	-6	LEU	-	EXPRESSION TAG	UNP Q9L1K2
A	-5	VAL	-	EXPRESSION TAG	UNP Q9L1K2
A	-4	PRO	-	EXPRESSION TAG	UNP Q9L1K2
A	-3	ARG	-	EXPRESSION TAG	UNP Q9L1K2
A	-2	GLY	-	EXPRESSION TAG	UNP Q9L1K2
A	-1	SER	-	EXPRESSION TAG	UNP Q9L1K2
A	0	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-19	MET	-	EXPRESSION TAG	UNP Q9L1K2

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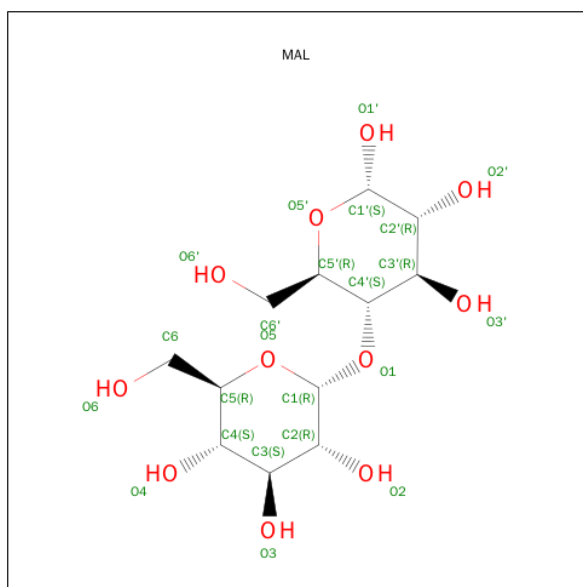
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP Q9L1K2
B	-17	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	-16	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	-15	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-14	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-13	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-12	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-11	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-10	HIS	-	EXPRESSION TAG	UNP Q9L1K2
B	-9	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	-8	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	-7	GLY	-	EXPRESSION TAG	UNP Q9L1K2
B	-6	LEU	-	EXPRESSION TAG	UNP Q9L1K2
B	-5	VAL	-	EXPRESSION TAG	UNP Q9L1K2
B	-4	PRO	-	EXPRESSION TAG	UNP Q9L1K2
B	-3	ARG	-	EXPRESSION TAG	UNP Q9L1K2
B	-2	GLY	-	EXPRESSION TAG	UNP Q9L1K2
B	-1	SER	-	EXPRESSION TAG	UNP Q9L1K2
B	0	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-19	MET	-	EXPRESSION TAG	UNP Q9L1K2
C	-18	GLY	-	EXPRESSION TAG	UNP Q9L1K2
C	-17	SER	-	EXPRESSION TAG	UNP Q9L1K2
C	-16	SER	-	EXPRESSION TAG	UNP Q9L1K2
C	-15	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-14	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-13	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-12	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-11	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-10	HIS	-	EXPRESSION TAG	UNP Q9L1K2
C	-9	SER	-	EXPRESSION TAG	UNP Q9L1K2
C	-8	SER	-	EXPRESSION TAG	UNP Q9L1K2
C	-7	GLY	-	EXPRESSION TAG	UNP Q9L1K2
C	-6	LEU	-	EXPRESSION TAG	UNP Q9L1K2
C	-5	VAL	-	EXPRESSION TAG	UNP Q9L1K2
C	-4	PRO	-	EXPRESSION TAG	UNP Q9L1K2
C	-3	ARG	-	EXPRESSION TAG	UNP Q9L1K2
C	-2	GLY	-	EXPRESSION TAG	UNP Q9L1K2
C	-1	SER	-	EXPRESSION TAG	UNP Q9L1K2
C	0	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-19	MET	-	EXPRESSION TAG	UNP Q9L1K2
D	-18	GLY	-	EXPRESSION TAG	UNP Q9L1K2
D	-17	SER	-	EXPRESSION TAG	UNP Q9L1K2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP Q9L1K2
D	-15	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-14	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-13	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-12	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-11	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-10	HIS	-	EXPRESSION TAG	UNP Q9L1K2
D	-9	SER	-	EXPRESSION TAG	UNP Q9L1K2
D	-8	SER	-	EXPRESSION TAG	UNP Q9L1K2
D	-7	GLY	-	EXPRESSION TAG	UNP Q9L1K2
D	-6	LEU	-	EXPRESSION TAG	UNP Q9L1K2
D	-5	VAL	-	EXPRESSION TAG	UNP Q9L1K2
D	-4	PRO	-	EXPRESSION TAG	UNP Q9L1K2
D	-3	ARG	-	EXPRESSION TAG	UNP Q9L1K2
D	-2	GLY	-	EXPRESSION TAG	UNP Q9L1K2
D	-1	SER	-	EXPRESSION TAG	UNP Q9L1K2
D	0	HIS	-	EXPRESSION TAG	UNP Q9L1K2

- Molecule 2 is SUGAR (MALTOSE) (three-letter code: MAL) (formula: C<sub>12</sub>H<sub>22</sub>O<sub>11</sub>).



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

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

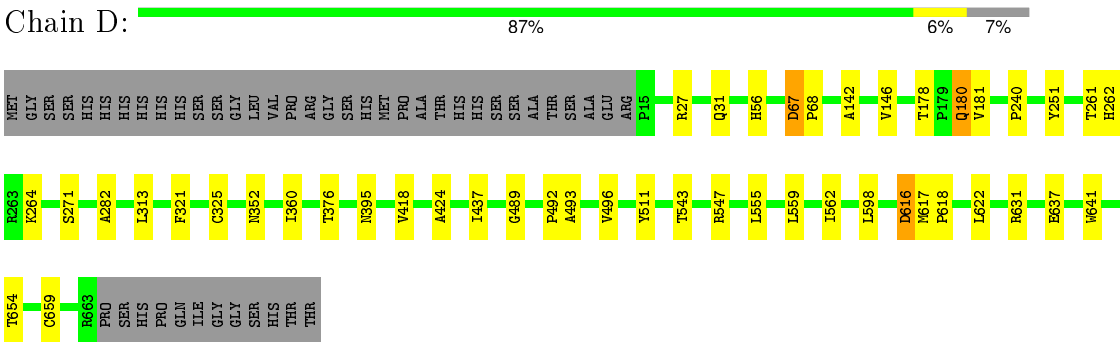
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	137	Total	O	0	0
			137	137		
3	B	118	Total	O	0	0
			118	118		
3	C	126	Total	O	0	0
			126	126		
3	D	105	Total	O	0	0
			105	105		



● Molecule 1: PUTATIVE GLUCANOHYDROLASE PEP1A







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.82Å 113.57Å 315.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.01 – 2.09 56.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (56.01-2.09) 98.7 (56.01-2.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0101	Depositor
R, $R_{free}$	0.204 , 0.228 (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 8.6	EDS
Estimated twinning fraction	0.516 for H, K, L 0.484 for K, H, -L 0.466 for k,h,-l	Xtriage
Reported twinning fraction	0.516 for H, K, L 0.484 for K, H, -L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.16$	Xtriage
Outliers	0 of 236803 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	20964	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.70	0/5253	0.75	4/7190 (0.1%)
1	B	0.69	1/5241 (0.0%)	0.75	1/7174 (0.0%)
1	C	0.72	0/5250	0.76	1/7186 (0.0%)
1	D	0.70	2/5249 (0.0%)	0.76	3/7185 (0.0%)
All	All	0.70	3/20993 (0.0%)	0.75	9/28735 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	325	CYS	CB-SG	-5.66	1.72	1.81
1	B	484	ALA	CA-CB	5.17	1.63	1.52
1	D	418	VAL	CB-CG1	5.08	1.63	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	67	ASP	CB-CG-OD1	6.83	124.44	118.30
1	B	67	ASP	CB-CG-OD1	6.57	124.21	118.30
1	A	67	ASP	CB-CG-OD1	6.48	124.14	118.30
1	D	555	LEU	CB-CG-CD2	-6.41	100.10	111.00
1	D	67	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	130	LEU	CB-CG-CD2	-6.16	100.53	111.00
1	D	27	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	137	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	87	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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	5101	0	4910	35	0
1	B	5090	0	4889	23	0
1	C	5098	0	4905	33	0
1	D	5097	0	4896	25	0
2	A	23	0	22	1	0
2	B	23	0	22	5	0
2	C	23	0	22	2	0
2	D	23	0	22	1	0
3	A	137	0	0	2	0
3	B	118	0	0	2	0
3	C	126	0	0	4	0
3	D	105	0	0	2	0
All	All	20964	0	19688	115	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 3.

All (115) 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:395:ASN:HD21	2:B:701:MAL:C1'	1.75	0.97
1:A:628:VAL:HG13	1:A:629:PRO:HD2	1.53	0.90
1:C:319:LEU:HD22	3:C:2064:HOH:O	1.82	0.79
1:B:82:ALA:HB3	1:B:85:THR:HG21	1.65	0.78
1:A:555:LEU:O	1:A:555:LEU:HD12	1.88	0.74
1:B:395:ASN:HD21	2:B:701:MAL:H1'	1.55	0.71
1:D:178:THR:OG1	1:D:181:VAL:HG23	1.91	0.69
1:C:617:MET:CE	1:C:622:LEU:HD12	2.23	0.69
1:B:395:ASN:ND2	2:B:701:MAL:O5'	2.26	0.68
1:A:395:ASN:ND2	2:A:701:MAL:O5'	2.26	0.67
1:B:395:ASN:ND2	2:B:701:MAL:C1'	2.56	0.65
1:D:178:THR:HB	1:D:180:GLN:HE21	1.62	0.65
1:A:18:VAL:HG12	1:A:19:GLY:O	1.98	0.64
1:C:480:ASP:OD2	2:C:701:MAL:O2'	2.17	0.63
1:D:395:ASN:HD21	2:D:701:MAL:C1'	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:514:TYR:HA	3:C:2103:HOH:O	1.97	0.63
1:C:617:MET:HE1	1:C:622:LEU:HD12	1.84	0.59
1:A:437:ILE:HD12	1:A:437:ILE:C	2.23	0.58
1:B:82:ALA:HB3	1:B:85:THR:CG2	2.34	0.58
1:C:482:LEU:HD22	1:C:529:TYR:CD2	2.40	0.56
1:A:482:LEU:HD22	1:A:529:TYR:CD2	2.41	0.56
1:C:617:MET:HE3	1:C:617:MET:HA	1.88	0.55
1:B:437:ILE:HD12	1:B:437:ILE:C	2.28	0.54
1:D:424:ALA:HB3	3:D:2076:HOH:O	2.08	0.54
1:A:255:ILE:HD12	1:A:293:ILE:CD1	2.38	0.53
1:A:377:VAL:HG23	3:A:2094:HOH:O	2.09	0.53
1:A:555:LEU:C	1:A:555:LEU:HD12	2.28	0.53
1:C:582:LYS:NZ	1:C:610:GLU:O	2.30	0.53
1:A:180:GLN:O	1:A:184:VAL:HG23	2.09	0.52
1:A:628:VAL:HG13	1:A:629:PRO:CD	2.35	0.52
1:C:458:TYR:CE2	1:C:462:LEU:HD11	2.45	0.52
1:A:452:LYS:NZ	1:A:582:LYS:O	2.41	0.51
1:B:395:ASN:ND2	2:B:701:MAL:H1'	2.22	0.51
1:C:482:LEU:HD22	1:C:529:TYR:CE2	2.46	0.50
1:C:600:VAL:O	1:C:656:ALA:HB1	2.11	0.50
1:A:421:LEU:HD11	1:A:443:TYR:CD1	2.46	0.50
1:D:437:ILE:HD12	1:D:437:ILE:C	2.32	0.49
1:D:598:LEU:HD23	1:D:641:TRP:HZ3	1.77	0.49
1:D:178:THR:HB	1:D:180:GLN:NE2	2.28	0.49
1:B:489:GLY:HA3	1:B:493:ALA:HB2	1.94	0.49
1:B:67:ASP:HB2	1:B:68:PRO:CD	2.43	0.49
1:C:282:ALA:HA	1:C:360:ILE:CG2	2.42	0.49
1:D:489:GLY:HA3	1:D:493:ALA:HB2	1.95	0.48
1:A:437:ILE:HD12	1:A:438:GLY:N	2.29	0.48
1:A:255:ILE:HD12	1:A:293:ILE:HD13	1.95	0.48
1:A:427:ARG:HB2	3:A:2100:HOH:O	2.13	0.48
1:B:495:GLU:O	1:B:499:VAL:HG23	2.14	0.48
1:C:437:ILE:C	1:C:437:ILE:HD12	2.34	0.47
1:D:598:LEU:HD23	1:D:641:TRP:CZ3	2.49	0.47
1:B:142:ALA:O	1:B:146:VAL:HG23	2.14	0.47
1:C:631:ARG:O	1:C:659:CYS:HA	2.15	0.47
1:D:492:PRO:O	1:D:496:VAL:HG23	2.14	0.47
1:D:180:GLN:NE2	1:D:180:GLN:H	2.12	0.47
1:A:623:ASP:HB3	1:A:625:HIS:CE1	2.50	0.47
1:C:395:ASN:ND2	2:C:701:MAL:O5'	2.49	0.46
1:D:261:THR:HG22	1:D:262:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:543:THR:HG23	3:D:2100:HOH:O	2.15	0.46
1:D:67:ASP:HB2	1:D:68:PRO:CD	2.45	0.46
1:A:631:ARG:O	1:A:659:CYS:HA	2.15	0.46
1:C:38:LYS:NZ	1:C:439:PHE:O	2.48	0.46
1:C:67:ASP:HB2	1:C:68:PRO:CD	2.46	0.46
1:B:220:ARG:O	1:B:537:LEU:HD22	2.15	0.46
1:C:82:ALA:HB3	1:C:85:THR:HG21	1.97	0.46
1:C:617:MET:N	1:C:618:PRO:CD	2.79	0.46
1:A:617:MET:N	1:A:618:PRO:CD	2.79	0.46
1:D:180:GLN:H	1:D:180:GLN:CD	2.20	0.45
1:D:631:ARG:O	1:D:659:CYS:HA	2.17	0.45
1:A:67:ASP:HB2	1:A:68:PRO:CD	2.46	0.45
1:C:489:GLY:HA3	1:C:493:ALA:HB2	1.99	0.45
1:A:482:LEU:HD22	1:A:529:TYR:CE2	2.53	0.44
1:B:180:GLN:O	1:B:184:VAL:HG23	2.17	0.44
1:C:251:TYR:HE1	1:C:320:ASP:HB2	1.82	0.44
1:B:35:ARG:NH1	3:B:2008:HOH:O	2.42	0.44
1:A:142:ALA:O	1:A:146:VAL:HG23	2.17	0.44
1:B:617:MET:N	1:B:618:PRO:CD	2.81	0.44
1:B:631:ARG:O	1:B:659:CYS:HA	2.17	0.44
1:A:437:ILE:CD1	1:A:437:ILE:C	2.86	0.43
1:B:423:GLU:HA	1:B:443:TYR:CD1	2.53	0.43
1:A:499:VAL:HG22	1:A:559:LEU:HD21	1.99	0.43
1:C:575:LEU:HD22	3:C:2109:HOH:O	2.19	0.43
1:C:504:LEU:HD23	1:C:504:LEU:HA	1.86	0.43
1:D:67:ASP:HB2	1:D:68:PRO:HD2	2.01	0.43
1:C:114:TRP:CZ2	1:C:135:GLY:HA3	2.54	0.43
1:A:424:ALA:O	1:A:431:MET:HE2	2.19	0.43
1:B:532:SER:HA	3:B:2107:HOH:O	2.19	0.43
1:A:421:LEU:HD21	1:A:443:TYR:CE1	2.54	0.42
1:A:397:HIS:H	1:A:397:HIS:CD2	2.38	0.42
1:D:142:ALA:O	1:D:146:VAL:HG23	2.20	0.42
1:A:631:ARG:HB2	1:A:662:LEU:HD21	2.01	0.42
1:D:559:LEU:HA	1:D:562:ILE:HD12	2.00	0.42
1:A:251:TYR:HE1	1:A:320:ASP:HB2	1.84	0.42
1:C:598:LEU:HD21	1:C:615:LEU:HD21	2.02	0.42
1:D:617:MET:HE3	1:D:622:LEU:HB2	2.00	0.42
1:D:240:PRO:HA	1:D:313:LEU:HD13	2.02	0.41
1:B:51:VAL:HG13	1:B:106:ALA:HB1	2.02	0.41
1:C:352:ASN:HA	1:D:56:HIS:NE2	2.35	0.41
1:A:261:THR:HG22	1:A:262:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:PHE:HA	1:A:509:GLY:O	2.21	0.41
1:C:617:MET:CE	1:C:622:LEU:CD1	2.96	0.41
1:B:67:ASP:HB2	1:B:68:PRO:HD2	2.01	0.41
1:C:53:ARG:NH1	3:C:2020:HOH:O	2.52	0.41
1:A:36:PRO:HA	1:A:201:PRO:HG2	2.03	0.41
1:B:459:LEU:HD13	1:B:459:LEU:HA	1.90	0.41
1:C:121:LYS:HD3	1:C:126:LEU:HD23	2.03	0.41
1:A:628:VAL:HG12	1:A:661:VAL:HG13	2.03	0.41
1:C:67:ASP:HB2	1:C:68:PRO:HD2	2.03	0.41
1:A:489:GLY:HA3	1:A:493:ALA:HB2	2.01	0.41
1:A:424:ALA:O	1:A:431:MET:CE	2.69	0.40
1:D:321:PHE:CZ	1:D:376:THR:HG23	2.56	0.40
1:C:220:ARG:O	1:C:537:LEU:HD22	2.21	0.40
1:B:251:TYR:HE1	1:B:320:ASP:HB2	1.85	0.40
1:D:617:MET:N	1:D:618:PRO:CD	2.83	0.40
1:D:282:ALA:HA	1:D:360:ILE:CG2	2.50	0.40
1:C:121:LYS:HD2	1:C:131:VAL:HG21	2.04	0.40
1:C:36:PRO:HA	1:C:201:PRO:HG2	2.03	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	647/695 (93%)	638 (99%)	8 (1%)	1 (0%)	52	53
1	B	647/695 (93%)	637 (98%)	9 (1%)	1 (0%)	52	53
1	C	647/695 (93%)	637 (98%)	9 (1%)	1 (0%)	52	53
1	D	647/695 (93%)	634 (98%)	12 (2%)	1 (0%)	52	53
All	All	2588/2780 (93%)	2546 (98%)	38 (2%)	4 (0%)	52	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	616	ASP
1	D	616	ASP
1	A	616	ASP
1	C	616	ASP

### 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	529/575 (92%)	519 (98%)	10 (2%)	65	70
1	B	526/575 (92%)	514 (98%)	12 (2%)	58	62
1	C	527/575 (92%)	513 (97%)	14 (3%)	52	56
1	D	527/575 (92%)	516 (98%)	11 (2%)	61	66
All	All	2109/2300 (92%)	2062 (98%)	47 (2%)	60	64

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	180	GLN
1	A	251	TYR
1	A	264	LYS
1	A	270	LEU
1	A	352	ASN
1	A	511	TYR
1	A	547	ARG
1	A	616	ASP
1	A	654	THR
1	B	23	VAL
1	B	31	GLN
1	B	180	GLN
1	B	251	TYR
1	B	270	LEU
1	B	271	SER
1	B	352	ASN
1	B	511	TYR

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Mol	Chain	Res	Type
1	B	547	ARG
1	B	616	ASP
1	B	643	ARG
1	B	654	THR
1	C	31	GLN
1	C	167	ARG
1	C	180	GLN
1	C	251	TYR
1	C	270	LEU
1	C	271	SER
1	C	323	LEU
1	C	352	ASN
1	C	511	TYR
1	C	547	ARG
1	C	582	LYS
1	C	616	ASP
1	C	637	GLU
1	C	654	THR
1	D	31	GLN
1	D	180	GLN
1	D	251	TYR
1	D	264	LYS
1	D	271	SER
1	D	352	ASN
1	D	511	TYR
1	D	547	ARG
1	D	616	ASP
1	D	637	GLU
1	D	654	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	HIS
1	A	397	HIS
1	A	436	GLN
1	B	262	HIS
1	B	395	ASN
1	B	436	GLN
1	C	397	HIS
1	C	436	GLN
1	D	31	GLN

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Mol	Chain	Res	Type
1	D	180	GLN
1	D	262	HIS
1	D	395	ASN
1	D	397	HIS
1	D	436	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 ⓘ

4 ligands are 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	A	701	-	24,24,24	0.89	0	35,35,35	1.55	9 (25%)
2	MAL	B	701	-	24,24,24	0.64	0	35,35,35	1.57	9 (25%)
2	MAL	C	701	-	24,24,24	0.77	0	35,35,35	1.73	8 (22%)
2	MAL	D	701	-	24,24,24	0.53	0	35,35,35	1.67	6 (17%)

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

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	MAL	O5'-C5'-C6'	-4.92	93.92	106.36
2	C	701	MAL	O3'-C3'-C2'	-4.20	100.88	110.34
2	C	701	MAL	C1-O1-C4'	-3.83	108.00	118.01
2	A	701	MAL	O3'-C3'-C2'	-3.21	103.10	110.34
2	D	701	MAL	O4-C4-C3	-3.11	103.33	110.34
2	A	701	MAL	C1-O1-C4'	-2.95	110.31	118.01
2	B	701	MAL	C1-O1-C4'	-2.94	110.32	118.01
2	C	701	MAL	O5'-C1'-C2'	-2.94	105.11	109.80
2	B	701	MAL	O4-C4-C3	-2.89	103.82	110.34
2	B	701	MAL	C1'-C2'-C3'	-2.25	107.08	110.43
2	B	701	MAL	C2'-C3'-C4'	-2.21	104.74	109.60
2	A	701	MAL	O3-C3-C2	-2.16	105.47	110.34
2	A	701	MAL	O1-C4'-C5'	-2.16	103.66	109.32
2	B	701	MAL	C6'-C5'-C4'	-2.07	107.23	113.25
2	A	701	MAL	O5'-C1'-C2'	-2.03	106.56	109.80
2	C	701	MAL	C1'-C2'-C3'	2.01	113.42	110.43
2	B	701	MAL	O2-C2-C3	2.03	114.91	110.34
2	A	701	MAL	O2-C2-C3	2.08	115.03	110.34
2	D	701	MAL	C1-O5-C5	2.16	117.94	113.75
2	A	701	MAL	C1-O5-C5	2.22	118.05	113.75
2	C	701	MAL	O4-C4-C5	2.27	115.24	109.24
2	B	701	MAL	O1-C1-O5	2.27	116.42	110.68
2	A	701	MAL	O1-C4'-C3'	2.34	113.21	107.17
2	D	701	MAL	O1'-C1'-C2'	2.40	115.65	109.21
2	C	701	MAL	O2'-C2'-C1'	2.55	115.43	109.82
2	D	701	MAL	C1-C2-C3	2.71	115.32	109.97
2	A	701	MAL	O3'-C3'-C4'	2.79	116.47	109.87
2	B	701	MAL	C1'-O5'-C5'	3.03	119.08	113.47
2	C	701	MAL	O1'-C1'-C2'	3.14	117.62	109.21
2	B	701	MAL	O5'-C5'-C4'	3.49	117.13	109.75
2	C	701	MAL	C1'-O5'-C5'	3.58	120.09	113.47
2	D	701	MAL	O5-C5-C4	3.99	117.17	109.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	MAL	1	0
2	B	701	MAL	5	0
2	C	701	MAL	2	0
2	D	701	MAL	1	0

## 5.7 Other polymers [i](#)

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 [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	649/695 (93%)	-0.53	0 <b>100</b> <b>100</b>	18, 28, 41, 59	0
1	B	649/695 (93%)	-0.48	1 (0%) <b>95</b> <b>96</b>	17, 26, 47, 58	0
1	C	649/695 (93%)	-0.49	0 <b>100</b> <b>100</b>	17, 28, 39, 50	0
1	D	649/695 (93%)	-0.45	0 <b>100</b> <b>100</b>	17, 26, 44, 51	0
All	All	2596/2780 (93%)	-0.49	1 (0%) <b>100</b> <b>100</b>	17, 27, 43, 59	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	ALA	2.5

### 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( $\text{\AA}^2$ )	Q<0.9
2	MAL	D	701	23/23	0.95	0.10	0.84	19,22,31,32	0
2	MAL	B	701	23/23	0.95	0.08	-0.14	19,25,30,35	0
2	MAL	C	701	23/23	0.96	0.08	-0.51	20,23,24,26	0
2	MAL	A	701	23/23	0.97	0.08	-0.59	19,24,31,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.