



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:23 AM GMT

PDB ID : 3OSR  
Title : Maltose-bound maltose sensor engineered by insertion of circularly permuted green fluorescent protein into E. coli maltose binding protein at position 311  
Authors : Echevarria, I.M.; Marvin, J.S.; Looger, L.L.; Schreiter, E.R.  
Deposited on : 2010-09-09  
Resolution : 2.00 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

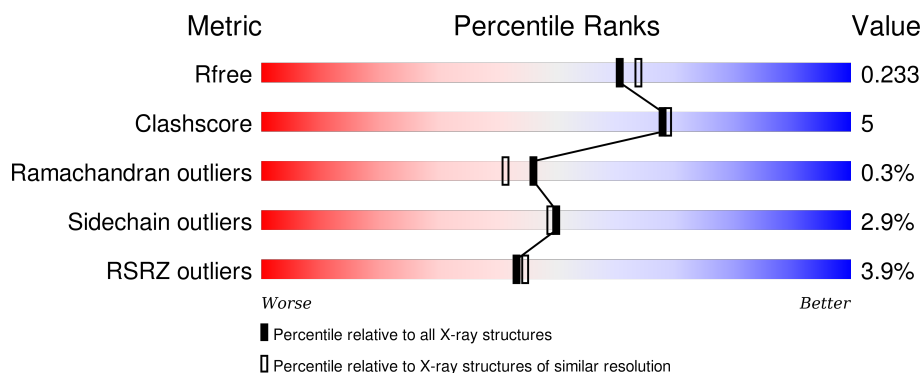
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

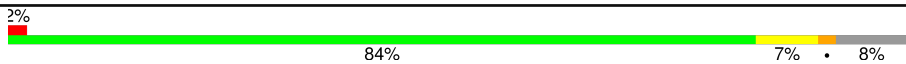
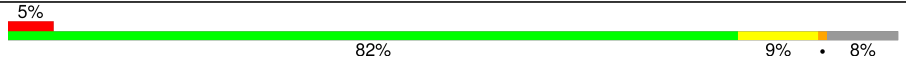
The reported resolution of this entry is 2.00 Å.

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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	653	
1	B	653	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10100 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 Maltose-binding periplasmic protein, Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	604	Total	C	N	O	S	0	1	0
			4752	3046	787	907	12			
1	B	601	Total	C	N	O	S	0	3	0
			4743	3040	785	906	12			

There are 118 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	EXPRESSION TAG	UNP P0AEX9
A	-34	ARG	-	EXPRESSION TAG	UNP P0AEX9
A	-33	GLY	-	EXPRESSION TAG	UNP P0AEX9
A	-32	SER	-	EXPRESSION TAG	UNP P0AEX9
A	-31	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-30	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-29	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-28	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-27	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-26	HIS	-	EXPRESSION TAG	UNP P0AEX9
A	-25	GLY	-	EXPRESSION TAG	UNP P0AEX9
A	-24	MET	-	EXPRESSION TAG	UNP P0AEX9
A	-23	ALA	-	EXPRESSION TAG	UNP P0AEX9
A	-22	SER	-	EXPRESSION TAG	UNP P0AEX9
A	-21	MET	-	EXPRESSION TAG	UNP P0AEX9
A	-20	THR	-	EXPRESSION TAG	UNP P0AEX9
A	-19	GLY	-	EXPRESSION TAG	UNP P0AEX9
A	-18	GLY	-	EXPRESSION TAG	UNP P0AEX9
A	-17	GLN	-	EXPRESSION TAG	UNP P0AEX9
A	-16	GLN	-	EXPRESSION TAG	UNP P0AEX9
A	-15	MET	-	EXPRESSION TAG	UNP P0AEX9
A	-14	GLY	-	EXPRESSION TAG	UNP P0AEX9
A	-13	ARG	-	EXPRESSION TAG	UNP P0AEX9
A	-12	ASP	-	EXPRESSION TAG	UNP P0AEX9
A	-11	LEU	-	EXPRESSION TAG	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	TYR	-	EXPRESSION TAG	UNP P0AEX9
A	-9	ASP	-	EXPRESSION TAG	UNP P0AEX9
A	-8	ASP	-	EXPRESSION TAG	UNP P0AEX9
A	-7	ASP	-	EXPRESSION TAG	UNP P0AEX9
A	-6	ASP	-	EXPRESSION TAG	UNP P0AEX9
A	-5	LYS	-	EXPRESSION TAG	UNP P0AEX9
A	-4	ASP	-	EXPRESSION TAG	UNP P0AEX9
A	-3	ARG	-	EXPRESSION TAG	UNP P0AEX9
A	-2	TRP	-	EXPRESSION TAG	UNP P0AEX9
A	-1	GLY	-	EXPRESSION TAG	UNP P0AEX9
A	0	SER	-	EXPRESSION TAG	UNP P0AEX9
A	312	GLY	-	LINKER	UNP P0AEX9
A	313	GLY	-	LINKER	UNP P0AEX9
A	325	ARG	LYS	CONFLICT	UNP P42212
A	330	ALA	VAL	CONFLICT	UNP P42212
A	342	GLY	SER	CONFLICT	UNP P42212
A	347	TYR	ASP	CONFLICT	UNP P42212
A	373	LYS	ALA	CONFLICT	UNP P42212
A	398	LEU	HIS	CONFLICT	UNP P42212
A	406	GLY	-	LINKER	UNP P42212
A	407	GLY	-	LINKER	UNP P42212
A	408	THR	-	LINKER	UNP P42212
A	409	GLY	-	LINKER	UNP P42212
A	410	GLY	-	LINKER	UNP P42212
A	411	SER	-	LINKER	UNP P42212
A	412	MET	-	LINKER	UNP P42212
A	413	VAL	-	LINKER	UNP P42212
A	476	LEU	PHE	CONFLICT	UNP P42212
A	478	C12	SER	CHROMOPHORE	UNP P42212
A	478	C12	TYR	CHROMOPHORE	UNP P42212
A	478	C12	GLY	CHROMOPHORE	UNP P42212
A	505	ILE	VAL	CONFLICT	UNP P42212
A	557	PHE	TYR	CONFLICT	UNP P42212
A	609	ASP	ALA	CONFLICT	UNP P0AEX9
B	-35	MET	-	EXPRESSION TAG	UNP P0AEX9
B	-34	ARG	-	EXPRESSION TAG	UNP P0AEX9
B	-33	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	-32	SER	-	EXPRESSION TAG	UNP P0AEX9
B	-31	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-30	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-29	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-28	HIS	-	EXPRESSION TAG	UNP P0AEX9

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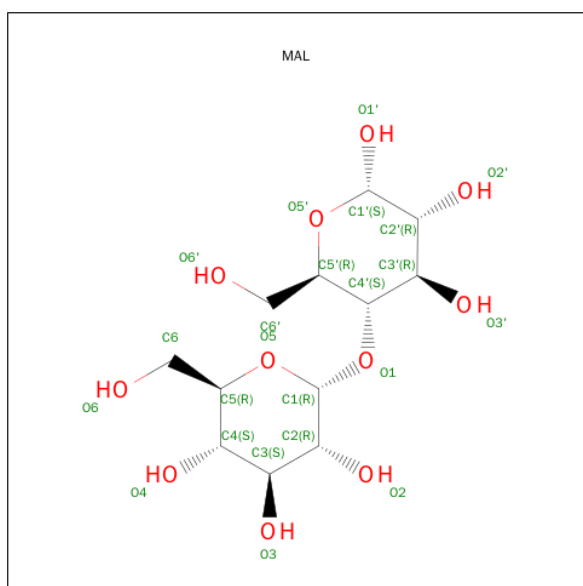
Chain	Residue	Modelled	Actual	Comment	Reference
B	-27	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-26	HIS	-	EXPRESSION TAG	UNP P0AEX9
B	-25	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	-24	MET	-	EXPRESSION TAG	UNP P0AEX9
B	-23	ALA	-	EXPRESSION TAG	UNP P0AEX9
B	-22	SER	-	EXPRESSION TAG	UNP P0AEX9
B	-21	MET	-	EXPRESSION TAG	UNP P0AEX9
B	-20	THR	-	EXPRESSION TAG	UNP P0AEX9
B	-19	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	-18	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	-17	GLN	-	EXPRESSION TAG	UNP P0AEX9
B	-16	GLN	-	EXPRESSION TAG	UNP P0AEX9
B	-15	MET	-	EXPRESSION TAG	UNP P0AEX9
B	-14	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	-13	ARG	-	EXPRESSION TAG	UNP P0AEX9
B	-12	ASP	-	EXPRESSION TAG	UNP P0AEX9
B	-11	LEU	-	EXPRESSION TAG	UNP P0AEX9
B	-10	TYR	-	EXPRESSION TAG	UNP P0AEX9
B	-9	ASP	-	EXPRESSION TAG	UNP P0AEX9
B	-8	ASP	-	EXPRESSION TAG	UNP P0AEX9
B	-7	ASP	-	EXPRESSION TAG	UNP P0AEX9
B	-6	ASP	-	EXPRESSION TAG	UNP P0AEX9
B	-5	LYS	-	EXPRESSION TAG	UNP P0AEX9
B	-4	ASP	-	EXPRESSION TAG	UNP P0AEX9
B	-3	ARG	-	EXPRESSION TAG	UNP P0AEX9
B	-2	TRP	-	EXPRESSION TAG	UNP P0AEX9
B	-1	GLY	-	EXPRESSION TAG	UNP P0AEX9
B	0	SER	-	EXPRESSION TAG	UNP P0AEX9
B	312	GLY	-	LINKER	UNP P0AEX9
B	313	GLY	-	LINKER	UNP P0AEX9
B	325	ARG	LYS	CONFLICT	UNP P42212
B	330	ALA	VAL	CONFLICT	UNP P42212
B	342	GLY	SER	CONFLICT	UNP P42212
B	347	TYR	ASP	CONFLICT	UNP P42212
B	373	LYS	ALA	CONFLICT	UNP P42212
B	398	LEU	HIS	CONFLICT	UNP P42212
B	406	GLY	-	LINKER	UNP P42212
B	407	GLY	-	LINKER	UNP P42212
B	408	THR	-	LINKER	UNP P42212
B	409	GLY	-	LINKER	UNP P42212
B	410	GLY	-	LINKER	UNP P42212
B	411	SER	-	LINKER	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	412	MET	-	LINKER	UNP P42212
B	413	VAL	-	LINKER	UNP P42212
B	476	LEU	PHE	CONFLICT	UNP P42212
B	478	C12	SER	CHROMOPHORE	UNP P42212
B	478	C12	TYR	CHROMOPHORE	UNP P42212
B	478	C12	GLY	CHROMOPHORE	UNP P42212
B	505	ILE	VAL	CONFLICT	UNP P42212
B	557	PHE	TYR	CONFLICT	UNP P42212
B	609	ASP	ALA	CONFLICT	UNP P0AEX9

- 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	B	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	302	Total	O	0	0
			302	302		
3	B	257	Total	O	0	0
			257	257		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.83Å 74.81Å 171.50Å 90.00° 97.52° 90.00°	Depositor
Resolution (Å)	34.24 – 2.00 32.65 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.24-2.00) 100.0 (32.65-2.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.33 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.183 , 0.226 0.193 , 0.233	Depositor DCC
$R_{free}$ test set	4825 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 47.5	EDS
Estimated twinning fraction	0.033 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 96455 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: C12, 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	1.08	3/4846 (0.1%)	0.93	8/6563 (0.1%)
1	B	1.01	5/4843 (0.1%)	0.87	5/6559 (0.1%)
All	All	1.04	8/9689 (0.1%)	0.90	13/13122 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	SER	CB-OG	-6.63	1.33	1.42
1	A	246	VAL	CB-CG2	-5.66	1.41	1.52
1	A	389	GLU	CG-CD	5.48	1.60	1.51
1	B	288	GLU	CB-CG	5.35	1.62	1.52
1	B	288	GLU	CG-CD	5.19	1.59	1.51
1	A	78	GLU	CB-CG	5.15	1.61	1.52
1	B	211	SER	CB-OG	-5.09	1.35	1.42
1	B	291	GLU	CG-CD	-5.04	1.44	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	ARG	NE-CZ-NH2	12.38	126.49	120.30
1	A	335	ARG	NE-CZ-NH1	-11.87	114.37	120.30
1	A	148	MET	CG-SD-CE	-7.47	88.24	100.20
1	B	287	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	128	THR	N-CA-CB	-5.85	99.18	110.30
1	A	374	LEU	CB-CG-CD1	5.68	120.65	111.00
1	A	128	THR	OG1-CB-CG2	5.58	122.83	110.00
1	B	335	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	A	485	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	B	335	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	233	SER	CB-CA-C	-5.25	100.13	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	GLU	C-N-CA	-5.22	108.64	121.70
1	B	89	LEU	CB-CG-CD2	5.20	119.84	111.00

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	4752	0	4670	45	0
1	B	4743	0	4659	43	0
2	A	23	0	21	0	0
2	B	23	0	21	0	0
3	A	302	0	0	18	0
3	B	257	0	0	9	0
All	All	10100	0	9371	88	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 5.

All (88) 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:295:LYS:HD2	3:B:760:HOH:O	1.29	1.25
1:B:300:GLY:HA3	3:B:750:HOH:O	1.69	0.92
1:B:335:ARG:HB3	1:B:343:VAL:HG21	1.54	0.86
1:A:577:GLU:CB	3:A:762:HOH:O	2.25	0.85
1:A:128:THR:HG21	3:A:918:HOH:O	1.77	0.83
1:A:577:GLU:HB3	3:A:762:HOH:O	1.79	0.81
1:A:148:MET:HE3	1:A:222:THR:HB	1.67	0.77
1:B:31:THR:HG23	1:B:33:ILE:HG12	1.67	0.76
1:A:43:LEU:HD12	1:A:43:LEU:C	2.13	0.69
1:B:335:ARG:HB3	1:B:343:VAL:CG2	2.26	0.66
1:A:65:ASP:HB3	1:A:579:MET:HE3	1.78	0.65
1:A:128:THR:HB	1:A:131:GLU:OE1	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LEU:HD12	1:A:431:ASP:N	2.12	0.65
1:B:288:GLU:HG2	3:B:783:HOH:O	1.98	0.64
1:A:577:GLU:HB2	3:A:762:HOH:O	1.95	0.62
1:A:246:VAL:HG21	1:A:571:GLU:OE2	2.00	0.62
1:B:189:LYS:HE3	3:B:820:HOH:O	2.01	0.60
1:A:148:MET:CE	3:A:685:HOH:O	2.50	0.60
1:B:295:LYS:HD3	1:B:295:LYS:C	2.23	0.59
1:B:367:TYR:CE1	1:B:394:ALA:HB3	2.38	0.59
1:A:175:LYS:HB2	3:A:817:HOH:O	2.02	0.58
1:A:325:ARG:HD2	3:A:769:HOH:O	2.02	0.58
1:B:295:LYS:HD3	1:B:296:ASP:N	2.19	0.57
1:B:370:THR:HG23	1:B:391:VAL:HG22	1.86	0.56
1:A:170:LYS:HE2	3:A:821:HOH:O	2.06	0.56
1:B:31:THR:HG22	1:B:33:ILE:H	1.72	0.55
1:A:430:LEU:HD12	1:A:430:LEU:C	2.27	0.55
1:A:147:LEU:HG	1:A:204:MET:HE2	1.90	0.54
1:B:192:LEU:O	1:B:196:VAL:HG23	2.08	0.54
1:B:27:PHE:O	1:B:31:THR:HB	2.07	0.54
1:B:31:THR:CG2	1:B:33:ILE:H	2.20	0.54
1:A:246:VAL:HG22	1:A:571:GLU:CD	2.28	0.54
1:B:153:GLU:OE1	1:B:593:ARG:NH1	2.40	0.53
1:A:6:LYS:HD3	3:A:777:HOH:O	2.08	0.53
1:B:381:LYS:N	3:B:850:HOH:O	2.43	0.51
1:B:430:LEU:HD12	1:B:431:ASP:N	2.26	0.51
1:A:531:LEU:C	1:A:531:LEU:HD13	2.31	0.51
1:B:619:LYS:CG	1:B:619:LYS:O	2.59	0.50
1:A:505:ILE:CD1	1:A:523:GLU:HG2	2.43	0.48
1:A:505:ILE:HD13	1:A:523:GLU:HG2	1.96	0.47
1:B:465:LEU:HD22	1:B:469:TRP:CD2	2.50	0.47
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.50	0.46
1:B:335:ARG:HD2	3:B:691:HOH:O	2.14	0.46
1:A:246:VAL:CG2	1:A:571:GLU:OE2	2.63	0.46
1:A:128:THR:HG22	1:A:131:GLU:H	1.81	0.46
1:A:92:PHE:HZ	1:A:110:VAL:HG21	1.81	0.46
1:A:388:LEU:HD13	1:A:455:THR:HG22	1.98	0.45
1:B:185:ASN:O	1:B:189:LYS:HG3	2.16	0.45
1:B:1:LYS:O	1:B:1:LYS:HG2	2.16	0.45
1:B:619:LYS:HG2	1:B:619:LYS:O	2.17	0.45
1:B:392:THR:HG22	1:B:393:ALA:O	2.15	0.45
1:A:148:MET:HE2	3:A:685:HOH:O	2.11	0.45
1:A:246:VAL:CG2	1:A:571:GLU:CD	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LYS:CE	3:A:772:HOH:O	2.65	0.44
1:B:68:GLY:HA3	1:B:581:ASN:O	2.17	0.44
1:B:468:PRO:HD3	1:B:548:ILE:O	2.17	0.44
1:B:189:LYS:CE	3:B:820:HOH:O	2.63	0.44
1:B:251:LYS:HE3	3:B:801:HOH:O	2.16	0.44
1:B:184:ASP:HB2	1:B:614:GLN:HB2	2.00	0.44
1:A:370:THR:HG22	3:A:722:HOH:O	2.18	0.44
1:B:361:LEU:HD13	1:B:492:GLN:HA	2.00	0.44
1:B:43:LEU:C	1:B:43:LEU:HD12	2.37	0.43
1:A:545:ASP:O	1:A:552:LYS:NZ	2.28	0.43
1:B:317:VAL:O	1:B:367:TYR:HB2	2.18	0.43
1:A:127:LYS:NZ	3:A:907:HOH:O	2.51	0.43
1:B:390:PHE:HA	1:B:452:GLY:O	2.18	0.43
1:A:370:THR:HG21	1:A:478:C12:CE1	2.49	0.42
1:B:291:GLU:HG3	1:B:291:GLU:O	2.18	0.42
1:A:576:GLY:O	1:A:577:GLU:HG3	2.19	0.42
1:B:531:LEU:C	1:B:531:LEU:HD13	2.39	0.42
1:A:128:THR:CG2	1:A:131:GLU:H	2.32	0.42
1:B:47:PHE:N	1:B:48:PRO:HD2	2.35	0.42
1:A:78:GLU:CD	3:A:752:HOH:O	2.58	0.41
1:B:229:PRO:HA	1:B:232:TRP:CE2	2.55	0.41
1:A:430:LEU:HD12	1:A:431:ASP:C	2.41	0.41
1:A:148:MET:HE1	3:A:685:HOH:O	2.19	0.41
1:B:465:LEU:HD22	1:B:469:TRP:CE2	2.55	0.41
1:A:45:GLU:HG3	3:A:905:HOH:O	2.20	0.41
1:A:148:MET:HE1	3:A:785:HOH:O	2.20	0.41
1:B:497:LYS:NZ	3:B:640:HOH:O	2.53	0.41
1:A:298:PRO:HD3	3:A:795:HOH:O	2.21	0.41
1:A:246:VAL:HG23	1:A:246:VAL:H	1.66	0.40
1:B:363:PRO:HB3	1:B:493:HIS:O	2.21	0.40
1:A:372:SER:OG	1:A:389:GLU:OE2	2.30	0.40
1:B:578:ILE:HG23	1:B:578:ILE:O	2.20	0.40
1:A:83:LYS:HE2	1:A:87:ASP:OD1	2.20	0.40
1:A:92:PHE:CZ	1:A:110:VAL:HG21	2.57	0.40
1:B:122:LEU:HD11	1:B:135:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	598/653 (92%)	584 (98%)	13 (2%)	1 (0%)	52	48
1	B	597/653 (91%)	588 (98%)	7 (1%)	2 (0%)	46	41
All	All	1195/1306 (92%)	1172 (98%)	20 (2%)	3 (0%)	46	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	173	ASN
1	A	173	ASN
1	B	168	ALA

### 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	499/537 (93%)	481 (96%)	18 (4%)	42	39
1	B	499/537 (93%)	488 (98%)	11 (2%)	60	62
All	All	998/1074 (93%)	969 (97%)	29 (3%)	50	49

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	92	PHE
1	A	128	THR

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Mol	Chain	Res	Type
1	A	138	GLU
1	A	140	LYS
1	A	170	LYS
1	A	175	LYS
1	A	204	MET
1	A	343	VAL
1	A	373	LYS
1	A	374	LEU
1	A	397	THR
1	A	430	LEU
1	A	456	LEU
1	A	519	LYS
1	A	586	SER
1	A	593	ARG
1	A	611	LYS
1	B	31	THR
1	B	127	LYS
1	B	233	SER
1	B	258	PHE
1	B	291	GLU
1	B	295	LYS
1	B	369	SER
1	B	373	LYS
1	B	415	LYS
1	B	444	GLU
1	B	548	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	HIS
1	B	315	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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$
1	C12	A	478	-	20,23,23	1.11	1 (5%)	18,32,32	2.31	3 (16%)
1	C12	B	478	-	20,23,23	1.49	3 (15%)	18,32,32	1.99	2 (11%)

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
1	C12	A	478	-	-	0/7/15/15	0/2/2/2
1	C12	B	478	-	-	0/7/15/15	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	478	C12	CB2-CA2	-4.45	1.47	1.51
1	A	478	C12	CB2-CA2	-3.51	1.48	1.51
1	B	478	C12	CA3-N3	-2.43	1.44	1.49
1	B	478	C12	CA1-N1	-2.26	1.43	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	C12	CB2-CG2-CD2	-2.03	114.69	120.90
1	A	478	C12	C3-CA3-N3	2.29	116.08	112.37
1	B	478	C12	C3-CA3-N3	2.30	116.10	112.37
1	B	478	C12	CG2-CB2-CA2	7.26	127.20	112.58
1	A	478	C12	CG2-CB2-CA2	8.67	130.04	112.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	478	C12	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 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	700	-	24,24,24	0.86	1 (4%)	35,35,35	1.36	5 (14%)
2	MAL	B	700	-	24,24,24	0.81	0	35,35,35	1.39	5 (14%)

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	700	-	-	0/8/48/48	0/2/2/2
2	MAL	B	700	-	-	0/8/48/48	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	MAL	O5'-C5'	-2.42	1.38	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	700	MAL	O1'-C1'-O5'	-3.75	100.00	110.25
2	B	700	MAL	C4-C3-C2	-3.07	105.05	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	MAL	C4-C3-C2	-2.58	105.97	110.79
2	A	700	MAL	O1'-C1'-O5'	-2.48	103.47	110.25
2	B	700	MAL	O5-C1-C2	-2.24	105.67	110.28
2	A	700	MAL	C1-O5-C5	-2.11	109.64	113.75
2	B	700	MAL	O5-C5-C6	-2.01	101.27	106.36
2	A	700	MAL	O5-C5-C4	2.49	114.36	109.68
2	B	700	MAL	O5'-C1'-C2'	3.67	115.64	109.80
2	A	700	MAL	O5'-C1'-C2'	4.34	116.72	109.80

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 [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 ⓘ

### 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<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	603/653 (92%)	-0.09	15 (2%) 61 61	8, 19, 39, 55	0
1	B	600/653 (91%)	0.09	32 (5%) 30 32	11, 23, 51, 72	0
All	All	1203/1306 (92%)	-0.00	47 (3%) 43 45	8, 21, 44, 72	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	489	HIS	6.0
1	B	359	PRO	5.3
1	B	360	VAL	5.3
1	B	173	ASN	5.1
1	B	358	GLY	4.9
1	B	488	ASP	4.5
1	B	172	GLU	4.5
1	B	490	MET	4.2
1	B	619	LYS	4.0
1	B	357	ASP	3.9
1	B	326	ASN	3.9
1	B	325	ARG	3.7
1	A	357	ASP	3.6
1	B	487	PRO	3.5
1	A	173	ASN	3.5
1	B	491	LYS	3.4
1	A	172	GLU	3.4
1	B	492	GLN	3.3
1	A	323	LYS	3.2
1	A	489	HIS	3.2
1	A	415	LYS	3.2
1	B	381	LYS	3.2
1	B	-2	TRP	3.1
1	B	361	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	486	TYR	3.0
1	A	324	GLN	2.9
1	B	355	ILE	2.8
1	B	493	HIS	2.8
1	B	184	ASP	2.7
1	B	174	GLY	2.7
1	A	326	ASN	2.6
1	A	358	GLY	2.6
1	B	611	LYS	2.5
1	B	364	ASP	2.5
1	A	381	LYS	2.5
1	B	367	TYR	2.4
1	B	614	GLN	2.4
1	B	327	GLY	2.4
1	B	323	LYS	2.3
1	B	362	LEU	2.3
1	A	339	GLU	2.2
1	A	-2	TRP	2.2
1	A	488	ASP	2.1
1	A	382	ARG	2.1
1	B	607	ASP	2.1
1	A	480	VAL	2.1
1	B	451	TYR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	C12	A	478	22/22	0.95	0.16	-	7,16,20,21	0
1	C12	B	478	22/22	0.95	0.15	-	14,20,21,24	0

## 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	A	700	23/23	0.97	0.15	0.57	2,8,13,15	0
2	MAL	B	700	23/23	0.96	0.15	0.03	5,12,17,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.