



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:14 AM GMT

PDB ID : 3LDK  
Title : Crystal Structure of A. japonicus CB05  
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Deposited on : 2010-01-13  
Resolution : 2.20 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

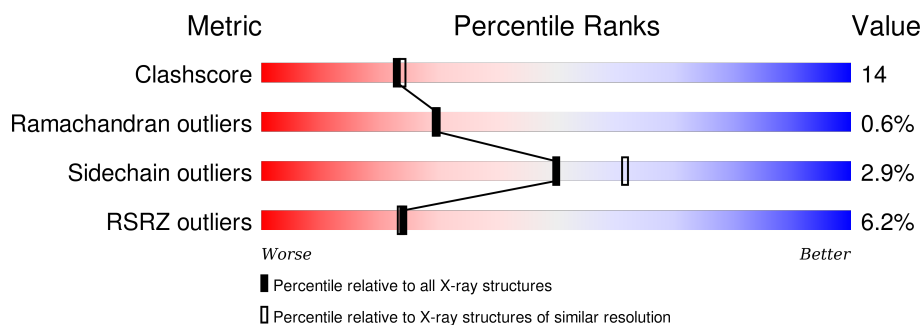
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	634	<div> <div>6%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

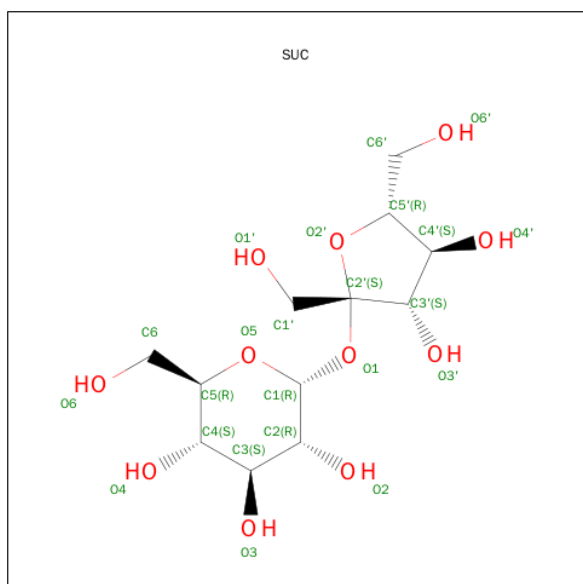
There are 3 unique types of molecules in this entry. The entry contains 5134 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fructosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	634	Total	C	N	O	S	0	0	0
			4883	3091	824	965	3			

- Molecule 2 is SUGAR (SUCROSE) (three-letter code: SUC) (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		

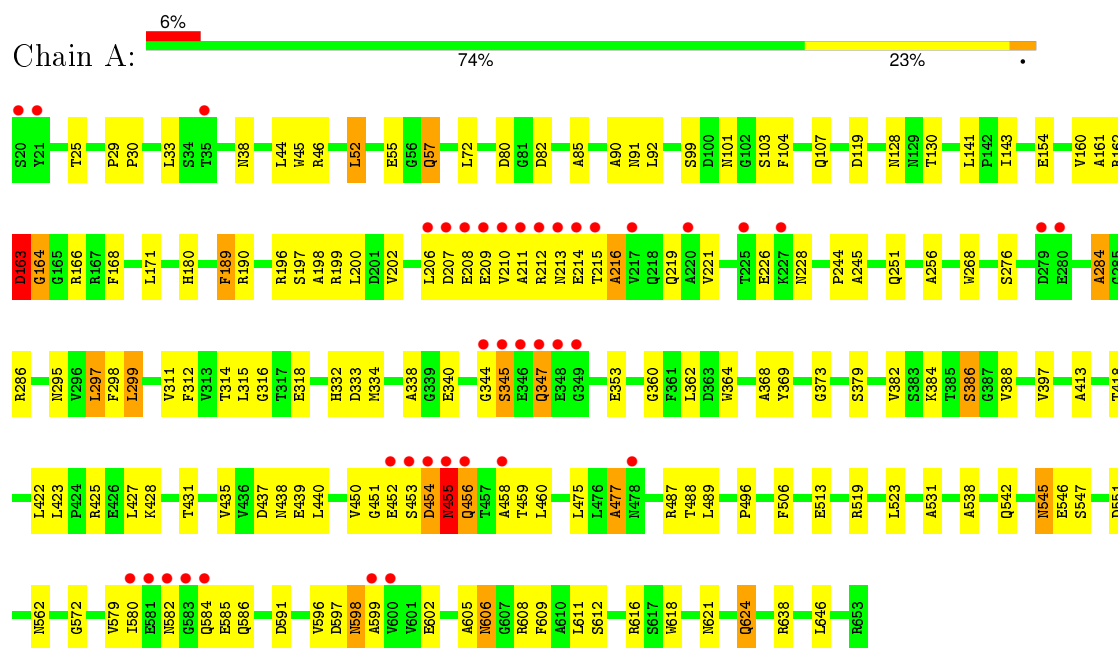
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	228	Total	O	0	0
			228	228		

### 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: Fructosyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.35Å 110.97Å 66.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 24.84 – 2.20	Depositor EDS
% Data completeness (in resolution range)	88.6 (30.00-2.20) 88.7 (24.84-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.43 (at 2.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.224 , 0.264 0.238 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	28.4	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 36134 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5134	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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: SUC

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	0.51	6/5014 (0.1%)	0.74	7/6858 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	ASP	C-N	6.49	1.44	1.33
1	A	189	PHE	C-N	5.85	1.47	1.34
1	A	545	ASN	C-N	5.71	1.47	1.34
1	A	216	ALA	C-N	5.59	1.47	1.34
1	A	284	ALA	C-N	5.53	1.43	1.33
1	A	101	ASN	C-N	-5.08	1.24	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	SER	O-C-N	5.96	132.23	122.70
1	A	454	ASP	N-CA-C	-5.56	96.00	111.00
1	A	52	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	608	ARG	O-C-N	-5.33	114.17	122.70
1	A	455	ASN	CA-C-N	-5.22	105.72	117.20
1	A	164	GLY	C-N-CA	5.19	133.20	122.30
1	A	477	ALA	O-C-N	-5.12	114.50	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	ASP	Mainchain
1	A	455	ASN	Mainchain,Peptide
1	A	477	ALA	Mainchain

## 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	4883	0	4609	129	0
2	A	23	0	22	1	0
3	A	228	0	0	2	0
All	All	5134	0	4631	129	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 14.

All (129) 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:454:ASP:HB2	1:A:456:GLN:CG	1.67	1.25
1:A:454:ASP:CB	1:A:456:GLN:HG2	1.84	1.08
1:A:45:TRP:HB3	1:A:599:ALA:HB2	1.40	1.02
1:A:45:TRP:HB3	1:A:599:ALA:CB	1.97	0.95
1:A:344:GLY:HA2	1:A:353:GLU:OE1	1.77	0.85
1:A:454:ASP:HB2	1:A:456:GLN:HG2	0.87	0.84
1:A:454:ASP:O	1:A:455:ASN:HB2	1.76	0.82
1:A:207:ASP:HB2	1:A:210:VAL:HB	1.64	0.80
1:A:216:ALA:HA	1:A:219:GLN:OE1	1.83	0.79
1:A:531:ALA:O	1:A:624:GLN:HB2	1.81	0.79
1:A:164:GLY:HA3	1:A:166:ARG:NH1	2.00	0.76
1:A:295:ASN:HD21	1:A:373:GLY:H	1.33	0.76
1:A:33:LEU:H	1:A:562:ASN:HD21	1.31	0.75
1:A:295:ASN:ND2	1:A:373:GLY:H	1.85	0.75
1:A:45:TRP:CB	1:A:599:ALA:HB2	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:VAL:HG13	1:A:458:ALA:HB1	1.70	0.72
1:A:332:HIS:HD2	1:A:369:TYR:CE1	2.08	0.71
1:A:496:PRO:HB2	1:A:624:GLN:HE22	1.55	0.71
1:A:251:GLN:OE1	1:A:256:ALA:HA	1.91	0.71
1:A:475:LEU:HD22	1:A:646:LEU:HD22	1.73	0.70
1:A:213:ASN:HD22	1:A:215:THR:HB	1.56	0.70
1:A:332:HIS:HB3	1:A:369:TYR:CE2	2.27	0.69
1:A:452:GLU:O	1:A:458:ALA:HA	1.93	0.69
1:A:213:ASN:ND2	1:A:216:ALA:H	1.90	0.68
1:A:379:SER:O	1:A:384:LYS:HE2	1.93	0.68
1:A:454:ASP:CB	1:A:456:GLN:CG	2.58	0.67
1:A:46:ARG:O	1:A:598:ASN:ND2	2.30	0.65
1:A:332:HIS:HB3	1:A:369:TYR:CD2	2.32	0.64
1:A:435:VAL:HG21	1:A:460:LEU:HD13	1.79	0.63
1:A:538:ALA:HB3	1:A:551:ASP:HB3	1.80	0.62
1:A:29:PRO:HB3	1:A:618:TRP:CE2	2.34	0.61
1:A:85:ALA:HA	1:A:104:PHE:HA	1.83	0.60
1:A:45:TRP:CE2	1:A:616:ARG:HB3	2.37	0.60
1:A:513:GLU:OE1	1:A:638:ARG:HD2	2.02	0.59
1:A:439:GLU:H	1:A:439:GLU:CD	2.06	0.59
1:A:208:GLU:O	1:A:212:ARG:HG2	2.02	0.58
1:A:332:HIS:CD2	1:A:369:TYR:CE1	2.92	0.58
1:A:450:VAL:CG1	1:A:458:ALA:HB1	2.34	0.57
1:A:523:LEU:HD23	1:A:523:LEU:C	2.24	0.57
1:A:57:GLN:HG3	1:A:80:ASP:HA	1.87	0.57
1:A:506:PHE:CZ	1:A:596:VAL:HG21	2.40	0.56
1:A:196:ARG:HD3	1:A:226:GLU:OE2	2.06	0.56
1:A:295:ASN:HB2	1:A:314:THR:OG1	2.05	0.55
1:A:284:ALA:HB2	1:A:360:GLY:HA2	1.87	0.55
1:A:312:PHE:CE1	1:A:338:ALA:HB2	2.42	0.55
1:A:580:ILE:HA	1:A:584:GLN:O	2.07	0.55
1:A:298:PHE:CE1	1:A:311:VAL:HG22	2.42	0.54
1:A:29:PRO:HB3	1:A:618:TRP:CD2	2.42	0.54
1:A:316:GLY:HA2	1:A:333:ASP:O	2.07	0.54
1:A:199:ARG:HG3	1:A:199:ARG:HH11	1.73	0.54
1:A:57:GLN:HB2	1:A:418:THR:HB	1.90	0.54
1:A:606:ASN:N	1:A:606:ASN:HD22	2.06	0.54
1:A:82:ASP:OD2	1:A:107:GLN:NE2	2.42	0.53
1:A:591:ASP:H	1:A:606:ASN:HD21	1.57	0.52
1:A:154:GLU:OE2	1:A:190:ARG:HD3	2.09	0.52
1:A:605:ALA:HB3	1:A:609:PHE:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:THR:HA	1:A:460:LEU:O	2.10	0.52
1:A:435:VAL:HB	1:A:458:ALA:O	2.10	0.52
1:A:202:VAL:HG21	1:A:221:VAL:HG22	1.90	0.52
1:A:579:VAL:O	1:A:585:GLU:HA	2.10	0.52
1:A:591:ASP:H	1:A:606:ASN:ND2	2.08	0.52
1:A:318:GLU:OE2	2:A:1:SUC:O3	2.26	0.52
1:A:30:PRO:HG2	1:A:33:LEU:HD23	1.92	0.51
1:A:99:SER:OG	1:A:103:SER:HA	2.10	0.51
1:A:162:ARG:O	1:A:163:ASP:HB3	2.10	0.51
1:A:128:ASN:O	1:A:130:THR:HG23	2.11	0.51
1:A:438:ASN:OD1	1:A:440:LEU:HB2	2.11	0.50
1:A:25:THR:HG21	1:A:44:LEU:HD13	1.92	0.50
1:A:198:ALA:O	1:A:202:VAL:HG23	2.12	0.50
1:A:164:GLY:HA3	1:A:166:ARG:HH11	1.75	0.50
1:A:451:GLY:N	1:A:459:THR:O	2.42	0.49
1:A:315:LEU:N	1:A:315:LEU:HD23	2.27	0.49
1:A:297:LEU:HD12	1:A:297:LEU:N	2.28	0.49
1:A:161:ALA:HB2	1:A:168:PHE:CZ	2.47	0.49
1:A:582:ASN:C	1:A:584:GLN:N	2.65	0.48
1:A:213:ASN:HD21	1:A:216:ALA:HB2	1.79	0.48
1:A:207:ASP:HB2	1:A:210:VAL:CB	2.40	0.47
1:A:206:LEU:HB2	1:A:211:ALA:HB2	1.96	0.47
1:A:298:PHE:HE1	1:A:311:VAL:HG22	1.80	0.47
1:A:244:PRO:O	1:A:245:ALA:HB2	2.15	0.47
1:A:215:THR:O	1:A:219:GLN:HG3	2.15	0.46
1:A:91:ASN:O	1:A:92:LEU:HB3	2.16	0.46
1:A:602:GLU:HG2	1:A:612:SER:OG	2.15	0.46
1:A:38:ASN:OD1	1:A:413:ALA:HB1	2.15	0.46
1:A:33:LEU:H	1:A:562:ASN:ND2	2.06	0.46
1:A:597:ASP:O	1:A:598:ASN:CB	2.62	0.45
1:A:585:GLU:HG2	1:A:586:GLN:N	2.31	0.45
1:A:364:TRP:CE3	1:A:572:GLY:HA2	2.52	0.45
1:A:344:GLY:O	1:A:347:GLN:OE1	2.35	0.45
1:A:340:GLU:CD	1:A:340:GLU:N	2.70	0.45
1:A:130:THR:OG1	1:A:160:VAL:HG13	2.16	0.45
1:A:199:ARG:HG3	1:A:199:ARG:NH1	2.32	0.44
1:A:202:VAL:HG21	1:A:221:VAL:CG2	2.48	0.44
1:A:364:TRP:HB2	1:A:611:LEU:HD13	1.99	0.44
1:A:180:HIS:HA	1:A:189:PHE:CZ	2.52	0.44
1:A:276:SER:CB	1:A:286:ARG:HA	2.48	0.44
1:A:488:THR:O	1:A:489:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HD12	3:A:686:HOH:O	2.18	0.44
1:A:299:LEU:HG	1:A:428:LYS:HA	1.99	0.44
1:A:542:GLN:O	1:A:546:GLU:CA	2.65	0.43
1:A:460:LEU:HD12	1:A:460:LEU:N	2.33	0.43
1:A:397:VAL:HB	1:A:422:LEU:HD12	2.00	0.43
1:A:312:PHE:CD1	1:A:338:ALA:HB2	2.53	0.43
1:A:90:ALA:O	1:A:382:VAL:HA	2.18	0.43
1:A:332:HIS:C	1:A:369:TYR:CE2	2.92	0.43
1:A:160:VAL:HG23	1:A:171:LEU:HD21	2.01	0.43
1:A:368:ALA:O	1:A:369:TYR:HB2	2.18	0.42
1:A:334:MET:HG3	1:A:362:LEU:HB3	2.01	0.42
1:A:332:HIS:CB	1:A:369:TYR:CE2	3.00	0.42
1:A:542:GLN:O	1:A:546:GLU:HA	2.18	0.42
1:A:197:SER:HB3	1:A:200:LEU:HD12	2.02	0.42
1:A:386:SER:OG	1:A:388:VAL:HG23	2.19	0.42
1:A:598:ASN:HB3	1:A:599:ALA:H	1.62	0.42
1:A:545:ASN:OD1	1:A:547:SER:HB2	2.20	0.42
1:A:582:ASN:C	1:A:584:GLN:H	2.23	0.41
1:A:454:ASP:HB2	1:A:456:GLN:CD	2.34	0.41
1:A:384:LYS:HB2	3:A:797:HOH:O	2.20	0.41
1:A:487:ARG:HD3	1:A:489:LEU:HD21	2.02	0.41
1:A:597:ASP:O	1:A:598:ASN:HB2	2.20	0.41
1:A:423:LEU:O	1:A:425:ARG:HG3	2.21	0.41
1:A:276:SER:HB2	1:A:286:ARG:HA	2.03	0.41
1:A:141:LEU:HD23	1:A:143:ILE:HG13	2.03	0.41
1:A:332:HIS:HB3	1:A:369:TYR:CZ	2.56	0.41
1:A:57:GLN:HE21	1:A:80:ASP:H	1.68	0.41
1:A:519:ARG:HG2	1:A:519:ARG:HH11	1.86	0.40
1:A:435:VAL:HA	1:A:579:VAL:HG12	2.03	0.40
1:A:332:HIS:CA	1:A:369:TYR:CE2	3.04	0.40
1:A:437:ASP:OD2	1:A:453:SER:OG	2.39	0.40
1:A:621:ASN:HD22	1:A:621:ASN:H	1.70	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	632/634 (100%)	584 (92%)	44 (7%)	4 (1%)	30 29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	GLN
1	A	598	ASN
1	A	455	ASN
1	A	214	GLU

### 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	516/516 (100%)	501 (97%)	15 (3%)	50 62

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	55	GLU
1	A	57	GLN
1	A	119	ASP
1	A	209	GLU
1	A	228	ASN
1	A	268	TRP
1	A	297	LEU
1	A	299	LEU
1	A	345	SER
1	A	347	GLN
1	A	386	SER
1	A	427	LEU

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Mol	Chain	Res	Type
1	A	606	ASN
1	A	624	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	74	HIS
1	A	156	GLN
1	A	213	ASN
1	A	295	ASN
1	A	332	HIS
1	A	415	GLN
1	A	511	GLN
1	A	562	ASN
1	A	606	ASN
1	A	621	ASN
1	A	624	GLN
1	A	639	ASN

### 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	SUC	A	1	-	24,24,24	0.88	1 (4%)	36,36,36	2.12	6 (16%)

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	SUC	A	1	-	-	0/12/51/51	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	SUC	O5-C1	2.62	1.48	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	SUC	C2'-O1-C1	-3.45	108.45	117.53
2	A	1	SUC	C6-C5-C4	-2.63	106.53	113.02
2	A	1	SUC	C6'-C5'-C4'	-2.19	109.90	115.08
2	A	1	SUC	O1-C2'-C3'	-2.03	100.97	108.04
2	A	1	SUC	O1-C2'-C1'	2.61	118.05	109.69
2	A	1	SUC	O6-C6-C5	10.57	146.25	111.33

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
2	A	1	SUC	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

### 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	634/634 (100%)	0.14	39 (6%)	24 23	22, 34, 68, 113	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	345	SER	8.7
1	A	212	ARG	8.4
1	A	211	ALA	7.8
1	A	20	SER	6.3
1	A	207	ASP	6.2
1	A	206	LEU	5.7
1	A	214	GLU	5.6
1	A	347	GLN	5.3
1	A	346	GLU	5.1
1	A	348	GLU	5.0
1	A	208	GLU	4.8
1	A	213	ASN	4.6
1	A	349	GLY	4.6
1	A	215	THR	4.5
1	A	21	TYR	4.4
1	A	456	GLN	4.1
1	A	453	SER	4.1
1	A	455	ASN	3.8
1	A	599	ALA	3.8
1	A	452	GLU	3.6
1	A	209	GLU	3.6
1	A	584	GLN	3.5
1	A	454	ASP	3.5
1	A	583	GLY	3.1
1	A	210	VAL	3.1
1	A	582	ASN	2.9
1	A	279	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	581	GLU	2.9
1	A	227	LYS	2.7
1	A	458	ALA	2.6
1	A	478	ASN	2.6
1	A	280	GLU	2.3
1	A	580	ILE	2.3
1	A	35	THR	2.3
1	A	225	THR	2.2
1	A	217	VAL	2.1
1	A	344	GLY	2.1
1	A	600	VAL	2.0
1	A	220	ALA	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( $\text{\AA}^2$ )	Q<0.9
2	SUC	A	1	23/23	0.91	0.14	0.52	21,29,34,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.