



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 05:09 AM UTC

PDB ID : 3LFI / pdb_00003lfi
Title : Crystal structure of fructosyltransferase (wild-type) from *A. japonicus* in complex with glucose
Authors : Chuankhayan, P.; Chen, C.J.; Chiang, C.M.
Deposited on : 2010-01-17
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

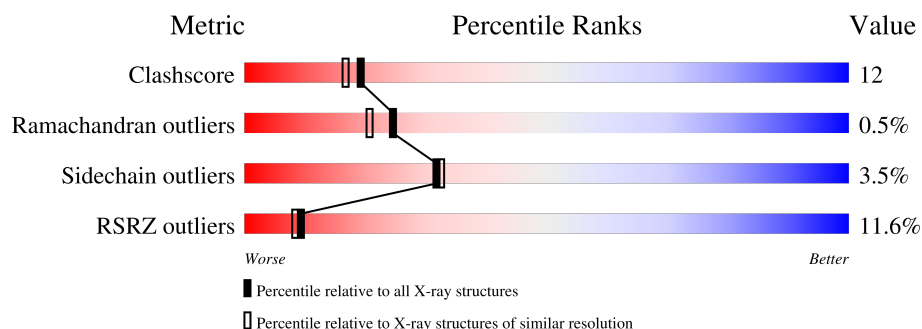
1 Overall quality at a glance

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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
1	B	634	

2 Entry composition [i](#)

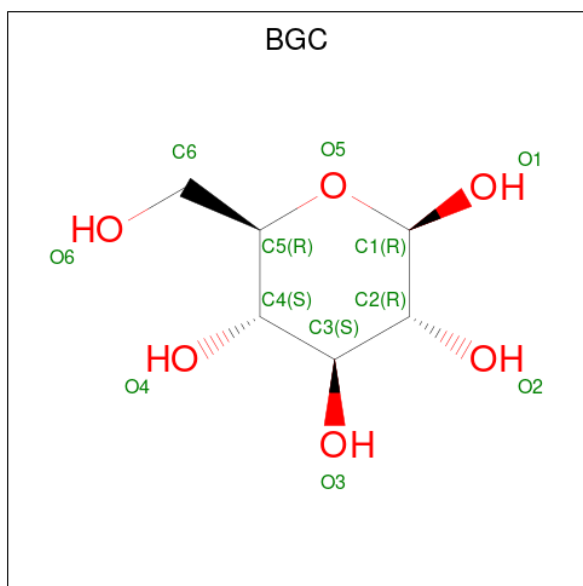
There are 3 unique types of molecules in this entry. The entry contains 10139 atoms, of which 0 are hydrogens and 0 are deuteriums.

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			
1	B	634	Total	C	N	O	S	0	0	0
			4883	3091	824	965	3			

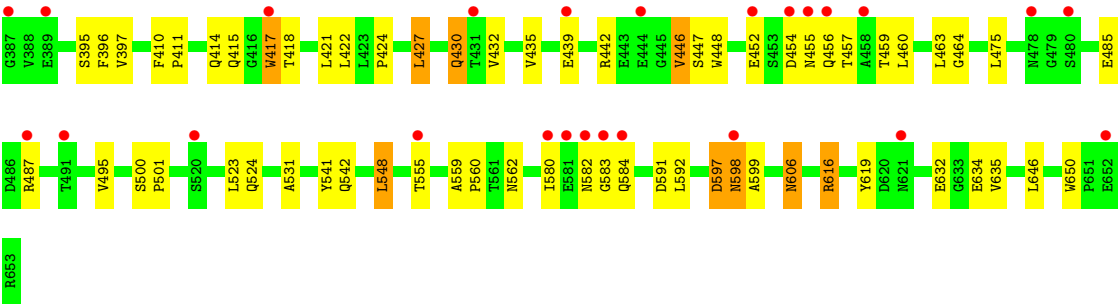
- Molecule 2 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	176	Total 176	O 176	0	0
3	B	173	Total 173	O 173	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.95Å 110.25Å 129.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.8 (30.00-2.00) 93.7 (30.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.56 (at 1.95Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.255 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10139	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0240e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: BGC

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	0.46	2/5014 (0.0%)	0.96	31/6858 (0.5%)
1	B	0.43	3/5014 (0.1%)	0.93	24/6858 (0.3%)
All	All	0.45	5/10028 (0.0%)	0.94	55/13716 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	THR	C-N	-12.99	1.22	1.33
1	B	292	GLU	C-N	-8.43	1.22	1.33
1	A	50	HIS	C-N	-8.18	1.25	1.33
1	B	597	ASP	C-N	6.82	1.43	1.33
1	B	598	ASN	C-N	6.17	1.43	1.33

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	ILE	N-CA-C	-7.36	99.52	107.77
1	B	123	ILE	N-CA-C	-7.24	100.38	107.55
1	B	122	VAL	N-CA-C	7.02	117.94	108.11
1	A	347	GLN	CA-C-N	-6.85	112.54	122.06
1	A	347	GLN	C-N-CA	-6.85	112.54	122.06
1	B	26	THR	N-CA-C	-6.77	104.70	114.12
1	A	597	ASP	CA-C-N	6.51	133.92	122.66
1	A	597	ASP	C-N-CA	6.51	133.92	122.66
1	B	61	PRO	N-CA-C	-6.50	101.69	111.57
1	A	26	THR	N-CA-C	-6.39	104.73	113.30
1	A	347	GLN	O-C-N	6.34	131.02	122.59
1	A	616	ARG	N-CA-C	6.21	118.93	109.62
1	A	362	LEU	N-CA-C	-6.16	104.47	112.23
1	A	61	PRO	N-CA-C	-6.11	102.29	111.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	ALA	N-CA-C	-6.09	105.70	113.01
1	B	619	TYR	N-CA-C	6.07	119.03	110.23
1	A	122	VAL	N-CA-C	6.04	117.18	108.48
1	B	362	LEU	N-CA-C	-5.96	104.72	112.23
1	B	531	ALA	N-CA-C	5.93	119.38	109.95
1	A	597	ASP	O-C-N	-5.85	114.80	122.59
1	A	650	TRP	CA-C-N	5.84	125.70	119.28
1	A	650	TRP	C-N-CA	5.84	125.70	119.28
1	A	299	LEU	N-CA-C	5.77	119.46	110.17
1	B	616	ARG	N-CA-C	5.73	118.21	109.62
1	B	60	ASP	N-CA-C	5.64	116.51	109.57
1	B	357	SER	N-CA-C	-5.58	106.82	113.97
1	A	357	SER	N-CA-C	-5.53	106.43	114.12
1	A	528	GLU	N-CA-C	-5.48	99.96	108.90
1	A	335	LEU	N-CA-C	5.48	118.57	110.46
1	A	187	THR	N-CA-C	-5.47	106.44	113.23
1	A	598	ASN	CB-CA-C	-5.44	110.32	116.63
1	A	592	LEU	N-CA-C	5.43	118.66	109.76
1	A	548	LEU	N-CA-C	-5.41	100.48	109.46
1	A	138	VAL	N-CA-C	5.40	115.73	108.17
1	B	335	LEU	N-CA-C	5.36	118.39	110.46
1	B	442	ARG	N-CA-C	5.32	119.48	113.15
1	A	532	SER	N-CA-C	-5.32	101.75	108.45
1	B	378	ALA	N-CA-C	-5.29	106.08	112.54
1	A	293	THR	CA-C-N	-5.27	114.86	120.92
1	A	293	THR	C-N-CA	-5.27	114.86	120.92
1	A	531	ALA	N-CA-C	5.25	118.30	109.95
1	B	548	LEU	N-CA-C	-5.21	100.81	109.46
1	A	556	SER	N-CA-C	5.21	116.90	108.41
1	B	650	TRP	CA-C-N	5.21	124.83	119.05
1	B	650	TRP	C-N-CA	5.21	124.83	119.05
1	B	236	SER	N-CA-C	5.19	118.27	109.76
1	B	370	ALA	N-CA-C	5.17	118.58	111.54
1	B	321	GLY	N-CA-C	-5.17	104.65	112.41
1	B	592	LEU	N-CA-C	5.14	118.19	109.76
1	B	299	LEU	N-CA-C	5.13	118.43	110.17
1	A	370	ALA	N-CA-C	5.09	118.47	111.54
1	B	177	ILE	N-CA-C	-5.06	98.81	109.34
1	A	275	SER	N-CA-C	-5.06	103.36	110.35
1	B	42	PHE	N-CA-C	5.01	117.40	111.33
1	B	555	THR	N-CA-C	5.01	116.43	111.07

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	4883	0	4601	102	0
1	B	4883	0	4601	121	0
2	A	12	0	11	1	0
2	B	12	0	12	1	0
3	A	176	0	0	0	0
3	B	173	0	0	0	0
All	All	10139	0	9225	223	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 12.

All (223) 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:454:ASP:HB2	1:B:456:GLN:HE21	1.33	0.92
1:B:206:LEU:HB2	1:B:211:ALA:HB2	1.54	0.89
1:B:454:ASP:HB2	1:B:456:GLN:NE2	1.91	0.85
1:B:452:GLU:HG2	1:B:459:THR:HB	1.60	0.83
1:A:45:TRP:HB2	1:A:599:ALA:HB2	1.62	0.80
1:B:162:ARG:HG3	1:B:169:ASP:OD2	1.80	0.80
1:A:606:ASN:N	1:A:606:ASN:HD22	1.80	0.79
1:A:454:ASP:HB2	1:A:456:GLN:NE2	1.97	0.79
1:B:45:TRP:C	1:B:598:ASN:ND2	2.41	0.77
1:B:45:TRP:HE1	1:B:415:GLN:NE2	1.82	0.77
1:B:33:LEU:H	1:B:562:ASN:HD21	1.34	0.75
1:A:456:GLN:NE2	1:A:457:THR:H	1.85	0.75
1:B:45:TRP:NE1	1:B:415:GLN:NE2	2.35	0.75
1:A:45:TRP:HE1	1:A:415:GLN:NE2	1.84	0.74
1:B:456:GLN:NE2	1:B:457:THR:H	1.84	0.74
1:A:513:GLU:OE2	1:A:638:ARG:HD2	1.88	0.74
1:A:591:ASP:H	1:A:606:ASN:HD21	1.36	0.73
1:B:45:TRP:CD1	1:B:415:GLN:NE2	2.57	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:LEU:N	1:B:299:LEU:HD12	2.04	0.71
1:A:295:ASN:ND2	1:A:373:GLY:H	1.88	0.71
1:A:45:TRP:NE1	1:A:415:GLN:NE2	2.38	0.71
1:A:45:TRP:HB2	1:A:599:ALA:CB	2.21	0.71
1:A:454:ASP:HB2	1:A:456:GLN:HE21	1.56	0.70
1:A:456:GLN:CD	1:A:457:THR:H	1.98	0.70
1:B:606:ASN:N	1:B:606:ASN:HD22	1.90	0.69
1:B:345:SER:OG	1:B:346:GLU:N	2.23	0.69
1:B:456:GLN:CD	1:B:457:THR:H	2.00	0.69
1:A:50:HIS:ND1	1:A:597:ASP:OD2	2.25	0.69
1:B:295:ASN:ND2	1:B:373:GLY:H	1.91	0.69
1:A:292:GLU:OE2	2:A:1:BGC:H1	1.92	0.69
1:A:33:LEU:H	1:A:562:ASN:HD21	1.39	0.68
1:A:45:TRP:CD1	1:A:415:GLN:NE2	2.61	0.68
1:A:162:ARG:HG3	1:A:169:ASP:OD2	1.94	0.68
1:B:295:ASN:HD21	1:B:373:GLY:H	1.39	0.67
1:B:46:ARG:N	1:B:598:ASN:ND2	2.43	0.67
1:B:45:TRP:HA	1:B:598:ASN:ND2	2.10	0.67
1:B:446:VAL:HG13	1:B:447:SER:N	2.09	0.67
1:B:212:ARG:NE	1:B:343:VAL:HG11	2.09	0.67
1:B:591:ASP:H	1:B:606:ASN:HD21	1.43	0.66
1:B:212:ARG:HE	1:B:343:VAL:HG11	1.60	0.66
1:A:591:ASP:H	1:A:606:ASN:ND2	1.95	0.65
1:A:606:ASN:HD22	1:A:606:ASN:H	1.45	0.65
1:A:295:ASN:HD21	1:A:373:GLY:H	1.44	0.65
1:B:299:LEU:HD13	1:B:312:PHE:CD2	2.32	0.65
1:A:485:GLU:O	1:A:487:ARG:HG3	1.97	0.64
1:A:452:GLU:HG2	1:A:459:THR:HB	1.78	0.64
1:A:45:TRP:CB	1:A:599:ALA:HB2	2.27	0.63
1:B:591:ASP:H	1:B:606:ASN:ND2	1.96	0.63
1:A:299:LEU:HG	1:A:428:LYS:HA	1.81	0.62
1:B:292:GLU:OE2	2:B:2:BGC:H1	1.99	0.61
1:B:213:ASN:ND2	1:B:216:ALA:H	1.99	0.61
1:B:45:TRP:HA	1:B:598:ASN:CG	2.25	0.61
1:B:320:SER:HA	1:B:330:SER:OG	2.01	0.60
1:B:45:TRP:CA	1:B:598:ASN:ND2	2.66	0.59
1:A:446:VAL:HG13	1:A:447:SER:N	2.16	0.59
1:B:207:ASP:C	1:B:209:GLU:H	2.08	0.59
1:A:37:PRO:HD2	1:A:40:THR:HG21	1.83	0.59
1:B:446:VAL:HG11	1:B:448:TRP:CE2	2.38	0.58
1:A:446:VAL:HG11	1:A:448:TRP:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:SER:HA	1:A:330:SER:OG	2.04	0.58
1:A:582:ASN:C	1:A:584:GLN:H	2.10	0.58
1:B:42:PHE:O	1:B:417:TRP:CZ3	2.57	0.57
1:B:524:GLN:HG2	1:B:542:GLN:HG3	1.86	0.57
1:A:347:GLN:HE22	1:A:349:GLY:HA3	1.70	0.56
1:A:486:ASP:OD2	1:A:638:ARG:HG2	2.05	0.56
1:B:173:GLN:OE1	1:B:174:GLY:O	2.23	0.56
1:B:42:PHE:O	1:B:417:TRP:HZ3	1.88	0.56
1:B:206:LEU:CB	1:B:211:ALA:HB2	2.33	0.55
1:B:251:GLN:OE1	1:B:256:ALA:HA	2.06	0.55
1:A:207:ASP:HB2	1:A:210:VAL:HG23	1.89	0.55
1:A:269:TRP:CZ3	1:A:271:GLU:OE2	2.60	0.55
1:B:297:LEU:CB	1:B:299:LEU:HD11	2.36	0.55
1:A:487:ARG:NH2	1:A:495:VAL:HG11	2.23	0.54
1:A:212:ARG:HE	1:A:343:VAL:HG11	1.73	0.53
1:B:118:PHE:HB2	1:B:136:THR:HB	1.89	0.53
1:B:45:TRP:CD1	1:B:415:GLN:HE22	2.24	0.53
1:A:439:GLU:CD	1:A:439:GLU:H	2.16	0.53
1:A:208:GLU:O	1:A:212:ARG:HG2	2.10	0.52
1:B:297:LEU:HB3	1:B:299:LEU:HD11	1.92	0.52
1:B:396:PHE:CE1	1:B:424:PRO:HG3	2.45	0.52
1:A:580:ILE:HD11	1:A:583:GLY:HA2	1.92	0.51
1:B:315:LEU:HD23	1:B:315:LEU:N	2.24	0.51
1:A:582:ASN:C	1:A:584:GLN:N	2.67	0.51
1:B:523:LEU:HA	1:B:632:GLU:HB2	1.92	0.51
1:A:213:ASN:O	1:A:217:VAL:HG23	2.11	0.51
1:B:299:LEU:HD13	1:B:312:PHE:HB2	1.92	0.51
1:B:45:TRP:HB2	1:B:599:ALA:CB	2.41	0.51
1:B:582:ASN:C	1:B:584:GLN:H	2.19	0.51
1:A:269:TRP:CH2	1:A:271:GLU:OE2	2.64	0.50
1:B:213:ASN:HD21	1:B:216:ALA:HB2	1.75	0.50
1:B:606:ASN:HD22	1:B:606:ASN:H	1.57	0.50
1:A:42:PHE:O	1:A:417:TRP:HZ3	1.94	0.50
1:A:42:PHE:O	1:A:417:TRP:CZ3	2.65	0.50
1:A:315:LEU:N	1:A:315:LEU:HD23	2.26	0.50
1:B:456:GLN:CD	1:B:457:THR:N	2.69	0.50
1:A:251:GLN:OE1	1:A:256:ALA:HA	2.12	0.50
1:A:296:VAL:C	1:A:297:LEU:HD12	2.37	0.49
1:B:33:LEU:H	1:B:562:ASN:ND2	2.07	0.49
1:B:45:TRP:CD1	1:B:415:GLN:HE21	2.28	0.49
1:B:269:TRP:CH2	1:B:271:GLU:OE2	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:VAL:HB	1:A:422:LEU:HD12	1.94	0.49
1:A:45:TRP:CD1	1:A:415:GLN:HE21	2.31	0.49
1:B:299:LEU:N	1:B:299:LEU:CD1	2.74	0.49
1:B:432:VAL:HB	1:B:460:LEU:HB2	1.95	0.49
1:A:213:ASN:HD21	1:A:216:ALA:CB	2.26	0.49
1:B:410:PHE:CG	1:B:411:PRO:HD2	2.48	0.48
1:A:173:GLN:OE1	1:A:174:GLY:O	2.32	0.48
1:A:198:ALA:HB2	1:A:224:TRP:CD2	2.48	0.48
1:B:130:THR:OG1	1:B:160:VAL:HG13	2.13	0.48
1:A:423:LEU:O	1:A:425:ARG:HG3	2.14	0.48
1:B:200:LEU:HD21	1:B:341:VAL:HG11	1.94	0.48
1:A:118:PHE:HB2	1:A:136:THR:HB	1.96	0.48
1:B:45:TRP:CE3	1:B:616:ARG:HB3	2.48	0.48
1:B:213:ASN:HD21	1:B:216:ALA:CB	2.27	0.48
1:B:430:GLN:HG2	1:B:464:GLY:HA3	1.95	0.48
1:B:244:PRO:HB2	1:B:291:PHE:CD1	2.49	0.47
1:B:269:TRP:CZ3	1:B:271:GLU:OE2	2.67	0.47
1:A:57:GLN:HG3	1:A:80:ASP:HA	1.96	0.47
1:B:198:ALA:HB2	1:B:224:TRP:CD2	2.49	0.47
1:A:454:ASP:O	1:A:455:ASN:HB2	2.15	0.47
1:B:523:LEU:C	1:B:523:LEU:HD23	2.40	0.46
1:B:128:ASN:O	1:B:130:THR:HG23	2.15	0.46
1:A:277:TRP:HB3	1:A:284:ALA:HB3	1.96	0.46
1:B:454:ASP:O	1:B:455:ASN:HB2	2.14	0.46
1:A:264:TYR:CZ	1:A:266:GLY:HA2	2.51	0.46
1:B:344:GLY:HA3	1:B:350:ALA:O	2.16	0.46
1:A:396:PHE:CE1	1:A:424:PRO:HG3	2.50	0.46
1:B:207:ASP:C	1:B:209:GLU:N	2.73	0.46
1:B:46:ARG:N	1:B:598:ASN:HD22	2.13	0.46
1:A:29:PRO:HB3	1:A:618:TRP:CD2	2.51	0.45
1:B:326:PRO:O	1:B:327:GLN:HB2	2.16	0.45
1:B:410:PHE:CD1	1:B:411:PRO:HD2	2.51	0.45
1:B:454:ASP:C	1:B:456:GLN:H	2.24	0.45
1:A:311:VAL:HG21	1:A:341:VAL:HG23	1.97	0.45
1:B:485:GLU:O	1:B:487:ARG:HG3	2.17	0.45
1:A:197:SER:HB2	1:A:298:PHE:CZ	2.51	0.45
1:A:326:PRO:O	1:A:327:GLN:HB2	2.16	0.45
1:B:397:VAL:HB	1:B:422:LEU:HD12	1.98	0.45
1:B:299:LEU:CD1	1:B:312:PHE:HB2	2.47	0.45
1:A:45:TRP:CD1	1:A:415:GLN:HE22	2.31	0.45
1:A:430:GLN:HG2	1:A:464:GLY:HA3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:SER:C	1:A:523:LEU:H	2.25	0.45
1:B:395:SER:HB2	1:B:427:LEU:HD22	1.98	0.45
1:A:487:ARG:HD3	1:A:627:PHE:CZ	2.51	0.45
1:B:175:PRO:HG2	1:B:178:ALA:HB2	1.97	0.45
1:A:226:GLU:OE2	1:A:306:PRO:HG3	2.17	0.45
1:A:297:LEU:HD12	1:A:297:LEU:N	2.32	0.45
1:A:410:PHE:CG	1:A:411:PRO:HD2	2.52	0.45
1:A:446:VAL:HG21	1:A:448:TRP:CZ2	2.52	0.44
1:A:487:ARG:HD3	1:A:627:PHE:CE2	2.52	0.44
1:B:213:ASN:O	1:B:217:VAL:HG23	2.17	0.44
1:A:250:ARG:O	1:A:251:GLN:C	2.59	0.44
1:A:417:TRP:CD1	1:A:418:THR:N	2.86	0.44
1:A:432:VAL:HG12	1:A:435:VAL:CG2	2.48	0.44
1:B:37:PRO:HD2	1:B:40:THR:HG21	1.99	0.44
1:A:634:GLU:HG2	1:A:635:VAL:N	2.32	0.44
1:B:446:VAL:CG1	1:B:447:SER:N	2.75	0.44
1:B:46:ARG:C	1:B:598:ASN:HD22	2.26	0.44
1:B:58:ILE:HG13	1:B:77:PHE:CD1	2.53	0.44
1:B:99:SER:OG	1:B:103:SER:HA	2.17	0.44
1:A:538:ALA:HB3	1:A:551:ASP:HB3	2.00	0.43
1:A:299:LEU:HB3	1:A:429:VAL:HG23	1.99	0.43
1:B:487:ARG:NH2	1:B:495:VAL:HG11	2.32	0.43
1:B:297:LEU:HB2	1:B:299:LEU:HD11	1.99	0.43
1:B:33:LEU:O	1:B:414:GLN:HG2	2.18	0.43
1:B:61:PRO:O	1:B:62:CYS:HB3	2.19	0.43
1:B:439:GLU:CD	1:B:439:GLU:H	2.27	0.43
1:B:45:TRP:NE1	1:B:415:GLN:HE22	2.11	0.43
1:A:452:GLU:CG	1:A:459:THR:HB	2.47	0.43
1:A:200:LEU:HD21	1:A:341:VAL:HG11	2.00	0.43
1:A:364:TRP:HB2	1:A:611:LEU:HD13	2.00	0.43
1:B:126:GLY:HA2	1:B:259:PHE:CZ	2.54	0.43
1:B:197:SER:HB2	1:B:298:PHE:CZ	2.54	0.43
1:B:597:ASP:O	1:B:598:ASN:CB	2.67	0.43
1:A:45:TRP:NE1	1:A:415:GLN:HE22	2.16	0.43
1:A:542:GLN:HG2	1:A:544:SER:OG	2.19	0.43
1:B:45:TRP:HB2	1:B:599:ALA:HB2	2.00	0.43
1:B:548:LEU:HD23	1:B:548:LEU:HA	1.90	0.42
1:B:311:VAL:HG21	1:B:341:VAL:HG23	2.01	0.42
1:A:29:PRO:HB3	1:A:618:TRP:CE2	2.54	0.42
1:B:475:LEU:HD22	1:B:646:LEU:HD22	2.00	0.42
1:A:213:ASN:HD21	1:A:216:ALA:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:HIS:NE2	1:A:602:GLU:OE2	2.35	0.42
1:A:269:TRP:CH2	1:A:356:PRO:HG2	2.55	0.42
1:A:99:SER:OG	1:A:103:SER:HA	2.19	0.42
1:A:128:ASN:O	1:A:130:THR:HG23	2.20	0.42
1:B:580:ILE:HG23	1:B:580:ILE:O	2.20	0.42
1:A:244:PRO:HB2	1:A:291:PHE:CD1	2.54	0.42
1:B:417:TRP:CD1	1:B:418:THR:N	2.88	0.42
1:B:500:SER:HB3	1:B:501:PRO:HD2	2.02	0.42
1:A:332:HIS:HB3	1:A:369:TYR:CD2	2.54	0.41
1:A:456:GLN:CD	1:A:457:THR:N	2.73	0.41
1:B:296:VAL:C	1:B:297:LEU:HD12	2.45	0.41
1:B:446:VAL:HG21	1:B:448:TRP:CZ2	2.55	0.41
1:B:312:PHE:CE1	1:B:338:ALA:HB2	2.55	0.41
1:B:580:ILE:HD11	1:B:583:GLY:HA2	2.02	0.41
1:B:208:GLU:N	1:B:208:GLU:OE1	2.54	0.41
1:B:210:VAL:O	1:B:210:VAL:HG12	2.19	0.41
1:A:344:GLY:O	1:A:345:SER:C	2.62	0.41
1:A:609:PHE:CD2	1:A:609:PHE:C	2.98	0.41
1:B:264:TYR:CZ	1:B:266:GLY:HA2	2.55	0.41
1:B:634:GLU:HG2	1:B:635:VAL:N	2.36	0.41
1:A:446:VAL:HG13	1:A:448:TRP:CD2	2.56	0.41
1:B:379:SER:O	1:B:384:LYS:HE2	2.21	0.41
1:A:278:GLY:HA2	1:A:445:GLY:HA3	2.02	0.41
1:B:250:ARG:O	1:B:251:GLN:C	2.62	0.41
1:A:32:ASN:ND2	1:A:35:THR:HG23	2.35	0.41
1:B:45:TRP:NE1	1:B:415:GLN:HE21	2.17	0.41
1:B:321:GLY:O	1:B:324:ILE:HD13	2.21	0.41
1:B:45:TRP:CB	1:B:599:ALA:HB2	2.50	0.41
1:B:50:HIS:HD2	1:B:421:LEU:O	2.04	0.41
1:B:380:SER:O	1:B:384:LYS:HG3	2.21	0.41
1:B:524:GLN:HA	1:B:541:TYR:O	2.20	0.41
1:B:559:ALA:N	1:B:560:PRO:CD	2.84	0.41
1:A:130:THR:OG1	1:A:160:VAL:HG13	2.21	0.40
1:A:438:ASN:HB2	1:A:439:GLU:OE2	2.21	0.40
1:A:475:LEU:HD22	1:A:646:LEU:HD22	2.02	0.40
1:A:559:ALA:N	1:A:560:PRO:CD	2.84	0.40
1:B:57:GLN:HG3	1:B:80:ASP:HA	2.04	0.40
1:A:379:SER:O	1:A:384:LYS:HE2	2.21	0.40
1:B:45:TRP:HB2	1:B:599:ALA:HB3	2.03	0.40
1:B:432:VAL:HG12	1:B:435:VAL:CG2	2.52	0.40
1:A:552:ARG:HD3	1:A:568:PHE:O	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	632/634 (100%)	596 (94%)	32 (5%)	4 (1%)	21	17
1	B	632/634 (100%)	589 (93%)	41 (6%)	2 (0%)	36	35
All	All	1264/1268 (100%)	1185 (94%)	73 (6%)	6 (0%)	24	21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	345	SER
1	B	345	SER
1	A	347	GLN
1	B	208	GLU
1	A	215	THR
1	A	344	GLY

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	515/517 (100%)	495 (96%)	20 (4%)	28	28
1	B	515/517 (100%)	499 (97%)	16 (3%)	35	37
All	All	1030/1034 (100%)	994 (96%)	36 (4%)	32	32

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	57	GLN
1	A	111	LYS
1	A	137	SER
1	A	173	GLN
1	A	181	PRO
1	A	199	ARG
1	A	208	GLU
1	A	269	TRP
1	A	297	LEU
1	A	299	LEU
1	A	347	GLN
1	A	348	GLU
1	A	417	TRP
1	A	427	LEU
1	A	430	GLN
1	A	446	VAL
1	A	456	GLN
1	A	463	LEU
1	A	606	ASN
1	B	45	TRP
1	B	52	LEU
1	B	57	GLN
1	B	173	GLN
1	B	199	ARG
1	B	208	GLU
1	B	269	TRP
1	B	297	LEU
1	B	299	LEU
1	B	347	GLN
1	B	417	TRP
1	B	427	LEU
1	B	430	GLN
1	B	446	VAL
1	B	463	LEU
1	B	606	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN

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Mol	Chain	Res	Type
1	A	156	GLN
1	A	213	ASN
1	A	295	ASN
1	A	415	GLN
1	A	430	GLN
1	A	434	ASN
1	A	456	GLN
1	A	511	GLN
1	A	562	ASN
1	A	606	ASN
1	A	636	GLN
1	A	639	ASN
1	B	39	ASN
1	B	57	GLN
1	B	156	GLN
1	B	213	ASN
1	B	295	ASN
1	B	415	GLN
1	B	430	GLN
1	B	456	GLN
1	B	511	GLN
1	B	562	ASN
1	B	598	ASN
1	B	606	ASN
1	B	639	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

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	BGC	A	1	-	12,12,12	0.63	0	17,17,17	2.62	3 (17%)
2	BGC	B	2	-	12,12,12	0.46	0	17,17,17	0.71	0

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	BGC	A	1	-	-	2/2/22/22	0/1/1/1
2	BGC	B	2	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	BGC	O6-C6-C5	9.90	145.03	111.33
2	A	1	BGC	C1-C2-C3	-2.43	105.40	110.36
2	A	1	BGC	C3-C4-C5	2.33	114.46	110.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	BGC	C4-C5-C6-O6
2	A	1	BGC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	BGC	1	0
2	B	2	BGC	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 ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	634/634 (100%)	0.61	76 (11%) 9 8	8, 20, 58, 109	0
1	B	634/634 (100%)	0.53	71 (11%) 10 9	8, 19, 56, 104	0
All	All	1268/1268 (100%)	0.57	147 (11%) 9 8	8, 19, 58, 109	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	21	TYR	9.8
1	B	21	TYR	9.2
1	A	20	SER	7.3
1	A	211	ALA	6.8
1	B	344	GLY	5.6
1	A	210	VAL	5.5
1	B	345	SER	5.3
1	B	210	VAL	5.1
1	A	349	GLY	5.0
1	A	345	SER	5.0
1	A	22	HIS	4.9
1	A	45	TRP	4.8
1	B	45	TRP	4.8
1	B	211	ALA	4.8
1	A	343	VAL	4.5
1	B	208	GLU	4.4
1	B	417	TRP	4.4
1	B	349	GLY	4.4
1	B	22	HIS	4.4
1	A	227	LYS	4.4
1	A	344	GLY	4.4
1	B	213	ASN	4.3
1	A	598	ASN	4.3
1	B	228	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	215	THR	4.2
1	B	20	SER	4.2
1	B	456	GLN	4.2
1	A	208	GLU	4.2
1	B	269	TRP	4.0
1	A	213	ASN	4.0
1	B	206	LEU	4.0
1	B	214	GLU	4.0
1	A	456	GLN	4.0
1	B	584	GLN	4.0
1	A	417	TRP	3.9
1	B	216	ALA	3.9
1	A	228	ASN	3.9
1	A	580	ILE	3.9
1	A	219	GLN	3.9
1	A	223	GLY	3.9
1	B	581	GLU	3.8
1	B	346	GLU	3.7
1	A	597	ASP	3.7
1	A	217	VAL	3.7
1	B	217	VAL	3.7
1	B	227	LYS	3.7
1	B	205	SER	3.7
1	B	454	ASP	3.7
1	B	225	THR	3.6
1	B	212	ARG	3.6
1	A	346	GLU	3.6
1	A	269	TRP	3.6
1	A	583	GLY	3.6
1	B	580	ILE	3.5
1	A	226	GLU	3.5
1	B	444	GLU	3.5
1	B	207	ASP	3.4
1	B	218	GLN	3.4
1	A	491	THR	3.3
1	A	206	LEU	3.3
1	B	583	GLY	3.3
1	A	480	SER	3.3
1	A	214	GLU	3.3
1	B	491	THR	3.2
1	A	207	ASP	3.2
1	B	487	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	216	ALA	3.1
1	B	340	GLU	3.1
1	B	219	GLN	3.1
1	A	584	GLN	3.1
1	A	225	THR	3.0
1	A	455	ASN	3.0
1	A	454	ASP	3.0
1	A	348	GLU	3.0
1	A	347	GLN	3.0
1	A	582	ASN	3.0
1	A	212	ARG	2.9
1	A	218	GLN	2.9
1	A	224	TRP	2.9
1	A	162	ARG	2.8
1	B	439	GLU	2.8
1	A	215	THR	2.8
1	B	431	THR	2.8
1	B	582	ASN	2.8
1	B	598	ASN	2.8
1	B	209	GLU	2.7
1	A	431	THR	2.7
1	A	652	GLU	2.6
1	B	347	GLN	2.6
1	A	209	GLU	2.6
1	B	279	ASP	2.6
1	B	480	SER	2.6
1	B	324	ILE	2.5
1	B	222	ASP	2.5
1	B	220	ALA	2.5
1	A	324	ILE	2.5
1	A	222	ASP	2.5
1	A	279	ASP	2.5
1	A	220	ALA	2.5
1	A	353	GLU	2.5
1	B	452	GLU	2.5
1	B	35	THR	2.5
1	B	455	ASN	2.5
1	A	389	GLU	2.4
1	A	581	GLU	2.4
1	A	444	GLU	2.4
1	A	490	GLN	2.4
1	A	101	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	452	GLU	2.4
1	A	435	VAL	2.4
1	B	226	GLU	2.4
1	A	387	GLY	2.3
1	A	487	ARG	2.3
1	A	638	ARG	2.3
1	B	387	GLY	2.3
1	A	69	SER	2.3
1	B	348	GLU	2.3
1	B	555	THR	2.3
1	A	621	ASN	2.3
1	A	591	ASP	2.3
1	B	223	GLY	2.3
1	B	652	GLU	2.2
1	A	203	LEU	2.2
1	B	322	LEU	2.2
1	A	439	GLU	2.2
1	B	280	GLU	2.2
1	A	281	GLY	2.2
1	B	458	ALA	2.2
1	A	205	SER	2.2
1	B	621	ASN	2.2
1	A	40	THR	2.2
1	B	31	THR	2.2
1	B	281	GLY	2.2
1	B	389	GLU	2.2
1	B	343	VAL	2.1
1	A	453	SER	2.1
1	B	69	SER	2.1
1	B	101	ASN	2.1
1	A	520	SER	2.1
1	B	302	GLU	2.0
1	A	322	LEU	2.0
1	B	478	ASN	2.0
1	A	457	THR	2.0
1	B	341	VAL	2.0
1	B	520	SER	2.0
1	A	23	LEU	2.0
1	A	31	THR	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	B	2	12/12	0.74	0.16	25,25,25,25	0
2	BGC	A	1	12/12	0.78	0.14	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.