Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:15 AM GMT

PDB ID	:	3LFI
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

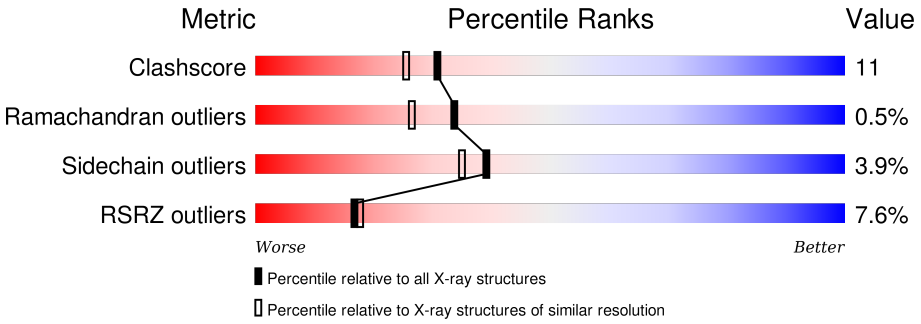
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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))
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 >=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 <=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	8% 78% 21%
1	B	634	8% 78% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BGC	A	1	-	-	-	X
2	BGC	B	2	-	-	-	X

2 Entry composition

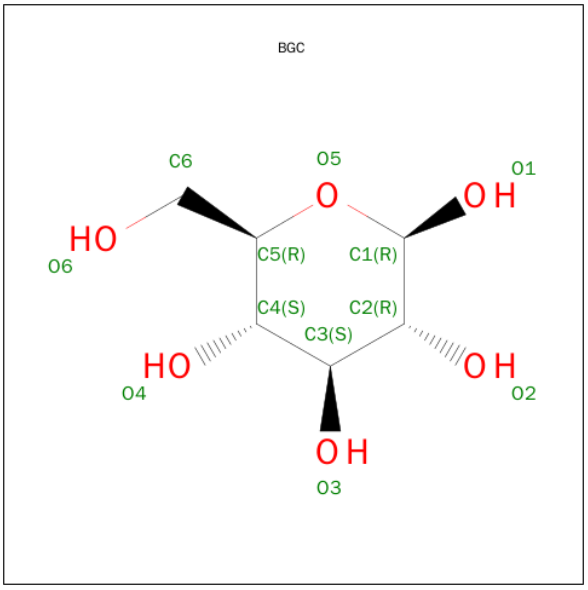
There are 3 unique types of molecules in this entry. The entry contains 10139 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



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.

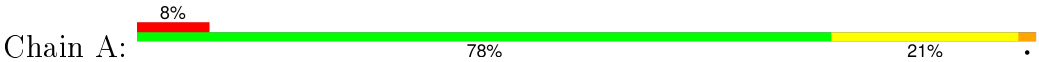
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	176	Total O 176 176	0	0
3	B	173	Total O 173 173	0	0

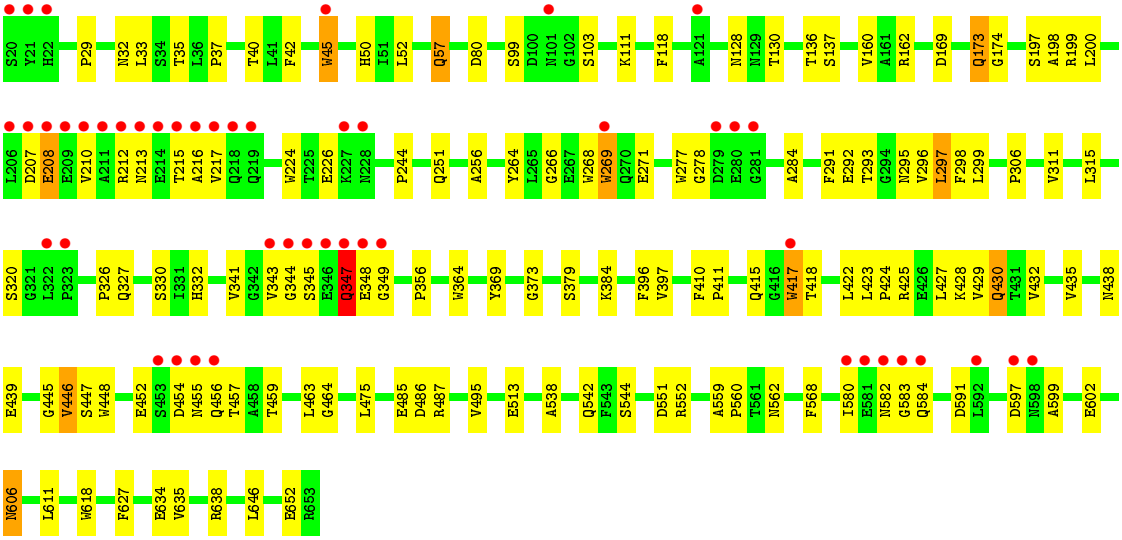
3 Residue-property plots (i)

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

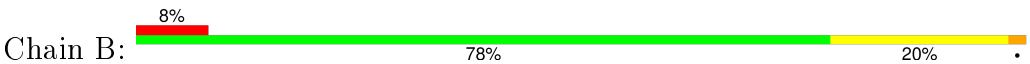
Chain A:

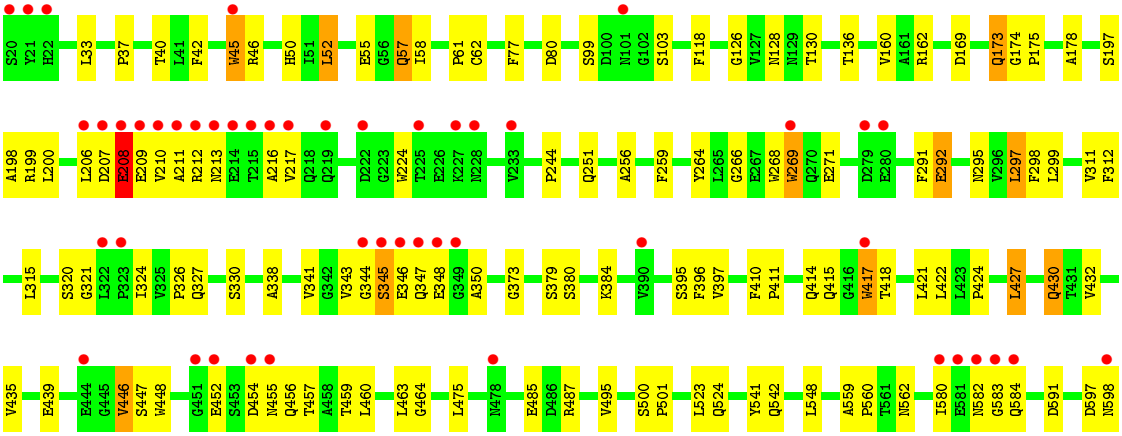




- Molecule 1: Fructosyltransferase

Chain B:






A599
N606
R616
E632
G633
E634
V635
L646
E652
R653

4 Data and refinement statistics (i)

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 27.06 – 1.95	Depositor EDS
% Data completeness (in resolution range)	93.8 (30.00-2.00) 92.5 (27.06-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.56 (at 1.95Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.226 , 0.255 0.227 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	18.4	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	5 of 101087 reflections (0.005%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.38	1/5014 (0.0%)	0.66	1/6858 (0.0%)
1	B	0.37	1/5014 (0.0%)	0.64	1/6858 (0.0%)
All	All	0.38	2/10028 (0.0%)	0.65	2/13716 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	THR	C-N	-5.88	1.22	1.33
1	B	292	GLU	C-N	-5.12	1.22	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	347	GLN	O-C-N	5.20	131.02	122.70
1	B	52	LEU	CA-CB-CG	5.19	127.23	115.30

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	4883	0	4601	95	0
1	B	4883	0	4601	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	208	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 11.

All (208) 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:HD22	1:A:606:ASN:N	1.80	0.79
1:A:454:ASP:HB2	1:A:456:GLN:NE2	1.97	0.79
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:C	1:B:598:ASN:ND2	2.41	0.72
1:B:45:TRP:CD1	1:B:415:GLN:NE2	2.57	0.72
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:B:606:ASN:HD22	1:B:606:ASN:N	1.90	0.69
1:B:345:SER:OG	1:B:346:GLU:N	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:456:GLN:CD	1:A:457:THR:H	1.98	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:B:456:GLN:CD	1:B:457:THR:H	2.00	0.65
1:B:299:LEU:HD13	1:B:312:PHE:CD2	2.32	0.65
1:A:295:ASN:HD21	1:A:373:GLY:H	1.44	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:A:446:VAL:HG13	1:A:447:SER:N	2.16	0.60
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: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
1:A:320:SER:HA	1:A:330:SER:OG	2.04	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:B:45:TRP:HA	1:B:598:ASN:CG	2.25	0.57
1:A:486:ASP:OD2	1:A:638:ARG:HG2	2.05	0.56
1:A:347:GLN:HE22	1:A:349:GLY:HA3	1.70	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:B:297:LEU:CB	1:B:299:LEU:HD11	2.36	0.55
1:A:269:TRP:CZ3	1:A:271:GLU:OE2	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ASP:C	1:B:209:GLU:H	2.08	0.54
1:A:487:ARG:NH2	1:A:495:VAL:HG11	2.23	0.54
1:A:582:ASN:C	1:A:584:GLN:H	2.10	0.53
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: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:B:523:LEU:HA	1:B:632:GLU:HB2	1.92	0.51
1:B:299:LEU:HD13	1:B:312:PHE:HB2	1.92	0.51
1:A:213:ASN:O	1:A:217:VAL:HG23	2.11	0.51
1:B:45:TRP:HB2	1:B:599:ALA:CB	2.41	0.51
1:B:213:ASN:HD21	1:B:216:ALA:HB2	1.75	0.50
1:A:269:TRP:CH2	1:A:271:GLU:OE2	2.64	0.50
1:B:606:ASN:H	1:B:606:ASN:HD22	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:A:251:GLN:OE1	1:A:256:ALA:HA	2.12	0.50
1:B:33:LEU:H	1:B:562:ASN:ND2	2.07	0.49
1:B:269:TRP:CH2	1:B:271:GLU:OE2	2.65	0.49
1:A:397:VAL:HB	1:A:422:LEU:HD12	1.94	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:606:ASN:N	1:A:606:ASN:ND2	2.53	0.48
1:B:130:THR:OG1	1:B:160:VAL:HG13	2.13	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: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: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:A:118:PHE:HB2	1:A:136:THR:HB	1.96	0.48
1:A:439:GLU:H	1:A:439:GLU:CD	2.16	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:446:VAL:CG1	1:B:447:SER:N	2.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ASN:C	1:A:584:GLN:N	2.67	0.47
1:B:269:TRP:CZ3	1:B:271:GLU:OE2	2.67	0.47
1:A:454:ASP:O	1:A:455:ASN:HB2	2.15	0.47
1:B:198:ALA:HB2	1:B:224:TRP:CD2	2.49	0.47
1:A:57:GLN:HG3	1:A:80:ASP:HA	1.96	0.47
1:B:454:ASP:O	1:B:455:ASN:HB2	2.14	0.47
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: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:46:ARG:N	1:B:598:ASN:HD22	2.13	0.46
1:B:410:PHE:CD1	1:B:411:PRO:HD2	2.51	0.45
1:B:326:PRO:O	1:B:327:GLN:HB2	2.16	0.45
1:A:29:PRO:HB3	1:A:618:TRP:CD2	2.51	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:296:VAL:C	1:A:297:LEU:HD12	2.37	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:A:197:SER:HB2	1:A:298:PHE:CZ	2.51	0.45
1:B:299:LEU:CD1	1:B:312:PHE:HB2	2.47	0.45
1:A:430:GLN:HG2	1:A:464:GLY:HA3	1.97	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:582:ASN:C	1:B:584:GLN:H	2.19	0.45
1:B:175:PRO:HG2	1:B:178:ALA:HB2	1.97	0.45
1:A:297:LEU:HD12	1:A:297:LEU:N	2.32	0.45
1:A:226:GLU:OE2	1:A:306:PRO:HG3	2.17	0.45
1:A:410:PHE:CG	1:A:411:PRO:HD2	2.52	0.45
1:B:456:GLN:CD	1:B:457:THR:N	2.69	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:446:VAL:HG21	1:A:448:TRP:CZ2	2.52	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:597:ASP:O	1:B:598:ASN:CB	2.67	0.43
1:B:210:VAL:O	1:B:210:VAL:HG12	2.19	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:45:TRP:HB2	1:B:599:ALA:HB2	2.00	0.43
1:A:542:GLN:HG2	1:A:544:SER:OG	2.19	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
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:B:580:ILE:HG23	1:B:580:ILE:O	2.20	0.42
1:A:128:ASN:O	1:A:130:THR:HG23	2.20	0.42
1:A:99:SER:OG	1:A:103:SER:HA	2.19	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:244:PRO:HB2	1:A:291:PHE:CD1	2.54	0.42
1:B:446:VAL:HG21	1:B:448:TRP:CZ2	2.55	0.41
1:A:332:HIS:HB3	1:A:369:TYR:CD2	2.54	0.41
1:B:523:LEU:HD23	1:B:523:LEU:C	2.40	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: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:321:GLY:O	1:B:324:ILE:HD13	2.21	0.41
1:A:32:ASN:ND2	1:A:35:THR:HG23	2.35	0.41
1:B:454:ASP:C	1:B:456:GLN:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:TRP:CB	1:B:599:ALA:HB2	2.50	0.41
1:B:524:GLN:HA	1:B:541:TYR:O	2.20	0.41
1:B:380:SER:O	1:B:384:LYS:HG3	2.21	0.41
1:B:50:HIS:HD2	1:B:421:LEU:O	2.04	0.41
1:B:559:ALA:N	1:B:560:PRO:CD	2.84	0.41
1:A:438:ASN:HB2	1:A:439:GLU:OE2	2.21	0.40
1:A:130:THR:OG1	1:A:160:VAL:HG13	2.21	0.40
1:A:475:LEU:HD22	1:A:646:LEU:HD22	2.02	0.40
1:B:57:GLN:HG3	1:B:80:ASP:HA	2.04	0.40
1:A:559:ALA:N	1:A:560:PRO:CD	2.84	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:207:ASP:C	1:B:209:GLU:N	2.73	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

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%)	596 (94%)	32 (5%)	4 (1%)	30	22
1	B	632/634 (100%)	589 (93%)	41 (6%)	2 (0%)	46	41
All	All	1264/1268 (100%)	1185 (94%)	73 (6%)	6 (0%)	34	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	345	SER
1	B	345	SER
1	A	347	GLN

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Mol	Chain	Res	Type
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%)	39	35
1	B	515/517 (100%)	495 (96%)	20 (4%)	39	35
All	All	1030/1034 (100%)	990 (96%)	40 (4%)	39	35

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	TRP
1	A	52	LEU
1	A	57	GLN
1	A	111	LYS
1	A	137	SER
1	A	173	GLN
1	A	199	ARG
1	A	208	GLU
1	A	268	TRP
1	A	269	TRP
1	A	297	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	463	LEU
1	A	606	ASN
1	A	652	GLU

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Mol	Chain	Res	Type
1	B	45	TRP
1	B	52	LEU
1	B	55	GLU
1	B	57	GLN
1	B	173	GLN
1	B	199	ARG
1	B	208	GLU
1	B	268	TRP
1	B	269	TRP
1	B	297	LEU
1	B	347	GLN
1	B	348	GLU
1	B	417	TRP
1	B	427	LEU
1	B	430	GLN
1	B	439	GLU
1	B	446	VAL
1	B	463	LEU
1	B	606	ASN
1	B	652	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	57	GLN
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	639	ASN
1	B	39	ASN
1	B	57	GLN
1	B	156	GLN
1	B	213	ASN
1	B	295	ASN

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Mol	Chain	Res	Type
1	B	415	GLN
1	B	430	GLN
1	B	434	ASN
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 carbohydrates 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	0.62	0	17,17,17	2.75	3 (17%)
2	BGC	B	2	-	12,12,12	0.42	0	17,17,17	0.80	1 (5%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	BGC	C1-C2-C3	-3.38	105.40	110.43
2	B	2	BGC	C1-C2-C3	-2.44	106.79	110.43
2	A	1	BGC	C3-C4-C5	2.45	114.46	110.20
2	A	1	BGC	O6-C6-C5	10.20	145.03	111.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	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, 95^{th} 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%)	0.39	48 (7%)	17	18	8, 20, 58, 109	0
1	B	634/634 (100%)	0.37	48 (7%)	17	18	8, 19, 56, 104	0
All	All	1268/1268 (100%)	0.38	96 (7%)	17	18	8, 19, 58, 109	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	SER	12.2
1	A	21	TYR	11.6
1	B	345	SER	9.1
1	B	21	TYR	8.7
1	B	20	SER	8.3
1	B	346	GLU	7.8
1	B	212	ARG	7.5
1	A	346	GLU	7.4
1	A	208	GLU	7.2
1	A	211	ALA	7.0
1	A	212	ARG	6.8
1	B	208	GLU	6.7
1	A	345	SER	6.7
1	B	211	ALA	6.3
1	A	217	VAL	6.2
1	A	209	GLU	5.9
1	B	344	GLY	5.9
1	A	214	GLU	5.7
1	A	207	ASP	5.5
1	B	210	VAL	5.5
1	B	209	GLU	5.4
1	B	206	LEU	5.4
1	B	213	ASN	5.3
1	B	347	GLN	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	348	GLU	5.2
1	B	214	GLU	5.1
1	B	215	THR	5.1
1	B	348	GLU	5.1
1	B	45	TRP	4.8
1	A	45	TRP	4.7
1	A	347	GLN	4.4
1	B	279	ASP	4.3
1	A	454	ASP	4.2
1	B	207	ASP	4.2
1	B	227	LYS	4.1
1	B	454	ASP	4.1
1	A	227	LYS	4.1
1	A	210	VAL	4.1
1	A	349	GLY	4.0
1	B	349	GLY	3.9
1	A	455	ASN	3.9
1	A	580	ILE	3.9
1	A	215	THR	3.9
1	B	455	ASN	3.9
1	A	213	ASN	3.8
1	B	216	ALA	3.8
1	A	279	ASP	3.7
1	A	216	ALA	3.7
1	B	101	ASN	3.6
1	A	228	ASN	3.4
1	A	206	LEU	3.4
1	A	456	GLN	3.2
1	B	269	TRP	3.2
1	A	219	GLN	3.2
1	A	583	GLY	3.1
1	A	598	ASN	3.0
1	B	225	THR	3.0
1	A	417	TRP	2.9
1	B	451	GLY	2.9
1	B	417	TRP	2.9
1	A	22	HIS	2.8
1	B	219	GLN	2.8
1	B	584	GLN	2.8
1	A	581	GLU	2.8
1	B	322	LEU	2.7
1	B	478	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	344	GLY	2.7
1	B	280	GLU	2.7
1	B	452	GLU	2.6
1	B	598	ASN	2.6
1	A	597	ASP	2.6
1	B	583	GLY	2.5
1	A	101	ASN	2.5
1	A	281	GLY	2.5
1	B	217	VAL	2.5
1	B	581	GLU	2.4
1	A	323	PRO	2.4
1	B	22	HIS	2.4
1	B	228	ASN	2.4
1	A	453	SER	2.4
1	B	390	VAL	2.3
1	B	233	VAL	2.3
1	B	323	PRO	2.3
1	A	322	LEU	2.3
1	B	222	ASP	2.3
1	B	582	ASN	2.3
1	A	280	GLU	2.3
1	A	343	VAL	2.2
1	A	582	ASN	2.2
1	A	218	GLN	2.1
1	A	584	GLN	2.1
1	B	444	GLU	2.1
1	A	121	ALA	2.1
1	A	592	LEU	2.1
1	B	580	ILE	2.0
1	A	269	TRP	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

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^{th} 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^2)	Q<0.9
2	BGC	B	2	12/12	0.71	0.23	9.45	25,25,25,25	0
2	BGC	A	1	12/12	0.80	0.19	5.71	24,24,24,24	0

6.5 Other polymers

There are no such residues in this entry.