



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:16 AM GMT

PDB ID : 2GDV  
Title : Sucrose phosphorylase from BIFIDOBACTERIUM ADOLESCENTIS reacted with sucrose  
Authors : Skov, L.K.; Mirza, O.; Gajhede, M.; Katsrup, J.S.  
Deposited on : 2006-03-17  
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](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

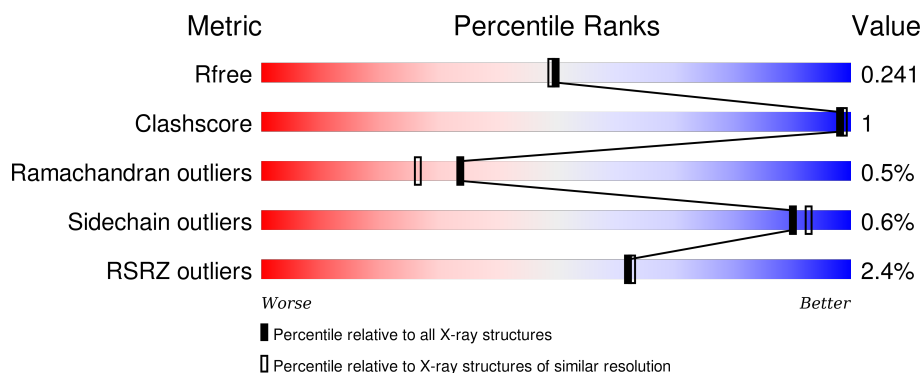
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

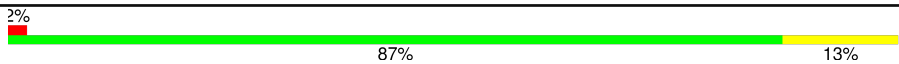

The reported resolution of this entry is 2.00 Å.

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	504	
1	B	504	

## 2 Entry composition [i](#)

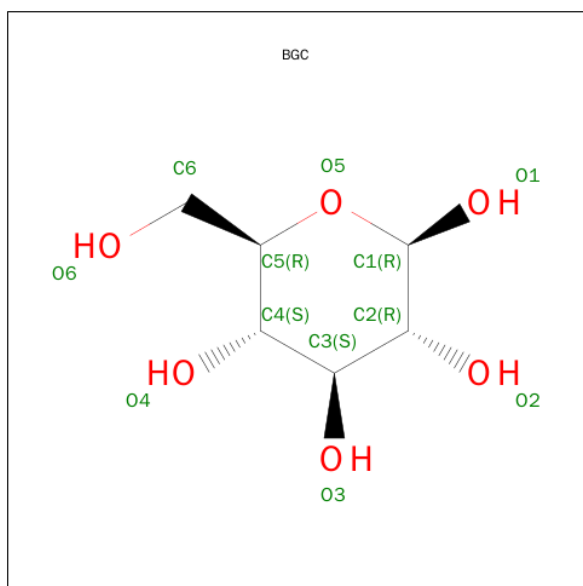
There are 3 unique types of molecules in this entry. The entry contains 8959 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 sucrose phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			3965	2507	671	774	13			
1	B	504	Total	C	N	O	S	0	0	0
			3965	2507	671	774	13			

- 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
			11	6	5		
2	B	1	Total	C	O	0	0
			12	6	6		

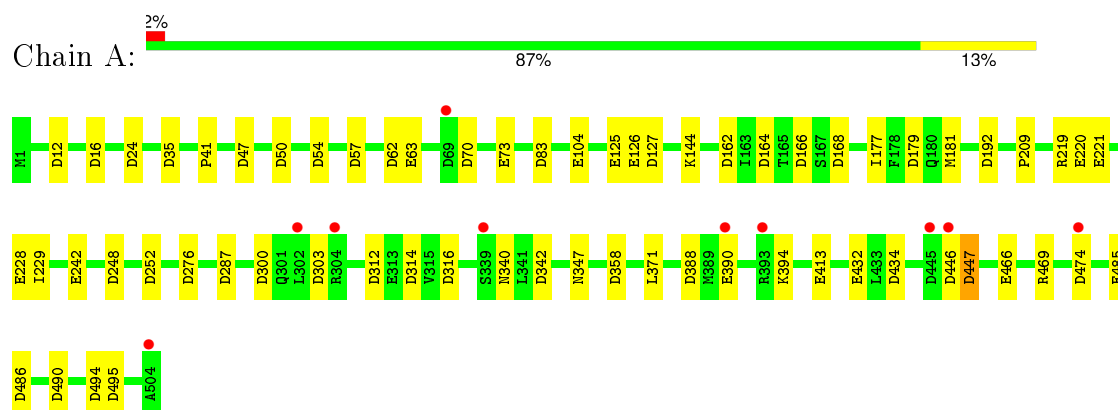
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	504	Total 504	O 504	0	0
3	B	502	Total 502	O 502	0	0

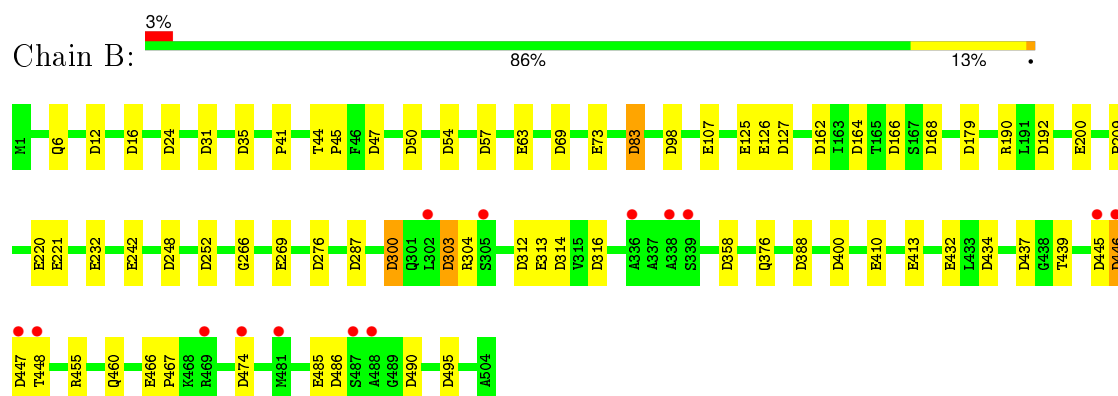
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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: sucrose phosphorylase



- Molecule 1: sucrose phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.74Å 103.07Å 150.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.00 19.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.89-2.00) 99.4 (19.89-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 1.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.198 , 0.237 0.204 , 0.241	Depositor DCC
$R_{free}$ test set	4028 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 80298 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8959	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.66	1/4059 (0.0%)	1.63	93/5519 (1.7%)
1	B	0.64	0/4059	1.65	109/5519 (2.0%)
All	All	0.65	1/8118 (0.0%)	1.64	202/11038 (1.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	ASP	CG-OD2	7.94	1.43	1.25

All (202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	ASP	CB-CG-OD1	-35.81	86.07	118.30
1	A	276	ASP	CB-CG-OD2	35.67	150.40	118.30
1	B	276	ASP	CB-CG-OD2	-22.53	98.02	118.30
1	B	276	ASP	CB-CG-OD1	22.49	138.54	118.30
1	A	300	ASP	CB-CG-OD1	22.39	138.45	118.30
1	A	300	ASP	CB-CG-OD2	-21.98	98.52	118.30
1	B	434	ASP	CB-CG-OD1	20.50	136.75	118.30
1	B	445	ASP	CB-CG-OD1	20.50	136.75	118.30
1	B	445	ASP	CB-CG-OD2	-20.33	100.00	118.30
1	B	434	ASP	CB-CG-OD2	-18.86	101.33	118.30
1	A	434	ASP	CB-CG-OD1	18.79	135.21	118.30
1	A	434	ASP	CB-CG-OD2	-17.55	102.50	118.30
1	A	54	ASP	CB-CG-OD2	-17.26	102.77	118.30
1	A	54	ASP	CB-CG-OD1	17.23	133.81	118.30
1	B	446	ASP	CB-CG-OD1	15.34	132.11	118.30
1	B	495	ASP	CB-CG-OD1	15.11	131.90	118.30
1	B	447	ASP	CB-CG-OD2	15.10	131.89	118.30
1	B	474	ASP	CB-CG-OD1	14.53	131.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ASP	CB-CG-OD1	14.37	131.23	118.30
1	B	447	ASP	CB-CG-OD1	-14.34	105.39	118.30
1	B	314	ASP	CB-CG-OD1	14.18	131.06	118.30
1	A	166	ASP	CB-CG-OD1	14.15	131.04	118.30
1	A	127	ASP	CB-CG-OD2	-14.13	105.58	118.30
1	B	474	ASP	CB-CG-OD2	-13.91	105.78	118.30
1	B	495	ASP	CB-CG-OD2	-13.78	105.90	118.30
1	B	446	ASP	CB-CG-OD2	-13.55	106.11	118.30
1	B	314	ASP	CB-CG-OD2	-13.48	106.17	118.30
1	A	166	ASP	CB-CG-OD2	-13.43	106.21	118.30
1	B	54	ASP	CB-CG-OD2	-13.40	106.24	118.30
1	B	303	ASP	CB-CG-OD1	13.37	130.33	118.30
1	B	69	ASP	CB-CG-OD1	13.31	130.28	118.30
1	A	50	ASP	CB-CG-OD1	13.23	130.21	118.30
1	B	54	ASP	CB-CG-OD1	12.98	129.99	118.30
1	B	303	ASP	CB-CG-OD2	-12.94	106.66	118.30
1	A	168	ASP	CB-CG-OD1	12.94	129.94	118.30
1	B	300	ASP	CB-CG-OD1	12.76	129.79	118.30
1	B	486	ASP	CB-CG-OD1	12.74	129.77	118.30
1	B	69	ASP	CB-CG-OD2	-12.71	106.86	118.30
1	B	16	ASP	CB-CG-OD1	12.68	129.71	118.30
1	A	168	ASP	CB-CG-OD2	-12.52	107.03	118.30
1	A	50	ASP	CB-CG-OD2	-12.50	107.05	118.30
1	A	316	ASP	CB-CG-OD1	12.42	129.48	118.30
1	B	127	ASP	CB-CG-OD1	12.42	129.48	118.30
1	A	16	ASP	CB-CG-OD1	12.36	129.43	118.30
1	B	168	ASP	CB-CG-OD1	12.26	129.33	118.30
1	B	16	ASP	CB-CG-OD2	-12.12	107.39	118.30
1	A	447	ASP	CB-CG-OD1	11.79	128.92	118.30
1	A	316	ASP	CB-CG-OD2	-11.79	107.69	118.30
1	A	16	ASP	CB-CG-OD2	-11.76	107.72	118.30
1	B	300	ASP	CB-CG-OD2	-11.75	107.73	118.30
1	B	127	ASP	CB-CG-OD2	-11.70	107.77	118.30
1	B	490	ASP	CB-CG-OD1	11.68	128.81	118.30
1	B	12	ASP	CB-CG-OD2	-11.66	107.81	118.30
1	B	168	ASP	CB-CG-OD2	-11.55	107.90	118.30
1	B	490	ASP	CB-CG-OD2	-11.55	107.91	118.30
1	B	242	GLU	CG-CD-OE2	-11.39	95.52	118.30
1	B	12	ASP	CB-CG-OD1	11.38	128.54	118.30
1	B	486	ASP	CB-CG-OD2	-11.33	108.11	118.30
1	B	242	GLU	CG-CD-OE1	11.29	140.88	118.30
1	A	447	ASP	CB-CG-OD2	-11.19	108.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	ASP	CB-CG-OD1	10.76	127.98	118.30
1	A	179	ASP	CB-CG-OD1	10.72	127.95	118.30
1	A	35	ASP	CB-CG-OD1	10.61	127.85	118.30
1	A	221	GLU	CG-CD-OE1	10.47	139.24	118.30
1	A	312	ASP	CB-CG-OD1	10.46	127.72	118.30
1	B	179	ASP	CB-CG-OD1	10.44	127.69	118.30
1	A	432	GLU	CG-CD-OE1	10.31	138.91	118.30
1	A	388	ASP	CB-CG-OD1	10.30	127.57	118.30
1	A	221	GLU	CG-CD-OE2	-10.29	97.72	118.30
1	A	314	ASP	CB-CG-OD1	10.15	127.44	118.30
1	B	287	ASP	CB-CG-OD1	10.03	127.33	118.30
1	B	388	ASP	CB-CG-OD1	9.95	127.25	118.30
1	B	248	ASP	CB-CG-OD1	9.94	127.25	118.30
1	B	179	ASP	CB-CG-OD2	-9.88	109.41	118.30
1	B	400	ASP	CB-CG-OD1	9.87	127.18	118.30
1	B	312	ASP	CB-CG-OD1	9.86	127.17	118.30
1	A	432	GLU	CG-CD-OE2	-9.84	98.63	118.30
1	A	490	ASP	CB-CG-OD1	9.82	127.14	118.30
1	B	192	ASP	CB-CG-OD2	9.81	127.13	118.30
1	A	179	ASP	CB-CG-OD2	-9.80	109.48	118.30
1	B	126	GLU	CG-CD-OE1	9.80	137.91	118.30
1	B	232	GLU	CG-CD-OE2	-9.80	98.70	118.30
1	A	126	GLU	CG-CD-OE1	9.79	137.87	118.30
1	A	312	ASP	CB-CG-OD2	-9.64	109.63	118.30
1	B	126	GLU	CG-CD-OE2	-9.55	99.20	118.30
1	B	200	GLU	CG-CD-OE1	9.54	137.37	118.30
1	A	358	ASP	CB-CG-OD1	9.50	126.85	118.30
1	A	164	ASP	CB-CG-OD1	9.49	126.84	118.30
1	B	232	GLU	CG-CD-OE1	9.42	137.13	118.30
1	A	70	ASP	CB-CG-OD1	9.41	126.77	118.30
1	B	192	ASP	CB-CG-OD1	-9.27	109.96	118.30
1	A	35	ASP	CB-CG-OD2	-9.22	110.00	118.30
1	B	248	ASP	CB-CG-OD2	-9.13	110.08	118.30
1	A	358	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	B	312	ASP	CB-CG-OD2	-9.08	110.12	118.30
1	A	126	GLU	CG-CD-OE2	-9.06	100.17	118.30
1	A	303	ASP	CB-CG-OD2	-8.97	110.23	118.30
1	B	35	ASP	CB-CG-OD1	8.79	126.21	118.30
1	A	314	ASP	CB-CG-OD2	-8.76	110.42	118.30
1	B	400	ASP	CB-CG-OD2	-8.69	110.48	118.30
1	A	388	ASP	CB-CG-OD2	-8.68	110.49	118.30
1	A	162	ASP	CB-CG-OD1	8.63	126.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ASP	CB-CG-OD2	-8.57	110.59	118.30
1	B	269	GLU	CG-CD-OE1	8.49	135.27	118.30
1	B	269	GLU	CG-CD-OE2	-8.42	101.46	118.30
1	A	390	GLU	CG-CD-OE1	8.41	135.12	118.30
1	A	490	ASP	CB-CG-OD2	-8.35	110.78	118.30
1	A	486	ASP	CB-CG-OD1	8.35	125.81	118.30
1	A	287	ASP	CB-CG-OD1	8.30	125.77	118.30
1	A	342	ASP	CB-CG-OD1	8.30	125.77	118.30
1	B	287	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	B	200	GLU	CG-CD-OE2	-8.27	101.77	118.30
1	B	98	ASP	CB-CG-OD1	8.08	125.58	118.30
1	B	50	ASP	CB-CG-OD1	8.07	125.57	118.30
1	A	390	GLU	CG-CD-OE2	-8.07	102.17	118.30
1	B	24	ASP	CB-CG-OD1	8.04	125.53	118.30
1	A	162	ASP	CB-CG-OD2	-7.95	111.14	118.30
1	A	495	ASP	CB-CG-OD1	7.94	125.45	118.30
1	A	47	ASP	CB-CG-OD1	7.83	125.35	118.30
1	A	242	GLU	CG-CD-OE2	-7.70	102.91	118.30
1	A	242	GLU	CG-CD-OE1	7.67	133.64	118.30
1	A	342	ASP	CB-CG-OD2	-7.65	111.41	118.30
1	A	164	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	B	24	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	B	98	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	B	388	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	B	166	ASP	CB-CG-OD1	7.38	124.95	118.30
1	B	437	ASP	CB-CG-OD1	7.27	124.84	118.30
1	B	31	ASP	CB-CG-OD1	7.26	124.83	118.30
1	A	57	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	12	ASP	CB-CG-OD1	7.19	124.77	118.30
1	B	485	GLU	CG-CD-OE2	7.11	132.53	118.30
1	A	485	GLU	CG-CD-OE1	7.10	132.50	118.30
1	A	485	GLU	CG-CD-OE2	-7.00	104.30	118.30
1	B	35	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	B	358	ASP	CB-CG-OD1	6.95	124.55	118.30
1	B	413	GLU	CG-CD-OE1	6.93	132.15	118.30
1	A	287	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	B	485	GLU	CG-CD-OE1	-6.90	104.50	118.30
1	A	24	ASP	CB-CG-OD1	6.88	124.50	118.30
1	B	162	ASP	CB-CG-OD2	6.87	124.48	118.30
1	B	316	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	47	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	A	12	ASP	CB-CG-OD2	-6.72	112.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	221	GLU	CG-CD-OE1	6.71	131.72	118.30
1	A	486	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	A	495	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	A	413	GLU	CG-CD-OE1	6.66	131.61	118.30
1	B	83	ASP	CB-CG-OD1	-6.64	112.32	118.30
1	A	73	GLU	CG-CD-OE1	6.60	131.50	118.30
1	A	220	GLU	CG-CD-OE1	6.55	131.39	118.30
1	B	50	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	B	437	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	B	166	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	B	413	GLU	CG-CD-OE2	-6.40	105.50	118.30
1	A	73	GLU	CG-CD-OE2	-6.39	105.51	118.30
1	A	24	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	B	252	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	413	GLU	CG-CD-OE2	-6.36	105.58	118.30
1	B	221	GLU	CG-CD-OE2	-6.32	105.67	118.30
1	B	107	GLU	CG-CD-OE1	6.25	130.81	118.30
1	A	104	GLU	CG-CD-OE1	6.24	130.78	118.30
1	A	220	GLU	CG-CD-OE2	-6.23	105.84	118.30
1	A	104	GLU	CG-CD-OE2	-6.15	105.99	118.30
1	B	125	GLU	CG-CD-OE1	6.14	130.59	118.30
1	B	164	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	410	GLU	CG-CD-OE1	-6.02	106.25	118.30
1	B	107	GLU	CG-CD-OE2	-5.94	106.42	118.30
1	A	83	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	B	125	GLU	CG-CD-OE2	-5.90	106.50	118.30
1	B	47	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	494	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	57	ASP	CB-CG-OD1	5.85	123.57	118.30
1	B	31	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	B	410	GLU	CG-CD-OE2	5.81	129.92	118.30
1	B	316	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	B	432	GLU	CG-CD-OE1	5.74	129.77	118.30
1	B	162	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	B	358	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	A	474	ASP	CB-CG-OD1	5.53	123.27	118.30
1	A	63	GLU	CG-CD-OE1	5.49	129.28	118.30
1	B	220	GLU	CG-CD-OE1	5.49	129.27	118.30
1	B	63	GLU	CG-CD-OE1	5.48	129.25	118.30
1	A	228	GLU	CG-CD-OE2	-5.47	107.36	118.30
1	A	83	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	313	GLU	CG-CD-OE1	5.45	129.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	466	GLU	CG-CD-OE1	5.41	129.12	118.30
1	A	125	GLU	CG-CD-OE1	5.40	129.10	118.30
1	A	228	GLU	CG-CD-OE1	5.36	129.01	118.30
1	A	57	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	B	432	GLU	CG-CD-OE2	-5.32	107.66	118.30
1	B	73	GLU	CG-CD-OE2	-5.31	107.69	118.30
1	A	125	GLU	CG-CD-OE2	-5.30	107.70	118.30
1	A	63	GLU	CG-CD-OE2	-5.27	107.76	118.30
1	B	63	GLU	CG-CD-OE2	-5.27	107.76	118.30
1	B	466	GLU	CG-CD-OE2	-5.22	107.87	118.30
1	B	220	GLU	CG-CD-OE2	-5.21	107.87	118.30
1	A	248	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	73	GLU	CG-CD-OE1	5.13	128.56	118.30
1	A	62	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	252	ASP	CB-CG-OD1	5.06	122.85	118.30

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	3965	0	3823	9	0
1	B	3965	0	3823	8	0
2	A	11	0	10	0	0
2	B	12	0	12	0	0
3	A	504	0	0	0	0
3	B	502	0	0	0	0
All	All	8959	0	7668	15	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 1.

All (15) 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:340:ASN:ND2	1:A:347:ASN:HD21	2.00	0.59
1:A:144:LYS:NZ	1:B:304:ARG:HH21	2.06	0.52
1:B:266:GLY:HA2	1:B:467:PRO:HB2	1.92	0.52
1:B:455:ARG:HH11	1:B:460:GLN:NE2	2.09	0.51
1:A:219:ARG:HA	1:A:229:ILE:HG13	1.95	0.49
1:A:340:ASN:HD21	1:A:347:ASN:ND2	2.13	0.47
1:B:6:GLN:HB2	1:B:376:GLN:HG2	1.99	0.45
1:B:44:THR:HA	1:B:45:PRO:HA	1.94	0.43
1:A:340:ASN:HD21	1:A:347:ASN:HD21	1.64	0.43
1:B:83:ASP:OD1	1:B:190:ARG:HD3	2.19	0.42
1:A:371:LEU:HA	1:A:371:LEU:HD23	1.97	0.41
1:A:466:GLU:O	1:A:469:ARG:HG2	2.20	0.41
1:A:144:LYS:HZ1	1:B:304:ARG:HH21	1.69	0.41
1:A:177:ILE:O	1:A:181:MET:HG2	2.21	0.40
1:B:300:ASP:HB3	1:B:303:ASP:O	2.21	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	502/504 (100%)	490 (98%)	9 (2%)	3 (1%)	30	22
1	B	502/504 (100%)	484 (96%)	16 (3%)	2 (0%)	39	33
All	All	1004/1008 (100%)	974 (97%)	25 (2%)	5 (0%)	34	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	448	THR
1	A	446	ASP
1	A	447	ASP
1	A	41	PRO

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Mol	Chain	Res	Type
1	B	41	PRO

### 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	428/428 (100%)	426 (100%)	2 (0%)	92	94
1	B	428/428 (100%)	425 (99%)	3 (1%)	88	91
All	All	856/856 (100%)	851 (99%)	5 (1%)	90	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	PRO
1	A	394	LYS
1	B	209	PRO
1	B	439	THR
1	B	446	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
1	A	340	ASN
1	B	79	ASN
1	B	97	GLN
1	B	267	HIS
1	B	347	ASN
1	B	460	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	700	1	11,11,12	1.71	4 (36%)	14,15,17	1.84	2 (14%)
2	BGC	B	701	-	12,12,12	0.32	0	17,17,17	0.98	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	700	1	-	0/2/19/22	0/1/1/1
2	BGC	B	701	-	-	0/2/22/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	BGC	O5-C1	2.19	1.47	1.43
2	A	700	BGC	C1-C2	2.59	1.58	1.52
2	A	700	BGC	O5-C5	2.96	1.50	1.43
2	A	700	BGC	C2-C3	3.23	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	701	BGC	C1-C2-C3	-2.76	106.32	110.43
2	A	700	BGC	C1-C2-C3	3.87	114.12	109.54
2	A	700	BGC	C1-O5-C5	5.18	118.82	112.25

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	504/504 (100%)	0.04	10 (1%) 68 69	15, 24, 40, 65	0
1	B	504/504 (100%)	0.03	14 (2%) 56 57	12, 23, 50, 76	0
All	All	1008/1008 (100%)	0.03	24 (2%) 62 63	12, 24, 46, 76	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	446	ASP	6.0
1	B	446	ASP	5.7
1	B	338	ALA	3.5
1	B	487	SER	3.4
1	B	447	ASP	3.3
1	B	448	THR	3.1
1	B	336	ALA	3.0
1	A	504	ALA	3.0
1	A	302	LEU	2.8
1	B	474	ASP	2.7
1	B	445	ASP	2.7
1	A	304	ARG	2.6
1	A	390	GLU	2.6
1	B	305	SER	2.5
1	A	474	ASP	2.5
1	B	469	ARG	2.4
1	A	69	ASP	2.4
1	A	393	ARG	2.3
1	B	339	SER	2.3
1	A	445	ASP	2.2
1	B	302	LEU	2.2
1	B	488	ALA	2.1
1	B	481	MET	2.1
1	A	339	SER	2.1

## 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	BGC	A	700	11/12	0.87	0.14	1.59	23,28,30,30	0
2	BGC	B	701	12/12	0.97	0.08	-0.58	16,18,21,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.