



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:51 PM UTC

PDB ID : 2GBP / pdb_00002gbp
Title : SUGAR AND SIGNAL-TRANSDUCER BINDING SITES OF THE ES-
CHERICHIA COLI GALACTOSE CHEMORECEPTOR PROTEIN
Authors : Vyas, N.K.; Vyas, M.N.; Quioco, F.A.
Deposited on : 1989-02-23
Resolution : 1.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

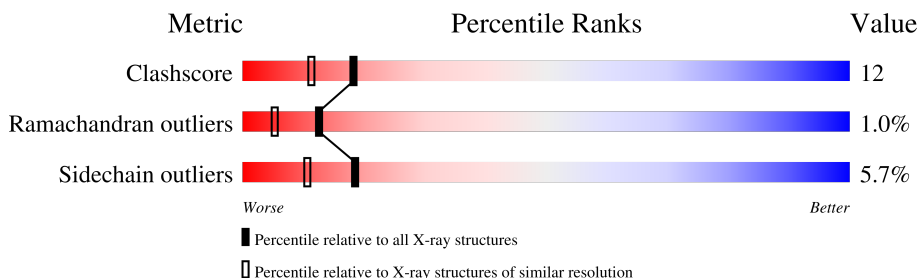
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	309	

2 Entry composition [i](#)

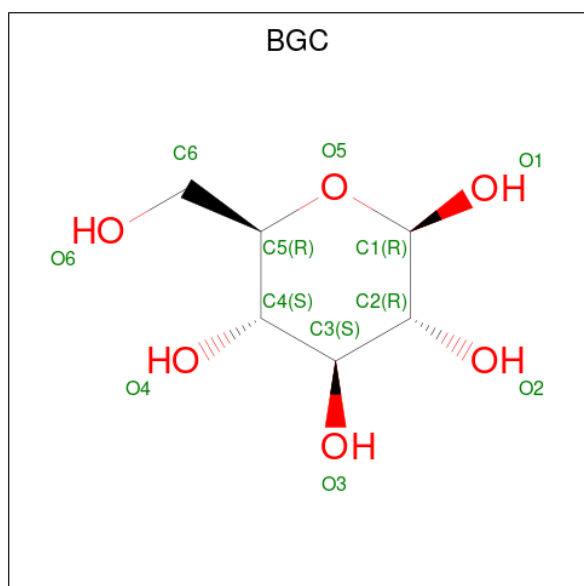
There are 4 unique types of molecules in this entry. The entry contains 2575 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-GALACTOSE/D-GLUCOSE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2348	1473	406	463	6			

- 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		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is water.

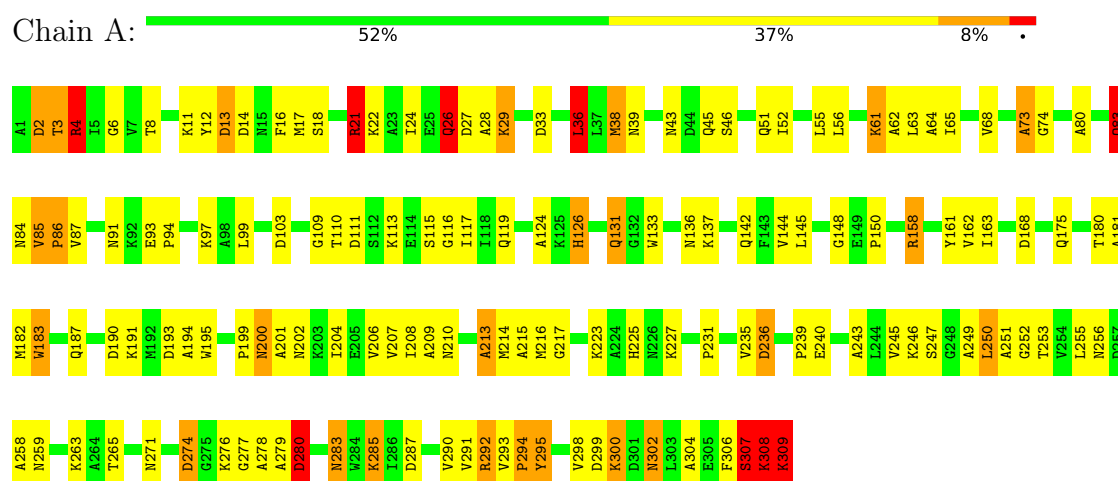
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	214	Total 214	O 214	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

• Molecule 1: D-GALACTOSE/D-GLUCOSE BINDING PROTEIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.00Å 37.05Å 61.57Å 90.00° 106.80° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.146 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2575	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	1.68	21/2384 (0.9%)	2.43	150/3229 (4.6%)

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	3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	GLY	N-CA	9.29	1.58	1.45
1	A	252	GLY	CA-C	7.05	1.59	1.51
1	A	215	ALA	N-CA	6.52	1.54	1.46
1	A	6	GLY	CA-C	6.29	1.58	1.52
1	A	256	ASN	N-CA	5.97	1.53	1.46
1	A	181	ALA	CA-C	5.89	1.60	1.52
1	A	213	ALA	N-CA	5.67	1.53	1.46
1	A	110	THR	CA-CB	5.63	1.63	1.53
1	A	207	VAL	N-CA	5.53	1.52	1.46
1	A	195	TRP	N-CA	5.50	1.53	1.46
1	A	204	ILE	CA-CB	5.50	1.60	1.54
1	A	150	PRO	C-O	5.45	1.30	1.23
1	A	148	GLY	N-CA	5.30	1.51	1.45
1	A	74	GLY	N-CA	5.27	1.52	1.45
1	A	199	PRO	C-O	5.25	1.30	1.24
1	A	62	ALA	N-CA	5.20	1.52	1.46
1	A	17	MET	N-CA	5.17	1.52	1.46
1	A	180	THR	C-O	5.15	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	ARG	N-CA	5.13	1.52	1.46
1	A	137	LYS	C-O	5.04	1.30	1.24
1	A	163	ILE	N-CA	5.03	1.52	1.46

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ASN	CA-CB-CG	-16.36	96.24	112.60
1	A	68	VAL	N-CA-C	-11.50	100.28	110.74
1	A	2	ASP	CA-C-O	10.39	132.99	120.62
1	A	280	ASP	CA-CB-CG	-10.31	102.29	112.60
1	A	119	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	A	252	GLY	O-C-N	9.05	133.01	123.87
1	A	51	GLN	OE1-CD-NE2	8.79	131.39	122.60
1	A	21	ARG	CD-NE-CZ	-8.77	112.12	124.40
1	A	28	ALA	CA-C-O	-8.60	111.44	120.55
1	A	306	PHE	CA-CB-CG	-8.52	105.28	113.80
1	A	256	ASN	N-CA-C	-8.41	93.81	108.20
1	A	193	ASP	CA-C-N	8.21	131.12	120.44
1	A	193	ASP	C-N-CA	8.21	131.12	120.44
1	A	276	LYS	CA-C-O	-7.99	109.67	119.18
1	A	278	ALA	CA-C-O	-7.96	112.00	120.92
1	A	29	LYS	N-CA-CB	7.84	122.53	110.14
1	A	292	ARG	CD-NE-CZ	-7.74	113.56	124.40
1	A	126	HIS	CA-CB-CG	-7.71	106.09	113.80
1	A	119	GLN	CA-C-O	-7.61	112.83	120.82
1	A	39	ASN	OD1-CG-ND2	-7.56	115.04	122.60
1	A	131	GLN	CA-CB-CG	7.50	129.10	114.10
1	A	109	GLY	O-C-N	7.50	132.45	122.70
1	A	307	SER	O-C-N	7.45	131.66	122.86
1	A	256	ASN	CB-CA-C	7.41	122.63	110.78
1	A	43	ASN	OD1-CG-ND2	-7.37	115.23	122.60
1	A	116	GLY	O-C-N	7.21	129.11	122.19
1	A	309	LYS	CA-C-O	-7.13	108.67	120.80
1	A	239	PRO	CA-C-N	7.09	129.78	120.28
1	A	239	PRO	C-N-CA	7.09	129.78	120.28
1	A	245	VAL	N-CA-C	-6.96	103.99	110.53
1	A	309	LYS	N-CA-CB	6.92	122.27	110.50
1	A	308	LYS	CA-C-N	6.80	133.94	121.70
1	A	308	LYS	C-N-CA	6.80	133.94	121.70
1	A	287	ASP	CB-CA-C	6.79	120.87	110.62
1	A	14	ASP	N-CA-C	-6.77	99.81	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ALA	O-C-N	6.71	128.98	122.07
1	A	195	TRP	CA-C-O	-6.71	113.44	120.55
1	A	265	THR	O-C-N	6.60	128.87	122.07
1	A	86	PRO	CA-C-N	-6.54	113.90	122.99
1	A	86	PRO	C-N-CA	-6.54	113.90	122.99
1	A	93	GLU	N-CA-C	6.53	119.08	109.42
1	A	29	LYS	CB-CA-C	-6.50	97.86	110.46
1	A	307	SER	N-CA-CB	6.45	119.46	110.17
1	A	291	VAL	CA-C-O	-6.44	113.70	120.39
1	A	247	SER	CB-CA-C	-6.35	98.47	110.67
1	A	276	LYS	N-CA-C	6.35	121.03	113.28
1	A	4	ARG	CD-NE-CZ	-6.33	115.54	124.40
1	A	231	PRO	O-C-N	6.31	131.08	123.13
1	A	119	GLN	O-C-N	6.28	128.54	122.07
1	A	27	ASP	O-C-N	6.24	128.73	122.12
1	A	158	ARG	NE-CZ-NH2	-6.23	113.59	119.20
1	A	142	GLN	N-CA-C	-6.22	98.39	108.41
1	A	277	GLY	N-CA-C	-6.21	98.46	113.18
1	A	199	PRO	O-C-N	-6.20	114.23	122.22
1	A	259	ASN	OD1-CG-ND2	-6.16	116.44	122.60
1	A	309	LYS	N-CA-C	-6.16	93.76	111.00
1	A	213	ALA	CA-C-O	-6.10	114.08	120.55
1	A	274	ASP	CA-C-O	-6.07	111.93	119.28
1	A	283	ASN	CA-CB-CG	-6.05	106.55	112.60
1	A	246	LYS	CA-C-N	6.02	129.47	120.31
1	A	246	LYS	C-N-CA	6.02	129.47	120.31
1	A	36	LEU	CA-C-O	-6.02	113.86	120.43
1	A	187	GLN	O-C-N	6.02	128.50	122.12
1	A	64	ALA	N-CA-C	-6.01	97.33	108.02
1	A	168	ASP	O-C-N	5.97	128.45	122.12
1	A	131	GLN	N-CA-C	-5.92	105.91	113.01
1	A	103	ASP	CA-CB-CG	-5.91	106.69	112.60
1	A	117	ILE	CA-C-O	-5.90	114.50	121.05
1	A	195	TRP	O-C-N	5.88	128.36	122.12
1	A	51	GLN	CG-CD-NE2	-5.86	107.61	116.40
1	A	258	ALA	CA-C-O	-5.86	114.34	120.55
1	A	200	ASN	CB-CA-C	-5.84	99.98	110.37
1	A	236	ASP	O-C-N	5.84	130.35	122.59
1	A	68	VAL	N-CA-CB	5.83	117.64	110.64
1	A	87	VAL	CB-CA-C	5.82	118.83	110.33
1	A	26	GLN	CG-CD-NE2	-5.80	107.70	116.40
1	A	52	ILE	O-C-N	5.80	127.50	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	LYS	CA-C-N	5.78	128.02	120.28
1	A	263	LYS	C-N-CA	5.78	128.02	120.28
1	A	276	LYS	CA-C-N	-5.76	110.12	121.41
1	A	276	LYS	C-N-CA	-5.76	110.12	121.41
1	A	12	TYR	CA-C-N	-5.73	112.70	122.56
1	A	12	TYR	C-N-CA	-5.73	112.70	122.56
1	A	85	VAL	CA-C-N	5.71	125.61	119.85
1	A	85	VAL	C-N-CA	5.71	125.61	119.85
1	A	251	ALA	CA-C-O	5.68	126.49	119.79
1	A	4	ARG	O-C-N	5.67	129.68	123.27
1	A	175	GLN	OE1-CD-NE2	5.65	128.25	122.60
1	A	227	LYS	CG-CD-CE	5.65	124.29	111.30
1	A	46	SER	CA-CB-OG	-5.65	99.81	111.10
1	A	309	LYS	CB-CA-C	5.64	120.81	110.10
1	A	65	ILE	O-C-N	5.62	129.08	123.18
1	A	249	ALA	CA-C-N	5.57	130.69	123.00
1	A	249	ALA	C-N-CA	5.57	130.69	123.00
1	A	239	PRO	O-C-N	-5.55	115.86	122.24
1	A	73	ALA	O-C-N	5.54	128.00	122.12
1	A	294	PRO	O-C-N	5.54	129.88	123.06
1	A	83	GLN	O-C-N	5.54	128.89	122.19
1	A	193	ASP	CA-C-O	-5.53	115.01	120.82
1	A	253	THR	CA-CB-CG2	5.52	119.89	110.50
1	A	63	LEU	CA-C-O	-5.49	114.77	120.70
1	A	29	LYS	O-C-N	5.47	128.44	122.20
1	A	309	LYS	CA-CB-CG	-5.46	103.18	114.10
1	A	3	THR	O-C-N	5.45	129.40	123.13
1	A	250	LEU	CA-C-O	-5.45	114.44	120.38
1	A	209	ALA	O-C-N	-5.43	116.12	123.19
1	A	306	PHE	O-C-N	5.43	130.28	122.13
1	A	210	ASN	CA-CB-CG	5.41	118.01	112.60
1	A	11	LYS	CA-C-O	5.40	126.57	119.98
1	A	190	ASP	CA-C-O	-5.38	114.72	120.42
1	A	255	LEU	CA-C-O	-5.37	114.36	120.58
1	A	56	LEU	O-C-N	5.35	127.79	122.12
1	A	161	TYR	CA-CB-CG	-5.34	104.28	113.90
1	A	162	VAL	N-CA-C	-5.34	105.33	110.72
1	A	295	TYR	CA-C-O	-5.29	115.47	121.72
1	A	13	ASP	CA-CB-CG	-5.29	107.31	112.60
1	A	308	LYS	CA-C-O	5.29	128.07	120.51
1	A	2	ASP	N-CA-C	5.28	116.75	109.15
1	A	64	ALA	CA-C-O	-5.27	114.64	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ASN	CA-CB-CG	-5.27	107.33	112.60
1	A	206	VAL	CA-C-N	-5.26	116.67	123.19
1	A	206	VAL	C-N-CA	-5.26	116.67	123.19
1	A	124	ALA	O-C-N	-5.25	116.63	122.09
1	A	243	ALA	CA-C-N	5.24	128.28	120.31
1	A	243	ALA	C-N-CA	5.24	128.28	120.31
1	A	183	TRP	N-CA-CB	-5.21	104.65	113.15
1	A	16	PHE	CA-CB-CG	-5.20	108.60	113.80
1	A	136	ASN	OD1-CG-ND2	5.20	127.80	122.60
1	A	39	ASN	CA-CB-CG	5.19	117.79	112.60
1	A	110	THR	N-CA-C	5.17	116.84	109.14
1	A	84	ASN	OD1-CG-ND2	5.15	127.75	122.60
1	A	8	THR	N-CA-CB	5.15	119.33	110.68
1	A	144	VAL	N-CA-C	-5.15	100.47	108.86
1	A	214	MET	O-C-N	5.14	128.01	122.15
1	A	225	HIS	CA-CB-CG	5.13	118.94	113.80
1	A	11	LYS	N-CA-CB	5.12	118.77	110.32
1	A	45	GLN	O-C-N	5.12	128.21	122.22
1	A	285	LYS	CA-C-O	5.11	125.85	120.54
1	A	161	TYR	N-CA-C	5.08	119.19	112.89
1	A	84	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	204	ILE	N-CA-C	5.06	115.63	109.30
1	A	235	VAL	CA-CB-CG2	5.06	119.00	110.40
1	A	290	VAL	CA-C-N	5.05	129.82	123.10
1	A	290	VAL	C-N-CA	5.05	129.82	123.10
1	A	148	GLY	N-CA-C	-5.05	102.88	112.27
1	A	56	LEU	N-CA-C	-5.04	105.78	111.28
1	A	80	ALA	O-C-N	5.04	127.90	122.15
1	A	217	GLY	N-CA-C	-5.04	106.32	112.77
1	A	280	ASP	OD1-CG-OD2	5.01	134.93	122.90
1	A	246	LYS	CA-CB-CG	5.01	124.11	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	ARG	Sidechain
1	A	21	ARG	Sidechain
1	A	4	ARG	Sidechain

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	2348	0	2348	57	0
2	A	12	0	12	0	0
3	A	1	0	0	0	0
4	A	214	0	0	15	0
All	All	2575	0	2360	57	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 (57) 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:85:VAL:O	4:A:507:HOH:O	1.55	1.23
1:A:85:VAL:C	4:A:507:HOH:O	1.85	1.20
1:A:61:LYS:HG2	4:A:348:HOH:O	1.39	1.18
1:A:26:GLN:HE22	1:A:29:LYS:NZ	1.62	0.97
1:A:26:GLN:HE22	1:A:29:LYS:HZ1	1.12	0.95
1:A:308:LYS:HA	4:A:526:HOH:O	1.71	0.89
1:A:4:ARG:HB2	1:A:61:LYS:HZ2	1.45	0.82
1:A:21:ARG:HG3	1:A:38:MET:HE1	1.66	0.76
1:A:309:LYS:HB2	4:A:525:HOH:O	1.98	0.62
1:A:4:ARG:HB2	1:A:61:LYS:NZ	2.15	0.60
1:A:13:ASP:OD2	1:A:13:ASP:N	2.29	0.59
1:A:21:ARG:HG2	1:A:21:ARG:HH11	1.68	0.59
1:A:283:ASN:ND2	1:A:283:ASN:O	2.37	0.58
1:A:111:ASP:OD1	4:A:509:HOH:O	2.16	0.58
1:A:94:PRO:HG2	1:A:99:LEU:HD13	1.86	0.57
1:A:26:GLN:NE2	1:A:29:LYS:NZ	2.45	0.56
1:A:21:ARG:HG3	1:A:38:MET:CE	2.34	0.55
1:A:4:ARG:H	1:A:61:LYS:HD2	1.72	0.55
1:A:4:ARG:H	1:A:61:LYS:NZ	2.05	0.54
1:A:182:MET:O	1:A:183:TRP:HB2	2.08	0.54
1:A:300:LYS:HE3	1:A:300:LYS:CA	2.39	0.53
1:A:126:HIS:HB3	1:A:133:TRP:CH2	2.45	0.51
1:A:274:ASP:OD2	4:A:488:HOH:O	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ASP:H	1:A:302:ASN:HD21	1.59	0.51
1:A:2:ASP:HA	1:A:33:ASP:O	2.10	0.51
1:A:21:ARG:NE	4:A:494:HOH:O	2.28	0.51
1:A:86:PRO:N	4:A:507:HOH:O	2.26	0.51
1:A:3:THR:HA	1:A:61:LYS:HD3	1.94	0.50
1:A:4:ARG:H	1:A:61:LYS:CD	2.25	0.50
1:A:145:LEU:HA	1:A:208:ILE:O	2.12	0.49
1:A:200:ASN:O	1:A:201:ALA:C	2.56	0.48
1:A:298:VAL:HA	1:A:302:ASN:HD21	1.79	0.48
1:A:300:LYS:HE3	1:A:300:LYS:HA	1.95	0.48
1:A:83:GLN:NE2	4:A:328:HOH:O	2.47	0.48
1:A:86:PRO:CA	4:A:507:HOH:O	2.59	0.48
1:A:285:LYS:O	1:A:285:LYS:HG3	2.13	0.47
1:A:279:ALA:O	1:A:280:ASP:C	2.55	0.47
1:A:86:PRO:HA	4:A:507:HOH:O	2.14	0.46
1:A:299:ASP:H	1:A:302:ASN:ND2	2.11	0.46
1:A:191:LYS:HE3	4:A:515:HOH:O	2.15	0.46
1:A:308:LYS:H	1:A:308:LYS:HG3	1.31	0.45
1:A:131:GLN:HB3	4:A:510:HOH:O	2.17	0.44
1:A:21:ARG:HH11	1:A:21:ARG:CG	2.27	0.43
1:A:73:ALA:HB2	1:A:94:PRO:HB3	2.00	0.43
1:A:293:VAL:HA	1:A:294:PRO:HD3	1.88	0.43
1:A:223:LYS:O	4:A:408:HOH:O	2.20	0.43
1:A:213:ALA:HA	1:A:216:MET:HE2	2.01	0.43
1:A:18:SER:O	1:A:22:LYS:HG3	2.19	0.42
1:A:24:ILE:HG22	1:A:36:LEU:HD21	2.02	0.41
1:A:302:ASN:H	1:A:302:ASN:HD22	1.68	0.41
1:A:292:ARG:HH11	1:A:292:ARG:HD3	1.56	0.41
1:A:115:SER:HB3	1:A:295:TYR:CZ	2.56	0.41
1:A:250:LEU:HD12	1:A:250:LEU:HA	1.86	0.41
1:A:283:ASN:C	1:A:283:ASN:HD22	2.26	0.41
1:A:271:ASN:HD22	1:A:271:ASN:HA	1.69	0.41
1:A:4:ARG:CB	1:A:61:LYS:HZ2	2.24	0.40
1:A:307:SER:O	1:A:308:LYS:C	2.64	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	307/309 (99%)	297 (97%)	7 (2%)	3 (1%)	12 5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	ASP
1	A	308	LYS
1	A	304	ALA

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	245/245 (100%)	231 (94%)	14 (6%)	18 11

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	36	LEU
1	A	38	MET
1	A	55	LEU
1	A	61	LYS
1	A	83	GLN
1	A	97	LYS
1	A	113	LYS

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Mol	Chain	Res	Type
1	A	240	GLU
1	A	280	ASP
1	A	300	LYS
1	A	302	ASN
1	A	307	SER
1	A	309	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	39	ASN
1	A	83	GLN
1	A	119	GLN
1	A	131	GLN
1	A	187	GLN
1	A	200	ASN
1	A	260	ASN
1	A	271	ASN
1	A	283	ASN
1	A	302	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	310	-	12,12,12	1.26	2 (16%)	17,17,17	2.03	5 (29%)

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	310	-	-	0/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	310	BGC	O2-C2	2.30	1.48	1.43
2	A	310	BGC	O5-C1	2.25	1.48	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	310	BGC	O5-C1-C2	-6.33	99.17	110.30
2	A	310	BGC	O2-C2-C1	-2.58	103.29	109.25
2	A	310	BGC	O1-C1-O5	-2.39	103.32	110.41
2	A	310	BGC	C1-O5-C5	2.13	117.78	113.65
2	A	310	BGC	C4-C3-C2	-2.10	107.14	110.83

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.