



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:00 PM UTC

PDB ID : 1J0Y / pdb_00001j0y
Title : Beta-amylase from *Bacillus cereus* var. *mycoides* in complex with glucose
Authors : Oyama, T.; Miyake, H.; Kusunoki, M.; Nitta, Y.
Deposited on : 2002-11-25
Resolution : 2.10 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

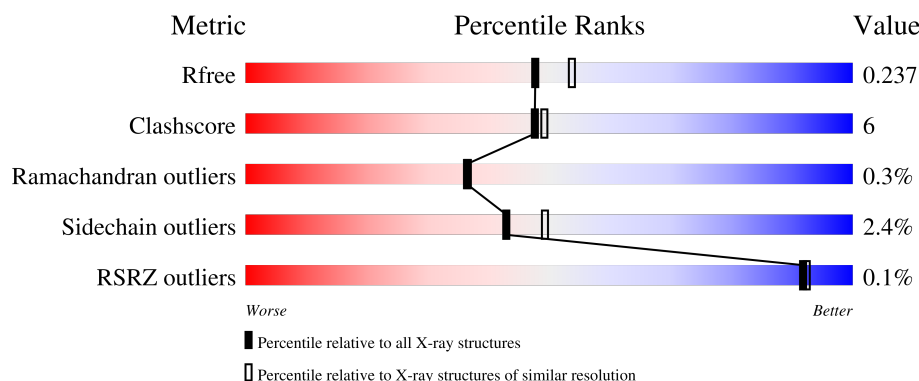
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	516	 80% 19% .
1	B	516	 81% 18% .
1	C	516	 81% 18% .
1	D	516	 82% 16% .

2 Entry composition [i](#)

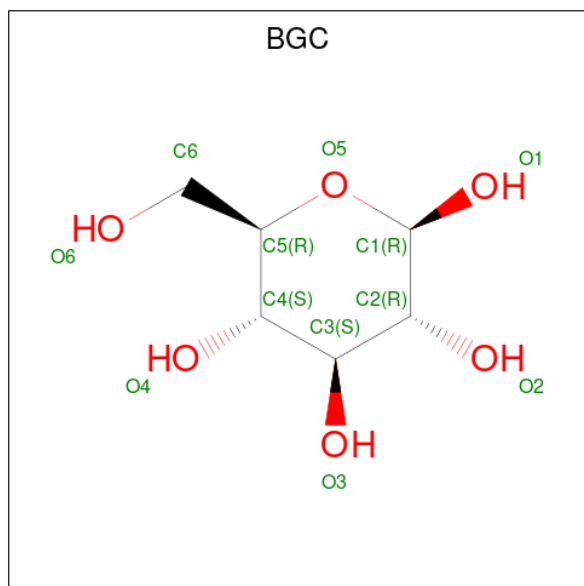
There are 4 unique types of molecules in this entry. The entry contains 17163 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			
1	B	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			
1	C	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			
1	D	516	Total	C	N	O	S	0	0	0
			4119	2645	676	781	17			

- 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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	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		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

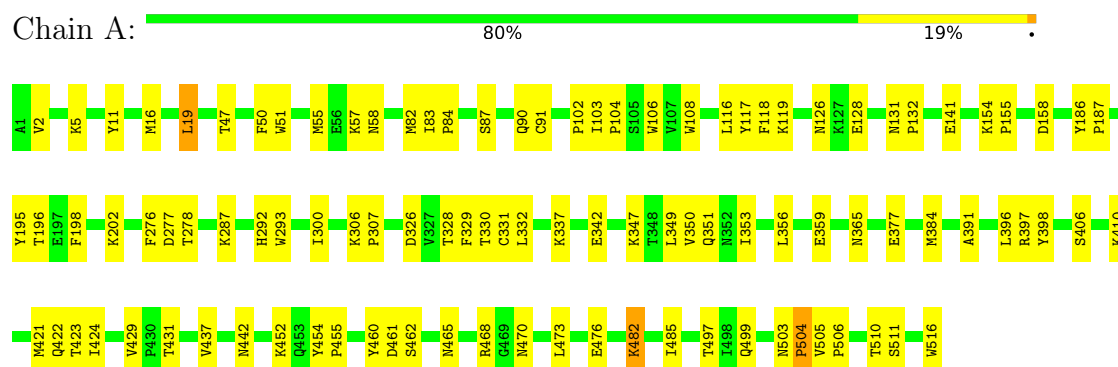
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	162	Total	O	0	0
			162	162		
4	B	145	Total	O	0	0
			145	145		
4	C	169	Total	O	0	0
			169	169		
4	D	159	Total	O	0	0
			159	159		

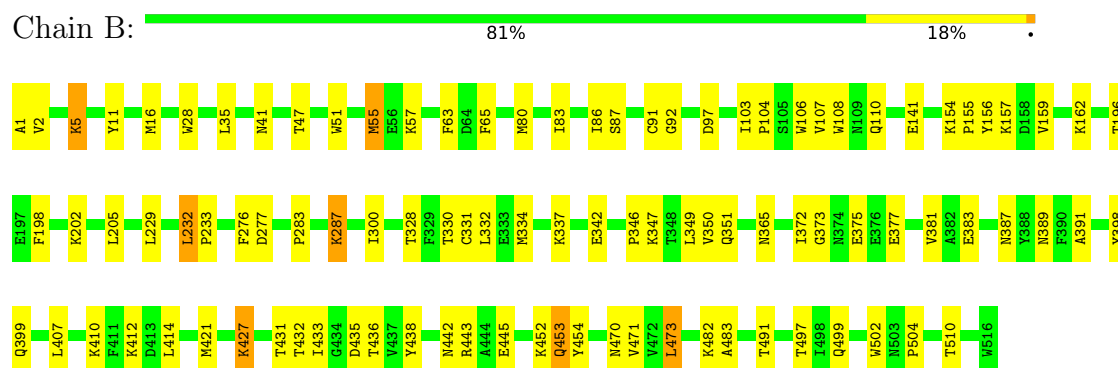
3 Residue-property plots

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 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.

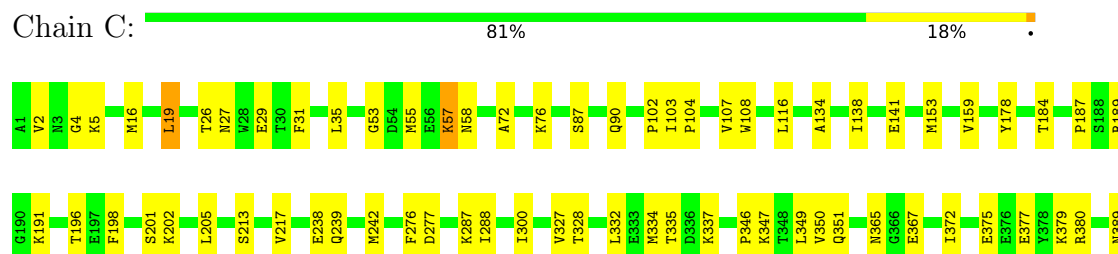
• Molecule 1: Beta-amylase

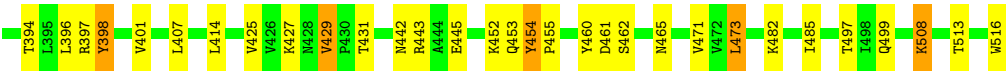


• Molecule 1: Beta-amylase

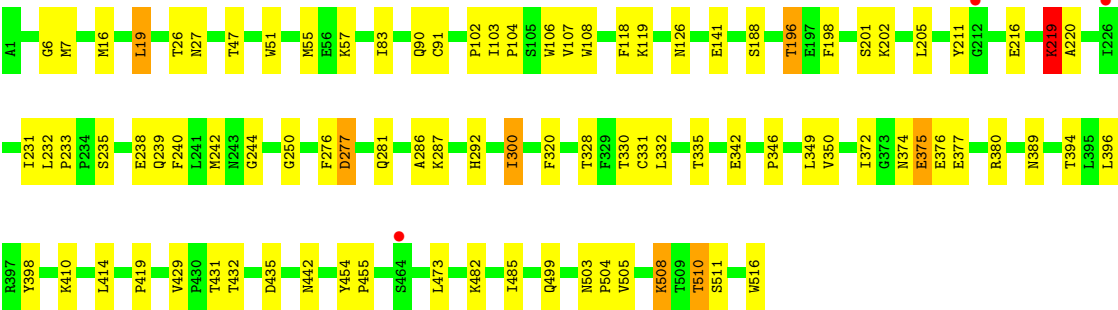
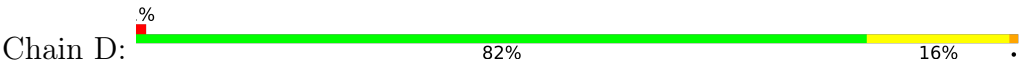


• Molecule 1: Beta-amylase





● Molecule 1: Beta-amylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.90Å 112.90Å 146.20Å 90.00° 105.80° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10 8.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	75.7 (8.00-2.10) 74.3 (8.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 2.00Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.179 , 0.236 0.179 , 0.237	Depositor DCC
R_{free} test set	6673 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 67.9	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	0.96	EDS
Total number of atoms	17163	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 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	0.47	0/4234	0.93	20/5751 (0.3%)
1	B	0.46	0/4234	0.93	18/5751 (0.3%)
1	C	0.47	0/4234	0.94	18/5751 (0.3%)
1	D	0.46	0/4234	0.93	16/5751 (0.3%)
All	All	0.46	0/16936	0.93	72/23004 (0.3%)

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	57	LYS	N-CA-C	8.72	120.41	111.07
1	C	277	ASP	N-CA-C	8.36	120.08	110.97
1	C	58	ASN	N-CA-C	8.09	122.41	112.54
1	A	57	LYS	N-CA-C	7.83	119.51	110.97
1	C	442	ASN	N-CA-C	7.75	119.36	111.07
1	A	58	ASN	N-CA-C	7.45	120.46	111.82
1	D	342	GLU	N-CA-C	7.30	119.31	111.36
1	B	277	ASP	N-CA-C	7.29	119.86	111.11
1	B	57	LYS	N-CA-C	7.27	118.99	111.14
1	A	442	ASN	N-CA-C	7.26	119.28	111.36
1	C	55	MET	N-CA-C	7.26	120.24	111.82
1	D	505	VAL	N-CA-C	-6.90	102.19	108.95
1	D	277	ASP	N-CA-C	6.87	118.42	111.07
1	D	442	ASN	N-CA-C	6.82	118.71	111.28
1	D	292	HIS	N-CA-C	6.66	121.15	112.89
1	A	505	VAL	N-CA-C	-6.62	102.46	108.95
1	A	196	THR	N-CA-C	-6.49	101.80	110.55
1	D	276	PHE	N-CA-C	6.48	122.26	113.97
1	B	337	LYS	N-CA-C	-6.45	103.47	112.12
1	A	277	ASP	N-CA-C	6.32	118.73	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	PHE	N-CA-C	6.26	121.58	113.88
1	C	337	LYS	N-CA-C	-6.19	103.64	112.13
1	D	55	MET	N-CA-C	6.14	120.50	112.89
1	C	116	LEU	N-CA-C	6.09	118.89	111.82
1	B	28	TRP	N-CA-C	5.99	117.81	111.28
1	A	55	MET	N-CA-C	5.89	120.20	112.89
1	C	189	ARG	N-CA-C	-5.89	102.76	110.53
1	D	196	THR	N-CA-C	-5.88	101.81	110.52
1	D	414	LEU	N-CA-C	5.87	118.56	111.40
1	B	497	THR	N-CA-C	5.85	118.13	111.11
1	B	141	GLU	N-CA-C	5.80	117.28	111.07
1	B	196	THR	N-CA-C	-5.79	102.34	110.50
1	D	389	ASN	N-CA-C	5.73	119.57	112.58
1	A	342	GLU	N-CA-C	5.71	118.44	111.82
1	B	342	GLU	N-CA-C	5.64	118.36	111.82
1	A	326	ASP	N-CA-C	-5.63	102.95	110.55
1	B	454	TYR	N-CA-C	5.58	122.15	109.81
1	C	57	LYS	N-CA-C	5.57	117.15	111.14
1	A	337	LYS	N-CA-C	-5.56	103.06	111.34
1	B	55	MET	N-CA-C	5.54	119.76	112.89
1	B	442	ASN	N-CA-C	5.45	118.14	111.82
1	D	141	GLU	N-CA-C	5.41	116.85	111.07
1	A	276	PHE	N-CA-C	5.39	119.99	113.41
1	C	334	MET	N-CA-C	5.37	118.47	110.52
1	C	454	TYR	N-CA-C	5.34	121.61	109.81
1	B	334	MET	N-CA-C	5.34	118.70	110.42
1	C	87	SER	N-CA-C	5.33	118.03	108.17
1	A	497	THR	N-CA-C	5.31	116.76	110.97
1	A	141	GLU	N-CA-C	5.31	116.75	111.07
1	A	50	PHE	N-CA-C	-5.29	98.63	107.99
1	A	87	SER	N-CA-C	5.27	117.92	108.17
1	A	476	GLU	N-CA-C	5.24	118.82	111.74
1	D	6	GLY	N-CA-C	-5.23	105.59	112.81
1	B	232	LEU	N-CA-C	5.21	114.13	108.14
1	D	300	ILE	CA-C-N	5.20	126.01	119.98
1	D	300	ILE	C-N-CA	5.20	126.01	119.98
1	C	389	ASN	N-CA-C	5.19	118.89	112.24
1	A	292	HIS	N-CA-C	5.17	119.64	113.23
1	C	429	VAL	N-CA-C	5.16	112.25	107.56
1	A	116	LEU	N-CA-C	5.14	119.26	112.89
1	B	414	LEU	N-CA-C	5.13	118.00	111.69
1	B	87	SER	N-CA-C	5.12	117.64	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	414	LEU	N-CA-C	5.11	117.98	111.69
1	C	497	THR	N-CA-C	5.10	117.24	111.02
1	B	453	GLN	N-CA-C	5.09	120.14	113.88
1	C	141	GLU	N-CA-C	5.07	116.80	111.28
1	C	196	THR	N-CA-C	-5.05	103.86	110.53
1	B	389	ASN	N-CA-C	5.05	118.68	111.92
1	A	195	TYR	N-CA-C	5.05	118.75	112.59
1	A	158	ASP	N-CA-C	5.04	117.50	111.71
1	C	276	PHE	N-CA-C	5.01	120.38	113.97
1	D	375	GLU	N-CA-C	5.01	117.47	111.71

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	4119	0	3984	43	0
1	B	4119	0	3984	46	0
1	C	4119	0	3984	48	0
1	D	4119	0	3984	44	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	162	0	0	1	0
4	B	145	0	0	2	0
4	C	169	0	0	2	0
4	D	159	0	0	1	0
All	All	17163	0	15984	181	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 6.

All (181) 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:431:THR:HG23	1:B:435:ASP:HB2	1.44	0.97
1:D:198:PHE:O	1:D:202:LYS:HG2	1.88	0.73
1:B:421:MET:SD	1:B:470:ASN:HB3	2.31	0.71
1:B:1:ALA:HB3	1:B:5:LYS:HG3	1.74	0.69
1:B:2:VAL:O	1:B:5:LYS:HG2	1.93	0.69
1:A:82:MET:HE2	1:A:84:PRO:HG3	1.73	0.69
1:D:7:MET:HE2	1:D:419:PRO:HB3	1.77	0.66
1:C:429:VAL:HG12	1:C:431:THR:HG23	1.78	0.65
1:A:103:ILE:HD11	1:A:108:TRP:CZ2	2.33	0.64
1:B:372:ILE:HG23	1:B:377:GLU:HB2	1.80	0.64
1:B:482:LYS:HG2	1:B:499:GLN:HA	1.80	0.63
1:B:156:TYR:O	1:B:159:VAL:HG22	2.00	0.62
1:B:162:LYS:HG3	1:B:283:PRO:O	2.00	0.61
1:B:107:VAL:O	1:B:110:GLN:HG2	2.00	0.61
1:C:300:ILE:HG13	1:C:300:ILE:O	2.00	0.60
1:C:198:PHE:O	1:C:202:LYS:HG2	2.01	0.60
1:B:198:PHE:O	1:B:202:LYS:HG2	2.02	0.59
1:C:184:THR:HG21	1:C:191:LYS:HG3	1.83	0.59
1:B:41:ASN:HA	1:B:412:LYS:HD3	1.84	0.59
1:C:2:VAL:O	1:C:5:LYS:HE2	2.03	0.59
1:A:2:VAL:O	1:A:5:LYS:HG2	2.04	0.58
1:D:335:THR:HG23	1:D:380:ARG:HD3	1.86	0.58
1:C:238:GLU:HG2	1:C:242:MET:HE2	1.86	0.57
1:A:452:LYS:HD3	1:A:452:LYS:C	2.29	0.57
1:D:16:MET:HG2	4:D:4745:HOH:O	2.06	0.56
1:D:238:GLU:HG2	1:D:242:MET:HE2	1.88	0.56
1:A:198:PHE:O	1:A:202:LYS:HG2	2.06	0.55
1:A:429:VAL:HG12	1:A:431:THR:HG23	1.89	0.55
1:A:90:GLN:HG3	1:A:102:PRO:HA	1.89	0.54
1:A:287:LYS:HG2	1:A:328:THR:HB	1.88	0.54
1:B:383:GLU:O	1:B:387:ASN:HB2	2.07	0.54
1:B:154:LYS:HB3	1:B:155:PRO:HD3	1.91	0.53
1:D:346:PRO:O	1:D:350:VAL:HG23	2.09	0.53
1:D:300:ILE:HG13	1:D:300:ILE:O	2.09	0.52
1:D:372:ILE:HG23	1:D:377:GLU:HB2	1.91	0.52
1:C:239:GLN:HA	1:C:242:MET:HE3	1.91	0.52
1:D:287:LYS:HG2	1:D:328:THR:HB	1.91	0.52
1:A:421:MET:SD	1:A:470:ASN:HB3	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LYS:HG3	1:B:328:THR:HB	1.91	0.52
1:D:375:GLU:HB3	1:D:410:LYS:HD3	1.92	0.51
1:C:287:LYS:HG2	1:C:328:THR:HB	1.93	0.51
1:C:103:ILE:HD11	1:C:108:TRP:CZ2	2.46	0.50
1:D:454:TYR:N	1:D:455:PRO:HD2	2.27	0.50
1:A:16:MET:HE3	1:A:396:LEU:HB2	1.93	0.50
1:D:118:PHE:HB2	1:D:126:ASN:HB3	1.93	0.50
1:C:347:LYS:O	1:C:351:GLN:HG3	2.12	0.50
1:B:433:ILE:H	1:B:433:ILE:HD12	1.76	0.49
1:C:443:ARG:HB3	1:C:445:GLU:OE1	2.12	0.49
1:D:482:LYS:HG3	1:D:499:GLN:HA	1.94	0.49
1:B:103:ILE:HD11	1:B:108:TRP:CZ2	2.47	0.49
1:D:429:VAL:HG12	1:D:431:THR:HG23	1.94	0.49
1:C:367:GLU:HG2	1:C:394:THR:HB	1.94	0.49
1:C:90:GLN:HG3	1:C:102:PRO:HA	1.94	0.49
1:C:471:VAL:HG12	1:C:473:LEU:HD13	1.95	0.49
1:D:374:ASN:OD1	1:D:376:GLU:HB2	2.12	0.49
1:C:104:PRO:HB2	1:C:107:VAL:HG23	1.93	0.49
1:B:11:TYR:HA	1:B:391:ALA:O	2.12	0.49
1:C:178:TYR:HB3	4:C:3620:HOH:O	2.12	0.49
1:D:51:TRP:CZ2	1:D:91:CYS:SG	3.06	0.49
1:A:482:LYS:HG3	1:A:499:GLN:HA	1.94	0.49
1:D:119:LYS:HB2	1:D:196:THR:HG23	1.95	0.49
1:A:306:LYS:HB2	1:A:307:PRO:HD3	1.93	0.49
1:A:454:TYR:N	1:A:455:PRO:HD2	2.28	0.49
1:B:452:LYS:HZ2	1:B:453:GLN:HG3	1.78	0.49
1:C:31:PHE:CZ	1:C:35:LEU:HD11	2.47	0.48
1:A:104:PRO:HB3	1:A:106:TRP:NE1	2.28	0.48
1:C:482:LYS:CG	1:C:499:GLN:HA	2.43	0.48
1:B:92:GLY:HA2	1:B:97:ASP:HB3	1.95	0.48
1:B:347:LYS:O	1:B:351:GLN:HG3	2.12	0.48
1:A:351:GLN:HG2	1:A:384:MET:HE1	1.96	0.48
1:C:76:LYS:HB2	1:C:159:VAL:HG11	1.95	0.48
1:A:429:VAL:HG11	1:A:437:VAL:HG21	1.96	0.48
1:B:373:GLY:HA2	1:B:407:LEU:HD11	1.95	0.48
1:D:16:MET:CE	1:D:396:LEU:HB2	2.44	0.48
1:C:201:SER:O	1:C:205:LEU:HD13	2.14	0.47
1:A:300:ILE:O	1:A:300:ILE:HG13	2.14	0.47
1:B:86:ILE:HD12	1:B:86:ILE:N	2.29	0.47
1:C:53:GLY:O	1:C:57:LYS:HB2	2.14	0.47
1:D:231:ILE:O	1:D:232:LEU:HD23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:PHE:CE2	1:A:350:VAL:HG22	2.50	0.47
1:D:232:LEU:HB3	1:D:233:PRO:HD2	1.96	0.47
1:A:118:PHE:HB2	1:A:126:ASN:HB3	1.97	0.47
1:B:51:TRP:CZ2	1:B:91:CYS:SG	3.08	0.47
1:C:335:THR:HG23	1:C:380:ARG:HD3	1.95	0.47
1:D:104:PRO:HB3	1:D:106:TRP:NE1	2.30	0.47
1:D:454:TYR:N	1:D:455:PRO:CD	2.78	0.47
1:B:104:PRO:HB3	1:B:106:TRP:NE1	2.30	0.47
1:A:330:THR:O	1:A:331:CYS:HB2	2.14	0.47
1:B:427:LYS:HB3	1:B:427:LYS:NZ	2.29	0.46
1:D:240:PHE:HA	1:D:244:GLY:HA3	1.97	0.46
1:D:104:PRO:HB2	1:D:107:VAL:HG23	1.97	0.46
1:A:47:THR:HG22	1:A:83:ILE:HB	1.97	0.46
1:D:432:THR:HG22	1:D:435:ASP:OD2	2.15	0.46
1:B:452:LYS:HZ2	1:B:453:GLN:CG	2.29	0.46
1:C:482:LYS:HG3	1:C:499:GLN:HA	1.98	0.46
1:D:47:THR:HG22	1:D:83:ILE:HB	1.98	0.46
1:C:508:LYS:N	1:C:508:LYS:HD3	2.31	0.45
1:A:347:LYS:O	1:A:351:GLN:HG3	2.16	0.45
1:A:117:TYR:HB2	1:A:126:ASN:O	2.16	0.45
1:C:16:MET:HG3	1:C:394:THR:HG22	1.99	0.45
1:D:277:ASP:O	1:D:281:GLN:HG3	2.16	0.45
1:A:485:ILE:HG13	1:A:516:TRP:CH2	2.51	0.45
1:B:365:ASN:HB3	4:B:2621:HOH:O	2.16	0.45
1:D:90:GLN:HG3	1:D:102:PRO:HA	1.99	0.45
1:C:346:PRO:O	1:C:350:VAL:HG23	2.17	0.45
1:C:454:TYR:N	1:C:455:PRO:HD2	2.32	0.45
1:A:424:ILE:O	1:A:468:ARG:HA	2.17	0.45
1:C:184:THR:CG2	1:C:191:LYS:HG3	2.46	0.45
1:A:454:TYR:N	1:A:455:PRO:CD	2.80	0.45
1:A:460:TYR:CE2	1:A:462:SER:HA	2.52	0.45
1:D:201:SER:O	1:D:205:LEU:HG	2.17	0.45
1:C:16:MET:CE	1:C:396:LEU:HB2	2.47	0.45
1:B:471:VAL:O	1:B:473:LEU:HD22	2.17	0.44
1:C:4:GLY:HA2	1:C:455:PRO:O	2.16	0.44
1:B:346:PRO:O	1:B:350:VAL:HG23	2.17	0.44
1:C:427:LYS:HE2	1:C:513:THR:HG21	1.99	0.44
1:D:330:THR:O	1:D:331:CYS:HB2	2.18	0.44
1:C:425:VAL:O	1:C:513:THR:HA	2.17	0.44
1:C:461:ASP:O	1:C:465:ASN:N	2.50	0.44
1:D:216:GLU:O	1:D:219:LYS:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:LEU:HG	1:D:91:CYS:SG	2.58	0.44
1:B:35:LEU:HB3	1:B:80:MET:HG3	1.99	0.43
1:B:432:THR:HG22	1:B:433:ILE:N	2.33	0.43
1:D:219:LYS:HZ3	1:D:220:ALA:H	1.66	0.43
1:B:16:MET:SD	4:B:2742:HOH:O	2.62	0.43
1:D:103:ILE:HD11	1:D:108:TRP:CZ2	2.53	0.43
1:D:211:TYR:O	1:D:216:GLU:HB2	2.18	0.43
1:D:485:ILE:HG13	1:D:516:TRP:CH2	2.53	0.43
1:A:406:SER:O	1:A:410:LYS:HG2	2.18	0.43
1:C:72:ALA:HB2	1:C:153:MET:HE1	1.99	0.43
1:C:407:LEU:HD23	1:C:407:LEU:HA	1.89	0.43
1:A:90:GLN:HB3	1:A:128:GLU:HB2	1.99	0.43
1:A:422:GLN:HE22	1:A:506:PRO:HG2	1.84	0.43
1:D:240:PHE:CE1	1:D:250:GLY:HA2	2.54	0.43
1:D:508:LYS:HD2	1:D:508:LYS:H	1.83	0.43
1:C:365:ASN:HB3	4:C:3653:HOH:O	2.19	0.43
1:A:154:LYS:HB3	1:A:155:PRO:HD3	1.99	0.43
1:A:356:LEU:O	1:A:359:GLU:HG2	2.19	0.43
1:B:300:ILE:HG13	1:B:300:ILE:O	2.19	0.43
1:C:460:TYR:CZ	1:C:462:SER:HA	2.54	0.42
1:D:119:LYS:HB2	1:D:196:THR:CG2	2.49	0.42
1:B:47:THR:HG22	1:B:83:ILE:HB	2.01	0.42
1:A:186:TYR:HD1	1:A:293:TRP:CD2	2.37	0.42
1:B:482:LYS:CG	1:B:499:GLN:HA	2.48	0.42
1:B:16:MET:SD	1:B:47:THR:OG1	2.75	0.42
1:B:433:ILE:HD12	1:B:433:ILE:N	2.34	0.42
1:A:329:PHE:HE2	1:A:350:VAL:HG22	1.85	0.42
1:B:375:GLU:HB3	1:B:410:LYS:HG2	2.02	0.42
1:C:453:GLN:C	1:C:455:PRO:HD2	2.45	0.42
1:A:11:TYR:HA	1:A:391:ALA:O	2.20	0.42
1:C:288:ILE:HD12	1:C:327:VAL:HG21	2.02	0.42
1:A:16:MET:CE	1:A:396:LEU:HB2	2.50	0.41
1:A:423:THR:O	1:A:511:SER:HA	2.20	0.41
1:B:55:MET:O	1:B:63:PHE:HA	2.20	0.41
1:B:438:TYR:O	1:B:483:ALA:HA	2.20	0.41
1:C:134:ALA:O	1:C:138:ILE:HG12	2.20	0.41
1:B:330:THR:O	1:B:331:CYS:HB2	2.21	0.41
1:C:213:SER:O	1:C:217:VAL:HG23	2.21	0.41
1:C:372:ILE:HG23	1:C:377:GLU:HB2	2.01	0.41
1:A:19:LEU:HD13	1:A:397:ARG:NH1	2.36	0.41
1:B:443:ARG:HB3	1:B:445:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:HD13	1:C:397:ARG:CZ	2.51	0.41
1:C:452:LYS:HE3	1:C:452:LYS:HB3	1.81	0.41
1:A:51:TRP:CZ2	1:A:91:CYS:SG	3.14	0.41
1:A:131:ASN:HA	1:A:132:PRO:HD2	1.94	0.41
1:A:365:ASN:HB3	4:A:1615:HOH:O	2.20	0.41
1:D:286:ALA:HB3	1:D:320:PHE:HE2	1.85	0.41
1:D:510:THR:HB	1:D:511:SER:H	1.71	0.41
1:A:461:ASP:O	1:A:465:ASN:N	2.54	0.41
1:B:232:LEU:HB3	1:B:233:PRO:CD	2.51	0.41
1:B:377:GLU:O	1:B:381:VAL:HG23	2.21	0.40
1:D:16:MET:HG3	1:D:394:THR:HG22	2.03	0.40
1:D:503:ASN:HA	1:D:504:PRO:HA	1.83	0.40
1:B:63:PHE:HB3	1:B:65:PHE:CE1	2.56	0.40
1:C:27:ASN:OD1	1:C:29:GLU:HB2	2.20	0.40
1:C:375:GLU:O	1:C:379:LYS:HG3	2.21	0.40
1:C:397:ARG:HG2	1:C:398:TYR:N	2.36	0.40
1:D:26:THR:HG23	1:D:27:ASN:N	2.36	0.40
1:C:485:ILE:HG13	1:C:516:TRP:CH2	2.56	0.40
1:A:503:ASN:HA	1:A:504:PRO:HA	1.77	0.40
1:B:399:GLN:CD	1:B:399:GLN:H	2.29	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	514/516 (100%)	490 (95%)	23 (4%)	1 (0%)	43	44
1	B	514/516 (100%)	489 (95%)	24 (5%)	1 (0%)	43	44
1	C	514/516 (100%)	495 (96%)	17 (3%)	2 (0%)	30	28
1	D	514/516 (100%)	494 (96%)	18 (4%)	2 (0%)	30	28
All	All	2056/2064 (100%)	1968 (96%)	82 (4%)	6 (0%)	36	36

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	398	TYR
1	D	398	TYR
1	A	398	TYR
1	C	398	TYR
1	D	219	LYS
1	C	26	THR

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	440/440 (100%)	428 (97%)	12 (3%)	39	45
1	B	440/440 (100%)	426 (97%)	14 (3%)	34	38
1	C	440/440 (100%)	433 (98%)	7 (2%)	55	64
1	D	440/440 (100%)	430 (98%)	10 (2%)	44	51
All	All	1760/1760 (100%)	1717 (98%)	43 (2%)	43	49

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	119	LYS
1	A	187	PRO
1	A	278	THR
1	A	332	LEU
1	A	349	LEU
1	A	353	ILE
1	A	377	GLU
1	A	473	LEU
1	A	482	LYS
1	A	504	PRO
1	A	510	THR
1	B	5	LYS
1	B	157	LYS

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Mol	Chain	Res	Type
1	B	205	LEU
1	B	229	LEU
1	B	287	LYS
1	B	332	LEU
1	B	349	LEU
1	B	427	LYS
1	B	436	THR
1	B	473	LEU
1	B	491	THR
1	B	502	TRP
1	B	504	PRO
1	B	510	THR
1	C	19	LEU
1	C	187	PRO
1	C	332	LEU
1	C	349	LEU
1	C	401	VAL
1	C	473	LEU
1	C	508	LYS
1	D	19	LEU
1	D	188	SER
1	D	219	LYS
1	D	235	SER
1	D	239	GLN
1	D	332	LEU
1	D	349	LEU
1	D	473	LEU
1	D	508	LYS
1	D	510	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	109	ASN
1	A	243	ASN
1	A	352	ASN
1	A	470	ASN
1	A	478	ASN
1	B	40	GLN
1	B	110	GLN
1	B	193	GLN

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Mol	Chain	Res	Type
1	B	389	ASN
1	B	453	GLN
1	B	465	ASN
1	C	73	GLN
1	C	352	ASN
1	C	428	ASN
1	C	470	ASN
1	D	94	ASN
1	D	239	GLN
1	D	274	ASN
1	D	311	ASN
1	D	453	GLN
1	D	463	HIS
1	D	470	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	D	4601	-	12,12,12	0.33	0	17,17,17	0.46	0
2	BGC	B	2601	-	12,12,12	0.40	0	17,17,17	0.43	0
2	BGC	A	1601	-	12,12,12	0.29	0	17,17,17	0.40	0
2	BGC	C	3601	-	12,12,12	0.40	0	17,17,17	0.43	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	D	4601	-	-	0/2/22/22	0/1/1/1
2	BGC	B	2601	-	-	0/2/22/22	0/1/1/1
2	BGC	A	1601	-	-	0/2/22/22	0/1/1/1
2	BGC	C	3601	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	516/516 (100%)	-0.85	0 100 100	10, 20, 42, 62	0
1	B	516/516 (100%)	-0.70	0 100 100	9, 21, 45, 65	0
1	C	516/516 (100%)	-0.77	0 100 100	9, 21, 43, 65	0
1	D	516/516 (100%)	-0.68	3 (0%) 85 87	10, 21, 42, 62	0
All	All	2064/2064 (100%)	-0.75	3 (0%) 92 92	9, 21, 43, 65	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	212	GLY	3.5
1	D	464	SER	2.2
1	D	226	ILE	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 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	A	1601	12/12	0.96	0.04	11,20,24,34	0
2	BGC	B	2601	12/12	0.96	0.05	13,18,24,32	0
2	BGC	C	3601	12/12	0.96	0.05	14,19,22,29	0
2	BGC	D	4601	12/12	0.96	0.05	14,19,23,24	0
3	CA	B	701	1/1	0.97	0.02	12,12,12,12	0
3	CA	C	701	1/1	0.98	0.03	13,13,13,13	0
3	CA	A	701	1/1	0.99	0.02	16,16,16,16	0
3	CA	D	701	1/1	0.99	0.02	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.