



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:32 PM GMT

PDB ID : 1U0A
Title : Crystal structure of the engineered beta-1,3-1,4-endoglucanase H(A16-M) in complex with beta-glucan tetrasaccharide
Authors : Gaiser, O.J.; Piotukh, K.; Ponnuswamy, M.N.; Planas, A.; Borriss, R.; Heinemann, U.
Deposited on : 2004-07-13
Resolution : 1.64 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 ⓘ symbol.

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

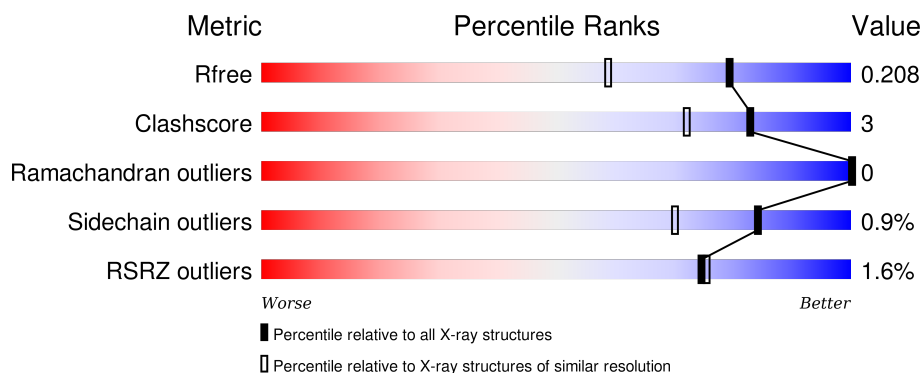
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	1953 (1.66-1.62)
Clashscore	102246	2091 (1.66-1.62)
Ramachandran outliers	100387	2052 (1.66-1.62)
Sidechain outliers	100360	2052 (1.66-1.62)
RSRZ outliers	91569	1955 (1.66-1.62)

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 $\leq 5\%$. 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	214	<div> <div>2%</div> <div>93%</div> <div>7%</div> </div>
1	B	214	<div> <div>%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>
1	C	214	<div> <div>%</div> <div>91%</div> <div>9%</div> </div>
1	D	214	<div> <div>2%</div> <div>96%</div> <div>.</div> </div>

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	4011	X	-	-	-
2	BGC	B	4021	X	-	-	-
2	BGC	C	4031	X	-	-	-
2	BGC	D	4041	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8629 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-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	3	0
			1703	1093	276	329	5			
1	B	214	Total	C	N	O	S	0	6	0
			1715	1099	278	333	5			
1	C	214	Total	C	N	O	S	0	5	0
			1711	1098	278	330	5			
1	D	214	Total	C	N	O	S	0	7	0
			1717	1101	278	333	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLN	-	SEE REMARK 999	UNP P23904
A	2	THR	-	SEE REMARK 999	UNP P23904
A	3	GLY	-	SEE REMARK 999	UNP P23904
A	4	GLY	-	SEE REMARK 999	UNP P23904
A	5	SER	-	SEE REMARK 999	UNP P23904
A	6	PHE	-	SEE REMARK 999	UNP P23904
A	7	PHE	-	SEE REMARK 999	UNP P23904
A	8	GLU	-	SEE REMARK 999	UNP P23904
A	9	PRO	-	SEE REMARK 999	UNP P23904
A	10	PHE	-	SEE REMARK 999	UNP P23904
A	11	ASN	-	SEE REMARK 999	UNP P23904
A	12	SER	-	SEE REMARK 999	UNP P23904
A	13	TYR	-	SEE REMARK 999	UNP P23904
A	14	ASN	-	SEE REMARK 999	UNP P23904
A	15	SER	-	SEE REMARK 999	UNP P23904
A	16	GLY	-	SEE REMARK 999	UNP P23904
A	105	GLN	GLU	ENGINEERED	UNP P23904
A	109	GLN	GLU	ENGINEERED	UNP P23904
B	301	GLN	-	SEE REMARK 999	UNP P23904
B	302	THR	-	SEE REMARK 999	UNP P23904
B	303	GLY	-	SEE REMARK 999	UNP P23904

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Chain	Residue	Modelled	Actual	Comment	Reference
B	304	GLY	-	SEE REMARK 999	UNP P23904
B	305	SER	-	SEE REMARK 999	UNP P23904
B	306	PHE	-	SEE REMARK 999	UNP P23904
B	307	PHE	-	SEE REMARK 999	UNP P23904
B	308	GLU	-	SEE REMARK 999	UNP P23904
B	309	PRO	-	SEE REMARK 999	UNP P23904
B	310	PHE	-	SEE REMARK 999	UNP P23904
B	311	ASN	-	SEE REMARK 999	UNP P23904
B	312	SER	-	SEE REMARK 999	UNP P23904
B	313	TYR	-	SEE REMARK 999	UNP P23904
B	314	ASN	-	SEE REMARK 999	UNP P23904
B	315	SER	-	SEE REMARK 999	UNP P23904
B	316	GLY	-	SEE REMARK 999	UNP P23904
B	405	GLN	GLU	ENGINEERED	UNP P23904
B	409	GLN	GLU	ENGINEERED	UNP P23904
C	601	GLN	-	SEE REMARK 999	UNP P23904
C	602	THR	-	SEE REMARK 999	UNP P23904
C	603	GLY	-	SEE REMARK 999	UNP P23904
C	604	GLY	-	SEE REMARK 999	UNP P23904
C	605	SER	-	SEE REMARK 999	UNP P23904
C	606	PHE	-	SEE REMARK 999	UNP P23904
C	607	PHE	-	SEE REMARK 999	UNP P23904
C	608	GLU	-	SEE REMARK 999	UNP P23904
C	609	PRO	-	SEE REMARK 999	UNP P23904
C	610	PHE	-	SEE REMARK 999	UNP P23904
C	611	ASN	-	SEE REMARK 999	UNP P23904
C	612	SER	-	SEE REMARK 999	UNP P23904
C	613	TYR	-	SEE REMARK 999	UNP P23904
C	614	ASN	-	SEE REMARK 999	UNP P23904
C	615	SER	-	SEE REMARK 999	UNP P23904
C	616	GLY	-	SEE REMARK 999	UNP P23904
C	705	GLN	GLU	ENGINEERED	UNP P23904
C	709	GLN	GLU	ENGINEERED	UNP P23904
D	901	GLN	-	SEE REMARK 999	UNP P23904
D	902	THR	-	SEE REMARK 999	UNP P23904
D	903	GLY	-	SEE REMARK 999	UNP P23904
D	904	GLY	-	SEE REMARK 999	UNP P23904
D	905	SER	-	SEE REMARK 999	UNP P23904
D	906	PHE	-	SEE REMARK 999	UNP P23904
D	907	PHE	-	SEE REMARK 999	UNP P23904
D	908	GLU	-	SEE REMARK 999	UNP P23904
D	909	PRO	-	SEE REMARK 999	UNP P23904

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Chain	Residue	Modelled	Actual	Comment	Reference
D	910	PHE	-	SEE REMARK 999	UNP P23904
D	911	ASN	-	SEE REMARK 999	UNP P23904
D	912	SER	-	SEE REMARK 999	UNP P23904
D	913	TYR	-	SEE REMARK 999	UNP P23904
D	914	ASN	-	SEE REMARK 999	UNP P23904
D	915	SER	-	SEE REMARK 999	UNP P23904
D	916	GLY	-	SEE REMARK 999	UNP P23904
D	1005	GLN	GLU	ENGINEERED	UNP P23904
D	1009	GLN	GLU	ENGINEERED	UNP P23904

- Molecule 2 is a polymer of unknown type called SUGAR (BGC-BGC-BGC-BGC).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total C O 45 24 21	0	0
2	B	4	Total C O 45 24 21	0	0
2	C	4	Total C O 45 24 21	0	0
2	D	4	Total C O 45 24 21	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0
4	A	2	Total Zn 2 2	0	0

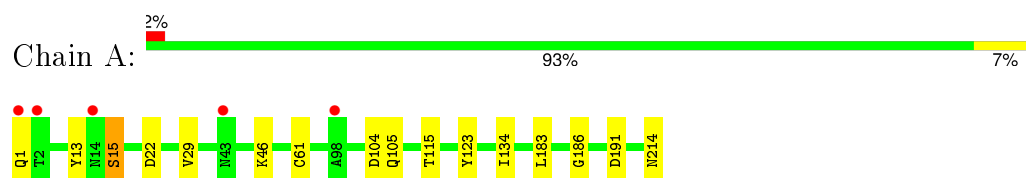
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	356	Total 356	O 356	0	0
5	B	426	Total 426	O 426	0	0
5	C	416	Total 416	O 416	0	0
5	D	398	Total 398	O 398	0	0

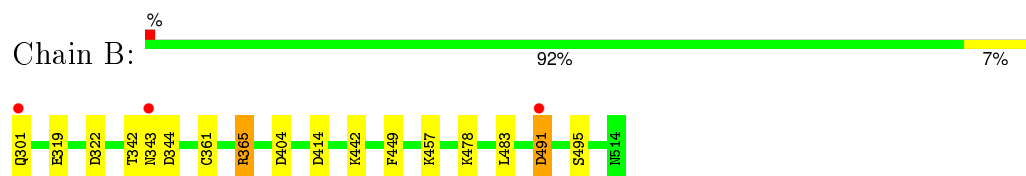
3 Residue-property plots [i](#)

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.

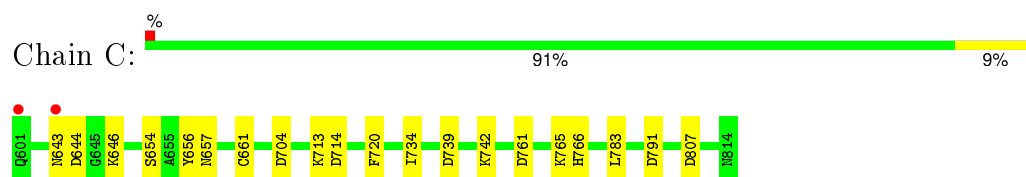
• Molecule 1: Beta-glucanase



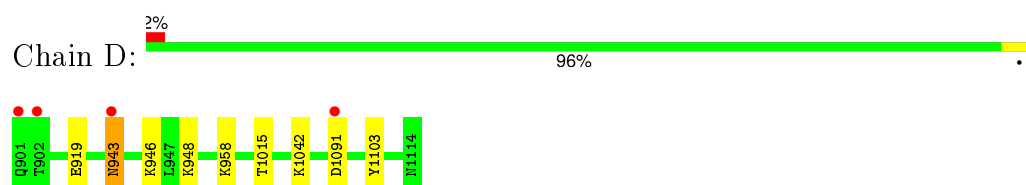
• Molecule 1: Beta-glucanase



• Molecule 1: Beta-glucanase



• Molecule 1: Beta-glucanase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.77Å 88.76Å 154.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.46 – 1.64 34.46 – 1.64	Depositor EDS
% Data completeness (in resolution range)	92.5 (34.46-1.64) 92.5 (34.46-1.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.64Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.161 , 0.197 0.174 , 0.208	Depositor DCC
R_{free} test set	8310 reflections (7.54%)	DCC
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 118568 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8629	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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, 0.375 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: ZN, BGC, CA

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	0.60	0/1774	0.81	3/2411 (0.1%)
1	B	0.61	0/1801	0.87	5/2447 (0.2%)
1	C	0.62	0/1792	0.82	6/2436 (0.2%)
1	D	0.62	0/1807	0.82	1/2455 (0.0%)
All	All	0.61	0/7174	0.83	15/9749 (0.2%)

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
2	A	1	0
2	B	1	0
2	C	1	0
2	D	1	0
All	All	4	0

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	491[A]	ASP	CB-CG-OD2	9.69	127.02	118.30
1	B	491[B]	ASP	CB-CG-OD2	9.69	127.02	118.30
1	A	104	ASP	CB-CG-OD2	7.24	124.82	118.30
1	B	322	ASP	CB-CG-OD2	6.50	124.15	118.30
1	C	791	ASP	CB-CG-OD2	5.85	123.56	118.30
1	C	739	ASP	CB-CG-OD2	5.75	123.48	118.30
1	C	807	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	704	ASP	CB-CG-OD2	5.63	123.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	714	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	22	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	404	ASP	CB-CG-OD2	5.32	123.08	118.30
1	D	1091	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	414	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	191	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	761	ASP	CB-CG-OD2	5.07	122.86	118.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	4011	BGC	C1
2	B	4021	BGC	C1
2	C	4031	BGC	C1
2	D	4041	BGC	C1

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	1703	0	1572	11	1
1	B	1715	0	1579	8	1
1	C	1711	0	1579	14	0
1	D	1717	0	1585	9	0
2	A	45	0	39	0	0
2	B	45	0	39	0	0
2	C	45	0	39	0	0
2	D	45	0	39	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	2	0	0	0	0
4	B	1	0	0	0	0
5	A	356	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	426	0	0	4	0
5	C	416	0	0	8	0
5	D	398	0	0	8	0
All	All	8629	0	6471	42	1

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 3.

All (42) 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:13:TYR:OH	1:A:15[A]:SER:OG	1.97	0.80
1:C:720:PHE:CE1	1:C:734[A]:ILE:HD12	2.19	0.77
1:A:13:TYR:CZ	1:A:15[A]:SER:OG	2.37	0.74
1:C:646:LYS:HE3	5:C:3318:HOH:O	1.89	0.73
1:C:720:PHE:HE1	1:C:734[A]:ILE:HD12	1.60	0.64
1:B:478[B]:LYS:HE3	5:B:3029:HOH:O	1.97	0.63
1:C:643:ASN:ND2	5:C:3333:HOH:O	2.33	0.60
1:B:342:THR:OG1	1:B:344[A]:ASP:OD1	2.19	0.59
1:C:657[B]:ASN:OD1	5:C:2762:HOH:O	2.17	0.57
1:D:946:LYS:HE3	5:D:3455:HOH:O	2.04	0.56
1:A:1:GLN:HA	1:A:1:GLN:HE21	1.71	0.55
1:A:13:TYR:OH	5:A:3454:HOH:O	2.18	0.55
1:C:644:ASP:HB2	5:C:3288:HOH:O	2.07	0.55
1:A:115:THR:HA	5:A:3325:HOH:O	2.07	0.55
1:D:958:LYS:NZ	5:D:3487:HOH:O	2.39	0.55
1:A:46:LYS:HE3	5:A:3539:HOH:O	2.07	0.55
1:D:1015:THR:HA	5:D:2365:HOH:O	2.07	0.54
1:C:713:LYS:NZ	5:C:2450:HOH:O	2.05	0.52
1:C:734[A]:ILE:HD11	1:C:766:HIS:HB2	1.93	0.51
1:B:319:GLU:HG3	1:B:365:ARG:HG3	1.93	0.49
1:A:1:GLN:HA	1:A:1:GLN:NE2	2.28	0.48
1:C:713:LYS:HE3	5:C:2846:HOH:O	2.13	0.48
1:C:661:CYS:HB2	1:C:783:LEU:O	2.14	0.48
1:C:742:LYS:HE3	5:C:3261:HOH:O	2.14	0.47
1:C:713:LYS:CE	5:C:2450:HOH:O	2.56	0.47
1:B:301:GLN:NE2	5:B:3001:HOH:O	2.47	0.47
1:D:919[B]:GLU:CD	5:D:2661:HOH:O	2.54	0.45
1:A:61:CYS:HB2	1:A:183:LEU:O	2.18	0.43
1:D:1042[B]:LYS:HD3	5:D:2892:HOH:O	2.18	0.43
1:C:734[A]:ILE:HD13	1:C:765:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:943[A]:ASN:ND2	5:D:3107:HOH:O	2.51	0.43
1:B:442[B]:LYS:NZ	5:B:3387:HOH:O	2.51	0.43
1:A:29:VAL:O	1:A:186:GLY:HA2	2.19	0.42
1:B:361:CYS:HB2	1:B:483:LEU:O	2.19	0.42
1:D:948:LYS:HE2	1:D:1103:TYR:CG	2.55	0.42
1:B:449:PHE:HA	1:B:457:LYS:O	2.20	0.42
1:D:946:LYS:NZ	5:D:2763:HOH:O	2.38	0.41
1:C:656:TYR:CE2	1:C:657[B]:ASN:ND2	2.88	0.41
1:A:134:ILE:HD13	1:A:134:ILE:HA	1.92	0.41
1:B:495[A]:SER:HB2	5:B:2395:HOH:O	2.20	0.41
1:A:105:GLN:HG2	1:A:123:TYR:HB2	2.03	0.41
1:D:1042[B]:LYS:HE3	5:D:2312:HOH:O	2.20	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ASN:O	1:B:301:GLN:N[2_565]	2.18	0.02

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	215/214 (100%)	209 (97%)	6 (3%)	0	100	100
1	B	218/214 (102%)	214 (98%)	4 (2%)	0	100	100
1	C	217/214 (101%)	213 (98%)	4 (2%)	0	100	100
1	D	219/214 (102%)	214 (98%)	5 (2%)	0	100	100
All	All	869/856 (102%)	850 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	179/176 (102%)	177 (99%)	2 (1%)	80	62
1	B	182/176 (103%)	177 (97%)	5 (3%)	52	22
1	C	181/176 (103%)	179 (99%)	2 (1%)	80	62
1	D	183/176 (104%)	181 (99%)	2 (1%)	80	62
All	All	725/704 (103%)	714 (98%)	11 (2%)	84	49

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15[A]	SER
1	A	15[B]	SER
1	B	343[A]	ASN
1	B	343[B]	ASN
1	B	365	ARG
1	B	491[A]	ASP
1	B	491[B]	ASP
1	C	654[A]	SER
1	C	654[B]	SER
1	D	943[A]	ASN
1	D	943[B]	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	152	GLN
1	A	214	ASN
1	B	301	GLN
1	C	668	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 ⓘ

16 carbohydrates 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	4011	2	11,11,12	0.82	0	14,15,17	2.70	3 (21%)
2	BGC	A	4012	2	11,11,12	0.88	0	14,15,17	2.29	4 (28%)
2	BGC	A	4013	2	11,11,12	1.07	1 (9%)	14,15,17	2.26	3 (21%)
2	BGC	A	4014	2	12,12,12	0.48	0	17,17,17	1.18	1 (5%)
2	BGC	B	4021	2	11,11,12	0.56	0	14,15,17	2.83	4 (28%)
2	BGC	B	4022	2	11,11,12	0.92	1 (9%)	14,15,17	2.49	3 (21%)
2	BGC	B	4023	2	11,11,12	1.15	1 (9%)	14,15,17	2.05	2 (14%)
2	BGC	B	4024	2	12,12,12	0.47	0	17,17,17	0.73	0
2	BGC	C	4031	2	11,11,12	0.73	0	14,15,17	2.70	3 (21%)
2	BGC	C	4032	2	11,11,12	0.71	0	14,15,17	2.58	3 (21%)
2	BGC	C	4033	2	11,11,12	0.94	1 (9%)	14,15,17	2.26	2 (14%)
2	BGC	C	4034	2	12,12,12	0.60	0	17,17,17	0.69	0
2	BGC	D	4041	2	11,11,12	0.62	0	14,15,17	2.57	4 (28%)
2	BGC	D	4042	2	11,11,12	0.96	1 (9%)	14,15,17	2.22	3 (21%)
2	BGC	D	4043	2	11,11,12	0.76	1 (9%)	14,15,17	2.06	3 (21%)
2	BGC	D	4044	2	12,12,12	0.66	0	17,17,17	1.08	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	4011	2	1/1/4/5	0/2/19/22	0/1/1/1
2	BGC	A	4012	2	-	0/2/19/22	0/1/1/1
2	BGC	A	4013	2	-	0/2/19/22	0/1/1/1
2	BGC	A	4014	2	-	0/2/22/22	0/1/1/1
2	BGC	B	4021	2	1/1/4/5	0/2/19/22	0/1/1/1
2	BGC	B	4022	2	-	0/2/19/22	0/1/1/1
2	BGC	B	4023	2	-	0/2/19/22	0/1/1/1
2	BGC	B	4024	2	-	0/2/22/22	0/1/1/1
2	BGC	C	4031	2	1/1/4/5	0/2/19/22	0/1/1/1
2	BGC	C	4032	2	-	0/2/19/22	0/1/1/1
2	BGC	C	4033	2	-	0/2/19/22	0/1/1/1
2	BGC	C	4034	2	-	0/2/22/22	0/1/1/1
2	BGC	D	4041	2	1/1/4/5	0/2/19/22	0/1/1/1
2	BGC	D	4042	2	-	0/2/19/22	0/1/1/1
2	BGC	D	4043	2	-	0/2/19/22	0/1/1/1
2	BGC	D	4044	2	-	0/2/22/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4023	BGC	O5-C1	-3.25	1.38	1.43
2	A	4013	BGC	O5-C1	-3.00	1.38	1.43
2	B	4022	BGC	O5-C1	-2.65	1.39	1.43
2	C	4033	BGC	O5-C1	-2.42	1.39	1.43
2	D	4043	BGC	O5-C1	-2.12	1.40	1.43
2	D	4042	BGC	O5-C1	-2.01	1.40	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4022	BGC	C1-O5-C5	-7.99	102.11	112.25
2	C	4033	BGC	C1-O5-C5	-6.71	103.73	112.25
2	B	4023	BGC	C1-O5-C5	-6.45	104.06	112.25
2	A	4013	BGC	C1-O5-C5	-6.41	104.11	112.25
2	D	4043	BGC	C1-O5-C5	-5.93	104.72	112.25
2	D	4041	BGC	C2-C3-C4	-4.88	102.75	111.04
2	A	4011	BGC	C2-C3-C4	-4.16	103.97	111.04
2	B	4021	BGC	C2-C3-C4	-3.89	104.44	111.04
2	C	4033	BGC	C1-C2-C3	-3.29	105.65	109.54
2	A	4014	BGC	C4-C3-C2	-3.25	104.72	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4013	BGC	C1-C2-C3	-3.22	105.73	109.54
2	A	4012	BGC	O4-C4-C3	-3.07	103.42	110.34
2	C	4031	BGC	C2-C3-C4	-3.03	105.89	111.04
2	D	4043	BGC	C1-C2-C3	-2.77	106.27	109.54
2	B	4022	BGC	O4-C4-C3	-2.46	104.79	110.34
2	D	4044	BGC	C1-C2-C3	-2.35	106.93	110.43
2	B	4023	BGC	O4-C4-C3	-2.35	105.04	110.34
2	D	4042	BGC	O4-C4-C3	-2.32	105.10	110.34
2	D	4041	BGC	C3-C4-C5	-2.13	106.48	110.20
2	B	4022	BGC	O2-C2-C1	2.19	113.59	109.21
2	A	4012	BGC	O2-C2-C1	2.21	113.63	109.21
2	D	4042	BGC	C1-C2-C3	2.25	112.20	109.54
2	D	4043	BGC	O5-C1-C2	2.67	115.19	110.86
2	C	4032	BGC	C1-O5-C5	2.70	115.67	112.25
2	A	4012	BGC	C1-C2-C3	2.88	112.94	109.54
2	C	4032	BGC	O2-C2-C1	3.14	115.49	109.21
2	A	4013	BGC	O5-C1-C2	3.30	116.21	110.86
2	B	4021	BGC	C1-C2-C3	3.90	114.16	109.54
2	A	4011	BGC	C1-O5-C5	4.02	117.35	112.25
2	D	4041	BGC	C1-O5-C5	4.07	117.41	112.25
2	B	4021	BGC	C1-O5-C5	4.22	117.60	112.25
2	C	4031	BGC	C1-O5-C5	5.79	119.60	112.25
2	D	4041	BGC	O5-C1-C2	6.13	120.80	110.86
2	A	4012	BGC	O5-C1-C2	6.61	121.58	110.86
2	D	4042	BGC	O5-C1-C2	6.75	121.80	110.86
2	C	4031	BGC	O5-C1-C2	7.27	122.66	110.86
2	C	4032	BGC	O5-C1-C2	7.60	123.19	110.86
2	B	4021	BGC	O5-C1-C2	7.62	123.21	110.86
2	A	4011	BGC	O5-C1-C2	7.97	123.78	110.86

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	4041	BGC	C1
2	A	4011	BGC	C1
2	C	4031	BGC	C1
2	B	4021	BGC	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	214/214 (100%)	0.13	5 (2%) 64 63	12, 19, 35, 55	0
1	B	214/214 (100%)	-0.15	3 (1%) 78 78	12, 17, 24, 46	0
1	C	214/214 (100%)	-0.11	2 (0%) 85 86	12, 18, 25, 45	0
1	D	214/214 (100%)	-0.17	4 (1%) 70 70	11, 16, 25, 47	0
All	All	856/856 (100%)	-0.07	14 (1%) 74 75	11, 18, 28, 55	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	GLN	6.6
1	D	901	GLN	5.4
1	C	601	GLN	4.7
1	A	43	ASN	4.0
1	C	643	ASN	3.7
1	B	301	GLN	3.6
1	B	343[A]	ASN	3.5
1	B	491[A]	ASP	3.3
1	A	14	ASN	3.0
1	A	2	THR	3.0
1	D	902	THR	2.9
1	D	943[A]	ASN	2.5
1	A	98	ALA	2.4
1	D	1091	ASP	2.3

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 ⓘ

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	BGC	A	4012	11/12	0.86	0.14	1.25	23,26,30,32	0
2	BGC	D	4042	11/12	0.95	0.09	1.01	17,21,24,28	0
2	BGC	C	4034	12/12	0.94	0.10	0.88	16,17,18,21	0
2	BGC	B	4022	11/12	0.95	0.08	0.58	15,19,22,23	0
2	BGC	C	4032	11/12	0.94	0.09	0.55	20,23,26,27	0
2	BGC	A	4013	11/12	0.92	0.09	0.29	17,19,22,22	0
2	BGC	D	4043	11/12	0.94	0.08	-0.17	15,17,20,21	0
2	BGC	D	4044	12/12	0.95	0.09	-0.18	15,16,18,19	0
2	BGC	A	4014	12/12	0.94	0.08	-0.49	15,18,19,19	0
2	BGC	B	4023	11/12	0.96	0.07	-0.56	14,15,16,18	0
2	BGC	B	4024	12/12	0.96	0.07	-0.93	13,14,15,15	0
2	BGC	C	4033	11/12	0.95	0.07	-1.38	17,19,20,21	0
2	BGC	D	4041	11/12	0.81	0.29	-	33,36,38,39	0
2	BGC	C	4031	11/12	0.72	0.28	-	31,34,36,36	0
2	BGC	B	4021	11/12	0.79	0.18	-	25,28,30,32	0
2	BGC	A	4011	11/12	0.64	0.32	-	35,38,40,41	0

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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	CA	D	5001	1/1	0.99	0.06	-1.20	13,13,13,13	0
3	CA	B	5002	1/1	0.98	0.06	-1.30	20,20,20,20	0
3	CA	A	5004	1/1	0.90	0.09	-1.40	27,27,27,27	0
3	CA	C	5003	1/1	0.98	0.04	-1.78	20,20,20,20	0
4	ZN	A	5005	1/1	1.00	0.06	-3.18	16,16,16,16	0
4	ZN	B	5006	1/1	1.00	0.04	-3.87	13,13,13,13	0
4	ZN	A	5011	1/1	0.99	0.07	-	23,23,23,23	0

6.5 Other polymers

There are no such residues in this entry.