



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 31, 2016 – 03:29 PM EDT

PDB ID : 5A94
Title : CRYSTAL STRUCTURE BETA-GLUCANASE SDGLUC5_26A FROM
SACCHAROPHAGUS DEGRADANS IN COMPLEX WITH TETRASAC-
CHARIDE A, form 1
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Berrin, J.G.; Garron, M.L.
Deposited on : 2015-07-17
Resolution : 1.99 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
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) : rb-20027107

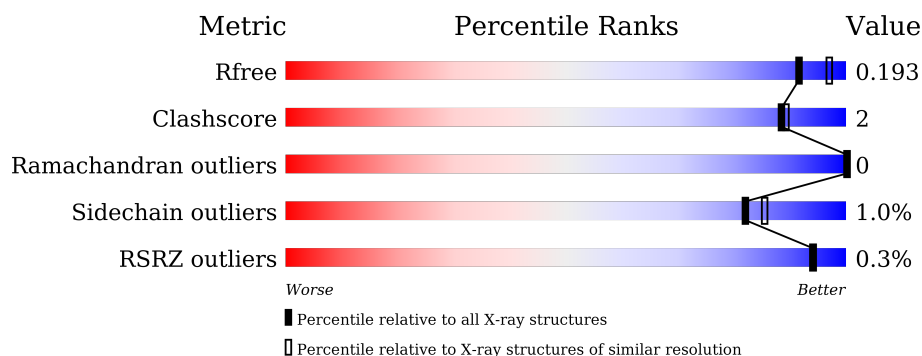
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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 ≥ 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	365	<div> <div>86%</div> <div>5%</div> <div>8%</div> </div>
1	B	365	<div> <div>85%</div> <div>7%</div> <div>8%</div> </div>
1	C	365	<div> <div>86%</div> <div>6%</div> <div>8%</div> </div>
1	D	365	<div> <div>85%</div> <div>6%</div> <div>8%</div> </div>
1	E	365	<div> <div>85%</div> <div>7%</div> <div>8%</div> </div>
1	F	365	<div> <div>86%</div> <div>5%</div> <div>8%</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	401	-	-	-	X
2	BGC	C	399	-	-	-	X
2	BGC	D	399	-	-	-	X
2	BGC	E	399	-	-	-	X
2	BGC	E	401	-	-	-	X
2	BGC	F	399	-	-	-	X
4	CL	A	403	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18380 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 PUTATIVE RETAINING B-GLYCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	2	0
			2775	1811	457	501	6			
1	B	336	Total	C	N	O	S	0	1	0
			2781	1814	460	501	6			
1	C	335	Total	C	N	O	S	0	0	0
			2767	1806	456	499	6			
1	D	334	Total	C	N	O	S	0	0	0
			2758	1800	454	498	6			
1	E	335	Total	C	N	O	S	0	2	0
			2775	1813	456	500	6			
1	F	335	Total	C	N	O	S	0	0	0
			2767	1806	456	499	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ARG	GLN	CLONING ARTIFACT	UNP Q21KE5
A	176	GLN	LYS	CLONING ARTIFACT	UNP Q21KE5
A	291	GLN	GLU	ENGINEERED MUTATION	UNP Q21KE5
B	82	ARG	GLN	CLONING ARTIFACT	UNP Q21KE5
B	176	GLN	LYS	CLONING ARTIFACT	UNP Q21KE5
B	291	GLN	GLU	ENGINEERED MUTATION	UNP Q21KE5
C	82	ARG	GLN	CLONING ARTIFACT	UNP Q21KE5
C	176	GLN	LYS	CLONING ARTIFACT	UNP Q21KE5
C	291	GLN	GLU	ENGINEERED MUTATION	UNP Q21KE5
D	82	ARG	GLN	CLONING ARTIFACT	UNP Q21KE5
D	176	GLN	LYS	CLONING ARTIFACT	UNP Q21KE5
D	291	GLN	GLU	ENGINEERED MUTATION	UNP Q21KE5
E	82	ARG	GLN	CLONING ARTIFACT	UNP Q21KE5
E	176	GLN	LYS	CLONING ARTIFACT	UNP Q21KE5
E	291	GLN	GLU	ENGINEERED MUTATION	UNP Q21KE5
F	82	ARG	GLN	CLONING ARTIFACT	UNP Q21KE5
F	176	GLN	LYS	CLONING ARTIFACT	UNP Q21KE5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	291	GLN	GLU	ENGINEERED MUTATION	UNP Q21KE5

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total C O 34 18 16	0	0
2	B	3	Total C O 34 18 16	0	0
2	C	3	Total C O 34 18 16	0	0
2	D	3	Total C O 34 18 16	0	0
2	E	3	Total C O 34 18 16	0	0
2	F	3	Total C O 34 18 16	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0
4	A	1	Total 1	Cl 1	0	0
4	F	1	Total 1	Cl 1	0	0

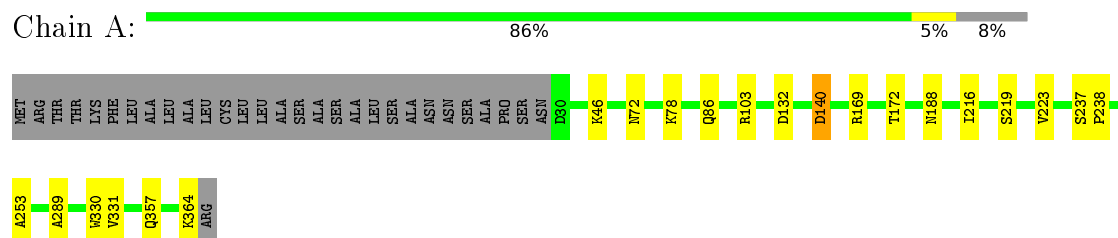
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	305	Total 305	O 305	0	0
5	B	259	Total 259	O 259	0	0
5	C	254	Total 254	O 254	0	0
5	D	217	Total 217	O 217	0	0
5	E	285	Total 285	O 285	0	0
5	F	221	Total 221	O 221	0	0

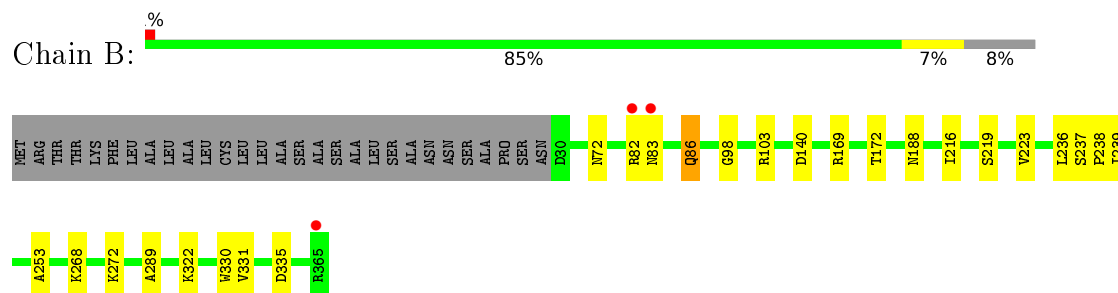
3 Residue-property plots [i](#)

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.

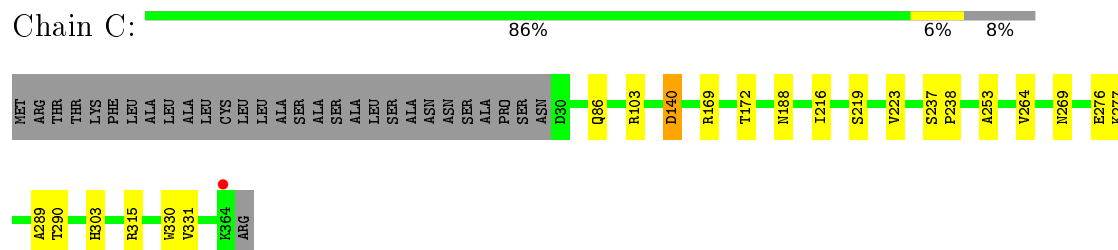
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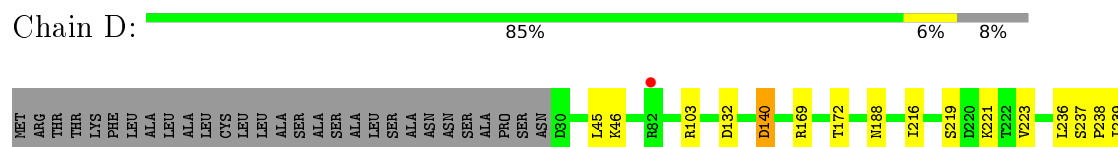
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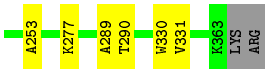


• Molecule 1: PUTATIVE RETAINING B-GLYCOSIDASE

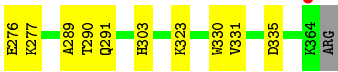
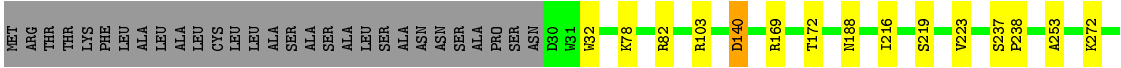
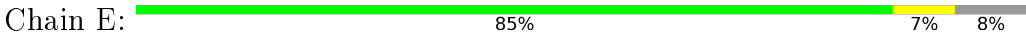


• Molecule 1: PUTATIVE RETAINING B-GLYCOSIDASE

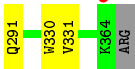
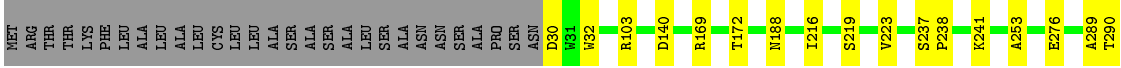
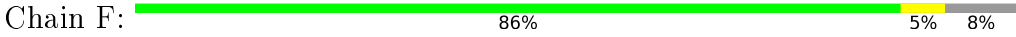




• Molecule 1: PUTATIVE RETAINING B-GLYCOSIDASE



• Molecule 1: PUTATIVE RETAINING B-GLYCOSIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	188.64Å 132.75Å 131.35Å 90.00° 133.78° 90.00°	Depositor
Resolution (Å)	47.42 – 1.99 47.42 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.42-1.99) 98.5 (47.42-1.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.179 , 0.190 0.184 , 0.193	Depositor DCC
R_{free} test set	8032 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.5	EDS
Estimated twinning fraction	0.772 for H, K, L 0.228 for H+4/2L, -K, -L 0.014 for h+2*l,k,-h-l 0.014 for k+l,h+l,-l 0.016 for -k+l,-h-l,-l 0.026 for -h+k-l,-l,-k 0.024 for -h-k-l,l,k 0.055 for h-k+l,l,-h-l 0.066 for -k-l,-h-l,k 0.046 for h+k+l,-l,-h-l 0.035 for k-l,h+l,-k 0.017 for h,-k,-h-l 0.157 for -h-2*l,-k,l	Xtriage
Reported twinning fraction	0.772 for H, K, L 0.228 for H+4/2L, -K, -L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 157773 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18380	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

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.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BGC, CL

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	0.48	0/2876	0.62	1/3921 (0.0%)
1	B	0.47	0/2879	0.61	0/3924
1	C	0.48	0/2862	0.61	0/3902
1	D	0.44	0/2853	0.60	0/3891
1	E	0.47	0/2876	0.61	1/3921 (0.0%)
1	F	0.44	0/2862	0.59	0/3902
All	All	0.47	0/17208	0.61	2/23461 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	LYS	CD-CE-NZ	6.69	127.09	111.70
1	E	78	LYS	CD-CE-NZ	6.57	126.81	111.70

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	2775	0	2686	12	0
1	B	2781	0	2693	14	0
1	C	2767	0	2675	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2758	0	2662	13	0
1	E	2775	0	2691	14	0
1	F	2767	0	2675	12	0
2	A	34	0	30	0	0
2	B	34	0	30	0	0
2	C	34	0	30	1	0
2	D	34	0	30	1	0
2	E	34	0	30	3	0
2	F	34	0	30	1	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
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	305	0	0	2	0
5	B	259	0	0	1	0
5	C	254	0	0	1	0
5	D	217	0	0	2	0
5	E	285	0	0	0	0
5	F	221	0	0	2	0
All	All	18380	0	16262	81	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 2.

All (81) 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:C:264:VAL:HG23	1:C:269:ASN:ND2	1.96	0.80
1:E:303:HIS:NE2	2:E:401:BGC:O6	2.23	0.71
1:A:46:LYS:HE2	1:A:132:ASP:HA	1.81	0.62
1:C:264:VAL:HG23	1:C:269:ASN:HD21	1.65	0.59
1:F:30:ASP:N	5:F:2001:HOH:O	2.38	0.57
1:C:315:ARG:HD2	5:C:2223:HOH:O	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:VAL:CG2	1:C:269:ASN:ND2	2.70	0.53
1:B:82:ARG:NH1	1:B:335:ASP:OD2	2.42	0.52
1:E:82:ARG:NH1	1:E:335:ASP:OD2	2.44	0.51
1:D:172:THR:CG2	1:D:219:SER:HB3	2.40	0.51
1:B:140:ASP:OD1	1:B:188:ASN:HB2	2.12	0.50
1:C:264:VAL:CG2	1:C:269:ASN:HD21	2.24	0.50
1:A:140:ASP:OD1	1:A:188:ASN:HB2	2.12	0.50
1:F:140:ASP:OD1	1:F:188:ASN:HB2	2.11	0.50
1:A:253:ALA:O	1:A:289:ALA:HA	2.12	0.49
1:C:140:ASP:OD1	1:C:188:ASN:HB2	2.12	0.49
1:E:253:ALA:O	1:E:289:ALA:HA	2.13	0.49
1:D:140:ASP:OD1	1:D:188:ASN:HB2	2.11	0.49
1:E:272:LYS:O	1:E:276:GLU:HG3	2.13	0.48
1:D:253:ALA:O	1:D:289:ALA:HA	2.13	0.48
1:A:357:GLN:HG2	5:A:2301:HOH:O	2.13	0.48
1:B:253:ALA:O	1:B:289:ALA:HA	2.13	0.48
1:F:172:THR:HG21	1:F:219:SER:HB3	1.96	0.48
1:E:140:ASP:OD1	1:E:188:ASN:HB2	2.14	0.47
1:C:253:ALA:O	1:C:289:ALA:HA	2.13	0.47
1:C:172:THR:HG21	1:C:219:SER:HB3	1.97	0.47
1:A:172:THR:HG21	1:A:219:SER:HB3	1.95	0.47
1:A:172:THR:CG2	1:A:219:SER:HB3	2.45	0.46
1:C:172:THR:CG2	1:C:219:SER:HB3	2.45	0.46
1:D:172:THR:HG21	1:D:219:SER:HB3	1.97	0.46
1:E:172:THR:HG21	1:E:219:SER:HB3	1.96	0.46
1:E:172:THR:CG2	1:E:219:SER:HB3	2.46	0.46
1:F:253:ALA:O	1:F:289:ALA:HA	2.15	0.46
1:A:330:TRP:CD2	1:A:331:VAL:HB	2.51	0.45
1:B:172:THR:HG21	1:B:219:SER:HB3	1.97	0.45
1:F:291:GLN:HE22	2:F:401:BGC:H1	1.81	0.45
1:E:291:GLN:HE22	2:E:401:BGC:H1	1.81	0.45
1:E:216:ILE:CG2	1:E:223:VAL:HG21	2.47	0.45
1:E:277:LYS:HD3	1:E:277:LYS:HA	1.88	0.45
1:B:172:THR:CG2	1:B:219:SER:HB3	2.46	0.45
1:B:216:ILE:CG2	1:B:223:VAL:HG21	2.47	0.45
1:C:303:HIS:CE1	2:C:401:BGC:H6	2.26	0.45
1:F:172:THR:CG2	1:F:219:SER:HB3	2.46	0.45
1:C:237:SER:N	1:C:238:PRO:CD	2.80	0.45
1:B:98:GLY:HA2	5:B:2063:HOH:O	2.16	0.45
1:B:268:LYS:HG2	1:B:272:LYS:HE2	1.98	0.44
1:B:330:TRP:CD2	1:B:331:VAL:HB	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:LYS:HE3	1:D:132:ASP:HA	1.97	0.44
1:A:216:ILE:CG2	1:A:223:VAL:HG21	2.47	0.44
1:A:237:SER:N	1:A:238:PRO:CD	2.80	0.44
1:D:103:ARG:NE	1:D:290:THR:HB	2.32	0.44
1:C:103:ARG:NE	1:C:290:THR:HB	2.33	0.44
1:C:330:TRP:CD2	1:C:331:VAL:HB	2.52	0.44
1:D:216:ILE:CG2	1:D:223:VAL:HG21	2.47	0.44
1:D:277:LYS:HD3	1:D:277:LYS:HA	1.81	0.43
1:F:103:ARG:NE	1:F:290:THR:HB	2.34	0.43
1:F:216:ILE:CG2	1:F:223:VAL:HG21	2.49	0.43
2:D:399:BGC:H6	1:E:32:TRP:HD1	1.63	0.43
1:B:272:LYS:HB2	1:B:272:LYS:HE3	1.82	0.43
1:C:216:ILE:CG2	1:C:223:VAL:HG21	2.47	0.43
1:D:237:SER:N	1:D:238:PRO:CD	2.81	0.43
1:C:264:VAL:HG23	1:C:269:ASN:HD22	1.77	0.42
1:B:83:ASN:O	1:B:86:GLN:NE2	2.52	0.42
1:B:237:SER:N	1:B:238:PRO:CD	2.82	0.42
1:F:330:TRP:CD2	1:F:331:VAL:HB	2.55	0.42
1:A:364:LYS:HB2	5:A:2304:HOH:O	2.18	0.42
1:D:45:LEU:HB2	5:D:2010:HOH:O	2.19	0.42
1:E:103:ARG:NE	1:E:290:THR:HB	2.35	0.41
1:D:45:LEU:HD12	5:D:2010:HOH:O	2.19	0.41
1:F:276:GLU:HB3	5:F:2150:HOH:O	2.20	0.41
1:A:72:ASN:OD1	1:A:103:ARG:HD3	2.21	0.41
1:F:237:SER:N	1:F:238:PRO:CD	2.83	0.41
2:E:399:BGC:C6	1:F:32:TRP:HD1	2.34	0.41
1:B:72:ASN:OD1	1:B:103:ARG:HD3	2.20	0.41
1:D:330:TRP:CD2	1:D:331:VAL:HB	2.56	0.41
1:B:236:LEU:O	1:B:239:ILE:HG12	2.21	0.41
1:D:236:LEU:O	1:D:239:ILE:HG12	2.21	0.40
1:A:330:TRP:HA	1:A:331:VAL:HA	1.93	0.40
1:C:277:LYS:HA	1:C:277:LYS:HD3	1.91	0.40
1:E:237:SER:N	1:E:238:PRO:CD	2.84	0.40
1:E:330:TRP:CD2	1:E:331:VAL:HB	2.56	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	335/365 (92%)	330 (98%)	5 (2%)	0	100	100
1	B	335/365 (92%)	330 (98%)	5 (2%)	0	100	100
1	C	333/365 (91%)	328 (98%)	5 (2%)	0	100	100
1	D	332/365 (91%)	327 (98%)	5 (2%)	0	100	100
1	E	335/365 (92%)	329 (98%)	6 (2%)	0	100	100
1	F	333/365 (91%)	329 (99%)	4 (1%)	0	100	100
All	All	2003/2190 (92%)	1973 (98%)	30 (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	296/317 (93%)	293 (99%)	3 (1%)	82	85
1	B	296/317 (93%)	293 (99%)	3 (1%)	82	85
1	C	294/317 (93%)	290 (99%)	4 (1%)	74	77
1	D	293/317 (92%)	290 (99%)	3 (1%)	82	85
1	E	296/317 (93%)	293 (99%)	3 (1%)	82	85
1	F	294/317 (93%)	292 (99%)	2 (1%)	88	91
All	All	1769/1902 (93%)	1751 (99%)	18 (1%)	82	85

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	140	ASP
1	A	169	ARG
1	B	86	GLN
1	B	169	ARG
1	B	322	LYS
1	C	86	GLN
1	C	140	ASP
1	C	169	ARG
1	C	276	GLU
1	D	140	ASP
1	D	169	ARG
1	D	221	LYS
1	E	140	ASP
1	E	169	ARG
1	E	323	LYS
1	F	169	ARG
1	F	241	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	357	GLN
1	D	357	GLN
1	E	357	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 ⓘ

18 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	399	2	12,12,12	0.81	0	17,17,17	2.05	5 (29%)
2	BGC	A	400	2	11,11,12	0.51	0	15,15,17	1.11	1 (6%)
2	BGC	A	401	2	11,11,12	0.52	0	15,15,17	0.89	0
2	BGC	B	399	2	12,12,12	0.73	0	17,17,17	1.45	3 (17%)
2	BGC	B	400	2	11,11,12	0.37	0	15,15,17	0.98	0
2	BGC	B	401	2	11,11,12	0.40	0	15,15,17	1.12	0
2	BGC	C	399	2	11,11,12	0.44	0	15,15,17	1.53	4 (26%)
2	BGC	C	400	2	11,11,12	0.66	0	15,15,17	1.32	2 (13%)
2	BGC	C	401	2	12,12,12	0.70	0	17,17,17	1.45	1 (5%)
2	BGC	D	399	2	11,11,12	0.61	0	15,15,17	1.88	5 (33%)
2	BGC	D	400	2	11,11,12	0.67	0	15,15,17	0.99	1 (6%)
2	BGC	D	401	2	12,12,12	0.76	0	17,17,17	1.65	4 (23%)
2	BGC	E	399	2	11,11,12	0.67	0	15,15,17	1.47	4 (26%)
2	BGC	E	400	2	11,11,12	0.83	0	15,15,17	0.99	1 (6%)
2	BGC	E	401	2	12,12,12	1.10	0	17,17,17	1.33	1 (5%)
2	BGC	F	399	2	11,11,12	0.67	0	15,15,17	1.30	3 (20%)
2	BGC	F	400	2	11,11,12	0.60	0	15,15,17	1.29	2 (13%)
2	BGC	F	401	2	12,12,12	0.79	0	17,17,17	1.39	3 (17%)

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	399	2	-	0/2/22/22	0/1/1/1
2	BGC	A	400	2	-	0/2/19/22	0/1/1/1
2	BGC	A	401	2	-	0/2/19/22	0/1/1/1
2	BGC	B	399	2	-	0/2/22/22	0/1/1/1
2	BGC	B	400	2	-	0/2/19/22	0/1/1/1
2	BGC	B	401	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	C	399	2	-	0/2/19/22	0/1/1/1
2	BGC	C	400	2	-	0/2/19/22	0/1/1/1
2	BGC	C	401	2	-	0/2/22/22	0/1/1/1
2	BGC	D	399	2	-	0/2/19/22	0/1/1/1
2	BGC	D	400	2	-	0/2/19/22	0/1/1/1
2	BGC	D	401	2	-	0/2/22/22	0/1/1/1
2	BGC	E	399	2	-	0/2/19/22	0/1/1/1
2	BGC	E	400	2	-	0/2/19/22	0/1/1/1
2	BGC	E	401	2	-	0/2/22/22	0/1/1/1
2	BGC	F	399	2	-	0/2/19/22	0/1/1/1
2	BGC	F	400	2	-	0/2/19/22	0/1/1/1
2	BGC	F	401	2	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	399	BGC	O1-C1-O5	-4.57	97.60	110.33
2	D	399	BGC	O5-C5-C6	-3.76	99.29	107.34
2	C	400	BGC	O5-C1-C2	-3.10	105.93	110.89
2	D	401	BGC	O1-C1-O5	-3.07	101.76	110.33
2	D	399	BGC	O6-C6-C5	-3.02	101.22	111.30
2	F	400	BGC	O3-C3-C2	-2.96	104.58	110.01
2	B	399	BGC	O5-C5-C4	-2.90	104.14	109.67
2	A	400	BGC	O3-C3-C2	-2.84	104.79	110.01
2	D	399	BGC	O3-C3-C4	-2.72	104.22	110.36
2	E	400	BGC	O3-C3-C2	-2.70	105.06	110.01
2	F	399	BGC	O6-C6-C5	-2.64	102.50	111.30
2	C	401	BGC	C3-C4-C5	-2.54	105.70	110.23
2	C	399	BGC	O5-C5-C6	-2.50	101.99	107.34
2	D	400	BGC	O3-C3-C2	-2.47	105.47	110.01
2	A	399	BGC	O2-C2-C3	-2.43	104.88	110.36
2	D	401	BGC	O2-C2-C3	-2.43	104.88	110.36
2	F	399	BGC	O5-C5-C4	-2.35	106.24	110.13
2	B	399	BGC	C3-C4-C5	-2.22	106.27	110.23
2	F	401	BGC	O1-C1-O5	-2.17	104.27	110.33
2	E	399	BGC	O2-C2-C1	-2.16	104.91	109.23
2	E	399	BGC	C2-C3-C4	-2.08	107.42	111.05
2	C	399	BGC	O6-C6-C5	-2.07	104.39	111.30
2	E	399	BGC	O2-C2-C3	2.13	114.47	110.19
2	C	399	BGC	C1-C2-C3	2.15	112.15	109.55
2	F	399	BGC	O4-C4-C3	2.20	115.31	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	BGC	C1-O5-C5	2.31	115.53	112.14
2	A	399	BGC	C1-O5-C5	2.46	118.26	113.54
2	F	401	BGC	O5-C1-C2	2.47	114.32	110.00
2	D	399	BGC	O5-C5-C4	2.49	114.26	110.13
2	D	401	BGC	O1-C1-C2	2.51	115.98	109.05
2	F	400	BGC	O2-C2-C1	2.62	114.48	109.23
2	E	401	BGC	O5-C1-C2	2.63	114.60	110.00
2	A	399	BGC	O5-C1-C2	2.71	114.75	110.00
2	B	399	BGC	C1-C2-C3	2.78	115.24	110.68
2	D	401	BGC	C1-C2-C3	2.90	115.43	110.68
2	A	399	BGC	O2-C2-C1	2.97	116.24	109.74
2	C	399	BGC	C1-O5-C5	2.97	116.50	112.14
2	F	401	BGC	C1-C2-C3	3.05	115.68	110.68
2	E	399	BGC	C1-O5-C5	3.16	116.79	112.14
2	D	399	BGC	C1-O5-C5	3.19	116.84	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	BGC	1	0
2	D	399	BGC	1	0
2	E	399	BGC	1	0
2	E	401	BGC	2	0
2	F	401	BGC	1	0

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 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 [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(Å²)	Q<0.9	
1	A	335/365 (91%)	-0.33	0	100	100	15, 20, 31, 48	0
1	B	336/365 (92%)	-0.27	3 (0%)	85	86	15, 21, 32, 55	0
1	C	335/365 (91%)	-0.27	1 (0%)	94	94	16, 22, 33, 57	0
1	D	334/365 (91%)	-0.18	1 (0%)	94	94	16, 24, 38, 48	0
1	E	335/365 (91%)	-0.30	1 (0%)	94	94	15, 20, 30, 53	0
1	F	335/365 (91%)	-0.22	1 (0%)	94	94	18, 23, 34, 59	0
All	All	2010/2190 (91%)	-0.26	7 (0%)	94	94	15, 22, 34, 59	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	365	ARG	4.6
1	D	82	ARG	3.3
1	E	364	LYS	3.2
1	C	364	LYS	2.9
1	B	82	ARG	2.7
1	F	364	LYS	2.6
1	B	83	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

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	E	399	11/12	0.70	0.32	7.25	29,34,37,38	0
2	BGC	D	399	11/12	0.80	0.18	7.00	28,30,31,33	0
2	BGC	A	401	11/12	0.79	0.21	4.73	25,28,30,32	0
2	BGC	C	399	11/12	0.92	0.17	3.16	27,30,34,37	0
2	BGC	F	399	11/12	0.82	0.19	2.97	26,30,33,36	0
2	BGC	E	401	12/12	0.83	0.14	2.54	22,25,27,30	0
2	BGC	B	399	12/12	0.85	0.12	1.94	21,24,29,29	0
2	BGC	B	401	11/12	0.87	0.14	1.44	25,26,32,34	0
2	BGC	D	401	12/12	0.90	0.11	1.05	24,28,30,31	0
2	BGC	A	399	12/12	0.90	0.11	1.04	21,23,25,26	0
2	BGC	A	400	11/12	0.89	0.12	0.98	17,20,22,24	0
2	BGC	F	401	12/12	0.91	0.10	-0.11	22,25,28,28	0
2	BGC	F	400	11/12	0.96	0.09	-0.39	19,20,23,25	0
2	BGC	C	401	12/12	0.92	0.09	-0.51	21,24,26,26	0
2	BGC	B	400	11/12	0.95	0.08	-0.54	18,21,23,24	0
2	BGC	D	400	11/12	0.95	0.09	-0.75	18,22,24,25	0
2	BGC	E	400	11/12	0.93	0.08	-0.76	18,21,23,24	0
2	BGC	C	400	11/12	0.93	0.08	-0.91	20,23,24,25	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
4	CL	A	403	1/1	1.00	0.10	2.47	21,21,21,21	0
4	CL	B	403	1/1	1.00	0.10	0.20	21,21,21,21	0
4	CL	E	403	1/1	1.00	0.10	0.12	23,23,23,23	0
3	MG	C	402	1/1	0.96	0.08	-0.30	26,26,26,26	0
3	MG	F	402	1/1	0.94	0.08	-0.74	26,26,26,26	0
3	MG	B	402	1/1	0.97	0.06	-1.23	25,25,25,25	0
3	MG	E	402	1/1	0.98	0.07	-1.44	22,22,22,22	0
4	CL	F	403	1/1	0.98	0.07	-2.39	24,24,24,24	0
3	MG	D	402	1/1	0.98	0.06	-2.75	26,26,26,26	0
4	CL	C	403	1/1	0.98	0.07	-2.78	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	A	402	1/1	0.97	0.05	-2.86	24,24,24,24	0
4	CL	D	403	1/1	0.99	0.07	-3.12	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.