



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 08:22 AM BST

PDB ID : 4GX0  
Title : Crystal structure of the GsuK L97D mutant  
Authors : Kong, C.; Zeng, W.; Ye, S.; Chen, L.; Sauer, D.B.; Lam, Y.; Derebe, M.G.; Jiang, Y.  
Deposited on : 2012-09-03  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

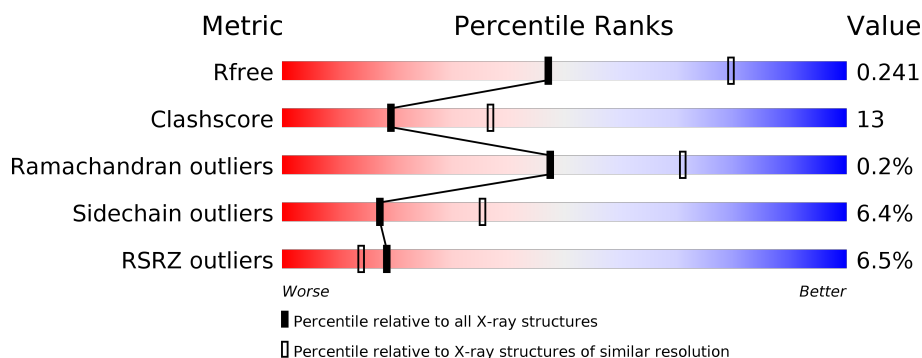
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	565	<div> <div>2%</div> <div> <div></div> <div>50%</div> <div>16%</div> <div>•</div> <div>34%</div> </div> </div>
1	B	565	<div> <div>11%</div> <div> <div></div> <div>66%</div> <div>29%</div> <div>• •</div> </div> </div>
1	C	565	<div> <div>5%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>• •</div> </div> </div>
1	D	565	<div> <div>3%</div> <div> <div></div> <div>49%</div> <div>16%</div> <div>•</div> <div>33%</div> </div> </div>
2	E	2	<div> <div></div> <div>100%</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
3	K	A	605	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14730 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 TrkA domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2922	1880	506	525	11			
1	B	547	Total	C	N	O	S	0	0	0
			4197	2687	725	770	15			
1	C	546	Total	C	N	O	S	0	0	0
			4188	2682	723	768	15			
1	D	376	Total	C	N	O	S	0	0	0
			2928	1883	507	527	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	expression tag	UNP Q74FS9
A	5	GLN	-	expression tag	UNP Q74FS9
A	6	ARG	-	expression tag	UNP Q74FS9
A	7	GLY	-	expression tag	UNP Q74FS9
A	8	SER	-	expression tag	UNP Q74FS9
A	52	ALA	GLU	engineered mutation	UNP Q74FS9
A	77	GLU	GLN	engineered mutation	UNP Q74FS9
A	97	ASP	LEU	engineered mutation	UNP Q74FS9
A	565	LEU	-	expression tag	UNP Q74FS9
A	566	VAL	-	expression tag	UNP Q74FS9
A	567	PRO	-	expression tag	UNP Q74FS9
A	568	ARG	-	expression tag	UNP Q74FS9
B	4	MET	-	expression tag	UNP Q74FS9
B	5	GLN	-	expression tag	UNP Q74FS9
B	6	ARG	-	expression tag	UNP Q74FS9
B	7	GLY	-	expression tag	UNP Q74FS9
B	8	SER	-	expression tag	UNP Q74FS9
B	52	ALA	GLU	engineered mutation	UNP Q74FS9
B	77	GLU	GLN	engineered mutation	UNP Q74FS9
B	97	ASP	LEU	engineered mutation	UNP Q74FS9
B	565	LEU	-	expression tag	UNP Q74FS9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	566	VAL	-	expression tag	UNP Q74FS9
B	567	PRO	-	expression tag	UNP Q74FS9
B	568	ARG	-	expression tag	UNP Q74FS9
C	4	MET	-	expression tag	UNP Q74FS9
C	5	GLN	-	expression tag	UNP Q74FS9
C	6	ARG	-	expression tag	UNP Q74FS9
C	7	GLY	-	expression tag	UNP Q74FS9
C	8	SER	-	expression tag	UNP Q74FS9
C	52	ALA	GLU	engineered mutation	UNP Q74FS9
C	77	GLU	GLN	engineered mutation	UNP Q74FS9
C	97	ASP	LEU	engineered mutation	UNP Q74FS9
C	565	LEU	-	expression tag	UNP Q74FS9
C	566	VAL	-	expression tag	UNP Q74FS9
C	567	PRO	-	expression tag	UNP Q74FS9
C	568	ARG	-	expression tag	UNP Q74FS9
D	4	MET	-	expression tag	UNP Q74FS9
D	5	GLN	-	expression tag	UNP Q74FS9
D	6	ARG	-	expression tag	UNP Q74FS9
D	7	GLY	-	expression tag	UNP Q74FS9
D	8	SER	-	expression tag	UNP Q74FS9
D	52	ALA	GLU	engineered mutation	UNP Q74FS9
D	77	GLU	GLN	engineered mutation	UNP Q74FS9
D	97	ASP	LEU	engineered mutation	UNP Q74FS9
D	565	LEU	-	expression tag	UNP Q74FS9
D	566	VAL	-	expression tag	UNP Q74FS9
D	567	PRO	-	expression tag	UNP Q74FS9
D	568	ARG	-	expression tag	UNP Q74FS9

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total K 1 1	0	0
3	A	5	Total K 5 5	0	0
3	D	1	Total K 1 1	0	0
3	C	5	Total K 5 5	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	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

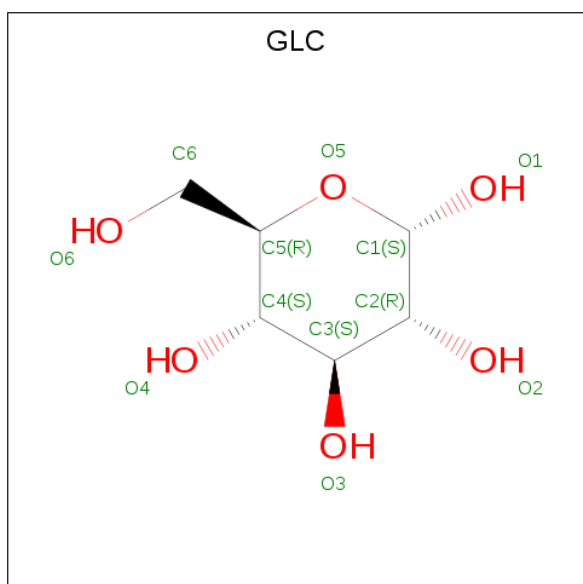
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ca 1 1	0	0
5	A	1	Total Ca 1 1	0	0
5	C	2	Total Ca 2 2	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			12	6	6		
7	B	1	Total	C	O	0	0
			12	6	6		
7	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 8 is water.

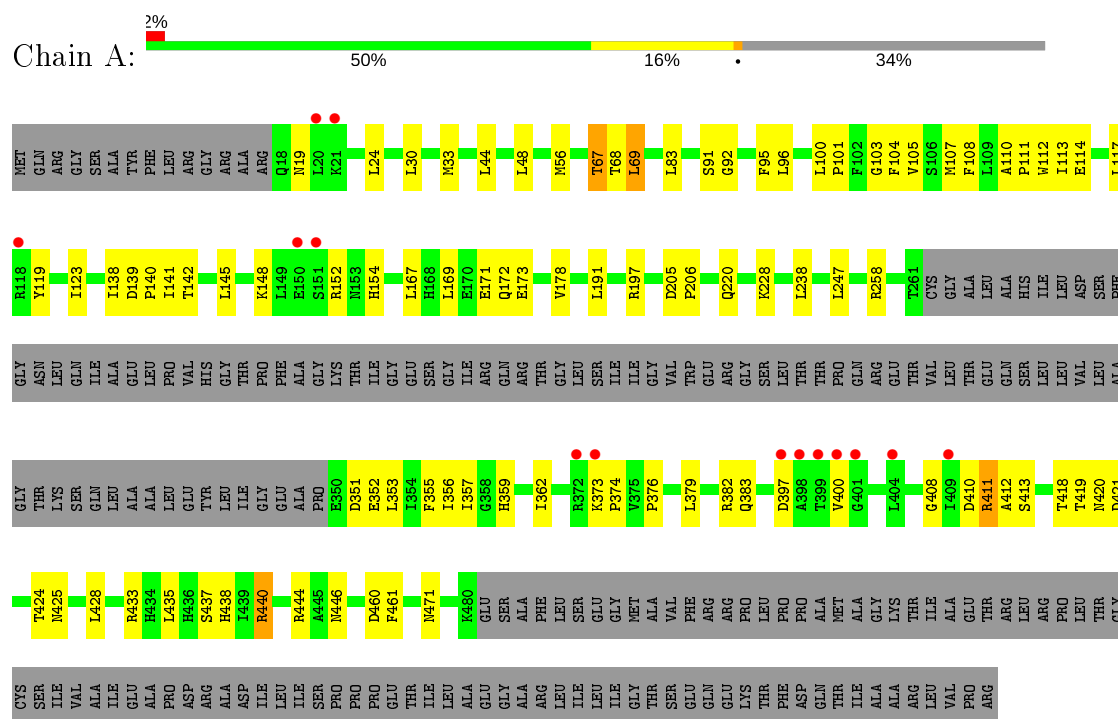
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	94	Total	O	0	0
			94	94		
8	B	99	Total	O	0	0
			99	99		
8	C	116	Total	O	0	0
			116	116		
8	D	82	Total	O	0	0
			82	82		



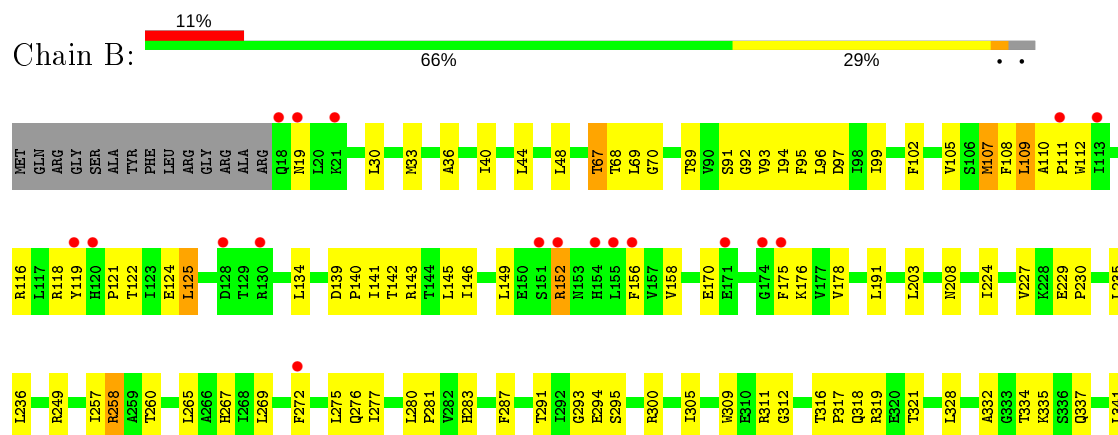
### 3 Residue-property plots [i](#)

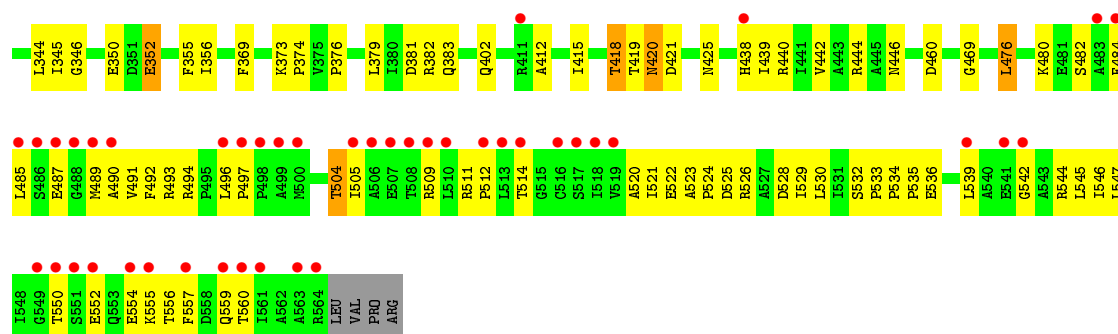
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

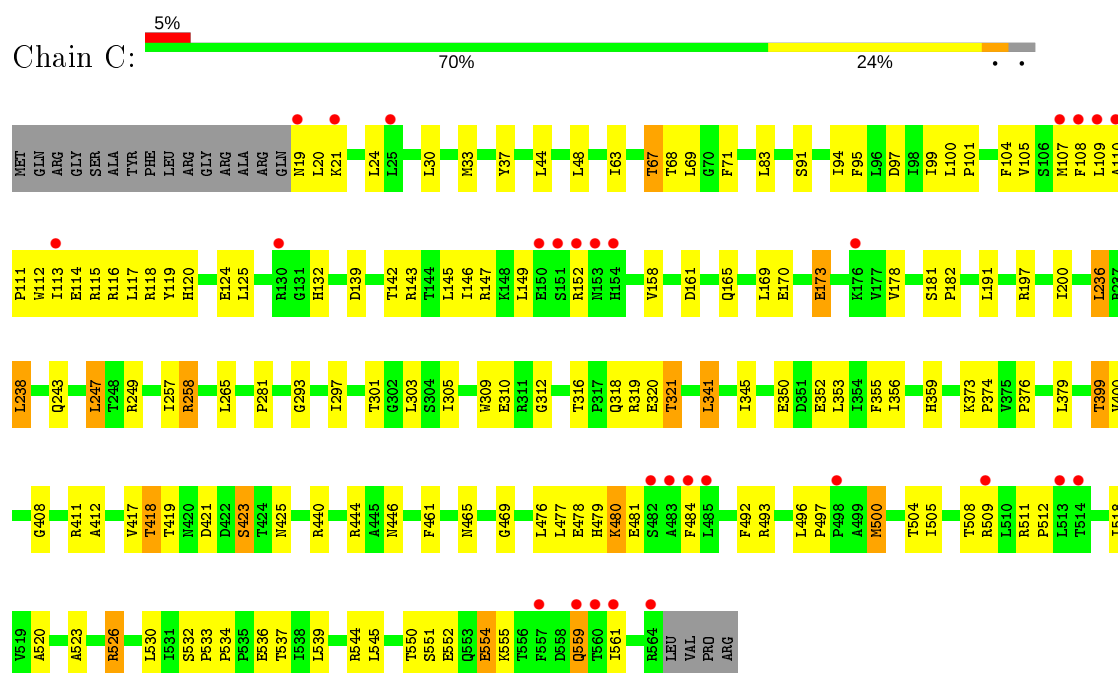


- Molecule 1: TrkA domain protein

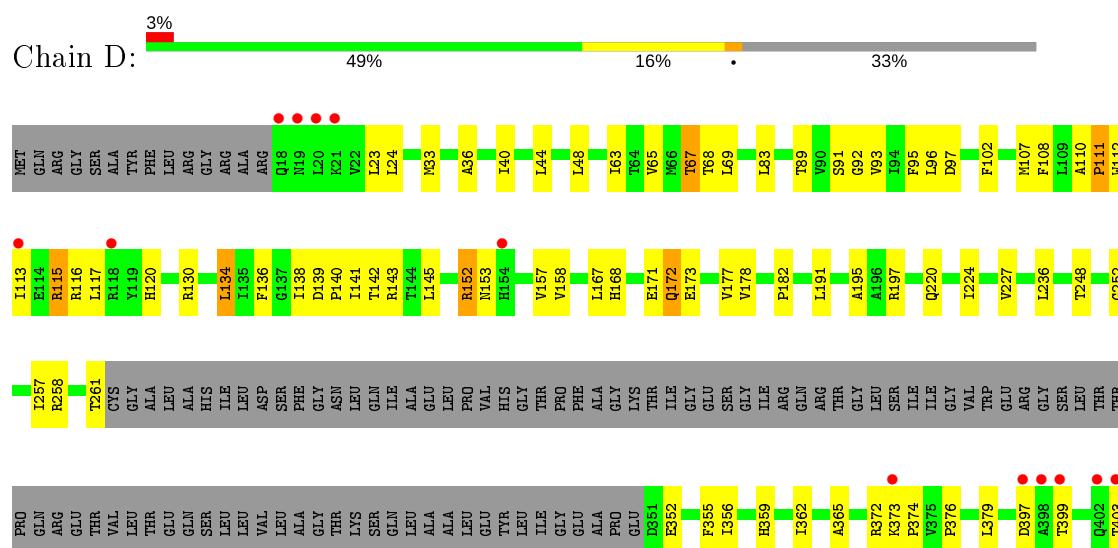


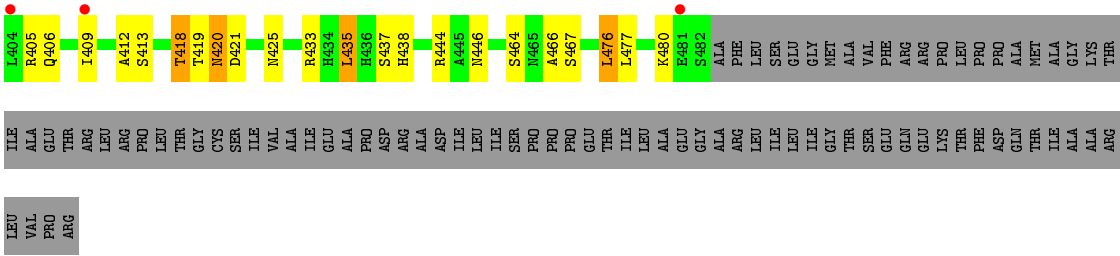


• Molecule 1: TrkA domain protein



• Molecule 1: TrkA domain protein





● Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E: 100%

GLC1  
GLC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	232.93Å 111.67Å 164.13Å 90.00° 134.47° 90.00°	Depositor
Resolution (Å)	30.94 – 2.60 49.63 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.6 (30.94-2.60) 94.6 (49.63-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.203 , 0.249 0.194 , 0.241	Depositor DCC
$R_{free}$ test set	4375 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.7	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 64.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.047 for h+2*l,k,-h-l 0.008 for h,-k,-h-l 0.018 for -h-2*l,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14730	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5581e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: K, ZN, GLC, CA, PO4

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	0.28	0/2982	0.41	0/4060
1	B	0.27	0/4280	0.42	0/5829
1	C	0.23	0/4271	0.42	0/5817
1	D	0.23	0/2988	0.41	0/4068
All	All	0.25	0/14521	0.41	0/19774

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2922	0	2955	70	0
1	B	4197	0	4267	125	0
1	C	4188	0	4259	117	0
1	D	2928	0	2960	78	0
2	E	23	0	21	0	0
3	A	5	0	0	0	0
3	B	1	0	0	0	0
3	C	5	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
6	A	5	0	0	1	0
6	B	10	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
7	B	24	0	22	0	0
7	D	12	0	11	0	0
8	A	94	0	0	0	0
8	B	99	0	0	0	0
8	C	116	0	0	2	0
8	D	82	0	0	2	0
All	All	14730	0	14495	371	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 13.

All (371) 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:493:ARG:HD2	1:C:544:ARG:HD3	1.44	1.00
1:D:130:ARG:HG3	1:D:195:ALA:HB1	1.48	0.95
1:C:112:TRP:CH2	1:D:113:ILE:HD13	2.11	0.86
1:B:352:GLU:O	1:B:376:PRO:HG2	1.76	0.85
1:D:33:MET:HE1	1:D:91:SER:HB3	1.59	0.83
1:C:33:MET:HE1	1:C:91:SER:HB3	1.60	0.83
1:C:105:VAL:HG13	1:C:109:LEU:HD23	1.61	0.82
1:B:493:ARG:HD3	1:B:544:ARG:HD2	1.59	0.82
1:B:496:LEU:HD22	1:B:497:PRO:HD2	1.64	0.80
1:A:352:GLU:O	1:A:376:PRO:HG2	1.84	0.77
1:C:119:TYR:HE2	1:C:170:GLU:HG3	1.50	0.77
1:C:112:TRP:HH2	1:D:113:ILE:HD13	1.49	0.76
1:B:33:MET:HE1	1:B:91:SER:HB3	1.65	0.76
1:C:352:GLU:O	1:C:376:PRO:HG2	1.87	0.75
1:A:419:THR:HG22	1:A:421:ASP:H	1.51	0.75
1:B:119:TYR:CE2	1:B:170:GLU:HG3	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:VAL:HG11	1:A:191:LEU:HD21	1.70	0.74
1:C:500:MET:HG3	1:C:508:THR:HG21	1.70	0.73
1:C:496:LEU:HD22	1:C:497:PRO:HD2	1.69	0.73
1:B:230:PRO:HB3	1:B:249:ARG:HH11	1.54	0.72
1:A:104:PHE:HE1	1:B:102:PHE:HD1	1.38	0.72
1:B:496:LEU:HD23	1:B:545:LEU:HD11	1.71	0.72
1:D:112:TRP:CE3	1:D:113:ILE:HG13	2.25	0.72
1:B:419:THR:HG22	1:B:421:ASP:H	1.54	0.71
1:B:334:THR:H	1:B:337:GLN:NE2	1.89	0.71
1:B:119:TYR:HE2	1:B:170:GLU:HG3	1.56	0.71
1:C:505:ILE:HD13	1:C:518:ILE:HG21	1.71	0.70
1:B:146:ILE:HG21	1:B:175:PHE:CD2	2.25	0.70
1:C:419:THR:HG22	1:C:421:ASP:H	1.56	0.70
1:D:143:ARG:HH22	1:D:172:GLN:HE22	1.38	0.70
1:C:113:ILE:HG13	1:C:117:LEU:HD23	1.74	0.70
1:C:496:LEU:HD21	1:C:539:LEU:HD23	1.74	0.69
1:C:69:LEU:HD23	1:D:68:THR:HA	1.72	0.69
1:B:146:ILE:HG21	1:B:175:PHE:HD2	1.57	0.69
1:D:143:ARG:HH22	1:D:172:GLN:NE2	1.90	0.69
1:B:139:ASP:HB2	1:B:140:PRO:HD2	1.74	0.68
1:B:523:ALA:HB3	1:B:526:ARG:HB2	1.76	0.68
1:A:110:ALA:HB3	1:A:111:PRO:HD3	1.76	0.68
1:B:203:LEU:H	1:B:208:ASN:HD21	1.41	0.68
1:B:224:ILE:HD11	1:B:480:LYS:HE2	1.77	0.67
1:C:105:VAL:O	1:C:109:LEU:HB3	1.94	0.67
1:D:419:THR:HG22	1:D:421:ASP:H	1.59	0.67
1:C:112:TRP:CH2	1:D:113:ILE:HG21	2.29	0.66
1:C:119:TYR:CE2	1:C:170:GLU:HG3	2.31	0.66
1:A:444:ARG:NH2	1:A:446:ASN:HD21	1.93	0.66
1:C:551:SER:O	1:C:555:LYS:HD3	1.95	0.65
1:A:171:GLU:HG3	1:A:172:GLN:N	2.13	0.64
1:C:115:ARG:HD3	1:C:120:HIS:CE1	2.32	0.64
1:D:139:ASP:HB2	1:D:140:PRO:HD2	1.80	0.63
1:C:112:TRP:CZ3	1:C:113:ILE:HB	2.34	0.63
1:D:113:ILE:HG23	1:D:117:LEU:HD12	1.81	0.63
1:A:113:ILE:HG13	1:A:114:GLU:N	2.12	0.63
1:B:149:LEU:HB2	1:B:156:PHE:HE1	1.64	0.62
1:A:419:THR:HB	1:A:425:ASN:OD1	2.00	0.62
1:A:92:GLY:O	1:A:96:LEU:HB2	1.99	0.62
1:C:111:PRO:O	1:C:115:ARG:HG3	1.98	0.62
1:C:419:THR:H	1:C:425:ASN:HD21	1.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:THR:HB	1:B:425:ASN:OD1	2.00	0.61
1:C:496:LEU:HD23	1:C:545:LEU:HD11	1.82	0.61
1:B:112:TRP:HE1	1:B:116:ARG:NH1	1.98	0.61
1:B:345:ILE:HB	1:B:346:GLY:HA2	1.82	0.61
1:D:36:ALA:O	1:D:40:ILE:HG13	2.00	0.61
1:C:112:TRP:CE3	1:C:113:ILE:HB	2.35	0.61
1:D:110:ALA:HB3	1:D:111:PRO:HD3	1.83	0.61
1:B:67:THR:O	1:B:68:THR:OG1	2.18	0.60
1:C:318:GLN:HB2	1:C:321:THR:HG22	1.81	0.60
1:D:352:GLU:O	1:D:376:PRO:HG2	2.00	0.60
1:B:272:PHE:CD2	1:B:490:ALA:HB2	2.37	0.60
1:B:110:ALA:HB3	1:B:111:PRO:HD3	1.82	0.60
1:C:480:LYS:HE2	1:C:481:GLU:HG2	1.82	0.60
1:C:523:ALA:HB3	1:C:526:ARG:HG3	1.84	0.59
1:C:418:THR:HG22	1:C:444:ARG:HH11	1.68	0.59
1:A:356:ILE:HB	1:A:379:LEU:HD23	1.84	0.58
1:B:511:ARG:N	1:B:512:PRO:HD2	2.18	0.58
1:C:178:VAL:HG11	1:C:191:LEU:HD21	1.84	0.58
1:A:171:GLU:HG3	1:A:172:GLN:H	1.67	0.58
1:B:149:LEU:HB2	1:B:156:PHE:CE1	2.38	0.58
1:B:44:LEU:O	1:B:48:LEU:HB2	2.04	0.58
1:A:444:ARG:CZ	1:A:446:ASN:HD21	2.17	0.58
1:C:511:ARG:HB3	1:C:512:PRO:HD3	1.87	0.57
1:B:272:PHE:CE2	1:B:490:ALA:HB2	2.39	0.57
1:A:103:GLY:O	1:A:107:MET:HB3	2.04	0.57
1:C:63:ILE:O	1:C:67:THR:HB	2.05	0.57
1:B:484:PHE:HA	1:B:487:GLU:HB3	1.87	0.57
1:C:419:THR:HB	1:C:425:ASN:ND2	2.20	0.57
1:C:419:THR:HB	1:C:425:ASN:HD21	1.68	0.57
1:B:525:ASP:O	1:B:526:ARG:HG3	2.04	0.57
1:C:500:MET:HE3	1:C:508:THR:HB	1.86	0.57
1:C:142:THR:O	1:C:146:ILE:HG13	2.05	0.57
1:C:318:GLN:H	1:C:321:THR:HG21	1.70	0.57
1:B:149:LEU:HD12	1:B:156:PHE:HZ	1.70	0.56
1:A:19:ASN:HB3	1:A:107:MET:CE	2.36	0.56
1:A:411:ARG:HD3	1:A:411:ARG:H	1.69	0.56
1:B:139:ASP:HB2	1:B:140:PRO:CD	2.34	0.56
1:B:504:THR:HG23	1:B:535:PRO:O	2.04	0.56
1:D:44:LEU:O	1:D:48:LEU:HB2	2.05	0.56
1:A:19:ASN:HB3	1:A:107:MET:HE2	1.88	0.56
1:C:265:LEU:HD21	1:C:341:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:GLN:HB2	1:B:321:THR:OG1	2.06	0.56
1:D:138:ILE:HD11	1:D:143:ARG:HG2	1.87	0.55
1:D:419:THR:HB	1:D:425:ASN:OD1	2.07	0.55
1:D:139:ASP:HB2	1:D:140:PRO:CD	2.37	0.55
1:C:309:TRP:CZ2	1:C:312:GLY:HA2	2.40	0.55
1:A:139:ASP:HB2	1:A:140:PRO:CD	2.37	0.55
1:B:440:ARG:NH2	1:B:460:ASP:HB3	2.22	0.54
1:B:493:ARG:O	1:B:494:ARG:HD2	2.07	0.54
1:C:509:ARG:C	1:C:512:PRO:HD2	2.26	0.54
1:C:112:TRP:HH2	1:D:113:ILE:HG21	1.69	0.54
1:C:444:ARG:HE	1:C:465:ASN:HD21	1.56	0.54
1:D:111:PRO:O	1:D:115:ARG:HG2	2.08	0.54
1:B:356:ILE:HB	1:B:379:LEU:HD23	1.90	0.53
1:A:437:SER:OG	1:A:438:HIS:HD2	1.90	0.53
1:B:555:LYS:N	1:B:555:LYS:HD2	2.23	0.53
1:C:170:GLU:O	1:C:173:GLU:HB2	2.08	0.53
1:D:444:ARG:NH2	1:D:446:ASN:HD21	2.05	0.53
1:A:33:MET:HE1	1:A:91:SER:HB3	1.91	0.53
1:B:141:ILE:HD12	1:B:469:GLY:HA3	1.89	0.53
1:C:318:GLN:H	1:C:321:THR:CG2	2.21	0.53
1:A:56:MET:O	1:A:56:MET:HE3	2.09	0.52
1:C:418:THR:HG22	1:C:444:ARG:NH1	2.24	0.52
1:D:138:ILE:HD12	1:D:142:THR:OG1	2.10	0.52
1:D:437:SER:OG	1:D:438:HIS:HD2	1.90	0.52
1:A:69:LEU:CD2	1:B:70:GLY:HA3	2.39	0.52
1:C:500:MET:HE1	1:C:561:ILE:HD11	1.92	0.52
1:A:67:THR:HG21	1:B:89:THR:CG2	2.39	0.52
1:B:257:ILE:HG22	1:B:369:PHE:CZ	2.44	0.52
1:B:520:ALA:HB1	1:B:529:ILE:HD11	1.92	0.52
1:B:526:ARG:HE	1:B:528:ASP:HB2	1.74	0.52
1:A:19:ASN:O	1:A:107:MET:HE3	2.10	0.52
1:B:265:LEU:HD21	1:B:341:LEU:CD2	2.40	0.52
1:B:265:LEU:HD21	1:B:341:LEU:HD23	1.92	0.52
1:B:275:LEU:HD23	1:B:491:VAL:HG22	1.90	0.52
1:C:21:LYS:HA	1:C:24:LEU:CD2	2.41	0.51
1:C:67:THR:HG21	1:D:89:THR:CG2	2.40	0.51
1:A:104:PHE:CE1	1:B:102:PHE:HD1	2.25	0.51
1:C:301:THR:CG2	1:C:303:LEU:HG	2.40	0.51
1:A:228:LYS:HD2	1:A:228:LYS:N	2.25	0.51
1:B:309:TRP:CZ2	1:B:312:GLY:HA2	2.45	0.51
1:C:423:SER:HB2	8:C:806:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:476:LEU:O	1:D:480:LYS:HB2	2.11	0.51
1:A:138:ILE:HD12	1:A:142:THR:OG1	2.10	0.51
1:C:350:GLU:HA	1:C:350:GLU:OE2	2.10	0.51
1:D:178:VAL:HG11	1:D:191:LEU:HD21	1.93	0.51
1:C:359:HIS:CG	1:C:359:HIS:O	2.63	0.51
1:A:69:LEU:HD22	1:B:70:GLY:HA3	1.93	0.51
1:C:418:THR:HG23	1:C:444:ARG:HD3	1.92	0.51
1:A:408:GLY:C	1:A:410:ASP:H	2.14	0.51
1:B:230:PRO:HB3	1:B:249:ARG:NH1	2.24	0.51
1:A:139:ASP:HB2	1:A:140:PRO:HD2	1.92	0.51
1:C:110:ALA:N	1:C:111:PRO:HD2	2.26	0.50
1:C:356:ILE:HB	1:C:379:LEU:HD23	1.93	0.50
1:C:418:THR:CG2	1:C:444:ARG:HD3	2.42	0.50
1:B:281:PRO:HB2	1:B:283:HIS:CD2	2.47	0.50
1:B:122:THR:HG21	1:B:176:LYS:HE2	1.92	0.50
1:C:108:PHE:HA	1:C:111:PRO:HG2	1.93	0.50
1:D:397:ASP:O	1:D:403:THR:HG21	2.11	0.50
1:B:36:ALA:O	1:B:40:ILE:HG13	2.12	0.50
1:D:63:ILE:O	1:D:67:THR:HB	2.11	0.50
1:D:92:GLY:O	1:D:96:LEU:HB2	2.11	0.50
1:D:405:ARG:HA	1:D:409:ILE:HG22	1.94	0.50
1:A:138:ILE:HG21	1:A:169:LEU:HD11	1.94	0.50
1:B:293:GLY:HA3	1:B:319:ARG:HG2	1.94	0.50
1:B:524:PRO:HG3	1:B:542:GLY:C	2.32	0.49
1:B:227:VAL:HG22	1:B:229:GLU:H	1.76	0.49
1:D:168:HIS:O	1:D:171:GLU:HG3	2.11	0.49
1:C:71:PHE:HZ	1:D:65:VAL:HG22	1.76	0.49
1:C:20:LEU:H	1:C:20:LEU:HD22	1.77	0.49
1:C:115:ARG:HD3	1:C:120:HIS:NE2	2.28	0.49
1:C:33:MET:HE2	1:C:37:TYR:CE1	2.48	0.49
1:A:352:GLU:HG3	1:A:413:SER:OG	2.12	0.49
1:C:554:GLU:OE1	1:C:555:LYS:HD2	2.13	0.49
1:A:104:PHE:HE1	1:B:102:PHE:CD1	2.25	0.49
1:A:67:THR:O	1:A:68:THR:OG1	2.27	0.49
1:C:124:GLU:HG2	1:C:125:LEU:N	2.27	0.49
1:A:362:ILE:HD12	1:A:444:ARG:CZ	2.43	0.49
1:C:108:PHE:HA	1:C:111:PRO:CG	2.42	0.49
1:C:497:PRO:HG2	1:C:500:MET:HB2	1.94	0.49
1:A:420:ASN:HB3	6:A:608:PO4:O1	2.13	0.48
1:D:248:THR:HG23	8:D:770:HOH:O	2.13	0.48
1:A:440:ARG:HA	1:A:460:ASP:OD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:PRO:HB2	1:B:536:GLU:OE1	2.13	0.48
1:D:477:LEU:O	1:D:480:LYS:HB3	2.12	0.48
1:B:521:ILE:HG13	1:B:533:PRO:HG2	1.95	0.48
1:B:438:HIS:CD2	1:B:439:ILE:HG23	2.48	0.48
1:C:67:THR:O	1:C:68:THR:OG1	2.27	0.48
1:A:172:GLN:O	1:A:173:GLU:HG3	2.14	0.48
1:A:444:ARG:NH2	1:A:446:ASN:ND2	2.61	0.48
1:B:419:THR:HG22	1:B:421:ASP:N	2.24	0.48
1:D:112:TRP:HE3	1:D:113:ILE:HG13	1.75	0.48
1:C:257:ILE:HG23	1:C:281:PRO:HG3	1.95	0.48
1:C:417:VAL:HG12	1:C:425:ASN:ND2	2.29	0.48
1:D:433:ARG:O	1:D:433:ARG:HD3	2.13	0.48
1:B:105:VAL:HA	1:B:109:LEU:HB2	1.96	0.47
1:C:301:THR:HG22	1:C:303:LEU:HG	1.96	0.47
1:A:119:TYR:HB2	1:B:118:ARG:HH12	1.79	0.47
1:B:482:SER:HA	1:B:485:LEU:HB2	1.97	0.47
1:C:399:THR:HG22	1:C:400:VAL:HG23	1.96	0.47
1:A:152:ARG:HB2	1:A:154:HIS:CE1	2.49	0.47
1:B:381:ASP:OD2	1:B:382:ARG:N	2.48	0.47
1:B:550:THR:C	1:B:552:GLU:H	2.16	0.47
1:C:173:GLU:HA	1:C:173:GLU:OE2	2.14	0.47
1:C:408:GLY:O	1:C:411:ARG:HG2	2.13	0.47
1:D:134:LEU:HD12	1:D:157:VAL:HB	1.97	0.47
1:A:355:PHE:CE1	1:A:412:ALA:HB2	2.49	0.47
1:B:178:VAL:HG11	1:B:191:LEU:HD21	1.96	0.47
1:B:418:THR:HG23	1:B:444:ARG:HD3	1.97	0.47
1:B:532:SER:N	1:B:533:PRO:HD3	2.29	0.47
1:B:276:GLN:O	1:B:332:ALA:HA	2.15	0.47
1:C:258:ARG:O	1:C:440:ARG:HD3	2.14	0.47
1:C:200:ILE:HD11	1:C:477:LEU:HD11	1.97	0.47
1:D:107:MET:O	1:D:111:PRO:HG2	2.15	0.47
1:A:67:THR:HG21	1:B:89:THR:HG21	1.95	0.47
1:B:287:PHE:HD2	1:B:295:SER:HB2	1.80	0.47
1:D:444:ARG:HH21	1:D:446:ASN:HD21	1.63	0.46
1:A:119:TYR:CG	1:A:167:LEU:HD13	2.50	0.46
1:B:281:PRO:HB2	1:B:283:HIS:HD2	1.80	0.46
1:D:355:PHE:CE1	1:D:412:ALA:HB2	2.50	0.46
1:D:173:GLU:OE2	1:D:177:VAL:HG23	2.16	0.46
1:B:520:ALA:HB3	1:B:546:ILE:HB	1.96	0.46
1:B:514:THR:HG21	1:B:557:PHE:HD1	1.81	0.46
1:D:418:THR:CG2	1:D:444:ARG:HD3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:THR:O	1:B:283:HIS:HE1	1.98	0.46
1:D:252:GLY:HA3	1:D:365:ALA:HB3	1.98	0.46
1:D:115:ARG:HG2	1:D:115:ARG:H	1.61	0.46
1:B:112:TRP:HE1	1:B:116:ARG:CZ	2.29	0.46
1:D:112:TRP:CZ3	1:D:113:ILE:HG13	2.51	0.46
1:D:355:PHE:CD1	1:D:412:ALA:HB2	2.51	0.46
1:D:136:PHE:CD1	1:D:182:PRO:HB3	2.51	0.45
1:D:93:VAL:O	1:D:97:ASP:HB2	2.15	0.45
1:B:337:GLN:HE22	1:B:493:ARG:HH12	1.64	0.45
1:B:92:GLY:O	1:B:96:LEU:HB2	2.16	0.45
1:B:267:HIS:HE1	1:B:276:GLN:OE1	1.99	0.45
1:C:113:ILE:HG13	1:C:117:LEU:CD2	2.43	0.45
1:B:415:ILE:HG13	1:B:439:ILE:HD12	1.98	0.45
1:B:444:ARG:NH2	1:B:446:ASN:HD21	2.15	0.45
1:A:104:PHE:CD1	1:A:108:PHE:CZ	3.05	0.45
1:A:373:LYS:HB2	1:A:374:PRO:CA	2.47	0.45
1:C:341:LEU:O	1:C:345:ILE:HG12	2.17	0.45
1:A:419:THR:HG22	1:A:421:ASP:N	2.27	0.45
1:C:197:ARG:NH2	1:C:480:LYS:HD2	2.32	0.45
1:C:419:THR:CB	1:C:425:ASN:HD21	2.30	0.45
1:C:117:LEU:HD11	1:D:117:LEU:HB2	1.98	0.45
1:A:148:LYS:NZ	1:A:471:ASN:HA	2.32	0.45
1:B:334:THR:H	1:B:337:GLN:HE21	1.62	0.45
1:C:120:HIS:O	1:C:120:HIS:CG	2.70	0.45
1:B:559:GLN:HG3	1:B:560:THR:N	2.31	0.45
1:B:91:SER:O	1:B:95:PHE:HD2	2.00	0.45
1:D:464:SER:HB3	1:D:467:SER:OG	2.17	0.45
1:B:265:LEU:HD22	1:B:280:LEU:HD13	1.99	0.44
1:C:161:ASP:HB3	1:C:182:PRO:HD3	2.00	0.44
1:B:556:THR:HG22	1:B:560:THR:OG1	2.17	0.44
1:C:19:ASN:O	1:C:107:MET:HE3	2.16	0.44
1:C:534:PRO:HB2	1:C:536:GLU:OE1	2.18	0.44
1:C:444:ARG:NH2	1:C:446:ASN:HD21	2.15	0.44
1:C:559:GLN:H	1:C:559:GLN:NE2	2.15	0.44
1:C:181:SER:HA	1:C:182:PRO:HD3	1.88	0.44
1:D:110:ALA:HA	1:D:113:ILE:HD12	1.99	0.44
1:A:373:LYS:HB2	1:A:374:PRO:C	2.38	0.44
1:B:119:TYR:CE1	1:B:121:PRO:HG3	2.52	0.44
1:C:165:GLN:O	1:C:169:LEU:HG	2.17	0.44
1:B:93:VAL:O	1:B:97:ASP:HB2	2.18	0.44
1:D:115:ARG:HB3	1:D:120:HIS:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ILE:HG21	1:A:428:LEU:HD13	2.00	0.44
1:C:107:MET:O	1:C:111:PRO:HG3	2.18	0.44
1:A:119:TYR:H	1:B:118:ARG:HH12	1.64	0.44
1:D:115:ARG:HH21	1:D:120:HIS:CE1	2.36	0.44
1:D:141:ILE:HD13	1:D:466:ALA:HA	1.99	0.44
1:A:359:HIS:CG	1:A:359:HIS:O	2.71	0.43
1:C:480:LYS:HG2	1:C:481:GLU:HG2	2.00	0.43
1:C:550:THR:HG21	1:C:552:GLU:OE1	2.18	0.43
1:D:359:HIS:O	1:D:359:HIS:CG	2.70	0.43
1:B:476:LEU:HD12	1:B:476:LEU:HA	1.78	0.43
1:A:141:ILE:HD13	1:A:247:LEU:HD13	2.00	0.43
1:B:505:ILE:HG13	1:B:539:LEU:HD11	1.99	0.43
1:B:267:HIS:CE1	1:B:276:GLN:OE1	2.72	0.43
1:B:489:MET:HG2	1:B:550:THR:HA	2.00	0.43
1:C:100:LEU:HB3	1:C:101:PRO:HD3	2.01	0.43
1:C:91:SER:O	1:C:95:PHE:HD2	2.01	0.43
1:D:420:ASN:HA	1:D:444:ARG:NH2	2.33	0.43
1:A:112:TRP:CE3	1:A:113:ILE:HG22	2.54	0.43
1:C:373:LYS:HG3	1:C:373:LYS:O	2.18	0.43
1:B:418:THR:HG22	1:B:444:ARG:HH11	1.84	0.43
1:A:424:THR:O	1:A:428:LEU:HG	2.19	0.43
1:B:208:ASN:HA	1:B:208:ASN:HD22	1.65	0.43
1:D:158:VAL:HG22	1:D:177:VAL:HG22	2.01	0.43
1:D:373:LYS:HG3	1:D:373:LYS:O	2.19	0.43
1:B:124:GLU:HG2	1:B:125:LEU:N	2.34	0.43
1:C:297:ILE:HB	1:C:305:ILE:HD11	2.00	0.43
1:B:311:ARG:HA	1:B:311:ARG:HD3	1.90	0.43
1:C:258:ARG:HG2	1:C:461:PHE:CD1	2.54	0.43
1:C:532:SER:N	1:C:533:PRO:HD3	2.34	0.43
1:B:300:ARG:HH11	1:B:344:LEU:HD13	1.83	0.42
1:C:478:GLU:HG3	1:C:479:HIS:CD2	2.54	0.42
1:D:356:ILE:HB	1:D:379:LEU:HD23	1.99	0.42
1:A:408:GLY:O	1:A:411:ARG:HD3	2.19	0.42
1:B:335:LYS:HB2	1:B:335:LYS:HE3	1.87	0.42
1:D:167:LEU:HD23	1:D:167:LEU:C	2.40	0.42
1:B:492:PHE:CZ	1:B:547:LEU:HB2	2.54	0.42
1:B:556:THR:O	1:B:556:THR:HG22	2.20	0.42
1:C:238:LEU:HA	1:C:238:LEU:HD23	1.79	0.42
1:D:143:ARG:HD2	8:D:758:HOH:O	2.18	0.42
1:C:419:THR:N	1:C:425:ASN:HD21	2.16	0.42
1:C:44:LEU:O	1:C:48:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:O	1:A:48:LEU:HB2	2.18	0.42
1:B:291:THR:OG1	1:B:294:GLU:HB2	2.20	0.42
1:C:520:ALA:HA	1:C:530:LEU:O	2.19	0.42
1:D:352:GLU:HG3	1:D:413:SER:OG	2.20	0.42
1:A:411:ARG:H	1:A:411:ARG:CD	2.33	0.42
1:D:224:ILE:HD13	1:D:476:LEU:HB3	2.00	0.42
1:D:91:SER:O	1:D:95:PHE:HD1	2.02	0.42
1:B:520:ALA:HA	1:B:530:LEU:O	2.20	0.42
1:C:143:ARG:O	1:C:147:ARG:HG3	2.19	0.42
1:D:143:ARG:HH12	1:D:172:GLN:NE2	2.18	0.42
1:D:67:THR:O	1:D:68:THR:OG1	2.33	0.42
1:B:402:GLN:OE1	1:B:402:GLN:HA	2.20	0.42
1:B:355:PHE:CD1	1:B:412:ALA:HB2	2.55	0.42
1:C:492:PHE:CD2	1:C:554:GLU:HG3	2.55	0.42
1:C:293:GLY:HA3	1:C:319:ARG:HG3	2.01	0.42
1:C:497:PRO:O	1:C:500:MET:HB2	2.20	0.42
1:A:100:LEU:N	1:A:101:PRO:HD2	2.34	0.41
1:A:258:ARG:HG3	1:A:461:PHE:CD1	2.55	0.41
1:A:91:SER:O	1:A:95:PHE:HD1	2.03	0.41
1:B:419:THR:HG22	1:B:420:ASN:N	2.34	0.41
1:B:305:ILE:O	1:B:317:PRO:HG3	2.20	0.41
1:B:109:LEU:HD13	1:B:109:LEU:HA	1.91	0.41
1:D:362:ILE:HD12	1:D:444:ARG:NH1	2.36	0.41
1:A:108:PHE:C	1:A:111:PRO:HD2	2.40	0.41
1:B:142:THR:O	1:B:146:ILE:HG13	2.20	0.41
1:B:373:LYS:H	1:B:374:PRO:HA	1.85	0.41
1:C:100:LEU:HB3	1:C:101:PRO:CD	2.50	0.41
1:B:496:LEU:HD22	1:B:497:PRO:CD	2.43	0.41
1:C:236:LEU:HA	1:C:236:LEU:HD12	1.83	0.41
1:A:205:ASP:HB2	1:A:206:PRO:HD3	2.03	0.41
1:B:95:PHE:O	1:B:96:LEU:HD12	2.21	0.41
1:C:94:ILE:O	1:C:99:ILE:HG12	2.20	0.41
1:D:152:ARG:HD3	1:D:152:ARG:N	2.35	0.41
1:D:23:LEU:HD23	1:D:24:LEU:N	2.36	0.41
1:B:492:PHE:CD2	1:B:554:GLU:HG3	2.55	0.41
1:D:399:THR:O	1:D:399:THR:HG22	2.20	0.41
1:A:104:PHE:CD2	1:A:105:VAL:N	2.89	0.41
1:A:108:PHE:HA	1:A:111:PRO:HD2	2.03	0.41
1:B:149:LEU:HA	1:B:152:ARG:HG2	2.02	0.41
1:C:243:GLN:HG2	8:C:742:HOH:O	2.21	0.41
1:D:112:TRP:CD1	1:D:116:ARG:HD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ILE:O	1:B:99:ILE:HG12	2.21	0.41
1:C:21:LYS:HA	1:C:24:LEU:HD23	2.01	0.41
1:A:382:ARG:HG3	1:A:383:GLN:HG3	2.03	0.41
1:C:19:ASN:HB3	1:C:107:MET:HE2	2.03	0.41
1:B:107:MET:HG3	1:B:108:PHE:N	2.36	0.40
1:C:110:ALA:O	1:C:114:GLU:HG3	2.21	0.40
1:C:71:PHE:CZ	1:D:65:VAL:HG22	2.55	0.40
1:A:107:MET:HG2	1:A:108:PHE:HD2	1.87	0.40
1:A:119:TYR:HB2	1:B:118:ARG:HH22	1.86	0.40
1:B:19:ASN:HB3	1:B:107:MET:SD	2.61	0.40
1:B:269:LEU:HD23	1:B:277:ILE:HD12	2.03	0.40
1:B:44:LEU:HB3	1:B:48:LEU:HD12	2.02	0.40
1:B:505:ILE:CG1	1:B:539:LEU:HD11	2.51	0.40
1:C:373:LYS:HE3	1:C:373:LYS:HB2	1.84	0.40
1:C:355:PHE:CD1	1:C:412:ALA:HB2	2.56	0.40
1:D:355:PHE:CD1	1:D:409:ILE:HD12	2.57	0.40
1:A:397:ASP:OD1	1:A:400:VAL:HG23	2.22	0.40
1:C:247:LEU:HD21	1:C:469:GLY:HA2	2.02	0.40
1:C:504:THR:HA	1:C:537:THR:O	2.21	0.40
1:D:257:ILE:O	1:D:261:THR:HG23	2.21	0.40
1:D:405:ARG:HH12	1:D:435:LEU:HD11	1.86	0.40
1:C:480:LYS:HE2	1:C:481:GLU:CG	2.51	0.40
1:D:419:THR:HG22	1:D:420:ASN:N	2.36	0.40
1:A:123:ILE:HD12	1:A:123:ILE:O	2.21	0.40
1:B:258:ARG:HB3	1:B:442:VAL:HG21	2.03	0.40
1:B:522:GLU:HB3	1:B:529:ILE:HG13	2.03	0.40
1:D:139:ASP:CB	1:D:140:PRO:CD	2.99	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	371/565 (66%)	353 (95%)	18 (5%)	0	100	100
1	B	545/565 (96%)	514 (94%)	31 (6%)	0	100	100
1	C	544/565 (96%)	520 (96%)	23 (4%)	1 (0%)	47	71
1	D	372/565 (66%)	354 (95%)	16 (4%)	2 (0%)	29	52
All	All	1832/2260 (81%)	1741 (95%)	88 (5%)	3 (0%)	47	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	374	PRO
1	D	374	PRO
1	D	111	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/463 (68%)	296 (95%)	17 (5%)	22	44
1	B	448/463 (97%)	424 (95%)	24 (5%)	22	44
1	C	447/463 (96%)	412 (92%)	35 (8%)	12	25
1	D	314/463 (68%)	292 (93%)	22 (7%)	15	30
All	All	1522/1852 (82%)	1424 (94%)	98 (6%)	17	35

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	30	LEU
1	A	67	THR
1	A	69	LEU
1	A	83	LEU
1	A	117	LEU
1	A	145	LEU
1	A	197	ARG

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Mol	Chain	Res	Type
1	A	220	GLN
1	A	238	LEU
1	A	351	ASP
1	A	353	LEU
1	A	411	ARG
1	A	418	THR
1	A	433	ARG
1	A	435	LEU
1	A	440	ARG
1	B	30	LEU
1	B	67	THR
1	B	69	LEU
1	B	107	MET
1	B	109	LEU
1	B	125	LEU
1	B	134	LEU
1	B	143	ARG
1	B	145	LEU
1	B	152	ARG
1	B	158	VAL
1	B	235	LEU
1	B	236	LEU
1	B	258	ARG
1	B	316	THR
1	B	328	LEU
1	B	350	GLU
1	B	352	GLU
1	B	383	GLN
1	B	418	THR
1	B	420	ASN
1	B	476	LEU
1	B	504	THR
1	B	509	ARG
1	C	30	LEU
1	C	67	THR
1	C	83	LEU
1	C	97	ASP
1	C	104	PHE
1	C	116	ARG
1	C	118	ARG
1	C	132	HIS
1	C	139	ASP

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Mol	Chain	Res	Type
1	C	145	LEU
1	C	149	LEU
1	C	152	ARG
1	C	158	VAL
1	C	173	GLU
1	C	236	LEU
1	C	238	LEU
1	C	247	LEU
1	C	249	ARG
1	C	258	ARG
1	C	310	GLU
1	C	316	THR
1	C	320	GLU
1	C	321	THR
1	C	341	LEU
1	C	353	LEU
1	C	399	THR
1	C	418	THR
1	C	423	SER
1	C	476	LEU
1	C	480	LYS
1	C	484	PHE
1	C	500	MET
1	C	526	ARG
1	C	554	GLU
1	C	559	GLN
1	D	67	THR
1	D	69	LEU
1	D	83	LEU
1	D	102	PHE
1	D	108	PHE
1	D	115	ARG
1	D	134	LEU
1	D	145	LEU
1	D	152	ARG
1	D	153	ASN
1	D	172	GLN
1	D	197	ARG
1	D	220	GLN
1	D	227	VAL
1	D	236	LEU
1	D	258	ARG

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Mol	Chain	Res	Type
1	D	372	ARG
1	D	406	GLN
1	D	418	THR
1	D	420	ASN
1	D	435	LEU
1	D	476	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	154	HIS
1	A	406	GLN
1	A	438	HIS
1	A	446	ASN
1	B	208	ASN
1	B	267	HIS
1	B	274	ASN
1	B	283	HIS
1	B	337	GLN
1	B	406	GLN
1	B	420	ASN
1	B	434	HIS
1	B	446	ASN
1	C	276	GLN
1	C	318	GLN
1	C	406	GLN
1	C	425	ASN
1	C	446	ASN
1	C	471	ASN
1	C	479	HIS
1	C	559	GLN
1	D	120	HIS
1	D	154	HIS
1	D	172	GLN
1	D	406	GLN
1	D	438	HIS
1	D	446	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 ⓘ

2 monosaccharides 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	GLC	E	1	2	12,12,12	1.71	2 (16%)	17,17,17	1.08	1 (5%)
2	GLC	E	2	2	11,11,12	2.36	3 (27%)	15,15,17	1.50	3 (20%)

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	GLC	E	1	2	-	2/2/22/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	GLC	C2-C3	-5.38	1.44	1.52
2	E	1	GLC	C3-C2	-4.37	1.41	1.52
2	E	2	GLC	C4-C3	-4.16	1.41	1.52
2	E	2	GLC	O5-C1	-2.37	1.39	1.43
2	E	1	GLC	C4-C3	-2.31	1.46	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	GLC	C1-C2-C3	2.81	113.12	109.67
2	E	1	GLC	O3-C3-C2	-2.46	104.66	110.35
2	E	2	GLC	O3-C3-C2	-2.32	105.55	109.99
2	E	2	GLC	O5-C5-C6	2.28	110.77	107.20

There are no chirality outliers.

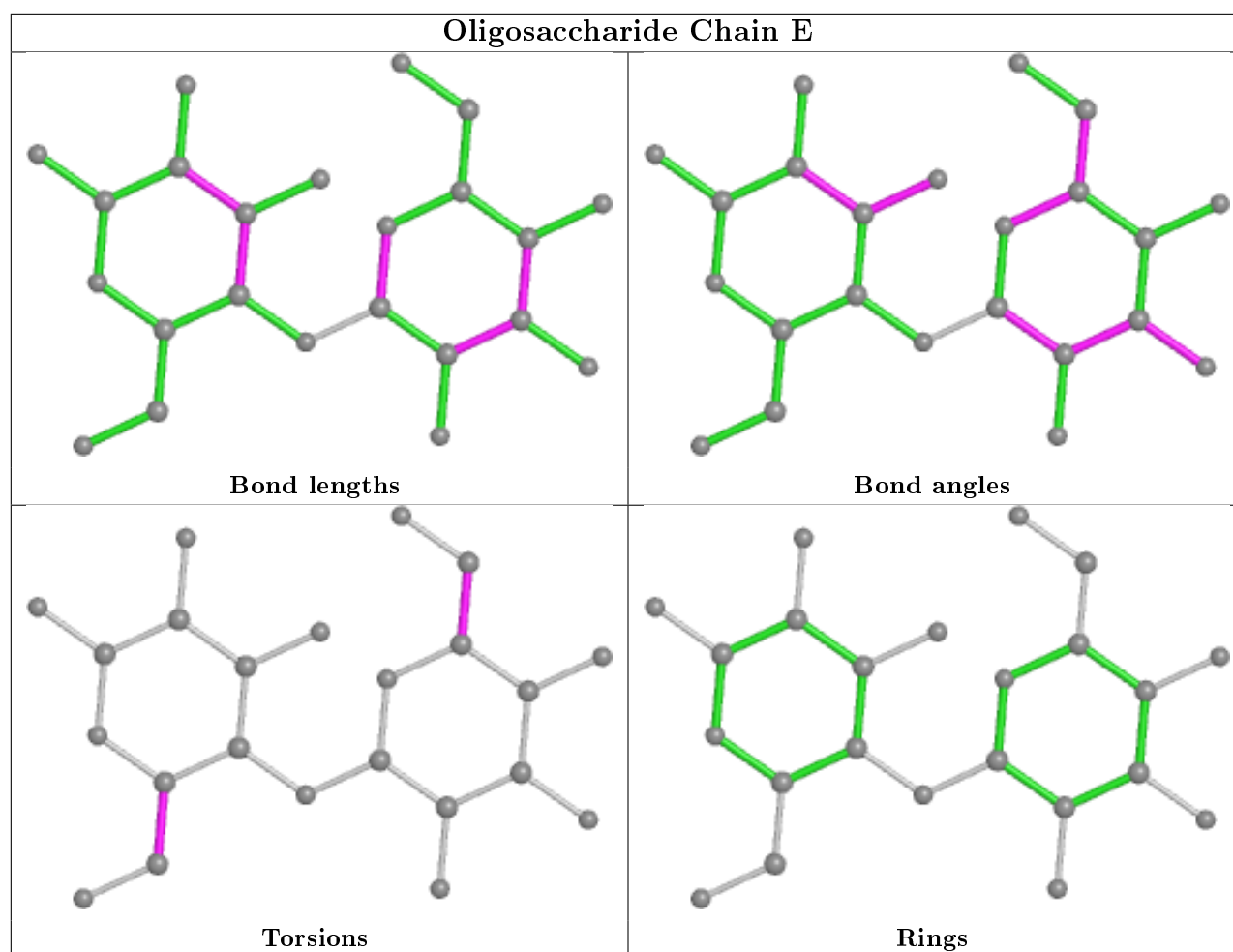
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	GLC	O5-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 20 are monoatomic - leaving 8 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	$\# Z  > 2$
6	PO4	B	604	-	4,4,4	0.85	0	6,6,6	0.44	0
6	PO4	C	609	-	4,4,4	0.89	0	6,6,6	0.48	0
7	GLC	B	606	-	12,12,12	1.77	2 (16%)	17,17,17	1.17	1 (5%)
6	PO4	D	603	-	4,4,4	0.89	0	6,6,6	0.45	0
6	PO4	A	608	-	4,4,4	0.88	0	6,6,6	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GLC	B	607	-	12,12,12	1.82	2 (16%)	17,17,17	1.22	1 (5%)
6	PO4	B	605	-	4,4,4	0.92	0	6,6,6	0.53	0
7	GLC	D	604	-	12,12,12	1.79	2 (16%)	17,17,17	1.12	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
7	GLC	D	604	-	-	2/2/22/22	0/1/1/1
7	GLC	B	607	-	-	1/2/22/22	0/1/1/1
7	GLC	B	606	-	-	2/2/22/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	607	GLC	C4-C3	-4.05	1.42	1.52
7	D	604	GLC	C4-C3	-3.97	1.42	1.52
7	B	606	GLC	C4-C3	-3.91	1.42	1.52
7	B	607	GLC	C3-C2	-3.46	1.43	1.52
7	D	604	GLC	C3-C2	-3.38	1.43	1.52
7	B	606	GLC	C3-C2	-3.38	1.43	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	607	GLC	O3-C3-C4	-2.12	105.44	110.35
7	D	604	GLC	O3-C3-C4	-2.08	105.55	110.35
7	B	606	GLC	O3-C3-C4	-2.02	105.67	110.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	604	GLC	O5-C5-C6-O6
7	B	606	GLC	O5-C5-C6-O6
7	B	607	GLC	O5-C5-C6-O6
7	B	606	GLC	C4-C5-C6-O6
7	D	604	GLC	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	608	PO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	375/565 (66%)	0.11	14 (3%) 41 34	31, 54, 126, 191	0
1	B	547/565 (96%)	0.42	61 (11%) 5 3	33, 63, 163, 243	0
1	C	546/565 (96%)	0.15	28 (5%) 28 22	35, 64, 131, 210	0
1	D	376/565 (66%)	0.11	16 (4%) 35 28	31, 55, 137, 200	0
All	All	1844/2260 (81%)	0.21	119 (6%) 18 14	31, 60, 142, 243	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	398	ALA	10.1
1	B	516	CYS	9.8
1	D	398	ALA	9.6
1	B	564	ARG	8.9
1	B	563	ALA	8.4
1	B	174	GLY	7.7
1	B	561	ILE	7.4
1	A	399	THR	7.3
1	B	499	ALA	6.4
1	D	404	LEU	6.4
1	A	21	LYS	5.9
1	B	510	LEU	5.6
1	B	512	PRO	5.6
1	B	509	ARG	5.5
1	B	485	LEU	5.5
1	B	508	THR	5.3
1	A	404	LEU	5.3
1	B	484	PHE	5.1
1	B	513	LEU	5.1
1	A	409	ILE	4.9
1	C	113	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	560	THR	4.7
1	B	507	GLU	4.7
1	A	373	LYS	4.6
1	D	18	GLN	4.5
1	C	509	ARG	4.4
1	B	19	ASN	4.3
1	C	21	LYS	4.3
1	C	151	SER	4.3
1	B	505	ILE	4.1
1	B	557	PHE	4.1
1	B	506	ALA	4.0
1	D	399	THR	4.0
1	B	549	GLY	4.0
1	B	113	ILE	4.0
1	B	486	SER	3.9
1	D	113	ILE	3.8
1	B	120	HIS	3.8
1	B	152	ARG	3.8
1	B	175	PHE	3.8
1	B	542	GLY	3.7
1	B	483	ALA	3.7
1	D	21	LYS	3.7
1	B	539	LEU	3.6
1	B	555	LYS	3.6
1	C	561	ILE	3.6
1	A	397	ASP	3.5
1	B	489	MET	3.4
1	B	518	ILE	3.4
1	C	154	HIS	3.4
1	B	18	GLN	3.4
1	B	151	SER	3.3
1	C	130	ARG	3.3
1	B	496	LEU	3.3
1	B	559	GLN	3.2
1	D	402	GLN	3.2
1	B	487	GLU	3.1
1	C	514	THR	3.1
1	A	401	GLY	3.1
1	C	153	ASN	3.1
1	A	151	SER	3.1
1	B	171	GLU	3.1
1	B	21	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	108	PHE	3.0
1	B	119	TYR	3.0
1	D	403	THR	3.0
1	C	484	PHE	2.9
1	B	128	ASP	2.9
1	B	519	VAL	2.9
1	B	517	SER	2.8
1	B	154	HIS	2.8
1	B	514	THR	2.8
1	B	550	THR	2.8
1	B	497	PRO	2.8
1	C	564	ARG	2.7
1	B	554	GLU	2.7
1	C	107	MET	2.7
1	C	559	GLN	2.7
1	D	397	ASP	2.7
1	A	372	ARG	2.7
1	C	25	LEU	2.7
1	C	485	LEU	2.6
1	C	557	PHE	2.5
1	D	373	LYS	2.5
1	B	438	HIS	2.5
1	B	156	PHE	2.5
1	C	482	SER	2.5
1	B	488	GLY	2.5
1	B	490	ALA	2.5
1	B	130	ARG	2.4
1	D	19	ASN	2.4
1	B	498	PRO	2.4
1	B	411	ARG	2.4
1	C	560	THR	2.4
1	C	176	LYS	2.4
1	C	483	ALA	2.4
1	B	500	MET	2.4
1	D	118	ARG	2.4
1	B	552	GLU	2.4
1	B	155	LEU	2.4
1	C	150	GLU	2.3
1	D	154	HIS	2.3
1	D	481	GLU	2.2
1	C	152	ARG	2.2
1	C	110	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	513	LEU	2.2
1	B	272	PHE	2.2
1	A	20	LEU	2.1
1	D	20	LEU	2.1
1	C	498	PRO	2.1
1	C	19	ASN	2.1
1	A	118	ARG	2.1
1	B	551	SER	2.1
1	C	109	LEU	2.1
1	D	409	ILE	2.1
1	B	541	GLU	2.1
1	B	111	PRO	2.0
1	A	150	GLU	2.0
1	A	400	VAL	2.0

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

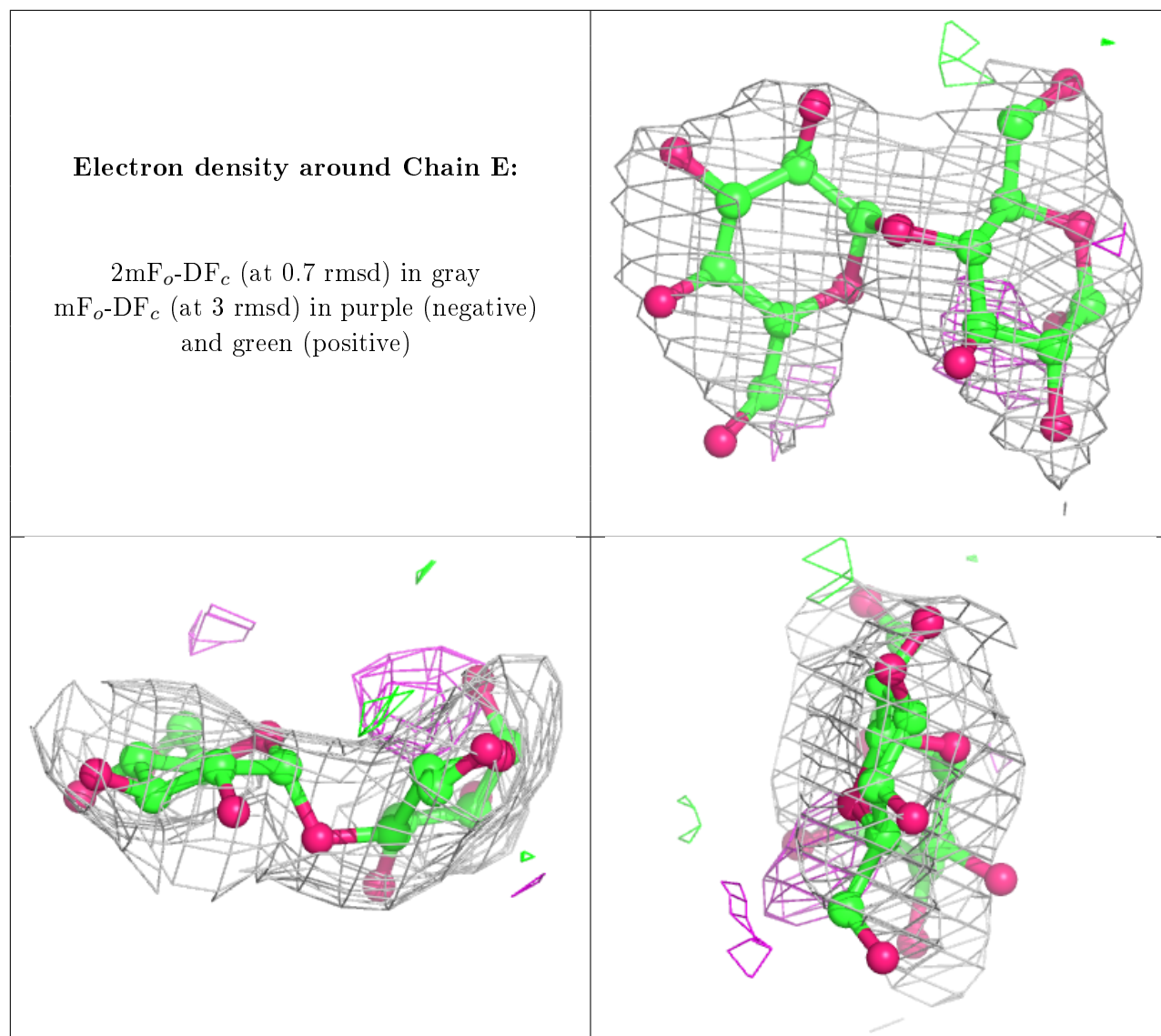
There are no non-standard protein/DNA/RNA residues in this entry.

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLC	E	2	11/12	0.72	0.25	131,134,138,138	0
2	GLC	E	1	12/12	0.86	0.27	80,109,120,124	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	K	A	605	1/1	0.51	0.60	131,131,131,131	1
3	K	C	604	1/1	0.62	0.34	82,82,82,82	1
6	PO4	D	603	5/5	0.78	0.19	127,130,136,136	0
3	K	B	603	1/1	0.81	1.07	185,185,185,185	1
7	GLC	B	607	12/12	0.83	0.16	100,133,139,140	0
7	GLC	D	604	12/12	0.83	0.24	89,121,130,136	0
7	GLC	B	606	12/12	0.83	0.14	74,113,121,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	K	A	601	1/1	0.85	0.14	58,58,58,58	1
6	PO4	B	604	5/5	0.86	0.17	88,97,105,108	0
6	PO4	A	608	5/5	0.87	0.20	105,106,116,120	0
3	K	D	601	1/1	0.90	1.05	189,189,189,189	1
3	K	A	604	1/1	0.95	0.19	88,88,88,88	1
3	K	A	603	1/1	0.95	0.15	37,37,37,37	1
6	PO4	B	605	5/5	0.95	0.20	45,62,67,70	0
6	PO4	C	609	5/5	0.96	0.20	65,66,70,77	0
4	ZN	A	606	1/1	0.97	0.17	60,60,60,60	0
5	CA	C	606	1/1	0.97	0.12	50,50,50,50	0
3	K	A	602	1/1	0.98	0.25	42,42,42,42	1
5	CA	C	607	1/1	0.98	0.15	47,47,47,47	0
3	K	C	608	1/1	0.98	0.21	115,115,115,115	1
5	CA	B	602	1/1	0.99	0.14	49,49,49,49	0
5	CA	A	607	1/1	0.99	0.12	49,49,49,49	0
3	K	C	603	1/1	0.99	0.16	55,55,55,55	1
4	ZN	D	602	1/1	0.99	0.18	64,64,64,64	0
3	K	C	602	1/1	0.99	0.17	36,36,36,36	1
4	ZN	C	605	1/1	0.99	0.13	52,52,52,52	0
3	K	C	601	1/1	0.99	0.14	38,38,38,38	1
4	ZN	B	601	1/1	1.00	0.16	54,54,54,54	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.