wwPDB X-ray Structure Validation Summary Report (i)

Feb 18, 2024 – 09:54 PM EST

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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

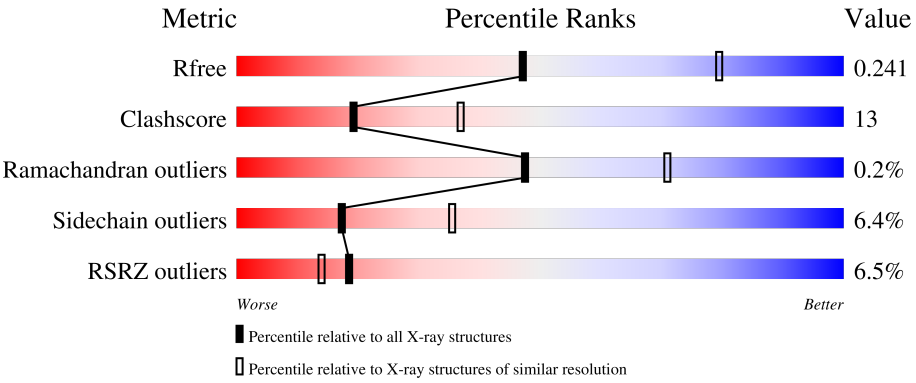
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 50% 16% 34%
1	B	565	11% 66% 29%
1	C	565	5% 70% 24%
1	D	565	3% 49% 16% 33%
2	E	2	100%

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 (i)

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	A	5	Total K 5 5	0	0
3	B	1	Total K 1 1	0	0
3	C	5	Total K 5 5	0	0
3	D	1	Total K 1 1	0	0

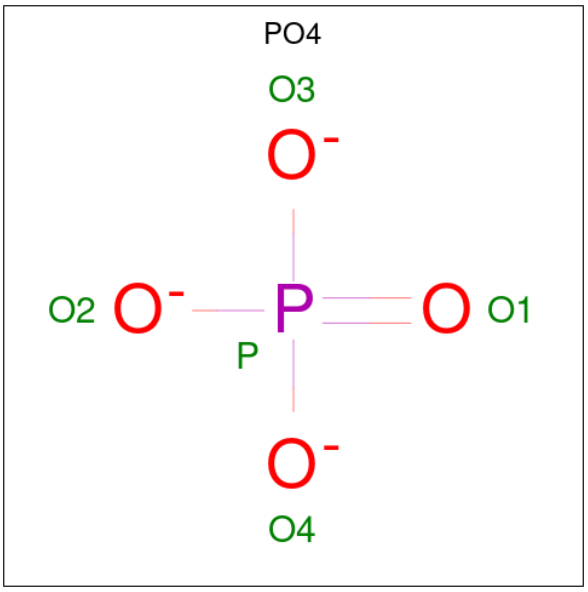
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

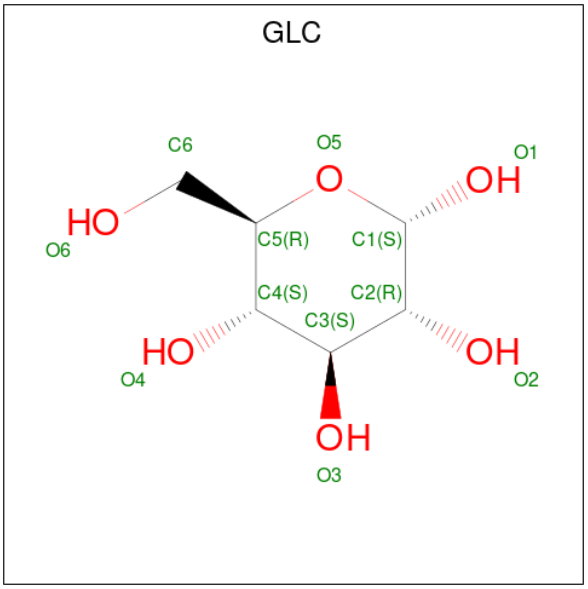
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0
5	C	2	Total Ca 2 2	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 7 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



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

- Molecule 8 is water.

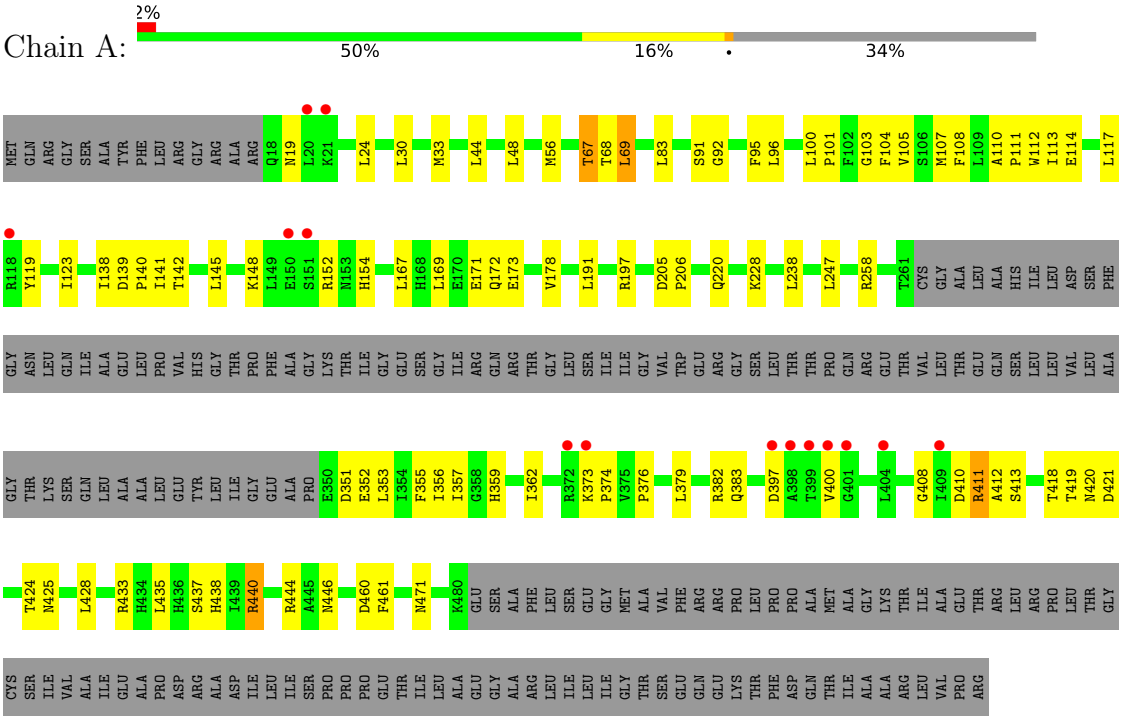
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	94	Total O 94 94	0	0
8	B	99	Total O 99 99	0	0
8	C	116	Total O 116 116	0	0
8	D	82	Total O 82 82	0	0

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.

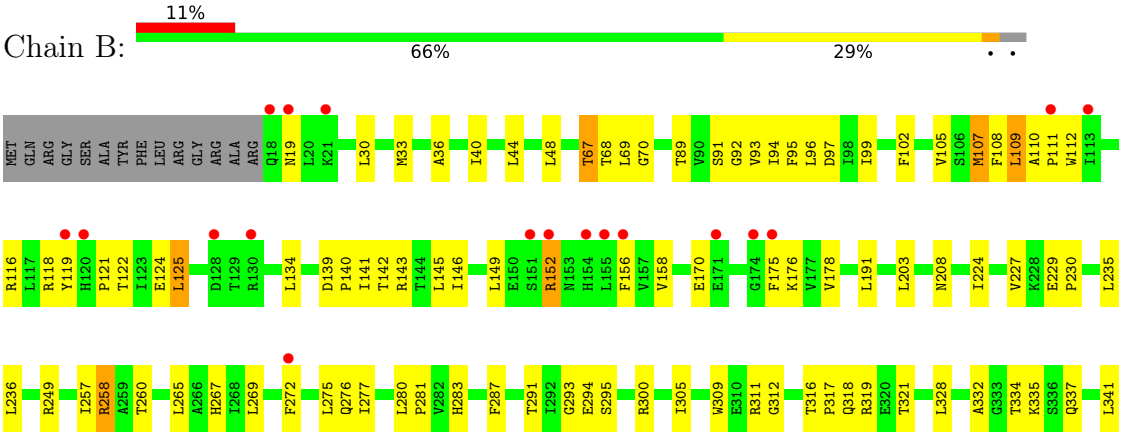
• Molecule 1: TrkA domain protein

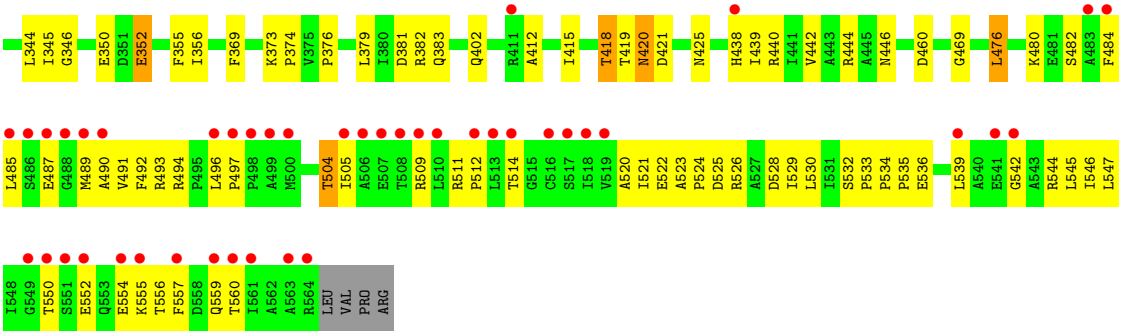
Chain A:



• Molecule 1: TrkA domain protein

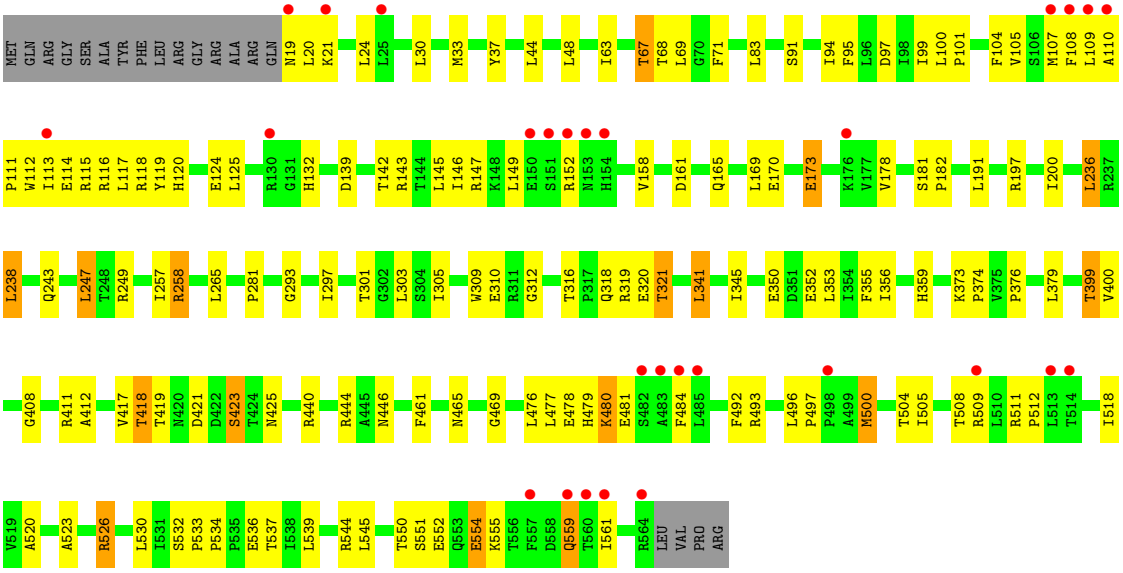
Chain B:





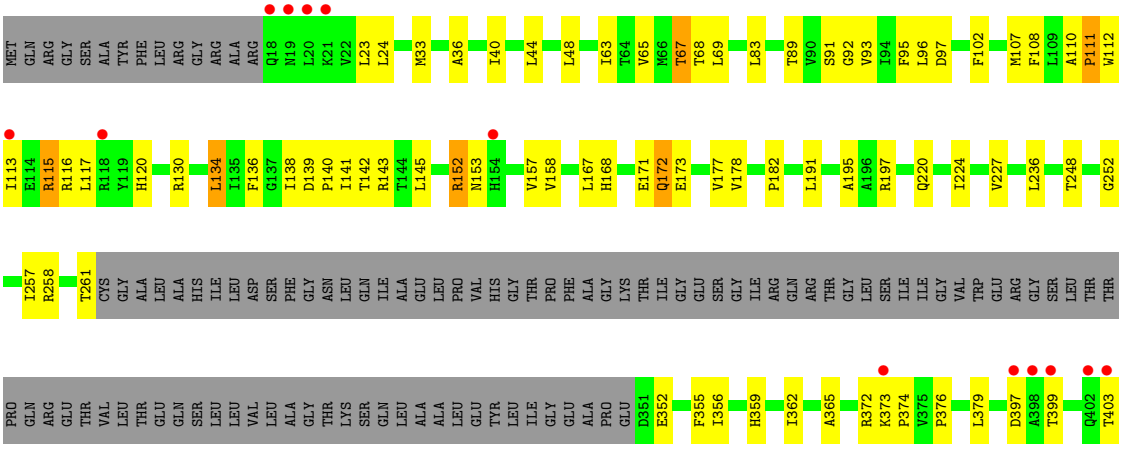
• Molecule 1: TrkA domain protein

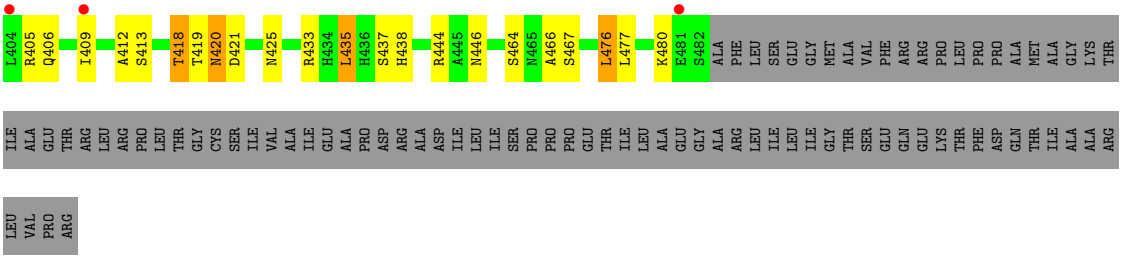
Chain C:



• Molecule 1: TrkA domain protein

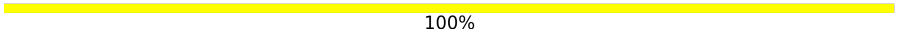
Chain D:





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

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	57.7	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 64.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, K, PO4, CA, ZN

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

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.

The worst 5 of 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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	247	LEU
1	C	484	PHE
1	C	258	ARG
1	C	353	LEU
1	C	559	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	276	GLN
1	D	446	ASN
1	C	425	ASN
1	D	172	GLN
1	C	406	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

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(^{o})	Ideal(^{o})
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:

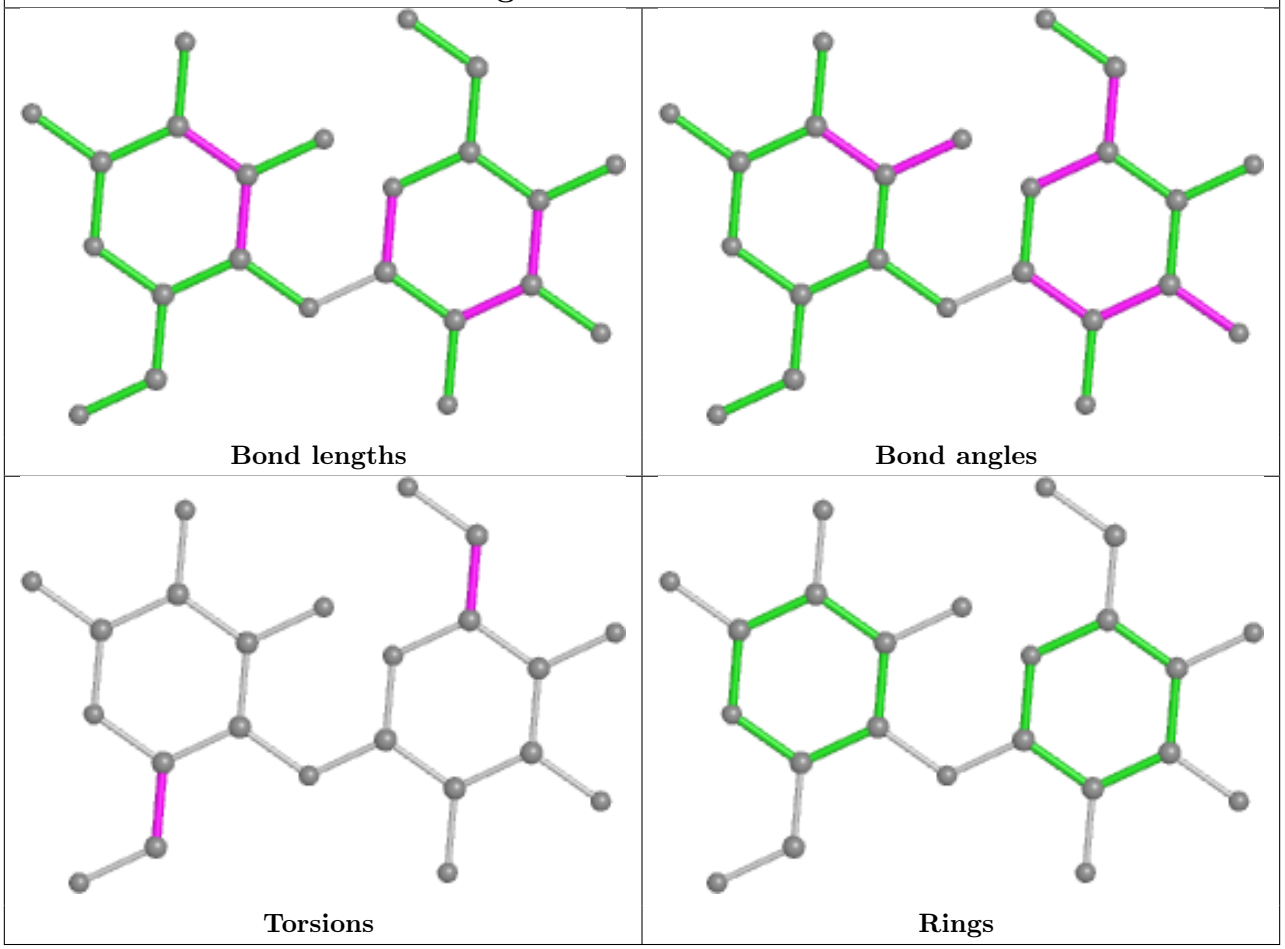
Mol	Chain	Res	Type	Atoms
2	E	2	GLC	O5-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6

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.

Oligosaccharide Chain E



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	D	603	-	4,4,4	0.89	0	6,6,6	0.45	0
7	GLC	D	604	-	12,12,12	1.79	2 (16%)	17,17,17	1.12	1 (5%)
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
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	B	606	-	12,12,12	1.77	2 (16%)	17,17,17	1.17	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	B	606	-	-	2/2/22/22	0/1/1/1
7	GLC	D	604	-	-	2/2/22/22	0/1/1/1
7	GLC	B	607	-	-	1/2/22/22	0/1/1/1

The worst 5 of 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

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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^{th} 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	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

The worst 5 of 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

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

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

6.3 Carbohydrates

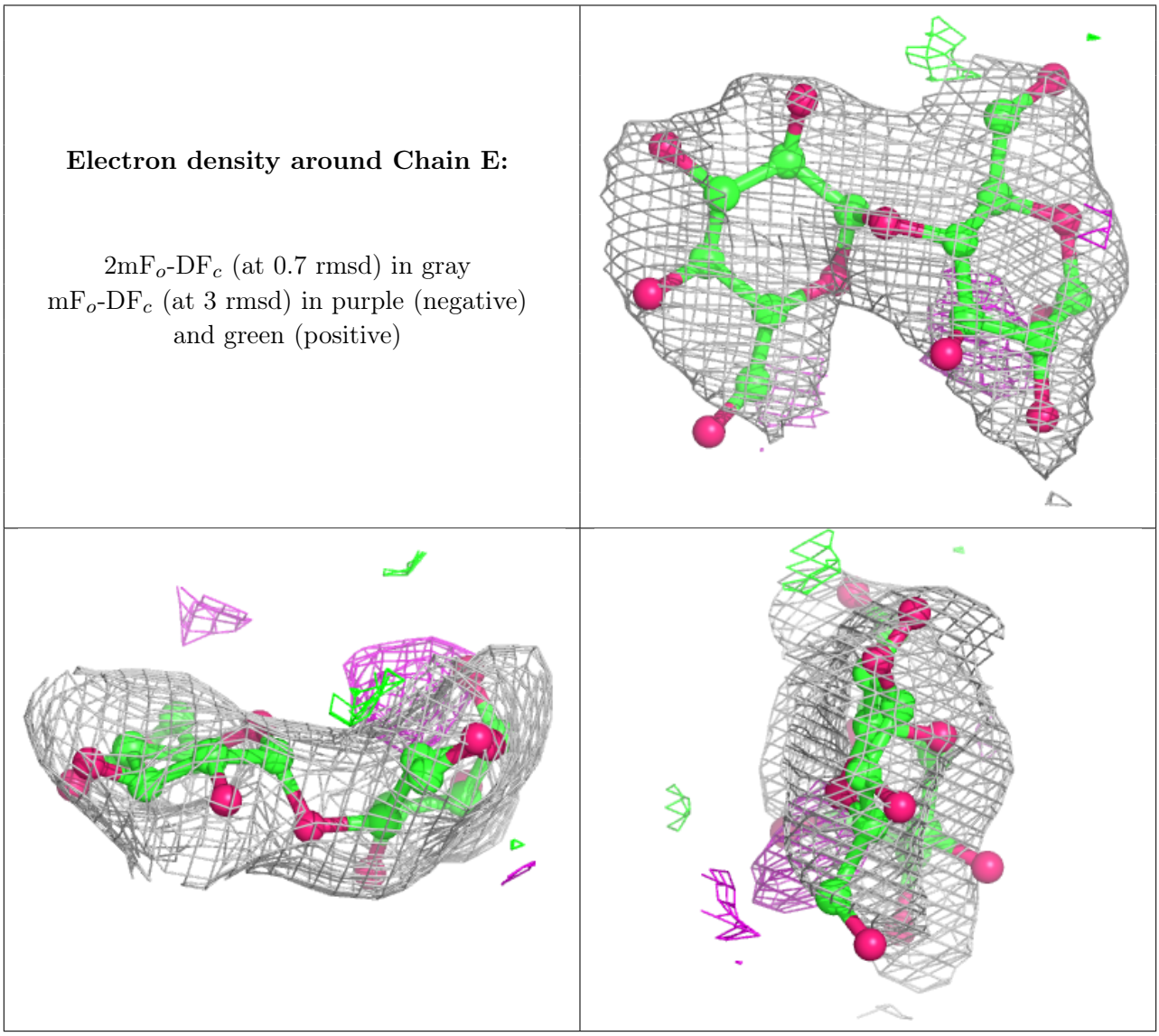
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	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.

Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



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. The B-factors column lists the minimum, median, 95^{th} 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^2)	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GLC	B	606	12/12	0.83	0.14	74,113,121,123	0
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
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
6	PO4	B	605	5/5	0.95	0.20	45,62,67,70	0
3	K	A	603	1/1	0.95	0.15	37,37,37,37	1
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
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
3	K	A	602	1/1	0.98	0.25	42,42,42,42	1
4	ZN	C	605	1/1	0.99	0.13	52,52,52,52	0
4	ZN	D	602	1/1	0.99	0.18	64,64,64,64	0
5	CA	A	607	1/1	0.99	0.12	49,49,49,49	0
5	CA	B	602	1/1	0.99	0.14	49,49,49,49	0
3	K	C	602	1/1	0.99	0.17	36,36,36,36	1
3	K	C	603	1/1	0.99	0.16	55,55,55,55	1
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 (i)

There are no such residues in this entry.