



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 10:39 pm GMT

PDB ID : 3HM8  
Title : Crystal structure of the C-terminal Hexokinase domain of human HK3  
Authors : Nedyalkova, L.; Tong, Y.; Rabeh, W.; Tempel, W.; Landry, R.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Bochkarev, A.; Park, H.; Structural Genomics Consortium (SGC)  
Deposited on : 2009-05-28  
Resolution : 2.80 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

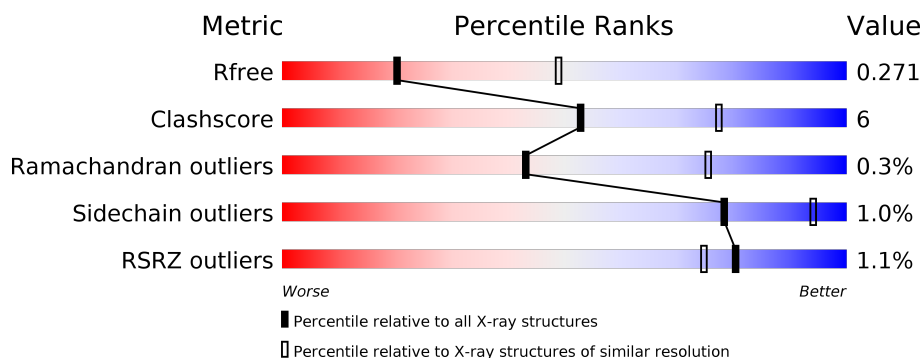
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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. 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	445	<div> <div>85%</div> <div>14%</div> <div>•</div> </div>
1	B	445	<div> <div>%</div> <div>88%</div> <div>11%</div> <div>•</div> </div>
1	C	445	<div> <div>%</div> <div>85%</div> <div>13%</div> <div>•</div> </div>
1	D	445	<div> <div>2%</div> <div>87%</div> <div>11%</div> <div>•</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12633 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.

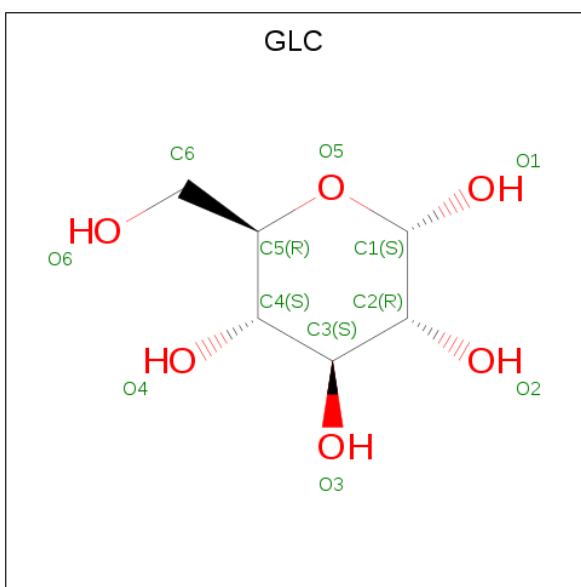
- Molecule 1 is a protein called Hexokinase-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3206	2012	555	617	22			
1	B	441	Total	C	N	O	S	0	0	0
			3117	1959	546	590	22			
1	C	436	Total	C	N	O	S	0	0	0
			3116	1962	537	596	21			
1	D	437	Total	C	N	O	S	0	0	0
			3082	1934	534	592	22			

There are 8 discrepancies between the modelled and reference sequences:

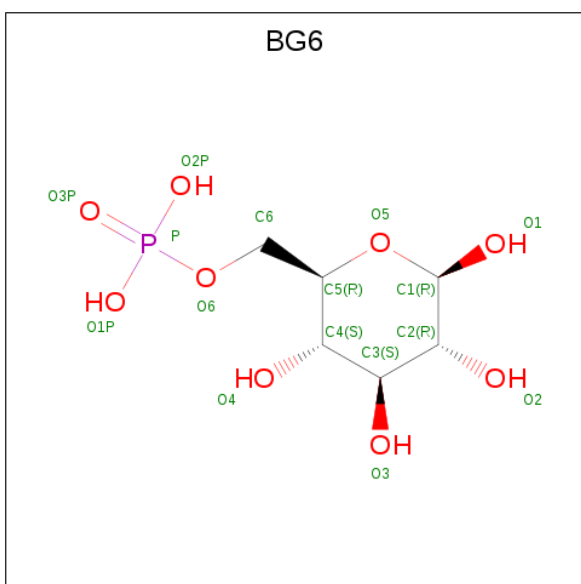
Chain	Residue	Modelled	Actual	Comment	Reference
A	478	GLY	-	EXPRESSION TAG	UNP P52790
A	479	SER	-	EXPRESSION TAG	UNP P52790
B	478	GLY	-	EXPRESSION TAG	UNP P52790
B	479	SER	-	EXPRESSION TAG	UNP P52790
C	478	GLY	-	EXPRESSION TAG	UNP P52790
C	479	SER	-	EXPRESSION TAG	UNP P52790
D	478	GLY	-	EXPRESSION TAG	UNP P52790
D	479	SER	-	EXPRESSION TAG	UNP P52790

- Molecule 2 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

- Molecule 3 is BETA-D-GLUCOSE-6-PHOSPHATE (three-letter code: BG6) (formula:  $C_6H_{13}O_9P$ ).

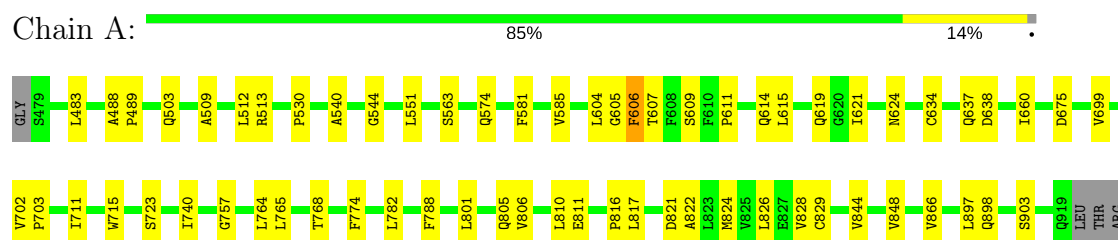


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 16	C 6	O 9	P 1	0	0
3	B	1	Total 16	C 6	O 9	P 1	0	0
3	C	1	Total 16	C 6	O 9	P 1	0	0
3	D	1	Total 16	C 6	O 9	P 1	0	0

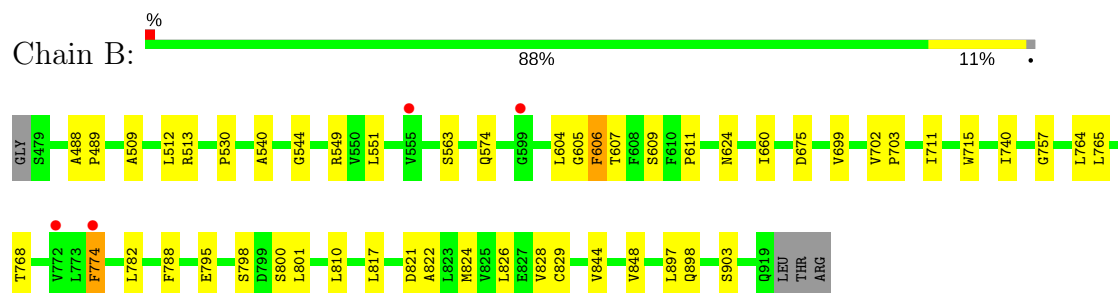
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

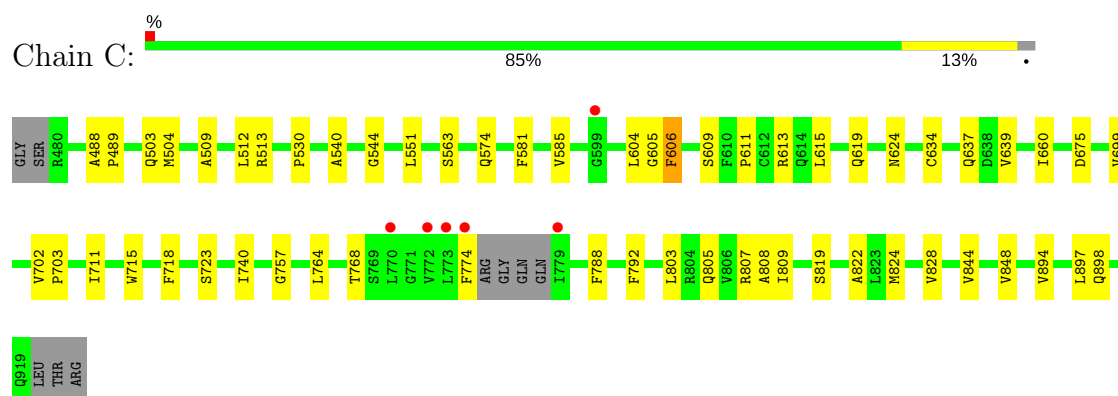
#### • Molecule 1: Hexokinase-3



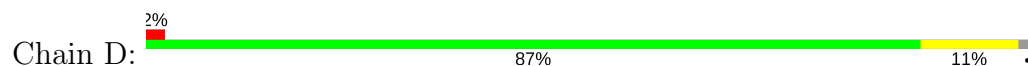
#### • Molecule 1: Hexokinase-3

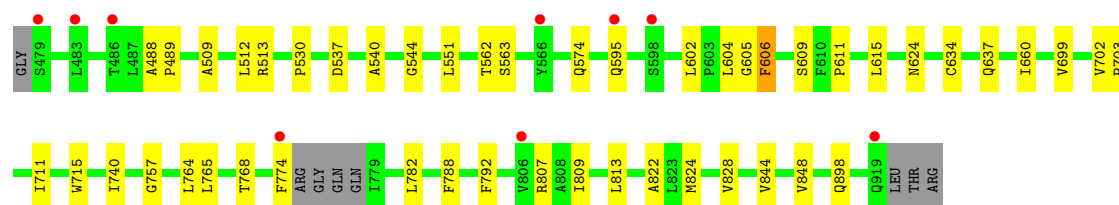


#### • Molecule 1: Hexokinase-3



#### • Molecule 1: Hexokinase-3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.90Å 83.90Å 323.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-2.80) 97.2 (20.00-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.245 , 0.270 0.249 , 0.271	Depositor DCC
$R_{free}$ test set	1502 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.9	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 26.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.076 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: GLC, BG6

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	0.62	1/3249 (0.0%)	0.57	0/4407
1	B	0.55	1/3160 (0.0%)	0.55	0/4295
1	C	0.55	0/3158	0.54	0/4288
1	D	0.52	0/3124	0.54	0/4250
All	All	0.56	2/12691 (0.0%)	0.55	0/17240

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	829	CYS	CB-SG	-6.89	1.70	1.82
1	B	829	CYS	CB-SG	-5.17	1.73	1.81

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	3206	0	3098	48	0
1	B	3117	0	2950	32	0
1	C	3116	0	2967	40	0
1	D	3082	0	2884	31	0
2	A	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
3	A	16	0	11	0	0
3	B	16	0	11	0	0
3	C	16	0	11	0	0
3	D	16	0	11	0	0
All	All	12633	0	11991	145	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (145) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:VAL:HG13	1:A:703:PRO:HD2	1.61	0.83
1:B:702:VAL:HG13	1:B:703:PRO:HD2	1.61	0.83
1:C:702:VAL:HG13	1:C:703:PRO:HD2	1.61	0.81
1:D:702:VAL:HG13	1:D:703:PRO:HD2	1.62	0.79
1:D:562:THR:HG21	1:D:595:GLN:HE22	1.48	0.78
1:A:810:LEU:HD13	1:A:817:LEU:HD11	1.66	0.76
1:C:551:LEU:HD23	1:C:563:SER:HB3	1.68	0.75
1:B:551:LEU:HD23	1:B:563:SER:HB3	1.69	0.73
1:D:551:LEU:HD23	1:D:563:SER:HB3	1.68	0.73
1:C:503:GLN:NE2	1:C:723:SER:HB2	2.05	0.72
1:A:551:LEU:HD23	1:A:563:SER:HB3	1.70	0.71
1:A:817:LEU:HD13	1:A:822:ALA:HA	1.73	0.70
1:A:615:LEU:HD12	1:A:615:LEU:N	2.09	0.68
1:D:574:GLN:NE2	1:D:740:ILE:HD11	2.12	0.64
1:A:574:GLN:NE2	1:A:740:ILE:HD11	2.12	0.64
1:A:824:MET:O	1:A:828:VAL:HG23	1.98	0.63
1:A:483:LEU:HD22	1:A:824:MET:HG2	1.81	0.62
1:C:574:GLN:NE2	1:C:740:ILE:HD11	2.15	0.62
1:A:810:LEU:HD13	1:A:817:LEU:CD1	2.29	0.62
1:B:574:GLN:NE2	1:B:740:ILE:HD11	2.16	0.60
1:C:768:THR:HG22	1:C:774:PHE:HD2	1.66	0.60
1:A:606:PHE:HB3	1:A:660:ILE:HD13	1.82	0.60
1:C:824:MET:O	1:C:828:VAL:HG23	2.02	0.60
1:A:503:GLN:NE2	1:A:723:SER:HB2	2.18	0.59
1:A:768:THR:HG22	1:A:774:PHE:HD2	1.66	0.59
1:D:551:LEU:HD23	1:D:563:SER:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:PHE:HB3	1:B:660:ILE:HD13	1.86	0.57
1:A:638:ASP:OD2	1:C:615:LEU:HD21	2.04	0.57
1:D:606:PHE:HB3	1:D:660:ILE:HD13	1.85	0.57
1:C:606:PHE:HB3	1:C:660:ILE:HD13	1.86	0.57
1:C:540:ALA:HB3	1:C:551:LEU:HB2	1.87	0.57
1:A:699:VAL:HG22	1:A:711:ILE:HD11	1.87	0.56
1:D:699:VAL:HG22	1:D:711:ILE:HD11	1.87	0.56
1:B:699:VAL:HG22	1:B:711:ILE:HD11	1.87	0.56
1:C:699:VAL:HG22	1:C:711:ILE:HD11	1.88	0.56
1:C:581:PHE:O	1:C:585:VAL:HG23	2.04	0.56
1:B:551:LEU:HD23	1:B:563:SER:CB	2.35	0.56
1:D:540:ALA:HB3	1:D:551:LEU:HB2	1.88	0.55
1:C:503:GLN:HE21	1:C:723:SER:HB2	1.71	0.55
1:C:551:LEU:HD23	1:C:563:SER:CB	2.33	0.55
1:A:540:ALA:HB3	1:A:551:LEU:HB2	1.87	0.55
1:A:551:LEU:HD23	1:A:563:SER:CB	2.35	0.55
1:A:614:GLN:C	1:A:615:LEU:HD12	2.28	0.55
1:A:509:ALA:O	1:A:513:ARG:HG3	2.08	0.54
1:B:764:LEU:O	1:B:768:THR:HG23	2.08	0.54
1:B:540:ALA:HB3	1:B:551:LEU:HB2	1.90	0.53
1:D:768:THR:HG22	1:D:774:PHE:HD2	1.74	0.52
1:A:488:ALA:HB3	1:A:489:PRO:HD3	1.92	0.51
1:B:765:LEU:HD23	1:B:782:LEU:HD23	1.91	0.51
1:A:619:GLN:HB2	1:C:615:LEU:HD22	1.91	0.51
1:C:803:LEU:HD21	1:C:819:SER:HB3	1.92	0.51
1:D:764:LEU:O	1:D:768:THR:HG23	2.11	0.51
1:C:764:LEU:O	1:C:768:THR:HG23	2.10	0.51
1:D:792:PHE:CD1	1:D:813:LEU:HD11	2.45	0.51
1:D:807:ARG:HG2	1:D:822:ALA:HB2	1.92	0.51
1:A:621:ILE:HD11	1:C:615:LEU:HD13	1.93	0.51
1:B:544:GLY:HA3	1:B:609:SER:OG	2.11	0.51
1:C:544:GLY:HA3	1:C:609:SER:OG	2.11	0.51
1:D:615:LEU:N	1:D:615:LEU:HD12	2.25	0.51
1:D:544:GLY:HA3	1:D:609:SER:OG	2.11	0.50
1:D:509:ALA:O	1:D:513:ARG:HG3	2.11	0.49
1:A:512:LEU:HD21	1:A:711:ILE:CD1	2.42	0.49
1:D:757:GLY:HA3	1:D:788:PHE:O	2.12	0.49
1:C:702:VAL:CG1	1:C:703:PRO:HD2	2.39	0.49
1:B:774:PHE:CZ	1:B:817:LEU:HD21	2.48	0.49
1:B:810:LEU:HD12	1:B:817:LEU:HD12	1.95	0.49
1:A:544:GLY:HA3	1:A:609:SER:OG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:LEU:O	1:A:768:THR:HG23	2.14	0.48
1:B:702:VAL:HG13	1:B:703:PRO:CD	2.40	0.48
1:C:509:ALA:O	1:C:513:ARG:HG3	2.13	0.48
1:C:488:ALA:HB3	1:C:489:PRO:HD3	1.95	0.47
1:B:512:LEU:HD21	1:B:711:ILE:HD13	1.97	0.47
1:A:512:LEU:HD21	1:A:711:ILE:HD13	1.95	0.47
1:C:792:PHE:HE1	1:C:809:ILE:HG22	1.79	0.47
1:A:581:PHE:O	1:A:585:VAL:HG23	2.13	0.47
1:A:611:PRO:HD2	1:A:624:ASN:O	2.15	0.47
1:B:795:GLU:O	1:B:801:LEU:HD12	2.15	0.47
1:B:702:VAL:CG1	1:B:703:PRO:HD2	2.39	0.46
1:B:512:LEU:HD21	1:B:711:ILE:CD1	2.45	0.46
1:A:702:VAL:CG1	1:A:703:PRO:HD2	2.39	0.46
1:A:757:GLY:HA3	1:A:788:PHE:O	2.15	0.46
1:C:512:LEU:HD21	1:C:711:ILE:CD1	2.45	0.46
1:D:512:LEU:HD21	1:D:711:ILE:CD1	2.45	0.46
1:D:611:PRO:HD2	1:D:624:ASN:O	2.15	0.46
1:B:509:ALA:O	1:B:513:ARG:HG3	2.15	0.46
1:A:637:GLN:OE1	1:C:613:ARG:NH2	2.49	0.46
1:D:792:PHE:HE1	1:D:809:ILE:HG22	1.81	0.46
1:A:817:LEU:HD13	1:A:822:ALA:CA	2.45	0.46
1:B:549:ARG:HD2	1:B:551:LEU:HD21	1.97	0.46
1:C:844:VAL:O	1:C:848:VAL:HG22	2.16	0.46
1:A:817:LEU:HD22	1:A:821:ASP:HB3	1.98	0.45
1:B:817:LEU:HD13	1:B:822:ALA:HA	1.97	0.45
1:A:574:GLN:HE21	1:A:740:ILE:HD11	1.80	0.45
1:C:604:LEU:HD23	1:C:605:GLY:N	2.32	0.45
1:B:488:ALA:HB3	1:B:489:PRO:HD3	1.98	0.45
1:A:675:ASP:OD2	1:A:897:LEU:HD11	2.16	0.45
1:A:768:THR:HG22	1:A:774:PHE:CD2	2.50	0.45
1:D:604:LEU:HD23	1:D:605:GLY:N	2.32	0.45
1:A:634:CYS:O	1:A:637:GLN:HB2	2.17	0.45
1:D:488:ALA:HB3	1:D:489:PRO:HD3	1.99	0.44
1:C:611:PRO:HD2	1:C:624:ASN:O	2.17	0.44
1:C:634:CYS:O	1:C:637:GLN:HB2	2.17	0.44
1:D:702:VAL:HG13	1:D:703:PRO:CD	2.40	0.44
1:D:574:GLN:HE21	1:D:740:ILE:HD11	1.80	0.44
1:A:866:VAL:HG12	1:A:897:LEU:O	2.15	0.44
1:A:604:LEU:HD23	1:A:605:GLY:N	2.31	0.44
1:B:817:LEU:HD22	1:B:821:ASP:HB3	1.98	0.44
1:A:615:LEU:CD1	1:A:615:LEU:N	2.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:512:LEU:HD21	1:C:711:ILE:HD13	1.99	0.44
1:C:574:GLN:HE21	1:C:740:ILE:HD11	1.80	0.44
1:A:621:ILE:HD11	1:C:615:LEU:CD1	2.48	0.44
1:D:634:CYS:O	1:D:637:GLN:HB2	2.18	0.44
1:A:844:VAL:O	1:A:848:VAL:HG22	2.18	0.43
1:B:826:LEU:HA	1:B:826:LEU:HD12	1.92	0.43
1:C:807:ARG:HG2	1:C:822:ALA:HB2	2.00	0.43
1:C:675:ASP:OD2	1:C:897:LEU:HD11	2.19	0.43
1:B:611:PRO:HD2	1:B:624:ASN:O	2.19	0.43
1:D:512:LEU:HD21	1:D:711:ILE:HD13	1.99	0.43
1:D:844:VAL:O	1:D:848:VAL:HG22	2.18	0.43
1:C:504:MET:HE2	1:C:718:PHE:CD2	2.54	0.43
1:D:765:LEU:HD23	1:D:782:LEU:HD23	2.01	0.43
1:A:702:VAL:HG13	1:A:703:PRO:CD	2.39	0.43
1:C:757:GLY:HA3	1:C:788:PHE:O	2.19	0.43
1:B:604:LEU:HD23	1:B:605:GLY:N	2.33	0.43
1:B:675:ASP:OD2	1:B:897:LEU:HD11	2.18	0.43
1:B:757:GLY:HA3	1:B:788:PHE:O	2.19	0.43
1:A:615:LEU:HD22	1:C:619:GLN:HB2	2.01	0.43
1:D:702:VAL:CG1	1:D:703:PRO:HD2	2.39	0.43
1:B:607:THR:HG21	1:B:903:SER:CB	2.50	0.42
1:C:702:VAL:HG13	1:C:703:PRO:CD	2.39	0.42
1:B:798:SER:OG	1:B:800:SER:OG	2.35	0.42
1:C:805:GLN:O	1:C:808:ALA:HB3	2.19	0.42
1:D:562:THR:CG2	1:D:595:GLN:HE22	2.22	0.42
1:B:574:GLN:HE21	1:B:740:ILE:HD11	1.83	0.42
1:C:848:VAL:HG11	1:C:894:VAL:HG21	2.02	0.41
1:B:824:MET:O	1:B:828:VAL:HG23	2.19	0.41
1:B:844:VAL:O	1:B:848:VAL:HG22	2.19	0.41
1:A:801:LEU:HD22	1:A:805:GLN:HB3	2.02	0.41
1:A:765:LEU:HD23	1:A:782:LEU:HD23	2.03	0.41
1:D:824:MET:O	1:D:828:VAL:HG23	2.20	0.41
1:A:811:GLU:HG3	1:A:816:PRO:HA	2.02	0.41
1:C:639:VAL:HG23	1:C:660:ILE:HD11	2.03	0.41
1:A:607:THR:HG21	1:A:903:SER:CB	2.51	0.40
1:D:537:ASP:O	1:D:602:LEU:HD22	2.20	0.40
1:A:806:VAL:HG21	1:A:826:LEU:HD22	2.04	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	439/445 (99%)	424 (97%)	14 (3%)	1 (0%)	49	81
1	B	439/445 (99%)	423 (96%)	14 (3%)	2 (0%)	31	65
1	C	432/445 (97%)	420 (97%)	11 (2%)	1 (0%)	49	81
1	D	433/445 (97%)	419 (97%)	13 (3%)	1 (0%)	49	81
All	All	1743/1780 (98%)	1686 (97%)	52 (3%)	5 (0%)	43	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	774	PHE
1	A	530	PRO
1	B	530	PRO
1	C	530	PRO
1	D	530	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	321/365 (88%)	318 (99%)	3 (1%)	81	95
1	B	296/365 (81%)	293 (99%)	3 (1%)	78	94
1	C	301/365 (82%)	298 (99%)	3 (1%)	78	94
1	D	293/365 (80%)	290 (99%)	3 (1%)	78	94
All	All	1211/1460 (83%)	1199 (99%)	12 (1%)	78	94

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	606	PHE
1	A	715	TRP
1	A	898	GLN
1	B	606	PHE
1	B	715	TRP
1	B	898	GLN
1	C	606	PHE
1	C	715	TRP
1	C	898	GLN
1	D	606	PHE
1	D	715	TRP
1	D	898	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	503	GLN
1	A	574	GLN
1	A	651	GLN
1	A	698	ASN
1	B	574	GLN
1	B	698	ASN
1	C	574	GLN
1	C	698	ASN
1	D	595	GLN
1	D	698	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

8 ligands 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	A	1001	-	12,12,12	1.26	2 (16%)	17,17,17	1.00	0
3	BG6	A	1002	-	16,16,16	1.48	3 (18%)	24,24,24	0.92	2 (8%)
2	GLC	B	1001	-	12,12,12	1.16	1 (8%)	17,17,17	0.84	0
3	BG6	B	1002	-	16,16,16	1.52	3 (18%)	24,24,24	1.00	2 (8%)
2	GLC	C	1001	-	12,12,12	0.98	1 (8%)	17,17,17	0.77	0
3	BG6	C	1002	-	16,16,16	1.54	3 (18%)	24,24,24	0.96	2 (8%)
2	GLC	D	1001	-	12,12,12	1.03	1 (8%)	17,17,17	0.69	0
3	BG6	D	1002	-	16,16,16	1.70	3 (18%)	24,24,24	1.03	2 (8%)

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	A	1001	-	-	0/2/22/22	0/1/1/1
3	BG6	A	1002	-	-	0/6/26/26	0/1/1/1
2	GLC	B	1001	-	-	0/2/22/22	0/1/1/1
3	BG6	B	1002	-	-	0/6/26/26	0/1/1/1
2	GLC	C	1001	-	-	0/2/22/22	0/1/1/1
3	BG6	C	1002	-	-	0/6/26/26	0/1/1/1
2	GLC	D	1001	-	-	0/2/22/22	0/1/1/1
3	BG6	D	1002	-	-	0/6/26/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1002	BG6	C4-C3	2.04	1.57	1.52
3	A	1002	BG6	P-O2P	2.04	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	BG6	O5-C1	2.11	1.48	1.42
3	A	1002	BG6	O5-C1	2.11	1.48	1.42
3	D	1002	BG6	P-O2P	2.18	1.63	1.54
3	C	1002	BG6	P-O2P	2.24	1.63	1.54
3	B	1002	BG6	O5-C1	2.35	1.48	1.42
2	C	1001	GLC	C6-C5	2.35	1.59	1.51
2	A	1001	GLC	O1-C1	2.49	1.47	1.39
2	D	1001	GLC	C6-C5	2.55	1.60	1.51
2	A	1001	GLC	C6-C5	2.64	1.60	1.51
2	B	1001	GLC	C6-C5	2.73	1.61	1.51
3	B	1002	BG6	P-O3P	2.85	1.60	1.50
3	B	1002	BG6	P-O2P	3.09	1.67	1.54
3	C	1002	BG6	P-O3P	3.46	1.62	1.50
3	A	1002	BG6	P-O3P	3.51	1.62	1.50
3	D	1002	BG6	P-O3P	4.20	1.64	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1002	BG6	O5-C5-C6	2.06	110.75	106.64
3	C	1002	BG6	O1P-P-O6	2.35	112.99	106.73
3	B	1002	BG6	O1P-P-O6	2.38	113.08	106.73
3	B	1002	BG6	O5-C5-C6	2.46	111.56	106.64
3	A	1002	BG6	O1P-P-O6	2.53	113.45	106.73
3	D	1002	BG6	O5-C5-C6	2.67	111.98	106.64
3	D	1002	BG6	O1P-P-O6	2.68	113.86	106.73
3	C	1002	BG6	O5-C5-C6	2.77	112.17	106.64

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

### 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	441/445 (99%)	-0.23	0 <b>100</b> <b>100</b>	54, 69, 98, 117	0
1	B	441/445 (99%)	-0.11	4 (0%) <b>84</b> <b>79</b>	61, 89, 128, 148	0
1	C	436/445 (97%)	-0.09	6 (1%) <b>75</b> <b>69</b>	58, 82, 141, 162	0
1	D	437/445 (98%)	-0.12	9 (2%) <b>63</b> <b>54</b>	69, 91, 138, 151	0
All	All	1755/1780 (98%)	-0.14	19 (1%) <b>80</b> <b>75</b>	54, 83, 131, 162	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	599	GLY	4.6
1	D	598	SER	4.3
1	C	770	LEU	3.6
1	D	486	THR	3.2
1	D	774	PHE	3.2
1	C	774	PHE	3.2
1	D	479	SER	3.1
1	C	772	VAL	2.7
1	D	919	GLN	2.7
1	C	599	GLY	2.7
1	D	483	LEU	2.6
1	C	773	LEU	2.4
1	B	772	VAL	2.4
1	B	774	PHE	2.3
1	B	555	VAL	2.2
1	D	806	VAL	2.2
1	C	779	ILE	2.1
1	D	595	GLN	2.1
1	D	566	TYR	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](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
3	BG6	D	1002	16/16	0.94	0.20	76,79,83,84	0
3	BG6	B	1002	16/16	0.95	0.17	65,69,73,74	0
2	GLC	A	1001	12/12	0.96	0.18	54,55,56,57	0
2	GLC	B	1001	12/12	0.96	0.16	66,67,71,71	0
2	GLC	D	1001	12/12	0.96	0.15	69,71,72,72	0
3	BG6	A	1002	16/16	0.96	0.17	58,60,65,65	0
3	BG6	C	1002	16/16	0.96	0.15	69,73,76,79	0
2	GLC	C	1001	12/12	0.97	0.17	60,61,63,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.