



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 21, 2016 – 05:03 PM EDT

PDB ID : 5HEX
Title : Crystal Structure of Human Hexokinase 2 with cmpd 30, a 2-amino-6-benzenesulfonamide glucosamine
Authors : Campobasso, N.; Zhao, B.; Smallwood, A.
Deposited on : 2016-01-06
Resolution : 2.73 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

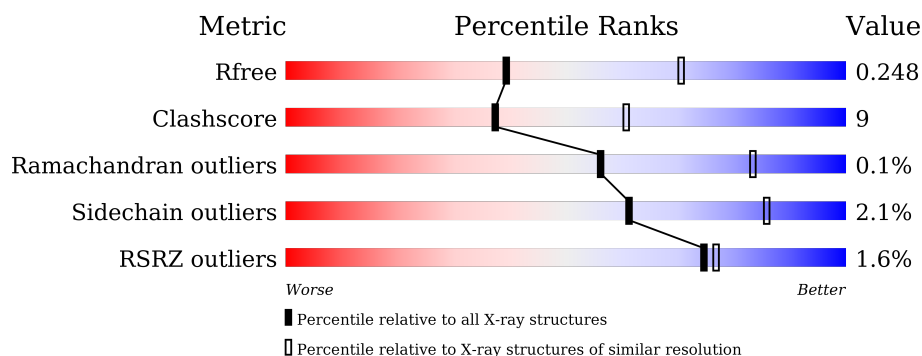
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	923	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>• 5%</div> </div> </div>
1	B	923	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13830 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-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	880	Total	C	N	O	S	0	1	0
			6771	4245	1191	1274	61			
1	B	891	Total	C	N	O	S	0	0	0
			6847	4293	1195	1297	62			

There are 44 discrepancies between the modelled and reference sequences:

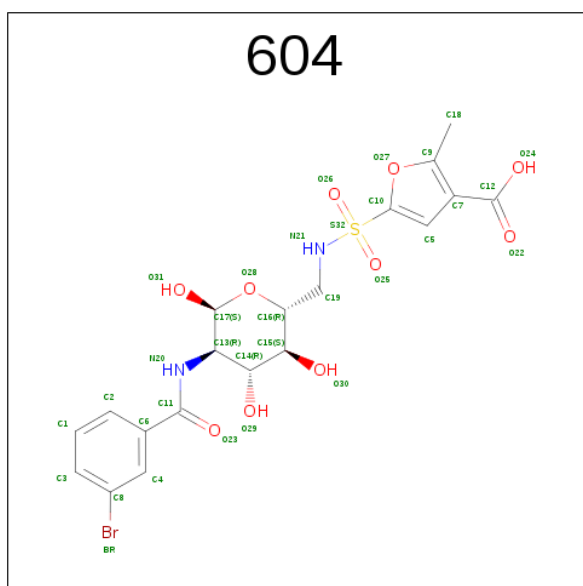
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP P52789
A	-4	GLY	-	expression tag	UNP P52789
A	-3	SER	-	expression tag	UNP P52789
A	-2	SER	-	expression tag	UNP P52789
A	-1	HIS	-	expression tag	UNP P52789
A	0	HIS	-	expression tag	UNP P52789
A	1	HIS	-	expression tag	UNP P52789
A	2	HIS	-	expression tag	UNP P52789
A	3	HIS	-	expression tag	UNP P52789
A	4	HIS	-	expression tag	UNP P52789
A	5	SER	-	expression tag	UNP P52789
A	6	SER	-	expression tag	UNP P52789
A	7	GLY	-	expression tag	UNP P52789
A	8	LEU	-	expression tag	UNP P52789
A	9	GLU	-	expression tag	UNP P52789
A	10	ASN	-	expression tag	UNP P52789
A	11	LEU	-	expression tag	UNP P52789
A	12	TYR	-	expression tag	UNP P52789
A	13	PHE	-	expression tag	UNP P52789
A	14	GLN	-	expression tag	UNP P52789
A	15	GLY	-	expression tag	UNP P52789
A	16	SER	-	expression tag	UNP P52789
B	-5	MET	-	initiating methionine	UNP P52789
B	-4	GLY	-	expression tag	UNP P52789
B	-3	SER	-	expression tag	UNP P52789

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP P52789
B	-1	HIS	-	expression tag	UNP P52789
B	0	HIS	-	expression tag	UNP P52789
B	1	HIS	-	expression tag	UNP P52789
B	2	HIS	-	expression tag	UNP P52789
B	3	HIS	-	expression tag	UNP P52789
B	4	HIS	-	expression tag	UNP P52789
B	5	SER	-	expression tag	UNP P52789
B	6	SER	-	expression tag	UNP P52789
B	7	GLY	-	expression tag	UNP P52789
B	8	LEU	-	expression tag	UNP P52789
B	9	GLU	-	expression tag	UNP P52789
B	10	ASN	-	expression tag	UNP P52789
B	11	LEU	-	expression tag	UNP P52789
B	12	TYR	-	expression tag	UNP P52789
B	13	PHE	-	expression tag	UNP P52789
B	14	GLN	-	expression tag	UNP P52789
B	15	GLY	-	expression tag	UNP P52789
B	16	SER	-	expression tag	UNP P52789

- Molecule 2 is 5-[[[(2 {R},3 {S},4 {R},5 {R},6 {S})-5-[(3-bromophenyl)carbonylamino]-3,4,6-tris(oxidanyl)oxan-2-yl]methylsulfamoyl]-2-methyl-furan-3-carboxylic acid (three-letter code: 604) (formula: C₁₉H₂₁BrN₂O₁₀S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	S	0	0
			33	1	19	2	10	1		

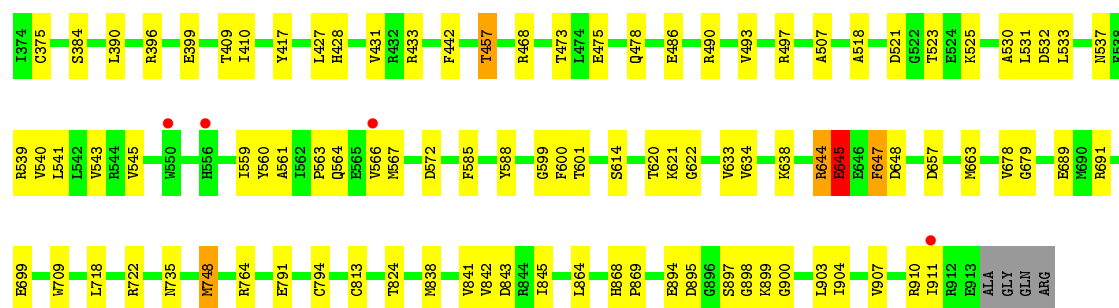
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	S	0	0
			33	1	19	2	10	1		
2	B	1	Total	Br	C	N	O	S	0	0
			30	1	16	2	10	1		
2	B	1	Total	Br	C	N	O	S	0	0
			33	1	19	2	10	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	0
			31	31		
3	B	52	Total	O	0	0
			52	52		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.03Å 154.89Å 114.83Å 90.00° 96.34° 90.00°	Depositor
Resolution (Å)	114.12 – 2.73 114.12 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.8 (114.12-2.73) 93.8 (114.12-2.73)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.190 , 0.252 0.187 , 0.248	Depositor DCC
R_{free} test set	2770 reflections (4.88%)	DCC
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 19.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 59896 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13830	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 604

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	0.47	3/6878 (0.0%)	0.73	8/9262 (0.1%)
1	B	0.47	0/6952	0.67	2/9365 (0.0%)
All	All	0.47	3/13830 (0.0%)	0.70	10/18627 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	386	CYS	CB-SG	-7.50	1.69	1.82
1	A	691	ARG	CZ-NH1	-5.14	1.26	1.33
1	A	691	ARG	NE-CZ	-5.11	1.26	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	846	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	A	846	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	A	423	PHE	CB-CG-CD1	6.81	125.57	120.80
1	B	645	GLU	N-CA-C	6.28	127.97	111.00
1	A	305	LEU	CA-CB-CG	5.93	128.93	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	523	THR	Peptide
1	A	646	GLU	Peptide
1	B	622	GLY	Peptide
1	B	644	ARG	Peptide
1	B	645	GLU	Peptide

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	6771	0	6696	157	0
1	B	6847	0	6763	98	0
2	A	66	0	0	2	0
2	B	63	0	0	2	0
3	A	31	0	0	4	0
3	B	52	0	0	1	0
All	All	13830	0	13459	253	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 9.

The worst 5 of 253 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:865:TYR:HH	1:A:876:HIS:HE2	1.01	0.96
1:A:153:THR:HG21	1:A:449:SER:HB2	1.49	0.95
1:B:663:MET:HG3	1:B:904:ILE:HG12	1.54	0.89
1:B:240:GLU:CD	1:B:396:ARG:HH12	1.77	0.86
1:B:239:MET:HG3	1:B:254:ARG:HH21	1.37	0.86

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	875/923 (95%)	850 (97%)	25 (3%)	0	100	100
1	B	887/923 (96%)	870 (98%)	16 (2%)	1 (0%)	56	83
All	All	1762/1846 (95%)	1720 (98%)	41 (2%)	1 (0%)	56	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	648	ASP

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	719/782 (92%)	705 (98%)	14 (2%)	65	87
1	B	729/782 (93%)	713 (98%)	16 (2%)	60	85
All	All	1448/1564 (93%)	1418 (98%)	30 (2%)	61	86

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	910	ARG
1	B	190	ARG
1	B	748	MET
1	B	168	LEU
1	B	261	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	110	GLN
1	A	478	GLN
1	A	609	ASN

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](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	604	A	1001	-	27,35,35	1.83	2 (7%)	34,52,52	1.32	2 (5%)
2	604	A	1002	-	27,35,35	1.69	2 (7%)	34,52,52	1.56	5 (14%)
2	604	B	1001	-	23,31,35	2.32	4 (17%)	26,45,52	2.13	9 (34%)
2	604	B	1002	-	27,35,35	1.71	2 (7%)	34,52,52	1.53	7 (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	604	A	1001	-	-	0/14/44/44	0/2/3/3
2	604	A	1002	-	-	0/14/44/44	0/2/3/3
2	604	B	1001	-	-	0/14/42/44	0/1/2/3
2	604	B	1002	-	-	0/14/44/44	0/2/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	604	C4-C6	-3.67	1.38	1.52
2	A	1001	604	C10-S32	-2.16	1.73	1.76
2	B	1002	604	O26-S32	2.02	1.45	1.43
2	B	1001	604	O25-S32	2.07	1.45	1.43
2	A	1002	604	O25-S32	2.11	1.45	1.43

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	604	O26-S32-C10	-6.31	97.47	107.64
2	A	1002	604	C17-O28-C16	-4.21	105.49	113.54
2	A	1001	604	O26-S32-C10	-4.12	101.00	107.64
2	B	1002	604	C19-N21-S32	-3.86	112.52	119.80
2	B	1001	604	O25-S32-C10	-3.55	101.92	107.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	604	2	0
2	B	1002	604	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	880/923 (95%)	0.10	22 (2%) 61 63	21, 47, 80, 100	0
1	B	891/923 (96%)	-0.07	7 (0%) 87 88	19, 36, 70, 94	0
All	All	1771/1846 (95%)	0.02	29 (1%) 74 77	19, 41, 77, 100	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	895	ASP	3.5
1	B	178	SER	3.3
1	A	641	ILE	3.3
1	A	499	LEU	3.2
1	A	602	PHE	3.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	604	A	1001	33/33	0.96	0.18	-0.02	24,35,42,73	0
2	604	A	1002	33/33	0.95	0.18	-0.19	36,45,72,147	0
2	604	B	1002	33/33	0.96	0.15	-0.49	27,33,51,111	0
2	604	B	1001	30/33	0.97	0.15	-0.65	21,29,46,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.