

wwPDB X-ray Structure Validation Summary Report (i)

Feb 11, 2024 – 08:42 PM EST

PDB ID	:	3DH4
Title	:	Crystal Structure of Sodium/Sugar symporter with bound Galactose from vib-
		rio parahaemolyticus
Authors	:	Abramson, J.; Faham, S.; Cascio, D.
Deposited on	:	2008-06-16
Resolution	:	2.70 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 (1)) 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: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.70 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	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 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%

Mol	Chain	Length	Quality of chain				
1	А	530	57%	34%	5% •		
1	В	530	58%	32%	6% •		
1	С	530	58%	32%	6% •		
1	D	530	58%	33%	5% •		



3DH4

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15472 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	519	Total	С	Ν	0	\mathbf{S}	0	0	0
1	A	512	3854	2579	580	675	20	0		
1	В	519	Total	С	Ν	0	S	0	0	0
1	I D	512	3854	2579	580	675	20			
1	C	519	Total	С	Ν	0	S	0	0	0
	512	3854	2579	580	675	20	0	0		
1 D	519	Total	С	Ν	0	S	0	0	0	
	512	3854	2579	580	675	20		0	U	

• Molecule 1 is a protein called Sodium/glucose cotransporter.

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	544	VAL	-	expression tag	UNP P96169
А	545	LEU	-	expression tag	UNP P96169
А	546	TYR	-	expression tag	UNP P96169
А	547	LYS	-	expression tag	UNP P96169
А	548	SER	-	expression tag	UNP P96169
А	549	GLY	-	expression tag	UNP P96169
А	550	GLY	-	expression tag	UNP P96169
А	551	SER	-	expression tag	UNP P96169
А	552	PRO	-	expression tag	UNP P96169
А	553	GLY	-	expression tag	UNP P96169
А	554	HIS	-	expression tag	UNP P96169
А	555	HIS	-	expression tag	UNP P96169
А	556	HIS	-	expression tag	UNP P96169
А	557	HIS	-	expression tag	UNP P96169
А	558	HIS	-	expression tag	UNP P96169
А	559	HIS	-	expression tag	UNP P96169
В	544	VAL	-	expression tag	UNP P96169
В	545	LEU	-	expression tag	UNP P96169
В	546	TYR	-	expression tag	UNP P96169
В	547	LYS	-	expression tag	UNP P96169
В	548	SER	-	expression tag	UNP P96169





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Chain	Residue	Modelled	Actual	Comment	Reference		
В	549	GLY	-	expression tag	UNP P96169		
В	550	GLY	-	expression tag	UNP P96169		
В	551	SER	-	expression tag	UNP P96169		
В	552	PRO	-	expression tag	UNP P96169		
В	553	GLY	-	expression tag	UNP P96169		
В	554	HIS	-	expression tag	UNP P96169		
В	555	HIS	-	expression tag	UNP P96169		
В	556	HIS	-	expression tag	UNP P96169		
В	557	HIS	-	expression tag	UNP P96169		
В	558	HIS	-	expression tag	UNP P96169		
В	559	HIS	-	expression tag	UNP P96169		
С	544	VAL	-	expression tag	UNP P96169		
С	545	LEU	-	expression tag	UNP P96169		
С	546	TYR	-	expression tag	UNP P96169		
С	547	LYS	-	expression tag	UNP P96169		
С	548	SER	-	expression tag	UNP P96169		
С	549	GLY	-	expression tag	UNP P96169		
С	550	GLY	-	expression tag	UNP P96169		
С	551	SER	-	expression tag	UNP P96169		
С	552	PRO	-	expression tag	UNP P96169		
С	553	GLY	-	expression tag	UNP P96169		
С	554	HIS	-	expression tag	UNP P96169		
С	555	HIS	-	expression tag	UNP P96169		
С	556	HIS	-	expression tag	UNP P96169		
С	557	HIS	-	expression tag	UNP P96169		
С	558	HIS	-	expression tag	UNP P96169		
С	559	HIS	-	expression tag	UNP P96169		
D	544	VAL	-	expression tag	UNP P96169		
D	545	LEU	-	expression tag	UNP P96169		
D	546	TYR	-	expression tag	UNP P96169		
D	547	LYS	-	expression tag	UNP P96169		
D	548	SER	-	expression tag	UNP P96169		
D	549	GLY	-	expression tag	UNP P96169		
D	550	GLY	-	expression tag	UNP P96169		
D	551	SER	-	expression tag	UNP P96169		
D	552	PRO	-	expression tag	UNP P96169		
D	553	GLY	-	expression tag	UNP P96169		
D	554	HIS	-	expression tag	UNP P96169		
D	555	HIS	-	expression tag	UNP P96169		
D	556	HIS	-	expression tag	UNP P96169		
D	557	HIS	-	expression tag	UNP P96169		
D	558	HIS	-	expression tag	UNP P96169		



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Chain	Residue	Modelled	Actual	Comment	Reference
D	559	HIS	-	expression tag	UNP P96169

• Molecule 2 is beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total C O 12 6 6	0	0
2	В	1	Total C O 12 6 6	0	0
2	С	1	Total C O 12 6 6	0	0
2	D	1	Total C O 12 6 6	0	0

• Molecule 3 is ERBIUM (III) ION (three-letter code: ER3) (formula: Er).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Er 2 2	0	0
3	D	2	Total Er 2 2	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Na 1 1	0	0
4	В	1	Total Na 1 1	0	0
4	С	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	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. 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. 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: Sodium/glucose cotransporter

 \bullet Molecule 1: Sodium/glucose cotransporter





552 F52

1493 1494 V544 1545 Y546 Y546 K647 SER GLY GLY HIS HIS HIS HIS F518 V519 V534 L535 A536 V537 L538 L538 Y539

• Molecule 1: Sodium/glucose cotransporter



• Molecule 1: Sodium/glucose cotransporter

Chain D:	58%	33%	5% •
X3 P52 P52 P52 W53 W54 W54 M55 A63 A63 A63 A63 A63 A63 A63 A63 A63 A63	675 576 576 184 184 194 196 196 7100 7100 7100 7100 7100 1100 7100	1107 E108 G110 G1110 F117 F122 F122	L126 K127 T128 A131 V132 F133 V132 F133 T135 S136
L137 Y138 Y141 N142 N143 L143 L143 L143 L146 L146 M153 L146 L146 L146 L146 L157 L146 L157 L166	A170 A176 T178 T178 T178 GLY GLY GLY SER ALA ALA ALA V186 V186 V186 V186 V186 V196 L196 L196 L196	Y206 M206 S222 K223 M224 V225 F232 F232 F232	P247 P247 1249 1249 A250 V251 1253 1253 1253
A259 N260 N260 N261 1261 1261 V263 V264 V264 V264 V264 V264 V264 V264 V265 V265 V265 V265 V265 V265 V265 V265	V280 A283 A283 A283 A283 V288 V288 V286 V286 V286 V295 V296 V301 V301 V302 V307 A307	A308 Y310 V310 S313 S313 A325 A325 A325 A325 A325 A325 A325 A32	L329 A333 A3336 A3356 A336 A336 7 A336 P340 P341
L342 L342 L346 L346 C349 G349 G349 G349 A361 A361 A361 A361 A361 A361 A361 A371 B372 B374 B374	1378 M379 M379 M379 1381 1381 7383 K383 K383 1385 K383 R389 C399 C399 C399 C399 C399 C399 C399 C	C411 L412 1413 A414 P415 P415 A416 L417 A423 A423 P425 P425	Y426 1427 1427 1427 1421 1431 1436 1436 1437
L4339 N441 V441 V441 V441 L443 L445 C445 C445 C449 C449 C455 A456 C455 A456 C455 C455 C455 C455 C455	1464 1464 1470 1471 1475 1474 1475 1475 1475 1475 1481 1483 1483 1487 1487	F489 T490 M491 V492 V493 1494 F496 F496 F496 S495 S499 S499	S500 D505 D505 D501 S512 V513 T514 F518



V519 V524 F524 F524 V534 V534 V534 V534 V534 V534 V534 V534 V534 V535 V545 V545 V545 V545 V545 V545 V546 V547 V547 V548 V547 V547 V547 V547 V547 V547 V547 V548 V547 V547 V547 V548



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	83.28Å 109.21Å 127.58Å	Depositor
a, b, c, α , β , γ	109.70° 92.02° 102.11°	Depositor
Bosolution (Å)	30.00 - 2.70	Depositor
Resolution (A)	29.50 - 2.70	EDS
% Data completeness	53.3 (30.00-2.70)	Depositor
(in resolution range)	91.3(29.50-2.70)	EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.45 (at 2.68 \text{\AA})$	Xtriage
Refinement program	REFMAC	Depositor
B B.	0.270 , 0.287	Depositor
n, n_{free}	0.330 , 0.340	DCC
R_{free} test set	5170 reflections (5.02%)	wwPDB-VP
Wilson B-factor $(Å^2)$	63.0	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.17, 32.5	EDS
L-test for $twinning^2$	$ < L >=0.43, < L^2>=0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15472	wwPDB-VP
Average B, all atoms $(Å^2)$	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: NA, GAL, ER3

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).

Mal	Chain	Bo	nd lengths	Bond angles		
IVIOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.48	0/3867	0.57	0/5279	
1	В	0.48	0/3867	0.57	0/5279	
1	С	0.48	1/3867~(0.0%)	0.57	0/5279	
1	D	0.47	0/3867	0.57	0/5279	
All	All	0.48	1/15468~(0.0%)	0.57	0/21116	

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	А	0	1
1	В	0	1
1	С	0	1
1	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	С	481	ASP	CB-CG	5.38	1.63	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	122	PHE	Peptide
	~		7	



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Mol	Chain	Res	Type	Group
1	В	122	PHE	Peptide
1	С	122	PHE	Peptide
1	D	122	PHE	Peptide

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	А	3854	0	3887	180	0
1	В	3854	0	3887	164	0
1	С	3854	0	3887	164	0
1	D	3854	0	3887	188	0
2	А	12	0	12	0	0
2	В	12	0	12	0	0
2	С	12	0	12	0	0
2	D	12	0	12	0	0
3	А	2	0	0	0	0
3	D	2	0	0	0	0
4	А	1	0	0	0	0
4	В	1	0	0	0	0
4	С	1	0	0	0	0
4	D	1	0	0	0	0
All	All	15472	0	15596	668	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 22.

The worst 5 of 668 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance} \ (\text{\AA}) \end{array}$	Clash overlap (Å)
1:B:103:LEU:HD11	1:B:275:LEU:HD13	1.36	1.06
1:A:103:LEU:HD11	1:A:275:LEU:HD13	1.42	1.01
1:C:103:LEU:HD11	1:C:275:LEU:HD13	1.39	1.01
1:D:103:LEU:HD11	1:D:275:LEU:HD13	1.42	1.00
1:C:505:ASP:HB2	1:D:513:VAL:HB	1.47	0.96



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	Pe	erce	entil	\mathbf{es}
1	А	491/530~(93%)	424 (86%)	53 (11%)	14 (3%)		4	10	
1	В	491/530~(93%)	417 (85%)	59 (12%)	15 (3%)		4	9	
1	С	491/530~(93%)	418 (85%)	59~(12%)	14 (3%)		4	10	
1	D	491/530~(93%)	421 (86%)	54 (11%)	16 (3%)		4	8	
All	All	1964/2120~(93%)	1680 (86%)	225 (12%)	59(3%)		4	10	

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	53	TRP
1	А	110	GLY
1	А	268	GLN
1	А	348	VAL
1	А	513	VAL

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		Outliers	Percentiles		
1	А	396/413~(96%)	357~(90%)	39 (10%)	8 18		
1	В	396/413~(96%)	357~(90%)	39~(10%)	8 18		
1	С	396/413~(96%)	356~(90%)	40 (10%)	7 17		



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	396/413~(96%)	356~(90%)	40 (10%)	7 17	
All	All	1584/1652~(96%)	1426 (90%)	158 (10%)	7 18	

 $5~{\rm of}~158$ residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	С	500	SER
1	D	397	ASN
1	D	60	LEU
1	D	204	THR
1	D	471	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such side chains are listed below:

Mol	Chain	Res	Type
1	В	425	GLN
1	D	272	GLN
1	С	245	ASN
1	D	425	GLN
1	D	142	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	Turne	Chain	Dec	Tinle	Bond lengths			Bond angles		
	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
2	GAL	С	701	-	12,12,12	0.55	0	$17,\!17,\!17$	0.63	0
2	GAL	В	701	-	12,12,12	0.55	0	$17,\!17,\!17$	0.58	0
2	GAL	А	701	-	12,12,12	0.55	0	17,17,17	0.60	0
2	GAL	D	701	-	12,12,12	0.55	0	17,17,17	0.61	0

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	GAL	С	701	-	-	0/2/22/22	0/1/1/1
2	GAL	В	701	-	-	0/2/22/22	0/1/1/1
2	GAL	А	701	-	-	0/2/22/22	0/1/1/1
2	GAL	D	701	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	В	1
	a	1. 1



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Mol	Chain	Number of breaks
1	С	1
1	А	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	В	19:UNK	С	47:ALA	N	17.80
1	С	19:UNK	С	47:ALA	N	17.80
1	A	19:UNK	С	47:ALA	N	17.79
1	D	19:UNK	С	47:ALA	N	17.78



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

