wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 04:01 pm BST

PDB ID	:	6HYC
Title	:	The structure of full-length human phenylalanine hydroxylase in complex with the cofactor and negative regulator tetrahydrobiopterin
Authors	:	Alcorlo Pages, M.; Flydal, I.M.
Deposited on	:	2018-10-19
Resolution	:	3.18 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 following versions of software and data (see references (1)) were used in the production of this report:

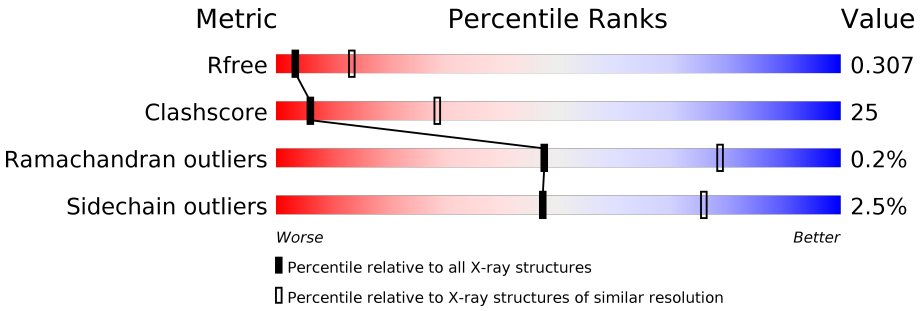
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.18 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)

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 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	A	452	56% 36% • 6%
1	B	452	54% 39% • 6%
1	C	452	50% 42% • 6%
1	D	452	49% 42% • 6%

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
2	H4B	D	501	-	-	X	-

2 Entry composition

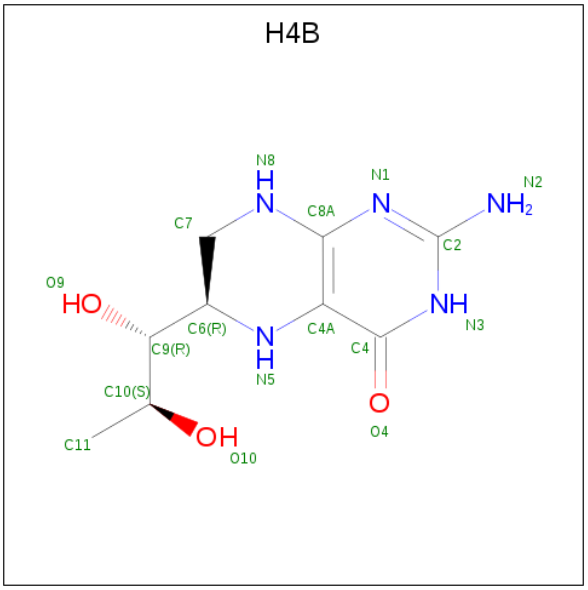
There are 3 unique types of molecules in this entry. The entry contains 13879 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phenylalanine-4-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	423	Total	C	N	O	S	0	4	0
			3477	2237	587	642	11			
1	A	423	Total	C	N	O	S	0	0	0
			3445	2213	583	638	11			
1	C	423	Total	C	N	O	S	0	0	0
			3446	2214	583	638	11			
1	B	424	Total	C	N	O	S	0	0	0
			3455	2219	584	641	11			

- Molecule 2 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			17	9	5	3		
2	C	1	Total	C	N	O	0	0
			17	9	5	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 3 is water.

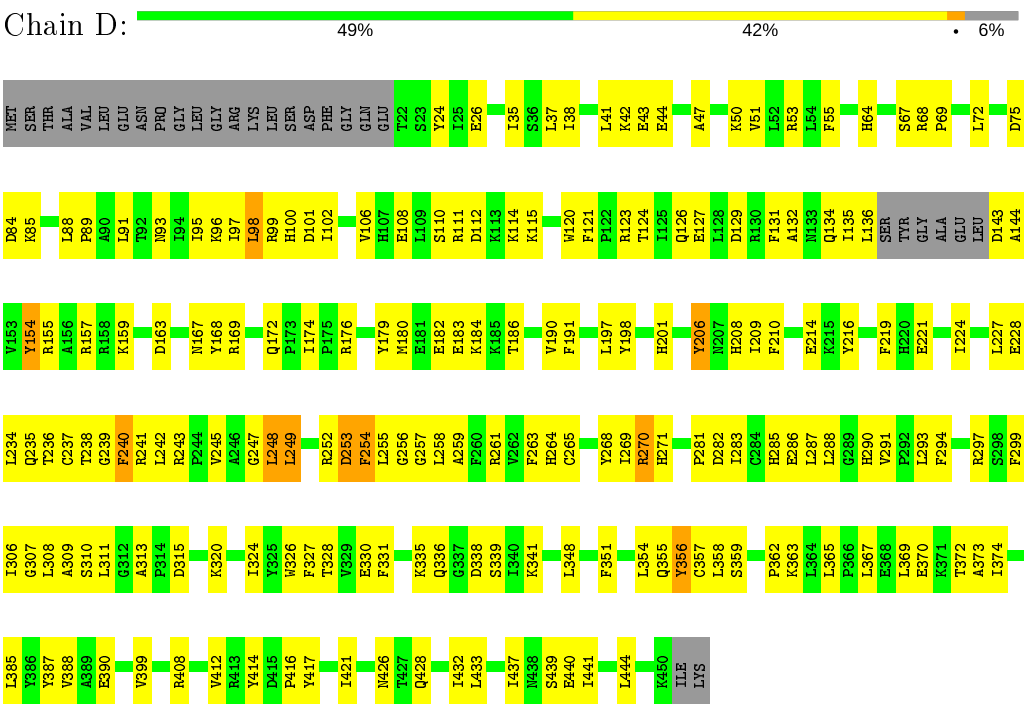
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	C	3	Total	O	0	0
			3	3		
3	B	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

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. 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.

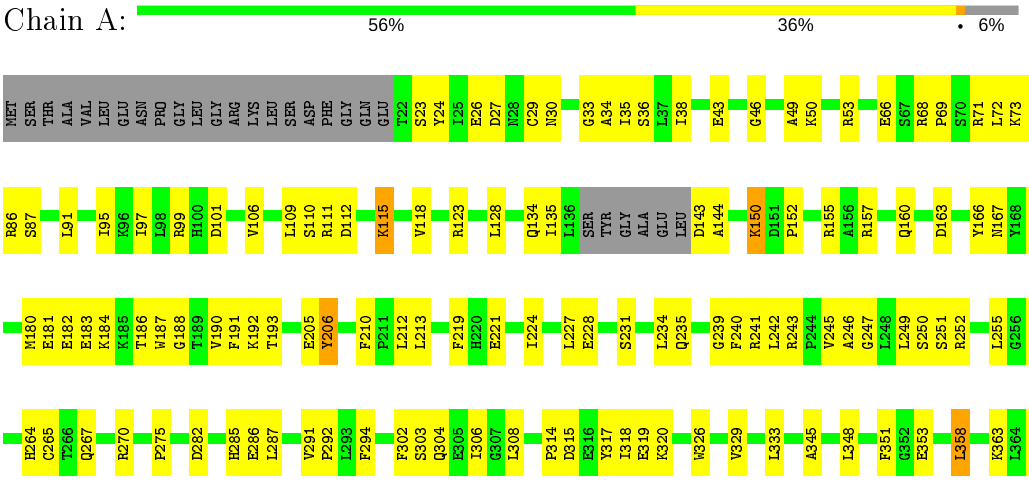
- Molecule 1: Phenylalanine-4-hydroxylase

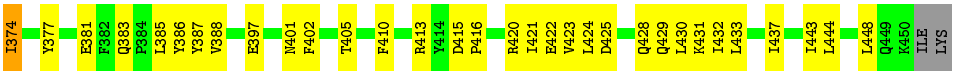
Chain D:



- Molecule 1: Phenylalanine-4-hydroxylase

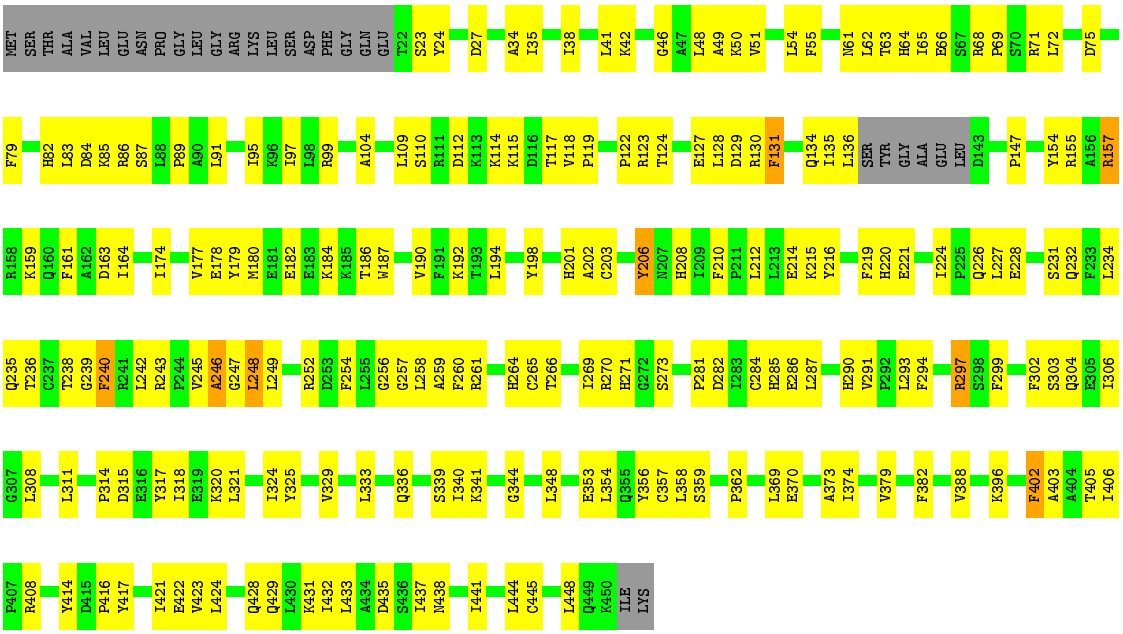
Chain A:





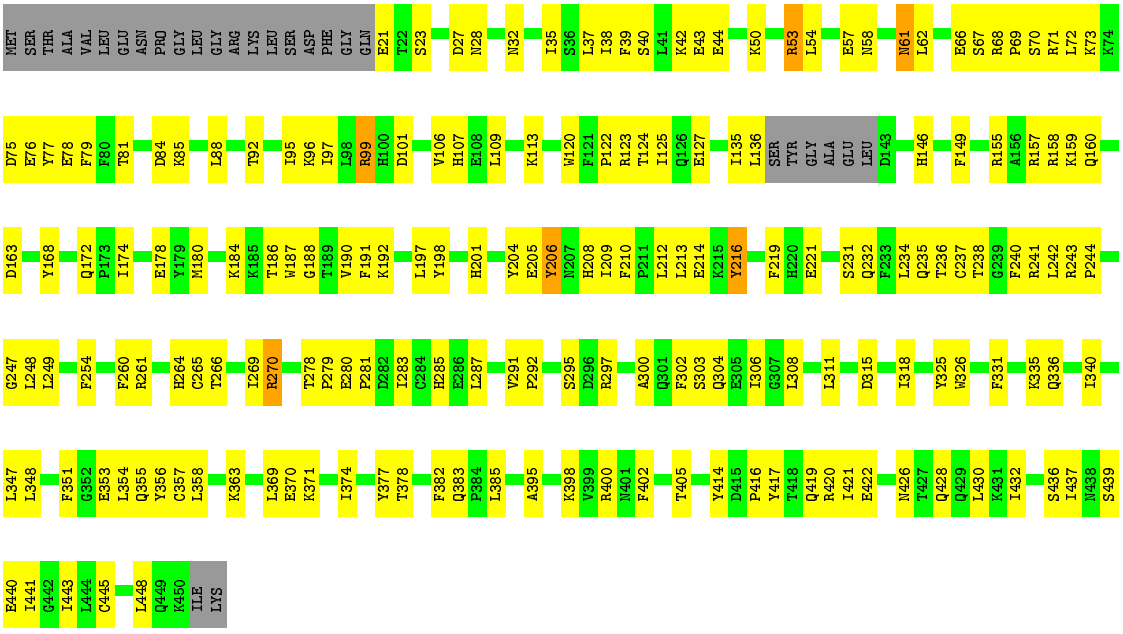
- Molecule 1: Phenylalanine-4-hydroxylase

Chain C:



- Molecule 1: Phenylalanine-4-hydroxylase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	101.94Å 101.37Å 203.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.92 – 3.18 49.18 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (33.92-3.18) 94.4 (49.18-2.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.262 , 0.311 0.267 , 0.307	Depositor DCC
R_{free} test set	2070 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	58.3	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , -48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.039 for -k,-h,-l 0.030 for k,h,-l 0.087 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	13879	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: H4B

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	0.31	0/3531	0.56	0/4778
1	B	0.32	0/3541	0.55	0/4792
1	C	0.31	0/3532	0.56	0/4780
1	D	0.33	0/3564	0.57	0/4823
All	All	0.32	0/14168	0.56	0/19173

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	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	254[A]	PHE	Mainchain

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	3445	0	3394	137	1
1	B	3455	0	3404	164	1
1	C	3446	0	3398	211	0
1	D	3477	0	3430	215	1
2	B	17	0	15	1	0
2	C	17	0	15	6	0
2	D	17	0	15	26	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
3	C	3	0	0	2	0
All	All	13879	0	13671	679	2

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 25.

The worst 5 of 679 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:D:254[A]:PHE:HE2	2:D:501:H4B:C2	1.20	1.55
1:D:254[A]:PHE:CE2	2:D:501:H4B:C4	2.02	1.41
1:D:254[A]:PHE:HE2	2:D:501:H4B:N3	1.20	1.35
1:C:178:GLU:CB	1:B:180:MET:HE2	1.56	1.35
1:D:254[A]:PHE:CE2	2:D:501:H4B:N3	1.94	1.34

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:ILE:CG2	1:D:441:ILE:CG2[2_556]	2.01	0.19
1:A:115:LYS:NZ	1:B:374:ILE:O[3_555]	2.06	0.14

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	419/452 (93%)	388 (93%)	30 (7%)	1 (0%)	47 78
1	B	420/452 (93%)	385 (92%)	35 (8%)	0	100 100
1	C	419/452 (93%)	387 (92%)	31 (7%)	1 (0%)	47 78
1	D	423/452 (94%)	395 (93%)	26 (6%)	2 (0%)	29 66
All	All	1681/1808 (93%)	1555 (92%)	122 (7%)	4 (0%)	47 78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	246	ALA
1	D	115	LYS
1	D	374	ILE
1	A	374	ILE

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	376/399 (94%)	369 (98%)	7 (2%)	57 80
1	B	377/399 (94%)	367 (97%)	10 (3%)	44 74
1	C	376/399 (94%)	369 (98%)	7 (2%)	57 80
1	D	379/399 (95%)	364 (96%)	15 (4%)	31 64
All	All	1508/1596 (94%)	1469 (97%)	39 (3%)	47 75

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LYS
1	A	358	LEU
1	B	240	PHE
1	A	150	LYS
1	A	206	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such

sidechains are listed below:

Mol	Chain	Res	Type
1	D	438	ASN
1	B	61	ASN
1	C	264	HIS
1	D	290	HIS
1	A	30	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)

3 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	H4B	C	501	-	16,18,18	1.65	2 (12%)	11,26,26	2.34	5 (45%)
2	H4B	B	501	-	16,18,18	1.64	2 (12%)	11,26,26	2.35	5 (45%)
2	H4B	D	501	-	16,18,18	1.64	2 (12%)	11,26,26	2.35	5 (45%)

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	H4B	C	501	-	-	4/8/17/17	0/2/2/2
2	H4B	B	501	-	-	2/8/17/17	0/2/2/2
2	H4B	D	501	-	-	2/8/17/17	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	H4B	C4-C4A	5.07	1.48	1.41
2	C	501	H4B	C4-C4A	5.06	1.48	1.41
2	D	501	H4B	C4-C4A	5.06	1.48	1.41
2	C	501	H4B	C4A-C8A	3.51	1.48	1.41
2	D	501	H4B	C4A-C8A	3.46	1.48	1.41

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	H4B	C4-C4A-N5	4.39	122.80	119.12
2	D	501	H4B	C4-C4A-N5	4.37	122.79	119.12
2	B	501	H4B	C4-C4A-N5	4.34	122.76	119.12
2	D	501	H4B	C4-N3-C2	3.97	122.23	115.93
2	C	501	H4B	C4-N3-C2	3.95	122.21	115.93

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	H4B	N5-C6-C9-O9
2	B	501	H4B	N5-C6-C9-O9
2	D	501	H4B	N5-C6-C9-O9
2	C	501	H4B	C7-C6-C9-O9
2	C	501	H4B	C7-C6-C9-C10

There are no ring outliers.

3 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	H4B	6	0
2	B	501	H4B	1	0
2	D	501	H4B	26	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

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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