wwPDB X-ray Structure Validation Summary Report (i)

Oct 17, 2023 – 10:11 PM EDT

PDB ID	:	2DTT
Title	:	Crystal structure of 6-pyruvoyl tetrahydrobiopterin synthase from Pyrococcus horikoshii OT3 complexed with (1'R,2'S)-biopterin
Authors	:	Bagautdinov, B.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2006-07-15
Resolution	:	2.20 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:

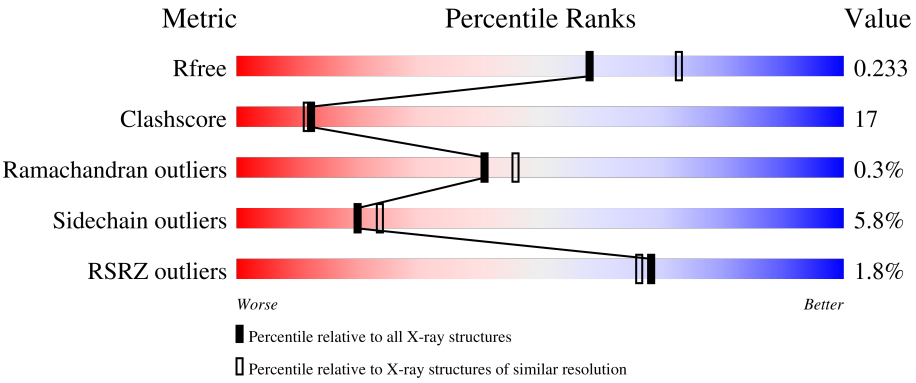
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	115	57% 32% 9%
1	B	115	3% 70% 29%
1	C	115	63% 26% 9%
1	D	115	50% 31% 9% 10%
1	E	115	68% 32%

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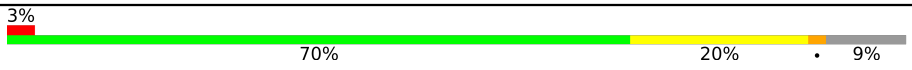
Mol	Chain	Length	Quality of chain
1	F	115	

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	A	1003	X	-	-	-
2	H4B	B	1001	X	-	-	-
2	H4B	C	1002	X	-	-	-
2	H4B	D	1006	X	-	-	-
2	H4B	E	1004	X	-	-	-
2	H4B	F	1005	X	-	-	-

2 Entry composition (i)

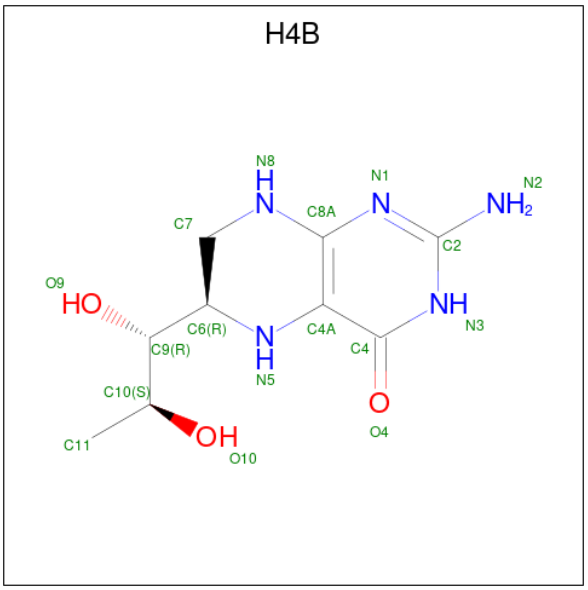
There are 3 unique types of molecules in this entry. The entry contains 5910 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hypothetical protein PH0634.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	0	0	0
			873	561	152	158	2			
1	B	115	Total	C	N	O	S	0	0	0
			956	614	166	174	2			
1	C	105	Total	C	N	O	S	0	0	0
			875	563	152	158	2			
1	D	104	Total	C	N	O	S	0	0	0
			868	558	151	157	2			
1	E	115	Total	C	N	O	S	0	0	0
			956	614	166	174	2			
1	F	105	Total	C	N	O	S	0	0	0
			875	563	152	158	2			

- 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	A	1	Total	C	N	O	0	0
			17	9	5	3		
2	B	1	Total	C	N	O	0	0
			17	9	5	3		
2	C	1	Total	C	N	O	0	0
			17	9	5	3		
2	D	1	Total	C	N	O	0	0
			17	9	5	3		
2	E	1	Total	C	N	O	0	0
			17	9	5	3		
2	F	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 3 is water.

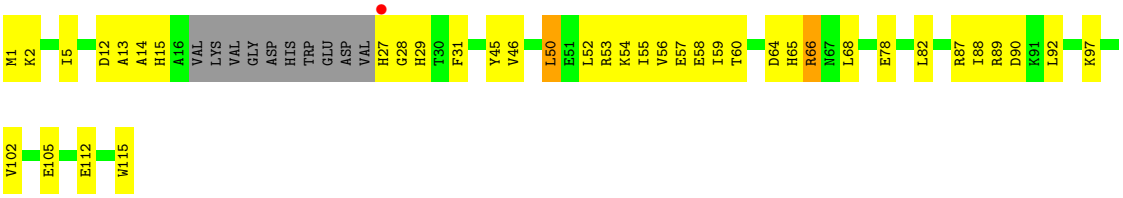
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	53	Total	O	0	0
			53	53		
3	B	98	Total	O	0	0
			98	98		
3	C	78	Total	O	0	0
			78	78		
3	D	29	Total	O	0	0
			29	29		
3	E	82	Total	O	0	0
			82	82		
3	F	65	Total	O	0	0
			65	65		

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.

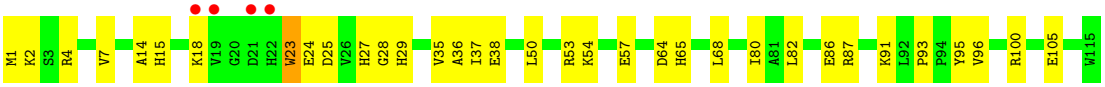
• Molecule 1: Hypothetical protein PH0634

Chain A:



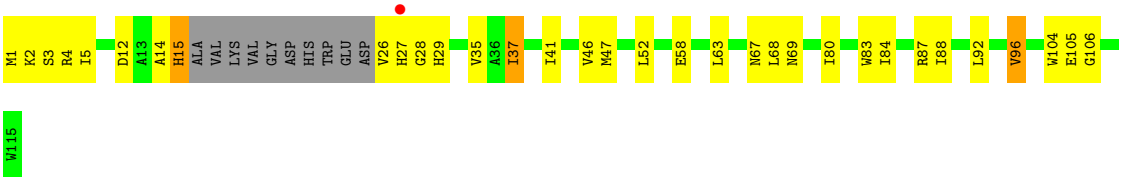
• Molecule 1: Hypothetical protein PH0634

Chain B:



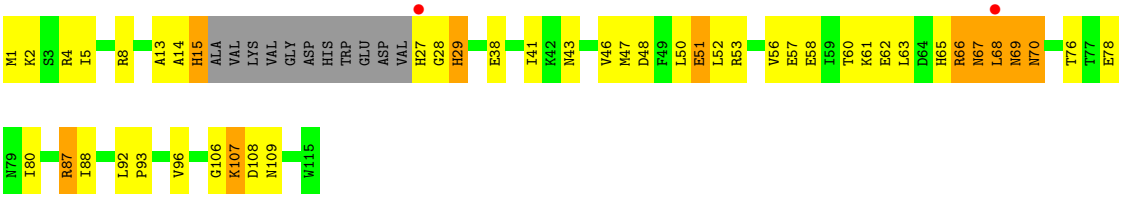
• Molecule 1: Hypothetical protein PH0634

Chain C:



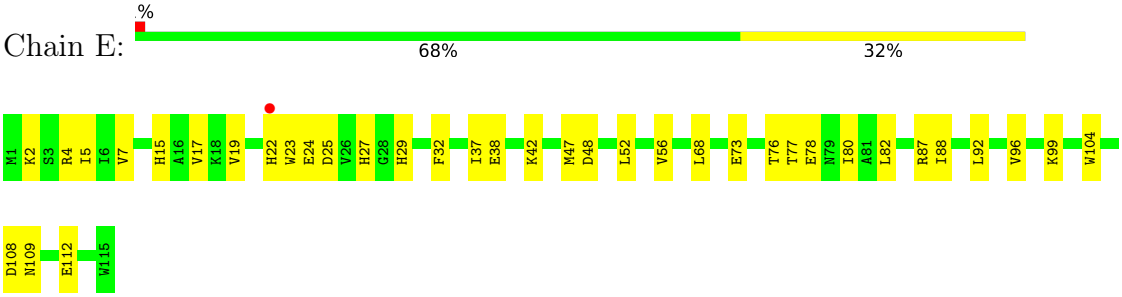
• Molecule 1: Hypothetical protein PH0634

Chain D:



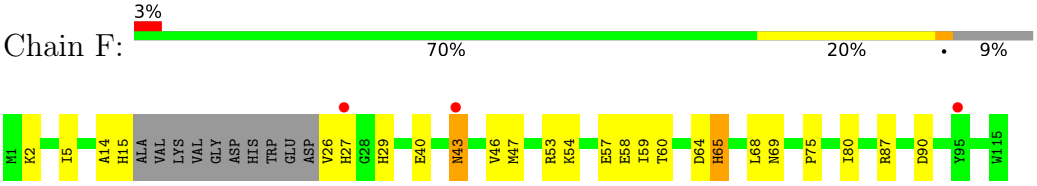
• Molecule 1: Hypothetical protein PH0634

Chain E:



• Molecule 1: Hypothetical protein PH0634

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	35.68Å 105.44Å 96.15Å 90.00° 90.95° 90.00°	Depositor
Resolution (Å)	35.68 – 2.20 46.23 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.4 (35.68-2.20) 90.4 (46.23-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.78 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.236 0.193 , 0.233	Depositor DCC
R_{free} test set	1637 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.249 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5910	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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	0.38	0/891	0.68	0/1200
1	B	0.49	1/978 (0.1%)	0.68	0/1321
1	C	0.38	0/893	0.68	0/1203
1	D	0.42	0/886	0.64	0/1193
1	E	0.32	0/978	0.60	0/1321
1	F	0.32	0/893	0.61	0/1203
All	All	0.39	1/5519 (0.0%)	0.65	0/7441

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	23	TRP	NE1-CE2	8.73	1.49	1.37

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	873	0	876	31	0
1	B	956	0	951	22	0
1	C	875	0	880	29	0
1	D	868	0	871	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	956	0	951	32	0
1	F	875	0	880	16	0
2	A	17	0	14	2	0
2	B	17	0	14	2	0
2	C	17	0	14	1	0
2	D	17	0	14	6	0
2	E	17	0	14	4	0
2	F	17	0	14	0	0
3	A	53	0	0	0	0
3	B	98	0	0	2	0
3	C	78	0	0	0	0
3	D	29	0	0	2	0
3	E	82	0	0	2	0
3	F	65	0	0	0	0
All	All	5910	0	5493	187	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 17.

The worst 5 of 187 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:63:LEU:HD22	1:D:68:LEU:HD21	1.23	1.11
1:D:63:LEU:HD22	1:D:68:LEU:CD2	1.81	1.09
1:E:77:THR:H	2:E:1004:H4B:HN3	1.02	0.94
1:D:27:HIS:HE1	2:D:1006:H4B:H113	1.35	0.90
1:D:29:HIS:CE1	2:D:1006:H4B:H111	2.09	0.87

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	101/115 (88%)	98 (97%)	3 (3%)	0	100 100
1	B	113/115 (98%)	111 (98%)	2 (2%)	0	100 100
1	C	101/115 (88%)	99 (98%)	2 (2%)	0	100 100
1	D	100/115 (87%)	94 (94%)	4 (4%)	2 (2%)	7 4
1	E	113/115 (98%)	110 (97%)	3 (3%)	0	100 100
1	F	101/115 (88%)	99 (98%)	2 (2%)	0	100 100
All	All	629/690 (91%)	611 (97%)	16 (2%)	2 (0%)	41 46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	68	LEU
1	D	67	ASN

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	94/103 (91%)	89 (95%)	5 (5%)	22 27
1	B	103/103 (100%)	101 (98%)	2 (2%)	57 71
1	C	95/103 (92%)	89 (94%)	6 (6%)	18 20
1	D	94/103 (91%)	84 (89%)	10 (11%)	6 6
1	E	103/103 (100%)	100 (97%)	3 (3%)	42 54
1	F	95/103 (92%)	87 (92%)	8 (8%)	11 11
All	All	584/618 (94%)	550 (94%)	34 (6%)	20 23

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	43	ASN
1	F	47	MET
1	F	65	HIS

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Mol	Chain	Res	Type
1	C	96	VAL
1	C	58	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	69	ASN
1	E	29	HIS
1	C	70	ASN
1	F	69	ASN
1	D	67	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)

6 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	A	1003	-	16,18,18	3.90	6 (37%)	11,26,26	2.40	5 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	H4B	F	1005	-	16,18,18	3.81	5 (31%)	11,26,26	2.36	5 (45%)
2	H4B	E	1004	-	16,18,18	3.85	5 (31%)	11,26,26	2.38	5 (45%)
2	H4B	D	1006	-	16,18,18	3.87	5 (31%)	11,26,26	2.43	5 (45%)
2	H4B	B	1001	-	16,18,18	3.86	5 (31%)	11,26,26	2.41	5 (45%)
2	H4B	C	1002	-	16,18,18	3.87	5 (31%)	11,26,26	2.41	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	A	1003	-	1/1/3/5	2/8/17/17	0/2/2/2
2	H4B	F	1005	-	1/1/3/5	2/8/17/17	0/2/2/2
2	H4B	E	1004	-	1/1/3/5	2/8/17/17	0/2/2/2
2	H4B	D	1006	-	1/1/3/5	3/8/17/17	0/2/2/2
2	H4B	B	1001	-	1/1/3/5	2/8/17/17	0/2/2/2
2	H4B	C	1002	-	1/1/3/5	2/8/17/17	0/2/2/2

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1004	H4B	C7-C6	-10.90	1.41	1.52
2	A	1003	H4B	C7-C6	-10.90	1.41	1.52
2	B	1001	H4B	C7-C6	-10.80	1.41	1.52
2	C	1002	H4B	C7-C6	-10.75	1.41	1.52
2	D	1006	H4B	C7-C6	-10.73	1.41	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1006	H4B	C4-C4A-N5	4.94	123.27	119.12
2	B	1001	H4B	C4-C4A-N5	4.70	123.06	119.12
2	E	1004	H4B	C4-C4A-N5	4.70	123.06	119.12
2	C	1002	H4B	C4-C4A-N5	4.61	122.99	119.12
2	A	1003	H4B	C4-C4A-N5	4.61	122.99	119.12

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1003	H4B	C6
2	B	1001	H4B	C6
2	C	1002	H4B	C6
2	D	1006	H4B	C6
2	E	1004	H4B	C6

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1003	H4B	C7-C6-C9-O9
2	A	1003	H4B	C7-C6-C9-C10
2	B	1001	H4B	N5-C6-C9-O9
2	C	1002	H4B	N5-C6-C9-O9
2	C	1002	H4B	N5-C6-C9-C10

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1003	H4B	2	0
2	E	1004	H4B	4	0
2	D	1006	H4B	6	0
2	B	1001	H4B	2	0
2	C	1002	H4B	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	105/115 (91%)	-0.48	1 (0%)	82	81	20, 36, 59, 84	0
1	B	115/115 (100%)	-0.53	4 (3%)	44	42	16, 26, 78, 110	0
1	C	105/115 (91%)	-0.57	1 (0%)	82	81	20, 34, 53, 87	0
1	D	104/115 (90%)	-0.08	2 (1%)	66	65	25, 45, 73, 90	0
1	E	115/115 (100%)	-0.51	1 (0%)	84	83	17, 28, 76, 106	0
1	F	105/115 (91%)	-0.51	3 (2%)	51	49	22, 34, 60, 99	0
All	All	649/690 (94%)	-0.45	12 (1%)	68	66	16, 33, 69, 110	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	HIS	5.5
1	B	22	HIS	4.4
1	B	19	VAL	4.4
1	E	22	HIS	3.8
1	D	27	HIS	3.4

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

There are no monosaccharides in this entry.

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
2	H4B	B	1001	17/17	0.78	0.36	81,96,106,107	0
2	H4B	E	1004	17/17	0.81	0.25	103,107,111,113	0
2	H4B	D	1006	17/17	0.87	0.20	50,62,87,88	0
2	H4B	C	1002	17/17	0.87	0.20	55,67,86,88	0
2	H4B	F	1005	17/17	0.91	0.20	47,62,84,84	0
2	H4B	A	1003	17/17	0.93	0.16	42,58,84,84	0

6.5 Other polymers

There are no such residues in this entry.