wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 06:47 am BST

PDB ID	:	5BZA
Title	:	Crystal structure of CbsA from Thermotoga neapolitana
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Deposited on	:	2015-06-11
Resolution	:	2.00 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:

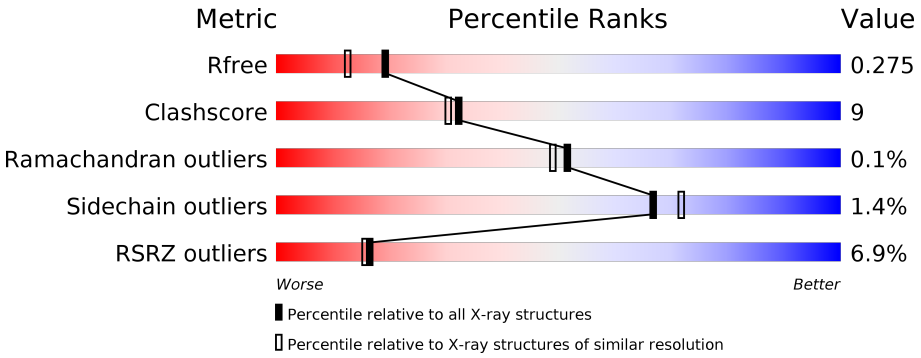
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

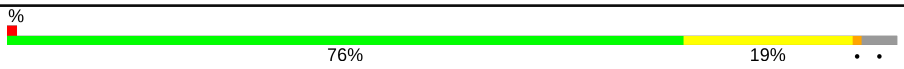
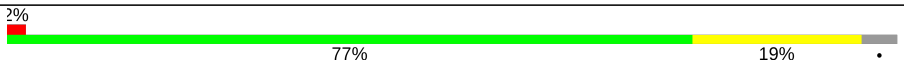
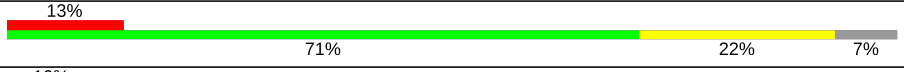
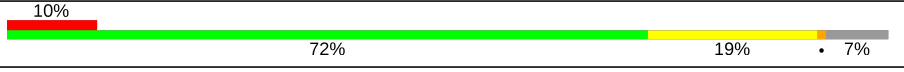
The reported resolution of this entry is 2.00 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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% 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	467	
1	B	467	
1	C	467	
1	D	467	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14692 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 Beta-N-acetylhexosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3559	2291	599	652	17			
1	B	450	Total	C	N	O	S	0	0	0
			3582	2304	602	659	17			
1	C	434	Total	C	N	O	S	0	0	0
			3462	2230	580	636	16			
1	D	432	Total	C	N	O	S	0	0	0
			3429	2216	567	631	15			

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	9	Total	Cd	0	0
			9	9		
2	A	8	Total	Cd	0	0
			8	8		
2	D	7	Total	Cd	0	0
			7	7		
2	C	9	Total	Cd	0	0
			9	9		

- Molecule 3 is water.

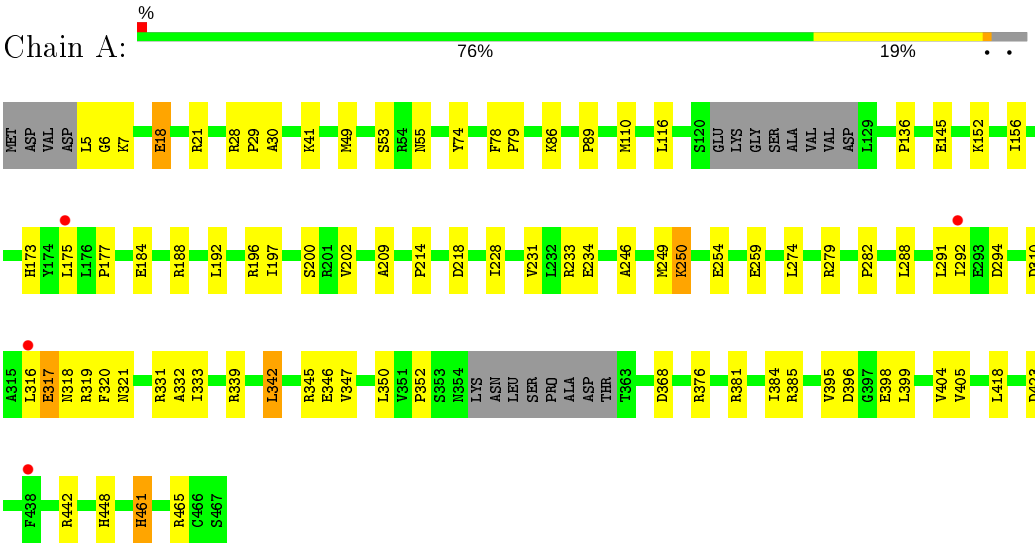
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	170	Total	O	0	0
			170	170		
3	B	221	Total	O	0	0
			221	221		
3	C	113	Total	O	0	0
			113	113		
3	D	123	Total	O	0	0
			123	123		

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 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.

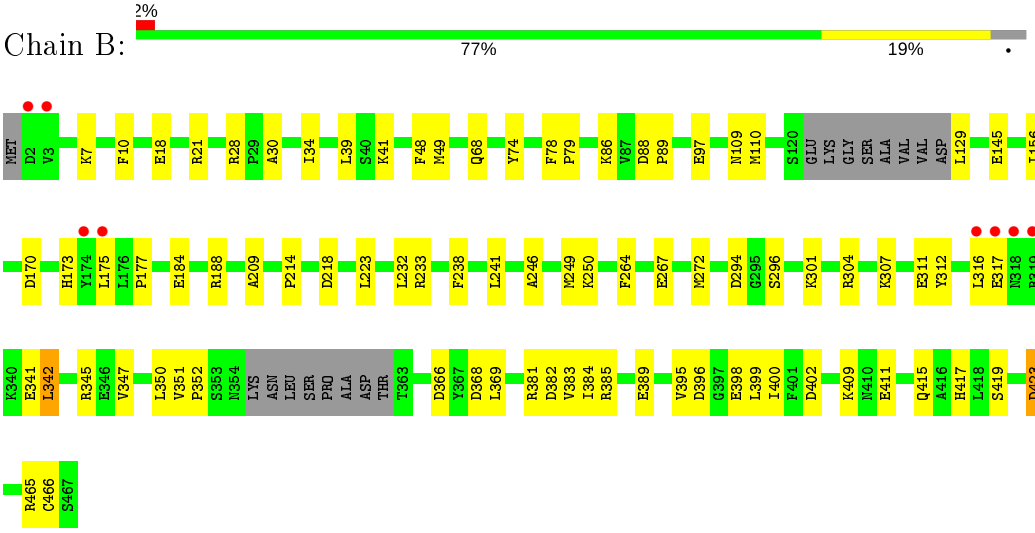
- Molecule 1: Beta-N-acetylhexosaminidase

Chain A:



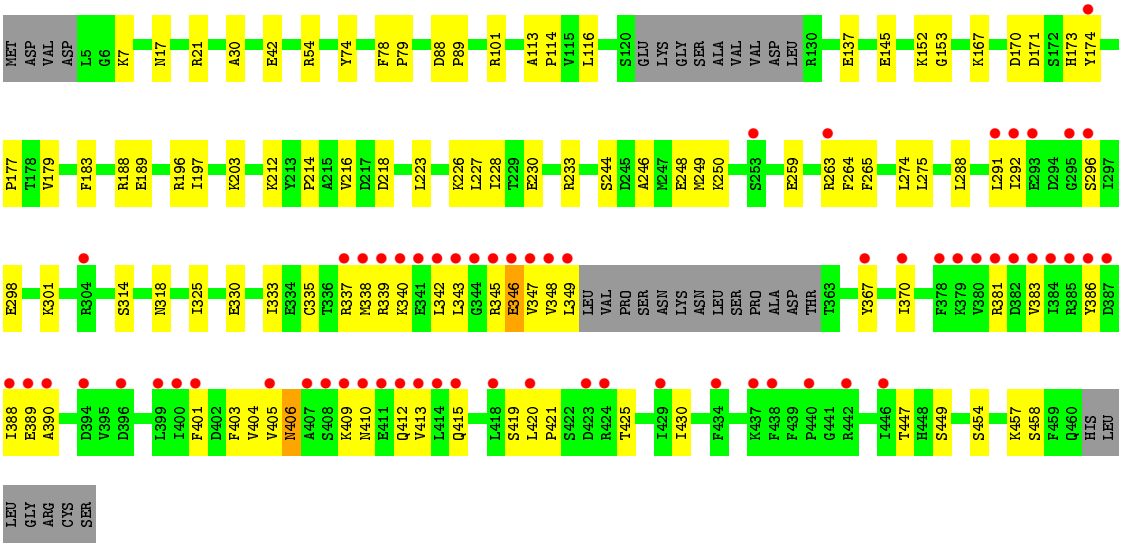
- Molecule 1: Beta-N-acetylhexosaminidase

Chain B:



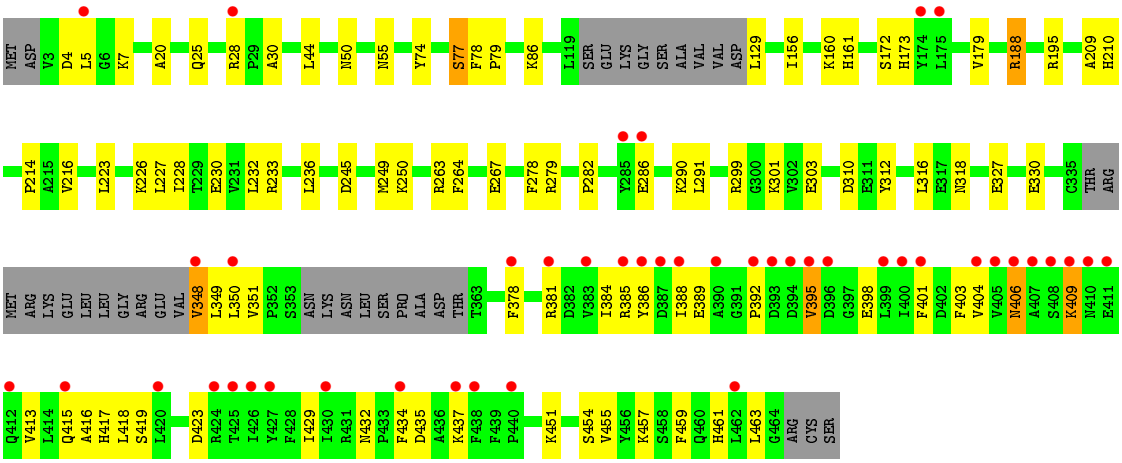
- Molecule 1: Beta-N-acetylhexosaminidase

Chain C:



- Molecule 1: Beta-N-acetylhexosaminidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	158.97Å 158.97Å 517.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.74 – 2.00 39.74 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.8 (39.74-2.00) 93.9 (39.74-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.238 , 0.276 0.239 , 0.275	Depositor DCC
R_{free} test set	2000 reflections (1.26%)	wwPDB-VP
Wilson B-factor (Å^2)	20.3	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14692	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7120e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CD

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	0.71	1/3636 (0.0%)	0.77	4/4906 (0.1%)
1	B	0.71	0/3659	0.76	2/4938 (0.0%)
1	C	0.58	0/3537	0.69	1/4771 (0.0%)
1	D	0.57	0/3505	0.67	2/4734 (0.0%)
All	All	0.65	1/14337 (0.0%)	0.73	9/19349 (0.0%)

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	C	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	GLU	CB-CG	5.09	1.61	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	LEU	CA-CB-CG	6.83	131.02	115.30
1	A	342	LEU	CA-CB-CG	6.07	129.25	115.30
1	D	188	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	D	5	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	342	LEU	CA-CB-CG	5.43	127.78	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	346	GLU	Peptide
1	D	409	LYS	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	A	3559	0	3556	62	1
1	B	3582	0	3573	61	1
1	C	3462	0	3454	64	1
1	D	3429	0	3411	65	1
2	A	8	0	0	0	0
2	B	9	0	0	0	0
2	C	9	0	0	0	0
2	D	7	0	0	0	0
3	A	170	0	0	5	0
3	B	221	0	0	12	0
3	C	113	0	0	4	0
3	D	123	0	0	3	0
All	All	14692	0	13994	247	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 9.

The worst 5 of 247 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:C:337:ARG:NH1	1:C:338:MET:O	1.88	1.06
1:C:389:GLU:O	1:C:409:LYS:NZ	1.89	1.05
1:B:18:GLU:OE1	1:B:21:ARG:NH1	1.94	1.00
1:A:234:GLU:N	3:A:601:HOH:O	2.06	0.89
1:C:420:LEU:HD12	1:C:421:PRO:HD2	1.54	0.89

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:PRO:O	1:D:188:ARG:NH1[4_556]	1.94	0.26
1:B:214:PRO:O	1:C:188:ARG:NH1[18_655]	2.04	0.16

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	441/467 (94%)	427 (97%)	13 (3%)	1 (0%)	47 44
1	B	444/467 (95%)	430 (97%)	13 (3%)	1 (0%)	47 44
1	C	428/467 (92%)	417 (97%)	11 (3%)	0	100 100
1	D	424/467 (91%)	413 (97%)	11 (3%)	0	100 100
All	All	1737/1868 (93%)	1687 (97%)	48 (3%)	2 (0%)	51 49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	317	GLU
1	A	317	GLU

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	389/406 (96%)	385 (99%)	4 (1%)	76 81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	392/406 (97%)	388 (99%)	4 (1%)	76 81
1	C	377/406 (93%)	370 (98%)	7 (2%)	57 61
1	D	374/406 (92%)	368 (98%)	6 (2%)	62 67
All	All	1532/1624 (94%)	1511 (99%)	21 (1%)	67 72

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	335	CYS
1	C	348	VAL
1	D	395	VAL
1	C	314	SER
1	D	406	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	50	ASN
1	D	406	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

Of 33 ligands modelled in this entry, 33 are monoatomic - leaving 0 for Mogul analysis.

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

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

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	447/467 (95%)	-0.05	5 (1%)	80	79	8, 17, 37, 69	0
1	B	450/467 (96%)	-0.04	8 (1%)	68	66	7, 17, 41, 67	0
1	C	434/467 (92%)	0.71	63 (14%)	2	2	10, 32, 117, 152	0
1	D	432/467 (92%)	0.47	45 (10%)	6	5	10, 28, 94, 115	0
All	All	1763/1868 (94%)	0.27	121 (6%)	16	16	7, 22, 89, 152	0

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	343	LEU	9.3
1	C	378	PHE	7.1
1	C	383	VAL	6.3
1	C	399	LEU	5.9
1	D	388	ILE	5.8

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 carbohydrates 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	CD	C	501	1/1	0.49	0.10	134,134,134,134	0
2	CD	C	509	1/1	0.82	0.05	124,124,124,124	0
2	CD	C	507	1/1	0.84	0.11	85,85,85,85	0
2	CD	D	501	1/1	0.86	0.04	83,83,83,83	0
2	CD	B	506	1/1	0.87	0.05	105,105,105,105	0
2	CD	D	507	1/1	0.88	0.04	116,116,116,116	0
2	CD	B	509	1/1	0.90	0.04	98,98,98,98	0
2	CD	C	506	1/1	0.91	0.03	119,119,119,119	0
2	CD	B	505	1/1	0.92	0.04	119,119,119,119	0
2	CD	C	504	1/1	0.92	0.05	105,105,105,105	0
2	CD	A	503	1/1	0.92	0.09	115,115,115,115	0
2	CD	C	508	1/1	0.92	0.07	88,88,88,88	0
2	CD	B	504	1/1	0.93	0.07	105,105,105,105	0
2	CD	A	507	1/1	0.94	0.05	78,78,78,78	0
2	CD	A	508	1/1	0.95	0.06	95,95,95,95	0
2	CD	D	503	1/1	0.95	0.06	65,65,65,65	0
2	CD	D	505	1/1	0.96	0.03	99,99,99,99	0
2	CD	B	507	1/1	0.96	0.09	71,71,71,71	0
2	CD	A	501	1/1	0.96	0.14	64,64,64,64	0
2	CD	A	504	1/1	0.97	0.03	98,98,98,98	0
2	CD	A	502	1/1	0.97	0.07	69,69,69,69	0
2	CD	C	503	1/1	0.97	0.08	74,74,74,74	0
2	CD	B	501	1/1	0.97	0.04	74,74,74,74	0
2	CD	C	502	1/1	0.97	0.10	52,52,52,52	0
2	CD	B	502	1/1	0.98	0.13	48,48,48,48	0
2	CD	D	506	1/1	0.98	0.10	74,74,74,74	0
2	CD	B	503	1/1	0.99	0.07	56,56,56,56	0
2	CD	D	502	1/1	0.99	0.11	46,46,46,46	0
2	CD	A	506	1/1	0.99	0.11	21,21,21,21	0
2	CD	B	508	1/1	0.99	0.09	26,26,26,26	0
2	CD	C	505	1/1	0.99	0.12	20,20,20,20	0
2	CD	A	505	1/1	0.99	0.09	60,60,60,60	0
2	CD	D	504	1/1	1.00	0.10	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.