



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 29, 2025 – 05:21 AM EDT

PDB ID : 3R6Q / pdb\_00003r6q  
Title : A triclinic-lattice structure of aspartase from Bacillus sp. YM55-1  
Authors : Fibriansah, G.; Puthan Veetil, V.; Poelarends, G.J.; Thunnissen, A.-M.W.H.  
Deposited on : 2011-03-22  
Resolution : 2.40 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

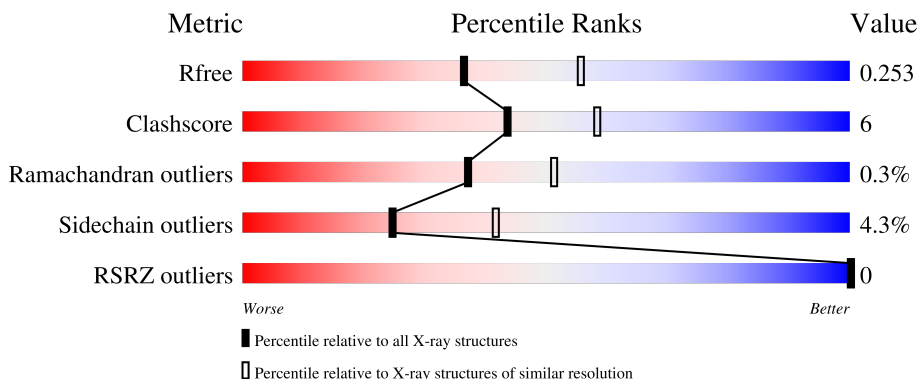
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	468	 82% 15% ..
1	B	468	 87% 12% .
1	C	468	 82% 16% ..
1	D	468	 85% 12% ..
1	E	468	 83% 16% .

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Mol	Chain	Length	Quality of chain
1	F	468	 84%13%..
1	G	468	 83%15%..
1	H	468	 81%17%..

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29459 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 Aspartase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	2	0
			3583	2262	605	694	22			
1	B	462	Total	C	N	O	S	0	0	0
			3568	2253	604	689	22			
1	C	462	Total	C	N	O	S	0	0	0
			3568	2253	604	689	22			
1	D	462	Total	C	N	O	S	0	0	0
			3568	2253	604	689	22			
1	E	462	Total	C	N	O	S	0	0	0
			3568	2253	604	689	22			
1	F	463	Total	C	N	O	S	0	0	0
			3576	2257	605	692	22			
1	G	462	Total	C	N	O	S	0	0	0
			3568	2253	604	689	22			
1	H	462	Total	C	N	O	S	0	0	0
			3568	2253	604	689	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	460	ILE	THR	conflict	UNP Q9LCC6
B	460	ILE	THR	conflict	UNP Q9LCC6
C	460	ILE	THR	conflict	UNP Q9LCC6
D	460	ILE	THR	conflict	UNP Q9LCC6
E	460	ILE	THR	conflict	UNP Q9LCC6
F	460	ILE	THR	conflict	UNP Q9LCC6
G	460	ILE	THR	conflict	UNP Q9LCC6
H	460	ILE	THR	conflict	UNP Q9LCC6

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0
2	D	1	Total 1	Ca 1	0	0
2	E	1	Total 1	Ca 1	0	0
2	H	1	Total 1	Ca 1	0	0

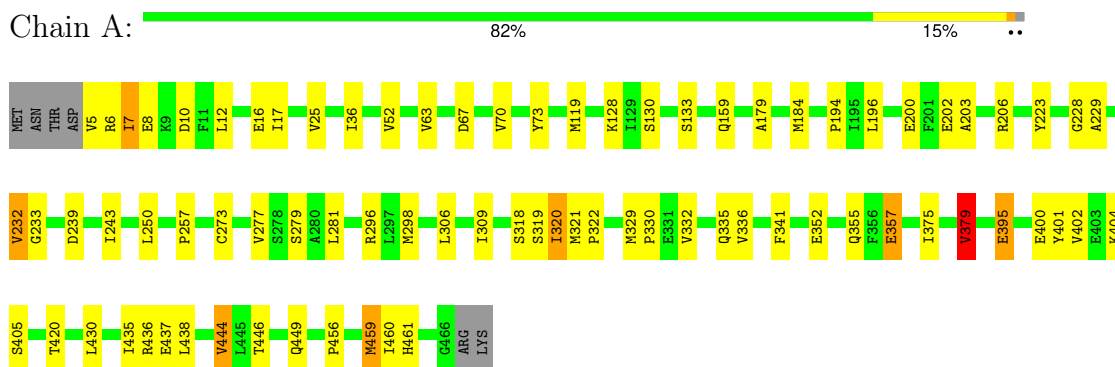
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total 128	O 128	0	0
3	B	104	Total 104	O 104	0	0
3	C	103	Total 103	O 103	0	0
3	D	128	Total 128	O 128	0	0
3	E	109	Total 109	O 109	0	0
3	F	113	Total 113	O 113	0	0
3	G	90	Total 90	O 90	0	0
3	H	113	Total 113	O 113	0	0

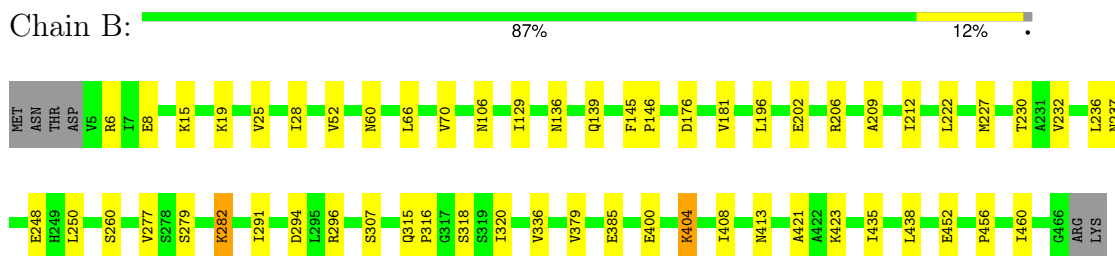
### 3 Residue-property plots [i](#)

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 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.

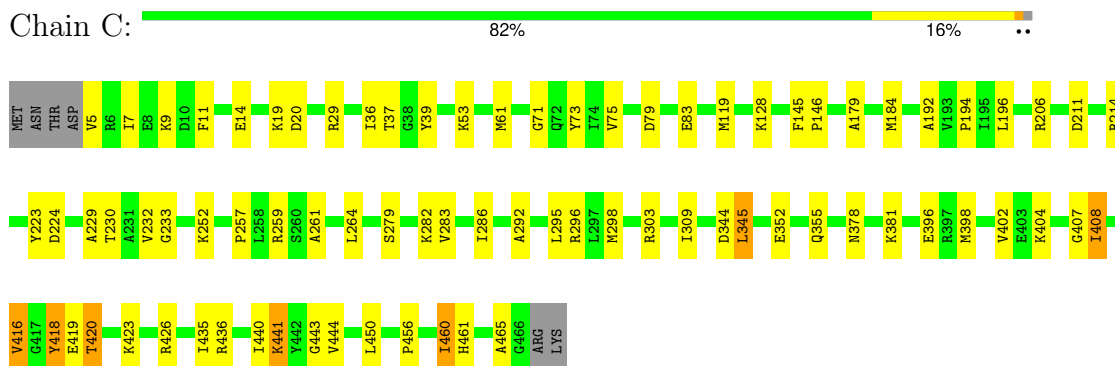
- Molecule 1: Aspartase



- Molecule 1: Aspartase



- Molecule 1: Aspartase

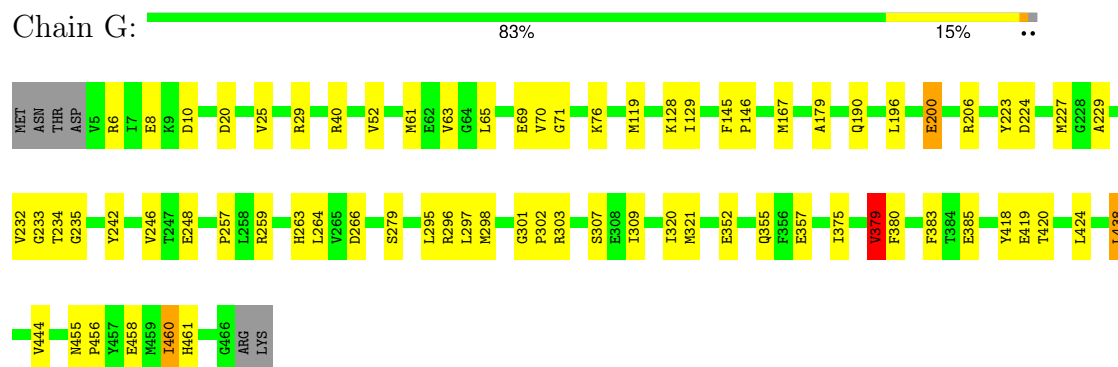


- Molecule 1: Aspartase

- Molecule 1: Aspartase

- Molecule 1: Aspartase

- Molecule 1: Aspartase



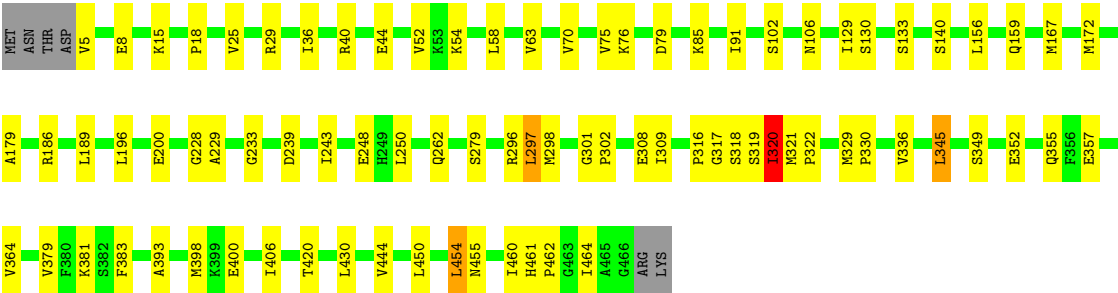
● Molecule 1: Aspartase

Chain H: 

81%

17%

..





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.59Å 118.19Å 140.23Å 89.85° 89.59° 76.51°	Depositor
Resolution (Å)	39.56 – 2.40 39.56 – 2.40	Depositor EDS
% Data completeness (in resolution range)	87.7 (39.56-2.40) 85.9 (39.56-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.199 , 0.253 0.200 , 0.253	Depositor DCC
$R_{free}$ test set	8118 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 11.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.438 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	29459	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.63	0/3645	0.89	2/4932 (0.0%)
1	B	0.63	0/3627	0.89	1/4908 (0.0%)
1	C	0.62	0/3627	0.91	0/4908
1	D	0.63	0/3627	0.89	2/4908 (0.0%)
1	E	0.64	1/3627 (0.0%)	0.90	2/4908 (0.0%)
1	F	0.62	0/3635	0.90	0/4919
1	G	0.60	0/3627	0.91	2/4908 (0.0%)
1	H	0.65	0/3627	0.90	2/4908 (0.0%)
All	All	0.63	1/29042 (0.0%)	0.90	11/39299 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	464	ILE	CA-CB	5.03	1.59	1.54

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	ILE	N-CA-C	7.15	117.22	106.42
1	D	379	VAL	CB-CA-C	-6.95	102.63	112.22
1	A	379	VAL	CB-CA-C	-6.17	103.71	112.22
1	E	362	GLU	CA-C-N	-5.83	112.49	118.85
1	E	362	GLU	C-N-CA	-5.83	112.49	118.85

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	3583	0	3596	52	0
1	B	3568	0	3585	34	0
1	C	3568	0	3585	53	0
1	D	3568	0	3585	46	0
1	E	3568	0	3585	52	0
1	F	3576	0	3589	47	0
1	G	3568	0	3585	42	0
1	H	3568	0	3585	64	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	H	1	0	0	0	0
3	A	128	0	0	0	0
3	B	104	0	0	0	0
3	C	103	0	0	2	0
3	D	128	0	0	1	0
3	E	109	0	0	0	0
3	F	113	0	0	1	0
3	G	90	0	0	1	0
3	H	113	0	0	1	0
All	All	29459	0	28695	342	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 6.

The worst 5 of 342 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:218:THR:HG23	1:D:277:VAL:HG22	1.27	1.11
1:H:336:VAL:HG21	1:H:379:VAL:HG11	1.35	1.08
1:E:184:MET:CE	1:E:402:VAL:HA	1.93	0.98
1:E:318:SER:HB2	1:E:321:MET:HB3	1.48	0.92
1:D:218:THR:CG2	1:D:277:VAL:HG22	2.01	0.90

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	462/468 (99%)	439 (95%)	21 (4%)	2 (0%)	30	44
1	B	460/468 (98%)	446 (97%)	12 (3%)	2 (0%)	30	44
1	C	460/468 (98%)	444 (96%)	13 (3%)	3 (1%)	19	29
1	D	460/468 (98%)	447 (97%)	12 (3%)	1 (0%)	44	59
1	E	460/468 (98%)	446 (97%)	13 (3%)	1 (0%)	44	59
1	F	461/468 (98%)	446 (97%)	14 (3%)	1 (0%)	44	59
1	G	460/468 (98%)	450 (98%)	10 (2%)	0	100	100
1	H	460/468 (98%)	445 (97%)	13 (3%)	2 (0%)	30	44
All	All	3683/3744 (98%)	3563 (97%)	108 (3%)	12 (0%)	37	51

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	408	ILE
1	C	465	ALA
1	B	408	ILE
1	H	464	ILE
1	B	230	THR

### 5.3.2 Protein sidechains

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	390/394 (99%)	375 (96%)	15 (4%)	28	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	388/394 (98%)	374 (96%)	14 (4%)	30	49
1	C	388/394 (98%)	370 (95%)	18 (5%)	23	39
1	D	388/394 (98%)	373 (96%)	15 (4%)	27	46
1	E	388/394 (98%)	368 (95%)	20 (5%)	19	34
1	F	389/394 (99%)	374 (96%)	15 (4%)	27	46
1	G	388/394 (98%)	371 (96%)	17 (4%)	24	41
1	H	388/394 (98%)	367 (95%)	21 (5%)	18	32
All	All	3107/3152 (99%)	2972 (96%)	135 (4%)	25	42

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	58	LEU
1	H	140	SER
1	H	406	ILE
1	D	29	ARG
1	D	9	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	415	HIS
1	G	26	GLN
1	H	169	GLN
1	C	461	HIS
1	C	451	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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	462/468 (98%)	-1.71	0 100 100	7, 20, 71, 79	2 (0%)
1	B	462/468 (98%)	-1.74	0 100 100	10, 26, 49, 69	0
1	C	462/468 (98%)	-1.68	0 100 100	8, 28, 55, 70	0
1	D	462/468 (98%)	-1.78	0 100 100	7, 21, 47, 60	0
1	E	462/468 (98%)	-1.75	0 100 100	8, 20, 70, 76	0
1	F	463/468 (98%)	-1.76	0 100 100	8, 26, 47, 66	0
1	G	462/468 (98%)	-1.72	0 100 100	8, 27, 53, 66	0
1	H	462/468 (98%)	-1.78	0 100 100	6, 22, 47, 60	0
All	All	3697/3744 (98%)	-1.74	0 100 100	6, 23, 56, 79	2 (0%)

There are no RSRZ outliers to report.

### 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 monosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	CA	A	469	1/1	0.99	0.03	42,42,42,42	0
2	CA	D	469	1/1	1.00	0.02	31,31,31,31	0
2	CA	E	469	1/1	1.00	0.02	38,38,38,38	0
2	CA	H	469	1/1	1.00	0.02	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.