



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 08:59 pm GMT

PDB ID : 1HL9  
Title : CRYSTAL STRUCTURE OF THERMOTOGA MARITIMA ALPHA-FUCOSIDASE IN COMPLEX WITH A MECHANISM BASED INHIBITOR  
Authors : Sulzenbacher, G.; Bignon, C.; Bourne, Y.; Henrissat, B.  
Deposited on : 2003-03-14  
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 4.02b-467  
Mogul : 1.8.4, 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

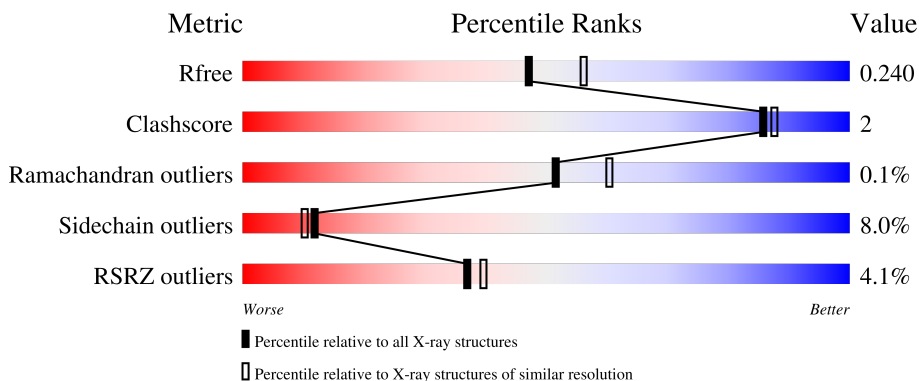
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	449	 2% 81% 11% • 6%
1	B	449	 6% 81% 13% • 5%

## 2 Entry composition [i](#)

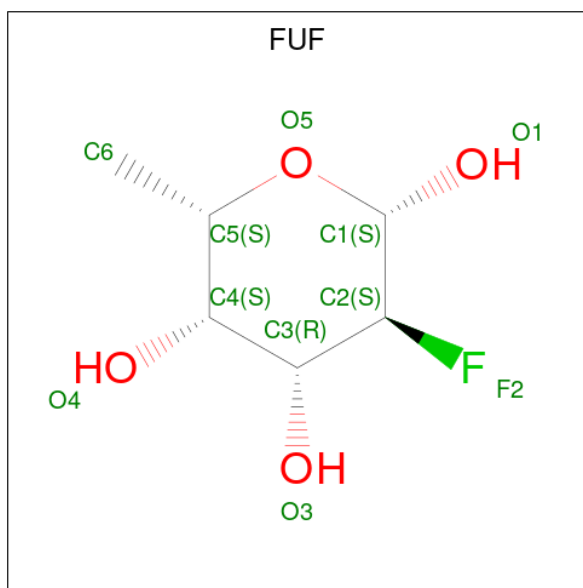
There are 3 unique types of molecules in this entry. The entry contains 7280 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PUTATIVE ALPHA-L-FUCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	421	Total 3490	C 2276	N 573	O 634	S 7	0	0	0
1	B	427	Total 3539	C 2308	N 583	O 641	S 7	0	0	0

- Molecule 2 is 2-deoxy-2-fluoro-beta-L-fucopyranose (three-letter code: FUF) (formula: C<sub>6</sub>H<sub>11</sub>FO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	O		
2	A	1	Total 21	C 12	F 2	O 7	0	1
2	B	1	Total 21	C 12	F 2	O 7	0	1

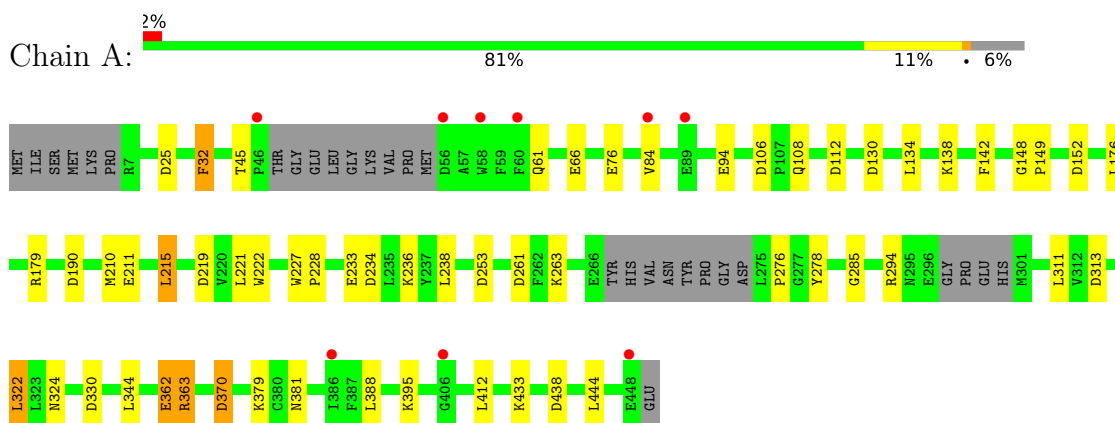
- Molecule 3 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	118	Total 118	O 118	0	0
3	B	91	Total 91	O 91	0	0

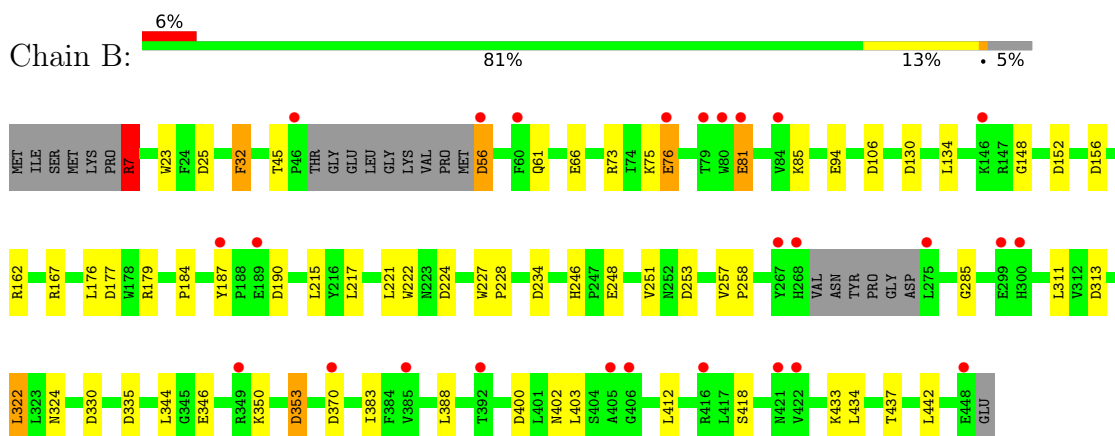
### 3 Residue-property plots [i](#)

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: PUTATIVE ALPHA-L-FUCOSIDASE



- Molecule 1: PUTATIVE ALPHA-L-FUCOSIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.16Å 172.16Å 167.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.25 20.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	90.8 (20.00-2.25) 88.8 (20.00-2.25)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.03 (at 2.26Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.181 , 0.229 0.201 , 0.240	Depositor DCC
$R_{free}$ test set	2918 reflections (7.28%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtrriage
Anisotropy	0.021	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7280	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.47	0/3587	0.78	13/4867 (0.3%)
1	B	0.46	1/3644 (0.0%)	0.76	16/4947 (0.3%)
All	All	0.47	1/7231 (0.0%)	0.77	29/9814 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	GLU	CD-OE2	5.19	1.31	1.25

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	B	313	ASP	CB-CG-OD2	7.08	124.67	118.30
1	A	330	ASP	CB-CG-OD2	7.05	124.65	118.30
1	A	130	ASP	CB-CG-OD2	6.66	124.29	118.30
1	A	370	ASP	CB-CG-OD2	6.56	124.20	118.30
1	A	219	ASP	CB-CG-OD2	6.46	124.11	118.30
1	B	177	ASP	CB-CG-OD2	6.27	123.95	118.30
1	A	152	ASP	CB-CG-OD2	6.23	123.91	118.30
1	B	330	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	353	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	25	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	234	ASP	CB-CG-OD2	5.96	123.66	118.30
1	B	162	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	234	ASP	CB-CG-OD2	5.89	123.61	118.30
1	B	152	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	190	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	156	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	106	ASP	CB-CG-OD2	5.68	123.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	370	ASP	CB-CG-OD2	5.66	123.40	118.30
1	B	335	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	253	ASP	CB-CG-OD2	5.46	123.21	118.30
1	B	130	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	313	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	438	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	190	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	261	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	56	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	253	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	106	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3490	0	3363	14	0
1	B	3539	0	3402	17	0
2	A	21	0	20	0	0
2	B	21	0	20	1	0
3	A	118	0	0	0	0
3	B	91	0	0	1	0
All	All	7280	0	6805	31	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 2.

All (31) 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:A:362:GLU:OE1	1:A:363:ARG:HD2	1.68	0.93
1:A:233:GLU:OE1	1:A:236:LYS:NZ	2.16	0.77
1:A:362:GLU:OE1	1:A:363:ARG:CD	2.35	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:LEU:HD23	1:B:437:THR:HG22	1.70	0.72
1:A:32:PHE:CD2	1:A:322:LEU:HD13	2.32	0.64
1:B:434:LEU:O	1:B:437:THR:HB	2.01	0.60
1:B:94:GLU:OE1	1:B:179:ARG:NH1	2.38	0.57
1:B:248:GLU:H	1:B:248:GLU:CD	2.06	0.57
1:B:7:ARG:HH11	1:B:7:ARG:CG	2.18	0.56
1:B:7:ARG:HH11	1:B:7:ARG:HG2	1.72	0.55
1:B:412:LEU:HD23	1:B:437:THR:CG2	2.37	0.54
1:B:75:LYS:O	1:B:76:GLU:HB2	2.07	0.54
1:A:210:MET:SD	1:A:238:LEU:HD23	2.50	0.51
1:A:179:ARG:HH21	1:A:179:ARG:HG3	1.79	0.47
1:A:211:GLU:HG2	1:A:215:LEU:HD22	1.95	0.47
1:B:257:VAL:HB	1:B:258:PRO:CD	2.45	0.46
1:A:84:VAL:O	1:A:84:VAL:HG12	2.17	0.45
1:B:350:LYS:NZ	3:B:2083:HOH:O	2.46	0.45
1:A:276:PRO:HB3	1:A:278:TYR:CE2	2.53	0.44
1:A:285:GLY:HA2	1:A:324:ASN:HB3	1.99	0.44
1:B:73:ARG:HB2	1:B:184:PRO:HB3	2.00	0.43
1:B:246:HIS:ND1	1:B:248:GLU:OE1	2.52	0.43
1:A:142:PHE:CE2	1:A:179:ARG:HD3	2.54	0.43
1:A:61:GLN:HE21	1:A:61:GLN:HB3	1.66	0.42
1:A:148:GLY:HA3	1:A:149:PRO:HD3	1.96	0.41
1:A:227:TRP:CG	1:A:228:PRO:HD2	2.55	0.41
1:B:32:PHE:CD2	1:B:322:LEU:HD13	2.56	0.41
1:B:224:ASP:OD1	2:B:1449[A]:FUF:H2	2.21	0.41
1:B:285:GLY:HA2	1:B:324:ASN:HB3	2.02	0.41
1:B:227:TRP:CG	1:B:228:PRO:HD2	2.55	0.40
1:B:23:TRP:CE3	1:B:167:ARG:HD2	2.55	0.40

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	412/449 (92%)	395 (96%)	17 (4%)	0	100	100
1	B	420/449 (94%)	403 (96%)	16 (4%)	1 (0%)	47	55
All	All	832/898 (93%)	798 (96%)	33 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	GLY

### 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	364/388 (94%)	336 (92%)	28 (8%)	13	11
1	B	369/388 (95%)	338 (92%)	31 (8%)	11	9
All	All	733/776 (94%)	674 (92%)	59 (8%)	12	10

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	PHE
1	A	45	THR
1	A	66	GLU
1	A	76	GLU
1	A	94	GLU
1	A	108	GLN
1	A	112	ASP
1	A	134	LEU
1	A	138	LYS
1	A	176	LEU
1	A	215	LEU
1	A	221	LEU
1	A	222	TRP
1	A	263	LYS
1	A	294	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	311	LEU
1	A	322	LEU
1	A	344	LEU
1	A	362	GLU
1	A	363	ARG
1	A	370	ASP
1	A	379	LYS
1	A	381	ASN
1	A	388	LEU
1	A	395	LYS
1	A	412	LEU
1	A	433	LYS
1	A	444	LEU
1	B	7	ARG
1	B	25	ASP
1	B	32	PHE
1	B	45	THR
1	B	56	ASP
1	B	61	GLN
1	B	66	GLU
1	B	76	GLU
1	B	81	GLU
1	B	85	LYS
1	B	134	LEU
1	B	176	LEU
1	B	187	TYR
1	B	215	LEU
1	B	217	LEU
1	B	221	LEU
1	B	222	TRP
1	B	251	VAL
1	B	311	LEU
1	B	322	LEU
1	B	344	LEU
1	B	346	GLU
1	B	353	ASP
1	B	383	ILE
1	B	388	LEU
1	B	400	ASP
1	B	402	ASN
1	B	403	LEU
1	B	418	SER

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Mol	Chain	Res	Type
1	B	433	LYS
1	B	442	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	90	ASN
1	A	108	GLN
1	A	402	ASN
1	B	61	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	KCX	A	338	1	9,11,12	1.01	0	5,12,14	0.65	0
1	KCX	B	338	1	7,8,12	0.56	0	3,8,14	0.56	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
1	KCX	A	338	1	-	1/9/10/12	-
1	KCX	B	338	1	-	0/6/7/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	338	KCX	CG-CD-CE-NZ

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	FUF	B	1449[A]	-	11,11,11	1.15	1 (9%)	14,16,16	0.81	1 (7%)
2	FUF	A	1449[A]	-	11,11,11	1.35	2 (18%)	14,16,16	0.96	1 (7%)
2	FUF	B	1449[B]	1	10,10,11	1.08	1 (10%)	9,14,16	1.82	2 (22%)
2	FUF	A	1449[B]	1	10,10,11	1.12	1 (10%)	9,14,16	1.94	2 (22%)

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	FUF	B	1449[A]	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUF	A	1449[A]	-	-	-	0/1/1/1
2	FUF	B	1449[B]	1	-	-	0/1/1/1
2	FUF	A	1449[B]	1	-	-	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1449[A]	FUF	C2-C3	3.09	1.55	1.52
2	B	1449[A]	FUF	C2-C3	2.61	1.54	1.52
2	A	1449[B]	FUF	C1-C2	2.35	1.55	1.52
2	A	1449[A]	FUF	C2-C1	2.15	1.54	1.52
2	B	1449[B]	FUF	C1-C2	2.05	1.55	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1449[B]	FUF	O5-C5-C4	4.93	118.36	109.52
2	B	1449[B]	FUF	O5-C5-C4	4.28	117.20	109.52
2	A	1449[B]	FUF	C1-O5-C5	2.54	118.54	112.78
2	B	1449[B]	FUF	C1-O5-C5	2.44	118.31	112.78
2	A	1449[A]	FUF	F2-C2-C3	2.24	110.84	108.85
2	B	1449[A]	FUF	F2-C2-C3	2.05	110.67	108.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1449[A]	FUF	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<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	420/449 (93%)	-0.17	9 (2%) 63 66	22, 36, 59, 75	0
1	B	426/449 (94%)	0.10	26 (6%) 21 23	25, 43, 77, 93	0
All	All	846/898 (94%)	-0.03	35 (4%) 37 40	22, 39, 72, 93	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	405	ALA	5.9
1	B	268	HIS	5.5
1	B	267	TYR	5.4
1	A	56	ASP	4.5
1	B	46	PRO	3.8
1	A	84	VAL	3.8
1	B	84	VAL	3.6
1	B	300	HIS	3.4
1	B	76	GLU	3.4
1	A	406	GLY	3.2
1	B	299	GLU	3.1
1	A	46	PRO	3.0
1	B	80	TRP	3.0
1	B	416	ARG	3.0
1	B	60	PHE	3.0
1	B	189	GLU	2.9
1	A	58	TRP	2.9
1	B	56	ASP	2.8
1	B	275	LEU	2.7
1	A	448	GLU	2.7
1	B	406	GLY	2.7
1	B	392	THR	2.5
1	B	421	ASN	2.5
1	B	81	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	370	ASP	2.3
1	B	385	VAL	2.2
1	B	422	VAL	2.2
1	B	79	THR	2.1
1	B	146	LYS	2.1
1	A	60	PHE	2.1
1	B	187	TYR	2.1
1	A	386	ILE	2.1
1	B	349	ARG	2.1
1	A	89	GLU	2.0
1	B	448	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	KCX	B	338	9/13	0.91	0.16	45,48,56,60	0
1	KCX	A	338	12/13	0.92	0.10	48,53,57,58	0

## 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(Å <sup>2</sup> )	Q<0.9
2	FUF	A	1449[A]	11/11	0.91	0.18	35,36,37,37	11
2	FUF	A	1449[B]	10/11	0.91	0.18	35,36,37,37	10
2	FUF	B	1449[A]	11/11	0.94	0.12	37,38,38,39	11
2	FUF	B	1449[B]	10/11	0.94	0.12	36,38,39,40	10



## 6.5 Other polymers [i](#)

There are no such residues in this entry.