



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 08:52 AM BST

PDB ID : 1OIN  
Title : Family 1 b-glucosidase from *Thermotoga maritima*  
Authors : Gloster, T.; Zechel, D.L.; Boraston, A.B.; Boraston, C.M.; Macdonald, J.M.;  
Tilbrook, D.M.; Stick, R.V.; Davies, G.J.  
Deposited on : 2003-06-19  
Resolution : 2.15 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1  
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) : 2.13.1

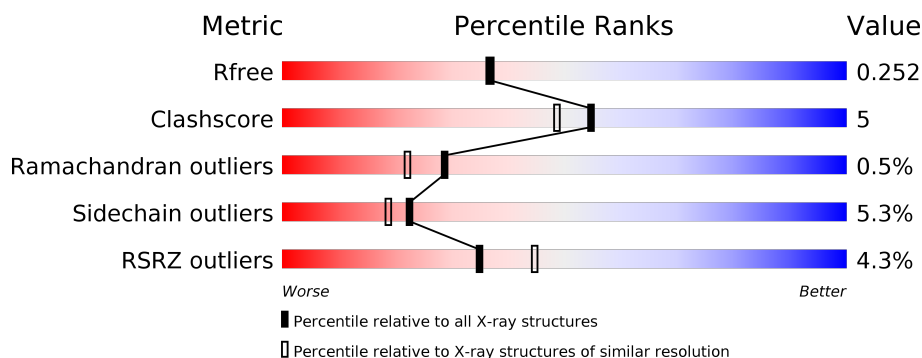
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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  $\geq 3$ , 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	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>• 6%</div> </div> </div>
1	B	468	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• 5%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7550 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-GLUCOSIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	1	0
			3576	2326	603	641	6			
1	B	443	Total	C	N	O	S	0	0	0
			3539	2302	590	641	6			

There are 46 discrepancies between the modelled and reference sequences:

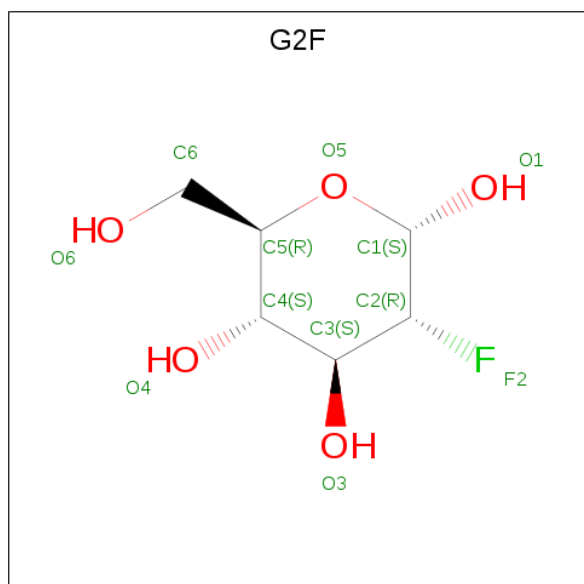
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q08638
A	-20	GLY	-	expression tag	UNP Q08638
A	-19	SER	-	expression tag	UNP Q08638
A	-18	SER	-	expression tag	UNP Q08638
A	-17	HIS	-	expression tag	UNP Q08638
A	-16	HIS	-	expression tag	UNP Q08638
A	-15	HIS	-	expression tag	UNP Q08638
A	-14	HIS	-	expression tag	UNP Q08638
A	-13	HIS	-	expression tag	UNP Q08638
A	-12	HIS	-	expression tag	UNP Q08638
A	-11	SER	-	expression tag	UNP Q08638
A	-10	SER	-	expression tag	UNP Q08638
A	-9	GLY	-	expression tag	UNP Q08638
A	-8	LEU	-	expression tag	UNP Q08638
A	-7	VAL	-	expression tag	UNP Q08638
A	-6	PRO	-	expression tag	UNP Q08638
A	-5	ARG	-	expression tag	UNP Q08638
A	-4	GLY	-	expression tag	UNP Q08638
A	-3	SER	-	expression tag	UNP Q08638
A	-2	HIS	-	expression tag	UNP Q08638
A	-1	MET	-	expression tag	UNP Q08638
A	0	ALA	-	expression tag	UNP Q08638
A	1	SER	-	expression tag	UNP Q08638
B	-21	MET	-	expression tag	UNP Q08638
B	-20	GLY	-	expression tag	UNP Q08638

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	SER	-	expression tag	UNP Q08638
B	-18	SER	-	expression tag	UNP Q08638
B	-17	HIS	-	expression tag	UNP Q08638
B	-16	HIS	-	expression tag	UNP Q08638
B	-15	HIS	-	expression tag	UNP Q08638
B	-14	HIS	-	expression tag	UNP Q08638
B	-13	HIS	-	expression tag	UNP Q08638
B	-12	HIS	-	expression tag	UNP Q08638
B	-11	SER	-	expression tag	UNP Q08638
B	-10	SER	-	expression tag	UNP Q08638
B	-9	GLY	-	expression tag	UNP Q08638
B	-8	LEU	-	expression tag	UNP Q08638
B	-7	VAL	-	expression tag	UNP Q08638
B	-6	PRO	-	expression tag	UNP Q08638
B	-5	ARG	-	expression tag	UNP Q08638
B	-4	GLY	-	expression tag	UNP Q08638
B	-3	SER	-	expression tag	UNP Q08638
B	-2	HIS	-	expression tag	UNP Q08638
B	-1	MET	-	expression tag	UNP Q08638
B	0	ALA	-	expression tag	UNP Q08638
B	1	SER	-	expression tag	UNP Q08638

- Molecule 2 is 2-deoxy-2-fluoro-alpha-D-glucopyranose (three-letter code: G2F) (formula:  $C_6H_{11}FO_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	O	0	0
			11	6	1	4		
2	B	1	Total	C	F	O	0	0
			11	6	1	4		

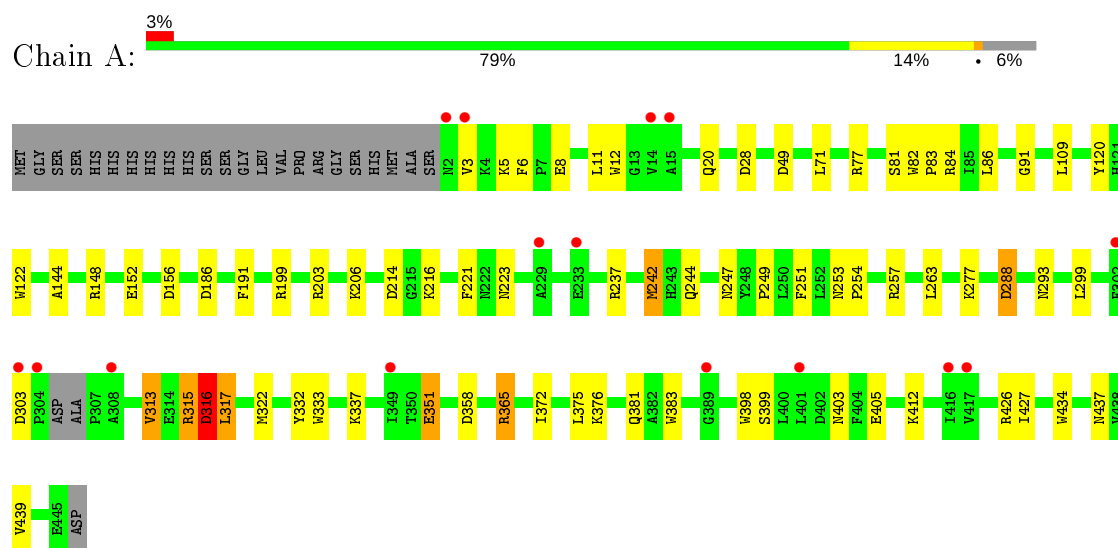
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	224	Total	O	0	0
			224	224		
3	B	189	Total	O	0	0
			189	189		

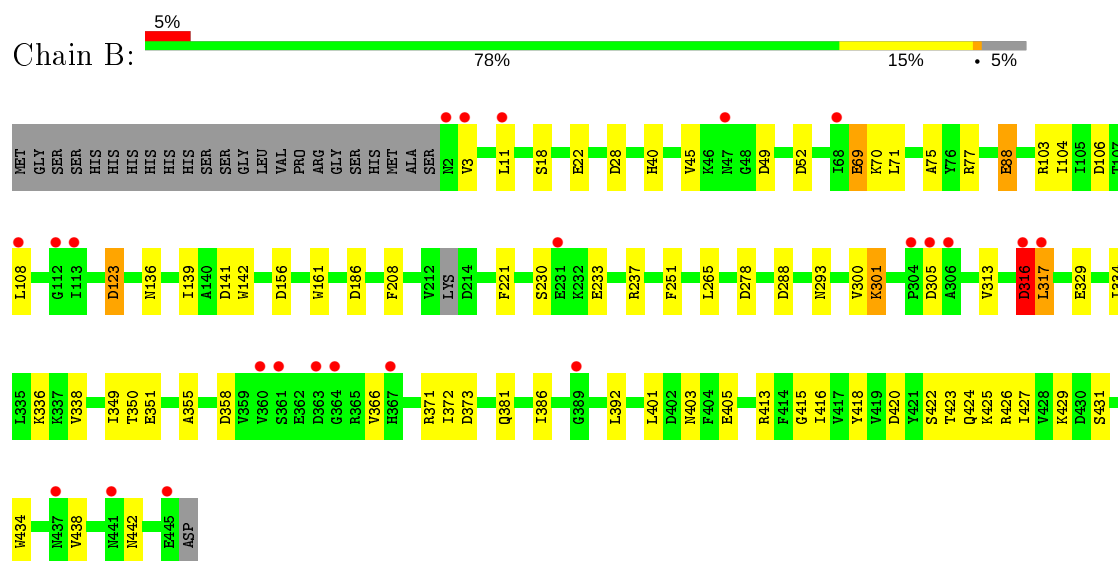
### 3 Residue-property plots [i](#)

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: BETA-GLUCOSIDASE A



#### • Molecule 1: BETA-GLUCOSIDASE A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.91Å 94.98Å 113.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.55 – 2.15 24.43 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (72.55-2.15) 99.7 (24.43-2.15)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.41 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.201 , 0.256 0.199 , 0.252	Depositor DCC
$R_{free}$ test set	2878 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7550	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: G2F

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	0.91	3/3692 (0.1%)	0.90	9/5019 (0.2%)
1	B	0.87	0/3651	0.90	12/4974 (0.2%)
All	All	0.89	3/7343 (0.0%)	0.90	21/9993 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	TYR	CE2-CZ	6.16	1.46	1.38
1	A	351	GLU	CD-OE2	5.22	1.31	1.25
1	A	191	PHE	CE2-CZ	5.05	1.47	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ASP	CB-CG-OD2	7.05	124.64	118.30
1	A	49	ASP	CB-CG-OD2	6.96	124.56	118.30
1	B	316	ASP	CB-CG-OD2	6.62	124.26	118.30
1	B	278	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	49	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	28	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	186	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	365	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	186	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	358	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	288	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	305	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	52	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	214	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	156	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	156	ASP	CB-CG-OD2	5.28	123.06	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	373	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	106	ASP	CB-CG-OD2	5.18	122.97	118.30
1	B	141	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	28	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	199	ARG	NE-CZ-NH1	5.14	122.87	120.30

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	3576	0	3386	35	1
1	B	3539	0	3295	37	0
2	A	11	0	9	0	0
2	B	11	0	9	0	0
3	A	224	0	0	1	0
3	B	189	0	0	3	0
All	All	7550	0	6699	72	1

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 5.

All (72) 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:242:MET:CE	1:A:242:MET:HA	2.01	0.91
1:A:244:GLN:HE22	1:A:263:LEU:H	1.20	0.83
1:A:242:MET:HA	1:A:242:MET:HE3	1.71	0.73
1:A:242:MET:HA	1:A:242:MET:HE2	1.70	0.73
1:A:144:ALA:HB2	1:A:203[A]:ARG:HG2	1.72	0.69
1:B:104:ILE:O	1:B:108:LEU:HD12	1.95	0.67
1:A:244:GLN:NE2	1:A:263:LEU:H	1.95	0.65
1:B:371:ARG:HH12	1:B:429:LYS:NZ	1.95	0.63
1:A:426:ARG:O	1:A:427:ILE:HD13	1.99	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LEU:HG	1:B:75:ALA:HB2	1.85	0.59
1:B:88:GLU:HG2	3:B:2053:HOH:O	2.01	0.58
1:A:148:ARG:O	1:A:152:GLU:HG2	2.03	0.58
1:B:371:ARG:HH12	1:B:429:LYS:HZ2	1.53	0.56
1:B:316:ASP:O	1:B:317:LEU:O	2.24	0.56
1:A:316:ASP:O	1:A:317:LEU:O	2.24	0.55
1:B:40:HIS:CE1	3:B:2032:HOH:O	2.60	0.54
1:B:426:ARG:O	1:B:427:ILE:HD13	2.07	0.54
1:A:437:ASN:HB3	3:A:2217:HOH:O	2.08	0.54
1:B:301:LYS:HD2	1:B:313:VAL:CG2	2.38	0.53
1:A:322:MET:SD	1:A:412:LYS:HG3	2.49	0.52
1:A:299:LEU:HB2	1:A:315:ARG:HD3	1.93	0.51
1:B:18:SER:O	1:B:22:GLU:HG3	2.12	0.49
1:A:293:ASN:CG	1:A:351:GLU:HB2	2.32	0.49
1:B:418:TYR:HB3	1:B:427:ILE:HB	1.94	0.49
1:B:372:ILE:HG13	1:B:431:SER:HA	1.93	0.49
1:A:12:TRP:HB3	1:A:439:VAL:HG22	1.94	0.49
1:B:358:ASP:HB3	1:B:366:VAL:HG11	1.94	0.48
1:B:358:ASP:HB3	1:B:366:VAL:CG1	2.43	0.48
1:B:434:TRP:O	1:B:438:VAL:HG23	2.14	0.48
1:A:216:LYS:HD3	1:A:288:ASP:HB3	1.96	0.47
1:B:40:HIS:HE1	3:B:2032:HOH:O	1.94	0.47
1:B:69:GLU:HG3	1:B:70:LYS:N	2.29	0.47
1:A:293:ASN:OD1	1:A:351:GLU:HB2	2.15	0.47
1:A:376:LYS:HB2	1:A:434:TRP:CZ2	2.50	0.47
1:B:123:ASP:N	1:B:123:ASP:OD1	2.48	0.47
1:A:299:LEU:HD23	1:A:313:VAL:HG13	1.97	0.47
1:B:293:ASN:CG	1:B:351:GLU:HB2	2.35	0.47
1:B:136:ASN:O	1:B:139:ILE:HG22	2.15	0.47
1:B:416:ILE:C	1:B:429:LYS:HD2	2.35	0.46
1:A:82:TRP:N	1:A:83:PRO:HD2	2.31	0.46
1:B:329:GLU:HA	1:B:381:GLN:HE21	1.80	0.46
1:A:332:TYR:CB	1:A:381:GLN:HE21	2.30	0.45
1:B:405:GLU:HG3	1:B:405:GLU:O	2.16	0.45
1:A:303:ASP:OD1	1:A:303:ASP:C	2.55	0.45
1:A:251:PHE:C	1:A:254:PRO:HD2	2.37	0.45
1:A:20:GLN:O	1:A:403:ASN:HB2	2.17	0.44
1:B:11:LEU:HD12	1:B:11:LEU:HA	1.52	0.44
1:B:371:ARG:NH1	1:B:429:LYS:HZ2	2.14	0.44
1:B:221:PHE:CE1	1:B:251:PHE:HB2	2.53	0.44
1:A:81:SER:HB3	1:A:84:ARG:HG3	2.00	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:TRP:CD1	1:B:208:PHE:HE1	2.35	0.43
1:B:336:LYS:HD2	1:B:336:LYS:HA	1.70	0.43
1:A:405:GLU:HG3	1:A:405:GLU:O	2.18	0.43
1:A:247:ASN:C	1:A:249:PRO:CD	2.86	0.43
1:B:442:ASN:O	1:B:442:ASN:OD1	2.36	0.43
1:A:122:TRP:CD1	1:A:122:TRP:N	2.85	0.43
1:B:265:LEU:HD23	1:B:265:LEU:HA	1.91	0.42
1:B:423:THR:O	1:B:424:GLN:HB2	2.19	0.42
1:A:223:ASN:HA	1:A:247:ASN:OD1	2.20	0.42
1:B:233:GLU:O	1:B:237:ARG:HG3	2.19	0.42
1:B:371:ARG:NH1	1:B:415:GLY:O	2.52	0.42
1:B:355:ALA:HA	1:B:413:ARG:O	2.19	0.42
1:A:6:PHE:CZ	1:A:383:TRP:HB2	2.56	0.41
1:A:299:LEU:HD22	1:A:315:ARG:HD3	2.02	0.41
1:A:398:TRP:HA	1:A:399:SER:HA	1.85	0.41
1:B:139:ILE:HA	1:B:142:TRP:CE3	2.55	0.41
1:B:420:ASP:OD2	1:B:423:THR:HG23	2.20	0.41
1:A:332:TYR:HB3	1:A:381:GLN:HE21	1.86	0.41
1:B:349:ILE:HG12	1:B:392:LEU:HD11	2.02	0.41
1:A:221:PHE:CE1	1:A:251:PHE:HB2	2.56	0.41
1:A:247:ASN:C	1:A:249:PRO:HD2	2.42	0.40
1:A:333:TRP:CZ2	1:A:337:LYS:HG3	2.56	0.40

All (1) 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:A:91:GLY:O	1:A:365:ARG:NH2[4_555]	2.13	0.07

## 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	439/468 (94%)	419 (95%)	18 (4%)	2 (0%)	29	22
1	B	439/468 (94%)	420 (96%)	17 (4%)	2 (0%)	29	22
All	All	878/936 (94%)	839 (96%)	35 (4%)	4 (0%)	29	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	ASP
1	A	317	LEU
1	B	316	ASP
1	B	317	LEU

### 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	362/399 (91%)	343 (95%)	19 (5%)	23	19
1	B	352/399 (88%)	333 (95%)	19 (5%)	22	18
All	All	714/798 (90%)	676 (95%)	38 (5%)	22	19

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	5	LYS
1	A	8	GLU
1	A	11	LEU
1	A	71	LEU
1	A	77	ARG
1	A	86	LEU
1	A	109	LEU
1	A	206	LYS
1	A	237	ARG
1	A	242	MET
1	A	253	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	257	ARG
1	A	277	LYS
1	A	313	VAL
1	A	315	ARG
1	A	316	ASP
1	A	372	ILE
1	A	375	LEU
1	B	3	VAL
1	B	45	VAL
1	B	69	GLU
1	B	71	LEU
1	B	77	ARG
1	B	88	GLU
1	B	103	ARG
1	B	123	ASP
1	B	230	SER
1	B	300	VAL
1	B	301	LYS
1	B	334	ILE
1	B	338	VAL
1	B	350	THR
1	B	386	ILE
1	B	401	LEU
1	B	403	ASN
1	B	422	SER
1	B	425	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	GLN
1	A	246	ASN
1	A	352	ASN
1	A	381	GLN
1	B	352	ASN
1	B	381	GLN
1	B	403	ASN

### 5.3.3 RNA ⓘ

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](#)

2 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	G2F	A	1446	1	11,11,12	1.28	2 (18%)	10,15,17	1.43	2 (20%)
2	G2F	B	1446	1	11,11,12	0.57	0	10,15,17	1.51	3 (30%)

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	G2F	A	1446	1	-	0/2/19/22	0/1/1/1
2	G2F	B	1446	1	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1446	G2F	C2-C3	2.25	1.54	1.51
2	A	1446	G2F	C1-C2	2.13	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	1446	G2F	C1-O5-C5	3.13	116.44	112.19
2	B	1446	G2F	O3-C3-C4	2.64	116.45	110.35
2	A	1446	G2F	O3-C3-C4	2.64	116.44	110.35
2	B	1446	G2F	C3-C4-C5	-2.20	106.31	110.24
2	A	1446	G2F	C3-C4-C5	-2.15	106.41	110.24

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 ⓘ

### 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	442/468 (94%)	0.09	15 (3%) 45 53	22, 39, 63, 71	0
1	B	443/468 (94%)	0.22	23 (5%) 27 35	23, 41, 62, 72	0
All	All	885/936 (94%)	0.15	38 (4%) 35 45	22, 40, 63, 72	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	360	VAL	5.4
1	B	445	GLU	4.3
1	B	361	SER	4.0
1	A	233	GLU	3.8
1	B	2	ASN	3.7
1	B	68	ILE	3.6
1	A	3	VAL	3.5
1	A	302	PHE	3.3
1	B	317	LEU	3.3
1	B	363	ASP	3.3
1	A	2	ASN	3.1
1	A	229	ALA	3.1
1	B	367	HIS	3.0
1	B	389	GLY	3.0
1	B	47	ASN	3.0
1	B	441	ASN	2.8
1	B	364	GLY	2.7
1	B	231	GLU	2.7
1	A	308	ALA	2.6
1	A	416	ILE	2.6
1	B	113	ILE	2.5
1	A	303	ASP	2.4
1	B	316	ASP	2.4
1	B	305	ASP	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	3	VAL	2.3
1	B	112	GLY	2.3
1	A	349	ILE	2.2
1	A	401	LEU	2.2
1	A	417	VAL	2.2
1	A	14	VAL	2.1
1	B	306	ALA	2.1
1	B	437	ASN	2.1
1	B	304	PRO	2.1
1	B	11	LEU	2.1
1	A	304	PRO	2.1
1	A	15	ALA	2.1
1	A	389	GLY	2.0
1	B	108	LEU	2.0

## 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	G2F	B	1446	11/12	0.96	0.08	32,35,40,40	0
2	G2F	A	1446	11/12	0.97	0.06	24,25,27,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.