



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2023 – 08:30 AM EDT

PDB ID : 3JUR  
Title : The crystal structure of a hyperthermoactive Exopolygalacturonase from *Thermotoga maritima*  
Authors : Pijning, T.; van Pouderooyen, G.; Kluskens, L.D.; van der Oost, J.; Dijkstra, B.W.  
Deposited on : 2009-09-15  
Resolution : 2.05 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  
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

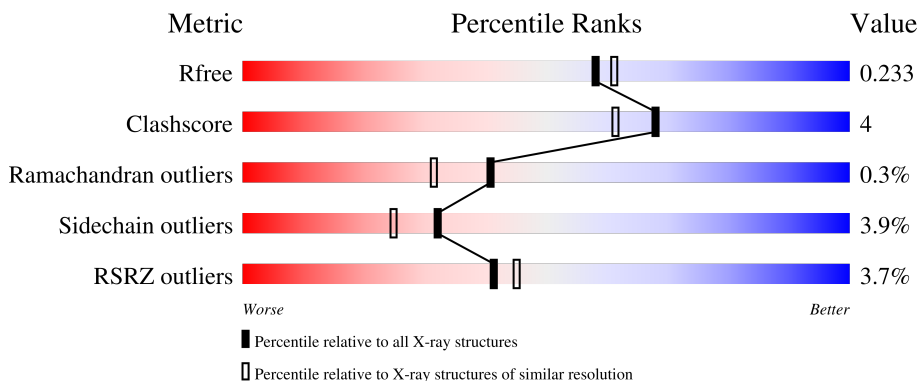
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


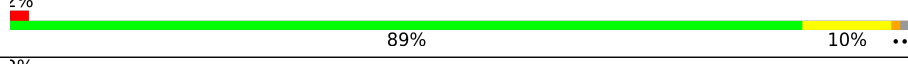
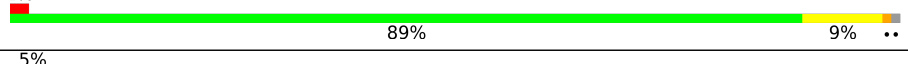

The reported resolution of this entry is 2.05 Å.

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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	448	 6% 87% 11% ..
1	B	448	 2% 89% 10% ..
1	C	448	 2% 89% 9% ..
1	D	448	 5% 86% 12% .

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15294 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 Exo-poly-alpha-D-galacturonosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	444	3528	2233	616	665	14	0	1	0
1	B	444	3533	2234	619	666	14	0	2	0
1	C	444	3532	2233	620	665	14	0	2	0
1	D	446	3545	2243	618	669	15	0	1	0


There are 4 discrepancies between the modelled and reference sequences:

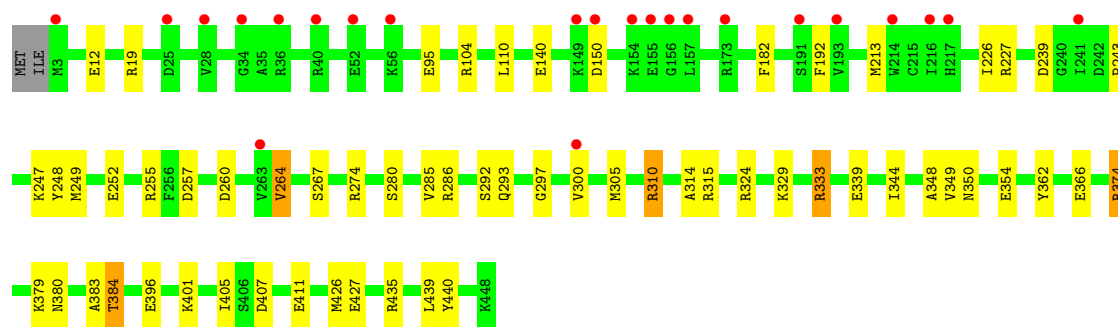
Chain	Residue	Modelled	Actual	Comment	Reference
A	216	ILE	VAL	conflict	UNP Q9WYR8
B	216	ILE	VAL	conflict	UNP Q9WYR8
C	216	ILE	VAL	conflict	UNP Q9WYR8
D	216	ILE	VAL	conflict	UNP Q9WYR8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	239	Total 239	O 239	0	0
2	B	365	Total 365	O 365	0	0
2	C	283	Total 283	O 283	0	0
2	D	269	Total 269	O 269	0	0



Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.27Å 155.90Å 200.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.43 – 2.05 33.89 – 2.05	Depositor EDS
% Data completeness (in resolution range)	91.3 (34.43-2.05) 91.3 (33.89-2.05)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.05Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.175 , 0.220 0.186 , 0.233	Depositor DCC
$R_{free}$ test set	5742 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtrriage
Anisotropy	0.083	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15294	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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](#)

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	0.42	0/3596	0.57	1/4852 (0.0%)
1	B	0.46	0/3603	0.59	0/4860
1	C	0.42	0/3602	0.58	0/4859
1	D	0.41	0/3613	0.56	0/4874
All	All	0.43	0/14414	0.57	1/19445 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	LEU	CA-CB-CG	5.48	127.91	115.30

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	3528	0	3538	28	0
1	B	3533	0	3548	25	0
1	C	3532	0	3548	28	0
1	D	3545	0	3553	28	0
2	A	239	0	0	3	0
2	B	365	0	0	1	0
2	C	283	0	0	3	0
2	D	269	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15294	0	14187	107	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 4.

All (107) 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:350:ASN:H	1:A:384:THR:HG22	1.39	0.85
1:C:350:ASN:H	1:C:384:THR:HG22	1.43	0.84
1:D:350:ASN:H	1:D:384:THR:HG22	1.46	0.79
1:B:435:ARG:NH2	1:D:411:GLU:OE1	2.28	0.67
1:D:274:ARG:NH2	1:D:333:ARG:O	2.28	0.66
1:C:384:THR:HG23	2:C:770:HOH:O	1.97	0.65
1:C:97:TYR:CE1	1:C:116:LEU:HD22	2.33	0.63
1:C:384:THR:CG2	2:C:770:HOH:O	2.49	0.61
1:B:28:VAL:HG13	1:B:33:PHE:HE2	1.69	0.57
1:B:20:GLU:OE2	1:B:227[B]:ARG:NH1	2.38	0.56
1:C:361:ARG:NH2	1:C:420:GLU:OE1	2.40	0.55
1:A:192:PHE:HB3	1:A:215:CYS:O	2.07	0.55
1:B:324:ARG:HA	1:B:354:GLU:O	2.09	0.53
1:A:20:GLU:OE2	1:A:227:ARG:NH1	2.42	0.52
1:A:28:VAL:HG13	1:A:33:PHE:HE2	1.74	0.52
1:D:226:ILE:HD12	1:D:249:MET:CE	2.40	0.51
1:C:315:ARG:HA	1:C:344:ILE:O	2.11	0.50
1:A:324:ARG:HA	1:A:354:GLU:O	2.12	0.50
1:C:20:GLU:HG2	2:C:888:HOH:O	2.10	0.50
1:A:380:ASN:HA	1:A:407:ASP:O	2.12	0.50
1:B:216:ILE:HD11	1:B:229:ILE:HD13	1.93	0.49
1:D:310:ARG:HA	1:D:339:GLU:O	2.12	0.49
1:A:333:ARG:HD2	2:A:450:HOH:O	2.13	0.49
1:A:239:ASP:OD1	1:A:260:ASP:HB3	2.12	0.49
1:A:348:ALA:O	1:A:383:ALA:HA	2.11	0.49
1:B:28:VAL:HG13	1:B:33:PHE:CE2	2.48	0.49
1:C:270:ASP:OD1	1:C:334:ARG:HD3	2.14	0.48
1:B:374:ARG:HA	1:B:401:LYS:O	2.14	0.48
1:D:243:PRO:HG3	1:D:249:MET:HE1	1.96	0.48
1:D:333:ARG:HD3	1:D:366:GLU:O	2.13	0.47
1:B:192:PHE:HB3	1:B:215:CYS:O	2.15	0.47
1:D:252:GLU:HA	1:D:286:ARG:O	2.14	0.47
1:D:315:ARG:HA	1:D:344:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLU:HA	1:A:227:ARG:O	2.14	0.47
1:C:6:LEU:HB3	1:C:342:PHE:CZ	2.50	0.47
1:D:19:ARG:NH1	2:D:571:HOH:O	2.40	0.46
1:D:324:ARG:HA	1:D:354:GLU:O	2.15	0.46
1:A:315:ARG:HA	1:A:344:ILE:O	2.15	0.46
1:C:310:ARG:HA	1:C:339:GLU:O	2.16	0.46
1:A:374:ARG:HA	1:A:401:LYS:O	2.16	0.46
1:C:257:ASP:HA	1:C:292:SER:HB2	1.98	0.46
1:B:252:GLU:HA	1:B:286:ARG:O	2.17	0.45
1:A:320:MET:HG2	1:A:349:VAL:HG13	1.97	0.45
1:A:435:ARG:NH2	2:A:974:HOH:O	2.40	0.45
1:B:315:ARG:HA	1:B:344:ILE:O	2.16	0.45
1:C:176:PRO:HG2	1:C:179:GLU:HB2	1.98	0.45
1:D:239:ASP:OD1	1:D:260:ASP:HB3	2.17	0.45
1:B:411[A]:GLU:OE1	1:B:411[A]:GLU:HA	2.17	0.44
1:C:264:VAL:HG13	1:C:300:VAL:HB	1.99	0.44
1:D:257:ASP:HA	1:D:292:SER:HB2	1.97	0.44
1:D:264:VAL:HG13	1:D:300:VAL:HB	1.99	0.44
1:D:110:LEU:HD12	1:D:182:PHE:CD2	2.52	0.44
1:D:405:ILE:O	1:D:426:MET:HA	2.17	0.44
1:A:264:VAL:HG13	1:A:300:VAL:HB	2.00	0.43
1:A:310:ARG:HA	1:A:339:GLU:O	2.18	0.43
1:B:66:GLU:CD	1:B:66:GLU:H	2.21	0.43
1:C:339:GLU:HA	1:C:374:ARG:O	2.19	0.43
1:A:166:LYS:O	1:A:170:MET:HG3	2.18	0.43
1:C:281:GLU:HA	1:C:310:ARG:O	2.19	0.43
1:A:243:PRO:HD2	1:A:264:VAL:O	2.18	0.43
1:B:216:ILE:CD1	1:B:229:ILE:HD13	2.48	0.43
1:B:239:ASP:OD1	1:B:260:ASP:HB3	2.19	0.43
1:C:192:PHE:HB3	1:C:215:CYS:O	2.19	0.43
1:A:19:ARG:NH2	2:A:472:HOH:O	2.51	0.42
1:C:261:ASP:CB	1:C:264:VAL:HG22	2.49	0.42
1:C:374:ARG:HA	1:C:401:LYS:O	2.19	0.42
1:D:380:ASN:HA	1:D:407:ASP:O	2.20	0.42
1:D:226:ILE:HD12	1:D:249:MET:HE3	2.00	0.42
1:B:300:VAL:HG11	1:B:329:LYS:HE2	2.01	0.42
1:A:300:VAL:HG22	1:A:327:ARG:HB3	2.00	0.42
1:B:428:ASN:HB2	2:B:758:HOH:O	2.19	0.42
1:A:164:VAL:O	1:A:168:LYS:HG2	2.20	0.42
1:C:383:ALA:HB3	1:C:410:ILE:HG12	2.01	0.42
1:B:333:ARG:HG3	1:B:366:GLU:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ASP:HA	1:A:292:SER:HB2	2.01	0.42
1:C:170:MET:HB2	1:C:170:MET:HE3	1.87	0.42
1:B:281:GLU:HA	1:B:310:ARG:O	2.20	0.41
1:D:247:LYS:HE2	1:D:248:TYR:CE2	2.54	0.41
1:D:396:GLU:HG3	2:D:470:HOH:O	2.20	0.41
1:A:286:ARG:HA	1:A:315:ARG:O	2.20	0.41
1:B:227[A]:ARG:HG2	1:B:228:ASN:OD1	2.20	0.41
1:B:418:LEU:C	1:B:418:LEU:HD23	2.41	0.41
1:C:261:ASP:HB2	1:C:264:VAL:CG2	2.50	0.41
1:C:239:ASP:OD1	1:C:260:ASP:HB3	2.20	0.41
1:D:348:ALA:O	1:D:383:ALA:HA	2.20	0.41
1:D:426:MET:HB2	1:D:439:LEU:HB3	2.03	0.41
1:A:204:GLU:OE2	1:A:227:ARG:NH2	2.53	0.41
1:A:252:GLU:HA	1:A:286:ARG:O	2.20	0.41
1:A:281:GLU:HA	1:A:310:ARG:O	2.21	0.41
1:B:405:ILE:O	1:B:426:MET:HA	2.20	0.41
1:C:324:ARG:HA	1:C:354:GLU:O	2.21	0.41
1:D:297:GLY:HA2	1:D:324:ARG:O	2.20	0.41
1:A:107:GLY:HA2	1:A:244:GLU:OE1	2.21	0.40
1:B:228:ASN:HA	1:B:253:LYS:O	2.21	0.40
1:B:13:GLU:HG2	1:B:282:TYR:CE1	2.56	0.40
1:B:411[A]:GLU:OE2	1:D:411:GLU:HG3	2.20	0.40
1:C:246:CYS:O	1:C:280:SER:HA	2.20	0.40
1:C:247:LYS:HG3	1:C:281:GLU:HG3	2.03	0.40
1:C:167:LEU:HA	1:C:170:MET:HE2	2.03	0.40
1:D:285:VAL:O	1:D:314:ALA:HA	2.21	0.40
1:D:427:GLU:OE2	1:D:440[B]:TYR:OH	2.35	0.40
1:A:178:GLU:CD	1:A:178:GLU:H	2.25	0.40
1:D:329:LYS:HD2	1:D:362:TYR:CE1	2.56	0.40
1:D:374:ARG:HA	1:D:401:LYS:O	2.22	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	443/448 (99%)	419 (95%)	23 (5%)	1 (0%)	47	39
1	B	444/448 (99%)	416 (94%)	27 (6%)	1 (0%)	47	39
1	C	444/448 (99%)	421 (95%)	22 (5%)	1 (0%)	47	39
1	D	445/448 (99%)	424 (95%)	19 (4%)	2 (0%)	34	24
All	All	1776/1792 (99%)	1680 (95%)	91 (5%)	5 (0%)	41	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	213	MET
1	C	213	MET
1	A	213	MET
1	D	213	MET
1	D	267	SER

### 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	387/390 (99%)	370 (96%)	17 (4%)	28	21
1	B	388/390 (100%)	376 (97%)	12 (3%)	40	33
1	C	388/390 (100%)	376 (97%)	12 (3%)	40	33
1	D	389/390 (100%)	370 (95%)	19 (5%)	25	17
All	All	1552/1560 (100%)	1492 (96%)	60 (4%)	32	25

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	28	VAL
1	A	40	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	175	THR
1	A	192	PHE
1	A	253	LYS
1	A	255	ARG
1	A	264	VAL
1	A	280	SER
1	A	305	MET
1	A	316	ASN
1	A	349	VAL
1	A	368	GLU
1	A	374	ARG
1	A	384	THR
1	A	420	GLU
1	A	447	LEU
1	B	5	GLU
1	B	48	LYS
1	B	104	ARG
1	B	140	GLU
1	B	166	LYS
1	B	173	ARG
1	B	192	PHE
1	B	280	SER
1	B	305	MET
1	B	310	ARG
1	B	379	LYS
1	B	435	ARG
1	C	20	GLU
1	C	48	LYS
1	C	165	LYS
1	C	192	PHE
1	C	255	ARG
1	C	264	VAL
1	C	305	MET
1	C	374	ARG
1	C	384	THR
1	C	420	GLU
1	C	423	GLN
1	C	448	LYS
1	D	12	GLU
1	D	95	GLU
1	D	104	ARG
1	D	140	GLU

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Mol	Chain	Res	Type
1	D	150	ASP
1	D	192	PHE
1	D	227	ARG
1	D	255	ARG
1	D	264	VAL
1	D	280	SER
1	D	293	GLN
1	D	305	MET
1	D	310	ARG
1	D	333	ARG
1	D	349	VAL
1	D	374	ARG
1	D	379	LYS
1	D	384	THR
1	D	435	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	194	GLN
1	C	293	GLN
1	D	293	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](#)

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](#)

There are no ligands in this entry.

## 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	444/448 (99%)	0.19	26 (5%) 22 24	20, 24, 31, 38	0
1	B	444/448 (99%)	-0.03	8 (1%) 68 71	17, 23, 30, 39	0
1	C	444/448 (99%)	-0.01	9 (2%) 65 69	18, 23, 29, 40	0
1	D	446/448 (99%)	0.16	23 (5%) 27 29	19, 24, 30, 42	0
All	All	1778/1792 (99%)	0.08	66 (3%) 41 45	17, 24, 30, 42	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	157	LEU	3.7
1	A	36	ARG	3.4
1	A	173	ARG	3.2
1	B	156	GLY	3.1
1	D	3	MET	3.0
1	C	265	ILE	3.0
1	A	264	VAL	2.9
1	D	173	ARG	2.9
1	A	265	ILE	2.9
1	D	40	ARG	2.9
1	D	34	GLY	2.8
1	A	193	VAL	2.8
1	C	263	VAL	2.8
1	C	40	ARG	2.7
1	A	241	ILE	2.7
1	A	301	ILE	2.7
1	D	241	ILE	2.7
1	A	117	VAL	2.6
1	D	263	VAL	2.6
1	B	264	VAL	2.6
1	D	154	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	56	LYS	2.6
1	A	440[A]	TYR	2.5
1	C	301	ILE	2.5
1	A	40	ARG	2.5
1	A	218	PRO	2.5
1	A	192	PHE	2.5
1	D	156	GLY	2.5
1	D	214	TRP	2.5
1	B	193	VAL	2.5
1	B	265	ILE	2.5
1	C	241	ILE	2.5
1	D	193	VAL	2.4
1	D	155	GLU	2.4
1	A	368	GLU	2.4
1	C	328	LEU	2.4
1	C	300	VAL	2.4
1	C	193	VAL	2.4
1	A	187	TYR	2.4
1	A	216	ILE	2.4
1	C	216	ILE	2.4
1	A	195	PHE	2.4
1	D	300	VAL	2.3
1	A	151	PHE	2.3
1	A	157	LEU	2.3
1	D	216	ILE	2.3
1	B	241	ILE	2.3
1	D	25	ASP	2.3
1	A	328	LEU	2.2
1	A	243	PRO	2.2
1	A	19	ARG	2.2
1	D	28	VAL	2.2
1	D	36	ARG	2.1
1	A	214	TRP	2.1
1	B	301	ILE	2.1
1	A	149	LYS	2.1
1	D	191	SER	2.1
1	D	52	GLU	2.0
1	A	300	VAL	2.0
1	B	117	VAL	2.0
1	A	150	ASP	2.0
1	D	149	LYS	2.0
1	A	95	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	217	HIS	2.0
1	B	326	LEU	2.0
1	D	150	ASP	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.