



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:59 PM GMT

PDB ID : 4B3L
Title : Family 1 6-phospho-beta-D glycosidase from Streptococcus pyogenes
Authors : Stepper, J.; Dabin, J.; Ekloef, J.M.; Thongpoo, P.; Kongsaree, P.T.; Taylor, E.J.; Turkenburg, J.P.; Brumer, H.; Davies, G.J.
Deposited on : 2012-07-24
Resolution : 2.51 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

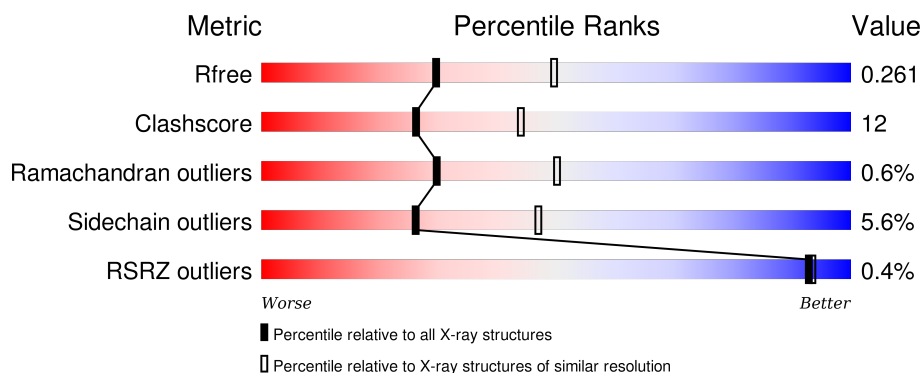
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	479	 74% 21% . .
1	B	479	 77% 17% . . .
1	C	479	 71% 23% . .
1	D	479	 77% 17% . .
1	E	479	 70% 22% . .

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Mol	Chain	Length	Quality of chain
1	F	479	<div><div><div>%</div><div><div></div><div>58%</div><div>33%</div><div>6%</div><div>•</div></div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22619 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			
1	B	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			
1	C	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			
1	D	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			
1	E	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			
1	F	461	Total	C	N	O	S	0	0	0
			3767	2435	636	686	10			

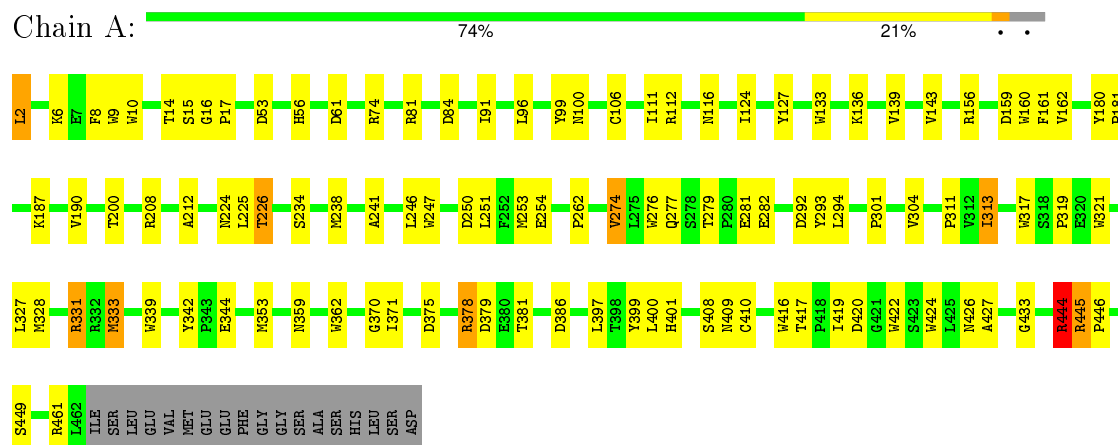
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		
2	B	4	Total	O	0	0
			4	4		
2	C	3	Total	O	0	0
			3	3		
2	D	5	Total	O	0	0
			5	5		
2	E	1	Total	O	0	0
			1	1		
2	F	3	Total	O	0	0
			3	3		

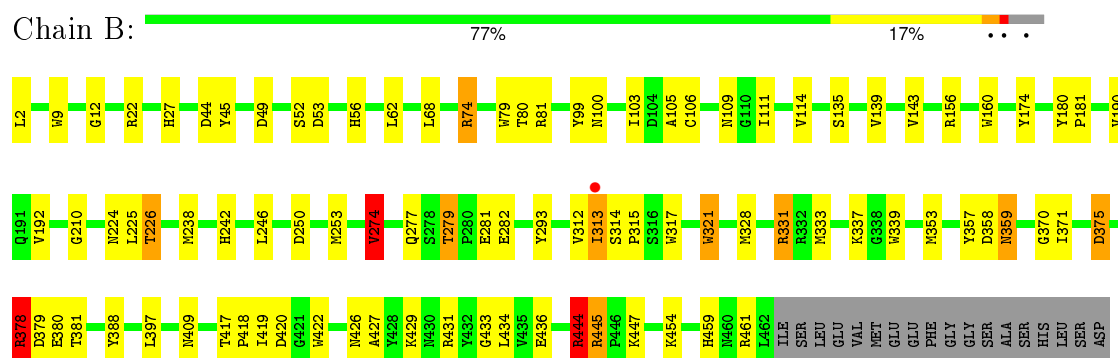
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

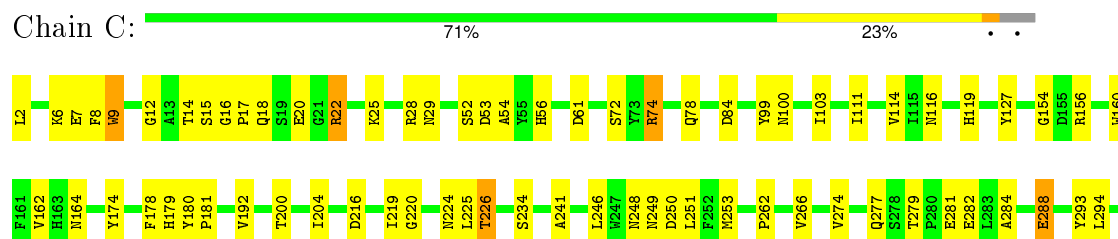
• Molecule 1: BETA-GLUCOSIDASE

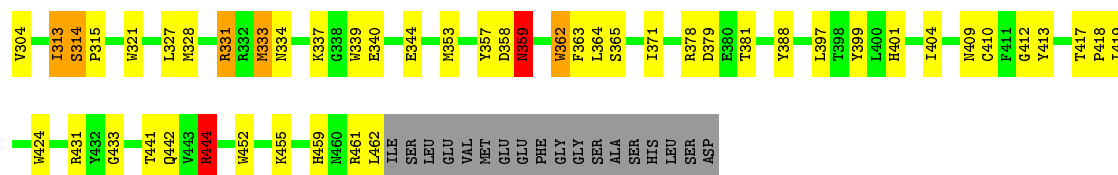


• Molecule 1: BETA-GLUCOSIDASE



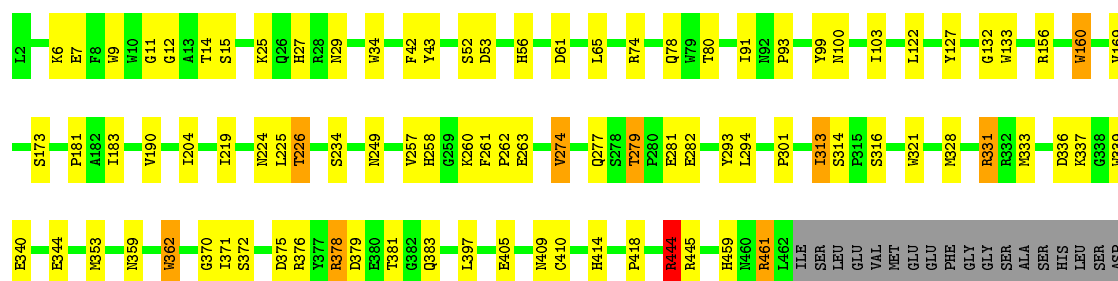
• Molecule 1: BETA-GLUCOSIDASE





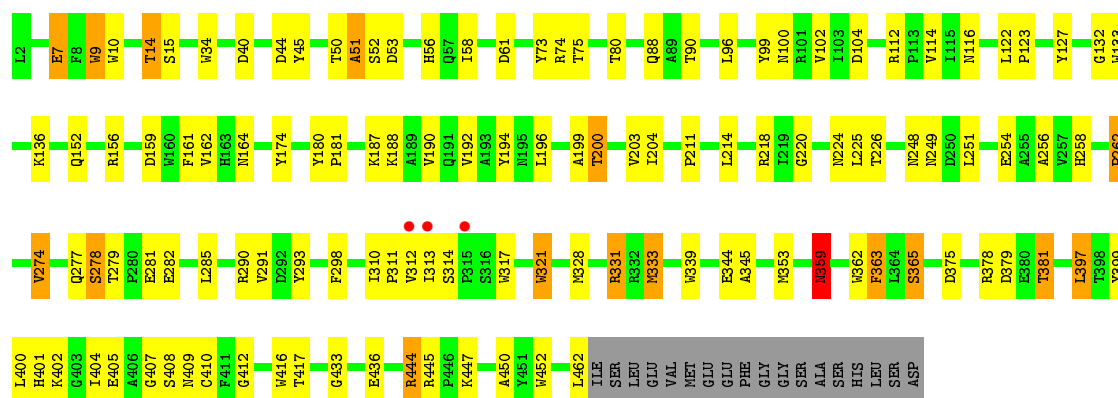
• Molecule 1: BETA-GLUCOSIDASE

Chain D: 77% 17%



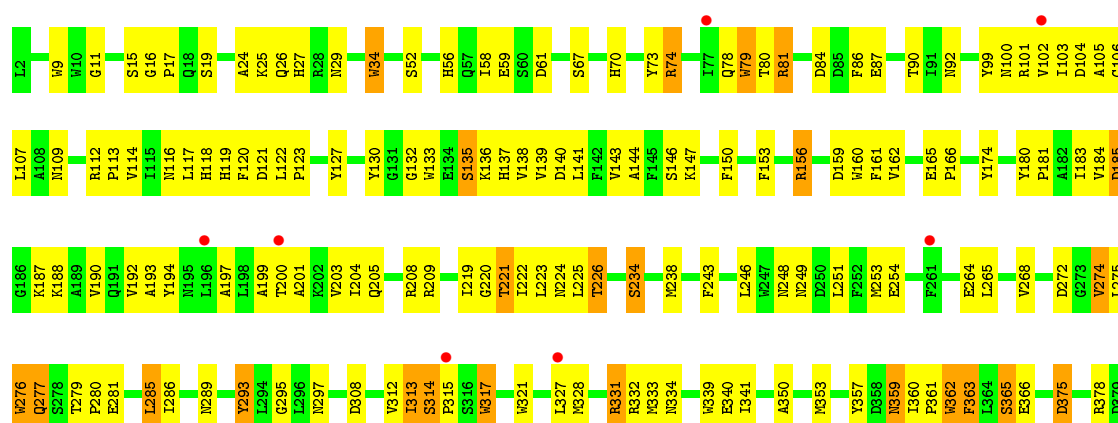
• Molecule 1: BETA-GLUCOSIDASE

Chain E: 70% 22%



• Molecule 1: BETA-GLUCOSIDASE

Chain F: 58% 33% 6%



E380	E381	E382	E383	E384	E389	E393	E397	E405	E409	E410	E411	E412	E413	E414	E415	E416	E417	E418	E419	E420	E421	E422	E433	E434	E435	E436	E444	E445	E446	E447	E461	E462	ILE	SER	LEU	GLU	VAL	MET	GLU	GLU	PHE	GLY	GLY	SER	ALA	SER	HIS	LEU	SER	ASP
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.83Å 198.04Å 107.88Å 90.00° 118.51° 90.00°	Depositor
Resolution (Å)	94.75 – 2.51 99.02 – 2.51	Depositor EDS
% Data completeness (in resolution range)	99.5 (94.75-2.51) 99.3 (99.02-2.51)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0025	Depositor
R, R_{free}	0.205 , 0.261 0.205 , 0.261	Depositor DCC
R_{free} test set	6762 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.023 for -h-l,k,h 0.023 for l,k,-h-l 0.032 for h,-k,-h-l 0.034 for -h-l,-k,l 0.087 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 134562 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22619	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.87	8/3891 (0.2%)	0.88	7/5304 (0.1%)
1	B	0.89	7/3891 (0.2%)	0.88	6/5304 (0.1%)
1	C	0.86	7/3891 (0.2%)	0.89	8/5304 (0.2%)
1	D	0.86	6/3891 (0.2%)	0.85	1/5304 (0.0%)
1	E	0.82	6/3891 (0.2%)	0.84	0/5304
1	F	0.91	8/3891 (0.2%)	0.91	2/5304 (0.0%)
All	All	0.87	42/23346 (0.2%)	0.87	24/31824 (0.1%)

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	TRP	CD2-CE2	6.69	1.49	1.41
1	D	339	TRP	CD2-CE2	6.69	1.49	1.41
1	E	339	TRP	CD2-CE2	6.51	1.49	1.41
1	F	34	TRP	CD2-CE2	6.50	1.49	1.41
1	B	339	TRP	CD2-CE2	6.48	1.49	1.41

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	444	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	C	444	ARG	NE-CZ-NH1	8.95	124.77	120.30
1	C	444	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	C	431	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	B	429	LYS	CD-CE-NZ	-6.62	96.47	111.70

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	3767	0	3574	78	0
1	B	3767	0	3574	74	0
1	C	3767	0	3574	79	0
1	D	3767	0	3574	64	0
1	E	3767	0	3574	93	0
1	F	3767	0	3574	155	0
2	A	1	0	0	0	0
2	B	4	0	0	2	0
2	C	3	0	0	0	0
2	D	5	0	0	0	0
2	E	1	0	0	0	0
2	F	3	0	0	0	0
All	All	22619	0	21444	540	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 12.

The worst 5 of 540 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:B:224:ASN:OD1	1:B:226:THR:HG23	1.35	1.23
1:F:331:ARG:CG	1:F:331:ARG:HH11	1.47	1.22
1:B:331:ARG:CG	1:B:331:ARG:HH11	1.54	1.16
1:A:224:ASN:OD1	1:A:226:THR:HG23	1.46	1.16
1:F:331:ARG:HG2	1:F:331:ARG:HH11	1.10	1.15

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	459/479 (96%)	438 (95%)	20 (4%)	1 (0%)	52	75
1	B	459/479 (96%)	429 (94%)	26 (6%)	4 (1%)	21	37
1	C	459/479 (96%)	425 (93%)	32 (7%)	2 (0%)	39	61
1	D	459/479 (96%)	424 (92%)	34 (7%)	1 (0%)	52	75
1	E	459/479 (96%)	425 (93%)	30 (6%)	4 (1%)	21	37
1	F	459/479 (96%)	409 (89%)	46 (10%)	4 (1%)	21	37
All	All	2754/2874 (96%)	2550 (93%)	188 (7%)	16 (1%)	30	50

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	359	ASN
1	B	375	ASP
1	D	336	ASP
1	E	274	VAL
1	E	359	ASN

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	389/404 (96%)	373 (96%)	16 (4%)	37	63
1	B	389/404 (96%)	372 (96%)	17 (4%)	35	60
1	C	389/404 (96%)	369 (95%)	20 (5%)	29	52
1	D	389/404 (96%)	369 (95%)	20 (5%)	29	52
1	E	389/404 (96%)	370 (95%)	19 (5%)	31	55
1	F	389/404 (96%)	351 (90%)	38 (10%)	10	19
All	All	2334/2424 (96%)	2204 (94%)	130 (6%)	26	47

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	263	GLU
1	D	461	ARG
1	F	363	PHE
1	D	277	GLN
1	D	331	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	297	ASN
1	D	179	HIS
1	F	249	ASN
1	C	359	ASN
1	D	56	HIS

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 carbohydrates 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, 95th 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	461/479 (96%)	-0.24	0 100 100	24, 40, 63, 93	1 (0%)
1	B	461/479 (96%)	-0.29	1 (0%) 95 96	25, 41, 63, 84	1 (0%)
1	C	461/479 (96%)	-0.24	0 100 100	26, 44, 67, 91	1 (0%)
1	D	461/479 (96%)	-0.27	0 100 100	25, 42, 64, 82	1 (0%)
1	E	461/479 (96%)	-0.15	3 (0%) 89 90	28, 48, 70, 103	2 (0%)
1	F	461/479 (96%)	0.11	7 (1%) 76 79	27, 53, 75, 97	2 (0%)
All	All	2766/2874 (96%)	-0.18	11 (0%) 93 93	24, 45, 69, 103	8 (0%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	315	PRO	4.3
1	F	200	THR	3.2
1	B	313	ILE	2.8
1	E	312	VAL	2.7
1	F	77	ILE	2.5

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 carbohydrates 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.