



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:53 PM GMT

PDB ID : 5BY3
Title : A novel family GH115 4-O-Methyl-alpha-glucuronidase, BtGH115A, with specificity for decorated arabinogalactans
Authors : Lammerts van Bueren, A.; Davies, G.J.; Turkenburg, J.P.
Deposited on : 2015-06-10
Resolution : 2.44 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
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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

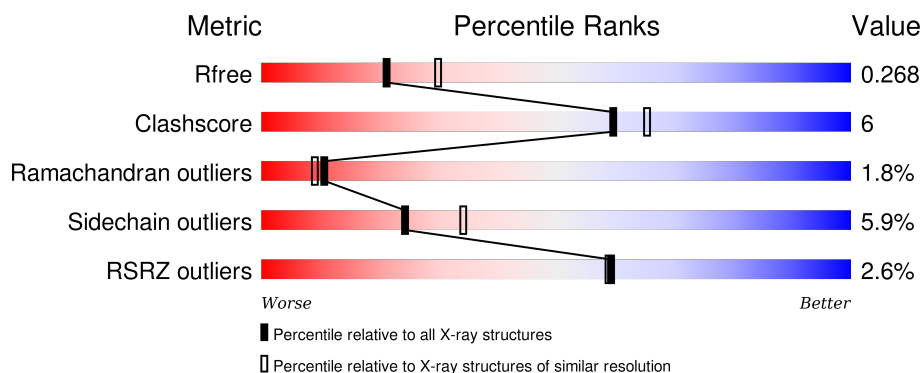
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.44 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	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

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	783	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6184 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 BtGH115A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	759	6078	3857	1057	1136	8	20	0	3	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q8A3J6
A	2	ALA	-	expression tag	UNP Q8A3J6
A	3	HIS	-	expression tag	UNP Q8A3J6
A	4	HIS	-	expression tag	UNP Q8A3J6
A	5	HIS	-	expression tag	UNP Q8A3J6
A	6	HIS	-	expression tag	UNP Q8A3J6
A	7	HIS	-	expression tag	UNP Q8A3J6
A	8	HIS	-	expression tag	UNP Q8A3J6
A	9	SER	-	expression tag	UNP Q8A3J6
A	10	ALA	-	expression tag	UNP Q8A3J6
A	11	ALA	-	expression tag	UNP Q8A3J6
A	12	LEU	-	expression tag	UNP Q8A3J6
A	13	GLU	-	expression tag	UNP Q8A3J6
A	14	VAL	-	expression tag	UNP Q8A3J6
A	15	LEU	-	expression tag	UNP Q8A3J6
A	16	PHE	-	expression tag	UNP Q8A3J6

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		

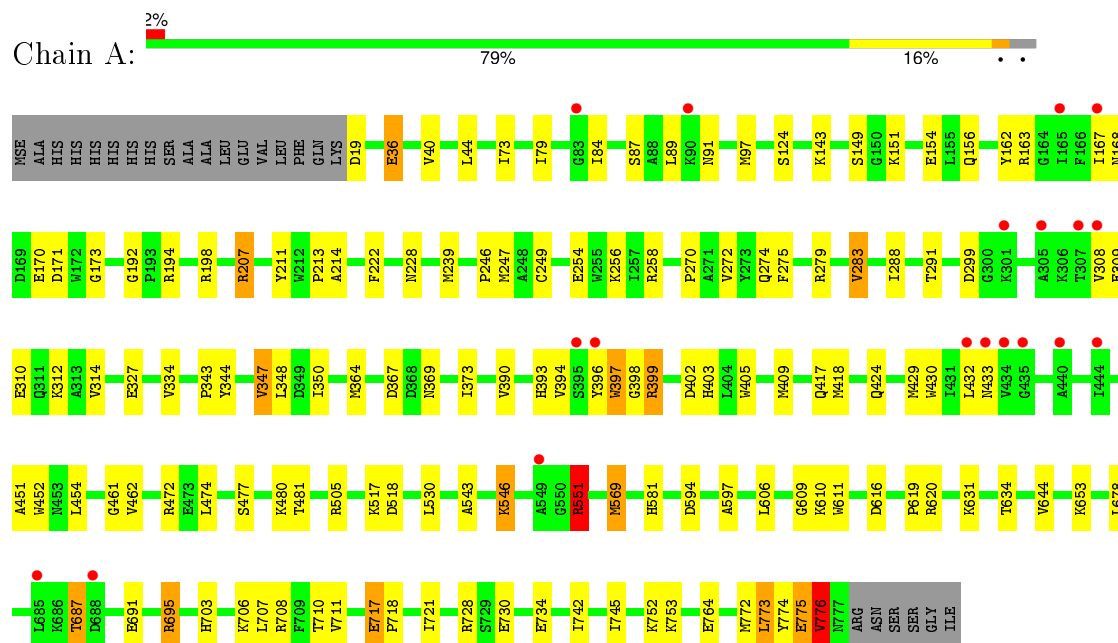
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	99	Total	O	0	1
			100	100		

3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: BtGH115A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.77Å 102.30Å 122.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.44 40.83 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.44) 99.9 (40.83-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.189 , 0.266 0.198 , 0.268	Depositor DCC
R_{free} test set	1630 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 32158 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6184	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

Bond lengths and bond angles in the following residue types are not validated in this section: NI, SO4

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	0.69	0/6206	0.90	12/8367 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	569	MSE	CG-SE-CE	6.99	114.27	98.90
1	A	207	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	198	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	A	198	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	163	ARG	CG-CD-NE	-6.25	98.68	111.80
1	A	399	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	551	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	A	143	LYS	CD-CE-NZ	-5.39	99.31	111.70
1	A	606	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	706	LYS	N-CA-C	5.31	125.34	111.00
1	A	609	GLY	N-CA-C	-5.18	100.15	113.10
1	A	409	MSE	CG-SE-CE	-5.03	87.84	98.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	461	GLY	Peptide

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	6078	0	6015	69	0
2	A	5	0	0	0	0
3	A	1	0	0	0	0
4	A	100	0	0	1	0
All	All	6184	0	6015	69	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.

All (69) 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:156:GLN:HE21	1:A:452:TRP:HE1	1.34	0.74
1:A:167:ILE:HD13	1:A:211:TYR:HE1	1.54	0.73
1:A:405:TRP:CZ3	1:A:569:MSE:HE3	2.25	0.71
1:A:347:VAL:HA	1:A:350:ILE:HG22	1.73	0.68
1:A:170:GLU:OE2	1:A:214:ALA:HB1	1.94	0.67
1:A:156:GLN:NE2	1:A:452:TRP:HE1	1.92	0.66
1:A:168:ASN:HD22	1:A:433:ASN:HD21	1.44	0.66
1:A:162:TYR:HB2	1:A:429:MSE:HG3	1.78	0.65
1:A:610:LYS:HE2	1:A:611:TRP:CZ2	2.32	0.65
1:A:246:PRO:O	1:A:291:THR:O	2.17	0.62
1:A:399:ARG:HD2	1:A:728:ARG:HE	1.65	0.62
1:A:691:GLU:O	1:A:773:LEU:O	2.20	0.60
1:A:424:GLN:HE22	1:A:703:HIS:CE1	2.19	0.59
1:A:721:ILE:HD11	1:A:745:ILE:HD12	1.83	0.59
1:A:310:GLU:O	1:A:314:VAL:HG23	2.03	0.58
1:A:424:GLN:NE2	1:A:703:HIS:CE1	2.73	0.56
1:A:644:VAL:HG23	1:A:773:LEU:HB3	1.88	0.56
1:A:258:ARG:NH2	1:A:275:PHE:O	2.39	0.55
1:A:211:TYR:CZ	1:A:213:PRO:HA	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ASP:HA	1:A:373:ILE:HA	1.89	0.54
1:A:347:VAL:HA	1:A:350:ILE:CG2	2.39	0.53
1:A:343:PRO:HD2	1:A:364:MSE:O	2.09	0.52
1:A:343:PRO:HA	1:A:347:VAL:HG22	1.90	0.52
1:A:36:GLU:HG2	1:A:40:VAL:HG21	1.92	0.52
1:A:424:GLN:HE22	1:A:703:HIS:HE1	1.57	0.51
1:A:695:ARG:HD2	1:A:742:ILE:HG12	1.92	0.51
1:A:247:MSE:H	1:A:249:CYS:HB2	1.77	0.50
1:A:344:TYR:O	1:A:347:VAL:CG1	2.61	0.49
1:A:270:PRO:O	1:A:274:GLN:HG3	2.13	0.48
1:A:272:VAL:O	1:A:275:PHE:HB3	2.14	0.48
1:A:390:VAL:CG1	1:A:418:MSE:HE1	2.44	0.48
1:A:505:ARG:HH22	1:A:730:GLU:CD	2.16	0.48
1:A:327:GLU:HG2	1:A:334:VAL:HG13	1.96	0.48
1:A:283:VAL:HG13	1:A:288:ILE:HG13	1.96	0.47
1:A:543:ALA:O	1:A:546:LYS:HG2	2.14	0.47
1:A:390:VAL:HG11	1:A:418:MSE:HE1	1.96	0.47
1:A:373:ILE:H	1:A:417:GLN:NE2	2.13	0.46
1:A:254:GLU:OE2	1:A:279:ARG:NH2	2.43	0.46
1:A:530:LEU:HD23	1:A:530:LEU:HA	1.80	0.46
1:A:312:LYS:CB	1:A:350:ILE:HD11	2.46	0.46
1:A:430:TRP:CE3	1:A:451:ALA:HB2	2.51	0.46
1:A:222:PHE:CE1	1:A:228:ASN:HB3	2.51	0.45
1:A:89:LEU:HD11	1:A:97:MSE:HB2	1.98	0.45
1:A:397:TRP:C	1:A:397:TRP:CD1	2.90	0.45
1:A:167:ILE:HD13	1:A:211:TYR:CE1	2.42	0.45
1:A:308:VAL:O	1:A:350:ILE:HD13	2.17	0.45
1:A:710:THR:HB	1:A:718:PRO:HB2	1.99	0.45
1:A:222:PHE:CE2	1:A:239:MSE:HE2	2.53	0.44
1:A:594:ASP:O	1:A:597:ALA:HB3	2.18	0.44
1:A:472:ARG:O	1:A:551:ARG:NH2	2.52	0.43
1:A:518:ASP:OD2	1:A:581:HIS:HE1	2.00	0.43
1:A:405:TRP:CZ3	1:A:569:MSE:CE	2.99	0.43
1:A:721:ILE:HD11	1:A:745:ILE:CD1	2.47	0.43
1:A:394:VAL:HG13	1:A:432:LEU:HD11	1.99	0.43
1:A:616:ASP:O	1:A:619:PRO:HD3	2.18	0.43
1:A:44:LEU:HD23	1:A:44:LEU:HA	1.80	0.42
1:A:344:TYR:O	1:A:347:VAL:HG13	2.18	0.42
1:A:396:TYR:CE2	1:A:398:GLY:HA3	2.54	0.42
1:A:168:ASN:HA	4:A:954:HOH:O	2.20	0.42
1:A:192:GLY:C	1:A:228:ASN:HD21	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:GLU:HA	1:A:718:PRO:HD2	1.90	0.41
1:A:373:ILE:H	1:A:417:GLN:HE21	1.69	0.41
1:A:396:TYR:HB3	1:A:403:HIS:CE1	2.56	0.41
1:A:775:GLU:O	1:A:776:VAL:HG22	2.20	0.41
1:A:343:PRO:HB2	1:A:348:LEU:HA	2.03	0.41
1:A:312:LYS:CA	1:A:350:ILE:HD11	2.51	0.41
1:A:369:ASN:HD22	1:A:393:HIS:CE1	2.39	0.41
1:A:344:TYR:O	1:A:347:VAL:HG12	2.21	0.40
1:A:79:ILE:HA	1:A:79:ILE:HD13	1.96	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	760/783 (97%)	700 (92%)	45 (6%)	15 (2%)	9 7

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	GLU
1	A	774	TYR
1	A	776	VAL
1	A	73	ILE
1	A	87	SER
1	A	687	THR
1	A	707	LEU
1	A	753	LYS
1	A	775	GLU
1	A	653	LYS
1	A	764	GLU
1	A	717	GLU

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Mol	Chain	Res	Type
1	A	91[A]	ASN
1	A	91[B]	ASN
1	A	173	GLY

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	648/644 (101%)	610 (94%)	38 (6%)	24	34

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

Mol	Chain	Res	Type
1	A	19	ASP
1	A	36	GLU
1	A	84	ILE
1	A	124	SER
1	A	149	SER
1	A	151	LYS
1	A	171	ASP
1	A	194	ARG
1	A	207	ARG
1	A	256	LYS
1	A	283	VAL
1	A	299	ASP
1	A	309	GLU
1	A	347	VAL
1	A	397	TRP
1	A	402	ASP
1	A	454	LEU
1	A	462	VAL
1	A	474	LEU
1	A	477	SER
1	A	480	LYS
1	A	481	THR
1	A	517	LYS

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Mol	Chain	Res	Type
1	A	546	LYS
1	A	551	ARG
1	A	620	ARG
1	A	631	LYS
1	A	634	THR
1	A	678	LEU
1	A	687	THR
1	A	695	ARG
1	A	708	ARG
1	A	711	VAL
1	A	734	GLU
1	A	752	LYS
1	A	772	MSE
1	A	773	LEU
1	A	776	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	168	ASN
1	A	228	ASN
1	A	369	ASN
1	A	416	GLN
1	A	417	GLN
1	A	424	GLN
1	A	581	HIS
1	A	602	HIS
1	A	626	ASN
1	A	699	ASN
1	A	703	HIS

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	SO4	A	801	-	4,4,4	0.46	0	6,6,6	0.24	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
2	SO4	A	801	-	-	0/0/0/0	0/0/0/0

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	739/783 (94%)	-0.21	19 (2%) 59 59	30, 50, 84, 109	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	434	VAL	4.7
1	A	432	LEU	3.5
1	A	549	ALA	3.0
1	A	308	VAL	2.9
1	A	307	THR	2.8
1	A	83	GLY	2.8
1	A	440	ALA	2.8
1	A	435	GLY	2.6
1	A	165	ILE	2.6
1	A	688	ASP	2.5
1	A	90	LYS	2.3
1	A	444	ILE	2.2
1	A	685	LEU	2.2
1	A	395	SER	2.2
1	A	305	ALA	2.1
1	A	167	ILE	2.1
1	A	301	LYS	2.1
1	A	396	TYR	2.0
1	A	433	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
3	NI	A	802	1/1	0.99	0.12	-1.91	63,63,63,63	0
2	SO4	A	801	5/5	0.93	0.12	-	83,92,104,105	0

6.5 Other polymers [i](#)

There are no such residues in this entry.