



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:19 PM GMT

PDB ID : 1F1S  
Title : CRYSTAL STRUCTURE OF STREPTOCOCCUS AGALACTIAE  
HYALURONATE LYASE AT 2.1 ANGSTROM RESOLUTION.  
Authors : Li, S.; Jedrzejas, M.J.  
Deposited on : 2000-05-19  
Resolution : 2.10 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (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

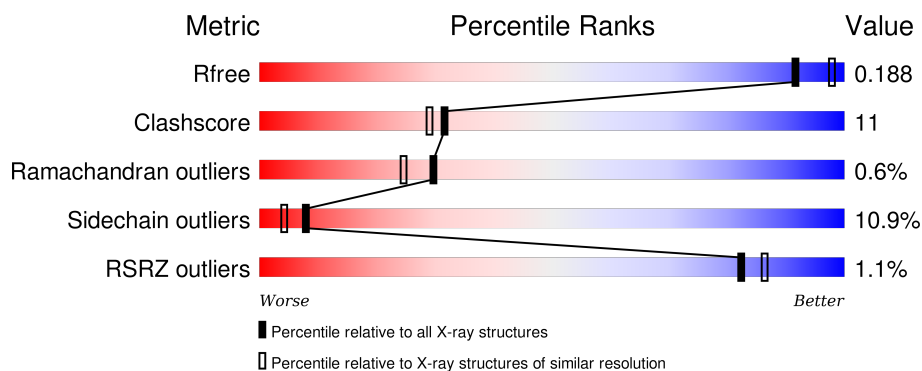
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	814	<div> <div></div> <div>75%</div> <div>20%</div> <div>5%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7051 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 HYALURONATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	814	Total	C	N	O	S	0	0	0
			6513	4101	1108	1286	18			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	ALA	GLY	SEE REMARK 999	UNP Q53591
A	248	THR	PRO	SEE REMARK 999	UNP Q53591
A	280	ASN	THR	SEE REMARK 999	UNP Q53591
A	288	ALA	GLY	SEE REMARK 999	UNP Q53591
A	583	THR	ALA	SEE REMARK 999	UNP Q53591
A	688	PHE	LEU	SEE REMARK 999	UNP Q53591
A	689	TRP	GLY	SEE REMARK 999	UNP Q53591
A	882	GLN	LEU	SEE REMARK 999	UNP Q53591
A	894	MET	LEU	SEE REMARK 999	UNP Q53591

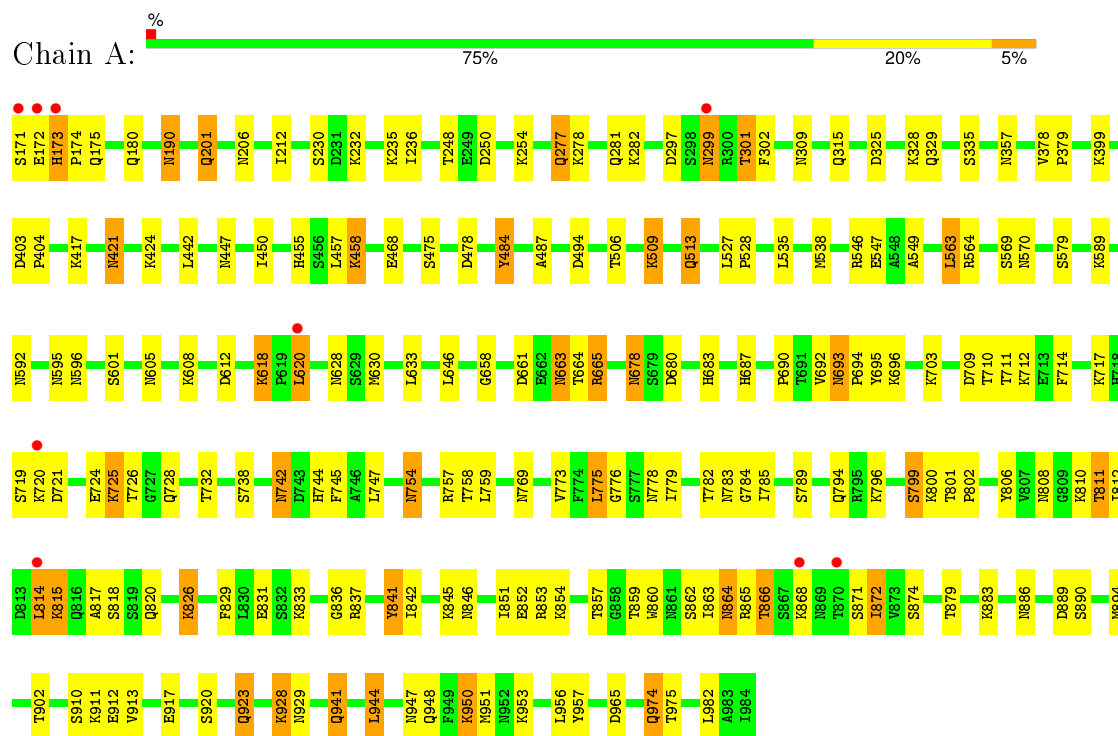
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	538	Total	O	0	0
			538	538		

### 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: HYALURONATE LYASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.27Å 156.76Å 237.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 47.73 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-2.10) 97.0 (47.73-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 2.10Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.191 , 0.253 0.195 , 0.188	Depositor DCC
$R_{free}$ test set	1097 reflections (2.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 61.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 54836 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7051	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.32	0/6640	0.57	0/8987

There are no bond length outliers.

There are no bond angle outliers.

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	6513	0	6402	138	0
2	A	538	0	0	0	0
All	All	7051	0	6402	138	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 11.

All (138) 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:864:ASN:ND2	1:A:866:THR:HB	1.78	0.98
1:A:808:ASN:HD21	1:A:826:LYS:H	0.96	0.95
1:A:190:ASN:H	1:A:190:ASN:HD22	1.16	0.93
1:A:864:ASN:HD21	1:A:866:THR:HB	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:ASN:H	1:A:794:GLN:HE22	1.08	0.92
1:A:299:ASN:HD22	1:A:299:ASN:C	1.76	0.90
1:A:808:ASN:ND2	1:A:826:LYS:H	1.74	0.86
1:A:421:ASN:H	1:A:421:ASN:HD22	1.23	0.85
1:A:742:ASN:HD22	1:A:744:HIS:H	1.24	0.82
1:A:173:HIS:O	1:A:175:GLN:HG2	1.79	0.82
1:A:628:ASN:HD21	1:A:738:SER:H	1.25	0.80
1:A:683:HIS:HE1	1:A:796:LYS:H	1.31	0.79
1:A:277:GLN:HE22	1:A:281:GLN:NE2	1.85	0.74
1:A:817:ALA:HA	1:A:853:ARG:O	1.89	0.72
1:A:941:GLN:HA	1:A:941:GLN:HE21	1.53	0.72
1:A:301:THR:HG22	1:A:302:PHE:HD2	1.54	0.72
1:A:513:GLN:H	1:A:513:GLN:HE21	1.38	0.70
1:A:563:LEU:HD13	1:A:605:ASN:HB3	1.74	0.70
1:A:683:HIS:CE1	1:A:796:LYS:H	2.10	0.70
1:A:808:ASN:HD21	1:A:826:LYS:N	1.80	0.66
1:A:190:ASN:ND2	1:A:248:THR:H	1.94	0.66
1:A:301:THR:HG22	1:A:302:PHE:CD2	2.29	0.66
1:A:944:LEU:HD12	1:A:947:ASN:HA	1.76	0.65
1:A:309:ASN:H	1:A:315:GLN:NE2	1.94	0.65
1:A:277:GLN:HE22	1:A:281:GLN:HE21	1.43	0.65
1:A:779:ILE:O	1:A:889:ASP:HB2	1.97	0.64
1:A:628:ASN:HD21	1:A:738:SER:N	1.95	0.64
1:A:175:GLN:H	1:A:357:ASN:HD21	1.42	0.64
1:A:309:ASN:H	1:A:315:GLN:HE22	1.44	0.64
1:A:421:ASN:H	1:A:421:ASN:ND2	1.96	0.63
1:A:974:GLN:HG3	1:A:975:THR:HG23	1.80	0.62
1:A:857:THR:HG22	1:A:874:SER:HB3	1.80	0.62
1:A:190:ASN:HD21	1:A:248:THR:H	1.46	0.62
1:A:299:ASN:C	1:A:299:ASN:ND2	2.49	0.61
1:A:693:ASN:HD22	1:A:693:ASN:C	2.03	0.61
1:A:693:ASN:N	1:A:794:GLN:HE22	1.91	0.61
1:A:974:GLN:HG3	1:A:975:THR:N	2.15	0.60
1:A:912:GLU:HA	1:A:928:LYS:HG2	1.82	0.60
1:A:754:ASN:HD21	1:A:758:THR:H	1.48	0.60
1:A:864:ASN:HD22	1:A:866:THR:H	1.50	0.60
1:A:190:ASN:H	1:A:190:ASN:ND2	1.93	0.60
1:A:678:ASN:HB2	1:A:836:GLY:O	2.02	0.58
1:A:773:VAL:HG12	1:A:775:LEU:HD13	1.84	0.58
1:A:742:ASN:HD21	1:A:745:PHE:HD1	1.51	0.58
1:A:754:ASN:HD21	1:A:758:THR:N	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:THR:HG22	1:A:872:ILE:HA	1.87	0.57
1:A:175:GLN:H	1:A:357:ASN:ND2	2.03	0.57
1:A:829:PHE:CE2	1:A:831:GLU:HB2	2.40	0.56
1:A:711:THR:HG21	1:A:865:ARG:NH1	2.21	0.56
1:A:678:ASN:ND2	1:A:680:ASP:H	2.02	0.56
1:A:658:GLY:H	1:A:728:GLN:NE2	2.02	0.56
1:A:742:ASN:ND2	1:A:744:HIS:H	1.98	0.55
1:A:468:GLU:HG3	1:A:478:ASP:HA	1.88	0.55
1:A:806:TYR:CE2	1:A:811:THR:HG23	2.42	0.54
1:A:403:ASP:N	1:A:404:PRO:HD2	2.22	0.54
1:A:941:GLN:HE21	1:A:941:GLN:CA	2.20	0.54
1:A:329:GLN:HB3	1:A:335:SER:OG	2.07	0.54
1:A:693:ASN:ND2	1:A:695:TYR:H	2.06	0.54
1:A:230:SER:HB3	1:A:236:ILE:HD13	1.90	0.53
1:A:721:ASP:HB2	1:A:724:GLU:HB3	1.91	0.53
1:A:703:LYS:HE3	1:A:759:LEU:HB2	1.91	0.53
1:A:547:GLU:HG3	1:A:860:TRP:CE2	2.43	0.53
1:A:173:HIS:O	1:A:174:PRO:C	2.45	0.53
1:A:173:HIS:N	1:A:174:PRO:CD	2.72	0.52
1:A:468:GLU:CG	1:A:478:ASP:HA	2.39	0.52
1:A:815:LYS:HB2	1:A:815:LYS:HZ2	1.73	0.52
1:A:678:ASN:HD22	1:A:678:ASN:C	2.13	0.52
1:A:678:ASN:HD22	1:A:680:ASP:H	1.57	0.52
1:A:853:ARG:HH11	1:A:853:ARG:HG2	1.74	0.51
1:A:421:ASN:N	1:A:421:ASN:HD22	1.90	0.51
1:A:494:ASP:O	1:A:564:ARG:NH2	2.43	0.51
1:A:812:ILE:HD12	1:A:814:LEU:HD13	1.94	0.50
1:A:421:ASN:ND2	1:A:421:ASN:N	2.56	0.50
1:A:814:LEU:HD12	1:A:820:GLN:OE1	2.12	0.50
1:A:592:ASN:O	1:A:595:ASN:HB2	2.13	0.49
1:A:442:LEU:HD23	1:A:450:ILE:HD11	1.93	0.49
1:A:664:THR:OG1	1:A:863:ILE:HA	2.13	0.49
1:A:174:PRO:HA	1:A:357:ASN:ND2	2.27	0.49
1:A:513:GLN:NE2	1:A:513:GLN:H	2.09	0.49
1:A:297:ASP:OD2	1:A:299:ASN:ND2	2.45	0.49
1:A:250:ASP:O	1:A:254:LYS:HG3	2.13	0.49
1:A:513:GLN:HE21	1:A:513:GLN:N	2.08	0.49
1:A:776:GLY:O	1:A:890:SER:HB2	2.11	0.49
1:A:378:VAL:HB	1:A:379:PRO:HD3	1.93	0.49
1:A:714:PHE:HA	1:A:717:LYS:NZ	2.28	0.48
1:A:190:ASN:HD22	1:A:190:ASN:N	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:ASN:HD22	1:A:695:TYR:H	1.61	0.48
1:A:747:LEU:HD23	1:A:956:LEU:HB3	1.95	0.48
1:A:829:PHE:HE2	1:A:831:GLU:HB2	1.78	0.48
1:A:665:ARG:HD3	1:A:709:ASP:OD1	2.13	0.48
1:A:721:ASP:O	1:A:725:LYS:HB2	2.14	0.47
1:A:951:MET:HG2	1:A:957:TYR:CE2	2.49	0.47
1:A:758:THR:HA	1:A:782:THR:OG1	2.13	0.47
1:A:661:ASP:HB3	1:A:865:ARG:HB2	1.95	0.47
1:A:814:LEU:HD21	1:A:851:ILE:HG22	1.97	0.47
1:A:687:HIS:C	1:A:690:PRO:HD2	2.36	0.46
1:A:974:GLN:CG	1:A:975:THR:HG23	2.46	0.46
1:A:757:ARG:HG2	1:A:757:ARG:HH11	1.81	0.45
1:A:799:SER:O	1:A:802:PRO:HD3	2.17	0.45
1:A:693:ASN:H	1:A:794:GLN:NE2	1.92	0.45
1:A:201:GLN:HB2	1:A:201:GLN:HE21	1.56	0.45
1:A:683:HIS:HE1	1:A:796:LYS:N	2.08	0.45
1:A:171:SER:O	1:A:173:HIS:N	2.47	0.45
1:A:633:LEU:HB3	1:A:646:LEU:HB2	1.98	0.45
1:A:917:GLU:O	1:A:923:GLN:HA	2.17	0.45
1:A:579:SER:OG	1:A:618:LYS:HD2	2.17	0.45
1:A:484:TYR:CD1	1:A:487:ALA:HB3	2.53	0.44
1:A:710:THR:HG23	1:A:726:THR:HG21	1.99	0.44
1:A:692:VAL:O	1:A:694:PRO:HD3	2.18	0.44
1:A:325:ASP:HA	1:A:328:LYS:HD2	1.98	0.44
1:A:458:LYS:HD3	1:A:458:LYS:HA	1.64	0.43
1:A:173:HIS:O	1:A:175:GLN:N	2.51	0.43
1:A:663:ASN:HA	1:A:663:ASN:HD22	1.66	0.43
1:A:928:LYS:HG3	1:A:929:ASN:N	2.33	0.43
1:A:859:THR:HG22	1:A:871:SER:O	2.18	0.43
1:A:841:TYR:CD1	1:A:841:TYR:N	2.87	0.43
1:A:527:LEU:N	1:A:528:PRO:CD	2.82	0.43
1:A:860:TRP:CE3	1:A:863:ILE:HD11	2.54	0.43
1:A:546:ARG:HB2	1:A:549:ALA:HB3	2.00	0.42
1:A:801:THR:CG2	1:A:833:LYS:HB2	2.50	0.42
1:A:475:SER:HB3	1:A:630:MET:HB3	2.01	0.42
1:A:171:SER:CB	1:A:173:HIS:NE2	2.82	0.42
1:A:570:ASN:HD22	1:A:570:ASN:HA	1.66	0.42
1:A:297:ASP:OD2	1:A:299:ASN:CG	2.59	0.42
1:A:944:LEU:CD2	1:A:950:LYS:HG3	2.50	0.42
1:A:941:GLN:HA	1:A:941:GLN:NE2	2.29	0.41
1:A:773:VAL:CG1	1:A:775:LEU:HD13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:LYS:NZ	1:A:758:THR:OG1	2.44	0.41
1:A:842:ILE:HD12	1:A:894:MET:HE3	2.02	0.41
1:A:944:LEU:HD21	1:A:950:LYS:HD2	2.03	0.41
1:A:783:ASN:CG	1:A:785:ILE:HD12	2.41	0.41
1:A:455:HIS:O	1:A:458:LYS:HB2	2.21	0.40
1:A:506:THR:O	1:A:509:LYS:HE2	2.21	0.40
1:A:608:LYS:O	1:A:612:ASP:HB2	2.21	0.40
1:A:696:LYS:HE3	1:A:879:THR:HG21	2.03	0.40
1:A:894:MET:SD	1:A:913:VAL:HG21	2.61	0.40
1:A:620:LEU:HG	1:A:620:LEU:H	1.66	0.40
1:A:678:ASN:HD21	1:A:680:ASP:HB3	1.86	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	812/814 (100%)	774 (95%)	33 (4%)	5 (1%)	30 24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	GLU
1	A	719	SER
1	A	784	GLY
1	A	769	ASN
1	A	173	HIS

### 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	728/729 (100%)	649 (89%)	79 (11%)	8 4

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	190	ASN
1	A	201	GLN
1	A	206	ASN
1	A	212	ILE
1	A	232	LYS
1	A	235	LYS
1	A	277	GLN
1	A	278	LYS
1	A	282	LYS
1	A	299	ASN
1	A	301	THR
1	A	399	LYS
1	A	417	LYS
1	A	421	ASN
1	A	424	LYS
1	A	447	ASN
1	A	457	LEU
1	A	458	LYS
1	A	484	TYR
1	A	509	LYS
1	A	513	GLN
1	A	535	LEU
1	A	538	MET
1	A	563	LEU
1	A	569	SER
1	A	589	LYS
1	A	596	ASN
1	A	601	SER
1	A	618	LYS

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Mol	Chain	Res	Type
1	A	620	LEU
1	A	663	ASN
1	A	665	ARG
1	A	678	ASN
1	A	693	ASN
1	A	712	LYS
1	A	720	LYS
1	A	725	LYS
1	A	732	THR
1	A	742	ASN
1	A	754	ASN
1	A	775	LEU
1	A	778	ASN
1	A	789	SER
1	A	799	SER
1	A	800	LYS
1	A	810	LYS
1	A	811	THR
1	A	814	LEU
1	A	815	LYS
1	A	818	SER
1	A	826	LYS
1	A	837	ARG
1	A	841	TYR
1	A	845	LYS
1	A	846	ASN
1	A	852	GLU
1	A	854	LYS
1	A	862	SER
1	A	864	ASN
1	A	866	THR
1	A	868	LYS
1	A	872	ILE
1	A	883	LYS
1	A	886	ASN
1	A	902	THR
1	A	910	SER
1	A	911	LYS
1	A	920	SER
1	A	923	GLN
1	A	928	LYS
1	A	941	GLN

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Mol	Chain	Res	Type
1	A	944	LEU
1	A	948	GLN
1	A	950	LYS
1	A	953	LYS
1	A	965	ASP
1	A	974	GLN
1	A	982	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	180	GLN
1	A	190	ASN
1	A	201	GLN
1	A	206	ASN
1	A	266	ASN
1	A	281	GLN
1	A	299	ASN
1	A	315	GLN
1	A	355	HIS
1	A	357	ASN
1	A	421	ASN
1	A	429	ASN
1	A	447	ASN
1	A	498	GLN
1	A	512	ASN
1	A	513	GLN
1	A	570	ASN
1	A	595	ASN
1	A	596	ASN
1	A	605	ASN
1	A	607	ASN
1	A	623	ASN
1	A	628	ASN
1	A	660	ASN
1	A	663	ASN
1	A	678	ASN
1	A	683	HIS
1	A	693	ASN
1	A	718	HIS
1	A	728	GLN

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Mol	Chain	Res	Type
1	A	742	ASN
1	A	754	ASN
1	A	762	GLN
1	A	778	ASN
1	A	787	ASN
1	A	794	GLN
1	A	808	ASN
1	A	846	ASN
1	A	856	GLN
1	A	861	ASN
1	A	864	ASN
1	A	875	ASN
1	A	882	GLN
1	A	886	ASN
1	A	923	GLN
1	A	941	GLN
1	A	946	ASN
1	A	960	GLN
1	A	967	GLN

### 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 ⓘ

There are no ligands in this entry.

### 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 [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	814/814 (100%)	-0.28	9 (1%) 82 86	10, 23, 48, 91	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	GLU	5.9
1	A	171	SER	5.6
1	A	173	HIS	5.5
1	A	620	LEU	3.0
1	A	814	LEU	3.0
1	A	870	THR	2.6
1	A	868	LYS	2.2
1	A	299	ASN	2.1
1	A	720	LYS	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 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.