



Full wwPDB X-ray Structure Validation Report

Oct 20, 2014 – 12:02 PM EDT

PDB ID : 4Q1Q
Title : Crystal structure of TibC-catalyzed hyper-glycosylated TibA55-350 fragment
Authors : Yao, Q.; Lu, Q.; Shao, F.
Deposited on : 2014-04-04
Resolution : 2.11 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

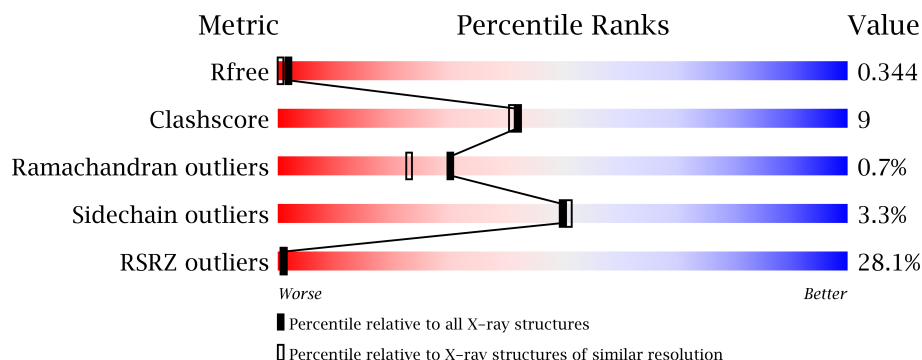
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance

The reported resolution of this entry is 2.11 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}	66092	3409 (2.14-2.10)
Clashscore	79885	4090 (2.14-2.10)
Ramachandran outliers	78287	4048 (2.14-2.10)
Sidechain outliers	78261	4049 (2.14-2.10)
RSRZ outliers	66119	3410 (2.14-2.10)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	305	
1	B	305	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	289	A	401	-	X
2	289	A	404	-	X
2	289	A	408	-	X
2	289	A	409	-	X
2	289	A	410	-	X
2	289	A	411	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	289	A	413	-	X
2	289	A	415	-	X
2	289	A	416	-	X
2	289	A	417	-	X
2	289	A	420	-	X
2	289	A	426	-	X
2	289	A	430	-	X
2	289	A	432	-	X
2	289	A	434	-	X
2	289	A	435	-	X
2	289	B	404	-	X
2	289	B	409	-	X
2	289	B	411	-	X
2	289	B	413	-	X
2	289	B	416	-	X
2	289	B	417	-	X
2	289	B	421	-	X
2	289	B	422	-	X
2	289	B	423	-	X
2	289	B	427	-	X
2	289	B	430	-	X
2	289	B	432	-	X
2	289	B	434	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4712 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

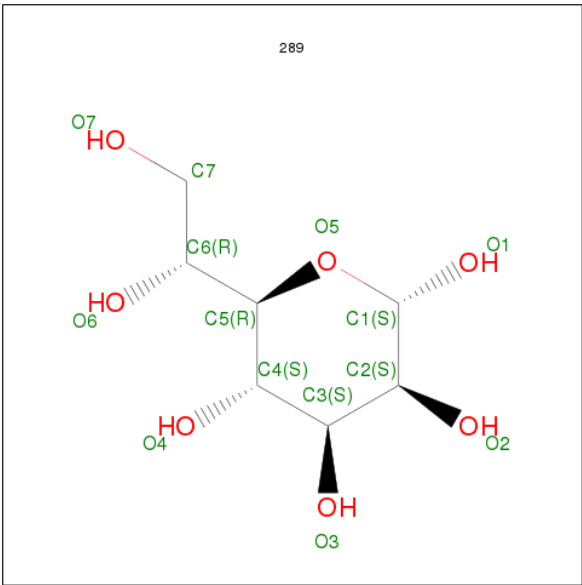
- Molecule 1 is a protein called Adhesin/invasin TibA autotransporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	Se	0	0	0
			1864	1102	345	413	4			
1	B	274	Total	C	N	O	Se	0	0	0
			1864	1102	345	413	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	MSE	-	EXPRESSION TAG	UNP Q9XD84
A	47	ASP	-	EXPRESSION TAG	UNP Q9XD84
A	48	TYR	-	EXPRESSION TAG	UNP Q9XD84
A	49	LYS	-	EXPRESSION TAG	UNP Q9XD84
A	50	ASP	-	EXPRESSION TAG	UNP Q9XD84
A	51	ASP	-	EXPRESSION TAG	UNP Q9XD84
A	52	ASP	-	EXPRESSION TAG	UNP Q9XD84
A	53	ASP	-	EXPRESSION TAG	UNP Q9XD84
A	54	LYS	-	EXPRESSION TAG	UNP Q9XD84
B	46	MSE	-	EXPRESSION TAG	UNP Q9XD84
B	47	ASP	-	EXPRESSION TAG	UNP Q9XD84
B	48	TYR	-	EXPRESSION TAG	UNP Q9XD84
B	49	LYS	-	EXPRESSION TAG	UNP Q9XD84
B	50	ASP	-	EXPRESSION TAG	UNP Q9XD84
B	51	ASP	-	EXPRESSION TAG	UNP Q9XD84
B	52	ASP	-	EXPRESSION TAG	UNP Q9XD84
B	53	ASP	-	EXPRESSION TAG	UNP Q9XD84
B	54	LYS	-	EXPRESSION TAG	UNP Q9XD84

- Molecule 2 is SUGAR (D-GLYCERO-ALPHA-D-MANNO-HEPTOPYRANOSE) (three-letter code: 289) (formula: C₇H₁₄O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		
2	A	1	Total	C	O	0	0
			13	7	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		
2	B	1	Total	C	O	0	0
			13	7	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 13 7 6	0	0
2	B	1	Total C O 13 7 6	0	0
2	B	1	Total C O 13 7 6	0	0
2	B	1	Total C O 13 7 6	0	0
2	B	1	Total C O 13 7 6	0	0
2	B	1	Total C O 13 7 6	0	0
2	B	1	Total C O 13 7 6	0	0
2	B	1	Total C O 13 7 6	0	0
2	B	1	Total C O 13 7 6	0	0
2	B	1	Total C O 13 7 6	0	0
2	B	1	Total C O 13 7 6	0	0
2	B	1	Total C O 13 7 6	0	0
2	B	1	Total C O 13 7 6	0	0
2	B	1	Total C O 13 7 6	0	0
2	B	1	Total C O 13 7 6	0	0

- Molecule 3 is water.

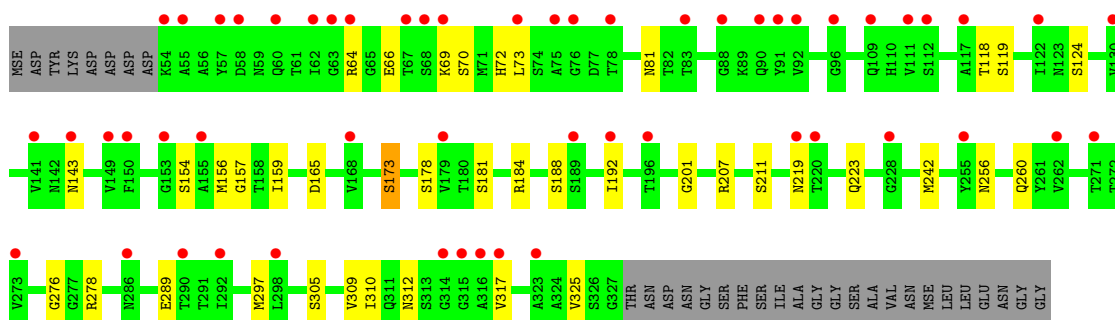
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	22	Total O 22 22	0	0
3	B	52	Total O 52 52	0	0

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.

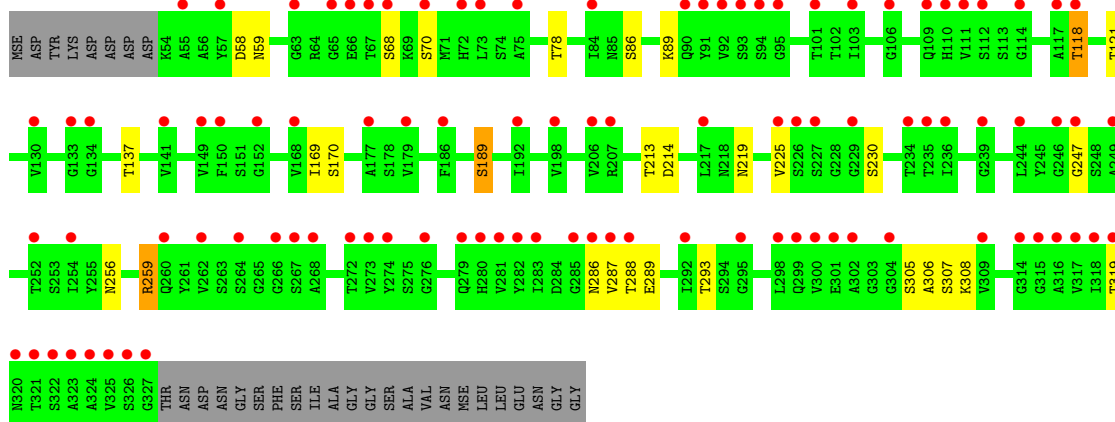
- Molecule 1: Adhesin/invasin TibA autotransporter

Chain A: 



- Molecule 1: Adhesin/invasin TibA autotransporter

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.81Å 62.17Å 97.29Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	19.87 – 2.11 19.86 – 2.11	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.87-2.11) 98.0 (19.86-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 2.11Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.205 , 0.248 0.334 , 0.344	Depositor DCC
R_{free} test set	1597 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.3	EDS
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 31556 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4712	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
289

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	0/1877	0.83	0/2530
1	B	0.35	0/1877	0.86	1/2530 (0.0%)
All	All	0.34	0/3754	0.84	1/5060 (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	B	259	ARG	NE-CZ-NH1	7.26	123.93	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1864	0	1737	26	4
1	B	1864	0	1737	19	2
2	A	455	0	419	32	6
2	B	455	0	407	24	9
3	A	22	0	0	0	0
3	B	52	0	0	1	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4712	0	4300	80	11

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (80) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:435:289:C2	2:B:435:289:C3	1.79	1.58
2:B:433:289:C3	2:B:433:289:C2	1.85	1.51
2:A:413:289:C5	2:A:413:289:O5	1.64	1.44
2:B:433:289:C5	2:B:433:289:O5	1.64	1.42
2:B:406:289:O2	2:B:408:289:O6	1.55	1.24
2:A:413:289:C4	2:A:413:289:O5	2.06	1.02
2:B:433:289:C5	2:B:433:289:C1	2.50	0.89
2:B:435:289:C3	2:B:435:289:H2	2.04	0.88
2:B:433:289:C4	2:B:433:289:C2	2.53	0.86
2:A:413:289:C5	2:A:413:289:C1	2.51	0.83
2:A:410:289:H3	2:A:434:289:O3	1.79	0.81
2:B:404:289:H2	2:B:406:289:O4	1.81	0.81
1:B:286:ASN:HA	1:B:305:SER:O	1.80	0.80
1:B:286:ASN:OD1	1:B:305:SER:HB3	1.83	0.78
2:A:412:289:O7	2:A:412:289:O4	2.04	0.75
2:B:433:289:C4	2:B:433:289:O5	2.35	0.75
2:B:435:289:C2	2:B:435:289:C4	2.62	0.75
1:A:154:SER:OG	2:A:434:289:O3	2.05	0.74
2:B:428:289:O6	3:B:549:HOH:O	2.05	0.74
2:A:406:289:HO3	2:A:406:289:HO6	1.29	0.73
1:B:287:VAL:O	1:B:306:ALA:HA	1.93	0.69
2:A:432:289:O4	2:A:433:289:H6	1.92	0.69
2:A:413:289:H4	2:A:413:289:O5	1.96	0.65
1:B:230:SER:HB2	2:B:416:289:O2	1.98	0.63
2:B:406:289:C2	2:B:408:289:O6	2.47	0.62
1:B:286:ASN:OD1	1:B:305:SER:CB	2.47	0.61
1:B:70:SER:HA	1:B:89:LYS:O	2.00	0.60
1:A:188:SER:HB3	2:A:412:289:H5	1.83	0.60
2:B:433:289:O5	2:B:433:289:H4	2.03	0.59
1:A:156:MSE:HB3	2:A:434:289:O2	2.03	0.59
1:A:81:ASN:OD1	2:A:430:289:H6	2.02	0.58
2:B:433:289:O5	2:B:433:289:C6	2.47	0.57
2:A:432:289:HO4	2:A:433:289:C7	2.17	0.57
2:B:404:289:H2	2:B:406:289:HO4	1.70	0.56
1:A:223:GLN:OE1	1:A:242:MSE:HG3	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:169:ILE:HD12	2:B:411:289:H2	1.88	0.55
1:B:287:VAL:HG22	1:B:306:ALA:HB2	1.89	0.55
2:B:433:289:C4	2:B:433:289:C1	2.85	0.55
1:A:154:SER:HB2	2:A:410:289:C5	2.37	0.54
1:B:256:ASN:HB2	2:B:425:289:H7A	1.90	0.53
1:A:188:SER:CB	2:A:412:289:H5	2.38	0.53
2:B:433:289:C5	2:B:433:289:C2	2.86	0.53
1:A:256:ASN:OD1	1:A:276:GLY:HA3	2.10	0.52
2:B:433:289:O4	2:B:433:289:H7	2.10	0.52
1:B:306:ALA:O	1:B:307:SER:HB3	2.10	0.52
2:A:406:289:C3	2:A:406:289:HO6	2.23	0.52
2:B:433:289:C2	2:B:433:289:O3	2.39	0.51
1:B:58:ASP:OD1	1:B:59:ASN:ND2	2.42	0.50
1:A:119:SER:HB3	2:A:431:289:H7	1.96	0.48
1:A:156:MSE:CB	2:A:434:289:O2	2.61	0.48
1:A:72:HIS:C	1:A:73:LEU:HD12	2.35	0.47
1:B:213:THR:HG22	1:B:214:ASP:OD2	2.14	0.47
1:A:154:SER:HB2	2:A:410:289:H5	1.97	0.46
2:A:413:289:O4	2:A:413:289:H7	2.15	0.46
1:A:278:ARG:HA	1:A:297:MSE:O	2.16	0.46
1:A:173:SER:HB2	2:A:410:289:O5	2.16	0.45
1:B:225:VAL:HG12	1:B:247:GLY:HA3	1.99	0.45
1:A:154:SER:CB	2:A:410:289:C5	2.94	0.45
2:A:412:289:C4	2:A:412:289:O7	2.63	0.44
2:A:413:289:C6	2:A:413:289:O5	2.55	0.43
1:A:188:SER:CB	2:A:412:289:C5	2.97	0.43
1:B:289:GLU:HA	1:B:308:LYS:O	2.18	0.43
1:A:165:ASP:OD1	1:A:184:ARG:HB2	2.19	0.43
1:B:219:ASN:CG	2:B:424:289:H7	2.39	0.43
2:A:425:289:C4	2:A:425:289:HO7	2.31	0.42
1:B:118:THR:CG2	2:B:432:289:O2	2.67	0.42
1:A:181:SER:HA	1:A:201:GLY:HA3	2.00	0.42
1:A:157:GLY:O	1:A:159:ILE:HD12	2.20	0.42
1:A:309:VAL:HG21	1:A:325:VAL:HG13	2.00	0.42
1:A:211:SER:OG	2:A:416:289:H7	2.19	0.42
1:A:207:ARG:NE	2:A:414:289:O2	2.45	0.42
1:A:219:ASN:ND2	2:A:424:289:O6	2.53	0.42
1:A:143:ASN:ND2	2:A:420:289:O3	2.53	0.41
1:A:173:SER:HA	1:A:192:ILE:O	2.21	0.41
1:A:242:MSE:SE	1:A:260:GLN:HE21	2.54	0.41
2:A:420:289:H7	2:A:420:289:H4	1.84	0.41
2:A:425:289:C4	2:A:425:289:O7	2.69	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:286:ASN:OD1	1:B:305:SER:OG	2.39	0.41
1:B:170:SER:HA	1:B:189:SER:O	2.22	0.40
1:B:288:THR:HA	1:B:307:SER:O	2.21	0.40

All (11) 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	Distance(Å)	Clash(Å)
1:A:312:ASN:OD1	3:B:549:HOH:O[2_656]	1.57	0.63
2:A:420:289:C7	2:B:416:289:O7[1_665]	1.59	0.61
2:A:403:289:O4	2:B:409:289:O7[1_665]	1.76	0.44
2:A:403:289:O3	2:B:409:289:O4[1_665]	1.81	0.39
2:A:408:289:O6	2:B:430:289:O3[1_655]	2.06	0.14
1:B:293:THR:OG1	2:B:420:289:O3[1_455]	2.06	0.14
2:A:420:289:C7	2:B:416:289:C7[1_665]	2.12	0.08
1:A:310:ILE:CG2	2:B:428:289:O7[2_656]	2.12	0.08
2:A:420:289:C4	2:B:416:289:O7[1_665]	2.14	0.06
1:A:289:GLU:OE1	2:B:424:289:O3[1_655]	2.18	0.02
1:A:317:VAL:N	1:B:319:THR:O[2_656]	2.19	0.01

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	272/305 (89%)	257 (94%)	13 (5%)	2 (1%)	30	23
1	B	272/305 (89%)	260 (96%)	10 (4%)	2 (1%)	30	23
All	All	544/610 (89%)	517 (95%)	23 (4%)	4 (1%)	30	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	124	SER

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Mol	Chain	Res	Type
1	B	86	SER
1	B	189	SER

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	197/216 (91%)	190 (96%)	7 (4%)	47	47
1	B	197/216 (91%)	191 (97%)	6 (3%)	53	55
All	All	394/432 (91%)	381 (97%)	13 (3%)	50	51

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	GLU
1	A	69	LYS
1	A	70	SER
1	A	118	THR
1	A	173	SER
1	A	178	SER
1	A	305	SER
1	B	68	SER
1	B	78	THR
1	B	118	THR
1	B	121	THR
1	B	137	THR
1	B	259	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	ASN
1	A	320	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

70 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	289	A	401	1	12,13,14	0.62	0	14,18,20	2.08	4 (28%)
2	289	A	402	1	12,13,14	0.59	0	14,18,20	1.24	2 (14%)
2	289	A	403	1	12,13,14	0.53	0	14,18,20	1.15	1 (7%)
2	289	A	404	1	12,13,14	0.54	0	14,18,20	1.71	2 (14%)
2	289	A	405	1	12,13,14	0.58	0	14,18,20	1.20	1 (7%)
2	289	A	406	1	12,13,14	0.56	0	14,18,20	1.41	3 (21%)
2	289	A	407	1	12,13,14	0.51	0	14,18,20	1.88	5 (35%)
2	289	A	408	1	12,13,14	0.53	0	14,18,20	1.08	0
2	289	A	409	1	12,13,14	0.57	0	14,18,20	1.88	5 (35%)
2	289	A	410	1	12,13,14	0.54	0	14,18,20	0.82	0
2	289	A	411	1	12,13,14	0.52	0	14,18,20	1.65	4 (28%)
2	289	A	412	1	12,13,14	0.59	0	14,18,20	2.36	5 (35%)
2	289	A	413	1	12,13,14	3.02	1 (8%)	14,18,20	3.84	2 (14%)
2	289	A	414	1	12,13,14	0.54	0	14,18,20	1.69	3 (21%)
2	289	A	415	1	12,13,14	0.51	0	14,18,20	1.33	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	289	A	416	1	12,13,14	0.59	0	14,18,20	1.66	3 (21%)
2	289	A	417	1	12,13,14	0.54	0	14,18,20	1.59	4 (28%)
2	289	A	418	1	12,13,14	0.55	0	14,18,20	1.55	3 (21%)
2	289	A	419	1	12,13,14	0.52	0	14,18,20	2.50	6 (42%)
2	289	A	420	1	12,13,14	0.54	0	14,18,20	0.84	2 (14%)
2	289	A	421	1	12,13,14	0.51	0	14,18,20	0.88	0
2	289	A	422	1	12,13,14	0.57	0	14,18,20	1.30	1 (7%)
2	289	A	423	1	12,13,14	0.51	0	14,18,20	1.27	1 (7%)
2	289	A	424	1	12,13,14	0.46	0	14,18,20	1.24	2 (14%)
2	289	A	425	1	12,13,14	0.55	0	14,18,20	2.37	6 (42%)
2	289	A	426	1	12,13,14	0.51	0	14,18,20	0.81	0
2	289	A	427	1	12,13,14	0.49	0	14,18,20	0.85	0
2	289	A	428	1	12,13,14	0.56	0	14,18,20	1.33	2 (14%)
2	289	A	429	1	12,13,14	0.58	0	14,18,20	1.47	2 (14%)
2	289	A	430	1	12,13,14	0.52	0	14,18,20	1.19	1 (7%)
2	289	A	431	1	12,13,14	0.52	0	14,18,20	0.76	0
2	289	A	432	1	12,13,14	0.56	0	14,18,20	0.81	1 (7%)
2	289	A	433	1	12,13,14	0.50	0	14,18,20	1.25	1 (7%)
2	289	A	434	1	12,13,14	2.34	4 (33%)	14,18,20	4.76	7 (50%)
2	289	A	435	1	12,13,14	0.53	0	14,18,20	1.05	0
2	289	B	401	1	12,13,14	0.57	0	14,18,20	1.42	3 (21%)
2	289	B	402	1	12,13,14	0.50	0	14,18,20	1.21	0
2	289	B	403	1	12,13,14	0.55	0	14,18,20	1.72	4 (28%)
2	289	B	404	1	12,13,14	0.54	0	14,18,20	1.14	1 (7%)
2	289	B	405	1	12,13,14	0.46	0	14,18,20	2.12	3 (21%)
2	289	B	406	1	12,13,14	0.53	0	14,18,20	0.82	0
2	289	B	407	1	12,13,14	0.56	0	14,18,20	2.23	5 (35%)
2	289	B	408	1	12,13,14	0.50	0	14,18,20	1.66	3 (21%)
2	289	B	409	1	12,13,14	0.51	0	14,18,20	1.13	1 (7%)
2	289	B	410	1	12,13,14	0.57	0	14,18,20	1.33	2 (14%)
2	289	B	411	1	12,13,14	0.55	0	14,18,20	1.08	1 (7%)
2	289	B	412	1	12,13,14	0.58	0	14,18,20	2.24	6 (42%)
2	289	B	413	1	12,13,14	0.48	0	14,18,20	2.49	5 (35%)
2	289	B	414	1	12,13,14	0.57	0	14,18,20	2.25	2 (14%)
2	289	B	415	1	12,13,14	0.68	1 (8%)	14,18,20	1.48	2 (14%)
2	289	B	416	1	12,13,14	4.42	4 (33%)	14,18,20	2.50	6 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	289	B	417	1	12,13,14	0.51	0	14,18,20	1.10	2 (14%)
2	289	B	418	1	12,13,14	0.52	0	14,18,20	1.49	2 (14%)
2	289	B	419	1	12,13,14	0.45	0	14,18,20	2.90	5 (35%)
2	289	B	420	1	12,13,14	0.55	0	14,18,20	2.36	5 (35%)
2	289	B	421	1	12,13,14	0.50	0	14,18,20	1.27	1 (7%)
2	289	B	422	1	12,13,14	0.50	0	14,18,20	1.29	2 (14%)
2	289	B	423	1	12,13,14	0.52	0	14,18,20	1.30	1 (7%)
2	289	B	424	1	12,13,14	0.60	0	14,18,20	2.37	7 (50%)
2	289	B	425	1	12,13,14	0.50	0	14,18,20	1.66	4 (28%)
2	289	B	426	1	12,13,14	0.56	0	14,18,20	3.30	7 (50%)
2	289	B	427	1	12,13,14	0.49	0	14,18,20	1.13	1 (7%)
2	289	B	428	1	12,13,14	0.51	0	14,18,20	2.02	3 (21%)
2	289	B	429	1	12,13,14	0.59	0	14,18,20	1.99	4 (28%)
2	289	B	430	1	12,13,14	0.51	0	14,18,20	1.76	5 (35%)
2	289	B	431	1	12,13,14	0.59	0	14,18,20	1.69	3 (21%)
2	289	B	432	1	12,13,14	0.53	0	14,18,20	1.52	3 (21%)
2	289	B	433	1	12,13,14	7.69	5 (41%)	14,18,20	3.81	5 (35%)
2	289	B	434	1	12,13,14	6.17	7 (58%)	14,18,20	4.63	11 (78%)
2	289	B	435	1	12,13,14	7.93	4 (33%)	14,18,20	7.94	8 (57%)

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	289	A	401	1	-	0/6/23/26	0/1/1/1
2	289	A	402	1	1/1/5/6	0/6/23/26	0/1/1/1
2	289	A	403	1	-	0/6/23/26	0/1/1/1
2	289	A	404	1	-	0/6/23/26	0/1/1/1
2	289	A	405	1	-	0/6/23/26	0/1/1/1
2	289	A	406	1	1/1/5/6	0/6/23/26	0/1/1/1
2	289	A	407	1	-	0/6/23/26	0/1/1/1
2	289	A	408	1	-	0/6/23/26	0/1/1/1
2	289	A	409	1	-	0/6/23/26	0/1/1/1
2	289	A	410	1	-	0/6/23/26	0/1/1/1
2	289	A	411	1	-	0/6/23/26	0/1/1/1
2	289	A	412	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	289	A	413	1	-	0/6/23/26	0/1/1/1
2	289	A	414	1	-	0/6/23/26	0/1/1/1
2	289	A	415	1	-	0/6/23/26	0/1/1/1
2	289	A	416	1	-	0/6/23/26	0/1/1/1
2	289	A	417	1	-	0/6/23/26	0/1/1/1
2	289	A	418	1	-	0/6/23/26	0/1/1/1
2	289	A	419	1	-	0/6/23/26	0/1/1/1
2	289	A	420	1	-	0/6/23/26	0/1/1/1
2	289	A	421	1	1/1/5/6	0/6/23/26	0/1/1/1
2	289	A	422	1	-	0/6/23/26	0/1/1/1
2	289	A	423	1	-	0/6/23/26	0/1/1/1
2	289	A	424	1	-	0/6/23/26	0/1/1/1
2	289	A	425	1	-	0/6/23/26	0/1/1/1
2	289	A	426	1	-	0/6/23/26	0/1/1/1
2	289	A	427	1	-	0/6/23/26	0/1/1/1
2	289	A	428	1	-	0/6/23/26	0/1/1/1
2	289	A	429	1	-	0/6/23/26	0/1/1/1
2	289	A	430	1	-	0/6/23/26	0/1/1/1
2	289	A	431	1	-	0/6/23/26	0/1/1/1
2	289	A	432	1	-	0/6/23/26	0/1/1/1
2	289	A	433	1	1/1/5/6	0/6/23/26	0/1/1/1
2	289	A	434	1	-	0/6/23/26	0/1/1/1
2	289	A	435	1	1/1/5/6	0/6/23/26	0/1/1/1
2	289	B	401	1	-	0/6/23/26	0/1/1/1
2	289	B	402	1	-	0/6/23/26	0/1/1/1
2	289	B	403	1	-	0/6/23/26	0/1/1/1
2	289	B	404	1	-	0/6/23/26	0/1/1/1
2	289	B	405	1	-	0/6/23/26	0/1/1/1
2	289	B	406	1	-	0/6/23/26	0/1/1/1
2	289	B	407	1	-	0/6/23/26	0/1/1/1
2	289	B	408	1	1/1/5/6	0/6/23/26	0/1/1/1
2	289	B	409	1	-	0/6/23/26	0/1/1/1
2	289	B	410	1	-	0/6/23/26	0/1/1/1
2	289	B	411	1	-	0/6/23/26	0/1/1/1
2	289	B	412	1	-	0/6/23/26	0/1/1/1
2	289	B	413	1	-	0/6/23/26	0/1/1/1
2	289	B	414	1	-	0/6/23/26	0/1/1/1
2	289	B	415	1	-	0/6/23/26	0/1/1/1
2	289	B	416	1	-	0/6/23/26	0/1/1/1
2	289	B	417	1	-	0/6/23/26	0/1/1/1
2	289	B	418	1	-	0/6/23/26	0/1/1/1
2	289	B	419	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	289	B	420	1	-	0/6/23/26	0/1/1/1
2	289	B	421	1	-	0/6/23/26	0/1/1/1
2	289	B	422	1	-	0/6/23/26	0/1/1/1
2	289	B	423	1	-	0/6/23/26	0/1/1/1
2	289	B	424	1	-	0/6/23/26	0/1/1/1
2	289	B	425	1	-	0/6/23/26	0/1/1/1
2	289	B	426	1	-	0/6/23/26	0/1/1/1
2	289	B	427	1	-	0/6/23/26	0/1/1/1
2	289	B	428	1	-	0/6/23/26	0/1/1/1
2	289	B	429	1	-	0/6/23/26	0/1/1/1
2	289	B	430	1	-	0/6/23/26	0/1/1/1
2	289	B	431	1	-	0/6/23/26	0/1/1/1
2	289	B	432	1	-	0/6/23/26	0/1/1/1
2	289	B	433	1	-	0/6/23/26	0/1/1/1
2	289	B	434	1	-	0/6/23/26	0/1/1/1
2	289	B	435	1	-	0/6/23/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	435	289	O3-C3	-22.31	0.88	1.43
2	B	434	289	C7-C6	-19.65	0.96	1.52
2	B	433	289	O3-C3	-16.80	1.02	1.43
2	B	433	289	C3-C2	16.21	1.85	1.52
2	B	435	289	C3-C2	13.27	1.79	1.52
2	B	416	289	C3-C2	-11.50	1.29	1.52
2	B	433	289	O5-C5	10.42	1.64	1.45
2	A	413	289	O5-C5	10.38	1.64	1.45
2	B	416	289	O2-C2	8.91	1.62	1.43
2	B	435	289	O2-C2	-7.96	1.26	1.43
2	B	434	289	C6-C5	-6.07	1.39	1.52
2	A	434	289	O3-C3	5.84	1.57	1.43
2	B	433	289	C4-C3	-5.45	1.38	1.52
2	B	433	289	O2-C2	5.02	1.54	1.43
2	A	434	289	O2-C2	4.09	1.52	1.43
2	B	434	289	C4-C5	-3.18	1.43	1.52
2	B	435	289	C4-C3	2.92	1.60	1.52
2	B	416	289	C4-C3	2.88	1.60	1.52
2	B	416	289	O4-C4	2.78	1.49	1.43
2	A	434	289	C4-C3	-2.64	1.45	1.52
2	B	434	289	C3-C2	2.39	1.57	1.52
2	A	434	289	C7-C6	2.20	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	434	289	O6-C6	2.19	1.48	1.43
2	B	434	289	O5-C5	2.13	1.49	1.45
2	B	434	289	O2-C2	-2.06	1.39	1.43
2	B	415	289	O5-C5	-2.00	1.42	1.45

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	435	289	O3-C3-C2	25.10	155.34	109.74
2	A	434	289	C4-C3-C2	14.91	127.23	110.61
2	A	413	289	O5-C5-C4	-13.39	80.78	109.16
2	B	434	289	O5-C5-C6	10.64	125.59	105.93
2	B	433	289	C3-C4-C5	9.24	129.63	109.59
2	B	435	289	C4-C3-C2	-8.32	101.33	110.61
2	B	433	289	C4-C3-C2	-7.24	102.53	110.61
2	B	413	289	O5-C5-C6	7.22	119.28	105.93
2	B	435	289	O4-C4-C3	-6.88	94.98	110.36
2	B	435	289	O3-C3-C4	-6.80	95.17	110.36
2	B	414	289	C6-C5-C4	-6.48	103.65	114.14
2	B	419	289	C4-C3-C2	-6.44	103.43	110.61
2	B	433	289	O5-C5-C4	-6.37	95.67	109.16
2	B	419	289	C6-C5-C4	-6.33	103.91	114.14
2	B	420	289	C6-C5-C4	6.10	124.01	114.14
2	B	426	289	O7-C7-C6	-6.08	97.74	111.06
2	A	419	289	C6-C5-C4	-5.96	104.50	114.14
2	B	424	289	O5-C5-C6	-5.92	94.99	105.93
2	A	434	289	O3-C3-C2	5.88	120.42	109.74
2	B	434	289	O3-C3-C2	5.77	120.22	109.74
2	B	426	289	O6-C6-C5	5.61	122.68	109.02
2	B	434	289	O7-C7-C6	-5.45	99.11	111.06
2	B	428	289	C6-C5-C4	-5.41	105.39	114.14
2	B	412	289	C3-C4-C5	5.38	121.27	109.59
2	B	435	289	C3-C4-C5	5.36	121.22	109.59
2	B	435	289	O2-C2-C3	5.35	121.44	110.10
2	B	426	289	C6-C5-C4	5.29	122.70	114.14
2	B	416	289	O3-C3-C2	4.97	118.76	109.74
2	A	412	289	C4-C3-C2	4.96	116.14	110.61
2	A	412	289	C6-C5-C4	4.75	121.84	114.14
2	B	405	289	C6-C5-C4	-4.73	106.48	114.14
2	B	426	289	O5-C5-C6	-4.62	97.40	105.93
2	A	425	289	C6-C5-C4	4.58	121.56	114.14
2	A	434	289	O3-C3-C4	-4.52	100.27	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	434	289	C3-C4-C5	4.51	119.37	109.59
2	A	413	289	C4-C3-C2	4.50	115.62	110.61
2	B	434	289	O3-C3-C4	4.47	120.35	110.36
2	B	405	289	O5-C5-C6	4.47	114.18	105.93
2	B	434	289	O2-C2-C3	-4.43	100.71	110.10
2	A	425	289	C7-C6-C5	4.26	121.03	112.19
2	B	407	289	O6-C6-C5	4.23	119.32	109.02
2	B	435	289	O5-C5-C4	4.20	118.07	109.16
2	B	416	289	O2-C2-C3	4.19	118.97	110.10
2	B	419	289	O5-C5-C6	4.14	113.57	105.93
2	B	408	289	O5-C5-C6	4.12	113.54	105.93
2	B	434	289	O4-C4-C3	-4.11	101.17	110.36
2	B	434	289	O6-C6-C7	-4.11	99.59	109.22
2	A	414	289	O4-C4-C3	-4.09	101.23	110.36
2	B	426	289	O4-C4-C3	-4.00	101.41	110.36
2	B	428	289	O5-C5-C6	3.96	113.25	105.93
2	B	414	289	O5-C5-C6	3.90	113.14	105.93
2	B	420	289	O5-C5-C6	-3.86	98.79	105.93
2	B	416	289	O4-C4-C5	-3.86	100.82	109.86
2	A	401	289	C6-C5-C4	3.85	120.38	114.14
2	B	430	289	C6-C5-C4	3.79	120.29	114.14
2	A	404	289	O4-C4-C3	-3.78	101.91	110.36
2	B	403	289	C6-C5-C4	-3.71	108.14	114.14
2	B	429	289	C4-C3-C2	3.68	114.71	110.61
2	B	433	289	O4-C4-C3	-3.66	102.18	110.36
2	B	407	289	O7-C7-C6	-3.65	103.06	111.06
2	A	401	289	O4-C4-C3	-3.62	102.27	110.36
2	A	411	289	C3-C4-C5	3.58	117.36	109.59
2	A	412	289	O2-C2-C3	3.58	117.68	110.10
2	B	413	289	O2-C2-C3	3.56	117.64	110.10
2	B	431	289	C4-C3-C2	3.55	114.57	110.61
2	A	429	289	C6-C5-C4	3.51	119.82	114.14
2	B	434	289	O6-C6-C5	3.47	117.48	109.02
2	A	409	289	C6-C5-C4	3.47	119.76	114.14
2	A	419	289	O3-C3-C2	3.47	116.04	109.74
2	A	434	289	O2-C2-C3	-3.44	102.82	110.10
2	A	425	289	C4-C3-C2	3.39	114.39	110.61
2	B	420	289	O4-C4-C3	-3.32	102.95	110.36
2	A	406	289	O5-C5-C6	3.31	112.05	105.93
2	A	416	289	C6-C5-C4	3.31	119.50	114.14
2	A	430	289	C4-C3-C2	3.29	114.27	110.61
2	B	405	289	O7-C7-C6	-3.25	103.94	111.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	412	289	C3-C4-C5	3.23	116.58	109.59
2	B	432	289	C6-C5-C4	3.22	119.36	114.14
2	B	407	289	O5-C5-C6	-3.21	100.00	105.93
2	B	416	289	O4-C4-C3	3.17	117.43	110.36
2	A	418	289	C6-C5-C4	3.15	119.24	114.14
2	B	429	289	C6-C5-C4	3.14	119.23	114.14
2	A	409	289	O4-C4-C3	-3.13	103.35	110.36
2	B	418	289	O7-C7-C6	-3.13	104.19	111.06
2	A	404	289	C3-C4-C5	3.12	116.34	109.59
2	A	419	289	O5-C5-C4	3.11	115.76	109.16
2	B	435	289	O4-C4-C5	3.11	117.15	109.86
2	B	423	289	O7-C7-C6	-3.05	104.38	111.06
2	B	415	289	O4-C4-C3	-3.04	103.56	110.36
2	A	407	289	O5-C5-C6	-3.04	100.31	105.93
2	B	408	289	O2-C2-C3	-3.02	103.69	110.10
2	A	434	289	C6-C5-C4	-3.01	109.27	114.14
2	B	434	289	C6-C5-C4	3.00	119.00	114.14
2	B	407	289	C6-C5-C4	3.00	119.00	114.14
2	B	412	289	C6-C5-C4	-3.00	109.30	114.14
2	A	403	289	C6-C5-C4	2.99	118.99	114.14
2	B	413	289	O3-C3-C2	2.99	115.17	109.74
2	A	407	289	C6-C5-C4	2.95	118.93	114.14
2	A	401	289	C3-C4-C5	2.95	115.98	109.59
2	A	405	289	C4-C3-C2	-2.94	107.33	110.61
2	B	425	289	O2-C2-C3	2.94	116.33	110.10
2	A	401	289	O7-C7-C6	2.92	117.44	111.06
2	B	401	289	C3-C4-C5	2.91	115.90	109.59
2	B	429	289	O4-C4-C5	2.89	116.64	109.86
2	A	416	289	C4-C3-C2	2.89	113.83	110.61
2	A	434	289	C3-C4-C5	-2.87	103.36	109.59
2	A	407	289	O6-C6-C5	2.86	115.99	109.02
2	A	425	289	O7-C7-C6	2.86	117.32	111.06
2	A	419	289	C4-C3-C2	-2.81	107.48	110.61
2	B	431	289	O4-C4-C3	-2.81	104.09	110.36
2	A	418	289	O5-C5-C6	-2.80	100.75	105.93
2	B	425	289	O4-C4-C3	-2.80	104.09	110.36
2	A	411	289	O4-C4-C3	-2.80	104.10	110.36
2	A	417	289	C4-C3-C2	-2.78	107.51	110.61
2	B	403	289	C4-C3-C2	2.77	113.69	110.61
2	A	409	289	O7-C7-C6	2.75	117.08	111.06
2	B	424	289	C7-C6-C5	-2.74	106.49	112.19
2	A	425	289	O4-C4-C3	-2.70	104.32	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	289	C4-C3-C2	2.69	113.61	110.61
2	B	416	289	O5-C5-C4	2.66	114.81	109.16
2	B	424	289	C6-C5-C4	2.66	118.44	114.14
2	B	412	289	O5-C5-C4	2.66	114.80	109.16
2	A	402	289	C6-C5-C4	2.65	118.43	114.14
2	B	421	289	O5-C5-C4	2.65	114.77	109.16
2	A	414	289	C6-C5-C4	2.64	118.42	114.14
2	A	422	289	O5-C5-C6	2.64	110.81	105.93
2	B	424	289	O7-C7-C6	-2.63	105.29	111.06
2	A	407	289	O4-C4-C3	-2.62	104.50	110.36
2	B	412	289	O4-C4-C3	-2.62	104.51	110.36
2	A	415	289	O4-C4-C5	2.62	115.99	109.86
2	B	434	289	O4-C4-C5	2.60	115.96	109.86
2	A	433	289	O3-C3-C2	2.60	114.46	109.74
2	B	426	289	C7-C6-C5	-2.60	106.79	112.19
2	B	410	289	C4-C3-C2	2.57	113.48	110.61
2	B	422	289	O5-C5-C6	2.57	110.68	105.93
2	B	412	289	O4-C4-C5	-2.57	103.83	109.86
2	B	425	289	C6-C5-C4	2.57	118.30	114.14
2	B	424	289	O6-C6-C5	2.55	115.23	109.02
2	B	430	289	O7-C7-C6	-2.55	105.47	111.06
2	B	419	289	O7-C7-C6	-2.54	105.50	111.06
2	B	404	289	C3-C4-C5	2.50	115.00	109.59
2	B	413	289	O5-C5-C4	-2.48	103.90	109.16
2	A	417	289	C6-C5-C4	2.47	118.14	114.14
2	B	429	289	O3-C3-C2	-2.47	105.26	109.74
2	B	422	289	C6-C5-C4	-2.42	110.24	114.14
2	B	418	289	C6-C5-C4	2.40	118.03	114.14
2	A	423	289	O7-C7-C6	-2.38	105.85	111.06
2	B	416	289	C6-C5-C4	-2.36	110.32	114.14
2	A	417	289	O5-C5-C6	-2.35	101.58	105.93
2	B	417	289	O5-C5-C6	2.34	110.25	105.93
2	B	424	289	C4-C3-C2	-2.33	108.01	110.61
2	A	419	289	O6-C6-C5	-2.33	103.35	109.02
2	B	401	289	O3-C3-C2	-2.31	105.55	109.74
2	A	409	289	C7-C6-C5	2.31	116.99	112.19
2	B	412	289	O5-C5-C6	2.31	110.19	105.93
2	B	408	289	C3-C4-C5	2.30	114.57	109.59
2	A	416	289	O5-C5-C4	-2.29	104.31	109.16
2	A	424	289	O4-C4-C5	2.29	115.22	109.86
2	B	409	289	O5-C5-C6	2.28	110.15	105.93
2	B	430	289	O3-C3-C2	2.27	113.87	109.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	415	289	C3-C4-C5	2.27	114.51	109.59
2	A	424	289	O4-C4-C3	-2.26	105.30	110.36
2	B	432	289	O2-C2-C3	2.25	114.88	110.10
2	B	411	289	O6-C6-C5	2.24	114.47	109.02
2	B	419	289	O5-C5-C4	2.24	113.91	109.16
2	B	401	289	C4-C3-C2	2.23	113.10	110.61
2	B	403	289	O5-C5-C4	2.23	113.89	109.16
2	A	428	289	O5-C5-C4	2.21	113.84	109.16
2	B	430	289	O2-C2-C3	2.20	114.77	110.10
2	B	432	289	O4-C4-C5	2.19	114.99	109.86
2	B	430	289	O4-C4-C5	2.17	114.95	109.86
2	B	426	289	O5-C5-C4	2.17	113.77	109.16
2	B	420	289	O5-C5-C4	-2.17	104.57	109.16
2	A	428	289	O4-C4-C5	-2.16	104.80	109.86
2	A	406	289	C3-C4-C5	2.15	114.26	109.59
2	A	417	289	O4-C4-C3	-2.14	105.58	110.36
2	A	434	289	C7-C6-C5	-2.13	107.75	112.19
2	A	418	289	O4-C4-C5	2.13	114.86	109.86
2	A	425	289	O5-C5-C6	2.12	109.85	105.93
2	A	406	289	C6-C5-C4	-2.11	110.73	114.14
2	B	413	289	C6-C5-C4	-2.10	110.74	114.14
2	B	427	289	O3-C3-C4	-2.10	105.67	110.36
2	B	410	289	C3-C4-C5	2.08	114.11	109.59
2	B	424	289	O3-C3-C4	2.08	115.01	110.36
2	A	412	289	O4-C4-C3	-2.08	105.70	110.36
2	A	432	289	O5-C5-C6	2.08	109.77	105.93
2	B	431	289	O4-C4-C5	2.07	114.72	109.86
2	B	433	289	C6-C5-C4	-2.07	110.80	114.14
2	A	402	289	O4-C4-C3	-2.06	105.75	110.36
2	A	411	289	O5-C5-C4	2.06	113.53	109.16
2	A	407	289	C3-C4-C5	2.05	114.04	109.59
2	B	428	289	O7-C7-C6	-2.05	106.56	111.06
2	A	420	289	C6-C5-C4	-2.05	110.83	114.14
2	A	414	289	O5-C5-C6	-2.04	102.17	105.93
2	B	425	289	O6-C6-C5	2.04	113.98	109.02
2	B	403	289	O3-C3-C4	-2.03	105.81	110.36
2	A	409	289	C4-C3-C2	2.02	112.86	110.61
2	A	419	289	O2-C2-C3	2.02	114.38	110.10
2	B	420	289	O6-C6-C5	2.01	113.91	109.02
2	A	429	289	O4-C4-C3	-2.01	105.87	110.36
2	B	417	289	C3-C4-C5	2.00	113.93	109.59
2	A	420	289	O5-C5-C6	2.00	109.63	105.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	407	289	O4-C4-C3	-2.00	105.89	110.36

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	433	289	C1
2	A	406	289	C1
2	A	402	289	C1
2	B	408	289	C1
2	A	421	289	C1
2	A	435	289	C1

There are no torsion outliers.

There are no ring outliers.

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	274/305 (89%)	1.37	54 (19%) 2 1	40, 55, 83, 95	0
1	B	274/305 (89%)	1.83	100 (36%) 1 1	33, 46, 76, 98	0
All	All	548/610 (89%)	1.60	154 (28%) 1 1	33, 51, 81, 98	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	GLY	16.3
1	A	76	GLY	8.6
1	A	111	VAL	5.6
1	B	326	SER	5.5
1	A	130	VAL	4.8
1	B	319	THR	4.8
1	B	320	ASN	4.7
1	A	92	VAL	4.6
1	A	64	ARG	4.5
1	B	298	LEU	4.3
1	B	324	ALA	4.3
1	B	73	LEU	4.1
1	A	58	ASP	4.1
1	B	300	VAL	4.0
1	A	149	VAL	4.0
1	B	321	THR	3.9
1	B	179	VAL	3.9
1	A	62	ILE	3.8
1	A	315	GLY	3.7
1	B	281	VAL	3.7
1	A	88	GLY	3.6
1	B	302	ALA	3.6
1	A	91	TYR	3.6
1	A	54	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	247	GLY	3.5
1	B	92	VAL	3.5
1	A	298	LEU	3.5
1	B	266	GLY	3.5
1	A	117	ALA	3.5
1	B	318	ILE	3.5
1	A	55	ALA	3.4
1	B	117	ALA	3.4
1	A	63	GLY	3.4
1	B	246	GLY	3.4
1	A	317	VAL	3.4
1	B	84	ILE	3.4
1	B	229	GLY	3.3
1	A	262	VAL	3.3
1	B	254	ILE	3.2
1	B	111	VAL	3.2
1	B	262	VAL	3.2
1	A	323	ALA	3.2
1	B	150	PHE	3.2
1	B	273	VAL	3.2
1	B	323	ALA	3.2
1	B	292	ILE	3.2
1	B	314	GLY	3.1
1	B	130	VAL	3.1
1	B	252	THR	3.1
1	B	186	PHE	3.1
1	B	315	GLY	3.1
1	B	217	LEU	3.1
1	B	91	TYR	3.0
1	B	67	THR	3.0
1	B	206	VAL	2.9
1	B	239	GLY	2.9
1	B	322	SER	2.9
1	A	290	THR	2.9
1	B	57	TYR	2.9
1	A	192	ILE	2.8
1	A	67	THR	2.8
1	B	95	GLY	2.8
1	B	168	VAL	2.8
1	B	133	GLY	2.8
1	A	179	VAL	2.7
1	B	141	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	234	THR	2.7
1	B	236	ILE	2.7
1	B	268	ALA	2.7
1	A	83	THR	2.7
1	A	255	TYR	2.7
1	B	90	GLN	2.7
1	B	63	GLY	2.7
1	B	101	THR	2.6
1	B	286	ASN	2.6
1	B	225	VAL	2.6
1	A	189	SER	2.6
1	A	109	GLN	2.6
1	A	96	GLY	2.6
1	B	295	GLY	2.6
1	A	90	GLN	2.6
1	B	112	SER	2.6
1	B	249	ALA	2.6
1	B	260	GLN	2.6
1	B	227	SER	2.5
1	B	276	GLY	2.5
1	B	285	GLY	2.5
1	A	57	TYR	2.5
1	B	198	VAL	2.5
1	A	69	LYS	2.5
1	B	134	GLY	2.5
1	A	60	GLN	2.5
1	A	273	VAL	2.5
1	A	314	GLY	2.5
1	B	244	LEU	2.5
1	B	309	VAL	2.5
1	B	317	VAL	2.5
1	B	109	GLN	2.5
1	A	73	LEU	2.4
1	B	75	ALA	2.4
1	B	72	HIS	2.4
1	B	114	GLY	2.4
1	B	235	THR	2.4
1	A	316	ALA	2.4
1	B	207	ARG	2.4
1	A	219	ASN	2.4
1	B	226	SER	2.4
1	B	68	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	118	THR	2.3
1	A	228	GLY	2.3
1	B	283	ILE	2.3
1	B	267	SER	2.3
1	B	288	THR	2.3
1	A	286	ASN	2.3
1	B	177	ALA	2.3
1	A	78	THR	2.3
1	B	325	VAL	2.3
1	B	316	ALA	2.3
1	A	220	THR	2.3
1	B	279	GLN	2.3
1	B	282	TYR	2.3
1	A	68	SER	2.3
1	A	143	ASN	2.3
1	B	192	ILE	2.3
1	A	292	ILE	2.2
1	B	103	ILE	2.2
1	B	301	GLU	2.2
1	A	153	GLY	2.2
1	B	66	GLU	2.2
1	A	155	ALA	2.2
1	B	149	VAL	2.2
1	A	196	THR	2.2
1	A	168	VAL	2.2
1	B	152	GLY	2.2
1	B	94	SER	2.2
1	B	274	TYR	2.1
1	B	110	HIS	2.1
1	B	287	VAL	2.1
1	A	122	ILE	2.1
1	A	271	THR	2.1
1	B	272	THR	2.1
1	B	65	GLY	2.1
1	A	112	SER	2.1
1	B	304	GLY	2.1
1	B	299	GLN	2.1
1	A	141	VAL	2.1
1	B	70	SER	2.1
1	B	264	SER	2.1
1	B	93	SER	2.0
1	A	150	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	75	ALA	2.0
1	B	55	ALA	2.0
1	B	280	HIS	2.0
1	B	106	GLY	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	289	B	413	13/14	0.32	30.33	74,88,101,105	0
2	289	A	401	13/14	0.34	14.86	93,99,109,111	0
2	289	A	434	13/14	0.44	8.13	86,93,101,102	0
2	289	B	422	13/14	0.28	4.61	63,71,79,81	0
2	289	A	435	13/14	0.42	4.52	98,114,121,124	0
2	289	A	409	13/14	0.36	4.23	80,95,106,112	0
2	289	A	408	13/14	0.30	3.53	76,87,100,106	0
2	289	A	404	13/14	0.32	3.47	78,98,108,114	0
2	289	A	416	13/14	0.26	3.45	75,80,95,106	0
2	289	A	410	13/14	0.33	3.43	64,80,94,96	0
2	289	B	411	13/14	0.34	3.22	80,87,100,100	0
2	289	A	411	13/14	0.33	3.15	77,92,105,110	0
2	289	B	430	13/14	0.26	3.11	75,81,89,93	0
2	289	A	417	13/14	0.27	3.02	49,61,81,82	0
2	289	B	417	13/14	0.33	2.90	84,92,104,118	0
2	289	A	415	13/14	0.23	2.72	62,68,88,89	0
2	289	A	430	13/14	0.25	2.61	66,76,94,97	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	289	A	432	13/14	0.30	2.60	106,114,124,128	0
2	289	A	426	13/14	0.30	2.46	69,78,88,94	0
2	289	B	416	13/14	0.34	2.40	96,114,120,129	0
2	289	B	427	13/14	0.32	2.38	49,56,60,63	0
2	289	A	413	13/14	0.29	2.20	117,121,127,128	0
2	289	B	434	13/14	0.38	2.15	88,101,124,125	0
2	289	B	423	13/14	0.23	2.15	53,60,77,83	0
2	289	B	421	13/14	0.23	2.13	61,73,80,80	0
2	289	B	432	13/14	0.32	2.12	88,101,109,117	0
2	289	B	404	13/14	0.30	2.11	72,85,96,97	0
2	289	B	409	13/14	0.37	2.10	105,115,124,129	0
2	289	A	420	13/14	0.29	2.03	81,95,101,101	0
2	289	A	406	13/14	0.25	1.96	77,86,101,101	0
2	289	A	422	13/14	0.25	1.78	71,82,92,94	0
2	289	A	421	13/14	0.26	1.67	83,90,101,103	0
2	289	A	433	13/14	0.26	1.63	95,100,106,106	0
2	289	B	425	13/14	0.27	1.62	51,56,73,76	0
2	289	B	435	13/14	0.38	1.57	94,107,115,131	0
2	289	A	403	13/14	0.43	1.47	89,101,117,117	0
2	289	B	424	13/14	0.26	1.33	48,55,67,69	0
2	289	A	425	13/14	0.22	1.23	66,74,95,101	0
2	289	B	408	13/14	0.28	1.21	90,103,112,124	0
2	289	B	401	13/14	0.33	1.17	86,98,102,111	0
2	289	B	433	13/14	0.27	1.14	91,99,105,112	0
2	289	A	419	13/14	0.18	1.04	57,65,74,77	0
2	289	B	412	13/14	0.28	1.01	71,93,108,116	0
2	289	B	406	13/14	0.28	1.01	78,88,100,105	0
2	289	B	415	13/14	0.29	0.85	73,79,92,94	0
2	289	A	414	13/14	0.19	0.77	60,66,87,89	0
2	289	B	402	13/14	0.30	0.72	58,67,90,105	0
2	289	B	410	13/14	0.26	0.64	54,70,84,86	0
2	289	B	418	13/14	0.24	0.61	44,51,64,70	0
2	289	B	426	13/14	0.24	0.43	47,56,66,67	0
2	289	B	428	13/14	0.25	0.34	67,74,85,94	0
2	289	B	420	13/14	0.18	0.03	40,44,71,74	0
2	289	A	431	13/14	0.19	0.02	74,81,90,95	0
2	289	A	427	13/14	0.22	-0.14	65,71,89,97	0
2	289	A	423	13/14	0.16	-0.22	76,80,87,93	0
2	289	B	429	13/14	0.16	-0.26	51,59,82,91	0
2	289	B	414	13/14	0.21	-0.34	49,65,82,93	0
2	289	A	428	13/14	0.20	-0.51	59,66,73,85	0
2	289	A	412	13/14	0.16	-0.52	73,84,89,99	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	289	B	403	13/14	0.22	-0.55	73,85,94,100	0
2	289	A	402	13/14	0.24	-0.67	62,73,83,88	0
2	289	A	424	13/14	0.15	-0.68	67,73,81,93	0
2	289	B	431	13/14	0.15	-0.91	58,65,72,74	0
2	289	A	418	13/14	0.11	-1.08	48,51,78,83	0
2	289	A	407	13/14	0.15	-1.08	56,65,76,88	0
2	289	A	429	13/14	0.14	-1.20	66,70,83,86	0
2	289	B	419	13/14	0.20	-1.21	54,59,72,72	0
2	289	A	405	13/14	0.16	-1.31	58,67,80,83	0
2	289	B	407	13/14	0.19	-1.68	47,56,71,89	0
2	289	B	405	13/14	0.18	-4.57	53,63,83,86	0

6.5 Other polymers ⓘ

There are no such residues in this entry.