



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:59 PM UTC

PDB ID : 4Q1Q / pdb_00004q1q
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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

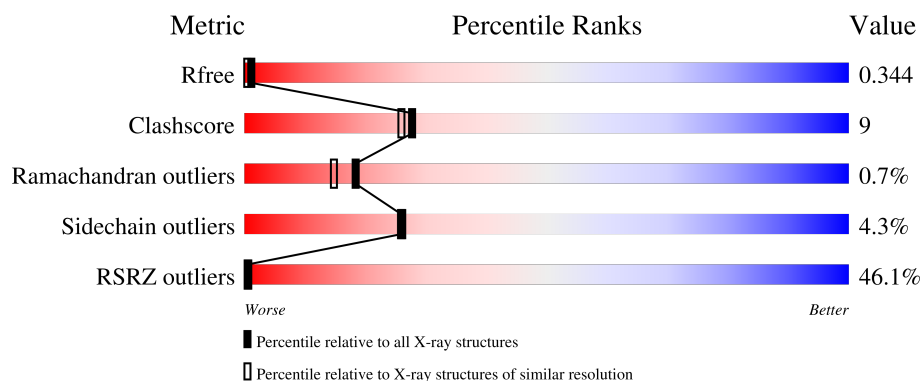
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	289	A	402	X	-	-	-
2	289	A	406	X	-	-	-
2	289	A	413	-	-	X	-
2	289	A	421	X	-	-	-
2	289	A	433	X	-	-	-
2	289	A	435	X	-	-	-
2	289	B	408	X	-	-	-
2	289	B	433	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4712 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.

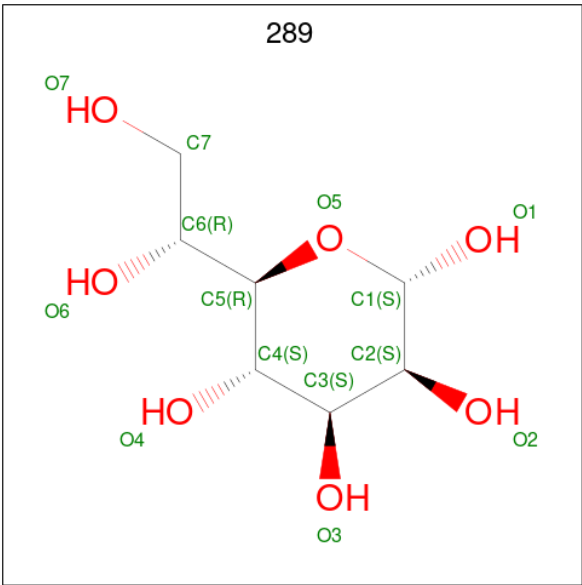
- Molecule 1 is a protein called Adhesin/invasin TibA autotransporter.

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 D-glycero-alpha-D-manno-heptopyranose (CCD ID: 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	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		

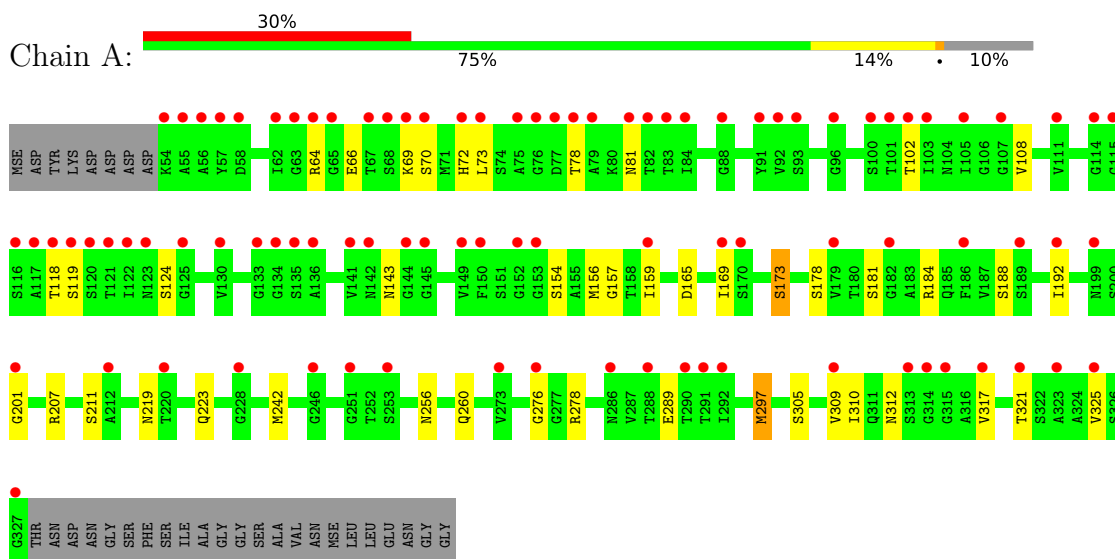
- Molecule 3 is water.

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

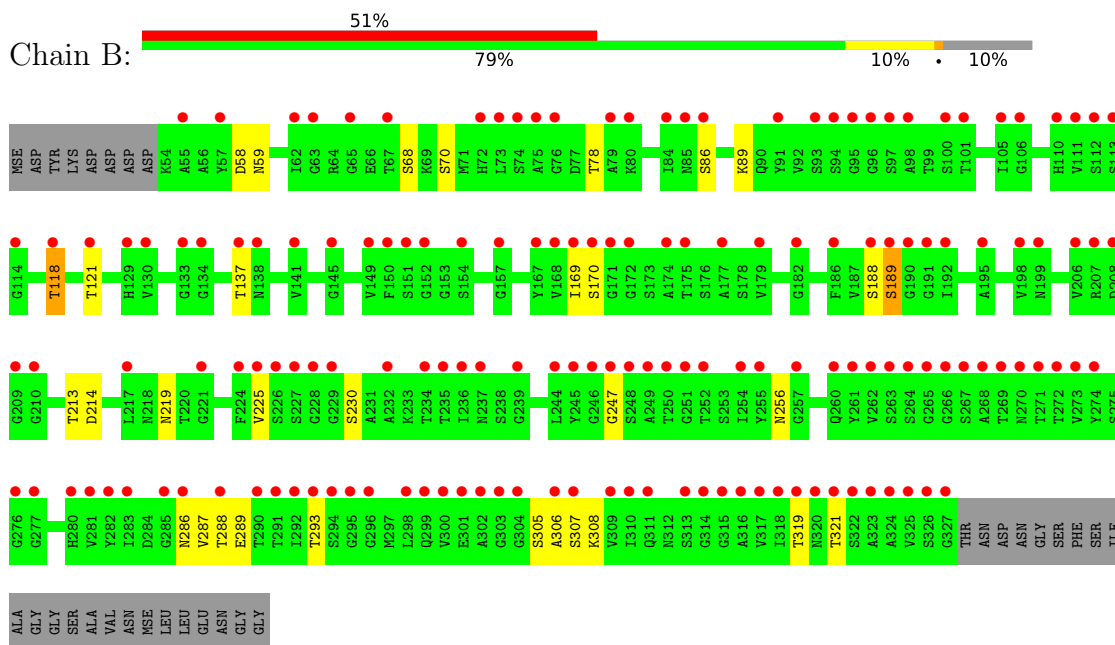
3 Residue-property plots

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



- Molecule 1: Adhesin/invasin TibA autotransporter



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 19.87 – 2.11	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.87-2.11) 97.8 (19.87-2.11)	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 0.336 , 0.344	Depositor DCC
R_{free} test set	1598 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	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.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.45	0/1877	1.09	2/2530 (0.1%)
1	B	0.47	0/1877	1.09	1/2530 (0.0%)
All	All	0.46	0/3754	1.09	3/5060 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	MSE	N-CA-C	5.42	118.29	108.69
1	B	188	SER	N-CA-C	5.42	116.21	108.74
1	A	108	VAL	N-CA-C	5.41	115.91	108.12

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	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

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 9.

All (80) 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)
2:B:435:289:C2	2:B:435:289:C3	1.79	1.58
2:B:433:289:C2	2:B:433:289:C3	1.85	1.51
2:A:413:289:O5	2:A:413:289:C5	1.64	1.44
2:B:433:289:O5	2:B:433:289:C5	1.64	1.42
2:B:406:289:O2	2:B:408:289:O6	1.55	1.24
2:A:413:289:O5	2:A:413:289:C4	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:C2	2:B:433:289:C4	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:O5	2:B:433:289:C4	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:O5	2:A:413:289:H4	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:B:404:289:H2	2:B:406:289:HO4	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLN:OE1	1:A:242:MSE:HG3	2.05	0.56
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:C1	2:B:433:289:C4	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:C2	2:B:433:289:C5	2.86	0.53
1:A:72:HIS:C	1:A:73:LEU:HD12	2.35	0.52
1:A:256:ASN:OD1	1:A:276:GLY:HA3	2.10	0.52
2:B:433:289:H7	2:B:433:289:O4	2.10	0.52
1:B:306:ALA:O	1:B:307:SER:HB3	2.10	0.52
2:A:406:289:HO6	2:A:406:289:C3	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:B:213:THR:HG22	1:B:214:ASP:OD2	2.14	0.47
1:B:219:ASN:CG	2:B:424:289:H7	2.39	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:O7	2:A:412:289:C4	2.63	0.44
2:A:413:289:O5	2:A:413:289:C6	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
2:A:432:289:O4	2:A:433:289:O7	2.33	0.43
2:A:425:289:HO7	2:A:425:289:C4	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:211:SER:OG	2:A:416:289:H7	2.19	0.42
1:A:309:VAL:HG21	1:A:325:VAL:HG13	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	Interatomic distance (Å)	Clash overlap (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
1:A:310:ILE:CG2	2:B:428:289:O7[2_656]	2.12	0.08
2:A:420:289:C7	2:B:416:289:C7[1_665]	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%)	18	15
1	B	272/305 (89%)	260 (96%)	10 (4%)	2 (1%)	18	15
All	All	544/610 (89%)	517 (95%)	23 (4%)	4 (1%)	18	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	124	SER
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%)	186 (94%)	11 (6%)	19	17
1	B	197/216 (91%)	191 (97%)	6 (3%)	36	40
All	All	394/432 (91%)	377 (96%)	17 (4%)	26	26

All (17) 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	78	THR
1	A	102	THR
1	A	118	THR
1	A	169	ILE
1	A	173	SER
1	A	178	SER
1	A	305	SER
1	A	321	THR
1	B	68	SER
1	B	78	THR
1	B	118	THR
1	B	121	THR
1	B	137	THR
1	B	321	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	123	ASN
1	A	127	HIS
1	A	142	ASN
1	A	161	ASN
1	A	219	ASN
1	A	312	ASN
1	A	320	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	413	1	13,13,14	0.49	0	16,18,20	1.66	3 (18%)
2	289	B	421	1	13,13,14	0.46	0	16,18,20	1.43	3 (18%)
2	289	A	428	1	13,13,14	0.20	0	16,18,20	1.90	4 (25%)
2	289	B	407	1	13,13,14	0.26	0	16,18,20	1.96	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	289	B	416	1	13,13,14	5.13	5 (38%)	16,18,20	3.39	7 (43%)
2	289	B	414	1	13,13,14	0.31	0	16,18,20	1.43	2 (12%)
2	289	A	430	1	13,13,14	0.29	0	16,18,20	1.09	0
2	289	B	426	1	13,13,14	0.25	0	16,18,20	3.00	6 (37%)
2	289	B	430	1	13,13,14	0.32	0	16,18,20	1.48	2 (12%)
2	289	B	422	1	13,13,14	0.27	0	16,18,20	1.08	0
2	289	A	414	1	13,13,14	0.28	0	16,18,20	1.59	2 (12%)
2	289	B	420	1	13,13,14	0.43	0	16,18,20	2.13	3 (18%)
2	289	A	433	1	13,13,14	0.31	0	16,18,20	1.25	3 (18%)
2	289	A	408	1	13,13,14	0.24	0	16,18,20	1.49	1 (6%)
2	289	A	410	1	13,13,14	0.24	0	16,18,20	0.48	0
2	289	A	402	1	13,13,14	0.33	0	16,18,20	1.17	1 (6%)
2	289	B	427	1	13,13,14	0.28	0	16,18,20	1.40	3 (18%)
2	289	A	419	1	13,13,14	0.21	0	16,18,20	1.96	5 (31%)
2	289	B	415	1	13,13,14	0.34	0	16,18,20	1.49	4 (25%)
2	289	A	416	1	13,13,14	0.45	0	16,18,20	1.50	2 (12%)
2	289	B	433	1	13,13,14	9.11	6 (46%)	16,18,20	3.72	7 (43%)
2	289	A	412	1	13,13,14	0.46	0	16,18,20	1.84	4 (25%)
2	289	B	431	1	13,13,14	0.30	0	16,18,20	1.45	3 (18%)
2	289	B	410	1	13,13,14	0.32	0	16,18,20	1.38	1 (6%)
2	289	B	435	1	13,13,14	8.17	5 (38%)	16,18,20	6.82	11 (68%)
2	289	B	403	1	13,13,14	0.33	0	16,18,20	1.20	0
2	289	A	417	1	13,13,14	0.34	0	16,18,20	2.04	3 (18%)
2	289	B	408	1	13,13,14	0.34	0	16,18,20	1.64	4 (25%)
2	289	A	425	1	13,13,14	0.40	0	16,18,20	1.99	6 (37%)
2	289	A	431	1	13,13,14	0.21	0	16,18,20	0.97	1 (6%)
2	289	A	401	1	13,13,14	0.39	0	16,18,20	2.13	5 (31%)
2	289	A	423	1	13,13,14	0.28	0	16,18,20	1.34	2 (12%)
2	289	A	405	1	13,13,14	0.24	0	16,18,20	1.33	2 (12%)
2	289	B	404	1	13,13,14	0.34	0	16,18,20	1.77	4 (25%)
2	289	A	407	1	13,13,14	0.28	0	16,18,20	1.48	3 (18%)
2	289	B	429	1	13,13,14	0.30	0	16,18,20	1.96	6 (37%)
2	289	B	434	1	13,13,14	7.38	7 (53%)	16,18,20	3.89	12 (75%)
2	289	A	409	1	13,13,14	0.44	0	16,18,20	1.58	4 (25%)
2	289	B	417	1	13,13,14	0.35	0	16,18,20	0.91	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	289	B	419	1	13,13,14	0.25	0	16,18,20	1.65	3 (18%)
2	289	A	418	1	13,13,14	0.40	0	16,18,20	1.21	1 (6%)
2	289	A	411	1	13,13,14	0.33	0	16,18,20	2.07	5 (31%)
2	289	A	406	1	13,13,14	0.38	0	16,18,20	1.11	1 (6%)
2	289	A	435	1	13,13,14	0.35	0	16,18,20	1.23	1 (6%)
2	289	A	404	1	13,13,14	0.25	0	16,18,20	1.63	4 (25%)
2	289	A	403	1	13,13,14	0.40	0	16,18,20	0.85	1 (6%)
2	289	B	423	1	13,13,14	0.23	0	16,18,20	1.27	2 (12%)
2	289	A	420	1	13,13,14	0.21	0	16,18,20	0.44	0
2	289	B	401	1	13,13,14	0.39	0	16,18,20	1.54	3 (18%)
2	289	B	405	1	13,13,14	0.21	0	16,18,20	1.34	1 (6%)
2	289	A	421	1	13,13,14	0.22	0	16,18,20	1.06	1 (6%)
2	289	B	412	1	13,13,14	0.36	0	16,18,20	2.56	8 (50%)
2	289	B	425	1	13,13,14	0.34	0	16,18,20	2.07	7 (43%)
2	289	B	432	1	13,13,14	0.39	0	16,18,20	1.44	4 (25%)
2	289	A	415	1	13,13,14	0.31	0	16,18,20	1.57	2 (12%)
2	289	A	429	1	13,13,14	0.24	0	16,18,20	1.45	2 (12%)
2	289	A	413	1	13,13,14	4.61	1 (7%)	16,18,20	4.40	2 (12%)
2	289	A	424	1	13,13,14	0.25	0	16,18,20	1.23	3 (18%)
2	289	B	418	1	13,13,14	0.28	0	16,18,20	1.43	1 (6%)
2	289	B	409	1	13,13,14	0.31	0	16,18,20	1.33	3 (18%)
2	289	B	424	1	13,13,14	0.30	0	16,18,20	2.12	6 (37%)
2	289	B	406	1	13,13,14	0.20	0	16,18,20	0.43	0
2	289	A	434	1	13,13,14	2.88	6 (46%)	16,18,20	4.16	9 (56%)
2	289	B	428	1	13,13,14	0.25	0	16,18,20	1.09	1 (6%)
2	289	A	432	1	13,13,14	0.22	0	16,18,20	0.46	0
2	289	B	411	1	13,13,14	0.37	0	16,18,20	1.59	2 (12%)
2	289	A	427	1	13,13,14	0.27	0	16,18,20	1.46	3 (18%)
2	289	B	402	1	13,13,14	0.17	0	16,18,20	1.55	2 (12%)
2	289	A	426	1	13,13,14	0.27	0	16,18,20	0.87	1 (6%)
2	289	A	422	1	13,13,14	0.21	0	16,18,20	1.17	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	289	B	413	1	-	4/6/23/26	0/1/1/1
2	289	B	421	1	-	4/6/23/26	0/1/1/1
2	289	A	428	1	-	4/6/23/26	0/1/1/1
2	289	B	407	1	-	6/6/23/26	0/1/1/1
2	289	B	416	1	-	0/6/23/26	0/1/1/1
2	289	B	414	1	-	6/6/23/26	0/1/1/1
2	289	A	430	1	-	3/6/23/26	0/1/1/1
2	289	B	426	1	-	2/6/23/26	0/1/1/1
2	289	B	430	1	-	3/6/23/26	0/1/1/1
2	289	B	422	1	-	0/6/23/26	0/1/1/1
2	289	A	414	1	-	1/6/23/26	0/1/1/1
2	289	B	420	1	-	4/6/23/26	0/1/1/1
2	289	A	433	1	1/1/5/6	4/6/23/26	0/1/1/1
2	289	A	408	1	-	4/6/23/26	0/1/1/1
2	289	A	410	1	-	1/6/23/26	0/1/1/1
2	289	A	402	1	1/1/5/6	2/6/23/26	0/1/1/1
2	289	B	427	1	-	1/6/23/26	0/1/1/1
2	289	A	419	1	-	4/6/23/26	0/1/1/1
2	289	B	415	1	-	4/6/23/26	0/1/1/1
2	289	A	416	1	-	2/6/23/26	0/1/1/1
2	289	B	433	1	-	0/6/23/26	0/1/1/1
2	289	A	412	1	-	3/6/23/26	0/1/1/1
2	289	B	431	1	-	6/6/23/26	0/1/1/1
2	289	B	410	1	-	6/6/23/26	0/1/1/1
2	289	B	435	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	A	417	1	-	4/6/23/26	0/1/1/1
2	289	B	403	1	-	3/6/23/26	0/1/1/1
2	289	A	425	1	-	6/6/23/26	0/1/1/1
2	289	A	431	1	-	0/6/23/26	0/1/1/1
2	289	A	401	1	-	2/6/23/26	0/1/1/1
2	289	A	423	1	-	3/6/23/26	0/1/1/1
2	289	A	405	1	-	1/6/23/26	0/1/1/1
2	289	B	404	1	-	3/6/23/26	0/1/1/1
2	289	A	407	1	-	4/6/23/26	0/1/1/1
2	289	B	429	1	-	2/6/23/26	0/1/1/1
2	289	B	434	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	289	A	409	1	-	4/6/23/26	0/1/1/1
2	289	B	417	1	-	1/6/23/26	0/1/1/1
2	289	B	419	1	-	4/6/23/26	0/1/1/1
2	289	A	418	1	-	6/6/23/26	0/1/1/1
2	289	A	411	1	-	4/6/23/26	0/1/1/1
2	289	A	406	1	1/1/5/6	6/6/23/26	0/1/1/1
2	289	A	435	1	1/1/5/6	5/6/23/26	0/1/1/1
2	289	A	404	1	-	0/6/23/26	0/1/1/1
2	289	A	403	1	-	4/6/23/26	0/1/1/1
2	289	B	423	1	-	4/6/23/26	0/1/1/1
2	289	A	420	1	-	1/6/23/26	0/1/1/1
2	289	B	401	1	-	1/6/23/26	0/1/1/1
2	289	B	405	1	-	2/6/23/26	0/1/1/1
2	289	A	421	1	1/1/5/6	0/6/23/26	0/1/1/1
2	289	B	412	1	-	4/6/23/26	0/1/1/1
2	289	B	425	1	-	6/6/23/26	0/1/1/1
2	289	B	432	1	-	4/6/23/26	0/1/1/1
2	289	A	415	1	-	2/6/23/26	0/1/1/1
2	289	A	429	1	-	4/6/23/26	0/1/1/1
2	289	A	413	1	-	1/6/23/26	0/1/1/1
2	289	A	424	1	-	4/6/23/26	0/1/1/1
2	289	B	418	1	-	6/6/23/26	0/1/1/1
2	289	B	409	1	-	0/6/23/26	0/1/1/1
2	289	B	424	1	-	5/6/23/26	0/1/1/1
2	289	B	406	1	-	0/6/23/26	0/1/1/1
2	289	A	434	1	-	0/6/23/26	0/1/1/1
2	289	B	428	1	-	4/6/23/26	0/1/1/1
2	289	A	432	1	-	1/6/23/26	0/1/1/1
2	289	B	411	1	-	2/6/23/26	1/1/1/1
2	289	A	427	1	-	4/6/23/26	0/1/1/1
2	289	B	402	1	-	4/6/23/26	0/1/1/1
2	289	A	426	1	-	5/6/23/26	0/1/1/1
2	289	A	422	1	-	1/6/23/26	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	434	289	C7-C6	-22.67	0.96	1.52
2	B	435	289	O3-C3	-21.82	0.88	1.43
2	B	433	289	C2-C3	21.62	1.85	1.52
2	B	435	289	C2-C3	17.75	1.79	1.52
2	B	433	289	O5-C5	16.58	1.64	1.43
2	A	413	289	O5-C5	16.53	1.64	1.43
2	B	433	289	O3-C3	-16.43	1.02	1.43
2	B	416	289	C2-C3	-14.87	1.29	1.52
2	B	434	289	O5-C1	-9.20	1.28	1.43
2	B	416	289	O2-C2	9.07	1.62	1.43
2	B	435	289	O2-C2	-7.86	1.26	1.43
2	B	434	289	C6-C5	-6.54	1.39	1.52
2	A	434	289	O3-C3	5.72	1.57	1.43
2	A	434	289	O5-C1	5.56	1.53	1.43
2	B	433	289	C4-C3	-5.54	1.38	1.52
2	B	433	289	O2-C2	5.16	1.54	1.43
2	B	434	289	O5-C5	5.15	1.49	1.43
2	B	416	289	C1-C2	4.42	1.62	1.52
2	A	434	289	O2-C2	4.23	1.52	1.43
2	B	434	289	C2-C3	3.42	1.57	1.52
2	B	434	289	C4-C5	-3.26	1.43	1.52
2	A	434	289	O5-C5	3.19	1.47	1.43
2	B	435	289	C4-C3	3.00	1.60	1.52
2	B	416	289	C4-C3	2.96	1.60	1.52
2	B	433	289	O5-C1	2.90	1.48	1.43
2	B	416	289	O4-C4	2.73	1.49	1.43
2	A	434	289	C4-C3	-2.67	1.45	1.52
2	A	434	289	C7-C6	2.58	1.58	1.52
2	B	434	289	O6-C6	2.40	1.48	1.43
2	B	435	289	C4-C5	2.12	1.58	1.52

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	435	289	O3-C3-C2	22.19	155.34	110.05
2	A	413	289	O5-C5-C4	-17.05	80.78	110.73
2	A	434	289	C1-C2-C3	-9.78	95.41	109.64
2	B	416	289	O2-C2-C1	-9.43	87.63	109.22
2	A	434	289	C2-C3-C4	9.31	127.23	110.86
2	B	433	289	C3-C4-C5	8.79	129.63	109.68
2	B	433	289	O5-C5-C4	-8.58	95.67	110.73
2	B	434	289	C1-O5-C5	7.72	124.14	111.48
2	B	435	289	O4-C4-C3	-6.53	94.98	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	435	289	O3-C3-C4	-6.45	95.17	110.38
2	B	426	289	O7-C7-C6	-6.39	97.74	111.16
2	B	420	289	C1-O5-C5	6.15	121.56	111.48
2	B	435	289	C1-C2-C3	5.97	118.33	109.64
2	B	434	289	O7-C7-C6	-5.73	99.11	111.16
2	B	426	289	O6-C6-C5	5.65	122.68	109.18
2	A	417	289	C1-C2-C3	-5.56	101.55	109.64
2	B	435	289	O2-C2-C3	5.45	121.44	110.15
2	B	435	289	C2-C3-C4	-5.42	101.33	110.86
2	B	416	289	C1-C2-C3	5.20	117.22	109.64
2	B	412	289	C3-C4-C5	5.10	121.27	109.68
2	B	435	289	C3-C4-C5	5.08	121.22	109.68
2	A	434	289	O3-C3-C2	5.08	120.42	110.05
2	B	411	289	C1-O5-C5	5.04	119.74	111.48
2	B	426	289	C1-C2-C3	-5.03	102.32	109.64
2	B	434	289	O3-C3-C2	4.98	120.22	110.05
2	B	425	289	C1-C2-C3	-4.79	102.67	109.64
2	B	433	289	C2-C3-C4	-4.73	102.53	110.86
2	B	434	289	O2-C2-C3	-4.56	100.71	110.15
2	A	411	289	C1-O5-C5	4.55	118.93	111.48
2	A	401	289	C1-O5-C5	4.52	118.88	111.48
2	A	425	289	C7-C6-C5	4.51	121.03	112.05
2	B	404	289	C1-C2-C3	-4.46	103.15	109.64
2	B	412	289	C1-C2-C3	-4.42	103.20	109.64
2	A	408	289	C1-O5-C5	4.37	118.64	111.48
2	A	415	289	C1-O5-C5	4.35	118.60	111.48
2	A	434	289	O3-C3-C4	-4.29	100.27	110.38
2	A	428	289	C1-C2-C3	-4.29	103.40	109.64
2	B	434	289	C3-C4-C5	4.27	119.37	109.68
2	B	416	289	O3-C3-C2	4.27	118.76	110.05
2	B	416	289	O2-C2-C3	4.26	118.97	110.15
2	B	407	289	O6-C6-C5	4.25	119.32	109.18
2	B	434	289	O3-C3-C4	4.23	120.35	110.38
2	B	419	289	C2-C3-C4	-4.23	103.43	110.86
2	B	424	289	C1-C2-C3	-4.21	103.51	109.64
2	B	435	289	O5-C5-C4	4.17	118.07	110.73
2	B	434	289	O6-C6-C7	-4.15	99.59	109.03
2	B	412	289	C1-O5-C5	-4.10	104.75	111.48
2	A	419	289	C1-C2-C3	-4.07	103.71	109.64
2	B	434	289	O4-C4-C3	-3.90	101.17	110.38
2	B	413	289	O5-C5-C4	-3.89	103.90	110.73
2	A	414	289	O4-C4-C3	-3.88	101.23	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	407	289	O7-C7-C6	-3.86	103.06	111.16
2	B	426	289	O4-C4-C3	-3.80	101.41	110.38
2	B	435	289	O5-C1-C2	3.74	119.72	110.79
2	A	428	289	C1-O5-C5	3.70	117.55	111.48
2	B	402	289	C1-C2-C3	-3.69	104.27	109.64
2	A	416	289	O5-C5-C4	-3.66	104.31	110.73
2	A	412	289	O2-C2-C3	3.64	117.68	110.15
2	B	413	289	O2-C2-C3	3.62	117.64	110.15
2	A	404	289	O4-C4-C3	-3.59	101.91	110.38
2	B	416	289	O4-C4-C5	-3.56	100.82	109.94
2	A	434	289	O2-C2-C3	-3.54	102.82	110.15
2	B	420	289	O5-C5-C4	-3.51	104.57	110.73
2	B	433	289	O4-C4-C3	-3.48	102.18	110.38
2	B	434	289	O6-C6-C5	3.47	117.48	109.18
2	B	426	289	C1-O5-C5	3.46	117.15	111.48
2	B	408	289	C1-C2-C3	3.45	114.67	109.64
2	A	401	289	O4-C4-C3	-3.44	102.27	110.38
2	B	405	289	O7-C7-C6	-3.43	103.94	111.16
2	A	417	289	O5-C1-C2	-3.41	102.66	110.79
2	B	404	289	O5-C1-C2	-3.40	102.67	110.79
2	B	433	289	C1-C2-C3	3.39	114.58	109.64
2	A	411	289	C3-C4-C5	3.38	117.36	109.68
2	A	427	289	C1-C2-C3	-3.37	104.74	109.64
2	B	429	289	C1-O5-C5	3.35	116.97	111.48
2	B	418	289	O7-C7-C6	-3.31	104.19	111.16
2	A	405	289	C1-C2-C3	-3.30	104.84	109.64
2	A	425	289	O5-C5-C4	-3.25	105.02	110.73
2	B	423	289	O7-C7-C6	-3.23	104.38	111.16
2	B	412	289	O5-C1-C2	-3.20	103.15	110.79
2	A	429	289	C1-C2-C3	-3.20	104.98	109.64
2	B	421	289	O5-C1-C2	-3.19	103.19	110.79
2	B	427	289	C1-C2-C3	-3.15	105.05	109.64
2	B	420	289	O4-C4-C3	-3.15	102.95	110.38
2	B	424	289	C1-O5-C5	3.12	116.59	111.48
2	B	408	289	O2-C2-C3	-3.12	103.69	110.15
2	B	433	289	C1-O5-C5	-3.09	106.41	111.48
2	A	412	289	C3-C4-C5	3.04	116.58	109.68
2	B	401	289	C1-C2-C3	-3.04	105.22	109.64
2	A	411	289	O5-C1-C2	3.02	117.98	110.79
2	B	410	289	C1-C2-C3	-3.01	105.26	109.64
2	A	434	289	O5-C5-C4	-3.00	105.45	110.73
2	A	412	289	C2-C3-C4	3.00	116.14	110.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	289	O7-C7-C6	2.99	117.44	111.16
2	B	416	289	O4-C4-C3	2.99	117.43	110.38
2	B	425	289	O2-C2-C3	2.98	116.33	110.15
2	A	409	289	O4-C4-C3	-2.98	103.35	110.38
2	B	412	289	O2-C2-C1	2.95	115.98	109.22
2	A	425	289	O7-C7-C6	2.94	117.32	111.16
2	A	404	289	C3-C4-C5	2.94	116.34	109.68
2	A	419	289	O3-C3-C2	2.93	116.04	110.05
2	B	429	289	O2-C2-C1	2.93	115.94	109.22
2	B	424	289	O5-C1-C2	-2.93	103.80	110.79
2	B	414	289	O2-C2-C1	2.93	115.92	109.22
2	A	434	289	O5-C1-C2	2.92	117.75	110.79
2	B	433	289	O5-C1-C2	2.89	117.69	110.79
2	B	415	289	O4-C4-C3	-2.89	103.56	110.38
2	A	419	289	O5-C5-C4	2.86	115.76	110.73
2	A	411	289	C1-C2-C3	2.85	113.80	109.64
2	A	407	289	O6-C6-C5	2.85	115.99	109.18
2	A	409	289	O7-C7-C6	2.82	117.08	111.16
2	B	435	289	O4-C4-C5	2.81	117.15	109.94
2	B	425	289	O5-C5-C4	-2.80	105.82	110.73
2	B	424	289	C7-C6-C5	-2.80	106.49	112.05
2	A	401	289	O5-C5-C4	-2.80	105.82	110.73
2	A	421	289	O5-C1-C2	-2.80	104.12	110.79
2	B	424	289	O7-C7-C6	-2.79	105.29	111.16
2	A	434	289	C3-C4-C5	-2.78	103.36	109.68
2	B	434	289	O5-C5-C4	-2.78	105.86	110.73
2	A	401	289	C3-C4-C5	2.78	115.98	109.68
2	B	431	289	O5-C5-C4	-2.75	105.90	110.73
2	B	401	289	C3-C4-C5	2.74	115.90	109.68
2	A	427	289	C1-O5-C5	2.71	115.92	111.48
2	A	413	289	C2-C3-C4	2.71	115.62	110.86
2	B	430	289	O7-C7-C6	-2.71	105.47	111.16
2	B	419	289	O7-C7-C6	-2.69	105.50	111.16
2	B	414	289	C1-O5-C5	2.67	115.86	111.48
2	B	415	289	C1-O5-C5	2.67	115.85	111.48
2	B	431	289	O4-C4-C3	-2.67	104.09	110.38
2	B	425	289	O4-C4-C3	-2.66	104.09	110.38
2	A	411	289	O4-C4-C3	-2.66	104.10	110.38
2	A	429	289	O5-C5-C4	-2.66	106.07	110.73
2	B	426	289	C7-C6-C5	-2.65	106.79	112.05
2	B	432	289	C1-C2-C3	-2.65	105.79	109.64
2	B	429	289	O4-C4-C5	2.62	116.64	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	423	289	C1-O5-C5	2.61	115.75	111.48
2	A	423	289	C1-C2-C3	-2.60	105.85	109.64
2	B	408	289	C1-O5-C5	2.57	115.69	111.48
2	A	425	289	O4-C4-C3	-2.57	104.32	110.38
2	B	432	289	O5-C5-C4	-2.54	106.27	110.73
2	B	424	289	O6-C6-C5	2.53	115.23	109.18
2	A	423	289	O7-C7-C6	-2.53	105.85	111.16
2	B	427	289	O5-C5-C4	-2.51	106.32	110.73
2	B	409	289	C1-C2-C3	-2.51	105.98	109.64
2	B	413	289	O3-C3-C2	2.50	115.17	110.05
2	B	429	289	O5-C5-C4	-2.50	106.33	110.73
2	B	402	289	C1-O5-C5	2.50	115.57	111.48
2	A	407	289	O4-C4-C3	-2.49	104.50	110.38
2	B	409	289	O5-C5-C4	-2.49	106.36	110.73
2	B	412	289	O4-C4-C3	-2.49	104.51	110.38
2	A	409	289	C7-C6-C5	2.48	116.99	112.05
2	A	433	289	O5-C1-C2	-2.46	104.92	110.79
2	B	409	289	O5-C1-C2	-2.46	104.93	110.79
2	B	415	289	O5-C5-C4	-2.46	106.42	110.73
2	B	407	289	C1-O5-C5	2.44	115.48	111.48
2	B	435	289	O2-C2-C1	-2.44	103.64	109.22
2	A	419	289	O6-C6-C5	-2.44	103.35	109.18
2	A	424	289	C1-C2-C3	-2.44	106.09	109.64
2	A	414	289	C1-C2-C3	-2.41	106.14	109.64
2	B	419	289	O2-C2-C1	2.41	114.73	109.22
2	A	404	289	C1-C2-C3	-2.40	106.15	109.64
2	A	409	289	O5-C5-C4	-2.39	106.53	110.73
2	A	426	289	C1-C2-C3	-2.39	106.17	109.64
2	B	412	289	O4-C4-C5	-2.38	103.83	109.94
2	B	434	289	C1-C2-C3	2.38	113.11	109.64
2	A	415	289	O4-C4-C5	2.36	115.99	109.94
2	A	416	289	C1-C2-C3	-2.35	106.22	109.64
2	A	433	289	O5-C5-C4	-2.35	106.60	110.73
2	B	434	289	O4-C4-C5	2.35	115.96	109.94
2	B	429	289	O3-C3-C2	-2.35	105.26	110.05
2	B	404	289	C3-C4-C5	2.35	115.00	109.68
2	A	427	289	O2-C2-C1	2.34	114.58	109.22
2	A	412	289	C1-C2-C3	-2.33	106.25	109.64
2	B	416	289	O5-C5-C4	2.32	114.81	110.73
2	B	412	289	O5-C5-C4	2.31	114.80	110.73
2	B	421	289	O5-C5-C4	2.30	114.77	110.73
2	B	432	289	O2-C2-C3	2.28	114.88	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	407	289	C1-C2-C3	-2.26	106.35	109.64
2	A	425	289	O2-C2-C1	2.24	114.35	109.22
2	B	430	289	O2-C2-C3	2.23	114.77	110.15
2	B	411	289	O6-C6-C5	2.22	114.47	109.18
2	B	401	289	O3-C3-C2	-2.21	105.55	110.05
2	A	428	289	O5-C1-C2	-2.20	105.55	110.79
2	B	425	289	O2-C2-C1	-2.19	104.20	109.22
2	B	429	289	C2-C3-C4	2.19	114.71	110.86
2	B	428	289	O7-C7-C6	-2.19	106.56	111.16
2	B	425	289	C1-O5-C5	2.18	115.05	111.48
2	A	435	289	O2-C2-C1	2.17	114.20	109.22
2	A	434	289	C7-C6-C5	-2.16	107.75	112.05
2	A	433	289	O3-C3-C2	2.16	114.46	110.05
2	B	408	289	C3-C4-C5	2.16	114.57	109.68
2	A	424	289	O4-C4-C3	-2.15	105.30	110.38
2	B	427	289	O5-C1-C2	-2.14	105.67	110.79
2	B	404	289	O2-C2-C1	2.14	114.13	109.22
2	B	415	289	C3-C4-C5	2.13	114.51	109.68
2	B	431	289	C2-C3-C4	2.11	114.57	110.86
2	A	431	289	O5-C1-C2	-2.10	105.78	110.79
2	A	403	289	C7-C6-C5	2.07	116.17	112.05
2	A	424	289	O4-C4-C5	2.06	115.22	109.94
2	A	418	289	O5-C1-C2	-2.05	105.89	110.79
2	B	417	289	C1-O5-C5	2.05	114.84	111.48
2	A	419	289	O2-C2-C3	2.04	114.38	110.15
2	B	421	289	O7-C7-C6	-2.04	106.88	111.16
2	A	404	289	O5-C5-C4	-2.04	107.16	110.73
2	A	417	289	O4-C4-C3	-2.03	105.58	110.38
2	A	402	289	C1-C2-C3	-2.03	106.69	109.64
2	A	406	289	C3-C4-C5	2.02	114.26	109.68
2	B	425	289	O6-C6-C5	2.01	113.98	109.18
2	A	405	289	C2-C3-C4	-2.01	107.33	110.86
2	A	428	289	O4-C4-C5	-2.01	104.80	109.94
2	A	425	289	C2-C3-C4	2.00	114.39	110.86
2	B	432	289	C7-C6-C5	2.00	116.04	112.05

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	402	289	C1
2	A	406	289	C1
2	A	421	289	C1

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

All (201) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	289	O6-C6-C7-O7
2	A	403	289	C4-C5-C6-C7
2	A	403	289	O5-C5-C6-O6
2	A	403	289	C4-C5-C6-O6
2	A	406	289	O6-C6-C7-O7
2	A	406	289	C5-C6-C7-O7
2	A	406	289	O5-C5-C6-C7
2	A	406	289	C4-C5-C6-C7
2	A	406	289	O5-C5-C6-O6
2	A	406	289	C4-C5-C6-O6
2	A	407	289	O5-C5-C6-C7
2	A	407	289	C4-C5-C6-C7
2	A	407	289	O5-C5-C6-O6
2	A	407	289	C4-C5-C6-O6
2	A	408	289	O5-C5-C6-C7
2	A	408	289	C4-C5-C6-C7
2	A	408	289	O5-C5-C6-O6
2	A	408	289	C4-C5-C6-O6
2	A	409	289	O5-C5-C6-C7
2	A	409	289	C4-C5-C6-C7
2	A	409	289	O5-C5-C6-O6
2	A	409	289	C4-C5-C6-O6
2	A	411	289	O5-C5-C6-C7
2	A	411	289	C4-C5-C6-C7
2	A	411	289	O5-C5-C6-O6
2	A	411	289	C4-C5-C6-O6
2	A	412	289	O6-C6-C7-O7
2	A	412	289	C5-C6-C7-O7
2	A	413	289	O5-C5-C6-O6
2	A	415	289	O6-C6-C7-O7
2	A	415	289	C5-C6-C7-O7
2	A	416	289	O6-C6-C7-O7
2	A	417	289	O5-C5-C6-C7
2	A	417	289	C4-C5-C6-C7
2	A	417	289	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	417	289	C4-C5-C6-O6
2	A	418	289	O6-C6-C7-O7
2	A	418	289	C5-C6-C7-O7
2	A	418	289	O5-C5-C6-C7
2	A	418	289	C4-C5-C6-C7
2	A	418	289	O5-C5-C6-O6
2	A	418	289	C4-C5-C6-O6
2	A	419	289	O5-C5-C6-C7
2	A	419	289	C4-C5-C6-C7
2	A	419	289	O5-C5-C6-O6
2	A	419	289	C4-C5-C6-O6
2	A	424	289	O5-C5-C6-C7
2	A	424	289	C4-C5-C6-C7
2	A	424	289	O5-C5-C6-O6
2	A	425	289	O6-C6-C7-O7
2	A	425	289	C5-C6-C7-O7
2	A	425	289	O5-C5-C6-C7
2	A	425	289	C4-C5-C6-C7
2	A	425	289	O5-C5-C6-O6
2	A	425	289	C4-C5-C6-O6
2	A	426	289	O5-C5-C6-O6
2	A	427	289	O5-C5-C6-C7
2	A	427	289	C4-C5-C6-C7
2	A	427	289	O5-C5-C6-O6
2	A	427	289	C4-C5-C6-O6
2	A	428	289	O5-C5-C6-C7
2	A	428	289	C4-C5-C6-C7
2	A	428	289	O5-C5-C6-O6
2	A	428	289	C4-C5-C6-O6
2	A	429	289	O5-C5-C6-C7
2	A	429	289	C4-C5-C6-C7
2	A	429	289	O5-C5-C6-O6
2	A	429	289	C4-C5-C6-O6
2	A	433	289	O5-C5-C6-C7
2	A	433	289	C4-C5-C6-C7
2	A	433	289	O5-C5-C6-O6
2	A	433	289	C4-C5-C6-O6
2	A	435	289	C4-C5-C6-C7
2	B	401	289	O5-C5-C6-O6
2	B	402	289	O6-C6-C7-O7
2	B	402	289	C5-C6-C7-O7
2	B	403	289	O6-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
2	B	404	289	C4-C5-C6-C7
2	B	404	289	O5-C5-C6-O6
2	B	404	289	C4-C5-C6-O6
2	B	405	289	O6-C6-C7-O7
2	B	405	289	C5-C6-C7-O7
2	B	407	289	C5-C6-C7-O7
2	B	407	289	O5-C5-C6-C7
2	B	407	289	C4-C5-C6-C7
2	B	407	289	O5-C5-C6-O6
2	B	407	289	C4-C5-C6-O6
2	B	410	289	O5-C5-C6-C7
2	B	410	289	C4-C5-C6-C7
2	B	410	289	O5-C5-C6-O6
2	B	410	289	C4-C5-C6-O6
2	B	411	289	O6-C6-C7-O7
2	B	411	289	C5-C6-C7-O7
2	B	412	289	O5-C5-C6-C7
2	B	412	289	C4-C5-C6-C7
2	B	412	289	O5-C5-C6-O6
2	B	412	289	C4-C5-C6-O6
2	B	413	289	O5-C5-C6-C7
2	B	413	289	O5-C5-C6-O6
2	B	413	289	C4-C5-C6-O6
2	B	414	289	O5-C5-C6-C7
2	B	414	289	C4-C5-C6-C7
2	B	414	289	O5-C5-C6-O6
2	B	414	289	C4-C5-C6-O6
2	B	418	289	O5-C5-C6-C7
2	B	418	289	C4-C5-C6-C7
2	B	418	289	O5-C5-C6-O6
2	B	418	289	C4-C5-C6-O6
2	B	419	289	C4-C5-C6-O6
2	B	420	289	O5-C5-C6-C7
2	B	420	289	C4-C5-C6-C7
2	B	420	289	O5-C5-C6-O6
2	B	420	289	C4-C5-C6-O6
2	B	421	289	O5-C5-C6-C7
2	B	421	289	C4-C5-C6-C7
2	B	421	289	O5-C5-C6-O6
2	B	421	289	C4-C5-C6-O6
2	B	423	289	O5-C5-C6-C7
2	B	423	289	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
2	B	423	289	O5-C5-C6-O6
2	B	423	289	C4-C5-C6-O6
2	B	424	289	O5-C5-C6-C7
2	B	424	289	C4-C5-C6-C7
2	B	424	289	O5-C5-C6-O6
2	B	424	289	C4-C5-C6-O6
2	B	425	289	O6-C6-C7-O7
2	B	425	289	O5-C5-C6-C7
2	B	425	289	C4-C5-C6-C7
2	B	425	289	O5-C5-C6-O6
2	B	425	289	C4-C5-C6-O6
2	B	426	289	O6-C6-C7-O7
2	B	426	289	C5-C6-C7-O7
2	B	428	289	O5-C5-C6-C7
2	B	428	289	C4-C5-C6-C7
2	B	428	289	O5-C5-C6-O6
2	B	428	289	C4-C5-C6-O6
2	B	429	289	C5-C6-C7-O7
2	B	430	289	C4-C5-C6-C7
2	B	430	289	O5-C5-C6-O6
2	B	431	289	O5-C5-C6-C7
2	B	431	289	C4-C5-C6-C7
2	B	431	289	O5-C5-C6-O6
2	B	431	289	C4-C5-C6-O6
2	B	432	289	O5-C5-C6-C7
2	B	432	289	C4-C5-C6-C7
2	B	432	289	O5-C5-C6-O6
2	B	432	289	C4-C5-C6-O6
2	A	401	289	O6-C6-C7-O7
2	A	426	289	O6-C6-C7-O7
2	B	407	289	O6-C6-C7-O7
2	B	410	289	O6-C6-C7-O7
2	B	414	289	O6-C6-C7-O7
2	B	429	289	O6-C6-C7-O7
2	B	431	289	O6-C6-C7-O7
2	A	402	289	C5-C6-C7-O7
2	A	416	289	C5-C6-C7-O7
2	A	435	289	C5-C6-C7-O7
2	B	403	289	C5-C6-C7-O7
2	B	414	289	C5-C6-C7-O7
2	A	435	289	O6-C6-C7-O7
2	A	401	289	C5-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
2	B	410	289	C5-C6-C7-O7
2	A	423	289	O6-C6-C7-O7
2	B	424	289	O6-C6-C7-O7
2	A	426	289	C5-C6-C7-O7
2	A	414	289	C5-C6-C7-O7
2	B	425	289	C5-C6-C7-O7
2	A	430	289	O6-C6-C7-O7
2	B	418	289	O6-C6-C7-O7
2	B	419	289	O6-C6-C7-O7
2	A	412	289	C4-C5-C6-C7
2	A	420	289	C4-C5-C6-C7
2	A	430	289	C4-C5-C6-C7
2	A	432	289	C4-C5-C6-C7
2	B	403	289	C4-C5-C6-C7
2	B	413	289	C4-C5-C6-C7
2	B	419	289	C4-C5-C6-C7
2	A	403	289	O5-C5-C6-C7
2	A	424	289	C4-C5-C6-O6
2	A	426	289	O5-C5-C6-C7
2	A	430	289	O5-C5-C6-C7
2	A	435	289	O5-C5-C6-O6
2	A	435	289	C4-C5-C6-O6
2	B	415	289	C4-C5-C6-O6
2	B	419	289	O5-C5-C6-C7
2	B	430	289	C4-C5-C6-O6
2	B	431	289	C5-C6-C7-O7
2	A	422	289	O6-C6-C7-O7
2	A	423	289	C5-C6-C7-O7
2	A	423	289	C4-C5-C6-C7
2	A	426	289	C4-C5-C6-C7
2	B	415	289	C4-C5-C6-C7
2	B	427	289	C4-C5-C6-C7
2	A	405	289	O5-C5-C6-C7
2	B	402	289	O5-C5-C6-C7
2	B	402	289	O5-C5-C6-O6
2	B	415	289	O5-C5-C6-C7
2	B	415	289	O5-C5-C6-O6
2	B	417	289	C4-C5-C6-O6
2	B	418	289	C5-C6-C7-O7
2	A	410	289	C5-C6-C7-O7

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	411	289	C1-C2-C3-C4-C5-O5

30 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	416	289	1	3
2	A	430	289	1	0
2	B	430	289	0	1
2	A	414	289	1	0
2	B	420	289	0	1
2	A	433	289	2	0
2	A	408	289	0	1
2	A	410	289	5	0
2	A	416	289	1	0
2	B	433	289	11	0
2	A	412	289	5	0
2	B	435	289	3	0
2	B	408	289	2	0
2	A	425	289	2	0
2	A	431	289	1	0
2	B	404	289	2	0
2	A	406	289	2	0
2	A	403	289	0	2
2	A	420	289	2	3
2	B	425	289	1	0
2	B	432	289	1	0
2	A	413	289	6	0
2	A	424	289	1	0
2	B	409	289	0	2
2	B	424	289	1	1
2	B	406	289	4	0
2	A	434	289	4	0
2	B	428	289	1	1
2	A	432	289	2	0
2	B	411	289	1	0

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	270/305 (88%)	1.73	92 (34%) 1 1	40, 55, 83, 95	0
1	B	270/305 (88%)	2.38	157 (58%) 0 0	33, 46, 76, 98	0
All	All	540/610 (88%)	2.06	249 (46%) 0 0	33, 51, 81, 98	0

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	327	GLY	7.7
1	A	76	GLY	6.5
1	B	73	LEU	6.0
1	B	321	THR	5.9
1	B	320	ASN	5.7
1	B	229	GLY	5.4
1	B	268	ALA	5.2
1	B	247	GLY	5.2
1	B	285	GLY	5.2
1	B	315	GLY	5.2
1	A	62	ILE	5.2
1	B	281	VAL	4.7
1	A	114	GLY	4.7
1	B	246	GLY	4.7
1	A	55	ALA	4.6
1	A	69	LYS	4.6
1	A	96	GLY	4.5
1	B	292	ILE	4.4
1	A	315	GLY	4.4
1	B	282	TYR	4.4
1	B	319	THR	4.4
1	B	179	VAL	4.4
1	B	286	ASN	4.3
1	B	266	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	150	PHE	4.2
1	B	190	GLY	4.2
1	B	239	GLY	4.1
1	B	323	ALA	4.1
1	B	324	ALA	4.1
1	B	314	GLY	4.0
1	B	252	THR	4.0
1	B	273	VAL	4.0
1	B	105	ILE	4.0
1	B	300	VAL	4.0
1	B	226	SER	3.9
1	B	267	SER	3.9
1	B	288	THR	3.9
1	B	262	VAL	3.9
1	B	232	ALA	3.9
1	B	322	SER	3.8
1	A	63	GLY	3.8
1	A	58	ASP	3.7
1	B	254	ILE	3.7
1	B	276	GLY	3.6
1	B	318	ILE	3.6
1	B	133	GLY	3.6
1	B	152	GLY	3.6
1	B	248	SER	3.6
1	A	83	THR	3.5
1	B	168	VAL	3.5
1	A	88	GLY	3.5
1	B	91	TYR	3.5
1	B	186	PHE	3.4
1	B	295	GLY	3.4
1	B	317	VAL	3.4
1	B	249	ALA	3.4
1	A	92	VAL	3.4
1	A	117	ALA	3.4
1	B	118	THR	3.4
1	B	296	GLY	3.4
1	B	309	VAL	3.3
1	A	91	TYR	3.3
1	B	177	ALA	3.3
1	A	78	THR	3.3
1	B	271	THR	3.3
1	B	311	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	171	GLY	3.3
1	A	103	ILE	3.3
1	A	73	LEU	3.3
1	A	288	THR	3.2
1	B	234	THR	3.2
1	B	290	THR	3.2
1	B	326	SER	3.2
1	B	130	VAL	3.2
1	B	149	VAL	3.2
1	A	84	ILE	3.2
1	B	93	SER	3.2
1	A	64	ARG	3.2
1	B	316	ALA	3.2
1	B	313	SER	3.2
1	B	270	ASN	3.2
1	B	98	ALA	3.1
1	A	228	GLY	3.1
1	A	79	ALA	3.1
1	A	93	SER	3.1
1	A	153	GLY	3.0
1	B	277	GLY	3.0
1	B	55	ALA	3.0
1	B	188	SER	3.0
1	A	276	GLY	3.0
1	B	251	GLY	3.0
1	B	265	GLY	3.0
1	A	56	ALA	3.0
1	A	70	SER	3.0
1	A	120	SER	3.0
1	B	264	SER	3.0
1	B	304	GLY	3.0
1	B	207	ARG	2.9
1	B	227	SER	2.9
1	B	298	LEU	2.9
1	B	228	GLY	2.9
1	A	100	SER	2.9
1	B	244	LEU	2.9
1	A	246	GLY	2.9
1	B	57	TYR	2.9
1	A	314	GLY	2.9
1	A	111	VAL	2.9
1	A	290	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	86	SER	2.9
1	B	112	SER	2.9
1	B	85	ASN	2.9
1	B	269	THR	2.8
1	A	105	ILE	2.8
1	B	189	SER	2.8
1	B	67	THR	2.8
1	B	169	ILE	2.8
1	B	310	ILE	2.8
1	A	57	TYR	2.8
1	B	95	GLY	2.8
1	B	302	ALA	2.8
1	B	206	VAL	2.8
1	B	100	SER	2.8
1	B	221	GLY	2.8
1	B	263	SER	2.7
1	B	141	VAL	2.7
1	B	280	HIS	2.7
1	A	122	ILE	2.7
1	A	192	ILE	2.7
1	A	186	PHE	2.7
1	B	129	HIS	2.7
1	A	141	VAL	2.7
1	B	72	HIS	2.6
1	B	151	SER	2.6
1	A	125	GLY	2.6
1	A	182	GLY	2.6
1	B	106	GLY	2.6
1	B	210	GLY	2.6
1	A	67	THR	2.6
1	A	220	THR	2.6
1	A	323	ALA	2.6
1	B	299	GLN	2.6
1	B	63	GLY	2.6
1	A	82	THR	2.6
1	B	291	THR	2.6
1	A	135	SER	2.6
1	B	170	SER	2.6
1	B	198	VAL	2.5
1	B	236	ILE	2.5
1	B	114	GLY	2.5
1	A	136	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	321	THR	2.5
1	B	94	SER	2.5
1	B	145	GLY	2.5
1	B	209	GLY	2.5
1	B	235	THR	2.5
1	B	65	GLY	2.5
1	B	80	LYS	2.5
1	B	138	ASN	2.5
1	B	167	TYR	2.5
1	B	301	GLU	2.5
1	A	68	SER	2.5
1	B	121	THR	2.5
1	B	250	THR	2.5
1	A	133	GLY	2.5
1	B	134	GLY	2.5
1	A	199	ASN	2.5
1	A	159	ILE	2.5
1	B	111	VAL	2.4
1	B	283	ILE	2.5
1	B	272	THR	2.4
1	B	174	ALA	2.4
1	B	217	LEU	2.4
1	A	107	GLY	2.4
1	B	199	ASN	2.4
1	A	130	VAL	2.4
1	A	179	VAL	2.4
1	A	119	SER	2.4
1	A	189	SER	2.4
1	B	274	TYR	2.4
1	B	307	SER	2.4
1	B	137	THR	2.4
1	B	306	ALA	2.4
1	B	172	GLY	2.4
1	A	150	PHE	2.4
1	B	294	SER	2.4
1	B	293	THR	2.4
1	B	195	ALA	2.4
1	A	169	ILE	2.4
1	A	72	HIS	2.4
1	A	286	ASN	2.3
1	B	257	GLY	2.3
1	B	84	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	149	VAL	2.3
1	A	121	THR	2.3
1	A	65	GLY	2.3
1	A	77	ASP	2.3
1	B	325	VAL	2.3
1	B	79	ALA	2.3
1	A	134	GLY	2.3
1	B	303	GLY	2.3
1	B	110	HIS	2.3
1	A	81	ASN	2.3
1	A	54	LYS	2.3
1	A	75	ALA	2.3
1	A	251	GLY	2.3
1	B	182	GLY	2.3
1	A	170	SER	2.2
1	B	74	SER	2.2
1	B	154	SER	2.2
1	A	309	VAL	2.2
1	A	115	GLY	2.2
1	A	327	GLY	2.2
1	B	96	GLY	2.2
1	B	255	TYR	2.2
1	A	313	SER	2.2
1	A	291	THR	2.2
1	B	225	VAL	2.2
1	B	75	ALA	2.2
1	B	192	ILE	2.2
1	A	273	VAL	2.2
1	A	144	GLY	2.2
1	B	76	GLY	2.2
1	B	191	GLY	2.2
1	A	116	SER	2.2
1	B	97	SER	2.2
1	B	245	TYR	2.2
1	A	123	ASN	2.2
1	A	317	VAL	2.1
1	A	145	GLY	2.1
1	A	152	GLY	2.1
1	B	113	SER	2.1
1	B	261	TYR	2.1
1	A	102	THR	2.1
1	A	118	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	101	THR	2.1
1	B	260	GLN	2.1
1	B	157	GLY	2.1
1	A	212	ALA	2.1
1	A	253	SER	2.1
1	A	142	ASN	2.1
1	B	208	ASP	2.1
1	B	175	THR	2.1
1	A	292	ILE	2.1
1	A	325	VAL	2.1
1	A	201	GLY	2.0
1	B	62	ILE	2.0
1	B	224	PHE	2.0
1	B	237	ASN	2.0
1	A	101	THR	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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	289	A	413	13/14	0.43	0.17	117,121,127,128	0
2	289	A	432	13/14	0.43	0.15	106,114,124,128	0
2	289	B	435	13/14	0.43	0.16	94,107,115,131	0
2	289	B	406	13/14	0.44	0.20	78,88,100,105	0
2	289	B	425	13/14	0.50	0.16	51,56,73,76	0
2	289	A	433	13/14	0.50	0.14	95,100,106,106	0
2	289	A	420	13/14	0.51	0.12	81,95,101,101	0
2	289	A	408	13/14	0.51	0.19	76,87,100,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	289	A	434	13/14	0.53	0.19	86,93,101,102	0
2	289	A	401	13/14	0.54	0.18	93,99,109,111	0
2	289	B	426	13/14	0.54	0.19	47,56,66,67	0
2	289	B	413	13/14	0.54	0.15	74,88,101,105	0
2	289	A	404	13/14	0.55	0.14	78,98,108,114	0
2	289	B	409	13/14	0.55	0.14	105,115,124,129	0
2	289	A	430	13/14	0.57	0.12	66,76,94,97	0
2	289	B	415	13/14	0.58	0.16	73,79,92,94	0
2	289	B	423	13/14	0.62	0.13	53,60,77,83	0
2	289	B	427	13/14	0.62	0.18	49,56,60,63	0
2	289	B	408	13/14	0.62	0.18	90,103,112,124	0
2	289	B	401	13/14	0.64	0.16	86,98,102,111	0
2	289	B	424	13/14	0.64	0.17	48,55,67,69	0
2	289	A	416	13/14	0.64	0.15	75,80,95,106	0
2	289	A	435	13/14	0.65	0.15	98,114,121,124	0
2	289	B	416	13/14	0.65	0.18	96,114,120,129	0
2	289	A	410	13/14	0.65	0.16	64,80,94,96	0
2	289	B	432	13/14	0.65	0.14	88,101,109,117	0
2	289	A	409	13/14	0.65	0.16	80,95,106,112	0
2	289	B	404	13/14	0.66	0.13	72,85,96,97	0
2	289	B	421	13/14	0.66	0.14	61,73,80,80	0
2	289	B	434	13/14	0.66	0.21	88,101,124,125	0
2	289	B	410	13/14	0.66	0.17	54,70,84,86	0
2	289	B	428	13/14	0.67	0.17	67,74,85,94	0
2	289	A	403	13/14	0.68	0.14	89,101,117,117	0
2	289	B	414	13/14	0.68	0.13	49,65,82,93	0
2	289	B	411	13/14	0.68	0.17	80,87,100,100	0
2	289	B	412	13/14	0.68	0.21	71,93,108,116	0
2	289	B	418	13/14	0.68	0.15	44,51,64,70	0
2	289	B	422	13/14	0.69	0.14	63,71,79,81	0
2	289	B	402	13/14	0.69	0.18	58,67,90,105	0
2	289	B	433	13/14	0.70	0.17	91,99,105,112	0
2	289	B	431	13/14	0.70	0.12	58,65,72,74	0
2	289	B	419	13/14	0.70	0.14	54,59,72,72	0
2	289	A	411	13/14	0.71	0.15	77,92,105,110	0
2	289	A	412	13/14	0.71	0.13	73,84,89,99	0
2	289	A	415	13/14	0.72	0.16	62,68,88,89	0
2	289	B	403	13/14	0.72	0.16	73,85,94,100	0
2	289	B	429	13/14	0.72	0.12	51,59,82,91	0
2	289	A	423	13/14	0.72	0.14	76,80,87,93	0
2	289	A	427	13/14	0.73	0.14	65,71,89,97	0
2	289	A	417	13/14	0.73	0.11	49,61,81,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	289	A	426	13/14	0.73	0.15	69,78,88,94	0
2	289	A	406	13/14	0.74	0.13	77,86,101,101	0
2	289	B	407	13/14	0.74	0.15	47,56,71,89	0
2	289	A	422	13/14	0.74	0.16	71,82,92,94	0
2	289	B	417	13/14	0.74	0.14	84,92,104,118	0
2	289	B	405	13/14	0.74	0.16	53,63,83,86	0
2	289	A	421	13/14	0.75	0.13	83,90,101,103	0
2	289	A	405	13/14	0.75	0.12	58,67,80,83	0
2	289	B	430	13/14	0.75	0.12	75,81,89,93	0
2	289	A	431	13/14	0.75	0.13	74,81,90,95	0
2	289	A	419	13/14	0.77	0.12	57,65,74,77	0
2	289	A	428	13/14	0.79	0.10	59,66,73,85	0
2	289	A	402	13/14	0.80	0.12	62,73,83,88	0
2	289	A	425	13/14	0.81	0.13	66,74,95,101	0
2	289	A	414	13/14	0.81	0.12	60,66,87,89	0
2	289	A	424	13/14	0.82	0.12	67,73,81,93	0
2	289	A	429	13/14	0.82	0.11	66,70,83,86	0
2	289	B	420	13/14	0.84	0.14	40,44,71,74	0
2	289	A	407	13/14	0.86	0.12	56,65,76,88	0
2	289	A	418	13/14	0.86	0.12	48,51,78,83	0

6.5 Other polymers

There are no such residues in this entry.