



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:54 PM GMT

PDB ID : 1GOH  
Title : NOVEL THIOETHER BOND REVEALED BY A 1.7 ANGSTROMS CRYSTAL STRUCTURE OF GALACTOSE OXIDASE  
Authors : Ito, N.; Phillips, S.E.V.; Knowles, P.F.  
Deposited on : 1993-09-30  
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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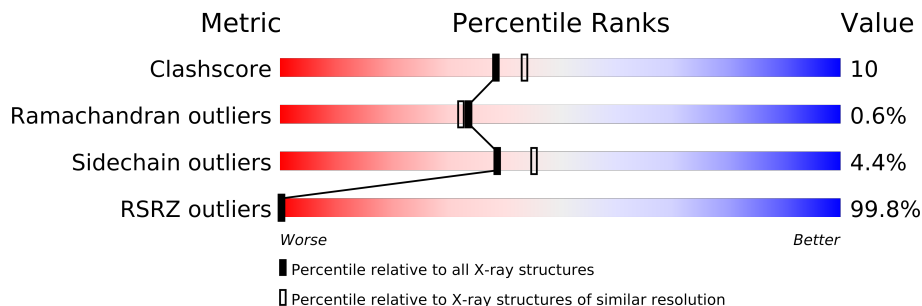
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
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) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	639	

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	NA	A	702	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5141 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 GALACTOSE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	0	0
			4830	3017	840	954	19			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is water.

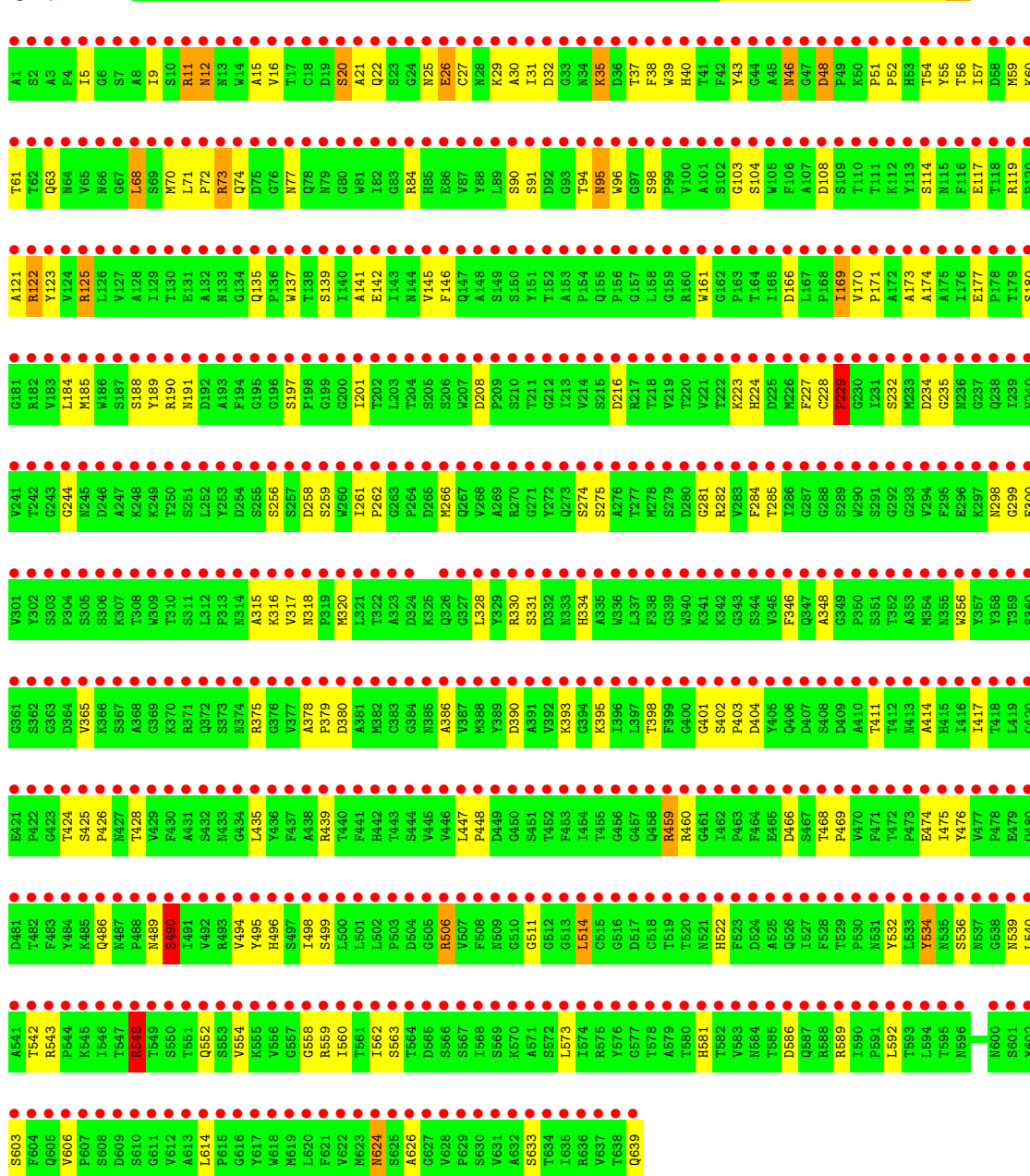
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	310	Total	O	0	0
			310	310		

### 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: GALACTOSE OXIDASE

Chain A:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.00Å 89.40Å 86.70Å 90.00° 117.80° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 9.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.20) 77.4 (9.99-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.19Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.156 , (Not available) 0.133 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	22.1	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.69 , 199.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 27365 reflections	Xtriage
$F_o, F_c$ correlation	0.32	EDS
Total number of atoms	5141	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: NA

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	0.99	1/4959 (0.0%)	1.73	66/6765 (1.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	490	SER	CA-CB	5.08	1.60	1.52

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	ARG	CD-NE-CZ	17.34	147.88	123.60
1	A	122	ARG	CD-NE-CZ	12.27	140.78	123.60
1	A	190	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	A	122	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	A	84	ARG	NE-CZ-NH2	-10.82	114.89	120.30
1	A	543	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	A	460	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	A	476	TYR	CB-CG-CD2	-8.62	115.83	121.00
1	A	68	LEU	CA-CB-CG	8.51	134.88	115.30
1	A	548	ARG	NE-CZ-NH2	8.48	124.54	120.30
1	A	282	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	A	543	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	A	119	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	A	20	SER	N-CA-CB	7.69	122.03	110.50
1	A	119	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	499	SER	N-CA-CB	7.63	121.94	110.50
1	A	125	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	A	330	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	26	GLU	CA-CB-CG	7.13	129.09	113.40
1	A	459	ARG	NE-CZ-NH2	-7.09	116.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	459	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	A	114	SER	N-CA-CB	6.51	120.27	110.50
1	A	48	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	A	70	MET	CG-SD-CE	6.42	110.47	100.20
1	A	404	ASP	O-C-N	6.42	132.96	122.70
1	A	300	GLU	OE1-CD-OE2	6.40	130.97	123.30
1	A	534	TYR	CB-CG-CD1	-6.33	117.20	121.00
1	A	258	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	506	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	559	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	190	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	633	SER	N-CA-CB	6.00	119.50	110.50
1	A	300	GLU	N-CA-CB	5.93	121.28	110.60
1	A	54	THR	N-CA-CB	-5.90	99.10	110.30
1	A	330	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	586	ASP	CB-CG-OD1	-5.82	113.06	118.30
1	A	606	VAL	CA-CB-CG1	-5.82	102.17	110.90
1	A	375	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	460	ARG	CD-NE-CZ	-5.76	115.54	123.60
1	A	35	LYS	CA-CB-CG	5.74	126.03	113.40
1	A	188	SER	O-C-N	5.63	131.71	122.70
1	A	386	ALA	CB-CA-C	5.56	118.44	110.10
1	A	119	ARG	CD-NE-CZ	5.55	131.37	123.60
1	A	108	ASP	CB-CA-C	5.54	121.48	110.40
1	A	224	HIS	N-CA-CB	-5.54	100.63	110.60
1	A	404	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	315	ALA	O-C-N	5.50	131.50	122.70
1	A	390	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	20	SER	O-C-N	5.38	131.30	122.70
1	A	104	SER	O-C-N	5.33	131.23	122.70
1	A	121	ALA	CB-CA-C	5.29	118.03	110.10
1	A	624	ASN	CB-CA-C	5.29	120.97	110.40
1	A	266	MET	CA-CB-CG	-5.27	104.33	113.30
1	A	73	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	169	ILE	O-C-N	5.23	131.07	122.70
1	A	380	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	318	ASN	CB-CA-C	5.18	120.75	110.40
1	A	614	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	586	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	589	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	208	ASP	CB-CG-OD2	5.13	122.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	LEU	O-C-N	5.07	130.81	122.70
1	A	11	ARG	CG-CD-NE	-5.03	101.24	111.80
1	A	84	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	232	SER	N-CA-CB	5.01	118.01	110.50

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	4830	0	4604	92	1
2	A	1	0	0	0	0
3	A	310	0	0	6	1
All	All	5141	0	4604	92	2

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 10.

All (92) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:22:GLN:HE21	1:A:46:ASN:HB2	1.32	0.94
1:A:35:LYS:HE3	1:A:71:LEU:HD21	1.58	0.86
1:A:22:GLN:NE2	1:A:46:ASN:HB2	1.92	0.84
1:A:122:ARG:HD3	1:A:123:TYR:CE1	2.22	0.75
1:A:417:ILE:HG12	1:A:428:THR:HG22	1.69	0.73
1:A:298:ASN:HD22	1:A:317:VAL:H	1.36	0.72
1:A:379:PRO:HD2	3:A:769:HOH:O	1.93	0.67
1:A:32:ASP:OD2	1:A:37:THR:OG1	2.11	0.65
1:A:60:LYS:HA	1:A:122:ARG:HH21	1.61	0.65
1:A:174:ALA:HB3	1:A:498:ILE:HD13	1.78	0.64
1:A:73:ARG:HD3	1:A:77:ASN:O	1.97	0.64
1:A:298:ASN:ND2	1:A:317:VAL:H	1.96	0.62
1:A:35:LYS:HE2	1:A:74:GLN:HG3	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:9:ILE:HD12	1:A:145:VAL:HG12	1.85	0.58
1:A:189:TYR:CD1	1:A:197:SER:HB2	2.38	0.58
1:A:552:GLN:HG3	3:A:961:HOH:O	2.04	0.57
1:A:475:ILE:HD12	1:A:486:GLN:CD	2.24	0.57
1:A:495:TYR:O	1:A:496:HIS:HB2	2.04	0.57
1:A:30:ALA:HB3	1:A:55:TYR:OH	2.05	0.56
1:A:146:PHE:CD1	1:A:146:PHE:N	2.73	0.56
1:A:71:LEU:HD12	1:A:72:PRO:HD2	1.87	0.56
1:A:30:ALA:O	1:A:142:GLU:HA	2.05	0.56
1:A:174:ALA:HA	1:A:184:LEU:O	2.06	0.55
1:A:171:PRO:HD2	1:A:511:GLY:HA2	1.89	0.55
1:A:21:ALA:HA	1:A:40:HIS:O	2.06	0.55
1:A:56:THR:HG21	1:A:125:ARG:HH21	1.70	0.55
1:A:11:ARG:NH1	1:A:31:ILE:HA	2.23	0.53
1:A:103:GLY:HA3	1:A:166:ASP:O	2.08	0.53
1:A:22:GLN:NE2	1:A:43:TYR:O	2.42	0.52
1:A:573:LEU:HG	1:A:592:LEU:HD11	1.92	0.52
1:A:170:VAL:HB	1:A:514:LEU:HD13	1.91	0.52
1:A:95:ASN:N	1:A:95:ASN:HD22	2.08	0.52
1:A:38:PHE:HB3	1:A:141:ALA:HA	1.92	0.52
1:A:439:ARG:NH2	1:A:474:GLU:HG3	2.25	0.51
1:A:560:ILE:O	1:A:603:SER:HA	2.10	0.51
1:A:328:LEU:HA	1:A:331:SER:OG	2.11	0.51
1:A:522:HIS:HD2	3:A:820:HOH:O	1.94	0.50
1:A:5:ILE:HD12	1:A:490:SER:HB3	1.93	0.50
1:A:227:PHE:O	1:A:244:GLY:HA3	2.11	0.50
1:A:548:ARG:O	1:A:562:ILE:HA	2.11	0.50
1:A:16:VAL:HG12	1:A:57:ILE:HG12	1.92	0.50
1:A:90:SER:HB2	1:A:96:TRP:CE3	2.47	0.49
1:A:317:VAL:O	1:A:320:MET:HG2	2.13	0.48
1:A:228:CYS:N	1:A:229:PRO:HD3	2.26	0.48
1:A:522:HIS:CD2	3:A:820:HOH:O	2.66	0.48
1:A:94:THR:HB	1:A:95:ASN:HD22	1.77	0.48
1:A:285:THR:O	1:A:299:GLY:HA2	2.14	0.47
1:A:39:TRP:O	1:A:139:SER:HA	2.14	0.47
1:A:539:ASN:HB3	3:A:893:HOH:O	2.13	0.47
1:A:174:ALA:CB	1:A:498:ILE:HD13	2.42	0.47
1:A:177:GLU:HB2	1:A:180:SER:OG	2.15	0.47
1:A:401:GLY:O	1:A:411:THR:HG22	2.15	0.47
1:A:235:GLY:HA3	1:A:281:GLY:HA3	1.97	0.47
1:A:189:TYR:HB2	1:A:201:ILE:HG23	1.96	0.47
1:A:624:ASN:OD1	1:A:626:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:425:SER:HA	1:A:426:PRO:HD2	1.81	0.46
1:A:61:THR:O	1:A:122:ARG:HA	2.15	0.46
1:A:275:SER:HA	1:A:284:PHE:O	2.16	0.46
1:A:59:MET:C	1:A:61:THR:H	2.18	0.46
1:A:554:VAL:HG22	1:A:558:GLY:HA3	1.98	0.46
1:A:169:ILE:HG22	1:A:191:ASN:HB2	1.96	0.45
1:A:123:TYR:CD1	1:A:123:TYR:N	2.84	0.45
1:A:15:ALA:HB2	1:A:60:LYS:HZ2	1.82	0.45
1:A:298:ASN:ND2	1:A:316:LYS:HA	2.32	0.44
1:A:378:ALA:HA	1:A:379:PRO:HD3	1.85	0.44
1:A:46:ASN:HA	1:A:46:ASN:HD22	1.50	0.44
1:A:356:TRP:O	1:A:365:VAL:HA	2.17	0.43
1:A:402:SER:HB2	1:A:403:PRO:HD2	2.00	0.43
1:A:506:ARG:HD3	3:A:819:HOH:O	2.18	0.43
1:A:173:ALA:O	1:A:185:MET:HA	2.18	0.43
1:A:334:HIS:CE1	1:A:581:HIS:HB3	2.53	0.43
1:A:94:THR:HB	1:A:95:ASN:ND2	2.34	0.43
1:A:59:MET:O	1:A:61:THR:HG22	2.19	0.43
1:A:393:LYS:HB2	1:A:395:LYS:HG2	2.00	0.42
1:A:554:VAL:CG2	1:A:558:GLY:HA3	2.49	0.42
1:A:117:GLU:OE2	1:A:490:SER:HB2	2.19	0.42
1:A:534:TYR:CE1	1:A:540:LEU:HD23	2.55	0.42
1:A:26:GLU:OE1	1:A:29:LYS:HE2	2.20	0.41
1:A:468:THR:N	1:A:469:PRO:CD	2.83	0.41
1:A:466:ASP:OD2	1:A:522:HIS:HE1	2.02	0.41
1:A:261:ILE:HA	1:A:262:PRO:HD3	1.85	0.41
1:A:161:TRP:CE2	1:A:489:ASN:HB3	2.55	0.41
1:A:59:MET:O	1:A:60:LYS:HB2	2.21	0.41
1:A:43:TYR:HA	1:A:48:ASP:OD1	2.21	0.41
1:A:21:ALA:HB1	1:A:26:GLU:HA	2.03	0.41
1:A:398:THR:O	1:A:414:ALA:HA	2.21	0.41
1:A:51:PRO:HA	1:A:52:PRO:C	2.41	0.40
1:A:61:THR:HG23	1:A:63:GLN:NE2	2.36	0.40
1:A:346:PHE:CE2	1:A:348:ALA:HB2	2.56	0.40
1:A:447:LEU:HA	1:A:448:PRO:HD3	1.89	0.40
1:A:22:GLN:O	1:A:25:ASN:N	2.49	0.40
1:A:424:THR:O	1:A:426:PRO:HD3	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:12:ASN:ND2	1:A:548:ARG:NH1[3_545]	2.14	0.06
3:A:836:HOH:O	3:A:958:HOH:O[2_656]	2.17	0.03

## 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	637/639 (100%)	604 (95%)	29 (5%)	4 (1%)	33 32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	514	LEU
1	A	494	VAL
1	A	229	PRO

### 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	526/526 (100%)	503 (96%)	23 (4%)	39 45

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	SER
1	A	27	CYS

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Mol	Chain	Res	Type
1	A	46	ASN
1	A	68	LEU
1	A	91	SER
1	A	95	ASN
1	A	98	SER
1	A	135	GLN
1	A	137	TRP
1	A	216	ASP
1	A	223	LYS
1	A	229	PRO
1	A	256	SER
1	A	259	SER
1	A	274	SER
1	A	459	ARG
1	A	490	SER
1	A	532	TYR
1	A	536	SER
1	A	542	THR
1	A	548	ARG
1	A	563	SER
1	A	639	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	46	ASN
1	A	78	GLN
1	A	95	ASN
1	A	298	ASN
1	A	427	ASN
1	A	522	HIS
1	A	552	GLN
1	A	597	ASN
1	A	600	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 ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	636/639 (99%)	11.49	635 (99%) 0 0	6, 21, 65, 100	0

All (635) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	451	SER	32.2
1	A	145	VAL	28.8
1	A	351	SER	28.3
1	A	541	ALA	27.2
1	A	97	GLY	27.0
1	A	14	TRP	26.9
1	A	322	THR	26.3
1	A	538	GLY	25.7
1	A	537	ASN	25.0
1	A	450	GLY	24.0
1	A	410	ALA	23.9
1	A	339	GLY	23.3
1	A	609	ASP	22.5
1	A	337	LEU	21.7
1	A	256	SER	21.7
1	A	638	THR	21.7
1	A	318	ASN	21.6
1	A	152	THR	21.6
1	A	539	ASN	21.5
1	A	348	ALA	21.2
1	A	553	SER	21.0
1	A	558	GLY	20.5
1	A	79	ASN	20.3
1	A	565	ASP	20.1
1	A	403	PRO	20.1
1	A	43	TYR	20.0
1	A	554	VAL	19.9

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Mol	Chain	Res	Type	RSRZ
1	A	143	ILE	19.9
1	A	389	TYR	19.7
1	A	613	ALA	19.7
1	A	606	VAL	19.5
1	A	381	ALA	19.3
1	A	340	TRP	19.2
1	A	349	GLY	19.2
1	A	151	TYR	19.1
1	A	542	THR	19.0
1	A	304	PRO	19.0
1	A	536	SER	19.0
1	A	95	ASN	19.0
1	A	315	ALA	18.8
1	A	429	VAL	18.8
1	A	388	MET	18.7
1	A	391	ALA	18.6
1	A	484	TYR	18.5
1	A	416	ILE	18.5
1	A	505	GLY	18.5
1	A	179	THR	18.4
1	A	398	THR	18.3
1	A	356	TRP	18.3
1	A	77	ASN	18.3
1	A	281	GLY	18.2
1	A	431	ALA	18.0
1	A	312	LEU	18.0
1	A	564	THR	17.8
1	A	611	GLY	17.8
1	A	535	ASN	17.8
1	A	96	TRP	17.7
1	A	309	TRP	17.7
1	A	376	GLY	17.7
1	A	317	VAL	17.7
1	A	183	VAL	17.6
1	A	595	THR	17.6
1	A	243	GLY	17.6
1	A	27	CYS	17.5
1	A	302	TYR	17.4
1	A	336	TRP	17.4
1	A	557	GLY	17.4
1	A	28	ASN	17.4
1	A	515	CYS	17.4

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Mol	Chain	Res	Type	RSRZ
1	A	635	ILE	17.4
1	A	422	PRO	17.4
1	A	560	ILE	17.4
1	A	31	ILE	17.3
1	A	301	VAL	17.3
1	A	396	ILE	17.3
1	A	425	SER	17.2
1	A	124	VAL	17.2
1	A	338	PHE	17.2
1	A	436	TYR	17.1
1	A	75	ASP	17.1
1	A	482	THR	17.0
1	A	419	LEU	16.9
1	A	23	SER	16.9
1	A	438	ALA	16.9
1	A	561	THR	16.9
1	A	610	SER	16.9
1	A	110	THR	16.9
1	A	544	PRO	16.9
1	A	64	ASN	16.9
1	A	478	PRO	16.9
1	A	37	THR	16.9
1	A	253	TYR	16.8
1	A	423	GLY	16.8
1	A	180	SER	16.7
1	A	345	VAL	16.7
1	A	150	SER	16.6
1	A	278	MET	16.5
1	A	353	ALA	16.4
1	A	19	ASP	16.4
1	A	76	GLY	16.4
1	A	39	TRP	16.3
1	A	284	PHE	16.2
1	A	612	VAL	16.2
1	A	432	SER	16.2
1	A	30	ALA	16.2
1	A	600	ASN	16.2
1	A	365	VAL	16.2
1	A	358	TYR	16.2
1	A	346	PHE	16.2
1	A	305	SER	16.1
1	A	417	ILE	16.1

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Mol	Chain	Res	Type	RSRZ
1	A	343	GLY	16.1
1	A	261	ILE	16.0
1	A	446	VAL	16.0
1	A	418	THR	15.9
1	A	430	PHE	15.9
1	A	307	LYS	15.9
1	A	549	THR	15.9
1	A	608	SER	15.9
1	A	548	ARG	15.9
1	A	59	MET	15.9
1	A	298	ASN	15.8
1	A	154	PRO	15.8
1	A	136	PRO	15.8
1	A	397	LEU	15.7
1	A	354	MET	15.7
1	A	368	ALA	15.7
1	A	475	ILE	15.7
1	A	444	SER	15.7
1	A	424	THR	15.6
1	A	452	THR	15.6
1	A	359	THR	15.5
1	A	352	THR	15.4
1	A	24	GLY	15.4
1	A	363	GLY	15.4
1	A	426	PRO	15.4
1	A	38	PHE	15.4
1	A	189	TYR	15.4
1	A	562	ILE	15.4
1	A	412	THR	15.3
1	A	8	ALA	15.3
1	A	392	VAL	15.3
1	A	344	SER	15.2
1	A	390	ASP	15.2
1	A	313	PRO	15.2
1	A	453	PHE	15.2
1	A	411	THR	15.1
1	A	212	GLY	15.0
1	A	146	PHE	15.0
1	A	286	ILE	15.0
1	A	33	GLY	15.0
1	A	311	SER	15.0
1	A	476	TYR	14.9

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Mol	Chain	Res	Type	RSRZ
1	A	12	ASN	14.9
1	A	264	PRO	14.8
1	A	299	GLY	14.8
1	A	477	VAL	14.8
1	A	303	SER	14.8
1	A	361	GLY	14.8
1	A	357	TYR	14.7
1	A	550	SER	14.7
1	A	364	ASP	14.6
1	A	551	THR	14.6
1	A	362	SER	14.6
1	A	161	TRP	14.5
1	A	378	ALA	14.5
1	A	100	VAL	14.5
1	A	596	ASN	14.5
1	A	153	ALA	14.4
1	A	414	ALA	14.4
1	A	158	LEU	14.4
1	A	148	ALA	14.3
1	A	308	THR	14.3
1	A	379	PRO	14.3
1	A	434	GLY	14.3
1	A	572	SER	14.3
1	A	442	HIS	14.3
1	A	428	THR	14.3
1	A	367	SER	14.3
1	A	34	ASN	14.2
1	A	394	GLY	14.2
1	A	481	ASP	14.1
1	A	377	VAL	14.1
1	A	156	PRO	14.1
1	A	400	GLY	14.1
1	A	65	VAL	14.1
1	A	268	VAL	14.1
1	A	287	GLY	14.1
1	A	568	ILE	14.0
1	A	306	SER	14.0
1	A	115	ASN	14.0
1	A	6	GLY	13.9
1	A	319	PRO	13.9
1	A	604	PHE	13.9
1	A	433	ASN	13.8

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Mol	Chain	Res	Type	RSRZ
1	A	547	THR	13.7
1	A	637	VAL	13.7
1	A	556	VAL	13.7
1	A	618	TRP	13.7
1	A	486	GLN	13.7
1	A	10	SER	13.7
1	A	15	ALA	13.6
1	A	147	GLN	13.6
1	A	196	GLY	13.6
1	A	602	TYR	13.6
1	A	127	VAL	13.6
1	A	262	PRO	13.6
1	A	335	ALA	13.5
1	A	369	GLY	13.5
1	A	594	LEU	13.5
1	A	350	PRO	13.5
1	A	149	SER	13.4
1	A	360	SER	13.4
1	A	300	GLU	13.4
1	A	157	GLY	13.4
1	A	534	TYR	13.4
1	A	626	ALA	13.4
1	A	68	LEU	13.4
1	A	267	GLN	13.3
1	A	355	ASN	13.3
1	A	576	TYR	13.3
1	A	472	THR	13.3
1	A	310	THR	13.3
1	A	525	ALA	13.3
1	A	71	LEU	13.2
1	A	634	THR	13.2
1	A	399	PHE	13.2
1	A	36	ASP	13.2
1	A	18	CYS	13.1
1	A	236	ASN	13.1
1	A	21	ALA	13.1
1	A	483	PHE	13.1
1	A	563	SER	13.1
1	A	427	ASN	13.1
1	A	420	GLY	13.0
1	A	32	ASP	13.0
1	A	170	VAL	13.0

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Mol	Chain	Res	Type	RSRZ
1	A	566	SER	13.0
1	A	257	SER	13.0
1	A	415	HIS	13.0
1	A	540	LEU	12.9
1	A	239	ILE	12.8
1	A	347	GLN	12.8
1	A	502	LEU	12.8
1	A	280	ASP	12.7
1	A	9	ILE	12.7
1	A	413	ASN	12.6
1	A	485	LYS	12.5
1	A	155	GLN	12.4
1	A	247	ALA	12.4
1	A	130	THR	12.4
1	A	470	VAL	12.4
1	A	94	THR	12.3
1	A	78	GLN	12.3
1	A	373	SER	12.3
1	A	316	LYS	12.3
1	A	503	PRO	12.2
1	A	629	PRO	12.2
1	A	435	LEU	12.2
1	A	240	VAL	12.2
1	A	615	PRO	12.2
1	A	185	MET	12.2
1	A	623	MET	12.2
1	A	29	LYS	12.1
1	A	624	ASN	12.1
1	A	570	LYS	12.1
1	A	619	MET	12.1
1	A	462	ILE	12.0
1	A	11	ARG	12.0
1	A	589	ARG	12.0
1	A	614	LEU	11.9
1	A	7	SER	11.9
1	A	186	TRP	11.9
1	A	26	GLU	11.8
1	A	372	GLN	11.8
1	A	106	PHE	11.8
1	A	98	SER	11.8
1	A	3	ALA	11.8
1	A	61	THR	11.8

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Mol	Chain	Res	Type	RSRZ
1	A	118	THR	11.8
1	A	320	MET	11.8
1	A	171	PRO	11.8
1	A	421	GLU	11.7
1	A	617	TYR	11.7
1	A	500	LEU	11.7
1	A	334	HIS	11.7
1	A	514	LEU	11.7
1	A	40	HIS	11.7
1	A	480	GLN	11.7
1	A	371	ARG	11.6
1	A	405	TYR	11.6
1	A	543	ARG	11.6
1	A	603	SER	11.6
1	A	605	GLN	11.6
1	A	89	LEU	11.6
1	A	35	LYS	11.5
1	A	559	ARG	11.5
1	A	569	SER	11.4
1	A	144	ASN	11.4
1	A	473	PRO	11.4
1	A	487	ASN	11.4
1	A	375	ARG	11.4
1	A	204	THR	11.4
1	A	62	THR	11.3
1	A	469	PRO	11.2
1	A	607	PRO	11.2
1	A	41	THR	11.2
1	A	479	GLU	11.2
1	A	528	PHE	11.2
1	A	471	PHE	11.1
1	A	393	LYS	11.1
1	A	579	ALA	11.1
1	A	70	MET	11.1
1	A	437	PHE	11.1
1	A	314	ASN	11.0
1	A	574	ILE	11.0
1	A	463	PRO	11.0
1	A	532	TYR	11.0
1	A	395	LYS	10.9
1	A	263	GLY	10.9
1	A	141	ALA	10.9

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Mol	Chain	Res	Type	RSRZ
1	A	636	ARG	10.9
1	A	341	LYS	10.9
1	A	639	GLN	10.8
1	A	495	TYR	10.8
1	A	409	ASP	10.8
1	A	252	LEU	10.8
1	A	374	ASN	10.8
1	A	555	LYS	10.7
1	A	628	VAL	10.7
1	A	622	VAL	10.7
1	A	455	THR	10.7
1	A	530	PRO	10.7
1	A	266	MET	10.6
1	A	187	SER	10.6
1	A	258	ASP	10.6
1	A	580	THR	10.5
1	A	120	PRO	10.5
1	A	173	ALA	10.5
1	A	573	LEU	10.5
1	A	48	ASP	10.5
1	A	119	ARG	10.5
1	A	370	LYS	10.5
1	A	342	LYS	10.4
1	A	385	ASN	10.4
1	A	87	VAL	10.3
1	A	45	ALA	10.3
1	A	191	ASN	10.3
1	A	134	GLY	10.3
1	A	590	ILE	10.3
1	A	246	ASP	10.3
1	A	99	PRO	10.2
1	A	497	SER	10.2
1	A	533	LEU	10.2
1	A	126	LEU	10.2
1	A	366	LYS	10.1
1	A	55	TYR	10.1
1	A	272	TYR	10.1
1	A	506	ARG	10.1
1	A	468	THR	10.0
1	A	529	THR	10.0
1	A	578	THR	10.0
1	A	279	SER	9.9

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Mol	Chain	Res	Type	RSRZ
1	A	104	SER	9.9
1	A	163	PRO	9.8
1	A	113	TYR	9.8
1	A	181	GLY	9.8
1	A	245	ASN	9.7
1	A	67	GLY	9.7
1	A	105	TRP	9.7
1	A	387	VAL	9.7
1	A	109	SER	9.7
1	A	488	PRO	9.7
1	A	82	ILE	9.7
1	A	466	ASP	9.7
1	A	169	ILE	9.6
1	A	260	TRP	9.6
1	A	218	THR	9.6
1	A	449	ASP	9.6
1	A	51	PRO	9.6
1	A	289	SER	9.5
1	A	402	SER	9.5
1	A	201	ILE	9.5
1	A	228	CYS	9.4
1	A	631	VAL	9.4
1	A	220	THR	9.4
1	A	203	LEU	9.4
1	A	271	GLY	9.4
1	A	383	CYS	9.4
1	A	42	PHE	9.3
1	A	129	ILE	9.2
1	A	142	GLU	9.2
1	A	175	ALA	9.2
1	A	103	GLY	9.2
1	A	254	ASP	9.2
1	A	282	ARG	9.1
1	A	524	ASP	9.1
1	A	489	ASN	9.1
1	A	571	ALA	9.1
1	A	210	SER	9.1
1	A	57	ILE	9.1
1	A	72	PRO	9.1
1	A	633	SER	9.0
1	A	227	PHE	9.0
1	A	4	PRO	9.0

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Mol	Chain	Res	Type	RSRZ
1	A	207	TRP	9.0
1	A	511	GLY	9.0
1	A	382	MET	9.0
1	A	174	ALA	8.9
1	A	632	ALA	8.9
1	A	81	TRP	8.8
1	A	283	VAL	8.8
1	A	616	GLY	8.8
1	A	552	GLN	8.8
1	A	88	TYR	8.8
1	A	531	ASN	8.8
1	A	93	GLY	8.7
1	A	248	LYS	8.7
1	A	22	GLN	8.7
1	A	518	CYS	8.6
1	A	128	ALA	8.6
1	A	285	THR	8.6
1	A	447	LEU	8.6
1	A	456	GLY	8.6
1	A	231	ILE	8.6
1	A	53	HIS	8.5
1	A	499	SER	8.5
1	A	443	THR	8.5
1	A	297	LYS	8.5
1	A	238	GLN	8.5
1	A	384	GLY	8.5
1	A	584	ASN	8.5
1	A	90	SER	8.4
1	A	290	TRP	8.4
1	A	321	LEU	8.4
1	A	54	THR	8.4
1	A	195	GLY	8.4
1	A	508	PHE	8.3
1	A	601	SER	8.3
1	A	625	SER	8.3
1	A	459	ARG	8.3
1	A	591	PRO	8.2
1	A	588	ARG	8.2
1	A	323	ALA	8.2
1	A	184	LEU	8.2
1	A	221	VAL	8.2
1	A	440	THR	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	25	ASN	8.2
1	A	159	GLY	8.2
1	A	273	GLN	8.2
1	A	5	ILE	8.2
1	A	329	TYR	8.1
1	A	401	GLY	8.1
1	A	211	THR	8.1
1	A	507	VAL	8.1
1	A	192	ASP	8.1
1	A	114	SER	8.0
1	A	107	ALA	8.0
1	A	454	ILE	8.0
1	A	494	VAL	8.0
1	A	251	SER	8.0
1	A	620	LEU	7.9
1	A	513	GLY	7.9
1	A	121	ALA	7.9
1	A	44	GLY	7.9
1	A	627	GLY	7.9
1	A	593	THR	7.9
1	A	219	VAL	7.8
1	A	585	THR	7.8
1	A	498	ILE	7.8
1	A	237	GLY	7.8
1	A	294	VAL	7.8
1	A	208	ASP	7.8
1	A	255	SER	7.7
1	A	523	PHE	7.7
1	A	139	SER	7.7
1	A	138	THR	7.7
1	A	582	THR	7.7
1	A	501	LEU	7.7
1	A	80	GLY	7.7
1	A	577	GLY	7.7
1	A	164	THR	7.7
1	A	84	ARG	7.7
1	A	545	LYS	7.6
1	A	20	SER	7.6
1	A	474	GLU	7.6
1	A	13	ASN	7.6
1	A	133	ASN	7.6
1	A	194	PHE	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	621	PHE	7.6
1	A	467	SER	7.6
1	A	265	ASP	7.6
1	A	464	PHE	7.5
1	A	209	PRO	7.5
1	A	630	SER	7.5
1	A	224	HIS	7.4
1	A	406	GLN	7.4
1	A	172	ALA	7.4
1	A	259	SER	7.3
1	A	73	ARG	7.3
1	A	583	VAL	7.3
1	A	235	GLY	7.3
1	A	132	ALA	7.3
1	A	168	PRO	7.3
1	A	293	GLY	7.2
1	A	439	ARG	7.2
1	A	202	THR	7.2
1	A	521	ASN	7.2
1	A	233	MET	7.2
1	A	46	ASN	7.2
1	A	586	ASP	7.1
1	A	165	ILE	7.1
1	A	461	GLY	7.1
1	A	288	GLY	7.1
1	A	408	SER	7.1
1	A	229	PRO	7.1
1	A	490	SER	7.0
1	A	182	ARG	7.0
1	A	69	SER	7.0
1	A	216	ASP	7.0
1	A	407	ASP	7.0
1	A	205	SER	6.9
1	A	116	PHE	6.9
1	A	66	ASN	6.9
1	A	496	HIS	6.8
1	A	519	THR	6.8
1	A	567	SER	6.8
1	A	16	VAL	6.8
1	A	460	ARG	6.8
1	A	527	ILE	6.8
1	A	592	LEU	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	178	PRO	6.7
1	A	522	HIS	6.7
1	A	546	ILE	6.7
1	A	135	GLN	6.7
1	A	140	ILE	6.7
1	A	188	SER	6.7
1	A	123	TYR	6.6
1	A	85	HIS	6.6
1	A	102	SER	6.6
1	A	520	THR	6.5
1	A	160	ARG	6.5
1	A	222	THR	6.5
1	A	575	ARG	6.5
1	A	226	MET	6.5
1	A	74	GLN	6.5
1	A	296	GLU	6.4
1	A	111	THR	6.4
1	A	327	GLY	6.4
1	A	56	THR	6.4
1	A	333	ASN	6.4
1	A	457	GLY	6.4
1	A	167	LEU	6.3
1	A	214	VAL	6.2
1	A	197	SER	6.2
1	A	328	LEU	6.2
1	A	112	LYS	6.2
1	A	292	GLY	6.2
1	A	491	ILE	6.2
1	A	2	SER	6.2
1	A	516	GLY	6.2
1	A	493	ARG	6.1
1	A	177	GLU	6.1
1	A	225	ASP	6.1
1	A	63	GLN	6.1
1	A	380	ASP	6.1
1	A	131	GLU	6.0
1	A	445	VAL	6.0
1	A	275	SER	6.0
1	A	274	SER	6.0
1	A	60	LYS	5.9
1	A	510	GLY	5.9
1	A	324	ASP	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	92	ASP	5.8
1	A	91	SER	5.8
1	A	125	ARG	5.8
1	A	244	GLY	5.8
1	A	232	SER	5.7
1	A	404	ASP	5.7
1	A	217	ARG	5.7
1	A	49	PRO	5.6
1	A	295	PHE	5.6
1	A	386	ALA	5.6
1	A	176	ILE	5.6
1	A	193	ALA	5.5
1	A	199	GLY	5.5
1	A	166	ASP	5.5
1	A	230	GLY	5.5
1	A	241	VAL	5.4
1	A	276	ALA	5.4
1	A	587	GLN	5.4
1	A	465	GLU	5.4
1	A	52	PRO	5.4
1	A	448	PRO	5.4
1	A	234	ASP	5.3
1	A	509	ASN	5.3
1	A	581	HIS	5.2
1	A	108	ASP	5.2
1	A	213	ILE	5.2
1	A	250	THR	5.0
1	A	137	TRP	5.0
1	A	83	GLY	5.0
1	A	277	THR	4.9
1	A	200	GLY	4.9
1	A	198	PRO	4.9
1	A	526	GLN	4.8
1	A	504	ASP	4.8
1	A	58	ASP	4.8
1	A	190	ARG	4.8
1	A	517	ASP	4.8
1	A	458	GLN	4.8
1	A	326	GLN	4.7
1	A	47	GLY	4.7
1	A	512	GLY	4.5
1	A	17	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	441	PHE	4.5
1	A	117	GLU	4.4
1	A	162	GLY	4.4
1	A	332	ASP	4.4
1	A	492	VAL	4.4
1	A	215	SER	4.2
1	A	330	ARG	4.2
1	A	242	THR	4.2
1	A	101	ALA	4.1
1	A	50	LYS	4.0
1	A	270	ARG	4.0
1	A	122	ARG	3.9
1	A	269	ALA	3.9
1	A	86	GLU	3.8
1	A	291	SER	3.6
1	A	206	SER	3.5
1	A	249	LYS	3.5
1	A	223	LYS	2.9
1	A	1	ALA	2.9
1	A	331	SER	2.4

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NA	A	702	1/1	1.22	2.17	20,20,20,20	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.