



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:54 PM GMT

PDB ID : 1GOG
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 : 1.90 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>

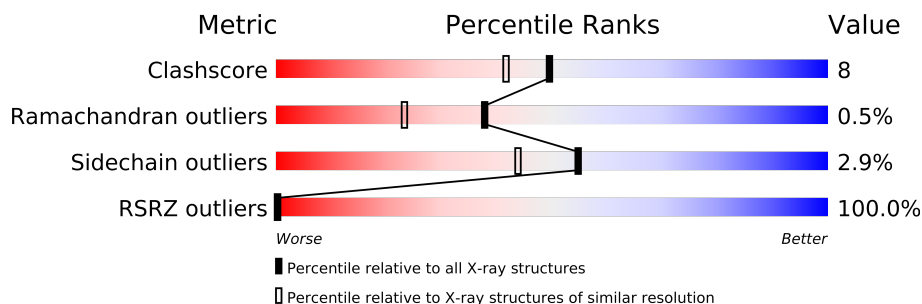
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 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 1.90 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	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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	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	CU	A	700	-	X
3	NA	A	702	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5142 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 COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

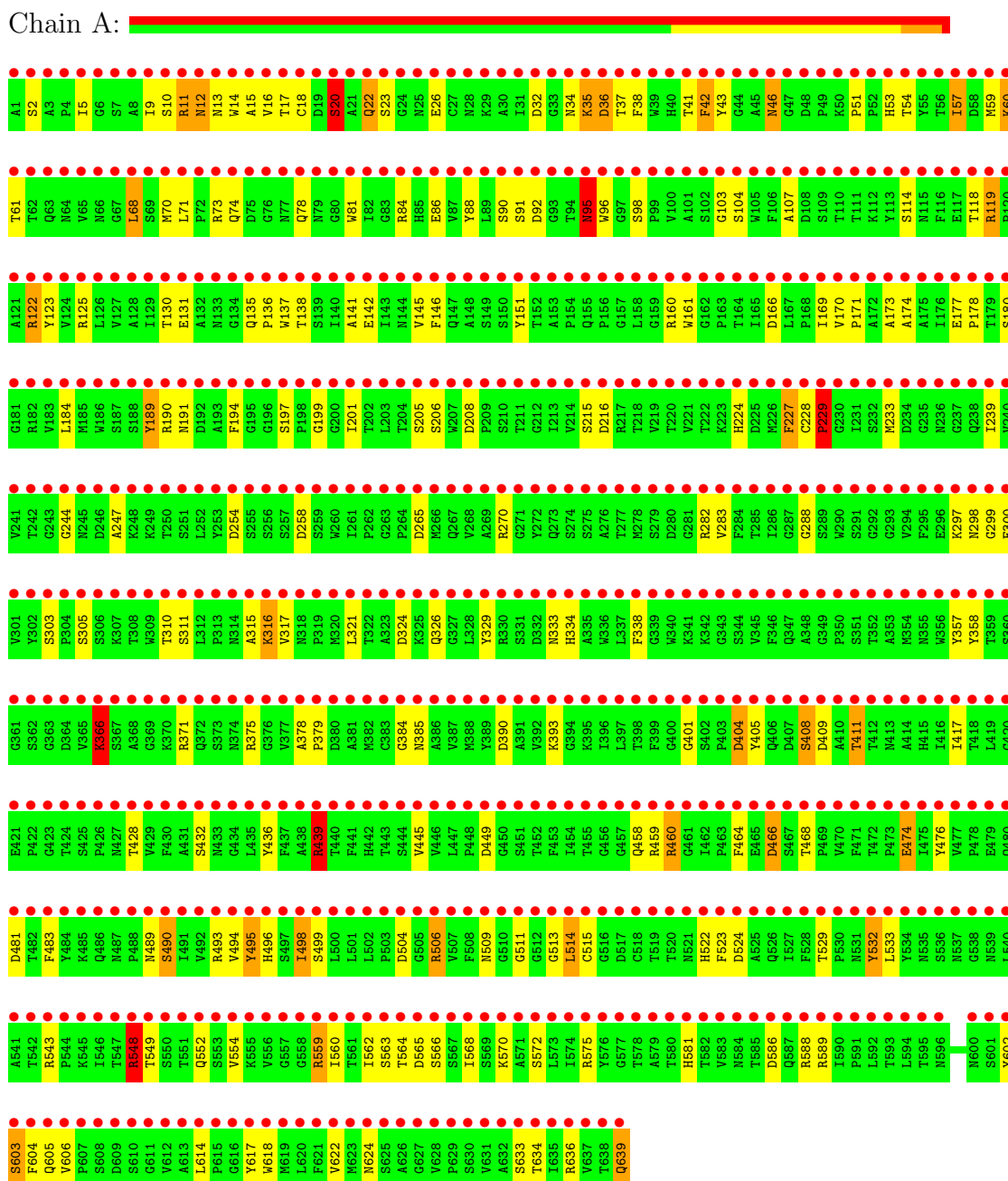
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	98.00Å 89.40Å 86.70Å 90.00° 117.80° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 9.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.90) 83.7 (9.99-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.90Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.170 , (Not available) 0.142 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.65 , 138.6	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 46302 reflections	Xtriage
F_o, F_c correlation	0.41	EDS
Total number of atoms	5142	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: NA, CU

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	1.13	3/4959 (0.1%)	2.19	189/6765 (2.8%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	436	TYR	CD1-CE1	5.64	1.47	1.39
1	A	303	SER	CB-OG	5.47	1.49	1.42
1	A	490	SER	CA-CB	5.02	1.60	1.52

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ARG	NE-CZ-NH2	-20.39	110.11	120.30
1	A	73	ARG	NE-CZ-NH1	18.43	129.52	120.30
1	A	460	ARG	NE-CZ-NH2	-16.14	112.23	120.30
1	A	543	ARG	NE-CZ-NH2	-15.75	112.43	120.30
1	A	548	ARG	CD-NE-CZ	15.45	145.23	123.60
1	A	190	ARG	NE-CZ-NH1	15.31	127.95	120.30
1	A	190	ARG	NE-CZ-NH2	-15.30	112.65	120.30
1	A	459	ARG	NE-CZ-NH1	15.16	127.88	120.30
1	A	493	ARG	NE-CZ-NH2	-14.66	112.97	120.30
1	A	282	ARG	NE-CZ-NH1	12.71	126.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	ASP	CB-CG-OD2	-12.39	107.15	118.30
1	A	119	ARG	NE-CZ-NH2	-12.28	114.16	120.30
1	A	543	ARG	NE-CZ-NH1	12.16	126.38	120.30
1	A	265	ASP	CB-CG-OD2	12.13	129.22	118.30
1	A	114	SER	N-CA-CB	11.54	127.80	110.50
1	A	73	ARG	NE-CZ-NH2	-11.43	114.59	120.30
1	A	460	ARG	NH1-CZ-NH2	10.95	131.45	119.40
1	A	338	PHE	CB-CG-CD2	-10.64	113.35	120.80
1	A	532	TYR	CB-CG-CD1	10.63	127.38	121.00
1	A	119	ARG	NE-CZ-NH1	10.55	125.58	120.30
1	A	216	ASP	CB-CA-C	9.94	130.28	110.40
1	A	532	TYR	CB-CG-CD2	-9.94	115.04	121.00
1	A	459	ARG	NE-CZ-NH2	-9.89	115.35	120.30
1	A	258	ASP	CB-CG-OD1	9.66	126.99	118.30
1	A	495	TYR	CB-CG-CD1	-9.56	115.26	121.00
1	A	11	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	A	523	PHE	CB-CG-CD1	9.34	127.33	120.80
1	A	589	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	122	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	A	604	PHE	CB-CG-CD2	-8.99	114.51	120.80
1	A	408	SER	N-CA-CB	-8.98	97.03	110.50
1	A	88	TYR	CB-CG-CD2	-8.90	115.66	121.00
1	A	189	TYR	CB-CG-CD1	8.73	126.24	121.00
1	A	375	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	405	TYR	CB-CG-CD1	8.66	126.19	121.00
1	A	125	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	A	404	ASP	CB-CG-OD2	-8.44	110.71	118.30
1	A	566	SER	O-C-N	8.41	136.15	122.70
1	A	20	SER	N-CA-CB	8.27	122.91	110.50
1	A	523	PHE	CB-CG-CD2	-8.17	115.08	120.80
1	A	409	ASP	CB-CG-OD2	-8.05	111.05	118.30
1	A	483	PHE	CB-CG-CD2	-8.01	115.20	120.80
1	A	476	TYR	CB-CG-CD2	-7.99	116.21	121.00
1	A	460	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	A	506	ARG	CD-NE-CZ	7.92	134.69	123.60
1	A	548	ARG	NE-CZ-NH2	7.76	124.18	120.30
1	A	432	SER	N-CA-CB	-7.59	99.12	110.50
1	A	404	ASP	CB-CG-OD1	7.57	125.11	118.30
1	A	565	ASP	CB-CG-OD1	7.49	125.04	118.30
1	A	493	ARG	NH1-CZ-NH2	7.49	127.63	119.40
1	A	160	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	A	92	ASP	CB-CG-OD1	7.46	125.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	SER	CB-CA-C	-7.45	95.94	110.10
1	A	390	ASP	OD1-CG-OD2	7.42	137.39	123.30
1	A	160	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	A	98	SER	N-CA-CB	-7.30	99.55	110.50
1	A	122	ARG	NH1-CZ-NH2	-7.03	111.67	119.40
1	A	36	ASP	O-C-N	7.01	133.91	122.70
1	A	474	GLU	OE1-CD-OE2	6.92	131.60	123.30
1	A	119	ARG	CD-NE-CZ	6.91	133.27	123.60
1	A	333	ASN	O-C-N	6.87	133.69	122.70
1	A	586	ASP	CB-CG-OD1	-6.84	112.14	118.30
1	A	84	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	A	466	ASP	CB-CG-OD1	6.80	124.42	118.30
1	A	371	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	A	495	TYR	N-CA-CB	-6.73	98.49	110.60
1	A	216	ASP	CB-CG-OD2	6.72	124.35	118.30
1	A	449	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	2	SER	CB-CA-C	6.67	122.77	110.10
1	A	589	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	216	ASP	CB-CG-OD1	-6.63	112.33	118.30
1	A	288	GLY	CA-C-O	-6.63	108.67	120.60
1	A	490	SER	N-CA-CB	-6.59	100.61	110.50
1	A	229	PRO	N-CA-CB	-6.49	95.46	102.60
1	A	118	THR	O-C-N	6.48	133.07	122.70
1	A	92	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	A	499	SER	N-CA-CB	6.46	120.19	110.50
1	A	375	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	409	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	385	ASN	CB-CG-OD1	-6.38	108.84	121.60
1	A	476	TYR	CD1-CE1-CZ	-6.36	114.08	119.80
1	A	122	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	A	254	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	617	TYR	O-C-N	6.28	132.75	122.70
1	A	270	ARG	CB-CA-C	-6.27	97.85	110.40
1	A	88	TYR	CG-CD2-CE2	-6.27	116.28	121.30
1	A	194	PHE	CB-CG-CD2	-6.25	116.42	120.80
1	A	173	ALA	N-CA-CB	6.22	118.80	110.10
1	A	311	SER	N-CA-CB	-6.21	101.18	110.50
1	A	282	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	199	GLY	CA-C-O	-6.19	109.46	120.60
1	A	624	ASN	CB-CA-C	6.17	122.74	110.40
1	A	84	ARG	NH1-CZ-NH2	6.15	126.17	119.40
1	A	602	TYR	CG-CD1-CE1	-6.11	116.41	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	ARG	CA-CB-CG	-6.10	99.98	113.40
1	A	224	HIS	N-CA-CB	-6.10	99.63	110.60
1	A	636	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	70	MET	CG-SD-CE	6.04	109.87	100.20
1	A	633	SER	N-CA-CB	6.01	119.52	110.50
1	A	636	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	617	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	A	411	THR	OG1-CB-CG2	-5.96	96.30	110.00
1	A	36	ASP	CB-CG-OD1	-5.96	112.94	118.30
1	A	602	TYR	CB-CG-CD1	-5.95	117.43	121.00
1	A	445	VAL	CG1-CB-CG2	-5.94	101.40	110.90
1	A	122	ARG	CD-NE-CZ	5.93	131.91	123.60
1	A	326	GLN	CA-CB-CG	5.91	126.40	113.40
1	A	54	THR	N-CA-CB	-5.86	99.17	110.30
1	A	524	ASP	N-CA-CB	-5.84	100.09	110.60
1	A	10	SER	N-CA-CB	5.83	119.24	110.50
1	A	95	ASN	O-C-N	5.82	132.02	122.70
1	A	215	SER	CA-CB-OG	5.80	126.85	111.20
1	A	366	LYS	N-CA-CB	-5.75	100.24	110.60
1	A	481	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	A	201	ILE	O-C-N	5.73	131.87	122.70
1	A	233	MET	CA-CB-CG	-5.73	103.56	113.30
1	A	572	SER	N-CA-CB	-5.71	101.93	110.50
1	A	283	VAL	CA-CB-CG2	5.71	119.46	110.90
1	A	26	GLU	CA-CB-CG	5.69	125.91	113.40
1	A	189	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	A	57	ILE	O-C-N	5.65	131.74	122.70
1	A	384	GLY	N-CA-C	-5.63	99.01	113.10
1	A	436	TYR	CD1-CE1-CZ	-5.63	114.73	119.80
1	A	104	SER	O-C-N	5.60	131.66	122.70
1	A	42	PHE	CB-CG-CD2	-5.58	116.90	120.80
1	A	559	ARG	CD-NE-CZ	-5.57	115.80	123.60
1	A	300	GLU	N-CA-CB	5.56	120.61	110.60
1	A	321	LEU	CB-CG-CD2	-5.55	101.56	111.00
1	A	86	GLU	OE1-CD-OE2	5.52	129.93	123.30
1	A	18	CYS	O-C-N	5.52	131.53	122.70
1	A	125	ARG	CD-NE-CZ	5.52	131.32	123.60
1	A	206	SER	CB-CA-C	-5.52	99.62	110.10
1	A	205	SER	CB-CA-C	5.51	120.58	110.10
1	A	572	SER	CB-CA-C	5.51	120.58	110.10
1	A	504	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	614	LEU	CB-CG-CD2	5.45	120.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	549	THR	N-CA-CB	5.43	120.61	110.30
1	A	315	ALA	N-CA-C	-5.41	96.39	111.00
1	A	428	THR	OG1-CB-CG2	-5.41	97.56	110.00
1	A	639	GLN	N-CA-CB	5.40	120.31	110.60
1	A	357	TYR	CG-CD1-CE1	-5.39	116.98	121.30
1	A	300	GLU	CB-CG-CD	-5.37	99.69	114.20
1	A	316	LYS	O-C-N	5.37	131.30	122.70
1	A	513	GLY	O-C-N	5.37	131.30	122.70
1	A	178	PRO	O-C-N	5.37	131.29	122.70
1	A	564	THR	CA-CB-OG1	-5.37	97.73	109.00
1	A	606	VAL	CA-CB-CG2	-5.35	102.87	110.90
1	A	130	THR	N-CA-CB	5.34	120.45	110.30
1	A	288	GLY	O-C-N	5.34	131.25	122.70
1	A	570	LYS	N-CA-CB	-5.34	100.99	110.60
1	A	602	TYR	CZ-CE2-CD2	-5.34	115.00	119.80
1	A	151	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	A	305	SER	CB-CA-C	5.33	120.23	110.10
1	A	329	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	A	88	TYR	CD1-CE1-CZ	-5.30	115.03	119.80
1	A	324	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	634	THR	OG1-CB-CG2	5.29	122.17	110.00
1	A	68	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	299	GLY	O-C-N	5.29	131.16	122.70
1	A	338	PHE	CB-CG-CD1	5.28	124.50	120.80
1	A	297	LYS	CD-CE-NZ	-5.28	99.57	111.70
1	A	310	THR	O-C-N	5.27	131.13	122.70
1	A	603	SER	CB-CA-C	-5.26	100.11	110.10
1	A	509	ASN	C-N-CA	-5.24	111.31	122.30
1	A	498	ILE	O-C-N	5.22	131.06	122.70
1	A	138	THR	CA-CB-OG1	-5.21	98.06	109.00
1	A	227	PHE	CB-CG-CD1	-5.21	117.16	120.80
1	A	417	ILE	CA-CB-CG1	-5.21	101.11	111.00
1	A	384	GLY	CA-C-O	5.19	129.94	120.60
1	A	208	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	495	TYR	CD1-CE1-CZ	-5.17	115.14	119.80
1	A	506	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	A	239	ILE	CA-CB-CG1	-5.17	101.17	111.00
1	A	390	ASP	CB-CA-C	5.17	120.74	110.40
1	A	22	GLN	CA-CB-CG	-5.15	102.06	113.40
1	A	588	ARG	CD-NE-CZ	5.14	130.79	123.60
1	A	107	ALA	O-C-N	5.14	130.92	122.70
1	A	476	TYR	CG-CD2-CE2	-5.13	117.19	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	589	ARG	O-C-N	5.13	130.91	122.70
1	A	495	TYR	CG-CD2-CE2	-5.12	117.20	121.30
1	A	378	ALA	N-CA-CB	-5.12	102.94	110.10
1	A	258	ASP	N-CA-CB	5.11	119.80	110.60
1	A	142	GLU	CG-CD-OE2	5.10	128.50	118.30
1	A	476	TYR	CD1-CG-CD2	5.09	123.50	117.90
1	A	60	LYS	CB-CA-C	-5.08	100.24	110.40
1	A	316	LYS	N-CA-CB	-5.06	101.50	110.60
1	A	146	PHE	CB-CG-CD1	5.03	124.32	120.80
1	A	35	LYS	CA-CB-CG	5.02	124.44	113.40
1	A	247	ALA	CA-C-O	-5.00	109.59	120.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	439	ARG	Sidechain

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	4603	72	1
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	310	0	0	5	0
All	All	5142	0	4603	72	1

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 8.

All (72) 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	1.15	1.07
1:A:22:GLN:HG3	1:A:42:PHE:HA	1.43	0.97

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:298:ASN:HD22	1:A:317:VAL:H	1.21	0.87
1:A:22:GLN:NE2	1:A:46:ASN:HB2	1.92	0.82
1:A:35:LYS:HE3	1:A:71:LEU:HD21	1.64	0.78
1:A:298:ASN:ND2	1:A:317:VAL:H	1.83	0.74
1:A:170:VAL:HB	1:A:514:LEU:HD13	1.79	0.63
1:A:298:ASN:HD22	1:A:317:VAL:N	1.97	0.60
1:A:20:SER:OG	4:A:999:HOH:O	2.17	0.60
1:A:522:HIS:HD2	4:A:822:HOH:O	1.85	0.58
1:A:379:PRO:HD2	4:A:770:HOH:O	2.04	0.58
1:A:466:ASP:OD2	1:A:522:HIS:HE1	1.87	0.57
1:A:171:PRO:HD2	1:A:511:GLY:HA2	1.85	0.56
1:A:32:ASP:OD2	1:A:37:THR:OG1	2.14	0.55
1:A:529:THR:HG23	1:A:533:LEU:HD12	1.88	0.55
1:A:174:ALA:HB3	1:A:498:ILE:HD13	1.89	0.55
1:A:174:ALA:CB	1:A:498:ILE:HD13	2.38	0.54
1:A:35:LYS:HE2	1:A:74:GLN:HG3	1.90	0.54
1:A:135:GLN:HB3	1:A:136:PRO:CD	2.38	0.53
1:A:174:ALA:HA	1:A:184:LEU:O	2.07	0.53
1:A:78:GLN:HG2	1:A:81:TRP:CH2	2.44	0.53
1:A:95:ASN:N	1:A:95:ASN:HD22	2.06	0.53
1:A:15:ALA:HB2	1:A:60:LYS:NZ	2.24	0.52
1:A:22:GLN:NE2	1:A:43:TYR:O	2.42	0.52
1:A:358:TYR:HE2	1:A:366:LYS:HB2	1.75	0.52
1:A:439:ARG:NH2	1:A:474:GLU:HG3	2.25	0.52
1:A:404:ASP:HB2	1:A:408:SER:HB2	1.93	0.51
1:A:506:ARG:HD3	4:A:821:HOH:O	2.10	0.51
1:A:5:ILE:HD12	1:A:490:SER:HB3	1.92	0.51
1:A:554:VAL:HG11	1:A:560:ILE:HD11	1.92	0.50
1:A:495:TYR:O	1:A:496:HIS:HB2	2.11	0.50
1:A:11:ARG:HG2	1:A:14:TRP:CH2	2.47	0.50
1:A:401:GLY:O	1:A:411:THR:HG22	2.12	0.50
1:A:228:CYS:N	1:A:229:PRO:HD3	2.25	0.50
1:A:131:GLU:HG3	1:A:137:TRP:O	2.12	0.49
1:A:298:ASN:ND2	1:A:316:LYS:HA	2.27	0.49
1:A:90:SER:HB2	1:A:96:TRP:CE3	2.47	0.49
1:A:13:ASN:HB3	1:A:60:LYS:HG3	1.95	0.48
1:A:59:MET:C	1:A:61:THR:H	2.16	0.48
1:A:103:GLY:HA3	1:A:166:ASP:O	2.14	0.47
1:A:135:GLN:HB3	1:A:136:PRO:HD2	1.96	0.47
1:A:122:ARG:HD3	1:A:123:TYR:CE1	2.50	0.47
1:A:227:PHE:O	1:A:244:GLY:HA3	2.15	0.47
1:A:177:GLU:HB2	1:A:180:SER:OG	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:9:ILE:HD12	1:A:145:VAL:HG12	1.98	0.45
1:A:169:ILE:HG22	1:A:191:ASN:HB2	1.98	0.45
1:A:458:GLN:HA	1:A:468:THR:O	2.15	0.45
1:A:95:ASN:N	1:A:95:ASN:ND2	2.64	0.45
1:A:189:TYR:CD1	1:A:197:SER:HB2	2.51	0.44
1:A:559:ARG:HG3	1:A:605:GLN:HG3	2.00	0.44
1:A:560:ILE:O	1:A:603:SER:HA	2.18	0.44
1:A:552:GLN:HG3	4:A:978:HOH:O	2.17	0.44
1:A:568:ILE:HD13	1:A:622:VAL:HB	1.99	0.44
1:A:170:VAL:HB	1:A:514:LEU:CD1	2.47	0.43
1:A:393:LYS:HD2	1:A:393:LYS:HA	1.95	0.43
1:A:334:HIS:CE1	1:A:581:HIS:HB3	2.53	0.43
1:A:35:LYS:HB2	1:A:35:LYS:HE3	1.93	0.43
1:A:575:ARG:HD2	1:A:618:TRP:CZ2	2.54	0.42
1:A:51:PRO:HD3	1:A:136:PRO:HA	2.01	0.42
1:A:38:PHE:HB3	1:A:141:ALA:HA	2.02	0.42
1:A:41:THR:HG21	1:A:53:HIS:CG	2.55	0.42
1:A:548:ARG:O	1:A:562:ILE:HA	2.20	0.42
1:A:460:ARG:HH11	1:A:460:ARG:HD2	1.56	0.41
1:A:61:THR:O	1:A:122:ARG:HA	2.20	0.41
1:A:16:VAL:HG12	1:A:57:ILE:HG12	2.01	0.41
1:A:34:ASN:OD1	1:A:36:ASP:HB2	2.21	0.41
1:A:22:GLN:HE21	1:A:46:ASN:CB	2.06	0.41
1:A:228:CYS:N	1:A:229:PRO:CD	2.84	0.41
1:A:161:TRP:CE2	1:A:489:ASN:HB3	2.56	0.41
1:A:46:ASN:HA	1:A:46:ASN:HD22	1.60	0.40
1:A:60:LYS:HA	1:A:122:ARG:HH21	1.85	0.40
1:A:464:PHE:CD1	1:A:515:CYS:HB3	2.56	0.40

All (1) 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:12:ASN:ND2	1:A:548:ARG:NH1[3_545]	2.14	0.06

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%)	610 (96%)	24 (4%)	3 (0%)	38 23

All (3) Ramachandran outliers are listed below:

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

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%)	511 (97%)	15 (3%)	55 44

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	20	SER
1	A	23	SER
1	A	46	ASN
1	A	68	LEU
1	A	91	SER
1	A	95	ASN
1	A	119	ARG
1	A	229	PRO
1	A	366	LYS
1	A	439	ARG
1	A	532	TYR
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	25	ASN
1	A	46	ASN
1	A	78	GLN
1	A	95	ASN
1	A	298	ASN
1	A	522	HIS
1	A	537	ASN
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 2 ligands modelled in this entry, 2 are 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, 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	636/639 (99%)	11.24	636 (100%) 0 0	6, 18, 56, 98	0

All (636) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	600	ASN	32.0
1	A	450	GLY	29.2
1	A	446	VAL	23.8
1	A	15	ALA	22.7
1	A	134	GLY	22.5
1	A	612	VAL	22.1
1	A	322	THR	21.9
1	A	389	TYR	21.9
1	A	183	VAL	21.6
1	A	595	THR	20.6
1	A	451	SER	20.5
1	A	62	THR	20.2
1	A	340	TRP	19.9
1	A	43	TYR	19.8
1	A	396	ILE	19.7
1	A	505	GLY	19.6
1	A	348	ALA	19.5
1	A	436	TYR	19.4
1	A	484	TYR	19.4
1	A	356	TRP	19.4
1	A	153	ALA	19.4
1	A	79	ASN	19.2
1	A	338	PHE	19.1
1	A	309	TRP	19.1
1	A	430	PHE	19.0
1	A	416	ILE	19.0
1	A	143	ILE	19.0

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Mol	Chain	Res	Type	RSRZ
1	A	417	ILE	18.9
1	A	358	TYR	18.9
1	A	353	ALA	18.8
1	A	77	ASN	18.7
1	A	476	TYR	18.7
1	A	558	GLY	18.7
1	A	301	VAL	18.6
1	A	310	THR	18.6
1	A	477	VAL	18.5
1	A	618	TRP	18.5
1	A	359	THR	18.5
1	A	336	TRP	18.3
1	A	557	GLY	18.3
1	A	346	PHE	18.3
1	A	429	VAL	18.3
1	A	419	LEU	18.2
1	A	97	GLY	18.2
1	A	475	ILE	18.2
1	A	281	GLY	18.1
1	A	145	VAL	18.0
1	A	152	THR	18.0
1	A	562	ILE	17.9
1	A	392	VAL	17.9
1	A	576	TYR	17.8
1	A	318	ASN	17.8
1	A	31	ILE	17.8
1	A	397	LEU	17.8
1	A	345	VAL	17.7
1	A	542	THR	17.7
1	A	369	GLY	17.7
1	A	14	TRP	17.7
1	A	365	VAL	17.6
1	A	124	VAL	17.6
1	A	158	LEU	17.5
1	A	554	VAL	17.4
1	A	378	ALA	17.4
1	A	532	TYR	17.4
1	A	534	TYR	17.3
1	A	388	MET	17.3
1	A	547	THR	17.2
1	A	38	PHE	17.2
1	A	549	THR	17.2

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Mol	Chain	Res	Type	RSRZ
1	A	121	ALA	17.1
1	A	635	ILE	17.1
1	A	431	ALA	17.1
1	A	357	TYR	17.1
1	A	368	ALA	17.0
1	A	146	PHE	16.9
1	A	247	ALA	16.9
1	A	312	LEU	16.8
1	A	483	PHE	16.8
1	A	556	VAL	16.8
1	A	304	PRO	16.8
1	A	398	THR	16.7
1	A	553	SER	16.7
1	A	573	LEU	16.6
1	A	638	THR	16.6
1	A	428	THR	16.5
1	A	426	PRO	16.5
1	A	411	THR	16.4
1	A	391	ALA	16.4
1	A	28	ASN	16.4
1	A	418	THR	16.3
1	A	37	THR	16.2
1	A	551	THR	16.2
1	A	539	ASN	16.2
1	A	317	VAL	16.2
1	A	561	THR	16.2
1	A	376	GLY	16.2
1	A	422	PRO	16.1
1	A	613	ALA	16.0
1	A	33	GLY	16.0
1	A	482	THR	16.0
1	A	9	ILE	15.9
1	A	315	ALA	15.8
1	A	423	GLY	15.8
1	A	536	SER	15.7
1	A	414	ALA	15.7
1	A	453	PHE	15.7
1	A	412	THR	15.7
1	A	550	SER	15.7
1	A	607	PRO	15.7
1	A	157	GLY	15.7
1	A	343	GLY	15.7

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Mol	Chain	Res	Type	RSRZ
1	A	377	VAL	15.6
1	A	478	PRO	15.6
1	A	424	THR	15.6
1	A	306	SER	15.6
1	A	515	CYS	15.5
1	A	89	LEU	15.5
1	A	299	GLY	15.5
1	A	432	SER	15.5
1	A	354	MET	15.3
1	A	610	SER	15.3
1	A	337	LEU	15.3
1	A	12	ASN	15.3
1	A	447	LEU	15.3
1	A	367	SER	15.2
1	A	75	ASP	15.2
1	A	264	PRO	15.2
1	A	313	PRO	15.1
1	A	151	TYR	15.1
1	A	564	THR	15.1
1	A	311	SER	15.1
1	A	261	ILE	15.0
1	A	604	PHE	15.0
1	A	399	PHE	15.0
1	A	361	GLY	14.9
1	A	623	MET	14.9
1	A	560	ILE	14.9
1	A	305	SER	14.8
1	A	394	GLY	14.8
1	A	373	SER	14.7
1	A	415	HIS	14.7
1	A	452	THR	14.7
1	A	596	ASN	14.7
1	A	308	THR	14.7
1	A	351	SER	14.6
1	A	319	PRO	14.6
1	A	8	ALA	14.5
1	A	379	PRO	14.5
1	A	39	TRP	14.5
1	A	434	GLY	14.5
1	A	486	GLN	14.5
1	A	363	GLY	14.4
1	A	180	SER	14.4

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Mol	Chain	Res	Type	RSRZ
1	A	339	GLY	14.4
1	A	425	SER	14.4
1	A	148	ALA	14.3
1	A	352	THR	14.3
1	A	381	ALA	14.2
1	A	565	ASP	14.2
1	A	284	PHE	14.2
1	A	141	ALA	14.1
1	A	7	SER	14.1
1	A	23	SER	14.0
1	A	344	SER	14.0
1	A	10	SER	14.0
1	A	544	PRO	14.0
1	A	240	VAL	13.9
1	A	507	VAL	13.9
1	A	64	ASN	13.9
1	A	236	ASN	13.8
1	A	360	SER	13.8
1	A	243	GLY	13.8
1	A	438	ALA	13.8
1	A	32	ASP	13.8
1	A	298	ASN	13.7
1	A	528	PHE	13.7
1	A	302	TYR	13.7
1	A	29	LYS	13.7
1	A	390	ASP	13.7
1	A	115	ASN	13.6
1	A	616	GLY	13.6
1	A	303	SER	13.6
1	A	537	ASN	13.6
1	A	527	ILE	13.6
1	A	34	ASN	13.6
1	A	307	LYS	13.4
1	A	602	TYR	13.4
1	A	420	GLY	13.4
1	A	626	ALA	13.4
1	A	72	PRO	13.4
1	A	481	ASP	13.4
1	A	364	ASP	13.3
1	A	98	SER	13.3
1	A	387	VAL	13.3
1	A	500	LEU	13.3

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Mol	Chain	Res	Type	RSRZ
1	A	150	SER	13.3
1	A	409	ASP	13.3
1	A	161	TRP	13.2
1	A	413	ASN	13.2
1	A	543	ARG	13.2
1	A	27	CYS	13.2
1	A	253	TYR	13.2
1	A	362	SER	13.2
1	A	179	THR	13.2
1	A	485	LYS	13.1
1	A	36	ASP	13.1
1	A	149	SER	13.1
1	A	606	VAL	13.1
1	A	24	GLY	13.0
1	A	156	PRO	13.0
1	A	622	VAL	13.0
1	A	174	ALA	13.0
1	A	13	ASN	13.0
1	A	427	ASN	13.0
1	A	614	LEU	13.0
1	A	535	ASN	13.0
1	A	76	GLY	12.9
1	A	355	ASN	12.9
1	A	96	TRP	12.8
1	A	541	ALA	12.8
1	A	410	ALA	12.8
1	A	127	VAL	12.7
1	A	568	ILE	12.7
1	A	88	TYR	12.7
1	A	91	SER	12.7
1	A	608	SER	12.7
1	A	30	ALA	12.7
1	A	257	SER	12.6
1	A	603	SER	12.6
1	A	624	ASN	12.6
1	A	155	GLN	12.6
1	A	433	ASN	12.5
1	A	105	TRP	12.5
1	A	234	ASP	12.5
1	A	591	PRO	12.5
1	A	61	THR	12.5
1	A	403	PRO	12.4

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Mol	Chain	Res	Type	RSRZ
1	A	488	PRO	12.4
1	A	634	THR	12.4
1	A	620	LEU	12.4
1	A	107	ALA	12.4
1	A	605	GLN	12.4
1	A	286	ILE	12.3
1	A	65	VAL	12.3
1	A	375	ARG	12.3
1	A	574	ILE	12.3
1	A	590	ILE	12.3
1	A	372	GLN	12.3
1	A	142	GLU	12.2
1	A	41	THR	12.1
1	A	283	VAL	12.1
1	A	609	ASP	12.1
1	A	555	LYS	12.1
1	A	45	ALA	12.1
1	A	349	GLY	12.0
1	A	470	VAL	12.0
1	A	625	SER	12.0
1	A	639	GLN	11.9
1	A	435	LEU	11.9
1	A	95	ASN	11.9
1	A	335	ALA	11.9
1	A	11	ARG	11.8
1	A	347	GLN	11.8
1	A	297	LYS	11.8
1	A	487	ASN	11.8
1	A	480	GLN	11.8
1	A	130	THR	11.8
1	A	501	LEU	11.8
1	A	154	PRO	11.7
1	A	395	LYS	11.7
1	A	472	THR	11.7
1	A	147	GLN	11.7
1	A	459	ARG	11.7
1	A	495	TYR	11.6
1	A	320	MET	11.6
1	A	118	THR	11.6
1	A	548	ARG	11.6
1	A	26	GLU	11.6
1	A	589	ARG	11.6

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Mol	Chain	Res	Type	RSRZ
1	A	393	LYS	11.5
1	A	479	GLU	11.5
1	A	54	THR	11.5
1	A	100	VAL	11.5
1	A	256	SER	11.5
1	A	212	GLY	11.5
1	A	258	ASP	11.5
1	A	628	VAL	11.5
1	A	113	TYR	11.4
1	A	55	TYR	11.4
1	A	502	LEU	11.4
1	A	21	ALA	11.4
1	A	341	LYS	11.4
1	A	637	VAL	11.4
1	A	559	ARG	11.4
1	A	316	LYS	11.4
1	A	552	GLN	11.3
1	A	540	LEU	11.3
1	A	473	PRO	11.3
1	A	421	GLU	11.3
1	A	165	ILE	11.3
1	A	371	ARG	11.3
1	A	6	GLY	11.3
1	A	525	ALA	11.2
1	A	611	GLY	11.2
1	A	170	VAL	11.2
1	A	437	PHE	11.2
1	A	3	ALA	11.2
1	A	350	PRO	11.1
1	A	370	LYS	11.1
1	A	282	ARG	11.1
1	A	572	SER	11.0
1	A	252	LEU	11.0
1	A	187	SER	11.0
1	A	342	LYS	11.0
1	A	42	PHE	11.0
1	A	181	GLY	11.0
1	A	175	ALA	10.9
1	A	35	LYS	10.9
1	A	366	LYS	10.9
1	A	592	LEU	10.8
1	A	267	GLN	10.8

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Mol	Chain	Res	Type	RSRZ
1	A	314	ASN	10.8
1	A	120	PRO	10.8
1	A	321	LEU	10.7
1	A	601	SER	10.7
1	A	300	GLU	10.7
1	A	468	THR	10.7
1	A	57	ILE	10.6
1	A	239	ILE	10.6
1	A	59	MET	10.5
1	A	18	CYS	10.5
1	A	139	SER	10.5
1	A	259	SER	10.5
1	A	400	GLY	10.5
1	A	106	PHE	10.4
1	A	214	VAL	10.4
1	A	103	GLY	10.4
1	A	538	GLY	10.4
1	A	263	GLY	10.3
1	A	585	THR	10.3
1	A	186	TRP	10.3
1	A	268	VAL	10.3
1	A	563	SER	10.3
1	A	287	GLY	10.2
1	A	408	SER	10.2
1	A	203	LEU	10.2
1	A	632	ALA	10.2
1	A	583	VAL	10.2
1	A	159	GLY	10.1
1	A	235	GLY	10.1
1	A	68	LEU	10.1
1	A	278	MET	10.1
1	A	571	ALA	10.0
1	A	402	SER	10.0
1	A	110	THR	10.0
1	A	189	TYR	10.0
1	A	449	ASP	10.0
1	A	374	ASN	10.0
1	A	463	PRO	10.0
1	A	636	ARG	10.0
1	A	90	SER	10.0
1	A	615	PRO	10.0
1	A	228	CYS	10.0

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Mol	Chain	Res	Type	RSRZ
1	A	260	TRP	9.9
1	A	569	SER	9.9
1	A	498	ILE	9.9
1	A	292	GLY	9.9
1	A	503	PRO	9.9
1	A	58	ASP	9.9
1	A	385	ASN	9.9
1	A	494	VAL	9.8
1	A	78	GLN	9.8
1	A	265	ASP	9.8
1	A	272	TYR	9.8
1	A	405	TYR	9.8
1	A	617	TYR	9.7
1	A	218	THR	9.7
1	A	442	HIS	9.7
1	A	546	ILE	9.7
1	A	93	GLY	9.7
1	A	467	SER	9.6
1	A	279	SER	9.6
1	A	499	SER	9.6
1	A	531	ASN	9.6
1	A	216	ASP	9.5
1	A	104	SER	9.5
1	A	280	ASP	9.5
1	A	471	PHE	9.5
1	A	266	MET	9.5
1	A	25	ASN	9.5
1	A	172	ALA	9.4
1	A	144	ASN	9.4
1	A	136	PRO	9.4
1	A	82	ILE	9.4
1	A	176	ILE	9.4
1	A	579	ALA	9.4
1	A	619	MET	9.3
1	A	386	ALA	9.3
1	A	594	LEU	9.3
1	A	5	ILE	9.3
1	A	46	ASN	9.3
1	A	173	ALA	9.2
1	A	210	SER	9.2
1	A	492	VAL	9.2
1	A	123	TYR	9.2

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Mol	Chain	Res	Type	RSRZ
1	A	508	PHE	9.2
1	A	111	THR	9.1
1	A	116	PHE	9.1
1	A	469	PRO	9.1
1	A	19	ASP	9.1
1	A	462	ILE	9.1
1	A	138	THR	9.0
1	A	458	GLN	9.0
1	A	518	CYS	9.0
1	A	87	VAL	8.9
1	A	334	HIS	8.9
1	A	132	ALA	8.9
1	A	514	LEU	8.9
1	A	248	LYS	8.9
1	A	207	TRP	8.8
1	A	444	SER	8.8
1	A	328	LEU	8.7
1	A	262	PRO	8.7
1	A	578	THR	8.7
1	A	200	GLY	8.7
1	A	126	LEU	8.6
1	A	273	GLN	8.6
1	A	455	THR	8.6
1	A	162	GLY	8.6
1	A	631	VAL	8.6
1	A	383	CYS	8.6
1	A	533	LEU	8.5
1	A	497	SER	8.5
1	A	329	TYR	8.5
1	A	70	MET	8.4
1	A	629	PRO	8.4
1	A	169	ILE	8.4
1	A	621	PHE	8.3
1	A	246	ASP	8.3
1	A	245	ASN	8.3
1	A	67	GLY	8.3
1	A	566	SER	8.3
1	A	509	ASN	8.3
1	A	443	THR	8.2
1	A	570	LYS	8.2
1	A	241	VAL	8.2
1	A	71	LEU	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	133	ASN	8.2
1	A	466	ASP	8.2
1	A	491	ILE	8.1
1	A	456	GLY	8.1
1	A	81	TRP	8.1
1	A	84	ARG	8.1
1	A	506	ARG	8.1
1	A	227	PHE	8.1
1	A	160	ARG	8.1
1	A	523	PHE	8.0
1	A	238	GLN	8.0
1	A	230	GLY	8.0
1	A	194	PHE	8.0
1	A	22	GLN	8.0
1	A	575	ARG	8.0
1	A	196	GLY	8.0
1	A	244	GLY	7.9
1	A	2	SER	7.9
1	A	580	THR	7.9
1	A	588	ARG	7.9
1	A	255	SER	7.9
1	A	191	ASN	7.9
1	A	285	THR	7.9
1	A	627	GLY	7.8
1	A	441	PHE	7.8
1	A	289	SER	7.8
1	A	448	PRO	7.8
1	A	511	GLY	7.8
1	A	53	HIS	7.8
1	A	524	ASP	7.8
1	A	193	ALA	7.7
1	A	295	PHE	7.7
1	A	221	VAL	7.7
1	A	251	SER	7.7
1	A	296	GLU	7.7
1	A	593	THR	7.7
1	A	114	SER	7.6
1	A	129	ILE	7.6
1	A	94	THR	7.6
1	A	56	THR	7.6
1	A	290	TRP	7.6
1	A	633	SER	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	69	SER	7.5
1	A	496	HIS	7.5
1	A	382	MET	7.5
1	A	204	THR	7.5
1	A	222	THR	7.4
1	A	530	PRO	7.4
1	A	125	ARG	7.4
1	A	581	HIS	7.4
1	A	529	THR	7.4
1	A	219	VAL	7.4
1	A	109	SER	7.3
1	A	168	PRO	7.3
1	A	184	LEU	7.3
1	A	464	PHE	7.3
1	A	526	GLN	7.3
1	A	489	ASN	7.3
1	A	384	GLY	7.2
1	A	20	SER	7.2
1	A	275	SER	7.2
1	A	401	GLY	7.2
1	A	16	VAL	7.2
1	A	80	GLY	7.2
1	A	213	ILE	7.2
1	A	323	ALA	7.2
1	A	99	PRO	7.2
1	A	521	ASN	7.1
1	A	380	ASP	7.1
1	A	63	GLN	7.1
1	A	51	PRO	7.0
1	A	128	ALA	7.0
1	A	217	ARG	7.0
1	A	4	PRO	7.0
1	A	164	THR	6.9
1	A	510	GLY	6.9
1	A	231	ILE	6.9
1	A	85	HIS	6.9
1	A	73	ARG	6.9
1	A	630	SER	6.9
1	A	40	HIS	6.9
1	A	177	GLU	6.9
1	A	288	GLY	6.8
1	A	101	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	178	PRO	6.8
1	A	274	SER	6.8
1	A	182	ARG	6.8
1	A	461	GLY	6.8
1	A	208	ASP	6.8
1	A	185	MET	6.8
1	A	586	ASP	6.8
1	A	439	ARG	6.7
1	A	119	ARG	6.7
1	A	140	ILE	6.7
1	A	195	GLY	6.7
1	A	224	HIS	6.7
1	A	567	SER	6.6
1	A	250	THR	6.6
1	A	513	GLY	6.6
1	A	137	TRP	6.6
1	A	163	PRO	6.5
1	A	242	THR	6.5
1	A	440	THR	6.5
1	A	294	VAL	6.5
1	A	201	ILE	6.5
1	A	171	PRO	6.4
1	A	582	THR	6.4
1	A	167	LEU	6.4
1	A	454	ILE	6.3
1	A	520	THR	6.3
1	A	74	GLN	6.3
1	A	52	PRO	6.3
1	A	270	ARG	6.3
1	A	102	SER	6.3
1	A	493	ARG	6.2
1	A	220	THR	6.2
1	A	215	SER	6.2
1	A	504	ASP	6.2
1	A	233	MET	6.2
1	A	232	SER	6.2
1	A	44	GLY	6.2
1	A	587	GLN	6.1
1	A	47	GLY	6.1
1	A	545	LYS	6.1
1	A	229	PRO	6.1
1	A	202	THR	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	211	THR	6.0
1	A	188	SER	6.0
1	A	269	ALA	6.0
1	A	584	ASN	6.0
1	A	225	ASP	5.9
1	A	333	ASN	5.9
1	A	519	THR	5.8
1	A	522	HIS	5.8
1	A	205	SER	5.8
1	A	404	ASP	5.8
1	A	407	ASP	5.8
1	A	50	LYS	5.7
1	A	516	GLY	5.7
1	A	324	ASP	5.7
1	A	135	GLN	5.5
1	A	293	GLY	5.5
1	A	326	GLN	5.5
1	A	209	PRO	5.4
1	A	276	ALA	5.4
1	A	192	ASP	5.4
1	A	112	LYS	5.4
1	A	249	LYS	5.4
1	A	577	GLY	5.3
1	A	92	ASP	5.3
1	A	254	ASP	5.3
1	A	237	GLY	5.3
1	A	460	ARG	5.3
1	A	66	ASN	5.2
1	A	327	GLY	5.2
1	A	108	ASP	5.1
1	A	490	SER	5.1
1	A	122	ARG	5.1
1	A	60	LYS	5.1
1	A	190	ARG	5.1
1	A	474	GLU	5.0
1	A	330	ARG	4.9
1	A	49	PRO	4.9
1	A	83	GLY	4.9
1	A	271	GLY	4.9
1	A	131	GLU	4.9
1	A	17	THR	4.9
1	A	206	SER	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	48	ASP	4.7
1	A	226	MET	4.7
1	A	277	THR	4.7
1	A	197	SER	4.6
1	A	457	GLY	4.6
1	A	223	LYS	4.6
1	A	117	GLU	4.5
1	A	445	VAL	4.5
1	A	332	ASP	4.4
1	A	198	PRO	4.4
1	A	406	GLN	4.3
1	A	199	GLY	4.3
1	A	512	GLY	4.0
1	A	166	ASP	4.0
1	A	86	GLU	3.9
1	A	331	SER	3.9
1	A	291	SER	3.7
1	A	465	GLU	3.6
1	A	517	ASP	3.5
1	A	325	LYS	3.5
1	A	1	ALA	3.2

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	CU	A	700	1/1	0.79	5.20	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NA	A	702	1/1	1.04	0.51	15,15,15,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.