



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 06:54 PM GMT

PDB ID : 1GOF
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 : 1.70 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>

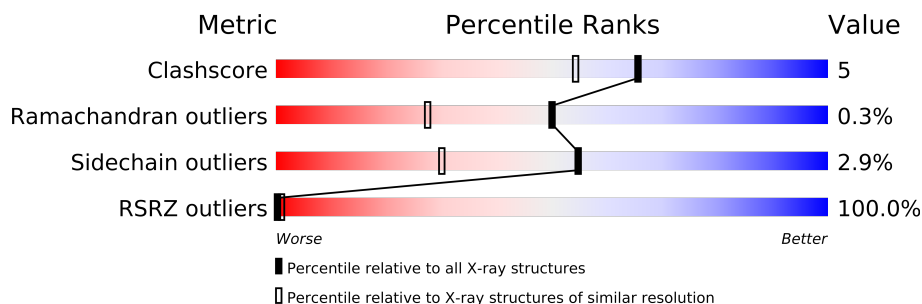
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.70 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	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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
4	ACY	A	701	-	X
4	ACY	A	703	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5156 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			

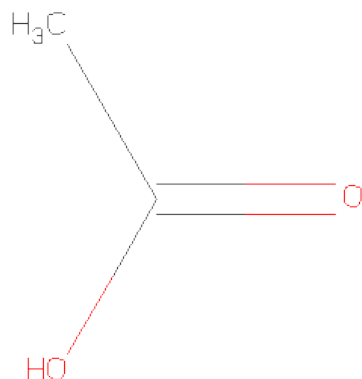
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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 ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

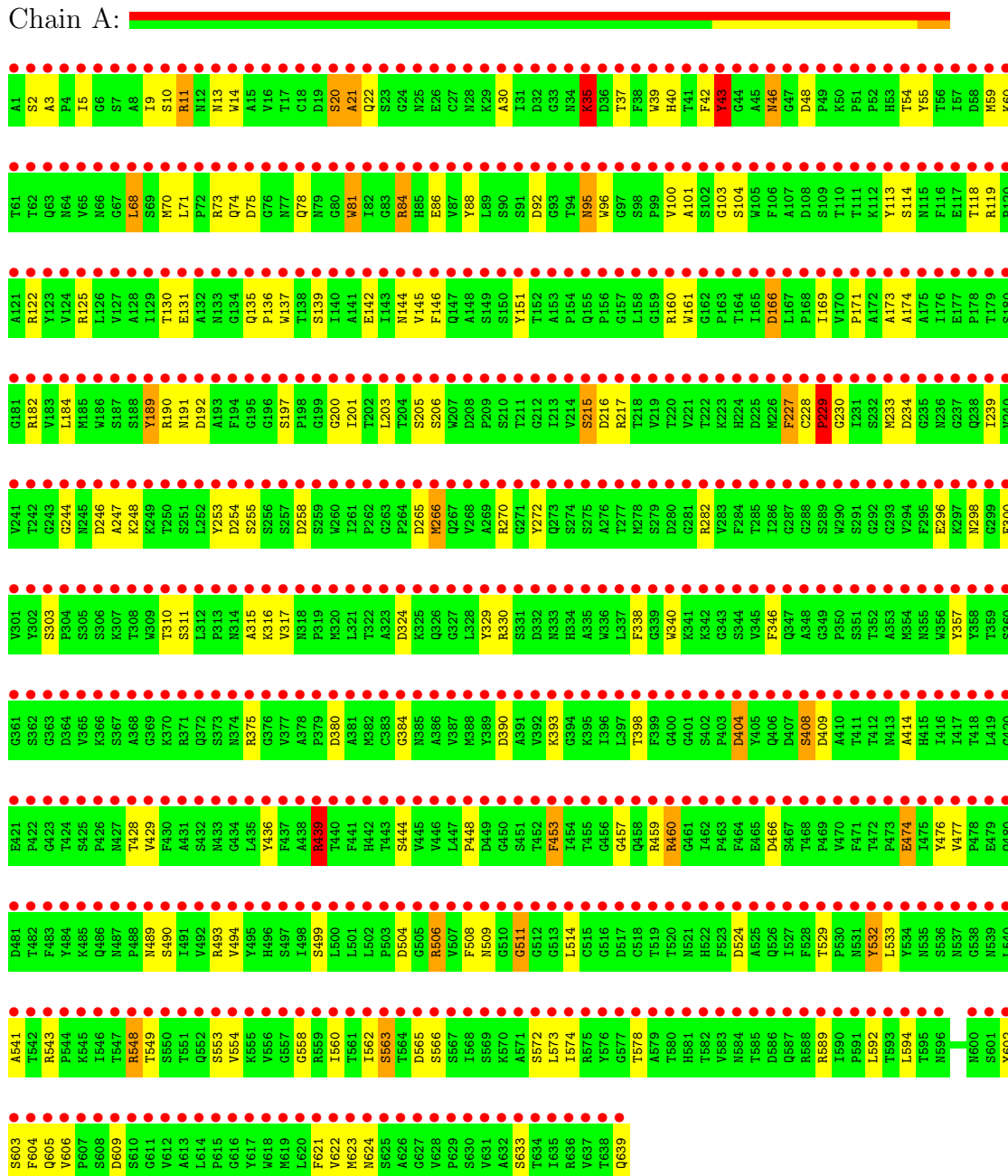
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	316	Total	O	0	0
			316	316		

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, α , β , γ	98.00Å 89.40Å 86.70Å 90.00° 117.80° 90.00°	Depositor
Resolution (Å)	10.00 – 1.70 9.99 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.70) 72.8 (9.99-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.70Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.177 , (Not available) 0.146 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.84 , 187.0	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 57090 reflections	Xtriage
F_o, F_c correlation	0.47	EDS
Total number of atoms	5156	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 6.26% 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, ACY, 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	1.07	3/4959 (0.1%)	2.10	175/6765 (2.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	SER	CB-OG	5.79	1.49	1.42
1	A	303	SER	CB-OG	5.25	1.49	1.42
1	A	86	GLU	CD-OE2	-5.16	1.20	1.25

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ARG	CD-NE-CZ	23.55	156.58	123.60
1	A	460	ARG	NE-CZ-NH2	-18.95	110.82	120.30
1	A	493	ARG	NE-CZ-NH2	-18.66	110.97	120.30
1	A	190	ARG	NE-CZ-NH1	17.59	129.10	120.30
1	A	459	ARG	NE-CZ-NH1	16.59	128.60	120.30
1	A	330	ARG	NE-CZ-NH1	16.56	128.58	120.30
1	A	282	ARG	NE-CZ-NH1	15.24	127.92	120.30
1	A	114	SER	N-CA-CB	12.98	129.97	110.50
1	A	73	ARG	NE-CZ-NH2	-11.13	114.74	120.30
1	A	459	ARG	NE-CZ-NH2	-10.83	114.89	120.30
1	A	453	PHE	CB-CG-CD2	-10.55	113.42	120.80
1	A	189	TYR	CB-CG-CD1	10.50	127.30	121.00
1	A	86	GLU	OE1-CD-OE2	10.41	135.79	123.30
1	A	506	ARG	NE-CZ-NH1	10.25	125.43	120.30
1	A	493	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	A	460	ARG	NH1-CZ-NH2	10.14	130.55	119.40
1	A	476	TYR	CB-CG-CD2	-10.13	114.92	121.00
1	A	330	ARG	NE-CZ-NH2	-10.11	115.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	SER	N-CA-CB	-10.05	95.42	110.50
1	A	227	PHE	CB-CG-CD1	-9.75	113.97	120.80
1	A	160	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	A	182	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	A	453	PHE	CB-CG-CD1	9.49	127.44	120.80
1	A	543	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	A	543	ARG	NE-CZ-NH1	9.38	124.99	120.30
1	A	504	ASP	CB-CG-OD2	9.28	126.65	118.30
1	A	160	ARG	NE-CZ-NH1	9.08	124.84	120.30
1	A	258	ASP	CB-CG-OD1	8.97	126.37	118.30
1	A	466	ASP	CB-CG-OD1	8.89	126.30	118.30
1	A	375	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	A	254	ASP	CB-CG-OD1	8.63	126.07	118.30
1	A	88	TYR	CB-CG-CD2	-8.35	115.99	121.00
1	A	633	SER	N-CA-CB	8.30	122.95	110.50
1	A	20	SER	N-CA-CB	8.13	122.70	110.50
1	A	316	LYS	O-C-N	8.09	135.63	122.70
1	A	543	ARG	CD-NE-CZ	7.79	134.50	123.60
1	A	200	GLY	N-CA-C	7.76	132.51	113.10
1	A	409	ASP	CB-CG-OD2	-7.74	111.34	118.30
1	A	548	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	563	SER	N-CA-CB	7.56	121.84	110.50
1	A	602	TYR	CB-CG-CD1	-7.53	116.48	121.00
1	A	118	THR	O-C-N	7.51	134.72	122.70
1	A	234	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	A	200	GLY	CA-C-O	7.50	134.09	120.60
1	A	439	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	234	ASP	CB-CG-OD1	7.41	124.97	118.30
1	A	73	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	A	474	GLU	OE1-CD-OE2	7.22	131.97	123.30
1	A	390	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	A	329	TYR	CB-CG-CD1	-7.17	116.70	121.00
1	A	20	SER	CB-CA-C	-7.14	96.54	110.10
1	A	104	SER	O-C-N	7.08	134.03	122.70
1	A	217	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	324	ASP	CB-CG-OD2	7.04	124.64	118.30
1	A	92	ASP	CB-CG-OD1	7.02	124.62	118.30
1	A	282	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	246	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	604	PHE	CB-CG-CD2	-6.90	115.97	120.80
1	A	508	PHE	CB-CG-CD1	-6.88	115.99	120.80
1	A	499	SER	N-CA-CB	6.87	120.81	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	TYR	CB-CG-CD1	-6.86	116.89	121.00
1	A	466	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	A	75	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	A	81	TRP	O-C-N	6.82	133.62	122.70
1	A	624	ASN	CB-CA-C	6.78	123.96	110.40
1	A	217	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	190	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	380	ASP	CB-CG-OD1	6.73	124.35	118.30
1	A	113	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	A	375	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	A	166	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	310	THR	O-C-N	6.56	133.19	122.70
1	A	429	VAL	CA-CB-CG2	6.50	120.65	110.90
1	A	173	ALA	N-CA-CB	6.49	119.19	110.10
1	A	459	ARG	CD-NE-CZ	6.49	132.69	123.60
1	A	84	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	477	VAL	CA-CB-CG1	-6.44	101.25	110.90
1	A	88	TYR	CB-CG-CD1	6.41	124.84	121.00
1	A	272	TYR	CB-CG-CD2	-6.41	117.16	121.00
1	A	602	TYR	CB-CG-CD2	6.34	124.81	121.00
1	A	189	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	A	558	GLY	CA-C-O	6.32	131.98	120.60
1	A	357	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	A	101	ALA	O-C-N	6.31	132.79	122.70
1	A	606	VAL	CG1-CB-CG2	6.29	120.97	110.90
1	A	460	ARG	CA-CB-CG	-6.23	99.70	113.40
1	A	119	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	566	SER	O-C-N	6.17	132.56	122.70
1	A	506	ARG	CD-NE-CZ	6.08	132.11	123.60
1	A	247	ALA	CB-CA-C	6.02	119.14	110.10
1	A	55	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	A	589	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	605	GLN	O-C-N	5.94	132.20	122.70
1	A	96	TRP	CA-CB-CG	-5.92	102.46	113.70
1	A	48	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	338	PHE	CB-CG-CD2	-5.89	116.68	120.80
1	A	457	GLY	CA-C-O	5.87	131.17	120.60
1	A	227	PHE	CG-CD2-CE2	-5.85	114.36	120.80
1	A	436	TYR	CZ-CE2-CD2	-5.85	114.54	119.80
1	A	266	MET	CA-CB-CG	-5.83	103.38	113.30
1	A	216	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	84	ARG	NE-CZ-NH1	5.81	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	A	384	GLY	N-CA-C	-5.81	98.58	113.10
1	A	2	SER	CB-CA-C	5.78	121.07	110.10
1	A	436	TYR	CB-CG-CD2	-5.77	117.54	121.00
1	A	296	GLU	OE1-CD-OE2	5.77	130.22	123.30
1	A	511	GLY	CA-C-N	-5.77	104.67	116.20
1	A	246	ASP	O-C-N	5.75	131.89	122.70
1	A	37	THR	O-C-N	5.74	131.89	122.70
1	A	476	TYR	CD1-CG-CD2	5.74	124.22	117.90
1	A	70	MET	CG-SD-CE	5.64	109.23	100.20
1	A	621	PHE	CB-CG-CD2	-5.64	116.85	120.80
1	A	565	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	206	SER	N-CA-CB	5.61	118.91	110.50
1	A	233	MET	CA-CB-CG	-5.61	103.77	113.30
1	A	404	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	340	TRP	O-C-N	5.55	131.59	122.70
1	A	11	ARG	CG-CD-NE	-5.54	100.17	111.80
1	A	578	THR	CA-CB-OG1	-5.53	97.39	109.00
1	A	201	ILE	O-C-N	5.52	131.53	122.70
1	A	35	LYS	CA-CB-CG	5.49	125.47	113.40
1	A	43	TYR	N-CA-CB	5.49	120.47	110.60
1	A	476	TYR	CG-CD2-CE2	-5.49	116.91	121.30
1	A	346	PHE	CB-CG-CD2	-5.48	116.96	120.80
1	A	203	LEU	CB-CG-CD1	-5.47	101.70	111.00
1	A	606	VAL	N-CA-CB	-5.45	99.52	111.50
1	A	182	ARG	CA-CB-CG	-5.42	101.47	113.40
1	A	300	GLU	CB-CG-CD	-5.42	99.57	114.20
1	A	265	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	230	GLY	N-CA-C	-5.39	99.61	113.10
1	A	623	MET	CA-CB-CG	-5.38	104.16	113.30
1	A	404	ASP	O-C-N	5.35	131.26	122.70
1	A	606	VAL	CA-CB-CG2	-5.35	102.88	110.90
1	A	311	SER	N-CA-CB	-5.34	102.49	110.50
1	A	509	ASN	C-N-CA	-5.34	111.09	122.30
1	A	125	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	609	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	A	589	ARG	CD-NE-CZ	-5.31	116.16	123.60
1	A	436	TYR	CB-CG-CD1	5.30	124.18	121.00
1	A	541	ALA	CA-C-O	5.28	131.19	120.10
1	A	192	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	532	TYR	CB-CG-CD1	5.26	124.16	121.00
1	A	375	ARG	CD-NE-CZ	-5.25	116.25	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	565	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	524	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	A	622	VAL	CA-C-O	-5.22	109.13	120.10
1	A	553	SER	O-C-N	-5.22	114.35	122.70
1	A	130	THR	N-CA-CB	5.22	120.21	110.30
1	A	122	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	113	TYR	CG-CD1-CE1	-5.19	117.15	121.30
1	A	68	LEU	CB-CG-CD1	5.18	119.80	111.00
1	A	300	GLU	N-CA-CB	5.17	119.91	110.60
1	A	572	SER	CB-CA-C	5.16	119.91	110.10
1	A	122	ARG	NE-CZ-NH2	5.15	122.87	120.30
1	A	621	PHE	CG-CD1-CE1	-5.14	115.15	120.80
1	A	315	ALA	N-CA-C	-5.14	97.13	111.00
1	A	229	PRO	N-CA-CB	-5.13	96.96	102.60
1	A	200	GLY	CA-C-N	-5.11	105.95	117.20
1	A	144	ASN	O-C-N	5.10	130.87	122.70
1	A	393	LYS	C-N-CA	5.10	133.02	122.30
1	A	54	THR	N-CA-CB	-5.10	100.62	110.30
1	A	21	ALA	N-CA-CB	5.08	117.22	110.10
1	A	272	TYR	CZ-CE2-CD2	-5.08	115.22	119.80
1	A	338	PHE	CG-CD2-CE2	-5.08	115.21	120.80
1	A	190	ARG	NH1-CZ-NH2	-5.07	113.83	119.40
1	A	100	VAL	CG1-CB-CG2	5.06	119.00	110.90
1	A	239	ILE	CG1-CB-CG2	5.05	122.51	111.40
1	A	151	TYR	CB-CG-CD2	5.05	124.03	121.00
1	A	160	ARG	CB-CA-C	-5.04	100.31	110.40
1	A	3	ALA	O-C-N	5.03	130.65	121.10
1	A	270	ARG	CB-CA-C	-5.02	100.35	110.40
1	A	428	THR	OG1-CB-CG2	-5.02	98.45	110.00
1	A	594	LEU	CB-CG-CD2	-5.01	102.47	111.00
1	A	384	GLY	CA-C-O	5.00	129.61	120.60

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	4603	49	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	8	0	6	0	0
5	A	316	0	0	1	0
All	All	5156	0	4609	49	0

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 5.

All (49) 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	1.33	0.94
1:A:22:GLN:NE2	1:A:46:ASN:HB2	1.98	0.79
1:A:35:LYS:HE3	1:A:71:LEU:HD21	1.67	0.76
1:A:298:ASN:HD22	1:A:317:VAL:H	1.39	0.70
1:A:22:GLN:NE2	1:A:43:TYR:O	2.27	0.66
1:A:22:GLN:HG3	1:A:42:PHE:HA	1.79	0.65
1:A:298:ASN:ND2	1:A:317:VAL:H	1.94	0.64
1:A:448:PRO:HA	1:A:574:ILE:HD11	1.83	0.59
1:A:59:MET:O	1:A:60:LYS:HB2	2.02	0.59
1:A:35:LYS:HE2	1:A:74:GLN:HG3	1.87	0.56
1:A:22:GLN:NE2	1:A:43:TYR:H	2.05	0.55
1:A:171:PRO:HD2	1:A:511:GLY:HA2	1.91	0.53
1:A:529:THR:HG23	1:A:533:LEU:HD12	1.92	0.52
1:A:78:GLN:HG2	1:A:81:TRP:CH2	2.46	0.51
1:A:506:ARG:HD3	5:A:820:HOH:O	2.11	0.50
1:A:13:ASN:O	1:A:60:LYS:HG3	2.12	0.50
1:A:135:GLN:HB3	1:A:136:PRO:CD	2.42	0.49
1:A:39:TRP:O	1:A:139:SER:HA	2.14	0.48
1:A:554:VAL:HG11	1:A:560:ILE:HD11	1.94	0.48
1:A:228:CYS:N	1:A:229:PRO:HD3	2.27	0.48
1:A:404:ASP:HB2	1:A:408:SER:HB2	1.96	0.47
1:A:95:ASN:N	1:A:95:ASN:HD22	2.12	0.47
1:A:439:ARG:NH2	1:A:474:GLU:HG3	2.30	0.47
1:A:398:THR:O	1:A:414:ALA:HA	2.16	0.46
1:A:560:ILE:O	1:A:603:SER:HA	2.15	0.46
1:A:460:ARG:HH11	1:A:460:ARG:HD2	1.57	0.46
1:A:189:TYR:CD1	1:A:197:SER:HB2	2.51	0.45
1:A:248:LYS:HE3	1:A:266:MET:O	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:174:ALA:HA	1:A:184:LEU:O	2.16	0.45
1:A:573:LEU:HG	1:A:592:LEU:HD11	1.98	0.45
1:A:11:ARG:HG2	1:A:14:TRP:CZ3	2.51	0.45
1:A:298:ASN:HD22	1:A:317:VAL:N	2.11	0.45
1:A:103:GLY:HA3	1:A:166:ASP:O	2.17	0.45
1:A:161:TRP:CE2	1:A:489:ASN:HB3	2.52	0.44
1:A:135:GLN:HB3	1:A:136:PRO:HD2	1.98	0.44
1:A:205:SER:HA	1:A:215:SER:O	2.18	0.44
1:A:227:PHE:O	1:A:244:GLY:HA3	2.18	0.44
1:A:169:ILE:HG22	1:A:191:ASN:HB2	1.99	0.43
1:A:30:ALA:O	1:A:142:GLU:HA	2.18	0.43
1:A:146:PHE:CD1	1:A:146:PHE:N	2.86	0.42
1:A:9:ILE:HD12	1:A:145:VAL:HG12	2.01	0.42
1:A:253:TYR:CE2	1:A:255:SER:HA	2.54	0.42
1:A:549:THR:HG22	1:A:562:ILE:HG22	2.02	0.42
1:A:11:ARG:HG2	1:A:14:TRP:CH2	2.55	0.41
1:A:21:ALA:HA	1:A:40:HIS:O	2.21	0.41
1:A:131:GLU:HG3	1:A:137:TRP:O	2.21	0.41
1:A:444:SER:HA	1:A:453:PHE:O	2.21	0.41
1:A:95:ASN:N	1:A:95:ASN:ND2	2.69	0.40
1:A:5:ILE:HD12	1:A:490:SER:HB3	2.04	0.40

There are no symmetry-related clashes.

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%)	609 (96%)	26 (4%)	2 (0%)	50 27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	LEU
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 30

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

Mol	Chain	Res	Type
1	A	10	SER
1	A	20	SER
1	A	35	LYS
1	A	43	TYR
1	A	46	ASN
1	A	68	LEU
1	A	84	ARG
1	A	95	ASN
1	A	215	SER
1	A	229	PRO
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	12	ASN
1	A	22	GLN
1	A	25	ASN
1	A	63	GLN
1	A	78	GLN
1	A	95	ASN
1	A	298	ASN
1	A	413	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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
4	ACY	A	701	-	3,3,3	1.21	0	3,3,3	1.11	0
4	ACY	A	703	2	3,3,3	0.93	0	3,3,3	1.80	1 (33%)

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
4	ACY	A	701	-	-	0/0/0/0	0/0/0/0
4	ACY	A	703	2	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	703	ACY	OXT-C-O	2.45	131.94	121.96

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%)	13.92	636 (100%) 0 1	6, 18, 57, 98	0

All (636) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	TRP	35.0
1	A	351	SER	33.1
1	A	451	SER	30.8
1	A	336	TRP	29.8
1	A	14	TRP	29.2
1	A	183	VAL	29.0
1	A	389	TYR	28.8
1	A	43	TYR	27.2
1	A	340	TRP	26.8
1	A	436	TYR	26.7
1	A	381	ALA	26.5
1	A	301	VAL	26.4
1	A	403	PRO	26.2
1	A	302	TYR	26.1
1	A	322	THR	25.9
1	A	604	PHE	25.6
1	A	309	TRP	25.0
1	A	553	SER	24.8
1	A	356	TRP	24.7
1	A	243	GLY	24.7
1	A	419	LEU	24.4
1	A	475	ILE	24.3
1	A	97	GLY	24.2
1	A	317	VAL	24.2
1	A	152	THR	23.9
1	A	151	TYR	23.8
1	A	416	ILE	23.7

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Mol	Chain	Res	Type	RSRZ
1	A	484	TYR	23.7
1	A	635	ILE	23.7
1	A	612	VAL	23.6
1	A	450	GLY	23.5
1	A	453	PHE	23.5
1	A	145	VAL	23.3
1	A	161	TRP	23.3
1	A	257	SER	23.3
1	A	39	TRP	23.3
1	A	638	THR	23.3
1	A	253	TYR	23.2
1	A	348	ALA	23.2
1	A	337	LEU	23.2
1	A	110	THR	23.1
1	A	400	GLY	23.0
1	A	318	ASN	23.0
1	A	127	VAL	22.9
1	A	554	VAL	22.9
1	A	429	VAL	22.9
1	A	338	PHE	22.8
1	A	560	ILE	22.8
1	A	417	ILE	22.7
1	A	430	PHE	22.7
1	A	312	LEU	22.7
1	A	396	ILE	22.6
1	A	551	THR	22.6
1	A	281	GLY	22.5
1	A	358	TYR	22.5
1	A	397	LEU	22.4
1	A	618	TRP	22.3
1	A	398	THR	22.3
1	A	38	PHE	22.2
1	A	353	ALA	22.1
1	A	542	THR	22.1
1	A	537	ASN	22.1
1	A	346	PHE	21.8
1	A	8	ALA	21.7
1	A	143	ILE	21.7
1	A	594	LEU	21.6
1	A	240	VAL	21.6
1	A	376	GLY	21.4
1	A	146	PHE	21.4

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Mol	Chain	Res	Type	RSRZ
1	A	27	CYS	21.3
1	A	614	LEU	21.3
1	A	304	PRO	21.3
1	A	359	THR	21.2
1	A	158	LEU	21.1
1	A	31	ILE	21.1
1	A	437	PHE	21.1
1	A	410	ALA	21.1
1	A	515	CYS	21.1
1	A	77	ASN	21.0
1	A	65	VAL	21.0
1	A	558	GLY	20.9
1	A	378	ALA	20.9
1	A	549	THR	20.9
1	A	95	ASN	20.8
1	A	541	ALA	20.8
1	A	315	ALA	20.7
1	A	476	TYR	20.6
1	A	596	ASN	20.5
1	A	37	THR	20.3
1	A	562	ILE	20.2
1	A	392	VAL	20.2
1	A	15	ALA	20.2
1	A	483	PHE	20.2
1	A	153	ALA	20.2
1	A	391	ALA	20.2
1	A	576	TYR	20.2
1	A	357	TYR	20.1
1	A	477	VAL	20.1
1	A	124	VAL	20.0
1	A	616	GLY	19.9
1	A	557	GLY	19.9
1	A	345	VAL	19.7
1	A	438	ALA	19.7
1	A	9	ILE	19.7
1	A	412	THR	19.7
1	A	434	GLY	19.7
1	A	431	ALA	19.6
1	A	539	ASN	19.5
1	A	482	THR	19.5
1	A	595	THR	19.5
1	A	637	VAL	19.5

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Mol	Chain	Res	Type	RSRZ
1	A	23	SER	19.2
1	A	572	SER	19.2
1	A	30	ALA	19.2
1	A	263	GLY	19.2
1	A	363	GLY	19.1
1	A	435	LEU	19.0
1	A	377	VAL	18.9
1	A	388	MET	18.9
1	A	299	GLY	18.9
1	A	564	THR	18.9
1	A	339	GLY	18.8
1	A	411	THR	18.8
1	A	189	TYR	18.7
1	A	534	TYR	18.7
1	A	239	ILE	18.7
1	A	418	THR	18.7
1	A	368	ALA	18.7
1	A	284	PHE	18.6
1	A	561	THR	18.6
1	A	154	PRO	18.6
1	A	535	ASN	18.6
1	A	130	THR	18.6
1	A	343	GLY	18.5
1	A	379	PRO	18.5
1	A	556	VAL	18.5
1	A	532	TYR	18.4
1	A	79	ASN	18.4
1	A	170	VAL	18.3
1	A	354	MET	18.3
1	A	505	GLY	18.3
1	A	424	THR	18.2
1	A	423	GLY	18.2
1	A	256	SER	18.2
1	A	422	PRO	18.1
1	A	426	PRO	18.1
1	A	55	TYR	18.1
1	A	609	ASP	18.1
1	A	428	THR	18.0
1	A	446	VAL	18.0
1	A	478	PRO	18.0
1	A	148	ALA	18.0
1	A	514	LEU	17.9

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Mol	Chain	Res	Type	RSRZ
1	A	607	PRO	17.9
1	A	365	VAL	17.9
1	A	313	PRO	17.9
1	A	497	SER	17.9
1	A	602	TYR	17.9
1	A	606	VAL	17.8
1	A	486	GLN	17.8
1	A	98	SER	17.8
1	A	352	THR	17.7
1	A	306	SER	17.7
1	A	399	PHE	17.7
1	A	613	ALA	17.7
1	A	610	SER	17.6
1	A	550	SER	17.6
1	A	45	ALA	17.5
1	A	528	PHE	17.5
1	A	287	GLY	17.5
1	A	278	MET	17.4
1	A	305	SER	17.4
1	A	344	SER	17.3
1	A	150	SER	17.3
1	A	28	ASN	17.2
1	A	286	ILE	17.2
1	A	308	THR	17.2
1	A	425	SER	17.2
1	A	61	THR	17.2
1	A	62	THR	17.2
1	A	414	ALA	17.1
1	A	590	ILE	17.1
1	A	364	ASP	17.0
1	A	548	ARG	16.9
1	A	298	ASN	16.9
1	A	432	SER	16.9
1	A	59	MET	16.9
1	A	525	ALA	16.8
1	A	367	SER	16.8
1	A	603	SER	16.8
1	A	362	SER	16.7
1	A	75	ASP	16.7
1	A	462	ILE	16.7
1	A	568	ILE	16.7
1	A	311	SER	16.6

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Mol	Chain	Res	Type	RSRZ
1	A	187	SER	16.5
1	A	18	CYS	16.5
1	A	536	SER	16.5
1	A	440	THR	16.5
1	A	310	THR	16.4
1	A	319	PRO	16.4
1	A	565	ASP	16.4
1	A	452	THR	16.3
1	A	415	HIS	16.3
1	A	544	PRO	16.3
1	A	260	TRP	16.2
1	A	369	GLY	16.2
1	A	264	PRO	16.2
1	A	390	ASP	16.2
1	A	470	VAL	16.2
1	A	608	SER	16.2
1	A	34	ASN	16.1
1	A	361	GLY	16.1
1	A	12	ASN	16.1
1	A	113	TYR	16.1
1	A	19	ASP	16.0
1	A	394	GLY	16.0
1	A	180	SER	16.0
1	A	527	ILE	16.0
1	A	625	SER	16.0
1	A	115	ASN	15.9
1	A	471	PHE	15.8
1	A	33	GLY	15.8
1	A	626	ALA	15.8
1	A	360	SER	15.7
1	A	283	VAL	15.7
1	A	303	SER	15.5
1	A	149	SER	15.4
1	A	495	TYR	15.4
1	A	245	ASN	15.4
1	A	636	ARG	15.3
1	A	76	GLY	15.3
1	A	89	LEU	15.3
1	A	238	GLN	15.3
1	A	502	LEU	15.3
1	A	605	GLN	15.3
1	A	68	LEU	15.2

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Mol	Chain	Res	Type	RSRZ
1	A	320	MET	15.2
1	A	538	GLY	15.2
1	A	103	GLY	15.2
1	A	155	GLN	15.1
1	A	591	PRO	15.1
1	A	573	LEU	15.1
1	A	64	ASN	15.1
1	A	267	GLN	15.1
1	A	455	THR	15.0
1	A	157	GLY	15.0
1	A	355	ASN	15.0
1	A	147	GLN	15.0
1	A	6	GLY	15.0
1	A	32	ASP	15.0
1	A	335	ALA	15.0
1	A	570	LYS	14.9
1	A	156	PRO	14.9
1	A	485	LYS	14.9
1	A	347	GLN	14.9
1	A	10	SER	14.8
1	A	36	ASP	14.8
1	A	24	GLY	14.8
1	A	175	ALA	14.7
1	A	540	LEU	14.6
1	A	420	GLY	14.6
1	A	349	GLY	14.6
1	A	574	ILE	14.6
1	A	481	ASP	14.6
1	A	93	GLY	14.5
1	A	405	TYR	14.5
1	A	385	ASN	14.5
1	A	144	ASN	14.5
1	A	136	PRO	14.5
1	A	81	TRP	14.5
1	A	373	SER	14.5
1	A	413	ASN	14.5
1	A	159	GLY	14.4
1	A	552	GLN	14.4
1	A	100	VAL	14.3
1	A	2	SER	14.3
1	A	427	ASN	14.2
1	A	186	TRP	14.2

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Mol	Chain	Res	Type	RSRZ
1	A	214	VAL	14.2
1	A	592	LEU	14.2
1	A	29	LYS	14.1
1	A	547	THR	14.1
1	A	42	PHE	14.1
1	A	408	SER	14.1
1	A	235	GLY	14.0
1	A	11	ARG	14.0
1	A	488	PRO	14.0
1	A	26	GLU	13.9
1	A	583	VAL	13.9
1	A	624	ASN	13.9
1	A	71	LEU	13.9
1	A	16	VAL	13.9
1	A	563	SER	13.9
1	A	479	GLU	13.8
1	A	447	LEU	13.8
1	A	442	HIS	13.8
1	A	105	TRP	13.8
1	A	174	ALA	13.7
1	A	372	GLN	13.7
1	A	433	ASN	13.7
1	A	371	ARG	13.7
1	A	282	ARG	13.7
1	A	555	LYS	13.6
1	A	480	GLN	13.6
1	A	316	LYS	13.6
1	A	179	THR	13.6
1	A	589	ARG	13.5
1	A	375	ARG	13.4
1	A	35	LYS	13.4
1	A	487	ASN	13.4
1	A	280	ASP	13.4
1	A	384	GLY	13.4
1	A	272	TYR	13.4
1	A	252	LEU	13.4
1	A	227	PHE	13.4
1	A	169	ILE	13.3
1	A	262	PRO	13.3
1	A	87	VAL	13.3
1	A	559	ARG	13.3
1	A	472	THR	13.3

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Mol	Chain	Res	Type	RSRZ
1	A	500	LEU	13.3
1	A	207	TRP	13.3
1	A	402	SER	13.3
1	A	501	LEU	13.2
1	A	617	TYR	13.2
1	A	395	LYS	13.2
1	A	627	GLY	13.2
1	A	57	ILE	13.1
1	A	314	ASN	13.1
1	A	393	LYS	13.1
1	A	507	VAL	13.0
1	A	639	GLN	13.0
1	A	579	ALA	12.9
1	A	629	PRO	12.9
1	A	54	THR	12.9
1	A	374	ASN	12.9
1	A	82	ILE	12.9
1	A	350	PRO	12.9
1	A	295	PHE	12.9
1	A	334	HIS	12.9
1	A	204	THR	12.8
1	A	279	SER	12.8
1	A	47	GLY	12.7
1	A	191	ASN	12.7
1	A	247	ALA	12.7
1	A	292	GLY	12.7
1	A	268	VAL	12.7
1	A	236	ASN	12.6
1	A	342	LYS	12.6
1	A	421	GLU	12.6
1	A	94	THR	12.6
1	A	621	PHE	12.5
1	A	622	VAL	12.5
1	A	321	LEU	12.5
1	A	142	GLU	12.5
1	A	619	MET	12.4
1	A	366	LYS	12.4
1	A	41	THR	12.4
1	A	623	MET	12.4
1	A	261	ILE	12.3
1	A	387	VAL	12.3
1	A	307	LYS	12.3

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Mol	Chain	Res	Type	RSRZ
1	A	300	GLU	12.3
1	A	25	ASN	12.3
1	A	580	THR	12.3
1	A	611	GLY	12.3
1	A	184	LEU	12.2
1	A	499	SER	12.2
1	A	546	ILE	12.2
1	A	328	LEU	12.2
1	A	464	PHE	12.1
1	A	443	THR	12.1
1	A	370	LYS	12.1
1	A	341	LYS	12.1
1	A	218	THR	12.0
1	A	543	ARG	12.0
1	A	503	PRO	12.0
1	A	615	PRO	11.9
1	A	401	GLY	11.9
1	A	221	VAL	11.9
1	A	165	ILE	11.9
1	A	533	LEU	11.8
1	A	593	THR	11.8
1	A	231	ILE	11.8
1	A	530	PRO	11.8
1	A	123	TYR	11.7
1	A	254	ASP	11.7
1	A	386	ALA	11.7
1	A	498	ILE	11.7
1	A	121	ALA	11.7
1	A	578	THR	11.7
1	A	118	THR	11.6
1	A	91	SER	11.6
1	A	126	LEU	11.6
1	A	46	ASN	11.5
1	A	531	ASN	11.5
1	A	22	GLN	11.4
1	A	631	VAL	11.4
1	A	382	MET	11.4
1	A	203	LEU	11.4
1	A	473	PRO	11.4
1	A	116	PHE	11.3
1	A	3	ALA	11.3
1	A	258	ASP	11.3

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Mol	Chain	Res	Type	RSRZ
1	A	383	CYS	11.2
1	A	5	ILE	11.2
1	A	172	ALA	11.2
1	A	634	THR	11.2
1	A	523	PHE	11.2
1	A	138	THR	11.1
1	A	4	PRO	11.0
1	A	44	GLY	11.0
1	A	628	VAL	11.0
1	A	7	SER	11.0
1	A	469	PRO	11.0
1	A	511	GLY	11.0
1	A	444	SER	10.9
1	A	196	GLY	10.9
1	A	409	ASP	10.9
1	A	185	MET	10.8
1	A	233	MET	10.8
1	A	70	MET	10.8
1	A	244	GLY	10.8
1	A	173	ALA	10.7
1	A	492	VAL	10.6
1	A	275	SER	10.6
1	A	222	THR	10.6
1	A	529	THR	10.6
1	A	457	GLY	10.6
1	A	454	ILE	10.5
1	A	506	ARG	10.4
1	A	194	PHE	10.4
1	A	575	ARG	10.3
1	A	620	LEU	10.3
1	A	459	ARG	10.3
1	A	176	ILE	10.2
1	A	21	ALA	10.2
1	A	171	PRO	10.2
1	A	467	SER	10.2
1	A	219	VAL	10.1
1	A	518	CYS	10.1
1	A	329	TYR	10.1
1	A	104	SER	10.1
1	A	569	SER	10.1
1	A	290	TRP	10.0
1	A	248	LYS	10.0

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Mol	Chain	Res	Type	RSRZ
1	A	167	LEU	10.0
1	A	449	ASP	10.0
1	A	632	ALA	10.0
1	A	521	ASN	10.0
1	A	441	PHE	10.0
1	A	228	CYS	9.9
1	A	114	SER	9.9
1	A	181	GLY	9.9
1	A	111	THR	9.9
1	A	109	SER	9.9
1	A	182	ARG	9.8
1	A	380	ASP	9.8
1	A	285	THR	9.8
1	A	581	HIS	9.7
1	A	213	ILE	9.7
1	A	571	ALA	9.7
1	A	508	PHE	9.7
1	A	212	GLY	9.7
1	A	577	GLY	9.7
1	A	201	ILE	9.7
1	A	276	ALA	9.7
1	A	120	PRO	9.7
1	A	195	GLY	9.6
1	A	271	GLY	9.6
1	A	88	TYR	9.6
1	A	99	PRO	9.6
1	A	168	PRO	9.6
1	A	456	GLY	9.5
1	A	513	GLY	9.5
1	A	102	SER	9.5
1	A	125	ARG	9.4
1	A	585	THR	9.4
1	A	133	ASN	9.4
1	A	119	ARG	9.4
1	A	141	ALA	9.4
1	A	323	ALA	9.3
1	A	129	ILE	9.3
1	A	220	THR	9.2
1	A	297	LYS	9.2
1	A	242	THR	9.1
1	A	545	LYS	9.1
1	A	519	THR	9.1

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Mol	Chain	Res	Type	RSRZ
1	A	66	ASN	9.0
1	A	489	ASN	9.0
1	A	211	THR	9.0
1	A	193	ALA	8.9
1	A	491	ILE	8.8
1	A	50	LYS	8.8
1	A	327	GLY	8.8
1	A	461	GLY	8.8
1	A	224	HIS	8.8
1	A	468	THR	8.8
1	A	217	ARG	8.8
1	A	197	SER	8.7
1	A	56	THR	8.7
1	A	72	PRO	8.7
1	A	78	GLN	8.7
1	A	137	TRP	8.6
1	A	210	SER	8.6
1	A	135	GLN	8.6
1	A	51	PRO	8.6
1	A	80	GLY	8.6
1	A	90	SER	8.6
1	A	128	ALA	8.6
1	A	259	SER	8.6
1	A	633	SER	8.5
1	A	466	ASP	8.5
1	A	106	PHE	8.5
1	A	177	GLU	8.5
1	A	266	MET	8.5
1	A	522	HIS	8.5
1	A	588	ARG	8.5
1	A	216	ASP	8.4
1	A	630	SER	8.4
1	A	74	GLN	8.4
1	A	60	LYS	8.4
1	A	160	ARG	8.4
1	A	509	ASN	8.4
1	A	209	PRO	8.4
1	A	40	HIS	8.4
1	A	494	VAL	8.3
1	A	73	ARG	8.3
1	A	84	ARG	8.3
1	A	63	GLN	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	582	THR	8.3
1	A	251	SER	8.2
1	A	229	PRO	8.2
1	A	293	GLY	8.2
1	A	333	ASN	8.2
1	A	20	SER	8.2
1	A	132	ALA	8.2
1	A	122	ARG	8.1
1	A	162	GLY	8.0
1	A	460	ARG	8.0
1	A	230	GLY	8.0
1	A	439	ARG	8.0
1	A	139	SER	8.0
1	A	202	THR	7.9
1	A	566	SER	7.9
1	A	463	PRO	7.8
1	A	200	GLY	7.8
1	A	516	GLY	7.8
1	A	496	HIS	7.8
1	A	13	ASN	7.7
1	A	140	ILE	7.7
1	A	273	GLN	7.7
1	A	53	HIS	7.7
1	A	584	ASN	7.7
1	A	48	ASP	7.7
1	A	17	THR	7.7
1	A	246	ASP	7.7
1	A	448	PRO	7.6
1	A	190	ARG	7.6
1	A	326	GLN	7.6
1	A	164	THR	7.6
1	A	85	HIS	7.5
1	A	490	SER	7.5
1	A	324	ASP	7.4
1	A	134	GLY	7.4
1	A	567	SER	7.4
1	A	163	PRO	7.4
1	A	241	VAL	7.4
1	A	526	GLN	7.3
1	A	493	ARG	7.3
1	A	178	PRO	7.3
1	A	92	ASP	7.3

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Mol	Chain	Res	Type	RSRZ
1	A	192	ASP	7.3
1	A	296	GLU	7.2
1	A	234	ASP	7.2
1	A	524	ASP	7.2
1	A	101	ALA	7.2
1	A	69	SER	7.2
1	A	458	GLN	7.2
1	A	255	SER	7.1
1	A	226	MET	7.1
1	A	289	SER	7.0
1	A	474	GLU	7.0
1	A	504	ASP	7.0
1	A	107	ALA	7.0
1	A	265	ASP	7.0
1	A	117	GLU	7.0
1	A	188	SER	6.9
1	A	288	GLY	6.9
1	A	52	PRO	6.9
1	A	294	VAL	6.9
1	A	407	ASP	6.9
1	A	225	ASP	6.8
1	A	274	SER	6.8
1	A	250	THR	6.8
1	A	520	THR	6.8
1	A	112	LYS	6.7
1	A	587	GLN	6.7
1	A	232	SER	6.6
1	A	198	PRO	6.5
1	A	445	VAL	6.5
1	A	277	THR	6.4
1	A	67	GLY	6.3
1	A	206	SER	6.3
1	A	586	ASP	6.3
1	A	291	SER	6.3
1	A	83	GLY	6.2
1	A	510	GLY	6.2
1	A	512	GLY	6.1
1	A	1	ALA	6.1
1	A	131	GLU	6.1
1	A	270	ARG	6.0
1	A	330	ARG	6.0
1	A	199	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	208	ASP	5.9
1	A	205	SER	5.7
1	A	108	ASP	5.7
1	A	406	GLN	5.5
1	A	517	ASP	5.5
1	A	166	ASP	5.4
1	A	332	ASP	5.3
1	A	269	ALA	5.2
1	A	49	PRO	5.1
1	A	215	SER	5.0
1	A	404	ASP	4.9
1	A	331	SER	4.7
1	A	58	ASP	4.7
1	A	223	LYS	4.5
1	A	237	GLY	4.4
1	A	249	LYS	4.0
1	A	465	GLU	4.0
1	A	325	LYS	4.0
1	A	86	GLU	4.0
1	A	601	SER	3.7
1	A	600	ASN	2.5

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	0.67	0.79	22,22,22,22	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	1.09	0.79	22,22,22,22	0
4	ACY	A	703	4/4	0.58	0.49	18,28,39,40	0
4	ACY	A	701	4/4	0.93	-0.86	9,11,13,14	0

6.5 Other polymers

There are no such residues in this entry.