



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 07:45 am 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 X-ray Structure 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

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

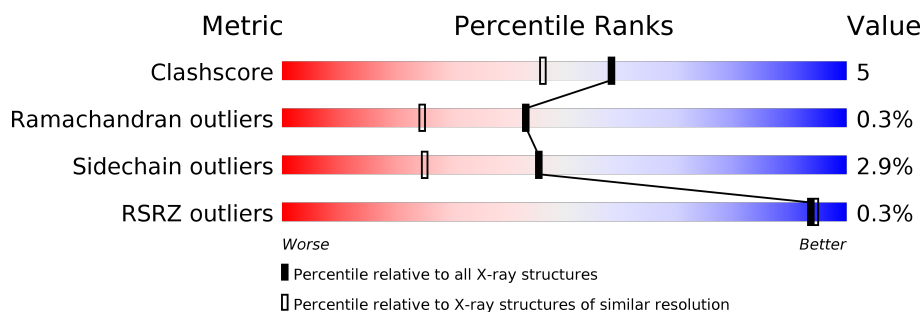
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 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	122126	4167 (1.70-1.70)
Ramachandran outliers	120053	4100 (1.70-1.70)
Sidechain outliers	120020	4100 (1.70-1.70)
RSRZ outliers	108989	3718 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	639	 71% <span style="float: right;">25%</span> . .

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5156 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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			

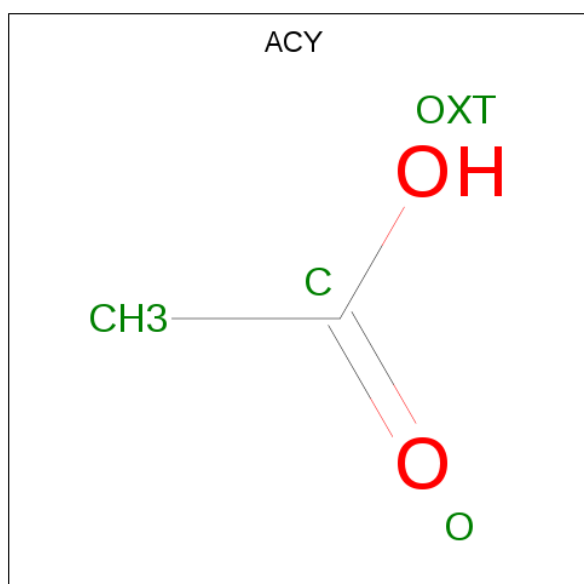
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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		

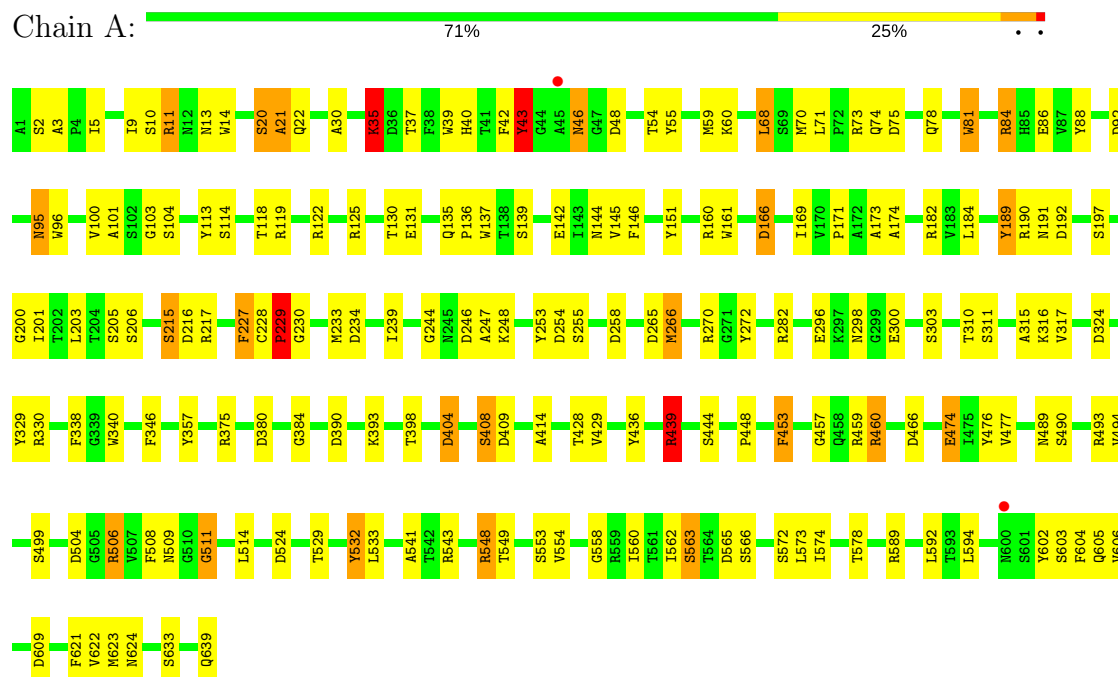
- Molecule 5 is water.

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: GALACTOSE OXIDASE



## 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 – 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*



*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:228:CYS:N	1:A:229:PRO:HD3	2.27	0.48
1:A:554:VAL:HG11	1:A:560:ILE:HD11	1.94	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
1:A:174:ALA:HA	1:A:184:LEU:O	2.16	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:103:GLY:HA3	1:A:166:ASP:O	2.17	0.45
1:A:298:ASN:HD22	1:A:317:VAL:N	2.11	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:131:GLU:HG3	1:A:137:TRP:O	2.21	0.41
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:444:SER:HA	1:A:453:PHE:O	2.21	0.41
1:A:5:ILE:HD12	1:A:490:SER:HB3	2.04	0.40
1:A:95:ASN:N	1:A:95:ASN:ND2	2.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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%)	43 25

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	LEU

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
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%)	45	25

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	95	ASN
1	A	298	ASN
1	A	413	ASN
1	A	597	ASN
1	A	600	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	-	1,3,3	5.22	1 (100%)	0,3,3	0.00	-
4	ACY	A	703	2	1,3,3	2.95	1 (100%)	0,3,3	0.00	-

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	ACY	CH3-C	2.95	1.52	1.48
4	A	701	ACY	CH3-C	5.22	1.55	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.85	2 (0%) 93 94	6, 18, 57, 98	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	600	ASN	48.9
1	A	45	ALA	4.6

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	NA	A	702	1/1	0.96	0.07	22,22,22,22	0
4	ACY	A	703	4/4	0.97	0.10	18,28,39,40	0
4	ACY	A	701	4/4	0.99	0.03	9,11,13,14	0
2	CU	A	700	1/1	1.00	0.04	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.