Full wwPDB X-ray Structure Validation Report (i)

Jul 18, 2023 – 04:06 PM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

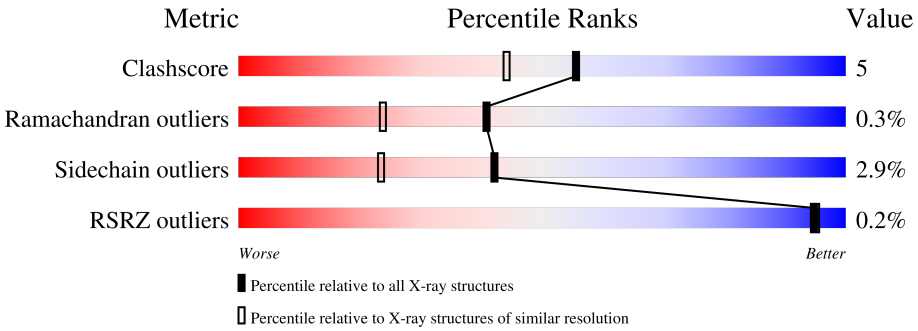
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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% 25%

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
			Total	C	N	O	S			
1	A	639	4830	3017	840	954	19	0	0	0

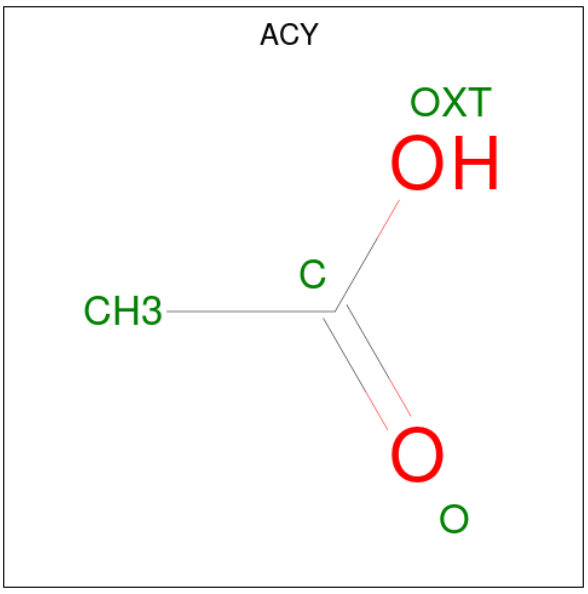
- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

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

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

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 5 is water.

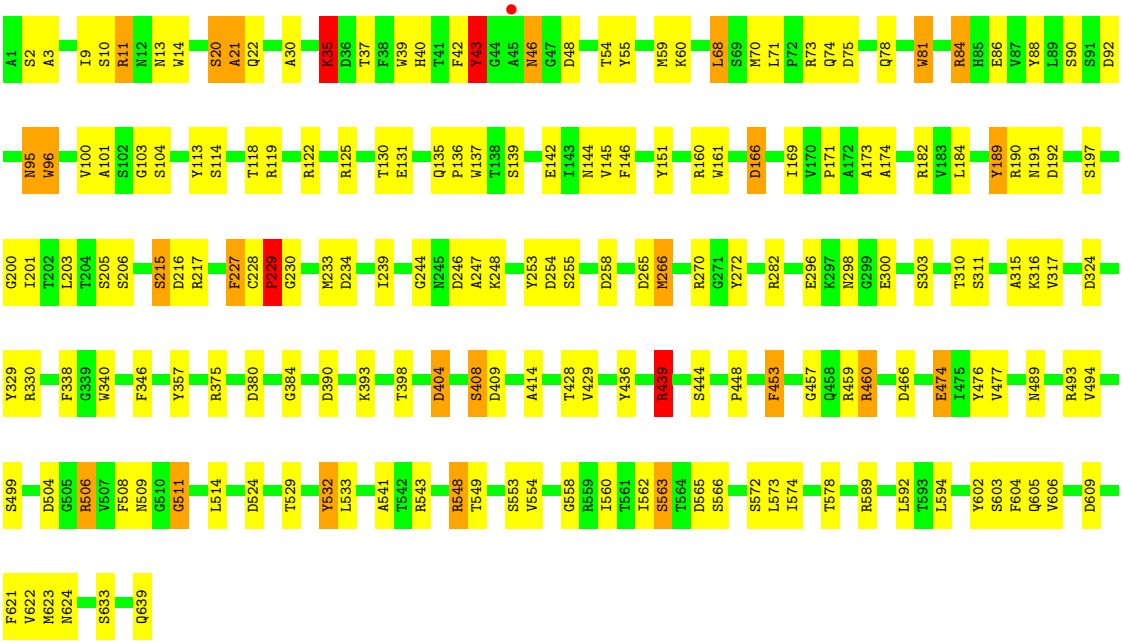
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	316	Total O 316 316	0	0

3 Residue-property plots (i)

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

- Molecule 1: GALACTOSE OXIDASE

Chain A:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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.	wwPDB-VP
Wilson B-factor (Å^2)	16.0	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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^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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CU, ACY, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.07	3/4959 (0.1%)	2.10	176/6765 (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	5.83	1.49	1.42
1	A	303	SER	CB-OG	5.24	1.49	1.42
1	A	86	GLU	CD-OE2	-5.13	1.20	1.25

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	84	ARG	CD-NE-CZ	23.57	156.59	123.60
1	A	460	ARG	NE-CZ-NH2	-19.01	110.80	120.30
1	A	493	ARG	NE-CZ-NH2	-18.66	110.97	120.30
1	A	190	ARG	NE-CZ-NH1	17.54	129.07	120.30
1	A	459	ARG	NE-CZ-NH1	16.59	128.59	120.30
1	A	330	ARG	NE-CZ-NH1	16.55	128.58	120.30
1	A	282	ARG	NE-CZ-NH1	15.16	127.88	120.30
1	A	114	SER	N-CA-CB	12.96	129.94	110.50
1	A	73	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	A	459	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	A	453	PHE	CB-CG-CD2	-10.56	113.41	120.80
1	A	189	TYR	CB-CG-CD1	10.53	127.32	121.00
1	A	86	GLU	OE1-CD-OE2	10.42	135.80	123.30
1	A	506	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	A	493	ARG	NE-CZ-NH1	10.16	125.38	120.30
1	A	476	TYR	CB-CG-CD2	-10.16	114.91	121.00
1	A	460	ARG	NH1-CZ-NH2	10.13	130.54	119.40
1	A	330	ARG	NE-CZ-NH2	-10.09	115.25	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	408	SER	N-CA-CB	-10.06	95.41	110.50
1	A	227	PHE	CB-CG-CD1	-9.78	113.96	120.80
1	A	160	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	A	182	ARG	NE-CZ-NH2	-9.53	115.53	120.30
1	A	453	PHE	CB-CG-CD1	9.48	127.44	120.80
1	A	543	ARG	NE-CZ-NH1	9.37	124.99	120.30
1	A	543	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	A	504	ASP	CB-CG-OD2	9.26	126.64	118.30
1	A	160	ARG	NE-CZ-NH1	9.09	124.85	120.30
1	A	258	ASP	CB-CG-OD1	8.97	126.38	118.30
1	A	466	ASP	CB-CG-OD1	8.92	126.33	118.30
1	A	375	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	A	254	ASP	CB-CG-OD1	8.64	126.08	118.30
1	A	88	TYR	CB-CG-CD2	-8.36	115.98	121.00
1	A	633	SER	N-CA-CB	8.30	122.95	110.50
1	A	20	SER	N-CA-CB	8.13	122.69	110.50
1	A	316	LYS	O-C-N	8.10	135.65	122.70
1	A	543	ARG	CD-NE-CZ	7.78	134.49	123.60
1	A	200	GLY	N-CA-C	7.76	132.50	113.10
1	A	409	ASP	CB-CG-OD2	-7.76	111.32	118.30
1	A	548	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	A	563	SER	N-CA-CB	7.55	121.83	110.50
1	A	234	ASP	CB-CG-OD2	-7.53	111.53	118.30
1	A	118	THR	O-C-N	7.52	134.73	122.70
1	A	439	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	A	602	TYR	CB-CG-CD1	-7.50	116.50	121.00
1	A	200	GLY	CA-C-O	7.50	134.10	120.60
1	A	73	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	A	234	ASP	CB-CG-OD1	7.41	124.97	118.30
1	A	474	GLU	OE1-CD-OE2	7.21	131.96	123.30
1	A	390	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	A	329	TYR	CB-CG-CD1	-7.17	116.69	121.00
1	A	20	SER	CB-CA-C	-7.13	96.55	110.10
1	A	217	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	A	104	SER	O-C-N	7.06	134.00	122.70
1	A	92	ASP	CB-CG-OD1	7.03	124.63	118.30
1	A	324	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	246	ASP	CB-CG-OD2	6.96	124.57	118.30
1	A	282	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	A	604	PHE	CB-CG-CD2	-6.93	115.95	120.80
1	A	499	SER	N-CA-CB	6.88	120.81	110.50
1	A	81	TRP	O-C-N	6.84	133.65	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	508	PHE	CB-CG-CD1	-6.84	116.01	120.80
1	A	466	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	A	151	TYR	CB-CG-CD1	-6.83	116.90	121.00
1	A	75	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	A	217	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	A	624	ASN	CB-CA-C	6.78	123.95	110.40
1	A	375	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	113	TYR	CB-CG-CD2	-6.69	116.98	121.00
1	A	380	ASP	CB-CG-OD1	6.67	124.31	118.30
1	A	190	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	166	ASP	CB-CG-OD1	6.62	124.25	118.30
1	A	310	THR	O-C-N	6.54	133.17	122.70
1	A	173	ALA	N-CA-CB	6.51	119.22	110.10
1	A	459	ARG	CD-NE-CZ	6.50	132.71	123.60
1	A	429	VAL	CA-CB-CG2	6.49	120.64	110.90
1	A	84	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	477	VAL	CA-CB-CG1	-6.45	101.22	110.90
1	A	272	TYR	CB-CG-CD2	-6.45	117.13	121.00
1	A	88	TYR	CB-CG-CD1	6.40	124.84	121.00
1	A	558	GLY	CA-C-O	6.31	131.96	120.60
1	A	357	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	A	189	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	A	101	ALA	O-C-N	6.29	132.76	122.70
1	A	602	TYR	CB-CG-CD2	6.29	124.77	121.00
1	A	606	VAL	CG1-CB-CG2	6.29	120.96	110.90
1	A	119	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	460	ARG	CA-CB-CG	-6.23	99.69	113.40
1	A	566	SER	O-C-N	6.16	132.55	122.70
1	A	506	ARG	CD-NE-CZ	6.09	132.12	123.60
1	A	247	ALA	CB-CA-C	6.04	119.16	110.10
1	A	55	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	A	589	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	605	GLN	O-C-N	5.92	132.17	122.70
1	A	96	TRP	CA-CB-CG	-5.92	102.46	113.70
1	A	338	PHE	CB-CG-CD2	-5.91	116.66	120.80
1	A	48	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	A	227	PHE	CG-CD2-CE2	-5.87	114.34	120.80
1	A	457	GLY	CA-C-O	5.86	131.15	120.60
1	A	266	MET	CA-CB-CG	-5.84	103.38	113.30
1	A	436	TYR	CZ-CE2-CD2	-5.82	114.56	119.80
1	A	84	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	384	GLY	N-CA-C	-5.80	98.59	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	119	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	436	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	A	476	TYR	CD1-CG-CD2	5.78	124.25	117.90
1	A	511	GLY	CA-C-N	-5.77	104.66	116.20
1	A	216	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	2	SER	CB-CA-C	5.76	121.05	110.10
1	A	37	THR	O-C-N	5.76	131.91	122.70
1	A	296	GLU	OE1-CD-OE2	5.74	130.19	123.30
1	A	246	ASP	O-C-N	5.71	131.84	122.70
1	A	621	PHE	CB-CG-CD2	-5.66	116.84	120.80
1	A	70	MET	CG-SD-CE	5.65	109.24	100.20
1	A	206	SER	N-CA-CB	5.61	118.91	110.50
1	A	565	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	233	MET	CA-CB-CG	-5.60	103.78	113.30
1	A	404	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	11	ARG	CG-CD-NE	-5.54	100.16	111.80
1	A	340	TRP	O-C-N	5.54	131.56	122.70
1	A	578	THR	CA-CB-OG1	-5.52	97.40	109.00
1	A	201	ILE	O-C-N	5.52	131.53	122.70
1	A	476	TYR	CG-CD2-CE2	-5.51	116.89	121.30
1	A	35	LYS	CA-CB-CG	5.49	125.49	113.40
1	A	43	TYR	N-CA-CB	5.47	120.45	110.60
1	A	203	LEU	CB-CG-CD1	-5.47	101.69	111.00
1	A	346	PHE	CB-CG-CD2	-5.46	116.98	120.80
1	A	606	VAL	N-CA-CB	-5.43	99.55	111.50
1	A	300	GLU	CB-CG-CD	-5.42	99.55	114.20
1	A	182	ARG	CA-CB-CG	-5.41	101.51	113.40
1	A	230	GLY	N-CA-C	-5.40	99.59	113.10
1	A	265	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	623	MET	CA-CB-CG	-5.38	104.16	113.30
1	A	404	ASP	O-C-N	5.37	131.29	122.70
1	A	606	VAL	CA-CB-CG2	-5.37	102.85	110.90
1	A	125	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	589	ARG	CD-NE-CZ	-5.33	116.14	123.60
1	A	311	SER	N-CA-CB	-5.32	102.52	110.50
1	A	509	ASN	C-N-CA	-5.31	111.15	122.30
1	A	532	TYR	CB-CG-CD1	5.31	124.19	121.00
1	A	609	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	541	ALA	CA-C-O	5.29	131.20	120.10
1	A	436	TYR	CB-CG-CD1	5.28	124.17	121.00
1	A	524	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	A	192	ASP	CB-CG-OD2	5.26	123.04	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	375	ARG	CD-NE-CZ	-5.25	116.24	123.60
1	A	565	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	130	THR	N-CA-CB	5.22	120.21	110.30
1	A	553	SER	O-C-N	-5.21	114.36	122.70
1	A	622	VAL	CA-C-O	-5.21	109.15	120.10
1	A	68	LEU	CB-CG-CD1	5.19	119.82	111.00
1	A	113	TYR	CG-CD1-CE1	-5.18	117.15	121.30
1	A	572	SER	CB-CA-C	5.16	119.90	110.10
1	A	300	GLU	N-CA-CB	5.15	119.88	110.60
1	A	621	PHE	CG-CD1-CE1	-5.14	115.15	120.80
1	A	122	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	A	229	PRO	N-CA-CB	-5.14	96.95	102.60
1	A	315	ALA	N-CA-C	-5.14	97.13	111.00
1	A	393	LYS	C-N-CA	5.12	133.06	122.30
1	A	122	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	200	GLY	CA-C-N	-5.11	105.96	117.20
1	A	54	THR	N-CA-CB	-5.09	100.63	110.30
1	A	272	TYR	CZ-CE2-CD2	-5.09	115.22	119.80
1	A	144	ASN	O-C-N	5.07	130.81	122.70
1	A	190	ARG	NH1-CZ-NH2	-5.07	113.82	119.40
1	A	21	ALA	N-CA-CB	5.07	117.20	110.10
1	A	338	PHE	CG-CD2-CE2	-5.06	115.23	120.80
1	A	100	VAL	CG1-CB-CG2	5.06	118.99	110.90
1	A	239	ILE	CG1-CB-CG2	5.05	122.51	111.40
1	A	160	ARG	CB-CA-C	-5.04	100.31	110.40
1	A	151	TYR	CB-CG-CD2	5.04	124.02	121.00
1	A	594	LEU	CB-CG-CD2	-5.03	102.46	111.00
1	A	3	ALA	O-C-N	5.02	130.64	121.10
1	A	11	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	270	ARG	CB-CA-C	-5.01	100.38	110.40
1	A	428	THR	OG1-CB-CG2	-5.01	98.47	110.00
1	A	384	GLY	CA-C-O	5.01	129.61	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4830	0	4603	48	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	48	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 (48) 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	0.93
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	0.74
1:A:298:ASN:HD22	1:A:317:VAL:H	1.39	0.68
1:A:22:GLN:NE2	1:A:43:TYR:O	2.27	0.67
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	0.65
1:A:448:PRO:HA	1:A:574:ILE:HD11	1.83	0.61
1:A:59:MET:O	1:A:60:LYS:HB2	2.02	0.59
1:A:35:LYS:HE2	1:A:74:GLN:HG3	1.86	0.57
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:78:GLN:HG2	1:A:81:TRP:CH2	2.46	0.51
1:A:529:THR:HG23	1:A:533:LEU:HD12	1.92	0.51
1:A:506:ARG:HD3	5:A:820:HOH:O	2.11	0.50
1:A:554:VAL:HG11	1:A:560:ILE:HD11	1.94	0.50
1:A:228:CYS:N	1:A:229:PRO:HD3	2.27	0.49
1:A:13:ASN:O	1:A:60:LYS:HG3	2.12	0.49
1:A:135:GLN:HB3	1:A:136:PRO:CD	2.42	0.49
1:A:404:ASP:HB2	1:A:408:SER:HB2	1.96	0.48
1:A:95:ASN:HD22	1:A:95:ASN:N	2.12	0.47
1:A:560:ILE:O	1:A:603:SER:HA	2.15	0.47
1:A:39:TRP:O	1:A:139:SER:HA	2.14	0.46
1:A:439:ARG:NH2	1:A:474:GLU:HG3	2.30	0.46
1:A:398:THR:O	1:A:414:ALA:HA	2.16	0.46
1:A:174:ALA:HA	1:A:184:LEU:O	2.16	0.46
1:A:161:TRP:CE2	1:A:489:ASN:HB3	2.52	0.45
1:A:573:LEU:HG	1:A:592:LEU:HD11	1.98	0.45
1:A:135:GLN:HB3	1:A:136:PRO:HD2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:GLY:HA3	1:A:166:ASP:O	2.17	0.45
1:A:169:ILE:HG22	1:A:191:ASN:HB2	1.99	0.44
1:A:189:TYR:CD1	1:A:197:SER:HB2	2.51	0.44
1:A:11:ARG:HG2	1:A:14:TRP:CZ3	2.51	0.44
1:A:30:ALA:O	1:A:142:GLU:HA	2.18	0.44
1:A:146:PHE:N	1:A:146:PHE:CD1	2.86	0.44
1:A:227:PHE:O	1:A:244:GLY:HA3	2.18	0.44
1:A:248:LYS:HE3	1:A:266:MET:O	2.17	0.43
1:A:460:ARG:HH11	1:A:460:ARG:HD2	1.57	0.43
1:A:205:SER:HA	1:A:215:SER:O	2.18	0.43
1:A:298:ASN:HD22	1:A:317:VAL:N	2.11	0.43
1:A:253:TYR:CE2	1:A:255:SER:HA	2.54	0.42
1:A:11:ARG:HG2	1:A:14:TRP:CH2	2.55	0.42
1:A:9:ILE:HD12	1:A:145:VAL:HG12	2.01	0.41
1:A:131:GLU:HG3	1:A:137:TRP:O	2.21	0.41
1:A:21:ALA:HA	1:A:40:HIS:O	2.21	0.41
1:A:549:THR:HG22	1:A:562:ILE:HG22	2.02	0.41
1:A:444:SER:HA	1:A:453:PHE:O	2.21	0.40
1:A:90:SER:HB2	1:A:96:TRP:CE3	2.57	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%)	41 24

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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%)	42 23

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

Sometimes 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	46	ASN
1	A	95	ASN
1	A	298	ASN
1	A	413	ASN
1	A	427	ASN
1	A	597	ASN
1	A	600	ASN

5.3.3 RNA

There are no RNA molecules 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 monosaccharides 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	703	2	3,3,3	1.03	0	3,3,3	2.01	2 (66%)
4	ACY	A	701	-	3,3,3	1.38	0	3,3,3	1.27	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	703	ACY	OXT-C-O	2.68	131.95	122.05
4	A	703	ACY	O-C-CH3	-2.21	113.72	122.33

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	639/639 (100%)	-0.92	1 (0%)	95	95	6, 18, 57, 98	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	ALA	4.6

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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	0.03	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.