Full wwPDB X-ray Structure Validation Report (i)

Jul 18, 2023 – 04:40 PM EDT

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 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 (1)) were used in the production of this report:

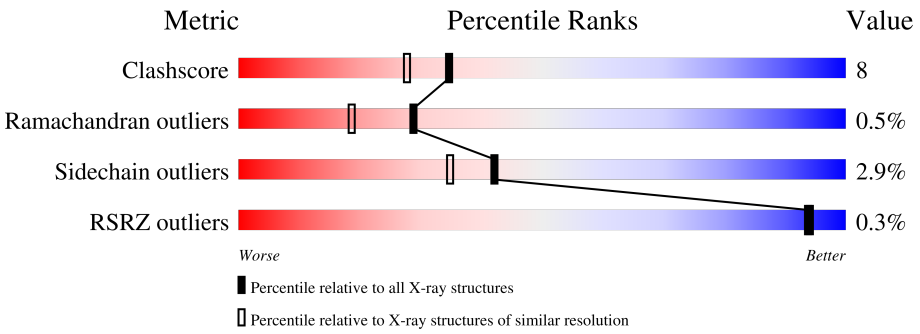
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 1.90 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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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	65% 29% 5% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5142 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 water.

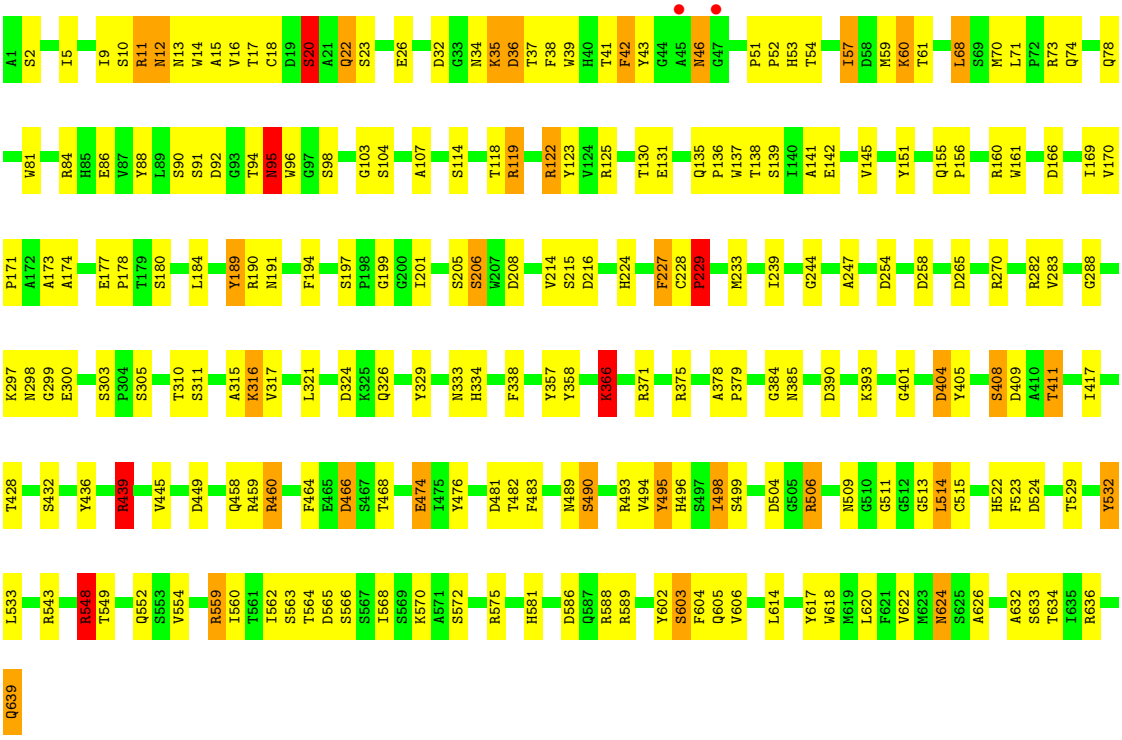
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	310	310	310	0	0

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 – 1.90 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
$< I/\sigma(I) >$ [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.	wwPDB-VP
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 56.7	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	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.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, 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	1.13	2/4959 (0.0%)	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	436	TYR	CD1-CE1	5.65	1.47	1.39
1	A	303	SER	CB-OG	5.48	1.49	1.42

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	84	ARG	NE-CZ-NH2	-20.34	110.13	120.30
1	A	73	ARG	NE-CZ-NH1	18.38	129.49	120.30
1	A	460	ARG	NE-CZ-NH2	-16.09	112.26	120.30
1	A	543	ARG	NE-CZ-NH2	-15.73	112.43	120.30
1	A	548	ARG	CD-NE-CZ	15.44	145.22	123.60
1	A	190	ARG	NE-CZ-NH2	-15.38	112.61	120.30
1	A	190	ARG	NE-CZ-NH1	15.37	127.98	120.30
1	A	459	ARG	NE-CZ-NH1	15.16	127.88	120.30
1	A	493	ARG	NE-CZ-NH2	-14.67	112.97	120.30
1	A	282	ARG	NE-CZ-NH1	12.74	126.67	120.30
1	A	390	ASP	CB-CG-OD2	-12.37	107.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	119	ARG	NE-CZ-NH2	-12.26	114.17	120.30
1	A	543	ARG	NE-CZ-NH1	12.12	126.36	120.30
1	A	265	ASP	CB-CG-OD2	12.11	129.19	118.30
1	A	114	SER	N-CA-CB	11.53	127.80	110.50
1	A	73	ARG	NE-CZ-NH2	-11.43	114.58	120.30
1	A	460	ARG	NH1-CZ-NH2	10.97	131.47	119.40
1	A	532	TYR	CB-CG-CD1	10.64	127.38	121.00
1	A	338	PHE	CB-CG-CD2	-10.60	113.38	120.80
1	A	119	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	A	532	TYR	CB-CG-CD2	-9.95	115.03	121.00
1	A	216	ASP	CB-CA-C	9.95	130.30	110.40
1	A	459	ARG	NE-CZ-NH2	-9.93	115.34	120.30
1	A	258	ASP	CB-CG-OD1	9.67	127.00	118.30
1	A	495	TYR	CB-CG-CD1	-9.56	115.26	121.00
1	A	11	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	A	523	PHE	CB-CG-CD1	9.34	127.34	120.80
1	A	589	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	A	122	ARG	NE-CZ-NH1	9.17	124.89	120.30
1	A	604	PHE	CB-CG-CD2	-9.02	114.48	120.80
1	A	408	SER	N-CA-CB	-8.98	97.03	110.50
1	A	88	TYR	CB-CG-CD2	-8.86	115.68	121.00
1	A	189	TYR	CB-CG-CD1	8.74	126.24	121.00
1	A	405	TYR	CB-CG-CD1	8.73	126.24	121.00
1	A	375	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	A	125	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	A	404	ASP	CB-CG-OD2	-8.47	110.68	118.30
1	A	566	SER	O-C-N	8.40	136.13	122.70
1	A	20	SER	N-CA-CB	8.26	122.89	110.50
1	A	523	PHE	CB-CG-CD2	-8.18	115.07	120.80
1	A	409	ASP	CB-CG-OD2	-8.06	111.05	118.30
1	A	460	ARG	NE-CZ-NH1	-8.06	116.27	120.30
1	A	483	PHE	CB-CG-CD2	-8.03	115.18	120.80
1	A	476	TYR	CB-CG-CD2	-7.97	116.22	121.00
1	A	506	ARG	CD-NE-CZ	7.91	134.68	123.60
1	A	548	ARG	NE-CZ-NH2	7.79	124.19	120.30
1	A	432	SER	N-CA-CB	-7.58	99.14	110.50
1	A	404	ASP	CB-CG-OD1	7.53	125.08	118.30
1	A	565	ASP	CB-CG-OD1	7.52	125.07	118.30
1	A	493	ARG	NH1-CZ-NH2	7.51	127.67	119.40
1	A	92	ASP	CB-CG-OD1	7.49	125.04	118.30
1	A	20	SER	CB-CA-C	-7.46	95.93	110.10
1	A	160	ARG	NE-CZ-NH1	7.45	124.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	390	ASP	OD1-CG-OD2	7.41	137.37	123.30
1	A	160	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	A	98	SER	N-CA-CB	-7.29	99.57	110.50
1	A	122	ARG	NH1-CZ-NH2	-7.05	111.65	119.40
1	A	36	ASP	O-C-N	7.01	133.92	122.70
1	A	119	ARG	CD-NE-CZ	6.92	133.28	123.60
1	A	474	GLU	OE1-CD-OE2	6.91	131.59	123.30
1	A	333	ASN	O-C-N	6.88	133.71	122.70
1	A	586	ASP	CB-CG-OD1	-6.86	112.12	118.30
1	A	84	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	A	371	ARG	NE-CZ-NH1	-6.81	116.90	120.30
1	A	466	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	495	TYR	N-CA-CB	-6.72	98.50	110.60
1	A	216	ASP	CB-CG-OD2	6.71	124.34	118.30
1	A	589	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	449	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	2	SER	CB-CA-C	6.66	122.76	110.10
1	A	216	ASP	CB-CG-OD1	-6.62	112.34	118.30
1	A	288	GLY	CA-C-O	-6.62	108.69	120.60
1	A	490	SER	N-CA-CB	-6.57	100.64	110.50
1	A	375	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	229	PRO	N-CA-CB	-6.50	95.45	102.60
1	A	92	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	118	THR	O-C-N	6.48	133.07	122.70
1	A	499	SER	N-CA-CB	6.42	120.12	110.50
1	A	409	ASP	CB-CG-OD1	6.39	124.06	118.30
1	A	385	ASN	CB-CG-OD1	-6.39	108.81	121.60
1	A	476	TYR	CD1-CE1-CZ	-6.36	114.08	119.80
1	A	122	ARG	NE-CZ-NH2	6.33	123.47	120.30
1	A	254	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	617	TYR	O-C-N	6.28	132.74	122.70
1	A	270	ARG	CB-CA-C	-6.27	97.87	110.40
1	A	88	TYR	CG-CD2-CE2	-6.26	116.30	121.30
1	A	194	PHE	CB-CG-CD2	-6.23	116.44	120.80
1	A	282	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	311	SER	N-CA-CB	-6.22	101.17	110.50
1	A	173	ALA	N-CA-CB	6.21	118.79	110.10
1	A	199	GLY	CA-C-O	-6.18	109.48	120.60
1	A	624	ASN	CB-CA-C	6.18	122.75	110.40
1	A	636	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	84	ARG	NH1-CZ-NH2	6.13	126.14	119.40
1	A	460	ARG	CA-CB-CG	-6.11	99.96	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	224	HIS	N-CA-CB	-6.10	99.62	110.60
1	A	602	TYR	CG-CD1-CE1	-6.06	116.45	121.30
1	A	70	MET	CG-SD-CE	6.06	109.89	100.20
1	A	636	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	A	633	SER	N-CA-CB	6.02	119.53	110.50
1	A	617	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	A	411	THR	OG1-CB-CG2	-5.96	96.30	110.00
1	A	36	ASP	CB-CG-OD1	-5.95	112.95	118.30
1	A	122	ARG	CD-NE-CZ	5.94	131.91	123.60
1	A	445	VAL	CG1-CB-CG2	-5.94	101.40	110.90
1	A	602	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	A	326	GLN	CA-CB-CG	5.89	126.36	113.40
1	A	54	THR	N-CA-CB	-5.86	99.16	110.30
1	A	524	ASP	N-CA-CB	-5.83	100.10	110.60
1	A	10	SER	N-CA-CB	5.80	119.20	110.50
1	A	95	ASN	O-C-N	5.80	131.98	122.70
1	A	215	SER	CA-CB-OG	5.80	126.86	111.20
1	A	366	LYS	N-CA-CB	-5.77	100.22	110.60
1	A	233	MET	CA-CB-CG	-5.74	103.54	113.30
1	A	201	ILE	O-C-N	5.73	131.88	122.70
1	A	572	SER	N-CA-CB	-5.72	101.92	110.50
1	A	481	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	189	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	A	283	VAL	CA-CB-CG2	5.70	119.45	110.90
1	A	26	GLU	CA-CB-CG	5.70	125.93	113.40
1	A	57	ILE	O-C-N	5.66	131.75	122.70
1	A	384	GLY	N-CA-C	-5.64	99.01	113.10
1	A	436	TYR	CD1-CE1-CZ	-5.63	114.73	119.80
1	A	104	SER	O-C-N	5.62	131.69	122.70
1	A	559	ARG	CD-NE-CZ	-5.57	115.81	123.60
1	A	86	GLU	OE1-CD-OE2	5.57	129.98	123.30
1	A	321	LEU	CB-CG-CD2	-5.55	101.56	111.00
1	A	42	PHE	CB-CG-CD2	-5.55	116.91	120.80
1	A	300	GLU	N-CA-CB	5.55	120.59	110.60
1	A	206	SER	CB-CA-C	-5.53	99.60	110.10
1	A	205	SER	CB-CA-C	5.52	120.59	110.10
1	A	18	CYS	O-C-N	5.51	131.52	122.70
1	A	572	SER	CB-CA-C	5.51	120.56	110.10
1	A	125	ARG	CD-NE-CZ	5.49	131.29	123.60
1	A	614	LEU	CB-CG-CD2	5.45	120.27	111.00
1	A	549	THR	N-CA-CB	5.44	120.63	110.30
1	A	504	ASP	CB-CG-OD2	5.43	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	315	ALA	N-CA-C	-5.42	96.36	111.00
1	A	428	THR	OG1-CB-CG2	-5.42	97.54	110.00
1	A	357	TYR	CG-CD1-CE1	-5.40	116.98	121.30
1	A	178	PRO	O-C-N	5.39	131.33	122.70
1	A	564	THR	CA-CB-OG1	-5.39	97.69	109.00
1	A	513	GLY	O-C-N	5.38	131.31	122.70
1	A	639	GLN	N-CA-CB	5.38	120.28	110.60
1	A	300	GLU	CB-CG-CD	-5.38	99.69	114.20
1	A	316	LYS	O-C-N	5.38	131.30	122.70
1	A	602	TYR	CZ-CE2-CD2	-5.37	114.97	119.80
1	A	151	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	A	606	VAL	CA-CB-CG2	-5.36	102.86	110.90
1	A	130	THR	N-CA-CB	5.35	120.47	110.30
1	A	570	LYS	N-CA-CB	-5.33	101.00	110.60
1	A	288	GLY	O-C-N	5.33	131.22	122.70
1	A	305	SER	CB-CA-C	5.32	120.21	110.10
1	A	88	TYR	CD1-CE1-CZ	-5.30	115.03	119.80
1	A	329	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	A	634	THR	OG1-CB-CG2	5.29	122.17	110.00
1	A	68	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	299	GLY	O-C-N	5.29	131.16	122.70
1	A	297	LYS	CD-CE-NZ	-5.27	99.58	111.70
1	A	603	SER	CB-CA-C	-5.26	100.10	110.10
1	A	310	THR	O-C-N	5.25	131.11	122.70
1	A	338	PHE	CB-CG-CD1	5.24	124.47	120.80
1	A	498	ILE	O-C-N	5.23	131.07	122.70
1	A	509	ASN	C-N-CA	-5.23	111.31	122.30
1	A	324	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	138	THR	CA-CB-OG1	-5.21	98.05	109.00
1	A	495	TYR	CD1-CE1-CZ	-5.21	115.11	119.80
1	A	384	GLY	CA-C-O	5.21	129.98	120.60
1	A	417	ILE	CA-CB-CG1	-5.21	101.11	111.00
1	A	227	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	A	239	ILE	CA-CB-CG1	-5.18	101.16	111.00
1	A	390	ASP	CB-CA-C	5.18	120.76	110.40
1	A	22	GLN	CA-CB-CG	-5.16	102.04	113.40
1	A	208	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	588	ARG	CD-NE-CZ	5.16	130.82	123.60
1	A	506	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	495	TYR	CG-CD2-CE2	-5.15	117.18	121.30
1	A	589	ARG	O-C-N	5.14	130.93	122.70
1	A	107	ALA	O-C-N	5.13	130.91	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	476	TYR	CG-CD2-CE2	-5.12	117.20	121.30
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	60	LYS	CB-CA-C	-5.08	100.24	110.40
1	A	378	ALA	N-CA-CB	-5.08	102.99	110.10
1	A	476	TYR	CD1-CG-CD2	5.08	123.49	117.90
1	A	316	LYS	N-CA-CB	-5.07	101.48	110.60
1	A	35	LYS	CA-CB-CG	5.03	124.46	113.40
1	A	482	THR	O-C-N	5.01	130.71	122.70
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 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	78	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	78	1

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 8.

All (78) 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	1.15	1.11
1:A:22:GLN:HG3	1:A:42:PHE:HA	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ASN:HD22	1:A:317:VAL:H	1.21	0.89
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	0.80
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	0.65
1:A:32:ASP:OD2	1:A:37:THR:OG1	2.14	0.62
1:A:20:SER:OG	4:A:999:HOH:O	2.17	0.60
1:A:298:ASN:HD22	1:A:317:VAL:N	1.97	0.58
1:A:171:PRO:HD2	1:A:511:GLY:HA2	1.85	0.58
1:A:522:HIS:HD2	4:A:822:HOH:O	1.86	0.58
1:A:379:PRO:HD2	4:A:770:HOH:O	2.04	0.57
1:A:466:ASP:OD2	1:A:522:HIS:HE1	1.87	0.57
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:HA	1:A:184:LEU:O	2.07	0.55
1:A:35:LYS:HE2	1:A:74:GLN:HG3	1.90	0.55
1:A:95:ASN:HD22	1:A:95:ASN:N	2.06	0.54
1:A:174:ALA:CB	1:A:498:ILE:HD13	2.38	0.53
1:A:78:GLN:HG2	1:A:81:TRP:CH2	2.44	0.53
1:A:135:GLN:HB3	1:A:136:PRO:CD	2.38	0.52
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:506:ARG:HD3	4:A:821:HOH:O	2.10	0.52
1:A:554:VAL:HG11	1:A:560:ILE:HD11	1.92	0.52
1:A:358:TYR:HE2	1:A:366:LYS:HB2	1.75	0.52
1:A:228:CYS:N	1:A:229:PRO:HD3	2.25	0.51
1:A:5:ILE:HD12	1:A:490:SER:HB3	1.92	0.51
1:A:404:ASP:HB2	1:A:408:SER:HB2	1.93	0.51
1:A:439:ARG:NH2	1:A:474:GLU:HG3	2.25	0.51
1:A:495:TYR:O	1:A:496:HIS:HB2	2.11	0.51
1:A:90:SER:HB2	1:A:96:TRP:CE3	2.47	0.50
1:A:131:GLU:HG3	1:A:137:TRP:O	2.12	0.50
1:A:401:GLY:O	1:A:411:THR:HG22	2.12	0.50
1:A:298:ASN:ND2	1:A:316:LYS:HA	2.27	0.49
1:A:11:ARG:HG2	1:A:14:TRP:CH2	2.47	0.49
1:A:59:MET:C	1:A:61:THR:H	2.16	0.49
1:A:13:ASN:HB3	1:A:60:LYS:HG3	1.95	0.48
1:A:103:GLY:HA3	1:A:166:ASP:O	2.14	0.47
1:A:227:PHE:O	1:A:244:GLY:HA3	2.15	0.47
1:A:458:GLN:HA	1:A:468:THR:O	2.15	0.47
1:A:135:GLN:HB3	1:A:136:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ILE:HD12	1:A:145:VAL:HG12	1.98	0.46
1:A:22:GLN:HE21	1:A:46:ASN:CB	2.06	0.46
1:A:169:ILE:HG22	1:A:191:ASN:HB2	1.98	0.46
1:A:122:ARG:HD3	1:A:123:TYR:CE1	2.50	0.46
1:A:177:GLU:HB2	1:A:180:SER:OG	2.16	0.46
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:568:ILE:HD13	1:A:622:VAL:HB	1.99	0.44
1:A:552:GLN:HG3	4:A:978:HOH:O	2.17	0.44
1:A:560:ILE:O	1:A:603:SER:HA	2.18	0.43
1:A:334:HIS:CE1	1:A:581:HIS:HB3	2.53	0.43
1:A:16:VAL:HG12	1:A:57:ILE:HG12	2.01	0.43
1:A:170:VAL:HB	1:A:514:LEU:CD1	2.47	0.43
1:A:575:ARG:HD2	1:A:618:TRP:CZ2	2.54	0.43
1:A:35:LYS:HE3	1:A:35:LYS:HB2	1.93	0.42
1:A:41:THR:HG21	1:A:53:HIS:CG	2.55	0.42
1:A:51:PRO:HD3	1:A:136:PRO:HA	2.01	0.41
1:A:61:THR:O	1:A:122:ARG:HA	2.20	0.41
1:A:460:ARG:HH11	1:A:460:ARG:HD2	1.56	0.41
1:A:60:LYS:HA	1:A:122:ARG:HH21	1.85	0.41
1:A:548:ARG:O	1:A:562:ILE:HA	2.20	0.41
1:A:155:GLN:HA	1:A:156:PRO:HD3	1.83	0.41
1:A:34:ASN:OD1	1:A:36:ASP:HB2	2.21	0.41
1:A:38:PHE:HB3	1:A:141:ALA:HA	2.02	0.41
1:A:620:LEU:O	1:A:632:ALA:HA	2.21	0.41
1:A:206:SER:O	1:A:214:VAL:HA	2.21	0.40
1:A:393:LYS:HA	1:A:393:LYS:HD2	1.95	0.40
1:A:624:ASN:OD1	1:A:626:ALA:HB3	2.21	0.40
1:A:94:THR:HB	1:A:95:ASN:HD22	1.86	0.40
1:A:464:PHE:CD1	1:A:515:CYS:HB3	2.56	0.40
1:A:559:ARG:HE	1:A:605:GLN:HG3	1.87	0.40
1:A:161:TRP:CE2	1:A:489:ASN:HB3	2.56	0.40
1:A:39:TRP:O	1:A:139:SER:HA	2.22	0.40
1:A:51:PRO:HA	1:A:52:PRO:C	2.42	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	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASN:ND2	1:A:548:ARG:NH1[3_545]	2.15	0.05

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%)	610 (96%)	24 (4%)	3 (0%)	29 18

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 (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 35

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

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Mol	Chain	Res	Type
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

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	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 (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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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.

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, 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	639/639 (100%)	-0.94	2 (0%)	94	94	6, 18, 56, 98	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	ALA	3.3
1	A	47	GLY	2.7

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 monosaccharides 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, 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	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	A	702	1/1	0.98	0.04	15,15,15,15	0
2	CU	A	700	1/1	1.00	0.04	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.