



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:23 AM UTC

PDB ID : 4BE3 / pdb_00004be3
Title : crystal structure of the exolytic PL7 alginate lyase AlyA5 from *Zobellia galac-*
tanivorans
Authors : Thomas, F.; Jeudy, A.; Michel, G.; Czjzek, M.
Deposited on : 2013-03-05
Resolution : 1.75 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

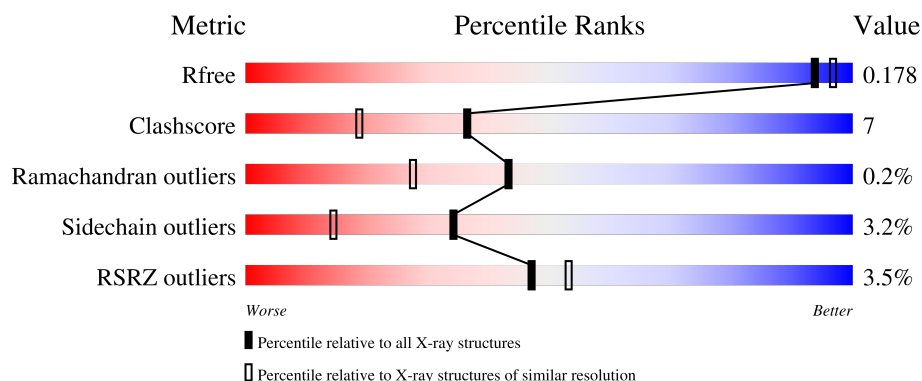
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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 $\leq 5\%$. 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	314	4% 71% 25% ..
1	B	314	4% 72% 19% 7% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SRT	A	400	X	X	-	-
4	TAR	B	400	-	X	-	-
5	TLA	B	401	-	X	-	-

2 Entry composition [i](#)

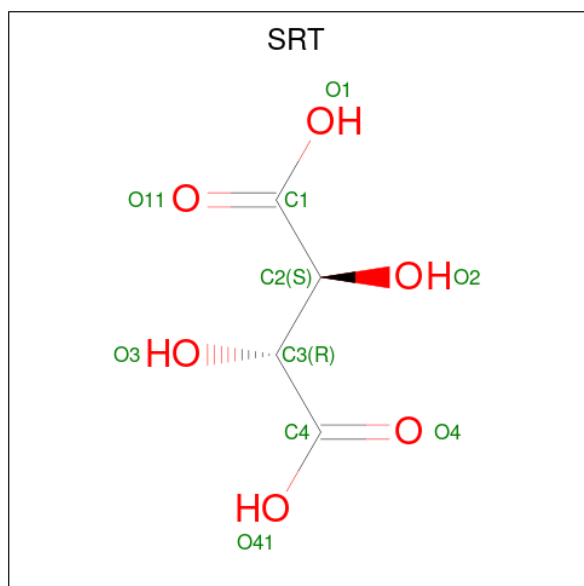
There are 6 unique types of molecules in this entry. The entry contains 5646 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALGINATE LYASE, FAMILY PL7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	6	0
			2505	1592	406	504	3			
1	B	312	Total	C	N	O	S	0	10	0
			2531	1610	411	507	3			

- Molecule 2 is S,R MESO-TARTARIC ACID (CCD ID: SRT) (formula: C₄H₆O₆).

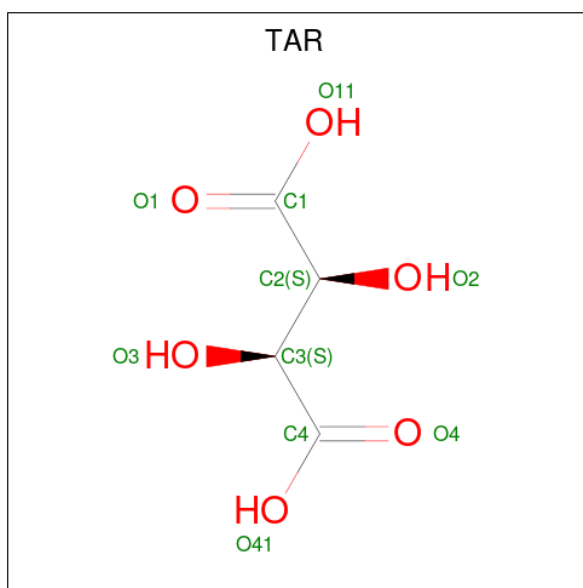


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

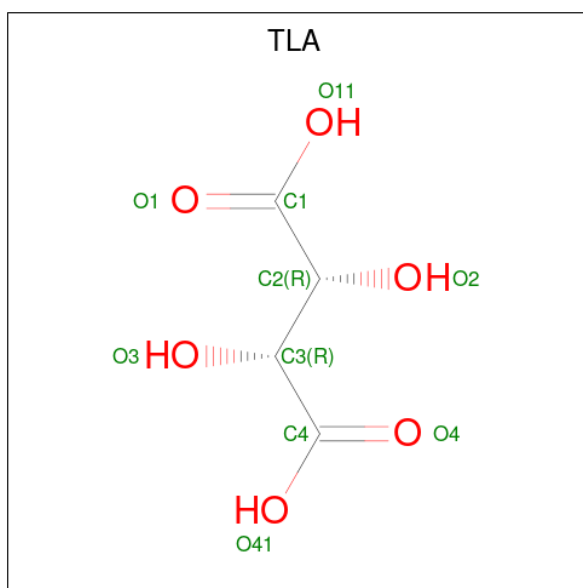
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 5 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	4	6		

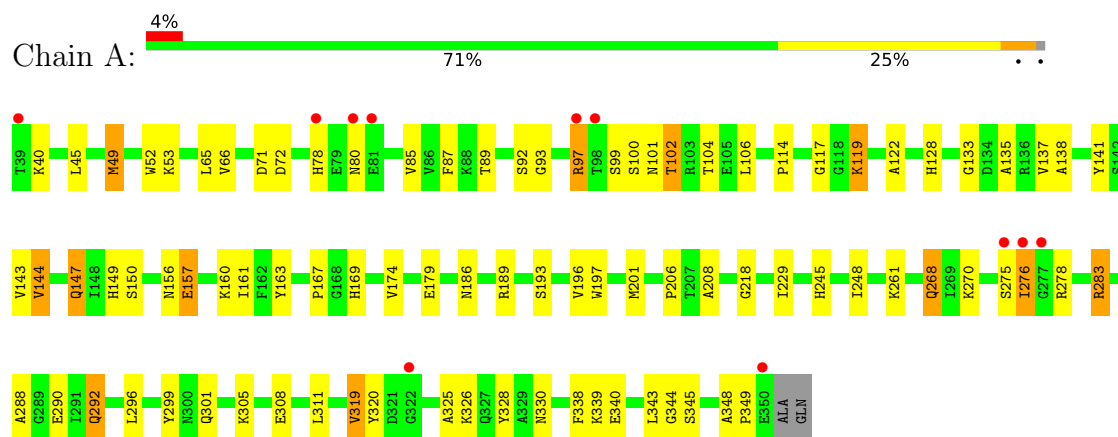
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	286	Total 286	O 286	0	0
6	B	293	Total 293	O 293	0	0

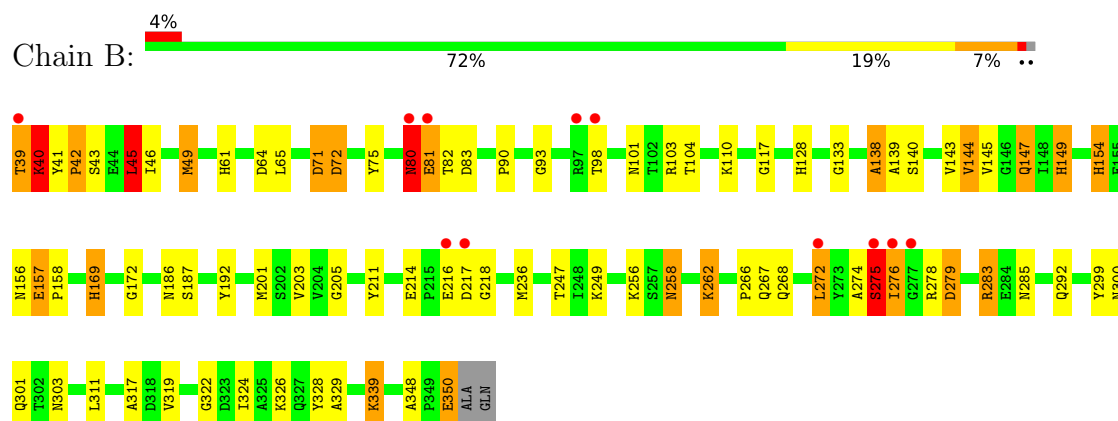
3 Residue-property plots [i](#)

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: ALGINATE LYASE, FAMILY PL7



• Molecule 1: ALGINATE LYASE, FAMILY PL7



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.42Å 93.91Å 130.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.95 – 1.75 41.95 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.95-1.75) 99.4 (41.95-1.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.156 , 0.178 0.156 , 0.178	Depositor DCC
R_{free} test set	5709 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5646	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SRT, TAR, TLA

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	2.01	55/2589 (2.1%)	1.64	25/3512 (0.7%)
1	B	1.94	48/2627 (1.8%)	1.72	37/3562 (1.0%)
All	All	1.98	103/5216 (2.0%)	1.68	62/7074 (0.9%)

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	B	0	1

All (103) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	VAL	C-O	10.13	1.35	1.24
1	B	278	ARG	N-CA	8.45	1.58	1.46
1	B	149	HIS	ND1-CE1	8.38	1.41	1.32
1	A	288	ALA	N-CA	8.32	1.56	1.46
1	B	267	GLN	CA-C	-8.23	1.41	1.52
1	B	192	TYR	N-CA	7.96	1.55	1.46
1	A	292	GLN	CD-OE1	7.73	1.38	1.23
1	B	268	GLN	CA-CB	7.61	1.65	1.53
1	A	149	HIS	ND1-CE1	7.49	1.40	1.32
1	A	344	GLY	N-CA	7.26	1.53	1.44
1	A	292	GLN	CA-CB	-7.23	1.41	1.53
1	A	128	HIS	ND1-CE1	7.16	1.39	1.32
1	B	268	GLN	N-CA	-7.11	1.37	1.46
1	B	205	GLY	N-CA	7.09	1.54	1.44
1	B	211	TYR	N-CA	6.91	1.51	1.45
1	A	137	VAL	N-CA	6.91	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	104	THR	C-O	6.77	1.31	1.24
1	B	301	GLN	CD-OE1	6.73	1.36	1.23
1	B	133	GLY	N-CA	6.71	1.52	1.45
1	B	128	HIS	ND1-CE1	6.66	1.39	1.32
1	B	203	VAL	N-CA	6.60	1.53	1.46
1	A	320	TYR	N-CA	6.54	1.56	1.46
1	A	49	MET	SD-CE	-6.48	1.63	1.79
1	A	93	GLY	N-CA	6.44	1.54	1.45
1	B	117	GLY	C-O	6.42	1.32	1.23
1	A	117	GLY	N-CA	6.41	1.53	1.45
1	B	279	ASP	N-CA	-6.35	1.38	1.46
1	A	270	LYS	N-CA	6.34	1.54	1.46
1	A	45	LEU	N-CA	6.29	1.54	1.46
1	A	290	GLU	C-O	6.29	1.31	1.24
1	B	187	SER	CA-C	6.25	1.61	1.52
1	A	101	ASN	C-O	6.18	1.31	1.23
1	A	349	PRO	CA-C	6.18	1.60	1.52
1	B	64[A]	ASP	CA-CB	6.12	1.61	1.53
1	B	64[B]	ASP	CA-CB	6.12	1.61	1.53
1	A	345	SER	CB-OG	-6.10	1.29	1.42
1	B	249	LYS	CA-C	-6.09	1.45	1.52
1	A	78	HIS	CE1-NE2	6.09	1.38	1.32
1	A	196	VAL	C-O	6.05	1.31	1.24
1	B	75	TYR	C-O	-6.01	1.18	1.24
1	B	49	MET	SD-CE	-6.00	1.64	1.79
1	A	85	VAL	N-CA	-5.94	1.39	1.46
1	B	275	SER	CA-CB	5.90	1.62	1.53
1	B	143	VAL	N-CA	5.90	1.53	1.46
1	B	169	HIS	CE1-NE2	5.89	1.38	1.32
1	B	43	SER	N-CA	5.87	1.53	1.46
1	A	133	GLY	N-CA	5.83	1.51	1.45
1	B	300	ASN	CA-C	-5.83	1.45	1.52
1	B	140	SER	CA-CB	5.81	1.63	1.53
1	B	93	GLY	N-CA	5.81	1.53	1.45
1	B	292	GLN	N-CA	5.81	1.53	1.45
1	A	278	ARG	N-CA	5.79	1.53	1.46
1	B	154	HIS	ND1-CE1	5.79	1.38	1.32
1	A	80	ASN	N-CA	5.75	1.53	1.46
1	A	104	THR	C-O	5.74	1.30	1.24
1	B	145	VAL	CA-CB	-5.73	1.48	1.54
1	B	110	LYS	N-CA	5.73	1.53	1.46
1	A	296	LEU	C-O	5.72	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	LEU	N-CA	5.70	1.53	1.45
1	B	72	ASP	N-CA	5.68	1.54	1.46
1	A	65	LEU	CA-CB	5.66	1.62	1.53
1	A	197	TRP	N-CA	5.65	1.52	1.46
1	B	217	ASP	CG-OD2	5.61	1.36	1.25
1	A	174	VAL	N-CA	5.61	1.52	1.46
1	B	147	GLN	N-CA	5.60	1.53	1.45
1	A	268	GLN	CD-OE1	5.60	1.34	1.23
1	A	78	HIS	CA-CB	5.59	1.61	1.53
1	A	119	LYS	CA-C	-5.59	1.45	1.52
1	A	245	HIS	ND1-CE1	5.58	1.38	1.32
1	A	78	HIS	CG-CD2	5.58	1.42	1.35
1	B	40	LYS	N-CA	-5.58	1.39	1.46
1	A	87	PHE	C-O	5.54	1.30	1.24
1	A	326	LYS	CA-C	5.53	1.59	1.52
1	A	340	GLU	C-O	5.52	1.30	1.23
1	A	65	LEU	CA-C	-5.51	1.45	1.52
1	A	157	GLU	CA-C	-5.51	1.46	1.52
1	A	283	ARG	CA-CB	-5.48	1.44	1.53
1	A	135	ALA	N-CA	5.48	1.53	1.46
1	A	102	THR	C-O	5.45	1.30	1.23
1	A	330	ASN	N-CA	5.41	1.52	1.46
1	A	325	ALA	CA-CB	5.38	1.61	1.53
1	B	169	HIS	CG-CD2	5.33	1.41	1.35
1	A	319	VAL	N-CA	5.28	1.51	1.46
1	B	98	THR	CA-CB	5.26	1.62	1.53
1	B	236	MET	CA-CB	5.26	1.60	1.53
1	A	122	ALA	N-CA	-5.24	1.39	1.45
1	B	98	THR	CA-C	5.23	1.59	1.52
1	B	247	THR	CA-C	-5.21	1.46	1.52
1	B	267	GLN	CA-CB	5.21	1.61	1.53
1	B	138	ALA	CA-C	5.20	1.59	1.52
1	B	317	ALA	N-CA	5.19	1.52	1.45
1	A	143	VAL	N-CA	5.18	1.52	1.46
1	B	139	ALA	N-CA	5.17	1.52	1.46
1	A	292	GLN	CA-C	-5.16	1.46	1.52
1	A	160	LYS	CA-C	5.15	1.58	1.52
1	A	45	LEU	C-O	-5.12	1.17	1.24
1	B	61	HIS	C-O	5.10	1.29	1.23
1	A	169	HIS	ND1-CE1	5.08	1.37	1.32
1	A	87	PHE	N-CA	-5.07	1.40	1.46
1	B	217	ASP	CG-OD1	5.06	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	329	ALA	CA-CB	5.05	1.61	1.53
1	A	218	GLY	N-CA	5.03	1.51	1.45
1	A	53	LYS	C-O	5.02	1.30	1.23

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	ILE	N-CA-C	9.98	122.48	112.90
1	A	292	GLN	CB-CG-CD	-9.31	96.78	112.60
1	A	133	GLY	N-CA-C	-9.10	100.13	110.96
1	A	283	ARG	NE-CZ-NH1	7.91	129.41	121.50
1	A	345	SER	CB-CA-C	7.60	122.51	109.51
1	A	283	ARG	CB-CG-CD	-7.49	94.06	111.30
1	A	345	SER	CA-CB-OG	-7.46	96.17	111.10
1	B	217	ASP	CA-C-N	-7.33	113.97	122.83
1	B	217	ASP	C-N-CA	-7.33	113.97	122.83
1	B	326	LYS	N-CA-C	-6.78	103.97	111.36
1	B	104	THR	N-CA-C	-6.59	96.49	108.02
1	B	274	ALA	CA-C-N	6.34	129.41	120.28
1	B	274	ALA	C-N-CA	6.34	129.41	120.28
1	B	39	THR	CA-C-N	-6.31	109.49	121.54
1	B	39	THR	C-N-CA	-6.31	109.49	121.54
1	B	258	ASN	CB-CA-C	-6.24	100.01	110.56
1	A	144	VAL	N-CA-CB	-6.15	103.61	110.99
1	A	348	ALA	CA-C-N	-6.15	113.43	119.76
1	A	348	ALA	C-N-CA	-6.15	113.43	119.76
1	B	272	LEU	N-CA-C	6.11	117.60	111.07
1	B	348	ALA	CA-C-N	-5.87	113.92	119.85
1	B	348	ALA	C-N-CA	-5.87	113.92	119.85
1	B	46	ILE	CA-C-O	5.81	124.83	120.88
1	B	49	MET	CG-SD-CE	-5.80	88.14	100.90
1	B	319	VAL	N-CA-C	-5.78	107.65	113.20
1	A	150	SER	CA-CB-OG	-5.68	99.73	111.10
1	B	279	ASP	CA-C-N	-5.66	114.14	120.53
1	B	279	ASP	C-N-CA	-5.66	114.14	120.53
1	B	275	SER	N-CA-CB	-5.57	101.64	110.22
1	A	339	LYS	CB-CG-CD	-5.52	98.60	111.30
1	A	301	GLN	CA-C-N	-5.52	115.43	122.77
1	A	301	GLN	C-N-CA	-5.52	115.43	122.77
1	A	338	PHE	CA-C-N	-5.37	113.72	122.26
1	A	338	PHE	C-N-CA	-5.37	113.72	122.26
1	B	339	LYS	N-CA-C	-5.35	106.43	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	GLU	CB-CA-C	-5.34	104.00	110.15
1	B	301	GLN	CA-C-N	-5.33	115.68	122.77
1	B	301	GLN	C-N-CA	-5.33	115.68	122.77
1	A	248	ILE	CB-CA-C	-5.33	102.75	110.63
1	A	206	PRO	N-CA-C	-5.32	106.78	114.18
1	A	283	ARG	CD-NE-CZ	5.27	131.78	124.40
1	A	208	ALA	CA-C-N	-5.25	114.23	122.79
1	A	208	ALA	C-N-CA	-5.25	114.23	122.79
1	A	163	TYR	N-CA-C	-5.24	99.90	108.76
1	A	99	SER	N-CA-C	5.24	117.21	108.99
1	B	71	ASP	CB-CA-C	-5.23	101.28	109.70
1	B	266	PRO	CB-CA-C	-5.22	104.55	111.23
1	B	144	VAL	N-CA-CB	-5.22	104.73	110.99
1	B	292	GLN	CA-CB-CG	5.21	124.52	114.10
1	B	311	LEU	CA-C-N	-5.20	116.21	122.35
1	B	311	LEU	C-N-CA	-5.20	116.21	122.35
1	B	217	ASP	O-C-N	-5.20	115.49	122.19
1	A	167	PRO	CB-CA-C	-5.17	104.79	111.46
1	B	158	PRO	CA-C-N	-5.14	114.09	121.95
1	B	158	PRO	C-N-CA	-5.14	114.09	121.95
1	B	322	GLY	N-CA-C	-5.12	108.18	115.30
1	B	256	LYS	N-CA-C	-5.06	99.05	107.80
1	B	45	LEU	CB-CG-CD1	5.04	125.83	110.70
1	A	141	TYR	CA-C-N	-5.03	114.38	122.82
1	A	141	TYR	C-N-CA	-5.03	114.38	122.82
1	B	64[A]	ASP	CB-CA-C	5.02	118.98	110.79
1	B	64[B]	ASP	CB-CA-C	5.02	118.98	110.79

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	103	ARG	Sidechain

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	2505	0	2382	27	0
1	B	2531	0	2422	44	0
2	A	10	0	2	0	0
3	B	1	0	0	0	0
4	B	10	0	3	0	0
5	B	10	0	2	0	0
6	A	286	0	0	2	0
6	B	293	0	0	7	0
All	All	5646	0	4811	71	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 7.

All (71) 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:B:80:ASN:ND2	1:B:81:GLU:H	1.35	1.25
1:B:80:ASN:HD22	1:B:81:GLU:N	1.36	1.21
1:B:283[A]:ARG:NH1	1:B:283[A]:ARG:HG2	1.56	1.07
1:B:350:GLU:HA	1:B:350:GLU:OE1	1.49	1.07
1:A:40:LYS:HG3	6:A:2001:HOH:O	1.58	1.02
1:A:193:SER:H	1:A:268:GLN:HE22	1.06	1.02
1:B:283[A]:ARG:HG2	1:B:283[A]:ARG:HH11	1.23	0.94
1:B:283[A]:ARG:HH11	1:B:283[A]:ARG:CG	1.79	0.92
1:B:40:LYS:O	6:B:2001:HOH:O	1.90	0.89
1:B:276:ILE:O	1:B:276:ILE:HG22	1.70	0.88
1:B:275:SER:HB2	6:B:2250:HOH:O	1.77	0.84
1:A:156:ASN:HD21	1:A:186:ASN:HD21	1.23	0.82
1:B:39:THR:HG22	1:B:40:LYS:N	2.01	0.75
1:B:101:ASN:HD21	1:B:303:ASN:HD22	1.34	0.73
1:B:149:HIS:HE1	6:B:2130:HOH:O	1.72	0.73
1:B:156:ASN:HD21	1:B:186:ASN:HD21	1.36	0.71
1:B:90:PRO:HG3	1:B:324[A]:ILE:HG12	1.72	0.70
1:B:276:ILE:O	1:B:276:ILE:CG2	2.40	0.70
1:B:39:THR:CG2	1:B:40:LYS:N	2.56	0.68
1:B:101:ASN:ND2	1:B:303:ASN:HD22	2.01	0.59
1:B:154:HIS:HD2	6:B:2141:HOH:O	1.86	0.58
1:B:262[B]:LYS:NZ	1:B:279:ASP:HB2	2.20	0.56
1:B:350:GLU:OE1	1:B:350:GLU:CA	2.36	0.54
1:A:276:ILE:HD11	1:A:311[B]:LEU:H	1.73	0.53
1:B:169:HIS:CG	1:B:214[A]:GLU:HG3	2.43	0.52
1:B:45:LEU:HD21	1:B:83:ASP:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ASN:ND2	1:B:81:GLU:N	2.17	0.51
1:B:258:ASN:ND2	6:B:2224:HOH:O	2.30	0.51
1:A:276:ILE:HD11	1:A:311[A]:LEU:H	1.75	0.50
1:B:339:LYS:NZ	6:B:2202:HOH:O	2.44	0.50
1:A:193:SER:H	1:A:268:GLN:NE2	1.90	0.50
1:B:147:GLN:HE21	1:B:157:GLU:HG2	1.77	0.50
1:B:90:PRO:HG3	1:B:324[B]:ILE:HD12	1.93	0.50
1:A:157:GLU:OE1	6:A:2153:HOH:O	2.19	0.49
1:A:138:ALA:HB1	1:A:201:MET:HG2	1.96	0.48
1:A:92:SER:HB3	1:A:319:VAL:HB	1.96	0.48
1:B:262[B]:LYS:HZ1	1:B:279:ASP:HB2	1.80	0.47
1:A:97:ARG:HH11	1:A:97:ARG:CB	2.27	0.47
1:A:275[B]:SER:HB2	1:A:311[B]:LEU:HD12	1.97	0.47
1:B:71:ASP:O	1:B:72:ASP:HB2	2.15	0.46
1:B:138:ALA:HB1	1:B:201:MET:HG2	1.97	0.46
1:B:39:THR:CG2	1:B:40:LYS:H	2.28	0.46
1:A:72:ASP:HB3	1:A:328:TYR:HE2	1.81	0.46
1:B:39:THR:HG21	1:B:45:LEU:HD13	1.97	0.45
1:B:283[B]:ARG:HG2	1:B:285[B]:ASN:OD1	2.17	0.45
1:A:179:GLU:OE2	1:A:189:ARG:HD2	2.17	0.45
1:A:89:THR:OG1	1:A:102:THR:HG22	2.17	0.45
1:A:147:GLN:HE21	1:A:157:GLU:HG2	1.82	0.45
1:B:149:HIS:HD2	1:B:157:GLU:OE2	2.00	0.44
1:A:100:SER:HB3	1:A:305:LYS:HD2	2.01	0.43
1:B:154:HIS:CD2	1:B:186:ASN:HB2	2.54	0.43
1:A:71:ASP:O	1:A:72:ASP:HB2	2.19	0.42
1:A:144:VAL:HB	1:A:299:TYR:HB3	2.01	0.42
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.94	0.42
1:A:52:TRP:CE2	1:A:343:LEU:HD11	2.54	0.42
1:B:144:VAL:HB	1:B:299:TYR:HB3	2.01	0.42
1:B:49:MET:HG3	1:B:65:LEU:HB2	2.01	0.42
1:A:308:GLU:H	1:A:308:GLU:CD	2.28	0.41
1:B:39:THR:O	1:B:40:LYS:CB	2.65	0.41
1:B:272:LEU:HD12	6:B:2168:HOH:O	2.20	0.41
1:B:283[A]:ARG:H	1:B:283[A]:ARG:HG3	1.40	0.41
1:A:114:PRO:HG3	1:A:292:GLN:NE2	2.36	0.41
1:A:275[B]:SER:HB2	1:A:311[B]:LEU:CD1	2.51	0.41
1:B:41:TYR:O	1:B:42:PRO:C	2.62	0.41
1:A:147:GLN:NE2	1:A:157:GLU:HG2	2.36	0.40
1:A:119:LYS:HA	1:A:229:ILE:O	2.21	0.40
1:A:144:VAL:HA	1:A:161:ILE:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:GLY:O	1:B:218:GLY:HA3	2.21	0.40
1:B:72:ASP:HB3	1:B:328:TYR:HE2	1.87	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	316/314 (101%)	309 (98%)	7 (2%)	0	100	100
1	B	320/314 (102%)	312 (98%)	7 (2%)	1 (0%)	36	21
All	All	636/628 (101%)	621 (98%)	14 (2%)	1 (0%)	43	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	80	ASN

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	272/267 (102%)	266 (98%)	6 (2%)	45	26
1	B	276/267 (103%)	263 (95%)	13 (5%)	23	6
All	All	548/534 (103%)	529 (96%)	19 (4%)	34	12

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	MET
1	A	97	ARG
1	A	147	GLN
1	A	261	LYS
1	A	276	ILE
1	A	283	ARG
1	B	40	LYS
1	B	42	PRO
1	B	45	LEU
1	B	80	ASN
1	B	81	GLU
1	B	82	THR
1	B	216	GLU
1	B	262[A]	LYS
1	B	262[B]	LYS
1	B	275	SER
1	B	283[A]	ARG
1	B	283[B]	ARG
1	B	350	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	147	GLN
1	A	181	ASN
1	A	186	ASN
1	A	258	ASN
1	A	268	GLN
1	A	292	GLN
1	A	301	GLN
1	B	80	ASN
1	B	101	ASN
1	B	147	GLN
1	B	149	HIS
1	B	154	HIS
1	B	186	ASN
1	B	258	ASN
1	B	301	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	TAR	B	400	-	9,9,9	1.14	1 (11%)	12,12,12	4.10	7 (58%)
2	SRT	A	400	-	9,9,9	2.10	4 (44%)	12,12,12	4.80	11 (91%)
5	TLA	B	401	-	9,9,9	2.47	4 (44%)	12,12,12	3.41	9 (75%)

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	TAR	B	400	-	-	10/12/12/12	-
2	SRT	A	400	-	1/1/4/4	6/12/12/12	-
5	TLA	B	401	-	-	3/12/12/12	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	401	TLA	C3-C4	-5.47	1.44	1.52
2	A	400	SRT	C3-C4	-4.16	1.46	1.52
5	B	401	TLA	O2-C2	-2.71	1.36	1.42
5	B	401	TLA	O11-C1	-2.71	1.22	1.30
2	A	400	SRT	O3-C3	-2.70	1.36	1.42
5	B	401	TLA	C2-C1	-2.46	1.49	1.52
4	B	400	TAR	O41-C4	-2.36	1.23	1.30
2	A	400	SRT	O41-C4	-2.26	1.23	1.30
2	A	400	SRT	C2-C1	-2.24	1.49	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	SRT	O3-C3-C2	-9.80	90.22	110.17
4	B	400	TAR	C2-C3-C4	8.09	127.76	109.82
2	A	400	SRT	O11-C1-C2	-6.75	103.63	121.62
2	A	400	SRT	O2-C2-C3	6.49	123.38	110.17
4	B	400	TAR	C3-C2-C1	6.06	123.25	109.82
4	B	400	TAR	O11-C1-C2	5.93	129.79	113.31
5	B	401	TLA	C3-C2-C1	5.71	122.47	109.82
4	B	400	TAR	O1-C1-C2	-5.11	108.01	121.62
5	B	401	TLA	C2-C3-C4	4.67	120.18	109.82
2	A	400	SRT	C2-C3-C4	4.27	119.28	109.82
5	B	401	TLA	O11-C1-C2	4.24	125.08	113.31
2	A	400	SRT	O1-C1-O11	4.15	133.49	124.08
5	B	401	TLA	O41-C4-C3	4.09	124.69	113.31
5	B	401	TLA	O4-C4-C3	-3.86	111.33	121.62
2	A	400	SRT	O2-C2-C1	3.65	118.50	110.69
4	B	400	TAR	O4-C4-C3	3.60	131.19	121.62
4	B	400	TAR	O41-C4-C3	-3.57	103.40	113.31
5	B	401	TLA	O2-C2-C1	3.52	118.22	110.69
2	A	400	SRT	C3-C2-C1	3.51	117.61	109.82
2	A	400	SRT	O1-C1-C2	3.35	122.63	113.31
5	B	401	TLA	O3-C3-C4	3.19	117.52	110.69
4	B	400	TAR	O2-C2-C1	2.74	116.54	110.69
2	A	400	SRT	O41-C4-O4	-2.69	117.97	124.08
2	A	400	SRT	O3-C3-C4	2.68	116.41	110.69
5	B	401	TLA	O11-C1-O1	-2.51	118.39	124.08
5	B	401	TLA	O1-C1-C2	-2.33	115.42	121.62
2	A	400	SRT	O41-C4-C3	2.32	119.77	113.31

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	400	SRT	C2

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	400	TAR	C1-C2-C3-C4
4	B	400	TAR	O3-C3-C4-O4
4	B	400	TAR	O3-C3-C4-O41
2	A	400	SRT	O11-C1-C2-O2
4	B	400	TAR	O1-C1-C2-O2
4	B	400	TAR	O11-C1-C2-O2
2	A	400	SRT	O2-C2-C3-O3
2	A	400	SRT	O2-C2-C3-C4
2	A	400	SRT	O1-C1-C2-O2
4	B	400	TAR	C1-C2-C3-O3
4	B	400	TAR	C2-C3-C4-O4
2	A	400	SRT	C1-C2-C3-O3
4	B	400	TAR	C2-C3-C4-O41
4	B	400	TAR	O2-C2-C3-O3
5	B	401	TLA	O2-C2-C3-O3
2	A	400	SRT	C1-C2-C3-C4
4	B	400	TAR	O2-C2-C3-C4
5	B	401	TLA	O3-C3-C4-O41
5	B	401	TLA	O3-C3-C4-O4

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, 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	312/314 (99%)	-0.12	11 (3%) 47 53	16, 26, 46, 74	15 (4%)
1	B	312/314 (99%)	-0.34	11 (3%) 47 53	15, 24, 45, 85	16 (5%)
All	All	624/628 (99%)	-0.23	22 (3%) 47 53	15, 25, 46, 85	31 (4%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	GLU	12.0
1	A	39	THR	11.7
1	B	81	GLU	10.2
1	A	81	GLU	9.0
1	B	275	SER	4.7
1	A	97	ARG	4.3
1	B	276	ILE	4.3
1	B	98	THR	3.6
1	B	80	ASN	3.5
1	A	276	ILE	2.8
1	B	217	ASP	2.6
1	B	39	THR	2.5
1	A	80	ASN	2.4
1	B	277	GLY	2.3
1	B	272	LEU	2.3
1	A	98	THR	2.2
1	B	97	ARG	2.2
1	A	78	HIS	2.2
1	A	277	GLY	2.1
1	B	216	GLU	2.1
1	A	322	GLY	2.0
1	A	275[A]	SER	2.0

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	TAR	B	400	10/10	0.85	0.12	36,58,68,77	0
2	SRT	A	400	10/10	0.91	0.11	24,26,31,32	10
5	TLA	B	401	10/10	0.95	0.09	19,21,25,28	10
3	NA	B	399	1/1	0.98	0.05	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.