



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:51 pm GMT

PDB ID : 4BE3  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

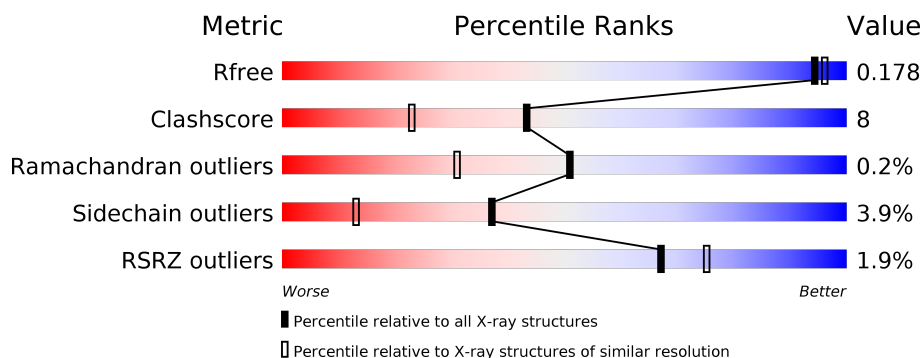
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (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 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	314	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>
1	B	314	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• • •</div> </div> </div>

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	-	-	-
3	NA	B	399	-	-	-	X
4	TAR	B	400	-	-	-	X

## 2 Entry composition [i](#)

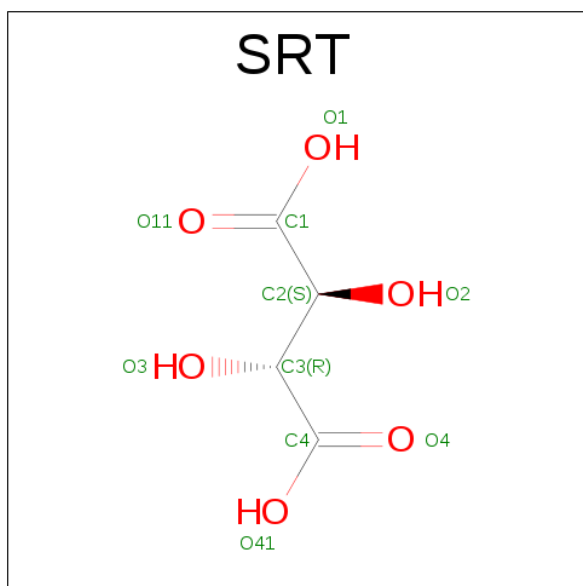
There are 6 unique types of molecules in this entry. The entry contains 5646 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: SRT) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).

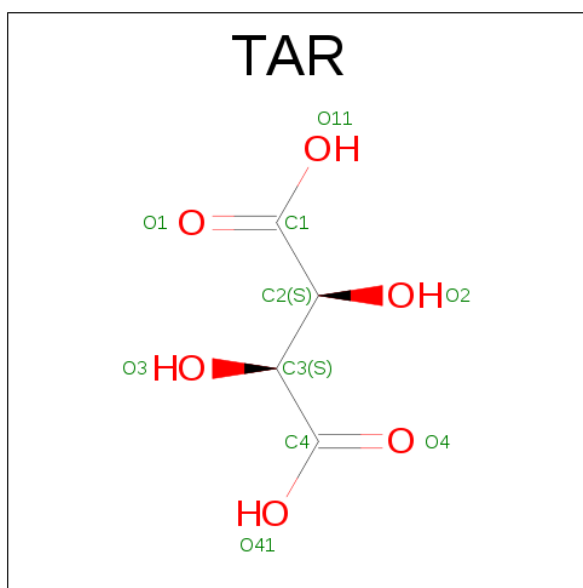


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		

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

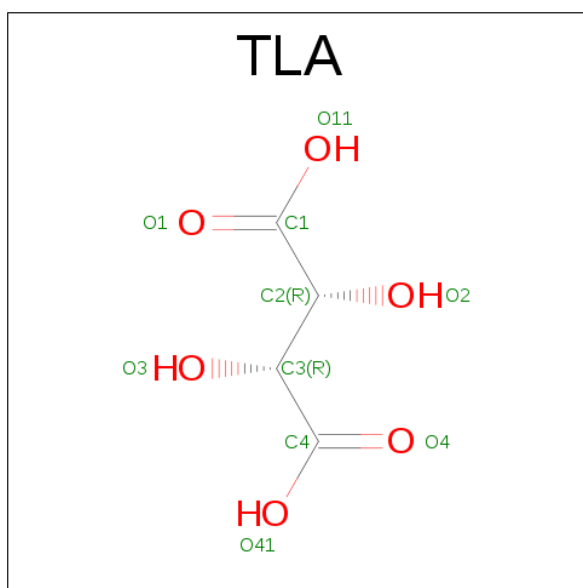
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is D(-)-TARTARIC ACID (three-letter code: 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 (three-letter code: TLA) (formula:  $C_4H_6O_6$ ).



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

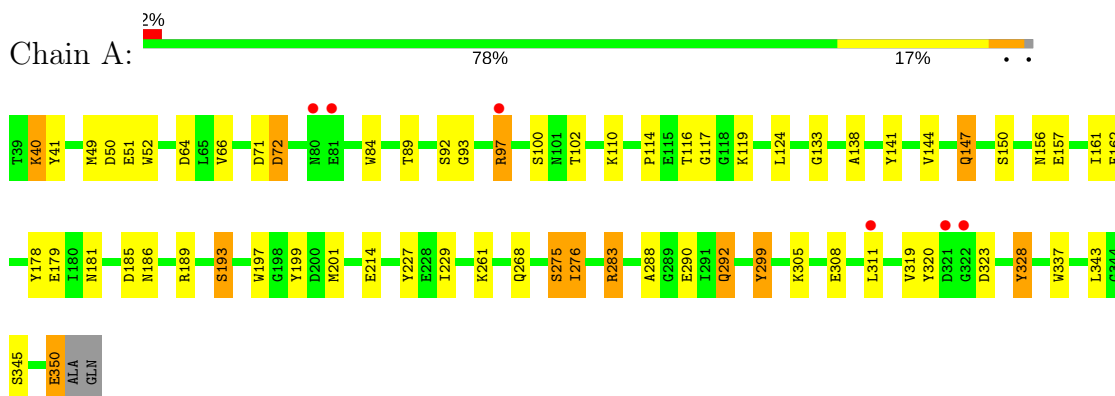
- Molecule 6 is water.

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

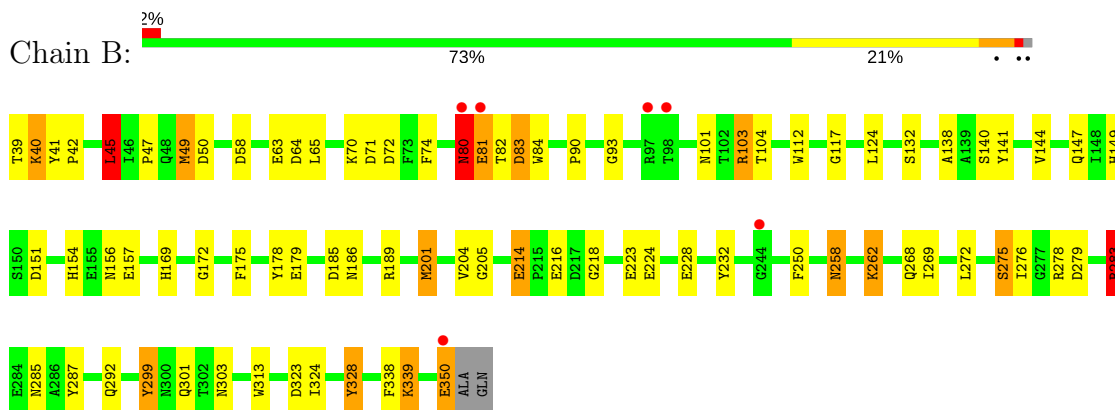
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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: 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.9	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 40.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<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, TLA, SRT, TAR

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	1.67	24/2589 (0.9%)	1.49	24/3512 (0.7%)
1	B	1.66	30/2627 (1.1%)	1.52	37/3562 (1.0%)
All	All	1.66	54/5216 (1.0%)	1.51	61/7074 (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 (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	SER	CB-OG	-9.47	1.29	1.42
1	B	41	TYR	CE2-CZ	-7.38	1.28	1.38
1	B	275	SER	CB-OG	7.37	1.51	1.42
1	A	51	GLU	CD-OE1	7.34	1.33	1.25
1	B	140	SER	CA-CB	6.88	1.63	1.52
1	B	214[A]	GLU	CD-OE1	-6.78	1.18	1.25
1	B	214[B]	GLU	CD-OE1	-6.78	1.18	1.25
1	B	275	SER	CA-CB	6.70	1.62	1.52
1	A	292	GLN	CD-OE1	6.49	1.38	1.24
1	B	287	TYR	CE1-CZ	6.41	1.46	1.38
1	A	66	VAL	C-O	6.35	1.35	1.23
1	A	320	TYR	CE2-CZ	6.33	1.46	1.38
1	B	223	GLU	CD-OE2	6.28	1.32	1.25
1	A	84	TRP	CD2-CE2	6.23	1.48	1.41
1	B	228	GLU	CD-OE1	-6.18	1.18	1.25
1	B	313	TRP	CD2-CE2	6.08	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	TYR	CD1-CE1	6.02	1.48	1.39
1	B	278	ARG	N-CA	5.98	1.58	1.46
1	B	112	TRP	CD2-CE2	5.98	1.48	1.41
1	B	313	TRP	CZ3-CH2	5.91	1.49	1.40
1	B	179	GLU	CD-OE2	5.91	1.32	1.25
1	A	214	GLU	CD-OE1	-5.88	1.19	1.25
1	B	338	PHE	CE2-CZ	5.84	1.48	1.37
1	B	132	SER	CB-OG	-5.82	1.34	1.42
1	A	93	GLY	N-CA	5.78	1.54	1.46
1	A	308	GLU	CD-OE2	5.75	1.31	1.25
1	B	63	GLU	CD-OE1	5.71	1.31	1.25
1	A	292	GLN	CA-CB	-5.65	1.41	1.53
1	B	301	GLN	CD-OE1	5.63	1.36	1.24
1	A	227	TYR	CG-CD1	5.61	1.46	1.39
1	A	150	SER	CB-OG	5.60	1.49	1.42
1	B	205	GLY	N-CA	5.58	1.54	1.46
1	B	74	PHE	CG-CD2	5.56	1.47	1.38
1	B	175	PHE	CG-CD1	5.47	1.47	1.38
1	A	193	SER	CA-CB	5.45	1.61	1.52
1	B	141	TYR	CE1-CZ	5.45	1.45	1.38
1	A	197	TRP	CD2-CE2	5.40	1.47	1.41
1	A	337	TRP	CG-CD1	5.39	1.44	1.36
1	A	199	TYR	CD1-CE1	5.38	1.47	1.39
1	B	117	GLY	C-O	5.37	1.32	1.23
1	B	287	TYR	CG-CD2	5.37	1.46	1.39
1	A	227	TYR	CE2-CZ	5.35	1.45	1.38
1	A	178	TYR	CE2-CZ	5.33	1.45	1.38
1	B	41	TYR	CG-CD2	5.25	1.46	1.39
1	A	117	GLY	N-CA	5.24	1.53	1.46
1	A	227	TYR	CD2-CE2	5.18	1.47	1.39
1	B	93	GLY	N-CA	5.16	1.53	1.46
1	A	328	TYR	CD1-CE1	5.15	1.47	1.39
1	B	84	TRP	CD2-CE2	5.13	1.47	1.41
1	A	290	GLU	CD-OE1	5.12	1.31	1.25
1	B	268	GLN	CA-CB	5.10	1.65	1.53
1	B	132	SER	CA-CB	5.05	1.60	1.52
1	A	288	ALA	N-CA	5.02	1.56	1.46
1	A	320	TYR	N-CA	5.01	1.56	1.46

All (61) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	ARG	NE-CZ-NH1	18.22	129.41	120.30
1	A	50	ASP	CB-CG-OD1	11.04	128.23	118.30
1	A	283	ARG	NE-CZ-NH2	-10.79	114.90	120.30
1	B	50	ASP	CB-CG-OD1	10.67	127.91	118.30
1	B	189	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	B	45	LEU	CB-CG-CD1	8.72	125.83	111.00
1	B	50	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	A	141	TYR	CB-CG-CD2	-7.82	116.31	121.00
1	B	323	ASP	CB-CG-OD1	7.65	125.18	118.30
1	B	49	MET	CG-SD-CE	-7.53	88.14	100.20
1	B	83	ASP	CB-CG-OD1	7.20	124.78	118.30
1	B	185	ASP	CB-CG-OD1	7.02	124.62	118.30
1	B	338	PHE	CB-CG-CD1	-7.01	115.89	120.80
1	B	269	ILE	CG1-CB-CG2	-6.87	96.29	111.40
1	A	283	ARG	CB-CG-CD	-6.75	94.06	111.60
1	A	323	ASP	CB-CG-OD1	6.74	124.36	118.30
1	B	299	TYR	CB-CG-CD2	-6.67	117.00	121.00
1	A	345	SER	CB-CA-C	6.53	122.51	110.10
1	B	250	PHE	CG-CD2-CE2	-6.27	113.91	120.80
1	A	64[A]	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	64[B]	ASP	CB-CG-OD1	6.15	123.83	118.30
1	B	224	GLU	OE1-CD-OE2	6.11	130.64	123.30
1	B	178	TYR	CB-CG-CD1	-6.10	117.34	121.00
1	A	72	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	B	339	LYS	CD-CE-NZ	-5.95	98.02	111.70
1	B	83	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	B	151	ASP	CB-CG-OD1	5.91	123.62	118.30
1	B	275	SER	N-CA-CB	-5.91	101.64	110.50
1	B	151	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	283	ARG	CD-NE-CZ	5.84	131.78	123.60
1	A	40	LYS	CD-CE-NZ	-5.77	98.43	111.70
1	B	189	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	201	MET	CG-SD-CE	-5.75	91.00	100.20
1	B	232	TYR	CB-CG-CD1	-5.75	117.55	121.00
1	B	141	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	A	110	LYS	CD-CE-NZ	-5.74	98.51	111.70
1	A	292	GLN	CB-CG-CD	-5.70	96.78	111.60
1	B	283[A]	ARG	CG-CD-NE	-5.68	99.87	111.80
1	B	283[B]	ARG	CG-CD-NE	-5.68	99.87	111.80
1	A	299	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	A	345	SER	CA-CB-OG	-5.57	96.17	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	ARG	NE-CZ-NH2	5.54	123.07	120.30
1	A	162	PHE	CB-CG-CD2	-5.52	116.93	120.80
1	A	185	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	64[A]	ASP	CB-CG-OD1	5.49	123.25	118.30
1	B	64[B]	ASP	CB-CG-OD1	5.49	123.25	118.30
1	A	116	THR	CA-CB-CG2	-5.44	104.78	112.40
1	B	58	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	104	THR	N-CA-C	-5.37	96.49	111.00
1	B	70	LYS	CD-CE-NZ	-5.34	99.42	111.70
1	B	287	TYR	CD1-CE1-CZ	-5.30	115.03	119.80
1	B	103	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	275[A]	SER	N-CA-CB	5.23	118.34	110.50
1	A	275[B]	SER	N-CA-CB	5.23	118.34	110.50
1	A	41	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	B	58	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	258	ASN	CB-CA-C	-5.20	100.01	110.40
1	A	133	GLY	N-CA-C	-5.19	100.13	113.10
1	A	141	TYR	CG-CD1-CE1	-5.16	117.17	121.30
1	B	204	VAL	CA-CB-CG2	5.13	118.60	110.90
1	B	292	GLN	CA-CB-CG	5.05	124.52	113.40

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	32	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	286	0	0	2	0
6	B	293	0	0	7	0
All	All	5646	0	4811	76	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 8.

All (76) 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:OE1	1:B:350:GLU:HA	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:A:97:ARG:HH11	1:A:97:ARG:HG2	1.27	0.98
1:B:283[A]:ARG:HH11	1:B:283[A]:ARG:HG2	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:HG22	1:B:276:ILE:O	1.70	0.88
1:A:97:ARG:CG	1:A:97:ARG:HH11	1.88	0.86
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:A:350:GLU:N	1:A:350:GLU:OE1	2.18	0.76
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:CG2	1:B:276:ILE:O	2.40	0.70
1:B:39:THR:CG2	1:B:40:LYS:N	2.56	0.68
1:A:350:GLU:CD	1:A:350:GLU:H	1.98	0.67
1:A:97:ARG:NH1	1:A:97:ARG:HG2	2.05	0.62
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:CA	1:B:350:GLU:OE1	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:258:ASN:ND2	6:B:2224:HOH:O	2.30	0.51
1:B:80:ASN:ND2	1:B:81:GLU:N	2.17	0.51
1:A:97:ARG:CG	1:A:97:ARG:NH1	2.60	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:A:97:ARG:CB	1:A:97:ARG:HH11	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:B:262[B]:LYS:HZ1	1:B:279:ASP:HB2	1.83	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:39:THR:O	1:B:40:LYS:CB	2.65	0.42
1:B:49:MET:HG3	1:B:65:LEU:HB2	2.01	0.42
1:B:272:LEU:HD12	6:B:2168:HOH:O	2.20	0.41
1:B:283[A]:ARG:HG3	1:B:283[A]:ARG:H	1.40	0.41
1:A:114:PRO:HG3	1:A:292:GLN:NE2	2.36	0.41
1:B:276:ILE:HG21	1:B:276:ILE:HD13	1.87	0.41
1:A:275[B]:SER:HB2	1:A:311[B]:LEU:CD1	2.51	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%)	44	24
All	All	636/628 (101%)	621 (98%)	14 (2%)	1 (0%)	51	31

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%)	263 (97%)	9 (3%)	43	18
1	B	276/267 (103%)	262 (95%)	14 (5%)	28	7
All	All	548/534 (103%)	525 (96%)	23 (4%)	37	11

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	MET
1	A	97	ARG
1	A	124	LEU
1	A	147	GLN
1	A	181	ASN
1	A	261	LYS
1	A	276	ILE
1	A	283	ARG
1	A	350	GLU
1	B	40	LYS
1	B	42	PRO
1	B	45	LEU
1	B	47	PRO
1	B	80	ASN
1	B	81	GLU
1	B	82	THR
1	B	124	LEU
1	B	216	GLU
1	B	262[A]	LYS
1	B	262[B]	LYS
1	B	283[A]	ARG
1	B	283[B]	ARG
1	B	350	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
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	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

### 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 carbohydrates 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	$\# Z  > 2$
2	SRT	A	400	-	3,9,9	1.85	1 (33%)	6,12,12	3.83	6 (100%)
4	TAR	B	400	-	3,9,9	0.79	0	6,12,12	3.61	3 (50%)
5	TLA	B	401	-	3,9,9	1.80	1 (33%)	6,12,12	2.77	4 (66%)

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
2	SRT	A	400	-	1/1/4/4	0/4/12/12	0/0/0/0
4	TAR	B	400	-	-	0/4/12/12	0/0/0/0
5	TLA	B	401	-	-	0/4/12/12	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	401	TLA	O2-C2	-2.94	1.36	1.42
2	A	400	SRT	O3-C3	-2.93	1.36	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	SRT	O3-C3-C2	-6.20	90.22	108.88
2	A	400	SRT	C1-C2-C3	2.09	117.61	113.11
2	A	400	SRT	O3-C3-C4	2.17	116.41	111.13
4	B	400	TAR	O2-C2-C1	2.22	116.54	111.13
5	B	401	TLA	O3-C3-C4	2.63	117.52	111.13
2	A	400	SRT	C4-C3-C2	2.87	119.28	113.11
5	B	401	TLA	O2-C2-C1	2.92	118.22	111.13
2	A	400	SRT	O2-C2-C1	3.03	118.50	111.13
5	B	401	TLA	C4-C3-C2	3.29	120.18	113.11
5	B	401	TLA	C1-C2-C3	4.35	122.47	113.11
4	B	400	TAR	C1-C2-C3	4.72	123.25	113.11
2	A	400	SRT	O2-C2-C3	4.81	123.38	108.88
4	B	400	TAR	C4-C3-C2	6.81	127.76	113.11

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	400	SRT	C2

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	312/314 (99%)	-0.20	6 (1%) 67 75	16, 27, 47, 74	9 (2%)
1	B	312/314 (99%)	-0.32	6 (1%) 67 75	15, 25, 46, 85	6 (1%)
All	All	624/628 (99%)	-0.26	12 (1%) 67 75	15, 26, 46, 85	15 (2%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	97	ARG	4.6
1	A	97	ARG	3.7
1	B	80	ASN	3.7
1	B	350	GLU	3.3
1	A	80	ASN	3.2
1	B	98	THR	3.0
1	A	81	GLU	2.6
1	B	81	GLU	2.6
1	A	322	GLY	2.2
1	A	311[A]	LEU	2.2
1	A	321	ASP	2.1
1	B	244	GLY	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	TAR	B	400	10/10	0.88	0.25	12.99	36,58,68,77	0
3	NA	B	399	1/1	0.98	0.13	8.06	20,20,20,20	0
2	SRT	A	400	10/10	0.95	0.10	0.55	24,26,31,32	10
5	TLA	B	401	10/10	0.96	0.09	0.06	19,21,25,28	10

## 6.5 Other polymers [i](#)

There are no such residues in this entry.