Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 06:29 PM JST

PDB ID	:	8IC6
Title	:	exo-beta-D-arabinanase ExoMA2 from Microbacterium arabinogalactanolyticum in complex with Tris
Authors	:	Fukushima, R.; Kashima, T.; Ishiwata, A.; Fujita, K.; Fushinobu, S.
Deposited on	:	2023-02-10
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:

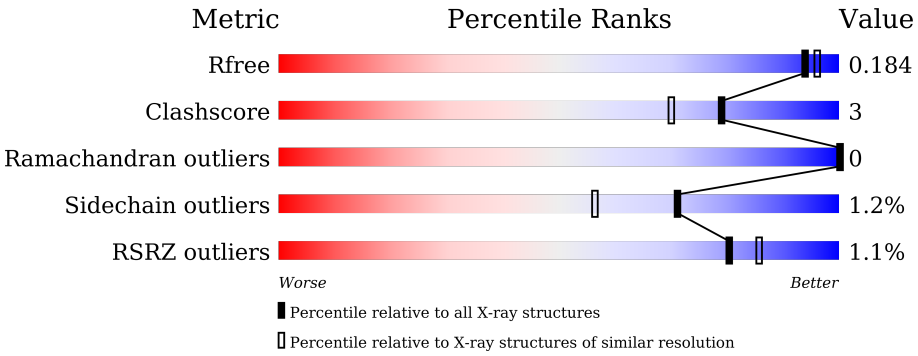
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

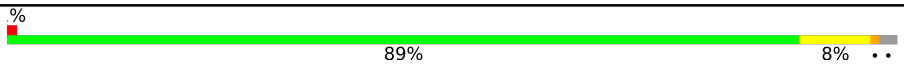
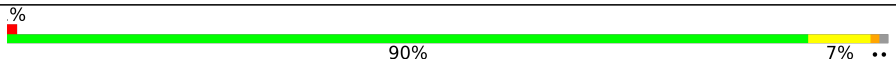
The reported resolution of this entry is 1.75 Å.

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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (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 <=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	867	
1	B	867	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15006 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.

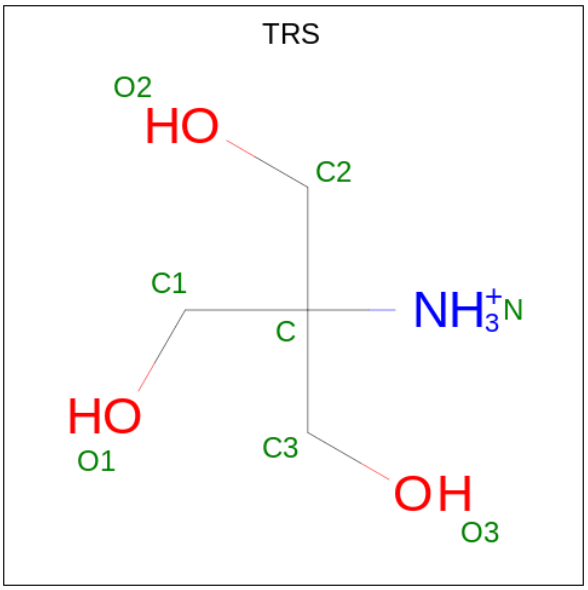
- Molecule 1 is a protein called exo-beta-D-arabinanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	855	Total	C	N	O	S	0	3	0
			6642	4179	1204	1248	11			
1	A	853	Total	C	N	O	S	0	3	0
			6632	4171	1205	1245	11			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

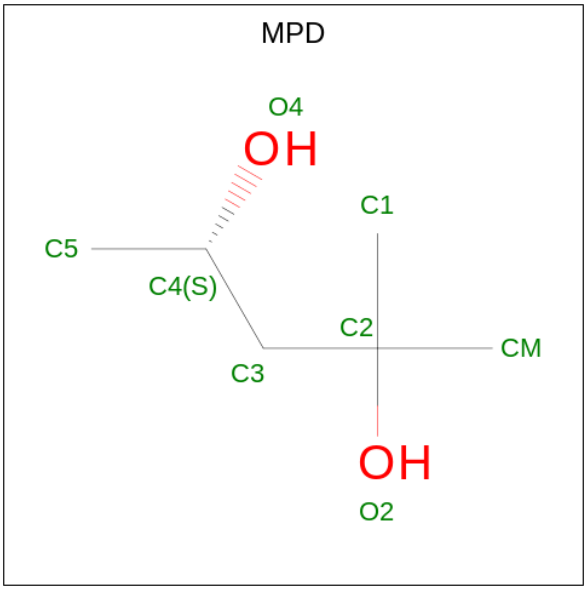
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	8	Total	Mg	0	0
			8	8		
2	A	7	Total	Mg	0	0
			7	7		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



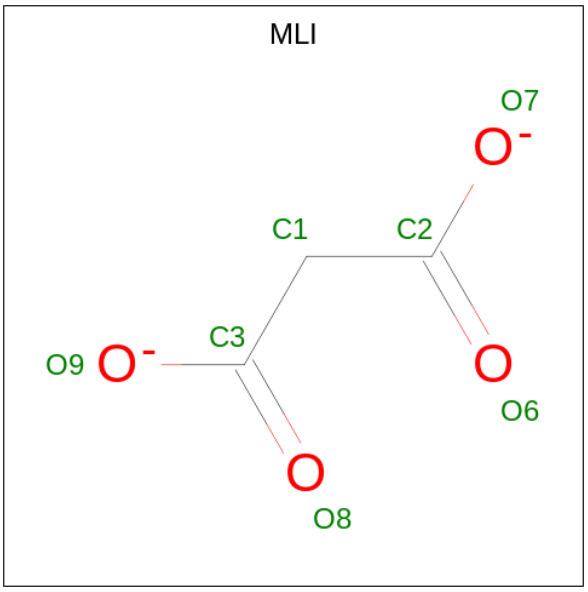
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 8 4 1 3	0	0
3	A	1	Total C N O 8 4 1 3	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 7 3 4	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is water.

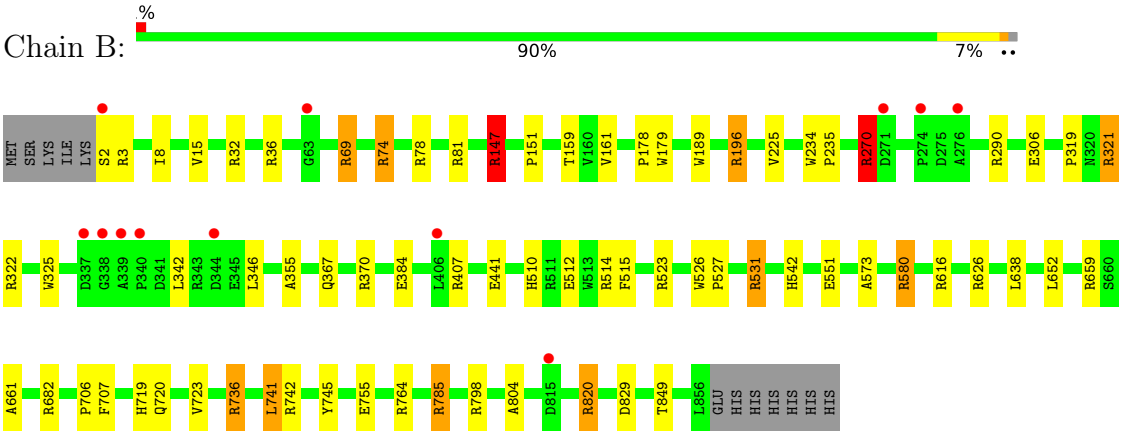
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	814	Total O 814 814	0	0
7	A	847	Total O 847 847	0	0

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.

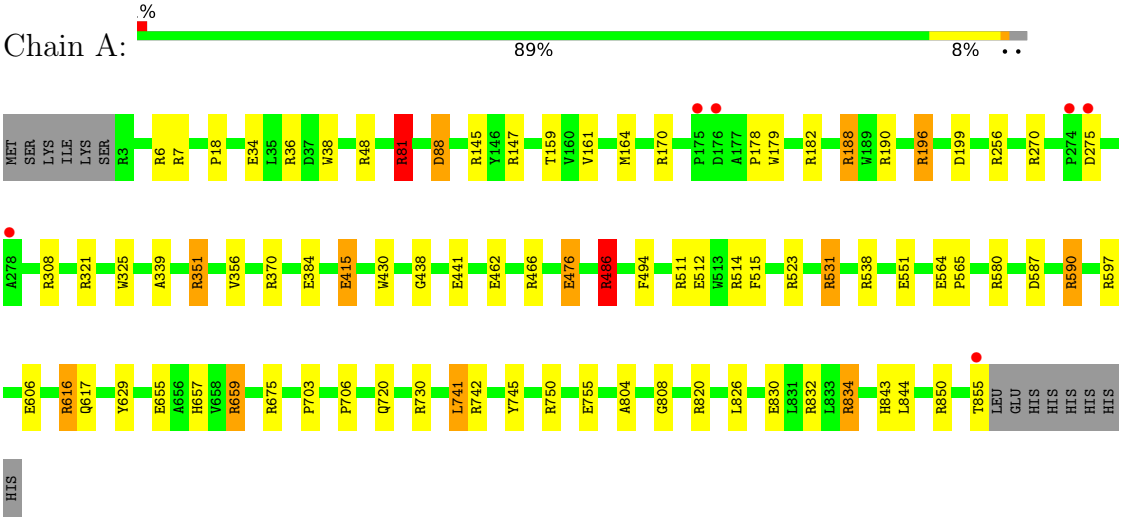
• Molecule 1: exo-beta-D-arabinanase

Chain B:



• Molecule 1: exo-beta-D-arabinanase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.55Å 97.51Å 139.98Å 90.00° 100.55° 90.00°	Depositor
Resolution (Å)	48.80 – 1.75 48.76 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.80-1.75) 100.0 (48.76-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.138 , 0.174 0.151 , 0.184	Depositor DCC
R_{free} test set	8854 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15006	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: CL, MPD, MG, TRS, MLI

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	0.79	8/6823 (0.1%)	1.11	37/9301 (0.4%)
1	B	0.75	5/6833 (0.1%)	1.08	24/9316 (0.3%)
All	All	0.77	13/13656 (0.1%)	1.10	61/18617 (0.3%)

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	13
1	B	0	13
All	All	0	26

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	415	GLU	CD-OE1	13.85	1.40	1.25
1	B	551	GLU	CD-OE1	-7.83	1.17	1.25
1	A	384	GLU	CD-OE1	7.53	1.33	1.25
1	B	551	GLU	CD-OE2	-7.03	1.18	1.25
1	A	34	GLU	CD-OE2	7.03	1.33	1.25
1	B	384	GLU	CD-OE1	6.79	1.33	1.25
1	B	384	GLU	CD-OE2	5.81	1.32	1.25
1	A	551	GLU	CD-OE2	-5.80	1.19	1.25
1	A	88	ASP	CG-OD1	5.79	1.38	1.25
1	A	476	GLU	CD-OE1	5.76	1.31	1.25
1	B	306	GLU	CD-OE1	5.65	1.31	1.25
1	A	462	GLU	CD-OE1	5.33	1.31	1.25
1	A	88	ASP	CG-OD2	5.21	1.37	1.25

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	188	ARG	NE-CZ-NH2	-19.67	110.47	120.30
1	B	32	ARG	NE-CZ-NH1	15.53	128.06	120.30
1	B	32	ARG	NE-CZ-NH2	-13.75	113.42	120.30
1	B	74	ARG	NE-CZ-NH2	-11.41	114.60	120.30
1	A	188	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	A	370	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	A	675	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	A	182	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	B	531	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	A	182	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	659	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	A	597	ARG	NE-CZ-NH1	-8.54	116.03	120.30
1	A	580	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	B	407	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	A	850	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	A	370	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	A	270	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	A	48	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	B	742	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	351[A]	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	351[B]	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	B	78	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	A	6	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	514	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	B	290	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	B	270	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	B	514	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	675	ARG	CB-CG-CD	-6.56	94.53	111.60
1	A	7	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	580	ARG	NE-CZ-NH2	6.51	123.56	120.30
1	A	750	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	531	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	170	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	190	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	A	486	ARG	CG-CD-NE	6.24	124.91	111.80
1	B	69[A]	ARG	CG-CD-NE	6.22	124.86	111.80
1	B	69[B]	ARG	CG-CD-NE	6.22	124.86	111.80
1	B	682	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	590	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	270	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	A	308	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	145	ARG	NE-CZ-NH1	5.76	123.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	199	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	511	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	290	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	7	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	147	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	145	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	764	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	321	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	B	580	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	A	81[A]	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	81[B]	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	69[A]	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	69[B]	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	742	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	626	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	538	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	256	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	A	855	THR	CA-CB-OG1	-5.07	98.36	109.00
1	B	407	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	ARG	Sidechain
1	A	196	ARG	Sidechain
1	A	351[A]	ARG	Sidechain
1	A	351[B]	ARG	Sidechain
1	A	36	ARG	Sidechain
1	A	466	ARG	Sidechain
1	A	486	ARG	Sidechain
1	A	523	ARG	Sidechain
1	A	616	ARG	Sidechain
1	A	81[A]	ARG	Sidechain
1	A	81[B]	ARG	Sidechain
1	A	834[A]	ARG	Sidechain
1	A	834[B]	ARG	Sidechain
1	B	147	ARG	Sidechain
1	B	196	ARG	Sidechain
1	B	270	ARG	Sidechain
1	B	36	ARG	Sidechain
1	B	531	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	659	ARG	Sidechain
1	B	69[A]	ARG	Sidechain
1	B	69[B]	ARG	Sidechain
1	B	736	ARG	Sidechain
1	B	74	ARG	Sidechain
1	B	785	ARG	Sidechain
1	B	81	ARG	Sidechain
1	B	820	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	6632	0	6308	37	0
1	B	6642	0	6320	35	0
2	A	7	0	0	0	0
2	B	8	0	0	0	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
4	A	16	0	28	2	0
4	B	16	0	28	4	0
5	B	7	0	2	0	0
6	A	1	0	0	0	0
7	A	847	0	0	5	0
7	B	814	0	0	10	0
All	All	15006	0	12710	73	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 3.

All (73) 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)
4:B:910:MPD:HM2	7:B:1055:HOH:O	1.73	0.89
1:A:830:GLU:OE2	1:A:832:ARG:NH1	2.22	0.71
1:B:322:ARG:HG3	1:B:322:ARG:HH11	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834[A]:ARG:NH1	7:A:1002:HOH:O	2.30	0.64
1:B:736:ARG:HD2	7:B:1012:HOH:O	1.99	0.62
1:B:321:ARG:NH1	4:B:912:MPD:H4	2.17	0.60
1:A:321:ARG:NH1	4:A:910:MPD:H4	2.17	0.59
1:A:655:GLU:HG2	1:A:659:ARG:NH2	2.19	0.57
1:B:745:TYR:CE2	1:B:755:GLU:HA	2.40	0.56
1:B:523:ARG:NH1	7:B:1010:HOH:O	2.37	0.56
1:A:834[A]:ARG:HD2	7:A:1686:HOH:O	2.09	0.53
1:B:542:HIS:HE1	7:B:1171:HOH:O	1.90	0.53
1:B:325:TRP:CD2	1:B:441:GLU:HB2	2.44	0.53
1:B:322:ARG:HH11	1:B:322:ARG:CG	2.19	0.53
1:B:736:ARG:NE	7:B:1012:HOH:O	2.39	0.51
1:B:515:PHE:O	1:B:804:ALA:HB2	2.10	0.51
1:B:322:ARG:CG	1:B:322:ARG:NH1	2.74	0.51
1:A:515:PHE:O	1:A:804:ALA:HB2	2.11	0.50
1:A:659:ARG:HG2	1:A:730:ARG:NH2	2.27	0.50
1:B:736:ARG:CD	7:B:1012:HOH:O	2.57	0.50
1:A:659:ARG:HD2	1:A:730:ARG:NH1	2.27	0.50
1:A:655:GLU:CG	1:A:659:ARG:NH2	2.75	0.50
1:B:189:TRP:CZ3	1:B:225:VAL:HG11	2.47	0.49
1:B:3:ARG:HA	7:B:1476:HOH:O	2.12	0.49
1:B:319:PRO:HB3	1:B:355:ALA:HB1	1.95	0.49
4:B:910:MPD:CM	7:B:1055:HOH:O	2.45	0.49
1:B:319:PRO:HB3	1:B:355:ALA:CB	2.43	0.48
1:A:88:ASP:OD1	7:A:1001:HOH:O	2.20	0.48
1:B:178:PRO:O	1:B:179:TRP:HB2	2.13	0.48
1:A:159:THR:HG22	1:A:161:VAL:HG23	1.96	0.48
1:A:325:TRP:CD2	1:A:441:GLU:HB2	2.49	0.47
1:A:38:TRP:CH2	1:A:164:MET:HE1	2.49	0.47
1:B:510:HIS:NE2	1:B:580:ARG:NH1	2.63	0.47
1:B:785:ARG:NH2	1:B:829:ASP:OD1	2.40	0.47
1:A:159:THR:HG22	1:A:161:VAL:CG2	2.45	0.46
1:A:826:LEU:O	1:A:843:HIS:HA	2.16	0.46
1:B:270:ARG:HA	1:A:494:PHE:CE2	2.50	0.46
1:B:321:ARG:HH11	4:B:912:MPD:H4	1.79	0.46
1:A:703:PRO:HG2	1:A:706:PRO:HB3	1.98	0.46
1:A:745:TYR:CE2	1:A:755:GLU:HA	2.51	0.45
1:B:849:THR:HG22	7:B:1005:HOH:O	2.16	0.45
1:A:655:GLU:CG	1:A:659:ARG:HH22	2.29	0.45
1:A:164:MET:HE2	1:A:164:MET:HB3	1.55	0.45
1:A:820:ARG:HD3	7:A:1582:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:GLN:NE2	1:B:370:ARG:HH22	2.16	0.44
1:A:476:GLU:H	1:A:476:GLU:CD	2.20	0.44
1:B:159:THR:HG22	1:B:161[A]:VAL:HG23	2.00	0.43
1:A:741:LEU:C	1:A:741:LEU:HD12	2.38	0.43
1:A:339:ALA:HB1	1:A:486:ARG:CZ	2.49	0.43
1:A:81[A]:ARG:NH1	7:A:1008:HOH:O	2.40	0.43
1:B:741:LEU:HD12	1:B:741:LEU:C	2.39	0.43
1:A:476:GLU:O	1:A:531:ARG:HD3	2.19	0.43
1:B:8:ILE:HG21	1:B:15:VAL:HG21	2.01	0.42
1:A:587:ASP:OD2	1:A:590:ARG:HD2	2.19	0.42
1:B:322:ARG:HD3	7:B:1346:HOH:O	2.19	0.42
1:B:798:ARG:CG	1:B:820:ARG:HH22	2.33	0.42
1:A:430:TRP:CE2	1:A:438:GLY:HA3	2.55	0.42
1:B:234:TRP:HB3	1:B:235:PRO:HD2	2.01	0.42
1:B:342:LEU:O	1:B:346:LEU:HG	2.20	0.42
1:A:178:PRO:O	1:A:179:TRP:HB2	2.21	0.41
1:A:325:TRP:HA	4:A:910:MPD:H53	2.01	0.41
1:A:565:PRO:HD2	1:A:629:TYR:OH	2.21	0.41
1:A:655:GLU:CD	1:A:659:ARG:HH22	2.23	0.41
1:A:808:GLY:HA3	1:A:820:ARG:O	2.20	0.41
1:B:719:HIS:O	1:B:723:VAL:HG23	2.21	0.41
1:A:606:GLU:OE1	1:A:657:HIS:ND1	2.46	0.41
1:A:147:ARG:HH11	1:A:147:ARG:HD2	1.71	0.41
1:B:706:PRO:O	1:B:707:PHE:C	2.59	0.41
1:A:356:VAL:CG2	1:A:415:GLU:HG2	2.51	0.41
1:B:526:TRP:HB3	1:B:527:PRO:HD3	2.03	0.41
1:B:573:ALA:HB2	1:B:652:LEU:HD11	2.03	0.40
1:B:638:LEU:HD11	1:B:661:ALA:HB3	2.04	0.40
1:A:564:GLU:HB3	1:A:617:GLN:HG3	2.03	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	854/867 (98%)	835 (98%)	19 (2%)	0	100	100
1	B	856/867 (99%)	832 (97%)	24 (3%)	0	100	100
All	All	1710/1734 (99%)	1667 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	662/673 (98%)	654 (99%)	8 (1%)	71	56
1	B	664/673 (99%)	656 (99%)	8 (1%)	71	56
All	All	1326/1346 (98%)	1310 (99%)	16 (1%)	71	56

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	SER
1	B	147	ARG
1	B	151	PRO
1	B	196	ARG
1	B	512	GLU
1	B	616	ARG
1	B	720	GLN
1	B	741	LEU
1	A	18	PRO
1	A	196	ARG
1	A	275	ASP
1	A	512	GLU
1	A	616	ARG
1	A	720	GLN
1	A	741	LEU
1	A	844	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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 23 ligands modelled in this entry, 16 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
5	MLI	B	911	-	6,6,6	3.21	4 (66%)	7,7,7	1.07	0
4	MPD	B	912	-	7,7,7	0.78	0	9,10,10	1.16	1 (11%)
4	MPD	B	910	-	7,7,7	0.23	0	9,10,10	0.42	0
4	MPD	A	911	-	7,7,7	0.32	0	9,10,10	0.59	0
4	MPD	A	910	-	7,7,7	0.76	0	9,10,10	1.48	2 (22%)
3	TRS	B	909	-	7,7,7	0.38	0	9,9,9	0.66	0
3	TRS	A	909	-	7,7,7	0.27	0	9,9,9	0.48	0

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
5	MLI	B	911	-	-	0/4/4/4	-
4	MPD	B	912	-	-	2/5/5/5	-
4	MPD	B	910	-	-	0/5/5/5	-
4	MPD	A	911	-	-	0/5/5/5	-
4	MPD	A	910	-	-	2/5/5/5	-
3	TRS	B	909	-	-	2/9/9/9	-
3	TRS	A	909	-	-	4/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	911	MLI	O6-C2	5.32	1.39	1.22
5	B	911	MLI	O8-C3	4.25	1.36	1.22
5	B	911	MLI	C1-C3	3.07	1.55	1.51
5	B	911	MLI	C1-C2	2.32	1.54	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	910	MPD	O2-C2-CM	-3.08	98.21	108.08
4	A	910	MPD	O4-C4-C3	2.39	121.01	111.36
4	B	912	MPD	O4-C4-C3	2.20	120.26	111.36

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	909	TRS	N-C-C1-O1
3	A	909	TRS	N-C-C3-O3
4	B	912	MPD	C2-C3-C4-O4
4	B	912	MPD	O2-C2-C3-C4
3	A	909	TRS	N-C-C2-O2
4	A	910	MPD	C2-C3-C4-O4
3	B	909	TRS	C3-C-C1-O1
3	A	909	TRS	C1-C-C2-O2
3	A	909	TRS	C3-C-C2-O2
4	A	910	MPD	O2-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	912	MPD	2	0
4	B	910	MPD	2	0
4	A	910	MPD	2	0

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	853/867 (98%)	-0.51	6 (0%)	87	92	14, 19, 35, 70	0
1	B	855/867 (98%)	-0.38	12 (1%)	75	82	14, 20, 37, 79	0
All	All	1708/1734 (98%)	-0.44	18 (1%)	80	86	14, 19, 36, 79	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	339	ALA	5.3
1	B	340	PRO	3.3
1	A	176	ASP	3.3
1	B	344	ASP	3.1
1	A	275	ASP	2.7
1	B	2	SER	2.7
1	A	278	ALA	2.7
1	B	63	GLY	2.6
1	B	274	PRO	2.6
1	B	337	ASP	2.6
1	B	338	GLY	2.4
1	A	274	PRO	2.3
1	B	276	ALA	2.3
1	A	175	PRO	2.2
1	B	406	LEU	2.1
1	B	271	ASP	2.1
1	B	815	ASP	2.1
1	A	855	THR	2.0

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 (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, 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
4	MPD	B	912	8/8	0.87	0.15	26,29,33,35	0
5	MLI	B	911	7/7	0.90	0.15	30,33,36,37	0
4	MPD	A	910	8/8	0.91	0.12	29,31,36,39	0
2	MG	B	908	1/1	0.93	0.20	40,40,40,40	0
4	MPD	B	910	8/8	0.94	0.11	27,34,40,42	0
2	MG	B	906	1/1	0.96	0.08	33,33,33,33	0
4	MPD	A	911	8/8	0.96	0.09	25,31,33,34	0
3	TRS	A	909	8/8	0.96	0.10	16,19,23,24	0
2	MG	B	905	1/1	0.97	0.04	33,33,33,33	0
2	MG	A	904	1/1	0.97	0.05	22,22,22,22	0
2	MG	A	905	1/1	0.97	0.06	31,31,31,31	0
3	TRS	B	909	8/8	0.97	0.09	16,20,22,22	0
2	MG	B	907	1/1	0.97	0.18	38,38,38,38	0
2	MG	A	907	1/1	0.98	0.22	35,35,35,35	0
2	MG	B	902	1/1	0.98	0.05	17,17,17,17	0
2	MG	A	903	1/1	0.99	0.22	32,32,32,32	0
2	MG	B	903	1/1	0.99	0.05	22,22,22,22	0
2	MG	B	904	1/1	0.99	0.03	18,18,18,18	0
2	MG	A	906	1/1	0.99	0.03	20,20,20,20	0
2	MG	B	901	1/1	0.99	0.05	23,23,23,23	0
2	MG	A	901	1/1	0.99	0.04	19,19,19,19	0
2	MG	A	902	1/1	1.00	0.05	20,20,20,20	0
6	CL	A	908	1/1	1.00	0.04	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.