



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:59 PM GMT

PDB ID : 4YZX
Title : C. bescii Family 3 pectate lyase double mutant K108A/D107N in complex with trigalacturonic acid
Authors : Alahuhta, P.M.; Lunin, V.V.
Deposited on : 2015-03-25
Resolution : 1.25 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : rb-20026982

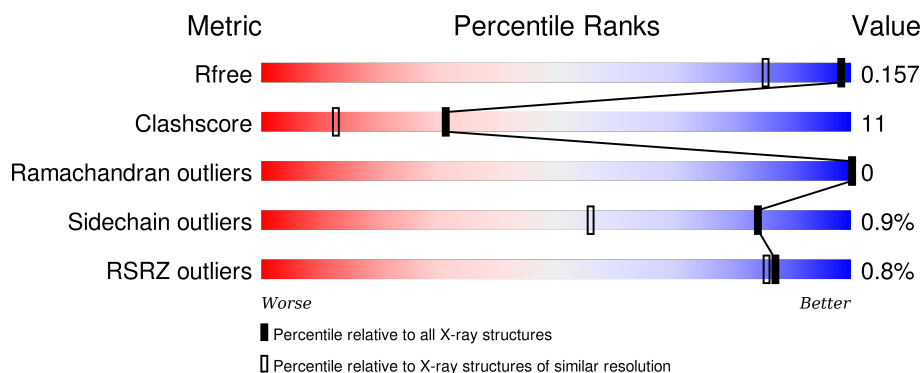
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.25 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}	91344	1442 (1.30-1.22)
Clashscore	102246	1530 (1.30-1.22)
Ramachandran outliers	100387	1467 (1.30-1.22)
Sidechain outliers	100360	1465 (1.30-1.22)
RSRZ outliers	91569	1442 (1.30-1.22)

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 ≥ 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	204	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 82%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 82% 14% </div> </div>
1	B	204	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 84%, yellow 12%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 84% 12% </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	CA	B	204	-	-	-	X
3	IMD	A	205	-	-	-	X
3	IMD	B	206	-	-	X	-
4	MPD	A	206	-	-	-	X
4	MPD	A	207	-	-	-	X
4	MPD	B	201	-	-	-	X
4	MPD	B	207	-	-	-	X
5	MRD	A	209	-	-	X	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4150 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 Pectate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	23	0
			1680	1050	290	333	7			
1	B	195	Total	C	N	O	S	0	22	0
			1656	1039	282	329	6			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP B9MKT4
A	-9	ALA	-	expression tag	UNP B9MKT4
A	-8	HIS	-	expression tag	UNP B9MKT4
A	-7	HIS	-	expression tag	UNP B9MKT4
A	-6	HIS	-	expression tag	UNP B9MKT4
A	-5	HIS	-	expression tag	UNP B9MKT4
A	-4	HIS	-	expression tag	UNP B9MKT4
A	-3	HIS	-	expression tag	UNP B9MKT4
A	-2	VAL	-	expression tag	UNP B9MKT4
A	-1	GLY	-	expression tag	UNP B9MKT4
A	0	THR	-	expression tag	UNP B9MKT4
A	107	ASN	ASP	engineered mutation	UNP B9MKT4
A	108	ALA	LYS	engineered mutation	UNP B9MKT4
B	-10	MET	-	expression tag	UNP B9MKT4
B	-9	ALA	-	expression tag	UNP B9MKT4
B	-8	HIS	-	expression tag	UNP B9MKT4
B	-7	HIS	-	expression tag	UNP B9MKT4
B	-6	HIS	-	expression tag	UNP B9MKT4
B	-5	HIS	-	expression tag	UNP B9MKT4
B	-4	HIS	-	expression tag	UNP B9MKT4
B	-3	HIS	-	expression tag	UNP B9MKT4
B	-2	VAL	-	expression tag	UNP B9MKT4
B	-1	GLY	-	expression tag	UNP B9MKT4
B	0	THR	-	expression tag	UNP B9MKT4
B	107	ASN	ASP	engineered mutation	UNP B9MKT4

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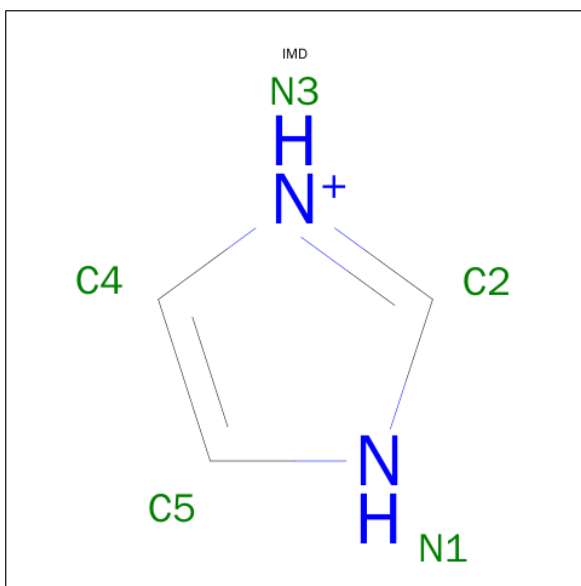
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Chain	Residue	Modelled	Actual	Comment	Reference
B	108	ALA	LYS	engineered mutation	UNP B9MKT4

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	4	Total Ca 4 4	0	0
2	A	4	Total Ca 4 4	0	0

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: C₃H₅N₂).



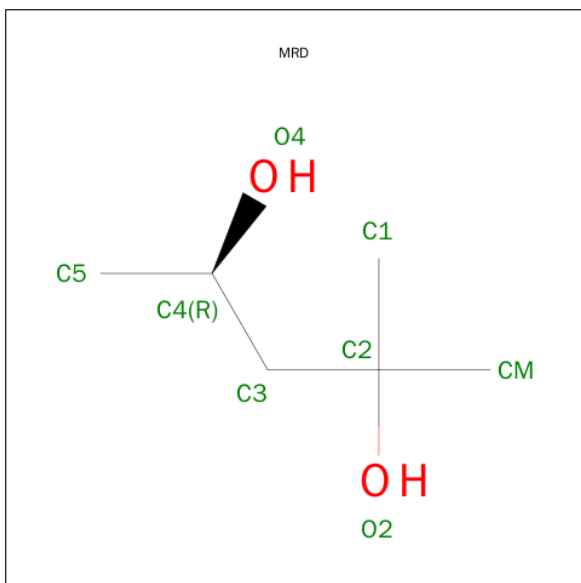
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 5 3 2	0	0
3	B	1	Total C N 5 3 2	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 5 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).

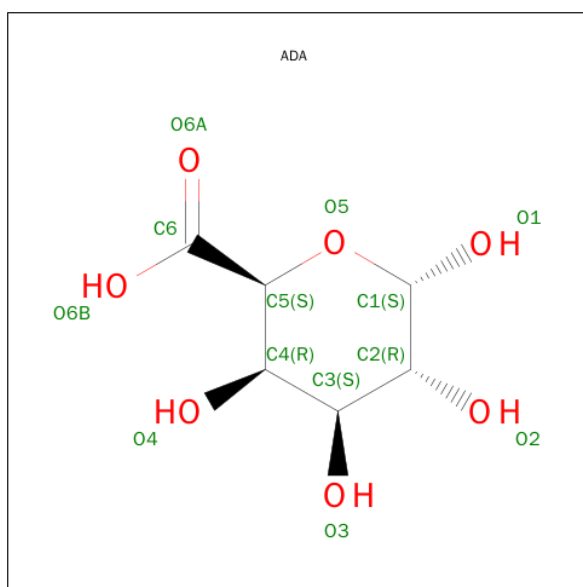


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		

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

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

- Molecule 7 is ALPHA-D-GALACTOPYRANURONIC ACID (three-letter code: ADA) (formula: C₆H₁₀O₇).



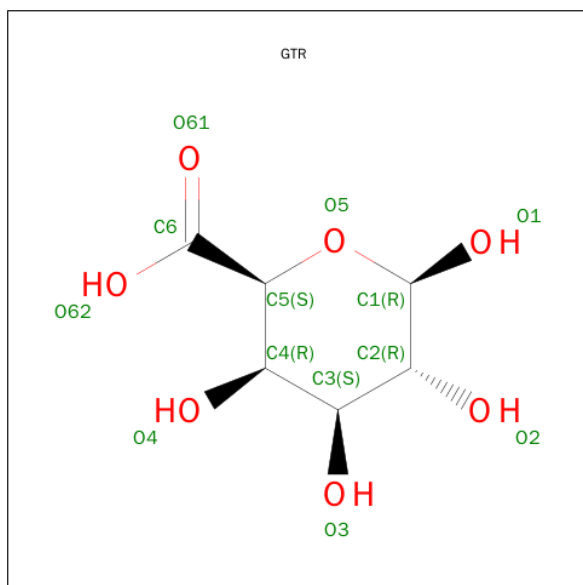
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	6	7		
7	A	1	Total	C	O	0	0
			12	6	6		
7	A	1	Total	C	O	0	0
			12	6	6		
7	B	1	Total	C	O	0	1
			13	6	7		
7	B	1	Total	C	O	0	1
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	1
			12	6	6		
7	B	1	Total	C	O	0	1
			12	6	6		
7	B	1	Total	C	O	0	1
			12	6	6		

- Molecule 8 is Beta-D-Galactopyranuronic acid (three-letter code: GTR) (formula: C₆H₁₀O₇).

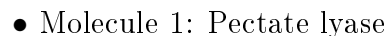


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	1
			13	6	7		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	292	Total	O	0	32
			324	324		
9	B	286	Total	O	0	25
			311	311		

- Molecule 1: Pectate lyase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.33 Å 36.35 Å 100.11 Å 90.00° 132.67° 90.00°	Depositor
Resolution (Å)	34.58 – 1.25 34.58 – 1.25	Depositor EDS
% Data completeness (in resolution range)	94.7 (34.58-1.25) 94.7 (34.58-1.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.25 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.110 , 0.156 0.110 , 0.157	Depositor DCC
R_{free} test set	4592 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	10.4	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 66.1	EDS
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 96370 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4150	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.20% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MPD, IMD, CL, CA, GTR, ADA, MRD

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	0.99	0/1705	0.98	3/2305 (0.1%)
1	B	0.95	0/1679	0.99	2/2269 (0.1%)
All	All	0.97	0/3384	0.98	5/4574 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	B	133	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	10	ASP	CB-CG-OD1	6.88	124.50	118.30
1	A	21	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	103	LYS	CD-CE-NZ	-5.44	99.18	111.70

There are no chirality outliers.

There are no planarity outliers.

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	1680	0	1663	29	0
1	B	1656	0	1651	33	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	5	2	0
3	B	5	0	5	4	0
4	A	16	0	28	0	0
4	B	16	0	28	3	0
5	A	16	0	28	8	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	37	0	21	0	0
7	B	61	0	34	0	0
8	B	13	0	8	1	0
9	A	324	0	0	24	0
9	B	311	0	0	29	0
All	All	4150	0	3471	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 11.

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:A:179[A]:LYS:N	9:A:303:HOH:O	1.64	1.27
1:B:38[A]:SER:OG	9:B:302:HOH:O	1.52	1.23
1:A:179[A]:LYS:CB	9:A:303:HOH:O	1.78	1.23
1:B:103[B]:LYS:HE2	9:B:512[B]:HOH:O	1.31	1.23
1:A:152[B]:ASN:ND2	9:A:305:HOH:O	1.72	1.21
1:A:179[A]:LYS:HB2	9:A:303:HOH:O	1.36	1.16
5:A:209:MRD:H1C3	9:A:534:HOH:O	1.42	1.15
1:A:176[B]:ASN:ND2	9:A:306:HOH:O	1.84	1.09
1:A:167[A]:GLU:OE1	9:A:304:HOH:O	1.68	1.08
5:A:209:MRD:HMC3	9:A:527[A]:HOH:O	1.55	1.06
5:A:209:MRD:C1	9:A:534:HOH:O	2.00	1.05
1:B:155[B]:LYS:NZ	9:B:303:HOH:O	1.66	1.01
1:B:152[A]:ASN:ND2	9:B:307:HOH:O	1.94	1.00
1:B:155[B]:LYS:CE	9:B:303:HOH:O	2.02	0.99
1:A:28[A]:ILE:CD1	9:A:414:HOH:O	2.10	0.97
3:B:206:IMD:N1	9:B:308:HOH:O	1.99	0.95
1:A:179[A]:LYS:CA	9:A:303:HOH:O	1.89	0.92
1:A:76[A]:ASN:ND2	9:A:307:HOH:O	2.02	0.91
8:B:212[B]:GTR:O2	9:B:306:HOH:O	1.89	0.91
1:B:180[A]:THR:OG1	9:B:305[A]:HOH:O	1.88	0.90
3:B:206:IMD:C5	9:B:308:HOH:O	2.21	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155[A]:LYS:NZ	9:A:308:HOH:O	2.08	0.87
1:A:124[B]:THR:HG21	9:A:463:HOH:O	1.76	0.84
1:B:155[A]:LYS:HD2	9:B:425:HOH:O	1.78	0.83
1:A:38[A]:SER:OG	1:A:40:ASN:OD1	1.96	0.82
4:B:201:MPD:H51	9:B:478:HOH:O	1.81	0.79
1:A:28[A]:ILE:HD11	9:A:414:HOH:O	1.75	0.79
1:B:103[B]:LYS:NZ	9:B:309:HOH:O	2.10	0.73
5:A:209:MRD:H5C3	9:A:498:HOH:O	1.89	0.72
1:B:155[B]:LYS:HD3	1:B:155[B]:LYS:N	2.05	0.71
1:B:124[A]:THR:CG2	9:B:307:HOH:O	2.39	0.69
1:B:155[A]:LYS:HD2	9:B:344:HOH:O	1.93	0.68
1:B:183:GLU:OE2	9:B:310:HOH:O	2.14	0.65
1:B:119[C]:LYS:NZ	3:B:206:IMD:HN1	1.95	0.64
5:A:209:MRD:CM	9:A:527[A]:HOH:O	2.30	0.64
5:A:209:MRD:CM	9:A:571:HOH:O	2.45	0.63
1:B:103[B]:LYS:CE	9:B:512[B]:HOH:O	2.09	0.62
1:B:103[A]:LYS:HD2	9:B:384:HOH:O	2.00	0.62
1:B:124[A]:THR:HG23	9:B:307:HOH:O	1.97	0.61
1:B:124[B]:THR:HG21	9:B:463:HOH:O	2.00	0.60
1:B:155[B]:LYS:HE3	9:B:303:HOH:O	1.87	0.59
1:A:155[A]:LYS:HD3	3:A:205:IMD:N3	2.17	0.59
5:A:209:MRD:HMC1	9:A:571:HOH:O	2.04	0.58
1:B:103[B]:LYS:CG	9:B:512[B]:HOH:O	2.50	0.56
1:A:23:LYS:NZ	9:A:312:HOH:O	2.37	0.56
1:B:119[C]:LYS:HZ3	3:B:206:IMD:HN1	1.54	0.54
1:A:165:VAL:HG22	9:A:469:HOH:O	2.07	0.54
1:B:155[A]:LYS:CD	9:B:344:HOH:O	2.53	0.53
1:A:103:LYS:CE	9:A:325[B]:HOH:O	2.56	0.52
1:A:124[B]:THR:HG22	1:A:150:THR:HB	1.91	0.51
1:A:58:ILE:HD11	1:A:66[B]:ILE:HD11	1.93	0.50
1:A:15[B]:LYS:HB2	1:A:18:GLN:HG3	1.94	0.49
4:B:207:MPD:C1	9:B:315:HOH:O	2.61	0.49
1:B:28[B]:ILE:HG22	1:B:28[B]:ILE:O	2.12	0.49
1:B:23:LYS:HE2	9:B:381:HOH:O	2.14	0.48
5:A:209:MRD:H1C2	9:A:375:HOH:O	2.14	0.48
1:A:45:PHE:HB2	1:A:66[B]:ILE:HD12	1.94	0.47
1:A:155[A]:LYS:CD	3:A:205:IMD:N3	2.78	0.46
1:A:130:LYS:HE2	1:A:160[A]:LYS:HD3	1.98	0.46
1:A:49[A]:LYS:HA	1:A:70:GLY:O	2.15	0.45
1:A:54:LYS:HA	1:A:75[B]:GLU:O	2.16	0.45
4:B:201:MPD:H52	4:B:201:MPD:O2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:HD11	1:B:56[B]:VAL:HG21	1.98	0.45
1:B:49[B]:LYS:HE2	9:B:554:HOH:O	2.17	0.44
1:A:179[B]:LYS:HE3	1:A:179[B]:LYS:HB2	1.37	0.44
1:B:98[B]:ILE:HG23	1:B:98[B]:ILE:O	2.17	0.44
1:B:13:ILE:CD1	9:B:564:HOH:O	2.65	0.43
1:B:130:LYS:HA	1:B:157:CYS:O	2.19	0.43
1:B:103[B]:LYS:HG3	9:B:512[B]:HOH:O	2.16	0.43
1:A:156[A]:SER:O	1:A:179[A]:LYS:HB3	2.19	0.42
1:A:124[B]:THR:CG2	9:A:463:HOH:O	2.51	0.42
1:B:49[B]:LYS:NZ	9:B:324:HOH:O	2.53	0.42
1:B:102:ALA:O	1:B:125:ALA:HA	2.20	0.42
1:B:49[A]:LYS:NZ	1:B:92:GLU:O	2.54	0.41
1:B:18[A]:GLN:NE2	9:B:318:HOH:O	2.47	0.41
1:A:130:LYS:HA	1:A:157:CYS:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	219/204 (107%)	207 (94%)	12 (6%)	0	100	100
1	B	216/204 (106%)	202 (94%)	14 (6%)	0	100	100
All	All	435/408 (107%)	409 (94%)	26 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	190/172 (110%)	189 (100%)	1 (0%)	92	72
1	B	187/172 (109%)	185 (99%)	2 (1%)	80	48
All	All	377/344 (110%)	374 (99%)	3 (1%)	84	61

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASP
1	B	64	ASP
1	B	85	ASP

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 10 are monoatomic - leaving 17 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
3	IMD	A	205	-	3,5,5	0.39	0	4,5,5	0.74	0
4	MPD	A	206	-	6,7,7	0.53	0	6,10,10	2.21	1 (16%)
4	MPD	A	207	-	6,7,7	0.53	0	6,10,10	1.01	0
5	MRD	A	208	-	6,7,7	0.39	0	6,10,10	0.90	0
5	MRD	A	209	-	6,7,7	0.59	0	6,10,10	0.92	0
7	ADA	A	211	7	10,13,13	1.66	3 (30%)	15,19,19	1.56	2 (13%)
7	ADA	A	212	2,7	9,12,13	1.76	2 (22%)	12,17,19	1.62	3 (25%)
7	ADA	A	213	2,7	9,12,13	2.22	2 (22%)	12,17,19	1.18	1 (8%)
4	MPD	B	201	-	6,7,7	0.42	0	6,10,10	0.75	0
3	IMD	B	206	-	3,5,5	0.41	0	4,5,5	0.92	0
4	MPD	B	207	-	6,7,7	0.44	0	6,10,10	1.32	1 (16%)
7	ADA	B	209[A]	7	10,13,13	0.84	0	15,19,19	1.57	3 (20%)
7	ADA	B	210[A]	2,7	9,12,13	2.35	2 (22%)	12,17,19	1.60	3 (25%)
7	ADA	B	211[A]	2,7	9,12,13	1.47	1 (11%)	12,17,19	0.79	0
8	GTR	B	212[B]	7	10,13,13	0.79	0	15,19,19	1.63	2 (13%)
7	ADA	B	213[B]	8,2,7	9,12,13	1.04	0	12,17,19	1.44	3 (25%)
7	ADA	B	214[B]	2,7	9,12,13	1.32	1 (11%)	12,17,19	0.85	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
3	IMD	A	205	-	-	0/0/0/0	0/1/1/1
4	MPD	A	206	-	-	0/5/5/5	0/0/0/0
4	MPD	A	207	-	-	0/5/5/5	0/0/0/0
5	MRD	A	208	-	-	0/5/5/5	0/0/0/0
5	MRD	A	209	-	-	0/5/5/5	0/0/0/0
7	ADA	A	211	7	-	0/0/24/24	0/1/1/1
7	ADA	A	212	2,7	-	0/0/21/24	0/1/1/1
7	ADA	A	213	2,7	-	0/0/21/24	0/1/1/1
4	MPD	B	201	-	-	0/5/5/5	0/0/0/0
3	IMD	B	206	-	-	0/0/0/0	0/1/1/1
4	MPD	B	207	-	-	0/5/5/5	0/0/0/0
7	ADA	B	209[A]	7	-	0/0/24/24	0/1/1/1
7	ADA	B	210[A]	2,7	-	0/0/21/24	0/1/1/1
7	ADA	B	211[A]	2,7	-	0/0/21/24	0/1/1/1
8	GTR	B	212[B]	7	-	0/0/24/24	0/1/1/1
7	ADA	B	213[B]	8,2,7	-	0/0/21/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADA	B	214[B]	2,7	-	0/0/21/24	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	213	ADA	O5-C5	-5.42	1.37	1.43
7	A	213	ADA	C2-C3	-2.80	1.48	1.52
7	A	211	ADA	O5-C1	-2.52	1.38	1.43
7	A	212	ADA	O4-C4	2.03	1.47	1.43
7	A	211	ADA	O2-C2	2.54	1.48	1.43
7	A	211	ADA	C3-C2	2.61	1.59	1.52
7	B	214[B]	ADA	O5-C5	3.30	1.47	1.43
7	B	211[A]	ADA	O5-C5	3.77	1.47	1.43
7	A	212	ADA	O5-C5	3.81	1.47	1.43
7	B	210[A]	ADA	O5-C5	4.17	1.47	1.43
7	B	210[A]	ADA	C2-C3	4.79	1.59	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	206	MPD	CM-C2-C1	-5.02	98.44	110.41
8	B	212[B]	GTR	C1-O5-C5	-4.77	105.21	112.22
7	B	209[A]	ADA	C1-C2-C3	-3.07	105.65	110.68
7	B	210[A]	ADA	O4-C4-C3	-2.76	104.13	110.36
8	B	212[B]	GTR	C1-C2-C3	-2.73	106.21	110.68
7	A	212	ADA	O4-C4-C3	-2.41	104.93	110.36
7	B	213[B]	ADA	O4-C4-C3	-2.05	105.72	110.36
7	A	213	ADA	C1-C2-C3	2.02	112.00	109.55
7	B	209[A]	ADA	C1-O5-C5	2.03	115.22	112.22
7	A	211	ADA	O3-C3-C4	2.11	115.12	110.36
7	B	210[A]	ADA	C6-C5-C4	2.13	118.72	112.61
7	B	209[A]	ADA	O3-C3-C4	2.35	115.66	110.36
7	A	212	ADA	C1-C2-C3	2.43	112.50	109.55
7	B	213[B]	ADA	C1-C2-C3	2.48	112.55	109.55
4	B	207	MPD	O2-C2-C1	2.91	118.73	108.01
7	B	213[B]	ADA	O4-C4-C5	2.96	116.03	110.40
7	B	210[A]	ADA	O4-C4-C5	3.23	116.55	110.40
7	A	212	ADA	O4-C4-C5	3.70	117.46	110.40
7	A	211	ADA	C1-O5-C5	4.71	119.15	112.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	205	IMD	2	0
5	A	209	MRD	8	0
4	B	201	MPD	2	0
3	B	206	IMD	4	0
4	B	207	MPD	1	0
8	B	212[B]	GTR	1	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 [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	198/204 (97%)	-0.61	2 (1%) 84 82	9, 12, 27, 57	3 (1%)
1	B	195/204 (95%)	-0.64	1 (0%) 91 90	8, 14, 27, 48	0
All	All	393/408 (96%)	-0.63	3 (0%) 87 86	8, 13, 27, 57	3 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-3	HIS	4.9
1	A	-2	VAL	4.3
1	B	0	THR	2.4

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	MPD	B	207	8/8	0.87	0.17	14.90	16,27,32,41	8
5	MRD	A	209	8/8	0.88	0.15	9.76	16,23,25,27	8
4	MPD	B	201	8/8	0.89	0.16	5.51	30,40,63,70	0
3	IMD	A	205	5/5	0.81	0.21	3.51	25,29,43,51	5
2	CA	B	204	1/1	1.00	0.06	2.83	11,11,11,11	0
4	MPD	A	206	8/8	0.93	0.11	2.44	28,36,54,95	0
4	MPD	A	207	8/8	0.93	0.09	2.39	26,37,46,49	0
3	IMD	B	206	5/5	0.89	0.10	1.20	43,50,59,65	5
5	MRD	A	208	8/8	0.96	0.09	0.42	22,24,34,37	0
7	ADA	A	213	12/13	0.98	0.05	-0.28	11,12,18,18	0
7	ADA	A	211	13/13	0.98	0.06	-0.55	15,18,24,27	0
7	ADA	A	212	12/13	0.98	0.04	-0.89	11,13,16,16	0
7	ADA	B	213[B]	12/13	0.99	0.04	-1.41	17,19,25,29	12
7	ADA	B	210[A]	12/13	0.99	0.04	-1.41	9,10,11,11	12
7	ADA	B	211[A]	12/13	0.99	0.04	-1.42	9,10,13,15	12
7	ADA	B	214[B]	12/13	0.99	0.04	-1.61	16,18,21,21	12
2	CA	A	203	1/1	1.00	0.04	-1.65	11,11,11,11	0
2	CA	B	205	1/1	1.00	0.03	-1.66	11,11,11,11	0
8	GTR	B	212[B]	13/13	0.99	0.04	-2.40	23,27,32,32	13
2	CA	A	204	1/1	1.00	0.03	-2.92	11,11,11,11	0
6	CL	B	208	1/1	1.00	0.03	-3.20	14,14,14,14	0
7	ADA	B	209[A]	13/13	0.99	0.03	-3.24	11,13,15,16	13
6	CL	A	210	1/1	1.00	0.03	-4.78	16,16,16,16	1
2	CA	A	202	1/1	1.00	0.04	-	12,12,12,12	0
2	CA	B	202	1/1	1.00	0.03	-	13,13,13,13	1
2	CA	B	203	1/1	1.00	0.04	-	12,12,12,12	0
2	CA	A	201	1/1	1.00	0.06	-	16,16,16,16	1

6.5 Other polymers ⓘ

There are no such residues in this entry.