



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:01 AM UTC

PDB ID : 3T9G / pdb_00003t9g
Title : The crystal structure of family 3 pectate lyase from *Caldicellulosiruptor bescii*
Authors : Alahuhta, P.M.; Lunin, V.V.
Deposited on : 2011-08-02
Resolution : 1.50 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

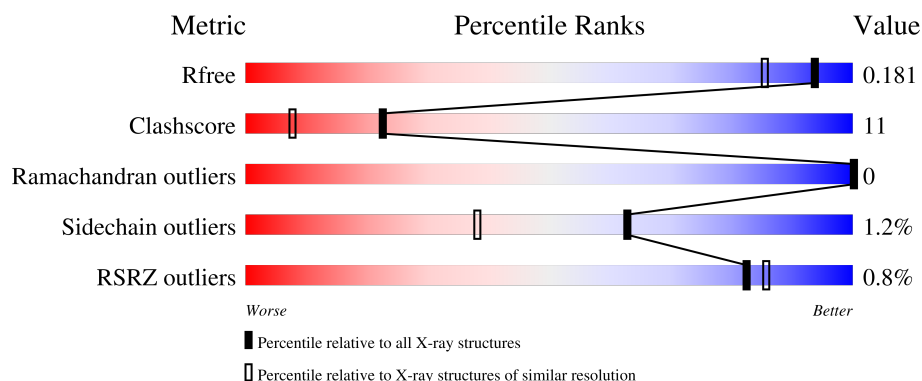
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	196	 2% 78% 20% .
1	B	196	 79% 19% ..

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
3	MRD	B	206	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 3980 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	196	Total	C	N	O	S	0	26	0
			1654	1047	276	325	6			
1	B	195	Total	C	N	O	S	0	21	0
			1632	1028	271	327	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	VAL	-	expression tag	UNP B9MKT4
A	-1	GLY	-	expression tag	UNP B9MKT4
A	0	THR	-	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

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

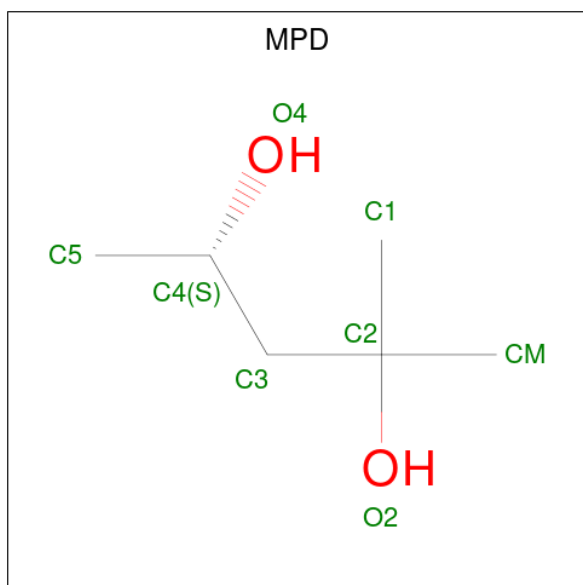
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



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

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



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	1
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).

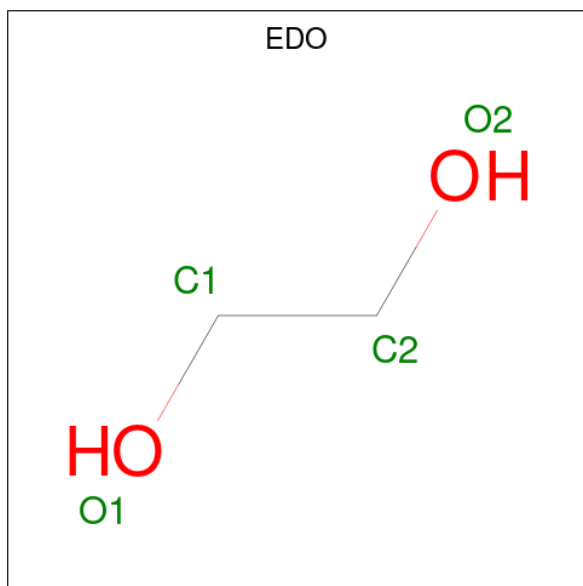


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			12	6	6		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	1
			12	6	6		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



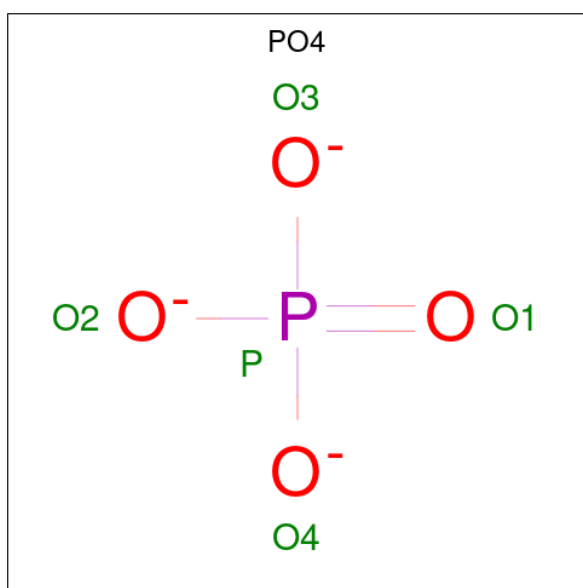
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

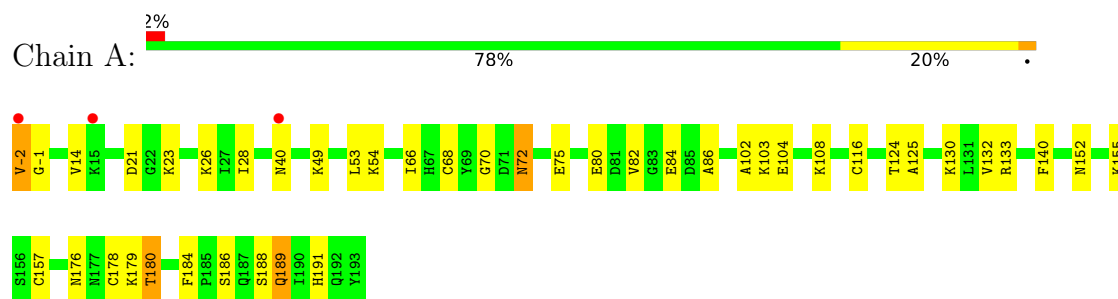
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	276	Total 293	O 293	0	17
11	B	250	Total 268	O 268	0	18

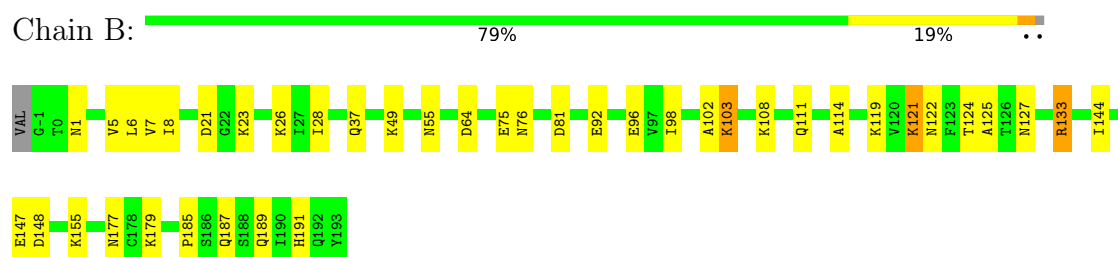
3 Residue-property plots [i](#)

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: Pectate lyase



• Molecule 1: Pectate lyase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	36.51Å 146.69Å 162.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.50 25.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.00-1.50) 99.6 (25.00-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.143 , 0.178 0.150 , 0.181	Depositor DCC
R_{free} test set	3552 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	11.4	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3980	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOL, CA, NA, ACT, EDO, PO4, MPD, 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	1.65	15/1715 (0.9%)	1.25	1/2319 (0.0%)
1	B	1.54	14/1680 (0.8%)	1.26	2/2270 (0.1%)
All	All	1.60	29/3395 (0.9%)	1.26	3/4589 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	GLN	CD-OE1	7.42	1.37	1.23
1	A	188	SER	C-O	-7.29	1.14	1.24
1	A	132	VAL	C-O	6.97	1.31	1.24
1	B	21	ASP	N-CA	-6.96	1.37	1.46
1	A	72	ASN	CA-C	-6.91	1.44	1.52
1	A	84	GLU	CD-OE1	6.66	1.38	1.25
1	A	14	VAL	N-CA	-6.05	1.39	1.46
1	A	184	PHE	CA-C	5.97	1.60	1.52
1	A	49	LYS	CA-C	-5.88	1.45	1.52
1	A	140	PHE	CA-C	5.87	1.61	1.53
1	A	82	VAL	CA-CB	5.82	1.60	1.54
1	B	144	ILE	CA-CB	-5.79	1.47	1.54
1	B	7	VAL	CA-CB	-5.78	1.47	1.54
1	A	178	CYS	CA-C	-5.76	1.45	1.52
1	A	49	LYS	CD-CE	5.76	1.69	1.52
1	B	6	LEU	N-CA	-5.69	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	ASP	CA-C	-5.66	1.48	1.53
1	B	6	LEU	C-O	5.62	1.30	1.24
1	B	55	ASN	CA-C	-5.54	1.46	1.53
1	B	21	ASP	C-O	5.50	1.30	1.24
1	B	114	ALA	CA-CB	-5.39	1.46	1.53
1	B	191	HIS	C-O	-5.37	1.17	1.23
1	B	177	ASN	N-CA	5.33	1.53	1.46
1	B	1	ASN	N-CA	5.30	1.52	1.46
1	B	8	ILE	N-CA	-5.23	1.40	1.46
1	A	21	ASP	N-CA	-5.19	1.39	1.46
1	A	191	HIS	N-CA	-5.08	1.39	1.45
1	B	127	ASN	N-CA	5.06	1.53	1.46
1	A	86	ALA	N-CA	5.03	1.52	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	ARG	NE-CZ-NH2	6.91	125.42	119.20
1	A	184	PHE	O-C-N	5.91	126.37	121.35
1	B	64	ASP	OD1-CG-OD2	5.54	136.19	122.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40[B]	ASN	Peptide

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	1654	0	1665	26	0
1	B	1632	0	1624	37	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	16	0	28	3	0
3	B	16	0	28	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	16	0	28	1	0
4	B	16	0	28	1	0
5	A	1	0	0	0	0
5	B	3	0	0	0	0
6	A	18	0	24	3	0
6	B	18	0	24	3	0
7	B	1	0	0	0	0
8	B	8	0	12	3	0
9	B	8	0	6	0	0
10	B	10	0	0	0	0
11	A	293	0	0	5	0
11	B	268	0	0	10	0
All	All	3980	0	3467	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 11.

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)
3:A:203:MRD:H1C3	3:A:203:MRD:C5	1.52	1.37
3:A:203:MRD:H5C2	3:A:203:MRD:C1	1.54	1.36
1:B:92[A]:GLU:OE1	11:B:528[A]:HOH:O	1.61	1.18
3:B:206:MRD:H1C1	3:B:206:MRD:C5	1.77	1.09
1:B:133:ARG:HH11	3:B:206:MRD:HMC1	1.23	1.01
1:A:133:ARG:HE	6:A:207[A]:GOL:H2	1.24	1.01
1:B:133:ARG:HE	3:B:206:MRD:H3C1	1.24	1.00
1:B:119[B]:LYS:HG2	1:B:121[B]:LYS:HG3	1.42	1.00
3:B:206:MRD:H5C3	3:B:206:MRD:C1	1.89	0.99
1:B:103[A]:LYS:HG2	6:B:212:GOL:H32	1.44	0.95
3:B:206:MRD:H1C1	3:B:206:MRD:H5C3	0.96	0.95
3:B:206:MRD:H3C2	11:B:359:HOH:O	1.76	0.85
3:B:206:MRD:H5C2	11:B:398[A]:HOH:O	1.84	0.78
1:B:103[A]:LYS:HG2	6:B:212:GOL:C3	2.15	0.76
1:B:133:ARG:NH1	3:B:206:MRD:HMC1	2.00	0.74
1:B:119[B]:LYS:HG2	1:B:121[B]:LYS:CG	2.18	0.71
1:B:133:ARG:HH11	3:B:206:MRD:CM	2.04	0.70
1:B:37[A]:GLN:OE1	11:B:483[A]:HOH:O	2.09	0.70
1:B:133:ARG:NE	3:B:206:MRD:H3C1	2.04	0.69
3:B:206:MRD:C5	3:B:206:MRD:C1	2.58	0.69
1:B:108:LYS:HE3	11:B:484:HOH:O	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:VAL:HG11	1:B:28[B]:ILE:HD12	1.75	0.68
1:A:186:SER:H	1:A:189:GLN:HE21	1.41	0.68
1:B:75[B]:GLU:HG3	1:B:98[B]:ILE:HG23	1.75	0.66
11:A:518:HOH:O	4:B:204[B]:MPD:HM3	1.97	0.63
1:A:70:GLY:H	1:A:72:ASN:HD21	1.46	0.63
1:A:103[B]:LYS:HG3	1:A:104:GLU:HG2	1.80	0.63
1:B:155:LYS:HG3	11:B:531:HOH:O	1.97	0.62
1:B:75[B]:GLU:O	1:B:76[B]:ASN:C	2.44	0.61
1:A:133:ARG:NE	6:A:207[A]:GOL:H2	2.07	0.60
1:A:186:SER:H	1:A:189:GLN:NE2	1.99	0.60
1:B:96[A]:GLU:HG2	1:B:119[A]:LYS:HD2	1.84	0.60
1:B:187[A]:GLN:HG2	8:B:208:EDO:H11	1.84	0.59
1:B:119[B]:LYS:CG	1:B:121[B]:LYS:HG3	2.26	0.58
1:B:187[A]:GLN:HG2	8:B:208:EDO:C1	2.34	0.58
1:B:179:LYS:HG2	11:B:507:HOH:O	2.06	0.56
1:B:121[B]:LYS:HE3	11:B:381:HOH:O	2.05	0.56
1:A:68:CYS:HB3	1:A:72:ASN:ND2	2.22	0.55
1:A:80:GLU:O	1:A:103[B]:LYS:HG2	2.07	0.54
1:A:108:LYS:HD3	11:A:569:HOH:O	2.07	0.53
1:B:103[A]:LYS:HG3	11:B:301:HOH:O	2.07	0.53
1:A:-2[A]:VAL:HG13	1:A:-1:GLY:N	2.23	0.53
1:B:121[C]:LYS:HA	1:B:147:GLU:O	2.09	0.52
1:A:23[A]:LYS:HE2	11:A:489:HOH:O	2.11	0.50
1:A:152:ASN:HD21	1:A:176:ASN:HD22	1.59	0.49
1:B:108:LYS:HD2	1:B:111[A]:GLN:OE1	2.13	0.48
1:B:75[B]:GLU:HG3	1:B:98[B]:ILE:CG2	2.43	0.48
1:A:-2[A]:VAL:CG1	1:A:-1:GLY:N	2.75	0.47
1:B:23:LYS:HE2	11:B:450:HOH:O	2.14	0.47
1:A:116:CYS:HA	4:A:205:MPD:H13	1.95	0.47
1:A:152:ASN:ND2	1:A:176:ASN:HD22	2.13	0.47
1:B:121[A]:LYS:HE3	1:B:148:ASP:OD2	2.14	0.47
1:B:26:LYS:HE2	1:B:28[A]:ILE:HD11	1.97	0.46
3:A:203:MRD:H1C3	3:A:203:MRD:H5C2	0.62	0.46
1:B:102:ALA:O	1:B:125:ALA:HA	2.16	0.45
1:A:180[B]:THR:HG23	11:A:444:HOH:O	2.16	0.45
1:A:68:CYS:HB3	1:A:72:ASN:HD22	1.82	0.44
1:B:121[C]:LYS:HD2	1:B:122:ASN:N	2.32	0.44
1:A:179:LYS:HG2	1:A:180[A]:THR:HG23	2.00	0.44
1:B:119[B]:LYS:HG2	1:B:121[B]:LYS:CD	2.47	0.44
1:A:70:GLY:H	1:A:72:ASN:ND2	2.12	0.43
1:A:53:LEU:HD23	1:A:66:ILE:HD13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LYS:HA	1:A:157:CYS:O	2.19	0.43
1:B:124[A]:THR:HG22	6:B:212:GOL:O3	2.19	0.43
1:B:187[A]:GLN:NE2	8:B:208:EDO:O1	2.52	0.42
1:B:185:PRO:HD2	1:B:189:GLN:HE22	1.82	0.42
1:A:155[A]:LYS:HA	6:A:208:GOL:H2	2.01	0.42
1:A:102:ALA:O	1:A:125:ALA:HA	2.20	0.41
1:A:54:LYS:HA	1:A:75[A]:GLU:O	2.20	0.41
1:B:121[A]:LYS:CE	1:B:148:ASP:OD2	2.68	0.41
1:A:26:LYS:HE2	1:A:28[A]:ILE:HD11	2.03	0.40
1:A:124[A]:THR:HG23	11:A:502:HOH:O	2.22	0.40
1:B:49:LYS:HB2	1:B:49:LYS: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	219/196 (112%)	210 (96%)	9 (4%)	0	100	100
1	B	215/196 (110%)	199 (93%)	16 (7%)	0	100	100
All	All	434/392 (111%)	409 (94%)	25 (6%)	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	190/166 (114%)	186 (98%)	4 (2%)	47	19
1	B	186/166 (112%)	181 (97%)	5 (3%)	39	12
All	All	376/332 (113%)	367 (98%)	9 (2%)	63	15

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2[A]	VAL
1	A	-2[B]	VAL
1	A	180[A]	THR
1	A	180[B]	THR
1	B	103[A]	LYS
1	B	103[B]	LYS
1	B	121[A]	LYS
1	B	121[B]	LYS
1	B	121[C]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	137	ASN
1	A	152	ASN
1	A	174	ASN
1	A	177	ASN
1	A	189	GLN
1	B	137	ASN
1	B	176	ASN
1	B	189	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 7 are monoatomic - leaving 20 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	MRD	B	206	-	7,7,7	0.59	0	9,10,10	2.34	3 (33%)
9	ACT	B	215	-	3,3,3	0.68	0	3,3,3	1.35	0
6	GOL	B	213[A]	-	5,5,5	0.44	0	5,5,5	0.42	0
8	EDO	B	208	-	3,3,3	0.43	0	2,2,2	0.51	0
4	MPD	B	204[B]	-	7,7,7	0.30	0	9,10,10	0.28	0
9	ACT	B	214	-	3,3,3	0.88	0	3,3,3	1.16	0
6	GOL	A	207[A]	-	5,5,5	0.63	0	5,5,5	0.73	0
10	PO4	B	217	-	4,4,4	0.67	0	6,6,6	1.13	0
6	GOL	B	213[B]	-	5,5,5	0.47	0	5,5,5	0.41	0
10	PO4	B	216	-	4,4,4	1.11	0	6,6,6	0.86	0
6	GOL	B	212	-	5,5,5	0.38	0	5,5,5	0.43	0
6	GOL	A	207[B]	-	5,5,5	0.42	0	5,5,5	0.69	0
8	EDO	B	207	-	3,3,3	0.60	0	2,2,2	0.28	0
3	MRD	A	203	-	7,7,7	0.60	0	9,10,10	1.20	1 (11%)
3	MRD	A	202	-	7,7,7	0.64	0	9,10,10	1.27	2 (22%)
3	MRD	B	203[A]	-	7,7,7	0.74	0	9,10,10	0.64	0
4	MPD	B	205	-	7,7,7	0.53	0	9,10,10	0.80	0
4	MPD	A	204	-	7,7,7	0.55	0	9,10,10	0.82	0
4	MPD	A	205	-	7,7,7	0.87	1 (14%)	9,10,10	2.15	5 (55%)
6	GOL	A	208	-	5,5,5	0.44	0	5,5,5	0.26	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
6	GOL	A	207[B]	-	-	1/4/4/4	-
6	GOL	A	207[A]	-	-	2/4/4/4	-
3	MRD	B	203[A]	-	-	0/5/5/5	-
3	MRD	B	206	-	-	2/5/5/5	-
3	MRD	A	203	-	-	4/5/5/5	-
4	MPD	B	205	-	-	0/5/5/5	-
8	EDO	B	207	-	-	1/1/1/1	-
3	MRD	A	202	-	-	0/5/5/5	-
6	GOL	B	213[B]	-	-	2/4/4/4	-
6	GOL	B	213[A]	-	-	2/4/4/4	-
4	MPD	A	204	-	-	3/5/5/5	-
4	MPD	A	205	-	-	1/5/5/5	-
8	EDO	B	208	-	-	1/1/1/1	-
6	GOL	A	208	-	-	2/4/4/4	-
6	GOL	B	212	-	-	4/4/4/4	-
4	MPD	B	204[B]	-	-	0/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	205	MPD	O2-C2	2.04	1.49	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	206	MRD	CM-C2-C1	5.18	122.22	110.63
4	A	205	MPD	C1-C2-C3	3.60	125.71	110.20
3	B	206	MRD	O2-C2-C3	3.25	121.44	109.27
4	A	205	MPD	CM-C2-C1	-3.21	103.43	110.63
4	A	205	MPD	CM-C2-C3	-2.68	98.63	110.20
3	B	206	MRD	O2-C2-C1	-2.62	99.83	107.99
3	A	202	MRD	CM-C2-C3	2.22	119.78	110.20
4	A	205	MPD	O2-C2-CM	2.20	114.83	107.99
3	A	202	MRD	O2-C2-C3	-2.16	101.20	109.27
4	A	205	MPD	O2-C2-C1	-2.14	101.33	107.99
3	A	203	MRD	O4-C4-C5	2.11	118.53	109.45

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	203	MRD	C2-C3-C4-C5
4	A	205	MPD	C2-C3-C4-C5
6	A	208	GOL	O1-C1-C2-O2
6	A	208	GOL	O1-C1-C2-C3
6	B	213[B]	GOL	C1-C2-C3-O3
6	A	207[A]	GOL	O2-C2-C3-O3
6	A	207[A]	GOL	C1-C2-C3-O3
6	B	212	GOL	O1-C1-C2-C3
6	B	212	GOL	C1-C2-C3-O3
6	B	213[A]	GOL	C1-C2-C3-O3
6	B	212	GOL	O2-C2-C3-O3
6	B	213[A]	GOL	O2-C2-C3-O3
8	B	208	EDO	O1-C1-C2-O2
6	A	207[B]	GOL	O1-C1-C2-O2
6	B	212	GOL	O1-C1-C2-O2
6	B	213[B]	GOL	O2-C2-C3-O3
3	B	206	MRD	O2-C2-C3-C4
3	A	203	MRD	C1-C2-C3-C4
3	B	206	MRD	C2-C3-C4-C5
8	B	207	EDO	O1-C1-C2-O2
4	A	204	MPD	O2-C2-C3-C4
3	A	203	MRD	C2-C3-C4-O4
3	A	203	MRD	CM-C2-C3-C4
4	A	204	MPD	C1-C2-C3-C4
4	A	204	MPD	CM-C2-C3-C4

There are no ring outliers.

8 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	206	MRD	11	0
8	B	208	EDO	3	0
4	B	204[B]	MPD	1	0
6	A	207[A]	GOL	2	0
6	B	212	GOL	3	0
3	A	203	MRD	3	0
4	A	205	MPD	1	0
6	A	208	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	196/196 (100%)	-0.58	3 (1%) 72 75	4, 11, 18, 27	26 (13%)
1	B	195/196 (99%)	-0.64	0 100 100	3, 10, 19, 30	21 (10%)
All	All	391/392 (99%)	-0.61	3 (0%) 82 86	3, 10, 19, 30	47 (12%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-2[A]	VAL	4.4
1	A	40[A]	ASN	2.7
1	A	15[A]	LYS	2.1

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(Å ²)	Q<0.9
6	GOL	B	213[A]	6/6	0.73	0.20	54,55,56,57	6
6	GOL	B	213[B]	6/6	0.73	0.20	30,32,33,34	6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	EDO	B	207	4/4	0.74	0.15	39,42,42,46	0
6	GOL	B	212	6/6	0.75	0.16	22,31,36,38	6
4	MPD	B	204[B]	8/8	0.76	0.40	61,61,62,62	8
9	ACT	B	215	4/4	0.77	0.16	31,32,32,35	4
10	PO4	B	217	5/5	0.78	0.14	49,50,55,56	5
3	MRD	B	206	8/8	0.79	0.16	24,28,32,32	8
6	GOL	A	208	6/6	0.80	0.21	31,32,33,35	6
8	EDO	B	208	4/4	0.80	0.16	28,28,31,31	4
9	ACT	B	214	4/4	0.82	0.13	52,53,53,53	0
3	MRD	A	203	8/8	0.85	0.14	23,25,30,30	8
4	MPD	A	205	8/8	0.86	0.12	15,20,25,26	8
6	GOL	A	207[B]	6/6	0.90	0.12	20,23,25,27	6
10	PO4	B	216	5/5	0.90	0.10	35,38,41,45	5
6	GOL	A	207[A]	6/6	0.90	0.12	18,23,26,29	6
4	MPD	A	204	8/8	0.91	0.10	16,23,26,26	8
4	MPD	B	205	8/8	0.92	0.10	17,24,27,29	0
3	MRD	B	203[A]	8/8	0.93	0.08	12,17,22,23	8
3	MRD	A	202	8/8	0.94	0.08	21,25,28,28	0
5	NA	A	206	1/1	0.98	0.07	15,15,15,15	1
5	NA	B	209	1/1	0.98	0.03	9,9,9,9	1
5	NA	B	211	1/1	0.98	0.07	22,22,22,22	0
5	NA	B	210	1/1	0.99	0.06	25,25,25,25	0
7	CL	B	202	1/1	0.99	0.03	12,12,12,12	0
2	CA	B	201	1/1	1.00	0.02	7,7,7,7	0
2	CA	A	201	1/1	1.00	0.03	10,10,10,10	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.