



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:54 am GMT

PDB ID : 3T9G
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

<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 : 1.7.2 (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

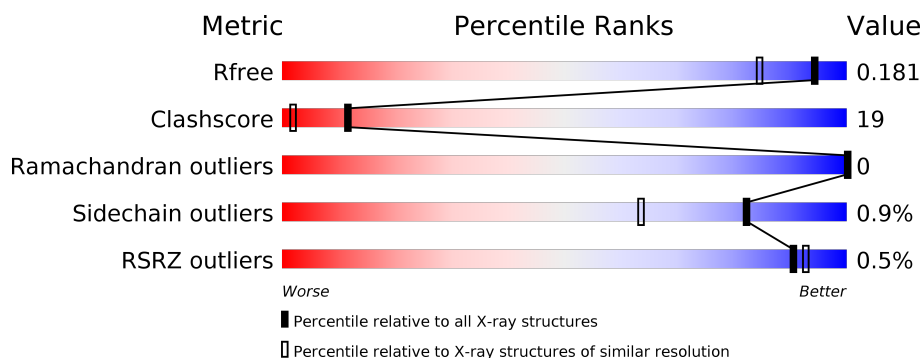
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	100719	2279 (1.50-1.50)
Clashscore	112137	2503 (1.50-1.50)
Ramachandran outliers	110173	2445 (1.50-1.50)
Sidechain outliers	110143	2443 (1.50-1.50)
RSRZ outliers	101464	2305 (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 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	196	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 76%, green 22%, grey 0%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 76% 22% . </div> </div>
1	B	196	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 81%, yellow 18%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 81% 18% .. </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
10	PO4	B	216	-	-	X	X
10	PO4	B	217	-	-	X	X
3	MRD	A	203	-	-	X	X
3	MRD	B	206	-	-	X	X
4	MPD	A	204	-	-	-	X
4	MPD	A	205	-	-	X	X
4	MPD	B	204[B]	-	-	-	X
6	GOL	A	207[A]	-	-	-	X
6	GOL	A	208	-	-	X	X
6	GOL	B	212	-	-	X	X
6	GOL	B	213[A]	-	-	-	X
8	EDO	B	208	-	-	X	-
9	ACT	B	214	-	-	-	X
9	ACT	B	215	-	-	-	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			

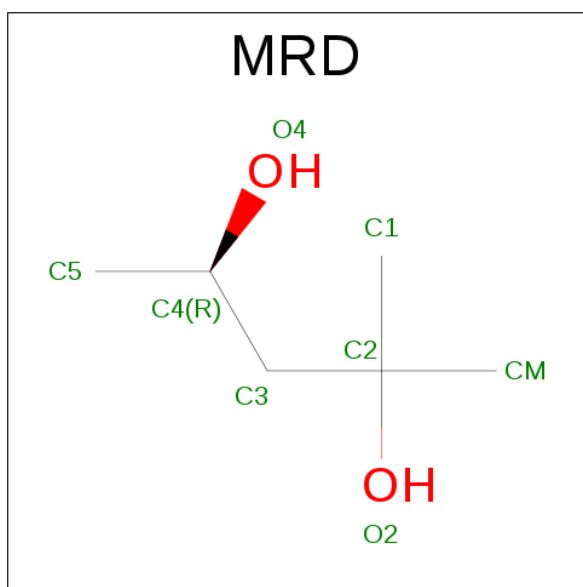
There are 6 discrepancies between the modelled and reference sequences:

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 (three-letter code: CA) (formula: Ca).

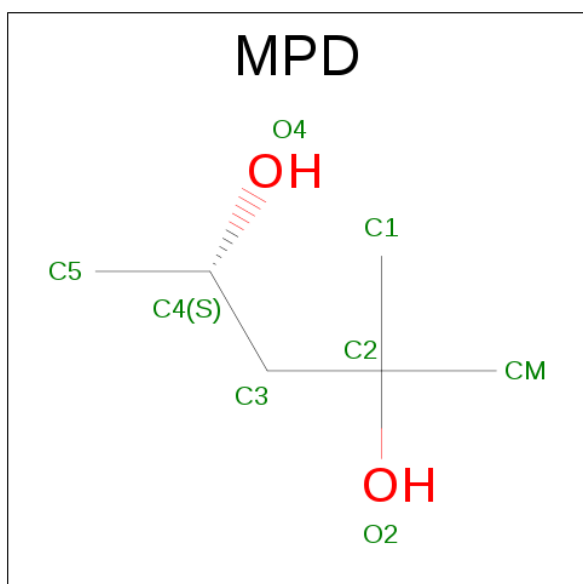
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: 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 (three-letter code: MPD) (formula: $C_6H_{14}O_2$).

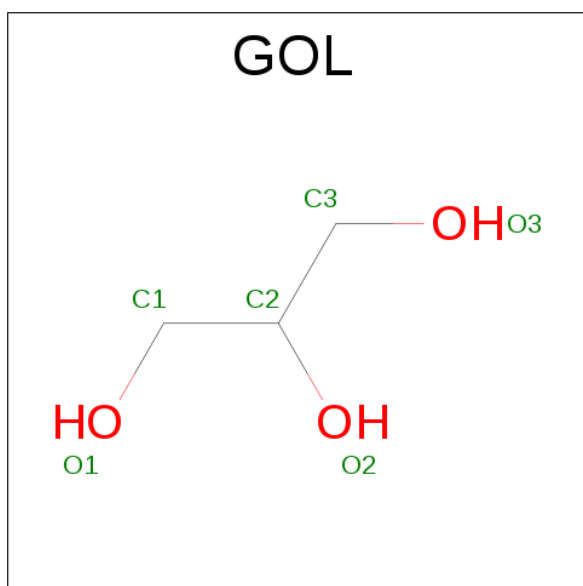


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	1
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

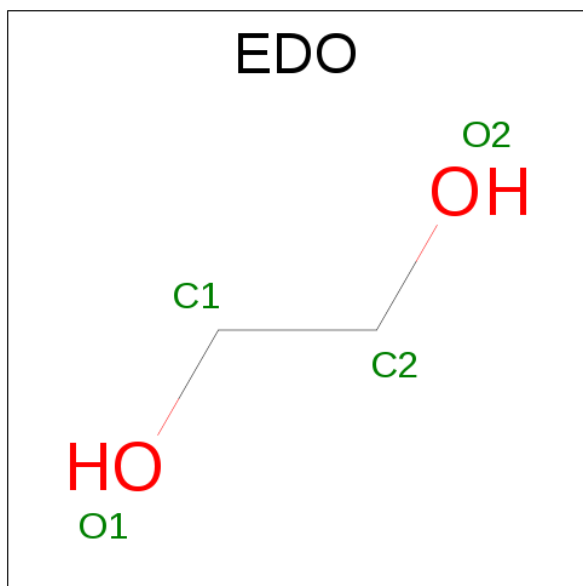


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			12	6	6		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	1
			12	6	6		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

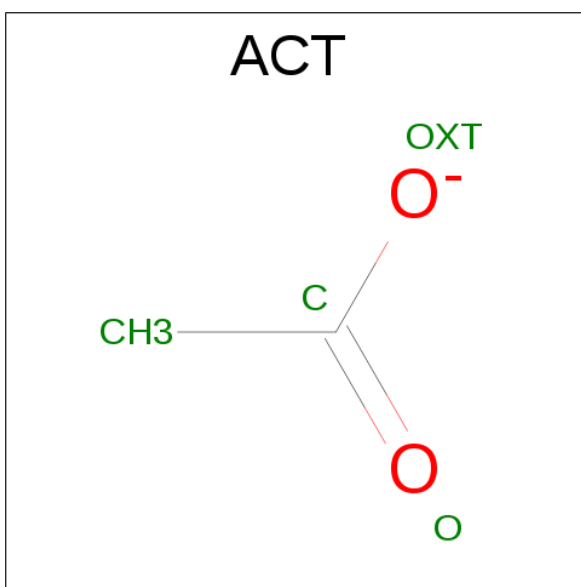
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



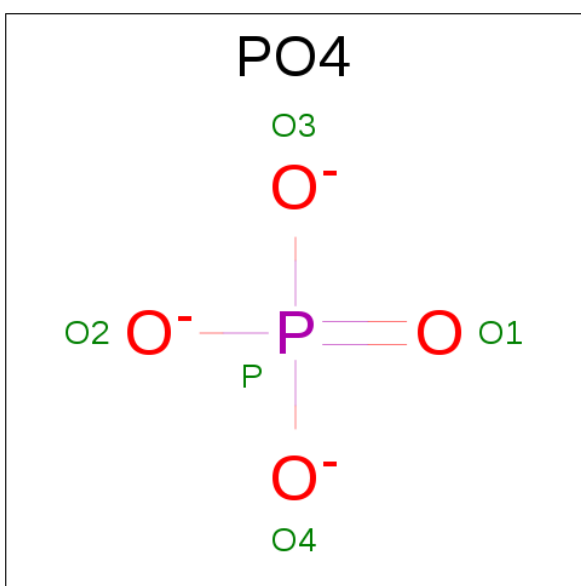
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is ACETATE ION (three-letter code: 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 (three-letter code: 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

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 35.77 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.00-1.50) 99.4 (35.77-1.50)	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	3526 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	11.4	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.6	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: GOL, MPD, CL, NA, CA, EDO, ACT, MRD, PO4

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	1.43	9/1715 (0.5%)	1.21	10/2319 (0.4%)
1	B	1.33	2/1680 (0.1%)	1.26	11/2270 (0.5%)
All	All	1.38	11/3395 (0.3%)	1.23	21/4589 (0.5%)

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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	GLU	CD-OE1	11.23	1.38	1.25
1	A	49	LYS	CD-CE	7.39	1.69	1.51
1	B	56[A]	VAL	CB-CG1	6.53	1.66	1.52
1	B	56[B]	VAL	CB-CG1	6.53	1.66	1.52
1	A	189	GLN	CD-OE1	6.22	1.37	1.24
1	A	145	TYR	CE1-CZ	-6.08	1.30	1.38
1	A	48[A]	GLU	CD-OE2	-5.71	1.19	1.25
1	A	48[B]	GLU	CD-OE2	-5.71	1.19	1.25
1	A	36	SER	CB-OG	-5.47	1.35	1.42
1	A	80	GLU	CB-CG	-5.31	1.42	1.52
1	A	49	LYS	CE-NZ	5.12	1.61	1.49

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	ASP	CB-CG-OD2	-11.13	108.28	118.30
1	B	21	ASP	CB-CG-OD1	10.59	127.83	118.30
1	B	133	ARG	NE-CZ-NH2	10.24	125.42	120.30
1	A	10	ASP	CB-CG-OD1	9.75	127.07	118.30
1	A	133	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	49	LYS	CD-CE-NZ	6.92	127.63	111.70
1	B	133	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	B	64	ASP	OD1-CG-OD2	6.78	136.19	123.30
1	B	34	ASP	CB-CG-OD1	6.63	124.27	118.30
1	B	34	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	A	71	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	69	TYR	CB-CG-CD2	6.28	124.77	121.00
1	A	21	ASP	CB-CG-OD1	5.95	123.65	118.30
1	B	193	TYR	CB-CG-CD1	5.90	124.54	121.00
1	B	71	ASP	CB-CG-OD1	5.72	123.44	118.30
1	A	10	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	133	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	118	PHE	CB-CG-CD1	-5.35	117.06	120.80
1	B	167	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	A	170	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	B	21	ASP	CB-CG-OD2	-5.00	113.80	118.30

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 [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	1654	0	1665	49	0
1	B	1632	0	1624	62	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	16	0	28	10	0
3	B	16	0	28	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	16	0	28	12	0
4	B	16	0	28	1	0
5	A	1	0	0	1	0
5	B	3	0	0	0	0
6	A	18	0	24	6	0
6	B	18	0	24	5	0
7	B	1	0	0	0	0
8	B	8	0	12	12	0
9	B	8	0	6	1	0
10	B	10	0	0	4	0
11	A	293	0	0	18	0
11	B	268	0	0	34	0
All	All	3980	0	3467	135	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 19.

All (135) 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
4:A:205:MPD:HM1	11:A:436:HOH:O	1.46	1.16
1:B:152[A]:ASN:ND2	11:B:535:HOH:O	1.77	1.15
10:B:216:PO4:O3	11:B:534:HOH:O	1.62	1.14
1:B:187[B]:GLN:OE1	8:B:208:EDO:H22	1.50	1.12
1:B:187[B]:GLN:OE1	8:B:208:EDO:C2	1.98	1.11
1:A:6[B]:LEU:HD13	3:A:203:MRD:HMC2	1.29	1.11
3:B:206:MRD:C5	3:B:206:MRD:H1C1	1.77	1.09
1:A:92[A]:GLU:HG3	4:A:205:MPD:C1	1.83	1.08
3:A:203:MRD:H5C1	11:A:558:HOH:O	1.55	1.06
1:A:92[A]:GLU:OE2	4:A:205:MPD:H11	1.56	1.06
1:A:76[B]:ASN:ND2	11:A:523:HOH:O	1.88	1.05
10:B:216:PO4:P	11:B:534:HOH:O	2.13	1.03
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
10:B:217:PO4:O2	11:B:545:HOH:O	1.80	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85[B]:ASP:OD2	11:B:484:HOH:O	1.82	0.96
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
1:B:92[A]:GLU:CD	11:B:468:HOH:O	2.03	0.95
1:A:6[B]:LEU:CD1	3:A:203:MRD:HMC2	1.97	0.94
1:A:6[B]:LEU:HD13	3:A:203:MRD:CM	1.97	0.94
1:A:92[A]:GLU:CD	4:A:205:MPD:H11	1.88	0.93
6:A:208:GOL:O1	11:A:506:HOH:O	1.87	0.91
1:B:76[B]:ASN:ND2	11:B:448:HOH:O	2.02	0.90
1:B:92[A]:GLU:OE1	11:B:468:HOH:O	1.88	0.90
1:A:92[A]:GLU:CG	4:A:205:MPD:C1	2.49	0.90
8:B:208:EDO:H22	11:B:533:HOH:O	1.72	0.90
8:B:208:EDO:C2	11:B:533:HOH:O	2.23	0.85
3:B:206:MRD:H3C2	11:B:359:HOH:O	1.76	0.85
1:A:85[A]:ASP:OD1	5:A:206:NA:NA	1.51	0.82
1:A:18[A]:GLN:OE1	11:A:344:HOH:O	2.01	0.79
1:A:92[A]:GLU:OE2	4:A:205:MPD:HM3	1.82	0.79
3:A:203:MRD:C5	11:A:558:HOH:O	2.21	0.79
3:B:206:MRD:H5C2	11:B:398[A]:HOH:O	1.84	0.78
1:A:92[A]:GLU:OE2	4:A:205:MPD:C1	2.31	0.78
10:B:217:PO4:P	11:B:545:HOH:O	2.39	0.77
1:B:121[B]:LYS:HD2	11:B:529:HOH:O	1.82	0.77
1:A:92[A]:GLU:CG	4:A:205:MPD:H11	2.13	0.76
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
9:B:215:ACT:C	11:B:482[B]:HOH:O	2.35	0.73
1:B:103[B]:LYS:HD2	11:B:401:HOH:O	1.89	0.72
1:A:92[A]:GLU:HG3	4:A:205:MPD:H12	1.71	0.72
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:A:92[A]:GLU:CG	4:A:205:MPD:H12	2.22	0.69
1:B:108:LYS:HE3	11:B:484:HOH:O	1.93	0.68
1:B:98[B]:ILE:HD11	11:B:547:HOH:O	1.92	0.68
1:A:180[B]:THR:HG21	11:A:356:HOH:O	1.92	0.68
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:111[B]:GLN:OE1	11:B:484:HOH:O	2.11	0.67
1:B:75[B]:GLU:HG3	1:B:98[B]:ILE:HG23	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187[B]:GLN:OE1	8:B:208:EDO:C1	2.44	0.65
1:B:92[A]:GLU:OE2	11:B:468:HOH:O	2.10	0.64
11:A:518:HOH:O	4:B:204[B]:MPD:HM3	1.97	0.63
1:B:121[B]:LYS:CE	11:B:529:HOH:O	2.45	0.63
1:A:70:GLY:H	1:A:72:ASN:HD21	1.46	0.63
6:A:208:GOL:C1	11:A:506:HOH:O	2.40	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:124[A]:THR:HG23	11:B:535:HOH:O	2.00	0.61
1:B:98[B]:ILE:CD1	11:B:547:HOH:O	2.47	0.61
1:B:121[B]:LYS:CD	11:B:529:HOH:O	2.45	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:A:92[A]:GLU:OE2	4:A:205:MPD:CM	2.51	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:121[B]:LYS:HE3	11:B:529:HOH:O	2.04	0.57
1:A:155[B]:LYS:HA	6:A:208:GOL:H2	1.86	0.56
1:B:75[B]:GLU:O	1:B:76[B]:ASN:C	2.44	0.56
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:B:124[A]:THR:CG2	11:B:535:HOH:O	2.54	0.55
1:A:68:CYS:HB3	1:A:72:ASN:ND2	2.22	0.55
1:A:119[B]:LYS:HG3	11:A:565:HOH:O	2.08	0.54
1:A:124[B]:THR:HG21	11:A:543:HOH:O	2.07	0.54
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:B:187[B]:GLN:NE2	8:B:208:EDO:O1	2.39	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:92[B]:GLU:HG3	11:A:434:HOH:O	2.09	0.52
3:A:203:MRD:O2	11:A:490[B]:HOH:O	2.18	0.50
1:A:23[A]:LYS:HE2	11:A:489:HOH:O	2.11	0.50
3:B:206:MRD:H1C3	11:B:540:HOH:O	2.12	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:103[B]:LYS:HG3	6:B:212:GOL:H32	1.95	0.48
1:B:75[B]:GLU:HG3	1:B:98[B]:ILE:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:119[B]:LYS:CG	11:A:565:HOH:O	2.64	0.46
3:A:203:MRD:H5C2	3:A:203:MRD:H1C3	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:B:187[B]:GLN:OE1	8:B:208:EDO:H21	2.02	0.45
1:A:6[B]:LEU:CD1	3:A:203:MRD:CM	2.75	0.44
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:130:LYS:HA	1:A:157:CYS:O	2.19	0.43
1:A:53:LEU:HD23	1:A:66:ILE:HD13	2.01	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:B:187[B]:GLN:CD	8:B:208:EDO:C1	2.88	0.42
1:A:155[A]:LYS:HA	6:A:208:GOL:H2	2.01	0.42
1:B:103[B]:LYS:CG	6:B:212:GOL:H32	2.50	0.42
1:A:102:ALA:O	1:A:125:ALA:HA	2.20	0.41
1:B:187[B]:GLN:NE2	8:B:208:EDO:C1	2.83	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:124[A]:THR:HG23	11:A:502:HOH:O	2.22	0.40
1:A:26:LYS:HE2	1:A:28[A]:ILE:HD11	2.03	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

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	219/196 (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 ⓘ

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%)	59	26
1	B	186/166 (112%)	183 (98%)	3 (2%)	68	39
All	All	376/332 (113%)	369 (98%)	7 (2%)	82	30

All (7) 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	121[A]	LYS
1	B	121[B]	LYS
1	B	121[C]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	152	ASN

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Mol	Chain	Res	Type
1	A	189	GLN
1	B	18	GLN
1	B	137	ASN
1	B	189	GLN

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, 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	A	202	-	7,7,7	0.56	0	9,10,10	1.19	1 (11%)
3	MRD	A	203	-	7,7,7	0.56	0	9,10,10	1.08	0
4	MPD	A	204	-	7,7,7	0.48	0	9,10,10	0.76	0
4	MPD	A	205	-	7,7,7	0.81	0	9,10,10	1.94	3 (33%)
6	GOL	A	207[A]	-	5,5,5	0.65	0	5,5,5	0.68	0
6	GOL	A	207[B]	-	5,5,5	0.39	0	5,5,5	0.63	0
6	GOL	A	208	-	5,5,5	0.48	0	5,5,5	0.22	0
3	MRD	B	203[A]	-	7,7,7	0.66	0	9,10,10	0.63	0
4	MPD	B	204[B]	-	7,7,7	0.26	0	9,10,10	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MPD	B	205	-	7,7,7	0.47	0	9,10,10	0.74	0
3	MRD	B	206	-	7,7,7	0.53	0	9,10,10	2.26	3 (33%)
8	EDO	B	207	-	3,3,3	0.61	0	2,2,2	0.26	0
8	EDO	B	208	-	3,3,3	0.43	0	2,2,2	0.51	0
6	GOL	B	212	-	5,5,5	0.35	0	5,5,5	0.39	0
6	GOL	B	213[A]	-	5,5,5	0.39	0	5,5,5	0.40	0
6	GOL	B	213[B]	-	5,5,5	0.44	0	5,5,5	0.36	0
9	ACT	B	214	-	1,3,3	2.19	1 (100%)	0,3,3	0.00	-
9	ACT	B	215	-	1,3,3	2.09	1 (100%)	0,3,3	0.00	-
10	PO4	B	216	-	4,4,4	1.03	0	6,6,6	0.72	0
10	PO4	B	217	-	4,4,4	0.67	0	6,6,6	0.95	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	MRD	A	202	-	-	0/5/5/5	0/0/0/0
3	MRD	A	203	-	-	0/5/5/5	0/0/0/0
4	MPD	A	204	-	-	0/5/5/5	0/0/0/0
4	MPD	A	205	-	-	0/5/5/5	0/0/0/0
6	GOL	A	207[A]	-	-	0/4/4/4	0/0/0/0
6	GOL	A	207[B]	-	-	0/4/4/4	0/0/0/0
6	GOL	A	208	-	-	0/4/4/4	0/0/0/0
3	MRD	B	203[A]	-	-	0/5/5/5	0/0/0/0
4	MPD	B	204[B]	-	-	0/5/5/5	0/0/0/0
4	MPD	B	205	-	-	0/5/5/5	0/0/0/0
3	MRD	B	206	-	-	0/5/5/5	0/0/0/0
8	EDO	B	207	-	-	0/1/1/1	0/0/0/0
8	EDO	B	208	-	-	0/1/1/1	0/0/0/0
6	GOL	B	212	-	-	0/4/4/4	0/0/0/0
6	GOL	B	213[A]	-	-	0/4/4/4	0/0/0/0
6	GOL	B	213[B]	-	-	0/4/4/4	0/0/0/0
9	ACT	B	214	-	-	0/0/0/0	0/0/0/0
9	ACT	B	215	-	-	0/0/0/0	0/0/0/0
10	PO4	B	216	-	-	0/0/0/0	0/0/0/0
10	PO4	B	217	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	215	ACT	CH3-C	2.09	1.51	1.48
9	B	214	ACT	CH3-C	2.19	1.51	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	205	MPD	CM-C2-C1	-3.13	103.43	110.42
3	B	206	MRD	O2-C2-C1	-2.36	99.83	108.00
4	A	205	MPD	CM-C2-C3	-2.30	98.63	110.08
3	A	202	MRD	O2-C2-C3	-2.19	101.20	109.88
3	B	206	MRD	O2-C2-C3	2.91	121.44	109.88
4	A	205	MPD	C1-C2-C3	3.14	125.71	110.08
3	B	206	MRD	CM-C2-C1	5.29	122.22	110.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	203	MRD	10	0
4	A	205	MPD	12	0
6	A	207[A]	GOL	2	0
6	A	208	GOL	4	0
4	B	204[B]	MPD	1	0
3	B	206	MRD	12	0
8	B	208	EDO	12	0
6	B	212	GOL	5	0
9	B	215	ACT	1	0
10	B	216	PO4	2	0
10	B	217	PO4	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 [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%)	-0.63	2 (1%) 82 85	6, 11, 20, 32	3 (1%)
1	B	195/196 (99%)	-0.66	0 100 100	6, 11, 19, 30	1 (0%)
All	All	391/392 (99%)	-0.65	2 (0%) 90 93	6, 11, 20, 32	4 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-2[A]	VAL	4.7
1	A	40[A]	ASN	4.5

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(Å ²)	Q<0.9
6	GOL	A	207[A]	6/6	0.92	0.13	10.06	18,23,26,29	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	GOL	A	208	6/6	0.72	0.25	8.93	31,32,33,35	6
10	PO4	B	216	5/5	0.88	0.11	6.67	35,38,41,45	5
3	MRD	B	206	8/8	0.90	0.12	5.61	24,28,32,32	8
9	ACT	B	214	4/4	0.88	0.12	5.51	52,53,53,53	0
10	PO4	B	217	5/5	0.81	0.16	5.43	49,50,55,56	5
6	GOL	B	212	6/6	0.80	0.17	5.16	22,31,36,38	6
4	MPD	A	204	8/8	0.90	0.11	4.59	16,23,26,26	8
3	MRD	A	203	8/8	0.86	0.14	4.37	23,25,30,30	8
9	ACT	B	215	4/4	0.73	0.16	4.23	31,32,32,35	4
6	GOL	B	213[A]	6/6	0.69	0.17	4.22	54,55,56,57	6
4	MPD	A	205	8/8	0.91	0.10	3.99	15,20,25,26	8
4	MPD	B	204[B]	8/8	0.91	0.15	2.87	61,61,62,62	8
3	MRD	B	203[A]	8/8	0.87	0.12	1.85	12,17,22,23	8
8	EDO	B	207	4/4	0.68	0.13	1.83	39,42,42,46	0
4	MPD	B	205	8/8	0.91	0.08	1.72	17,24,27,29	0
8	EDO	B	208	4/4	0.75	0.14	0.90	28,28,31,31	4
3	MRD	A	202	8/8	0.94	0.09	0.44	21,25,28,28	0
5	NA	B	209	1/1	0.98	0.09	0.19	9,9,9,9	1
7	CL	B	202	1/1	0.99	0.06	-1.46	12,12,12,12	0
2	CA	B	201	1/1	1.00	0.03	-1.85	7,7,7,7	0
2	CA	A	201	1/1	1.00	0.04	-2.82	10,10,10,10	0
5	NA	B	210	1/1	0.99	0.03	-3.29	25,25,25,25	0
5	NA	A	206	1/1	0.98	0.07	-	15,15,15,15	1
6	GOL	A	207[B]	6/6	0.92	0.13	-	20,23,25,27	6
6	GOL	B	213[B]	6/6	0.69	0.17	-	30,32,33,34	6
5	NA	B	211	1/1	0.98	0.11	-	22,22,22,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.