



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 11:04 PM UTC

PDB ID : 4J0D / pdb_00004j0d
Title : tannin acyl hydrolase from Lactobacillus plantarum (Cadmium)
Authors : Ren, B.; Wu, M.; Wang, Q.; Peng, X.; Wen, H.; Chen, Q.; McKinsty, W.J.
Deposited on : 2013-01-30
Resolution : 1.60 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

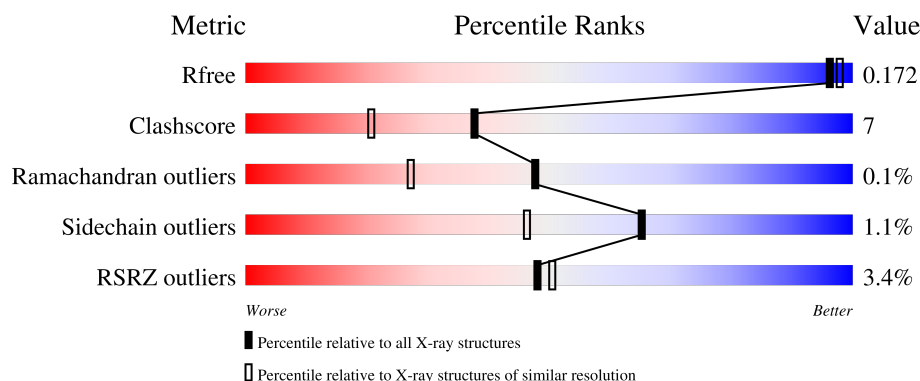
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	491	4% 85% 11% .
1	B	491	3% 87% 9% .

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	CD	B	502	-	-	-	X
3	PEG	A	503	-	X	X	-
3	PEG	A	505	-	-	X	-
3	PEG	B	508	-	-	X	-
3	PEG	B	511	-	-	X	-
5	PG4	B	503	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8177 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 Tannase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	10	0
			3638	2307	630	690	11			
1	B	470	Total	C	N	O	S	0	9	0
			3635	2308	628	687	12			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP B3Y018
A	-20	HIS	-	expression tag	UNP B3Y018
A	-19	HIS	-	expression tag	UNP B3Y018
A	-18	HIS	-	expression tag	UNP B3Y018
A	-17	HIS	-	expression tag	UNP B3Y018
A	-16	HIS	-	expression tag	UNP B3Y018
A	-15	HIS	-	expression tag	UNP B3Y018
A	-14	SER	-	expression tag	UNP B3Y018
A	-13	SER	-	expression tag	UNP B3Y018
A	-12	GLY	-	expression tag	UNP B3Y018
A	-11	VAL	-	expression tag	UNP B3Y018
A	-10	ASP	-	expression tag	UNP B3Y018
A	-9	LEU	-	expression tag	UNP B3Y018
A	-8	GLY	-	expression tag	UNP B3Y018
A	-7	THR	-	expression tag	UNP B3Y018
A	-6	GLU	-	expression tag	UNP B3Y018
A	-5	ASN	-	expression tag	UNP B3Y018
A	-4	LEU	-	expression tag	UNP B3Y018
A	-3	TYR	-	expression tag	UNP B3Y018
A	-2	PHE	-	expression tag	UNP B3Y018
A	-1	GLN	-	expression tag	UNP B3Y018
A	0	SER	-	expression tag	UNP B3Y018
B	-21	MET	-	expression tag	UNP B3Y018
B	-20	HIS	-	expression tag	UNP B3Y018
B	-19	HIS	-	expression tag	UNP B3Y018

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	expression tag	UNP B3Y018
B	-17	HIS	-	expression tag	UNP B3Y018
B	-16	HIS	-	expression tag	UNP B3Y018
B	-15	HIS	-	expression tag	UNP B3Y018
B	-14	SER	-	expression tag	UNP B3Y018
B	-13	SER	-	expression tag	UNP B3Y018
B	-12	GLY	-	expression tag	UNP B3Y018
B	-11	VAL	-	expression tag	UNP B3Y018
B	-10	ASP	-	expression tag	UNP B3Y018
B	-9	LEU	-	expression tag	UNP B3Y018
B	-8	GLY	-	expression tag	UNP B3Y018
B	-7	THR	-	expression tag	UNP B3Y018
B	-6	GLU	-	expression tag	UNP B3Y018
B	-5	ASN	-	expression tag	UNP B3Y018
B	-4	LEU	-	expression tag	UNP B3Y018
B	-3	TYR	-	expression tag	UNP B3Y018
B	-2	PHE	-	expression tag	UNP B3Y018
B	-1	GLN	-	expression tag	UNP B3Y018
B	0	SER	-	expression tag	UNP B3Y018

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

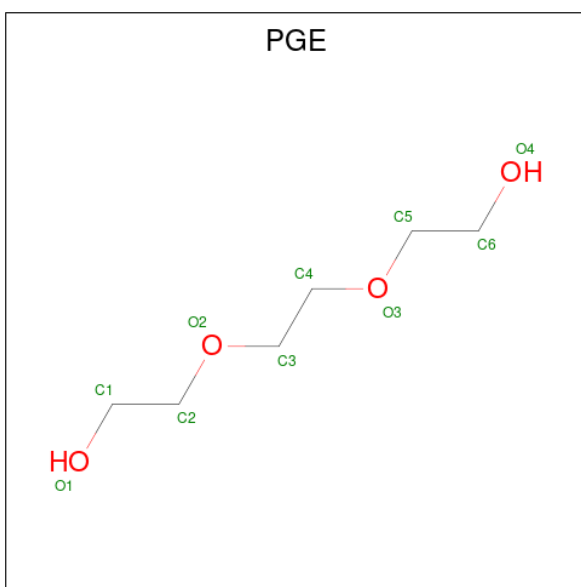
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cd 2 2	0	0
2	B	2	Total Cd 2 2	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



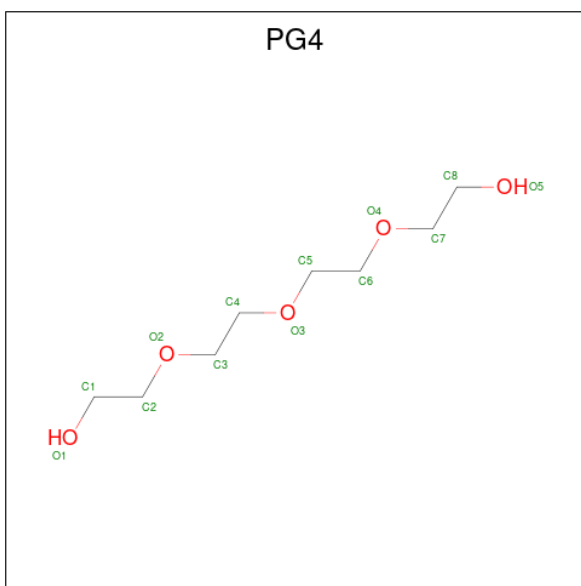
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total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

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		

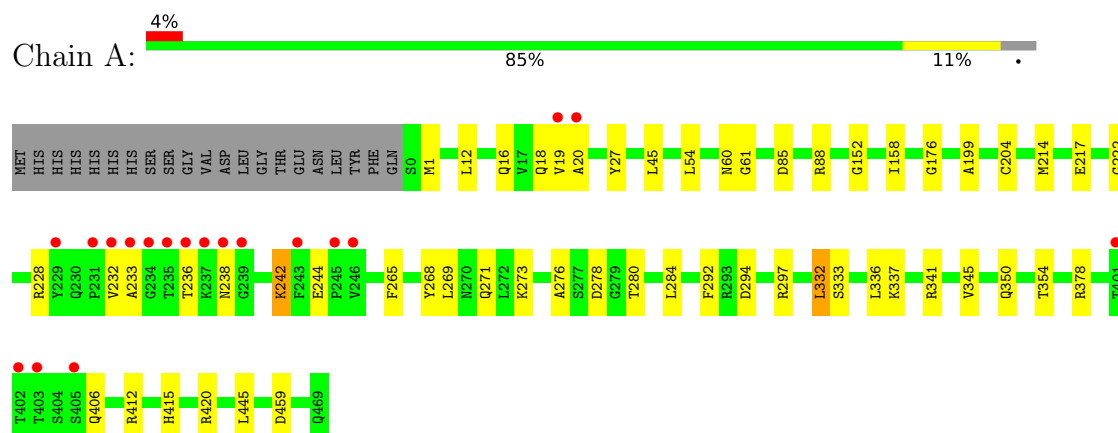
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	373	Total 373	O 373	0	0
6	B	414	Total 414	O 414	0	0

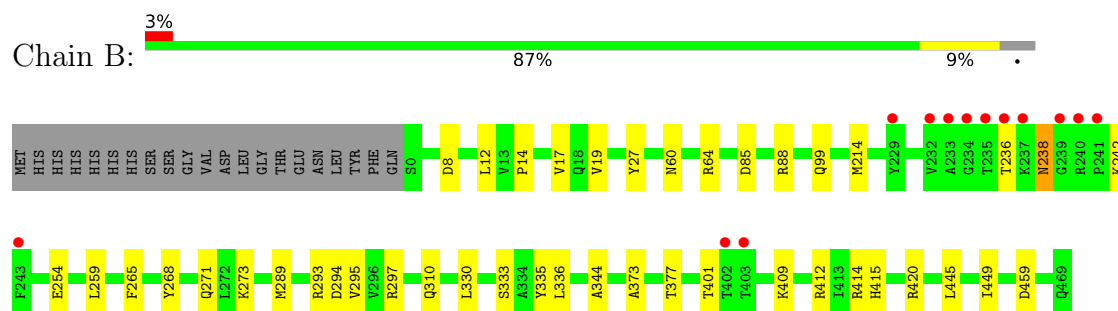
3 Residue-property plots

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: Tannase



• Molecule 1: Tannase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	46.94Å 62.92Å 84.07Å 70.58° 85.70° 78.96°	Depositor
Resolution (Å)	20.02 – 1.60 20.02 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.1 (20.02-1.60) 93.1 (20.02-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 1.60Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.143 , 0.175 0.141 , 0.172	Depositor DCC
R_{free} test set	1849 reflections (1.57%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8177	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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: PGE, PG4, PEG, CD

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	0.82	1/3743 (0.0%)	0.93	5/5106 (0.1%)
1	B	0.91	0/3744	0.95	1/5106 (0.0%)
All	All	0.87	1/7487 (0.0%)	0.94	6/10212 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	VAL	CA-CB	5.73	1.58	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ALA	N-CA-C	-6.48	92.86	111.00
1	A	345	VAL	N-CA-C	6.45	115.28	107.61
1	A	19	VAL	CB-CA-C	-5.86	101.68	111.29
1	A	222	GLY	N-CA-C	-5.39	108.28	114.69
1	A	204	CYS	O-C-N	5.19	123.92	121.53
1	B	449	ILE	CA-C-O	5.13	122.53	119.19

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	3638	0	3581	50	1
1	B	3635	0	3580	47	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	21	0	30	10	0
3	B	56	0	80	18	0
4	A	10	0	14	2	0
5	B	26	0	35	12	0
6	A	373	0	0	10	2
6	B	414	0	0	11	4
All	All	8177	0	7320	103	5

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 7.

All (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ASN:HB3	6:B:987:HOH:O	1.57	1.05
1:A:273:LYS:NZ	6:A:940:HOH:O	1.90	1.03
1:B:459:ASP:HB3	3:B:511:PEG:H41	1.34	1.01
1:A:294:ASP:OD1	1:A:297:ARG:NH2	1.98	0.96
1:B:294:ASP:OD1	1:B:297[A]:ARG:NH2	1.99	0.95
1:A:278:ASP:OD1	1:A:280[A]:THR:HG22	1.66	0.94
1:B:289[A]:MET:CE	6:B:981:HOH:O	2.21	0.89
1:B:273:LYS:NZ	6:B:973:HOH:O	2.07	0.87
5:B:504:PG4:H12	6:B:801:HOH:O	1.74	0.86
1:B:293:ARG:HE	5:B:503:PG4:H62	1.41	0.85
1:A:269[A]:LEU:HD21	1:A:292:PHE:CD2	2.13	0.84
5:B:504:PG4:O1	6:B:824:HOH:O	1.97	0.83
1:A:459:ASP:HB3	3:A:503:PEG:H21	1.61	0.82
1:A:61:GLY:H	3:A:505:PEG:H32	1.43	0.82
1:B:293:ARG:HH21	5:B:503:PG4:H41	1.42	0.82
1:B:336:LEU:HD12	5:B:503:PG4:H32	1.62	0.82
1:A:412:ARG:HH21	3:A:503:PEG:H21	1.47	0.79
1:B:64:ARG:HD2	3:B:509:PEG:H21	1.65	0.78
1:B:409:LYS:HB3	3:B:508:PEG:H41	1.67	0.77
1:A:61:GLY:H	3:A:505:PEG:C3	1.99	0.74
1:A:350[A]:GLN:OE1	1:A:354:THR:OG1	2.06	0.74
1:B:236:THR:HG1	1:B:238:ASN:CG	1.96	0.73
6:A:749:HOH:O	1:B:271:GLN:HG3	1.90	0.71
1:A:269[A]:LEU:HD21	1:A:292:PHE:CG	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ARG:HH21	5:B:503:PG4:C4	2.04	0.70
1:B:238:ASN:N	1:B:238:ASN:OD1	2.25	0.70
1:B:293:ARG:NE	5:B:503:PG4:H62	2.07	0.69
3:B:512:PEG:O1	6:B:952:HOH:O	2.10	0.68
1:A:61:GLY:N	3:A:505:PEG:H32	2.11	0.66
1:A:27:TYR:CG	1:A:54[B]:LEU:HD12	2.30	0.66
1:A:269[A]:LEU:HD23	1:A:284:LEU:CD1	2.26	0.66
1:A:332:LEU:HD13	4:A:504:PGE:H3	1.77	0.65
1:A:271:GLN:HG3	6:A:949:HOH:O	1.96	0.65
1:A:459:ASP:HB3	3:A:503:PEG:C2	2.28	0.64
1:B:409:LYS:NZ	3:B:508:PEG:H21	2.12	0.64
1:A:61:GLY:HA2	3:A:505:PEG:H12	1.80	0.64
1:A:16:GLN:NE2	6:A:875:HOH:O	2.05	0.63
1:A:214[B]:MET:HE3	1:A:265:PHE:HA	1.82	0.62
1:B:214[B]:MET:HE3	1:B:265:PHE:HA	1.82	0.62
1:A:228:ARG:NH1	6:A:873:HOH:O	2.32	0.62
1:A:333:SER:O	1:A:337:LYS:HG3	1.99	0.62
1:A:27:TYR:CD2	1:A:54[B]:LEU:HD12	2.38	0.58
1:B:459:ASP:CB	3:B:511:PEG:H41	2.22	0.58
1:B:293:ARG:HE	5:B:503:PG4:C6	2.16	0.57
1:B:412:ARG:HH21	3:B:511:PEG:H42	1.68	0.57
1:B:409:LYS:HZ2	3:B:508:PEG:H21	1.70	0.57
1:A:336:LEU:CD1	4:A:504:PGE:H32	2.35	0.57
1:A:158:ILE:HG12	1:A:199:ALA:HB3	1.86	0.56
1:A:214[B]:MET:HE1	1:A:268:TYR:CB	2.37	0.55
1:B:333:SER:OG	5:B:503:PG4:H31	2.06	0.55
1:A:152:GLY:O	6:A:639:HOH:O	2.18	0.54
1:A:236:THR:HG22	1:A:238:ASN:H	1.73	0.54
1:B:214[B]:MET:HE1	1:B:268:TYR:CB	2.37	0.54
1:B:64:ARG:HH11	3:B:509:PEG:H21	1.72	0.54
1:B:17:VAL:HG22	1:B:19:VAL:HG13	1.90	0.53
1:A:265:PHE:CE2	1:A:269[A]:LEU:HD22	2.44	0.53
1:B:409:LYS:HZ1	3:B:508:PEG:H42	1.73	0.53
1:B:373:ALA:O	1:B:377[B]:THR:HG23	2.08	0.53
1:B:293:ARG:NH2	5:B:503:PG4:H41	2.20	0.53
1:A:378:ARG:NH2	6:A:908:HOH:O	2.38	0.52
1:A:61:GLY:N	3:A:505:PEG:C3	2.69	0.51
1:A:214[A]:MET:HG3	6:A:638:HOH:O	2.11	0.51
1:A:378:ARG:NE	6:A:908:HOH:O	2.41	0.50
1:B:310:GLN:HG3	6:B:932:HOH:O	2.11	0.49
1:B:64:ARG:CD	3:B:509:PEG:H21	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:HIS:O	1:B:445:LEU:HA	2.13	0.48
1:A:85:ASP:HB3	1:A:88:ARG:HB2	1.96	0.48
1:A:278:ASP:OD1	1:A:280[B]:THR:HG23	2.14	0.47
1:A:269[A]:LEU:CD2	1:A:292:PHE:CD2	2.93	0.47
1:B:295:VAL:HG23	3:B:512:PEG:H21	1.95	0.47
1:A:18:GLN:NE2	6:A:875:HOH:O	2.34	0.47
1:B:289[A]:MET:HE2	6:B:981:HOH:O	2.03	0.47
1:B:214[B]:MET:HE2	1:B:214[B]:MET:HB2	1.82	0.47
1:B:8:ASP:OD2	6:B:873:HOH:O	2.21	0.46
1:B:295:VAL:CG2	3:B:512:PEG:H21	2.45	0.46
1:B:414:ARG:HH21	3:B:511:PEG:H42	1.81	0.46
1:A:12:LEU:HB3	1:A:27:TYR:HB3	1.97	0.46
1:B:214[A]:MET:HG3	6:B:632:HOH:O	2.15	0.46
1:A:415:HIS:O	1:A:445:LEU:HA	2.16	0.46
1:A:276:ALA:HB3	1:A:280[A]:THR:HG22	1.97	0.45
1:A:412:ARG:HH21	3:A:503:PEG:C2	2.23	0.45
1:A:232:VAL:HG22	1:A:242:LYS:HB2	1.96	0.45
1:A:176:GLY:O	1:A:406:GLN:HB3	2.16	0.45
1:B:330:LEU:HD11	1:B:335:TYR:HB2	1.99	0.45
1:A:278:ASP:CG	1:A:280[B]:THR:HG23	2.43	0.44
1:B:85:ASP:HB3	1:B:88:ARG:HB2	1.99	0.44
5:B:503:PG4:H41	5:B:503:PG4:H61	1.60	0.44
1:B:19:VAL:CG1	3:B:510:PEG:H42	2.48	0.44
1:A:236:THR:OG1	1:A:242:LYS:HD3	2.18	0.43
1:A:269[A]:LEU:HD23	1:A:284:LEU:HD11	2.01	0.43
1:A:276:ALA:HB3	1:A:280[A]:THR:CG2	2.49	0.43
1:B:401:THR:OG1	6:B:938:HOH:O	2.21	0.43
3:B:508:PEG:H21	3:B:508:PEG:H42	1.76	0.42
1:B:14:PRO:HB2	3:B:507:PEG:H32	2.02	0.42
1:A:217:GLU:OE2	1:A:341[B]:ARG:NH2	2.37	0.41
5:B:503:PG4:H61	5:B:503:PG4:H81	1.70	0.41
1:A:60:ASN:N	3:A:505:PEG:H32	2.35	0.41
1:A:269[A]:LEU:HD23	1:A:284:LEU:HD12	2.02	0.41
1:B:17:VAL:HG11	1:B:99:GLN:HG2	2.02	0.41
1:B:254:GLU:OE2	1:B:344:ALA:HB1	2.21	0.41
1:B:14:PRO:HB2	3:B:507:PEG:H11	2.03	0.40
1:A:45:LEU:C	1:A:45:LEU:HD12	2.47	0.40
1:B:12:LEU:HB3	1:B:27:TYR:HB3	2.03	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:956:HOH:O	6:B:974:HOH:O[1_455]	1.89	0.31
6:B:816:HOH:O	6:B:817:HOH:O[1_565]	1.97	0.23
6:B:872:HOH:O	6:B:907:HOH:O[1_545]	2.17	0.03
1:A:244:GLU:OE1	6:A:918:HOH:O[1_455]	2.19	0.01
6:A:959:HOH:O	6:B:767:HOH:O[1_556]	2.19	0.01

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	478/491 (97%)	467 (98%)	10 (2%)	1 (0%)	43	24
1	B	477/491 (97%)	466 (98%)	11 (2%)	0	100	100
All	All	955/982 (97%)	933 (98%)	21 (2%)	1 (0%)	48	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	ALA

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	379/389 (97%)	375 (99%)	4 (1%)	65	46
1	B	378/389 (97%)	374 (99%)	4 (1%)	65	46
All	All	757/778 (97%)	749 (99%)	8 (1%)	65	46

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	242	LYS
1	A	332	LEU
1	A	420	ARG
1	B	238	ASN
1	B	242	LYS
1	B	259	LEU
1	B	420	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	ASN
1	A	224	ASN
1	A	264	GLN
1	B	100	GLN
1	B	221	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	PEG	B	507	-	6,6,6	0.45	0	5,5,5	1.75	1 (20%)
3	PEG	B	505	-	6,6,6	0.55	0	5,5,5	0.96	0
3	PEG	A	505	-	6,6,6	0.72	0	5,5,5	1.74	2 (40%)
3	PEG	B	509	-	6,6,6	0.63	0	5,5,5	1.45	0
5	PG4	B	503	-	12,12,12	0.71	0	11,11,11	1.59	2 (18%)
3	PEG	A	506	-	6,6,6	0.57	0	5,5,5	1.46	1 (20%)
5	PG4	B	504	-	12,12,12	0.74	0	11,11,11	1.38	0
3	PEG	A	503	-	6,6,6	0.38	0	5,5,5	2.74	4 (80%)
3	PEG	B	510	-	6,6,6	0.53	0	5,5,5	1.67	1 (20%)
3	PEG	B	511	-	6,6,6	0.52	0	5,5,5	1.48	1 (20%)
4	PGE	A	504	-	9,9,9	0.67	0	8,8,8	1.36	1 (12%)
3	PEG	B	512	-	6,6,6	0.64	0	5,5,5	1.41	0
3	PEG	B	508	-	6,6,6	0.65	0	5,5,5	1.33	1 (20%)
3	PEG	B	506	-	6,6,6	0.37	0	5,5,5	1.37	1 (20%)

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	PEG	B	507	-	-	1/4/4/4	-
3	PEG	B	505	-	-	0/4/4/4	-
3	PEG	A	505	-	-	2/4/4/4	-
3	PEG	B	509	-	-	2/4/4/4	-
5	PG4	B	503	-	-	5/10/10/10	-
3	PEG	A	506	-	-	2/4/4/4	-
5	PG4	B	504	-	-	4/10/10/10	-
3	PEG	A	503	-	-	2/4/4/4	-
3	PEG	B	510	-	-	1/4/4/4	-
3	PEG	B	511	-	-	3/4/4/4	-
4	PGE	A	504	-	-	2/7/7/7	-
3	PEG	B	512	-	-	2/4/4/4	-
3	PEG	B	508	-	-	1/4/4/4	-
3	PEG	B	506	-	-	1/4/4/4	-

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	503	PEG	O2-C2-C1	3.81	126.91	110.11
3	A	503	PEG	O2-C3-C4	2.95	123.11	110.11
3	B	507	PEG	O2-C3-C4	2.83	122.59	110.11
3	B	506	PEG	C3-O2-C2	2.81	125.57	113.26
5	B	503	PG4	O2-C3-C4	2.81	123.14	110.35
4	A	504	PGE	O2-C2-C1	2.75	122.22	110.11
5	B	503	PG4	O3-C4-C3	2.63	122.36	110.35
3	A	503	PEG	C3-O2-C2	2.60	124.65	113.26
3	B	511	PEG	C3-O2-C2	2.57	124.51	113.26
3	A	505	PEG	O2-C2-C1	2.56	121.41	110.11
3	B	510	PEG	O2-C2-C1	2.44	120.88	110.11
3	A	506	PEG	O2-C2-C1	2.44	120.87	110.11
3	A	503	PEG	O1-C1-C2	2.21	124.84	111.82
3	A	505	PEG	O2-C3-C4	2.15	119.60	110.11
3	B	508	PEG	O2-C2-C1	2.11	119.42	110.11

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	506	PEG	C4-C3-O2-C2
3	B	508	PEG	C4-C3-O2-C2
5	B	503	PG4	C6-C5-O3-C4
4	A	504	PGE	C4-C3-O2-C2
4	A	504	PGE	O1-C1-C2-O2
3	A	503	PEG	O1-C1-C2-O2
3	A	503	PEG	O2-C3-C4-O4
3	B	507	PEG	O2-C3-C4-O4
5	B	503	PG4	C8-C7-O4-C6
3	A	505	PEG	O1-C1-C2-O2
3	B	509	PEG	O2-C3-C4-O4
3	B	511	PEG	O2-C3-C4-O4
5	B	503	PG4	O1-C1-C2-O2
5	B	504	PG4	O2-C3-C4-O3
3	A	506	PEG	O1-C1-C2-O2
3	B	510	PEG	O2-C3-C4-O4
3	B	512	PEG	C1-C2-O2-C3
5	B	504	PG4	O1-C1-C2-O2
3	B	511	PEG	C1-C2-O2-C3
3	B	509	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
5	B	504	PG4	O4-C7-C8-O5
5	B	504	PG4	O3-C5-C6-O4
3	B	512	PEG	O2-C3-C4-O4
3	B	511	PEG	O1-C1-C2-O2
3	B	506	PEG	O2-C3-C4-O4
5	B	503	PG4	C1-C2-O2-C3
3	A	505	PEG	C1-C2-O2-C3
5	B	503	PG4	O3-C5-C6-O4

There are no ring outliers.

11 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	507	PEG	2	0
3	A	505	PEG	6	0
3	B	509	PEG	3	0
5	B	503	PG4	10	0
5	B	504	PG4	2	0
3	A	503	PEG	4	0
3	B	510	PEG	1	0
3	B	511	PEG	4	0
4	A	504	PGE	2	0
3	B	512	PEG	3	0
3	B	508	PEG	5	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, 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	470/491 (95%)	-0.39	19 (4%)	42 44	6, 17, 45, 136	10 (2%)
1	B	470/491 (95%)	-0.59	13 (2%)	55 58	5, 14, 38, 124	9 (1%)
All	All	940/982 (95%)	-0.49	32 (3%)	48 50	5, 15, 41, 136	19 (2%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	THR	5.7
1	A	236	THR	5.0
1	A	20	ALA	4.2
1	A	237	LYS	4.0
1	A	238	ASN	3.8
1	B	233	ALA	3.7
1	A	229	TYR	3.2
1	A	233	ALA	3.2
1	B	402	THR	3.1
1	B	234	GLY	3.0
1	B	232	VAL	3.0
1	A	402	THR	3.0
1	B	243	PHE	2.8
1	A	405	SER	2.8
1	A	232	VAL	2.7
1	A	401	THR	2.7
1	A	403	THR	2.7
1	A	239	GLY	2.7
1	A	243	PHE	2.6
1	A	234	GLY	2.6
1	A	19	VAL	2.5
1	B	235	THR	2.5
1	B	229[A]	TYR	2.4
1	B	236	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	237	LYS	2.3
1	A	231	PRO	2.2
1	B	241	PRO	2.2
1	B	403	THR	2.2
1	B	240	ARG	2.2
1	B	239	GLY	2.2
1	A	246	VAL	2.2
1	A	245	PRO	2.2

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
3	PEG	B	507	7/7	0.75	0.15	33,42,46,46	0
2	CD	B	502	1/1	0.76	0.40	76,76,76,76	1
3	PEG	B	510	7/7	0.81	0.12	38,40,46,52	0
3	PEG	B	512	7/7	0.84	0.11	41,43,47,48	0
3	PEG	B	509	7/7	0.85	0.12	37,45,48,51	0
3	PEG	A	506	7/7	0.87	0.10	35,39,45,49	0
5	PG4	B	503	13/13	0.88	0.11	20,32,46,49	0
3	PEG	B	506	7/7	0.89	0.10	19,23,31,33	0
3	PEG	B	508	7/7	0.89	0.09	22,29,35,44	0
3	PEG	A	503	7/7	0.90	0.12	20,28,38,39	0
3	PEG	A	505	7/7	0.90	0.10	28,35,39,44	0
5	PG4	B	504	13/13	0.90	0.10	27,36,47,48	0
4	PGE	A	504	10/10	0.92	0.10	25,33,45,49	0
3	PEG	B	511	7/7	0.92	0.10	18,32,37,41	0
2	CD	A	502	1/1	0.92	0.14	27,27,27,27	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CD	A	501	1/1	0.93	0.08	35,35,35,35	1
3	PEG	B	505	7/7	0.94	0.07	19,22,26,27	0
2	CD	B	501	1/1	0.97	0.06	31,31,31,31	1

6.5 Other polymers [i](#)

There are no such residues in this entry.