



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 11:04 am BST

PDB ID : 5YGR
Title : Crystal structure of PLP bound Diaminopropionate ammonia lyase from *Salmonella typhimurium*
Authors : Geeta, D.; Shveta, B.; Shavithri, H.S.; Murthy, M.R.N.
Deposited on : 2017-09-25
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

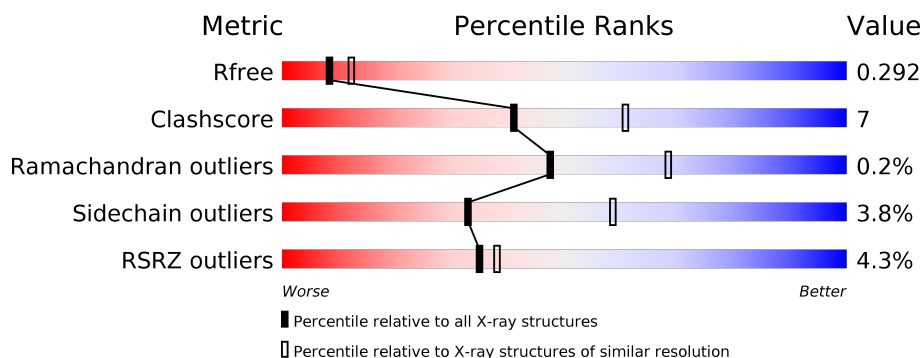
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	404	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>10%</div> <div>7%</div> </div> </div>
2	B	412	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>11%</div> </div> </div>
2	C	412	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>9%</div> <div>8%</div> </div> </div>
2	D	412	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>6%</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	504	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11693 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.

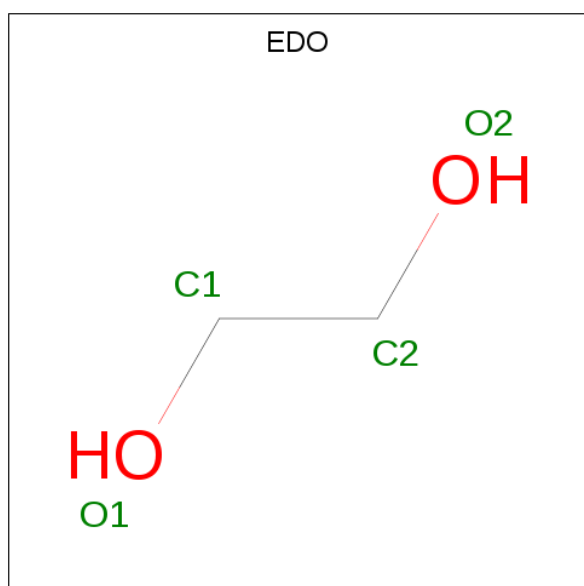
- Molecule 1 is a protein called Diaminopropionate ammonia lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	P	S	0	0	0
			2695	1690	471	515	1	18			

- Molecule 2 is a protein called Diaminopropionate ammonia lyase.

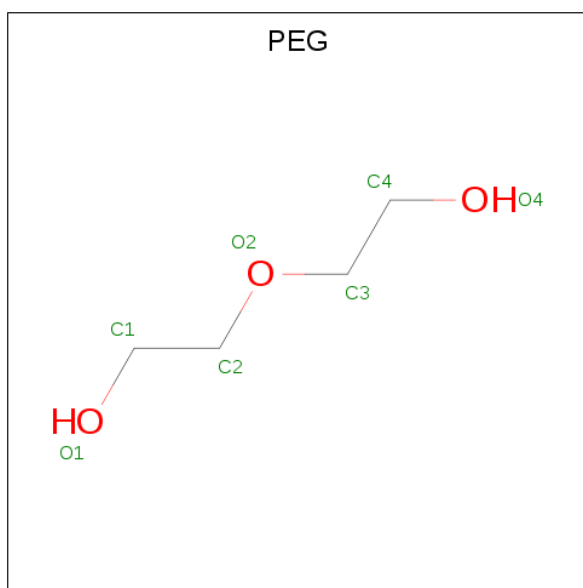
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	365	Total	C	N	O	P	S	0	1	0
			2632	1655	460	499	1	17			
2	C	380	Total	C	N	O	P	S	0	0	0
			2792	1760	485	527	1	19			
2	D	388	Total	C	N	O	P	S	0	4	0
			2893	1831	495	548	1	18			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	142	Total	O	0	0
			142	142		
6	B	144	Total	O	0	0
			144	144		
6	C	132	Total	O	0	0
			132	132		

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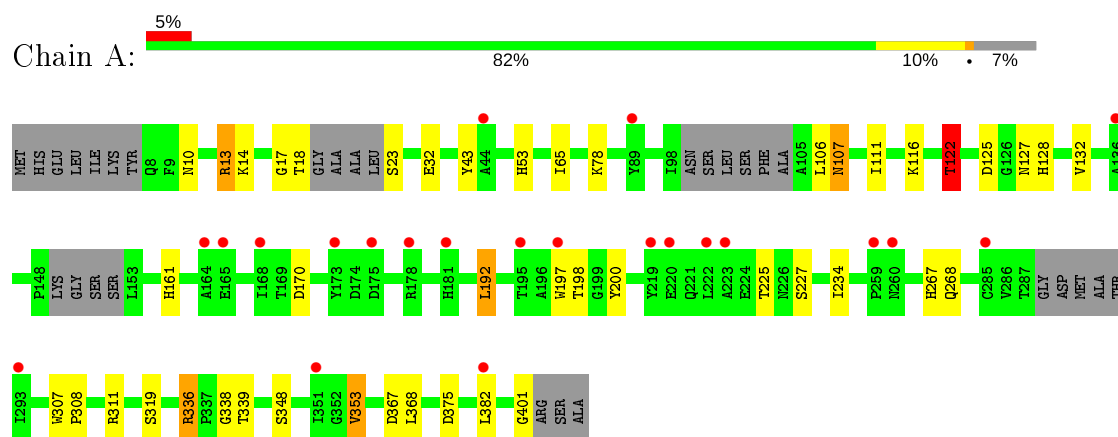
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	165	Total 165	O 165	0	0

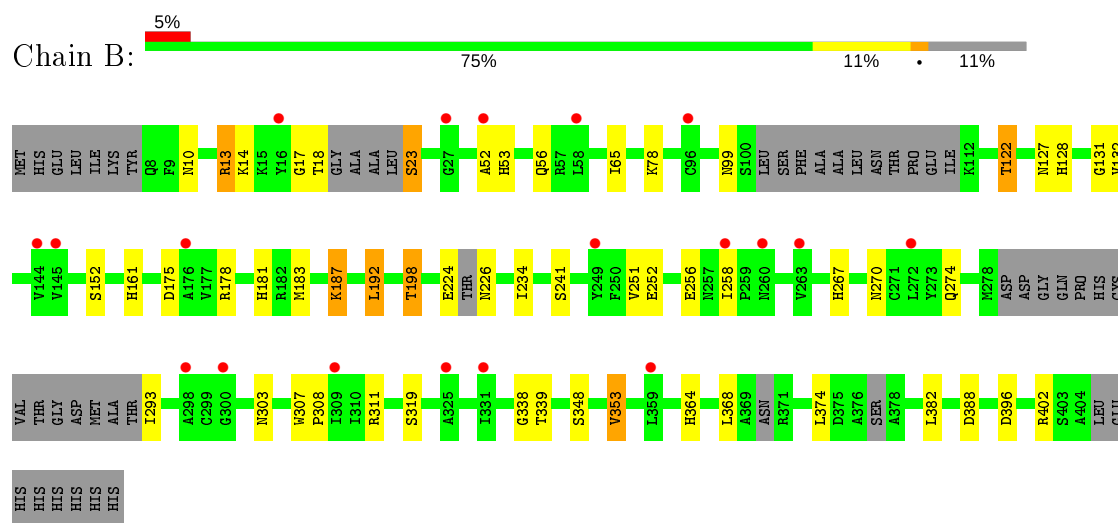
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

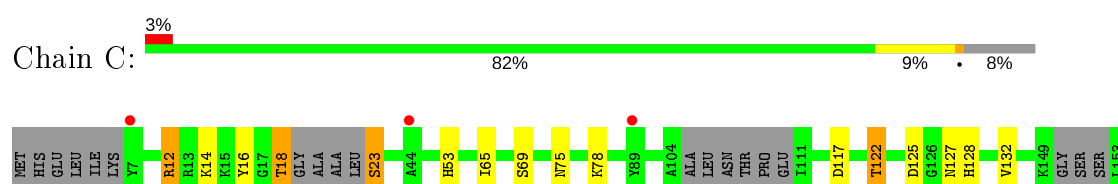
• Molecule 1: Diaminopropionate ammonia lyase

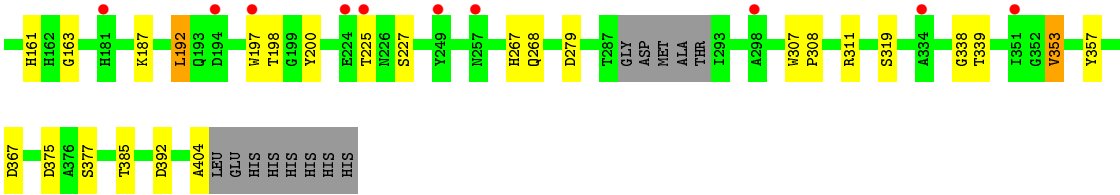


• Molecule 2: Diaminopropionate ammonia lyase

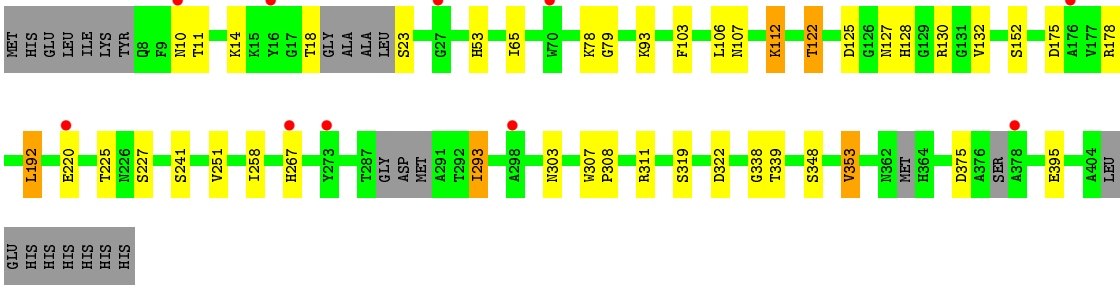
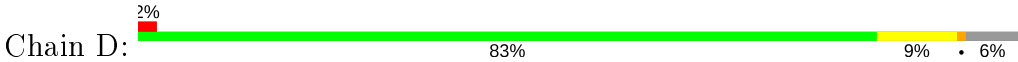


• Molecule 2: Diaminopropionate ammonia lyase





● Molecule 2: Diaminopropionate ammonia lyase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.89Å 128.44Å 138.10Å 90.00° 110.28° 90.00°	Depositor
Resolution (Å)	77.00 – 2.50 76.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (77.00-2.50) 99.9 (76.22-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.237 , 0.299 0.234 , 0.292	Depositor DCC
R_{free} test set	2802 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	1.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11693	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.85% 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: PO4, PEG, LLP, EDO

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	0.59	0/2727	0.69	1/3721 (0.0%)
2	B	0.59	1/2661 (0.0%)	0.69	0/3624
2	C	0.59	0/2825	0.69	0/3848
2	D	0.62	0/2934	0.72	3/3992 (0.1%)
All	All	0.60	1/11147 (0.0%)	0.70	4/15185 (0.0%)

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
2	B	0	1
2	C	0	1
2	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	187	LYS	C-N	-5.35	1.23	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	79	GLY	N-CA-C	-6.28	97.40	113.10
2	D	130	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	122	THR	CB-CA-C	-5.39	97.03	111.60
2	D	130	ARG	NE-CZ-NH1	5.15	122.88	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	338	GLY	Peptide
2	B	338	GLY	Peptide
2	C	338	GLY	Peptide
2	D	338	GLY	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	2695	0	2414	36	0
2	B	2632	0	2365	52	0
2	C	2792	0	2591	39	0
2	D	2893	0	2725	28	0
3	A	8	0	12	0	0
3	B	16	0	24	1	0
3	D	8	0	12	0	0
4	A	7	0	10	0	0
4	B	14	0	20	0	0
5	A	10	0	0	2	0
5	B	10	0	0	0	0
5	C	10	0	0	1	0
5	D	15	0	0	1	0
6	A	142	0	0	9	0
6	B	144	0	0	16	0
6	C	132	0	0	8	0
6	D	165	0	0	3	0
All	All	11693	0	10173	150	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 7.

All (150) 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)
2:C:78:LLP:H2'2	2:C:385:THR:OG1	1.16	1.27
2:C:18:THR:HG21	6:C:618:HOH:O	1.46	1.15
2:C:78:LLP:C2'	2:C:385:THR:OG1	2.04	1.05
2:B:293:ILE:CB	6:B:693:HOH:O	2.03	1.04
2:C:78:LLP:H2'2	2:C:385:THR:CB	1.92	0.99
1:A:268:GLN:CB	6:A:703:HOH:O	2.09	0.98
1:A:170:ASP:CB	6:A:707:HOH:O	2.13	0.94
2:B:198:THR:HG21	6:B:729:HOH:O	1.68	0.93
2:C:404:ALA:O	6:C:601:HOH:O	1.87	0.92
2:D:293:ILE:CB	6:D:703:HOH:O	2.18	0.91
2:B:270:ASN:CB	6:B:672:HOH:O	2.22	0.87
2:C:117:ASP:HB2	6:C:650:HOH:O	1.80	0.80
2:B:56:GLN:CB	6:D:740:HOH:O	2.29	0.80
2:D:293:ILE:CB	2:D:322:ASP:OD2	2.32	0.77
2:C:78:LLP:H5'1	2:C:78:LLP:NZ	2.01	0.76
2:C:78:LLP:H2'2	2:C:385:THR:HG1	1.47	0.75
2:D:78:LLP:H2'3	2:D:348:SER:HB2	1.77	0.66
2:B:122:THR:HG21	2:B:128:HIS:HE2	1.60	0.66
2:B:161:HIS:HD2	6:B:720:HOH:O	1.78	0.66
2:B:78:LLP:H2'3	2:B:348:SER:HB2	1.77	0.66
1:A:78:LLP:H2'3	1:A:348:SER:HB2	1.78	0.66
2:B:402:ARG:HB2	6:B:673:HOH:O	1.95	0.65
2:C:357:TYR:OH	2:D:395:GLU:OE1	2.09	0.62
2:C:125:ASP:N	5:C:501:PO4:O2	2.33	0.62
1:A:111:ILE:C	6:A:610:HOH:O	2.37	0.61
2:C:375:ASP:OD1	2:C:377:SER:OG	2.14	0.61
2:C:225:THR:HG1	2:C:227:SER:HG	1.49	0.60
1:A:336:ARG:NH2	2:B:388:ASP:OD2	2.34	0.60
2:C:392:ASP:CB	6:C:672:HOH:O	2.48	0.60
2:B:183:MET:O	2:B:187:LYS:HB2	2.02	0.59
2:B:274:GLN:CB	6:B:734:HOH:O	2.50	0.59
1:A:122:THR:CG2	1:A:192:LEU:O	2.50	0.59
2:D:122:THR:CG2	2:D:192:LEU:O	2.51	0.59
2:C:122:THR:CG2	2:C:192:LEU:O	2.51	0.58
1:A:225:THR:HG1	1:A:227:SER:HG	1.50	0.58
2:B:256:GLU:HB2	2:C:163:GLY:HA2	1.85	0.58
1:A:107:ASN:N	1:A:107:ASN:OD1	2.36	0.58
2:C:122:THR:HG21	2:C:128:HIS:NE2	2.19	0.57
1:A:13:ARG:HH11	1:A:13:ARG:HB2	1.70	0.57
2:B:122:THR:CG2	2:B:192:LEU:O	2.51	0.57
2:B:13:ARG:HB2	2:B:13:ARG:HH11	1.70	0.57
1:A:122:THR:HG21	1:A:128:HIS:NE2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:225:THR:HG1	2:D:227:SER:HG	1.52	0.57
2:D:53:HIS:CG	2:D:339:THR:HB	2.40	0.57
1:A:125:ASP:N	5:A:504:PO4:O1	2.33	0.56
2:D:122:THR:HG21	2:D:128:HIS:NE2	2.21	0.56
2:B:181:HIS:HD2	6:B:723:HOH:O	1.88	0.56
1:A:53:HIS:CG	1:A:339:THR:HB	2.42	0.55
2:B:53:HIS:CG	2:B:339:THR:HB	2.41	0.55
2:B:224:GLU:O	2:B:226:ASN:N	2.39	0.55
2:B:122:THR:HG21	2:B:128:HIS:NE2	2.21	0.55
2:C:53:HIS:CG	2:C:339:THR:HB	2.41	0.55
2:B:23:SER:HA	6:B:713:HOH:O	2.06	0.54
1:A:32:GLU:HG3	6:A:693:HOH:O	2.05	0.54
2:B:14:LYS:CD	2:B:311:ARG:O	2.56	0.54
2:B:198:THR:CG2	6:B:721:HOH:O	2.55	0.54
2:B:252:GLU:OE1	6:B:602:HOH:O	2.18	0.54
2:B:13:ARG:HH21	2:B:368:LEU:CD1	2.21	0.54
1:A:14:LYS:CD	1:A:311:ARG:O	2.56	0.54
2:B:13:ARG:NH2	2:B:368:LEU:CD1	2.70	0.53
2:C:16:TYR:CE2	2:C:279:ASP:OD1	2.62	0.53
2:D:14:LYS:CD	2:D:311:ARG:O	2.57	0.53
2:C:78:LLP:O3	2:C:127:ASN:ND2	2.38	0.53
1:A:13:ARG:NH2	1:A:368:LEU:CD1	2.72	0.52
2:C:23:SER:CB	6:C:690:HOH:O	2.58	0.52
2:B:78:LLP:OP4	2:B:78:LLP:C4'	2.59	0.51
2:C:14:LYS:CD	2:C:311:ARG:O	2.59	0.51
1:A:401:GLY:HA3	6:A:601:HOH:O	2.10	0.50
1:A:78:LLP:C4'	1:A:78:LLP:OP4	2.60	0.50
2:C:187:LYS:HA	6:C:625:HOH:O	2.12	0.49
2:C:122:THR:HG23	2:C:192:LEU:O	2.12	0.49
1:A:13:ARG:HH21	1:A:368:LEU:CD1	2.25	0.49
1:A:116:LYS:CB	6:A:605:HOH:O	2.60	0.49
2:B:198:THR:HB	6:B:721:HOH:O	2.11	0.49
2:D:125:ASP:HB2	5:D:503:PO4:O2	2.13	0.49
2:D:122:THR:HG23	2:D:192:LEU:O	2.12	0.49
1:A:122:THR:HG23	1:A:192:LEU:O	2.12	0.49
2:C:23:SER:HB2	6:C:690:HOH:O	2.13	0.49
2:B:122:THR:HG23	2:B:192:LEU:O	2.13	0.48
2:B:374:LEU:CA	6:B:670:HOH:O	2.61	0.48
2:D:78:LLP:OP4	2:D:78:LLP:C4'	2.61	0.48
2:D:78:LLP:H2'1	2:D:127:ASN:ND2	2.29	0.48
1:A:43:TYR:CD1	1:A:43:TYR:C	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:THR:CG2	6:C:618:HOH:O	2.27	0.47
1:A:78:LLP:H2'1	1:A:127:ASN:ND2	2.30	0.47
2:C:307:TRP:HB3	2:C:308:PRO:HD3	1.96	0.47
2:D:107:ASN:HA	2:D:112:LYS:NZ	2.30	0.47
2:D:307:TRP:HB3	2:D:308:PRO:HD3	1.96	0.47
2:C:78:LLP:C2'	2:C:385:THR:HG1	2.11	0.46
2:B:251:VAL:HG22	2:B:258:ILE:HG23	1.98	0.46
2:B:364[A]:HIS:CE1	6:B:702:HOH:O	2.68	0.46
2:D:93[B]:LYS:CA	2:D:93[B]:LYS:CE	2.93	0.46
2:D:132:VAL:HG22	2:D:192:LEU:HD23	1.98	0.46
1:A:307:TRP:HB3	1:A:308:PRO:HD3	1.98	0.46
2:C:267:HIS:HA	2:C:319:SER:HG	1.81	0.46
2:B:78:LLP:H2'1	2:B:127:ASN:ND2	2.31	0.45
2:D:11:THR:HG21	6:D:705:HOH:O	2.15	0.45
2:D:267:HIS:HA	2:D:319:SER:OG	2.16	0.45
2:B:307:TRP:HB3	2:B:308:PRO:HD3	1.98	0.45
1:A:65:ILE:HD11	1:A:353:VAL:HG13	1.98	0.45
1:A:267:HIS:HA	1:A:319:SER:HG	1.82	0.45
2:B:267:HIS:HA	2:B:319:SER:HG	1.81	0.45
2:B:364[A]:HIS:CD2	2:B:364[A]:HIS:O	2.69	0.45
2:B:65:ILE:HD11	2:B:353:VAL:HG13	1.99	0.45
2:B:131:GLY:HA3	6:B:661:HOH:O	2.17	0.44
1:A:267:HIS:HA	1:A:319:SER:OG	2.17	0.44
2:B:364[A]:HIS:HD2	2:B:364[A]:HIS:O	1.99	0.44
1:A:17:GLY:HA3	6:A:692:HOH:O	2.17	0.44
2:B:175:ASP:OD1	2:B:178:ARG:NH1	2.50	0.44
2:C:65:ILE:HD11	2:C:353:VAL:HG13	1.99	0.44
1:A:401:GLY:CA	6:A:601:HOH:O	2.64	0.44
2:B:267:HIS:HA	2:B:319:SER:OG	2.17	0.44
2:B:132:VAL:HG22	2:B:192:LEU:HD23	1.99	0.44
2:B:256:GLU:HG3	2:C:163:GLY:O	2.18	0.44
2:D:251:VAL:HG22	2:D:258:ILE:HG23	2.00	0.44
1:A:10:ASN:HB2	1:A:319:SER:HB3	2.00	0.44
1:A:111:ILE:CB	6:A:610:HOH:O	2.66	0.43
2:D:375:ASP:OD1	2:D:375:ASP:C	2.57	0.43
2:B:256:GLU:CG	2:C:163:GLY:O	2.67	0.43
2:C:375:ASP:OD1	2:C:375:ASP:C	2.57	0.43
2:C:267:HIS:HA	2:C:319:SER:OG	2.17	0.43
2:D:241:SER:OG	2:D:303:ASN:ND2	2.52	0.43
2:B:402:ARG:CB	6:B:673:HOH:O	2.60	0.43
1:A:132:VAL:HG22	1:A:192:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:SER:OG	2:B:303:ASN:ND2	2.52	0.42
2:B:52:ALA:HB3	3:B:502:EDO:C2	2.49	0.42
2:D:65:ILE:HD11	2:D:353:VAL:HG13	2.02	0.42
1:A:65:ILE:HD11	1:A:353:VAL:CG1	2.48	0.42
2:C:197:TRP:HB2	2:C:200:TYR:HB3	2.01	0.42
1:A:197:TRP:HB2	1:A:200:TYR:HB3	2.01	0.42
2:B:65:ILE:HD11	2:B:353:VAL:CG1	2.50	0.42
2:C:132:VAL:HG22	2:C:192:LEU:HD23	2.02	0.42
2:D:10:ASN:HB2	2:D:319:SER:HB3	2.01	0.42
2:D:93[B]:LYS:CA	2:D:93[B]:LYS:HE2	2.50	0.42
1:A:375:ASP:C	1:A:375:ASP:OD1	2.58	0.42
2:C:78:LLP:C5'	2:C:78:LLP:NZ	2.74	0.42
2:B:10:ASN:HB2	2:B:319:SER:HB3	2.03	0.41
2:C:65:ILE:HD11	2:C:353:VAL:CG1	2.50	0.41
2:B:303:ASN:C	2:B:303:ASN:OD1	2.59	0.41
1:A:128:HIS:N	5:A:504:PO4:O2	2.45	0.41
2:C:12:ARG:HH11	2:C:12:ARG:HB3	1.85	0.41
2:D:175:ASP:OD1	2:D:178:ARG:NH1	2.53	0.41
2:C:69:SER:O	2:C:75:ASN:HA	2.20	0.41
2:D:93[B]:LYS:HB2	2:D:93[B]:LYS:HE3	1.76	0.41
1:A:234:ILE:HB	1:A:382:LEU:CD2	2.50	0.41
2:D:65:ILE:HD11	2:D:353:VAL:CG1	2.51	0.41
2:B:17:GLY:HA3	6:B:706:HOH:O	2.21	0.41
2:B:234:ILE:HB	2:B:382:LEU:CD2	2.51	0.40
2:B:396:ASP:OD2	2:B:402:ARG:HD3	2.22	0.40
2:B:13:ARG:HH21	2:B:368:LEU:HD12	1.85	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	364/404 (90%)	351 (96%)	12 (3%)	1 (0%)	41	61
2	B	351/412 (85%)	335 (95%)	15 (4%)	1 (0%)	41	61
2	C	369/412 (90%)	354 (96%)	15 (4%)	0	100	100
2	D	381/412 (92%)	360 (94%)	20 (5%)	1 (0%)	41	61
All	All	1465/1640 (89%)	1400 (96%)	62 (4%)	3 (0%)	47	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	LEU
2	B	99	ASN
2	D	293	ILE

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	247/326 (76%)	236 (96%)	11 (4%)	27	51
2	B	239/334 (72%)	231 (97%)	8 (3%)	38	64
2	C	267/334 (80%)	257 (96%)	10 (4%)	34	60
2	D	282/334 (84%)	272 (96%)	10 (4%)	36	62
All	All	1035/1328 (78%)	996 (96%)	39 (4%)	33	58

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	18	THR
1	A	23	SER
1	A	107	ASN
1	A	122	THR
1	A	161	HIS
1	A	192	LEU
1	A	198	THR

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Mol	Chain	Res	Type
1	A	336	ARG
1	A	353	VAL
1	A	367	ASP
2	B	13	ARG
2	B	18	THR
2	B	23	SER
2	B	122	THR
2	B	152	SER
2	B	192	LEU
2	B	198	THR
2	B	353	VAL
2	C	12	ARG
2	C	18	THR
2	C	23	SER
2	C	122	THR
2	C	161	HIS
2	C	192	LEU
2	C	198	THR
2	C	268	GLN
2	C	353	VAL
2	C	367	ASP
2	D	18	THR
2	D	23	SER
2	D	103	PHE
2	D	106	LEU
2	D	112	LYS
2	D	122	THR
2	D	152	SER
2	D	192	LEU
2	D	220	GLU
2	D	353	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	GLN
2	C	99	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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
2	LLP	B	78	2	23,24,25	2.65	5 (21%)	25,32,34	1.85	5 (20%)
2	LLP	D	78	2	23,24,25	2.45	5 (21%)	25,32,34	1.69	4 (16%)
1	LLP	A	78	1	23,24,25	2.48	4 (17%)	25,32,34	1.98	6 (24%)
2	LLP	C	78	2	23,24,25	2.12	4 (17%)	25,32,34	2.10	8 (32%)

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
2	LLP	B	78	2	-	11/16/17/19	0/1/1/1
2	LLP	D	78	2	-	10/16/17/19	0/1/1/1
1	LLP	A	78	1	-	11/16/17/19	0/1/1/1
2	LLP	C	78	2	-	8/16/17/19	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	78	LLP	C3-C2	6.79	1.47	1.40
2	D	78	LLP	C4-C5	6.32	1.49	1.42
2	C	78	LLP	C4'-NZ	6.16	1.47	1.27
2	B	78	LLP	C4-C5	6.07	1.49	1.42
1	A	78	LLP	C4-C5	6.06	1.49	1.42
1	A	78	LLP	C3-C2	5.94	1.46	1.40
2	B	78	LLP	C4'-NZ	5.45	1.45	1.27
2	D	78	LLP	C3-C2	5.35	1.46	1.40
2	B	78	LLP	C4-C3	5.32	1.48	1.40
2	D	78	LLP	C4'-NZ	5.30	1.45	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	LLP	C4'-NZ	5.30	1.45	1.27
2	C	78	LLP	C3-C2	5.13	1.46	1.40
1	A	78	LLP	C4-C3	4.95	1.48	1.40
2	C	78	LLP	C4-C5	4.31	1.47	1.42
2	D	78	LLP	C4-C3	3.88	1.46	1.40
2	C	78	LLP	C4-C3	2.68	1.44	1.40
2	D	78	LLP	C4-C4'	2.67	1.51	1.46
2	B	78	LLP	C4-C4'	2.28	1.51	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	LLP	C4-C3-C2	-5.80	116.60	120.19
2	B	78	LLP	C4-C3-C2	-5.58	116.74	120.19
2	C	78	LLP	C4-C3-C2	-5.51	116.78	120.19
2	D	78	LLP	C4-C3-C2	-4.84	117.19	120.19
1	A	78	LLP	OP2-P-OP1	4.09	126.69	110.68
2	D	78	LLP	OP3-P-OP4	-3.28	97.99	106.73
2	D	78	LLP	C4-C4'-NZ	-3.28	109.25	124.31
2	B	78	LLP	OP3-P-OP4	-3.27	98.03	106.73
2	C	78	LLP	OP4-C5'-C5	3.20	115.45	109.35
1	A	78	LLP	OP4-P-OP1	-3.16	97.61	106.47
1	A	78	LLP	C4-C4'-NZ	-3.14	109.91	124.31
2	B	78	LLP	C4-C4'-NZ	-3.12	109.97	124.31
2	C	78	LLP	C3-C4-C5	-2.93	116.01	118.26
2	B	78	LLP	OP2-P-OP4	2.90	114.44	106.73
2	C	78	LLP	C2'-C2-C3	-2.89	117.32	120.89
1	A	78	LLP	OP2-P-OP4	-2.84	99.17	106.73
2	C	78	LLP	CE-NZ-C4'	2.74	127.31	118.90
2	D	78	LLP	OP2-P-OP4	2.70	113.92	106.73
2	C	78	LLP	C5'-C5-C6	-2.43	115.38	119.37
2	C	78	LLP	C4-C4'-NZ	-2.38	113.37	124.31
2	C	78	LLP	CD-CE-NZ	2.26	116.46	110.93
1	A	78	LLP	C6-N1-C2	2.26	123.34	119.17
2	B	78	LLP	C2'-C2-C3	-2.08	118.32	120.89

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	78	LLP	C4-C4'-NZ-CE
2	B	78	LLP	C4-C5-C5'-OP4

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Mol	Chain	Res	Type	Atoms
2	B	78	LLP	C6-C5-C5'-OP4
2	B	78	LLP	C5'-OP4-P-OP1
2	B	78	LLP	C5'-OP4-P-OP2
2	B	78	LLP	C5'-OP4-P-OP3
2	D	78	LLP	C4-C4'-NZ-CE
2	D	78	LLP	C4-C5-C5'-OP4
2	D	78	LLP	C6-C5-C5'-OP4
2	D	78	LLP	C5'-OP4-P-OP1
2	D	78	LLP	C5'-OP4-P-OP2
2	D	78	LLP	C5'-OP4-P-OP3
1	A	78	LLP	C4-C4'-NZ-CE
1	A	78	LLP	C4-C5-C5'-OP4
1	A	78	LLP	C6-C5-C5'-OP4
1	A	78	LLP	C5'-OP4-P-OP1
1	A	78	LLP	C5'-OP4-P-OP2
1	A	78	LLP	C5'-OP4-P-OP3
2	C	78	LLP	C4-C4'-NZ-CE
2	C	78	LLP	C5'-OP4-P-OP2
2	C	78	LLP	C5'-OP4-P-OP3
2	C	78	LLP	CG-CD-CE-NZ
2	C	78	LLP	CD-CE-NZ-C4'
2	C	78	LLP	CA-CB-CG-CD
1	A	78	LLP	CA-CB-CG-CD
2	B	78	LLP	CA-CB-CG-CD
2	B	78	LLP	CG-CD-CE-NZ
2	D	78	LLP	CG-CD-CE-NZ
1	A	78	LLP	CG-CD-CE-NZ
2	C	78	LLP	C5'-OP4-P-OP1
2	D	78	LLP	CA-CB-CG-CD
2	B	78	LLP	CD-CE-NZ-C4'
2	D	78	LLP	CD-CE-NZ-C4'
1	A	78	LLP	CD-CE-NZ-C4'
1	A	78	LLP	C-CA-CB-CG
2	C	78	LLP	C-CA-CB-CG
1	A	78	LLP	C3-C4-C4'-NZ
2	B	78	LLP	C3-C4-C4'-NZ
2	D	78	LLP	C3-C4-C4'-NZ
2	B	78	LLP	C-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	78	LLP	3	0
2	D	78	LLP	3	0
1	A	78	LLP	3	0
2	C	78	LLP	8	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

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	EDO	D	501	-	3,3,3	0.66	0	2,2,2	0.37	0
3	EDO	B	501	-	3,3,3	0.65	0	2,2,2	0.13	0
5	PO4	A	504	-	4,4,4	0.86	0	6,6,6	0.71	0
4	PEG	B	505	-	6,6,6	0.70	0	5,5,5	0.37	0
5	PO4	C	501	-	4,4,4	1.21	0	6,6,6	0.48	0
3	EDO	B	504	-	3,3,3	0.56	0	2,2,2	0.32	0
3	EDO	B	502	-	3,3,3	0.56	0	2,2,2	0.29	0
5	PO4	B	507	-	4,4,4	0.91	0	6,6,6	0.41	0
5	PO4	D	503	-	4,4,4	1.12	0	6,6,6	1.26	0
3	EDO	A	501	-	3,3,3	0.74	0	2,2,2	0.12	0
5	PO4	A	505	-	4,4,4	0.76	0	6,6,6	0.51	0
4	PEG	B	506	-	6,6,6	0.61	0	5,5,5	0.38	0
3	EDO	B	503	-	3,3,3	0.60	0	2,2,2	0.26	0
5	PO4	B	508	-	4,4,4	1.23	0	6,6,6	1.48	1 (16%)
5	PO4	D	505	-	4,4,4	0.79	0	6,6,6	0.50	0
3	EDO	D	502	-	3,3,3	0.51	0	2,2,2	0.19	0
3	EDO	A	502	-	3,3,3	0.68	0	2,2,2	0.05	0
5	PO4	C	502	-	4,4,4	0.81	0	6,6,6	1.13	0
5	PO4	D	504	-	4,4,4	1.02	0	6,6,6	0.94	0
4	PEG	A	503	-	6,6,6	0.64	0	5,5,5	0.30	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	EDO	D	501	-	-	1/1/1/1	-
3	EDO	B	501	-	-	1/1/1/1	-
4	PEG	B	505	-	-	1/4/4/4	-
3	EDO	B	504	-	-	1/1/1/1	-
3	EDO	A	501	-	-	1/1/1/1	-
4	PEG	B	506	-	-	1/4/4/4	-
3	EDO	B	503	-	-	1/1/1/1	-
3	EDO	B	502	-	-	1/1/1/1	-
3	EDO	D	502	-	-	1/1/1/1	-
3	EDO	A	502	-	-	0/1/1/1	-
4	PEG	A	503	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	508	PO4	O3-P-O1	-2.01	103.54	110.89

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	506	PEG	O1-C1-C2-O2
3	D	501	EDO	O1-C1-C2-O2
3	A	501	EDO	O1-C1-C2-O2
3	B	501	EDO	O1-C1-C2-O2
3	B	503	EDO	O1-C1-C2-O2
3	D	502	EDO	O1-C1-C2-O2
4	A	503	PEG	O2-C3-C4-O4
4	A	503	PEG	C1-C2-O2-C3
4	B	505	PEG	C4-C3-O2-C2
3	B	504	EDO	O1-C1-C2-O2
3	B	502	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	504	PO4	2	0
5	C	501	PO4	1	0
3	B	502	EDO	1	0
5	D	503	PO4	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 ⓘ

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	374/404 (92%)	0.72	22 (5%)	22 23	27, 44, 76, 93	0
2	B	364/412 (88%)	0.73	19 (5%)	27 29	27, 48, 74, 88	0
2	C	379/412 (91%)	0.62	13 (3%)	45 48	25, 41, 70, 92	0
2	D	387/412 (93%)	0.60	10 (2%)	56 59	24, 40, 62, 85	0
All	All	1504/1640 (91%)	0.67	64 (4%)	35 38	24, 43, 72, 93	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	7	TYR	4.6
1	A	222	LEU	4.5
2	B	27	GLY	3.8
2	D	27	GLY	3.5
2	C	257	ASN	3.4
2	B	52	ALA	3.3
1	A	168	ILE	3.3
2	D	16	TYR	3.3
1	A	285	CYS	3.2
2	D	176	ALA	3.2
1	A	259	PRO	3.1
2	D	298	ALA	2.9
2	B	144	VAL	2.8
2	B	58	LEU	2.8
1	A	44	ALA	2.8
2	D	220	GLU	2.8
2	C	224	GLU	2.7
2	C	194	ASP	2.7
2	C	44	ALA	2.7
2	D	273	TYR	2.7
2	B	96	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	181	HIS	2.7
2	B	300	GLY	2.6
2	B	331	ILE	2.6
2	B	359	LEU	2.6
1	A	181	HIS	2.5
2	B	309	ILE	2.5
1	A	195	THR	2.5
1	A	165	GLU	2.5
2	D	267	HIS	2.4
1	A	219	TYR	2.4
2	B	16	TYR	2.4
2	B	176	ALA	2.4
1	A	223	ALA	2.4
2	C	225	THR	2.4
2	C	197	TRP	2.3
2	B	260	ASN	2.3
2	B	145	VAL	2.3
1	A	89	TYR	2.3
1	A	164	ALA	2.3
1	A	351	ILE	2.3
2	D	378	ALA	2.3
2	C	334	ALA	2.2
2	B	263	VAL	2.2
1	A	293	ILE	2.2
2	B	298	ALA	2.2
2	D	10	ASN	2.2
2	C	249	TYR	2.2
2	B	325	ALA	2.2
1	A	382	LEU	2.2
1	A	136	ALA	2.2
2	C	298	ALA	2.2
1	A	173	TYR	2.2
1	A	220	GLU	2.2
1	A	260	ASN	2.2
2	D	70	TRP	2.1
2	C	351	ILE	2.1
2	C	89	TYR	2.1
1	A	197	TRP	2.1
1	A	175	ASP	2.1
1	A	178	ARG	2.1
2	B	272	LEU	2.0
2	B	258	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	249	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	LLP	B	78	24/25	0.94	0.26	36,40,46,50	0
2	LLP	D	78	24/25	0.94	0.24	27,34,38,43	0
2	LLP	C	78	24/25	0.94	0.18	28,35,45,60	0
1	LLP	A	78	24/25	0.95	0.18	30,33,37,38	0

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. 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	EDO	A	502	4/4	0.55	0.29	57,60,64,65	0
4	PEG	B	506	7/7	0.61	0.20	62,68,76,77	0
3	EDO	A	501	4/4	0.64	0.30	57,66,68,71	0
5	PO4	B	507	5/5	0.74	0.22	100,103,108,111	0
4	PEG	B	505	7/7	0.76	0.21	53,61,67,68	0
3	EDO	B	501	4/4	0.77	0.30	46,48,51,52	0
3	EDO	B	502	4/4	0.78	0.19	54,54,55,55	0
4	PEG	A	503	7/7	0.78	0.23	57,62,64,64	0
5	PO4	D	505	5/5	0.80	0.17	85,91,97,99	0
3	EDO	D	501	4/4	0.82	0.20	37,42,47,50	0
5	PO4	A	505	5/5	0.83	0.24	59,60,75,76	0
3	EDO	B	504	4/4	0.84	0.25	49,50,50,52	0
3	EDO	D	502	4/4	0.84	0.19	63,73,73,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	B	503	4/4	0.85	0.22	56,61,62,64	0
5	PO4	D	504	5/5	0.94	0.14	61,64,69,70	0
5	PO4	C	502	5/5	0.94	0.21	57,58,62,62	0
5	PO4	C	501	5/5	0.96	0.22	45,45,46,51	0
5	PO4	B	508	5/5	0.96	0.26	41,41,52,55	0
5	PO4	A	504	5/5	0.97	0.21	49,50,53,58	0
5	PO4	D	503	5/5	0.99	0.20	34,34,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.