



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 03:25 AM EDT

PDB ID : 3L6T  
Title : Crystal Structure of an N-terminal Mutant of the Plasmid pCU1 TraI Relaxase Domain  
Authors : Redinbo, M.R.; Nash, R.P.  
Deposited on : 2009-12-24  
Resolution : 1.93 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](mailto: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>.

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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 : 2.35  
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) : 2.35

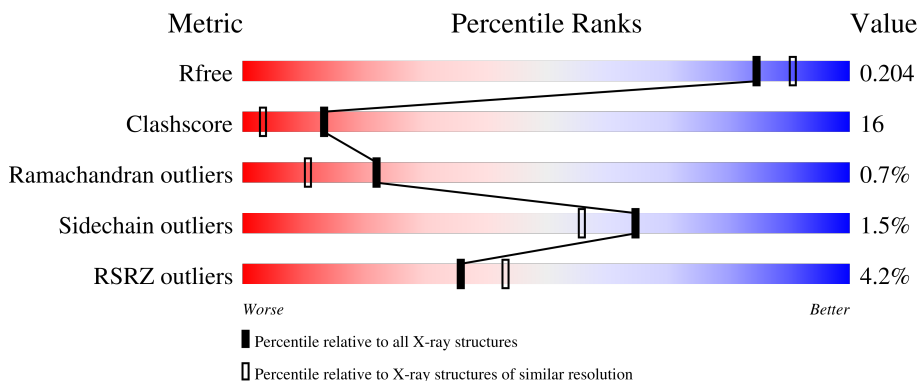
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.93 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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  $\geq 3$ , 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	302	 2% 55% 19% 25%
1	B	302	 4% 52% 15% 33%

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	EDO	B	307	-	-	X	-
5	CL	A	317	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 3986 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.

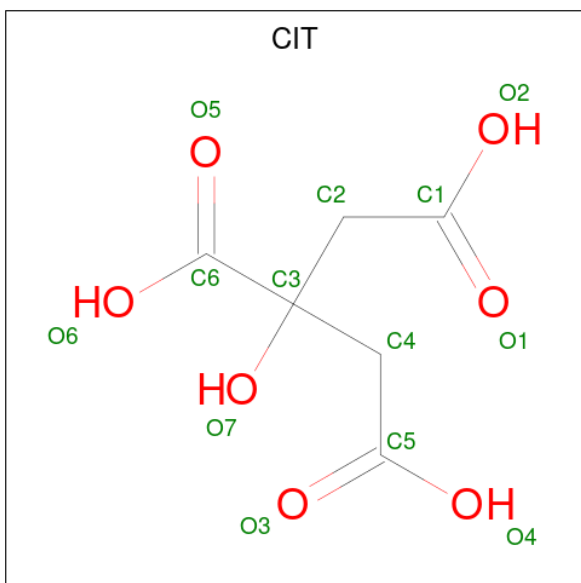
- Molecule 1 is a protein called Mobilization protein TraI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	226	Total 1852	C 1164	N 322	O 356	S 10	0	18	0
1	B	203	Total 1639	C 1024	N 292	O 313	S 10	0	10	0

There are 6 discrepancies between the modelled and reference sequences:

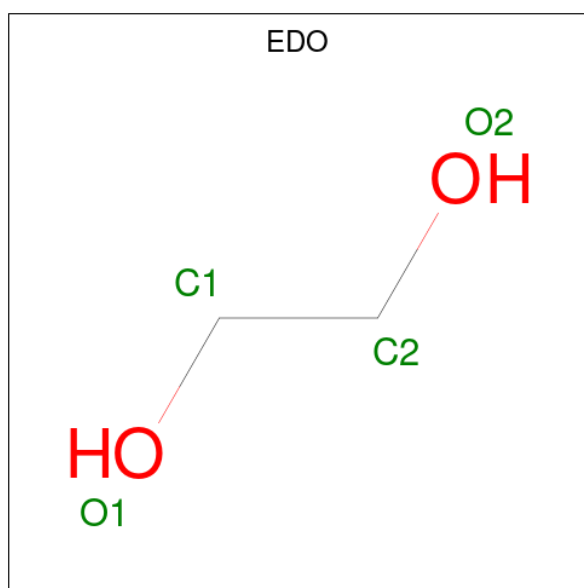
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9X4G2
A	-1	ASN	-	expression tag	UNP Q9X4G2
A	0	ALA	-	expression tag	UNP Q9X4G2
B	-2	SER	-	expression tag	UNP Q9X4G2
B	-1	ASN	-	expression tag	UNP Q9X4G2
B	0	ALA	-	expression tag	UNP Q9X4G2

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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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	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

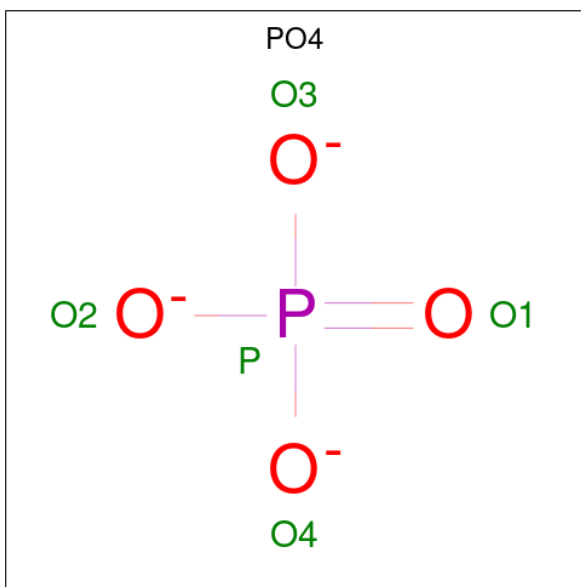
- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ni 1 1	0	0
4	B	1	Total Ni 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Cl 3 3	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	A	1	Total O P 5 4 1	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Na 1 1	0	0

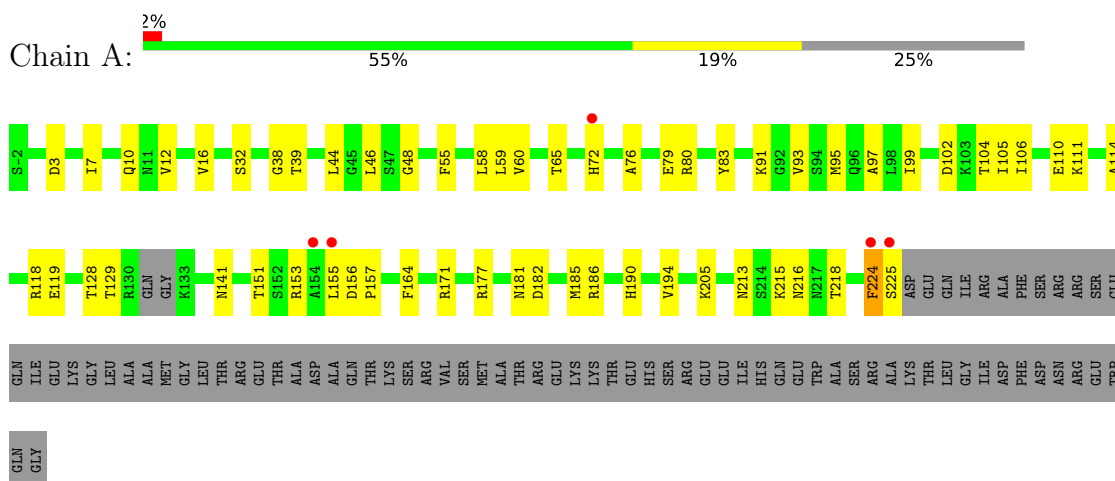
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	227	Total O 237 237	0	10
9	B	139	Total O 144 144	1	5

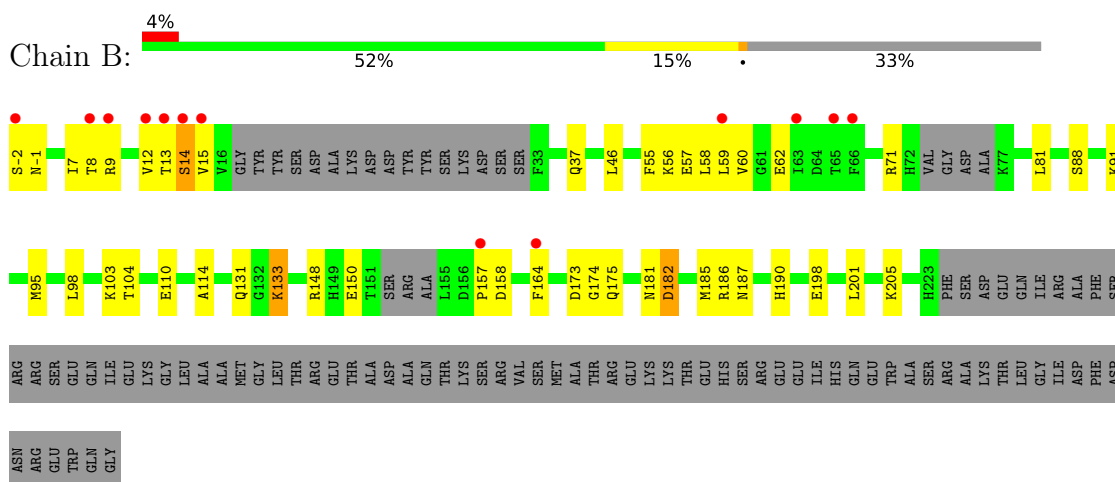
### 3 Residue-property plots [i](#)

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: Mobilization protein TraI



- Molecule 1: Mobilization protein TraI





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.38Å 58.66Å 86.53Å 90.00° 95.01° 90.00°	Depositor
Resolution (Å)	31.37 – 1.93 48.49 – 1.93	Depositor EDS
% Data completeness (in resolution range)	95.5 (31.37-1.93) 95.5 (48.49-1.93)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 1.92Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.168 , 0.204 0.165 , 0.204	Depositor DCC
$R_{free}$ test set	1823 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtrriage
Anisotropy	0.091	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 69.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3986	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL, EDO, PO4, NI, MG, CIT

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	0.34	0/1931	0.49	0/2604
1	B	0.31	0/1691	0.49	0/2277
All	All	0.33	0/3622	0.49	0/4881

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1852	0	1838	63	0
1	B	1639	0	1612	45	0
2	A	13	0	5	0	0
3	A	52	0	78	17	0
3	B	32	0	48	10	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	3	0	0	3	0
6	A	10	0	0	0	0
7	A	1	0	0	0	0
8	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	237	0	0	19	0
9	B	144	0	0	7	0
All	All	3986	0	3581	116	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 16.

All (116) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:HB	5:A:317:CL:CL	1.88	1.10
1:A:97:ALA:HB2	1:A:105[B]:ILE:HD12	1.36	1.04
1:B:12:VAL:HG11	1:B:81:LEU:HD12	1.55	0.87
1:A:72:HIS:CE1	1:A:79:GLU:HB2	2.10	0.86
1:B:198:GLU:HG2	3:B:305:EDO:O1	1.76	0.86
1:A:72:HIS:CE1	1:A:76:ALA:HA	2.14	0.82
1:B:7:ILE:HD12	1:B:164:PHE:HE1	1.51	0.75
1:B:164:PHE:HD1	3:B:307:EDO:HO1	1.34	0.75
1:A:48:GLY:HA2	3:A:303:EDO:H22	1.70	0.72
1:A:32:SER:HB3	9:A:435:HOH:O	1.90	0.70
1:B:91:LYS:O	1:B:95[B]:MET:HG3	1.93	0.68
1:B:15:VAL:HB	3:B:307:EDO:H12	1.74	0.68
1:B:-2:SER:HB3	1:B:88:SER:OG	1.94	0.68
9:A:323:HOH:O	1:B:-1:ASN:HB3	1.95	0.67
1:B:190:HIS:HB2	3:B:300:EDO:H21	1.78	0.65
1:B:7:ILE:HD12	1:B:164:PHE:CE1	2.30	0.65
1:A:12:VAL:HG11	3:A:312:EDO:H22	1.80	0.64
1:A:177:ARG:HD3	3:A:304:EDO:H22	1.79	0.63
1:B:8:THR:O	1:B:12:VAL:HG13	1.99	0.63
1:B:56:LYS:HA	1:B:59[A]:LEU:HD12	1.81	0.63
1:A:190:HIS:HB2	3:A:302:EDO:H12	1.82	0.61
1:B:103:LYS:HE3	9:B:422:HOH:O	2.00	0.61
1:B:164:PHE:HD1	3:B:307:EDO:O1	1.84	0.61
1:A:114:ALA:O	1:A:118[A]:ARG:HG3	2.03	0.59
1:A:72:HIS:NE2	1:A:79:GLU:HB2	2.17	0.59
1:B:91:LYS:NZ	1:B:157:PRO:HB2	2.19	0.57
1:B:131:GLN:O	1:B:133:LYS:HD2	2.04	0.57
1:A:38:GLY:HA2	3:A:307:EDO:H22	1.87	0.57
9:A:495:HOH:O	3:B:300:EDO:H22	2.05	0.57
1:A:205[A]:LYS:HG3	9:A:423:HOH:O	2.05	0.57
1:A:60:VAL:CG1	3:A:312:EDO:H12	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39[B]:THR:HG23	1:A:141:ASN:HA	1.87	0.56
1:A:151:THR:HG21	1:A:153:ARG:NH1	2.21	0.55
1:B:59[B]:LEU:HG	1:B:81:LEU:HD13	1.88	0.55
1:A:106:ILE:O	1:A:110[B]:GLU:HG3	2.05	0.55
1:A:151:THR:HG21	1:A:153:ARG:CZ	2.37	0.55
1:B:7:ILE:HD13	1:B:15:VAL:HG21	1.90	0.54
1:A:65[B]:THR:HG22	9:A:497:HOH:O	2.07	0.54
1:A:80:ARG:NH1	1:A:181:ASN:HD21	2.05	0.54
1:A:95[B]:MET:HE3	9:A:322:HOH:O	2.08	0.54
1:A:102:ASP:O	1:A:105[B]:ILE:HG22	2.08	0.54
1:A:55:PHE:CE2	1:A:59[B]:LEU:HD11	2.44	0.53
1:A:91[B]:LYS:HE2	9:A:322:HOH:O	2.08	0.53
1:A:118[B]:ARG:HG3	1:A:118[B]:ARG:NH1	2.23	0.53
1:B:55:PHE:O	1:B:59[A]:LEU:HG	2.10	0.52
1:A:44[B]:LEU:HD23	1:A:46:LEU:HD11	1.91	0.52
1:A:213:ASN:HB3	1:A:216[B]:ASN:HD21	1.73	0.52
1:B:182:ASP:HB3	1:B:186[B]:ARG:NH1	2.25	0.52
1:A:111:LYS:HD2	3:A:305:EDO:O1	2.09	0.52
1:A:216[B]:ASN:ND2	1:A:218:THR:OG1	2.45	0.50
1:A:55:PHE:CZ	1:A:59[B]:LEU:HD21	2.47	0.50
1:A:128[A]:THR:HG22	1:A:129:THR:N	2.26	0.50
1:A:118[B]:ARG:HD3	9:A:361:HOH:O	2.12	0.50
1:A:119:GLU:HG3	1:A:194:VAL:HG21	1.94	0.50
1:B:-2:SER:HB2	1:B:158:ASP:OD1	2.12	0.49
1:A:153:ARG:HG3	1:A:155:LEU:O	2.13	0.49
1:B:60:VAL:HG23	1:B:62:GLU:HG3	1.94	0.49
1:A:16:VAL:CB	5:A:317:CL:CL	2.80	0.48
1:B:173:ASP:O	1:B:173:ASP:OD1	2.30	0.48
3:A:305:EDO:H12	9:A:406:HOH:O	2.13	0.48
1:A:177:ARG:CD	3:A:304:EDO:H22	2.43	0.48
1:A:118[B]:ARG:HG3	1:A:118[B]:ARG:HH11	1.77	0.48
1:B:55:PHE:CE2	1:B:59[A]:LEU:HD11	2.48	0.48
1:B:57:GLU:HB2	1:B:62:GLU:HB2	1.95	0.48
1:B:15:VAL:HG12	9:B:365:HOH:O	2.14	0.47
1:A:44[B]:LEU:HG	9:A:448:HOH:O	2.14	0.47
1:A:44[B]:LEU:HD21	1:A:58:LEU:HD21	1.97	0.47
1:B:110:GLU:OE2	1:B:148:ARG:HD3	2.15	0.47
1:A:118[A]:ARG:HG2	3:A:307:EDO:C1	2.46	0.46
1:B:181:ASN:O	1:B:185:MET:HG2	2.15	0.46
1:B:12:VAL:CG1	1:B:81:LEU:HD12	2.36	0.46
1:A:3[A]:ASP:HB2	9:A:538:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LYS:HZ1	1:B:157:PRO:HB2	1.80	0.45
1:B:-2:SER:HB2	1:B:158:ASP:CG	2.36	0.45
1:A:83:TYR:CD1	1:A:185:MET:HE1	2.51	0.45
1:B:187:ASN:HA	3:B:300:EDO:O2	2.16	0.45
1:A:97:ALA:HB2	1:A:105[B]:ILE:HG23	1.98	0.45
3:A:302:EDO:H22	9:B:331:HOH:O	2.17	0.45
1:A:128[B]:THR:HG22	1:A:171:ARG:HD2	1.99	0.45
1:A:65[A]:THR:HG22	9:A:496:HOH:O	2.16	0.44
1:A:156:ASP:HA	9:A:322:HOH:O	2.17	0.44
1:B:37:GLN:HE22	1:B:114:ALA:HA	1.81	0.44
1:A:39[B]:THR:HG23	1:A:141:ASN:CB	2.48	0.44
1:B:98:LEU:HD22	1:B:150:GLU:HB3	2.00	0.44
1:B:9:ARG:HA	1:B:12:VAL:HG22	1.99	0.44
1:A:60:VAL:HG11	3:A:312:EDO:H12	2.00	0.43
1:A:215[B]:LYS:NZ	9:A:351:HOH:O	2.50	0.43
3:A:302:EDO:O2	3:B:305:EDO:O2	2.33	0.43
1:B:13:THR:O	1:B:14:SER:CB	2.66	0.43
3:B:305:EDO:H11	9:B:367:HOH:O	2.19	0.43
1:A:118[B]:ARG:HH11	1:A:118[B]:ARG:CG	2.31	0.43
1:B:46:LEU:HD11	1:B:58:LEU:HD11	1.99	0.43
1:A:7:ILE:HG13	1:A:164:PHE:HE1	1.84	0.43
3:A:310:EDO:H12	9:A:334:HOH:O	2.18	0.43
1:B:91:LYS:HZ1	1:B:95[B]:MET:HG2	1.82	0.43
1:A:48:GLY:CA	3:A:303:EDO:H22	2.44	0.43
1:A:93:VAL:HG13	1:A:105[B]:ILE:HG13	2.01	0.42
1:A:111:LYS:O	5:A:316:CL:CL	2.74	0.42
1:B:15:VAL:HB	3:B:307:EDO:C1	2.44	0.42
3:A:308:EDO:H11	9:A:411:HOH:O	2.20	0.42
1:B:104[B]:THR:HG21	9:B:395:HOH:O	2.19	0.42
3:A:306:EDO:H22	3:A:308:EDO:O1	2.20	0.42
9:A:539[B]:HOH:O	1:B:201[B]:LEU:HD21	2.18	0.42
1:A:72:HIS:CE1	1:A:76:ALA:CA	2.96	0.42
1:B:104[B]:THR:HG22	9:B:391:HOH:O	2.20	0.41
1:A:224:PHE:O	1:A:225:SER:C	2.58	0.41
1:A:99:ILE:HD11	1:A:157:PRO:HG3	2.01	0.41
1:A:118[B]:ARG:HG2	9:A:542:HOH:O	2.21	0.41
1:B:173:ASP:O	1:B:175:GLN:N	2.54	0.41
1:A:215[B]:LYS:HE2	9:A:535:HOH:O	2.20	0.41
1:B:205:LYS:HG3	9:B:420:HOH:O	2.21	0.41
1:A:182:ASP:O	1:A:186:ARG:HG2	2.21	0.41
1:A:181:ASN:OD1	1:A:181:ASN:C	2.58	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:ILE:CG2	1:B:12:VAL:HG12	2.52	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	241/302 (80%)	236 (98%)	4 (2%)	1 (0%)	34	24
1	B	206/302 (68%)	200 (97%)	4 (2%)	2 (1%)	15	6
All	All	447/604 (74%)	436 (98%)	8 (2%)	3 (1%)	22	11

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	PHE
1	B	14	SER
1	B	174	GLY

### 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	197/253 (78%)	195 (99%)	2 (1%)	76	71
1	B	172/253 (68%)	169 (98%)	3 (2%)	60	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	369/506 (73%)	364 (99%)	5 (1%)	65 58

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	104	THR
1	B	71	ARG
1	B	133	LYS
1	B	182	ASP

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

Mol	Chain	Res	Type
1	A	72	HIS
1	B	37	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 7 are monoatomic - leaving 24 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	EDO	A	308	-	3,3,3	0.47	0	2,2,2	0.72	0
3	EDO	A	309	-	3,3,3	0.47	0	2,2,2	0.84	0
3	EDO	A	312	-	3,3,3	0.50	0	2,2,2	0.80	0
3	EDO	B	301	-	3,3,3	0.48	0	2,2,2	0.71	0
3	EDO	B	304	-	3,3,3	0.47	0	2,2,2	0.87	0
6	PO4	A	318	-	4,4,4	0.91	0	6,6,6	0.46	0
3	EDO	A	301	-	3,3,3	0.45	0	2,2,2	0.61	0
6	PO4	A	319	8	4,4,4	0.92	0	6,6,6	0.44	0
3	EDO	B	302	4	3,3,3	0.44	0	2,2,2	0.62	0
2	CIT	A	300	4	12,12,12	2.78	5 (41%)	17,17,17	1.56	2 (11%)
3	EDO	A	304	-	3,3,3	0.48	0	2,2,2	0.92	0
3	EDO	A	302	-	3,3,3	0.47	0	2,2,2	0.74	0
3	EDO	A	311	-	3,3,3	0.47	0	2,2,2	0.83	0
3	EDO	A	313	-	3,3,3	0.47	0	2,2,2	0.66	0
3	EDO	B	305	-	3,3,3	0.48	0	2,2,2	0.69	0
3	EDO	B	306	-	3,3,3	0.46	0	2,2,2	0.84	0
3	EDO	A	310	-	3,3,3	0.47	0	2,2,2	0.79	0
3	EDO	B	303	-	3,3,3	0.47	0	2,2,2	0.88	0
3	EDO	A	305	-	3,3,3	0.48	0	2,2,2	0.50	0
3	EDO	A	306	-	3,3,3	0.47	0	2,2,2	0.78	0
3	EDO	A	303	-	3,3,3	0.49	0	2,2,2	0.81	0
3	EDO	B	307	-	3,3,3	0.46	0	2,2,2	0.67	0
3	EDO	A	307	-	3,3,3	0.47	0	2,2,2	0.77	0
3	EDO	B	300	-	3,3,3	0.50	0	2,2,2	0.76	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	A	308	-	-	1/1/1/1	-
3	EDO	A	309	-	-	1/1/1/1	-
3	EDO	A	312	-	-	1/1/1/1	-
3	EDO	B	301	-	-	1/1/1/1	-
3	EDO	B	304	-	-	1/1/1/1	-
3	EDO	A	301	-	-	1/1/1/1	-
3	EDO	B	302	4	-	1/1/1/1	-
2	CIT	A	300	4	-	2/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	304	-	-	0/1/1/1	-
3	EDO	A	302	-	-	1/1/1/1	-
3	EDO	A	311	-	-	1/1/1/1	-
3	EDO	A	313	-	-	0/1/1/1	-
3	EDO	B	305	-	-	1/1/1/1	-
3	EDO	B	306	-	-	1/1/1/1	-
3	EDO	A	310	-	-	1/1/1/1	-
3	EDO	B	303	-	-	1/1/1/1	-
3	EDO	A	305	-	-	0/1/1/1	-
3	EDO	A	306	-	-	1/1/1/1	-
3	EDO	A	303	-	-	0/1/1/1	-
3	EDO	B	307	-	-	1/1/1/1	-
3	EDO	A	307	-	-	0/1/1/1	-
3	EDO	B	300	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	CIT	O5-C6	5.44	1.39	1.22
2	A	300	CIT	O3-C5	5.38	1.40	1.22
2	A	300	CIT	O4-C5	-3.29	1.19	1.30
2	A	300	CIT	O6-C6	-3.08	1.18	1.30
2	A	300	CIT	O2-C1	2.63	1.39	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	300	CIT	O6-C6-C3	3.76	119.59	113.05
2	A	300	CIT	O4-C5-O3	-2.09	118.08	123.30

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	EDO	O1-C1-C2-O2
3	A	306	EDO	O1-C1-C2-O2
3	A	309	EDO	O1-C1-C2-O2
3	A	310	EDO	O1-C1-C2-O2
3	A	312	EDO	O1-C1-C2-O2
3	B	300	EDO	O1-C1-C2-O2
3	B	303	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	304	EDO	O1-C1-C2-O2
2	A	300	CIT	C3-C4-C5-O3
3	A	311	EDO	O1-C1-C2-O2
3	B	305	EDO	O1-C1-C2-O2
3	B	302	EDO	O1-C1-C2-O2
3	A	301	EDO	O1-C1-C2-O2
3	A	308	EDO	O1-C1-C2-O2
3	B	301	EDO	O1-C1-C2-O2
3	B	307	EDO	O1-C1-C2-O2
2	A	300	CIT	C3-C4-C5-O4
3	B	306	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	308	EDO	2	0
3	A	312	EDO	3	0
3	A	304	EDO	2	0
3	A	302	EDO	3	0
3	B	305	EDO	3	0
3	A	310	EDO	1	0
3	A	305	EDO	2	0
3	A	306	EDO	1	0
3	A	303	EDO	2	0
3	B	307	EDO	4	0
3	A	307	EDO	2	0
3	B	300	EDO	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	226/302 (74%)	0.04	5 (2%) 62 69	24, 38, 80, 107	9 (3%)
1	B	203/302 (67%)	0.16	13 (6%) 19 26	25, 47, 89, 114	6 (2%)
All	All	429/604 (71%)	0.10	18 (4%) 36 43	24, 41, 88, 114	15 (3%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	SER	4.9
1	A	224	PHE	4.8
1	B	-2	SER	4.7
1	B	65	THR	4.6
1	B	157	PRO	4.3
1	B	66	PHE	4.1
1	B	12	VAL	3.7
1	B	63	ILE	3.3
1	B	164	PHE	3.2
1	B	13	THR	3.1
1	B	9	ARG	3.0
1	A	154	ALA	2.8
1	A	72	HIS	2.6
1	B	15	VAL	2.1
1	A	155	LEU	2.1
1	B	14	SER	2.1
1	B	8	THR	2.0
1	B	59[A]	LEU	2.0

### 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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	EDO	A	306	4/4	0.71	0.36	66,67,67,67	1
3	EDO	A	304	4/4	0.76	0.21	58,61,66,68	0
3	EDO	B	306	4/4	0.76	0.34	71,72,72,72	0
3	EDO	A	310	4/4	0.78	0.17	89,90,91,91	0
3	EDO	B	305	4/4	0.79	0.23	60,66,67,69	0
3	EDO	A	303	4/4	0.80	0.23	62,63,64,65	0
5	CL	A	317	1/1	0.82	0.20	73,73,73,73	0
6	PO4	A	319	5/5	0.84	0.37	124,125,126,126	0
3	EDO	A	307	4/4	0.86	0.18	56,59,64,66	0
3	EDO	A	311	4/4	0.87	0.14	86,87,87,88	0
3	EDO	A	301	4/4	0.88	0.16	55,62,69,73	0
3	EDO	B	304	4/4	0.88	0.29	78,83,83,84	0
8	NA	A	321	1/1	0.88	0.16	52,52,52,52	0
3	EDO	A	308	4/4	0.89	0.37	58,66,71,73	0
3	EDO	A	313	4/4	0.89	0.20	55,57,57,60	0
3	EDO	B	303	4/4	0.89	0.35	65,73,77,82	0
3	EDO	B	307	4/4	0.90	0.35	74,75,76,78	0
3	EDO	A	305	4/4	0.90	0.30	61,62,65,65	0
3	EDO	B	300	4/4	0.92	0.30	46,51,56,60	0
3	EDO	B	302	4/4	0.93	0.07	53,58,65,68	0
3	EDO	B	301	4/4	0.93	0.15	41,51,59,64	0
5	CL	A	315	1/1	0.93	0.07	85,85,85,85	0
3	EDO	A	312	4/4	0.94	0.36	44,49,56,60	0
6	PO4	A	318	5/5	0.94	0.16	115,118,119,120	0
3	EDO	A	309	4/4	0.95	0.26	56,56,57,58	0
7	MG	A	320	1/1	0.96	0.08	47,47,47,47	0
5	CL	A	316	1/1	0.97	0.09	65,65,65,65	0
2	CIT	A	300	13/13	0.97	0.08	32,37,43,46	0
3	EDO	A	302	4/4	0.97	0.20	33,41,44,49	1
4	NI	B	308	1/1	0.99	0.09	48,48,48,48	0
4	NI	A	314	1/1	1.00	0.11	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.