



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:14 AM GMT

PDB ID : 2PY5  
Title : Phi29 DNA polymerase complexed with single-stranded DNA  
Authors : Berman, A.J.; Kamtekar, S.; Goodman, J.L.; Lazaro, J.M.; de Vega, M.;  
Blanco, L.; Salas, M.; Steitz, T.A.  
Deposited on : 2007-05-15  
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](mailto: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.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

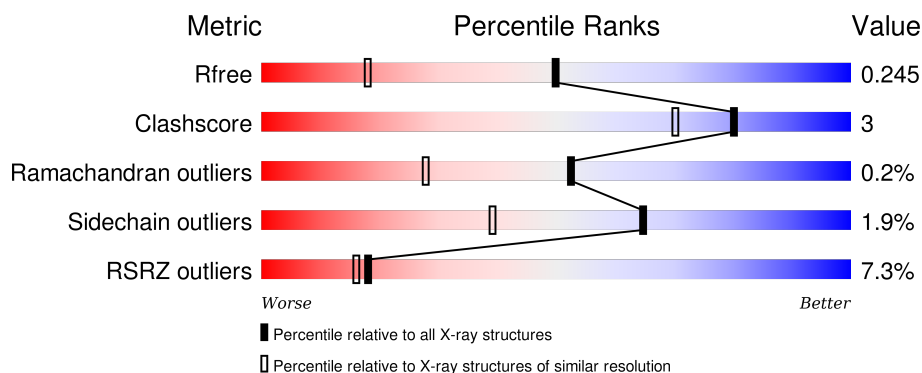
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	D	7	<div> <div>29%</div> <div> <div></div> <div>29%</div> <div>57%</div> <div>14%</div> </div> </div>
1	E	7	<div> <div>57%</div> <div>29%</div> <div>14%</div> </div>
1	J	7	<div> <div>71%</div> <div>14%</div> <div>14%</div> </div>
1	L	7	<div> <div>14%</div> <div>43%</div> <div>14%</div> <div>43%</div> </div>
1	Y	7	<div> <div>14%</div> <div>71%</div> <div>14%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
2	A	575	
2	B	575	

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	A	8004	-	-	-	X
3	EDO	A	8008	-	-	-	X
3	EDO	A	8010	-	-	-	X
3	EDO	A	8011	-	-	-	X
3	EDO	A	9012	-	-	-	X
3	EDO	A	9013	-	-	-	X
3	EDO	A	9014	-	-	-	X
3	EDO	B	8002	-	-	-	X
3	EDO	B	8006	-	-	-	X
3	EDO	B	9003	-	-	-	X
3	EDO	B	9009	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11400 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 DNA chain called 5'-d(GGACTTT)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	6	Total	C	N	O	P	0	0	0
			122	59	19	38	6			
1	Y	6	Total	C	N	O	P	0	0	0
			105	49	20	31	5			
1	D	6	Total	C	N	O	P	0	0	0
			121	59	22	35	5			
1	E	6	Total	C	N	O	P	0	0	0
			105	49	20	31	5			
1	L	4	Total	C	N	O	P	0	0	0
			79	39	9	27	4			

- Molecule 2 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	564	Total	C	N	O	S	28	11	0
			4650	3037	741	850	22			
2	B	562	Total	C	N	O	S	11	7	0
			4617	3014	737	844	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ALA	ASP	ENGINEERED	UNP P03680
A	66	ALA	ASP	ENGINEERED	UNP P03680
B	12	ALA	ASP	ENGINEERED	UNP P03680
B	66	ALA	ASP	ENGINEERED	UNP P03680

- 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	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	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	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	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
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	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	768	Total O 768 768	0	0
4	B	625	Total O 625 625	0	0
4	D	20	Total O 20 20	0	0
4	E	20	Total O 20 20	0	0
4	J	31	Total O 31 31	0	0
4	L	20	Total O 20 20	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Y	9	Total	O	0	0
			9	9		

### 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 errors 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: 5'-d(GGACTTT)-3'

Chain J: 



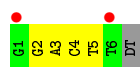
- Molecule 1: 5'-d(GGACTTT)-3'

Chain Y: 



- Molecule 1: 5'-d(GGACTTT)-3'

Chain D: 

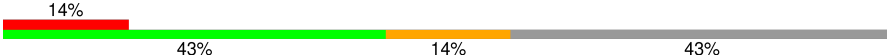


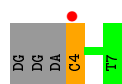
- Molecule 1: 5'-d(GGACTTT)-3'

Chain E: 



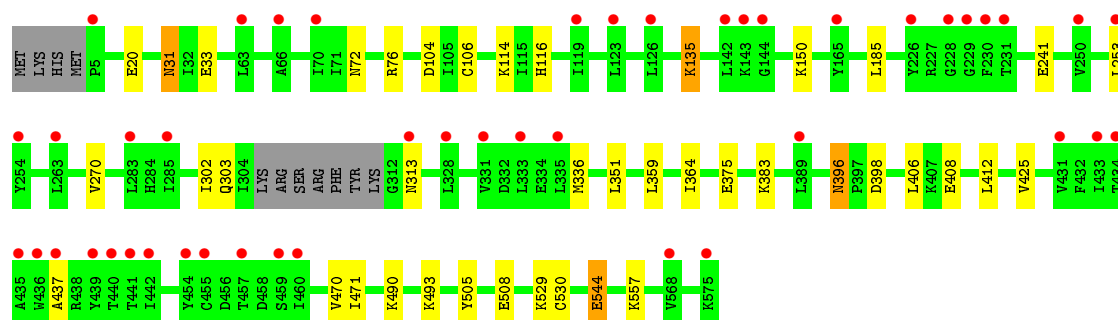
- Molecule 1: 5'-d(GGACTTT)-3'

Chain L: 

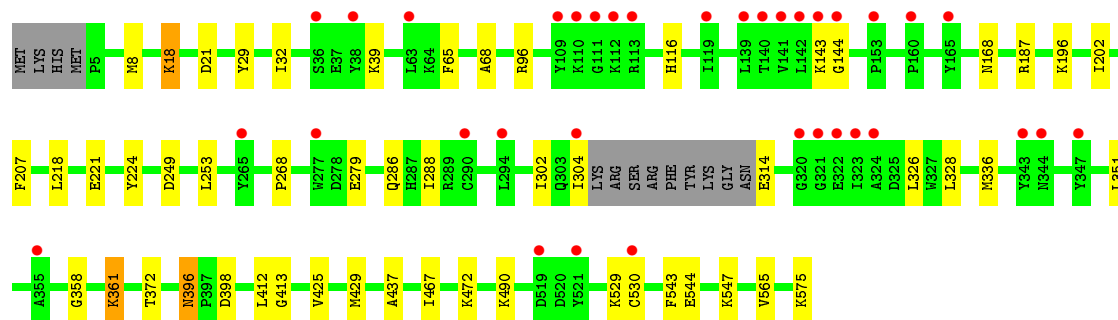
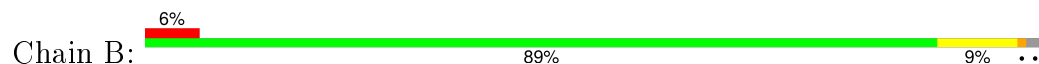


- Molecule 2: DNA polymerase

Chain A: 



• Molecule 2: DNA polymerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.20 Å   200.18 Å   66.99 Å 90.00°   109.40°   90.00°	Depositor
Resolution (Å)	40.59 – 1.60 40.58 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.8 (40.59-1.60) 97.8 (40.58-1.60)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 1.60 Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.164   ,   0.194 0.223   ,   0.245	Depositor DCC
$R_{free}$ test set	8622 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 172112 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	D	0.85	0/135	1.54	2/207 (1.0%)
1	E	0.95	0/117	1.52	2/180 (1.1%)
1	J	0.85	0/135	1.30	1/206 (0.5%)
1	L	1.19	1/86 (1.2%)	1.68	0/130
1	Y	0.69	0/117	1.29	1/180 (0.6%)
2	A	0.66	7/4801 (0.1%)	0.67	4/6477 (0.1%)
2	B	0.45	1/4755 (0.0%)	0.57	0/6418
All	All	0.59	9/10146 (0.1%)	0.71	10/13798 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	135	LYS	CB-CG	-19.61	0.99	1.52
2	A	544	GLU	CB-CG	-13.40	1.26	1.52
2	A	241	GLU	CB-CG	-9.14	1.34	1.52
2	B	314	GLU	CD-OE2	7.14	1.33	1.25
1	L	4	DC	C3'-O3'	-6.58	1.35	1.44
2	A	375	GLU	CG-CD	5.84	1.60	1.51
2	A	557	LYS	CB-CG	-5.70	1.37	1.52
2	A	408	GLU	CB-CG	-5.31	1.42	1.52
2	A	241	GLU	CG-CD	5.10	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	135	LYS	CA-CB-CG	15.16	146.76	113.40
1	D	3	DA	O4'-C1'-N9	-8.52	102.04	108.00
2	A	241	GLU	CA-CB-CG	8.12	131.25	113.40
2	A	544	GLU	CA-CB-CG	7.98	130.96	113.40
1	E	3	DA	O4'-C1'-N9	-7.82	102.53	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2	DG	O4'-C1'-N9	-7.81	102.53	108.00
2	A	408	GLU	CA-CB-CG	6.55	127.81	113.40
1	Y	1	DG	P-O3'-C3'	6.17	127.11	119.70
1	E	5	DT	O4'-C4'-C3'	6.04	109.63	106.00
1	J	5	DT	O4'-C1'-N1	-5.02	104.49	108.00

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	D	121	0	70	1	0
1	E	105	0	57	0	0
1	J	122	0	70	0	0
1	L	79	0	48	1	0
1	Y	105	0	57	0	0
2	A	4650	0	4683	25	0
2	B	4617	0	4642	39	0
3	A	72	0	108	4	0
3	B	36	0	54	0	0
4	A	768	0	0	4	2
4	B	625	0	0	4	2
4	D	20	0	0	0	0
4	E	20	0	0	0	0
4	J	31	0	0	0	0
4	L	20	0	0	1	0
4	Y	9	0	0	0	0
All	All	11400	0	9789	66	2

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 3.

All (66) 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:B:328:LEU:CD1	2:B:336:MET:HE1	1.79	1.12
2:B:328:LEU:HD11	2:B:336:MET:HE1	1.06	1.06
2:B:302:ILE:CD1	2:B:336:MET:HE2	1.99	0.93
2:B:302:ILE:HD11	2:B:336:MET:CE	2.05	0.87
2:A:72:ASN:HD22	2:A:76:ARG:HH12	1.31	0.78
2:B:328:LEU:HD11	2:B:336:MET:CE	2.03	0.77
2:A:106:CYS:SG	2:A:114:LYS:NZ	2.59	0.76
2:B:328:LEU:CD1	2:B:336:MET:CE	2.63	0.75
2:B:302:ILE:HD11	2:B:336:MET:HE3	1.67	0.74
2:B:302:ILE:CD1	2:B:336:MET:CE	2.65	0.72
2:A:529:LYS:O	2:A:530[B]:CYS:SG	2.48	0.70
2:B:372:THR:HG22	4:B:9498:HOH:O	1.91	0.70
2:B:396:ASN:HD22	2:B:398:ASP:H	1.39	0.69
2:B:302:ILE:HD12	2:B:336:MET:HE2	1.74	0.69
2:B:18:LYS:HG3	2:B:21:ASP:HB3	1.75	0.68
2:B:304:ILE:CD1	2:B:326:LEU:HD21	2.25	0.67
2:A:383:LYS:HG2	3:A:8001:EDO:H22	1.80	0.61
2:A:396:ASN:HD22	2:A:398:ASP:H	1.47	0.61
2:A:470[B]:VAL:HG13	4:A:9252:HOH:O	2.03	0.59
2:A:470[B]:VAL:HG23	2:A:471:ILE:HG23	1.85	0.58
2:B:218[B]:LEU:HD11	2:B:351:LEU:CD2	2.34	0.57
2:B:304:ILE:HD11	2:B:326:LEU:HD21	1.88	0.56
2:A:104:ASP:OD2	2:A:116:HIS:HD2	1.88	0.56
2:A:72:ASN:HD22	2:A:76:ARG:NH1	2.03	0.56
2:B:286:GLN:HG3	2:B:288:ILE:HG23	1.88	0.56
2:A:270:VAL:HG22	2:A:351[B]:LEU:CD2	2.36	0.55
2:A:529:LYS:C	2:A:530[B]:CYS:SG	2.84	0.55
2:A:359:LEU:HD23	3:A:9006:EDO:H12	1.87	0.55
2:B:187:ARG:HD2	2:B:196:LYS:HD2	1.89	0.54
2:B:218[B]:LEU:HD21	2:B:268:PRO:HG2	1.90	0.53
2:A:470[A]:VAL:HG23	4:A:9252:HOH:O	2.08	0.52
2:B:467:ILE:O	2:B:472:LYS:NZ	2.44	0.50
2:A:31:ASN:C	2:A:31:ASN:HD22	2.15	0.50
2:B:490:LYS:NZ	4:B:9424:HOH:O	2.46	0.48
2:B:8:MET:HB3	2:B:32:ILE:HD12	1.94	0.48
2:B:143:LYS:HG2	2:B:144:GLY:CA	2.44	0.48
2:B:253:LEU:HD21	2:B:437:ALA:HB1	1.96	0.47
2:A:406:LEU:HD23	2:A:412:LEU:HD23	1.97	0.47
2:B:218[B]:LEU:HD11	2:B:351:LEU:HD22	1.97	0.47
2:A:396:ASN:ND2	2:A:398:ASP:H	2.13	0.46
2:A:302:ILE:HD11	2:A:336:MET:HG3	1.98	0.46
2:B:65:PHE:CE1	2:B:565[B]:VAL:HG23	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:THR:CG2	4:B:9498:HOH:O	2.59	0.46
2:A:303:GLN:NE2	2:A:313:ASN:O	2.47	0.45
2:B:328:LEU:HD13	2:B:336:MET:CE	2.43	0.45
2:B:202:ILE:HD11	2:B:207:PHE:HD1	1.82	0.45
2:A:253:LEU:HD21	2:A:437:ALA:HB1	1.99	0.44
2:B:29:TYR:CZ	2:B:39:LYS:HB3	2.52	0.44
2:B:221:GLU:HA	2:B:224:TYR:CD1	2.53	0.44
2:B:187:ARG:HD2	2:B:196:LYS:CD	2.47	0.44
2:A:150[A]:LYS:NZ	4:A:9585:HOH:O	2.51	0.43
2:A:364:ILE:HG22	3:A:8012:EDO:H11	2.01	0.43
2:A:31:ASN:HD22	2:A:33:GLU:H	1.67	0.43
2:A:359:LEU:CD2	3:A:9006:EDO:H12	2.49	0.43
1:D:4:DC:H3'	1:D:5:DT:H71	1.99	0.43
2:B:529:LYS:O	2:B:530[B]:CYS:SG	2.74	0.43
2:B:304:ILE:HD13	2:B:326:LEU:HD21	2.00	0.43
2:B:168[A]:ASN:ND2	4:B:9316:HOH:O	2.52	0.43
2:A:493:LYS:HD2	4:A:9272:HOH:O	2.18	0.42
1:L:4:DC:OP1	4:L:999:HOH:O	2.22	0.42
2:B:412[B]:LEU:HD13	2:B:413:GLY:O	2.20	0.41
2:B:218[B]:LEU:HD11	2:B:351:LEU:HD21	2.02	0.41
2:B:68:ALA:CB	2:B:565[A]:VAL:HG23	2.52	0.40
2:A:490:LYS:HD3	2:A:505:TYR:OH	2.22	0.40
2:B:218[B]:LEU:HD21	2:B:268:PRO:CG	2.50	0.40
2:B:358:GLY:HA2	2:B:361:LYS:HD3	2.04	0.40

All (2) 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)
4:A:9650:HOH:O	4:B:9051:HOH:O[2_646]	1.61	0.59
4:A:9184:HOH:O	4:B:9568:HOH:O[2_646]	1.99	0.21

## 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	
2	A	571/575 (99%)	560 (98%)	10 (2%)	1 (0%)	52	28
2	B	565/575 (98%)	553 (98%)	11 (2%)	1 (0%)	52	28
All	All	1136/1150 (99%)	1113 (98%)	21 (2%)	2 (0%)	52	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	425	VAL
2	A	425	VAL

### 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	
2	A	506/506 (100%)	499 (99%)	7 (1%)	74	53
2	B	501/506 (99%)	488 (97%)	13 (3%)	54	25
All	All	1007/1012 (100%)	987 (98%)	20 (2%)	65	36

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	20	GLU
2	A	31	ASN
2	A	135	LYS
2	A	185	LEU
2	A	396	ASN
2	A	508	GLU
2	A	544	GLU
2	B	18	LYS
2	B	96	ARG
2	B	116	HIS
2	B	249[A]	ASP

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Mol	Chain	Res	Type
2	B	249[B]	ASP
2	B	279	GLU
2	B	361	LYS
2	B	396	ASN
2	B	429	MET
2	B	543	PHE
2	B	544	GLU
2	B	547	LYS
2	B	575	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	31	ASN
2	A	72	ASN
2	A	116	HIS
2	A	171	GLN
2	A	396	ASN
2	A	497	GLN
2	A	560	GLN
2	B	303	GLN
2	B	387	ASN
2	B	396	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

27 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	A	8001	-	3,3,3	0.59	0	2,2,2	0.44	0
3	EDO	A	8004	-	3,3,3	0.51	0	2,2,2	0.28	0
3	EDO	A	8008	-	3,3,3	0.51	0	2,2,2	0.23	0
3	EDO	A	8009	-	3,3,3	0.49	0	2,2,2	0.14	0
3	EDO	A	8010	-	3,3,3	0.45	0	2,2,2	0.47	0
3	EDO	A	8011	-	3,3,3	0.50	0	2,2,2	0.17	0
3	EDO	A	8012	-	3,3,3	0.39	0	2,2,2	0.41	0
3	EDO	A	8013	-	3,3,3	0.55	0	2,2,2	0.20	0
3	EDO	A	9001	-	3,3,3	0.49	0	2,2,2	0.24	0
3	EDO	A	9005	-	3,3,3	0.46	0	2,2,2	0.31	0
3	EDO	A	9006	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	A	9007	-	3,3,3	0.45	0	2,2,2	0.41	0
3	EDO	A	9008	-	3,3,3	0.50	0	2,2,2	0.23	0
3	EDO	A	9010	-	3,3,3	0.54	0	2,2,2	0.15	0
3	EDO	A	9011	-	3,3,3	0.46	0	2,2,2	0.26	0
3	EDO	A	9012	-	3,3,3	0.49	0	2,2,2	0.30	0
3	EDO	A	9013	-	3,3,3	0.54	0	2,2,2	0.21	0
3	EDO	A	9014	-	3,3,3	0.51	0	2,2,2	0.24	0
3	EDO	B	8002	-	3,3,3	0.45	0	2,2,2	0.31	0
3	EDO	B	8003	-	3,3,3	0.40	0	2,2,2	0.43	0
3	EDO	B	8005	-	3,3,3	0.44	0	2,2,2	0.37	0
3	EDO	B	8006	-	3,3,3	0.36	0	2,2,2	0.56	0
3	EDO	B	8007	-	3,3,3	0.50	0	2,2,2	0.40	0
3	EDO	B	9002	-	3,3,3	0.44	0	2,2,2	0.29	0
3	EDO	B	9003	-	3,3,3	0.46	0	2,2,2	0.38	0
3	EDO	B	9004	-	3,3,3	0.51	0	2,2,2	0.34	0
3	EDO	B	9009	-	3,3,3	0.51	0	2,2,2	0.27	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	8001	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	8004	-	-	0/1/1/1	0/0/0/0
3	EDO	A	8008	-	-	0/1/1/1	0/0/0/0
3	EDO	A	8009	-	-	0/1/1/1	0/0/0/0
3	EDO	A	8010	-	-	0/1/1/1	0/0/0/0
3	EDO	A	8011	-	-	0/1/1/1	0/0/0/0
3	EDO	A	8012	-	-	0/1/1/1	0/0/0/0
3	EDO	A	8013	-	-	0/1/1/1	0/0/0/0
3	EDO	A	9001	-	-	0/1/1/1	0/0/0/0
3	EDO	A	9005	-	-	0/1/1/1	0/0/0/0
3	EDO	A	9006	-	-	0/1/1/1	0/0/0/0
3	EDO	A	9007	-	-	0/1/1/1	0/0/0/0
3	EDO	A	9008	-	-	0/1/1/1	0/0/0/0
3	EDO	A	9010	-	-	0/1/1/1	0/0/0/0
3	EDO	A	9011	-	-	0/1/1/1	0/0/0/0
3	EDO	A	9012	-	-	0/1/1/1	0/0/0/0
3	EDO	A	9013	-	-	0/1/1/1	0/0/0/0
3	EDO	A	9014	-	-	0/1/1/1	0/0/0/0
3	EDO	B	8002	-	-	0/1/1/1	0/0/0/0
3	EDO	B	8003	-	-	0/1/1/1	0/0/0/0
3	EDO	B	8005	-	-	0/1/1/1	0/0/0/0
3	EDO	B	8006	-	-	0/1/1/1	0/0/0/0
3	EDO	B	8007	-	-	0/1/1/1	0/0/0/0
3	EDO	B	9002	-	-	0/1/1/1	0/0/0/0
3	EDO	B	9003	-	-	0/1/1/1	0/0/0/0
3	EDO	B	9004	-	-	0/1/1/1	0/0/0/0
3	EDO	B	9009	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	8001	EDO	1	0
3	A	8012	EDO	1	0
3	A	9006	EDO	2	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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, 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	D	6/7 (85%)	1.14	2 (33%) 0 0	27, 37, 57, 64	0
1	E	6/7 (85%)	0.17	0 100 100	27, 33, 46, 53	0
1	J	6/7 (85%)	-0.12	0 100 100	24, 32, 48, 66	0
1	L	4/7 (57%)	0.11	1 (25%) 1 1	26, 30, 31, 56	0
1	Y	6/7 (85%)	1.38	1 (16%) 2 2	32, 49, 68, 72	0
2	A	564/575 (98%)	0.55	45 (7%) 15 13	26, 32, 42, 66	8 (1%)
2	B	562/575 (97%)	0.42	35 (6%) 24 21	26, 33, 42, 59	3 (0%)
All	All	1154/1185 (97%)	0.49	84 (7%) 18 16	24, 33, 43, 72	11 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	144	GLY	8.1
2	A	5	PRO	6.1
2	B	343	TYR	5.6
2	B	141	VAL	5.3
2	B	140	THR	5.1
2	B	321	GLY	4.8
2	B	139	LEU	4.6
2	B	304	ILE	4.3
2	A	144	GLY	3.9
2	B	323	ILE	3.8
2	B	142	LEU	3.8
2	B	322	GLU	3.4
2	A	437	ALA	3.4
2	B	113	ARG	3.4
2	A	253	LEU	3.3
2	A	331	VAL	3.3
2	A	230	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
2	A	457	THR	3.3
2	B	519	ASP	3.2
2	A	333	LEU	3.2
2	B	165	TYR	3.2
2	A	433	ILE	3.2
2	A	165	TYR	3.1
2	A	254	TYR	3.1
2	A	142	LEU	3.1
2	A	434	THR	3.1
2	A	143	LYS	3.0
2	A	313	ASN	3.0
2	A	389	LEU	3.0
2	B	112	LYS	3.0
1	D	6	DT	2.9
2	B	290	CYS	2.9
1	Y	1	DG	2.8
2	A	229	GLY	2.8
2	A	328	LEU	2.8
2	B	38	TYR	2.7
2	B	347	TYR	2.7
2	B	320	GLY	2.7
2	B	277	TRP	2.7
2	B	63	LEU	2.6
2	A	441	THR	2.6
2	A	263	LEU	2.6
2	A	283	LEU	2.6
2	A	442	ILE	2.6
2	A	439	TYR	2.6
2	A	123	LEU	2.5
2	A	455	CYS	2.5
2	A	436	TRP	2.5
2	A	335	LEU	2.5
2	B	344	ASN	2.5
2	A	250	VAL	2.5
2	A	431	VAL	2.5
2	B	111	GLY	2.4
2	A	66	ALA	2.4
2	A	285	ILE	2.4
2	A	228	GLY	2.4
2	B	153	PRO	2.4
2	A	70	ILE	2.4
2	A	63	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	265	TYR	2.4
2	A	119	ILE	2.3
2	A	226	TYR	2.3
2	A	454	TYR	2.3
2	B	110	LYS	2.3
2	B	109	TYR	2.3
2	B	36	SER	2.3
2	A	440	THR	2.3
2	A	460	ILE	2.3
2	B	160	PRO	2.3
2	B	294	LEU	2.2
2	A	568	VAL	2.2
2	A	459[A]	SER	2.1
2	B	530[A]	CYS	2.1
2	B	324	ALA	2.1
2	A	231	THR	2.1
2	A	126	LEU	2.1
1	D	1	DG	2.1
1	L	4	DC	2.1
2	B	521	TYR	2.0
2	A	435	ALA	2.0
2	B	143	LYS	2.0
2	B	119	ILE	2.0
2	B	355	ALA	2.0
2	A	575	LYS	2.0

## 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 carbohydrates 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. 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	B	8006	4/4	0.76	0.43	27.23	41,42,44,49	0
3	EDO	A	8010	4/4	0.72	0.32	21.24	41,45,46,49	0
3	EDO	A	8008	4/4	0.72	0.28	7.98	55,55,56,56	0
3	EDO	B	8002	4/4	0.46	0.36	7.95	71,71,72,72	0
3	EDO	A	8011	4/4	0.84	0.22	6.76	40,40,41,42	0
3	EDO	A	9013	4/4	0.65	0.22	6.32	43,46,47,49	0
3	EDO	A	8004	4/4	0.74	0.21	4.44	76,76,76,77	0
3	EDO	B	9009	4/4	0.81	0.21	2.93	52,54,54,55	0
3	EDO	A	9012	4/4	0.69	0.19	2.43	53,54,56,57	0
3	EDO	B	9003	4/4	0.73	0.14	2.42	53,53,54,56	0
3	EDO	A	9014	4/4	0.82	0.20	2.35	45,49,50,52	0
3	EDO	A	8001	4/4	0.78	0.19	1.74	36,40,40,42	0
3	EDO	A	9011	4/4	0.92	0.22	1.09	32,38,40,44	0
3	EDO	B	9004	4/4	0.66	0.20	0.77	57,58,59,60	0
3	EDO	A	9010	4/4	0.73	0.20	-0.09	50,51,51,52	0
3	EDO	A	9008	4/4	0.92	0.09	-1.12	26,28,29,30	0
3	EDO	B	8003	4/4	0.84	0.39	-	36,42,45,49	0
3	EDO	B	8007	4/4	0.76	0.38	-	68,69,69,69	0
3	EDO	A	8013	4/4	0.76	0.26	-	58,59,59,59	0
3	EDO	A	9006	4/4	0.78	0.27	-	48,49,49,51	0
3	EDO	A	9005	4/4	0.81	0.15	-	50,51,51,54	0
3	EDO	B	8005	4/4	0.80	0.18	-	59,60,60,61	0
3	EDO	B	9002	4/4	0.75	0.20	-	46,47,47,49	0
3	EDO	A	8012	4/4	0.91	0.22	-	44,45,45,48	0
3	EDO	A	8009	4/4	0.85	0.29	-	45,48,49,51	0
3	EDO	A	9001	4/4	0.74	0.32	-	40,40,41,41	0
3	EDO	A	9007	4/4	0.79	0.15	-	40,41,42,42	0

## 6.5 Other polymers

There are no such residues in this entry.