



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:13 PM GMT

PDB ID : 4KXV  
Title : Human transketolase in covalent complex with donor ketose D-xylulose-5-phosphate, crystal 1  
Authors : Neumann, P.; Luedtke, S.; Ficner, R.; Tittmann, K.  
Deposited on : 2013-05-28  
Resolution : 0.97 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.

---

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

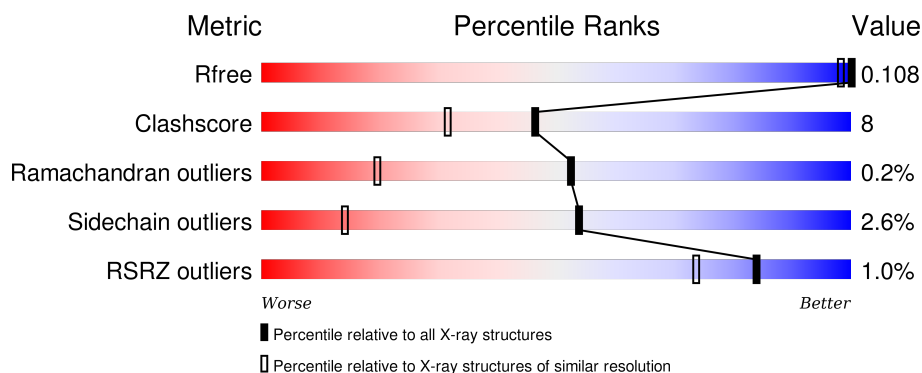
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 0.97 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	1291 (1.10-0.86)
Clashscore	102246	1390 (1.10-0.86)
Ramachandran outliers	100387	1301 (1.10-0.86)
Sidechain outliers	100360	1300 (1.10-0.86)
RSRZ outliers	91569	1295 (1.10-0.86)

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	A	637	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>84%</span> <span>11%</span> <span>• •</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	1002	-	-	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	1004	-	-	-	X
3	EDO	A	1005[A]	-	X	X	X
3	EDO	A	1005[B]	-	-	-	X
3	EDO	A	1006	-	X	-	X
3	EDO	A	1007	-	X	-	X
3	EDO	A	1008	-	X	-	X
3	EDO	A	1009	-	-	-	X
5	DX5	A	1012[B]	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6269 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 Transketolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	56	0
			5186	3263	908	987	28			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	624	LEU	-	EXPRESSION TAG	UNP P29401
A	625	VAL	-	EXPRESSION TAG	UNP P29401
A	626	PRO	-	EXPRESSION TAG	UNP P29401
A	627	ARG	-	EXPRESSION TAG	UNP P29401
A	628	GLY	-	EXPRESSION TAG	UNP P29401
A	629	SER	-	EXPRESSION TAG	UNP P29401
A	630	LEU	-	EXPRESSION TAG	UNP P29401
A	631	GLU	-	EXPRESSION TAG	UNP P29401
A	632	HIS	-	EXPRESSION TAG	UNP P29401
A	633	HIS	-	EXPRESSION TAG	UNP P29401
A	634	HIS	-	EXPRESSION TAG	UNP P29401
A	635	HIS	-	EXPRESSION TAG	UNP P29401
A	636	HIS	-	EXPRESSION TAG	UNP P29401
A	637	HIS	-	EXPRESSION TAG	UNP P29401

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

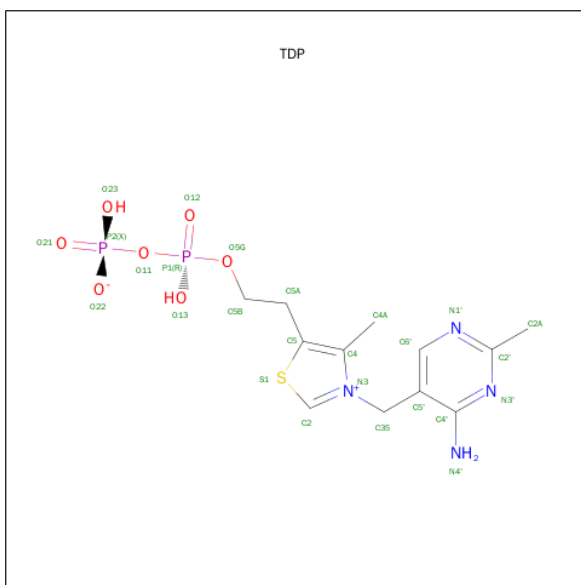
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

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



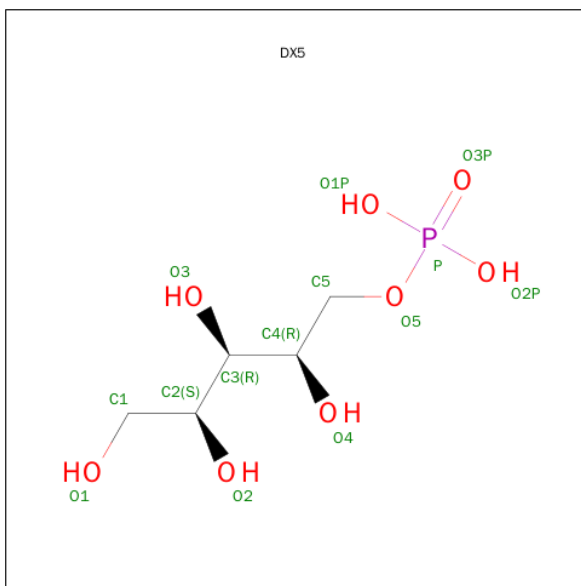
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	1
			8	4	4		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is THIAMIN DIPHOSPHATE (three-letter code: TDP) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	
									0
									0

- Molecule 5 is D-XYLITOL-5-PHOSPHATE (three-letter code: DX5) (formula:  $C_5H_{13}O_8P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P		
			24	8	14	2		
							0	1

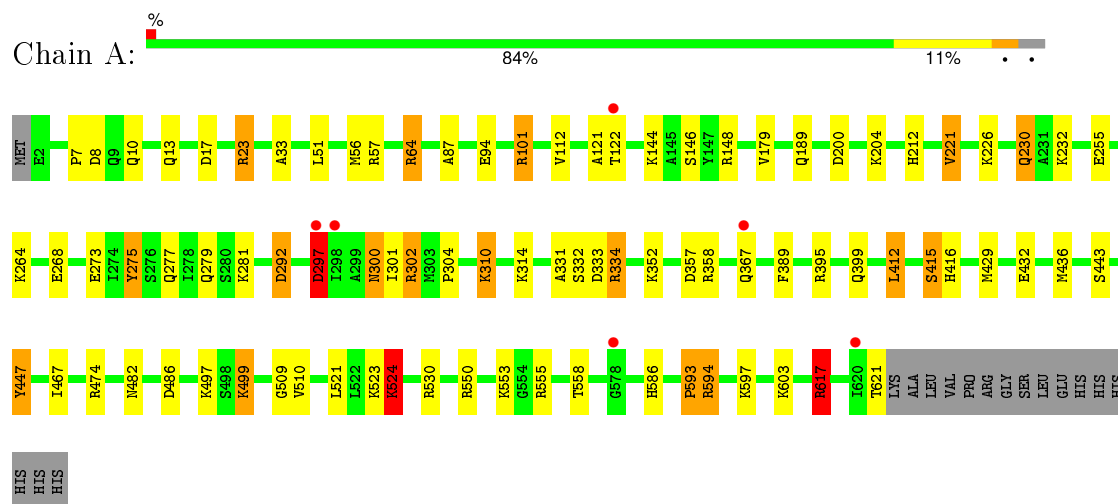
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	957	Total 992	O 992	0	51

### 3 Residue-property plots

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: Transketolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.67Å 85.98Å 73.00Å 90.00° 125.30° 90.00°	Depositor
Resolution (Å)	30.00 – 0.97 46.39 – 0.93	Depositor EDS
% Data completeness (in resolution range)	91.4 (30.00-0.97) 82.5 (46.39-0.93)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.00	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 0.94Å)	Xtriage
Refinement program	SHELXL-12	Depositor
R, $R_{free}$	0.094 , 0.114 0.090 , 0.108	Depositor DCC
$R_{free}$ test set	15421 reflections (5.42%)	DCC
Wilson B-factor (Å <sup>2</sup> )	6.2	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 76.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 321409 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	6269	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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: DX5, TDP, CA, 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	0.78	4/5286 (0.1%)	1.23	54/7147 (0.8%)

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	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122[A]	THR	C-N	-5.95	1.22	1.33
1	A	122[B]	THR	C-N	-5.95	1.22	1.33
1	A	415[A]	SER	CB-OG	-5.16	1.35	1.42
1	A	415[B]	SER	CB-OG	-5.16	1.35	1.42

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122[A]	THR	O-C-N	-11.81	103.13	123.20
1	A	122[B]	THR	O-C-N	-11.81	103.13	123.20
1	A	200	ASP	CB-CG-OD1	10.14	127.43	118.30
1	A	412[A]	LEU	CA-CB-CG	10.14	138.61	115.30
1	A	412[B]	LEU	CA-CB-CG	10.14	138.61	115.30
1	A	122[A]	THR	C-N-CA	9.95	143.20	122.30
1	A	122[B]	THR	C-N-CA	9.95	143.20	122.30
1	A	332	SER	N-CA-CB	-9.19	96.72	110.50
1	A	275[A]	TYR	CZ-CE2-CD2	-9.07	111.63	119.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275[B]	TYR	CZ-CE2-CD2	-9.07	111.63	119.80
1	A	221	VAL	CA-CB-CG1	8.76	124.03	110.90
1	A	121	ALA	O-C-N	-8.75	108.70	122.70
1	A	555	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	A	530	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	A	122[A]	THR	CA-C-N	8.29	132.77	116.20
1	A	122[B]	THR	CA-C-N	8.29	132.77	116.20
1	A	474	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	A	8	ASP	CB-CG-OD1	7.67	125.20	118.30
1	A	148	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	221	VAL	N-CA-CB	-7.28	95.48	111.50
1	A	333	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	275[A]	TYR	CG-CD2-CE2	7.01	126.91	121.30
1	A	275[B]	TYR	CG-CD2-CE2	7.01	126.91	121.30
1	A	121	ALA	CA-C-N	6.95	132.49	117.20
1	A	474	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	334	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	A	230	GLN	CB-CG-CD	6.45	128.38	111.60
1	A	617	ARG	CD-NE-CZ	6.44	132.62	123.60
1	A	221	VAL	CB-CA-C	6.43	123.63	111.40
1	A	334	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	A	273[A]	GLU	OE1-CD-OE2	-6.21	115.84	123.30
1	A	273[B]	GLU	OE1-CD-OE2	-6.21	115.84	123.30
1	A	64	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	57	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	57	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	302	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	A	486	ASP	CB-CG-OD1	-5.75	113.12	118.30
1	A	524	LYS	CA-CB-CG	5.67	125.88	113.40
1	A	395[A]	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	395[B]	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	23	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	101	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	148	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	A	17	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	297	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	357	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	121	ALA	C-N-CA	5.25	134.82	121.70
1	A	389	PHE	CB-CG-CD1	5.25	124.47	120.80
1	A	447	TYR	CB-CG-CD1	5.23	124.14	121.00
1	A	292	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	17	ASP	CB-CG-OD2	-5.07	113.73	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	594	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	23	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	221	VAL	CA-CB-CG2	5.05	118.48	110.90

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ARG	Sidechain
1	A	23	ARG	Sidechain
1	A	302	ARG	Sidechain
1	A	358	ARG	Sidechain
1	A	550	ARG	Sidechain
1	A	617	ARG	Sidechain

## 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	5186	0	5153	68	0
2	A	1	0	0	0	0
3	A	40	0	55	14	0
4	A	26	0	15	0	0
5	A	24	0	14	1	0
6	A	992	0	0	54	0
All	All	6269	0	5237	80	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 8.

All (80) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1006:EDO:C1	3:A:1006:EDO:C2	1.79	1.61
3:A:1002:EDO:C2	3:A:1002:EDO:C1	1.79	1.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1009:EDO:C2	3:A:1009:EDO:C1	1.76	1.58
3:A:1008:EDO:C1	3:A:1008:EDO:C2	1.91	1.48
1:A:436[A]:MET:HE1	6:A:7869:HOH:O	1.19	1.30
1:A:310:LYS:HG2	6:A:7934:HOH:O	1.30	1.29
3:A:1005[A]:EDO:O1	3:A:1005[A]:EDO:C1	1.80	1.28
1:A:314:LYS:HE2	6:A:7739[B]:HOH:O	1.25	1.27
3:A:1008:EDO:O1	3:A:1008:EDO:C1	1.88	1.21
3:A:1005[A]:EDO:O1	3:A:1005[A]:EDO:O2	1.66	1.13
3:A:1005[A]:EDO:O1	3:A:1005[A]:EDO:C2	2.04	1.04
1:A:275[B]:TYR:CE1	6:A:7490:HOH:O	2.11	1.02
1:A:232[B]:LYS:HE2	6:A:7762:HOH:O	1.66	0.96
1:A:232[B]:LYS:CE	6:A:7762:HOH:O	2.13	0.94
1:A:314:LYS:CE	6:A:7739[B]:HOH:O	1.93	0.92
1:A:255[B]:GLU:OE1	6:A:7241:HOH:O	1.87	0.91
1:A:204[B]:LYS:CD	6:A:7922:HOH:O	2.20	0.88
1:A:204[B]:LYS:HG2	6:A:7922:HOH:O	1.78	0.81
1:A:204[B]:LYS:HD3	6:A:7922:HOH:O	1.79	0.81
1:A:144:LYS:NZ	6:A:7760:HOH:O	1.94	0.80
1:A:352:LYS:HE3	6:A:7613:HOH:O	1.81	0.79
1:A:367:GLN:NE2	6:A:7477:HOH:O	2.14	0.79
1:A:275[B]:TYR:CZ	6:A:7490:HOH:O	2.34	0.77
1:A:87:ALA:HB3	3:A:1005[A]:EDO:H12	1.67	0.77
1:A:300[B]:ASN:ND2	6:A:7831:HOH:O	2.16	0.76
3:A:1006:EDO:O1	3:A:1006:EDO:C2	2.36	0.73
1:A:230:GLN:HG3	6:A:7706:HOH:O	1.88	0.73
1:A:334:ARG:HG2	6:A:7850:HOH:O	1.89	0.72
1:A:617:ARG:O	1:A:621:THR:HG23	1.89	0.71
1:A:603:LYS:HE3	6:A:7600:HOH:O	1.95	0.67
1:A:264[A]:LYS:HG3	6:A:7363[A]:HOH:O	1.93	0.67
1:A:521:LEU:O	1:A:524:LYS:HG3	1.97	0.64
1:A:268[A]:GLU:HG3	6:A:7484:HOH:O	2.01	0.61
1:A:64:ARG:HG3	6:A:7938:HOH:O	2.01	0.60
1:A:94[B]:GLU:HG3	6:A:7317:HOH:O	2.02	0.59
1:A:144:LYS:NZ	6:A:7877:HOH:O	2.15	0.58
1:A:33:ALA:O	3:A:1008:EDO:H11	2.04	0.58
1:A:499:LYS:HB2	6:A:7741[B]:HOH:O	2.04	0.56
1:A:144:LYS:HE2	6:A:7634:HOH:O	2.05	0.56
1:A:179:VAL:HG23	6:A:7707:HOH:O	2.05	0.55
3:A:1002:EDO:H22	6:A:7887:HOH:O	2.06	0.55
1:A:597:LYS:HE2	6:A:7683:HOH:O	2.06	0.55
1:A:367:GLN:HG2	1:A:399:GLN:OE1	2.09	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1009:EDO:H11	6:A:7866:HOH:O	2.09	0.52
1:A:301:ILE:HG23	6:A:7931:HOH:O	2.08	0.51
1:A:204[B]:LYS:CG	6:A:7922:HOH:O	2.35	0.50
1:A:304:PRO:HG3	6:A:7852:HOH:O	2.12	0.50
1:A:510[B]:VAL:HG23	6:A:7258:HOH:O	2.14	0.48
1:A:189:GLN:HE22	5:A:1012[A]:DX5:H3	1.79	0.48
1:A:310:LYS:HE3	6:A:7542:HOH:O	2.13	0.48
1:A:204[A]:LYS:HG2	6:A:7922:HOH:O	2.13	0.48
1:A:331:ALA:HB1	6:A:7931:HOH:O	2.14	0.48
1:A:334:ARG:NH2	6:A:7936:HOH:O	2.46	0.48
1:A:232[B]:LYS:HG3	6:A:7481:HOH:O	2.13	0.47
1:A:275[B]:TYR:HE1	6:A:7490:HOH:O	1.73	0.47
1:A:367:GLN:HG2	1:A:399:GLN:CD	2.36	0.47
1:A:7:PRO:HA	6:A:7913:HOH:O	2.14	0.46
1:A:212:HIS:CD2	1:A:232[B]:LYS:HD3	2.52	0.45
1:A:586[A]:HIS:CD2	6:A:7841:HOH:O	2.68	0.45
1:A:281:LYS:NZ	6:A:7939:HOH:O	2.50	0.45
1:A:482:ASN:ND2	6:A:7886:HOH:O	2.49	0.45
1:A:497:LYS:NZ	6:A:7767:HOH:O	2.51	0.44
1:A:297:ASP:OD1	1:A:334:ARG:HD2	2.18	0.44
1:A:617:ARG:NH2	6:A:7919:HOH:O	2.49	0.44
1:A:232[B]:LYS:NZ	6:A:7762:HOH:O	2.40	0.43
1:A:10[B]:GLN:HG3	6:A:7414:HOH:O	2.17	0.43
1:A:226:LYS:HE2	6:A:7811:HOH:O	2.17	0.43
1:A:64:ARG:NH2	6:A:7938:HOH:O	2.50	0.43
1:A:277:GLN:HG2	6:A:7763:HOH:O	2.18	0.43
1:A:51:LEU:O	1:A:56[B]:MET:HB2	2.19	0.42
1:A:443:SER:HA	1:A:467[A]:ILE:O	2.19	0.42
1:A:429:MET:SD	1:A:593[B]:PRO:HG2	2.60	0.42
1:A:415[B]:SER:O	1:A:416:HIS:HB2	2.19	0.42
3:A:1002:EDO:C2	3:A:1002:EDO:O1	2.62	0.42
1:A:558[A]:THR:HG22	6:A:7841:HOH:O	2.18	0.41
1:A:509:GLY:HA2	6:A:7894:HOH:O	2.20	0.41
1:A:146[B]:SER:OG	1:A:292:ASP:OD2	2.30	0.41
1:A:521:LEU:HD13	6:A:7267:HOH:O	2.20	0.41
1:A:13:GLN:NE2	1:A:279[A]:GLN:HG3	2.36	0.41
1:A:443:SER:HA	1:A:467[B]:ILE:O	2.21	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	674/637 (106%)	655 (97%)	17 (2%)	2 (0%)	46 16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	593[A]	PRO
1	A	593[B]	PRO

### 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	559/518 (108%)	544 (97%)	15 (3%)	52 13

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	VAL
1	A	221	VAL
1	A	297	ASP
1	A	300[A]	ASN
1	A	300[B]	ASN
1	A	310	LYS
1	A	412[A]	LEU
1	A	412[B]	LEU
1	A	432	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	447	TYR
1	A	499	LYS
1	A	523	LYS
1	A	524	LYS
1	A	553	LYS
1	A	594	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	61	GLN
1	A	99	ASN
1	A	189	GLN
1	A	272	GLN
1	A	483	ASN
1	A	502	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	1002	-	3,3,3	3.08	2 (66%)	2,2,2	1.04	0
3	EDO	A	1003	-	3,3,3	1.91	1 (33%)	2,2,2	0.67	0
3	EDO	A	1004	-	3,3,3	0.57	0	2,2,2	0.27	0
3	EDO	A	1005[A]	-	3,3,3	6.99	2 (66%)	2,2,2	3.59	1 (50%)
3	EDO	A	1005[B]	-	3,3,3	0.95	0	2,2,2	2.05	1 (50%)
3	EDO	A	1006	-	3,3,3	3.65	2 (66%)	2,2,2	2.26	2 (100%)
3	EDO	A	1007	-	3,3,3	2.09	1 (33%)	2,2,2	3.51	2 (100%)
3	EDO	A	1008	-	3,3,3	15.69	3 (100%)	2,2,2	4.04	1 (50%)
3	EDO	A	1009	-	3,3,3	3.14	2 (66%)	2,2,2	0.33	0
3	EDO	A	1010	-	3,3,3	2.39	1 (33%)	2,2,2	0.99	0
4	TDP	A	1011	2,5	21,27,27	1.02	2 (9%)	31,40,40	1.17	4 (12%)
5	DX5	A	1012[A]	4	13,13,13	2.04	4 (30%)	14,18,18	1.12	0
5	DX5	A	1012[B]	-	9,9,13	1.12	0	10,12,18	4.33	3 (30%)

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	1002	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1003	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1004	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1005[A]	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1005[B]	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1006	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1007	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1008	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1009	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1010	-	-	0/1/1/1	0/0/0/0
4	TDP	A	1011	2,5	-	0/16/17/17	0/2/2/2
5	DX5	A	1012[A]	4	-	0/16/16/16	0/0/0/0
5	DX5	A	1012[B]	-	-	0/8/8/16	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1005[A]	EDO	O2-C2	-9.68	0.89	1.42
3	A	1006	EDO	O2-C2	-4.56	1.17	1.42
5	A	1012[A]	DX5	O2-C2	-2.92	1.36	1.43
3	A	1003	EDO	O1-C1	-2.79	1.26	1.42
5	A	1012[A]	DX5	C4-C3	-2.20	1.49	1.53
4	A	1011	TDP	C4'-N3'	2.07	1.38	1.35
4	A	1011	TDP	C4-N3	2.84	1.42	1.39
3	A	1002	EDO	O1-C1	2.88	1.57	1.42
3	A	1009	EDO	O1-C1	3.21	1.59	1.42
3	A	1010	EDO	C2-C1	3.32	1.71	1.47
3	A	1007	EDO	O2-C2	3.38	1.60	1.42
5	A	1012[A]	DX5	C5-C4	3.53	1.57	1.51
3	A	1009	EDO	C2-C1	3.99	1.76	1.47
5	A	1012[A]	DX5	C2-C3	4.07	1.61	1.53
3	A	1006	EDO	C2-C1	4.36	1.79	1.47
3	A	1002	EDO	C2-C1	4.43	1.79	1.47
3	A	1008	EDO	C2-C1	5.98	1.91	1.47
3	A	1005[A]	EDO	O1-C1	7.16	1.80	1.42
3	A	1008	EDO	O1-C1	8.62	1.88	1.42
3	A	1008	EDO	O2-C2	25.08	2.77	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1008	EDO	O2-C2-C1	-5.48	73.28	112.54
3	A	1005[A]	EDO	O1-C1-C2	-4.76	78.44	112.54
3	A	1007	EDO	O2-C2-C1	-3.40	88.14	112.54
5	A	1012[B]	DX5	O1P-P-O3P	-3.24	100.14	110.58
4	A	1011	TDP	C4A-C4-N3	-2.94	118.66	122.59
3	A	1006	EDO	O1-C1-C2	-2.46	94.88	112.54
5	A	1012[B]	DX5	O2P-P-O3P	-2.41	102.82	110.58
3	A	1005[B]	EDO	O1-C1-C2	-2.37	95.51	112.54
4	A	1011	TDP	N1'-C2'-N3'	-2.10	121.71	125.60
3	A	1006	EDO	O2-C2-C1	2.03	127.11	112.54
4	A	1011	TDP	C5-C4-N3	2.50	113.20	107.69
4	A	1011	TDP	C6'-N1'-C2'	2.81	120.68	115.77
3	A	1007	EDO	O1-C1-C2	3.62	138.51	112.54
5	A	1012[B]	DX5	O5-P-O3P	12.79	139.70	107.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	EDO	3	0
3	A	1005[A]	EDO	4	0
3	A	1006	EDO	2	0
3	A	1008	EDO	3	0
3	A	1009	EDO	2	0
5	A	1012[A]	DX5	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 [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	620/637 (97%)	-0.63	6 (0%)	84 74	4, 7, 28, 93	16 (2%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	ILE	4.0
1	A	122[A]	THR	3.7
1	A	578	GLY	2.2
1	A	620	ILE	2.1
1	A	297	ASP	2.1
1	A	367	GLN	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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	A	1008	4/4	0.98	0.13	13.67	15,21,29,33	0
3	EDO	A	1006	4/4	0.94	0.09	5.96	15,19,19,22	0
3	EDO	A	1009	4/4	0.94	0.10	4.91	14,16,17,32	0
3	EDO	A	1007	4/4	0.90	0.10	4.44	23,25,35,38	0
3	EDO	A	1002	4/4	0.98	0.06	4.25	7,11,12,12	0
5	DX5	A	1012[B]	10/14	0.99	0.07	4.18	8,22,57,69	10
3	EDO	A	1005[A]	4/4	0.96	0.08	2.44	13,27,35,36	4
3	EDO	A	1004	4/4	0.99	0.05	2.27	8,11,12,14	0
3	EDO	A	1005[B]	4/4	0.96	0.08	2.22	7,10,13,16	4
5	DX5	A	1012[A]	14/14	0.99	0.07	1.94	3,5,7,8	14
3	EDO	A	1003	4/4	0.99	0.06	-0.07	6,10,11,12	0
4	TDP	A	1011	26/26	1.00	0.04	-0.43	3,4,5,5	0
2	CA	A	1001	1/1	1.00	0.03	-2.46	3,3,3,3	1
3	EDO	A	1010	4/4	0.86	0.10	-	19,26,40,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.