



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:57 am BST

PDB ID : 4CAZ
Title : CRYSTAL STRUCTURE OF BETAIN ALDEHYDE DEHYDROGENASE
FROM *Pseudomonas aeruginosa* IN COMPLEX WITH NADH
Authors : Gonzalez-Segura, L.; Diaz-Sanchez, A.G.; Rodriguez-Sotres, R.; Mujica-
Jimenez, C.; Munoz-Clares, R.A.
Deposited on : 2013-10-09
Resolution : 2.55 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
buster-report : 1.1.7 (2018)
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

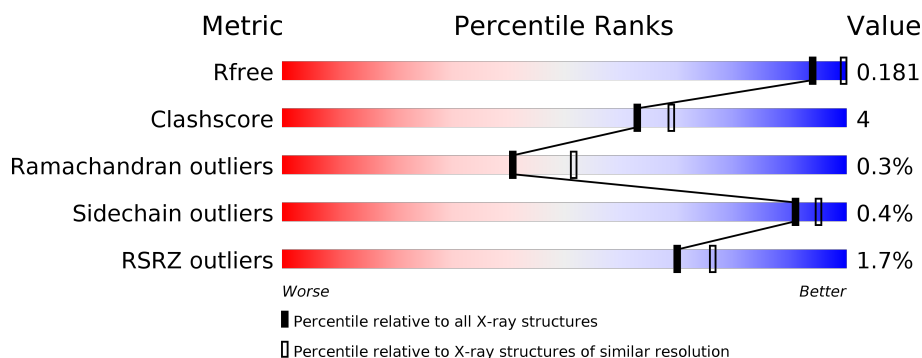
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	490	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	B	490	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>8%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	1502	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8475 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 BETAINE ALDEHYDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	8	0
			3814	2395	672	733	14			
1	B	489	Total	C	N	O	S	0	5	0
			3785	2375	665	731	14			

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



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

Continued on next page...

Continued from previous page...

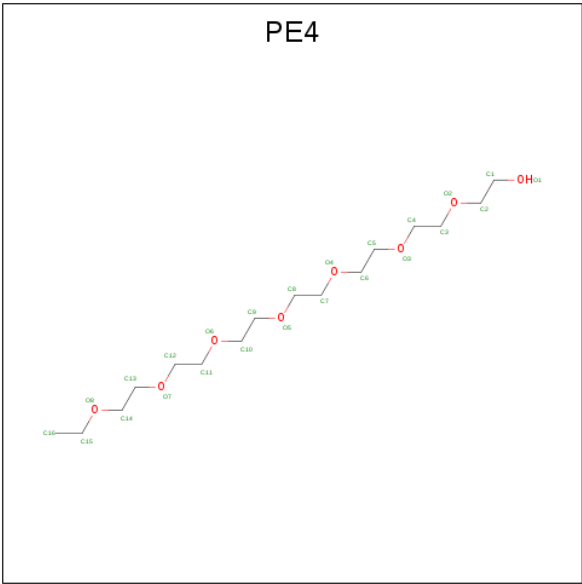
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			24	16	8		

Continued on next page...

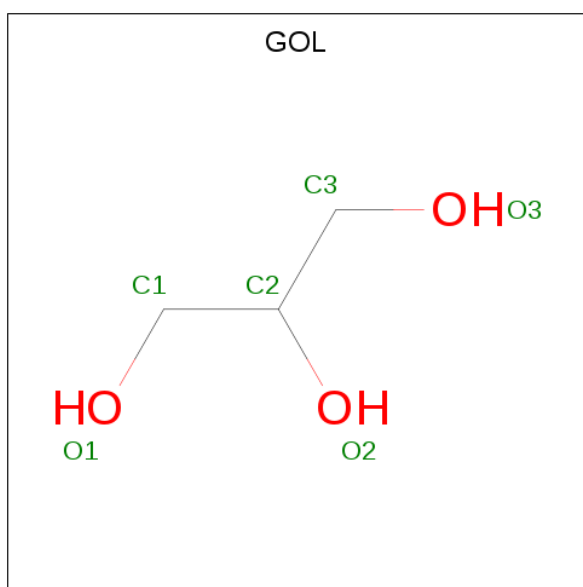
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			24	16	8		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	K	0	0
			3	3		
4	A	3	Total	K	0	0
			3	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



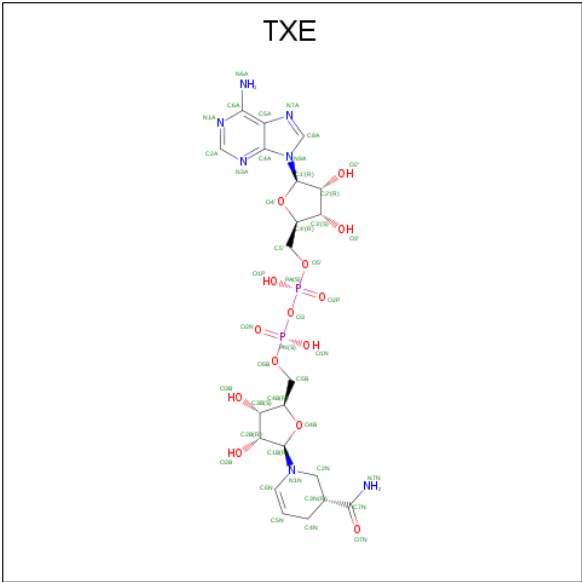
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is [[(2R,3S,4R,5R)-5-[(3R)-3-aminocarbonyl-3,4-dihydro-2H-pyridin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanidyl-phosphoryl] [(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl phosphate (three-letter code: TXE) (formula: C₂₁H₃₁N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
6	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

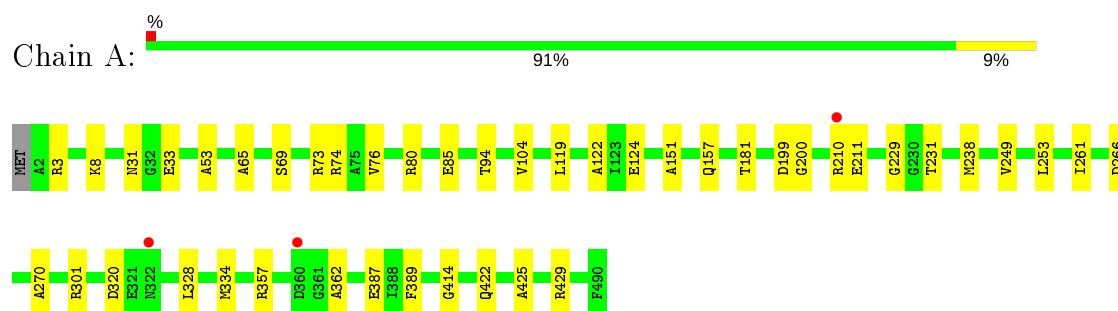
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	295	Total 295	O 295	0	0
7	B	203	Total 203	O 203	0	0

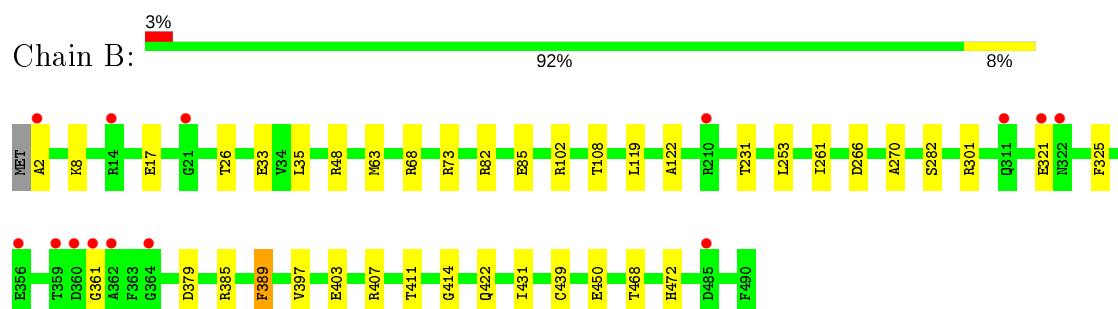
3 Residue-property plots [i](#)

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: BETAINES ALDEHYDE DEHYDROGENASE



• Molecule 1: BETAINES ALDEHYDE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.85Å 157.85Å 107.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.73 – 2.55 19.73 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.73-2.55) 99.1 (19.73-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 2.56Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.139 , 0.181 0.139 , 0.181	Depositor DCC
R_{free} test set	2537 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 78.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8475	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: PE4, GOL, K, EDO, TXE

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	0.40	0/3882	0.53	0/5260
1	B	0.36	0/3853	0.52	0/5221
All	All	0.38	0/7735	0.52	0/10481

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

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	3814	0	3786	38	0
1	B	3785	0	3751	28	0
2	A	84	0	126	14	0
2	B	56	0	84	3	0
3	A	24	0	33	2	0
3	B	24	0	34	2	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
5	A	66	0	88	5	0
5	B	30	0	40	1	0
6	A	44	0	28	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	44	0	28	1	0
7	A	295	0	0	6	0
7	B	203	0	0	5	1
All	All	8475	0	7998	69	1

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 4.

All (69) 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:73:ARG:HD3	1:B:73:ARG:HD3	1.60	0.83
1:A:73:ARG:NH1	7:A:2078:HOH:O	2.18	0.77
1:B:266:ASP:H	1:B:422:GLN:HE22	1.33	0.75
1:B:33:GLU:OE1	7:B:2003:HOH:O	2.07	0.72
1:B:102:ARG:NH1	1:B:321:GLU:OE2	2.26	0.69
1:A:357:ARG:HH12	2:A:1492:EDO:H11	1.58	0.67
1:A:3:ARG:NH1	1:A:33:GLU:OE2	2.31	0.64
1:A:8:LYS:NZ	7:A:2014:HOH:O	2.24	0.62
1:A:266:ASP:H	2:A:1510:EDO:HO1	1.46	0.62
1:A:429[B]:ARG:NH2	2:A:1499:EDO:O1	2.33	0.62
1:B:379:ASP:OD2	1:B:407:ARG:HD2	2.00	0.61
1:B:301:ARG:HH21	2:B:1494:EDO:H12	1.67	0.60
1:B:108:THR:HG21	2:B:1495:EDO:H22	1.87	0.56
3:B:1505:PE4:H141	3:B:1505:PE4:H32	1.86	0.56
3:A:1511:PE4:H102	3:A:1511:PE4:H163	1.88	0.56
1:A:429[B]:ARG:HE	2:A:1509:EDO:H21	1.72	0.55
1:A:238:MET:HG3	1:A:249[B]:VAL:HG11	1.88	0.55
1:A:119:LEU:HD21	1:B:122:ALA:HB2	1.91	0.53
1:A:65:ALA:HB2	2:A:1506:EDO:H12	1.89	0.53
1:B:397:VAL:O	1:B:407:ARG:NH2	2.42	0.53
1:A:231:THR:HA	1:A:253:LEU:HD13	1.92	0.52
1:A:157:GLN:HE22	5:A:1525:GOL:H11	1.75	0.52
1:B:450:GLU:OE1	5:B:1512:GOL:O3	2.28	0.51
1:B:385:ARG:NH1	7:B:2161:HOH:O	2.43	0.51
1:A:261[B]:ILE:HD12	1:A:270:ALA:HB1	1.94	0.50
2:A:1495:EDO:O1	7:A:2112:HOH:O	2.19	0.50
1:A:31:ASN:HD22	2:A:1503:EDO:H11	1.78	0.49
1:A:328:LEU:HD12	1:A:334:MET:HA	1.95	0.48
1:A:85:GLU:HG3	7:A:2091:HOH:O	2.15	0.47
1:B:468:THR:O	1:B:472:HIS:HD2	1.98	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:MET:O	1:B:68:ARG:NH1	2.48	0.47
5:A:1516:GOL:O1	7:A:2205:HOH:O	2.20	0.46
1:A:104:VAL:HG22	3:A:1511:PE4:H92	1.98	0.46
1:B:8:LYS:NZ	1:B:17:GLU:OE2	2.33	0.46
6:A:1526:TXE:H3'	7:A:2140:HOH:O	2.15	0.46
1:A:31:ASN:HD22	2:A:1503:EDO:C1	2.28	0.46
1:B:266:ASP:N	1:B:422:GLN:HE22	2.08	0.46
1:A:31:ASN:HB3	2:A:1503:EDO:H11	1.97	0.45
1:B:26:THR:HG23	1:B:35:LEU:HB2	1.98	0.45
1:A:387:GLU:OE1	6:A:1526:TXE:O2B	2.29	0.45
1:B:231:THR:HA	1:B:253:LEU:HD13	1.98	0.45
1:B:403:GLU:O	1:B:407:ARG:HG3	2.17	0.44
1:B:261[A]:ILE:HD12	1:B:270:ALA:HB1	1.98	0.44
1:A:53:ALA:HA	1:A:200:GLY:O	2.17	0.44
1:A:429[B]:ARG:HG3	2:A:1509:EDO:H12	1.99	0.44
1:A:362:ALA:HB1	5:A:1524:GOL:H31	2.00	0.44
1:A:69:SER:OG	1:A:73:ARG:NH2	2.49	0.44
1:B:2:ALA:HB2	7:B:2001:HOH:O	2.17	0.44
1:A:199:ASP:OD2	5:A:1521:GOL:H2	2.17	0.43
1:B:82:ARG:NH1	7:B:2055:HOH:O	2.40	0.43
1:A:151:ALA:CB	6:A:1526:TXE:H5N	2.48	0.43
1:A:122:ALA:HB2	1:B:119:LEU:HD21	2.01	0.43
1:B:282:SER:HA	1:B:325:PHE:CE2	2.53	0.43
1:B:431:ILE:HA	1:B:431:ILE:HD12	1.89	0.43
1:A:425:ALA:HB3	2:A:1499:EDO:H11	2.01	0.42
1:A:422:GLN:HB3	2:A:1510:EDO:O2	2.19	0.42
1:B:48:ARG:HH22	2:B:1491:EDO:H12	1.83	0.42
3:B:1505:PE4:H132	3:B:1505:PE4:H112	1.61	0.42
1:A:320:ASP:OD2	5:A:1516:GOL:H11	2.19	0.42
1:A:301:ARG:NH2	2:A:1504:EDO:O2	2.45	0.42
1:B:85:GLU:HG3	7:B:2053:HOH:O	2.20	0.42
1:A:229:GLY:C	6:A:1526:TXE:H1'A	2.41	0.41
1:A:74:ARG:HB2	2:A:1491:EDO:H12	2.03	0.41
1:B:431:ILE:HG13	1:B:439:CYS:HB3	2.01	0.41
1:B:389:PHE:CE1	6:B:1514:TXE:H2'A	2.56	0.41
1:A:210:ARG:HG3	1:A:211:GLU:HG3	2.03	0.41
1:A:94:THR:HG22	1:A:181:THR:HG21	2.03	0.41
1:A:122:ALA:O	1:A:124:GLU:HG3	2.22	0.40
1:A:76:VAL:O	1:A:80:ARG:HG2	2.21	0.40

All (1) 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)
7:B:2085:HOH:O	7:B:2190:HOH:O[5_555]	2.16	0.04

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	495/490 (101%)	480 (97%)	14 (3%)	1 (0%)	47	60
1	B	492/490 (100%)	473 (96%)	17 (4%)	2 (0%)	34	46
All	All	987/980 (101%)	953 (97%)	31 (3%)	3 (0%)	41	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	361	GLY
1	A	414	GLY
1	B	414	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	398/391 (102%)	397 (100%)	1 (0%)	92	96
1	B	395/391 (101%)	393 (100%)	2 (0%)	88	93
All	All	793/782 (101%)	790 (100%)	3 (0%)	91	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	389	PHE
1	B	389	PHE
1	B	411	THR

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

Mol	Chain	Res	Type
1	B	422	GLN
1	B	472	HIS

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](#)

Of 61 ligands modelled in this entry, 6 are monoatomic - leaving 55 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	$\# Z > 2$
2	EDO	A	1495	-	3,3,3	0.41	0	2,2,2	0.51	0
2	EDO	A	1506	-	3,3,3	0.52	0	2,2,2	0.27	0
5	GOL	B	1510	-	5,5,5	0.31	0	5,5,5	0.46	0
2	EDO	B	1504	-	3,3,3	0.41	0	2,2,2	0.63	0
5	GOL	B	1513	-	5,5,5	0.40	0	5,5,5	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	1500	-	3,3,3	0.47	0	2,2,2	0.23	0
6	TXE	A	1526	1	41,48,48	1.05	3 (7%)	44,73,73	1.40	7 (15%)
2	EDO	A	1505	-	3,3,3	0.57	0	2,2,2	0.07	0
2	EDO	B	1501	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	A	1493	-	3,3,3	0.46	0	2,2,2	0.44	0
2	EDO	B	1502	-	3,3,3	0.47	0	2,2,2	0.36	0
5	GOL	A	1517	-	5,5,5	0.25	0	5,5,5	0.24	0
5	GOL	B	1511	-	5,5,5	0.34	0	5,5,5	0.23	0
2	EDO	B	1493	-	3,3,3	0.45	0	2,2,2	0.53	0
5	GOL	A	1522	-	5,5,5	0.34	0	5,5,5	0.40	0
2	EDO	A	1507	-	3,3,3	0.45	0	2,2,2	0.37	0
2	EDO	B	1495	-	3,3,3	0.51	0	2,2,2	0.26	0
5	GOL	A	1515	-	5,5,5	0.25	0	5,5,5	0.30	0
5	GOL	A	1518	-	5,5,5	0.38	0	5,5,5	0.18	0
2	EDO	A	1527	-	3,3,3	0.46	0	2,2,2	0.35	0
5	GOL	A	1516	-	5,5,5	0.30	0	5,5,5	0.32	0
2	EDO	B	1499	-	3,3,3	0.51	0	2,2,2	0.18	0
2	EDO	A	1501	-	3,3,3	0.43	0	2,2,2	0.39	0
5	GOL	A	1524	-	5,5,5	0.37	0	5,5,5	0.39	0
2	EDO	B	1492	-	3,3,3	0.43	0	2,2,2	0.32	0
5	GOL	A	1520	-	5,5,5	0.36	0	5,5,5	0.39	0
3	PE4	A	1511	4	23,23,23	0.55	0	22,22,22	0.27	0
5	GOL	B	1509	-	5,5,5	0.26	0	5,5,5	0.44	0
2	EDO	A	1491	-	3,3,3	0.46	0	2,2,2	0.38	0
2	EDO	B	1491	-	3,3,3	0.47	0	2,2,2	0.38	0
2	EDO	A	1510	-	3,3,3	0.51	0	2,2,2	0.33	0
5	GOL	B	1512	-	5,5,5	0.34	0	5,5,5	0.37	0
2	EDO	B	1494	-	3,3,3	0.45	0	2,2,2	0.33	0
2	EDO	A	1496	-	3,3,3	0.49	0	2,2,2	0.23	0
5	GOL	A	1523	-	5,5,5	0.39	0	5,5,5	0.37	0
2	EDO	A	1492	-	3,3,3	0.44	0	2,2,2	0.35	0
2	EDO	B	1503	-	3,3,3	0.43	0	2,2,2	0.40	0
2	EDO	A	1494	-	3,3,3	0.45	0	2,2,2	0.39	0
2	EDO	A	1503	-	3,3,3	0.48	0	2,2,2	0.24	0
2	EDO	A	1508	-	3,3,3	0.43	0	2,2,2	0.38	0
2	EDO	A	1502	-	3,3,3	0.51	0	2,2,2	0.23	0
5	GOL	A	1525	-	5,5,5	0.35	0	5,5,5	0.49	0
2	EDO	B	1497	-	3,3,3	0.49	0	2,2,2	0.32	0
5	GOL	A	1521	-	5,5,5	0.28	0	5,5,5	0.27	0
2	EDO	B	1498	-	3,3,3	0.47	0	2,2,2	0.27	0
2	EDO	A	1497	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	A	1498	-	3,3,3	0.46	0	2,2,2	0.36	0
2	EDO	B	1496	-	3,3,3	0.41	0	2,2,2	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	1499	-	3,3,3	0.48	0	2,2,2	0.28	0
6	TXE	B	1514	1	41,48,48	1.05	3 (7%)	44,73,73	1.32	6 (13%)
5	GOL	A	1519	-	5,5,5	0.38	0	5,5,5	0.33	0
2	EDO	A	1504	-	3,3,3	0.42	0	2,2,2	0.41	0
2	EDO	A	1509	-	3,3,3	0.45	0	2,2,2	0.30	0
2	EDO	A	1500	-	3,3,3	0.45	0	2,2,2	0.38	0
3	PE4	B	1505	4	23,23,23	0.55	0	22,22,22	0.26	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
2	EDO	A	1495	-	-	0/1/1/1	-
2	EDO	A	1506	-	-	1/1/1/1	-
5	GOL	B	1510	-	-	2/4/4/4	-
2	EDO	B	1504	-	-	1/1/1/1	-
5	GOL	B	1513	-	-	0/4/4/4	-
2	EDO	B	1500	-	-	0/1/1/1	-
6	TXE	A	1526	1	-	5/26/72/72	0/5/5/5
2	EDO	A	1505	-	-	0/1/1/1	-
2	EDO	B	1501	-	-	0/1/1/1	-
2	EDO	A	1493	-	-	0/1/1/1	-
2	EDO	B	1502	-	-	0/1/1/1	-
5	GOL	A	1517	-	-	0/4/4/4	-
5	GOL	B	1511	-	-	2/4/4/4	-
2	EDO	B	1493	-	-	0/1/1/1	-
5	GOL	A	1522	-	-	0/4/4/4	-
2	EDO	A	1507	-	-	0/1/1/1	-
2	EDO	B	1495	-	-	1/1/1/1	-
5	GOL	A	1515	-	-	0/4/4/4	-
5	GOL	A	1518	-	-	4/4/4/4	-
2	EDO	A	1527	-	-	0/1/1/1	-
5	GOL	A	1516	-	-	0/4/4/4	-
2	EDO	B	1499	-	-	0/1/1/1	-
2	EDO	A	1501	-	-	1/1/1/1	-
5	GOL	A	1524	-	-	4/4/4/4	-
2	EDO	B	1492	-	-	0/1/1/1	-
5	GOL	A	1520	-	-	4/4/4/4	-
3	PE4	A	1511	4	-	10/21/21/21	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	1509	-	-	0/4/4/4	-
2	EDO	A	1491	-	-	0/1/1/1	-
2	EDO	B	1491	-	-	0/1/1/1	-
2	EDO	A	1510	-	-	0/1/1/1	-
5	GOL	B	1512	-	-	3/4/4/4	-
2	EDO	B	1494	-	-	0/1/1/1	-
2	EDO	A	1496	-	-	0/1/1/1	-
5	GOL	A	1523	-	-	1/4/4/4	-
2	EDO	A	1492	-	-	0/1/1/1	-
2	EDO	B	1503	-	-	0/1/1/1	-
2	EDO	A	1494	-	-	1/1/1/1	-
2	EDO	A	1503	-	-	0/1/1/1	-
2	EDO	A	1508	-	-	0/1/1/1	-
2	EDO	A	1502	-	-	0/1/1/1	-
5	GOL	A	1525	-	-	4/4/4/4	-
2	EDO	B	1497	-	-	0/1/1/1	-
5	GOL	A	1521	-	-	0/4/4/4	-
2	EDO	B	1498	-	-	0/1/1/1	-
2	EDO	A	1497	-	-	0/1/1/1	-
2	EDO	A	1498	-	-	0/1/1/1	-
2	EDO	B	1496	-	-	1/1/1/1	-
2	EDO	A	1499	-	-	1/1/1/1	-
6	TXE	B	1514	1	-	8/26/72/72	0/5/5/5
5	GOL	A	1519	-	-	0/4/4/4	-
2	EDO	A	1504	-	-	0/1/1/1	-
2	EDO	A	1509	-	-	0/1/1/1	-
2	EDO	A	1500	-	-	0/1/1/1	-
3	PE4	B	1505	4	-	8/21/21/21	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1526	TXE	PA-O2P	3.08	1.61	1.50
6	A	1526	TXE	PN-O2N	2.99	1.61	1.50
6	B	1514	TXE	PA-O2P	2.97	1.61	1.50
6	B	1514	TXE	PN-O2N	2.94	1.61	1.50
6	A	1526	TXE	C5A-C4A	2.73	1.48	1.40
6	B	1514	TXE	C5A-C4A	2.71	1.48	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1526	TXE	PN-O3-PA	-4.43	117.61	132.83
6	B	1514	TXE	N3A-C2A-N1A	-4.02	122.40	128.68
6	A	1526	TXE	N3A-C2A-N1A	-3.70	122.89	128.68
6	B	1514	TXE	PN-O3-PA	-3.67	120.23	132.83
6	A	1526	TXE	C2N-C3N-C7N	3.55	116.75	110.07
6	A	1526	TXE	C4A-C5A-N7A	-3.33	105.92	109.40
6	B	1514	TXE	C4A-C5A-N7A	-3.01	106.26	109.40
6	B	1514	TXE	C2N-C3N-C7N	2.78	115.30	110.07
6	B	1514	TXE	O4'-C1'-C2'	-2.46	103.33	106.93
6	A	1526	TXE	O4'-C1'-C2'	-2.43	103.37	106.93
6	A	1526	TXE	C3B-C2B-C1B	2.17	105.56	101.43
6	A	1526	TXE	C2A-N1A-C6A	2.09	122.33	118.75
6	B	1514	TXE	C3B-C2B-C1B	2.04	105.30	101.43

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1511	GOL	C1-C2-C3-O3
5	B	1511	GOL	O2-C2-C3-O3
5	A	1518	GOL	C1-C2-C3-O3
5	A	1524	GOL	O1-C1-C2-O2
5	A	1524	GOL	O1-C1-C2-C3
5	A	1524	GOL	C1-C2-C3-O3
5	A	1520	GOL	C1-C2-C3-O3
5	B	1512	GOL	O1-C1-C2-O2
5	B	1512	GOL	O1-C1-C2-C3
6	B	1514	TXE	C5'-O5'-PA-O3
6	B	1514	TXE	O4B-C1B-N1N-C2N
6	B	1514	TXE	C3B-C4B-C5B-O5B
5	A	1525	GOL	O1-C1-C2-C3
5	A	1525	GOL	C1-C2-C3-O3
6	A	1526	TXE	O4B-C1B-N1N-C2N
3	B	1505	PE4	C11-C12-O7-C13
3	B	1505	PE4	O4-C7-C8-O5
3	B	1505	PE4	O6-C11-C12-O7
3	A	1511	PE4	C6-C5-O3-C4
5	B	1510	GOL	C1-C2-C3-O3
5	A	1518	GOL	O1-C1-C2-C3
5	A	1520	GOL	O1-C1-C2-C3
5	B	1512	GOL	C1-C2-C3-O3
5	A	1518	GOL	O1-C1-C2-O2
5	A	1518	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

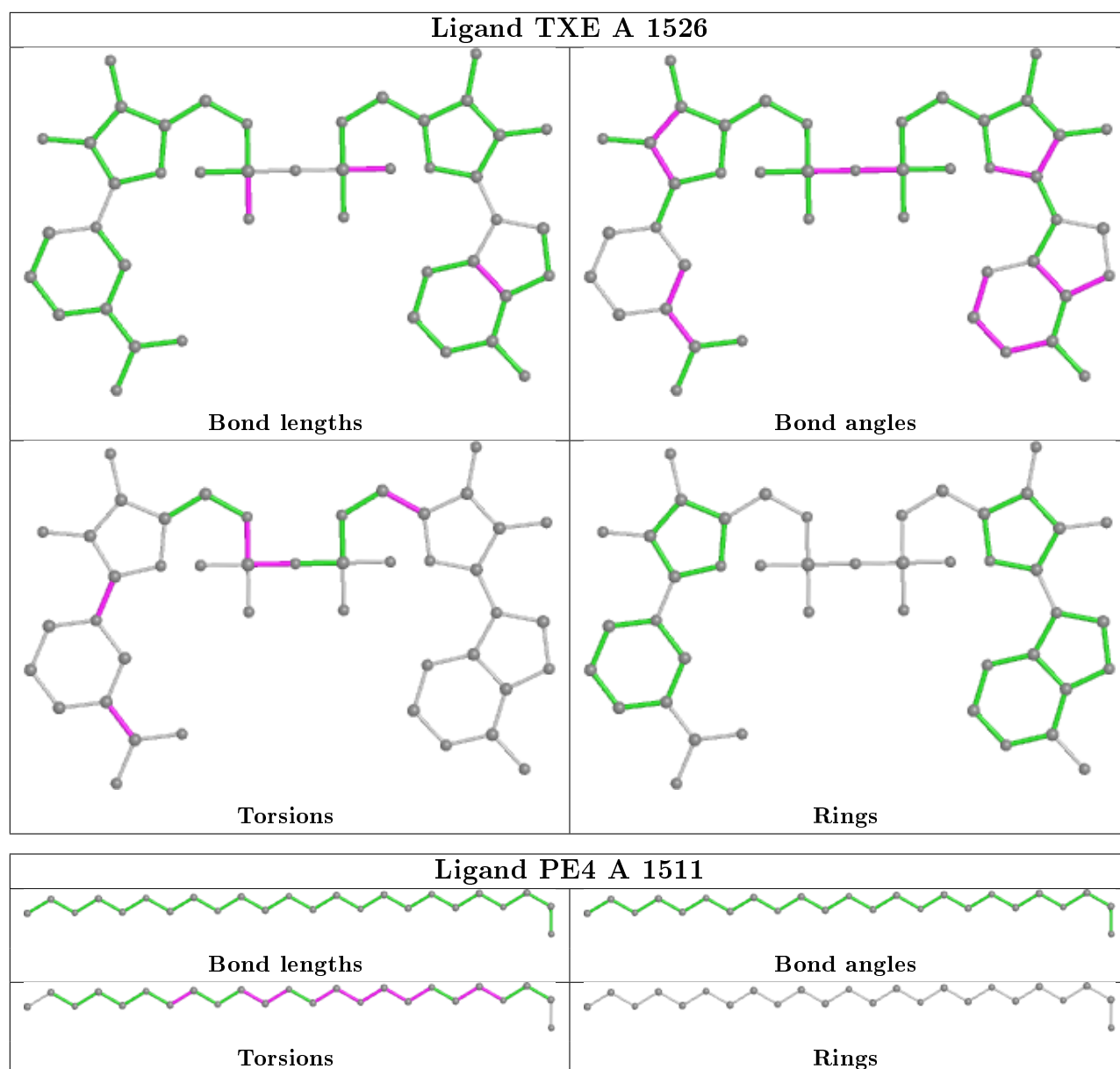
Mol	Chain	Res	Type	Atoms
5	A	1524	GOL	O2-C2-C3-O3
5	A	1520	GOL	O2-C2-C3-O3
5	A	1525	GOL	O2-C2-C3-O3
2	A	1501	EDO	O1-C1-C2-O2
3	A	1511	PE4	O6-C11-C12-O7
6	B	1514	TXE	O4B-C4B-C5B-O5B
3	A	1511	PE4	C8-C7-O4-C6
3	A	1511	PE4	O3-C5-C6-O4
5	A	1525	GOL	O1-C1-C2-O2
3	B	1505	PE4	O7-C13-C14-O8
3	A	1511	PE4	O4-C7-C8-O5
6	B	1514	TXE	PA-O3-PN-O5B
3	B	1505	PE4	C9-C10-O6-C11
6	B	1514	TXE	C4B-C5B-O5B-PN
3	A	1511	PE4	C10-C9-O5-C8
5	A	1520	GOL	O1-C1-C2-O2
6	B	1514	TXE	C5'-O5'-PA-O2P
2	A	1499	EDO	O1-C1-C2-O2
3	B	1505	PE4	O3-C5-C6-O4
3	A	1511	PE4	O2-C3-C4-O3
6	B	1514	TXE	PN-O3-PA-O1P
3	B	1505	PE4	C12-C11-O6-C10
3	B	1505	PE4	C4-C3-O2-C2
3	A	1511	PE4	C5-C6-O4-C7
3	A	1511	PE4	C4-C3-O2-C2
6	A	1526	TXE	PA-O3-PN-O2N
2	A	1506	EDO	O1-C1-C2-O2
5	A	1523	GOL	C1-C2-C3-O3
6	A	1526	TXE	O4'-C4'-C5'-O5'
6	A	1526	TXE	C2N-C3N-C7N-O7N
3	A	1511	PE4	O6-C10-C9-O5
2	B	1504	EDO	O1-C1-C2-O2
2	A	1494	EDO	O1-C1-C2-O2
2	B	1496	EDO	O1-C1-C2-O2
5	B	1510	GOL	O2-C2-C3-O3
6	A	1526	TXE	C5B-O5B-PN-O2N
2	B	1495	EDO	O1-C1-C2-O2

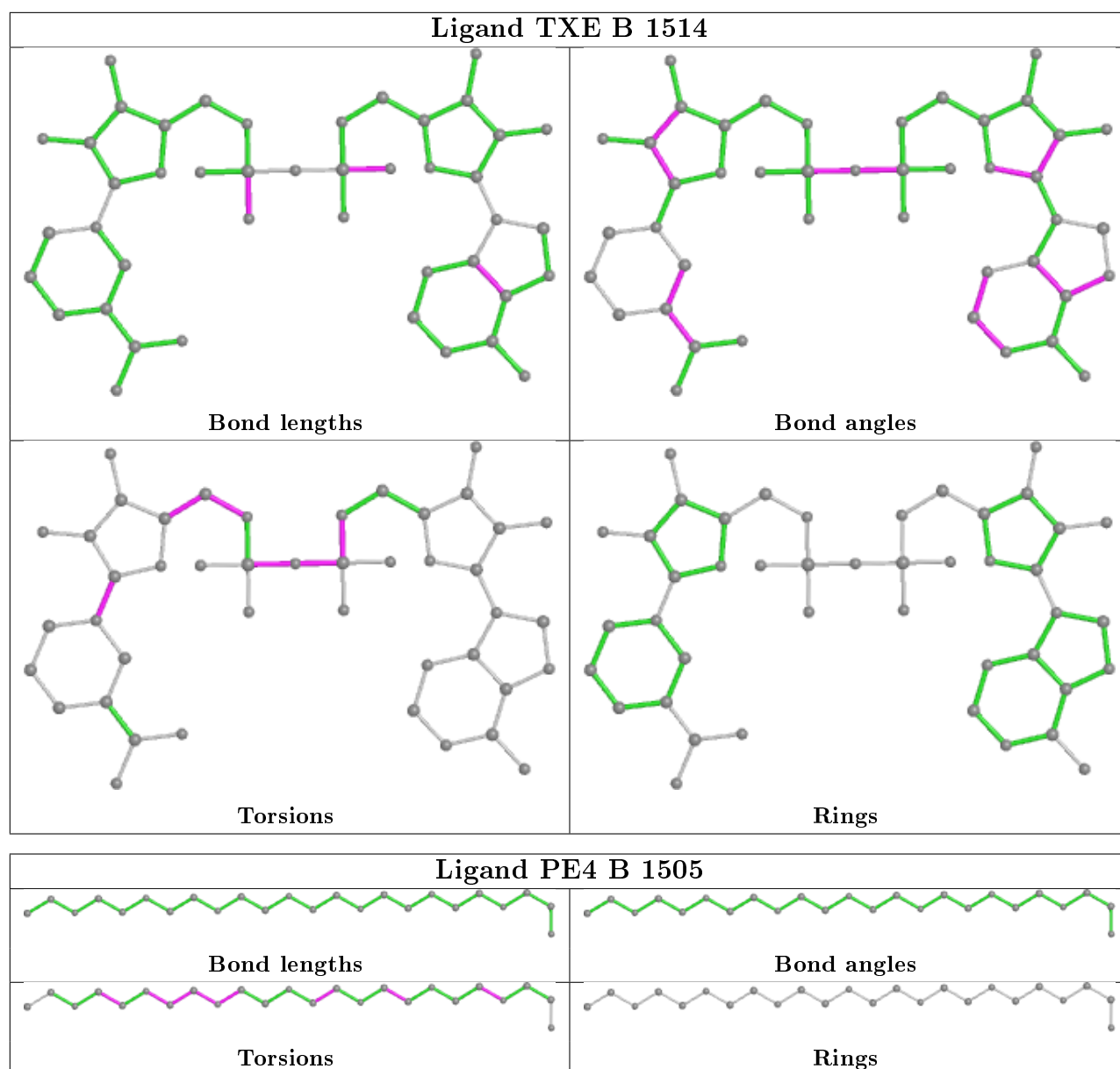
There are no ring outliers.

21 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1495	EDO	1	0
2	A	1506	EDO	1	0
6	A	1526	TXE	4	0
2	B	1495	EDO	1	0
5	A	1516	GOL	2	0
5	A	1524	GOL	1	0
3	A	1511	PE4	2	0
2	A	1491	EDO	1	0
2	B	1491	EDO	1	0
2	A	1510	EDO	2	0
5	B	1512	GOL	1	0
2	B	1494	EDO	1	0
2	A	1492	EDO	1	0
2	A	1503	EDO	3	0
5	A	1525	GOL	1	0
5	A	1521	GOL	1	0
2	A	1499	EDO	2	0
6	B	1514	TXE	1	0
2	A	1504	EDO	1	0
2	A	1509	EDO	2	0
3	B	1505	PE4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	489/490 (99%)	-0.51	3 (0%) 89 92	15, 28, 52, 77	0
1	B	489/490 (99%)	-0.32	14 (2%) 51 59	19, 39, 65, 90	0
All	All	978/980 (99%)	-0.41	17 (1%) 70 76	15, 32, 60, 90	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	210	ARG	4.2
1	B	359	THR	4.1
1	B	361	GLY	3.7
1	B	360	ASP	3.2
1	A	210	ARG	3.2
1	B	2	ALA	3.1
1	B	356	GLU	3.0
1	A	322	ASN	2.9
1	B	485	ASP	2.8
1	B	321	GLU	2.6
1	B	362	ALA	2.6
1	B	322	ASN	2.4
1	B	364	GLY	2.4
1	A	360	ASP	2.4
1	B	14	ARG	2.1
1	B	311	GLN	2.1
1	B	21	GLY	2.1

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. 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(\AA^2)	Q<0.9
2	EDO	A	1502	4/4	0.55	0.48	78,78,80,81	0
2	EDO	A	1506	4/4	0.72	0.36	54,58,68,70	0
2	EDO	A	1503	4/4	0.73	0.31	71,75,77,78	0
3	PE4	A	1511	24/24	0.76	0.22	62,76,83,86	0
2	EDO	A	1527	4/4	0.77	0.34	71,79,82,85	0
2	EDO	A	1500	4/4	0.77	0.27	62,66,75,86	0
5	GOL	B	1513	6/6	0.78	0.30	61,68,74,81	0
2	EDO	B	1500	4/4	0.78	0.28	66,69,69,71	0
2	EDO	B	1502	4/4	0.79	0.33	75,77,77,78	0
2	EDO	A	1501	4/4	0.79	0.23	83,83,84,86	0
2	EDO	A	1508	4/4	0.80	0.31	79,79,80,82	0
3	PE4	B	1505	24/24	0.80	0.24	62,79,96,99	0
2	EDO	A	1497	4/4	0.81	0.28	65,65,72,79	0
5	GOL	A	1516	6/6	0.82	0.20	59,73,75,75	0
2	EDO	B	1501	4/4	0.82	0.37	65,65,76,82	0
2	EDO	A	1495	4/4	0.82	0.48	62,64,65,76	0
2	EDO	A	1499	4/4	0.85	0.23	71,71,72,73	0
5	GOL	B	1511	6/6	0.85	0.29	69,81,84,91	0
2	EDO	A	1491	4/4	0.86	0.17	57,63,71,81	0
6	TXE	B	1514	44/44	0.86	0.26	45,78,109,197	44
2	EDO	B	1495	4/4	0.86	0.23	51,60,67,69	0
4	K	B	1508	1/1	0.87	0.17	68,68,68,68	0
5	GOL	B	1510	6/6	0.87	0.29	87,89,90,92	0
5	GOL	B	1512	6/6	0.87	0.19	52,61,64,66	0
2	EDO	A	1496	4/4	0.87	0.17	64,64,66,72	0
5	GOL	A	1523	6/6	0.88	0.32	59,68,74,74	0
5	GOL	A	1521	6/6	0.88	0.35	63,69,74,79	0
2	EDO	B	1499	4/4	0.88	0.19	53,62,66,71	0
5	GOL	A	1515	6/6	0.88	0.19	53,57,70,82	0
6	TXE	A	1526	44/44	0.89	0.25	47,70,114,199	44
2	EDO	B	1494	4/4	0.89	0.19	53,61,63,68	0
5	GOL	A	1517	6/6	0.89	0.29	75,76,80,80	0

Continued on next page...

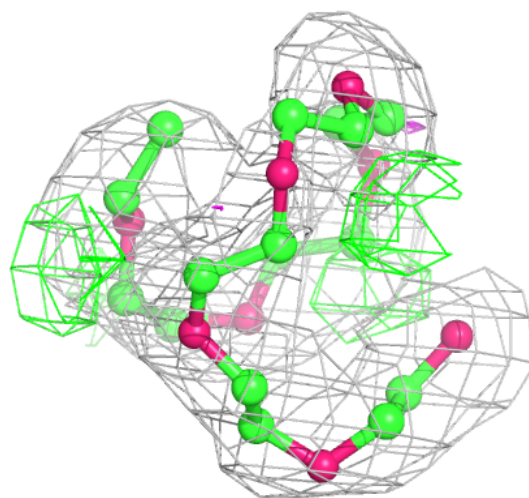
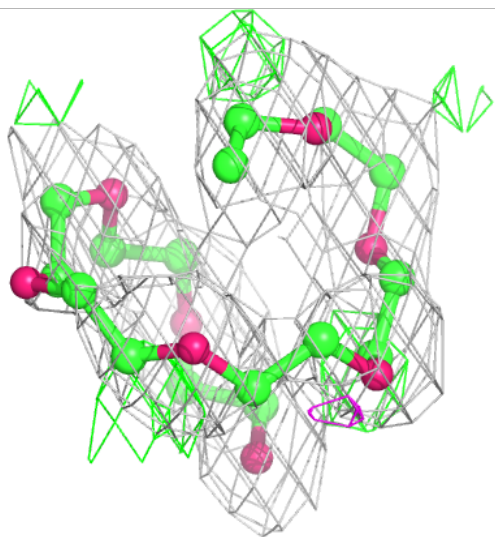
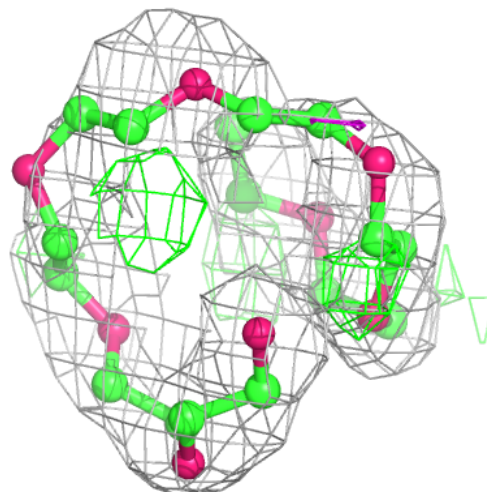
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	A	1510	4/4	0.90	0.19	57,60,62,64	0
2	EDO	A	1498	4/4	0.90	0.15	67,68,72,74	0
2	EDO	A	1494	4/4	0.90	0.32	58,60,62,68	0
5	GOL	A	1524	6/6	0.91	0.22	82,83,84,84	0
2	EDO	B	1491	4/4	0.91	0.30	64,66,68,71	0
5	GOL	A	1518	6/6	0.91	0.21	63,69,75,85	0
5	GOL	B	1509	6/6	0.91	0.19	70,75,81,92	0
2	EDO	A	1504	4/4	0.91	0.29	84,84,85,86	0
2	EDO	A	1509	4/4	0.91	0.20	74,78,80,85	0
2	EDO	B	1503	4/4	0.91	0.20	77,78,78,84	0
2	EDO	B	1498	4/4	0.91	0.27	68,69,70,70	0
5	GOL	A	1519	6/6	0.92	0.15	62,65,67,69	0
2	EDO	A	1492	4/4	0.92	0.21	61,63,64,65	0
2	EDO	A	1505	4/4	0.92	0.20	46,49,53,54	0
2	EDO	B	1504	4/4	0.92	0.34	52,55,61,73	0
4	K	A	1514	1/1	0.92	0.14	69,69,69,69	0
5	GOL	A	1522	6/6	0.93	0.27	74,75,83,90	0
2	EDO	A	1507	4/4	0.94	0.18	65,68,69,72	0
5	GOL	A	1520	6/6	0.94	0.15	52,76,84,84	0
2	EDO	B	1492	4/4	0.94	0.16	58,58,59,63	0
5	GOL	A	1525	6/6	0.95	0.14	56,58,60,66	0
2	EDO	B	1496	4/4	0.95	0.13	66,67,67,71	0
2	EDO	B	1497	4/4	0.95	0.28	35,47,57,66	0
2	EDO	B	1493	4/4	0.95	0.31	51,56,57,66	0
2	EDO	A	1493	4/4	0.96	0.14	46,47,55,58	0
4	K	A	1513	1/1	0.98	0.08	26,26,26,26	0
4	K	B	1507	1/1	0.98	0.08	35,35,35,35	0
4	K	B	1506	1/1	0.99	0.06	48,48,48,48	0
4	K	A	1512	1/1	1.00	0.11	31,31,31,31	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

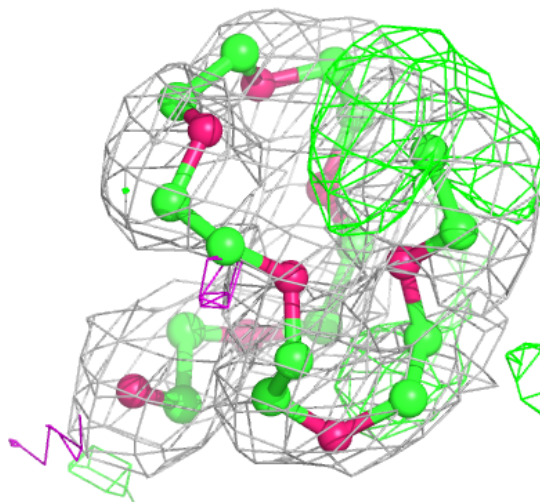
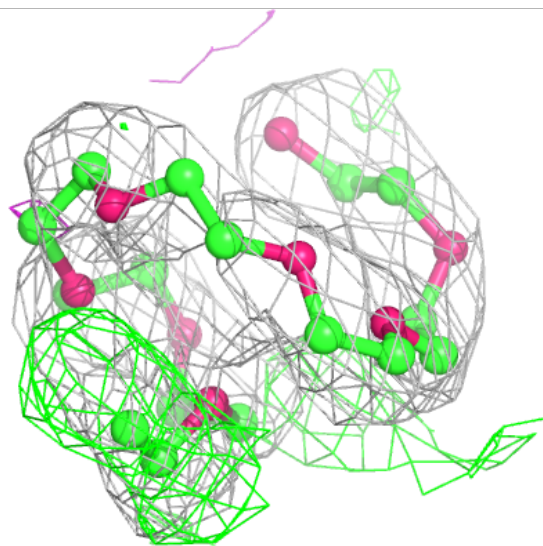
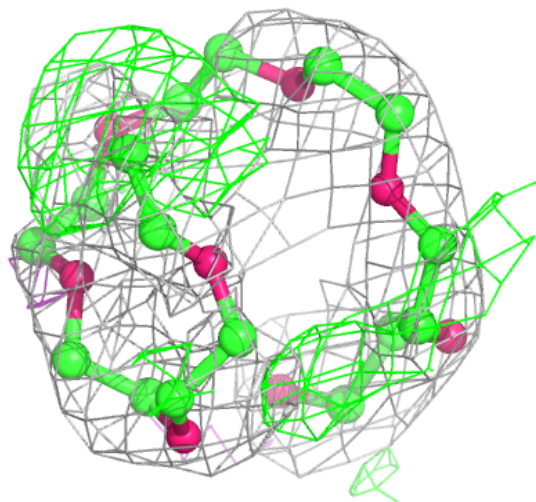
Electron density around PE4 A 1511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



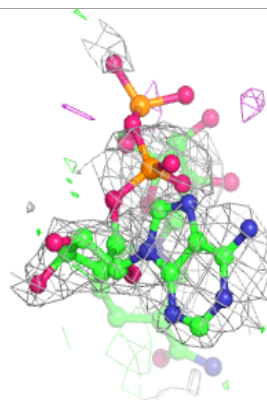
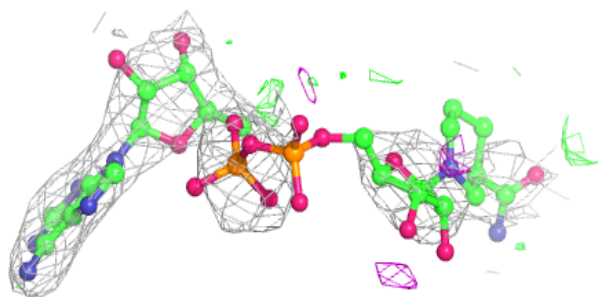
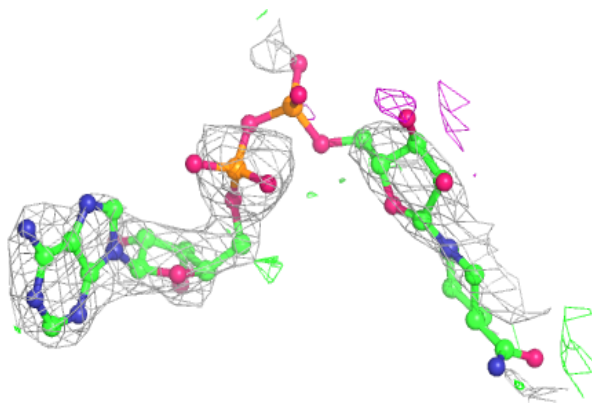
Electron density around PE4 B 1505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

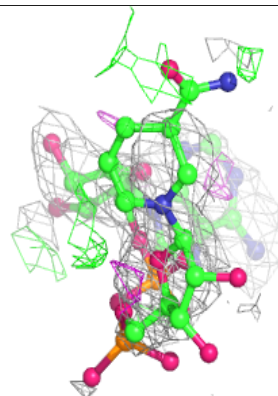
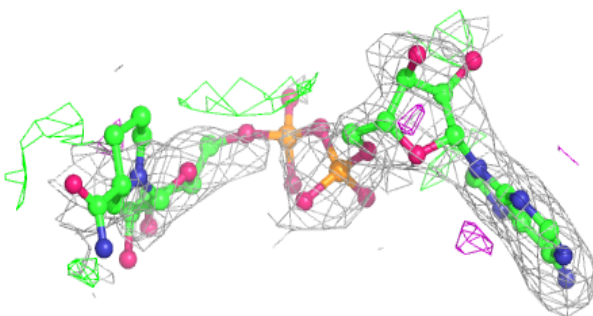
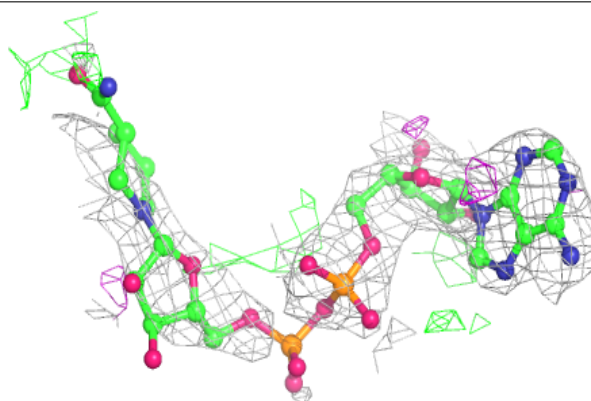


Electron density around TXE B 1514:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around TXE A 1526:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.