wwPDB X-ray Structure Validation Summary Report (i)

Sep 11, 2023 – 04:22 AM EDT

PDB ID	:	4KXY
Title	:	Human transketolase in complex with ThDP analogue (R)-2-(1,2-dihydroxyethyl)-3-deaza-ThDP
Authors	:	Neumann, P.; Luedtke, S.; Erixon, K.M.; Leeper, F.; Kluger, R.; Ficner, R.; Tittmann, K.
Deposited on	:	2013-05-28
Resolution	:	1.26 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

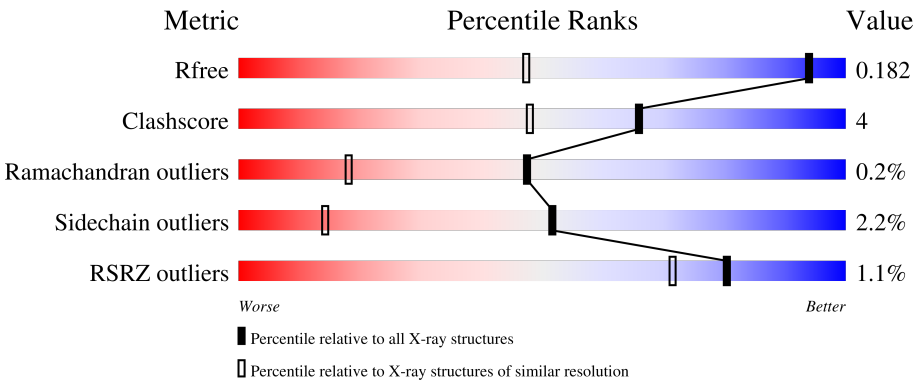
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.26 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	1023 (1.28-1.24)
Clashscore	141614	1060 (1.28-1.24)
Ramachandran outliers	138981	1029 (1.28-1.24)
Sidechain outliers	138945	1028 (1.28-1.24)
RSRZ outliers	127900	1004 (1.28-1.24)

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 >=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 <=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	% 84% 13% • •
1	B	637	% 85% 10% • •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11716 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
			Total	C	N	O	S			
1	A	620	5006	3156	874	950	26	0	34	0
1	B	620	5012	3158	878	949	27	0	34	0

There are 28 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
B	624	LEU	-	expression tag	UNP P29401
B	625	VAL	-	expression tag	UNP P29401
B	626	PRO	-	expression tag	UNP P29401
B	627	ARG	-	expression tag	UNP P29401
B	628	GLY	-	expression tag	UNP P29401
B	629	SER	-	expression tag	UNP P29401
B	630	LEU	-	expression tag	UNP P29401
B	631	GLU	-	expression tag	UNP P29401
B	632	HIS	-	expression tag	UNP P29401
B	633	HIS	-	expression tag	UNP P29401
B	634	HIS	-	expression tag	UNP P29401

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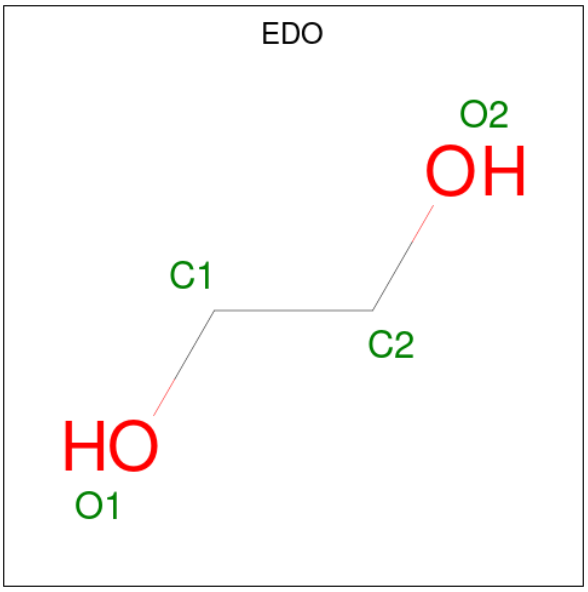
Chain	Residue	Modelled	Actual	Comment	Reference
B	635	HIS	-	expression tag	UNP P29401
B	636	HIS	-	expression tag	UNP P29401
B	637	HIS	-	expression tag	UNP P29401

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

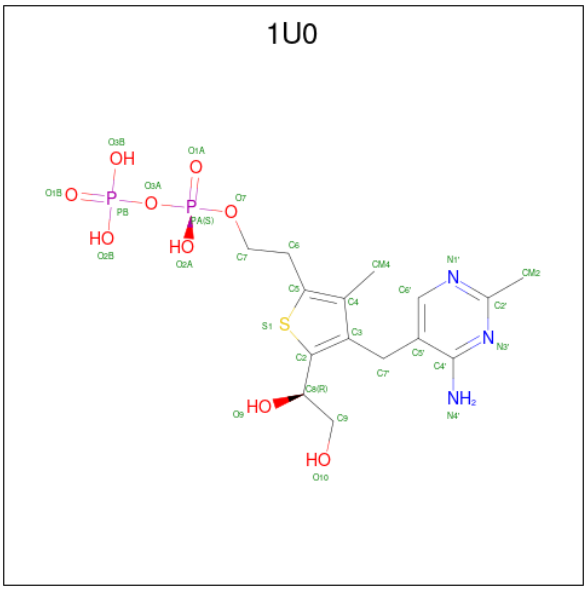
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	1	1	1	0	0
			Total	Ca		
3	B	1	1	1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

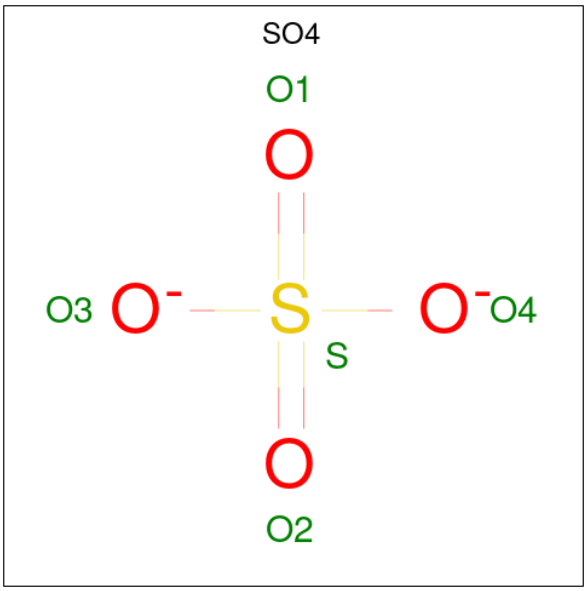
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	1	1	1	0	0
4	B	1	1	1	0	0

- Molecule 5 is 2-{4-[(4-amino-2-methylpyrimidin-5-yl)methyl]-5-[(1R)-1,2-dihydroxyethyl]-3-methylthiophen-2-yl}ethyl trihydrogen diphosphate (three-letter code: 1U0) (formula: $C_{15}H_{23}N_3O_9P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
5	A	1	32	16	3	10	2	1	0	1
5	B	1	32	16	3	10	2	1	0	1

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is water.

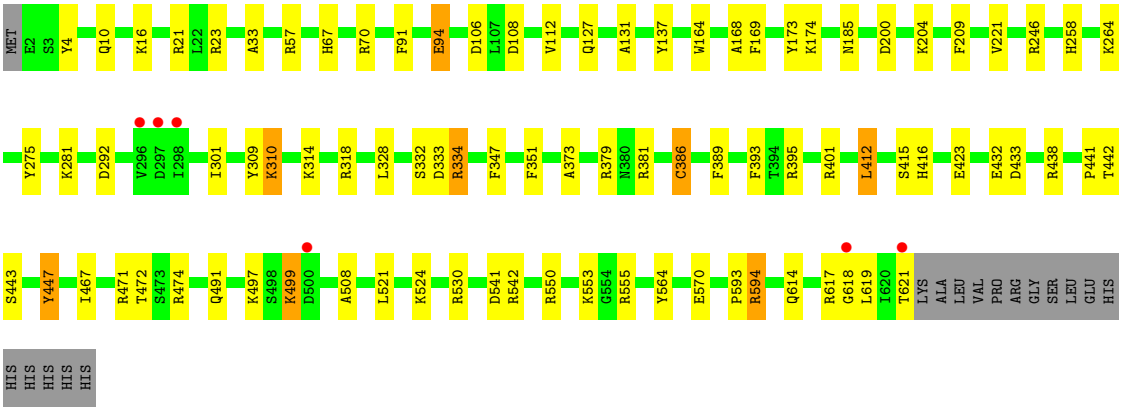
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	756	Total O 778 778	0	22
7	B	706	Total O 722 722	0	17

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.

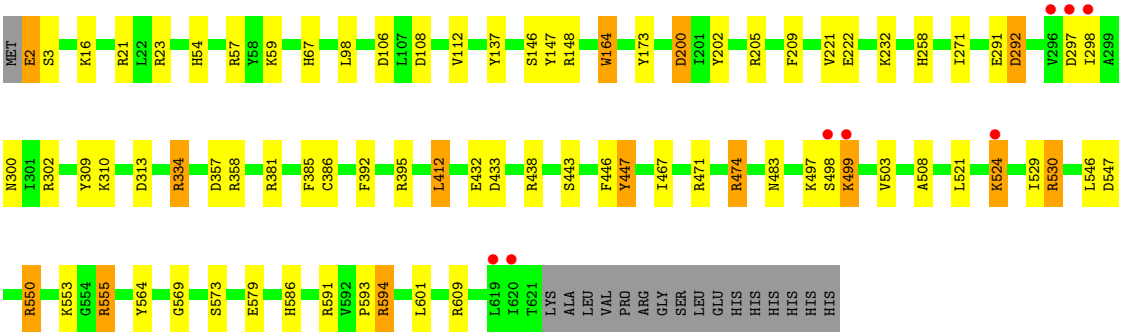
- Molecule 1: Transketolase

Chain A:



- Molecule 1: Transketolase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.15Å 86.05Å 92.73Å 90.00° 94.12° 90.00°	Depositor
Resolution (Å)	30.00 – 1.26 48.88 – 1.26	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-1.26) 89.7 (48.88-1.26)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 1.26Å)	Xtriage
Refinement program	SHELX, SHELXL	Depositor
R, R_{free}	0.154 , 0.204 0.149 , 0.182	Depositor DCC
R_{free} test set	13830 reflections (4.50%)	wwPDB-VP
Wilson B-factor (Å^2)	7.2	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 83.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	11716	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 89.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3396e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, SO4, EDO, 1U0, CA

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	0.64	0/5114	1.33	57/6915 (0.8%)
1	B	0.63	0/5121	1.38	68/6924 (1.0%)
All	All	0.64	0/10235	1.36	125/13839 (0.9%)

There are no bond length outliers.

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	395[A]	ARG	NE-CZ-NH2	15.57	128.09	120.30
1	B	395[B]	ARG	NE-CZ-NH2	15.57	128.09	120.30
1	B	381	ARG	NE-CZ-NH2	-12.65	113.98	120.30
1	A	334	ARG	NE-CZ-NH1	12.16	126.38	120.30
1	A	334	ARG	NE-CZ-NH2	-11.90	114.35	120.30

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	5006	0	5002	44	0
1	B	5012	0	5005	34	0
2	A	64	0	96	11	0
2	B	56	0	84	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	32	0	8	0	0
5	B	32	0	8	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	778	0	0	26	0
7	B	722	0	0	19	0
All	All	11716	0	10203	83	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 4.

The worst 5 of 83 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:B:16[C]:LYS:HE3	7:B:1729:HOH:O	1.69	0.92
1:B:357[B]:ASP:OD1	7:B:1480:HOH:O	1.98	0.80
1:B:271:ILE:HG21	7:B:1759:HOH:O	1.84	0.77
1:A:614:GLN:HG3	7:A:8594:HOH:O	1.86	0.76
2:B:1015:EDO:H22	7:B:1295:HOH:O	1.86	0.74

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	652/637 (102%)	631 (97%)	20 (3%)	1 (0%)	47 18
1	B	652/637 (102%)	634 (97%)	17 (3%)	1 (0%)	47 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1304/1274 (102%)	1265 (97%)	37 (3%)	2 (0%)	47 18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	593	PRO
1	A	593	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	536/518 (104%)	525 (98%)	11 (2%)	53 16
1	B	536/518 (104%)	521 (97%)	15 (3%)	43 7
All	All	1072/1036 (104%)	1046 (98%)	26 (2%)	52 11

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	98	LEU
1	B	412[A]	LEU
1	B	594	ARG
1	B	310	LYS
1	B	412[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	A	230	GLN
1	A	614	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 40 ligands modelled in this entry, 4 are monoatomic - leaving 36 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	B	1009	-	3,3,3	0.28	0	2,2,2	0.67	0
2	EDO	B	1008	-	3,3,3	0.50	0	2,2,2	0.89	0
6	SO4	B	1013	-	4,4,4	0.60	0	6,6,6	1.63	1 (16%)
2	EDO	B	1005	-	3,3,3	0.49	0	2,2,2	0.08	0
5	1U0	B	1006[A]	-	26,31,31	2.60	8 (30%)	32,46,46	2.35	12 (37%)
2	EDO	A	717[A]	-	3,3,3	0.37	0	2,2,2	0.41	0
2	EDO	B	1011[B]	-	3,3,3	0.28	0	2,2,2	0.40	0
2	EDO	B	1002	-	3,3,3	0.57	0	2,2,2	0.22	0
2	EDO	B	1003	-	3,3,3	0.46	0	2,2,2	0.36	0
2	EDO	B	1015	-	3,3,3	0.33	0	2,2,2	0.41	0
2	EDO	A	714	-	3,3,3	0.41	0	2,2,2	0.60	0
2	EDO	A	705	-	3,3,3	0.53	0	2,2,2	0.37	0
5	1U0	B	1006[B]	-	26,31,31	2.60	8 (30%)	32,46,46	2.33	12 (37%)
2	EDO	A	717[B]	-	3,3,3	0.39	0	2,2,2	0.77	0
2	EDO	B	1010	-	3,3,3	0.42	0	2,2,2	0.57	0
2	EDO	A	715	-	3,3,3	0.34	0	2,2,2	0.42	0
2	EDO	A	712	-	3,3,3	0.43	0	2,2,2	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	1U0	A	709[A]	-	26,31,31	2.68	9 (34%)	32,46,46	1.74	8 (25%)
2	EDO	A	701[A]	-	3,3,3	0.43	0	2,2,2	0.60	0
2	EDO	B	1004	-	3,3,3	0.55	0	2,2,2	0.56	0
6	SO4	A	716[B]	-	4,4,4	0.66	0	6,6,6	1.81	2 (33%)
2	EDO	A	710[A]	-	3,3,3	0.41	0	2,2,2	0.53	0
2	EDO	B	1017	-	3,3,3	0.28	0	2,2,2	0.47	0
2	EDO	B	1001	-	3,3,3	0.26	0	2,2,2	0.83	0
2	EDO	A	713	-	3,3,3	0.69	0	2,2,2	1.53	0
2	EDO	A	704	-	3,3,3	0.11	0	2,2,2	0.36	0
5	1U0	A	709[B]	-	26,31,31	2.67	8 (30%)	32,46,46	1.73	8 (25%)
2	EDO	A	701[B]	-	3,3,3	0.33	0	2,2,2	0.71	0
2	EDO	A	703	-	3,3,3	0.32	0	2,2,2	0.22	0
2	EDO	A	718	-	3,3,3	0.32	0	2,2,2	0.51	0
2	EDO	A	702	-	3,3,3	0.28	0	2,2,2	0.92	0
2	EDO	B	1011[A]	-	3,3,3	0.47	0	2,2,2	0.62	0
2	EDO	A	711	-	3,3,3	0.55	0	2,2,2	0.71	0
2	EDO	B	1016	-	3,3,3	0.26	0	2,2,2	1.01	0
2	EDO	B	1012	-	3,3,3	0.47	0	2,2,2	0.70	0
2	EDO	A	706	-	3,3,3	0.48	0	2,2,2	0.31	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	B	1009	-	-	0/1/1/1	-
2	EDO	B	1008	-	-	1/1/1/1	-
2	EDO	B	1005	-	-	0/1/1/1	-
5	1U0	B	1006[A]	-	-	3/18/23/23	0/2/2/2
2	EDO	A	717[A]	-	-	0/1/1/1	-
2	EDO	B	1011[B]	-	-	0/1/1/1	-
2	EDO	B	1002	-	-	0/1/1/1	-
2	EDO	B	1003	-	-	0/1/1/1	-
2	EDO	B	1015	-	-	1/1/1/1	-
2	EDO	A	714	-	-	0/1/1/1	-
2	EDO	A	705	-	-	0/1/1/1	-
5	1U0	B	1006[B]	-	-	2/18/23/23	0/2/2/2
2	EDO	A	717[B]	-	-	0/1/1/1	-
2	EDO	B	1010	-	-	0/1/1/1	-
2	EDO	A	715	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	712	-	-	0/1/1/1	-
5	1U0	A	709[A]	-	-	3/18/23/23	0/2/2/2
2	EDO	A	701[A]	-	-	0/1/1/1	-
2	EDO	B	1004	-	-	0/1/1/1	-
2	EDO	A	710[A]	-	-	1/1/1/1	-
2	EDO	B	1017	-	-	0/1/1/1	-
2	EDO	B	1001	-	-	0/1/1/1	-
2	EDO	A	713	-	-	1/1/1/1	-
2	EDO	A	704	-	-	0/1/1/1	-
5	1U0	A	709[B]	-	-	1/18/23/23	0/2/2/2
2	EDO	A	701[B]	-	-	0/1/1/1	-
2	EDO	A	703	-	-	0/1/1/1	-
2	EDO	A	718	-	-	1/1/1/1	-
2	EDO	A	702	-	-	0/1/1/1	-
2	EDO	B	1011[A]	-	-	1/1/1/1	-
2	EDO	A	711	-	-	1/1/1/1	-
2	EDO	B	1016	-	-	1/1/1/1	-
2	EDO	B	1012	-	-	1/1/1/1	-
2	EDO	A	706	-	-	0/1/1/1	-

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1006[A]	1U0	O9-C8	8.25	1.61	1.42
5	B	1006[B]	1U0	O9-C8	8.25	1.61	1.42
5	A	709[A]	1U0	O9-C8	7.94	1.60	1.42
5	A	709[B]	1U0	O9-C8	7.94	1.60	1.42
5	A	709[A]	1U0	C2-C8	6.64	1.58	1.51

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1006[A]	1U0	C7'-C5'-C6'	5.28	129.03	121.73
5	B	1006[B]	1U0	C7'-C5'-C6'	5.28	129.03	121.73
5	B	1006[A]	1U0	N1'-C2'-N3'	-4.67	117.51	125.54
5	B	1006[B]	1U0	N1'-C2'-N3'	-4.67	117.51	125.54
5	A	709[A]	1U0	C5'-C4'-N4'	-4.24	116.17	122.19

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	710[A]	EDO	O1-C1-C2-O2
5	A	709[A]	1U0	PA-O3A-PB-O2B
5	A	709[B]	1U0	PA-O3A-PB-O2B
5	B	1006[A]	1U0	PA-O3A-PB-O3B
5	B	1006[B]	1U0	PA-O3A-PB-O3B

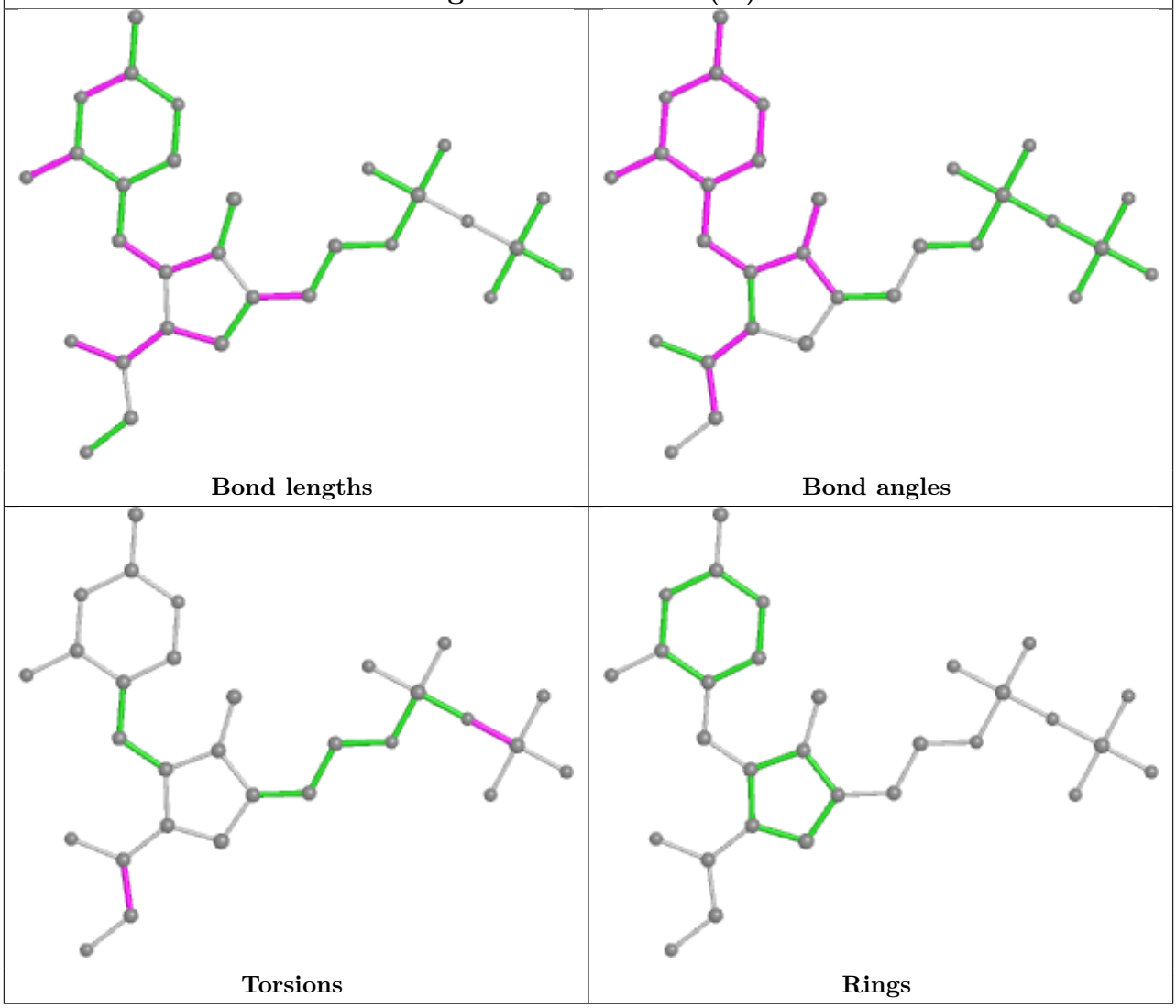
There are no ring outliers.

12 monomers are involved in 16 short contacts:

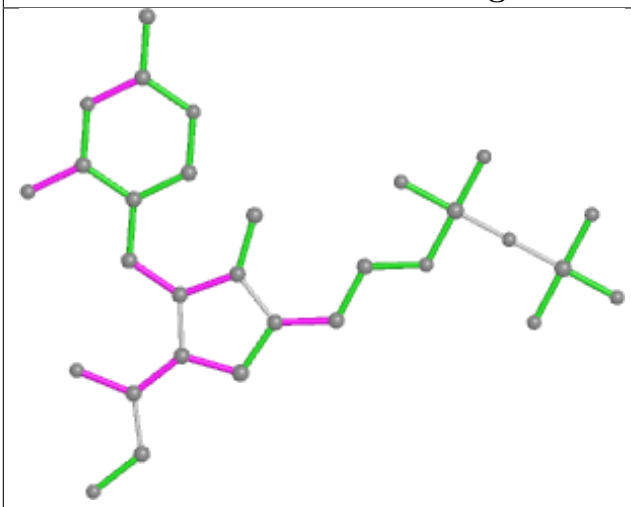
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1009	EDO	1	0
2	B	1008	EDO	3	0
2	A	717[A]	EDO	1	0
2	B	1015	EDO	1	0
2	A	717[B]	EDO	1	0
2	A	710[A]	EDO	2	0
2	A	713	EDO	1	0
2	A	704	EDO	1	0
2	A	701[B]	EDO	2	0
2	A	718	EDO	2	0
2	B	1011[A]	EDO	1	0
2	A	711	EDO	1	0

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 then 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.

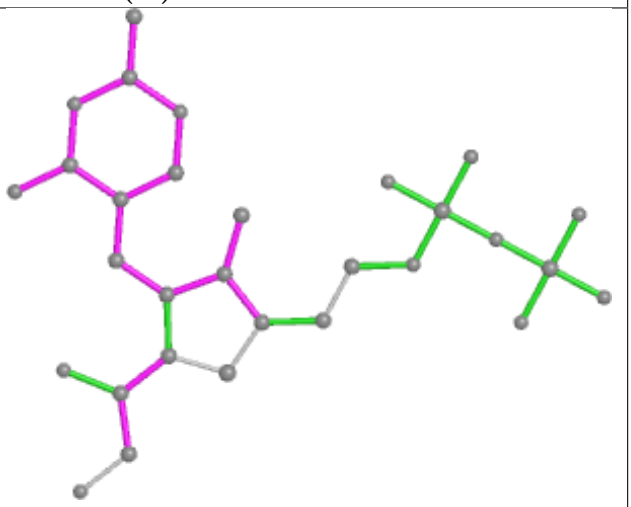
Ligand 1U0 B 1006 (A)



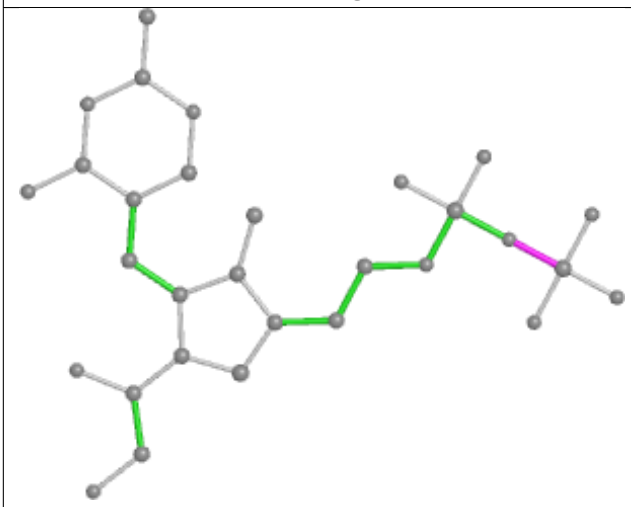
Ligand 1U0 B 1006 (B)



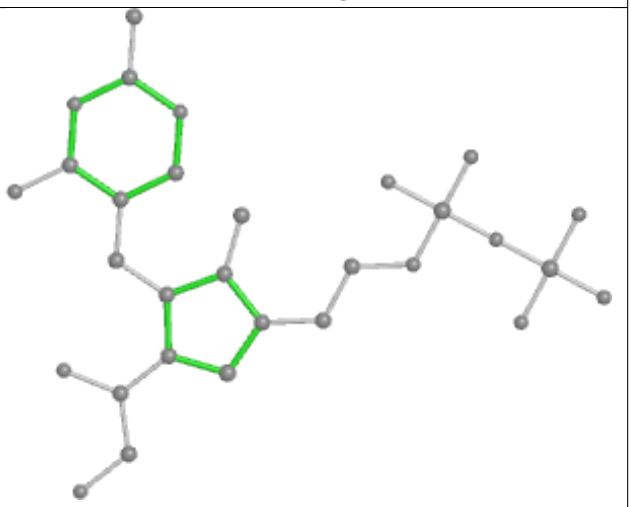
Bond lengths



Bond angles

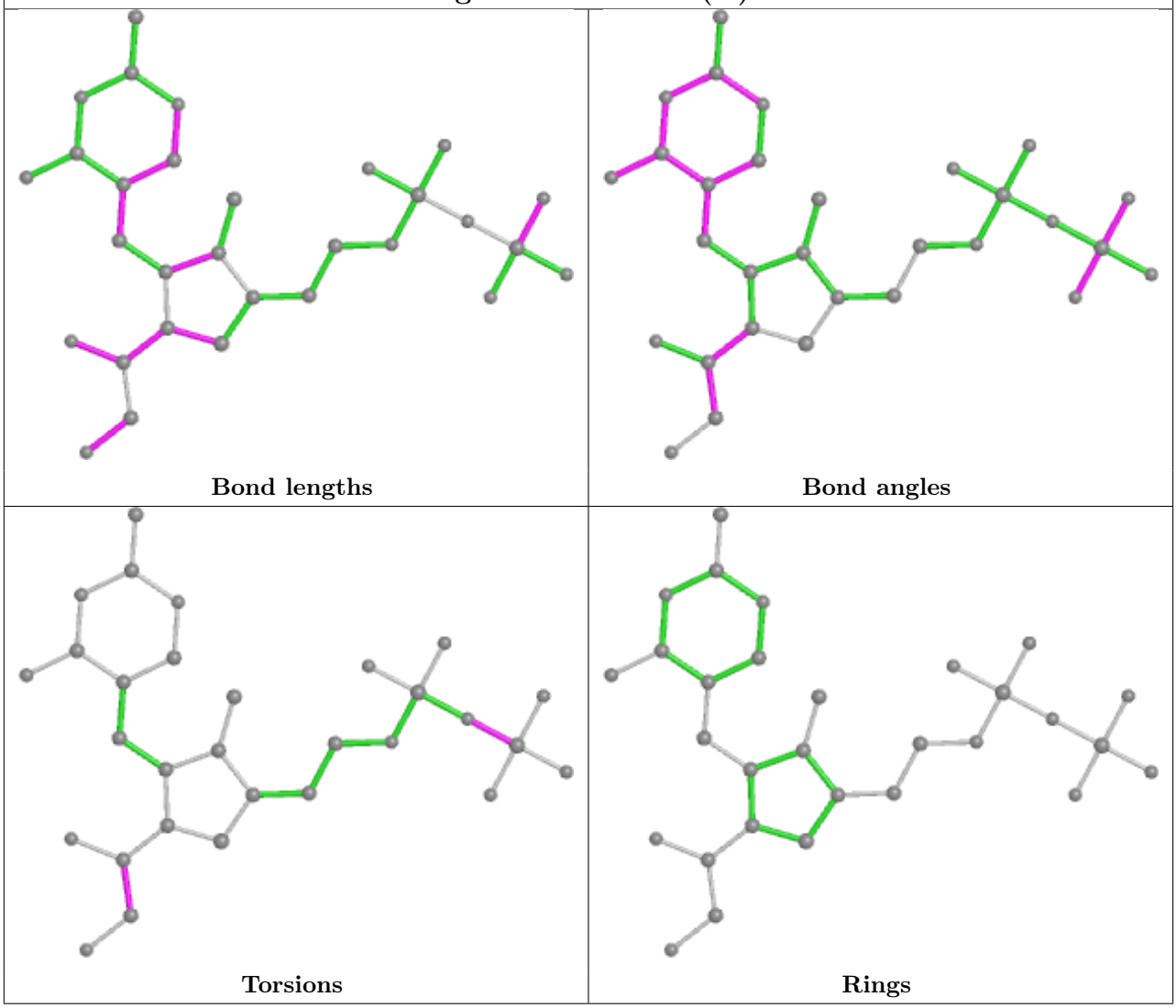


Torsions

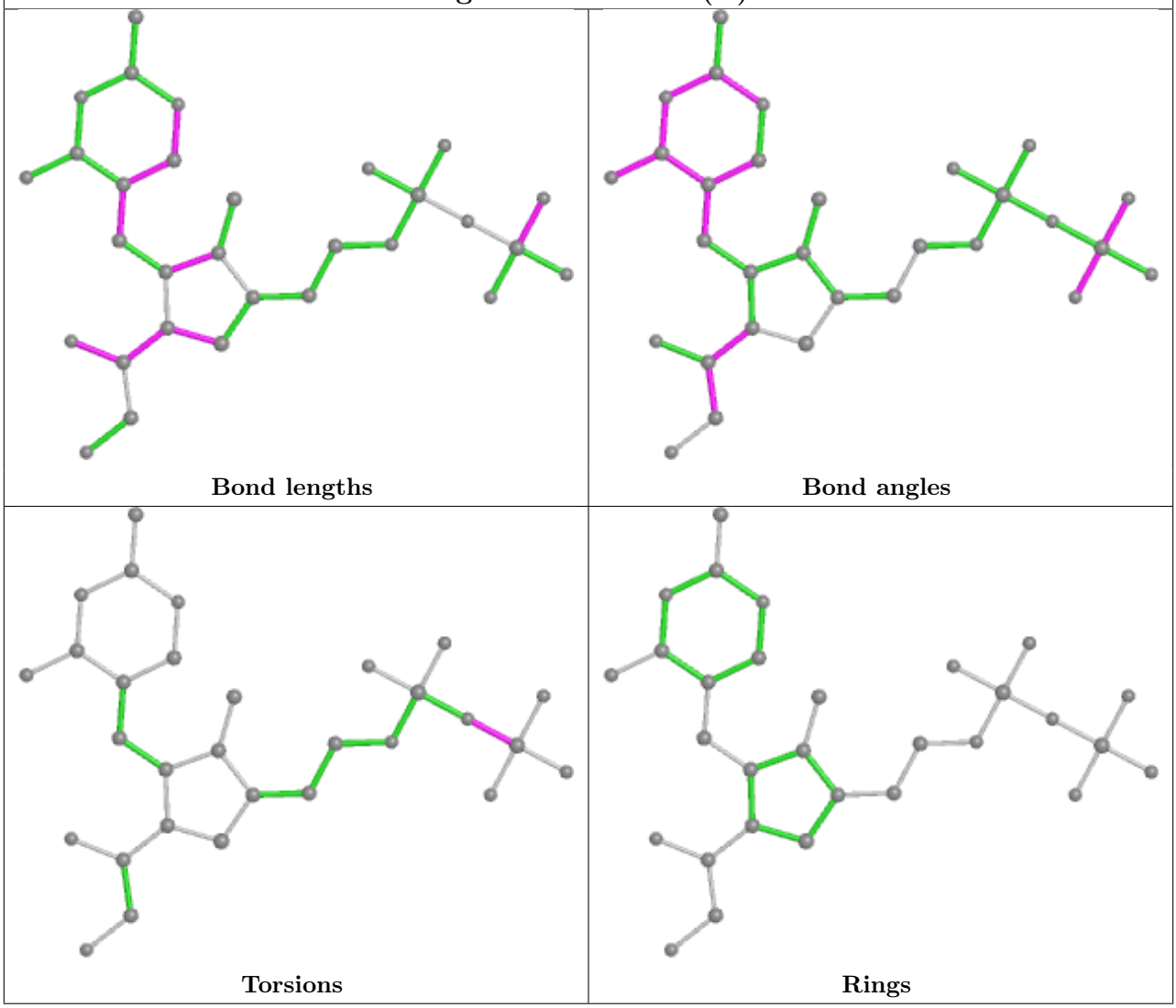


Rings

Ligand 1U0 A 709 (A)



Ligand 1U0 A 709 (B)



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, 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	620/637 (97%)	-0.48	6 (0%)	82	73	5, 9, 29, 73	0
1	B	620/637 (97%)	-0.40	8 (1%)	77	67	5, 11, 34, 75	0
All	All	1240/1274 (97%)	-0.44	14 (1%)	80	71	5, 10, 32, 75	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	298	ILE	5.1
1	B	620	ILE	4.4
1	A	298	ILE	4.1
1	A	296[A]	VAL	3.1
1	B	499	LYS	2.7

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.

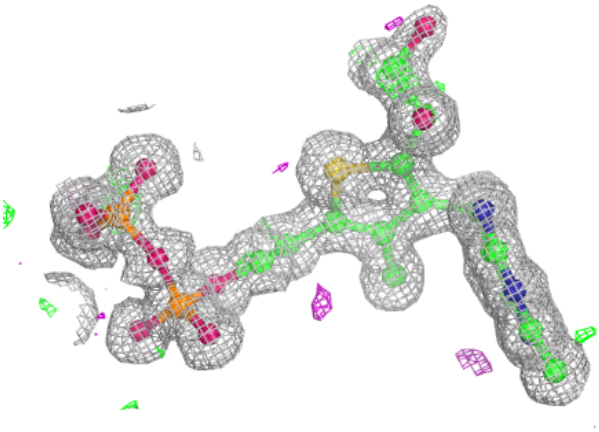
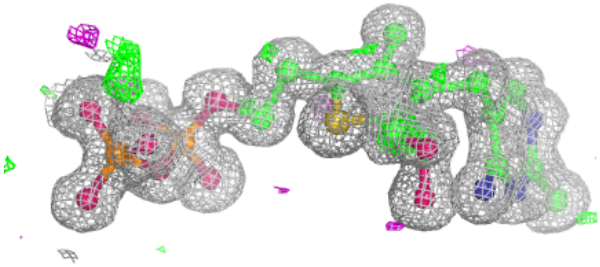
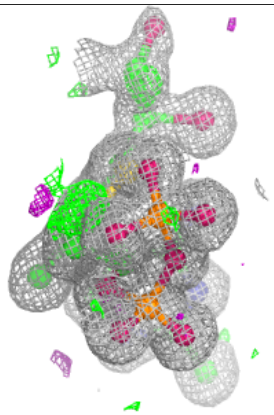
6.4 Ligands (i)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	A	710[A]	4/4	0.59	0.29	67,69,69,71	0
2	EDO	A	715	4/4	0.74	0.24	43,46,83,84	0
2	EDO	B	1017	4/4	0.74	0.13	47,49,53,54	0
2	EDO	A	718	4/4	0.83	0.21	28,66,70,87	0
6	SO4	A	716[B]	5/5	0.84	0.14	35,38,43,43	0
6	SO4	B	1013	5/5	0.86	0.15	41,46,47,49	0
2	EDO	B	1009	4/4	0.90	0.14	23,28,31,60	0
2	EDO	A	712	4/4	0.90	0.09	29,30,30,31	0
2	EDO	A	711	4/4	0.91	0.08	21,25,26,28	0
2	EDO	A	702	4/4	0.91	0.10	21,23,25,28	0
2	EDO	B	1011[B]	4/4	0.93	0.12	6,7,7,9	4
2	EDO	B	1001	4/4	0.93	0.07	19,19,22,32	0
2	EDO	A	714	4/4	0.93	0.09	20,22,23,23	0
2	EDO	B	1011[A]	4/4	0.93	0.12	19,21,31,59	4
2	EDO	B	1010	4/4	0.94	0.07	25,27,31,41	0
2	EDO	B	1015	4/4	0.95	0.12	16,40,42,45	0
2	EDO	A	717[B]	4/4	0.95	0.14	22,28,36,40	4
2	EDO	B	1003	4/4	0.95	0.08	13,22,23,23	0
2	EDO	A	717[A]	4/4	0.95	0.14	6,12,13,14	4
2	EDO	B	1008	4/4	0.96	0.09	13,17,18,19	0
2	EDO	B	1012	4/4	0.96	0.07	21,25,27,28	0
2	EDO	A	713	4/4	0.96	0.09	14,18,20,30	0
2	EDO	B	1016	4/4	0.97	0.09	14,23,27,32	0
2	EDO	A	701[B]	4/4	0.97	0.09	28,29,31,33	4
2	EDO	A	701[A]	4/4	0.97	0.09	8,8,11,11	4
2	EDO	A	703	4/4	0.97	0.07	9,12,13,14	0
2	EDO	A	704	4/4	0.98	0.05	11,16,18,21	0
2	EDO	B	1002	4/4	0.98	0.05	10,14,15,15	0
2	EDO	A	705	4/4	0.98	0.05	9,10,12,16	0
2	EDO	B	1004	4/4	0.98	0.07	11,14,15,17	0
2	EDO	A	706	4/4	0.98	0.05	11,17,17,18	0
5	1U0	A	709[B]	30/30	0.99	0.05	4,6,10,15	2
5	1U0	B	1006[A]	30/30	0.99	0.05	5,6,8,9	2
5	1U0	B	1006[B]	30/30	0.99	0.05	5,6,9,17	2
2	EDO	B	1005	4/4	0.99	0.05	8,11,12,13	0
5	1U0	A	709[A]	30/30	0.99	0.05	4,6,9,18	2
4	NA	A	708	1/1	1.00	0.02	7,7,7,7	0
4	NA	B	1014	1/1	1.00	0.04	11,11,11,11	0
3	CA	A	707	1/1	1.00	0.03	6,6,6,6	0
3	CA	B	1007	1/1	1.00	0.03	6,6,6,6	0

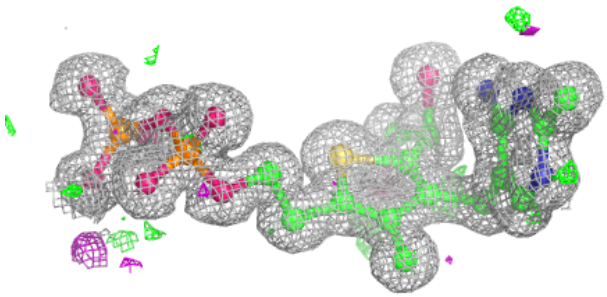
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

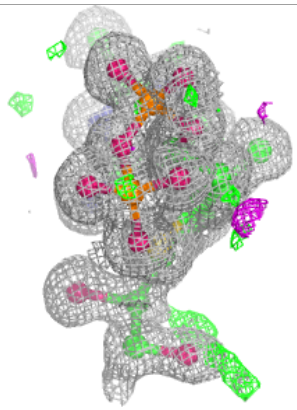
orientation to approximate a three-dimensional view.

Electron density around 1U0 A 709 (B): $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around 1U0 B 1006 (A):

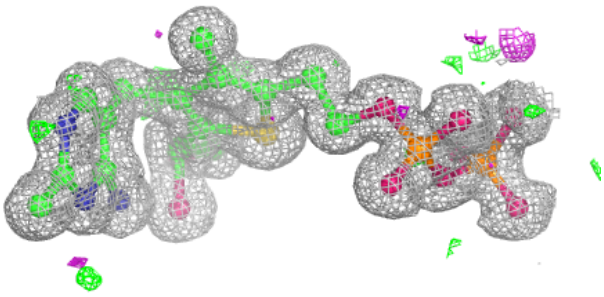
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

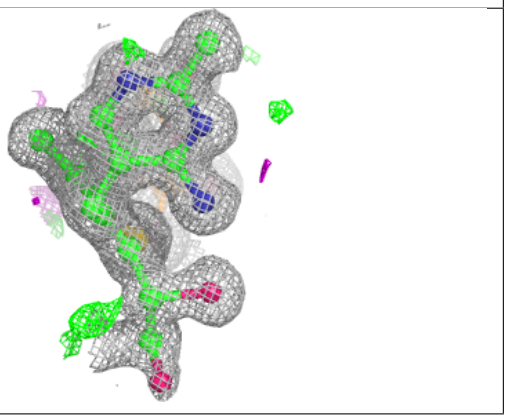


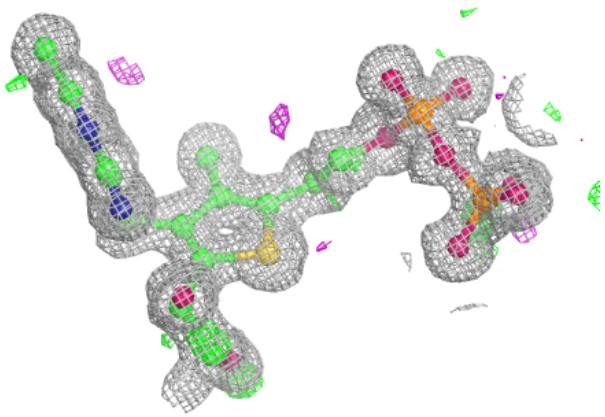
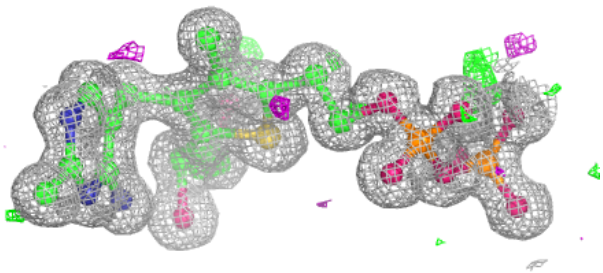
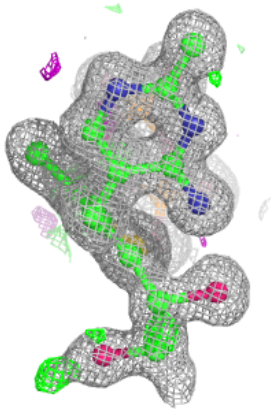


Electron density around 1U0 B 1006 (B):

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





Electron density around 1U0 A 709 (A): $2mF_o$-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 (i)

There are no such residues in this entry.