



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:05 AM UTC

PDB ID : 4KXY / pdb_00004kxy
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 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

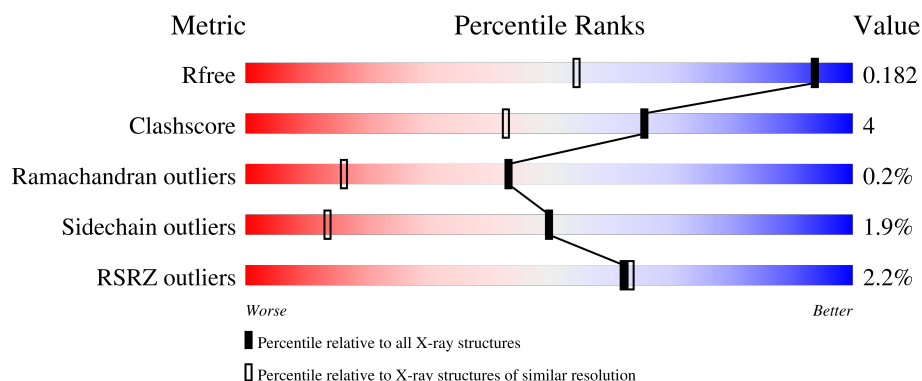
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

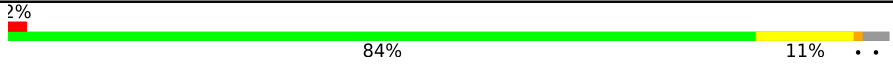
The reported resolution of this entry is 1.26 Å.

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}	180053	1693 (1.28-1.24)
Clashscore	190562	1730 (1.28-1.24)
Ramachandran outliers	187476	1695 (1.28-1.24)
Sidechain outliers	187428	1694 (1.28-1.24)
RSRZ outliers	180081	1693 (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 $\leq 5\%$. 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	
1	B	637	

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
1	A	620	Total	C	N	O	S	0	34	0
			5006	3156	874	950	26			
1	B	620	Total	C	N	O	S	0	34	0
			5012	3158	878	949	27			

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 (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

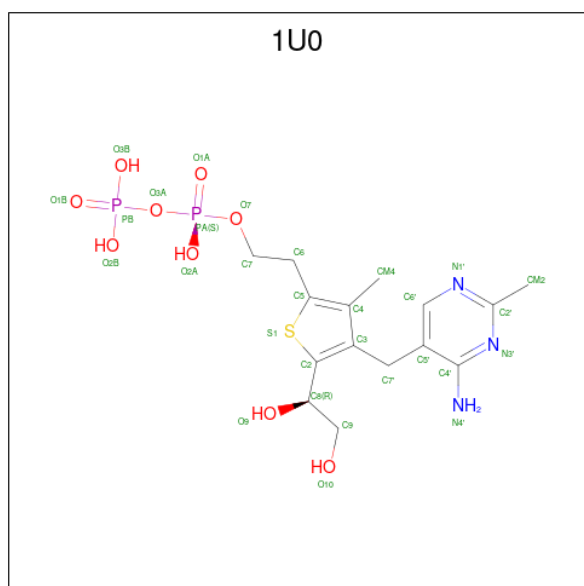
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is 2-{4-[(4-amino-2-methylpyrimidin-5-yl)methyl]-5-[(1R)-1,2-dihydroxyethyl]-3-methylthiophen-2-yl}ethyl trihydrogen diphosphate (CCD ID: 1U0) (formula: C₁₅H₂₃N₃O₉P₂S).



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

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

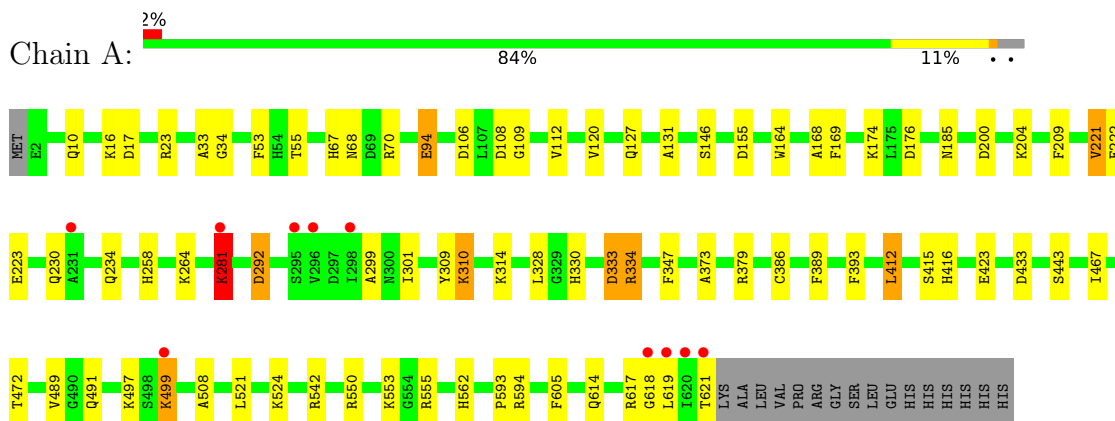
- Molecule 7 is water.

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

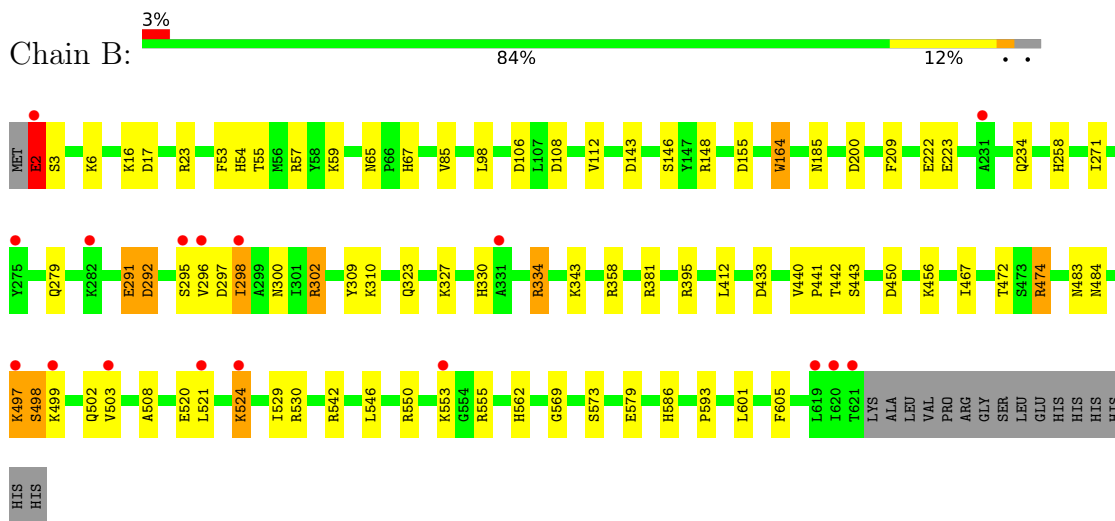
3 Residue-property plots [i](#)

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



• Molecule 1: Transketolase



4 Data and refinement statistics

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 30.00 – 1.26	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-1.26) 89.7 (30.00-1.26)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	13831 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)	0.35 , 74.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SO4, CA, EDO, 1U0

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	0.80	0/5114	1.51	66/6915 (1.0%)
1	B	0.78	2/5121 (0.0%)	1.54	71/6924 (1.0%)
All	All	0.79	2/10235 (0.0%)	1.52	137/13839 (1.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	258	HIS	CG-ND1	-5.83	1.31	1.38
1	B	67	HIS	CG-ND1	-5.47	1.32	1.38

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ASP	CA-C-N	15.86	137.58	119.98
1	A	108	ASP	C-N-CA	15.86	137.58	119.98
1	B	108	ASP	CA-C-N	14.10	135.51	120.00
1	B	108	ASP	C-N-CA	14.10	135.51	120.00
1	A	185	ASN	OD1-CG-ND2	-13.38	109.22	122.60
1	B	106	ASP	CA-C-N	10.05	137.15	122.08
1	B	106	ASP	C-N-CA	10.05	137.15	122.08
1	B	508	ALA	O-C-N	-9.80	112.25	123.33
1	A	108	ASP	O-C-N	-9.63	110.81	122.65
1	A	508	ALA	O-C-N	-9.56	112.77	123.48
1	A	605	PHE	CA-CB-CG	-9.35	104.45	113.80
1	B	508	ALA	CA-C-N	9.22	134.92	120.07
1	B	508	ALA	C-N-CA	9.22	134.92	120.07
1	A	106	ASP	CA-C-N	8.96	135.52	122.08
1	A	106	ASP	C-N-CA	8.96	135.52	122.08
1	B	222	GLU	CA-C-N	8.48	132.34	120.29
1	B	222	GLU	C-N-CA	8.48	132.34	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ASN	OD1-CG-ND2	-8.41	114.19	122.60
1	B	222	GLU	O-C-N	-8.19	112.81	122.15
1	B	395[A]	ARG	NE-CZ-NH2	8.06	126.45	119.20
1	B	395[B]	ARG	NE-CZ-NH2	8.06	126.45	119.20
1	B	106	ASP	O-C-N	-8.04	112.69	122.34
1	A	472	THR	CA-C-N	8.03	135.54	122.29
1	A	472	THR	C-N-CA	8.03	135.54	122.29
1	B	605	PHE	CA-CB-CG	-8.02	105.78	113.80
1	A	230	GLN	OE1-CD-NE2	-7.91	114.69	122.60
1	B	155	ASP	CA-CB-CG	7.70	120.30	112.60
1	B	292	ASP	CA-C-O	7.69	128.56	119.48
1	A	106	ASP	O-C-N	-7.67	113.13	122.34
1	A	67	HIS	CB-CG-CD2	7.44	140.87	131.20
1	A	550	ARG	NE-CZ-NH2	7.36	125.82	119.20
1	A	108	ASP	CA-C-O	7.30	130.34	121.94
1	A	489	VAL	O-C-N	-7.23	115.30	122.67
1	A	222	GLU	CA-C-N	7.13	129.84	120.28
1	A	222	GLU	C-N-CA	7.13	129.84	120.28
1	B	334	ARG	CD-NE-CZ	6.99	134.19	124.40
1	B	279	GLN	OE1-CD-NE2	6.97	129.57	122.60
1	A	292	ASP	O-C-N	-6.96	113.76	122.19
1	B	298	ILE	CB-CA-C	-6.88	99.81	111.37
1	B	108	ASP	O-C-N	-6.78	113.21	122.23
1	B	474	ARG	O-C-N	-6.76	113.54	121.32
1	B	298	ILE	N-CA-C	6.68	119.45	112.83
1	B	484	ASN	OD1-CG-ND2	-6.58	116.02	122.60
1	B	302	ARG	CD-NE-CZ	6.55	133.57	124.40
1	B	67	HIS	CB-CG-CD2	6.54	139.70	131.20
1	A	234	GLN	OE1-CD-NE2	6.49	129.09	122.60
1	B	292	ASP	O-C-N	-6.46	114.37	122.19
1	A	70	ARG	NE-CZ-NH1	-6.44	115.06	121.50
1	A	120	VAL	CA-C-O	6.39	127.83	120.67
1	A	281	LYS	CA-C-N	6.36	129.79	120.82
1	A	281	LYS	C-N-CA	6.36	129.79	120.82
1	B	292	ASP	CA-C-N	6.34	129.16	120.67
1	B	292	ASP	C-N-CA	6.34	129.16	120.67
1	A	120	VAL	O-C-N	-6.32	116.33	123.10
1	B	450	ASP	CA-CB-CG	6.26	118.86	112.60
1	B	65	ASN	CA-CB-CG	-6.24	106.36	112.60
1	B	164	TRP	CA-CB-CG	-6.17	101.87	113.60
1	B	258	HIS	ND1-CE1-NE2	-6.14	102.26	108.40
1	B	502	GLN	OE1-CD-NE2	6.09	128.69	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	ALA	N-CA-C	6.08	118.34	110.38
1	A	347	PHE	O-C-N	-6.08	112.25	122.03
1	B	258	HIS	ND1-CG-CD2	-6.07	100.03	106.10
1	A	164	TRP	CA-CB-CG	-6.07	102.08	113.60
1	A	221	VAL	CG1-CB-CG2	6.06	124.13	110.80
1	B	234[A]	GLN	OE1-CD-NE2	6.03	128.63	122.60
1	B	234[B]	GLN	OE1-CD-NE2	6.03	128.63	122.60
1	B	497	LYS	O-C-N	6.02	129.58	123.26
1	A	508	ALA	CA-C-O	5.99	127.47	120.89
1	A	222	GLU	O-C-N	-5.89	115.73	122.09
1	A	562	HIS	CA-CB-CG	5.88	119.68	113.80
1	B	53	PHE	CA-CB-CG	-5.88	107.92	113.80
1	B	85	VAL	N-CA-CB	5.88	119.40	110.58
1	B	55	THR	N-CA-C	5.87	118.56	111.40
1	A	53	PHE	CA-CB-CG	-5.87	107.94	113.80
1	A	594	ARG	NE-CZ-NH2	5.83	124.45	119.20
1	B	381	ARG	NE-CZ-NH2	-5.80	113.98	119.20
1	A	389	PHE	CA-CB-CG	5.75	119.56	113.80
1	A	347	PHE	CA-C-O	5.75	126.73	120.12
1	B	472	THR	CA-C-N	5.73	131.74	122.29
1	B	472	THR	C-N-CA	5.73	131.74	122.29
1	A	617	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	A	347	PHE	CA-C-N	5.61	130.09	120.72
1	A	347	PHE	C-N-CA	5.61	130.09	120.72
1	B	295	SER	CA-C-O	-5.60	114.89	121.16
1	A	109	GLY	O-C-N	5.58	127.55	122.19
1	B	258	HIS	CG-ND1-CE1	5.58	118.78	109.30
1	A	223	GLU	N-CA-C	-5.54	105.24	111.28
1	A	230	GLN	O-C-N	-5.54	116.90	123.22
1	B	6	LYS	O-C-N	5.53	126.01	121.31
1	B	330	HIS	N-CA-C	-5.53	106.03	112.89
1	B	2	GLU	CA-C-O	-5.53	111.41	120.80
1	A	17	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	333	ASP	CA-CB-CG	-5.51	107.08	112.60
1	B	143	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	498	SER	CA-C-O	5.45	127.11	121.28
1	A	508	ALA	CA-C-N	5.43	132.04	121.41
1	A	508	ALA	C-N-CA	5.43	132.04	121.41
1	B	296	VAL	O-C-N	-5.42	117.33	123.18
1	A	258	HIS	ND1-CE1-NE2	-5.40	103.00	108.40
1	A	334	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	B	54	HIS	CB-CG-CD2	5.38	138.19	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	ARG	CD-NE-CZ	5.37	131.91	124.40
1	A	334	ARG	CG-CD-NE	5.36	123.80	112.00
1	A	55	THR	N-CA-C	5.33	117.90	111.40
1	B	327	LYS	CA-C-N	-5.32	112.62	120.28
1	B	327	LYS	C-N-CA	-5.32	112.62	120.28
1	A	34	GLY	CA-C-O	5.27	125.12	119.06
1	B	291	GLU	N-CA-CB	-5.27	104.10	110.53
1	A	292	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	68	ASN	CA-CB-CG	5.20	117.80	112.60
1	A	258	HIS	ND1-CG-CD2	-5.20	100.90	106.10
1	A	176	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	330	HIS	CA-CB-CG	-5.19	108.61	113.80
1	A	120	VAL	CA-C-N	5.19	128.08	120.71
1	A	120	VAL	C-N-CA	5.19	128.08	120.71
1	B	358	ARG	NE-CZ-NH2	-5.18	114.54	119.20
1	A	555	ARG	NE-CZ-NH2	-5.18	114.54	119.20
1	B	292	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	54	HIS	ND1-CG-CD2	-5.15	100.95	106.10
1	B	148	ARG	CD-NE-CZ	5.13	131.59	124.40
1	B	562	HIS	CA-CB-CG	5.12	118.92	113.80
1	A	23	ARG	CG-CD-NE	-5.12	100.74	112.00
1	B	542	ARG	CA-C-O	-5.12	114.32	120.10
1	B	223	GLU	N-CA-C	-5.08	105.83	111.36
1	B	440	VAL	CA-C-O	5.07	122.13	119.14
1	B	323	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	A	230	GLN	N-CA-CB	-5.06	102.17	110.42
1	A	379	ARG	CD-NE-CZ	5.04	131.45	124.40
1	A	472	THR	O-C-N	-5.04	115.97	122.97
1	A	155	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	17	ASP	CA-CB-CG	5.03	117.62	112.60
1	B	520	GLU	CA-C-N	5.02	126.96	120.44
1	B	520	GLU	C-N-CA	5.02	126.96	120.44
1	B	23	ARG	CG-CD-NE	-5.02	100.96	112.00
1	A	542	ARG	NE-CZ-NH2	-5.02	114.69	119.20
1	A	234	GLN	CB-CG-CD	-5.01	104.08	112.60
1	B	343	LYS	N-CA-C	5.00	117.47	111.71

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	5006	0	5002	44	0
1	B	5012	0	5005	30	0
2	A	64	0	96	11	0
2	B	56	0	84	5	0
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	14	0
All	All	11716	0	10203	79	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.

All (79) 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: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
1:A:204:LYS:HG2	7:A:8737:HOH:O	1.87	0.72
1:A:209:PHE:HE1	2:B:1008:EDO:H22	1.56	0.71
1:A:334:ARG:HG2	7:A:8722:HOH:O	1.90	0.70
1:B:200:ASP:HB3	7:B:1803:HOH:O	1.92	0.69
1:A:16[B]:LYS:HE2	7:A:8465:HOH:O	1.95	0.66
1:A:333:ASP:O	2:A:718:EDO:H22	1.95	0.65
2:A:713:EDO:H22	1:B:209:PHE:HE1	1.60	0.65
1:B:521:LEU:O	1:B:524:LYS:HG3	1.96	0.65
1:A:524:LYS:HD3	7:A:8585:HOH:O	2.00	0.62
1:B:499:LYS:HD3	7:B:1666:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16[B]:LYS:CG	7:A:8662:HOH:O	2.49	0.60
1:B:499:LYS:HE2	7:B:1772:HOH:O	2.03	0.59
1:A:423:GLU:HG2	2:A:701[B]:EDO:H21	1.85	0.57
1:B:16[C]:LYS:HE2	7:B:1436:HOH:O	2.04	0.57
1:A:16[B]:LYS:CE	7:A:8662:HOH:O	2.51	0.57
1:A:393:PHE:CZ	1:A:412[A]:LEU:HG	2.39	0.57
1:A:200[B]:ASP:HB3	7:A:8737:HOH:O	2.04	0.57
1:B:553:LYS:HD3	1:B:555:ARG:NH1	2.20	0.56
1:A:16[B]:LYS:HG3	7:A:8292:HOH:O	2.08	0.53
1:A:16[B]:LYS:HE3	7:A:8662:HOH:O	2.08	0.53
1:A:127:GLN:OE1	2:A:717[B]:EDO:H12	2.08	0.53
2:A:718:EDO:H12	7:A:8602:HOH:O	2.09	0.53
1:A:16[B]:LYS:HG3	7:A:8662:HOH:O	2.10	0.52
1:A:393:PHE:CE1	1:A:412[A]:LEU:HG	2.45	0.52
1:A:94[B]:GLU:HG3	7:A:8490:HOH:O	2.09	0.51
1:A:314:LYS:HE3	7:A:8679:HOH:O	2.10	0.51
1:A:619:LEU:HD22	7:A:8496:HOH:O	2.09	0.51
1:A:16[B]:LYS:CD	7:A:8662:HOH:O	2.59	0.50
1:A:309[A]:TYR:O	1:A:310:LYS:HG2	2.11	0.50
1:A:415[B]:SER:O	1:A:416:HIS:HB2	2.12	0.50
2:A:701[B]:EDO:H12	7:A:8187:HOH:O	2.12	0.49
1:B:59:LYS:HE3	1:B:291:GLU:OE2	2.12	0.49
1:A:618:GLY:O	1:A:621:THR:OG1	2.30	0.49
1:A:281:LYS:HE2	7:A:8681:HOH:O	2.12	0.48
1:A:491:GLN:HB2	7:A:8719:HOH:O	2.13	0.48
1:A:131:ALA:HB2	2:A:717[A]:EDO:C1	2.45	0.47
1:A:168:ALA:HB3	2:A:710[A]:EDO:H22	1.96	0.47
1:A:200[A]:ASP:HB2	7:A:8737:HOH:O	2.14	0.47
1:B:441[B]:PRO:O	1:B:442[B]:THR:OG1	2.30	0.47
1:B:456:LYS:NZ	7:B:1725:HOH:O	2.49	0.46
1:A:499:LYS:HE2	1:A:499:LYS:H	1.80	0.46
1:A:521:LEU:O	1:A:524:LYS:HD3	2.16	0.46
1:B:573:SER:OG	1:B:586[B]:HIS:HE1	1.99	0.45
1:A:169:PHE:HB2	2:A:710[A]:EDO:H11	1.98	0.45
1:B:474:ARG:NH2	7:B:1724[A]:HOH:O	2.50	0.45
1:A:146[B]:SER:OG	1:A:292:ASP:OD2	2.30	0.45
1:B:300:ASN:ND2	7:B:1639:HOH:O	2.49	0.45
1:B:271:ILE:HD13	7:B:1759:HOH:O	2.16	0.44
1:B:297:ASP:O	1:B:334:ARG:NH2	2.50	0.44
1:B:498:SER:O	1:B:530:ARG:NH2	2.50	0.44
2:B:1008:EDO:O2	2:B:1009:EDO:H21	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:GLN:HE21	1:A:614:GLN:HB2	1.45	0.44
1:B:309:TYR:O	1:B:483[A]:ASN:ND2	2.48	0.44
1:A:33:ALA:O	2:B:1011[A]:EDO:H22	2.18	0.44
1:A:174[A]:LYS:NZ	7:A:8547:HOH:O	2.50	0.44
1:A:433:ASP:HB3	7:A:8179:HOH:O	2.17	0.44
1:B:164:TRP:CD1	2:B:1008:EDO:H21	2.52	0.44
1:B:499:LYS:HG3	7:B:1772:HOH:O	2.17	0.44
1:A:373:ALA:HB2	1:A:386[A]:CYS:SG	2.58	0.43
2:A:704:EDO:H11	7:A:8638:HOH:O	2.19	0.43
1:A:443:SER:HA	1:A:467:ILE:O	2.19	0.43
1:B:2:GLU:N	7:B:1660:HOH:O	2.52	0.43
1:A:10[B]:GLN:HG2	2:A:711:EDO:C2	2.49	0.42
1:A:264:LYS:NZ	7:A:8692:HOH:O	2.50	0.42
1:B:443:SER:HA	1:B:467:ILE:O	2.19	0.42
1:A:497:LYS:NZ	7:A:8305:HOH:O	2.50	0.42
1:B:503[A]:VAL:HG12	1:B:529:ILE:HG22	2.02	0.42
1:B:16[C]:LYS:HG3	7:B:1231:HOH:O	2.19	0.41
1:B:146[B]:SER:OG	1:B:292:ASP:OD2	2.30	0.41
1:B:546:LEU:O	1:B:550:ARG:HG3	2.20	0.41
1:B:569:GLY:HA3	1:B:586[A]:HIS:CE1	2.54	0.41
1:B:550:ARG:NH2	1:B:579:GLU:OE1	2.54	0.41
1:B:2:GLU:N	1:B:2:GLU:OE2	2.53	0.41
1:A:310:LYS:HA	7:A:8512:HOH:O	2.20	0.40
1:B:433:ASP:HB3	7:B:1456:HOH:O	2.20	0.40
1:A:301:ILE:HG22	1:A:328:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	652/637 (102%)	631 (97%)	20 (3%)	1 (0%)	43 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	652/637 (102%)	634 (97%)	17 (3%)	1 (0%)	43	16
All	All	1304/1274 (102%)	1265 (97%)	37 (3%)	2 (0%)	43	16

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	536/518 (104%)	526 (98%)	10 (2%)	50	13
1	B	536/518 (104%)	523 (98%)	13 (2%)	43	9
All	All	1072/1036 (104%)	1049 (98%)	23 (2%)	50	11

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94[A]	GLU
1	A	94[B]	GLU
1	A	112	VAL
1	A	221	VAL
1	A	281	LYS
1	A	310	LYS
1	A	412[A]	LEU
1	A	412[B]	LEU
1	A	499	LYS
1	A	553	LYS
1	B	2	GLU
1	B	3[A]	SER
1	B	3[B]	SER
1	B	98	LEU

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Mol	Chain	Res	Type
1	B	112	VAL
1	B	298	ILE
1	B	302	ARG
1	B	310	LYS
1	B	412[A]	LEU
1	B	412[B]	LEU
1	B	497	LYS
1	B	524	LYS
1	B	601	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	A	233	HIS
1	A	265	ASN
1	A	323	GLN
1	A	428	GLN
1	A	477	ASN
1	A	614	GLN
1	B	203	GLN
1	B	265	ASN
1	B	269	GLN
1	B	368	ASN
1	B	428	GLN
1	B	477	ASN
1	B	482	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

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	A	718	-	3,3,3	0.32	0	2,2,2	0.50	0
2	EDO	B	1002	-	3,3,3	0.57	0	2,2,2	0.23	0
5	1U0	B	1006[B]	-	27,31,31	2.64	7 (25%)	36,46,46	2.69	16 (44%)
2	EDO	A	710[A]	-	3,3,3	0.42	0	2,2,2	0.52	0
2	EDO	A	701[A]	-	3,3,3	0.43	0	2,2,2	0.61	0
2	EDO	B	1009	-	3,3,3	0.27	0	2,2,2	0.61	0
2	EDO	B	1015	-	3,3,3	0.32	0	2,2,2	0.45	0
2	EDO	A	717[A]	-	3,3,3	0.38	0	2,2,2	0.44	0
2	EDO	A	712	-	3,3,3	0.44	0	2,2,2	0.86	0
2	EDO	A	701[B]	-	3,3,3	0.33	0	2,2,2	0.73	0
2	EDO	B	1001	-	3,3,3	0.26	0	2,2,2	0.84	0
2	EDO	A	713	-	3,3,3	0.70	0	2,2,2	1.39	0
2	EDO	A	711	-	3,3,3	0.55	0	2,2,2	0.73	0
2	EDO	B	1017	-	3,3,3	0.28	0	2,2,2	0.45	0
2	EDO	A	717[B]	-	3,3,3	0.39	0	2,2,2	0.78	0
2	EDO	B	1012	-	3,3,3	0.47	0	2,2,2	0.64	0
6	SO4	B	1013	-	4,4,4	0.68	0	6,6,6	1.59	1 (16%)
2	EDO	A	715	-	3,3,3	0.35	0	2,2,2	0.46	0
2	EDO	B	1008	-	3,3,3	0.47	0	2,2,2	0.80	0
2	EDO	B	1003	-	3,3,3	0.46	0	2,2,2	0.33	0
2	EDO	B	1005	-	3,3,3	0.47	0	2,2,2	0.08	0
2	EDO	A	706	-	3,3,3	0.48	0	2,2,2	0.29	0
2	EDO	A	705	-	3,3,3	0.53	0	2,2,2	0.33	0
2	EDO	A	714	-	3,3,3	0.41	0	2,2,2	0.57	0
2	EDO	B	1004	-	3,3,3	0.56	0	2,2,2	0.52	0
2	EDO	A	702	-	3,3,3	0.28	0	2,2,2	0.93	0
2	EDO	B	1011[A]	-	3,3,3	0.47	0	2,2,2	0.64	0
6	SO4	A	716[B]	-	4,4,4	0.74	0	6,6,6	1.65	2 (33%)
2	EDO	A	704	-	3,3,3	0.10	0	2,2,2	0.30	0
2	EDO	B	1010	-	3,3,3	0.42	0	2,2,2	0.60	0
2	EDO	B	1011[B]	-	3,3,3	0.29	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	1U0	A	709[A]	-	27,31,31	2.54	9 (33%)	36,46,46	2.45	13 (36%)
5	1U0	A	709[B]	-	27,31,31	2.53	8 (29%)	36,46,46	2.45	13 (36%)
5	1U0	B	1006[A]	-	27,31,31	2.67	7 (25%)	36,46,46	2.65	16 (44%)
2	EDO	B	1016	-	3,3,3	0.26	0	2,2,2	0.98	0
2	EDO	A	703	-	3,3,3	0.31	0	2,2,2	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	718	-	-	1/1/1/1	-
2	EDO	B	1002	-	-	0/1/1/1	-
5	1U0	B	1006[B]	-	-	3/22/23/23	0/2/2/2
2	EDO	A	710[A]	-	-	1/1/1/1	-
2	EDO	A	701[A]	-	-	0/1/1/1	-
2	EDO	B	1009	-	-	0/1/1/1	-
2	EDO	B	1015	-	-	1/1/1/1	-
2	EDO	A	717[A]	-	-	0/1/1/1	-
2	EDO	A	712	-	-	0/1/1/1	-
2	EDO	A	701[B]	-	-	0/1/1/1	-
2	EDO	B	1001	-	-	0/1/1/1	-
2	EDO	A	713	-	-	1/1/1/1	-
2	EDO	A	711	-	-	1/1/1/1	-
2	EDO	B	1017	-	-	0/1/1/1	-
2	EDO	A	717[B]	-	-	0/1/1/1	-
2	EDO	B	1012	-	-	1/1/1/1	-
2	EDO	A	715	-	-	1/1/1/1	-
2	EDO	B	1008	-	-	1/1/1/1	-
2	EDO	B	1003	-	-	0/1/1/1	-
2	EDO	B	1005	-	-	0/1/1/1	-
2	EDO	A	706	-	-	0/1/1/1	-
2	EDO	A	705	-	-	0/1/1/1	-
2	EDO	A	714	-	-	0/1/1/1	-
2	EDO	B	1004	-	-	0/1/1/1	-
2	EDO	A	702	-	-	0/1/1/1	-
2	EDO	B	1011[A]	-	-	1/1/1/1	-
2	EDO	A	704	-	-	0/1/1/1	-
2	EDO	B	1010	-	-	0/1/1/1	-
2	EDO	B	1011[B]	-	-	0/1/1/1	-
5	1U0	A	709[A]	-	-	3/22/23/23	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1U0	A	709[B]	-	-	2/22/23/23	0/2/2/2
5	1U0	B	1006[A]	-	-	4/22/23/23	0/2/2/2
2	EDO	B	1016	-	-	1/1/1/1	-
2	EDO	A	703	-	-	0/1/1/1	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1006[A]	1U0	O9-C8	8.56	1.61	1.42
5	B	1006[B]	1U0	O9-C8	8.56	1.61	1.42
5	A	709[A]	1U0	O9-C8	8.24	1.60	1.42
5	A	709[B]	1U0	O9-C8	8.24	1.60	1.42
5	B	1006[A]	1U0	C3-C4	5.36	1.52	1.38
5	B	1006[B]	1U0	C3-C4	5.36	1.52	1.38
5	A	709[A]	1U0	C7'-C5'	-4.97	1.44	1.51
5	A	709[B]	1U0	C7'-C5'	-4.97	1.44	1.51
5	B	1006[A]	1U0	C7'-C3	4.46	1.57	1.51
5	B	1006[B]	1U0	C7'-C3	4.46	1.57	1.51
5	B	1006[A]	1U0	C9-C8	-4.25	1.45	1.51
5	B	1006[A]	1U0	C2-S1	3.86	1.80	1.73
5	B	1006[B]	1U0	C2-S1	3.86	1.80	1.73
5	B	1006[B]	1U0	C9-C8	-3.75	1.45	1.51
5	A	709[A]	1U0	C2-S1	3.68	1.80	1.73
5	A	709[B]	1U0	C2-S1	3.68	1.80	1.73
5	B	1006[A]	1U0	C2'-N3'	3.27	1.39	1.34
5	B	1006[B]	1U0	C2'-N3'	3.27	1.39	1.34
5	B	1006[A]	1U0	C4'-N4'	3.26	1.42	1.34
5	B	1006[B]	1U0	C4'-N4'	3.26	1.42	1.34
5	A	709[A]	1U0	C6'-C5'	3.26	1.44	1.37
5	A	709[B]	1U0	C6'-C5'	3.26	1.44	1.37
5	A	709[A]	1U0	C6'-N1'	3.13	1.40	1.34
5	A	709[B]	1U0	C6'-N1'	3.13	1.40	1.34
5	A	709[A]	1U0	C3-C4	3.09	1.47	1.38
5	A	709[B]	1U0	C3-C4	3.09	1.47	1.38
5	A	709[B]	1U0	C9-C8	2.69	1.56	1.51
5	A	709[A]	1U0	C9-C8	2.56	1.55	1.51
5	A	709[A]	1U0	O10-C9	2.37	1.52	1.42
5	A	709[A]	1U0	PB-O2B	-2.18	1.46	1.54
5	A	709[B]	1U0	PB-O2B	-2.18	1.46	1.54

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	709[A]	1U0	C4-C5-S1	-8.03	109.09	113.50
5	A	709[B]	1U0	C4-C5-S1	-8.03	109.09	113.50
5	B	1006[B]	1U0	O9-C8-C9	-6.96	95.43	109.97
5	B	1006[A]	1U0	O9-C8-C9	-6.65	96.08	109.97
5	A	709[B]	1U0	O9-C8-C9	-5.39	98.71	109.97
5	A	709[A]	1U0	O9-C8-C9	-5.35	98.79	109.97
5	B	1006[A]	1U0	N1'-C2'-N3'	-4.82	117.51	125.53
5	B	1006[B]	1U0	N1'-C2'-N3'	-4.82	117.51	125.53
5	B	1006[A]	1U0	C5-C4-C3	-4.69	108.88	112.43
5	B	1006[B]	1U0	C5-C4-C3	-4.69	108.88	112.43
5	A	709[A]	1U0	C5-C4-C3	4.51	115.86	112.43
5	A	709[B]	1U0	C5-C4-C3	4.51	115.86	112.43
5	A	709[A]	1U0	C5'-C4'-N4'	-4.43	116.17	122.14
5	A	709[B]	1U0	C5'-C4'-N4'	-4.43	116.17	122.14
5	B	1006[A]	1U0	C7'-C5'-C6'	4.34	129.03	122.19
5	B	1006[B]	1U0	C7'-C5'-C6'	4.34	129.03	122.19
5	B	1006[A]	1U0	C6'-C5'-C4'	-4.19	110.39	115.55
5	B	1006[B]	1U0	C6'-C5'-C4'	-4.19	110.39	115.55
5	B	1006[A]	1U0	N4'-C4'-N3'	-4.06	111.55	117.03
5	B	1006[B]	1U0	N4'-C4'-N3'	-4.06	111.55	117.03
5	B	1006[B]	1U0	O10-C9-C8	-3.62	103.03	111.95
5	B	1006[A]	1U0	CM2-C2'-N3'	3.53	122.42	117.13
5	B	1006[B]	1U0	CM2-C2'-N3'	3.53	122.42	117.13
5	B	1006[A]	1U0	C6-C5-C4	-3.23	126.48	130.78
5	B	1006[B]	1U0	C6-C5-C4	-3.23	126.48	130.78
5	B	1006[A]	1U0	C6'-N1'-C2'	3.13	121.22	116.07
5	B	1006[B]	1U0	C6'-N1'-C2'	3.13	121.22	116.07
5	B	1006[A]	1U0	C4-C5-S1	3.13	115.22	113.50
5	B	1006[B]	1U0	C4-C5-S1	3.13	115.22	113.50
5	B	1006[A]	1U0	O10-C9-C8	-3.09	104.33	111.95
5	A	709[A]	1U0	C6'-C5'-C4'	-3.00	111.86	115.55
5	A	709[B]	1U0	C6'-C5'-C4'	-3.00	111.86	115.55
5	B	1006[A]	1U0	C5'-C7'-C3	-2.95	109.17	114.05
5	B	1006[B]	1U0	C5'-C7'-C3	-2.95	109.17	114.05
5	A	709[A]	1U0	C7'-C5'-C4'	2.82	125.97	122.07
5	A	709[B]	1U0	C7'-C5'-C4'	2.82	125.97	122.07
5	B	1006[A]	1U0	C7'-C3-C4	-2.80	122.56	126.60
5	B	1006[B]	1U0	C7'-C3-C4	-2.80	122.56	126.60
5	A	709[A]	1U0	C5'-C7'-C3	-2.74	109.52	114.05
5	A	709[B]	1U0	C5'-C7'-C3	-2.74	109.52	114.05
5	B	1006[A]	1U0	CM2-C2'-N1'	2.70	120.07	117.20
5	B	1006[B]	1U0	CM2-C2'-N1'	2.70	120.07	117.20
5	B	1006[A]	1U0	CM4-C4-C3	-2.53	120.27	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1006[B]	1U0	CM4-C4-C3	-2.53	120.27	125.62
5	A	709[A]	1U0	C2-C3-C4	-2.52	111.24	113.24
5	A	709[B]	1U0	C2-C3-C4	-2.52	111.24	113.24
6	A	716[B]	SO4	O4-S-O3	2.51	122.38	108.54
5	A	709[A]	1U0	N4'-C4'-N3'	2.46	120.34	117.03
5	A	709[B]	1U0	N4'-C4'-N3'	2.46	120.34	117.03
6	A	716[B]	SO4	O3-S-O2	-2.45	96.74	109.56
5	A	709[A]	1U0	O2B-PB-O3B	2.43	116.91	107.80
5	A	709[B]	1U0	O2B-PB-O3B	2.43	116.91	107.80
5	B	1006[A]	1U0	C5'-C4'-N3'	2.33	124.73	121.31
5	B	1006[B]	1U0	C5'-C4'-N3'	2.33	124.73	121.31
5	A	709[A]	1U0	C2'-N3'-C4'	2.30	121.64	118.10
5	A	709[B]	1U0	C2'-N3'-C4'	2.30	121.64	118.10
5	A	709[A]	1U0	N1'-C2'-N3'	-2.25	121.79	125.53
5	A	709[B]	1U0	N1'-C2'-N3'	-2.25	121.79	125.53
6	B	1013	SO4	O3-S-O2	-2.19	98.11	109.56
5	A	709[A]	1U0	O10-C9-C8	-2.17	106.61	111.95
5	A	709[B]	1U0	O10-C9-C8	-2.02	106.96	111.95

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	709[A]	1U0	PA-O3A-PB-O2B
5	A	709[A]	1U0	S1-C2-C8-C9
5	A	709[B]	1U0	PA-O3A-PB-O2B
5	A	709[B]	1U0	S1-C2-C8-C9
5	B	1006[A]	1U0	PA-O3A-PB-O3B
5	B	1006[A]	1U0	S1-C2-C8-C9
5	B	1006[B]	1U0	PA-O3A-PB-O3B
5	B	1006[B]	1U0	S1-C2-C8-C9
2	A	710[A]	EDO	O1-C1-C2-O2
2	B	1011[A]	EDO	O1-C1-C2-O2
2	B	1015	EDO	O1-C1-C2-O2
5	A	709[A]	1U0	O9-C8-C9-O10
5	B	1006[A]	1U0	O9-C8-C9-O10
2	A	718	EDO	O1-C1-C2-O2
2	A	713	EDO	O1-C1-C2-O2
2	B	1012	EDO	O1-C1-C2-O2
5	B	1006[A]	1U0	PA-O3A-PB-O1B
5	B	1006[B]	1U0	PA-O3A-PB-O1B
2	A	711	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	715	EDO	O1-C1-C2-O2
2	B	1008	EDO	O1-C1-C2-O2
2	B	1016	EDO	O1-C1-C2-O2

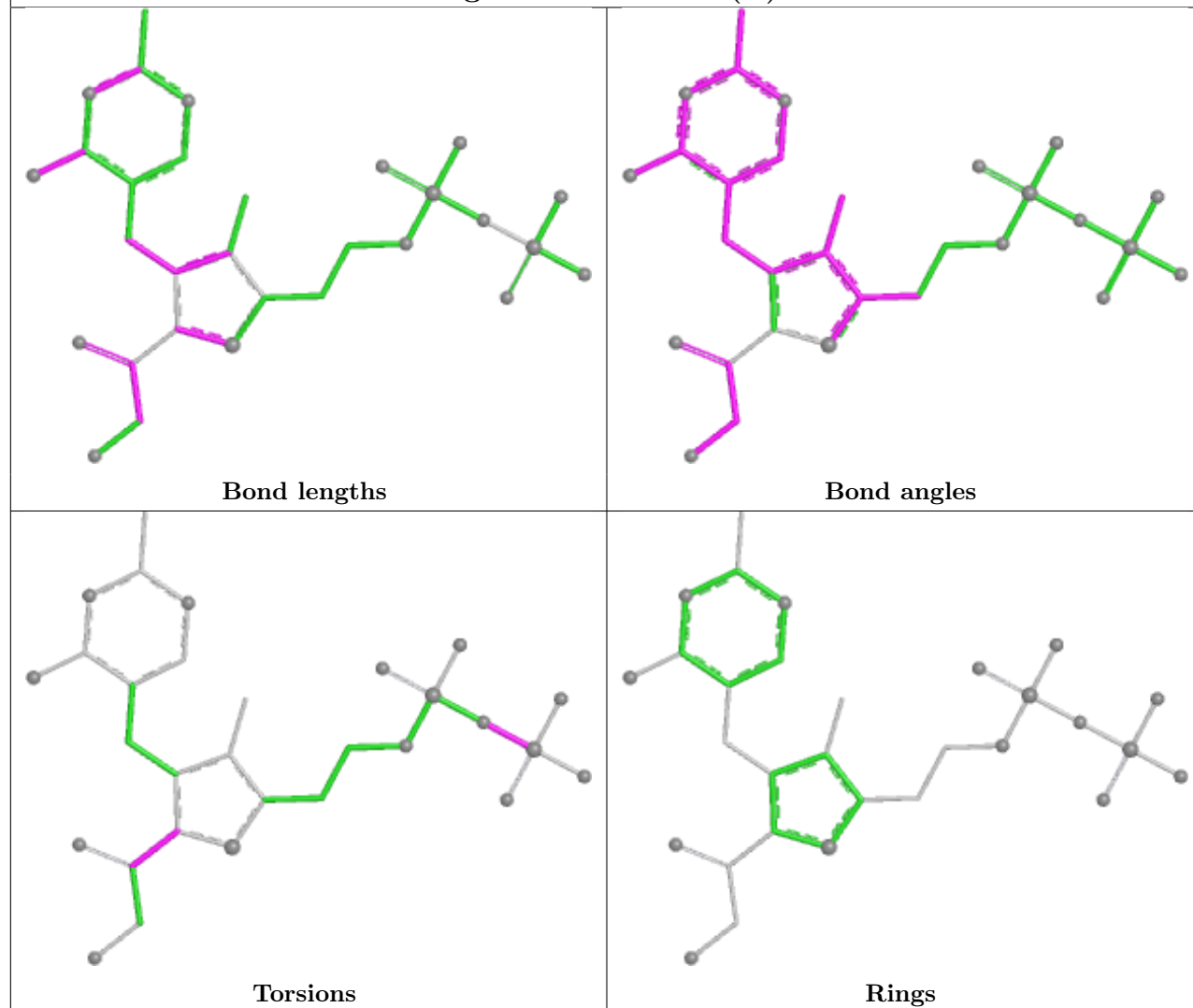
There are no ring outliers.

12 monomers are involved in 16 short contacts:

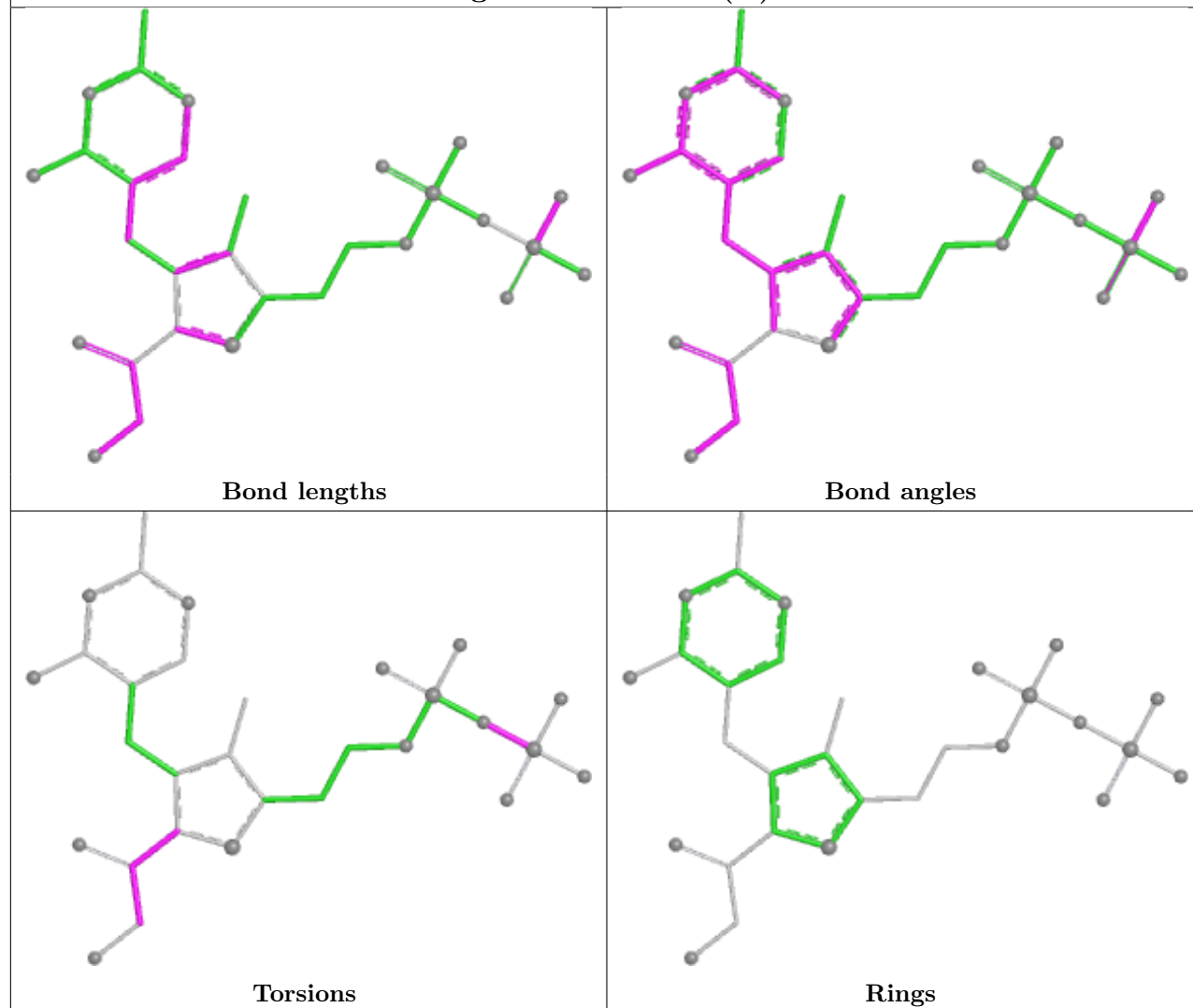
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	718	EDO	2	0
2	A	710[A]	EDO	2	0
2	B	1009	EDO	1	0
2	B	1015	EDO	1	0
2	A	717[A]	EDO	1	0
2	A	701[B]	EDO	2	0
2	A	713	EDO	1	0
2	A	711	EDO	1	0
2	A	717[B]	EDO	1	0
2	B	1008	EDO	3	0
2	B	1011[A]	EDO	1	0
2	A	704	EDO	1	0

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 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.

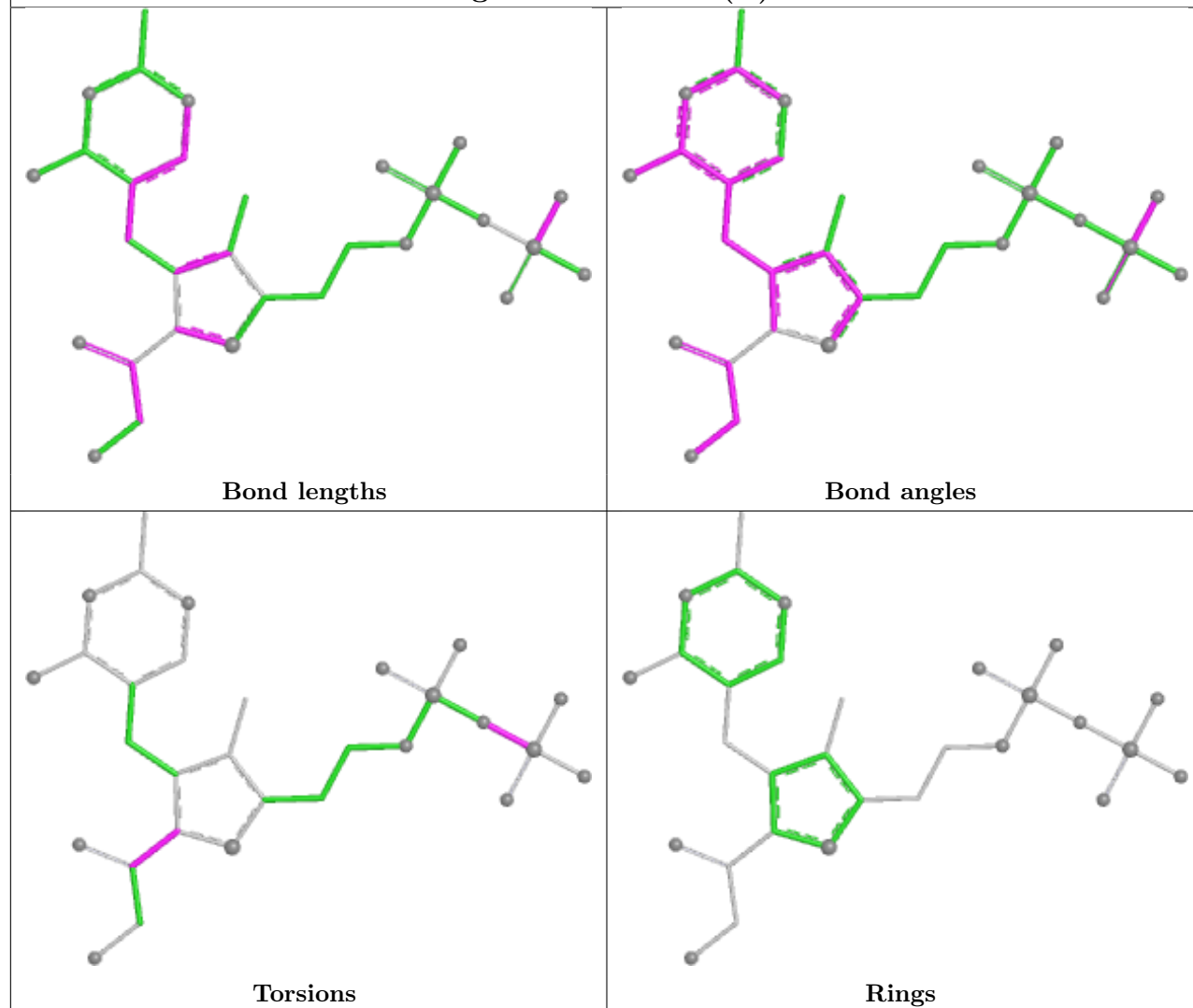
Ligand 1U0 B 1006 (B)

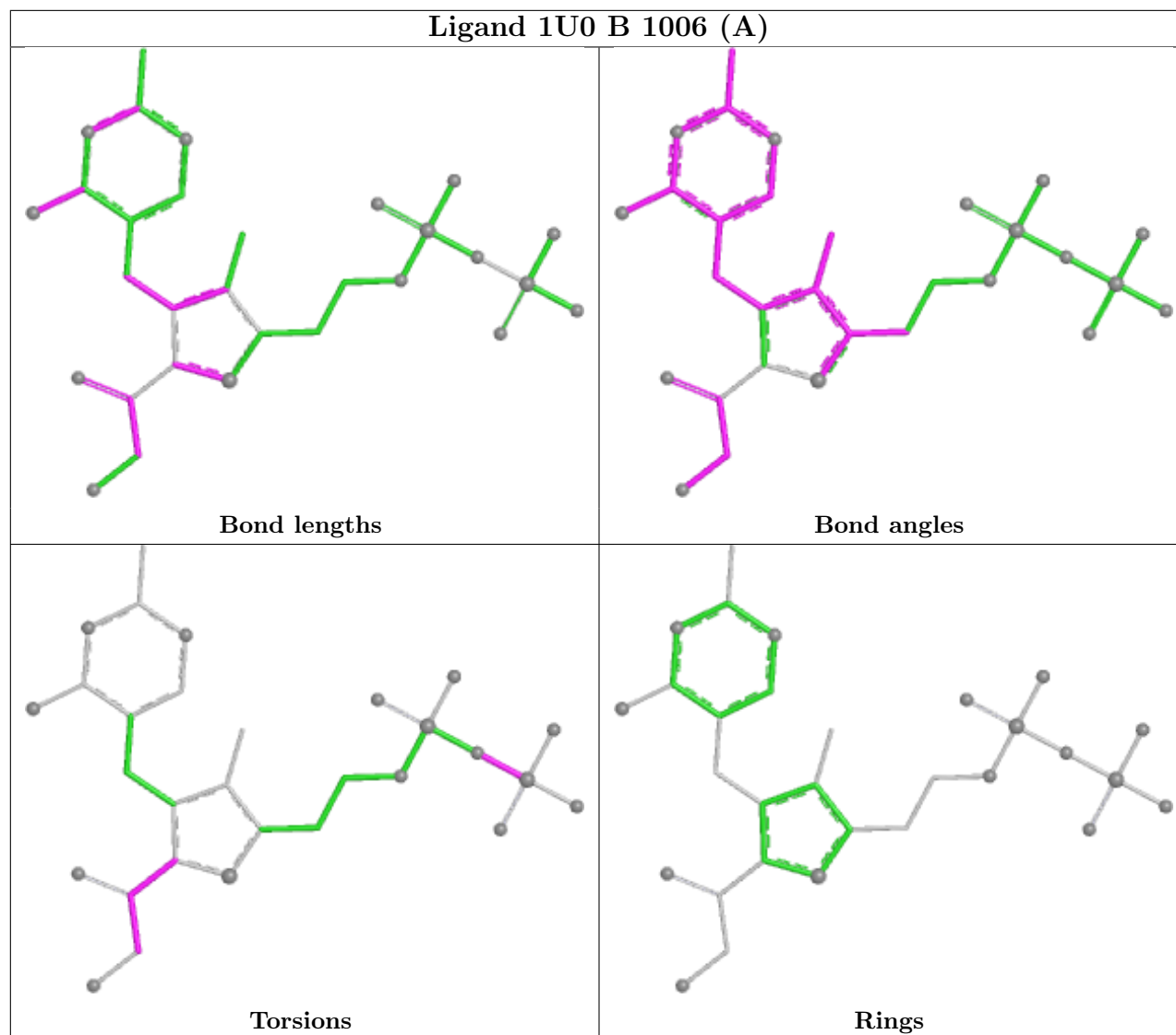


Ligand 1U0 A 709 (A)



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

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	620/637 (97%)	-0.28	10 (1%) 70 70	3, 9, 29, 73	34 (5%)
1	B	620/637 (97%)	-0.17	17 (2%) 56 58	3, 10, 34, 75	34 (5%)
All	All	1240/1274 (97%)	-0.23	27 (2%) 62 63	3, 10, 32, 75	68 (5%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	621	THR	5.4
1	B	621	THR	4.5
1	A	296[A]	VAL	4.1
1	A	619	LEU	3.9
1	A	620	ILE	3.5
1	B	503[A]	VAL	3.4
1	B	298	ILE	3.4
1	A	298	ILE	3.3
1	B	2	GLU	3.1
1	A	295[A]	SER	2.6
1	A	499	LYS	2.6
1	B	296	VAL	2.5
1	B	331	ALA	2.5
1	B	620	ILE	2.5
1	B	499	LYS	2.4
1	B	553	LYS	2.3
1	B	521	LEU	2.3
1	B	282	LYS	2.2
1	B	524	LYS	2.1
1	B	295	SER	2.1
1	A	231	ALA	2.1
1	B	275[A]	TYR	2.1
1	B	497	LYS	2.1
1	B	619	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	231[A]	ALA	2.0
1	A	281	LYS	2.0
1	A	618	GLY	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 oligosaccharides 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	715	4/4	0.81	0.29	43,46,83,84	0
2	EDO	A	718	4/4	0.83	0.21	28,66,70,87	0
2	EDO	B	1017	4/4	0.84	0.14	47,49,53,54	0
2	EDO	A	710[A]	4/4	0.85	0.22	67,69,69,71	0
6	SO4	B	1013	5/5	0.86	0.14	41,46,47,49	0
6	SO4	A	716[B]	5/5	0.88	0.13	35,38,43,43	0
2	EDO	B	1009	4/4	0.88	0.17	23,28,31,60	0
2	EDO	A	711	4/4	0.90	0.11	21,25,26,28	0
2	EDO	A	712	4/4	0.91	0.10	29,30,30,31	0
2	EDO	A	714	4/4	0.92	0.10	20,22,23,23	0
2	EDO	B	1011[A]	4/4	0.92	0.11	19,21,31,59	4
2	EDO	B	1011[B]	4/4	0.92	0.11	6,7,7,9	4
2	EDO	B	1015	4/4	0.93	0.12	16,40,42,45	0
2	EDO	B	1010	4/4	0.93	0.09	25,27,31,41	0
2	EDO	B	1001	4/4	0.93	0.08	19,19,22,32	0
2	EDO	A	702	4/4	0.93	0.09	21,23,25,28	0
2	EDO	B	1012	4/4	0.94	0.09	21,25,27,28	0
2	EDO	A	713	4/4	0.95	0.10	14,18,20,30	0
2	EDO	B	1003	4/4	0.95	0.09	13,22,23,23	0
2	EDO	B	1016	4/4	0.95	0.09	14,23,27,32	0

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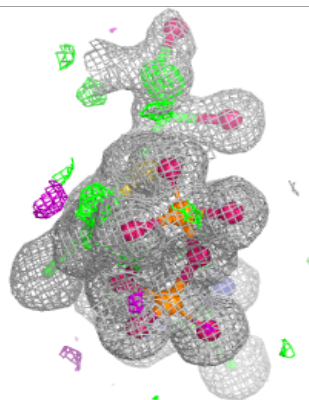
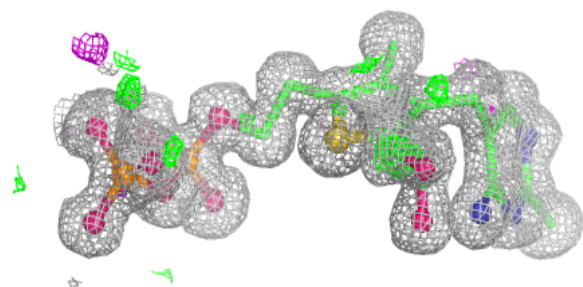
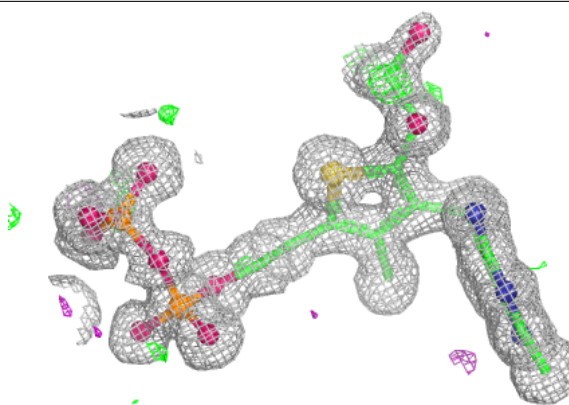
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	B	1008	4/4	0.96	0.11	13,17,18,19	0
2	EDO	A	717[B]	4/4	0.97	0.07	22,28,36,40	4
2	EDO	A	703	4/4	0.97	0.07	9,12,13,14	0
2	EDO	A	704	4/4	0.97	0.06	11,16,18,21	0
2	EDO	A	706	4/4	0.97	0.06	11,17,17,18	0
2	EDO	A	717[A]	4/4	0.97	0.07	6,12,13,14	4
2	EDO	B	1005	4/4	0.98	0.06	8,11,12,13	0
2	EDO	A	701[B]	4/4	0.98	0.04	28,29,31,33	4
2	EDO	A	701[A]	4/4	0.98	0.04	8,8,11,11	4
2	EDO	B	1002	4/4	0.98	0.05	10,14,15,15	0
2	EDO	A	705	4/4	0.98	0.06	9,10,12,16	0
2	EDO	B	1004	4/4	0.98	0.07	11,14,15,17	0
5	1U0	A	709[B]	30/30	0.99	0.03	4,6,10,15	2
5	1U0	B	1006[A]	30/30	0.99	0.03	5,6,8,9	2
5	1U0	B	1006[B]	30/30	0.99	0.03	5,6,9,17	2
4	NA	B	1014	1/1	0.99	0.04	11,11,11,11	0
5	1U0	A	709[A]	30/30	0.99	0.03	4,6,9,18	2
3	CA	B	1007	1/1	1.00	0.01	6,6,6,6	0
4	NA	A	708	1/1	1.00	0.02	7,7,7,7	0
3	CA	A	707	1/1	1.00	0.01	6,6,6,6	0

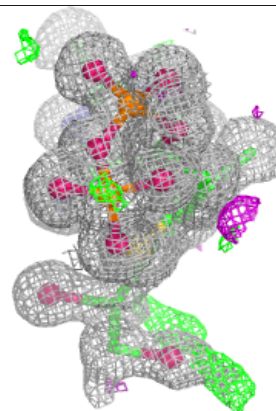
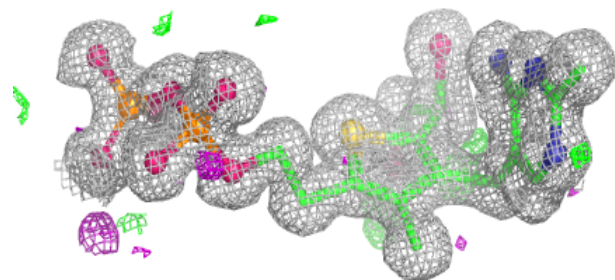
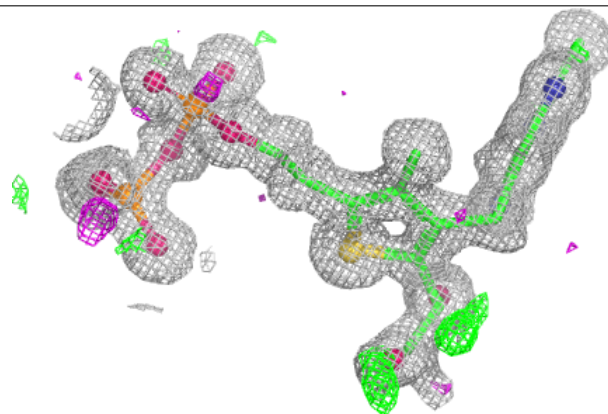
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

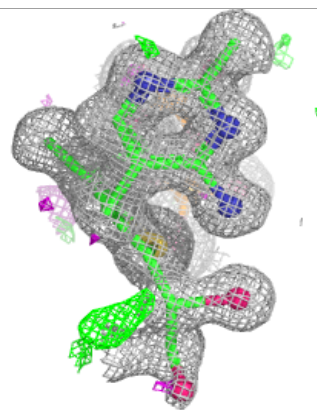
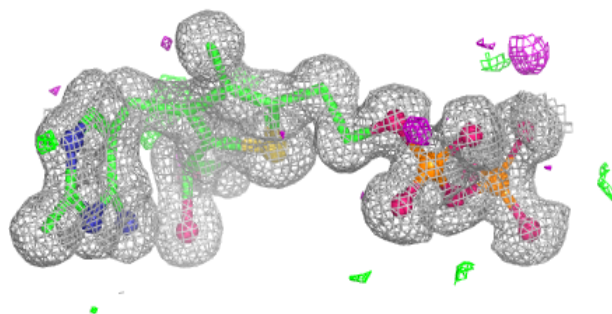
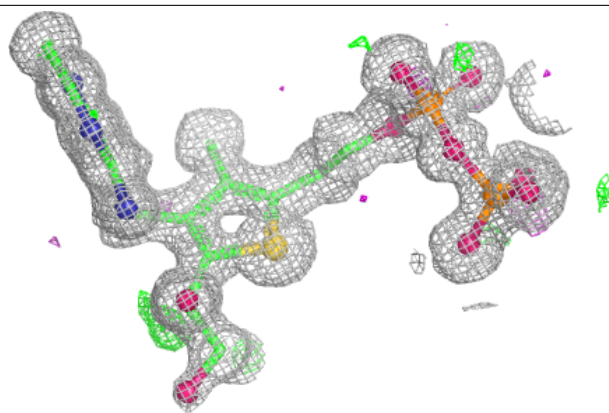
**Electron density around 1U0 B 1006 (A):**

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

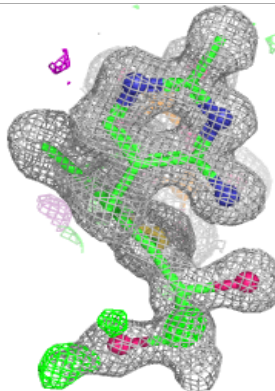
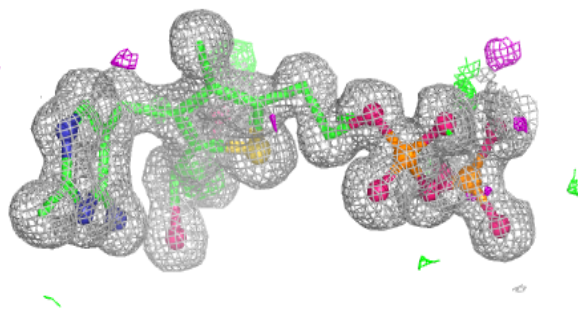
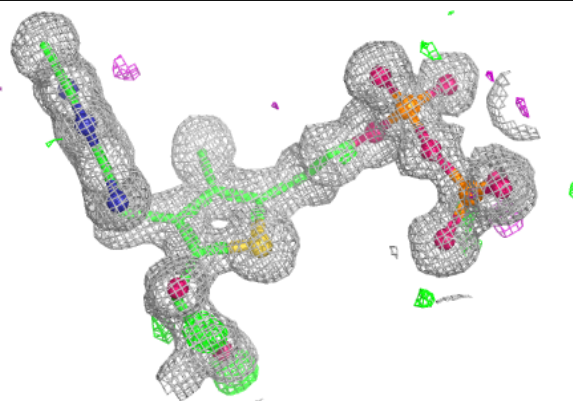


Electron density around 1U0 B 1006 (B):

$2mF_o-DF_c$ (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.