



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:25 am BST

PDB ID : 6FDI
Title : Crystal structure of human phosphodiesterase 4D2 catalytic domain with inhibitor NPD-226
Authors : Singh, A.K.; Brown, D.G.
Deposited on : 2017-12-24
Resolution : 1.90 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

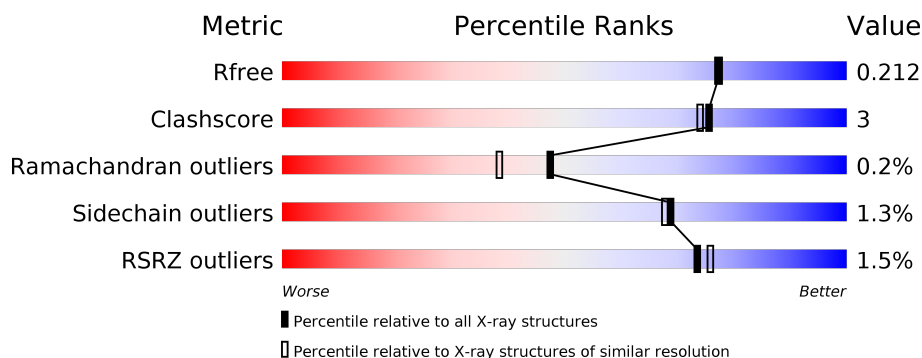
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	364	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>5%</div> <div>9%</div> </div> </div>
1	B	364	<div> <div></div> <div>84%</div> <div>5%</div> <div>11%</div> </div>
1	C	364	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>5%</div> <div>10%</div> </div> </div>
1	D	364	<div> <div></div> <div>79%</div> <div>10%</div> <div>11%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	B	505	-	-	X	-
4	EDO	B	516	-	-	-	X
5	PEG	D	511	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11904 atoms, of which 18 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	2	0
			2690	1702	462	512	14			
1	B	323	Total	C	N	O	S	0	0	0
			2613	1654	446	499	14			
1	C	326	Total	C	N	O	S	0	0	0
			2638	1668	450	506	14			
1	D	324	Total	C	N	O	S	0	1	0
			2632	1665	451	502	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	GLY	-	expression tag	UNP Q08499
A	76	SER	-	expression tag	UNP Q08499
A	77	HIS	-	expression tag	UNP Q08499
A	78	MET	-	expression tag	UNP Q08499
B	75	GLY	-	expression tag	UNP Q08499
B	76	SER	-	expression tag	UNP Q08499
B	77	HIS	-	expression tag	UNP Q08499
B	78	MET	-	expression tag	UNP Q08499
C	75	GLY	-	expression tag	UNP Q08499
C	76	SER	-	expression tag	UNP Q08499
C	77	HIS	-	expression tag	UNP Q08499
C	78	MET	-	expression tag	UNP Q08499
D	75	GLY	-	expression tag	UNP Q08499
D	76	SER	-	expression tag	UNP Q08499
D	77	HIS	-	expression tag	UNP Q08499
D	78	MET	-	expression tag	UNP Q08499

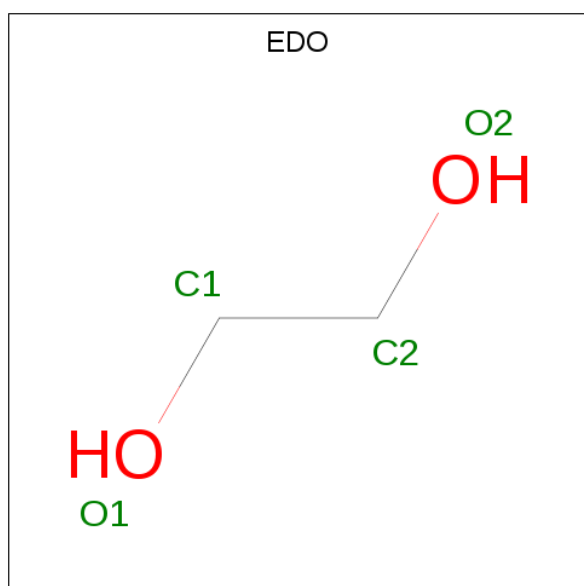
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O		0	0
			4	2	2			
4	B	1	Total	C	O		0	0
			4	2	2			
4	B	1	Total	C	O		0	0
			4	2	2			
4	B	1	Total	C	O		0	0
			4	2	2			
4	B	1	Total	C	O		0	0
			4	2	2			
4	B	1	Total	C	O		0	0
			4	2	2			
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	O		0	0
			4	2	2			
4	C	1	Total	C	O		0	0
			4	2	2			
4	C	1	Total	C	O		0	0
			4	2	2			
4	C	1	Total	C	O		0	0
			4	2	2			
4	C	1	Total	C	O		0	0
			4	2	2			
4	C	1	Total	C	O		0	0
			4	2	2			
4	C	1	Total	C	O		0	0
			4	2	2			
4	C	1	Total	C	O		0	0
			4	2	2			
4	C	1	Total	C	O		0	0
			4	2	2			
4	C	1	Total	C	O		0	0
			4	2	2			

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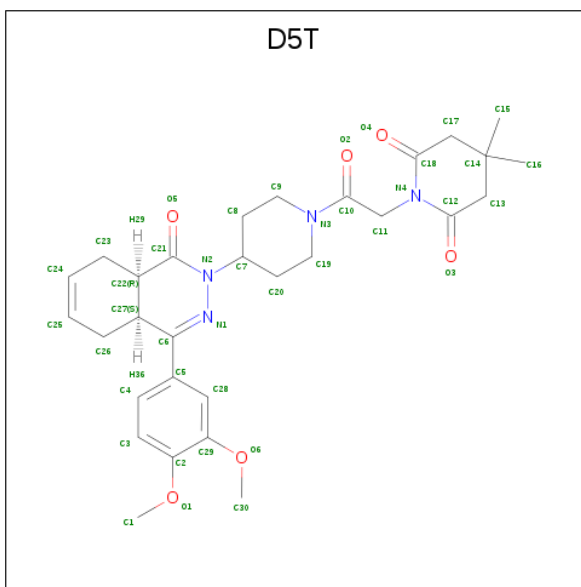
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	O		0	0
			4	2	2			
4	C	1	Total	C	O		0	0
			4	2	2			
4	D	1	Total	C	O		0	0
			4	2	2			
4	D	1	Total	C	O		0	0
			4	2	2			
4	D	1	Total	C	O		0	0
			4	2	2			
4	D	1	Total	C	O		0	0
			4	2	2			
4	D	1	Total	C	O		0	0
			4	2	2			
4	D	1	Total	C	O		0	0
			4	2	2			
4	D	1	Total	C	O		0	0
			4	2	2			
4	D	1	Total	C	O		0	0
			4	2	2			
4	D	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



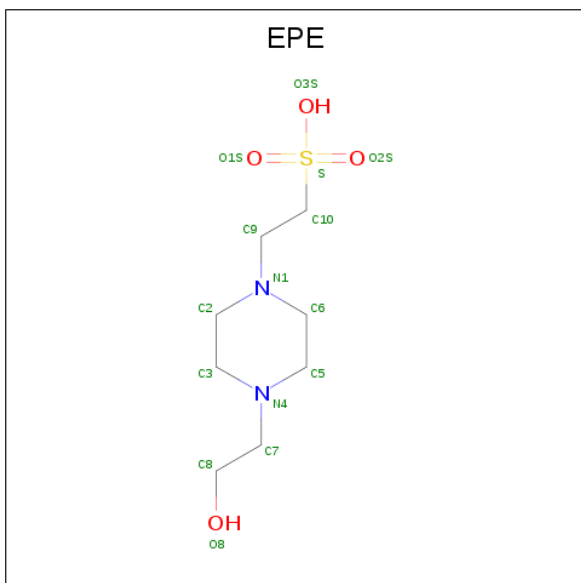
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 1-[2-[4-[(4 {a} {S},8 {a} {R})-4-(3,4-dimethoxyphenyl)-1-oxidanylidene-4 {a}, 5,8,8 {a}-tetrahydrophthalazin-2-yl]piperidin-1-yl]-2-oxidanylidene-ethyl]-4,4-dimethyl-piperidine-2,6-dione (three-letter code: D5T) (formula: C₃₀H₃₈N₄O₆).



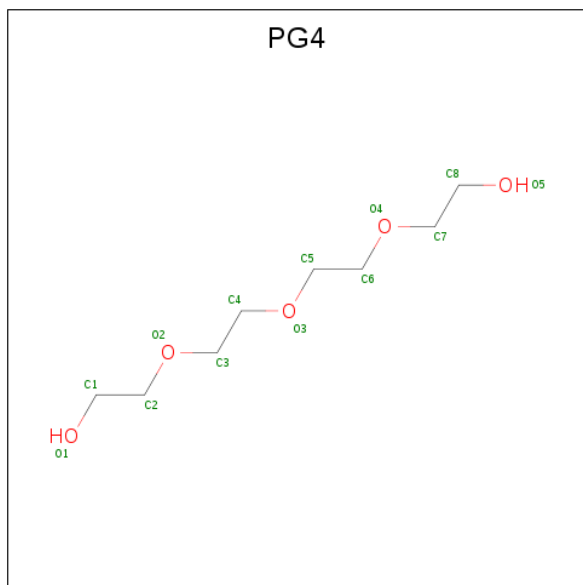
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			40	30	4	6		
6	B	1	Total	C	N	O	0	0
			40	30	4	6		
6	C	1	Total	C	N	O	0	0
			40	30	4	6		
6	D	1	Total	C	N	O	0	0
			40	30	4	6		

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

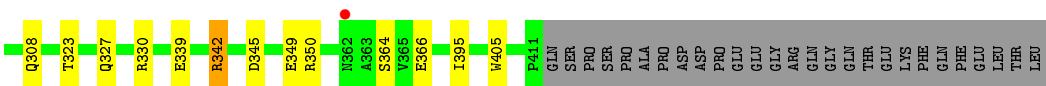
- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	220	Total	O	0	0
			220	220		
9	B	197	Total	O	0	0
			197	197		
9	C	150	Total	O	0	0
			150	150		
9	D	264	Total	O	0	0
			264	264		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.80Å 111.04Å 161.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.10 – 1.90 67.10 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (67.10-1.90) 100.0 (67.10-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.174 , 0.200 0.186 , 0.212	Depositor DCC
R_{free} test set	7136 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.6	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	0.96	EDS
Total number of atoms	11904	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: MG, PEG, ZN, EDO, PG4, EPE, D5T

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	0.82	0/2746	0.89	13/3729 (0.3%)
1	B	0.70	0/2667	0.76	3/3624 (0.1%)
1	C	0.69	1/2692 (0.0%)	0.84	8/3658 (0.2%)
1	D	0.87	2/2687 (0.1%)	0.81	4/3651 (0.1%)
All	All	0.78	3/10792 (0.0%)	0.83	28/14662 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	243	GLU	CD-OE2	-6.04	1.19	1.25
1	D	366	GLU	CD-OE2	-5.40	1.19	1.25
1	D	339	GLU	CD-OE2	-5.23	1.20	1.25

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	116	ARG	NE-CZ-NH2	11.93	126.27	120.30
1	A	350[A]	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	A	350[B]	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	C	116	ARG	NE-CZ-NH1	-8.36	116.12	120.30
1	A	330	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	A	330	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	D	105[A]	HIS	N-CA-CB	6.95	123.11	110.60
1	D	105[B]	HIS	N-CA-CB	6.95	123.11	110.60
1	A	342	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	342	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	C	330	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	221	LEU	CB-CG-CD2	6.03	121.25	111.00
1	D	342	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	C	348	ARG	NE-CZ-NH2	-5.82	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	PHE	CB-CG-CD2	-5.65	116.84	120.80
1	A	223	TYR	CB-CG-CD2	5.62	124.37	121.00
1	C	330	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	D	108	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	108	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	350[A]	ARG	CG-CD-NE	-5.37	100.52	111.80
1	A	350[B]	ARG	CG-CD-NE	-5.37	100.52	111.80
1	C	349	GLU	CB-CA-C	-5.25	99.90	110.40
1	A	223	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	C	296	GLY	N-CA-C	5.11	125.87	113.10
1	C	346	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	350[A]	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	A	350[B]	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	B	201	ASP	CB-CG-OD1	5.00	122.80	118.30

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	2690	0	2643	13	0
1	B	2613	0	2570	8	0
1	C	2638	0	2591	19	0
1	D	2632	0	2584	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	84	0	126	1	0
4	B	44	6	66	6	0
4	C	56	0	84	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	52	12	78	5	0
5	A	7	0	10	0	0
5	B	7	0	10	0	0
5	D	21	0	30	6	0
6	A	40	0	0	0	0
6	B	40	0	0	0	0
6	C	40	0	0	0	0
6	D	40	0	0	0	0
7	B	15	0	17	1	0
7	C	15	0	17	0	0
8	D	13	0	18	2	0
9	A	220	0	0	1	0
9	B	197	0	0	0	0
9	C	150	0	0	2	0
9	D	264	0	0	0	0
All	All	11886	18	10844	68	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 3.

All (68) 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:D:162:ASN:OD1	4:D:520:EDO:H12	1.71	0.90
1:D:153:TYR:O	5:D:509:PEG:H41	1.73	0.88
1:D:244:GLU:HA	5:D:511:PEG:H31	1.63	0.79
1:D:262:LYS:HD3	4:D:506:EDO:H22	1.63	0.79
1:D:245:ASN:H	5:D:511:PEG:H31	1.49	0.78
4:B:505:EDO:H11	1:D:215:THR:HG22	1.70	0.74
1:D:158:ALA:H	1:D:342:ARG:HH12	1.36	0.72
9:A:611:HOH:O	1:C:346:ARG:HD2	1.91	0.70
1:D:162:ASN:OD1	4:D:520:EDO:C1	2.39	0.69
1:C:132:LEU:HD22	1:C:139:VAL:HG22	1.75	0.69
1:D:245:ASN:H	5:D:511:PEG:C3	2.06	0.68
1:D:293:THR:HG22	1:D:299:LEU:HD23	1.79	0.64
1:C:181:LEU:CD2	1:C:298:LEU:HD12	2.31	0.60
1:D:150:GLU:O	5:D:509:PEG:H22	2.01	0.60
1:A:181:LEU:CD2	1:A:298:LEU:HD12	2.32	0.60
1:C:181:LEU:HD21	1:C:298:LEU:HD12	1.85	0.59
1:D:245:ASN:N	5:D:511:PEG:H31	2.17	0.58
1:C:132:LEU:CD2	1:C:139:VAL:HG22	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ARG:HD3	1:C:405:TRP:CH2	2.42	0.55
7:B:510:EPE:O8	7:B:510:EPE:H31	2.07	0.54
1:A:181:LEU:HD21	1:A:298:LEU:HD12	1.90	0.54
1:C:221:LEU:C	1:C:221:LEU:HD23	2.29	0.53
1:D:330:ARG:HD3	1:D:405:TRP:CZ3	2.45	0.52
1:A:270:ALA:HB1	1:A:279:LEU:HD11	1.92	0.51
1:D:270:ALA:HB1	1:D:279:LEU:HD11	1.92	0.51
1:C:409:THR:O	1:C:409:THR:HG22	2.11	0.51
1:C:223:TYR:OH	8:D:518:PG4:H71	2.11	0.49
1:B:270:ALA:HB1	1:B:279:LEU:HD11	1.93	0.49
1:C:345:ASP:O	1:C:349:GLU:HG3	2.12	0.49
1:C:162:ASN:ND2	4:C:506:EDO:H22	2.28	0.49
1:D:158:ALA:N	1:D:342:ARG:HH12	2.07	0.49
1:A:148:THR:O	1:A:152:HIS:HD2	1.96	0.48
1:C:261:ARG:HB2	4:C:508:EDO:H12	1.94	0.48
1:C:270:ALA:HB1	1:C:279:LEU:HD11	1.95	0.48
1:C:221:LEU:O	1:C:221:LEU:HD23	2.14	0.47
1:A:181:LEU:HD23	1:A:298:LEU:HD12	1.96	0.47
1:C:326:LEU:HB2	4:C:518:EDO:H12	1.97	0.47
1:D:286:MET:CE	1:D:308:GLN:OE1	2.63	0.47
1:D:303:TYR:CE1	4:D:506:EDO:H12	2.49	0.47
1:A:294:SER:O	1:A:295:SER:CB	2.63	0.46
1:A:294:SER:O	1:A:295:SER:HB3	2.15	0.46
1:D:330:ARG:HD3	1:D:405:TRP:CH2	2.50	0.45
1:C:139:VAL:HG23	9:C:704:HOH:O	2.16	0.45
1:D:345:ASP:O	1:D:349:GLU:HG3	2.17	0.45
1:D:115:ASN:HD21	4:D:520:EDO:C1	2.30	0.44
1:C:345:ASP:OD1	1:C:348:ARG:NH2	2.50	0.44
1:A:225:ASP:OD2	1:B:261:ARG:NH1	2.41	0.43
1:B:244:GLU:HB3	4:B:505:EDO:H12	1.99	0.43
1:D:222:MET:HA	8:D:518:PG4:C7	2.48	0.43
1:C:181:LEU:HD23	1:C:298:LEU:HD12	2.00	0.43
1:A:105[B]:HIS:HE1	1:A:107:PHE:HB2	1.84	0.43
4:B:505:EDO:C1	1:D:215:THR:HG22	2.43	0.43
4:C:518:EDO:H21	9:C:646:HOH:O	2.18	0.43
1:B:323:THR:HB	1:B:395:ILE:HG23	2.00	0.42
1:D:105[A]:HIS:HE1	1:D:107:PHE:HB2	1.85	0.42
4:B:505:EDO:O2	1:D:350:ARG:HB3	2.20	0.42
1:A:153:TYR:O	4:A:525:EDO:H11	2.20	0.42
1:B:113:SER:OG	1:B:116:ARG:HB2	2.21	0.41
1:D:323:THR:HB	1:D:395:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105[B]:HIS:CE1	1:A:107:PHE:HB2	2.56	0.41
1:A:350[A]:ARG:HD2	1:A:350[A]:ARG:HH11	1.55	0.41
1:B:244:GLU:O	4:B:505:EDO:O1	2.25	0.41
1:D:104:LEU:HD22	1:D:170:GLN:HG3	2.02	0.41
1:D:90:ASP:OD1	1:D:91:VAL:N	2.54	0.41
1:C:275:LYS:HD3	1:C:275:LYS:HA	1.96	0.40
1:B:144:THR:HG23	4:B:505:EDO:H22	2.02	0.40
1:A:158:ALA:H	1:A:342:ARG:HH12	1.69	0.40
1:B:286:MET:HE3	1:B:286:MET:HB2	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/364 (91%)	326 (99%)	4 (1%)	0	100	100
1	B	321/364 (88%)	319 (99%)	2 (1%)	0	100	100
1	C	324/364 (89%)	317 (98%)	5 (2%)	2 (1%)	25	15
1	D	323/364 (89%)	318 (98%)	5 (2%)	0	100	100
All	All	1298/1456 (89%)	1280 (99%)	16 (1%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	299	LEU
1	C	296	GLY

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	303/331 (92%)	300 (99%)	3 (1%)	76	76
1	B	295/331 (89%)	289 (98%)	6 (2%)	55	51
1	C	298/331 (90%)	296 (99%)	2 (1%)	84	84
1	D	297/331 (90%)	293 (99%)	4 (1%)	69	68
All	All	1193/1324 (90%)	1178 (99%)	15 (1%)	69	68

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

Mol	Chain	Res	Type
1	A	85	LYS
1	A	297	VAL
1	A	299	LEU
1	B	91	VAL
1	B	108	ARG
1	B	255	LYS
1	B	260	LEU
1	B	308	GLN
1	B	364	SER
1	C	87	GLU
1	C	364	SER
1	D	178	THR
1	D	260	LEU
1	D	327	GLN
1	D	364	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 79 ligands modelled in this entry, 8 are monoatomic - leaving 71 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	$\# Z > 2$
4	EDO	C	516	-	3,3,3	0.85	0	2,2,2	0.54	0
4	EDO	C	501	-	3,3,3	0.34	0	2,2,2	0.28	0
4	EDO	C	502	-	3,3,3	0.31	0	2,2,2	0.87	0
4	EDO	C	503	-	3,3,3	0.30	0	2,2,2	0.41	0
4	EDO	C	506	-	3,3,3	0.25	0	2,2,2	1.18	0
4	EDO	D	502	-	3,3,3	0.56	0	2,2,2	0.72	0
4	EDO	C	508	-	3,3,3	0.38	0	2,2,2	0.33	0
4	EDO	C	507	-	3,3,3	0.65	0	2,2,2	0.65	0
4	EDO	D	513	-	3,3,3	0.51	0	2,2,2	0.82	0
4	EDO	A	507	-	3,3,3	0.65	0	2,2,2	0.41	0
5	PEG	A	513	-	6,6,6	0.68	0	5,5,5	0.55	0
5	PEG	B	509	-	6,6,6	0.90	0	5,5,5	0.86	0
4	EDO	D	508	-	3,3,3	0.40	0	2,2,2	0.14	0
4	EDO	B	503	-	3,3,3	0.47	0	2,2,2	0.76	0
7	EPE	B	510	-	15,15,15	2.07	1 (6%)	18,20,20	1.58	3 (16%)
4	EDO	A	519	-	3,3,3	0.28	0	2,2,2	0.84	0
4	EDO	A	515	-	3,3,3	0.46	0	2,2,2	0.31	0
4	EDO	B	511	-	3,3,3	0.35	0	2,2,2	0.78	0
4	EDO	A	521	-	3,3,3	0.40	0	2,2,2	0.73	0
4	EDO	A	506	-	3,3,3	0.40	0	2,2,2	0.55	0
5	PEG	D	511	-	6,6,6	0.48	0	5,5,5	1.02	0
4	EDO	A	518	-	3,3,3	0.67	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	505	-	3,3,3	0.21	0	2,2,2	0.21	0
4	EDO	A	509	-	3,3,3	0.29	0	2,2,2	0.94	0
4	EDO	D	516	-	3,3,3	0.47	0	2,2,2	0.56	0
4	EDO	D	520	-	3,3,3	0.45	0	2,2,2	0.90	0
5	PEG	D	509	-	6,6,6	0.45	0	5,5,5	0.91	0
4	EDO	A	517	-	3,3,3	0.26	0	2,2,2	0.90	0
4	EDO	A	504	-	3,3,3	0.45	0	2,2,2	1.07	0
4	EDO	B	513	-	3,3,3	0.24	0	2,2,2	0.63	0
4	EDO	A	520	-	3,3,3	0.41	0	2,2,2	0.30	0
7	EPE	C	512	-	15,15,15	2.25	1 (6%)	18,20,20	1.84	6 (33%)
4	EDO	B	508	-	3,3,3	0.31	0	2,2,2	1.17	0
4	EDO	D	514	-	3,3,3	0.59	0	2,2,2	0.75	0
6	D5T	B	512	-	44,44,44	0.60	1 (2%)	55,65,65	1.80	5 (9%)
4	EDO	A	512	-	3,3,3	0.63	0	2,2,2	0.11	0
4	EDO	C	517	-	3,3,3	0.16	0	2,2,2	1.11	0
4	EDO	B	515	-	3,3,3	0.40	0	2,2,2	0.04	0
4	EDO	C	515	-	3,3,3	0.23	0	2,2,2	0.68	0
4	EDO	D	506	-	3,3,3	0.17	0	2,2,2	0.74	0
4	EDO	C	514	-	3,3,3	0.40	0	2,2,2	0.43	0
4	EDO	C	511	-	3,3,3	0.63	0	2,2,2	0.34	0
4	EDO	D	515	-	3,3,3	0.46	0	2,2,2	0.26	0
4	EDO	B	516	-	3,3,3	0.18	0	2,2,2	0.70	0
4	EDO	C	510	-	3,3,3	0.36	0	2,2,2	0.57	0
4	EDO	A	522	-	3,3,3	0.44	0	2,2,2	0.37	0
4	EDO	D	519	-	3,3,3	0.47	0	2,2,2	0.22	0
6	D5T	C	513	-	44,44,44	0.70	1 (2%)	55,65,65	0.83	2 (3%)
4	EDO	A	510	-	3,3,3	0.45	0	2,2,2	0.10	0
6	D5T	A	514	-	44,44,44	0.46	0	55,65,65	0.69	1 (1%)
5	PEG	D	510	-	6,6,6	0.43	0	5,5,5	0.39	0
4	EDO	D	507	-	3,3,3	0.52	0	2,2,2	0.52	0
4	EDO	B	514	-	3,3,3	0.35	0	2,2,2	0.75	0
4	EDO	A	508	-	3,3,3	0.64	0	2,2,2	0.74	0
4	EDO	A	524	-	3,3,3	0.53	0	2,2,2	0.87	0
4	EDO	B	507	-	3,3,3	0.41	0	2,2,2	0.75	0
4	EDO	B	506	-	3,3,3	0.52	0	2,2,2	0.24	0
4	EDO	A	523	-	3,3,3	0.60	0	2,2,2	0.26	0
6	D5T	D	512	-	44,44,44	0.46	0	55,65,65	0.70	1 (1%)
4	EDO	A	511	-	3,3,3	0.47	0	2,2,2	0.36	0
4	EDO	C	518	-	3,3,3	0.59	0	2,2,2	0.35	0
4	EDO	A	525	-	3,3,3	0.68	0	2,2,2	0.32	0
4	EDO	D	505	-	3,3,3	0.37	0	2,2,2	0.09	0
4	EDO	A	503	-	3,3,3	0.50	0	2,2,2	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	501	-	3,3,3	0.22	0	2,2,2	0.85	0
4	EDO	D	517	-	3,3,3	0.27	0	2,2,2	0.85	0
4	EDO	C	509	-	3,3,3	0.25	0	2,2,2	0.56	0
4	EDO	A	516	-	3,3,3	0.34	0	2,2,2	1.02	0
8	PG4	D	518	-	12,12,12	1.11	0	11,11,11	1.11	1 (9%)
4	EDO	B	504	-	3,3,3	0.64	0	2,2,2	0.04	0
4	EDO	A	505	-	3,3,3	0.53	0	2,2,2	0.18	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
4	EDO	C	516	-	-	1/1/1/1	-
4	EDO	C	501	-	-	1/1/1/1	-
4	EDO	C	502	-	-	1/1/1/1	-
4	EDO	C	503	-	-	0/1/1/1	-
4	EDO	C	506	-	-	0/1/1/1	-
4	EDO	D	502	-	-	1/1/1/1	-
4	EDO	C	508	-	-	0/1/1/1	-
4	EDO	C	507	-	-	0/1/1/1	-
4	EDO	D	513	-	-	1/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
5	PEG	A	513	-	-	3/4/4/4	-
5	PEG	B	509	-	-	1/4/4/4	-
4	EDO	D	508	-	-	1/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
7	EPE	B	510	-	-	5/9/19/19	0/1/1/1
4	EDO	A	519	-	-	1/1/1/1	-
4	EDO	A	515	-	-	1/1/1/1	-
4	EDO	B	511	-	-	0/1/1/1	-
4	EDO	A	521	-	-	1/1/1/1	-
4	EDO	A	506	-	-	1/1/1/1	-
5	PEG	D	511	-	-	3/4/4/4	-
4	EDO	A	518	-	-	1/1/1/1	-
4	EDO	B	505	-	-	0/1/1/1	-
4	EDO	A	509	-	-	1/1/1/1	-
4	EDO	D	516	-	-	1/1/1/1	-
4	EDO	D	520	-	-	1/1/1/1	-
5	PEG	D	509	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	517	-	-	0/1/1/1	-
4	EDO	A	504	-	-	0/1/1/1	-
4	EDO	B	513	-	-	1/1/1/1	-
4	EDO	A	520	-	-	0/1/1/1	-
7	EPE	C	512	-	-	5/9/19/19	0/1/1/1
4	EDO	B	508	-	-	1/1/1/1	-
4	EDO	D	514	-	-	0/1/1/1	-
6	D5T	B	512	-	-	0/20/75/75	0/5/5/5
4	EDO	A	512	-	-	1/1/1/1	-
4	EDO	C	517	-	-	1/1/1/1	-
4	EDO	B	515	-	-	0/1/1/1	-
4	EDO	C	515	-	-	0/1/1/1	-
4	EDO	D	506	-	-	0/1/1/1	-
4	EDO	C	514	-	-	1/1/1/1	-
4	EDO	C	511	-	-	1/1/1/1	-
4	EDO	D	515	-	-	1/1/1/1	-
4	EDO	B	516	-	-	0/1/1/1	-
4	EDO	C	510	-	-	1/1/1/1	-
4	EDO	A	522	-	-	0/1/1/1	-
4	EDO	D	519	-	-	1/1/1/1	-
6	D5T	C	513	-	-	0/20/75/75	0/5/5/5
4	EDO	A	510	-	-	1/1/1/1	-
6	D5T	A	514	-	-	1/20/75/75	0/5/5/5
5	PEG	D	510	-	-	3/4/4/4	-
4	EDO	D	507	-	-	0/1/1/1	-
4	EDO	B	514	-	-	1/1/1/1	-
4	EDO	A	508	-	-	0/1/1/1	-
4	EDO	A	524	-	-	1/1/1/1	-
4	EDO	B	507	-	-	0/1/1/1	-
4	EDO	B	506	-	-	1/1/1/1	-
4	EDO	A	523	-	-	1/1/1/1	-
6	D5T	D	512	-	-	0/20/75/75	0/5/5/5
4	EDO	A	511	-	-	0/1/1/1	-
4	EDO	C	518	-	-	1/1/1/1	-
4	EDO	A	525	-	-	1/1/1/1	-
4	EDO	D	505	-	-	0/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
4	EDO	D	501	-	-	1/1/1/1	-
4	EDO	D	517	-	-	1/1/1/1	-
4	EDO	C	509	-	-	1/1/1/1	-
4	EDO	A	516	-	-	0/1/1/1	-
8	PG4	D	518	-	-	6/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	504	-	-	1/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	512	EPE	C10-S	-8.50	1.65	1.77
7	B	510	EPE	C10-S	-7.81	1.66	1.77
6	C	513	D5T	C11-N4	3.57	1.51	1.46
6	B	512	D5T	C11-N4	2.36	1.49	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	512	D5T	C18-N4-C12	-11.12	120.59	124.07
7	B	510	EPE	O2S-S-C10	4.99	112.93	106.92
7	C	512	EPE	O3S-S-O2S	-3.69	102.27	111.27
6	D	512	D5T	C6-N1-N2	-2.94	115.89	118.97
6	A	514	D5T	C6-N1-N2	-2.88	115.96	118.97
6	C	513	D5T	C11-C10-N3	2.87	120.69	117.08
6	B	512	D5T	C11-N4-C12	2.85	119.99	117.79
7	C	512	EPE	C9-N1-C2	-2.77	104.14	111.23
7	C	512	EPE	C7-N4-C3	-2.70	104.33	111.23
7	C	512	EPE	O2S-S-C10	2.67	110.13	106.92
6	B	512	D5T	C11-C10-N3	2.56	120.31	117.08
7	C	512	EPE	C9-N1-C6	2.37	117.30	111.23
6	B	512	D5T	C5-C6-N1	2.29	118.81	115.95
6	C	513	D5T	O2-C10-C11	-2.26	117.06	120.59
8	D	518	PG4	O4-C7-C8	2.23	119.86	110.07
7	B	510	EPE	O2S-S-O1S	-2.20	106.32	113.95
7	C	512	EPE	C3-C2-N1	2.16	115.07	110.64
7	B	510	EPE	C7-N4-C3	2.05	116.47	111.23
6	B	512	D5T	C11-N4-C18	2.02	119.35	117.79

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	510	EPE	C8-C7-N4-C3
7	C	512	EPE	C10-C9-N1-C6
7	C	512	EPE	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
5	D	511	PEG	C4-C3-O2-C2
5	A	513	PEG	O2-C3-C4-O4
5	D	510	PEG	O2-C3-C4-O4
4	A	518	EDO	O1-C1-C2-O2
8	D	518	PG4	O2-C3-C4-O3
7	B	510	EPE	C9-C10-S-O3S
5	A	513	PEG	O1-C1-C2-O2
5	D	509	PEG	O1-C1-C2-O2
5	D	510	PEG	O1-C1-C2-O2
8	D	518	PG4	O4-C7-C8-O5
7	B	510	EPE	C8-C7-N4-C5
4	A	512	EDO	O1-C1-C2-O2
4	A	523	EDO	O1-C1-C2-O2
4	C	510	EDO	O1-C1-C2-O2
4	A	510	EDO	O1-C1-C2-O2
4	C	518	EDO	O1-C1-C2-O2
4	A	525	EDO	O1-C1-C2-O2
5	D	511	PEG	O1-C1-C2-O2
5	D	511	PEG	O2-C3-C4-O4
8	D	518	PG4	O1-C1-C2-O2
4	B	506	EDO	O1-C1-C2-O2
4	C	509	EDO	O1-C1-C2-O2
4	D	517	EDO	O1-C1-C2-O2
4	A	507	EDO	O1-C1-C2-O2
4	A	515	EDO	O1-C1-C2-O2
4	C	516	EDO	O1-C1-C2-O2
4	C	517	EDO	O1-C1-C2-O2
4	D	519	EDO	O1-C1-C2-O2
4	B	504	EDO	O1-C1-C2-O2
5	D	509	PEG	C4-C3-O2-C2
8	D	518	PG4	C5-C6-O4-C7
8	D	518	PG4	C1-C2-O2-C3
8	D	518	PG4	C6-C5-O3-C4
4	D	516	EDO	O1-C1-C2-O2
4	B	508	EDO	O1-C1-C2-O2
4	A	524	EDO	O1-C1-C2-O2
7	B	510	EPE	C9-C10-S-O1S
7	B	510	EPE	C9-C10-S-O2S
5	A	513	PEG	C1-C2-O2-C3
5	D	510	PEG	C1-C2-O2-C3
4	C	501	EDO	O1-C1-C2-O2
4	D	502	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	D	513	EDO	O1-C1-C2-O2
4	A	519	EDO	O1-C1-C2-O2
4	D	520	EDO	O1-C1-C2-O2
4	B	513	EDO	O1-C1-C2-O2
4	C	511	EDO	O1-C1-C2-O2
4	A	521	EDO	O1-C1-C2-O2
7	C	512	EPE	C9-C10-S-O3S
7	C	512	EPE	C10-C9-N1-C2
4	C	514	EDO	O1-C1-C2-O2
4	B	514	EDO	O1-C1-C2-O2
4	D	508	EDO	O1-C1-C2-O2
4	A	506	EDO	O1-C1-C2-O2
4	A	509	EDO	O1-C1-C2-O2
5	B	509	PEG	O1-C1-C2-O2
6	A	514	D5T	O2-C10-N3-C19
7	C	512	EPE	S-C10-C9-N1
4	C	502	EDO	O1-C1-C2-O2
4	D	515	EDO	O1-C1-C2-O2
4	D	501	EDO	O1-C1-C2-O2

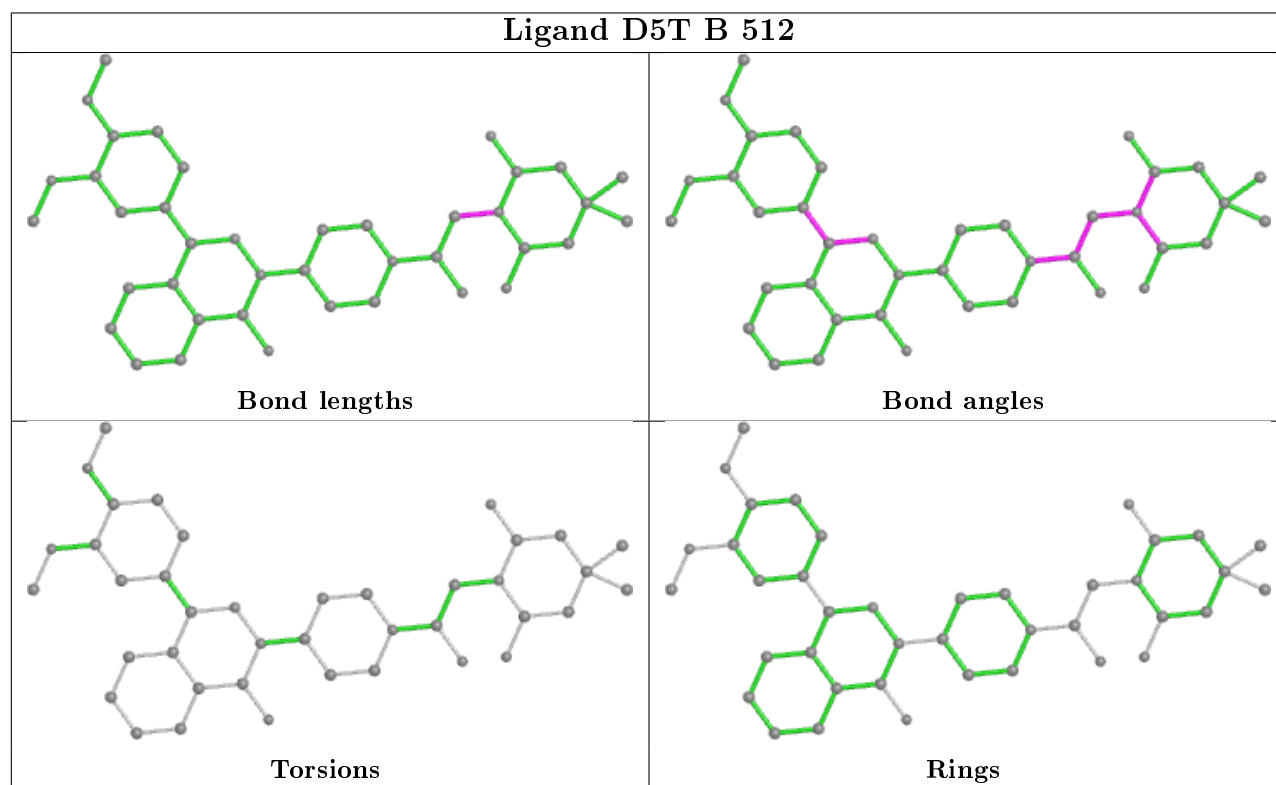
There are no ring outliers.

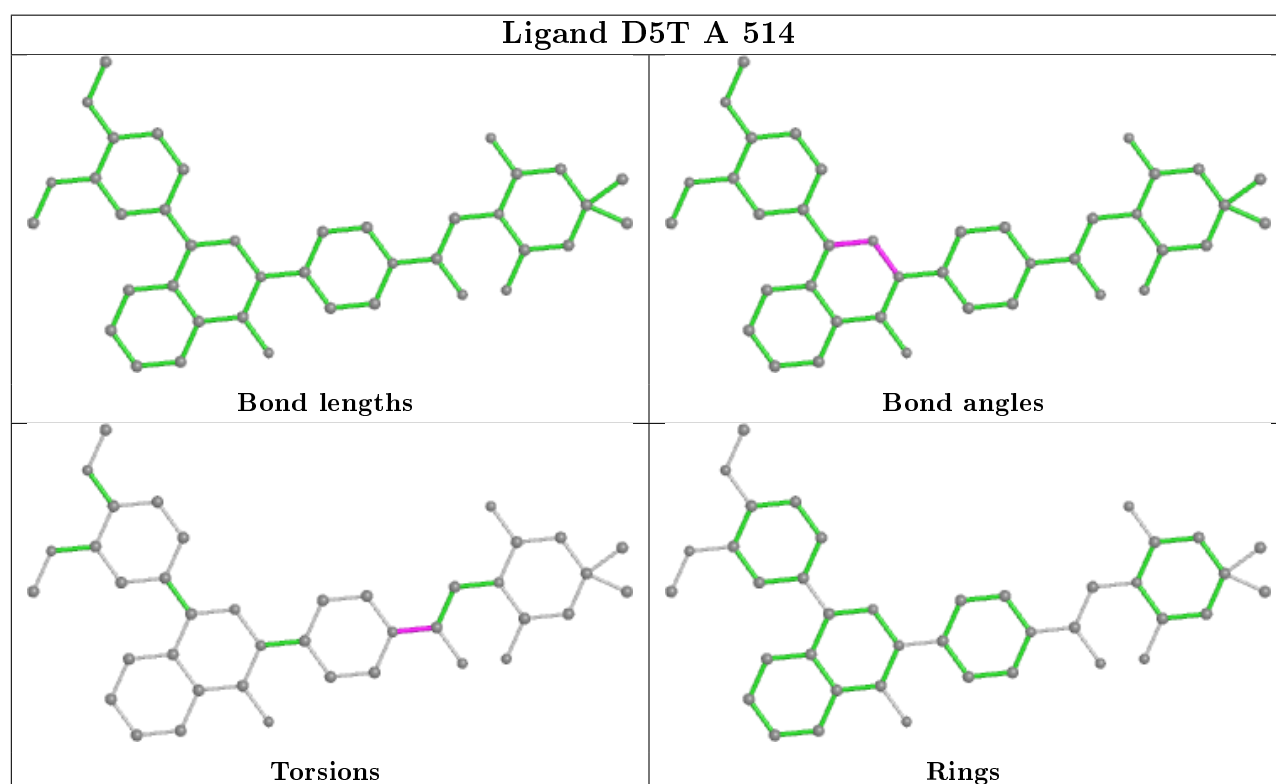
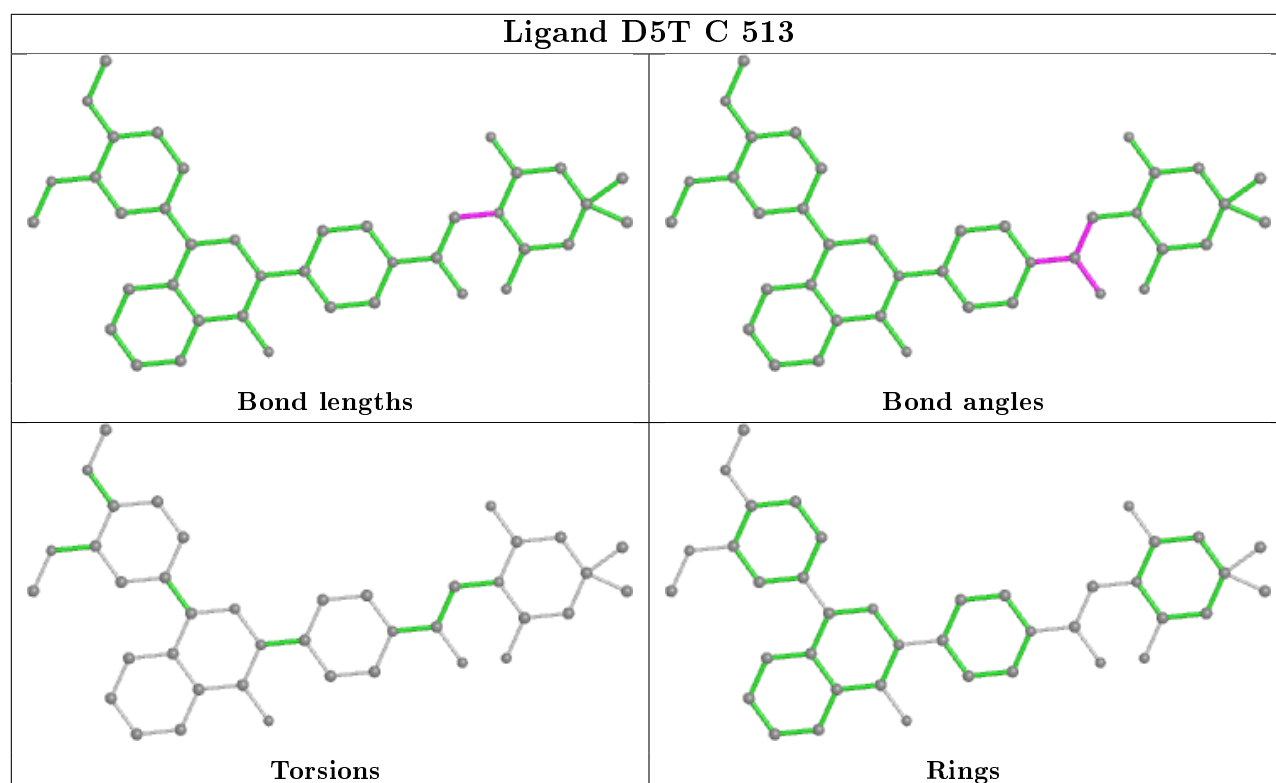
11 monomers are involved in 25 short contacts:

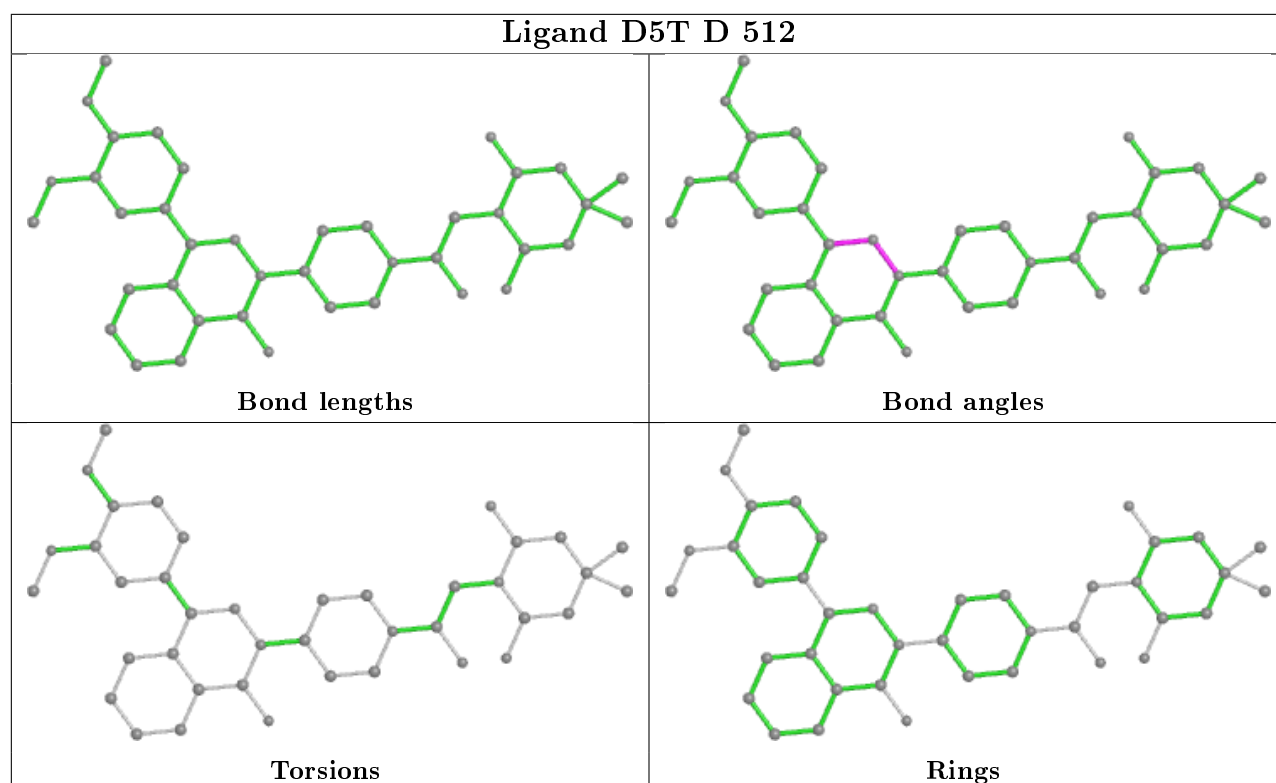
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	506	EDO	1	0
4	C	508	EDO	1	0
7	B	510	EPE	1	0
5	D	511	PEG	4	0
4	B	505	EDO	6	0
4	D	520	EDO	3	0
5	D	509	PEG	2	0
4	D	506	EDO	2	0
4	C	518	EDO	2	0
4	A	525	EDO	1	0
8	D	518	PG4	2	0

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	330/364 (90%)	0.02	7 (2%) 63 66	16, 27, 58, 106	0
1	B	323/364 (88%)	0.03	0 100 100	17, 33, 53, 81	0
1	C	326/364 (89%)	0.11	12 (3%) 41 44	18, 31, 62, 99	0
1	D	324/364 (89%)	-0.04	1 (0%) 94 94	14, 23, 43, 73	0
All	All	1303/1456 (89%)	0.03	20 (1%) 73 76	14, 29, 54, 106	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	SER	6.4
1	A	294	SER	5.2
1	C	294	SER	5.0
1	A	375	TYR	4.1
1	A	82	PHE	3.9
1	C	295	SER	3.8
1	C	293	THR	3.6
1	A	411	PRO	3.3
1	C	87	GLU	3.3
1	C	375	TYR	3.2
1	C	296	GLY	3.0
1	D	362	ASN	2.9
1	C	299	LEU	2.9
1	C	292	VAL	2.8
1	C	297	VAL	2.8
1	C	86	THR	2.5
1	C	298	LEU	2.5
1	C	301	ASP	2.4
1	A	296	GLY	2.2
1	A	353	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
8	PG4	D	518	13/13	0.68	0.30	39,46,67,71	0
4	EDO	A	512	4/4	0.70	0.23	54,57,60,63	0
4	EDO	A	518	4/4	0.70	0.25	51,55,58,62	0
5	PEG	D	509	7/7	0.74	0.19	36,45,54,56	0
4	EDO	C	511	4/4	0.75	0.20	52,56,59,59	0
4	EDO	A	511	4/4	0.76	0.26	69,74,75,80	0
4	EDO	A	525	4/4	0.76	0.23	50,50,54,57	0
4	EDO	A	523	4/4	0.76	0.15	53,54,58,59	0
4	EDO	B	514	4/4	0.79	0.23	45,57,59,59	0
4	EDO	D	506	4/4	0.79	0.21	46,48,49,60	0
4	EDO	C	517	4/4	0.80	0.29	50,52,58,61	0
4	EDO	B	516	4/4	0.80	0.52	20,20,20,20	0
4	EDO	C	501	4/4	0.81	0.18	43,49,51,52	0
4	EDO	A	524	4/4	0.81	0.18	42,46,49,52	0
4	EDO	C	516	4/4	0.81	0.34	36,56,58,70	0
4	EDO	A	517	4/4	0.81	0.18	53,55,59,64	0
5	PEG	D	510	7/7	0.81	0.30	48,61,66,69	0
4	EDO	D	520	4/4	0.83	0.47	20,20,20,20	0
4	EDO	A	522	4/4	0.84	0.22	38,44,46,49	0
4	EDO	C	502	4/4	0.84	0.19	54,55,59,66	0
4	EDO	B	506	4/4	0.84	0.27	49,51,53,56	0
6	D5T	A	514	40/40	0.85	0.18	21,26,67,71	0
4	EDO	D	519	4/4	0.85	0.45	20,20,20,20	0
4	EDO	D	501	4/4	0.86	0.26	43,62,63,64	0
4	EDO	C	514	4/4	0.87	0.17	43,44,53,59	0
5	PEG	A	513	7/7	0.87	0.22	33,56,62,62	0
4	EDO	C	509	4/4	0.87	0.14	53,53,56,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	C	518	4/4	0.87	0.28	50,52,56,61	0
4	EDO	B	507	4/4	0.88	0.14	51,52,53,55	0
5	PEG	D	511	7/7	0.88	0.21	27,40,52,54	0
7	EPE	B	510	15/15	0.88	0.18	50,74,86,87	0
4	EDO	A	506	4/4	0.88	0.29	47,52,57,68	0
4	EDO	A	520	4/4	0.89	0.14	40,45,51,53	0
4	EDO	C	510	4/4	0.89	0.16	44,46,49,52	0
4	EDO	A	505	4/4	0.89	0.12	51,52,54,55	0
4	EDO	A	509	4/4	0.90	0.19	43,55,56,62	0
4	EDO	C	515	4/4	0.90	0.24	53,55,57,59	0
6	D5T	D	512	40/40	0.90	0.14	20,25,66,71	0
4	EDO	B	511	4/4	0.90	0.16	41,42,47,47	0
4	EDO	A	516	4/4	0.90	0.17	39,44,46,57	0
4	EDO	B	505	4/4	0.90	0.39	40,46,50,54	0
4	EDO	A	515	4/4	0.91	0.15	35,38,39,47	0
4	EDO	B	515	4/4	0.91	0.17	27,37,48,57	0
4	EDO	D	508	4/4	0.91	0.17	35,40,44,50	0
4	EDO	C	503	4/4	0.91	0.13	45,46,49,49	0
4	EDO	C	508	4/4	0.91	0.14	56,56,57,58	0
4	EDO	A	507	4/4	0.92	0.14	32,40,44,55	0
4	EDO	A	519	4/4	0.92	0.14	30,33,36,40	0
5	PEG	B	509	7/7	0.92	0.29	42,53,57,58	0
4	EDO	C	506	4/4	0.92	0.18	39,43,53,57	0
4	EDO	A	508	4/4	0.93	0.09	32,42,43,44	0
4	EDO	D	517	4/4	0.93	0.15	52,56,57,59	0
4	EDO	B	508	4/4	0.93	0.17	42,44,45,46	0
4	EDO	A	510	4/4	0.93	0.20	60,61,64,67	0
4	EDO	D	505	4/4	0.93	0.11	24,25,26,28	0
7	EPE	C	512	15/15	0.94	0.19	28,63,79,82	0
4	EDO	B	513	4/4	0.94	0.22	46,48,48,57	0
6	D5T	C	513	40/40	0.94	0.12	22,27,65,68	0
4	EDO	D	516	4/4	0.95	0.15	32,33,34,37	0
4	EDO	D	502	4/4	0.95	0.09	32,32,34,35	0
4	EDO	A	504	4/4	0.95	0.11	29,36,37,41	0
4	EDO	A	521	4/4	0.95	0.10	27,31,31,32	0
4	EDO	C	507	4/4	0.95	0.12	30,31,31,37	0
6	D5T	B	512	40/40	0.95	0.11	20,23,63,67	0
4	EDO	D	514	4/4	0.95	0.10	27,27,29,30	0
4	EDO	D	515	4/4	0.96	0.13	28,31,32,33	0
4	EDO	B	504	4/4	0.96	0.18	37,46,47,55	0
4	EDO	D	513	4/4	0.96	0.11	31,35,36,37	0
4	EDO	B	503	4/4	0.97	0.10	22,24,28,31	0

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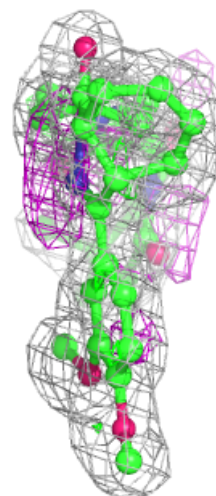
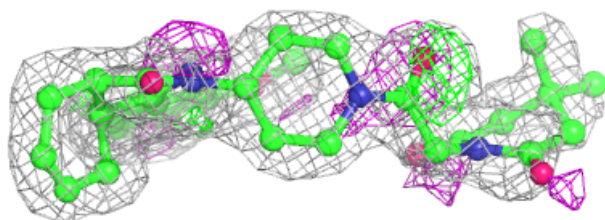
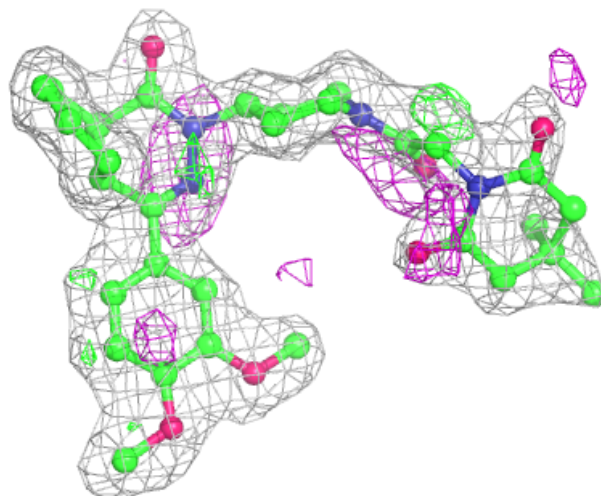
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	A	503	4/4	0.97	0.11	32,33,34,34	0
4	EDO	D	507	4/4	0.97	0.10	27,28,29,32	0
3	MG	D	504	1/1	0.97	0.13	15,15,15,15	0
3	MG	C	505	1/1	0.99	0.10	20,20,20,20	0
3	MG	B	502	1/1	0.99	0.12	20,20,20,20	0
2	ZN	D	503	1/1	0.99	0.09	21,21,21,21	0
2	ZN	B	501	1/1	0.99	0.08	26,26,26,26	0
2	ZN	A	501	1/1	1.00	0.08	23,23,23,23	0
3	MG	A	502	1/1	1.00	0.10	17,17,17,17	0
2	ZN	C	504	1/1	1.00	0.09	26,26,26,26	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.

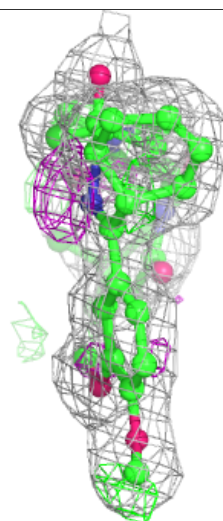
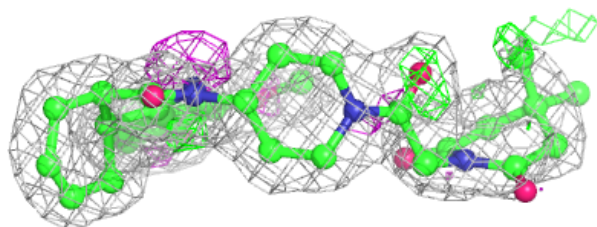
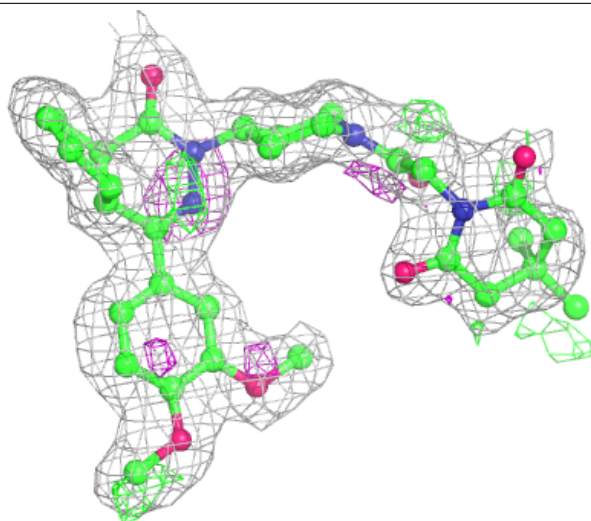
Electron density around D5T A 514:

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



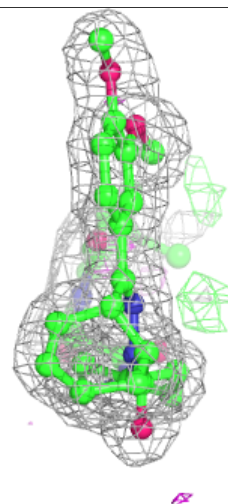
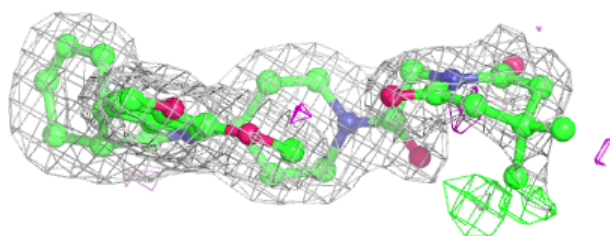
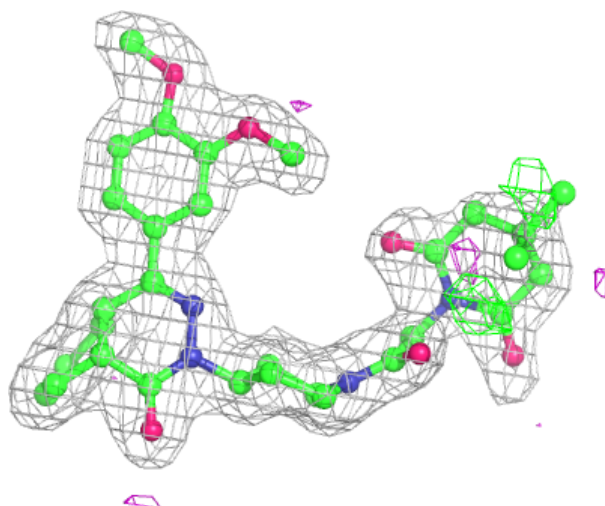
Electron density around D5T D 512:

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



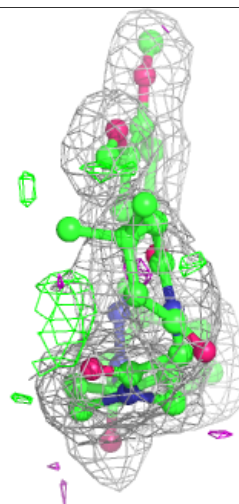
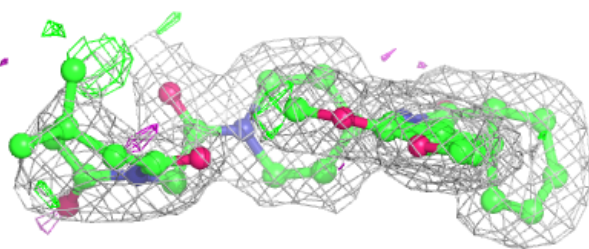
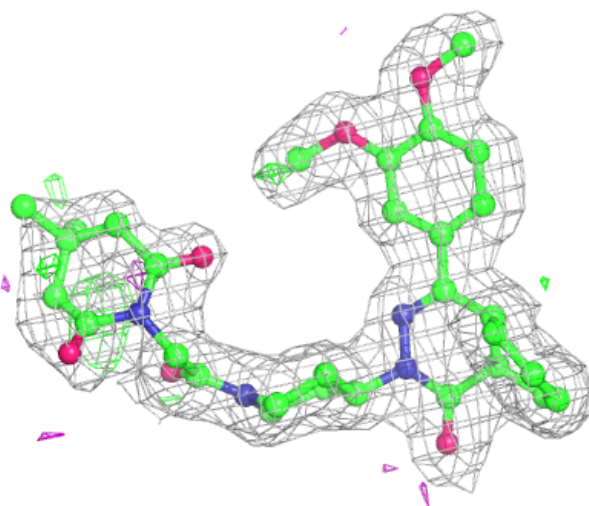
Electron density around D5T C 513:

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



Electron density around D5T B 512:

$2mF_o-DF_c$ (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.