



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:29 PM UTC

PDB ID : 6FT0 / pdb_00006ft0
Title : Crystal structure of human phosphodiesterase 4D2 catalytic domain with inhibitor NPD-425
Authors : Singh, A.K.; Brown, D.G.
Deposited on : 2018-02-20
Resolution : 2.10 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

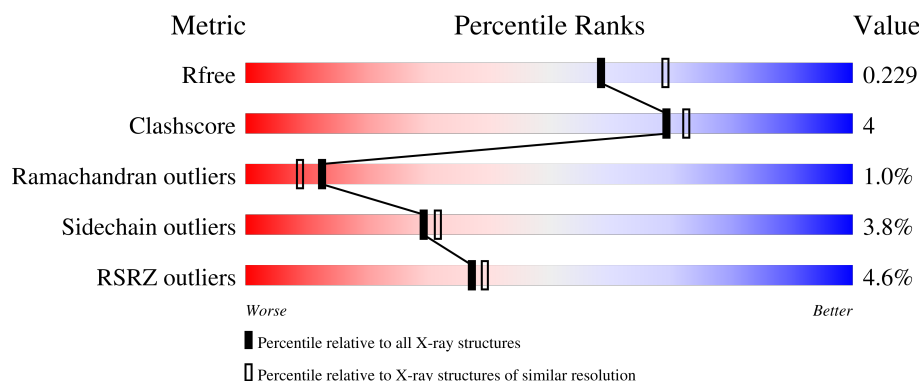
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

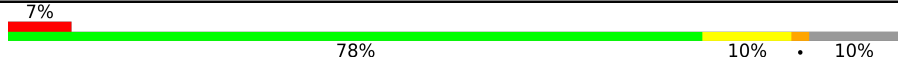
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	364	
1	B	364	
1	C	364	
1	D	364	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	E6E	B	509	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11547 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2658	1681	454	509	14			
1	B	324	Total	C	N	O	S	0	0	0
			2622	1659	448	501	14			
1	C	324	Total	C	N	O	S	0	0	0
			2622	1659	448	501	14			
1	D	324	Total	C	N	O	S	0	0	0
			2622	1659	448	501	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

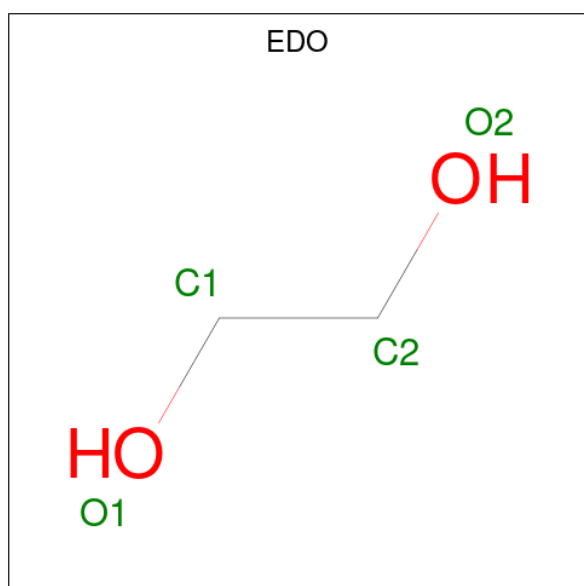
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: 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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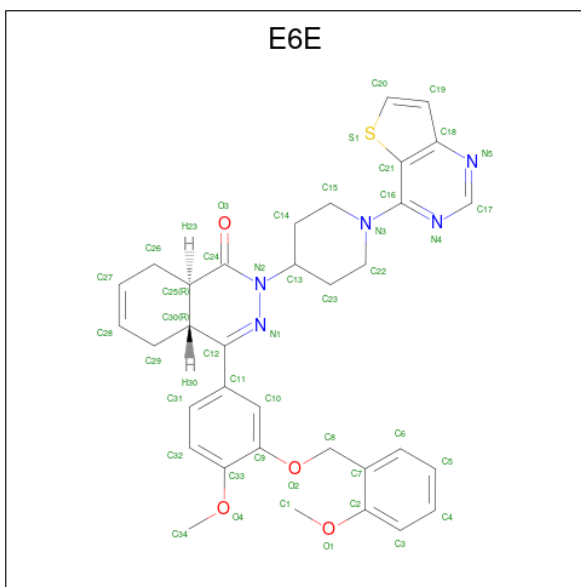
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

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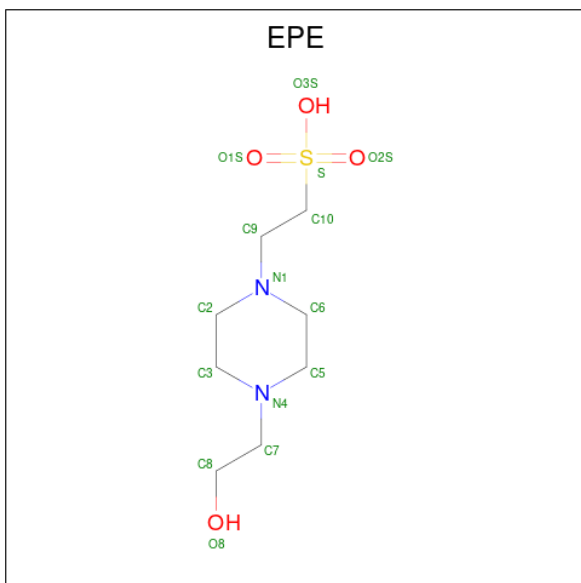
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total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

- Molecule 5 is 4-{4-methoxy-3-[(2-methoxyphenyl)methoxy]phenyl}-2-(1-{thieno[3,2-d]pyrimidin-4-yl}piperidin-4-yl)-1,2,4a,5,8,8a-hexahydrophthalazin-1-one (CCD ID: E6E) (formula: C₃₄H₃₅N₅O₄S) (labeled as "Ligand of Interest" by depositor).



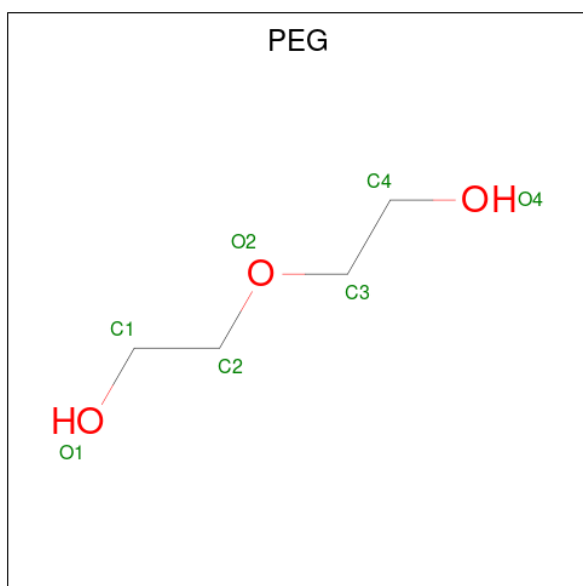
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			44	34	5	4	1		
5	B	1	Total	C	N	O	S	0	0
			44	34	5	4	1		
5	C	1	Total	C	N	O	S	0	0
			44	34	5	4	1		
5	D	1	Total	C	N	O	S	0	0
			44	34	5	4	1		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	151	Total	O	0	0
			151	151		
8	B	133	Total	O	0	0
			133	133		

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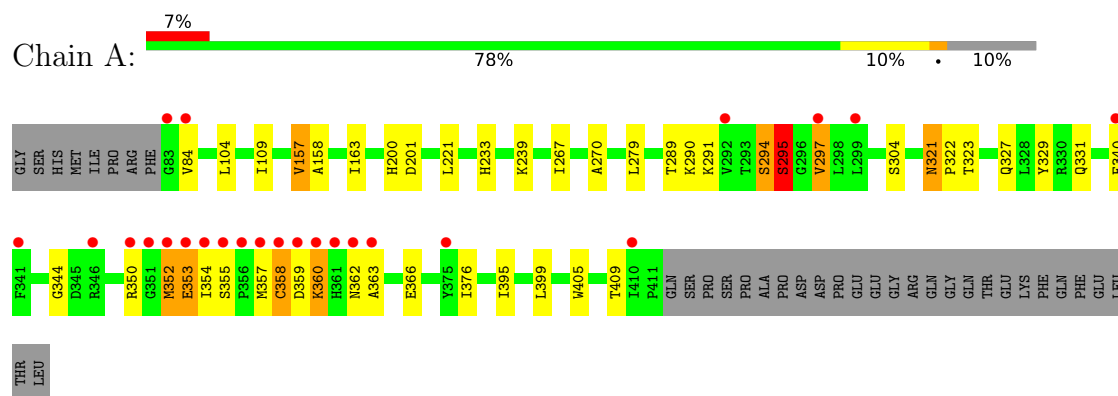
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	108	Total 108	O 108	0	0
8	D	183	Total 183	O 183	0	0

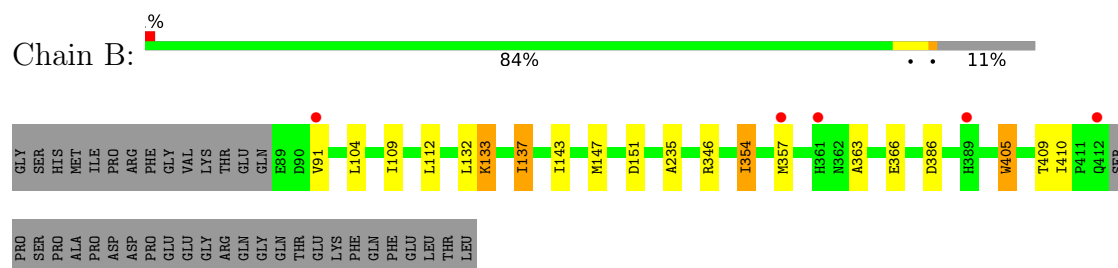
3 Residue-property plots [i](#)

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.

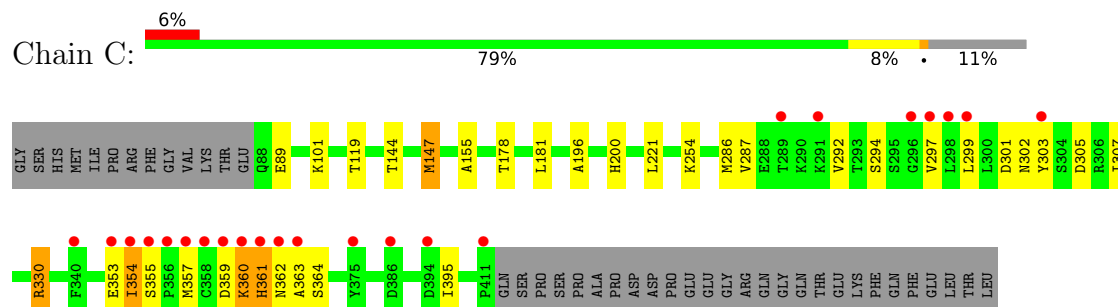
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



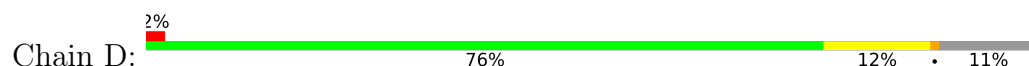
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

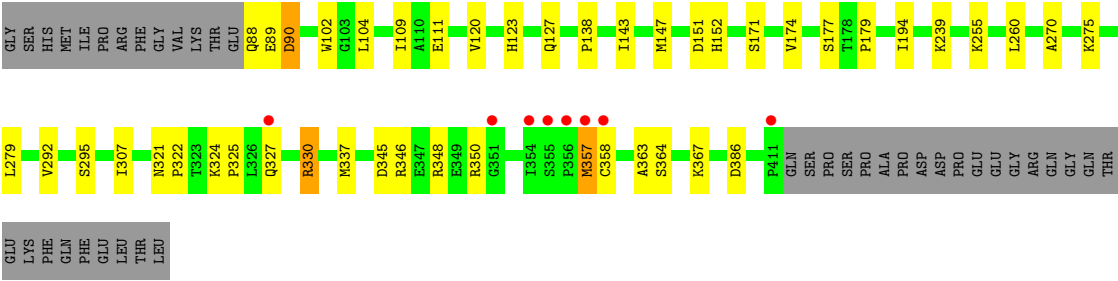


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.94Å 110.81Å 160.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.28 – 2.10 91.28 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (91.28-2.10) 100.0 (91.28-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.171 , 0.222 0.184 , 0.229	Depositor DCC
R_{free} test set	5318 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11547	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, EDO, MG, EPE, ZN, E6E

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	1.30	5/2712 (0.2%)	1.13	12/3684 (0.3%)
1	B	1.23	3/2676 (0.1%)	1.13	1/3636 (0.0%)
1	C	1.23	1/2676 (0.0%)	1.11	2/3636 (0.1%)
1	D	1.36	10/2676 (0.4%)	1.10	2/3636 (0.1%)
All	All	1.28	19/10740 (0.2%)	1.12	17/14592 (0.1%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	HIS	C-O	-7.04	1.15	1.24
1	D	151	ASP	C-O	-6.97	1.15	1.24
1	D	337	MET	C-O	-6.07	1.16	1.24
1	D	194	ILE	C-O	-6.06	1.17	1.24
1	D	138	PRO	C-O	-5.71	1.17	1.23
1	C	155	ALA	C-O	-5.69	1.17	1.24
1	A	157	VAL	C-O	-5.55	1.18	1.24
1	D	171	SER	C-O	5.49	1.30	1.24
1	B	137	ILE	CA-C	-5.41	1.48	1.53
1	A	344	GLY	N-CA	5.41	1.53	1.45
1	D	307	ILE	C-O	-5.34	1.17	1.24
1	A	163	ILE	C-O	-5.30	1.17	1.24
1	D	255	LYS	C-O	-5.16	1.18	1.24
1	B	405	TRP	C-O	5.14	1.30	1.24
1	D	120	VAL	C-O	-5.14	1.18	1.24
1	B	235	ALA	C-O	-5.11	1.18	1.24
1	D	177	SER	C-O	-5.11	1.17	1.24
1	A	321	ASN	C-O	-5.08	1.19	1.24
1	D	330	ARG	C-O	-5.05	1.18	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	HIS	N-CA-C	7.85	122.54	112.34
1	C	354	ILE	N-CA-C	7.57	118.50	106.32
1	C	301	ASP	N-CA-C	7.38	121.11	107.60
1	A	158	ALA	N-CA-C	6.91	118.89	111.36
1	A	295	SER	CB-CA-C	-6.79	96.91	110.42
1	A	290	LYS	N-CA-C	6.74	120.01	109.96
1	A	294	SER	CA-C-N	6.47	133.90	121.54
1	A	294	SER	C-N-CA	6.47	133.90	121.54
1	A	355	SER	CA-C-N	5.88	127.19	119.84
1	A	355	SER	C-N-CA	5.88	127.19	119.84
1	D	102	TRP	N-CA-C	-5.61	101.54	109.96
1	A	360	LYS	N-CA-C	-5.56	106.35	113.02
1	B	410	ILE	CB-CA-C	-5.54	104.78	110.71
1	D	363	ALA	N-CA-C	5.46	117.70	109.41
1	A	399	LEU	N-CA-C	-5.46	105.23	111.07
1	A	267	ILE	N-CA-C	5.20	115.41	110.42
1	A	376	ILE	CB-CA-C	-5.09	102.94	111.29

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	2658	0	2616	25	0
1	B	2622	0	2578	11	0
1	C	2622	0	2578	15	0
1	D	2622	0	2578	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	36	0	54	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	32	0	48	0	0
4	C	44	0	66	2	0
4	D	56	0	84	1	0
5	A	44	0	0	5	0
5	B	44	0	0	0	0
5	C	44	0	0	2	0
5	D	44	0	0	0	0
6	A	15	0	18	0	0
6	B	30	0	36	0	0
6	C	15	0	17	0	0
6	D	15	0	18	1	0
7	D	21	0	30	3	0
8	A	151	0	0	1	0
8	B	133	0	0	0	0
8	C	108	0	0	2	0
8	D	183	0	0	3	0
All	All	11547	0	10721	76	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 (76) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LYS:NZ	1:D:239:LYS:NZ	2.40	0.70
1:D:357:MET:N	1:D:357:MET:HE2	2.08	0.68
1:B:357:MET:HG3	1:B:363:ALA:HB1	1.78	0.66
1:C:119:THR:HG21	1:C:147:MET:HE3	1.78	0.65
1:A:239:LYS:NZ	1:D:239:LYS:HZ3	1.97	0.62
1:D:127:GLN:NE2	8:D:601:HOH:O	2.29	0.62
1:D:104:LEU:HD11	1:D:109:ILE:CD1	2.31	0.61
1:C:330:ARG:CG	1:C:330:ARG:HH11	2.13	0.61
1:C:286:MET:HE1	1:C:305:ASP:OD1	2.02	0.60
1:A:239:LYS:HZ3	1:D:239:LYS:NZ	2.03	0.56
1:A:289:THR:HG22	1:A:289:THR:O	2.03	0.56
1:D:346:ARG:NH2	8:D:602:HOH:O	2.38	0.56
5:A:509:E6E:C15	5:A:509:E6E:S1	2.93	0.56
1:D:174:VAL:HG12	7:D:512:PEG:H41	1.88	0.55
1:D:127:GLN:NE2	8:D:603:HOH:O	2.38	0.55
1:A:104:LEU:HD11	1:A:109:ILE:CD1	2.36	0.55
1:A:350:ARG:HG2	1:C:144:THR:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LEU:HD11	1:A:109:ILE:HD11	1.90	0.54
1:D:270:ALA:HB1	1:D:279:LEU:HD11	1.89	0.54
1:A:350:ARG:HD3	8:C:632:HOH:O	2.08	0.53
5:C:510:E6E:C15	5:C:510:E6E:S1	2.96	0.53
1:A:405:TRP:O	1:A:409:THR:HG23	2.07	0.53
5:A:509:E6E:C21	5:A:509:E6E:C1	2.85	0.53
1:D:88:GLN:HG3	1:D:90:ASP:HB2	1.89	0.52
1:B:143:ILE:HG22	1:B:147:MET:HE2	1.91	0.52
1:B:366:GLU:HG2	1:B:409:THR:OG1	2.10	0.52
1:D:104:LEU:HD11	1:D:109:ILE:HD11	1.93	0.51
1:A:239:LYS:NZ	1:D:239:LYS:HZ1	2.07	0.51
1:C:178:THR:CG2	1:C:181:LEU:HD12	2.41	0.51
1:C:330:ARG:CG	1:C:330:ARG:NH1	2.72	0.51
1:A:239:LYS:HZ1	1:D:239:LYS:NZ	2.06	0.51
1:B:104:LEU:HD11	1:B:109:ILE:HD11	1.94	0.50
1:A:340:PHE:HB3	1:A:358:CYS:SG	2.51	0.50
5:A:509:E6E:C1	5:A:509:E6E:C18	2.90	0.50
1:C:330:ARG:HH11	1:C:330:ARG:HG3	1.78	0.49
1:D:88:GLN:HG3	1:D:90:ASP:H	1.78	0.49
1:B:91:VAL:HG13	1:B:112:LEU:HD22	1.95	0.49
1:A:323:THR:HB	1:A:395:ILE:HG23	1.95	0.48
1:A:327:GLN:O	1:A:331:GLN:HG3	2.14	0.48
1:B:132:LEU:HD23	1:B:137:ILE:O	2.14	0.47
1:C:178:THR:HG21	1:C:181:LEU:HD12	1.96	0.46
1:D:357:MET:HE3	1:D:357:MET:HB2	1.72	0.46
1:B:133:LYS:HE3	1:B:133:LYS:HB2	1.44	0.46
1:D:143:ILE:HG22	1:D:147:MET:HE2	1.97	0.46
1:A:340:PHE:CD2	5:A:509:E6E:C5	2.98	0.46
1:C:303:TYR:CD2	1:C:303:TYR:C	2.93	0.46
1:A:321:ASN:HB2	1:A:322:PRO:HD3	1.99	0.45
1:B:405:TRP:O	1:B:409:THR:HG23	2.17	0.45
1:C:357:MET:HG3	5:C:510:E6E:N5	2.31	0.45
1:C:307:ILE:HD12	1:C:307:ILE:HA	1.90	0.45
4:A:504:EDO:H21	8:A:609:HOH:O	2.16	0.44
1:A:295:SER:HB3	1:A:297:VAL:HG13	1.99	0.44
7:D:513:PEG:H21	7:D:513:PEG:O4	2.18	0.44
1:D:345:ASP:OD1	1:D:348:ARG:NH2	2.49	0.44
1:A:350:ARG:HB3	8:C:634:HOH:O	2.17	0.44
1:A:340:PHE:HD2	5:A:509:E6E:C5	2.30	0.43
1:A:366:GLU:HG2	1:A:409:THR:OG1	2.18	0.43
1:C:286:MET:CE	1:C:305:ASP:OD1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:HIS:HE1	4:D:501:EDO:H22	1.83	0.43
1:D:123:HIS:ND1	7:D:518:PEG:H42	2.33	0.43
1:A:270:ALA:HB1	1:A:279:LEU:HD11	2.00	0.43
1:D:357:MET:HE2	1:D:357:MET:CA	2.48	0.43
1:A:201:ASP:HA	1:A:233:HIS:CD2	2.55	0.42
1:B:354:ILE:N	1:B:354:ILE:HD12	2.35	0.42
1:A:84:VAL:O	1:A:84:VAL:HG23	2.16	0.41
1:C:395:ILE:HD12	4:C:507:EDO:C1	2.50	0.41
1:D:330:ARG:HH11	1:D:330:ARG:HD3	1.70	0.41
1:B:151:ASP:OD2	1:D:350:ARG:NH2	2.41	0.41
1:C:395:ILE:HD12	4:C:507:EDO:H12	2.02	0.41
1:D:321:ASN:HB2	1:D:322:PRO:HD3	2.02	0.41
1:C:196:ALA:O	1:C:200:HIS:HB3	2.20	0.41
1:A:239:LYS:HZ3	1:D:239:LYS:HZ1	1.64	0.40
1:D:111:GLU:OE2	6:D:520:EPE:H32	2.21	0.40
1:D:324:LYS:HB3	1:D:325:PRO:HD2	2.03	0.40
1:A:329:TYR:CD1	1:A:329:TYR:C	2.98	0.40
1:B:104:LEU:HD11	1:B:109:ILE:CD1	2.51	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	327/364 (90%)	309 (94%)	13 (4%)	5 (2%)	8	4
1	B	322/364 (88%)	314 (98%)	8 (2%)	0	100	100
1	C	322/364 (88%)	302 (94%)	12 (4%)	8 (2%)	4	1
1	D	322/364 (88%)	314 (98%)	8 (2%)	0	100	100
All	All	1293/1456 (89%)	1239 (96%)	41 (3%)	13 (1%)	12	9

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	SER
1	A	352	MET
1	A	362	ASN
1	A	363	ALA
1	C	355	SER
1	C	361	HIS
1	C	362	ASN
1	C	302	ASN
1	C	360	LYS
1	C	363	ALA
1	A	353	GLU
1	C	364	SER
1	C	292	VAL

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	300/331 (91%)	287 (96%)	13 (4%)	26	27
1	B	296/331 (89%)	292 (99%)	4 (1%)	59	67
1	C	296/331 (89%)	281 (95%)	15 (5%)	21	21
1	D	296/331 (89%)	283 (96%)	13 (4%)	25	26
All	All	1188/1324 (90%)	1143 (96%)	45 (4%)	29	32

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	VAL
1	A	221	LEU
1	A	291	LYS
1	A	294	SER
1	A	297	VAL
1	A	304	SER
1	A	352	MET
1	A	353	GLU
1	A	354	ILE

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Mol	Chain	Res	Type
1	A	357	MET
1	A	358	CYS
1	A	359	ASP
1	A	360	LYS
1	B	133	LYS
1	B	346	ARG
1	B	354	ILE
1	B	386	ASP
1	C	89	GLU
1	C	101	LYS
1	C	147	MET
1	C	221	LEU
1	C	254	LYS
1	C	287	VAL
1	C	294	SER
1	C	297	VAL
1	C	299	LEU
1	C	330	ARG
1	C	353	GLU
1	C	354	ILE
1	C	359	ASP
1	C	360	LYS
1	C	361	HIS
1	D	89	GLU
1	D	90	ASP
1	D	179	PRO
1	D	260	LEU
1	D	275	LYS
1	D	292	VAL
1	D	295	SER
1	D	327	GLN
1	D	357	MET
1	D	358	CYS
1	D	364	SER
1	D	367	LYS
1	D	386	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	250	GLN

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Mol	Chain	Res	Type
1	A	278	ASN
1	A	312	ASN
1	A	407	GLN
1	B	210	GLN
1	B	242	GLN
1	B	308	GLN
1	B	312	ASN
1	B	321	ASN
1	B	362	ASN
1	B	407	GLN
1	C	210	GLN
1	C	250	GLN
1	C	302	ASN
1	C	312	ASN
1	C	331	GLN
1	D	210	GLN
1	D	258	GLN
1	D	321	ASN
1	D	369	GLN
1	D	389	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 62 ligands modelled in this entry, 8 are monoatomic - leaving 54 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	513	-	3,3,3	0.39	0	2,2,2	0.59	0
5	E6E	B	509	-	48,50,50	1.14	1 (2%)	56,71,71	1.46	9 (16%)
4	EDO	A	511	-	3,3,3	0.18	0	2,2,2	1.21	0
4	EDO	C	505	-	3,3,3	0.66	0	2,2,2	0.27	0
4	EDO	C	501	-	3,3,3	0.35	0	2,2,2	0.81	0
4	EDO	D	519	-	3,3,3	0.51	0	2,2,2	0.40	0
4	EDO	D	521	-	3,3,3	0.20	0	2,2,2	1.17	0
6	EPE	A	510	-	15,15,15	1.86	1 (6%)	19,20,20	1.98	3 (15%)
4	EDO	A	505	-	3,3,3	0.35	0	2,2,2	0.31	0
4	EDO	B	503	-	3,3,3	0.39	0	2,2,2	0.20	0
4	EDO	A	506	-	3,3,3	0.42	0	2,2,2	0.41	0
6	EPE	C	508	-	15,15,15	1.81	1 (6%)	19,20,20	3.64	6 (31%)
4	EDO	C	514	-	3,3,3	0.35	0	2,2,2	0.87	0
4	EDO	D	506	-	3,3,3	0.36	0	2,2,2	0.74	0
4	EDO	B	510	-	3,3,3	0.38	0	2,2,2	0.51	0
6	EPE	B	508	-	15,15,15	1.78	1 (6%)	19,20,20	1.54	2 (10%)
4	EDO	A	508	-	3,3,3	0.80	0	2,2,2	0.31	0
4	EDO	B	505	-	3,3,3	0.22	0	2,2,2	1.30	0
4	EDO	C	512	-	3,3,3	0.49	0	2,2,2	0.52	0
4	EDO	C	507	-	3,3,3	0.50	0	2,2,2	0.34	0
7	PEG	D	518	-	6,6,6	0.91	0	5,5,5	1.11	0
4	EDO	C	504	-	3,3,3	0.48	0	2,2,2	0.29	0
4	EDO	D	510	-	3,3,3	0.36	0	2,2,2	0.59	0
4	EDO	B	512	-	3,3,3	0.45	0	2,2,2	0.38	0
4	EDO	D	516	-	3,3,3	0.78	0	2,2,2	0.55	0
5	E6E	A	509	-	48,50,50	0.88	2 (4%)	56,71,71	1.58	8 (14%)
4	EDO	A	513	-	3,3,3	0.24	0	2,2,2	0.29	0
4	EDO	B	504	-	3,3,3	0.42	0	2,2,2	0.73	0
4	EDO	C	511	-	3,3,3	0.34	0	2,2,2	0.73	0
7	PEG	D	513	-	6,6,6	1.07	0	5,5,5	1.38	1 (20%)
5	E6E	D	517	-	48,50,50	1.07	1 (2%)	56,71,71	1.89	11 (19%)
4	EDO	C	515	-	3,3,3	0.29	0	2,2,2	0.41	0
5	E6E	C	510	-	48,50,50	0.93	3 (6%)	56,71,71	1.53	12 (21%)
6	EPE	B	511	-	15,15,15	1.81	1 (6%)	19,20,20	1.48	2 (10%)
4	EDO	D	514	-	3,3,3	0.61	0	2,2,2	0.14	0
4	EDO	A	503	-	3,3,3	0.33	0	2,2,2	0.72	0
4	EDO	D	511	-	3,3,3	0.29	0	2,2,2	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	C	509	-	3,3,3	0.75	0	2,2,2	0.27	0
4	EDO	C	506	-	3,3,3	0.50	0	2,2,2	0.10	0
4	EDO	D	515	-	3,3,3	0.40	0	2,2,2	0.76	0
4	EDO	B	513	-	3,3,3	0.32	0	2,2,2	0.89	0
4	EDO	D	501	-	3,3,3	0.38	0	2,2,2	0.67	0
4	EDO	D	505	-	3,3,3	0.43	0	2,2,2	0.84	0
4	EDO	A	512	-	3,3,3	0.59	0	2,2,2	0.08	0
7	PEG	D	512	-	6,6,6	0.63	0	5,5,5	1.19	1 (20%)
4	EDO	A	504	-	3,3,3	0.26	0	2,2,2	1.02	0
4	EDO	B	507	-	3,3,3	0.37	0	2,2,2	0.68	0
4	EDO	A	507	-	3,3,3	0.50	0	2,2,2	0.31	0
4	EDO	B	506	-	3,3,3	0.87	0	2,2,2	1.01	0
4	EDO	D	507	-	3,3,3	0.61	0	2,2,2	0.24	0
4	EDO	D	504	-	3,3,3	0.37	0	2,2,2	0.90	0
4	EDO	D	508	-	3,3,3	0.93	0	2,2,2	0.35	0
4	EDO	D	509	-	3,3,3	0.27	0	2,2,2	0.96	0
6	EPE	D	520	-	15,15,15	2.07	1 (6%)	19,20,20	2.56	7 (36%)

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	513	-	-	1/1/1/1	-
5	E6E	B	509	-	1/1/7/9	6/21/58/58	0/7/7/7
4	EDO	A	511	-	-	0/1/1/1	-
4	EDO	C	505	-	-	0/1/1/1	-
4	EDO	C	501	-	-	0/1/1/1	-
4	EDO	D	519	-	-	1/1/1/1	-
4	EDO	D	521	-	-	1/1/1/1	-
6	EPE	A	510	-	-	6/9/19/19	0/1/1/1
4	EDO	A	505	-	-	1/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	A	506	-	-	1/1/1/1	-
6	EPE	C	508	-	-	2/9/19/19	0/1/1/1
4	EDO	C	514	-	-	1/1/1/1	-
4	EDO	D	506	-	-	1/1/1/1	-
4	EDO	B	510	-	-	1/1/1/1	-
6	EPE	B	508	-	-	6/9/19/19	0/1/1/1
4	EDO	A	508	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	505	-	-	0/1/1/1	-
4	EDO	C	512	-	-	1/1/1/1	-
4	EDO	C	507	-	-	1/1/1/1	-
7	PEG	D	518	-	-	3/4/4/4	-
4	EDO	C	504	-	-	1/1/1/1	-
4	EDO	D	510	-	-	1/1/1/1	-
4	EDO	B	512	-	-	1/1/1/1	-
4	EDO	D	516	-	-	1/1/1/1	-
5	E6E	A	509	-	-	1/21/58/58	0/7/7/7
4	EDO	A	513	-	-	1/1/1/1	-
4	EDO	B	504	-	-	1/1/1/1	-
4	EDO	C	511	-	-	1/1/1/1	-
7	PEG	D	513	-	-	2/4/4/4	-
5	E6E	D	517	-	-	3/21/58/58	0/7/7/7
4	EDO	C	515	-	-	1/1/1/1	-
5	E6E	C	510	-	-	4/21/58/58	0/7/7/7
6	EPE	B	511	-	-	6/9/19/19	0/1/1/1
4	EDO	D	514	-	-	0/1/1/1	-
4	EDO	A	503	-	-	1/1/1/1	-
4	EDO	D	511	-	-	0/1/1/1	-
4	EDO	C	509	-	-	1/1/1/1	-
4	EDO	C	506	-	-	1/1/1/1	-
4	EDO	D	515	-	-	1/1/1/1	-
4	EDO	B	513	-	-	0/1/1/1	-
4	EDO	D	501	-	-	1/1/1/1	-
4	EDO	D	505	-	-	0/1/1/1	-
4	EDO	A	512	-	-	1/1/1/1	-
7	PEG	D	512	-	-	3/4/4/4	-
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	B	507	-	-	0/1/1/1	-
4	EDO	A	507	-	-	0/1/1/1	-
4	EDO	B	506	-	-	1/1/1/1	-
4	EDO	D	507	-	-	1/1/1/1	-
4	EDO	D	504	-	-	0/1/1/1	-
4	EDO	D	508	-	-	1/1/1/1	-
4	EDO	D	509	-	-	0/1/1/1	-
6	EPE	D	520	-	-	5/9/19/19	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	520	EPE	C10-S	-7.14	1.67	1.77
5	B	509	E6E	C29-C30	-6.57	1.42	1.53
6	B	511	EPE	C10-S	-6.53	1.68	1.77
6	A	510	EPE	C10-S	-6.44	1.68	1.77
6	C	508	EPE	C10-S	-6.18	1.68	1.77
6	B	508	EPE	C10-S	-6.16	1.69	1.77
5	D	517	E6E	C29-C30	-6.08	1.43	1.53
5	A	509	E6E	C29-C30	-4.01	1.47	1.53
5	C	510	E6E	C29-C30	-3.60	1.47	1.53
5	C	510	E6E	C18-C21	-3.40	1.36	1.40
5	A	509	E6E	C18-C21	-2.63	1.37	1.40
5	C	510	E6E	C23-C22	-2.11	1.46	1.52

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	508	EPE	O1S-S-C10	-10.53	90.82	106.73
6	C	508	EPE	O2S-S-C10	-7.86	94.85	106.73
5	D	517	E6E	C31-C11-C12	6.47	128.48	120.74
6	C	508	EPE	O3S-S-C10	-6.36	93.56	106.00
6	A	510	EPE	O2S-S-C10	6.28	116.21	106.73
5	A	509	E6E	C31-C11-C12	6.20	128.16	120.74
6	D	520	EPE	O2S-S-C10	6.11	115.95	106.73
5	A	509	E6E	C10-C11-C12	-5.81	113.02	120.24
5	D	517	E6E	C10-C11-C12	-5.77	113.07	120.24
6	B	508	EPE	O1S-S-C10	4.91	114.14	106.73
5	D	517	E6E	C26-C25-C30	4.57	118.42	110.59
6	D	520	EPE	O2S-S-O1S	-4.55	99.01	113.82
6	B	511	EPE	O3S-S-C10	4.42	114.65	106.00
5	C	510	E6E	C31-C11-C12	4.32	125.91	120.74
5	D	517	E6E	C11-C12-C30	4.24	128.00	120.10
6	D	520	EPE	C2-C3-N4	4.12	118.97	110.65
5	D	517	E6E	C24-N2-N1	-4.03	120.19	125.13
5	B	509	E6E	C14-C13-N2	3.96	115.23	110.89
5	C	510	E6E	C10-C11-C12	-3.96	115.32	120.24
6	A	510	EPE	C7-N4-C5	3.91	121.65	111.24
5	B	509	E6E	C31-C11-C12	3.70	125.18	120.74
5	C	510	E6E	C23-C13-N2	-3.70	106.85	110.89
5	B	509	E6E	C29-C30-C25	3.69	116.92	110.59
5	D	517	E6E	C17-N4-C16	3.51	120.41	111.83
5	B	509	E6E	C17-N4-C16	3.47	120.31	111.83
5	A	509	E6E	C29-C30-C25	3.43	116.47	110.59
6	D	520	EPE	C3-C2-N1	3.42	117.55	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	517	E6E	C23-C13-N2	3.39	114.60	110.89
6	C	508	EPE	O2S-S-O1S	3.35	124.72	113.82
5	B	509	E6E	C10-C11-C12	-3.30	116.14	120.24
5	C	510	E6E	C29-C30-C25	3.22	116.11	110.59
5	A	509	E6E	C26-C25-C30	3.21	116.10	110.59
6	D	520	EPE	O3S-S-O1S	3.21	119.42	111.40
5	C	510	E6E	C14-C13-N2	3.16	114.35	110.89
6	C	508	EPE	O3S-S-O2S	3.12	119.21	111.40
5	B	509	E6E	C24-N2-N1	-3.08	121.35	125.13
6	D	520	EPE	C5-N4-C3	3.06	115.43	108.84
6	B	511	EPE	O2S-S-O1S	-2.96	104.19	113.82
7	D	513	PEG	O2-C2-C1	2.86	122.72	110.11
5	D	517	E6E	C11-C12-N1	2.84	119.42	115.98
5	D	517	E6E	C14-C13-N2	-2.71	107.93	110.89
5	C	510	E6E	C24-N2-N1	-2.70	121.82	125.13
5	A	509	E6E	C17-N4-C16	2.61	118.22	111.83
5	B	509	E6E	C23-C13-N2	-2.59	108.06	110.89
6	C	508	EPE	C2-C3-N4	2.50	115.69	110.65
5	C	510	E6E	C17-N4-C16	2.48	117.88	111.83
5	B	509	E6E	C15-N3-C16	2.46	127.24	118.92
6	D	520	EPE	C7-N4-C3	2.43	117.70	111.24
5	C	510	E6E	C26-C25-C30	2.34	114.60	110.59
5	C	510	E6E	C30-C29-C28	-2.27	108.31	111.79
5	A	509	E6E	C24-N2-N1	-2.16	122.48	125.13
5	D	517	E6E	C22-N3-C16	2.16	126.24	118.92
5	A	509	E6E	C11-C12-C30	2.16	124.13	120.10
7	D	512	PEG	O2-C2-C1	2.13	119.49	110.11
6	B	508	EPE	O3S-S-C10	2.12	110.15	106.00
5	C	510	E6E	C18-C21-S1	2.11	112.92	110.75
5	C	510	E6E	C12-N1-N2	-2.09	116.78	118.97
6	A	510	EPE	O2S-S-O1S	-2.08	107.05	113.82
5	B	509	E6E	C26-C25-C30	2.06	114.12	110.59
5	A	509	E6E	C30-C29-C28	-2.02	108.69	111.79
5	D	517	E6E	C30-C29-C28	-2.01	108.70	111.79
5	C	510	E6E	C11-C12-C30	2.01	123.84	120.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	509	E6E	C30

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	510	EPE	C9-C10-S-O1S
6	A	510	EPE	C9-C10-S-O3S
6	B	511	EPE	C10-C9-N1-C6
6	B	511	EPE	S-C10-C9-N1
6	B	511	EPE	C9-C10-S-O2S
6	D	520	EPE	C9-C10-S-O2S
6	C	508	EPE	C8-C7-N4-C3
6	D	520	EPE	C8-C7-N4-C3
6	D	520	EPE	N4-C7-C8-O8
6	A	510	EPE	N4-C7-C8-O8
7	D	518	PEG	O2-C3-C4-O4
4	C	511	EDO	O1-C1-C2-O2
6	C	508	EPE	N4-C7-C8-O8
5	D	517	E6E	C3-C2-O1-C1
7	D	512	PEG	C4-C3-O2-C2
6	B	508	EPE	C9-C10-S-O3S
5	D	517	E6E	C7-C2-O1-C1
4	A	512	EDO	O1-C1-C2-O2
4	C	512	EDO	O1-C1-C2-O2
4	C	513	EDO	O1-C1-C2-O2
4	D	508	EDO	O1-C1-C2-O2
4	D	510	EDO	O1-C1-C2-O2
4	D	515	EDO	O1-C1-C2-O2
5	D	517	E6E	C7-C8-O2-C9
6	B	511	EPE	C9-C10-S-O3S
6	D	520	EPE	C9-C10-S-O3S
5	C	510	E6E	C7-C8-O2-C9
5	B	509	E6E	C7-C8-O2-C9
5	A	509	E6E	C7-C8-O2-C9
7	D	512	PEG	O2-C3-C4-O4
7	D	512	PEG	O1-C1-C2-O2
4	A	505	EDO	O1-C1-C2-O2
4	C	507	EDO	O1-C1-C2-O2
4	D	506	EDO	O1-C1-C2-O2
4	D	507	EDO	O1-C1-C2-O2
4	D	519	EDO	O1-C1-C2-O2
6	A	510	EPE	C10-C9-N1-C2
6	B	511	EPE	C10-C9-N1-C2
5	B	509	E6E	C3-C2-O1-C1
4	B	504	EDO	O1-C1-C2-O2
4	B	512	EDO	O1-C1-C2-O2
5	C	510	E6E	C14-C13-N2-C24
6	A	510	EPE	C9-C10-S-O2S

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Mol	Chain	Res	Type	Atoms
6	B	508	EPE	C9-C10-S-O1S
6	B	508	EPE	C9-C10-S-O2S
6	B	511	EPE	C9-C10-S-O1S
7	D	518	PEG	O1-C1-C2-O2
6	D	520	EPE	S-C10-C9-N1
7	D	513	PEG	C1-C2-O2-C3
4	A	503	EDO	O1-C1-C2-O2
5	B	509	E6E	N4-C16-N3-C15
7	D	513	PEG	O1-C1-C2-O2
5	C	510	E6E	C33-C9-O2-C8
6	B	508	EPE	N4-C7-C8-O8
6	A	510	EPE	C10-C9-N1-C6
6	B	508	EPE	C10-C9-N1-C2
5	B	509	E6E	C7-C2-O1-C1
7	D	518	PEG	C1-C2-O2-C3
4	C	504	EDO	O1-C1-C2-O2
4	D	501	EDO	O1-C1-C2-O2
5	B	509	E6E	C33-C9-O2-C8
4	B	510	EDO	O1-C1-C2-O2
4	C	506	EDO	O1-C1-C2-O2
4	C	514	EDO	O1-C1-C2-O2
4	D	521	EDO	O1-C1-C2-O2
4	A	506	EDO	O1-C1-C2-O2
4	A	513	EDO	O1-C1-C2-O2
4	C	509	EDO	O1-C1-C2-O2
4	D	516	EDO	O1-C1-C2-O2
6	B	508	EPE	C10-C9-N1-C6
4	A	504	EDO	O1-C1-C2-O2
4	B	506	EDO	O1-C1-C2-O2
5	C	510	E6E	C10-C9-O2-C8
4	C	515	EDO	O1-C1-C2-O2
5	B	509	E6E	C10-C9-O2-C8

There are no ring outliers.

9 monomers are involved in 15 short contacts:

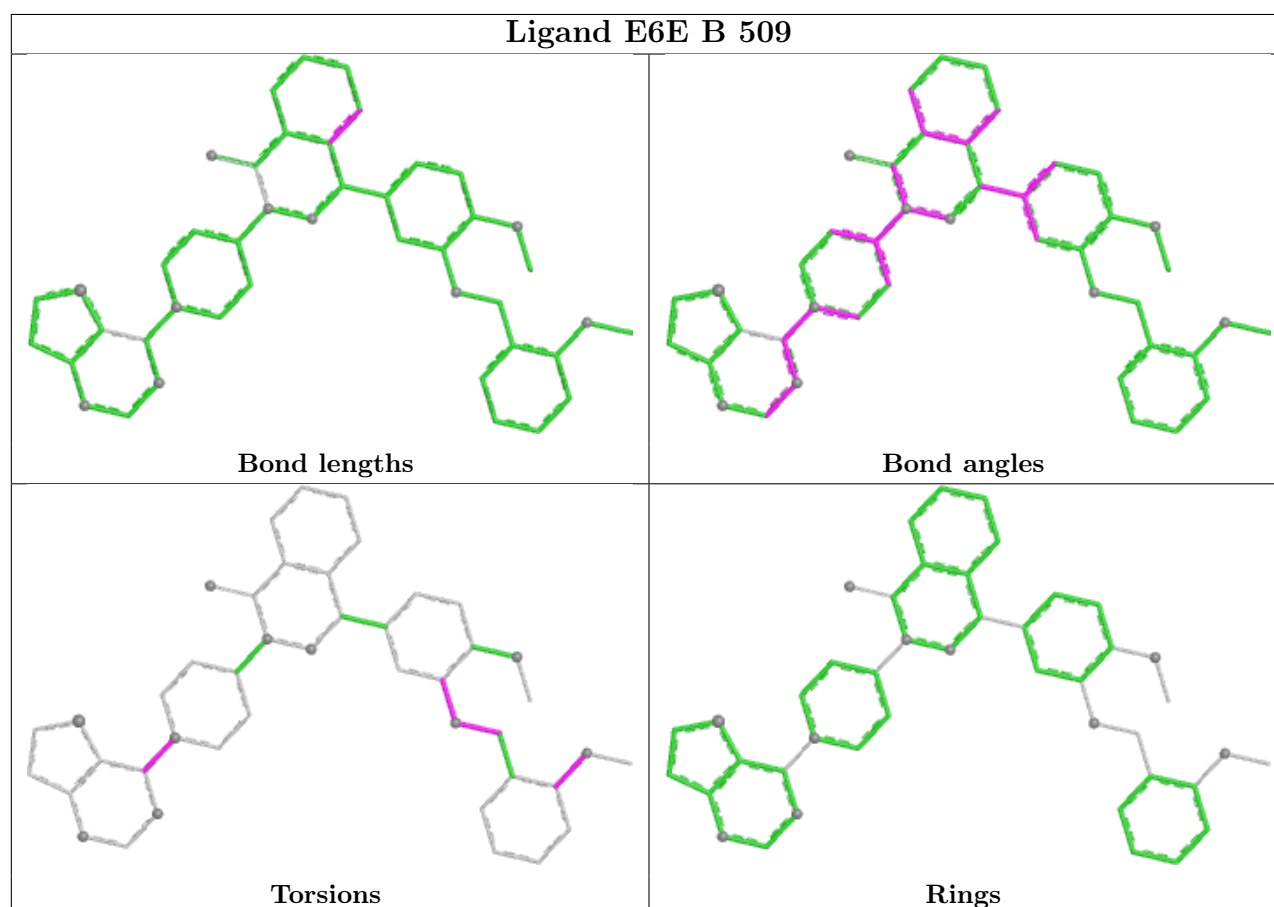
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	507	EDO	2	0
7	D	518	PEG	1	0
5	A	509	E6E	5	0
7	D	513	PEG	1	0
5	C	510	E6E	2	0

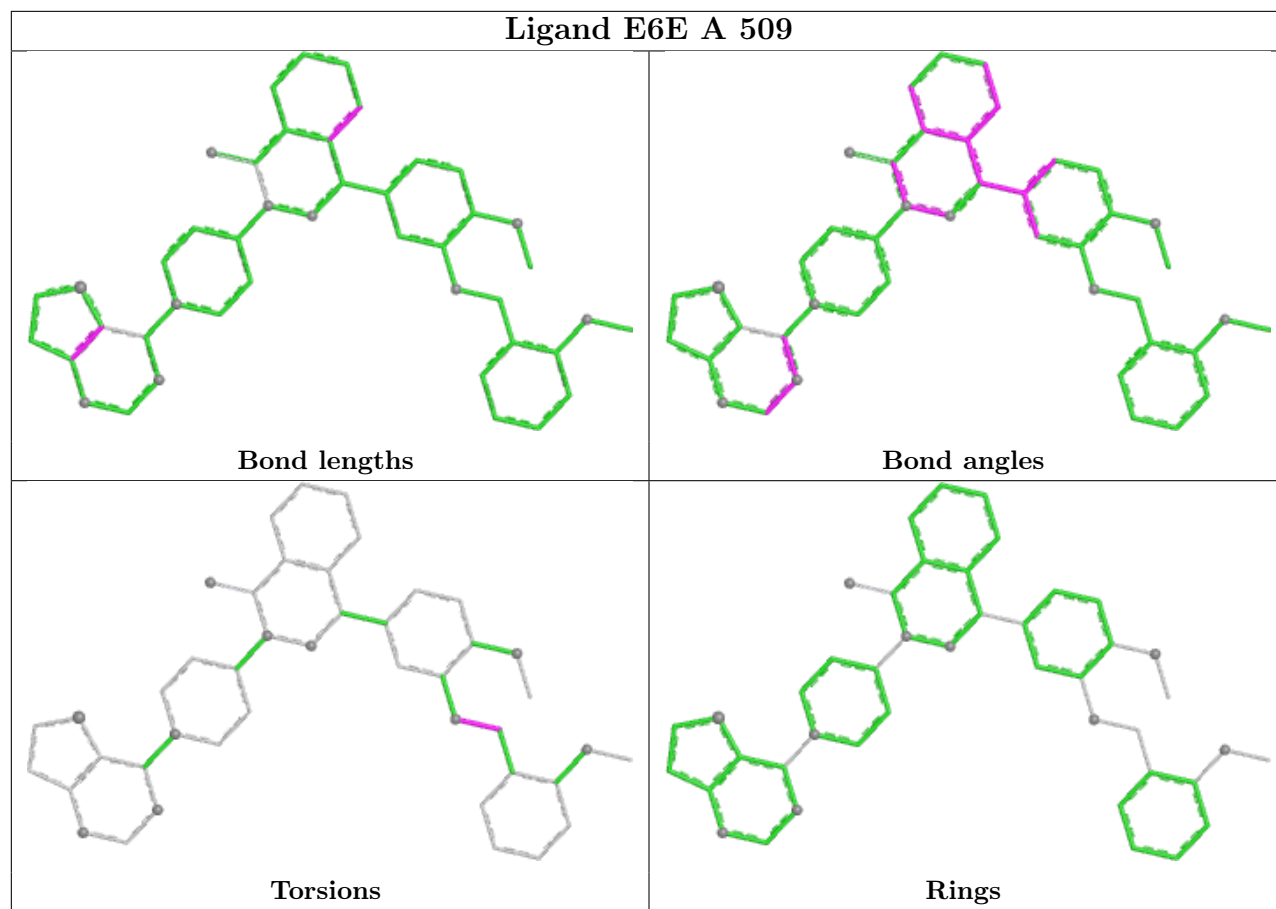
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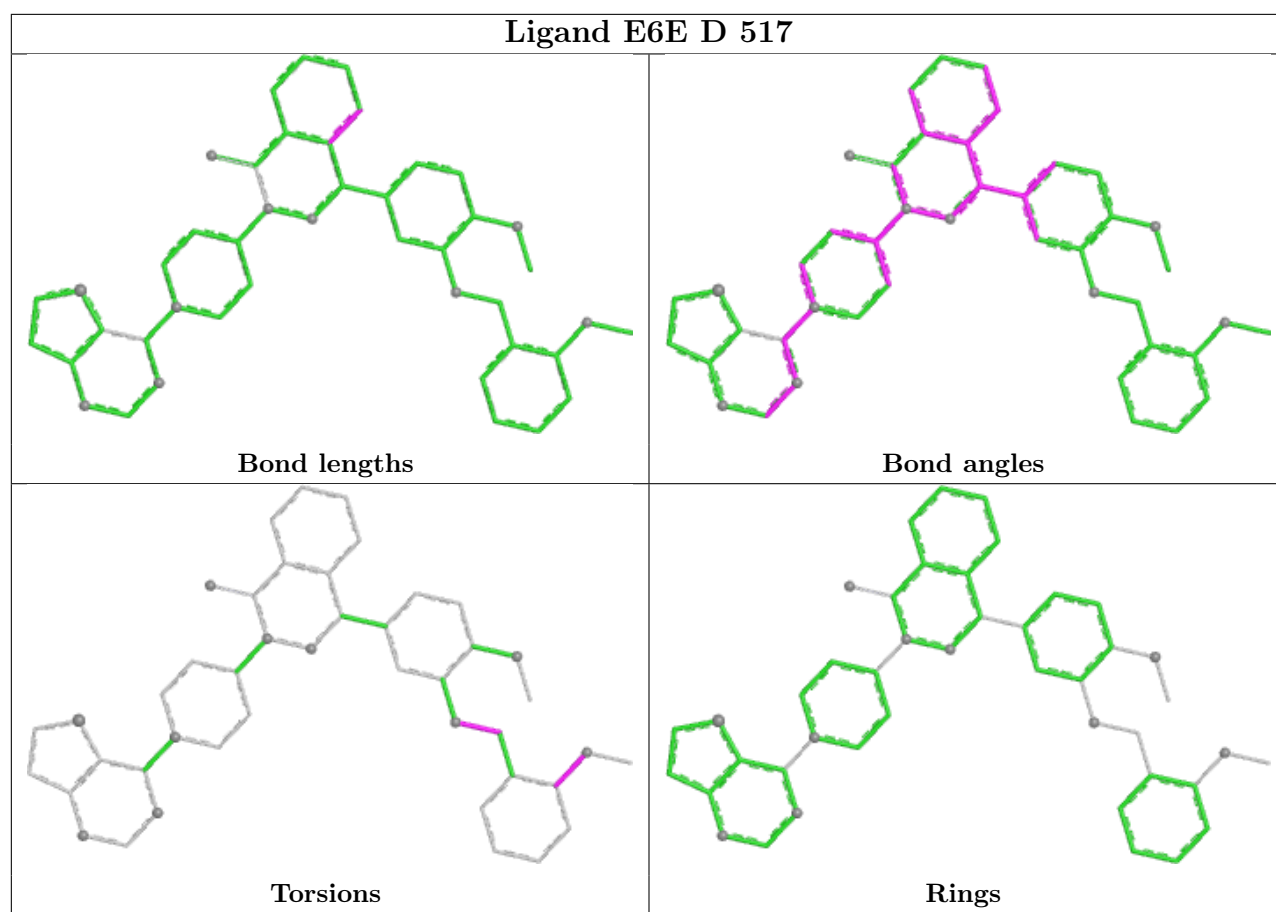
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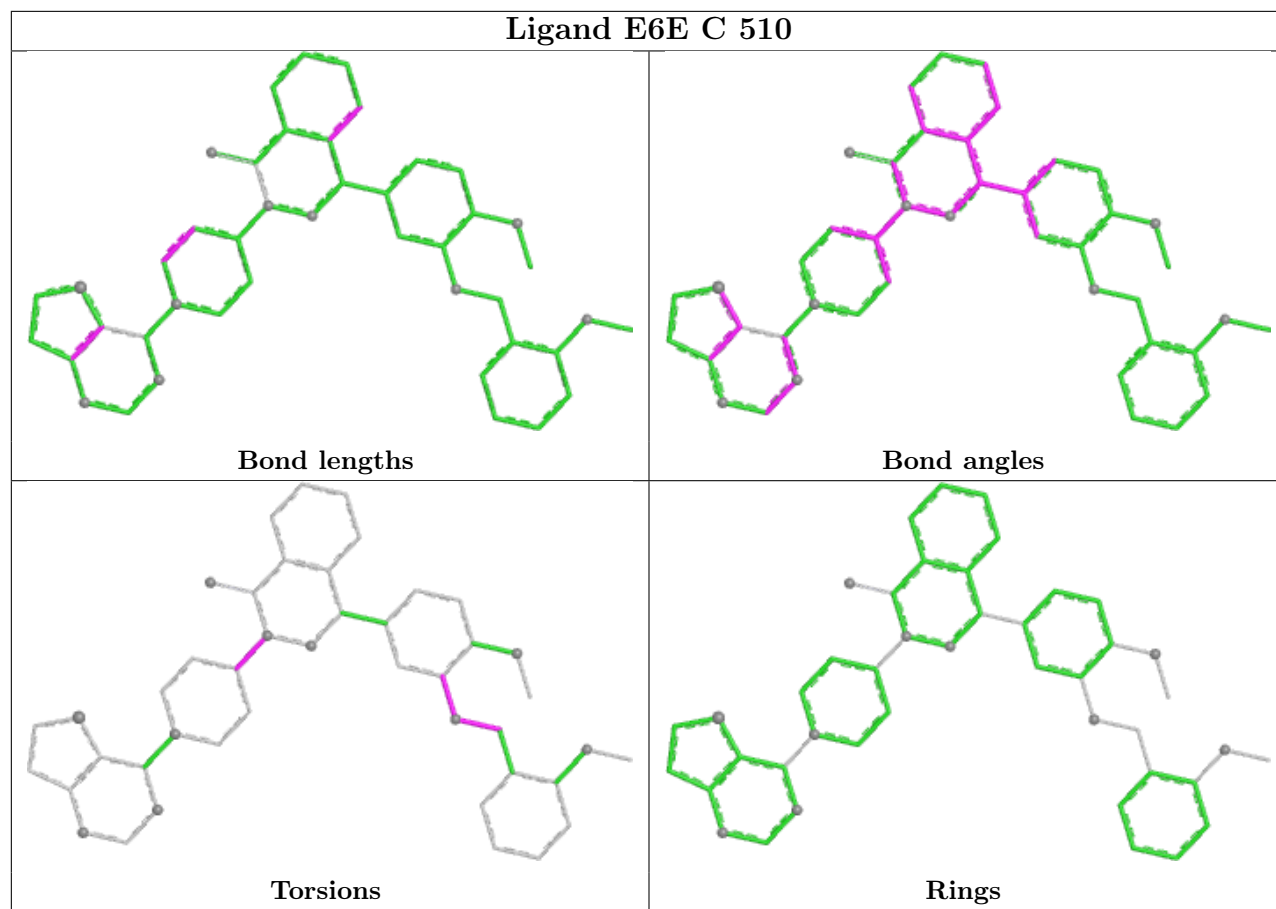
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	501	EDO	1	0
7	D	512	PEG	1	0
4	A	504	EDO	1	0
6	D	520	EPE	1	0

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.









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	329/364 (90%)	0.60	24 (7%) 21 22	25, 41, 77, 115	13 (3%)
1	B	324/364 (89%)	0.25	5 (1%) 72 74	27, 41, 64, 101	0
1	C	324/364 (89%)	0.67	23 (7%) 22 23	14, 41, 78, 106	11 (3%)
1	D	324/364 (89%)	-0.00	8 (2%) 58 61	23, 34, 67, 120	0
All	All	1301/1456 (89%)	0.38	60 (4%) 37 39	14, 40, 72, 120	24 (1%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	360	LYS	22.3
1	A	354	ILE	14.6
1	C	354	ILE	13.3
1	C	358	CYS	13.1
1	A	358	CYS	12.4
1	C	363	ALA	12.3
1	A	357	MET	11.5
1	A	356	PRO	11.5
1	C	356	PRO	10.7
1	C	357	MET	10.3
1	A	359	ASP	9.7
1	A	355	SER	9.2
1	A	360	LYS	9.1
1	A	363	ALA	8.6
1	A	352	MET	8.4
1	A	351	GLY	7.5
1	C	355	SER	7.5
1	C	361	HIS	7.2
1	C	362	ASN	7.2
1	A	361	HIS	7.1
1	C	359	ASP	6.6

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Mol	Chain	Res	Type	RSRZ
1	C	353	GLU	5.7
1	D	357	MET	5.5
1	A	340	PHE	5.0
1	A	353	GLU	4.9
1	B	412	GLN	4.5
1	B	357	MET	4.2
1	A	299	LEU	4.1
1	A	362	ASN	4.0
1	D	354	ILE	4.0
1	A	350	ARG	3.6
1	C	303	TYR	3.6
1	D	356	PRO	3.4
1	D	355	SER	3.2
1	D	351	GLY	3.1
1	C	298	LEU	2.9
1	A	375	TYR	2.9
1	C	375	TYR	2.8
1	A	341	PHE	2.7
1	D	358	CYS	2.6
1	C	297	VAL	2.6
1	B	389	HIS	2.5
1	D	327	GLN	2.5
1	B	91	VAL	2.4
1	A	292	VAL	2.4
1	B	361	HIS	2.4
1	A	410	ILE	2.3
1	C	299	LEU	2.3
1	C	296	GLY	2.3
1	A	346	ARG	2.2
1	C	291	LYS	2.2
1	A	84	VAL	2.2
1	C	340	PHE	2.1
1	A	83	GLY	2.1
1	C	394	ASP	2.1
1	C	289	THR	2.1
1	D	411	PRO	2.1
1	C	386	ASP	2.0
1	C	411	PRO	2.0
1	A	297	VAL	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($\text{\AA}^2$)	Q<0.9
4	EDO	C	512	4/4	0.79	0.15	67,67,69,77	0
4	EDO	B	507	4/4	0.82	0.14	62,68,70,74	0
4	EDO	B	513	4/4	0.83	0.19	63,64,66,68	0
4	EDO	B	506	4/4	0.84	0.17	56,59,62,67	0
4	EDO	C	511	4/4	0.84	0.17	64,70,70,76	0
4	EDO	B	504	4/4	0.84	0.18	63,65,68,69	0
4	EDO	C	514	4/4	0.84	0.18	66,67,69,73	0
4	EDO	D	514	4/4	0.84	0.18	61,64,66,69	0
5	E6E	A	509	44/44	0.84	0.17	46,64,109,115	0
6	EPE	B	508	15/15	0.84	0.19	65,87,96,100	0
4	EDO	D	507	4/4	0.85	0.19	64,70,72,79	0
4	EDO	A	512	4/4	0.85	0.18	72,72,80,83	0
4	EDO	C	504	4/4	0.85	0.32	98,100,101,103	0
4	EDO	C	505	4/4	0.85	0.19	64,65,71,73	0
7	PEG	D	518	7/7	0.85	0.18	63,66,71,72	0
4	EDO	D	515	4/4	0.86	0.18	63,64,66,70	0
4	EDO	C	509	4/4	0.86	0.20	53,68,69,70	0
4	EDO	D	510	4/4	0.86	0.16	59,60,72,78	0
4	EDO	D	506	4/4	0.86	0.18	56,58,59,61	0
4	EDO	B	512	4/4	0.87	0.15	63,66,68,73	0
4	EDO	B	505	4/4	0.87	0.14	51,53,53,58	0
4	EDO	D	519	4/4	0.88	0.17	53,61,65,72	0
4	EDO	D	521	4/4	0.88	0.17	52,53,53,57	0
4	EDO	C	507	4/4	0.88	0.14	57,58,61,65	0
6	EPE	A	510	15/15	0.88	0.17	54,92,104,105	0
4	EDO	C	501	4/4	0.88	0.16	48,59,64,77	0
7	PEG	D	513	7/7	0.88	0.15	41,42,55,55	0

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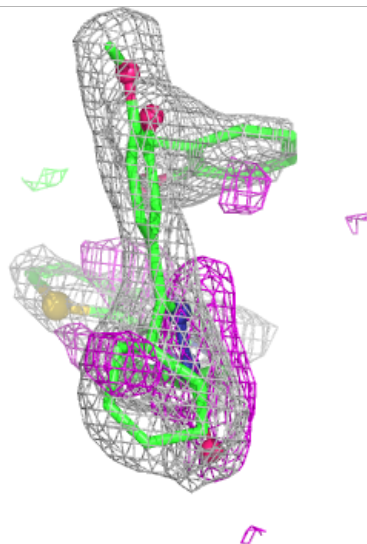
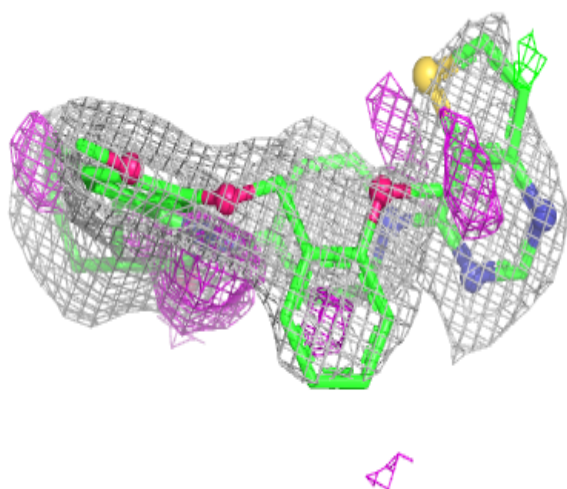
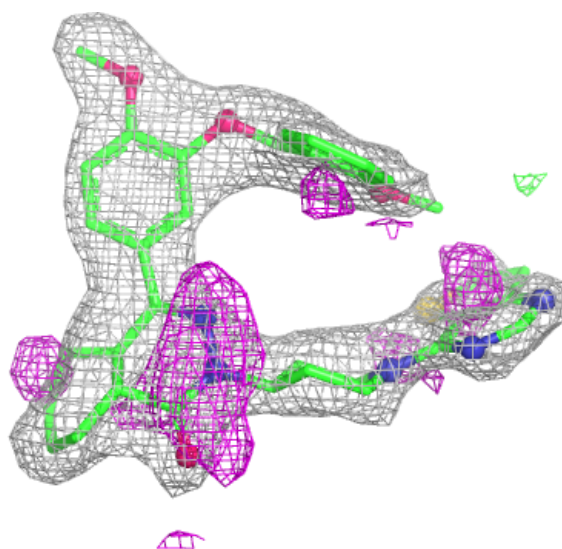
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	C	513	4/4	0.88	0.14	60,62,64,65	0
4	EDO	B	510	4/4	0.89	0.14	62,63,67,71	0
4	EDO	A	507	4/4	0.89	0.14	62,64,66,67	0
4	EDO	C	506	4/4	0.89	0.17	51,54,57,61	0
4	EDO	D	501	4/4	0.90	0.18	46,47,63,63	0
5	E6E	B	509	44/44	0.90	0.13	36,49,80,106	0
5	E6E	C	510	44/44	0.90	0.13	37,53,83,96	0
5	E6E	D	517	44/44	0.90	0.13	37,54,108,124	0
4	EDO	A	505	4/4	0.90	0.13	47,52,52,57	0
4	EDO	A	503	4/4	0.90	0.15	56,63,69,83	0
4	EDO	D	508	4/4	0.90	0.13	41,53,59,62	0
4	EDO	D	509	4/4	0.90	0.15	60,65,71,72	0
4	EDO	A	506	4/4	0.91	0.12	54,61,61,67	0
4	EDO	D	504	4/4	0.91	0.16	70,75,76,87	0
6	EPE	B	511	15/15	0.91	0.16	49,94,106,108	0
4	EDO	D	505	4/4	0.91	0.11	40,40,40,44	0
4	EDO	A	508	4/4	0.91	0.16	43,49,52,55	0
4	EDO	D	516	4/4	0.92	0.11	38,40,42,50	0
4	EDO	D	511	4/4	0.92	0.12	39,54,57,57	0
6	EPE	D	520	15/15	0.92	0.17	39,83,101,102	0
7	PEG	D	512	7/7	0.92	0.14	36,47,52,54	0
4	EDO	A	504	4/4	0.92	0.14	41,57,59,65	0
4	EDO	C	515	4/4	0.92	0.14	48,55,59,68	0
4	EDO	B	503	4/4	0.93	0.18	62,66,67,76	0
4	EDO	A	511	4/4	0.93	0.14	44,49,51,60	0
4	EDO	A	513	4/4	0.94	0.09	33,37,38,40	0
6	EPE	C	508	15/15	0.96	0.10	48,59,83,91	0
3	MG	A	502	1/1	0.98	0.09	18,18,18,18	0
2	ZN	A	501	1/1	0.99	0.02	35,35,35,35	0
2	ZN	C	502	1/1	1.00	0.01	35,35,35,35	0
2	ZN	D	502	1/1	1.00	0.01	31,31,31,31	0
2	ZN	B	501	1/1	1.00	0.03	35,35,35,35	0
3	MG	B	502	1/1	1.00	0.02	18,18,18,18	0
3	MG	C	503	1/1	1.00	0.04	19,19,19,19	0
3	MG	D	503	1/1	1.00	0.03	16,16,16,16	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.

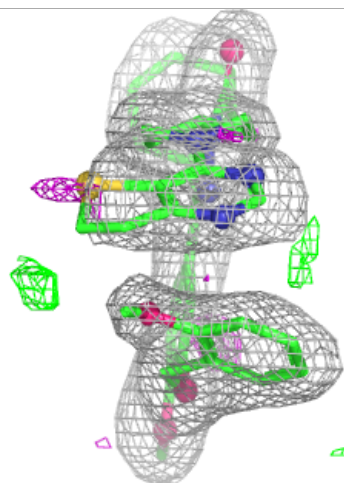
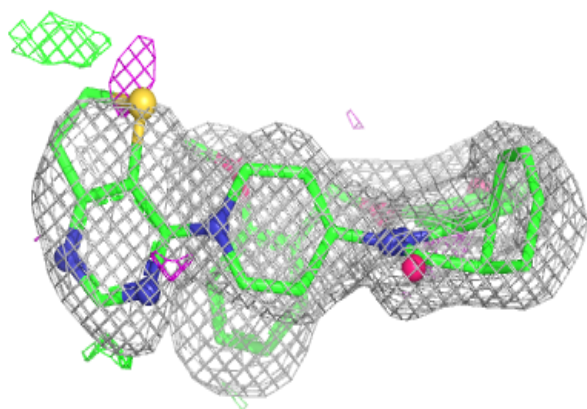
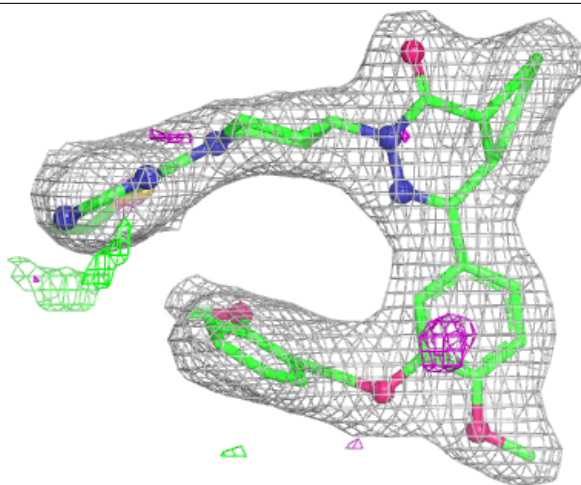
Electron density around E6E A 509:

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



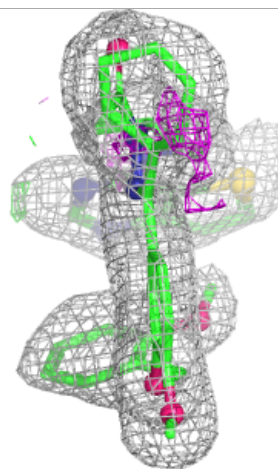
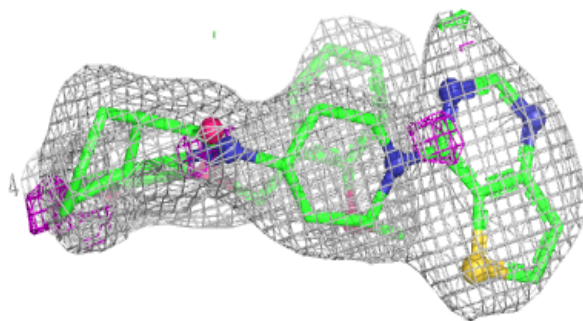
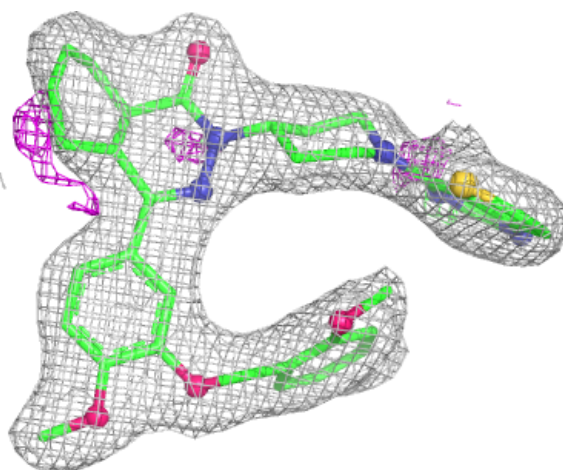
Electron density around E6E B 509:

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



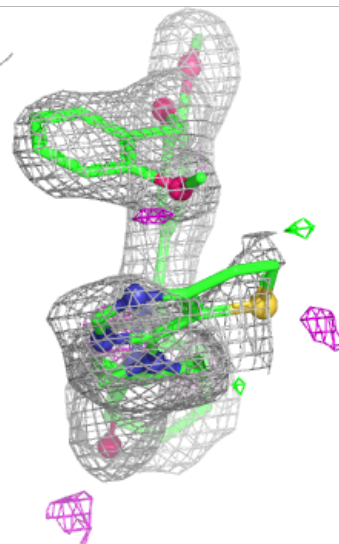
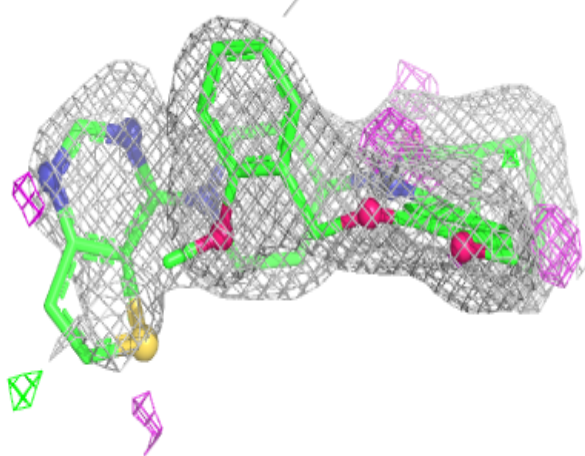
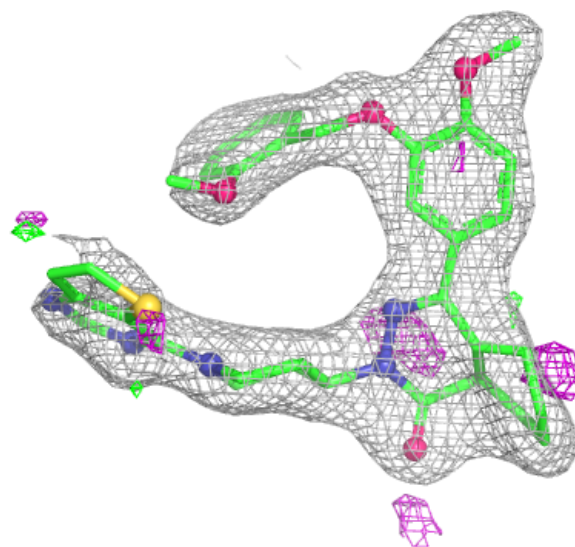
Electron density around E6E C 510:

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



Electron density around E6E D 517:

$2mF_o-DF_c$ (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.