



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:44 am BST

PDB ID : 6FET  
Title : Crystal structure of human phosphodiesterase 4D2 catalytic domain with inhibitor NPD-1439  
Authors : Singh, A.K.; Brown, D.G.  
Deposited on : 2018-01-03  
Resolution : 1.88 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](mailto: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

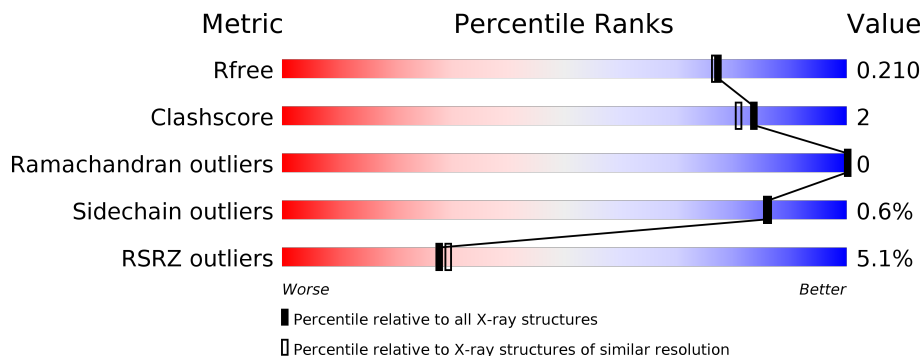
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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  $\geq 3$ , 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	 9% 83% 8% 10%
1	B	364	 2% 86% 11%
1	C	364	 5% 84% 5% 11%
1	D	364	 2% 83% 5% 11%

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
9	PG4	D	502	-	-	X	-

## 2 Entry composition i

There are 10 unique types of molecules in this entry. The entry contains 11731 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
			Total	C	N	O	S			
1	A	329	Total 2658	C 1681	N 454	O 509	S 14	0	0	0
1	B	323	Total 2613	C 1654	N 446	O 499	S 14	0	0	0
1	C	324	Total 2630	C 1663	N 450	O 503	S 14	0	1	0
1	D	324	Total 2622	C 1659	N 448	O 501	S 14	0	0	0

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

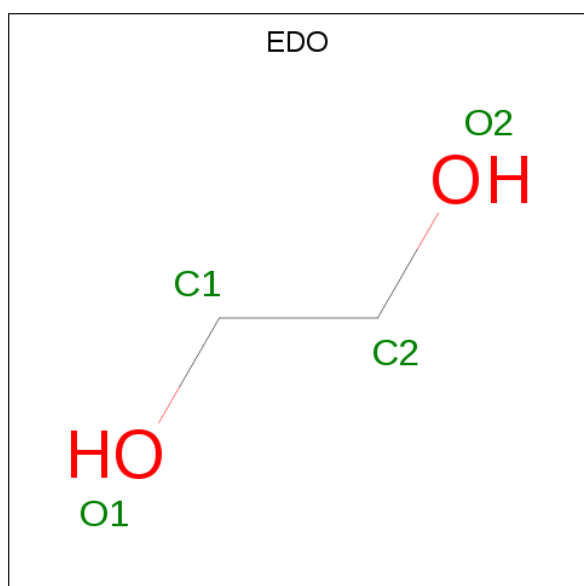
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

*Continued on next page...*

*Continued from previous page...*

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	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		

*Continued on next page...*

*Continued from previous page...*

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	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	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		

*Continued on next page...*

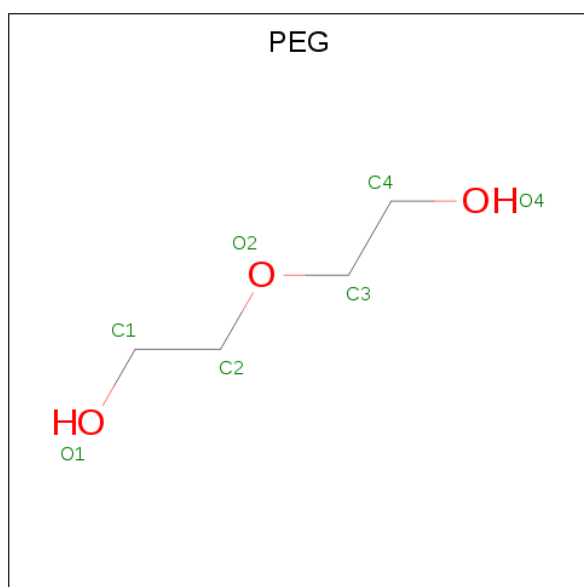




Continued from previous page...

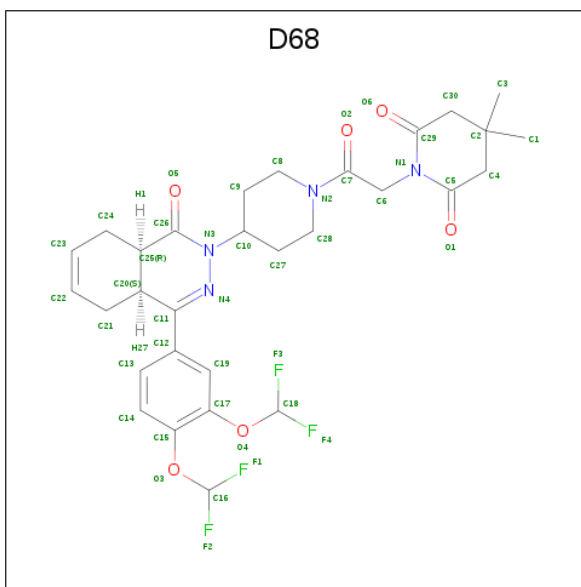
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



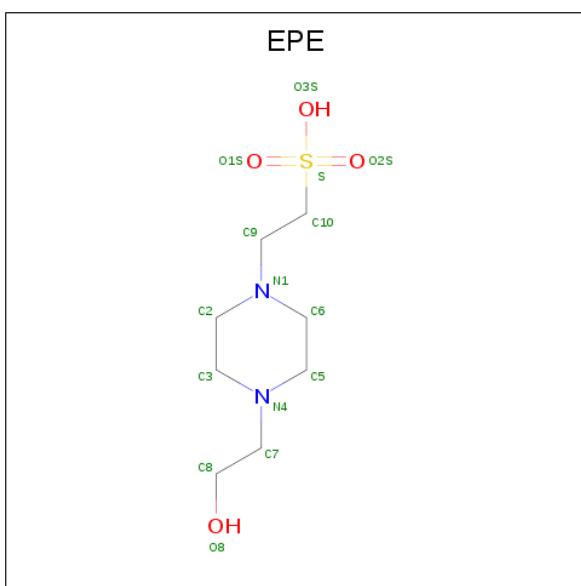
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 1-(2-{4-[(4aS,8aR)-4-[3,4-bis(difluoromethoxy)phenyl]-1-oxo-1,2,4a,5,8,8a-hexahydrophthalazin-2-yl]piperidin-1-yl}-2-oxoethyl)-4,4-dimethylpiperidine-2,6-dione (three-letter code: D68) (formula: C<sub>30</sub>H<sub>34</sub>F<sub>4</sub>N<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	F	N			O	
6	A	1	Total	44	30	4	4	6	0	0
6	B	1	Total	44	30	4	4	6	0	0
6	C	1	Total	44	30	4	4	6	0	0
6	D	1	Total	44	30	4	4	6	0	0

- Molecule 7 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).

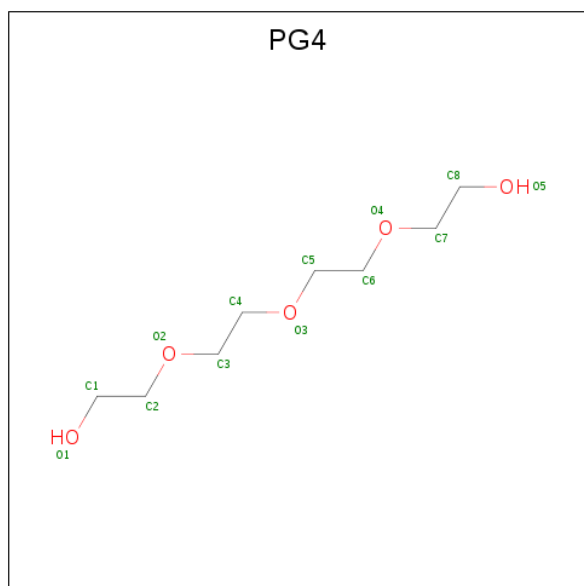


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
7	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 8 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ni	0	0
			1	1		
8	D	1	Total	Ni	0	0
			1	1		

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



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

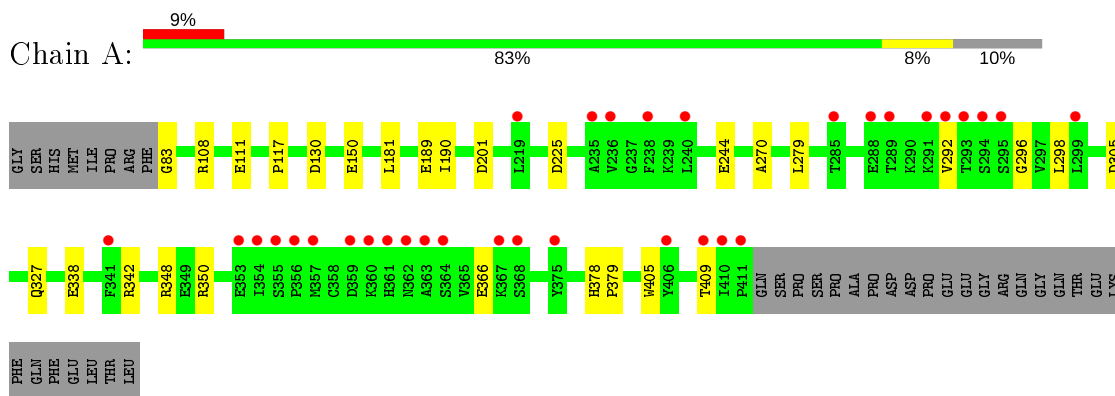
- Molecule 10 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
10	A	163	Total 163	O 163	0	0
10	B	169	Total 169	O 169	0	0
10	C	118	Total 118	O 118	0	0
10	D	175	Total 175	O 175	0	0

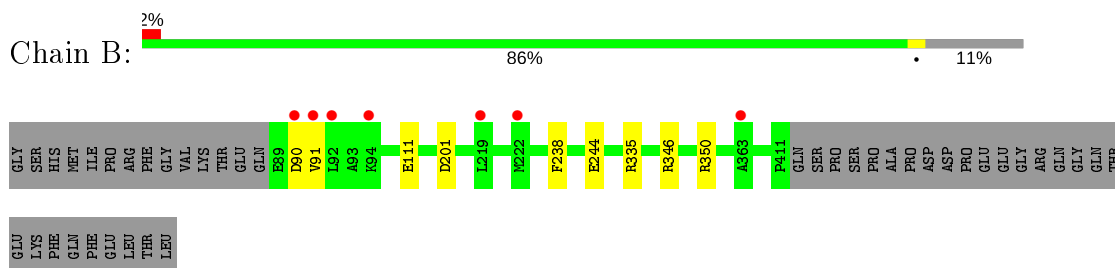
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

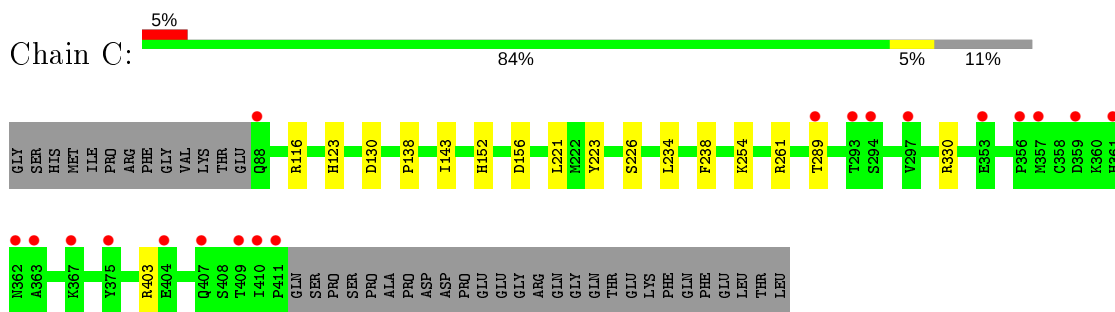
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



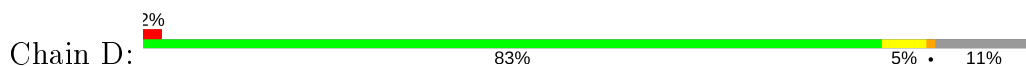
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

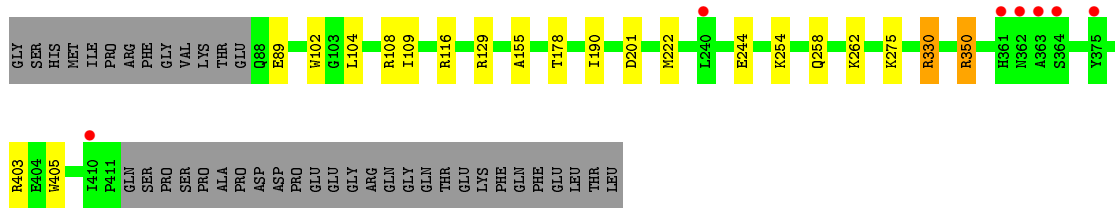


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- 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, $\alpha$ , $\beta$ , $\gamma$	97.19Å 110.71Å 161.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.35 – 1.88 55.35 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.9 (55.35-1.88) 100.0 (55.35-1.88)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.88Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.171 , 0.199 0.184 , 0.210	Depositor DCC
$R_{free}$ test set	7234 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtrriage
Anisotropy	0.384	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11731	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NI, ZN, PEG, MG, EDO, PG4, D68, EPE

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	0.91	1/2712 (0.0%)	0.88	7/3684 (0.2%)
1	B	0.89	0/2667	0.86	5/3624 (0.1%)
1	C	0.92	0/2684	0.88	6/3647 (0.2%)
1	D	1.03	1/2676 (0.0%)	0.91	10/3636 (0.3%)
All	All	0.94	2/10739 (0.0%)	0.88	28/14591 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	89	GLU	CG-CD	5.88	1.60	1.51
1	A	83	GLY	N-CA	5.05	1.53	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	116	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	D	330	ARG	NE-CZ-NH1	-9.20	115.70	120.30
1	C	116	ARG	NE-CZ-NH2	8.94	124.77	120.30
1	D	350	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	D	350	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	D	244	GLU	OE1-CD-OE2	-6.74	115.21	123.30
1	A	130	ASP	CB-CG-OD1	6.73	124.36	118.30
1	B	238	PHE	CB-CG-CD2	-6.54	116.22	120.80
1	B	201	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	201	ASP	CB-CG-OD1	6.14	123.82	118.30
1	A	225	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	D	330	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	C	403	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	C	156	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	201	ASP	CB-CG-OD1	5.49	123.24	118.30

*Continued on next page...*



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	348	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	C	330	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	C	130	ASP	CB-CG-OD1	5.35	123.11	118.30
1	D	108	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	D	201	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	330	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	D	403	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	305	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	D	102	TRP	C-N-CA	-5.12	111.55	122.30
1	A	350	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	244	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	B	335	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2658	0	2616	16	0
1	B	2613	0	2570	4	0
1	C	2630	0	2583	12	0
1	D	2622	0	2578	13	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	76	0	114	2	0
4	B	64	0	96	2	0
4	C	48	0	72	4	0
4	D	80	0	120	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	7	0	10	0	0
5	B	7	0	10	0	0
5	C	7	0	10	2	0
5	D	7	0	10	2	0
6	A	44	0	0	0	0
6	B	44	0	0	0	0
6	C	44	0	0	0	0
6	D	44	0	0	0	0
7	A	15	0	17	4	0
7	B	30	0	36	2	0
7	C	15	0	17	1	0
7	D	15	0	17	0	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
9	C	13	0	18	0	0
9	D	13	0	18	10	0
10	A	163	0	0	0	0
10	B	169	0	0	0	0
10	C	118	0	0	0	0
10	D	175	0	0	2	0
All	All	11731	0	10912	53	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 2.

All (53) 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)
9:D:502:PG4:H42	9:D:502:PG4:H11	1.45	0.99
9:D:502:PG4:H11	9:D:502:PG4:C4	2.07	0.83
1:D:222:MET:HA	9:D:502:PG4:H31	1.70	0.74
1:A:190:ILE:HD11	4:A:524:EDO:H22	1.72	0.70
1:A:111:GLU:OE1	7:A:518:EPE:H52	1.92	0.69
1:C:152:HIS:HE1	5:C:511:PEG:H22	1.58	0.68
1:C:261:ARG:HB2	4:C:508:EDO:H12	1.77	0.66
1:A:338:GLU:O	1:A:342:ARG:HG3	1.98	0.64
1:D:129:ARG:HB3	4:D:514:EDO:H22	1.80	0.62
4:B:508:EDO:H11	4:D:511:EDO:H21	1.83	0.59
1:B:111:GLU:OE1	7:B:513:EPE:H32	2.04	0.57
1:A:181:LEU:CD2	1:A:298:LEU:HD12	2.36	0.56
1:A:111:GLU:OE2	7:A:518:EPE:H72	2.05	0.55

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:PRO:HG2	4:C:509:EDO:H22	1.89	0.54
1:C:152:HIS:CE1	5:C:511:PEG:H22	2.43	0.53
9:D:502:PG4:C1	9:D:502:PG4:C4	2.84	0.51
9:D:502:PG4:O4	9:D:502:PG4:H41	2.10	0.51
1:D:275:LYS:NZ	10:D:603:HOH:O	2.42	0.51
1:B:346:ARG:HH22	4:B:508:EDO:H12	1.78	0.49
1:A:117:PRO:HD2	1:A:150:GLU:OE2	2.12	0.49
1:A:189:GLU:HG3	4:A:521:EDO:H22	1.95	0.48
1:B:244:GLU:OE2	1:C:254:LYS:NZ	2.46	0.48
1:A:378:HIS:HB3	1:A:379:PRO:HD3	1.96	0.48
1:A:181:LEU:HD23	1:A:298:LEU:HD12	1.95	0.47
1:C:238:PHE:CD2	9:D:502:PG4:H82	2.48	0.47
1:C:234:LEU:HB3	9:D:502:PG4:H62	1.95	0.47
1:D:262:LYS:HD3	4:D:507:EDO:C2	2.45	0.46
1:C:261:ARG:HB2	4:C:508:EDO:C1	2.44	0.45
1:A:111:GLU:OE2	7:A:518:EPE:H32	2.17	0.45
1:C:289:THR:O	1:C:289:THR:HG22	2.16	0.45
1:D:254:LYS:O	1:D:258:GLN:HG3	2.16	0.45
1:A:366:GLU:HG2	1:A:409:THR:OG1	2.16	0.45
1:D:104:LEU:HD11	1:D:109:ILE:CD1	2.47	0.45
1:A:181:LEU:HD21	1:A:298:LEU:HD12	1.99	0.44
1:D:155:ALA:HA	4:D:513:EDO:H11	2.00	0.44
7:C:512:EPE:H51	7:C:512:EPE:H81	1.77	0.43
1:D:190:ILE:HD13	4:D:514:EDO:H21	1.98	0.43
9:D:502:PG4:O1	9:D:502:PG4:H71	2.18	0.43
1:A:270:ALA:HB1	1:A:279:LEU:HD11	2.00	0.43
1:A:405:TRP:O	1:A:409:THR:HG23	2.19	0.42
1:C:223:TYR:OH	9:D:502:PG4:H32	2.19	0.42
1:A:111:GLU:CD	7:A:518:EPE:H52	2.39	0.42
1:C:123:HIS:ND1	1:C:143:ILE:HD11	2.35	0.42
4:D:510:EDO:C2	10:D:717:HOH:O	2.68	0.42
1:C:152:HIS:NE2	4:C:501:EDO:H12	2.34	0.41
1:D:178:THR:HA	5:D:519:PEG:H11	2.03	0.41
1:D:190:ILE:HD11	4:D:515:EDO:H12	2.03	0.41
1:D:104:LEU:HD11	1:D:109:ILE:HD11	2.02	0.40
1:D:222:MET:HA	9:D:502:PG4:C3	2.46	0.40
1:B:111:GLU:OE1	7:B:513:EPE:H81	2.21	0.40
1:A:292:VAL:CG1	1:A:296:GLY:HA2	2.50	0.40
1:D:330:ARG:HD2	1:D:405:TRP:CZ3	2.57	0.40
5:D:519:PEG:H31	5:D:519:PEG:H12	1.56	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%)	321 (98%)	6 (2%)	0	100	100
1	B	321/364 (88%)	318 (99%)	3 (1%)	0	100	100
1	C	323/364 (89%)	317 (98%)	6 (2%)	0	100	100
1	D	322/364 (88%)	316 (98%)	6 (2%)	0	100	100
All	All	1293/1456 (89%)	1272 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/331 (91%)	298 (99%)	2 (1%)	84	83
1	B	295/331 (89%)	293 (99%)	2 (1%)	84	83
1	C	297/331 (90%)	295 (99%)	2 (1%)	84	83
1	D	296/331 (89%)	295 (100%)	1 (0%)	92	92
All	All	1188/1324 (90%)	1181 (99%)	7 (1%)	86	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ARG
1	A	327	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	90	ASP
1	B	91	VAL
1	C	221	LEU
1	C	226	SER
1	D	350	ARG

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 92 ligands modelled in this entry, 10 are monoatomic - leaving 82 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	$\# Z  > 2$
5	PEG	A	510	-	6,6,6	0.41	0	5,5,5	1.00	0
4	EDO	B	520	-	3,3,3	0.80	0	2,2,2	0.58	0
4	EDO	A	507	-	3,3,3	0.18	0	2,2,2	0.61	0
5	PEG	C	511	-	6,6,6	0.29	0	5,5,5	0.89	0
4	EDO	B	515	-	3,3,3	0.28	0	2,2,2	0.27	0
4	EDO	D	516	-	3,3,3	0.52	0	2,2,2	1.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	A	524	-	3,3,3	0.27	0	2,2,2	0.13	0
4	EDO	D	508	-	3,3,3	0.29	0	2,2,2	1.25	0
4	EDO	A	520	-	3,3,3	0.56	0	2,2,2	0.37	0
4	EDO	A	504	-	3,3,3	0.96	0	2,2,2	0.22	0
4	EDO	A	521	-	3,3,3	0.26	0	2,2,2	0.63	0
4	EDO	C	513	-	3,3,3	0.79	0	2,2,2	0.76	0
4	EDO	D	517	-	3,3,3	0.15	0	2,2,2	1.34	0
4	EDO	B	521	-	3,3,3	1.06	0	2,2,2	0.82	0
4	EDO	C	517	-	3,3,3	0.29	0	2,2,2	0.57	0
4	EDO	B	510	-	3,3,3	0.49	0	2,2,2	1.21	0
4	EDO	C	501	-	3,3,3	0.28	0	2,2,2	0.69	0
9	PG4	D	502	-	12,12,12	0.51	0	11,11,11	1.14	2 (18%)
4	EDO	B	519	-	3,3,3	0.76	0	2,2,2	0.13	0
6	D68	C	515	-	48,48,48	0.67	1 (2%)	61,71,71	0.88	2 (3%)
4	EDO	D	507	-	3,3,3	0.29	0	2,2,2	0.85	0
4	EDO	D	509	-	3,3,3	0.60	0	2,2,2	0.96	0
4	EDO	D	511	-	3,3,3	0.40	0	2,2,2	0.84	0
4	EDO	A	506	-	3,3,3	0.27	0	2,2,2	1.41	0
4	EDO	B	506	-	3,3,3	0.42	0	2,2,2	1.05	0
6	D68	B	514	-	48,48,48	0.50	0	61,71,71	1.24	3 (4%)
4	EDO	A	515	-	3,3,3	0.33	0	2,2,2	1.29	0
9	PG4	C	514	-	12,12,12	0.68	0	11,11,11	0.94	0
4	EDO	A	514	-	3,3,3	0.40	0	2,2,2	1.52	0
4	EDO	C	507	-	3,3,3	0.28	0	2,2,2	1.20	0
4	EDO	B	508	-	3,3,3	0.36	0	2,2,2	0.58	0
4	EDO	B	516	-	3,3,3	0.24	0	2,2,2	1.26	0
4	EDO	B	518	-	3,3,3	0.48	0	2,2,2	0.59	0
4	EDO	B	517	-	3,3,3	0.35	0	2,2,2	0.51	0
4	EDO	C	518	-	3,3,3	0.28	0	2,2,2	0.51	0
7	EPE	D	521	-	15,15,15	2.92	3 (20%)	18,20,20	2.10	4 (22%)
4	EDO	D	525	-	3,3,3	0.62	0	2,2,2	0.36	0
4	EDO	D	513	-	3,3,3	0.17	0	2,2,2	0.73	0
4	EDO	D	522	-	3,3,3	0.56	0	2,2,2	0.47	0
4	EDO	D	512	-	3,3,3	0.33	0	2,2,2	0.22	0
4	EDO	A	512	-	3,3,3	0.39	0	2,2,2	0.28	0
4	EDO	C	508	-	3,3,3	0.21	0	2,2,2	0.59	0
4	EDO	A	516	-	3,3,3	0.27	0	2,2,2	0.91	0
4	EDO	C	506	-	3,3,3	0.15	0	2,2,2	0.35	0
7	EPE	B	513	-	15,15,15	2.07	1 (6%)	18,20,20	2.75	8 (44%)
7	EPE	B	507	-	15,15,15	1.25	1 (6%)	18,20,20	2.07	5 (27%)
4	EDO	B	509	-	3,3,3	0.22	0	2,2,2	0.66	0
4	EDO	D	501	-	3,3,3	0.31	0	2,2,2	1.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	B	522	-	3,3,3	0.28	0	2,2,2	0.37	0
4	EDO	A	519	-	3,3,3	0.41	0	2,2,2	0.80	0
6	D68	A	517	-	48,48,48	0.60	0	61,71,71	1.08	4 (6%)
4	EDO	D	526	-	3,3,3	0.77	0	2,2,2	0.21	0
4	EDO	D	514	-	3,3,3	0.40	0	2,2,2	0.75	0
7	EPE	C	512	-	15,15,15	2.60	2 (13%)	18,20,20	2.19	5 (27%)
4	EDO	A	509	-	3,3,3	0.28	0	2,2,2	1.79	0
4	EDO	A	513	-	3,3,3	0.15	0	2,2,2	0.40	0
4	EDO	A	508	-	3,3,3	0.63	0	2,2,2	0.82	0
4	EDO	C	516	-	3,3,3	0.48	0	2,2,2	0.50	0
4	EDO	D	503	-	3,3,3	0.34	0	2,2,2	0.59	0
4	EDO	B	503	-	3,3,3	0.50	0	2,2,2	0.71	0
4	EDO	D	515	-	3,3,3	0.43	0	2,2,2	0.31	0
4	EDO	D	510	-	3,3,3	0.35	0	2,2,2	0.53	0
5	PEG	D	519	-	6,6,6	0.54	0	5,5,5	0.80	0
4	EDO	D	506	-	3,3,3	0.61	0	2,2,2	0.36	0
4	EDO	A	511	-	3,3,3	0.61	0	2,2,2	0.45	0
4	EDO	B	511	-	3,3,3	0.55	0	2,2,2	0.24	0
4	EDO	C	502	-	3,3,3	0.44	0	2,2,2	1.04	0
4	EDO	A	523	-	3,3,3	0.54	0	2,2,2	0.50	0
4	EDO	A	503	-	3,3,3	0.54	0	2,2,2	0.56	0
4	EDO	B	505	-	3,3,3	0.46	0	2,2,2	0.54	0
7	EPE	A	518	-	15,15,15	2.70	2 (13%)	18,20,20	1.88	4 (22%)
5	PEG	B	512	-	6,6,6	0.92	0	5,5,5	1.65	2 (40%)
4	EDO	B	504	-	3,3,3	0.65	0	2,2,2	0.43	0
4	EDO	C	503	-	3,3,3	0.33	0	2,2,2	0.36	0
4	EDO	C	510	-	3,3,3	0.68	0	2,2,2	0.75	0
4	EDO	D	518	-	3,3,3	0.30	0	2,2,2	0.12	0
4	EDO	D	524	-	3,3,3	1.40	0	2,2,2	0.91	0
4	EDO	D	523	-	3,3,3	0.26	0	2,2,2	0.66	0
4	EDO	A	505	-	3,3,3	0.59	0	2,2,2	0.58	0
4	EDO	A	522	-	3,3,3	0.39	0	2,2,2	1.33	0
6	D68	D	520	-	48,48,48	0.71	2 (4%)	61,71,71	1.22	5 (8%)
4	EDO	C	509	-	3,3,3	0.16	0	2,2,2	1.09	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
5	PEG	A	510	-	-	4/4/4/4	-
4	EDO	B	520	-	-	0/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
5	PEG	C	511	-	-	3/4/4/4	-
4	EDO	B	515	-	-	1/1/1/1	-
4	EDO	D	516	-	-	1/1/1/1	-
4	EDO	A	524	-	-	1/1/1/1	-
4	EDO	D	508	-	-	0/1/1/1	-
4	EDO	A	520	-	-	1/1/1/1	-
4	EDO	A	504	-	-	0/1/1/1	-
4	EDO	A	521	-	-	0/1/1/1	-
4	EDO	C	513	-	-	0/1/1/1	-
4	EDO	D	517	-	-	0/1/1/1	-
4	EDO	B	521	-	-	0/1/1/1	-
4	EDO	C	517	-	-	1/1/1/1	-
4	EDO	B	510	-	-	1/1/1/1	-
4	EDO	C	501	-	-	1/1/1/1	-
9	PG4	D	502	-	-	9/10/10/10	-
4	EDO	B	519	-	-	0/1/1/1	-
6	D68	C	515	-	-	2/24/79/79	0/5/5/5
4	EDO	D	507	-	-	0/1/1/1	-
4	EDO	D	509	-	-	0/1/1/1	-
4	EDO	D	511	-	-	0/1/1/1	-
4	EDO	A	506	-	-	1/1/1/1	-
4	EDO	B	506	-	-	1/1/1/1	-
6	D68	B	514	-	-	2/24/79/79	0/5/5/5
4	EDO	A	515	-	-	0/1/1/1	-
9	PG4	C	514	-	-	4/10/10/10	-
4	EDO	A	514	-	-	0/1/1/1	-
4	EDO	C	507	-	-	1/1/1/1	-
4	EDO	B	508	-	-	0/1/1/1	-
4	EDO	B	516	-	-	0/1/1/1	-
4	EDO	B	518	-	-	1/1/1/1	-
4	EDO	B	517	-	-	1/1/1/1	-
4	EDO	C	518	-	-	1/1/1/1	-
7	EPE	D	521	-	-	2/9/19/19	0/1/1/1
4	EDO	D	525	-	-	1/1/1/1	-
4	EDO	D	513	-	-	0/1/1/1	-
4	EDO	D	522	-	-	1/1/1/1	-
4	EDO	D	512	-	-	1/1/1/1	-
4	EDO	A	512	-	-	0/1/1/1	-
4	EDO	C	508	-	-	0/1/1/1	-

Continued on next page...



Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	516	-	-	1/1/1/1	-
4	EDO	C	506	-	-	1/1/1/1	-
7	EPE	B	513	-	-	4/9/19/19	0/1/1/1
7	EPE	B	507	-	-	3/9/19/19	0/1/1/1
4	EDO	B	509	-	-	0/1/1/1	-
4	EDO	D	501	-	-	1/1/1/1	-
4	EDO	B	522	-	-	1/1/1/1	-
4	EDO	A	519	-	-	0/1/1/1	-
6	D68	A	517	-	-	2/24/79/79	0/5/5/5
4	EDO	D	526	-	-	1/1/1/1	-
4	EDO	D	514	-	-	1/1/1/1	-
7	EPE	C	512	-	-	6/9/19/19	0/1/1/1
4	EDO	A	509	-	-	1/1/1/1	-
4	EDO	A	513	-	-	0/1/1/1	-
4	EDO	A	508	-	-	0/1/1/1	-
4	EDO	C	516	-	-	0/1/1/1	-
4	EDO	D	503	-	-	1/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	D	515	-	-	1/1/1/1	-
4	EDO	D	510	-	-	1/1/1/1	-
5	PEG	D	519	-	-	2/4/4/4	-
4	EDO	D	506	-	-	0/1/1/1	-
4	EDO	A	511	-	-	1/1/1/1	-
4	EDO	B	511	-	-	1/1/1/1	-
4	EDO	C	502	-	-	1/1/1/1	-
4	EDO	A	523	-	-	1/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
4	EDO	B	505	-	-	0/1/1/1	-
7	EPE	A	518	-	-	5/9/19/19	0/1/1/1
5	PEG	B	512	-	-	2/4/4/4	-
4	EDO	B	504	-	-	0/1/1/1	-
4	EDO	C	503	-	-	1/1/1/1	-
4	EDO	C	510	-	-	0/1/1/1	-
4	EDO	D	518	-	-	0/1/1/1	-
4	EDO	D	524	-	-	1/1/1/1	-
4	EDO	D	523	-	-	0/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-
4	EDO	A	522	-	-	1/1/1/1	-
6	D68	D	520	-	-	2/24/79/79	0/5/5/5
4	EDO	C	509	-	-	0/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	521	EPE	C10-S	-10.41	1.62	1.77
7	A	518	EPE	C10-S	-9.84	1.63	1.77
7	C	512	EPE	C10-S	-9.49	1.64	1.77
7	B	513	EPE	C10-S	-7.49	1.66	1.77
7	B	507	EPE	C10-S	-3.84	1.72	1.77
7	D	521	EPE	O1S-S	-3.17	1.35	1.45
6	D	520	D68	C6-N1	2.63	1.50	1.46
6	D	520	D68	C21-C20	-2.58	1.49	1.53
7	A	518	EPE	O3S-S	-2.53	1.38	1.47
7	D	521	EPE	O3S-S	-2.30	1.39	1.47
6	C	515	D68	N3-N4	-2.13	1.33	1.37
7	C	512	EPE	O3S-S	-2.02	1.40	1.47

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	513	EPE	O2S-S-C10	7.82	116.33	106.92
7	A	518	EPE	O2S-S-C10	6.57	114.83	106.92
7	D	521	EPE	O1S-S-C10	6.08	114.24	106.92
7	C	512	EPE	O3S-S-C10	5.94	115.38	105.77
7	B	507	EPE	O1S-S-C10	4.86	112.77	106.92
6	B	514	D68	C13-C12-C11	4.75	126.38	120.75
7	C	512	EPE	O2S-S-C10	4.69	112.56	106.92
7	B	507	EPE	O2S-S-C10	4.56	112.40	106.92
6	B	514	D68	C17-O4-C18	4.51	134.70	118.77
6	D	520	D68	C13-C12-C11	4.45	126.03	120.75
7	D	521	EPE	O2S-S-O1S	-4.18	99.49	113.95
7	B	513	EPE	O2S-S-O1S	-4.10	99.77	113.95
6	D	520	D68	C17-O4-C18	4.07	133.13	118.77
7	B	513	EPE	O3S-S-O1S	4.03	121.12	111.27
6	A	517	D68	C17-O4-C18	3.88	132.47	118.77
7	B	513	EPE	O3S-S-O2S	-3.23	103.38	111.27
7	B	507	EPE	C2-C3-N4	3.16	117.13	110.64
6	C	515	D68	C29-N1-C5	3.01	125.01	124.07
7	C	512	EPE	C9-N1-C2	-2.75	104.21	111.23
7	D	521	EPE	O3S-S-C10	2.74	110.19	105.77
6	C	515	D68	C17-O4-C18	2.72	128.38	118.77
6	B	514	D68	O5-C26-N3	-2.72	118.33	121.64
7	D	521	EPE	O2S-S-C10	2.64	110.10	106.92
5	B	512	PEG	C3-O2-C2	2.58	124.45	113.29
7	B	513	EPE	C2-C3-N4	2.56	115.90	110.64
6	D	520	D68	C29-N1-C5	-2.56	123.27	124.07

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	517	D68	C27-C10-N3	2.53	113.66	110.86
6	A	517	D68	C13-C12-C11	2.51	123.72	120.75
5	B	512	PEG	O2-C3-C4	2.50	121.07	110.07
7	A	518	EPE	O3S-S-O2S	-2.45	105.29	111.27
7	B	507	EPE	O2S-S-O1S	-2.43	105.52	113.95
7	B	513	EPE	C7-N4-C3	2.42	117.42	111.23
7	C	512	EPE	O2S-S-O1S	-2.31	105.94	113.95
7	C	512	EPE	C3-C2-N1	2.27	115.30	110.64
7	B	513	EPE	O3S-S-C10	2.24	109.38	105.77
6	D	520	D68	C6-N1-C29	2.20	119.48	117.79
6	A	517	D68	C9-C8-N2	-2.19	107.49	110.82
7	B	513	EPE	C5-N4-C3	2.19	113.75	108.83
7	A	518	EPE	C7-N4-C3	-2.18	105.65	111.23
6	D	520	D68	O4-C17-C19	2.17	128.69	123.79
7	B	507	EPE	C6-C5-N4	2.09	114.93	110.64
9	D	502	PG4	O2-C2-C1	2.07	119.18	110.07
7	A	518	EPE	C9-N1-C2	-2.06	105.95	111.23
9	D	502	PG4	C3-O2-C2	2.04	122.15	113.29

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	521	EPE	C8-C7-N4-C3
7	B	507	EPE	C9-C10-S-O2S
7	B	507	EPE	C9-C10-S-O3S
7	B	513	EPE	C8-C7-N4-C3
7	B	513	EPE	C9-C10-S-O2S
7	C	512	EPE	C10-C9-N1-C6
7	C	512	EPE	C8-C7-N4-C5
7	C	512	EPE	C9-C10-S-O2S
7	A	518	EPE	S-C10-C9-N1
7	A	518	EPE	C9-C10-S-O1S
7	A	518	EPE	C9-C10-S-O3S
5	B	512	PEG	C4-C3-O2-C2
9	D	502	PG4	C1-C2-O2-C3
4	B	510	EDO	O1-C1-C2-O2
4	D	503	EDO	O1-C1-C2-O2
9	D	502	PG4	C4-C3-O2-C2
5	D	519	PEG	C1-C2-O2-C3
5	D	519	PEG	O2-C3-C4-O4
5	A	510	PEG	O1-C1-C2-O2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	A	511	EDO	O1-C1-C2-O2
4	D	512	EDO	O1-C1-C2-O2
4	D	515	EDO	O1-C1-C2-O2
4	C	502	EDO	O1-C1-C2-O2
4	C	507	EDO	O1-C1-C2-O2
4	C	503	EDO	O1-C1-C2-O2
4	D	524	EDO	O1-C1-C2-O2
4	D	526	EDO	O1-C1-C2-O2
5	C	511	PEG	O2-C3-C4-O4
5	B	512	PEG	O2-C3-C4-O4
9	D	502	PG4	C6-C5-O3-C4
6	C	515	D68	F4-C18-O4-C17
6	D	520	D68	F3-C18-O4-C17
6	B	514	D68	F3-C18-O4-C17
6	A	517	D68	F3-C18-O4-C17
7	B	513	EPE	S-C10-C9-N1
7	C	512	EPE	S-C10-C9-N1
9	C	514	PG4	O2-C3-C4-O3
7	B	513	EPE	C9-C10-S-O3S
4	D	516	EDO	O1-C1-C2-O2
4	D	514	EDO	O1-C1-C2-O2
4	A	509	EDO	O1-C1-C2-O2
4	C	501	EDO	O1-C1-C2-O2
9	D	502	PG4	O2-C3-C4-O3
7	A	518	EPE	C8-C7-N4-C5
9	C	514	PG4	C5-C6-O4-C7
5	A	510	PEG	C1-C2-O2-C3
5	C	511	PEG	C4-C3-O2-C2
5	C	511	PEG	C1-C2-O2-C3
9	D	502	PG4	O1-C1-C2-O2
7	C	512	EPE	C9-C10-S-O3S
7	B	507	EPE	C9-C10-S-O1S
7	C	512	EPE	C9-C10-S-O1S
7	A	518	EPE	C9-C10-S-O2S
6	D	520	D68	F4-C18-O4-C17
6	B	514	D68	F4-C18-O4-C17
6	A	517	D68	F4-C18-O4-C17
9	D	502	PG4	C3-C4-O3-C5
9	C	514	PG4	C6-C5-O3-C4
5	A	510	PEG	O2-C3-C4-O4
9	D	502	PG4	O4-C7-C8-O5
4	D	525	EDO	O1-C1-C2-O2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	D	501	EDO	O1-C1-C2-O2
4	B	522	EDO	O1-C1-C2-O2
4	D	510	EDO	O1-C1-C2-O2
4	A	507	EDO	O1-C1-C2-O2
9	D	502	PG4	C8-C7-O4-C6
4	C	506	EDO	O1-C1-C2-O2
4	B	511	EDO	O1-C1-C2-O2
4	B	518	EDO	O1-C1-C2-O2
4	A	520	EDO	O1-C1-C2-O2
4	A	522	EDO	O1-C1-C2-O2
6	C	515	D68	F3-C18-O4-C17
9	D	502	PG4	C5-C6-O4-C7
5	A	510	PEG	C4-C3-O2-C2
4	D	522	EDO	O1-C1-C2-O2
4	C	518	EDO	O1-C1-C2-O2
4	A	506	EDO	O1-C1-C2-O2
4	B	506	EDO	O1-C1-C2-O2
4	C	517	EDO	O1-C1-C2-O2
4	A	516	EDO	O1-C1-C2-O2
4	A	523	EDO	O1-C1-C2-O2
9	C	514	PG4	O1-C1-C2-O2
4	B	517	EDO	O1-C1-C2-O2
4	B	515	EDO	O1-C1-C2-O2
4	A	524	EDO	O1-C1-C2-O2
7	D	521	EPE	C9-C10-S-O1S

There are no ring outliers.

18 monomers are involved in 35 short contacts:

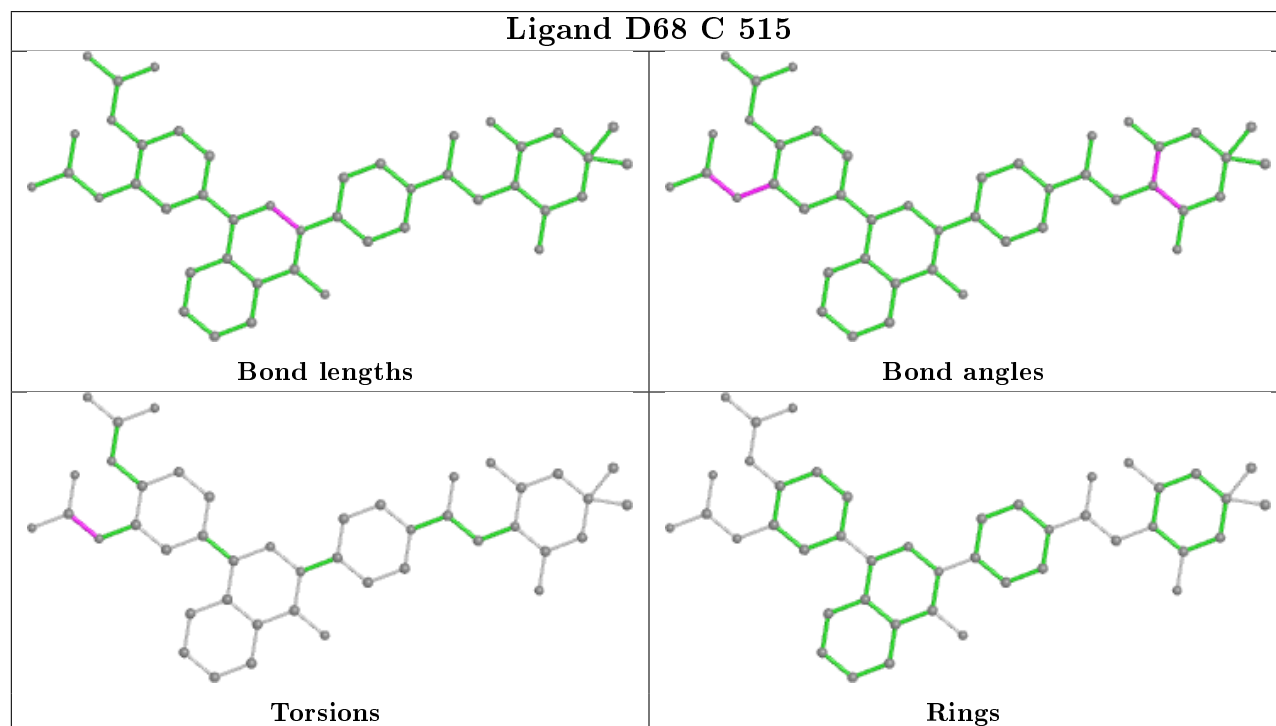
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	511	PEG	2	0
4	A	524	EDO	1	0
4	A	521	EDO	1	0
4	C	501	EDO	1	0
9	D	502	PG4	10	0
4	D	507	EDO	1	0
4	D	511	EDO	1	0
4	B	508	EDO	2	0
4	D	513	EDO	1	0
4	C	508	EDO	2	0
7	B	513	EPE	2	0
4	D	514	EDO	2	0

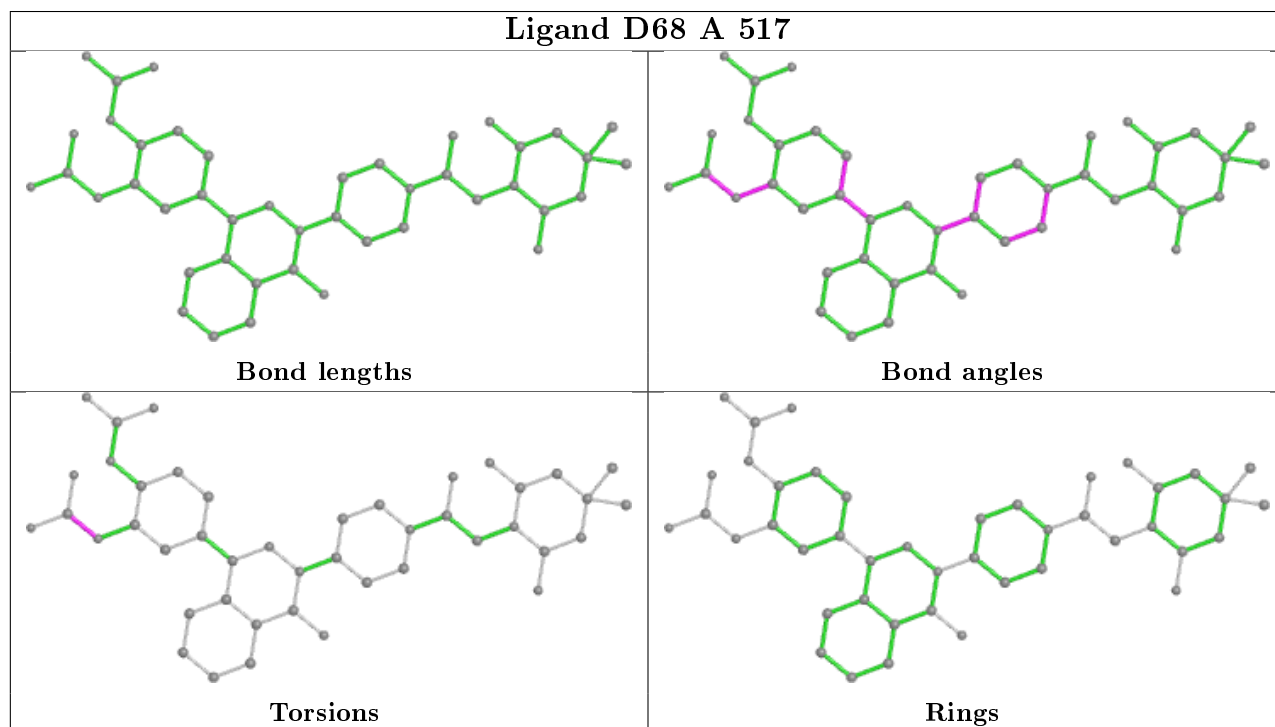
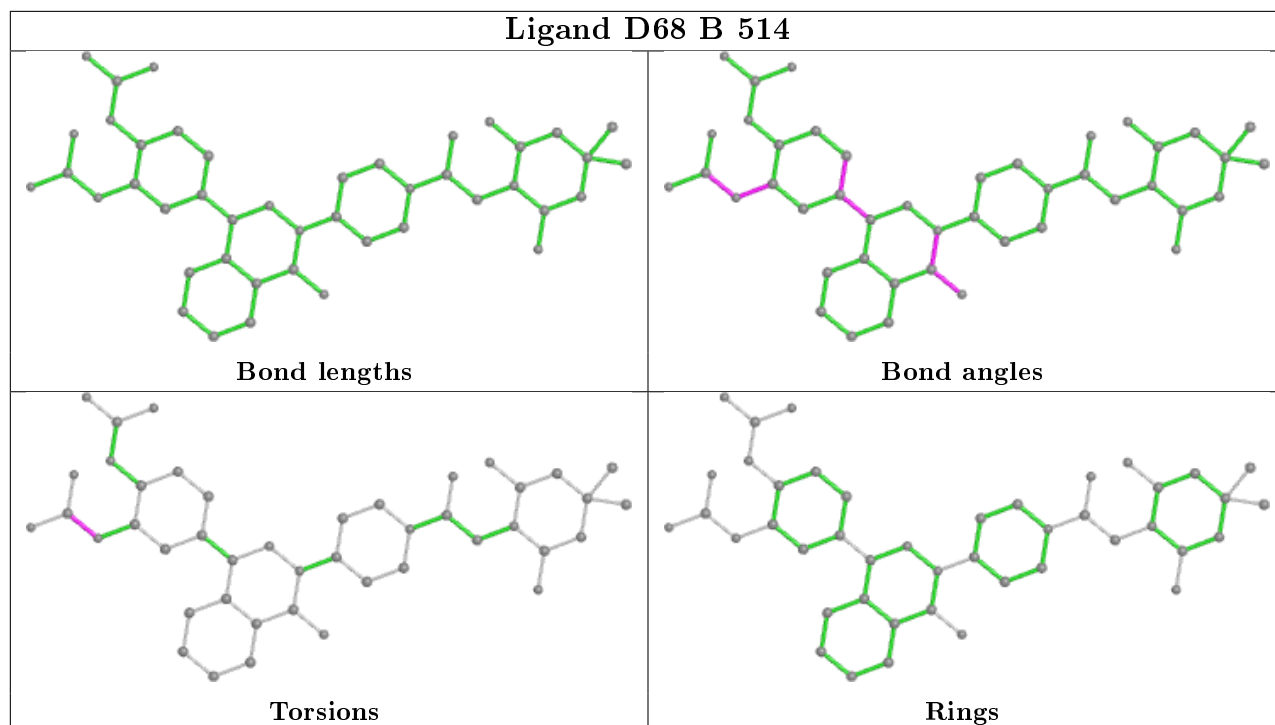
*Continued on next page...*

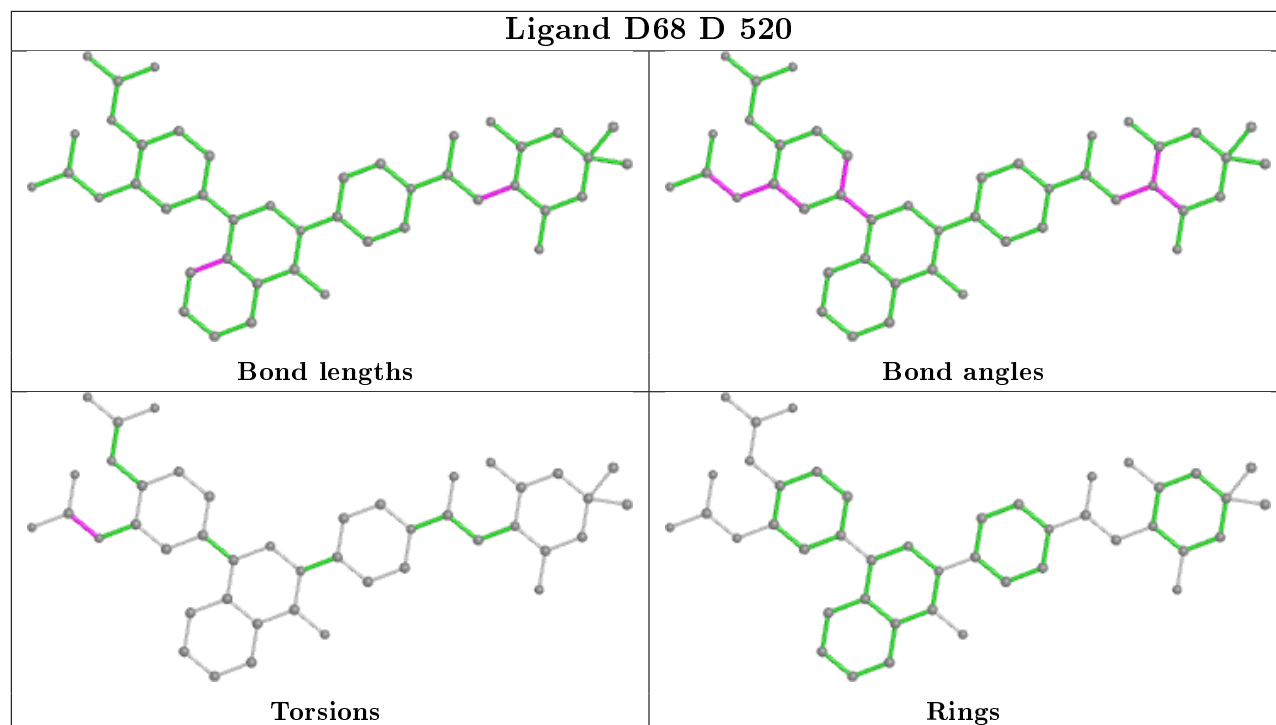
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	512	EPE	1	0
4	D	515	EDO	1	0
4	D	510	EDO	1	0
5	D	519	PEG	2	0
7	A	518	EPE	4	0
4	C	509	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.







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	329/364 (90%)	0.46	33 (10%) 7 7	24, 38, 70, 106	0
1	B	323/364 (88%)	-0.02	7 (2%) 62 63	24, 39, 58, 86	0
1	C	324/364 (89%)	0.20	19 (5%) 22 24	25, 40, 72, 94	0
1	D	324/364 (89%)	-0.07	7 (2%) 62 63	22, 32, 54, 78	0
All	All	1300/1456 (89%)	0.15	66 (5%) 28 29	22, 37, 66, 106	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	SER	7.9
1	A	411	PRO	6.6
1	A	362	ASN	6.3
1	A	363	ALA	5.4
1	C	356	PRO	5.2
1	A	410	ILE	4.8
1	C	410	ILE	4.7
1	A	295	SER	4.6
1	C	411	PRO	4.6
1	A	375	TYR	4.6
1	A	293	THR	4.6
1	C	362	ASN	4.4
1	C	363	ALA	4.3
1	D	363	ALA	4.3
1	D	362	ASN	3.9
1	A	353	GLU	3.9
1	A	361	HIS	3.9
1	A	356	PRO	3.9
1	C	294	SER	3.7
1	C	375	TYR	3.5
1	C	361	HIS	3.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	357	MET	3.1
1	B	90	ASP	3.1
1	D	375	TYR	3.0
1	A	357	MET	3.0
1	B	91	VAL	2.9
1	B	363	ALA	2.9
1	A	364	SER	2.8
1	A	354	ILE	2.8
1	A	360	LYS	2.7
1	C	359	ASP	2.7
1	A	359	ASP	2.6
1	A	219	LEU	2.5
1	B	219	LEU	2.5
1	A	292	VAL	2.5
1	A	291	LYS	2.5
1	A	288	GLU	2.5
1	D	361	HIS	2.5
1	D	364	SER	2.5
1	A	341	PHE	2.5
1	A	289	THR	2.5
1	C	353	GLU	2.5
1	C	409	THR	2.4
1	B	222	MET	2.4
1	A	409	THR	2.4
1	C	289	THR	2.4
1	A	367	LYS	2.4
1	A	236	VAL	2.3
1	C	407	GLN	2.3
1	A	285	THR	2.3
1	A	406	TYR	2.3
1	A	235	ALA	2.3
1	C	367	LYS	2.2
1	B	92	LEU	2.2
1	C	88	GLN	2.2
1	C	404	GLU	2.2
1	C	293	THR	2.1
1	A	238	PHE	2.1
1	A	355	SER	2.1
1	A	368	SER	2.1
1	A	240	LEU	2.1
1	D	240	LEU	2.1
1	C	297	VAL	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	299	LEU	2.0
1	D	410	ILE	2.0
1	B	94	LYS	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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	EDO	B	519	4/4	0.52	0.35	68,75,85,86	0
4	EDO	B	517	4/4	0.56	0.33	75,81,87,89	0
4	EDO	D	524	4/4	0.65	0.25	42,48,54,55	0
4	EDO	B	508	4/4	0.67	0.25	47,55,57,62	0
4	EDO	D	522	4/4	0.73	0.15	63,66,69,71	0
9	PG4	D	502	13/13	0.73	0.27	39,50,65,66	0
5	PEG	A	510	7/7	0.75	0.24	62,72,75,81	0
4	EDO	D	526	4/4	0.75	0.17	55,58,59,65	0
5	PEG	B	512	7/7	0.77	0.21	56,60,62,64	0
5	PEG	C	511	7/7	0.78	0.18	55,67,77,83	0
4	EDO	D	525	4/4	0.79	0.25	68,70,73,75	0
4	EDO	D	509	4/4	0.79	0.19	47,48,54,65	0
4	EDO	C	513	4/4	0.81	0.43	58,66,71,77	0
4	EDO	A	520	4/4	0.84	0.15	59,60,67,75	0
4	EDO	D	514	4/4	0.84	0.14	29,37,48,50	0
4	EDO	A	506	4/4	0.85	0.20	68,68,70,71	0
4	EDO	C	518	4/4	0.85	0.19	57,59,66,72	0
4	EDO	A	503	4/4	0.85	0.17	65,69,70,71	0
4	EDO	C	510	4/4	0.86	0.14	52,56,57,59	0
4	EDO	B	504	4/4	0.86	0.33	53,64,65,65	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	PG4	C	514	13/13	0.87	0.14	61,64,76,88	0
4	EDO	D	513	4/4	0.87	0.18	43,43,50,59	0
4	EDO	A	519	4/4	0.87	0.20	62,66,69,70	0
4	EDO	B	521	4/4	0.87	0.23	39,46,53,53	0
4	EDO	A	504	4/4	0.88	0.22	37,43,43,43	0
4	EDO	B	516	4/4	0.88	0.26	56,61,63,83	0
4	EDO	B	509	4/4	0.89	0.13	45,54,60,66	0
4	EDO	C	501	4/4	0.89	0.27	49,55,59,69	0
4	EDO	D	501	4/4	0.89	0.17	54,58,60,63	0
4	EDO	B	520	4/4	0.89	0.15	38,56,59,61	0
4	EDO	D	518	4/4	0.89	0.12	44,49,53,59	0
4	EDO	B	511	4/4	0.89	0.14	52,59,68,75	0
4	EDO	D	523	4/4	0.90	0.14	58,59,59,63	0
4	EDO	A	516	4/4	0.90	0.17	50,53,55,59	0
4	EDO	A	523	4/4	0.90	0.16	64,73,74,76	0
4	EDO	A	524	4/4	0.90	0.14	39,59,61,67	0
4	EDO	C	506	4/4	0.91	0.18	52,54,65,75	0
4	EDO	A	513	4/4	0.91	0.13	38,42,42,47	0
4	EDO	A	514	4/4	0.91	0.25	48,48,51,57	0
4	EDO	C	508	4/4	0.91	0.28	59,60,64,65	0
4	EDO	A	522	4/4	0.91	0.12	56,60,60,62	0
4	EDO	D	503	4/4	0.92	0.10	54,60,61,62	0
4	EDO	A	509	4/4	0.92	0.13	50,59,59,62	0
4	EDO	C	516	4/4	0.92	0.15	53,54,55,65	0
4	EDO	A	508	4/4	0.92	0.11	37,39,40,46	0
4	EDO	B	506	4/4	0.92	0.13	56,56,57,63	0
4	EDO	A	507	4/4	0.92	0.20	42,59,62,68	0
4	EDO	D	508	4/4	0.93	0.14	51,53,59,64	0
6	D68	A	517	44/44	0.93	0.17	35,42,73,80	0
4	EDO	C	517	4/4	0.93	0.18	44,50,58,69	0
4	EDO	B	518	4/4	0.93	0.15	70,71,71,73	0
6	D68	C	515	44/44	0.93	0.14	33,40,70,81	0
5	PEG	D	519	7/7	0.93	0.18	37,41,51,59	0
4	EDO	A	511	4/4	0.93	0.12	43,48,53,59	0
4	EDO	D	516	4/4	0.94	0.13	34,37,41,50	0
4	EDO	D	511	4/4	0.94	0.26	42,43,47,60	0
4	EDO	C	507	4/4	0.94	0.19	58,62,63,74	0
4	EDO	B	503	4/4	0.94	0.13	44,46,49,49	0
4	EDO	D	510	4/4	0.94	0.12	39,44,53,61	0
4	EDO	B	515	4/4	0.94	0.08	66,68,72,72	0
4	EDO	C	502	4/4	0.94	0.14	49,51,52,63	0
4	EDO	D	517	4/4	0.95	0.14	50,57,62,67	0

*Continued on next page...*

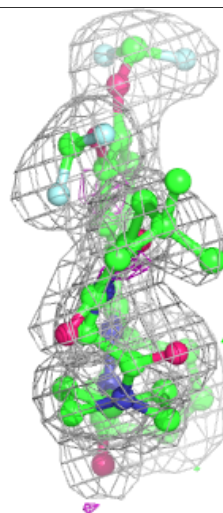
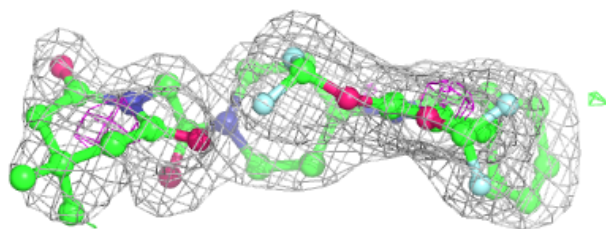
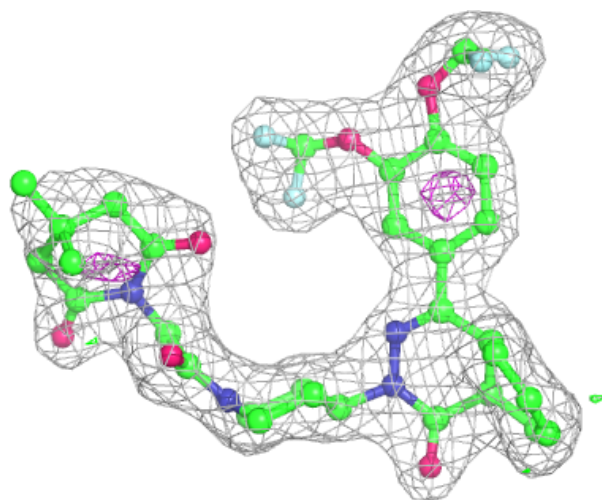
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	A	521	4/4	0.95	0.15	40,53,59,66	0
4	EDO	A	505	4/4	0.95	0.35	54,59,60,66	0
4	EDO	A	515	4/4	0.95	0.15	38,53,57,66	0
4	EDO	D	507	4/4	0.95	0.17	53,56,66,82	0
4	EDO	B	505	4/4	0.95	0.32	60,62,66,67	0
4	EDO	C	503	4/4	0.95	0.12	56,57,66,66	0
6	D68	D	520	44/44	0.95	0.11	29,35,61,67	0
6	D68	B	514	44/44	0.95	0.11	30,36,60,70	0
4	EDO	C	509	4/4	0.95	0.14	62,62,65,83	0
4	EDO	B	522	4/4	0.95	0.11	47,50,50,55	0
4	EDO	D	515	4/4	0.95	0.10	29,44,45,47	0
4	EDO	B	510	4/4	0.96	0.17	43,53,58,59	0
4	EDO	A	512	4/4	0.96	0.15	41,47,50,59	0
7	EPE	B	507	15/15	0.96	0.11	50,56,63,66	0
7	EPE	B	513	15/15	0.96	0.20	47,76,94,100	0
4	EDO	D	506	4/4	0.96	0.10	33,34,37,39	0
7	EPE	A	518	15/15	0.97	0.21	44,81,90,92	0
7	EPE	D	521	15/15	0.97	0.13	38,67,82,84	0
7	EPE	C	512	15/15	0.97	0.13	42,51,65,78	0
3	MG	C	505	1/1	0.98	0.14	23,23,23,23	0
8	NI	D	527	1/1	0.98	0.11	29,29,29,29	1
4	EDO	D	512	4/4	0.98	0.07	46,48,48,49	0
3	MG	D	505	1/1	0.99	0.15	20,20,20,20	0
8	NI	A	525	1/1	0.99	0.07	41,41,41,41	0
3	MG	A	502	1/1	0.99	0.14	23,23,23,23	0
2	ZN	D	504	1/1	1.00	0.11	29,29,29,29	0
3	MG	B	502	1/1	1.00	0.16	22,22,22,22	0
2	ZN	A	501	1/1	1.00	0.08	33,33,33,33	0
2	ZN	B	501	1/1	1.00	0.07	32,32,32,32	0
2	ZN	C	504	1/1	1.00	0.09	34,34,34,34	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.

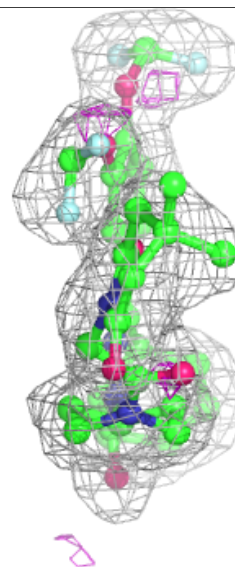
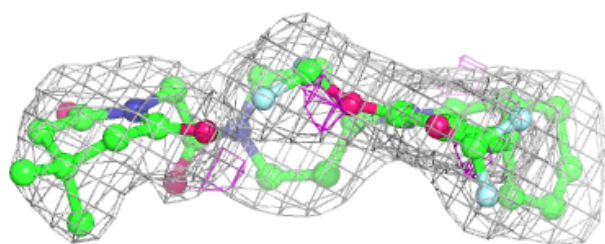
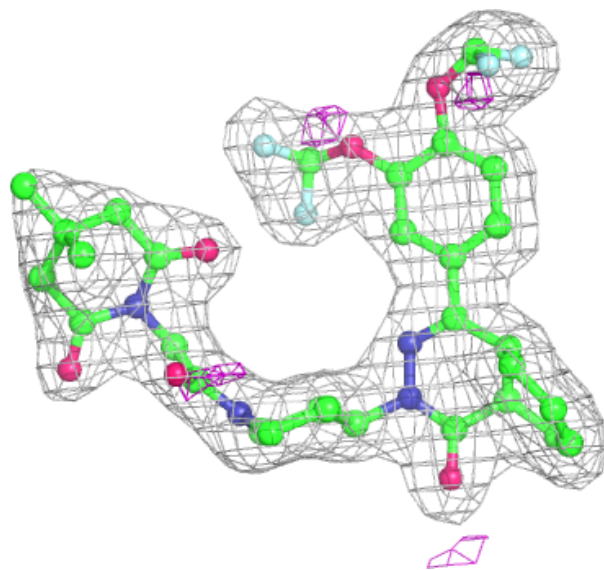
**Electron density around D68 A 517:**

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



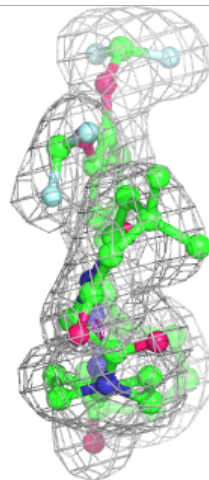
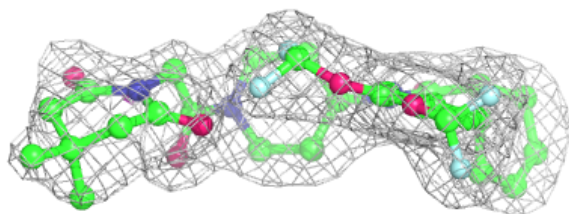
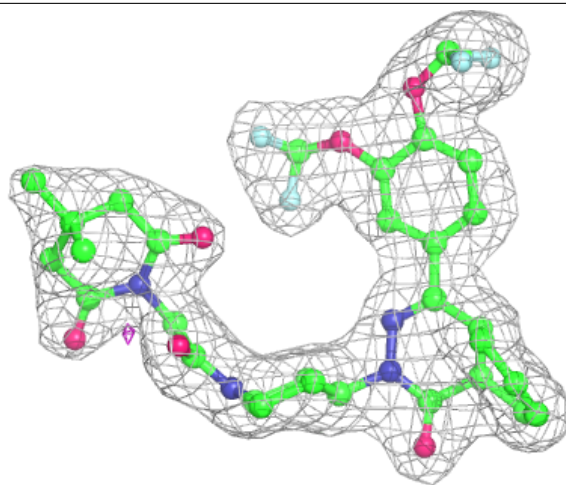
**Electron density around D68 C 515:**

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

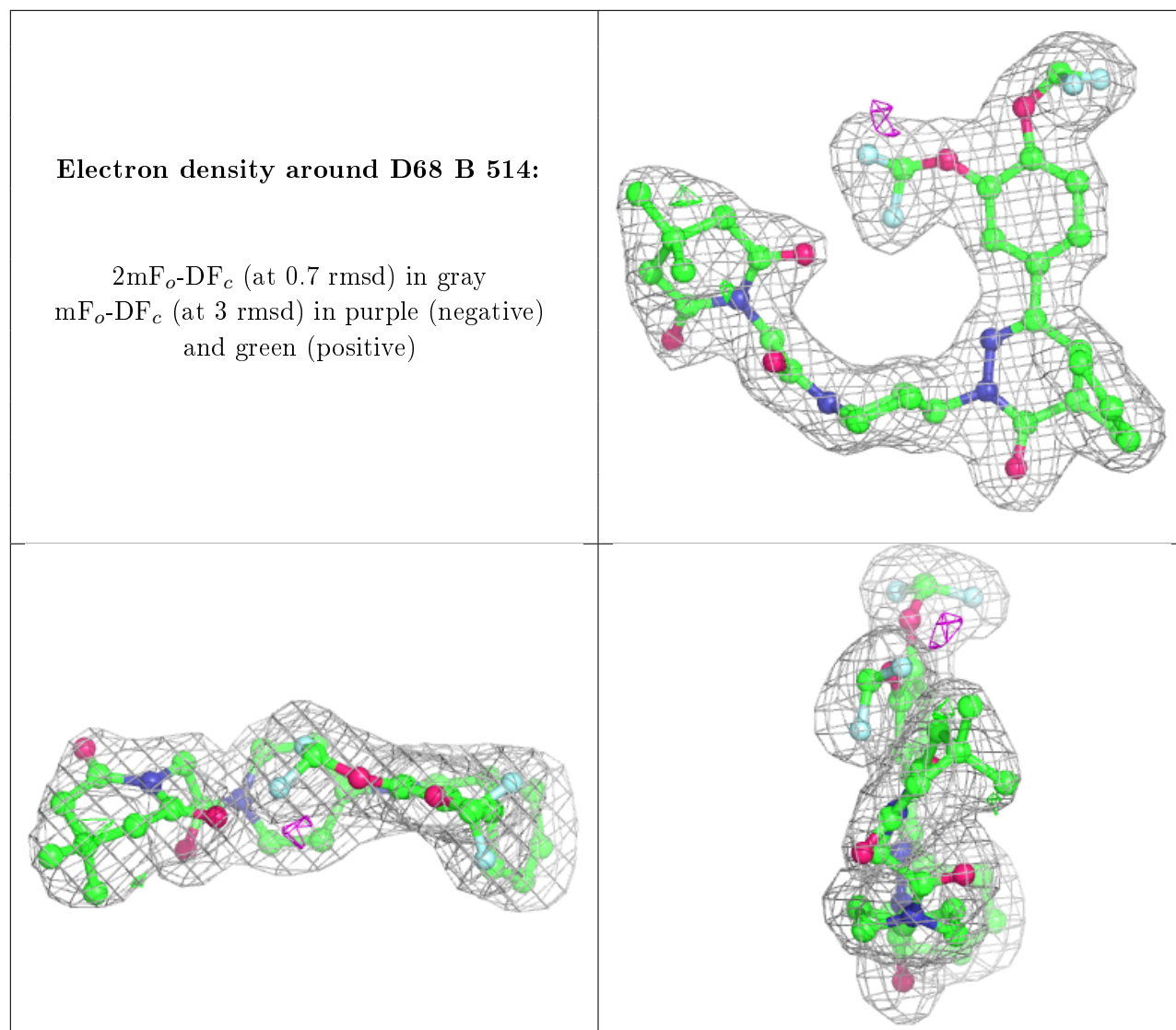


**Electron density around D68 D 520:**

$2mF_o-DF_c$  (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.