



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 09:30 pm BST

PDB ID : 6FE7
Title : Crystal structure of human phosphodiesterase 4D2 catalytic domain with inhibitor NPD-356
Authors : Singh, A.K.; Brown, D.G.
Deposited on : 2017-12-29
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

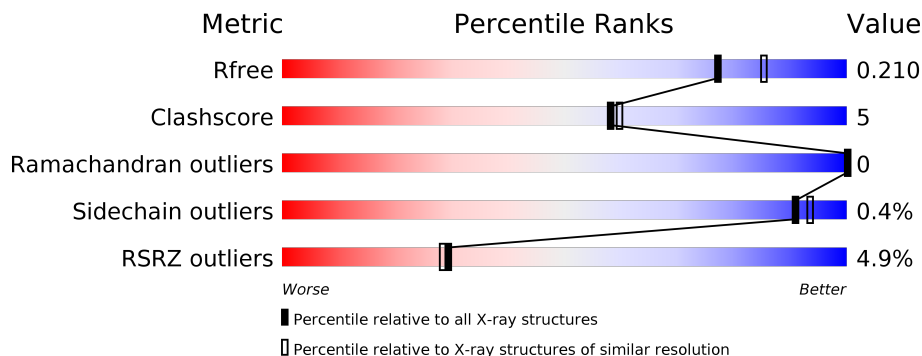
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	
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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	C	512	-	-	-	X
4	EDO	D	522	-	X	-	-
8	PG4	C	521	-	-	X	-

2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 11789 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	330	2669	1690	455	510	14	0	0	0
1	B	323	2619	1657	447	501	14	0	1	0
1	C	324	2622	1659	448	501	14	0	0	0
1	D	324	2622	1659	448	501	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

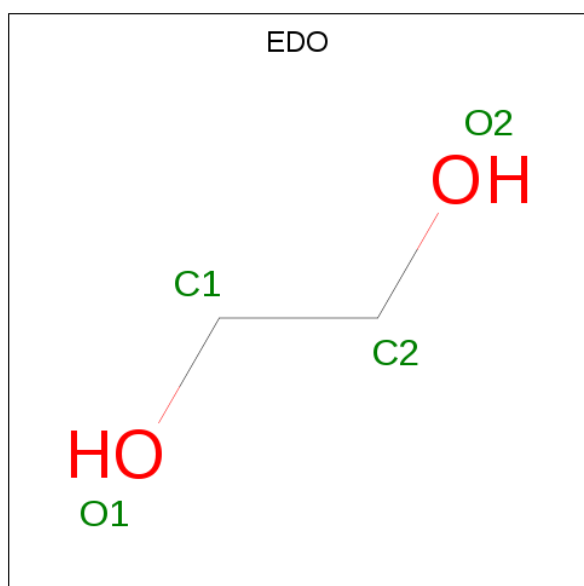
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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: C₂H₆O₂).



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

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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	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		

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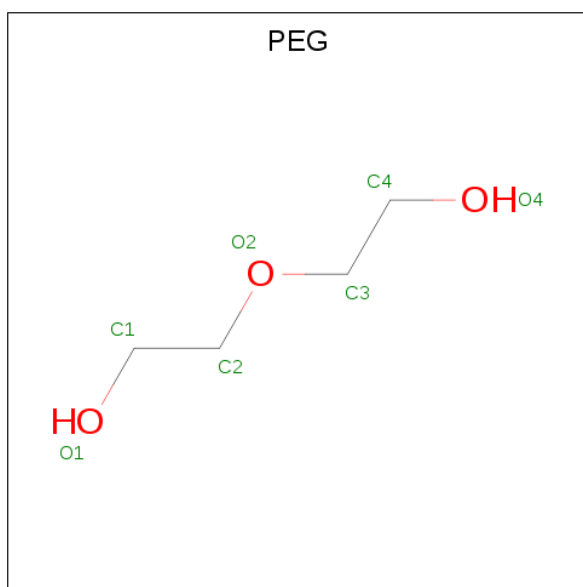
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total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

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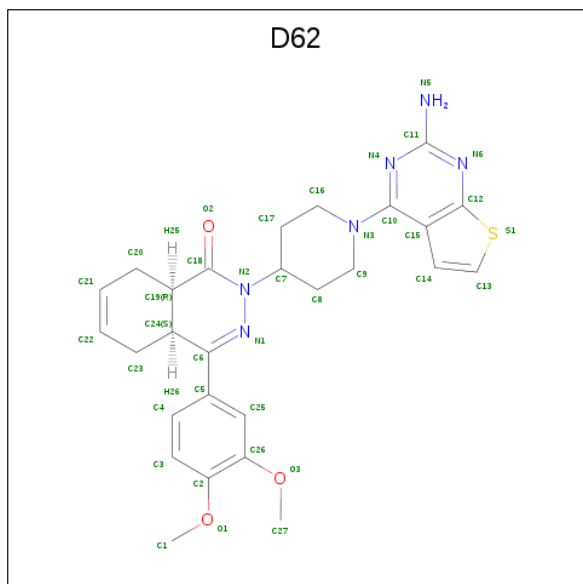
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	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 DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



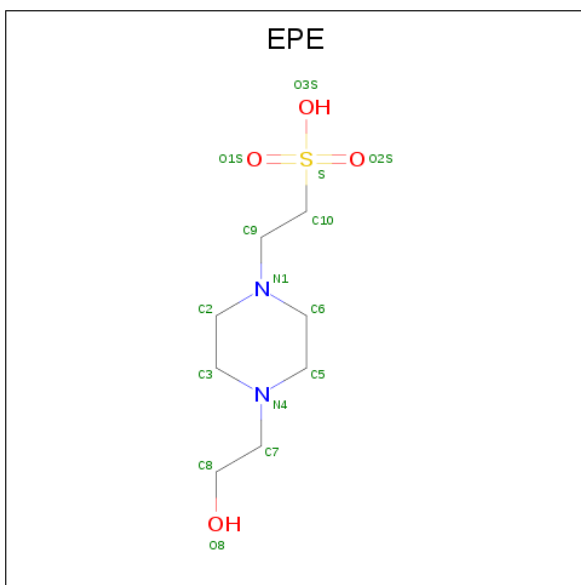
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0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

- Molecule 6 is (4a*S*,8a*R*)-2-(1-{2-aminothieno[2,3-*d*]pyrimidin-4-yl}piperidin-4-yl)-4-(3,4-dimethoxyphenyl)-1,2,4a,5,8,8a-hexahydrophthalazin-1-one (three-letter code: D62) (formula: C₂₇H₃₀N₆O₃S).



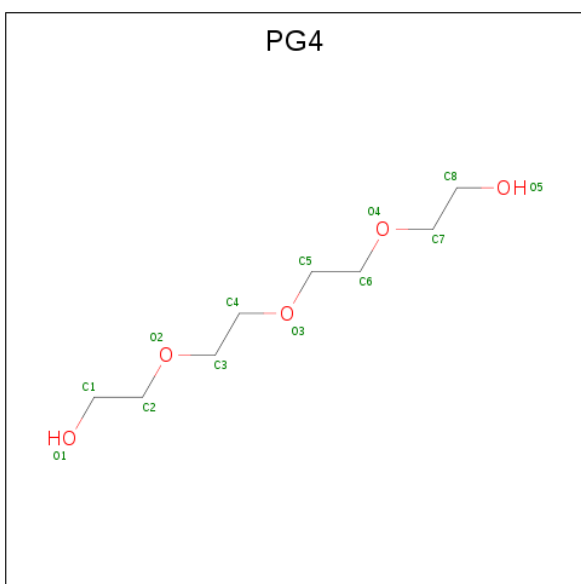
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	A	1	Total	C	N	O	S	0	0
			37	27	6	3	1		
6	B	1	Total	C	N	O	S	0	0
			37	27	6	3	1		
6	C	1	Total	C	N	O	S	0	0
			37	27	6	3	1		
6	D	1	Total	C	N	O	S	0	0
			37	27	6	3	1		

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



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

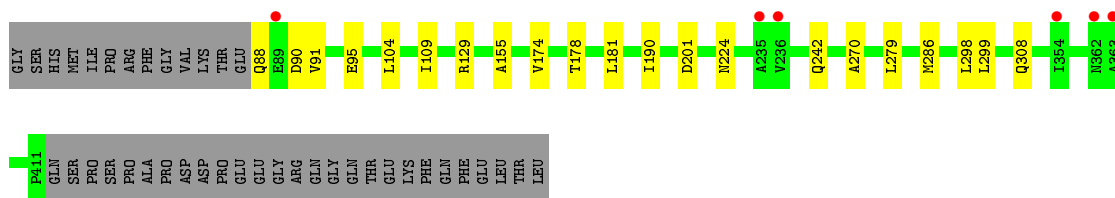
- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	172	Total	O	0	0
			172	172		
9	B	182	Total	O	0	0
			182	182		
9	C	119	Total	O	0	0
			119	119		
9	D	197	Total	O	0	0
			197	197		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.22Å 111.03Å 160.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.30 – 2.00 54.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.30-2.00) 100.0 (54.30-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.170 , 0.200 0.182 , 0.210	Depositor DCC
R_{free} test set	6067 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtrriage
Anisotropy	0.192	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11789	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: ZN, PEG, MG, EDO, PG4, EPE, D62

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	0.97	1/2724 (0.0%)	0.88	5/3700 (0.1%)
1	B	0.88	0/2673	0.83	0/3632
1	C	0.86	1/2676 (0.0%)	0.84	1/3636 (0.0%)
1	D	0.91	1/2676 (0.0%)	0.87	1/3636 (0.0%)
All	All	0.91	3/10749 (0.0%)	0.85	7/14604 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	GLU	CD-OE1	-5.47	1.19	1.25
1	D	95	GLU	CD-OE2	-5.13	1.20	1.25
1	C	364	SER	CB-OG	5.11	1.48	1.42

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ASP	CB-CG-OD2	12.36	129.42	118.30
1	A	201	ASP	CB-CG-OD1	-9.67	109.59	118.30
1	A	330	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	C	350	ARG	NE-CZ-NH1	-7.17	116.72	120.30
1	A	330	ARG	NE-CZ-NH2	5.78	123.19	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	2669	0	2625	21	0
1	B	2619	0	2574	18	0
1	C	2622	0	2578	43	0
1	D	2622	0	2578	19	0
2	A	1	0	0	1	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	60	0	90	4	0
4	B	60	0	90	1	0
4	C	56	0	84	3	0
4	D	56	0	84	4	0
5	A	42	0	60	5	0
5	B	7	0	10	2	0
5	C	14	0	20	3	0
5	D	35	0	50	2	0
6	A	37	0	0	2	0
6	B	37	0	0	0	0
6	C	37	0	0	0	0
6	D	37	0	0	0	0
7	A	15	0	18	1	0
7	B	30	0	36	4	0
7	C	15	0	18	4	0
7	D	15	0	17	2	0
8	C	26	0	36	14	0
9	A	172	0	0	2	0
9	B	182	0	0	4	0
9	C	119	0	0	3	0
9	D	197	0	0	0	0
All	All	11789	0	10968	107	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 5.

The worst 5 of 107 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:C:111:GLU:OE2	7:C:514:EPE:H32	1.65	0.95
1:B:111:GLU:OE1	7:B:521:EPE:H72	1.74	0.87
1:B:386:ASP:OD2	4:B:504:EDO:H22	1.75	0.87
1:C:116:ARG:HE	1:C:147:MET:CE	1.90	0.84
1:A:342:ARG:NH2	1:A:346:ARG:HH21	1.76	0.83

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	328/364 (90%)	321 (98%)	7 (2%)	0	100	100
1	B	322/364 (88%)	317 (98%)	5 (2%)	0	100	100
1	C	322/364 (88%)	318 (99%)	4 (1%)	0	100	100
1	D	322/364 (88%)	316 (98%)	6 (2%)	0	100	100
All	All	1294/1456 (89%)	1272 (98%)	22 (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	301/331 (91%)	300 (100%)	1 (0%)	92	95
1	B	296/331 (89%)	295 (100%)	1 (0%)	92	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	296/331 (89%)	293 (99%)	3 (1%)	76	81
1	D	296/331 (89%)	296 (100%)	0	100	100
All	All	1189/1324 (90%)	1184 (100%)	5 (0%)	91	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	LEU
1	B	89	GLU
1	C	94	LYS
1	C	116	ARG
1	C	330	ARG

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

Mol	Chain	Res	Type
1	A	224	ASN
1	A	308	GLN
1	B	231	ASN

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 91 ligands modelled in this entry, 8 are monoatomic - leaving 83 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	503	-	3,3,3	0.42	0	2,2,2	0.47	0
4	EDO	A	507	-	3,3,3	0.29	0	2,2,2	1.50	0
4	EDO	C	507	-	3,3,3	0.43	0	2,2,2	0.41	0
4	EDO	B	505	-	3,3,3	0.45	0	2,2,2	0.52	0
4	EDO	A	521	-	3,3,3	0.52	0	2,2,2	0.76	0
5	PEG	A	511	-	6,6,6	0.40	0	5,5,5	0.59	0
5	PEG	A	518	-	6,6,6	0.61	0	5,5,5	0.68	0
4	EDO	A	515	-	3,3,3	1.18	0	2,2,2	0.43	0
5	PEG	D	518	-	6,6,6	1.08	0	5,5,5	1.30	0
6	D62	C	520	-	40,42,42	0.74	2 (5%)	45,61,61	1.21	3 (6%)
4	EDO	D	505	-	3,3,3	0.49	0	2,2,2	0.45	0
4	EDO	A	509	-	3,3,3	0.54	0	2,2,2	0.37	0
4	EDO	C	512	-	3,3,3	0.96	0	2,2,2	0.69	0
5	PEG	B	508	-	6,6,6	0.77	0	5,5,5	1.39	1 (20%)
4	EDO	D	514	-	3,3,3	1.04	0	2,2,2	0.58	0
4	EDO	C	509	-	3,3,3	0.30	0	2,2,2	0.43	0
4	EDO	A	523	-	3,3,3	0.50	0	2,2,2	0.88	0
4	EDO	C	510	-	3,3,3	0.18	0	2,2,2	0.92	0
4	EDO	B	504	-	3,3,3	0.27	0	2,2,2	0.62	0
7	EPE	B	509	-	15,15,15	1.33	1 (6%)	18,20,20	2.44	7 (38%)
6	D62	D	517	-	40,42,42	0.83	1 (2%)	45,61,61	1.33	3 (6%)
4	EDO	A	514	-	3,3,3	0.53	0	2,2,2	0.78	0
5	PEG	A	510	-	6,6,6	0.51	0	5,5,5	0.73	0
7	EPE	B	521	-	15,15,15	2.04	1 (6%)	18,20,20	1.12	3 (16%)
4	EDO	D	520	-	3,3,3	0.32	0	2,2,2	0.90	0
4	EDO	A	508	-	3,3,3	0.44	0	2,2,2	0.38	0
6	D62	A	520	-	40,42,42	0.82	2 (5%)	45,61,61	1.17	5 (11%)
4	EDO	D	506	-	3,3,3	0.32	0	2,2,2	1.15	0
5	PEG	A	517	-	6,6,6	0.53	0	5,5,5	0.52	0
4	EDO	D	515	-	3,3,3	0.46	0	2,2,2	1.32	0
4	EDO	B	503	-	3,3,3	0.43	0	2,2,2	1.19	0
4	EDO	B	506	-	3,3,3	0.37	0	2,2,2	1.48	1 (50%)
4	EDO	D	521	-	3,3,3	0.61	0	2,2,2	0.88	0
4	EDO	C	501	-	3,3,3	0.54	0	2,2,2	0.19	0
4	EDO	B	507	-	3,3,3	0.29	0	2,2,2	1.55	0
8	PG4	C	502	-	12,12,12	1.03	0	11,11,11	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	507	-	3,3,3	0.46	0	2,2,2	0.46	0
5	PEG	A	516	-	6,6,6	0.72	0	5,5,5	1.15	0
4	EDO	A	512	-	3,3,3	0.31	0	2,2,2	1.23	0
5	PEG	C	519	-	6,6,6	0.91	0	5,5,5	1.22	0
4	EDO	A	504	-	3,3,3	0.40	0	2,2,2	0.92	0
4	EDO	D	504	-	3,3,3	0.77	0	2,2,2	0.21	0
5	PEG	A	519	-	6,6,6	0.43	0	5,5,5	0.45	0
4	EDO	D	512	-	3,3,3	0.47	0	2,2,2	0.23	0
5	PEG	D	509	-	6,6,6	0.98	0	5,5,5	1.64	1 (20%)
4	EDO	D	501	-	3,3,3	0.76	0	2,2,2	0.36	0
4	EDO	B	520	-	3,3,3	0.42	0	2,2,2	0.64	0
4	EDO	A	505	-	3,3,3	0.51	0	2,2,2	0.25	0
5	PEG	D	519	-	6,6,6	0.48	0	5,5,5	1.28	0
4	EDO	B	512	-	3,3,3	0.09	0	2,2,2	1.11	0
4	EDO	C	511	-	3,3,3	0.61	0	2,2,2	0.64	0
4	EDO	B	518	-	3,3,3	0.83	0	2,2,2	0.28	0
8	PG4	C	521	-	12,12,12	1.26	2 (16%)	11,11,11	1.58	2 (18%)
4	EDO	A	506	-	3,3,3	0.71	0	2,2,2	1.03	0
4	EDO	D	513	-	3,3,3	0.79	0	2,2,2	1.16	0
5	PEG	D	510	-	6,6,6	0.34	0	5,5,5	0.89	0
7	EPE	D	523	-	15,15,15	2.99	4 (26%)	18,20,20	1.82	6 (33%)
4	EDO	B	517	-	3,3,3	0.19	0	2,2,2	1.37	0
4	EDO	B	510	-	3,3,3	0.48	0	2,2,2	0.87	0
4	EDO	C	504	-	3,3,3	0.44	0	2,2,2	0.16	0
4	EDO	C	517	-	3,3,3	0.32	0	2,2,2	0.69	0
4	EDO	B	513	-	3,3,3	0.58	0	2,2,2	0.68	0
4	EDO	A	522	-	3,3,3	0.58	0	2,2,2	0.47	0
4	EDO	A	503	-	3,3,3	0.36	0	2,2,2	0.73	0
6	D62	B	516	-	40,42,42	0.76	1 (2%)	45,61,61	1.14	6 (13%)
4	EDO	A	525	-	3,3,3	0.77	0	2,2,2	0.11	0
4	EDO	C	522	-	3,3,3	0.45	0	2,2,2	0.47	0
7	EPE	C	514	-	15,15,15	2.03	1 (6%)	18,20,20	1.10	3 (16%)
4	EDO	C	515	-	3,3,3	0.86	0	2,2,2	0.34	0
4	EDO	D	511	-	3,3,3	0.47	0	2,2,2	0.86	0
4	EDO	C	508	-	3,3,3	0.47	0	2,2,2	0.62	0
4	EDO	B	514	-	3,3,3	0.77	0	2,2,2	0.29	0
4	EDO	B	511	-	3,3,3	0.69	0	2,2,2	1.20	0
4	EDO	C	516	-	3,3,3	1.03	0	2,2,2	0.88	0
7	EPE	A	524	-	15,15,15	2.38	1 (6%)	18,20,20	2.82	7 (38%)
4	EDO	B	515	-	3,3,3	0.36	0	2,2,2	0.53	0
4	EDO	C	518	-	3,3,3	0.29	0	2,2,2	0.69	0
5	PEG	C	513	-	6,6,6	0.52	0	5,5,5	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	513	-	3,3,3	0.27	0	2,2,2	1.50	1 (50%)
4	EDO	B	519	-	3,3,3	0.29	0	2,2,2	1.12	0
4	EDO	D	522	-	3,3,3	2.63	3 (100%)	2,2,2	2.36	2 (100%)
5	PEG	D	508	-	6,6,6	0.49	0	5,5,5	1.21	0
4	EDO	D	516	-	3,3,3	0.51	0	2,2,2	1.29	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	503	-	-	1/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
4	EDO	C	507	-	-	1/1/1/1	-
4	EDO	B	505	-	-	1/1/1/1	-
4	EDO	A	521	-	-	1/1/1/1	-
5	PEG	A	511	-	-	4/4/4/4	-
5	PEG	A	518	-	-	2/4/4/4	-
4	EDO	A	515	-	-	0/1/1/1	-
5	PEG	D	518	-	-	1/4/4/4	-
6	D62	C	520	-	-	2/16/53/53	0/6/6/6
4	EDO	D	505	-	-	0/1/1/1	-
4	EDO	A	509	-	-	1/1/1/1	-
4	EDO	C	512	-	-	1/1/1/1	-
5	PEG	B	508	-	-	1/4/4/4	-
4	EDO	D	514	-	-	0/1/1/1	-
4	EDO	C	509	-	-	0/1/1/1	-
4	EDO	A	523	-	-	1/1/1/1	-
4	EDO	C	510	-	-	1/1/1/1	-
4	EDO	B	504	-	-	1/1/1/1	-
7	EPE	B	509	-	-	3/9/19/19	0/1/1/1
6	D62	D	517	-	-	2/16/53/53	0/6/6/6
4	EDO	A	514	-	-	1/1/1/1	-
5	PEG	A	510	-	-	3/4/4/4	-
7	EPE	B	521	-	-	2/9/19/19	0/1/1/1
4	EDO	D	520	-	-	1/1/1/1	-
4	EDO	A	508	-	-	1/1/1/1	-
6	D62	A	520	-	-	1/16/53/53	0/6/6/6
4	EDO	D	506	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	517	-	-	3/4/4/4	-
4	EDO	D	515	-	-	1/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	B	506	-	-	0/1/1/1	-
4	EDO	D	521	-	-	1/1/1/1	-
4	EDO	C	501	-	-	1/1/1/1	-
4	EDO	B	507	-	-	1/1/1/1	-
8	PG4	C	502	-	-	5/10/10/10	-
4	EDO	D	507	-	-	1/1/1/1	-
5	PEG	A	516	-	-	3/4/4/4	-
4	EDO	A	512	-	-	0/1/1/1	-
5	PEG	C	519	-	-	2/4/4/4	-
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	D	504	-	-	0/1/1/1	-
5	PEG	A	519	-	-	1/4/4/4	-
4	EDO	D	512	-	-	1/1/1/1	-
5	PEG	D	509	-	-	3/4/4/4	-
4	EDO	D	501	-	-	1/1/1/1	-
4	EDO	B	520	-	-	1/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-
5	PEG	D	519	-	-	3/4/4/4	-
4	EDO	B	512	-	-	1/1/1/1	-
4	EDO	C	511	-	-	0/1/1/1	-
4	EDO	B	518	-	-	1/1/1/1	-
8	PG4	C	521	-	-	7/10/10/10	-
4	EDO	A	506	-	-	0/1/1/1	-
4	EDO	D	513	-	-	0/1/1/1	-
5	PEG	D	510	-	-	0/4/4/4	-
7	EPE	D	523	-	-	3/9/19/19	0/1/1/1
4	EDO	B	517	-	-	0/1/1/1	-
4	EDO	B	510	-	-	0/1/1/1	-
4	EDO	C	504	-	-	1/1/1/1	-
4	EDO	C	517	-	-	1/1/1/1	-
4	EDO	B	513	-	-	0/1/1/1	-
4	EDO	A	522	-	-	1/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
6	D62	B	516	-	-	2/16/53/53	0/6/6/6
4	EDO	A	525	-	-	0/1/1/1	-
4	EDO	C	522	-	-	0/1/1/1	-
7	EPE	C	514	-	-	6/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	515	-	-	0/1/1/1	-
4	EDO	D	511	-	-	1/1/1/1	-
4	EDO	C	508	-	-	1/1/1/1	-
4	EDO	B	514	-	-	0/1/1/1	-
4	EDO	B	511	-	-	1/1/1/1	-
4	EDO	C	516	-	-	0/1/1/1	-
7	EPE	A	524	-	-	3/9/19/19	0/1/1/1
4	EDO	B	515	-	-	1/1/1/1	-
4	EDO	C	518	-	-	1/1/1/1	-
5	PEG	C	513	-	-	3/4/4/4	-
4	EDO	A	513	-	-	0/1/1/1	-
4	EDO	B	519	-	-	1/1/1/1	-
4	EDO	D	522	-	-	0/1/1/1	-
5	PEG	D	508	-	-	3/4/4/4	-
4	EDO	D	516	-	-	0/1/1/1	-

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	523	EPE	C10-S	-10.83	1.62	1.77
7	A	524	EPE	C10-S	-8.72	1.65	1.77
7	C	514	EPE	C10-S	-7.66	1.66	1.77
7	B	521	EPE	C10-S	-7.66	1.66	1.77
7	B	509	EPE	C10-S	-4.18	1.71	1.77

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	524	EPE	O3S-S-C10	7.35	117.65	105.77
7	A	524	EPE	O2S-S-C10	-6.90	98.60	106.92
7	B	509	EPE	O2S-S-C10	4.93	112.85	106.92
7	B	509	EPE	O1S-S-C10	4.90	112.81	106.92
6	D	517	D62	C8-C7-N2	-4.25	106.15	110.86

There are no chirality outliers.

5 of 101 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	516	D62	N4-C10-N3-C9
4	D	507	EDO	O1-C1-C2-O2
7	C	514	EPE	C10-C9-N1-C6

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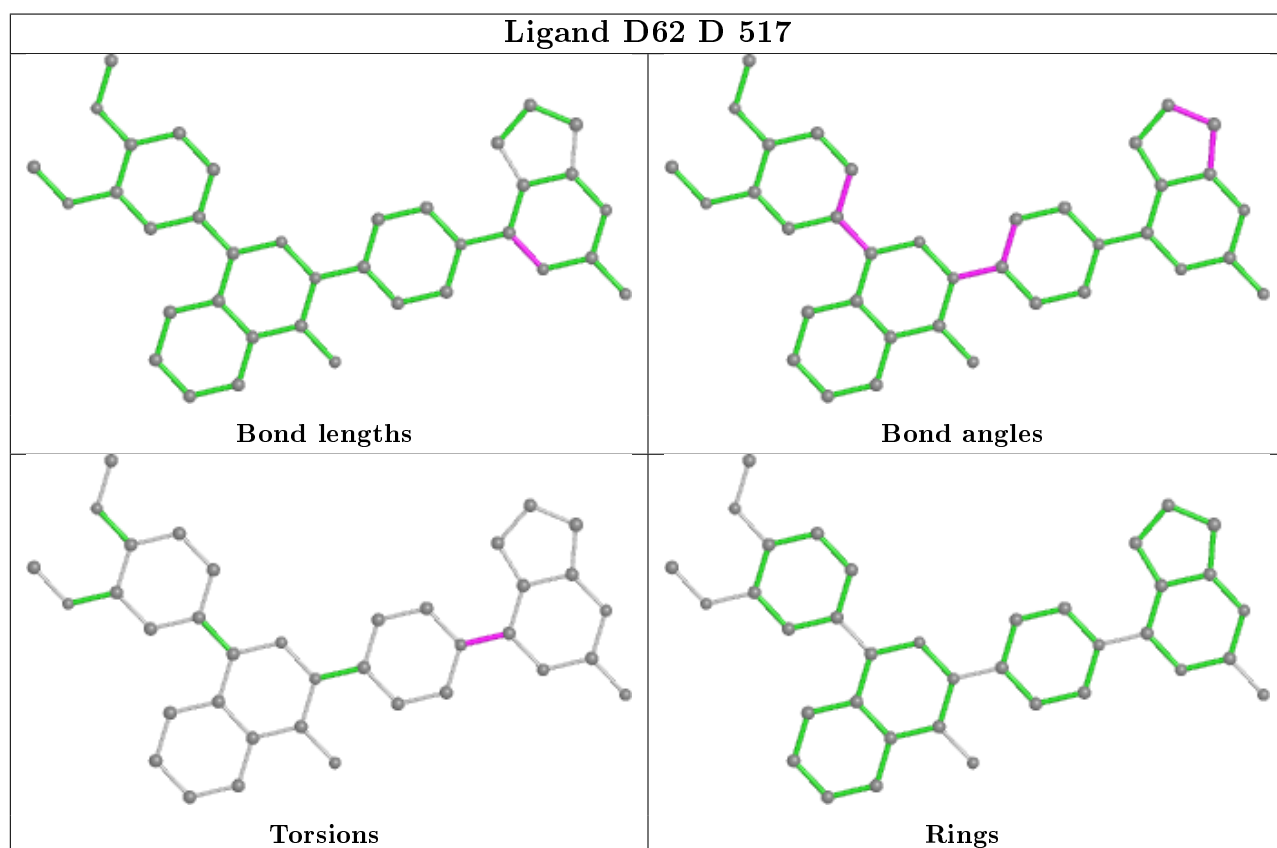
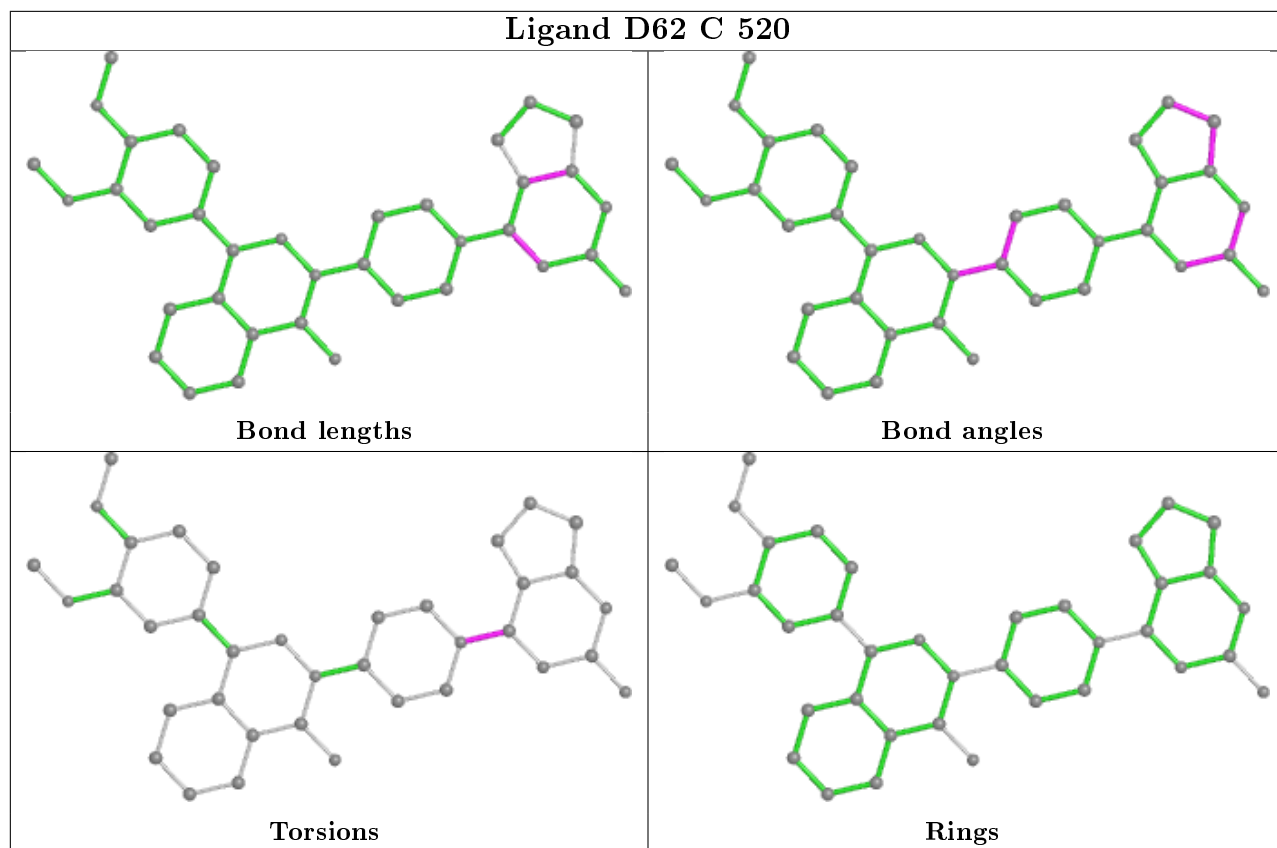
Mol	Chain	Res	Type	Atoms
7	C	514	EPE	S-C10-C9-N1
7	C	514	EPE	C9-C10-S-O2S

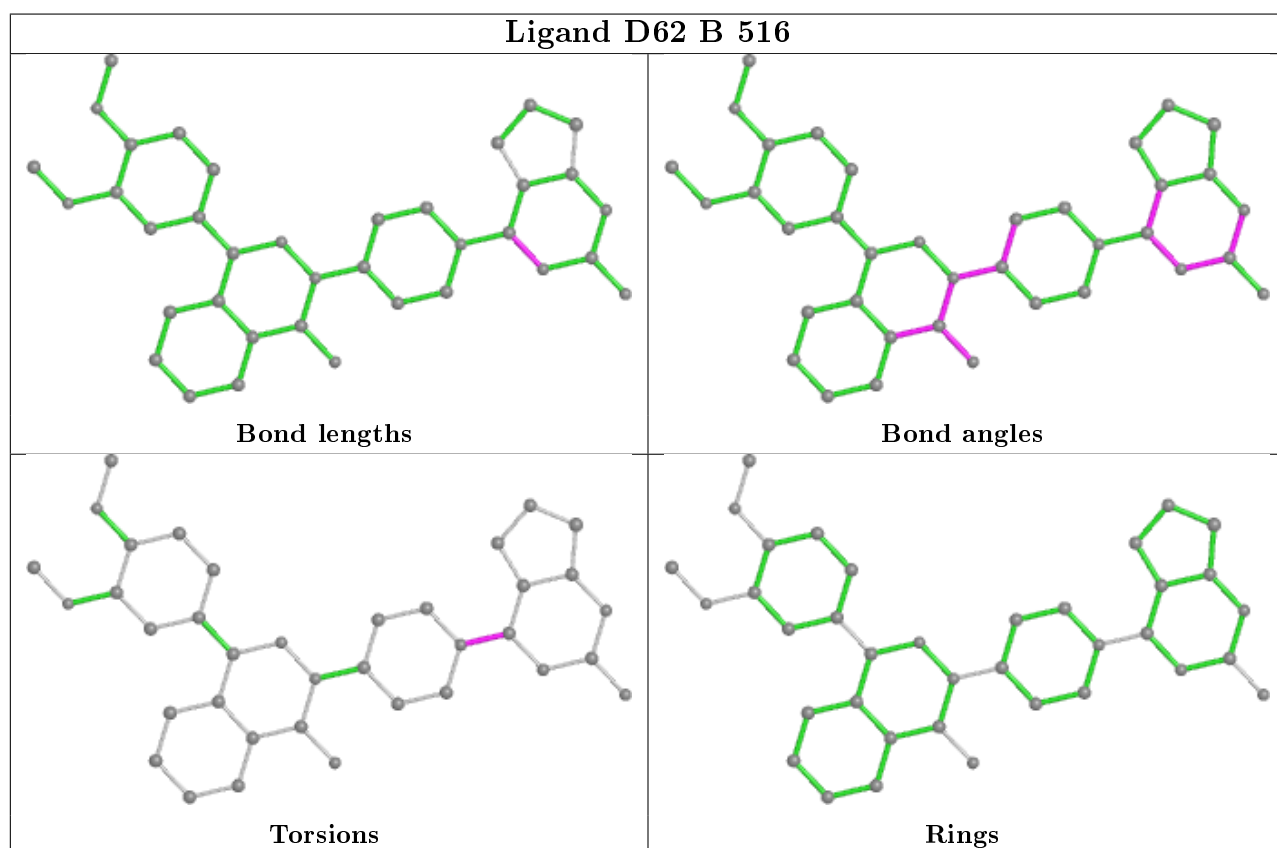
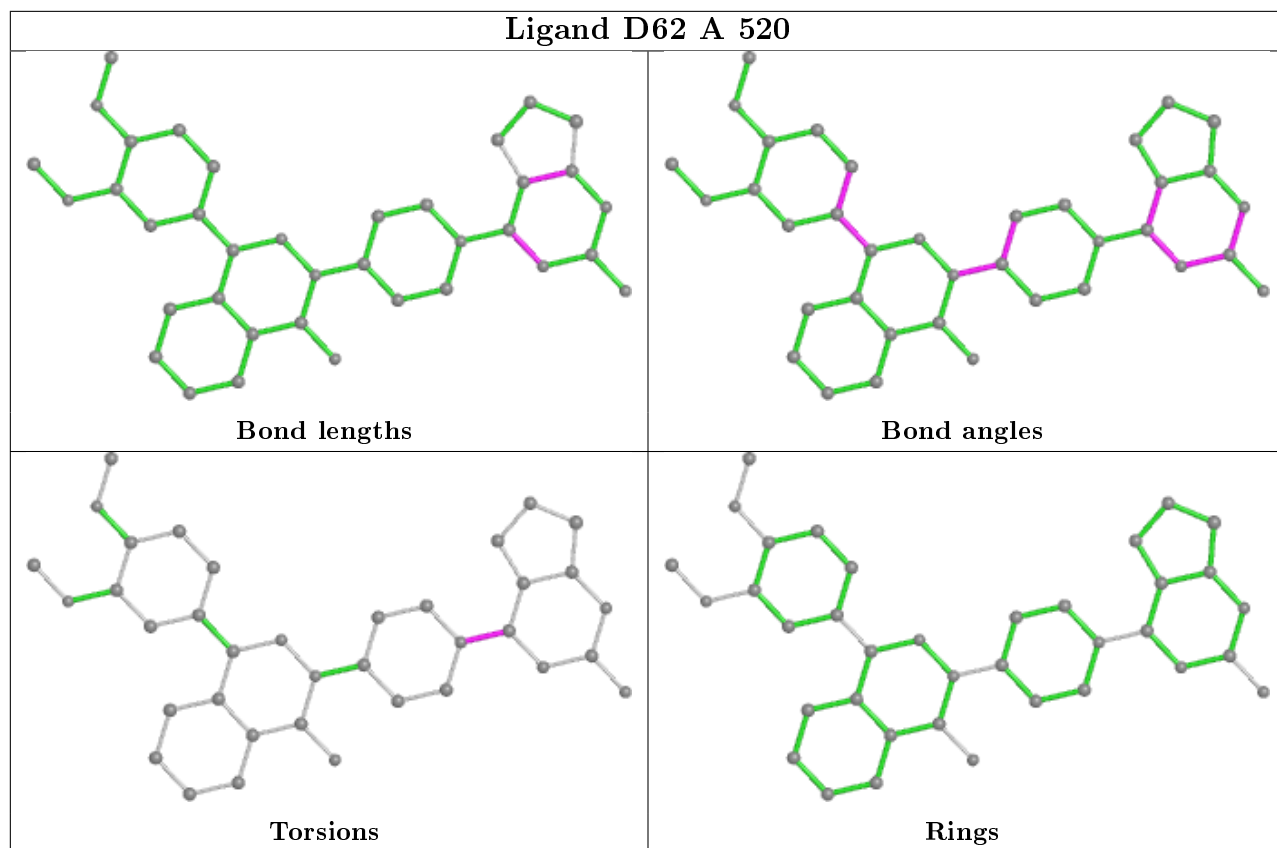
There are no ring outliers.

21 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	521	EDO	1	0
5	A	518	PEG	1	0
5	B	508	PEG	2	0
4	C	509	EDO	1	0
4	B	504	EDO	1	0
7	B	521	EPE	4	0
4	A	508	EDO	1	0
6	A	520	D62	2	0
5	A	517	PEG	2	0
4	D	521	EDO	3	0
8	C	502	PG4	4	0
5	A	516	PEG	2	0
5	C	519	PEG	3	0
5	D	519	PEG	2	0
8	C	521	PG4	10	0
4	D	513	EDO	1	0
7	D	523	EPE	2	0
4	A	525	EDO	2	0
7	C	514	EPE	4	0
4	C	515	EDO	2	0
7	A	524	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	330/364 (90%)	0.38	30 (9%) 9 8	24, 37, 67, 98	0
1	B	323/364 (88%)	0.12	10 (3%) 49 48	25, 40, 60, 91	0
1	C	324/364 (89%)	0.21	18 (5%) 24 23	25, 40, 73, 92	0
1	D	324/364 (89%)	-0.09	6 (1%) 66 65	23, 31, 54, 83	0
All	All	1301/1456 (89%)	0.16	64 (4%) 29 28	23, 37, 65, 98	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	294	SER	6.1
1	A	411	PRO	5.8
1	A	362	ASN	5.3
1	A	410	ILE	4.8
1	C	363	ALA	4.6

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, 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(\AA^2)	Q<0.9
4	EDO	C	512	4/4	0.63	0.58	63,68,70,75	0
4	EDO	A	525	4/4	0.69	0.35	58,64,64,70	0
5	PEG	C	519	7/7	0.71	0.24	43,57,66,75	0
5	PEG	D	518	7/7	0.75	0.19	50,56,60,68	0
8	PG4	C	502	13/13	0.76	0.33	46,73,84,85	0
4	EDO	B	514	4/4	0.76	0.21	57,62,69,69	0
5	PEG	D	509	7/7	0.78	0.29	44,55,69,75	0
5	PEG	A	511	7/7	0.79	0.28	44,68,77,80	0
4	EDO	D	522	4/4	0.79	0.21	39,40,45,48	0
4	EDO	A	509	4/4	0.79	0.23	66,67,72,76	0
5	PEG	A	519	7/7	0.80	0.16	58,64,71,73	0
4	EDO	D	506	4/4	0.80	0.24	51,52,53,61	0
5	PEG	D	508	7/7	0.81	0.18	43,60,69,72	0
8	PG4	C	521	13/13	0.81	0.28	38,46,59,65	0
4	EDO	B	517	4/4	0.82	0.37	66,69,75,79	0
4	EDO	D	513	4/4	0.82	0.23	43,45,47,55	0
4	EDO	B	505	4/4	0.82	0.23	54,58,63,63	0
4	EDO	C	503	4/4	0.83	0.83	73,78,78,84	0
5	PEG	A	510	7/7	0.84	0.19	55,71,76,78	0
5	PEG	A	518	7/7	0.84	0.38	59,63,70,71	0
4	EDO	B	510	4/4	0.84	0.62	54,57,62,62	0
4	EDO	B	504	4/4	0.84	0.30	70,75,77,82	0
4	EDO	A	508	4/4	0.85	0.31	60,69,69,80	0
4	EDO	C	501	4/4	0.85	0.48	48,48,60,66	0
4	EDO	D	515	4/4	0.86	0.25	53,65,68,76	0
4	EDO	B	518	4/4	0.86	0.35	48,54,57,67	0
4	EDO	C	516	4/4	0.86	0.16	43,47,50,52	0
4	EDO	C	515	4/4	0.86	0.25	58,66,70,70	0
5	PEG	B	508	7/7	0.86	0.40	49,67,72,80	0
4	EDO	D	520	4/4	0.87	0.20	64,65,68,74	0
6	D62	A	520	37/37	0.87	0.18	32,40,96,104	0
4	EDO	C	510	4/4	0.87	0.23	59,67,72,72	0
4	EDO	C	518	4/4	0.88	0.18	64,64,67,77	0
4	EDO	B	513	4/4	0.88	0.55	47,55,62,63	0
4	EDO	B	511	4/4	0.88	0.27	52,58,58,62	0
4	EDO	D	521	4/4	0.89	0.24	34,42,48,51	0
4	EDO	A	503	4/4	0.89	0.23	51,53,54,56	0
6	D62	C	520	37/37	0.90	0.15	33,39,100,107	0
5	PEG	A	516	7/7	0.90	0.20	39,59,73,75	0
4	EDO	A	521	4/4	0.90	0.14	54,65,68,78	0
4	EDO	C	508	4/4	0.90	0.16	57,58,63,66	0
4	EDO	A	522	4/4	0.90	0.47	49,56,64,69	0
4	EDO	B	515	4/4	0.90	0.20	50,54,61,65	0

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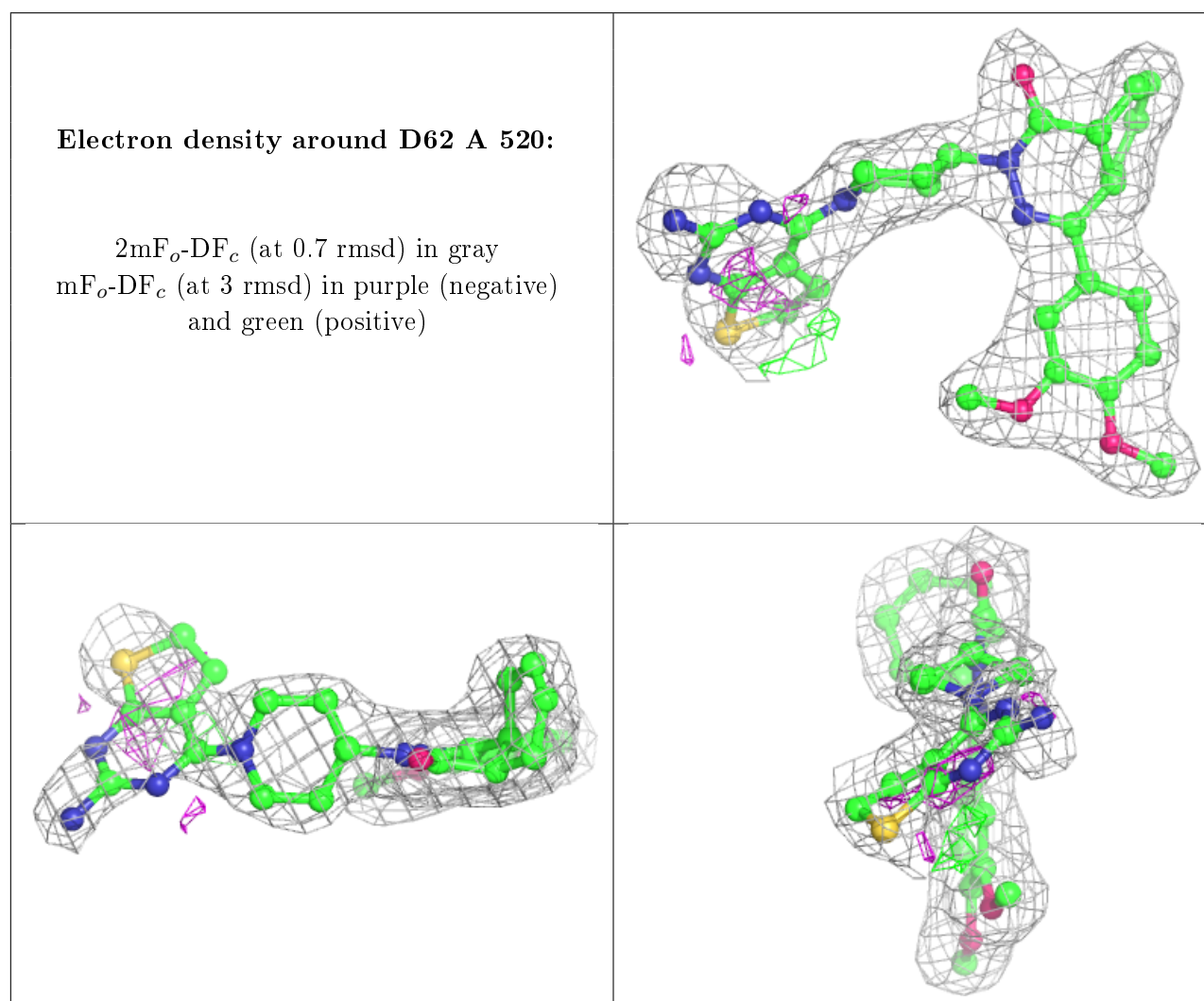
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	A	523	4/4	0.90	0.23	51,56,56,58	0
4	EDO	B	512	4/4	0.90	0.16	60,62,67,80	0
4	EDO	A	514	4/4	0.91	0.13	49,50,55,57	0
5	PEG	C	513	7/7	0.91	0.12	53,58,64,68	0
4	EDO	B	520	4/4	0.91	0.19	50,52,59,65	0
4	EDO	C	511	4/4	0.91	0.14	52,56,60,61	0
4	EDO	B	507	4/4	0.91	0.22	52,55,61,62	0
5	PEG	D	510	7/7	0.91	0.21	56,69,80,92	0
4	EDO	B	519	4/4	0.91	0.28	63,63,68,70	0
4	EDO	A	504	4/4	0.91	0.27	53,65,67,78	0
4	EDO	D	501	4/4	0.91	0.13	51,53,53,54	0
4	EDO	C	517	4/4	0.91	0.11	66,67,71,76	0
4	EDO	C	509	4/4	0.92	0.25	54,55,59,59	0
4	EDO	C	504	4/4	0.92	0.17	51,56,56,60	0
4	EDO	A	515	4/4	0.92	0.28	36,48,53,53	0
7	EPE	B	521	15/15	0.93	0.23	52,77,92,93	0
4	EDO	C	507	4/4	0.93	0.19	52,52,63,63	0
6	D62	D	517	37/37	0.93	0.12	26,32,74,89	0
4	EDO	D	504	4/4	0.93	0.13	31,32,32,33	0
4	EDO	A	505	4/4	0.93	0.18	42,49,54,65	0
5	PEG	A	517	7/7	0.93	0.17	31,43,48,53	0
4	EDO	B	503	4/4	0.93	0.14	37,41,41,43	0
4	EDO	A	506	4/4	0.93	0.11	39,43,46,50	0
4	EDO	D	514	4/4	0.93	0.13	30,41,43,47	0
4	EDO	C	522	4/4	0.94	0.21	49,49,58,68	0
4	EDO	B	506	4/4	0.94	0.12	54,57,60,62	0
5	PEG	D	519	7/7	0.94	0.22	37,42,49,51	0
4	EDO	D	511	4/4	0.94	0.35	42,43,43,61	0
4	EDO	A	512	4/4	0.94	0.26	44,47,48,49	0
6	D62	B	516	37/37	0.94	0.12	27,33,74,78	0
4	EDO	D	505	4/4	0.95	0.09	41,43,43,48	0
4	EDO	A	513	4/4	0.95	0.21	45,51,53,64	0
4	EDO	A	507	4/4	0.95	0.15	50,61,65,67	0
4	EDO	D	507	4/4	0.95	0.16	38,50,52,55	0
4	EDO	D	516	4/4	0.95	0.14	37,39,45,47	0
7	EPE	B	509	15/15	0.96	0.14	53,62,70,73	0
7	EPE	A	524	15/15	0.96	0.23	44,77,92,96	0
2	ZN	A	501	1/1	0.97	0.07	33,33,33,33	0
4	EDO	D	512	4/4	0.97	0.07	38,41,43,46	0
7	EPE	D	523	15/15	0.97	0.14	36,72,91,103	0
7	EPE	C	514	15/15	0.98	0.15	40,46,80,101	0
3	MG	B	502	1/1	0.98	0.17	22,22,22,22	0

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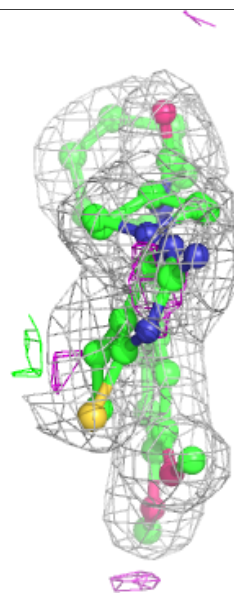
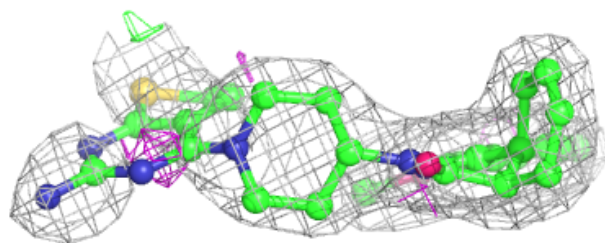
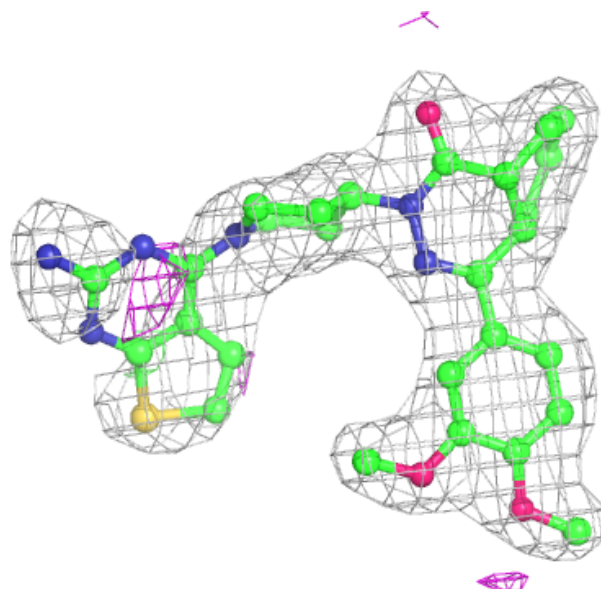
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	B	501	1/1	0.99	0.08	33,33,33,33	0
3	MG	A	502	1/1	0.99	0.15	19,19,19,19	0
3	MG	D	503	1/1	0.99	0.15	18,18,18,18	0
2	ZN	C	505	1/1	1.00	0.10	33,33,33,33	0
3	MG	C	506	1/1	1.00	0.17	21,21,21,21	0
2	ZN	D	502	1/1	1.00	0.11	30,30,30,30	0

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.



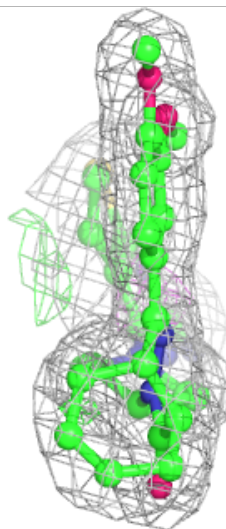
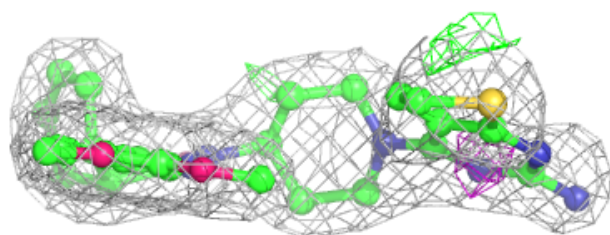
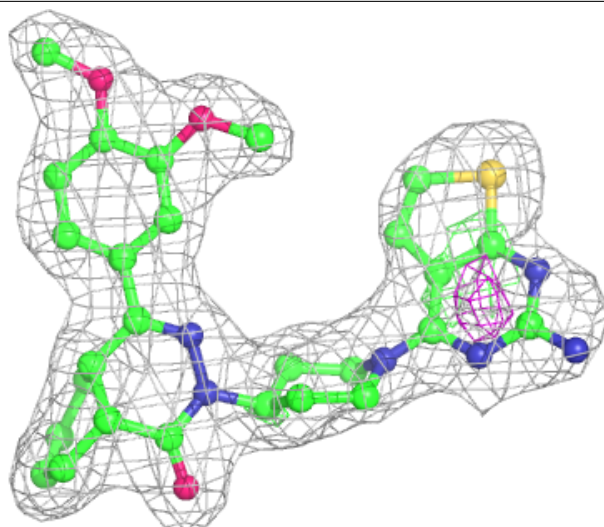
Electron density around D62 C 520:

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



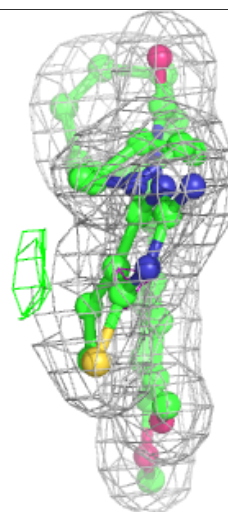
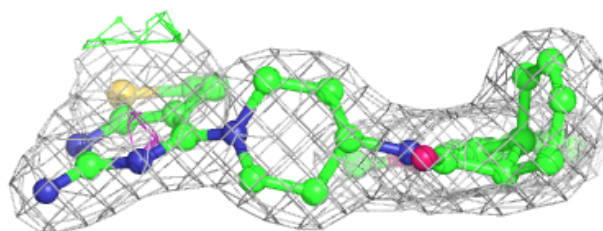
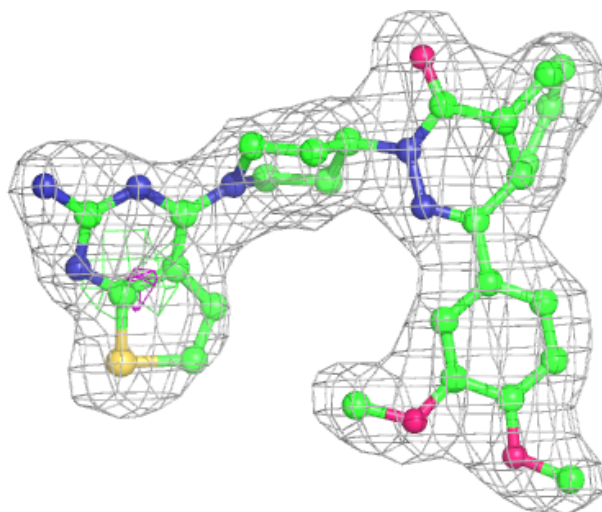
Electron density around D62 D 517:

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



Electron density around D62 B 516:

$2mF_o-DF_c$ (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.