wwPDB X-ray Structure Validation Summary Report (i)

Jan 8, 2024 – 04:54 am GMT

PDB ID	:	6FTW
Title	:	Crystal structure of human phosphodiesterase 4D2 catalytic domain with inhibitor NPD-048
Authors	:	Singh, A.K.; Brown, D.G.
Deposited on	:	2018-02-24
Resolution	:	2.16 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 (i) 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 (i)) were used in the production of this report:

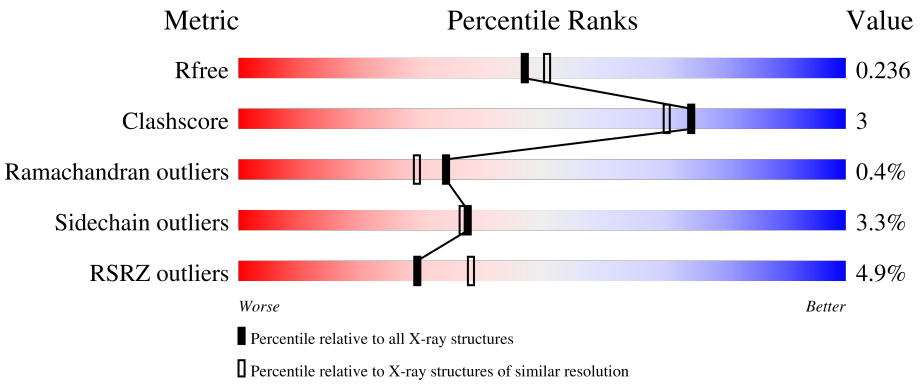
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 <=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	7%, 82%, 8% • 9%
1	B	364	2%, 81%, 7%, 11%
1	C	364	5%, 79%, 9% • 11%
1	D	364	4%, 82%, 7%, 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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	514	-	-	-	X
4	EDO	C	510	-	-	-	X
5	EPE	B	508	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11460 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	331	2680	1696	459	511	14	0	0	0
1	B	324	2628	1662	449	503	14	0	1	0
1	C	324	2622	1659	448	501	14	0	0	0
1	D	325	2631	1664	450	503	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

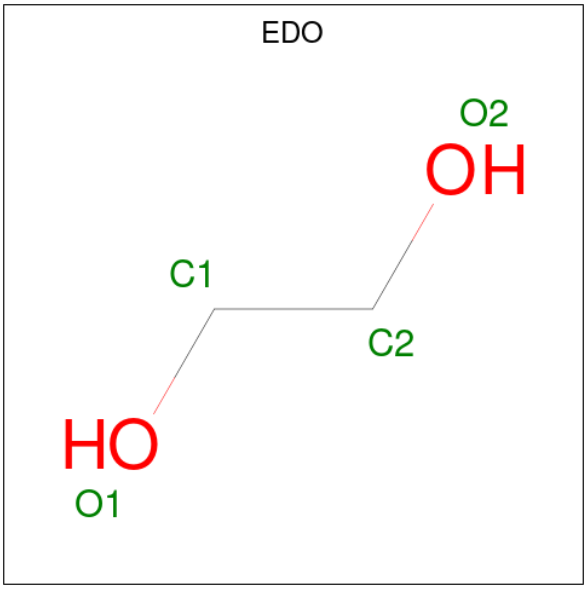
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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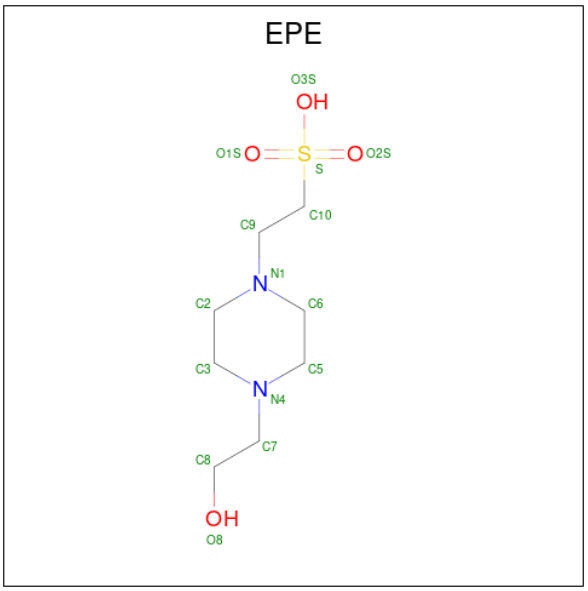
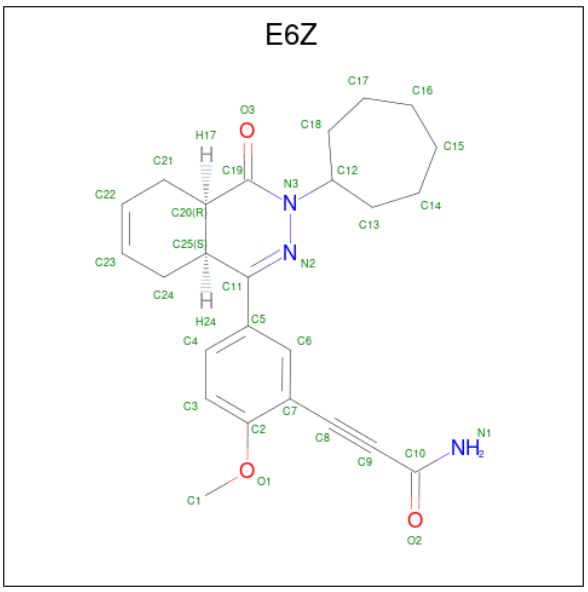
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	C	1	4	2	2	0	0
			Total	C	O		
4	C	1	4	2	2	0	0
			Total	C	O		
4	C	1	4	2	2	0	0
			Total	C	O		
4	C	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C	O		
4	D	1	4	2	2	0	0
			Total	C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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 6 is 3-{5-[(4aR,8aS)-3-cycloheptyl-4-oxo-3,4,4a,5,8,8a-hexahydrophthalazin-1-yl]-2-methoxyphenyl}prop-2-ynamide (three-letter code: E6Z) (formula: $C_{25}H_{29}N_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	31	25	3	3	0	0
6	B	1	31	25	3	3	0	0
6	C	1	31	25	3	3	0	0
6	D	1	31	25	3	3	0	0

- Molecule 7 is water.

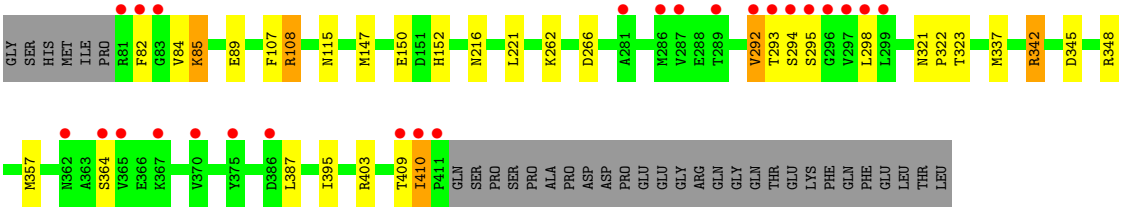
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	156	156	156	0	0
7	B	121	121	121	0	0
7	C	98	98	98	0	0
7	D	176	176	176	0	0

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.

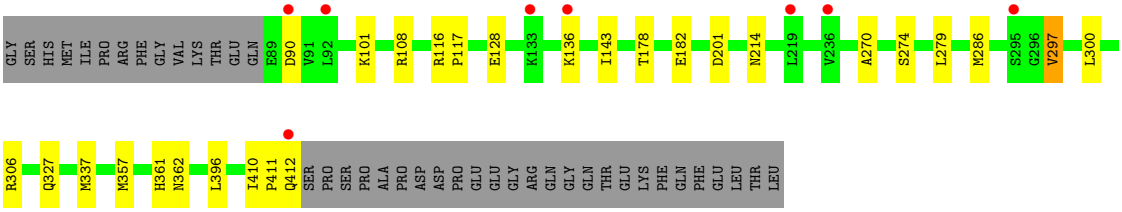
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain A:



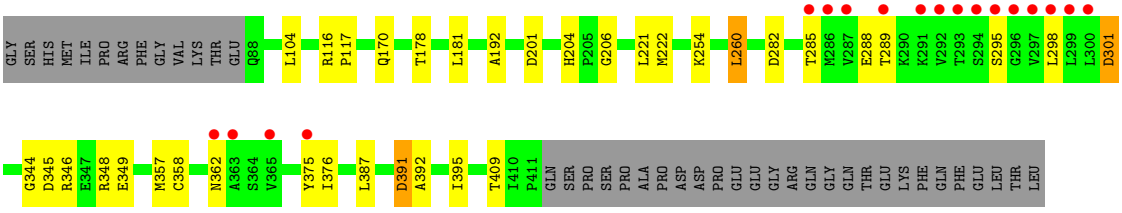
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain B:



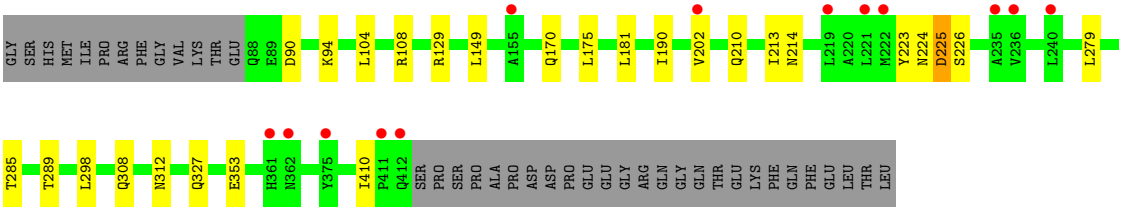
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain C:



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

Chain D:


GLY
SER
HIS
MET
ILE
PRO
ARG
PHE
GLY
VAL
LYS
THR
GLU
Q88
E89
D90
K94
L104
R108
R129
L149
A155
Q170
L175
L181
I190
V202
Q210
I213
N214
L219
A220
L221
M222
Y223
N224
D225
S226
A235
V236
L240
L279
T285
T289
L298
Q308
N312
Q327
E353
H361
N362
Y375
I410
P411
Q412
SER
PRO
SER
PRO
ALA
PRO
ASP
ASP
PRO
GLU
GLU
GLY
ARG
GLN
GLY
GLN
THR
GLU
LYS
PHE
GLN
PHE
GLU
LEU
THR
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.14Å 111.43Å 160.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.00 – 2.16 65.00 – 2.16	Depositor EDS
% Data completeness (in resolution range)	99.9 (65.00-2.16) 99.9 (65.00-2.16)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.182 , 0.233 0.192 , 0.236	Depositor DCC
R_{free} test set	4729 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11460	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: EPE, MG, ZN, EDO, E6Z

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	0.88	0/2735	0.84	1/3714 (0.0%)
1	B	0.81	0/2682	0.87	2/3644 (0.1%)
1	C	0.83	0/2676	0.84	2/3636 (0.1%)
1	D	0.95	0/2685	0.85	1/3648 (0.0%)
All	All	0.87	0/10778	0.85	6/14642 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	201	ASP	CB-CG-OD1	9.07	126.46	118.30
1	A	266	ASP	CB-CG-OD1	6.32	123.98	118.30
1	B	201	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	C	201	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	C	201	ASP	CB-CG-OD1	5.41	123.17	118.30

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	2680	0	2638	24	0
1	B	2628	0	2582	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2622	0	2578	20	0
1	D	2631	0	2586	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	52	0	78	5	0
4	B	20	0	30	2	0
4	C	36	0	54	1	0
4	D	48	0	72	3	0
5	A	15	0	17	2	0
5	B	15	0	18	1	0
5	C	15	0	18	0	0
5	D	15	0	18	0	0
6	A	31	0	0	1	0
6	B	31	0	0	1	0
6	C	31	0	0	1	0
6	D	31	0	0	0	0
7	A	156	0	0	3	0
7	B	121	0	0	1	0
7	C	98	0	0	1	0
7	D	176	0	0	1	0
All	All	11460	0	10689	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 69 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:MET:SD	6:B:509:E6Z:N1	2.24	1.09
1:C:345:ASP:OD2	1:C:348:ARG:NH2	1.89	1.06
1:A:342:ARG:HH11	1:A:342:ARG:HG2	1.29	0.96
1:B:214:ASN:HD22	4:B:506:EDO:H11	1.38	0.87
1:C:204:HIS:HD2	1:C:206:GLY:H	1.26	0.84

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	329/364 (90%)	318 (97%)	8 (2%)	3 (1%)	17	11
1	B	323/364 (89%)	310 (96%)	12 (4%)	1 (0%)	41	37
1	C	322/364 (88%)	312 (97%)	9 (3%)	1 (0%)	41	37
1	D	323/364 (89%)	312 (97%)	11 (3%)	0	100	100
All	All	1297/1456 (89%)	1252 (96%)	40 (3%)	5 (0%)	34	29

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	ASP
1	C	301	ASP
1	A	292	VAL
1	A	82	PHE
1	A	294	SER

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	302/331 (91%)	291 (96%)	11 (4%)	35	33
1	B	297/331 (90%)	285 (96%)	12 (4%)	31	29
1	C	296/331 (89%)	286 (97%)	10 (3%)	37	35
1	D	297/331 (90%)	290 (98%)	7 (2%)	49	51
All	All	1192/1324 (90%)	1152 (97%)	40 (3%)	38	35

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	288	GLU
1	D	108	ARG
1	C	295	SER
1	C	391	ASP
1	D	226	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	204	HIS
1	C	231	ASN
1	D	321	ASN
1	D	214	ASN
1	D	224	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 55 ligands modelled in this entry, 8 are monoatomic - leaving 47 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	509	-	3,3,3	1.11	0	2,2,2	0.70	0
4	EDO	C	508	-	3,3,3	0.37	0	2,2,2	1.16	0
4	EDO	D	503	-	3,3,3	0.59	0	2,2,2	0.60	0
4	EDO	D	512	-	3,3,3	0.57	0	2,2,2	0.25	0
6	E6Z	B	509	-	33,34,34	0.75	1 (3%)	35,47,47	0.88	1 (2%)
4	EDO	B	504	-	3,3,3	0.39	0	2,2,2	0.29	0
4	EDO	B	507	-	3,3,3	0.54	0	2,2,2	0.19	0
5	EPE	A	515	-	15,15,15	2.47	2 (13%)	18,20,20	2.25	6 (33%)
4	EDO	A	514	-	3,3,3	0.44	0	2,2,2	0.51	0
4	EDO	D	507	-	3,3,3	0.70	0	2,2,2	0.29	0
6	E6Z	D	516	-	33,34,34	0.74	0	35,47,47	0.89	1 (2%)
4	EDO	B	505	-	3,3,3	0.49	0	2,2,2	0.30	0
4	EDO	C	513	-	3,3,3	0.67	0	2,2,2	0.35	0
4	EDO	C	510	-	3,3,3	2.01	1 (33%)	2,2,2	0.81	0
5	EPE	B	508	-	15,15,15	1.86	1 (6%)	18,20,20	1.65	1 (5%)
4	EDO	D	506	-	3,3,3	0.52	0	2,2,2	0.35	0
4	EDO	C	506	-	3,3,3	0.92	0	2,2,2	0.97	0
4	EDO	C	504	-	3,3,3	0.78	0	2,2,2	0.74	0
4	EDO	D	510	-	3,3,3	0.23	0	2,2,2	0.56	0
4	EDO	A	503	-	3,3,3	0.38	0	2,2,2	1.23	0
4	EDO	C	507	-	3,3,3	0.57	0	2,2,2	0.56	0
5	EPE	D	514	-	15,15,15	1.82	1 (6%)	18,20,20	1.51	4 (22%)
4	EDO	C	503	-	3,3,3	0.36	0	2,2,2	0.56	0
4	EDO	A	504	-	3,3,3	0.66	0	2,2,2	0.19	0
4	EDO	A	511	-	3,3,3	0.32	0	2,2,2	1.01	0
4	EDO	D	511	-	3,3,3	0.42	0	2,2,2	0.87	0
4	EDO	D	513	-	3,3,3	0.40	0	2,2,2	0.80	0
4	EDO	A	510	-	3,3,3	0.96	0	2,2,2	0.75	0
4	EDO	B	503	-	3,3,3	0.33	0	2,2,2	1.21	0
4	EDO	D	515	-	3,3,3	0.89	0	2,2,2	0.25	0
4	EDO	A	516	-	3,3,3	0.43	0	2,2,2	0.09	0
4	EDO	D	505	-	3,3,3	0.24	0	2,2,2	0.91	0
4	EDO	A	508	-	3,3,3	0.50	0	2,2,2	0.42	0
4	EDO	A	506	-	3,3,3	0.41	0	2,2,2	0.84	0
4	EDO	A	513	-	3,3,3	0.57	0	2,2,2	0.44	0
5	EPE	C	511	-	15,15,15	1.70	1 (6%)	18,20,20	1.37	3 (16%)
4	EDO	A	509	-	3,3,3	0.37	0	2,2,2	0.46	0
4	EDO	A	507	-	3,3,3	0.64	0	2,2,2	0.55	0
4	EDO	A	512	-	3,3,3	0.48	0	2,2,2	0.42	0
6	E6Z	A	517	-	33,34,34	0.68	0	35,47,47	0.80	1 (2%)
4	EDO	B	506	-	3,3,3	0.49	0	2,2,2	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	A	505	-	3,3,3	0.45	0	2,2,2	0.44	0
4	EDO	D	509	-	3,3,3	0.55	0	2,2,2	0.18	0
6	E6Z	C	512	-	33,34,34	0.81	1 (3%)	35,47,47	1.14	2 (5%)
4	EDO	D	504	-	3,3,3	0.16	0	2,2,2	1.48	0
4	EDO	D	508	-	3,3,3	0.41	0	2,2,2	0.09	0
4	EDO	C	505	-	3,3,3	0.45	0	2,2,2	0.62	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	509	-	-	1/1/1/1	-
4	EDO	C	508	-	-	0/1/1/1	-
4	EDO	D	503	-	-	1/1/1/1	-
4	EDO	D	512	-	-	1/1/1/1	-
6	E6Z	B	509	-	-	3/10/51/51	0/4/4/4
4	EDO	B	504	-	-	0/1/1/1	-
4	EDO	B	507	-	-	0/1/1/1	-
5	EPE	A	515	-	-	3/9/19/19	0/1/1/1
4	EDO	A	514	-	-	0/1/1/1	-
4	EDO	D	507	-	-	1/1/1/1	-
6	E6Z	D	516	-	-	2/10/51/51	0/4/4/4
4	EDO	B	505	-	-	1/1/1/1	-
4	EDO	C	513	-	-	0/1/1/1	-
4	EDO	C	510	-	-	1/1/1/1	-
5	EPE	B	508	-	-	5/9/19/19	0/1/1/1
4	EDO	D	506	-	-	0/1/1/1	-
4	EDO	C	506	-	-	1/1/1/1	-
4	EDO	C	504	-	-	1/1/1/1	-
4	EDO	D	510	-	-	0/1/1/1	-
4	EDO	A	503	-	-	0/1/1/1	-
4	EDO	C	507	-	-	1/1/1/1	-
5	EPE	D	514	-	-	8/9/19/19	0/1/1/1
4	EDO	C	503	-	-	0/1/1/1	-
4	EDO	A	504	-	-	0/1/1/1	-
4	EDO	A	511	-	-	0/1/1/1	-
4	EDO	D	511	-	-	1/1/1/1	-
4	EDO	D	513	-	-	1/1/1/1	-
4	EDO	A	510	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	D	515	-	-	0/1/1/1	-
4	EDO	A	516	-	-	0/1/1/1	-
4	EDO	D	505	-	-	0/1/1/1	-
4	EDO	A	508	-	-	0/1/1/1	-
4	EDO	A	506	-	-	1/1/1/1	-
4	EDO	A	513	-	-	1/1/1/1	-
5	EPE	C	511	-	-	0/9/19/19	0/1/1/1
4	EDO	A	509	-	-	0/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
4	EDO	A	512	-	-	0/1/1/1	-
6	E6Z	A	517	-	-	2/10/51/51	0/4/4/4
4	EDO	B	506	-	-	0/1/1/1	-
4	EDO	A	505	-	-	1/1/1/1	-
4	EDO	D	509	-	-	1/1/1/1	-
6	E6Z	C	512	-	-	2/10/51/51	0/4/4/4
4	EDO	D	504	-	-	0/1/1/1	-
4	EDO	D	508	-	-	1/1/1/1	-
4	EDO	C	505	-	-	0/1/1/1	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	515	EPE	C10-S	-9.04	1.64	1.77
5	B	508	EPE	C10-S	-6.88	1.67	1.77
5	D	514	EPE	C10-S	-6.71	1.68	1.77
5	C	511	EPE	C10-S	-5.86	1.69	1.77
4	C	510	EDO	O2-C2	3.21	1.58	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	508	EPE	O3S-S-C10	6.08	115.61	105.77
5	A	515	EPE	O3S-S-C10	5.24	114.24	105.77
6	C	512	E6Z	C4-C5-C11	4.22	125.75	120.75
5	A	515	EPE	O1S-S-C10	4.05	111.79	106.92
5	D	514	EPE	O3S-S-C10	3.80	111.91	105.77

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	508	EPE	C10-C9-N1-C6
5	B	508	EPE	S-C10-C9-N1
5	D	514	EPE	N4-C7-C8-O8
5	D	514	EPE	S-C10-C9-N1
5	D	514	EPE	C9-C10-S-O1S

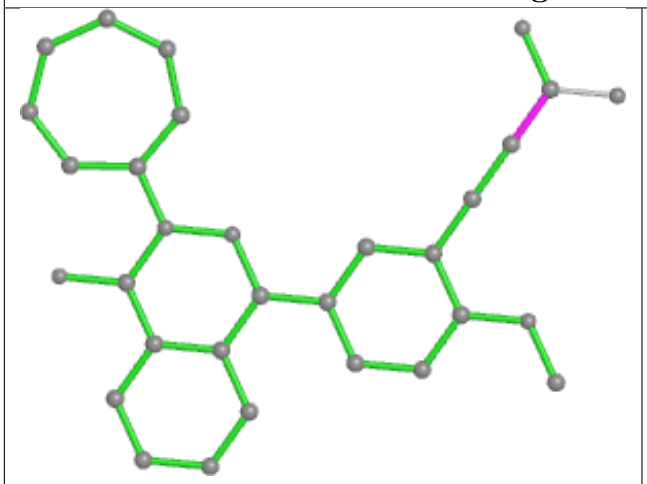
There are no ring outliers.

12 monomers are involved in 17 short contacts:

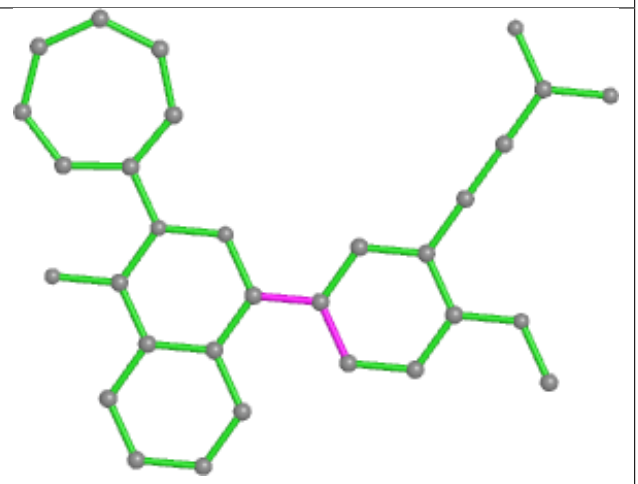
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	509	E6Z	1	0
5	A	515	EPE	2	0
4	C	510	EDO	1	0
5	B	508	EPE	1	0
4	D	510	EDO	2	0
4	A	510	EDO	3	0
4	A	513	EDO	1	0
4	A	512	EDO	1	0
6	A	517	E6Z	1	0
4	B	506	EDO	2	0
6	C	512	E6Z	1	0
4	D	508	EDO	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

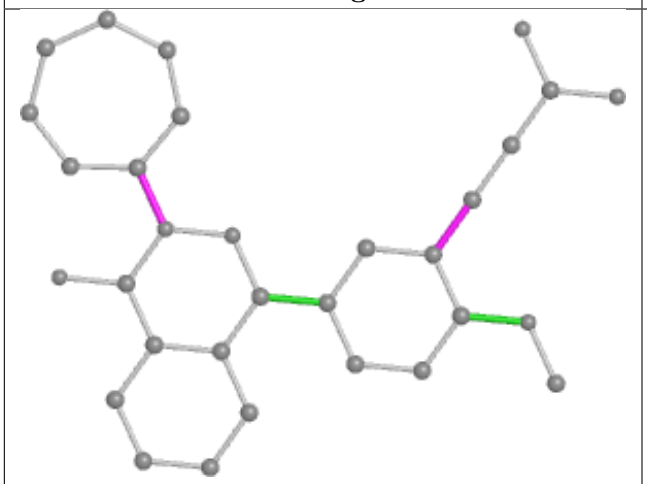
Ligand E6Z B 509



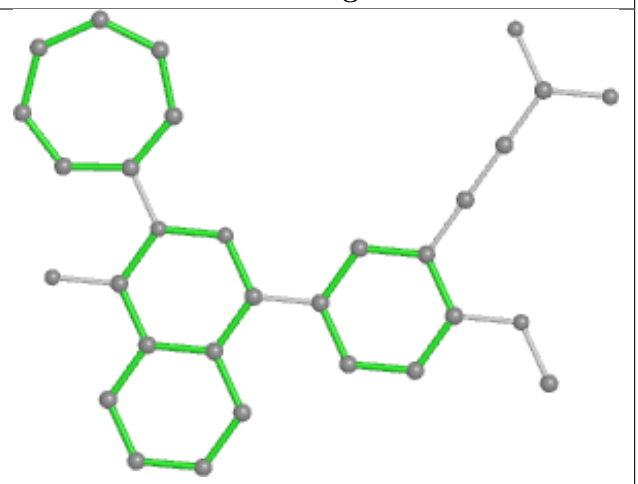
Bond lengths



Bond angles

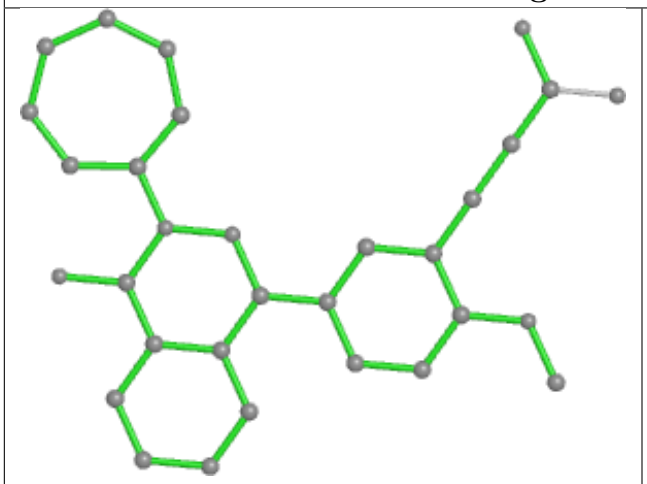


Torsions

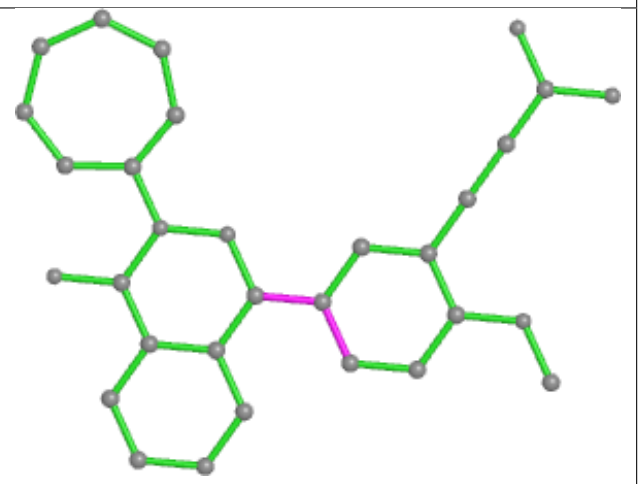


Rings

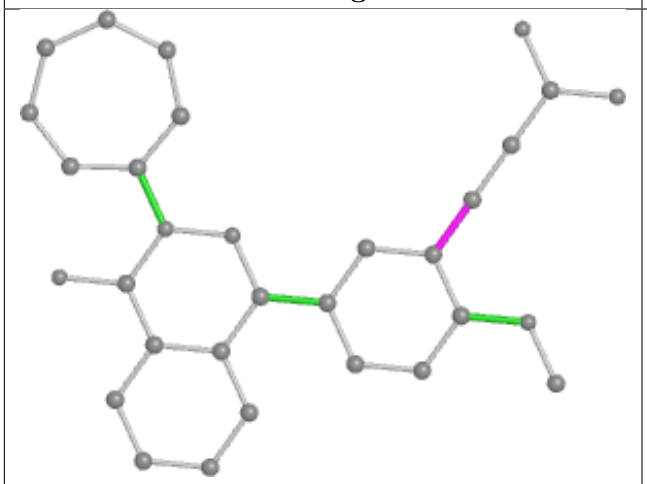
Ligand E6Z D 516



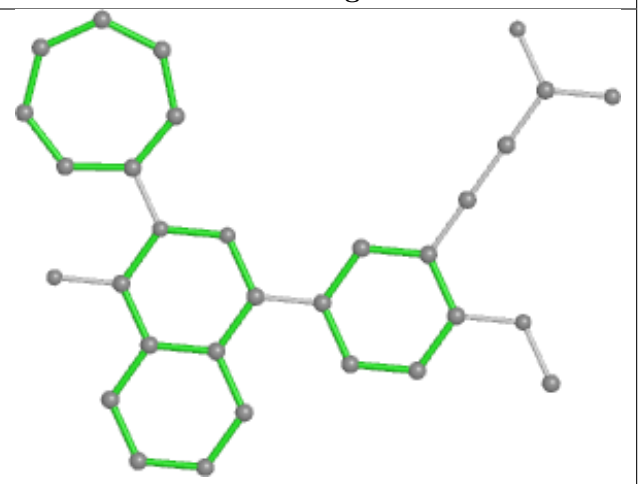
Bond lengths



Bond angles

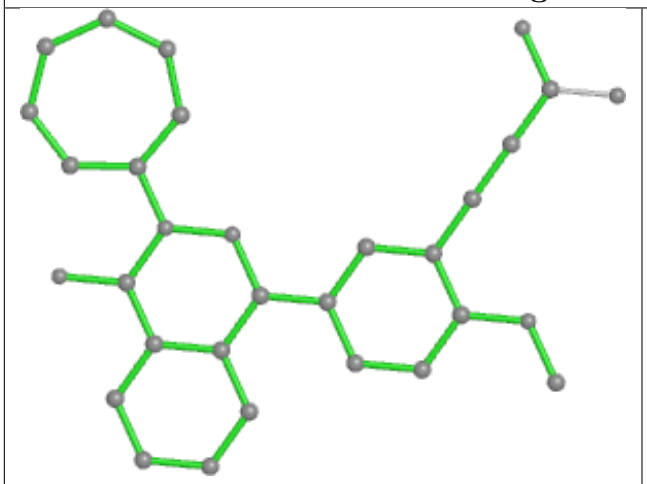


Torsions

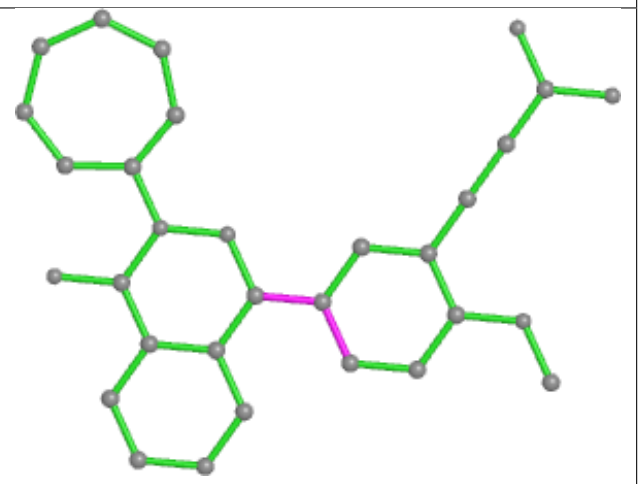


Rings

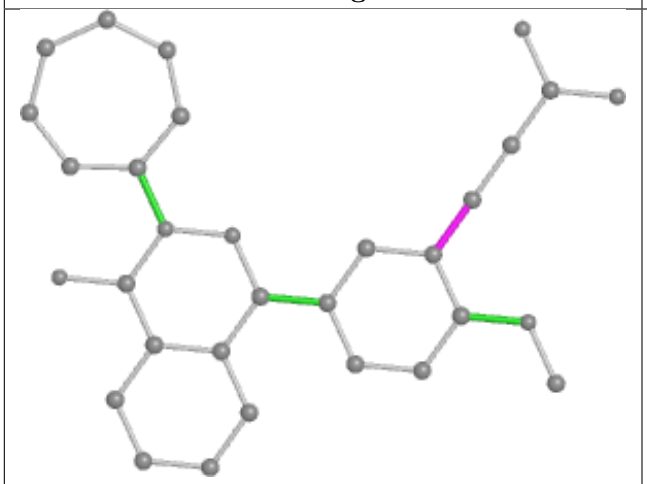
Ligand E6Z A 517



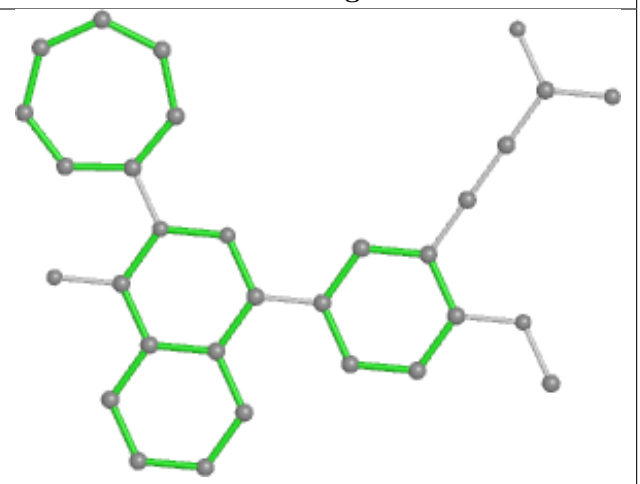
Bond lengths



Bond angles

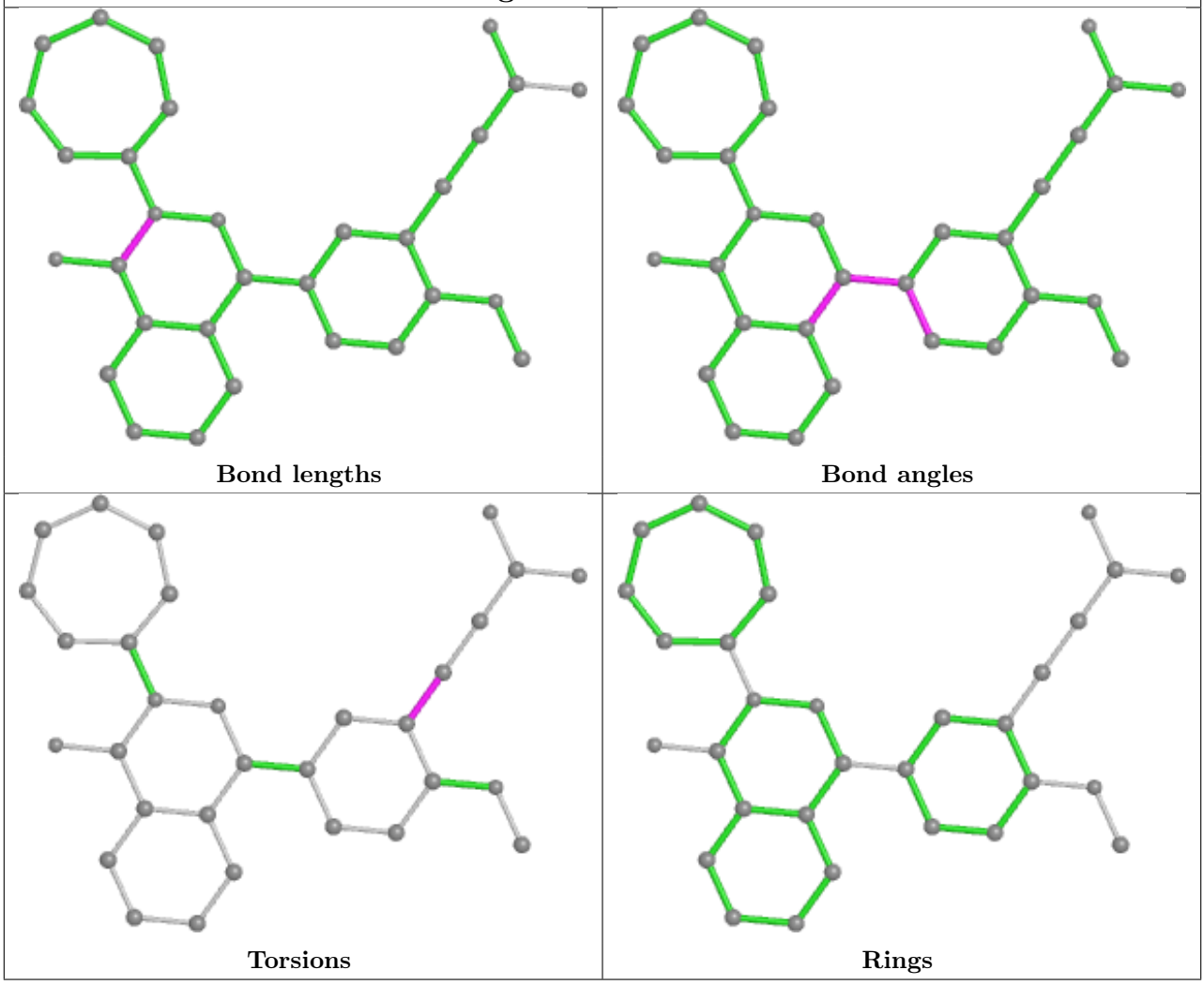


Torsions



Rings

Ligand E6Z C 512



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 (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	331/364 (90%)	0.24	25 (7%)	13	19	27, 41, 75, 122	0
1	B	324/364 (89%)	0.12	8 (2%)	57	65	29, 53, 76, 107	0
1	C	324/364 (89%)	0.14	18 (5%)	24	33	29, 50, 84, 123	0
1	D	325/364 (89%)	0.05	13 (4%)	38	47	26, 38, 66, 90	0
All	All	1304/1456 (89%)	0.13	64 (4%)	29	38	26, 46, 75, 123	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	412	GLN	5.3
1	C	294	SER	5.0
1	C	296	GLY	4.8
1	B	412	GLN	4.4
1	A	295	SER	4.2

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	514	4/4	0.59	0.47	108,111,113,118	0
4	EDO	C	510	4/4	0.60	0.45	97,107,113,130	0
4	EDO	D	512	4/4	0.76	0.25	67,80,81,82	0
4	EDO	B	505	4/4	0.77	0.25	77,80,82,87	0
5	EPE	B	508	15/15	0.77	0.61	64,73,103,113	11
4	EDO	C	513	4/4	0.79	0.18	59,59,64,65	0
4	EDO	D	510	4/4	0.79	0.20	41,44,48,54	0
4	EDO	C	507	4/4	0.82	0.20	60,63,64,68	0
4	EDO	A	512	4/4	0.84	0.17	56,56,65,71	0
5	EPE	A	515	15/15	0.85	0.27	46,117,144,147	0
4	EDO	A	506	4/4	0.85	0.29	68,68,70,73	0
4	EDO	A	504	4/4	0.86	0.14	67,72,73,77	0
4	EDO	C	509	4/4	0.86	0.24	51,53,53,56	0
4	EDO	A	513	4/4	0.86	0.26	54,62,73,81	0
4	EDO	C	505	4/4	0.86	0.40	63,65,66,76	0
6	E6Z	D	516	31/31	0.86	0.18	48,57,77,82	0
4	EDO	D	515	4/4	0.87	0.36	40,41,45,59	0
4	EDO	C	508	4/4	0.88	0.15	50,55,56,68	0
4	EDO	C	504	4/4	0.88	0.10	57,59,65,68	0
6	E6Z	A	517	31/31	0.88	0.28	43,58,71,81	0
6	E6Z	B	509	31/31	0.88	0.12	46,57,68,69	0
6	E6Z	C	512	31/31	0.88	0.19	45,52,70,76	0
4	EDO	D	507	4/4	0.88	0.35	60,69,70,75	0
5	EPE	D	514	15/15	0.89	0.48	42,58,68,73	11
4	EDO	C	503	4/4	0.89	0.26	69,74,75,78	0
4	EDO	D	504	4/4	0.89	0.24	63,63,66,76	0
4	EDO	C	506	4/4	0.89	0.18	52,58,58,60	0
4	EDO	B	507	4/4	0.89	0.53	59,64,70,71	0
4	EDO	D	505	4/4	0.90	0.19	42,44,50,60	0
4	EDO	D	513	4/4	0.91	0.21	71,80,86,86	0
4	EDO	A	509	4/4	0.91	0.16	38,42,44,47	0
4	EDO	A	503	4/4	0.91	0.14	57,59,63,78	0
4	EDO	D	509	4/4	0.92	0.33	63,67,71,72	0
4	EDO	A	507	4/4	0.92	0.14	46,54,58,61	0
4	EDO	A	510	4/4	0.92	0.23	38,43,51,53	0
4	EDO	D	503	4/4	0.92	0.14	48,49,49,50	0
4	EDO	D	506	4/4	0.93	0.11	41,43,43,43	0
4	EDO	B	506	4/4	0.94	0.21	42,50,51,57	0
4	EDO	A	505	4/4	0.94	0.20	42,61,64,65	0
4	EDO	D	508	4/4	0.94	0.17	46,47,49,49	0
4	EDO	A	508	4/4	0.95	0.10	46,56,60,63	0
4	EDO	A	516	4/4	0.95	0.15	36,40,40,40	0
4	EDO	B	503	4/4	0.95	0.18	43,45,48,55	0

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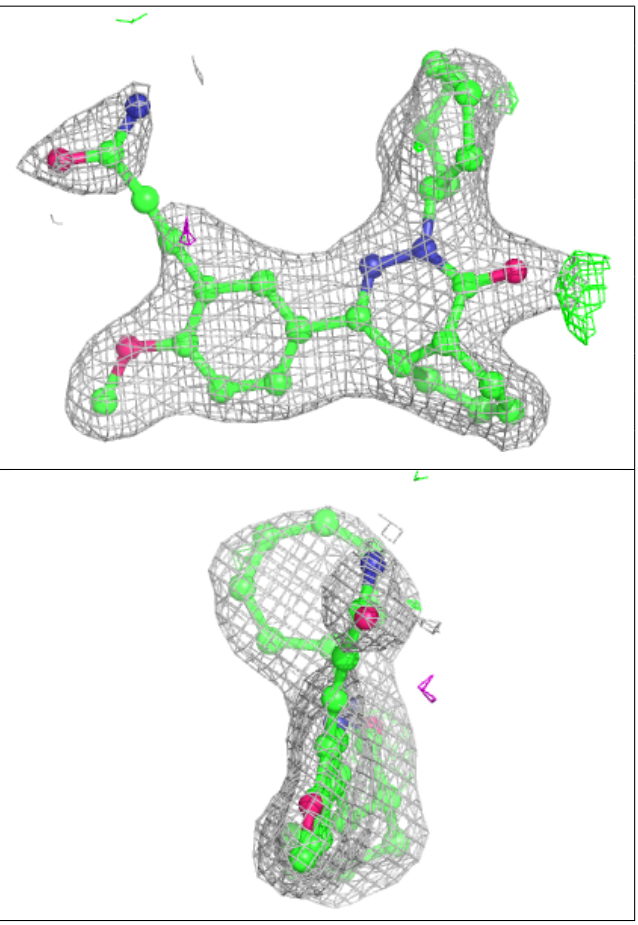
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	511	4/4	0.95	0.18	43,45,46,47	0
5	EPE	C	511	15/15	0.95	0.22	54,94,110,111	0
4	EDO	D	511	4/4	0.96	0.15	35,43,44,49	0
4	EDO	B	504	4/4	0.96	0.38	53,55,59,60	0
3	MG	B	502	1/1	0.97	0.14	32,32,32,32	0
3	MG	D	502	1/1	0.98	0.15	29,29,29,29	0
3	MG	A	502	1/1	0.99	0.11	26,26,26,26	0
2	ZN	B	501	1/1	0.99	0.08	44,44,44,44	0
3	MG	C	502	1/1	0.99	0.08	27,27,27,27	0
2	ZN	A	501	1/1	1.00	0.10	36,36,36,36	0
2	ZN	C	501	1/1	1.00	0.10	41,41,41,41	0
2	ZN	D	501	1/1	1.00	0.12	38,38,38,38	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.

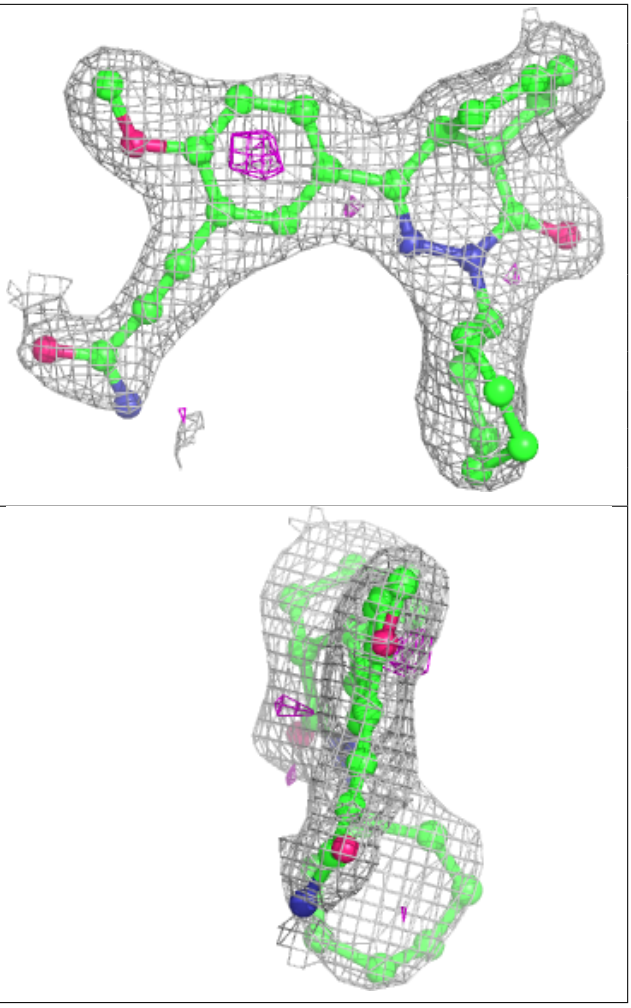
Electron density around E6Z D 516:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



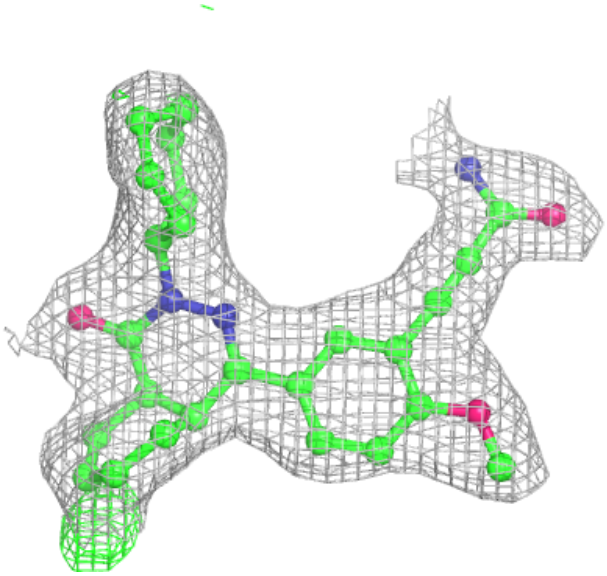
Electron density around E6Z A 517:

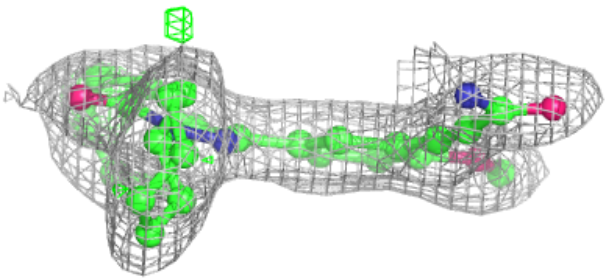
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

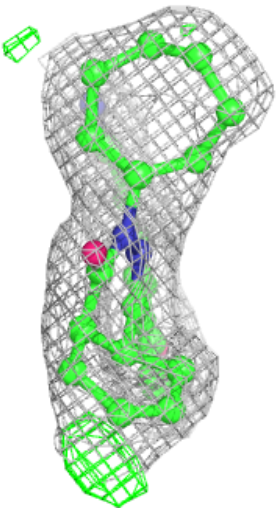


Electron density around E6Z B 509:

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

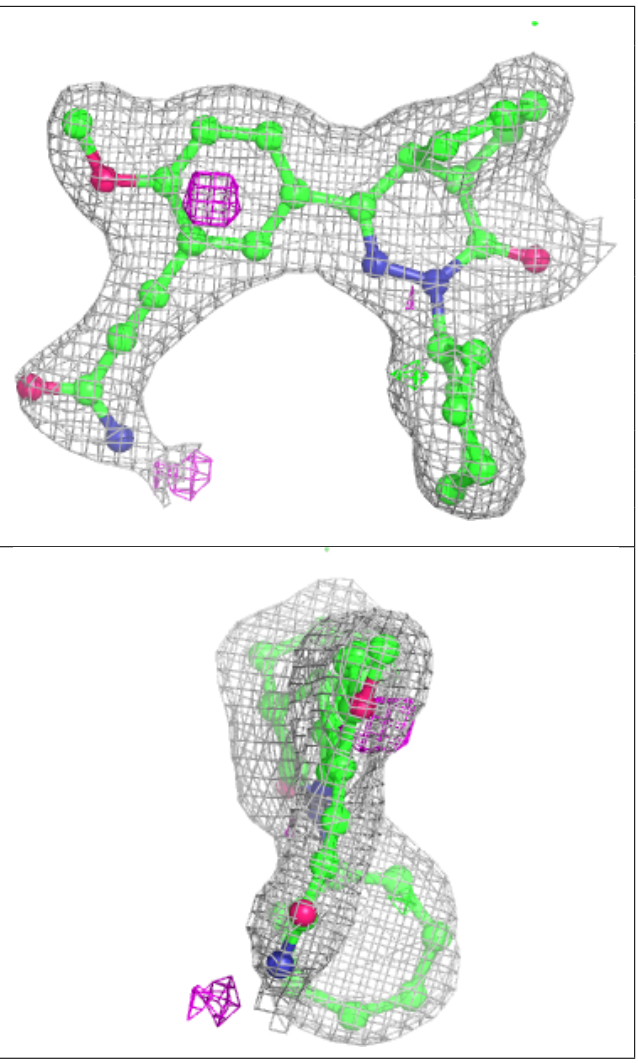






Electron density around E6Z C 512:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.