wwPDB X-ray Structure Validation Summary Report (i)

Jan 14, 2024 – 01:25 am GMT

PDB ID	:	6HWO
Title	:	Crystal structure of human phosphodiesterase 4D2 catalytic domain with inhibitor NPD-1335
Authors	:	Singh, A.K.; Brown, D.G.
Deposited on	:	2018-10-12
Resolution	:	1.99 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:

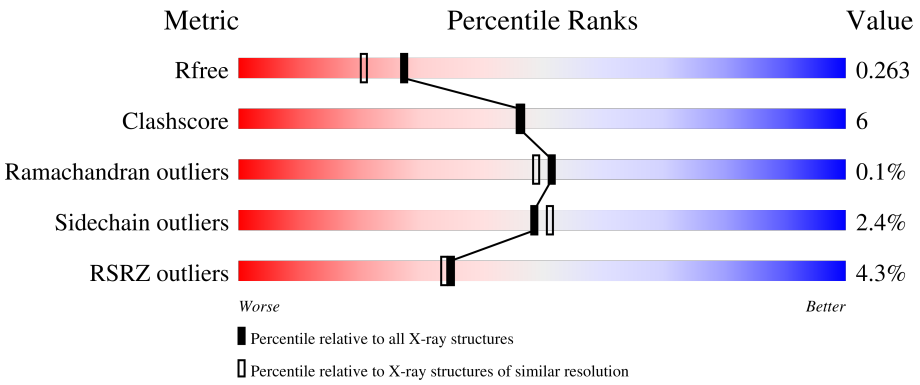
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 1.99 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 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	6% 77% 12% • 10%
1	B	364	2% 80% 8% • 12%
1	C	364	5% 76% 12% • 11%
1	D	364	2% 79% 10% 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
2	EDO	D	520	-	-	X	-
8	DMS	D	502	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 11546 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.

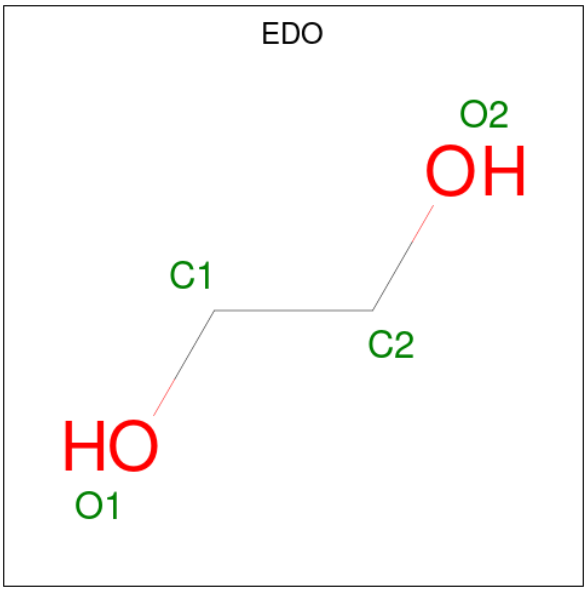
- Molecule 1 is a protein called cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	327	2643	1670	452	507	14	0	0	0
1	B	321	2604	1650	445	494	15	0	1	0
1	C	324	2624	1659	448	503	14	0	0	0
1	D	324	2630	1663	449	504	14	0	1	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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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

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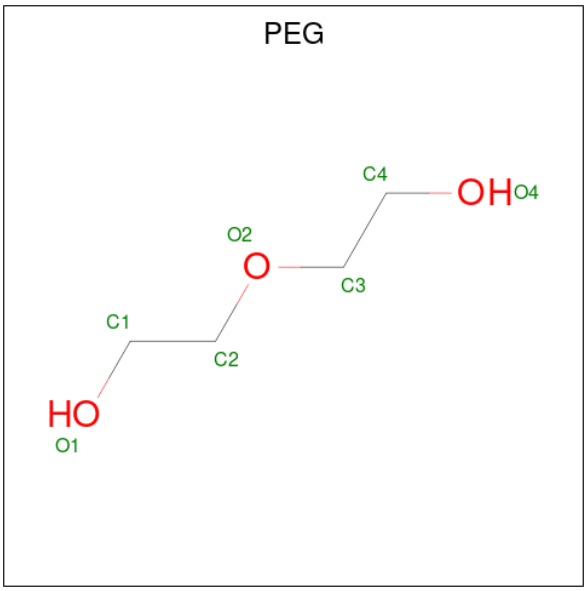
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	D	1	4	2	2	0	0
			Total	C	O		
2	D	1	4	2	2	0	0
			Total	C	O		
2	D	1	4	2	2	0	0
			Total	C	O		
2	D	1	4	2	2	0	0
			Total	C	O		
2	D	1	4	2	2	0	0
			Total	C	O		
2	D	1	4	2	2	0	0
			Total	C	O		
2	D	1	4	2	2	0	0
			Total	C	O		
2	D	1	4	2	2	0	0
			Total	C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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

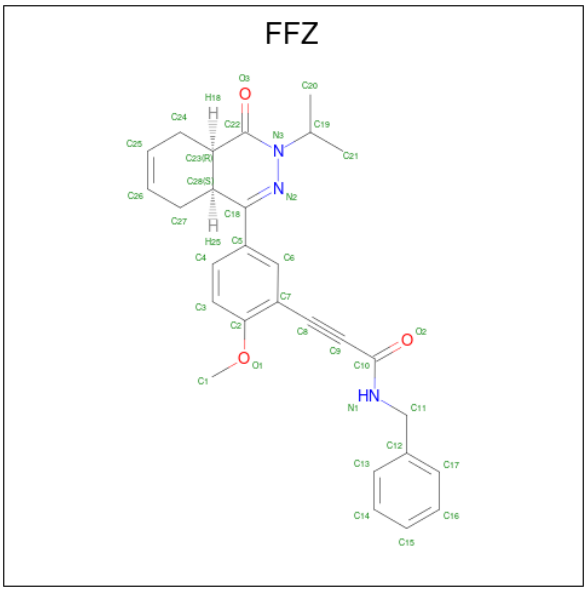


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	7	4	3	0	0
			Total	C	O		
3	A	1	7	4	3	0	0
			Total	C	O		
3	B	1	7	4	3	0	0
			Total	C	O		
3	C	1	7	4	3	0	0
			Total	C	O		
3	D	1	7	4	3	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is 3-[5-[(4aR,8aS)-4-OXIDANYLIDENE-3-PROPAN-2-YL-4a,5,8,8a-TETRAHYDROPHTHALAZIN-1-YL]-2-METHOXY-PHENYL]-N-(PHENYLMETHYL)PROP-2-YNAMIDE (three-letter code: FFZ) (formula: $C_{28}H_{29}N_3O_3$) (labeled as "Ligand of Interest" by depositor).

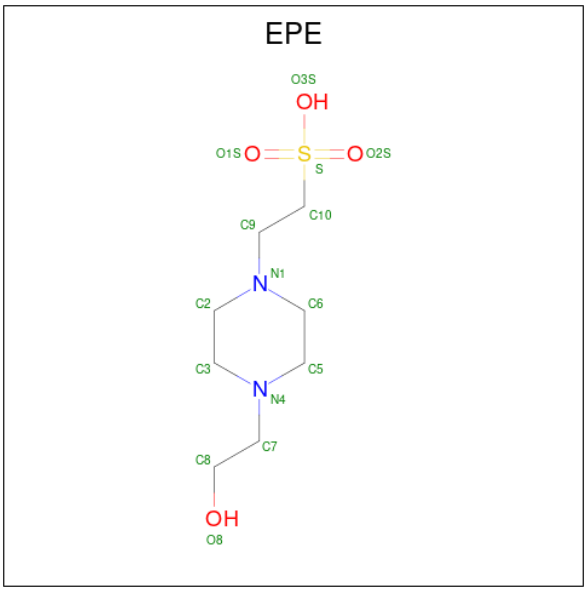


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	34	28	3	3	0	0
5	B	1	34	28	3	3	0	0
5	C	1	34	28	3	3	0	0
5	D	1	34	28	3	3	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

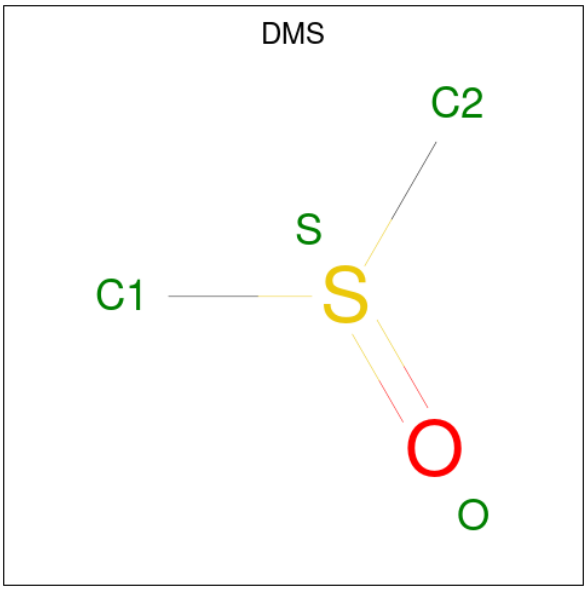
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	1	1	1	0	0
6	B	1	1	1	0	0
6	C	1	1	1	0	0
6	D	1	1	1	0	0

- Molecule 7 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		
7	A	1	15	8	2	4	1	0	0
7	B	1	15	8	2	4	1	0	0
7	C	1	15	8	2	4	1	0	0
7	D	1	15	8	2	4	1	0	0

- Molecule 8 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

- Molecule 9 is water.

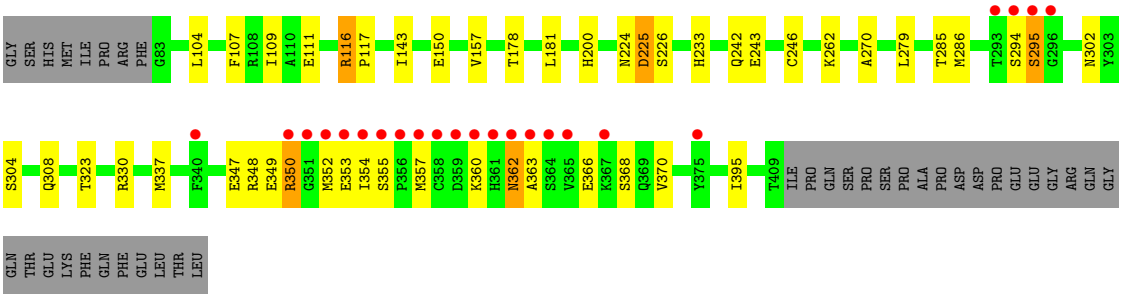
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	145	145	145	0	0
			Total	O		
9	B	129	129	129	0	0
			Total	O		
9	C	124	124	124	0	0
			Total	O		
9	D	192	192	192	0	0

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.

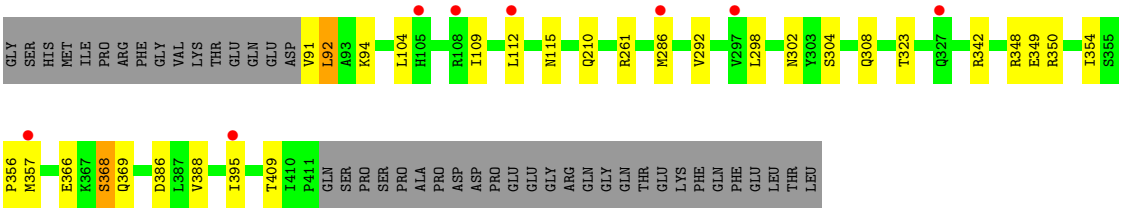
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain A:



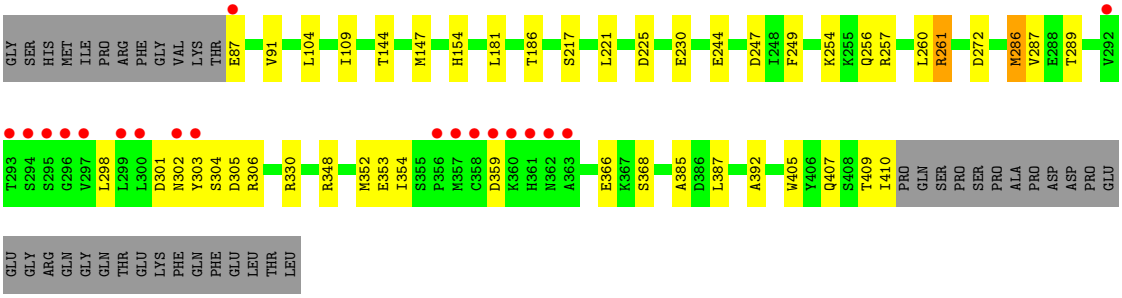
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain B:



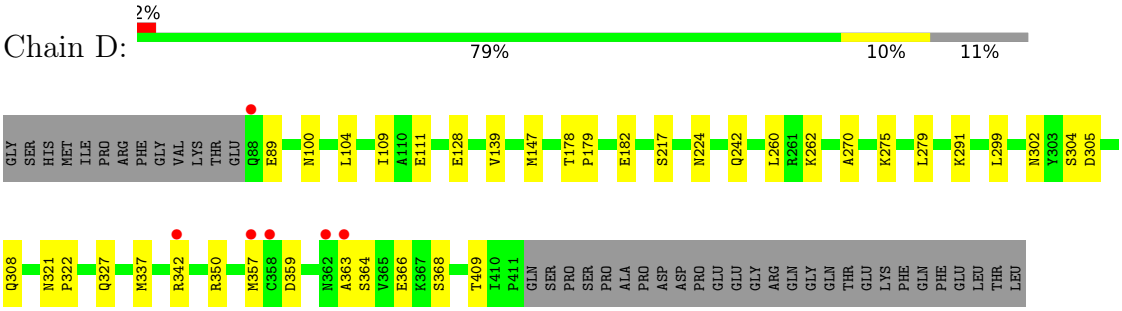
• Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

Chain C:



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

Chain D:


2%
79%
10%
11%
GLY SER HIS MET ILE PRO ARG PHE GLY VAL LYS THR GLU Q88 E89 N100 L104 I109 A110 E111 E128 V139 M147 T178 P179 E182 S217 N224 Q242 L260 R261 K262 A270 K275 L279 K291 L299 N302 Y303 S304 D305
Q308 N321 P322 Q327 M337 R342 R350 M357 C358 D359 N362 A363 S364 V365 E366 K367 S368 T409 I410 P411 GLN 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	98.47Å 110.85Å 160.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.19 – 1.99 73.62 – 1.99	Depositor EDS
% Data completeness (in resolution range)	97.9 (80.19-1.99) 98.0 (73.62-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.198 , 0.255 0.211 , 0.263	Depositor DCC
R_{free} test set	5954 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11546	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: MG, EPE, DMS, EDO, FFZ, ZN, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	1.01	0/2696	0.84	3/3661 (0.1%)
1	B	0.96	0/2658	0.85	0/3611
1	C	0.93	0/2677	0.89	2/3636 (0.1%)
1	D	1.07	0/2684	0.83	1/3647 (0.0%)
All	All	0.99	0/10715	0.85	6/14555 (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	C	261	ARG	NE-CZ-NH2	8.10	124.35	120.30
1	C	261	ARG	NE-CZ-NH1	-6.78	116.91	120.30
1	A	330	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	225	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	330	ARG	NE-CZ-NH1	5.33	122.97	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	2643	0	2598	46	0
1	B	2604	0	2568	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2624	0	2577	41	0
1	D	2630	0	2581	38	0
2	A	60	0	90	2	0
2	B	40	0	60	3	0
2	C	36	0	54	3	0
2	D	68	0	102	5	0
3	A	14	0	20	1	0
3	B	7	0	10	3	0
3	C	7	0	10	3	0
3	D	7	0	10	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	34	0	0	2	0
5	B	34	0	0	3	0
5	C	34	0	0	0	0
5	D	34	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	15	0	17	4	0
7	B	15	0	18	0	0
7	C	15	0	17	0	0
7	D	15	0	17	6	0
8	B	4	0	6	1	0
8	D	8	0	12	5	0
9	A	145	0	0	3	0
9	B	129	0	0	4	0
9	C	124	0	0	3	0
9	D	192	0	0	2	0
All	All	11546	0	10767	137	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 6.

The worst 5 of 137 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:MET:HE2	1:D:357:MET:CE	1.72	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:MET:CE	1:D:357:MET:HE3	1.81	1.08
1:A:349:GLU:HG2	1:C:147:MET:HE2	1.36	1.04
1:D:291:LYS:H	2:D:520:EDO:H22	1.23	1.02
1:A:349:GLU:CD	1:C:147:MET:CE	2.35	0.95

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	325/364 (89%)	308 (95%)	16 (5%)	1 (0%)	41	37
1	B	320/364 (88%)	306 (96%)	14 (4%)	0	100	100
1	C	322/364 (88%)	310 (96%)	12 (4%)	0	100	100
1	D	323/364 (89%)	315 (98%)	8 (2%)	0	100	100
All	All	1290/1456 (89%)	1239 (96%)	50 (4%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	ASN

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	298/331 (90%)	290 (97%)	8 (3%)	44	46
1	B	294/331 (89%)	287 (98%)	7 (2%)	49	51
1	C	296/331 (89%)	288 (97%)	8 (3%)	44	46
1	D	297/331 (90%)	292 (98%)	5 (2%)	60	65
All	All	1185/1324 (90%)	1157 (98%)	28 (2%)	49	51

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	386	ASP
1	D	364	SER
1	C	286	MET
1	D	178	THR
1	C	261	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	308	GLN
1	D	312	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 75 ligands modelled in this entry, 8 are monoatomic - leaving 67 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	$\#\|Z\| > 2$
2	EDO	D	508	-	3,3,3	0.67	0	2,2,2	0.57	0
5	FFZ	C	510	-	35,37,37	0.85	1 (2%)	39,51,51	0.76	1 (2%)
2	EDO	A	515	-	3,3,3	0.35	0	2,2,2	0.68	0
2	EDO	B	515	-	3,3,3	0.50	0	2,2,2	0.59	0
2	EDO	D	506	-	3,3,3	0.80	0	2,2,2	0.31	0
2	EDO	D	513	-	3,3,3	0.73	0	2,2,2	0.69	0
2	EDO	A	504	-	3,3,3	0.97	0	2,2,2	0.74	0
2	EDO	D	522	-	3,3,3	0.39	0	2,2,2	0.47	0
2	EDO	C	507	-	3,3,3	0.33	0	2,2,2	0.31	0
2	EDO	D	521	-	3,3,3	1.44	0	2,2,2	0.96	0
2	EDO	A	502	-	3,3,3	0.27	0	2,2,2	1.36	0
2	EDO	A	501	-	3,3,3	0.23	0	2,2,2	0.14	0
2	EDO	A	503	-	3,3,3	0.65	0	2,2,2	0.52	0
2	EDO	D	518	-	3,3,3	0.37	0	2,2,2	0.76	0
2	EDO	A	519	-	3,3,3	0.59	0	2,2,2	0.38	0
2	EDO	B	501	-	3,3,3	0.36	0	2,2,2	0.18	0
2	EDO	B	504	-	3,3,3	0.61	0	2,2,2	0.44	0
5	FFZ	A	513	-	35,37,37	0.71	1 (2%)	39,51,51	0.85	1 (2%)
2	EDO	C	502	-	3,3,3	0.37	0	2,2,2	0.06	0
2	EDO	D	511	-	3,3,3	0.10	0	2,2,2	1.32	0
5	FFZ	D	515	-	35,37,37	0.81	1 (2%)	39,51,51	1.02	2 (5%)
2	EDO	C	513	-	3,3,3	0.51	0	2,2,2	0.93	0
5	FFZ	B	512	-	35,37,37	0.89	1 (2%)	39,51,51	0.84	1 (2%)
2	EDO	A	508	-	3,3,3	0.66	0	2,2,2	0.22	0
2	EDO	A	512	-	3,3,3	0.32	0	2,2,2	0.40	0
2	EDO	B	514	-	3,3,3	0.15	0	2,2,2	1.12	0
3	PEG	A	521	-	6,6,6	0.95	0	5,5,5	1.61	2 (40%)
8	DMS	B	510	-	3,3,3	0.43	0	3,3,3	0.61	0
2	EDO	D	517	-	3,3,3	0.29	0	2,2,2	0.05	0
7	EPE	C	503	-	15,15,15	1.81	2 (13%)	18,20,20	5.19	7 (38%)
8	DMS	D	507	-	3,3,3	0.51	0	3,3,3	1.08	0
2	EDO	D	501	-	3,3,3	0.48	0	2,2,2	0.91	0
2	EDO	D	504	-	3,3,3	0.66	0	2,2,2	0.37	0
8	DMS	D	502	-	3,3,3	0.89	0	3,3,3	0.41	0
2	EDO	D	505	-	3,3,3	0.20	0	2,2,2	0.82	0
2	EDO	B	505	-	3,3,3	0.59	0	2,2,2	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EDO	D	514	-	3,3,3	0.61	0	2,2,2	0.26	0
2	EDO	A	516	-	3,3,3	0.30	0	2,2,2	0.28	0
2	EDO	D	510	-	3,3,3	0.33	0	2,2,2	0.42	0
2	EDO	C	508	-	3,3,3	1.26	0	2,2,2	1.00	0
7	EPE	A	520	-	15,15,15	3.04	1 (6%)	18,20,20	2.36	4 (22%)
2	EDO	B	509	-	3,3,3	0.42	0	2,2,2	0.47	0
2	EDO	A	517	-	3,3,3	0.33	0	2,2,2	0.42	0
2	EDO	A	518	-	3,3,3	0.34	0	2,2,2	0.83	0
2	EDO	D	519	-	3,3,3	0.37	0	2,2,2	1.05	0
2	EDO	C	501	-	3,3,3	0.72	0	2,2,2	0.61	0
2	EDO	C	504	-	3,3,3	0.65	0	2,2,2	0.22	0
2	EDO	A	511	-	3,3,3	0.80	0	2,2,2	0.63	0
3	PEG	A	509	-	6,6,6	0.94	0	5,5,5	1.01	0
2	EDO	B	502	-	3,3,3	0.45	0	2,2,2	0.34	0
2	EDO	D	509	-	3,3,3	0.34	0	2,2,2	0.38	0
2	EDO	A	507	-	3,3,3	0.16	0	2,2,2	0.74	0
2	EDO	A	506	-	3,3,3	0.56	0	2,2,2	0.68	0
2	EDO	B	507	-	3,3,3	0.69	0	2,2,2	0.14	0
3	PEG	C	511	-	6,6,6	0.45	0	5,5,5	1.30	1 (20%)
2	EDO	B	503	-	3,3,3	0.34	0	2,2,2	0.44	0
2	EDO	D	520	-	3,3,3	0.18	0	2,2,2	0.87	0
2	EDO	A	505	-	3,3,3	0.95	0	2,2,2	0.65	0
2	EDO	D	503	-	3,3,3	0.90	0	2,2,2	1.06	0
3	PEG	D	524	-	6,6,6	1.05	0	5,5,5	1.42	0
2	EDO	C	505	-	3,3,3	0.38	0	2,2,2	0.57	0
7	EPE	D	523	-	15,15,15	2.97	2 (13%)	18,20,20	1.78	4 (22%)
3	PEG	B	511	-	6,6,6	0.95	0	5,5,5	1.50	1 (20%)
2	EDO	B	506	-	3,3,3	0.31	0	2,2,2	0.66	0
7	EPE	B	516	-	15,15,15	1.89	1 (6%)	18,20,20	1.75	5 (27%)
2	EDO	C	514	-	3,3,3	0.45	0	2,2,2	1.63	0
2	EDO	C	506	-	3,3,3	0.41	0	2,2,2	0.06	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
2	EDO	D	508	-	-	0/1/1/1	-
5	FFZ	C	510	-	-	2/17/47/47	0/4/4/4
2	EDO	A	515	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	515	-	-	0/1/1/1	-
2	EDO	D	506	-	-	1/1/1/1	-
2	EDO	D	513	-	-	0/1/1/1	-
2	EDO	A	504	-	-	1/1/1/1	-
2	EDO	D	522	-	-	1/1/1/1	-
2	EDO	C	507	-	-	1/1/1/1	-
2	EDO	D	521	-	-	1/1/1/1	-
2	EDO	A	502	-	-	0/1/1/1	-
2	EDO	A	501	-	-	0/1/1/1	-
2	EDO	A	503	-	-	1/1/1/1	-
2	EDO	D	518	-	-	1/1/1/1	-
2	EDO	A	519	-	-	1/1/1/1	-
2	EDO	B	501	-	-	1/1/1/1	-
2	EDO	B	504	-	-	1/1/1/1	-
5	FFZ	A	513	-	-	4/17/47/47	0/4/4/4
2	EDO	C	502	-	-	1/1/1/1	-
2	EDO	D	511	-	-	1/1/1/1	-
5	FFZ	D	515	-	-	2/17/47/47	0/4/4/4
2	EDO	C	513	-	-	1/1/1/1	-
5	FFZ	B	512	-	-	2/17/47/47	0/4/4/4
2	EDO	A	508	-	-	1/1/1/1	-
2	EDO	A	512	-	-	0/1/1/1	-
2	EDO	B	514	-	-	0/1/1/1	-
3	PEG	A	521	-	-	1/4/4/4	-
2	EDO	D	517	-	-	1/1/1/1	-
7	EPE	C	503	-	-	1/9/19/19	0/1/1/1
2	EDO	D	501	-	-	1/1/1/1	-
2	EDO	D	504	-	-	0/1/1/1	-
2	EDO	D	505	-	-	1/1/1/1	-
2	EDO	B	505	-	-	1/1/1/1	-
2	EDO	D	514	-	-	1/1/1/1	-
2	EDO	A	516	-	-	1/1/1/1	-
2	EDO	D	510	-	-	1/1/1/1	-
2	EDO	C	508	-	-	0/1/1/1	-
7	EPE	A	520	-	-	8/9/19/19	0/1/1/1
2	EDO	B	509	-	-	0/1/1/1	-
2	EDO	A	517	-	-	0/1/1/1	-
2	EDO	A	518	-	-	0/1/1/1	-
2	EDO	D	519	-	-	0/1/1/1	-
2	EDO	C	501	-	-	0/1/1/1	-
2	EDO	C	504	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	511	-	-	1/1/1/1	-
3	PEG	A	509	-	-	1/4/4/4	-
2	EDO	B	502	-	-	0/1/1/1	-
2	EDO	D	509	-	-	0/1/1/1	-
2	EDO	A	507	-	-	1/1/1/1	-
2	EDO	A	506	-	-	0/1/1/1	-
2	EDO	B	507	-	-	0/1/1/1	-
3	PEG	C	511	-	-	2/4/4/4	-
2	EDO	B	503	-	-	0/1/1/1	-
2	EDO	D	520	-	-	0/1/1/1	-
2	EDO	A	505	-	-	1/1/1/1	-
2	EDO	D	503	-	-	1/1/1/1	-
3	PEG	D	524	-	-	4/4/4/4	-
2	EDO	C	505	-	-	1/1/1/1	-
7	EPE	D	523	-	-	3/9/19/19	0/1/1/1
3	PEG	B	511	-	-	2/4/4/4	-
2	EDO	B	506	-	-	0/1/1/1	-
7	EPE	B	516	-	-	5/9/19/19	0/1/1/1
2	EDO	C	514	-	-	0/1/1/1	-
2	EDO	C	506	-	-	0/1/1/1	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	520	EPE	C10-S	-11.58	1.61	1.77
7	D	523	EPE	C10-S	-10.83	1.62	1.77
7	B	516	EPE	C10-S	-6.50	1.68	1.77
7	C	503	EPE	C10-S	-6.17	1.68	1.77
5	C	510	FFZ	C9-C10	-4.00	1.42	1.45

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	503	EPE	O2S-S-C10	-15.10	88.73	106.92
7	C	503	EPE	O1S-S-C10	-10.40	94.39	106.92
7	C	503	EPE	O3S-S-C10	-10.15	89.35	105.77
7	A	520	EPE	O2S-S-C10	7.46	115.90	106.92
7	B	516	EPE	O2S-S-C10	5.19	113.16	106.92

There are no chirality outliers.

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	515	EDO	O1-C1-C2-O2
2	D	501	EDO	O1-C1-C2-O2
7	A	520	EPE	C8-C7-N4-C5
7	A	520	EPE	C9-C10-S-O1S
7	A	520	EPE	C9-C10-S-O2S

There are no ring outliers.

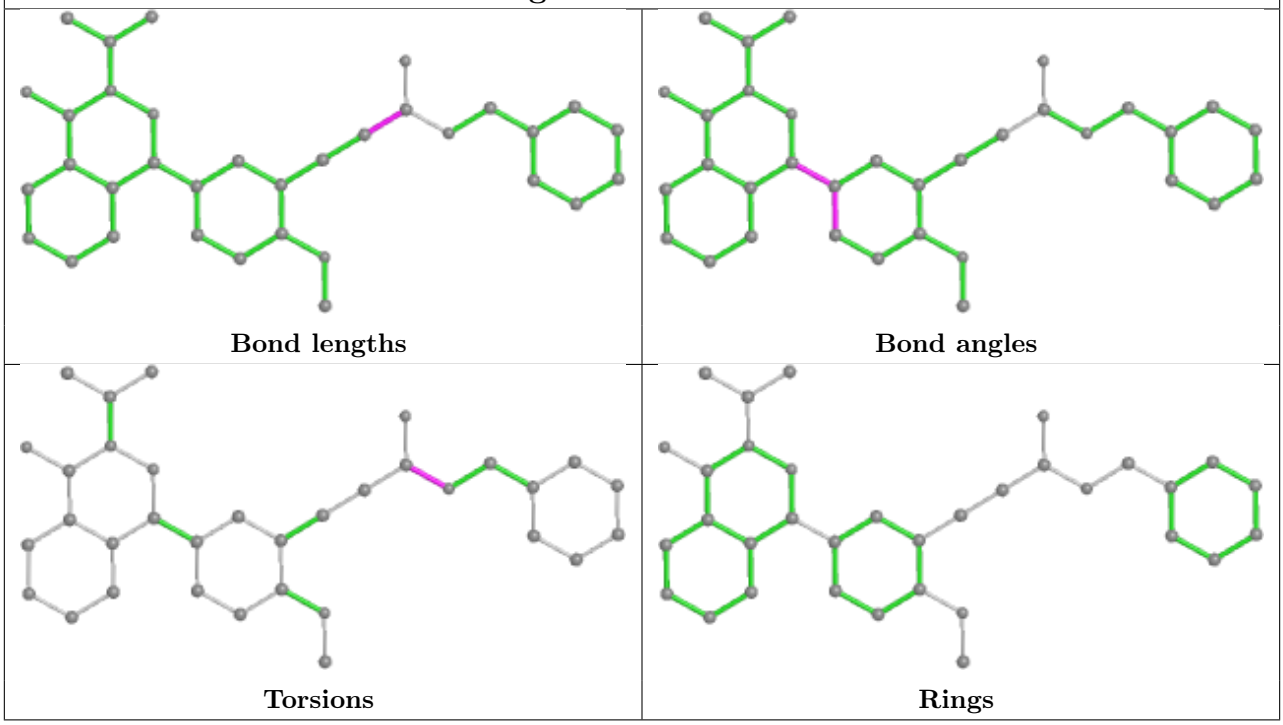
21 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	EDO	1	0
2	B	501	EDO	1	0
5	A	513	FFZ	2	0
5	D	515	FFZ	1	0
2	C	513	EDO	1	0
5	B	512	FFZ	3	0
3	A	521	PEG	1	0
8	B	510	DMS	1	0
2	D	517	EDO	1	0
8	D	502	DMS	5	0
2	B	505	EDO	1	0
2	C	508	EDO	1	0
7	A	520	EPE	4	0
3	C	511	PEG	3	0
2	D	520	EDO	4	0
2	A	505	EDO	1	0
3	D	524	PEG	1	0
7	D	523	EPE	6	0
3	B	511	PEG	3	0
2	B	506	EDO	1	0
2	C	506	EDO	1	0

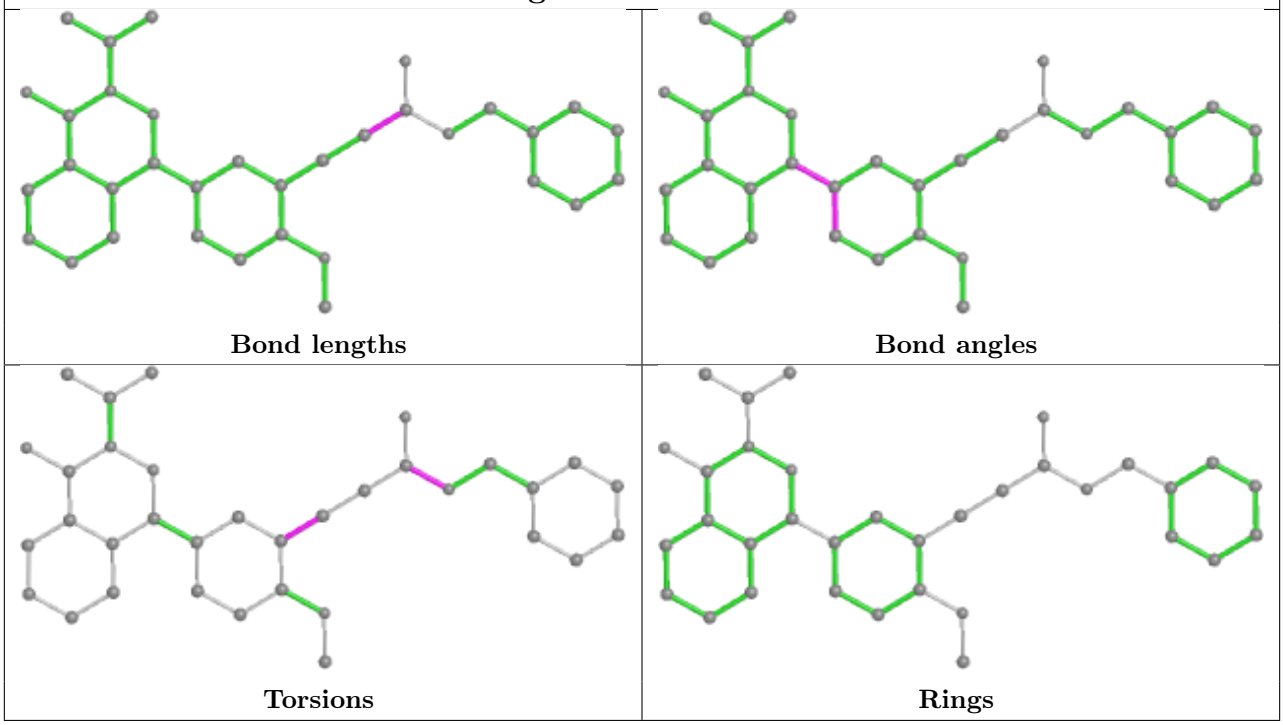
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

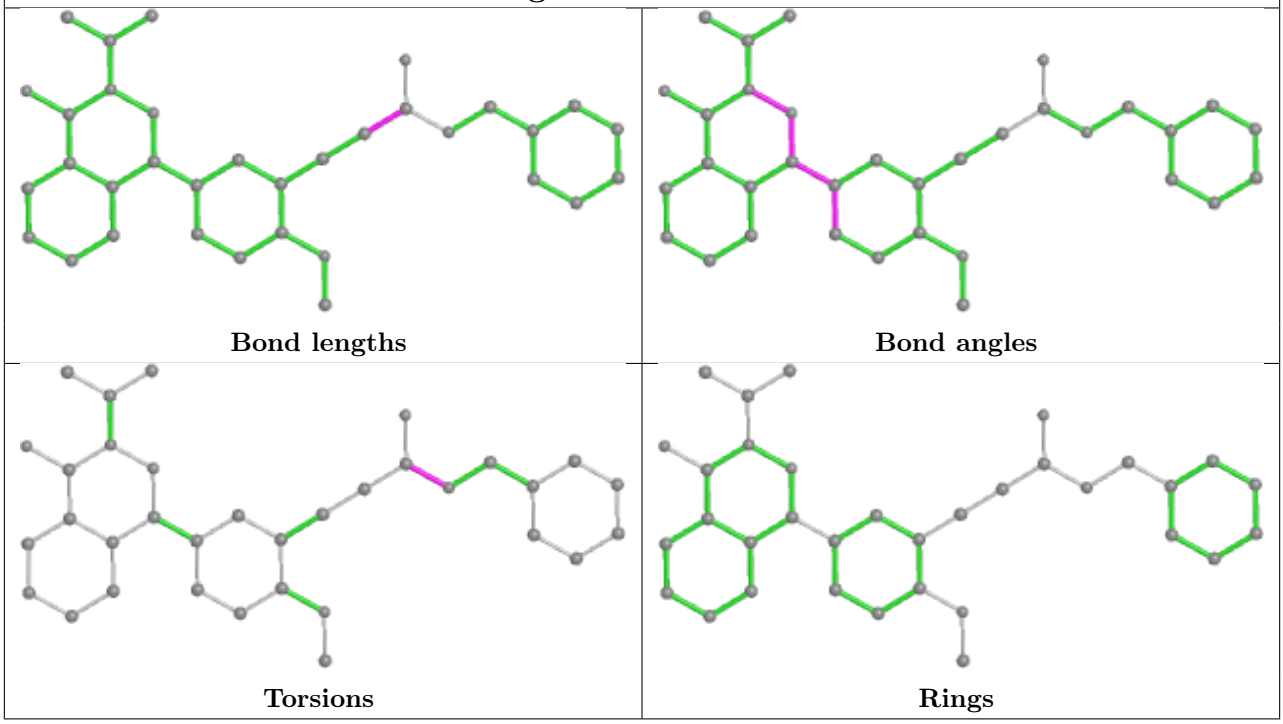
Ligand FFZ C 510



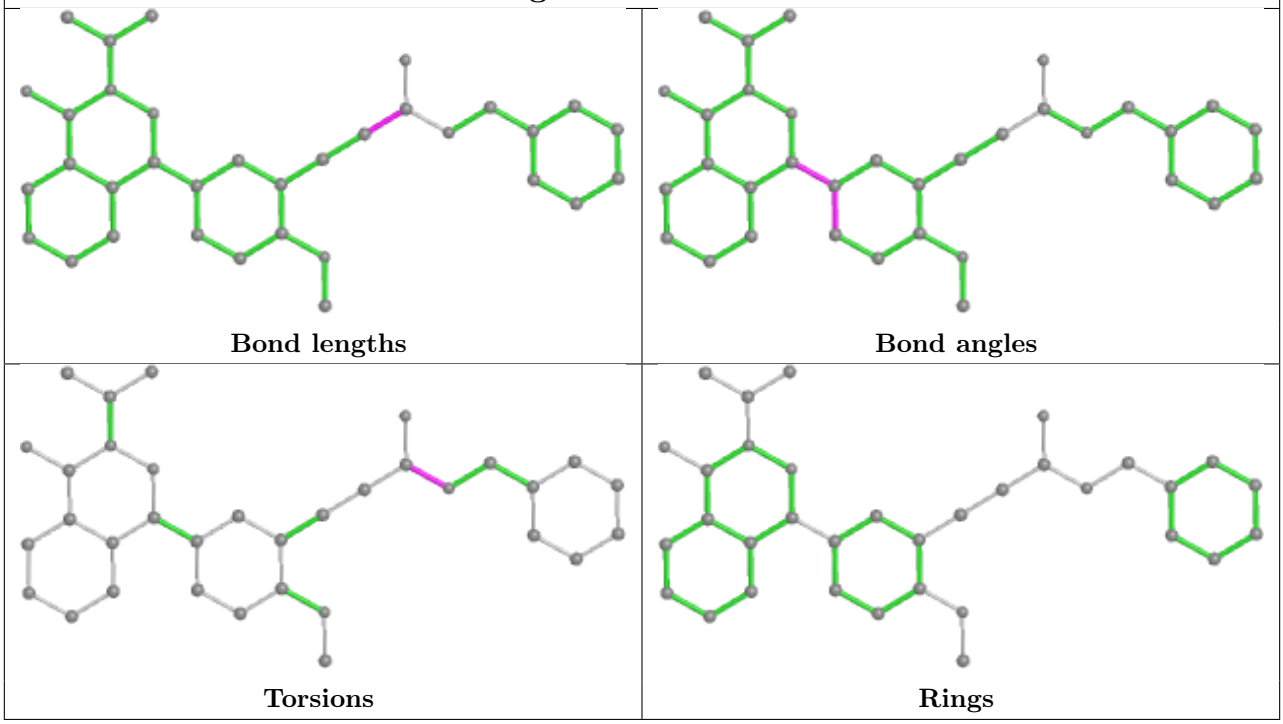
Ligand FFZ A 513



Ligand FFZ D 515



Ligand FFZ B 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	327/364 (89%)	0.46	23 (7%)	16	15	22, 40, 104, 147	0
1	B	321/364 (88%)	0.29	8 (2%)	57	56	25, 43, 66, 92	0
1	C	324/364 (89%)	0.46	19 (5%)	22	21	23, 42, 91, 117	0
1	D	324/364 (89%)	0.26	6 (1%)	66	65	20, 32, 67, 94	0
All	All	1296/1456 (89%)	0.37	56 (4%)	35	34	20, 39, 78, 147	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	ALA	9.2
1	C	357	MET	8.0
1	A	361	HIS	7.5
1	A	357	MET	7.2
1	C	294	SER	6.3

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
2	EDO	D	513	4/4	0.55	0.20	58,62,62,66	0
3	PEG	D	524	7/7	0.57	0.29	48,52,64,64	0
5	FFZ	A	513	34/34	0.61	0.33	56,77,99,104	0
2	EDO	C	508	4/4	0.66	0.26	50,51,57,59	0
3	PEG	C	511	7/7	0.66	0.28	31,35,47,50	0
2	EDO	C	507	4/4	0.70	0.29	47,50,53,62	0
2	EDO	A	508	4/4	0.71	0.17	62,63,65,68	0
2	EDO	B	507	4/4	0.75	0.27	59,70,71,74	0
8	DMS	D	502	4/4	0.75	0.36	95,98,107,111	0
2	EDO	C	504	4/4	0.76	0.15	58,63,65,67	0
2	EDO	A	505	4/4	0.77	0.35	47,56,57,57	0
3	PEG	A	521	7/7	0.77	0.20	53,59,74,75	0
3	PEG	B	511	7/7	0.79	0.30	49,61,66,68	0
2	EDO	D	510	4/4	0.80	0.25	45,61,63,78	0
2	EDO	D	521	4/4	0.80	0.19	39,49,50,52	0
2	EDO	A	504	4/4	0.81	0.17	36,49,55,57	0
2	EDO	C	513	4/4	0.81	0.30	57,68,72,75	0
2	EDO	D	508	4/4	0.81	0.18	45,55,62,66	0
2	EDO	A	503	4/4	0.82	0.24	56,69,73,81	0
2	EDO	D	509	4/4	0.83	0.15	51,53,57,63	0
3	PEG	A	509	7/7	0.83	0.21	43,59,71,73	0
2	EDO	D	503	4/4	0.83	0.22	40,47,52,53	0
5	FFZ	C	510	34/34	0.83	0.17	43,55,73,75	0
2	EDO	B	504	4/4	0.83	0.26	63,76,78,81	0
2	EDO	C	505	4/4	0.84	0.19	66,74,78,79	0
2	EDO	B	502	4/4	0.84	0.50	68,70,72,75	0
2	EDO	A	519	4/4	0.84	0.12	67,71,71,79	0
5	FFZ	D	515	34/34	0.85	0.18	42,52,82,84	0
2	EDO	D	514	4/4	0.85	0.16	47,52,58,62	0
2	EDO	A	517	4/4	0.86	0.14	52,62,63,65	0
2	EDO	C	514	4/4	0.86	0.18	47,51,51,61	0
2	EDO	B	505	4/4	0.87	0.38	58,60,60,63	0
2	EDO	B	514	4/4	0.87	0.22	54,54,55,62	0
2	EDO	A	518	4/4	0.88	0.20	57,60,62,66	0
2	EDO	B	506	4/4	0.88	0.30	58,63,64,66	0
8	DMS	D	507	4/4	0.88	0.22	87,90,95,96	0
2	EDO	C	501	4/4	0.89	0.34	51,59,61,61	0
2	EDO	C	502	4/4	0.89	0.18	51,59,60,65	0
2	EDO	A	516	4/4	0.89	0.16	52,53,54,57	0
5	FFZ	B	512	34/34	0.89	0.17	42,51,86,87	0
2	EDO	B	515	4/4	0.90	0.24	56,56,57,61	0
2	EDO	D	511	4/4	0.90	0.23	53,56,59,66	0
2	EDO	A	506	4/4	0.90	0.20	45,53,55,59	0

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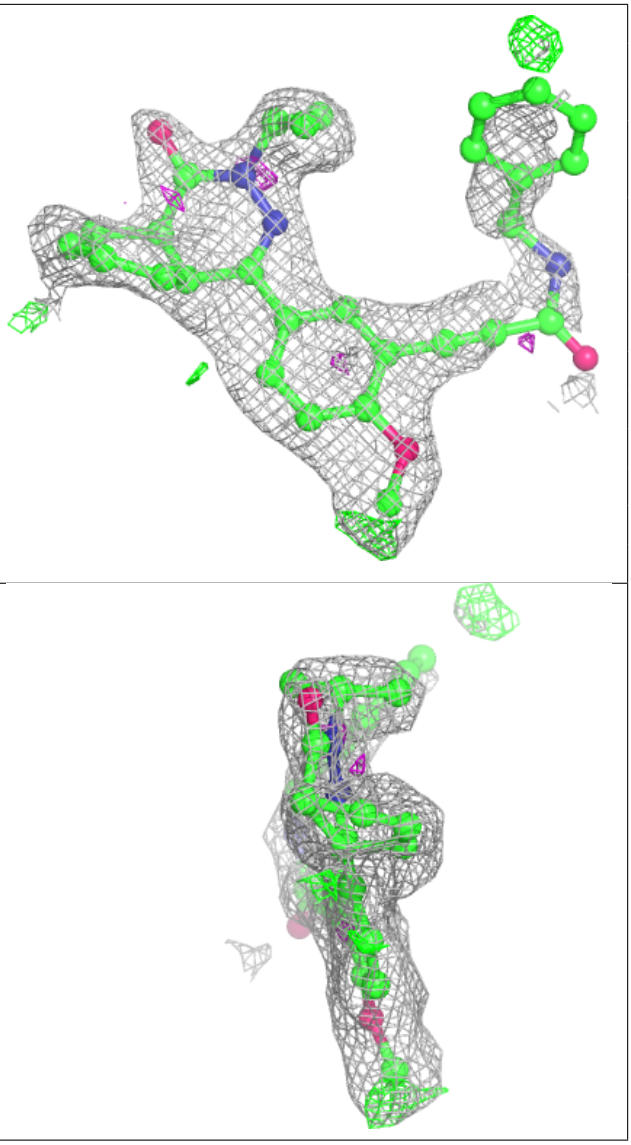
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	A	515	4/4	0.90	0.23	39,51,53,57	0
2	EDO	B	501	4/4	0.91	0.45	48,56,61,64	0
2	EDO	D	518	4/4	0.91	0.17	52,58,59,63	0
2	EDO	A	511	4/4	0.92	0.12	38,38,38,41	0
2	EDO	D	519	4/4	0.92	0.14	36,37,39,46	0
2	EDO	B	503	4/4	0.93	0.13	54,54,56,64	0
2	EDO	B	509	4/4	0.93	0.21	43,51,56,65	0
2	EDO	D	517	4/4	0.93	0.14	42,43,45,51	0
2	EDO	C	506	4/4	0.93	0.27	54,54,57,64	0
8	DMS	B	510	4/4	0.93	0.24	82,84,85,92	0
2	EDO	A	501	4/4	0.93	0.13	33,33,33,36	0
2	EDO	D	520	4/4	0.93	0.16	60,65,76,80	0
7	EPE	B	516	15/15	0.94	0.27	47,102,116,117	0
2	EDO	A	502	4/4	0.94	0.14	34,37,37,42	0
2	EDO	D	506	4/4	0.94	0.17	38,47,48,50	0
7	EPE	A	520	15/15	0.94	0.20	57,90,99,102	0
2	EDO	D	505	4/4	0.95	0.17	37,43,43,44	0
2	EDO	D	522	4/4	0.95	0.18	53,55,58,67	0
2	EDO	D	501	4/4	0.95	0.14	35,36,42,42	0
2	EDO	D	504	4/4	0.95	0.12	36,36,36,39	0
2	EDO	A	507	4/4	0.96	0.18	44,46,49,54	0
2	EDO	A	512	4/4	0.96	0.16	36,48,48,51	0
7	EPE	D	523	15/15	0.96	0.19	38,77,92,98	0
7	EPE	C	503	15/15	0.97	0.13	41,52,71,76	0
6	MG	A	514	1/1	0.98	0.18	21,21,21,21	0
6	MG	C	512	1/1	0.99	0.16	18,18,18,18	0
4	ZN	B	508	1/1	0.99	0.09	34,34,34,34	0
4	ZN	A	510	1/1	0.99	0.13	34,34,34,34	0
6	MG	B	513	1/1	0.99	0.13	18,18,18,18	0
4	ZN	C	509	1/1	1.00	0.12	32,32,32,32	0
6	MG	D	516	1/1	1.00	0.17	18,18,18,18	0
4	ZN	D	512	1/1	1.00	0.14	29,29,29,29	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.

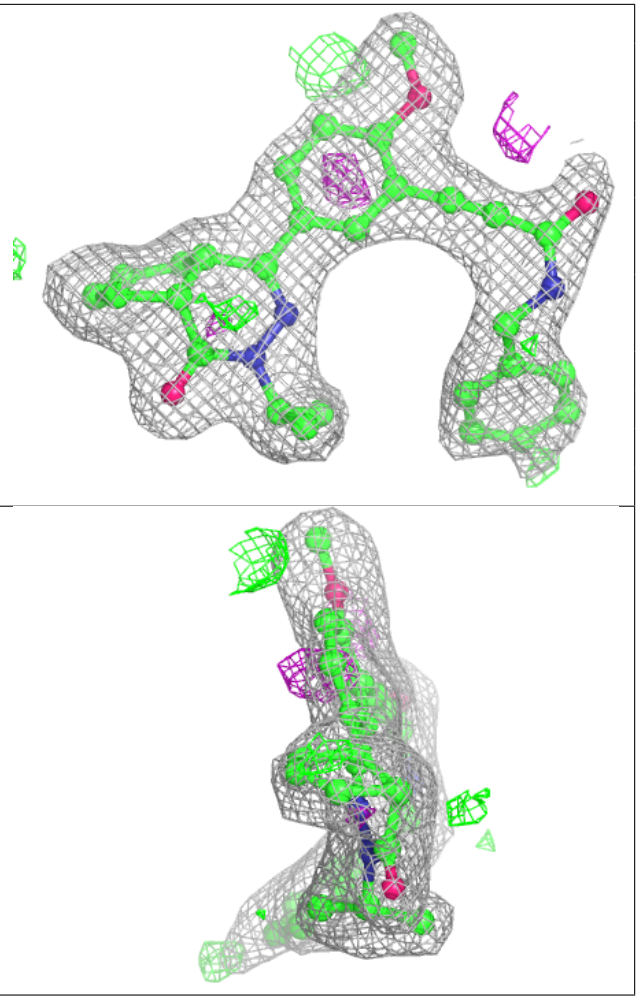
Electron density around FFZ A 513:

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



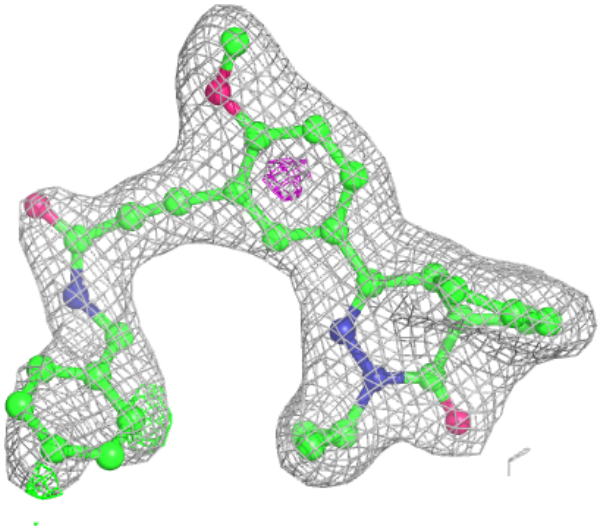
Electron density around FFZ C 510:

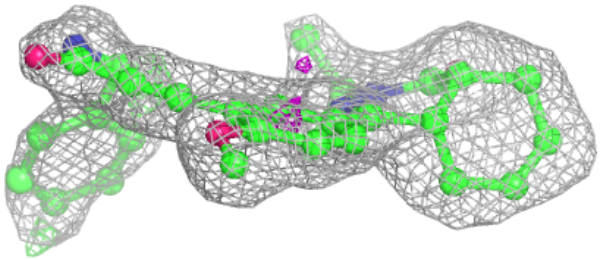
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

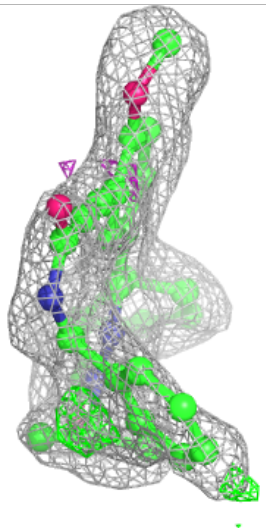


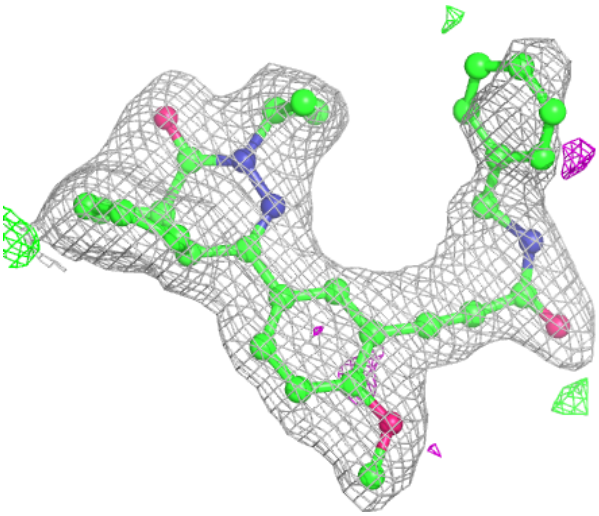
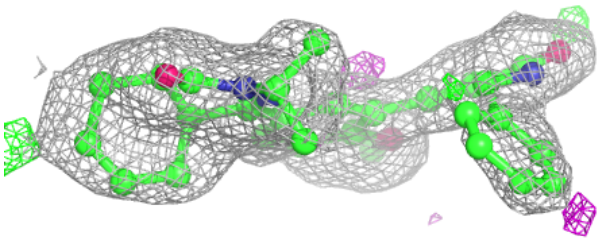
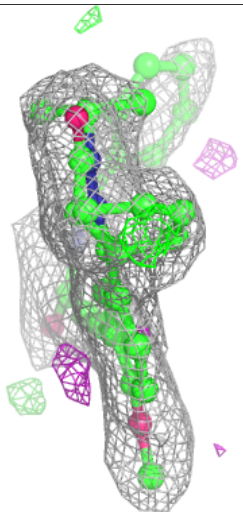
Electron density around FFZ D 515:

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







Electron density around FFZ B 512: 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.