wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 09:34 pm GMT

PDB ID	:	4C8R
Title	:	Human gamma-butyrobetaine dioxygenase (BBOX1) in complex with Ni(II) and N-(3-hydroxypicolinoyl)-S-(pyridin-2-ylmethyl)-L-cysteine (AR692B)
Authors	:	Chowdhury, R.; Rydzik, A.M.; Kochan, G.T.; McDonough, M.A.; Schofield, C.J.
Deposited on	:	2013-10-01
Resolution	:	2.82 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:

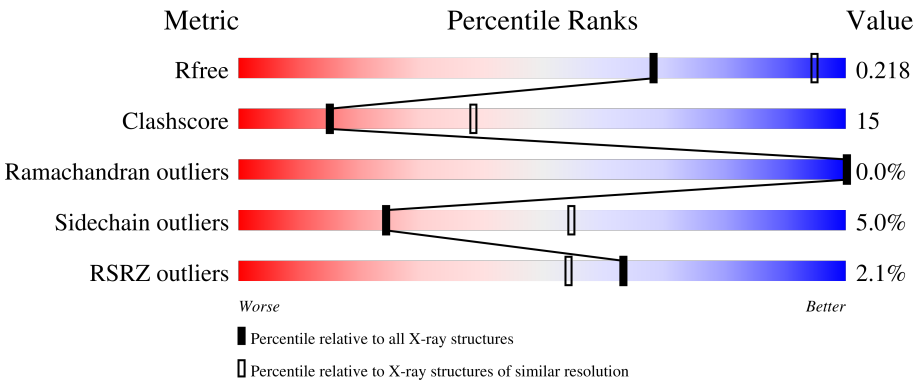
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	388	% 70% 27% • •
1	B	388	% 68% 29% • •
1	C	388	% 69% 27% • •
1	D	388	3% 64% 33% • •

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Mol	Chain	Length	Quality of chain
1	E	388	6% 64% 33%
1	F	388	2% 61% 37%

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	6YT	A	601	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 19352 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 GAMMA-BUTYROBETAINE DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	384	3116	1995	533	573	15	0	0	0
1	B	384	3130	2006	535	574	15	0	0	0
1	C	384	3117	1997	530	576	14	0	0	0
1	D	384	3109	1995	535	565	14	0	0	0
1	E	384	3097	1986	532	565	14	0	0	0
1	F	384	3109	1997	531	567	14	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP O75936
B	0	SER	-	expression tag	UNP O75936
C	0	SER	-	expression tag	UNP O75936
D	0	SER	-	expression tag	UNP O75936
E	0	SER	-	expression tag	UNP O75936
F	0	SER	-	expression tag	UNP O75936

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

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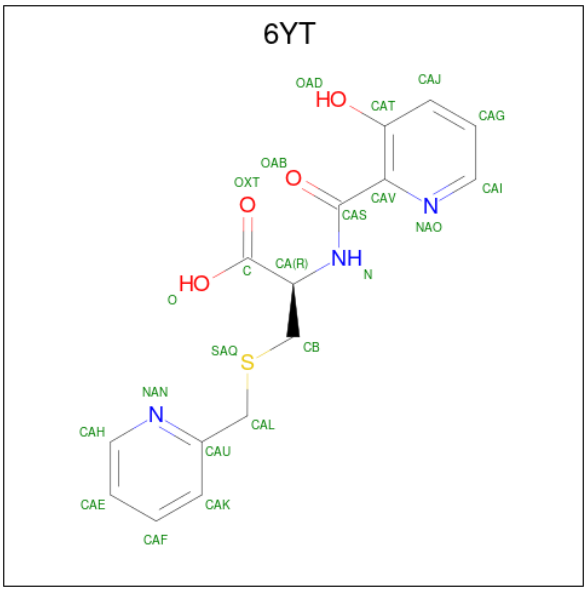
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Ni 1 1	0	0
2	E	1	Total Ni 1 1	0	0
2	F	1	Total Ni 1 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

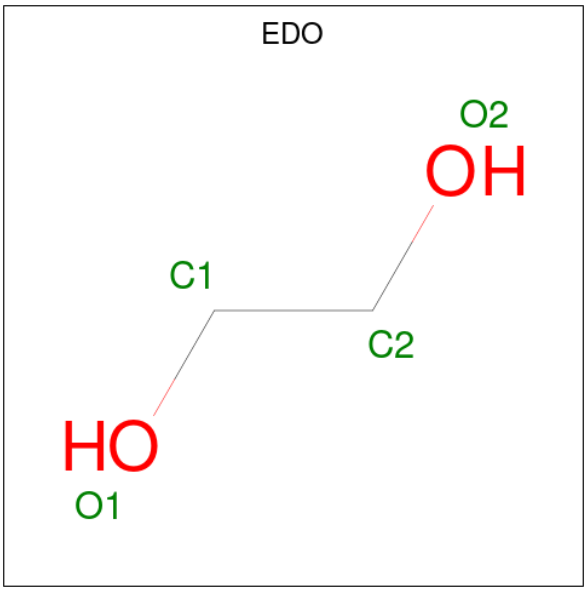
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0

- Molecule 4 is N-(3-hydroxypicolinoyl)-S-(pyridin-2-ylmethyl)-L-cysteine (three-letter code: 6YT) (formula: $C_{15}H_{15}N_3O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	23	15	3	4	1	0	0
4	B	1	23	15	3	4	1	0	0
4	C	1	23	15	3	4	1	0	0
4	D	1	23	15	3	4	1	0	0
4	E	1	23	15	3	4	1	0	0
4	F	1	23	15	3	4	1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	C	1	4	2	2	0	0
			Total	C	O		
5	C	1	4	2	2	0	0
			Total	C	O		
5	C	1	4	2	2	0	0
			Total	C	O		
5	E	1	4	2	2	0	0
			Total	C	O		
5	E	1	4	2	2	0	0
			Total	C	O		
5	E	1	4	2	2	0	0
			Total	C	O		
5	F	1	4	2	2	0	0
			Total	C	O		
5	F	1	4	2	2	0	0

- Molecule 6 is water.

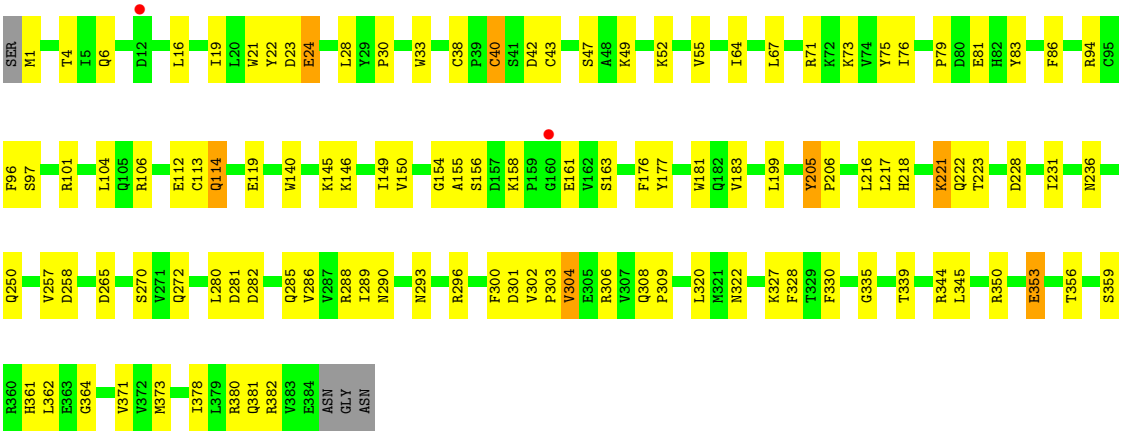
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	106	106	106	0	0
			Total	O		
6	B	95	95	95	0	0
			Total	O		
6	C	90	90	90	0	0
			Total	O		
6	D	60	60	60	0	0
			Total	O		
6	E	52	52	52	0	0
			Total	O		
6	F	65	65	65	0	0

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.

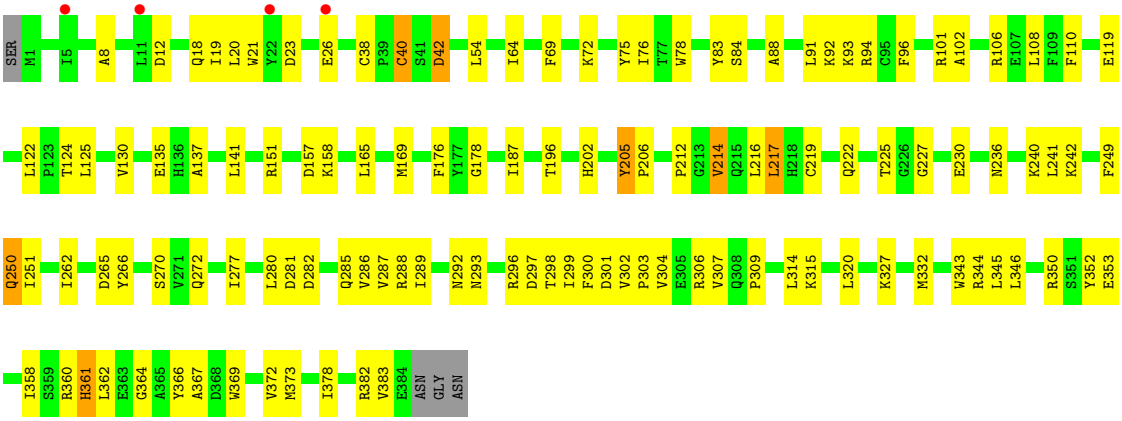
• Molecule 1: GAMMA-BUTYROBETAINE DIOXYGENASE

Chain A:



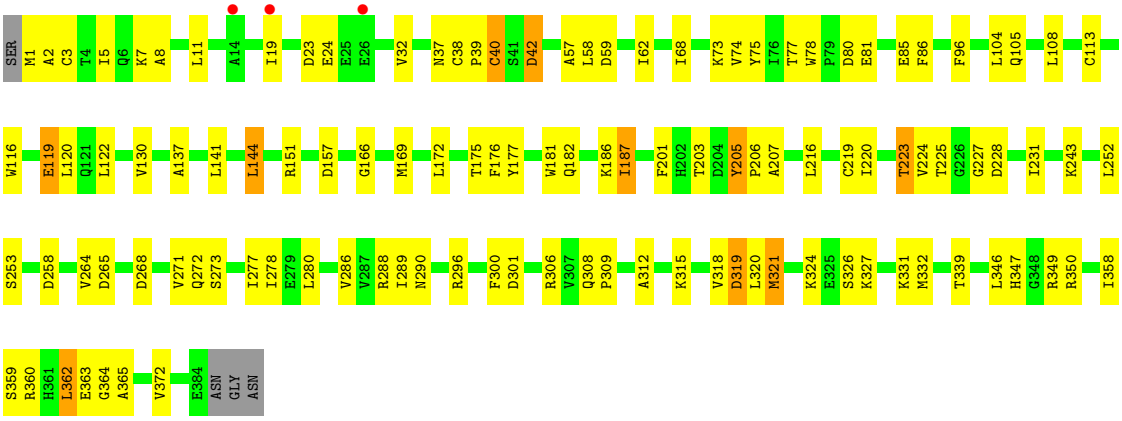
• Molecule 1: GAMMA-BUTYROBETAINE DIOXYGENASE

Chain B:



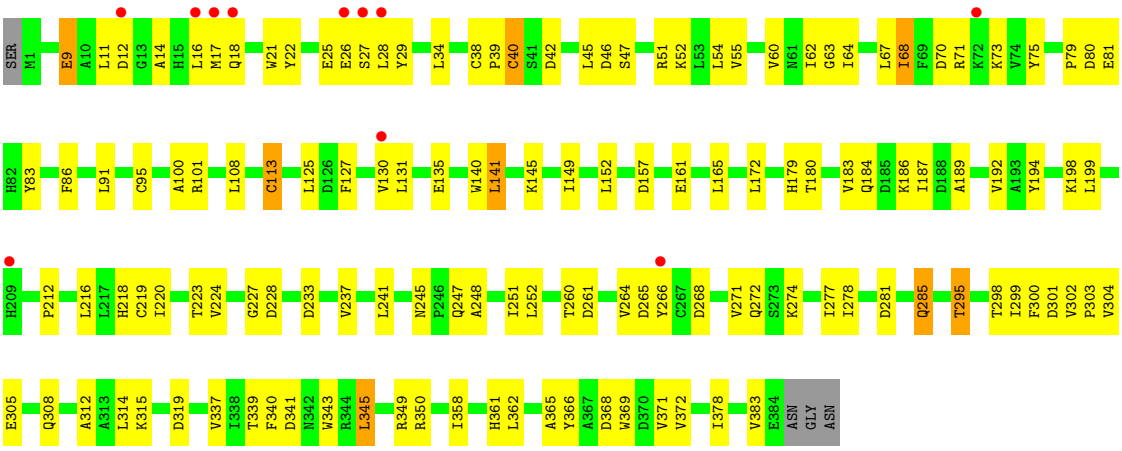
• Molecule 1: GAMMA-BUTYROBETAINE DIOXYGENASE

Chain C:



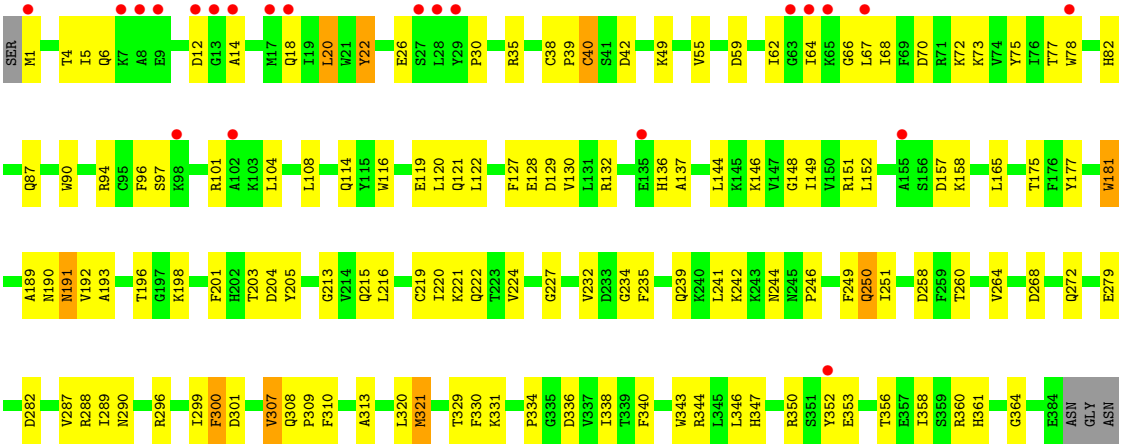
- Molecule 1: GAMMA-BUTYROBETAINE DIOXYGENASE

Chain D:



- Molecule 1: GAMMA-BUTYROBETAINE DIOXYGENASE

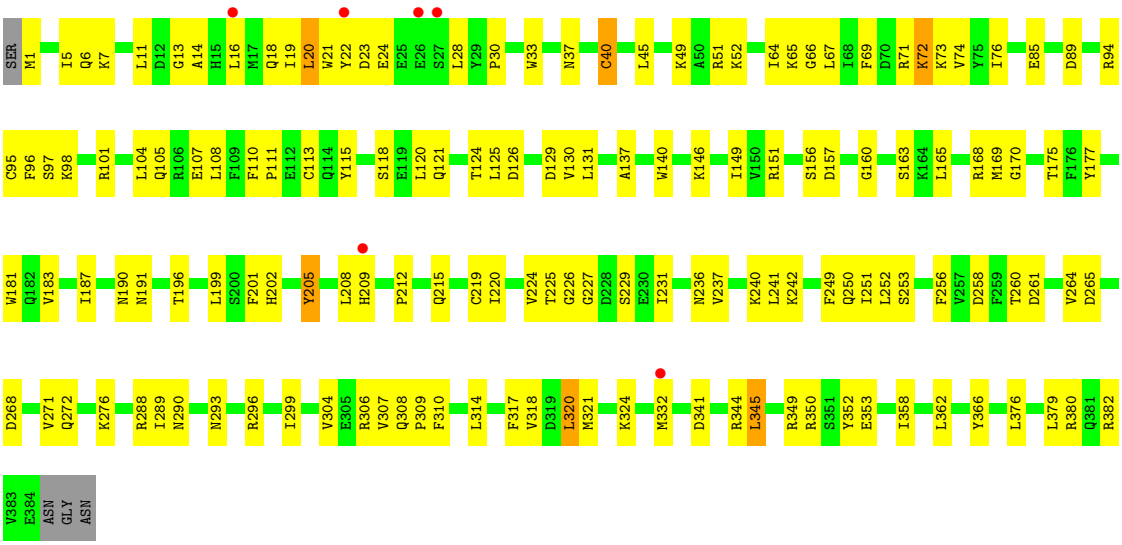
Chain E:



- Molecule 1: GAMMA-BUTYROBETAINE DIOXYGENASE

Chain F:

2%
61%
37%


SER M1 I5 Q6 K7 L11 D12 G13 A14 H15 L16 M17 Q18 I19 L20 W21 Y22 D23 E24 E25 E26 S27 L28 Y29 P30 W33 N37 C40 L45 K49 A50 R51 K52 I64 K65 G66 L67 I68 F69 D70 R71 K72 K73 V74 Y75 I76 E85 D89 R94
C95 F96 S97 K98 R101 L104 Q105 R106 E107 L108 F109 F110 P111 E112 C113 Q114 Y115 S118 E119 L120 Q121 T124 L125 D126 D129 V130 L131 A137 W140 K146 I149 V150 R151 S156 D157 G160 S163 K164 L165 R168 M169 G170 T175 F176 Y177
W181 Q182 V183 I187 N190 N191 T196 L199 S200 F201 H202 Y205 L208 H209 P212 Q215 C219 I220 V224 T225 G226 G227 D228 S229 E230 I231 N236 V237 K240 L241 K242 F249 Q250 I251 L252 S253 F256 V257 D258 F259 T260 D261 V264 D265
D268 V271 Q272 K276 R288 I289 N290 N293 R296 I299 V304 E305 R306 V307 Q308 P309 F310 L314 F317 V318 D319 L320 M321 K324 M332 D341 R344 L345 R349 R350 S351 Y352 E353 I358 L362 Y366 L376 L379 R380 Q381 R382
V383 E384 ASN GLY ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	195.74Å 91.66Å 167.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.42 – 2.82 48.94 – 2.82	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.42-2.82) 96.9 (48.94-2.82)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.81Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.215 , 0.244 0.217 , 0.218	Depositor DCC
R_{free} test set	3576 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	58.8	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19352	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2781e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: ZN, EDO, 6YT, NI

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	0.47	0/3193	0.65	1/4323 (0.0%)
1	B	0.48	0/3208	0.65	0/4341
1	C	0.45	0/3195	0.62	0/4327
1	D	0.44	0/3187	0.61	0/4315
1	E	0.43	0/3175	0.59	0/4302
1	F	0.43	0/3187	0.60	0/4315
All	All	0.45	0/19145	0.62	1/25923 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	24	GLU	CB-CA-C	-6.00	98.40	110.40

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	3116	0	3043	84	0
1	B	3130	0	3070	91	0
1	C	3117	0	3031	91	0
1	D	3109	0	3042	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3097	0	3012	110	0
1	F	3109	0	3042	121	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
2	E	1	0	0	0	0
2	F	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
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	23	0	14	7	0
4	B	23	0	14	5	0
4	C	23	0	14	0	0
4	D	23	0	14	1	0
4	E	23	0	14	0	0
4	F	23	0	14	2	0
5	A	12	0	18	0	0
5	B	8	0	12	0	0
5	C	16	0	24	1	0
5	E	12	0	18	2	0
5	F	8	0	12	0	0
6	A	106	0	0	5	0
6	B	95	0	0	2	0
6	C	90	0	0	5	0
6	D	60	0	0	4	0
6	E	52	0	0	2	0
6	F	65	0	0	5	0
All	All	19352	0	18408	564	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 15.

The worst 5 of 564 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:F:199:LEU:HD21	1:F:349:ARG:HB3	1.34	1.09
1:B:93:LYS:HE2	1:B:94:ARG:HH12	1.32	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:VAL:HG12	1:F:358:ILE:HA	1.56	0.85
1:B:93:LYS:HE2	1:B:94:ARG:NH1	1.92	0.85
1:C:219:CYS:HB2	1:C:332:MET:HE2	1.59	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	382/388 (98%)	353 (92%)	29 (8%)	0	100	100
1	B	382/388 (98%)	349 (91%)	33 (9%)	0	100	100
1	C	382/388 (98%)	341 (89%)	41 (11%)	0	100	100
1	D	382/388 (98%)	356 (93%)	26 (7%)	0	100	100
1	E	382/388 (98%)	349 (91%)	33 (9%)	0	100	100
1	F	382/388 (98%)	355 (93%)	26 (7%)	1 (0%)	41	70
All	All	2292/2328 (98%)	2103 (92%)	188 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	170	GLY

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	336/343 (98%)	316 (94%)	20 (6%)	19	47
1	B	339/343 (99%)	326 (96%)	13 (4%)	33	65
1	C	335/343 (98%)	315 (94%)	20 (6%)	19	47
1	D	333/343 (97%)	314 (94%)	19 (6%)	20	49
1	E	330/343 (96%)	313 (95%)	17 (5%)	23	53
1	F	333/343 (97%)	322 (97%)	11 (3%)	38	70
All	All	2006/2058 (98%)	1906 (95%)	100 (5%)	24	55

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	47	SER
1	D	372	VAL
1	F	379	LEU
1	D	113	CYS
1	D	228	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	272	GLN
1	F	222	GLN
1	E	333	ASN
1	F	182	GLN
1	F	347	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 12 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EDO	E	702	-	3,3,3	0.58	0	2,2,2	0.27	0
5	EDO	E	703	-	3,3,3	0.52	0	2,2,2	0.25	0
5	EDO	C	702	-	3,3,3	0.55	0	2,2,2	0.25	0
5	EDO	A	703	-	3,3,3	0.53	0	2,2,2	0.28	0
5	EDO	B	702	-	3,3,3	0.48	0	2,2,2	0.34	0
5	EDO	B	701	-	3,3,3	0.52	0	2,2,2	0.30	0
4	6YT	A	601	2	24,24,24	2.34	4 (16%)	27,31,31	1.34	4 (14%)
5	EDO	F	702	-	3,3,3	0.53	0	2,2,2	0.30	0
5	EDO	F	701	-	3,3,3	0.49	0	2,2,2	0.32	0
4	6YT	F	601	2	24,24,24	2.23	4 (16%)	27,31,31	1.30	5 (18%)
5	EDO	C	701	-	3,3,3	0.53	0	2,2,2	0.31	0
5	EDO	A	702	-	3,3,3	0.54	0	2,2,2	0.26	0
5	EDO	C	704	-	3,3,3	0.47	0	2,2,2	0.37	0
5	EDO	A	701	-	3,3,3	0.62	0	2,2,2	0.21	0
5	EDO	C	703	-	3,3,3	0.54	0	2,2,2	0.29	0
4	6YT	E	601	2	24,24,24	2.16	3 (12%)	27,31,31	1.23	5 (18%)
4	6YT	D	601	2	24,24,24	2.20	4 (16%)	27,31,31	1.17	2 (7%)
4	6YT	C	601	2	24,24,24	2.19	4 (16%)	27,31,31	1.08	2 (7%)
4	6YT	B	601	2	24,24,24	2.34	4 (16%)	27,31,31	1.34	4 (14%)
5	EDO	E	701	-	3,3,3	0.50	0	2,2,2	0.28	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	E	702	-	-	0/1/1/1	-
5	EDO	E	703	-	-	1/1/1/1	-
5	EDO	C	702	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	703	-	-	1/1/1/1	-
5	EDO	B	702	-	-	1/1/1/1	-
5	EDO	B	701	-	-	0/1/1/1	-
4	6YT	A	601	2	-	5/18/18/18	0/2/2/2
5	EDO	F	702	-	-	0/1/1/1	-
5	EDO	F	701	-	-	0/1/1/1	-
4	6YT	F	601	2	-	5/18/18/18	0/2/2/2
5	EDO	C	701	-	-	0/1/1/1	-
5	EDO	A	702	-	-	1/1/1/1	-
5	EDO	C	704	-	-	0/1/1/1	-
5	EDO	A	701	-	-	0/1/1/1	-
5	EDO	C	703	-	-	0/1/1/1	-
4	6YT	E	601	2	-	7/18/18/18	0/2/2/2
4	6YT	D	601	2	-	7/18/18/18	0/2/2/2
4	6YT	C	601	2	-	6/18/18/18	0/2/2/2
4	6YT	B	601	2	-	5/18/18/18	0/2/2/2
5	EDO	E	701	-	-	0/1/1/1	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	6YT	CAV-CAS	-8.00	1.38	1.50
4	A	601	6YT	CAV-CAS	-7.98	1.38	1.50
4	F	601	6YT	CAV-CAS	-7.73	1.39	1.50
4	D	601	6YT	CAV-CAS	-7.09	1.39	1.50
4	C	601	6YT	CAV-CAS	-6.97	1.40	1.50

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	601	6YT	CAH-NAN-CAU	2.43	120.75	117.42
4	A	601	6YT	CAL-CAU-NAN	2.35	120.28	116.68
4	B	601	6YT	CAL-CAU-NAN	2.35	120.28	116.68
4	F	601	6YT	CB-SAQ-CAL	-2.25	96.47	101.25
4	F	601	6YT	CAL-CAU-NAN	2.23	120.09	116.68

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	6YT	N-CAS-CAV-NAO
4	A	601	6YT	N-CAS-CAV-CAT
4	A	601	6YT	OAB-CAS-CAV-NAO
4	A	601	6YT	OAB-CAS-CAV-CAT
4	B	601	6YT	N-CAS-CAV-NAO

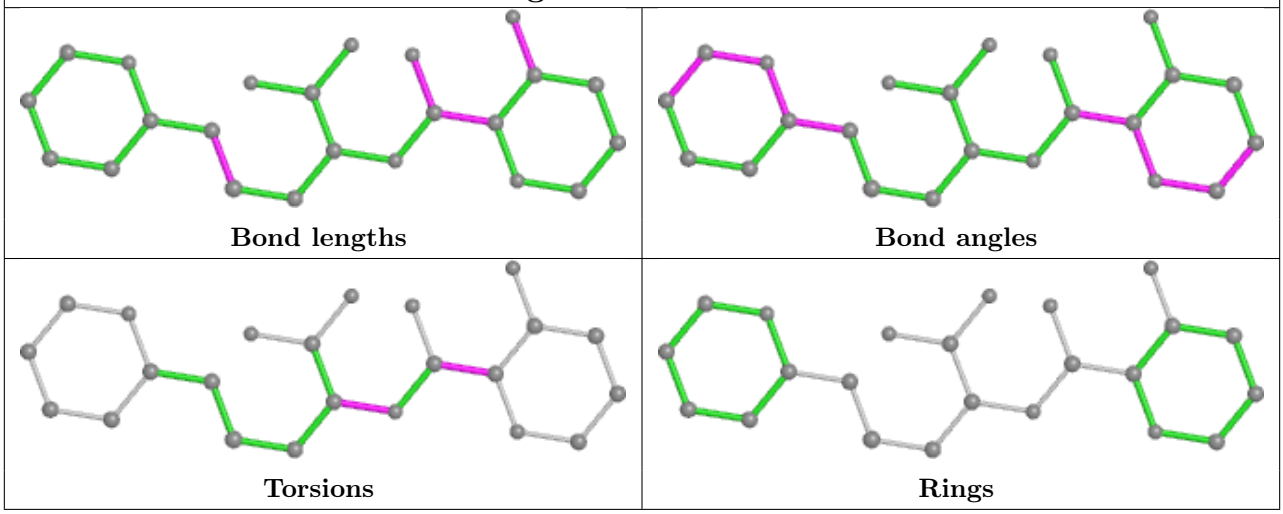
There are no ring outliers.

6 monomers are involved in 18 short contacts:

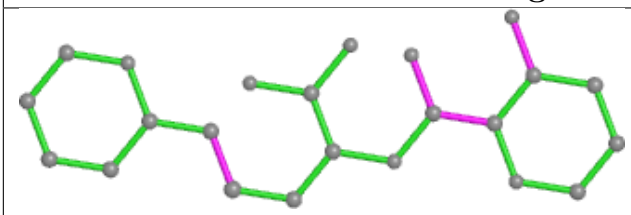
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	703	EDO	2	0
4	A	601	6YT	7	0
4	F	601	6YT	2	0
5	C	704	EDO	1	0
4	D	601	6YT	1	0
4	B	601	6YT	5	0

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.

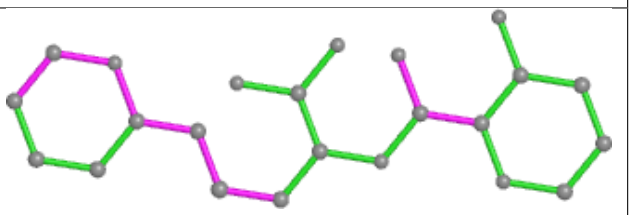
Ligand 6YT A 601



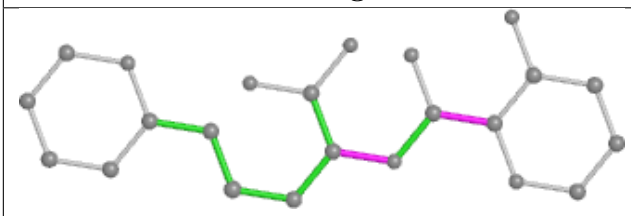
Ligand 6YT F 601



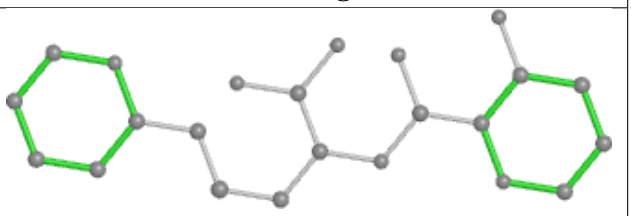
Bond lengths



Bond angles

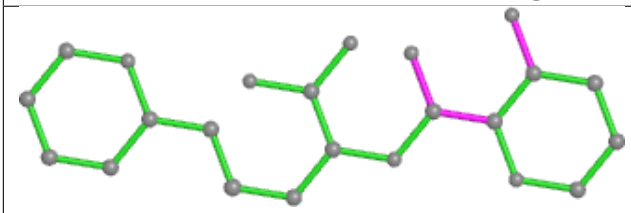


Torsions

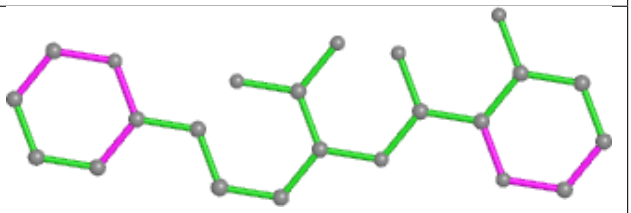


Rings

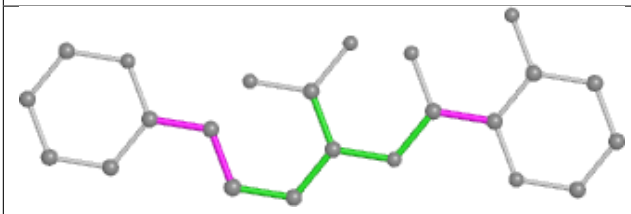
Ligand 6YT E 601



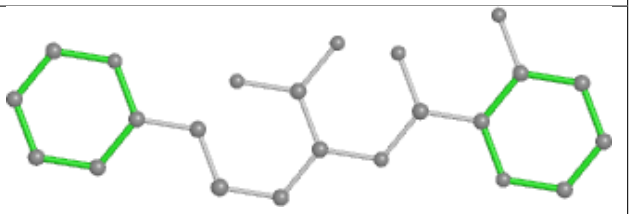
Bond lengths



Bond angles

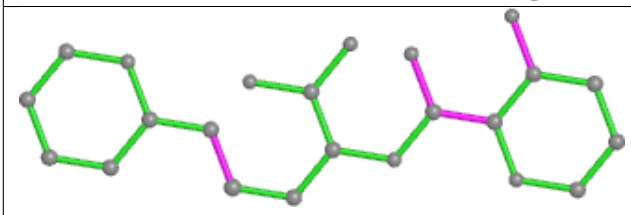


Torsions

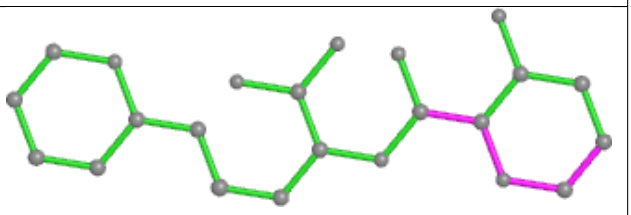


Rings

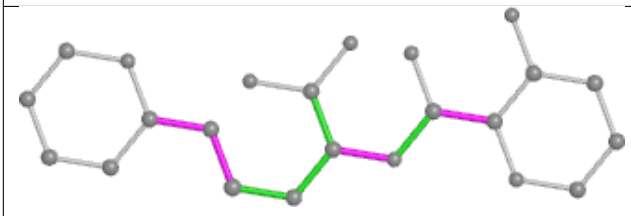
Ligand 6YT D 601



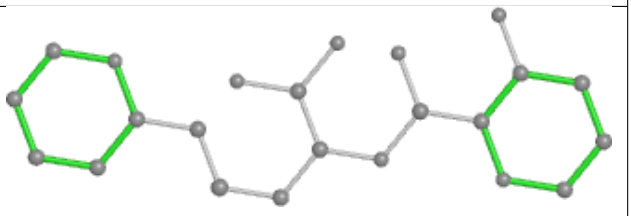
Bond lengths



Bond angles

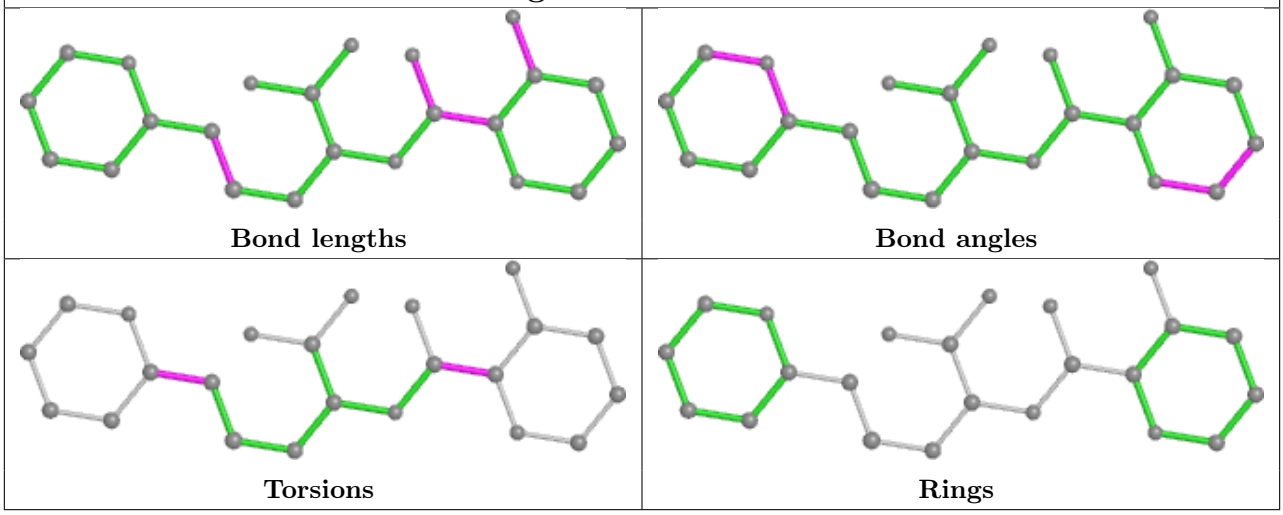


Torsions

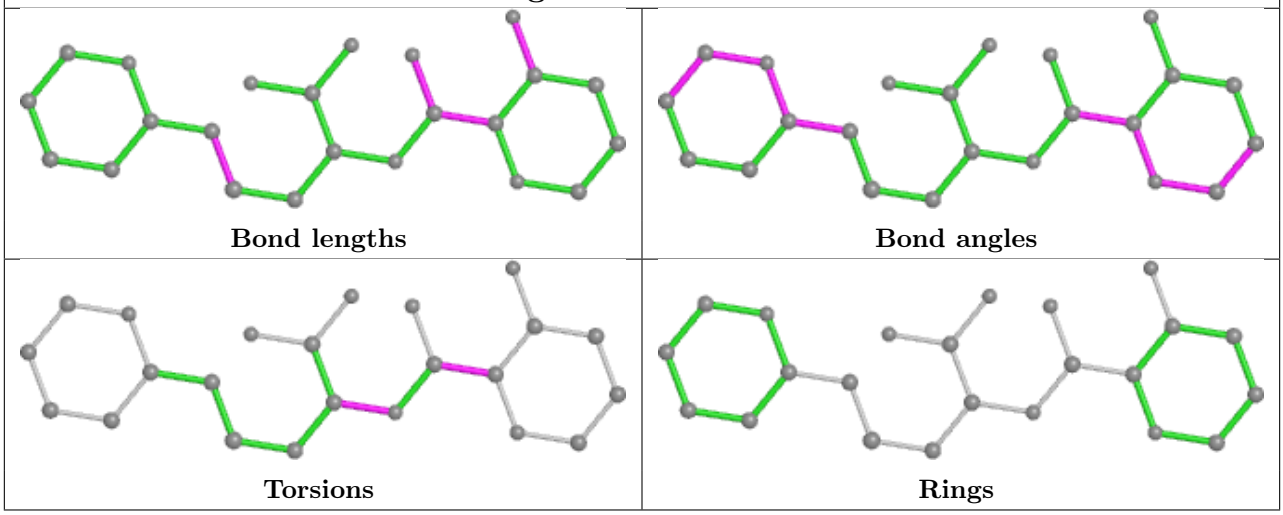


Rings

Ligand 6YT C 601



Ligand 6YT B 601



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	384/388 (98%)	-0.14	2 (0%)	91	88	36, 55, 80, 95	0
1	B	384/388 (98%)	-0.10	4 (1%)	82	77	34, 53, 76, 91	0
1	C	384/388 (98%)	-0.01	3 (0%)	86	82	27, 61, 82, 109	0
1	D	384/388 (98%)	0.11	11 (2%)	51	41	37, 65, 98, 113	1 (0%)
1	E	384/388 (98%)	0.16	22 (5%)	23	15	43, 72, 103, 113	0
1	F	384/388 (98%)	0.01	6 (1%)	72	65	40, 64, 85, 98	1 (0%)
All	All	2304/2328 (98%)	0.01	48 (2%)	63	54	27, 61, 90, 113	2 (0%)

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	8	ALA	4.0
1	D	72	LYS	4.0
1	E	64	ILE	3.9
1	E	67	LEU	3.5
1	D	18	GLN	3.4

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)

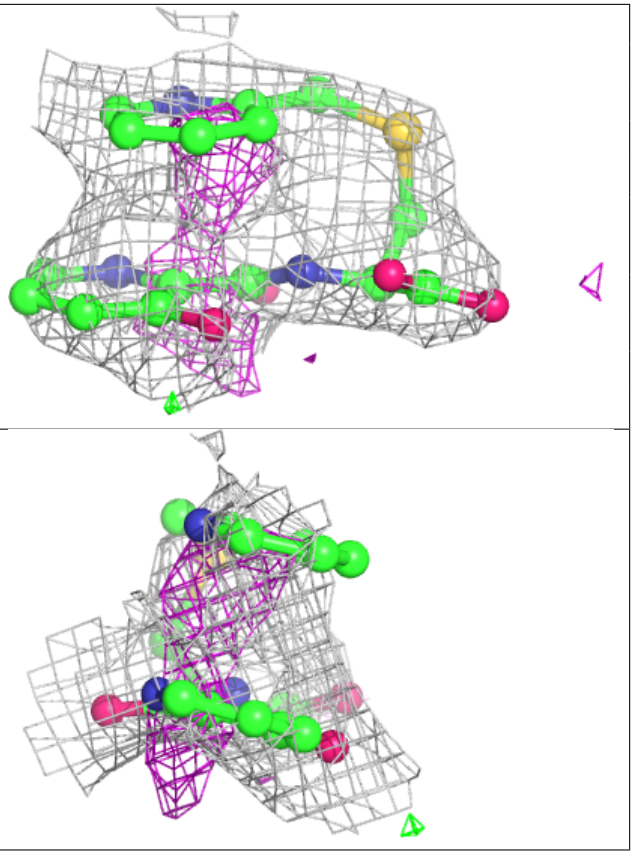
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	C	704	4/4	0.78	0.23	62,63,64,65	0
5	EDO	C	702	4/4	0.82	0.27	82,83,84,84	0
5	EDO	E	701	4/4	0.84	0.37	72,72,73,73	0
4	6YT	C	601	23/23	0.86	0.28	98,100,100,101	0
5	EDO	E	702	4/4	0.86	0.16	72,76,77,79	0
5	EDO	C	703	4/4	0.87	0.23	71,72,72,73	0
5	EDO	C	701	4/4	0.87	0.35	73,73,73,74	0
4	6YT	B	601	23/23	0.88	0.27	98,100,100,101	0
4	6YT	F	601	23/23	0.88	0.34	94,97,100,101	0
5	EDO	A	701	4/4	0.88	0.23	61,63,64,65	0
5	EDO	F	701	4/4	0.88	0.24	78,79,79,80	0
5	EDO	A	702	4/4	0.89	0.26	68,68,69,70	0
4	6YT	E	601	23/23	0.89	0.29	94,97,101,101	0
5	EDO	B	701	4/4	0.90	0.21	62,63,63,63	0
4	6YT	D	601	23/23	0.91	0.22	80,84,91,91	0
5	EDO	E	703	4/4	0.93	0.16	54,58,59,60	0
4	6YT	A	601	23/23	0.93	0.22	98,100,100,101	0
5	EDO	A	703	4/4	0.94	0.15	60,62,62,63	0
5	EDO	B	702	4/4	0.94	0.15	62,64,64,65	0
5	EDO	F	702	4/4	0.94	0.17	63,65,65,65	0
2	NI	B	501	1/1	0.96	0.14	70,70,70,70	0
2	NI	E	501	1/1	0.97	0.08	81,81,81,81	0
3	ZN	E	502	1/1	0.97	0.17	95,95,95,95	0
2	NI	F	501	1/1	0.98	0.14	49,49,49,49	0
2	NI	A	501	1/1	0.98	0.14	76,76,76,76	0
3	ZN	B	502	1/1	0.99	0.18	55,55,55,55	0
3	ZN	C	502	1/1	0.99	0.17	63,63,63,63	0
2	NI	C	501	1/1	0.99	0.14	67,67,67,67	0
3	ZN	F	502	1/1	0.99	0.16	63,63,63,63	0
2	NI	D	501	1/1	0.99	0.15	54,54,54,54	0
3	ZN	A	502	1/1	0.99	0.15	52,52,52,52	0
3	ZN	D	502	1/1	1.00	0.12	67,67,67,67	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.

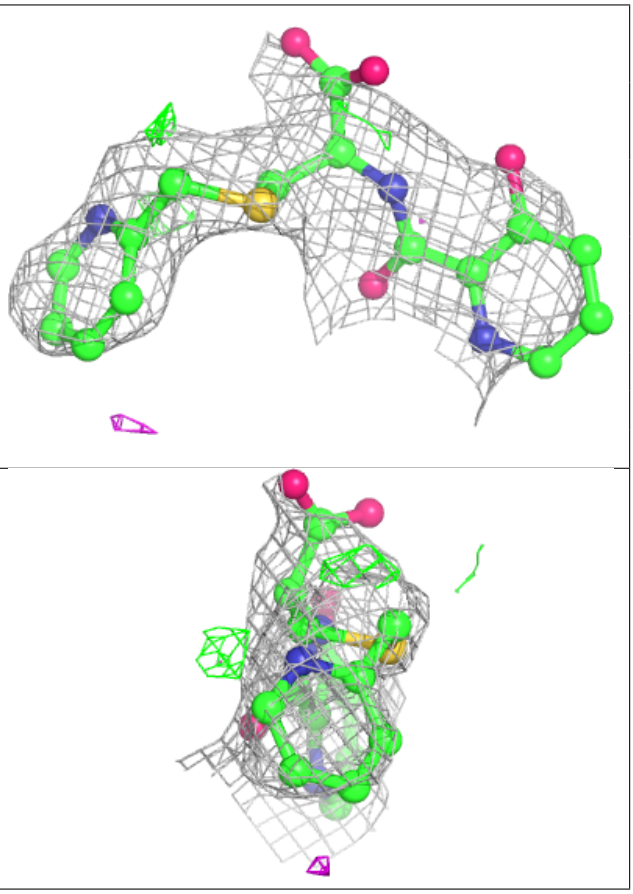
Electron density around 6YT C 601:

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



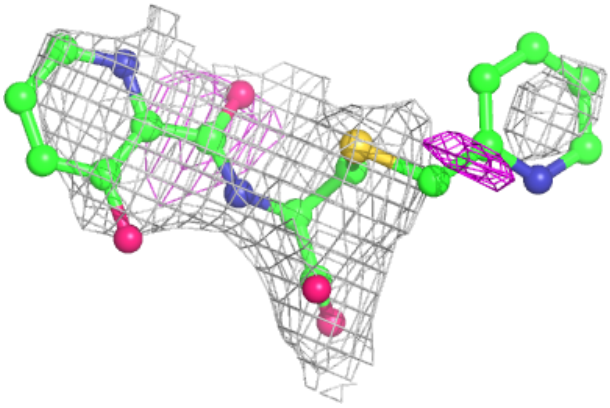
Electron density around 6YT B 601:

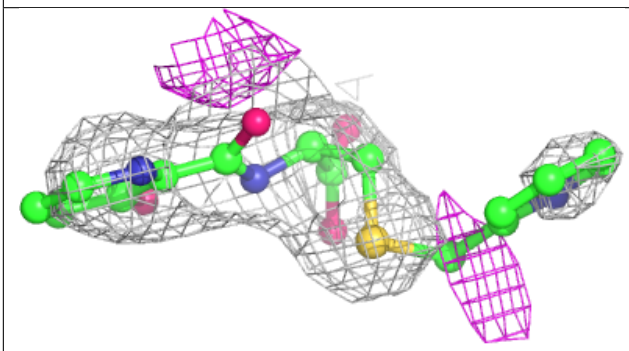
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

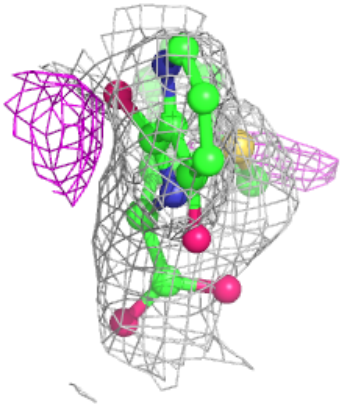


Electron density around 6YT F 601:

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







Electron density around 6YT E 601:

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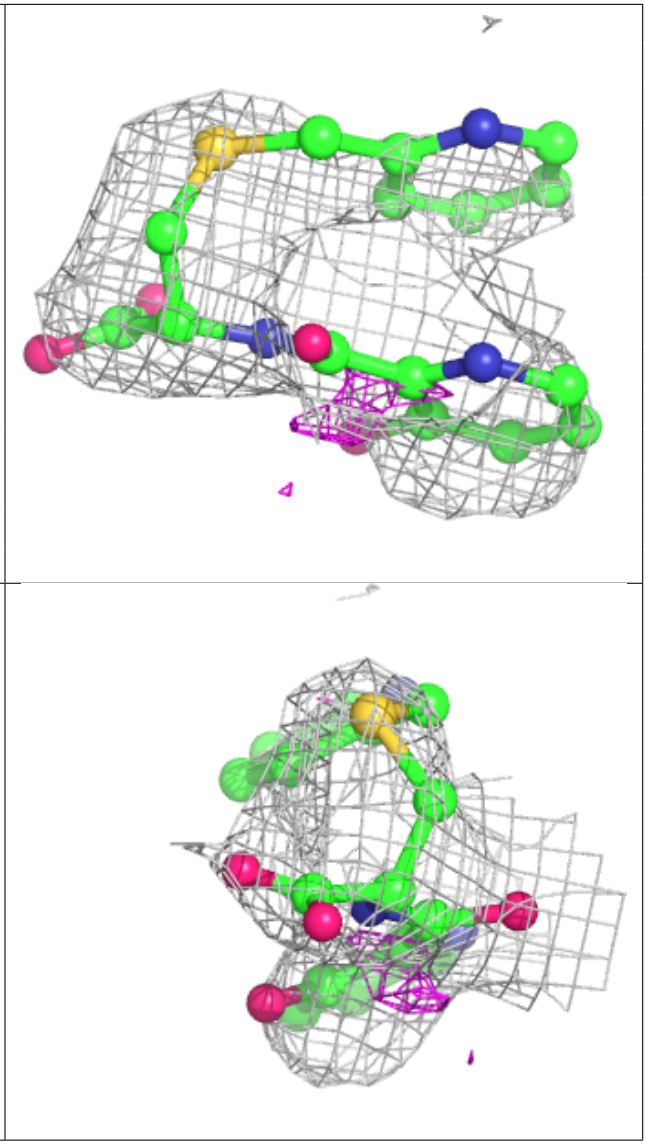
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 6YT D 601:

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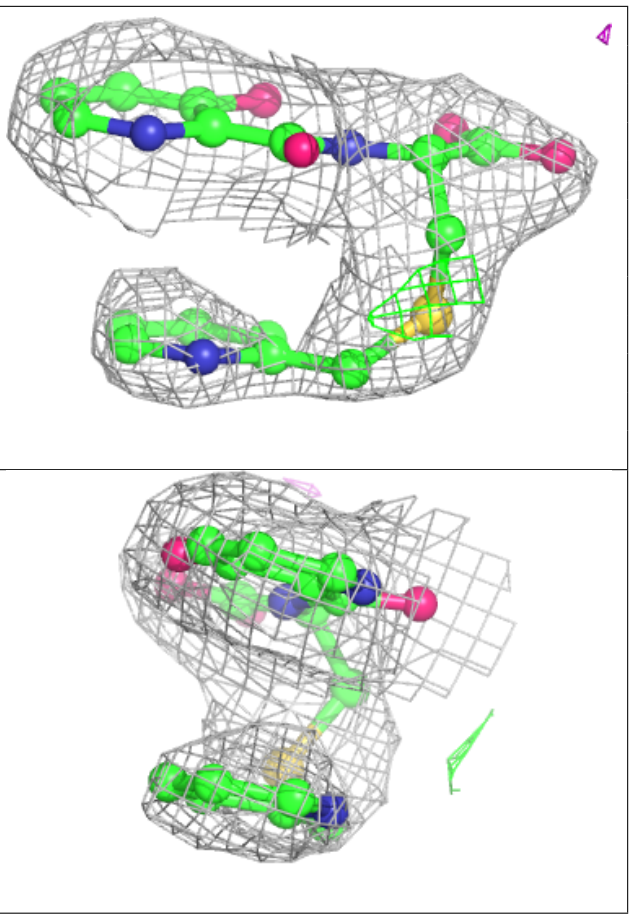
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 6YT A 601:

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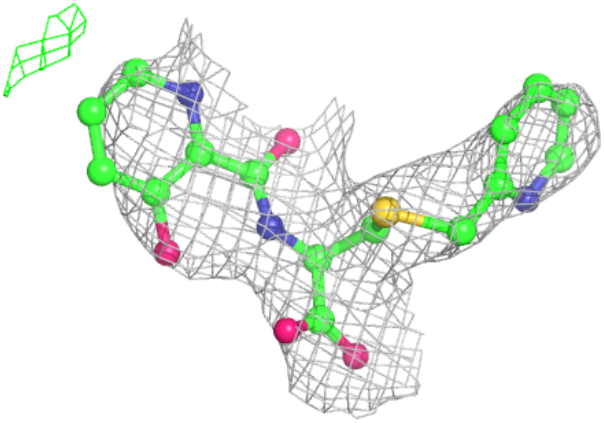
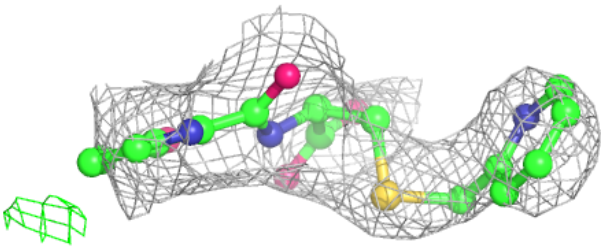
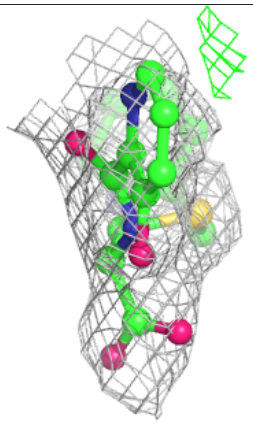
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.