



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 01:34 PM BST

PDB ID : 6U6C
Title : Crystal structure of tryptophan synthase from *M. tuberculosis* - aminoacylate- and GSK2-bound form
Authors : Chang, C.; Michalska, K.; Maltseva, N.I.; Jedrzejczak, R.; McCarren, P.; Nag, P.P.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2019-08-29
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13

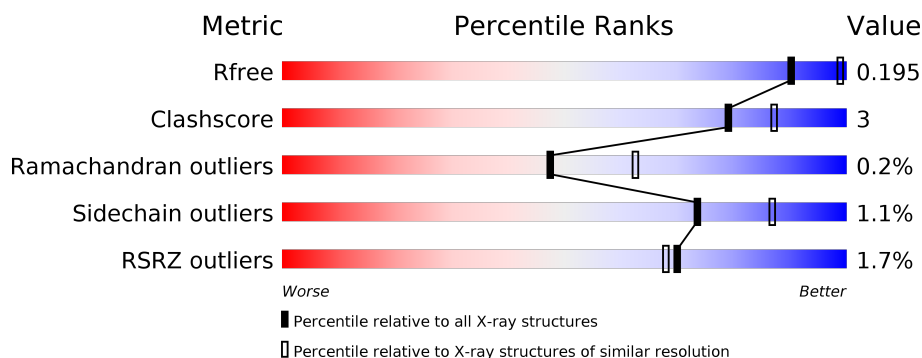
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	276	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>•</div> <div>10%</div> </div> </div>
1	C	276	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>7%</div> <div>10%</div> </div> </div>
1	E	276	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>5%</div> <div>11%</div> </div> </div>
1	G	276	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>6%</div> <div>10%</div> </div> </div>
2	B	410	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div>•</div> </div> </div>
2	D	410	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	410	
2	H	410	

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
12	ALA	E	301	-	-	-	X
3	FMT	A	301	-	-	-	X
3	FMT	B	520	-	-	-	X
3	FMT	C	302	-	-	-	X
3	FMT	G	307	-	-	-	X
3	FMT	H	508	-	-	X	-
3	FMT	H	511	-	-	-	X
3	FMT	H	524	-	-	-	X
3	FMT	H	526	-	-	-	X
5	ACT	A	310	-	-	X	-
5	ACT	F	818	-	-	X	-
9	PEG	G	309	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 21418 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 Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	1	0
			1807	1134	324	343	6			
1	C	249	Total	C	N	O	S	0	1	0
			1811	1136	324	345	6			
1	E	245	Total	C	N	O	S	0	1	0
			1784	1120	320	338	6			
1	G	249	Total	C	N	O	S	0	2	0
			1818	1140	328	344	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	HIS	-	expression tag	UNP P9WFY1
A	272	HIS	-	expression tag	UNP P9WFY1
A	273	HIS	-	expression tag	UNP P9WFY1
A	274	HIS	-	expression tag	UNP P9WFY1
A	275	HIS	-	expression tag	UNP P9WFY1
A	276	HIS	-	expression tag	UNP P9WFY1
C	271	HIS	-	expression tag	UNP P9WFY1
C	272	HIS	-	expression tag	UNP P9WFY1
C	273	HIS	-	expression tag	UNP P9WFY1
C	274	HIS	-	expression tag	UNP P9WFY1
C	275	HIS	-	expression tag	UNP P9WFY1
C	276	HIS	-	expression tag	UNP P9WFY1
E	271	HIS	-	expression tag	UNP P9WFY1
E	272	HIS	-	expression tag	UNP P9WFY1
E	273	HIS	-	expression tag	UNP P9WFY1
E	274	HIS	-	expression tag	UNP P9WFY1
E	275	HIS	-	expression tag	UNP P9WFY1
E	276	HIS	-	expression tag	UNP P9WFY1
G	271	HIS	-	expression tag	UNP P9WFY1
G	272	HIS	-	expression tag	UNP P9WFY1
G	273	HIS	-	expression tag	UNP P9WFY1

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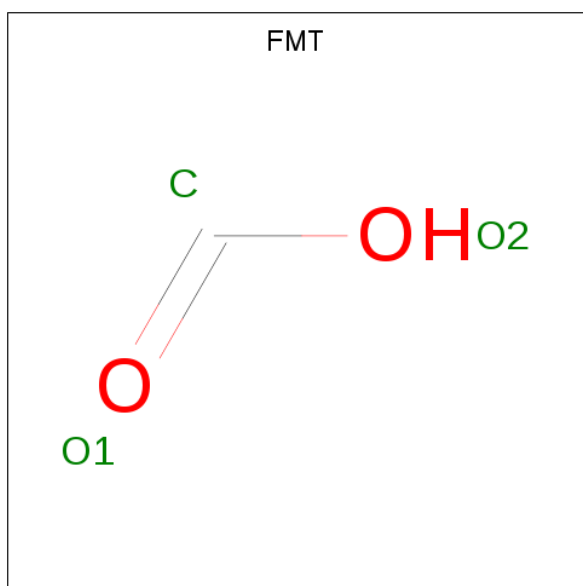
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Chain	Residue	Modelled	Actual	Comment	Reference
G	274	HIS	-	expression tag	UNP P9WFY1
G	275	HIS	-	expression tag	UNP P9WFY1
G	276	HIS	-	expression tag	UNP P9WFY1

- Molecule 2 is a protein called Tryptophan synthase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	8	0
			3083	1919	565	586	13			
2	D	404	Total	C	N	O	S	0	4	0
			3046	1901	553	579	13			
2	F	404	Total	C	N	O	S	0	3	0
			3036	1896	551	576	13			
2	H	404	Total	C	N	O	S	0	13	0
			3106	1940	564	588	14			

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		
3	E	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	F	1	Total 3	C 1	O 2	0	0
3	G	1	Total 3	C 1	O 2	0	0
3	G	1	Total 3	C 1	O 2	0	0
3	G	1	Total 3	C 1	O 2	0	0
3	G	1	Total 3	C 1	O 2	0	0

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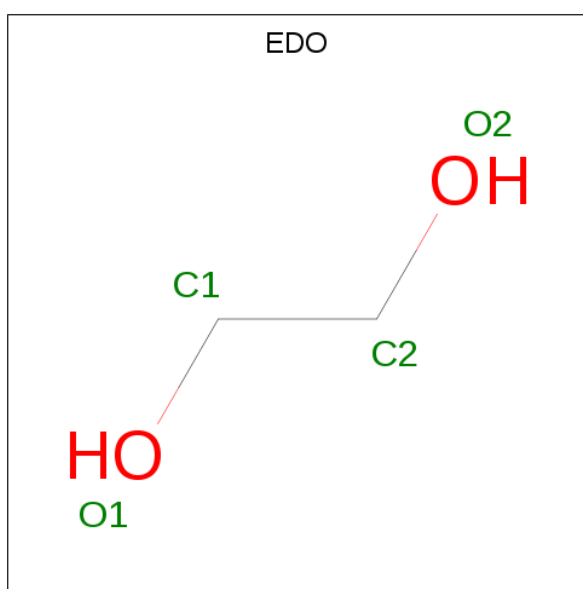
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	C	O	0	0
			3	1	2		
3	G	1	Total	C	O	0	0
			3	1	2		
3	G	1	Total	C	O	0	0
			3	1	2		
3	G	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		
3	H	1	Total	C	O	0	0
			3	1	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



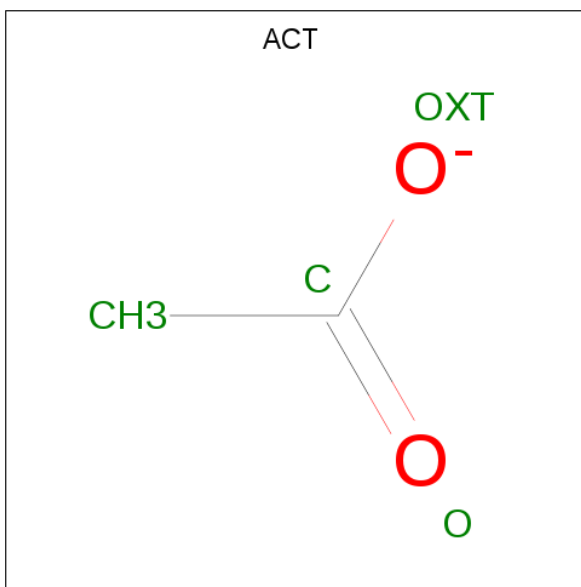
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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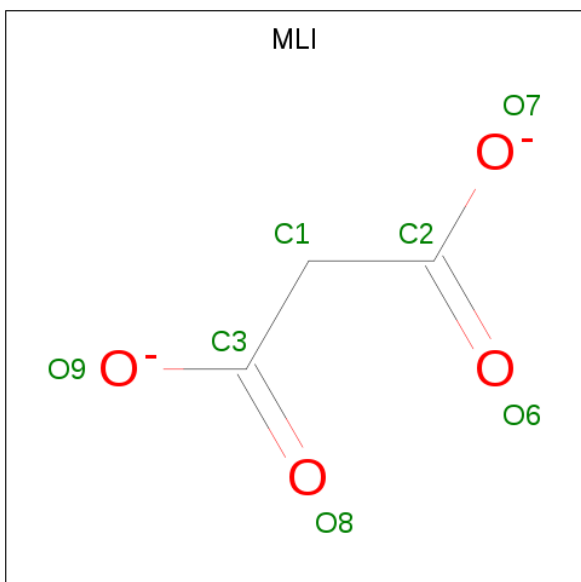
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



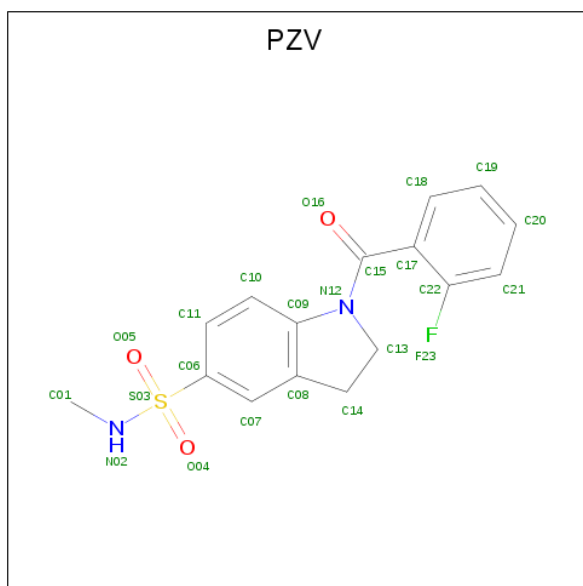
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	3	4		
6	C	1	Total	C	O	0	0
			7	3	4		
6	E	1	Total	C	O	0	0
			7	3	4		
6	F	1	Total	C	O	0	0
			7	3	4		
6	G	1	Total	C	O	0	0
			7	3	4		
6	H	1	Total	C	O	0	0
			7	3	4		

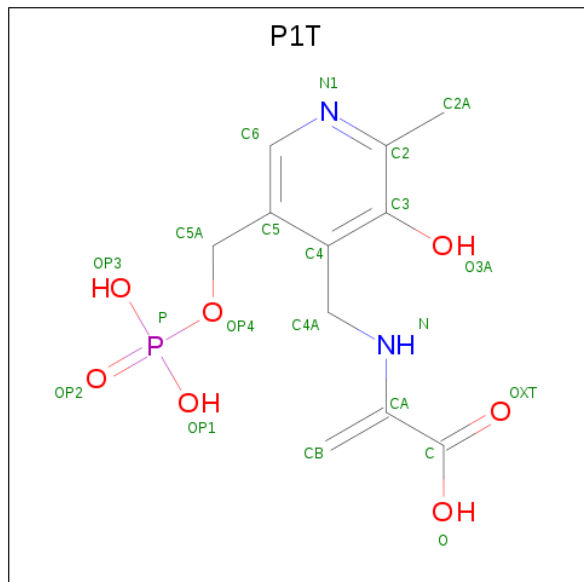
- Molecule 7 is 1-(2-fluorobenzene-1-carbonyl)-N-methyl-2,3-dihydro-1H-indole-5-sulfonamide (three-letter code: PZV) (formula: C₁₆H₁₅FN₂O₃S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	B	1	Total	C	F	N	O	S	0	0
			23	16	1	2	3	1		
7	D	1	Total	C	F	N	O	S	0	0
			23	16	1	2	3	1		
7	F	1	Total	C	F	N	O	S	0	0
			23	16	1	2	3	1		
7	H	1	Total	C	F	N	O	S	0	0
			23	16	1	2	3	1		

- Molecule 8 is 2-[(3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PY

RIDIN-4-YL}METHYL)AMINO]ACRYLIC ACID (three-letter code: P1T) (formula: $C_{11}H_{15}N_2O_7P$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
8	D	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
8	F	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
8	H	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

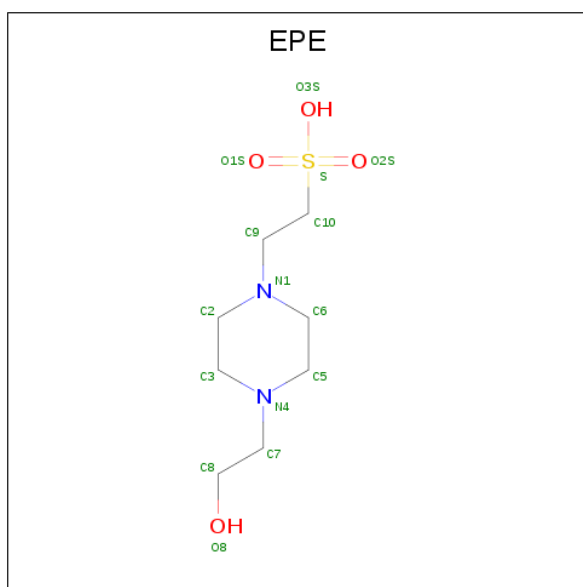


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			7	4	3		
9	F	1	Total	C	O	0	0
			7	4	3		
9	G	1	Total	C	O	0	0
			7	4	3		
9	H	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

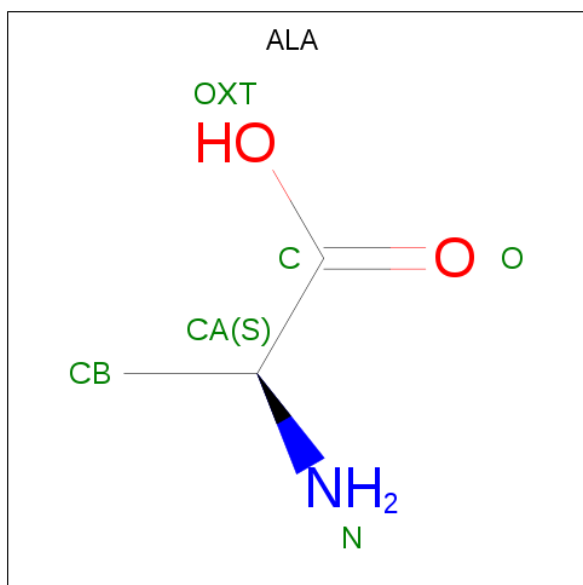
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	G	1	Total	K	0	0
			1	1		
10	D	3	Total	K	0	0
			3	3		
10	H	1	Total	K	0	0
			1	1		
10	B	1	Total	K	0	0
			1	1		
10	C	1	Total	K	0	0
			1	1		
10	F	1	Total	K	0	0
			1	1		

- Molecule 11 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



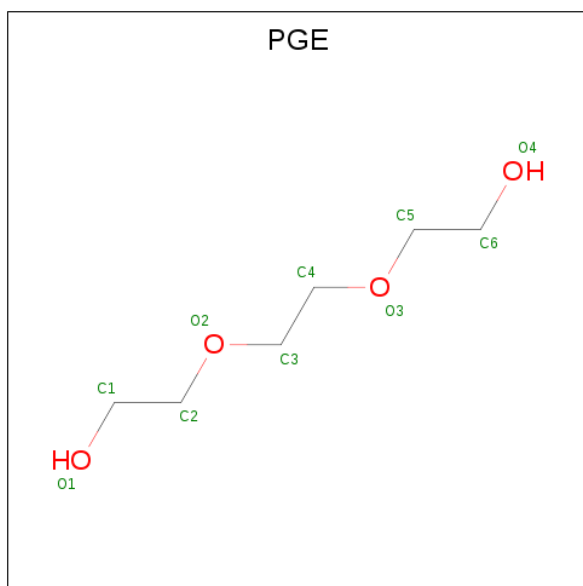
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
11	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
11	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
11	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 12 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	E	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 13 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	F	1	Total	C	O	0	0
			10	6	4		
13	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 14 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	F	1	Total	Na	0	0
			1	1		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	107	Total	O	0	0
			107	107		
15	B	201	Total	O	0	0
			201	201		
15	C	113	Total	O	0	0
			113	113		

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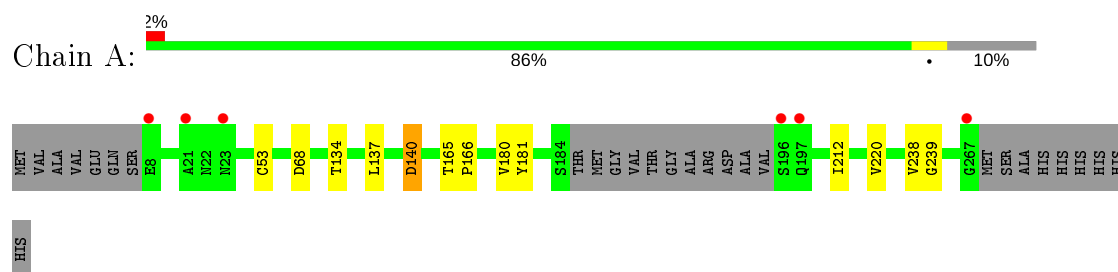
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	D	202	Total 202	O 202	0	0
15	E	71	Total 71	O 71	0	0
15	F	181	Total 181	O 181	0	0
15	G	124	Total 124	O 124	0	0
15	H	196	Total 196	O 196	0	0

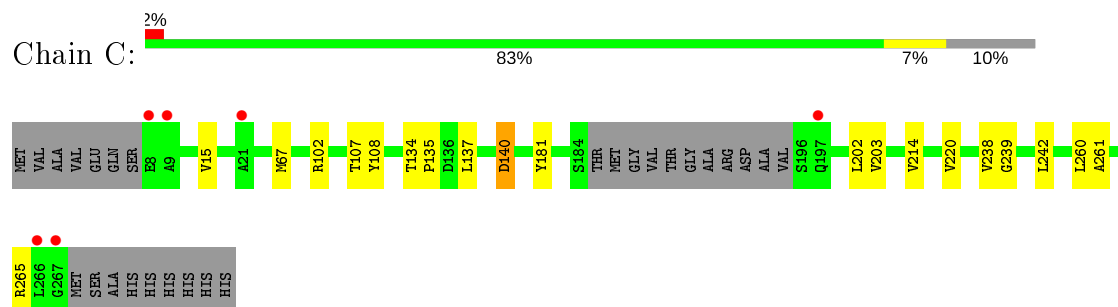
3 Residue-property plots [i](#)

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.

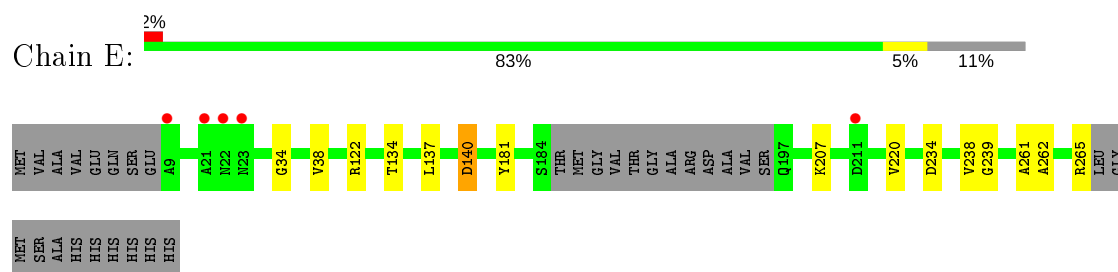
- Molecule 1: Tryptophan synthase alpha chain



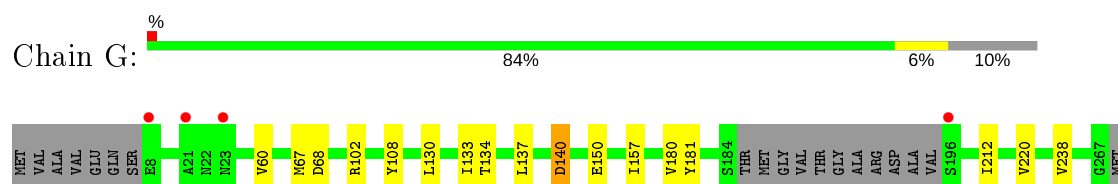
- Molecule 1: Tryptophan synthase alpha chain

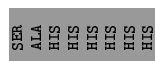


- Molecule 1: Tryptophan synthase alpha chain

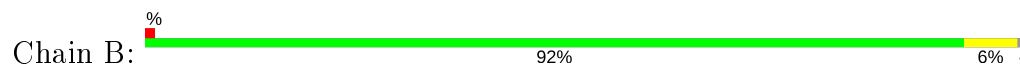


- Molecule 1: Tryptophan synthase alpha chain

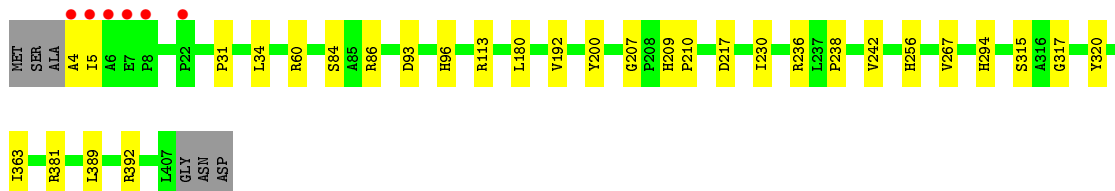




- Molecule 2: Tryptophan synthase beta chain



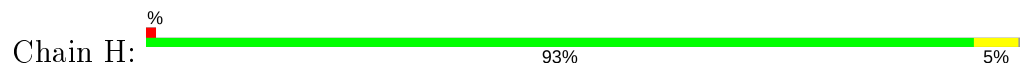
- Molecule 2: Tryptophan synthase beta chain



- Molecule 2: Tryptophan synthase beta chain



- Molecule 2: Tryptophan synthase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.11Å 159.23Å 164.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.40 29.88 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.88-2.40) 99.5 (29.88-2.40)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.153 , 0.195 0.153 , 0.195	Depositor DCC
R_{free} test set	2691 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21418	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PZV, NA, FMT, MLI, EDO, PGE, P1T, ACT, PEG, EPE, K

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	0.28	0/1836	0.46	0/2505
1	C	0.27	0/1840	0.46	0/2510
1	E	0.27	0/1813	0.45	0/2474
1	G	0.28	0/1847	0.45	0/2519
2	B	0.30	0/3144	0.47	0/4260
2	D	0.29	0/3107	0.49	0/4210
2	F	0.29	0/3098	0.48	0/4199
2	H	0.29	0/3170	0.48	0/4295
All	All	0.29	0/19855	0.47	0/26972

There are no bond length outliers.

There are no bond angle outliers.

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	1807	0	1826	7	0
1	C	1811	0	1830	12	0
1	E	1784	0	1805	8	0
1	G	1818	0	1838	11	0
2	B	3083	0	2974	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3046	0	2963	21	0
2	F	3036	0	2952	16	0
2	H	3106	0	3005	18	0
3	A	24	0	8	0	0
3	B	54	0	18	0	0
3	C	12	0	4	1	0
3	D	45	0	15	2	0
3	E	6	0	2	0	0
3	F	48	0	16	3	0
3	G	24	0	8	0	0
3	H	63	0	21	3	0
4	A	4	0	6	0	0
4	B	28	0	41	1	0
4	C	12	0	16	2	0
4	D	8	0	12	0	0
4	E	4	0	6	0	0
4	F	12	0	18	1	0
4	G	8	0	12	3	0
4	H	20	0	30	1	0
5	A	8	0	6	2	0
5	F	8	0	6	2	0
5	H	4	0	3	0	0
6	A	7	0	2	0	0
6	C	7	0	2	1	0
6	E	7	0	2	0	0
6	F	7	0	2	0	0
6	G	7	0	2	0	0
6	H	7	0	2	0	0
7	B	23	0	0	0	0
7	D	23	0	0	0	0
7	F	23	0	0	0	0
7	H	23	0	0	0	0
8	B	21	0	12	1	0
8	D	21	0	12	2	0
8	F	21	0	11	1	0
8	H	21	0	11	0	0
9	B	7	0	10	0	0
9	F	7	0	10	1	0
9	G	7	0	10	0	0
9	H	7	0	10	3	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	3	0	0	0	0
10	F	1	0	0	0	0
10	G	1	0	0	0	0
10	H	1	0	0	0	0
11	B	30	0	36	1	0
11	F	15	0	17	1	0
11	H	15	0	18	1	0
12	E	5	0	4	1	0
13	F	20	0	28	8	0
14	F	1	0	0	0	0
15	A	107	0	0	0	0
15	B	201	0	0	5	0
15	C	113	0	0	0	0
15	D	202	0	0	3	0
15	E	71	0	0	1	0
15	F	181	0	0	2	0
15	G	124	0	0	0	0
15	H	196	0	0	4	0
All	All	21418	0	19642	111	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.

All (111) 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)
2:F:28:ARG:HH22	13:F:809:PGE:H3	1.49	0.78
9:F:829:PEG:H32	2:H:138:ALA:HA	1.70	0.73
2:B:339[B]:ARG:NH1	15:B:601:HOH:O	2.22	0.68
4:C:306:EDO:H11	6:C:307:MLI:H11	1.76	0.67
2:D:381:ARG:NE	15:D:601:HOH:O	2.27	0.66
1:A:165:THR:HA	5:A:310:ACT:H3	1.80	0.64
2:F:42:THR:HG21	13:F:809:PGE:H2	1.78	0.64
2:H:144:CYS:H	9:H:513:PEG:H21	1.64	0.62
2:F:378[B]:GLU:OE1	15:F:901:HOH:O	2.16	0.61
2:H:144:CYS:N	9:H:513:PEG:H21	2.16	0.60
1:A:68:ASP:O	2:B:189:ARG:NH2	2.36	0.59
2:F:42:THR:HB	13:F:809:PGE:H4	1.84	0.59
2:D:84:SER:HB3	13:F:801:PGE:H42	1.85	0.59
2:D:230:ILE:HG21	2:D:238:PRO:HD3	1.84	0.58
2:D:315:SER:HB2	2:D:363:ILE:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:LYS:NZ	1:E:234:ASP:OD2	2.37	0.57
2:D:180:LEU:HD23	2:D:320:TYR:HB2	1.88	0.55
1:E:262:ALA:O	12:E:301:ALA:N	2.39	0.55
2:F:312[B]:HIS:ND1	5:F:818:ACT:OXT	2.37	0.55
1:C:140:ASP:OD1	1:C:140:ASP:N	2.41	0.54
2:D:96:HIS:CE1	3:D:512:FMT:H	2.42	0.54
1:A:140:ASP:OD1	1:A:140:ASP:N	2.41	0.54
1:G:140:ASP:OD1	1:G:140:ASP:N	2.39	0.53
2:H:129:HIS:CE1	2:H:203:GLY:HA2	2.43	0.53
1:G:220:VAL:HB	1:G:238:VAL:HG22	1.90	0.53
1:C:238:VAL:HG21	1:C:260:LEU:HD13	1.92	0.52
1:G:134:THR:HB	1:G:137:LEU:HB3	1.91	0.52
2:B:62[B]:GLN:HE22	2:B:103:ASN:HA	1.74	0.52
1:A:134:THR:HB	1:A:137:LEU:HB3	1.92	0.51
1:G:68:ASP:O	2:H:189:ARG:NH1	2.40	0.51
1:C:261:ALA:O	1:C:265:ARG:NH1	2.41	0.51
2:D:236[B]:ARG:NH1	15:D:603:HOH:O	2.40	0.51
1:A:180:VAL:HG23	1:A:212:ILE:HD13	1.94	0.50
2:D:242:VAL:HG12	2:D:267:VAL:HB	1.93	0.50
1:E:220:VAL:HB	1:E:238:VAL:HG22	1.94	0.50
2:B:45:TYR:OH	2:B:217:ASP:OD2	2.30	0.50
2:D:93:ASP:HB2	2:D:392:ARG:HB3	1.94	0.49
1:G:180:VAL:HG23	1:G:212:ILE:HD13	1.95	0.49
2:H:134:ALA:O	9:H:513:PEG:O4	2.30	0.49
2:B:272:ALA:HB2	2:B:340:PRO:HB2	1.95	0.49
1:G:108:TYR:HE2	4:G:312:EDO:H12	1.77	0.49
2:H:123:GLU:HG3	2:H:184:ILE:HG12	1.94	0.49
1:E:261:ALA:O	1:E:265:ARG:NH2	2.46	0.48
2:F:95:ASN:HA	3:F:823:FMT:H	1.95	0.48
1:A:220:VAL:HB	1:A:238:VAL:HG22	1.96	0.47
2:F:151:ILE:HG21	5:F:818:ACT:H3	1.95	0.47
2:H:272:ALA:HB2	2:H:340:PRO:HB2	1.95	0.47
1:C:15:VAL:HG22	1:C:102:ARG:HH11	1.80	0.47
1:G:133:ILE:HG12	1:G:157:ILE:HB	1.96	0.47
2:H:381[B]:ARG:NH1	15:H:611:HOH:O	2.45	0.47
1:C:67[A]:MET:SD	2:D:31:PRO:HB3	2.55	0.47
2:D:317:GLY:HA2	8:D:505:P1T:HB1	1.97	0.47
1:C:220:VAL:HB	1:C:238:VAL:HG22	1.97	0.47
2:F:18:HIS:CG	4:F:812:EDO:H22	2.50	0.47
2:H:316:ALA:H	3:H:508:FMT:C	2.29	0.46
2:B:123:GLU:HG3	2:B:184:ILE:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:LEU:HB2	3:C:302:FMT:H	1.98	0.45
8:F:805:P1T:N	8:F:805:P1T:O3A	2.48	0.45
1:G:67[A]:MET:SD	2:H:31:PRO:HB3	2.56	0.45
2:B:315:SER:HB2	2:B:363:ILE:HG22	1.99	0.45
8:B:502:P1T:N	8:B:502:P1T:O3A	2.48	0.45
2:D:86:ARG:HD2	13:F:801:PGE:H62	1.97	0.45
1:G:102[B]:ARG:HD3	1:G:130:LEU:HD11	1.98	0.45
1:E:134:THR:HB	1:E:137:LEU:HB3	1.98	0.45
2:B:280:ARG:NH2	15:B:610:HOH:O	2.47	0.44
2:B:402:LYS:HG3	2:B:407:LEU:HD12	1.99	0.44
1:C:203:VAL:HG22	1:C:214:VAL:HG11	2.00	0.44
2:D:60[A]:ARG:NH2	3:D:516:FMT:O2	2.46	0.44
2:F:375:LEU:HA	2:F:378[A]:GLU:HG2	1.99	0.44
1:E:34:GLY:HA2	1:E:38:VAL:HA	1.99	0.44
2:D:4:ALA:N	15:D:608:HOH:O	2.51	0.44
1:C:107:THR:O	1:C:135:PRO:HD2	2.18	0.43
1:G:108:TYR:CE2	4:G:312:EDO:H12	2.54	0.43
2:B:406:LEU:HD21	11:B:530:EPE:H51	2.00	0.43
2:F:272:ALA:HB2	2:F:340:PRO:HB2	2.01	0.43
1:G:60:VAL:O	4:G:312:EDO:H11	2.18	0.43
2:B:339[A]:ARG:NH2	15:B:614:HOH:O	2.51	0.43
1:C:134:THR:HB	1:C:137:LEU:HB3	1.98	0.43
2:D:84:SER:O	13:F:801:PGE:H5	2.18	0.43
11:F:830:EPE:H31	11:F:830:EPE:H81	1.60	0.43
1:E:140:ASP:N	1:E:140:ASP:OD1	2.50	0.43
1:C:238:VAL:HG12	1:C:242:LEU:HG	2.00	0.43
2:B:52[C]:GLN:NE2	15:B:612:HOH:O	2.48	0.42
2:D:113:ARG:HD3	2:D:113:ARG:HA	1.92	0.42
2:H:123:GLU:HG3	2:H:184:ILE:CG1	2.49	0.42
4:B:526:EDO:H12	15:B:733:HOH:O	2.19	0.42
2:D:207:GLY:HA2	2:D:294:HIS:O	2.18	0.42
2:D:5:ILE:HG23	2:D:217:ASP:HB3	2.01	0.42
2:H:305:ASP:HB2	4:H:512:EDO:H11	2.00	0.42
15:F:939:HOH:O	11:H:532:EPE:H52	2.20	0.42
2:D:389:LEU:HA	2:D:389:LEU:HD12	1.95	0.42
1:A:166:PRO:HD3	5:A:310:ACT:H3	2.02	0.42
2:F:100:HIS:NE2	2:F:250:ASN:HB3	2.34	0.42
2:H:156:GLN:CD	3:H:508:FMT:H	2.40	0.42
2:F:355:ARG:NH2	3:F:806:FMT:O2	2.51	0.42
8:D:505:P1T:O3A	8:D:505:P1T:N	2.51	0.41
1:C:108:TYR:CE2	4:C:303:EDO:H21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:236:ARG:CZ	13:F:801:PGE:H32	2.51	0.41
2:H:80:GLN:HB2	15:H:634:HOH:O	2.21	0.41
1:E:122:ARG:HD3	15:E:442:HOH:O	2.21	0.41
2:B:230:ILE:HG21	2:B:238:PRO:HD3	2.02	0.41
2:F:189:ARG:HH22	3:F:817:FMT:C	2.31	0.40
2:D:34:LEU:HG	2:D:192:VAL:HG22	2.03	0.40
2:F:34:LEU:HG	2:F:192:VAL:HG22	2.02	0.40
13:F:801:PGE:H4	13:F:801:PGE:H22	1.66	0.40
2:H:32:GLU:OE1	15:H:601:HOH:O	2.22	0.40
2:H:392:ARG:NH2	15:H:604:HOH:O	2.28	0.40
2:F:123:GLU:HG3	2:F:184:ILE:HG12	2.03	0.40
2:H:74:GLU:OE1	3:H:518:FMT:O1	2.40	0.40
2:B:181:LYS:HD3	2:B:321:PRO:HG3	2.03	0.40
2:D:209:HIS:ND1	2:D:210:PRO:HA	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	246/276 (89%)	242 (98%)	3 (1%)	1 (0%)	34	48
1	C	246/276 (89%)	242 (98%)	3 (1%)	1 (0%)	34	48
1	E	242/276 (88%)	240 (99%)	1 (0%)	1 (0%)	34	48
1	G	247/276 (90%)	242 (98%)	5 (2%)	0	100	100
2	B	412/410 (100%)	401 (97%)	9 (2%)	2 (0%)	29	41
2	D	406/410 (99%)	397 (98%)	9 (2%)	0	100	100
2	F	405/410 (99%)	393 (97%)	12 (3%)	0	100	100
2	H	415/410 (101%)	406 (98%)	8 (2%)	1 (0%)	47	62
All	All	2619/2744 (95%)	2563 (98%)	50 (2%)	6 (0%)	47	62

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	6	ALA
1	A	239	GLY
1	C	239	GLY
2	B	8	PRO
2	H	8	PRO
1	E	239	GLY

5.3.2 Protein sidechains ⓘ

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	179/200 (90%)	176 (98%)	3 (2%)	60	78
1	C	180/200 (90%)	178 (99%)	2 (1%)	73	87
1	E	177/200 (88%)	175 (99%)	2 (1%)	73	87
1	G	180/200 (90%)	177 (98%)	3 (2%)	60	78
2	B	303/302 (100%)	300 (99%)	3 (1%)	76	88
2	D	302/302 (100%)	300 (99%)	2 (1%)	84	92
2	F	301/302 (100%)	298 (99%)	3 (1%)	76	88
2	H	306/302 (101%)	304 (99%)	2 (1%)	84	92
All	All	1928/2008 (96%)	1908 (99%)	20 (1%)	73	88

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	CYS
1	A	140	ASP
1	A	181	TYR
2	B	12	ASP
2	B	196	ASP
2	B	200	TYR
1	C	140	ASP
1	C	181	TYR

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Mol	Chain	Res	Type
2	D	200	TYR
2	D	256	HIS
1	E	140	ASP
1	E	181	TYR
2	F	5	ILE
2	F	200	TYR
2	F	300	LEU
1	G	140	ASP
1	G	150	GLU
1	G	181	TYR
2	H	200	TYR
2	H	348	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	144	GLN

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 155 ligands modelled in this entry, 9 are monoatomic - leaving 146 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	$\# Z > 2$
3	FMT	H	501	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	505	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	309	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	D	511	-	3,3,3	0.47	0	2,2,2	0.31	0
3	FMT	G	305	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	306	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	513	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	G	302	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	517	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	E	304	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	E	303	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	F	806	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	510	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	F	817	-	0,2,2	0.00	-	0,1,1	0.00	-
13	PGE	F	809	-	9,9,9	0.33	0	8,8,8	0.28	0
9	PEG	B	506	-	6,6,6	0.12	0	5,5,5	0.10	0
5	ACT	H	506	-	1,3,3	6.90	1 (100%)	0,3,3	0.00	-
7	PZV	H	502	-	24,25,25	1.83	4 (16%)	32,37,37	3.30	8 (25%)
6	MLI	E	302	-	0,6,6	0.00	-	0,7,7	0.00	-
3	FMT	B	531	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	F	819	-	3,3,3	0.48	0	2,2,2	0.25	0
3	FMT	B	512	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	H	528	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	302	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	301	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	C	301	-	3,3,3	0.49	0	2,2,2	0.16	0
3	FMT	B	517	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	F	816	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	H	509	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	A	304	-	3,3,3	0.47	0	2,2,2	0.30	0
3	FMT	F	815	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	303	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	515	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	F	828	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	502	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	C	306	10	3,3,3	0.47	0	2,2,2	0.20	0
3	FMT	H	507	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	H	517	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	503	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	509	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PZV	B	501	-	24,25,25	1.86	7 (29%)	32,37,37	3.03	8 (25%)
3	FMT	H	515	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	H	511	-	0,2,2	0.00	-	0,1,1	0.00	-
13	PGE	F	801	-	9,9,9	0.33	0	8,8,8	0.47	0
6	MLI	H	530	-	0,6,6	0.00	-	0,7,7	0.00	-
5	ACT	F	808	-	1,3,3	6.62	1 (100%)	0,3,3	0.00	-
6	MLI	F	827	-	0,6,6	0.00	-	0,7,7	0.00	-
3	FMT	A	308	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	H	520	-	3,3,3	0.54	0	2,2,2	0.03	0
3	FMT	F	823	-	0,2,2	0.00	-	0,1,1	0.00	-
9	PEG	H	513	-	6,6,6	0.12	0	5,5,5	0.08	0
3	FMT	F	820	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	B	516	-	3,3,3	0.45	0	2,2,2	0.42	0
11	EPE	B	527	-	15,15,15	1.99	1 (6%)	18,20,20	1.13	1 (5%)
3	FMT	D	515	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	514	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	504	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	307	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	507	-	0,2,2	0.00	-	0,1,1	0.00	-
6	MLI	A	311	-	0,6,6	0.00	-	0,7,7	0.00	-
4	EDO	F	812	-	3,3,3	0.44	0	2,2,2	0.34	0
3	FMT	D	506	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	H	525	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	F	810	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	F	807	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	E	305	-	3,3,3	0.48	0	2,2,2	0.29	0
11	EPE	B	530	-	15,15,15	1.76	1 (6%)	18,20,20	1.69	3 (16%)
3	FMT	D	504	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	H	533	-	3,3,3	0.51	0	2,2,2	0.12	0
3	FMT	C	304	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	F	804	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	H	522	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	G	301	-	0,2,2	0.00	-	0,1,1	0.00	-
11	EPE	F	830	-	15,15,15	2.02	1 (6%)	18,20,20	1.54	3 (16%)
3	FMT	B	513	-	0,2,2	0.00	-	0,1,1	0.00	-
9	PEG	F	829	-	6,6,6	0.12	0	5,5,5	0.09	0
4	EDO	B	503	-	3,3,3	0.43	0	2,2,2	0.44	0
3	FMT	G	303	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	H	505	-	3,3,3	0.47	0	2,2,2	0.29	0
3	FMT	G	307	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	H	518	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	F	814	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	509	-	3,3,3	0.46	0	2,2,2	0.33	0
3	FMT	C	305	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	524	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	523	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	521	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	F	822	-	3,3,3	0.47	0	2,2,2	0.32	0
4	EDO	H	521	-	3,3,3	0.46	0	2,2,2	0.34	0
3	FMT	H	510	-	0,2,2	0.00	-	0,1,1	0.00	-
7	PZV	D	501	-	24,25,25	1.83	4 (16%)	32,37,37	2.97	9 (28%)
3	FMT	F	811	-	0,2,2	0.00	-	0,1,1	0.00	-
8	P1T	F	805	-	18,21,21	2.84	1 (5%)	23,30,30	1.37	1 (4%)
3	FMT	B	521	-	0,2,2	0.00	-	0,1,1	0.00	-
8	P1T	H	504	-	18,21,21	2.76	1 (5%)	23,30,30	1.36	1 (4%)
3	FMT	B	518	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	G	310	-	3,3,3	0.54	0	2,2,2	0.14	0
3	FMT	F	821	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	B	511	-	3,3,3	0.48	0	2,2,2	0.25	0
5	ACT	F	818	-	1,3,3	5.77	1 (100%)	0,3,3	0.00	-
3	FMT	H	529	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	514	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	H	508	-	0,2,2	0.00	-	0,1,1	0.00	-
11	EPE	H	532	-	15,15,15	1.90	1 (6%)	18,20,20	1.17	3 (16%)
4	EDO	C	303	10	3,3,3	0.42	0	2,2,2	0.35	0
3	FMT	D	516	-	0,2,2	0.00	-	0,1,1	0.00	-
9	PEG	G	309	-	6,6,6	0.14	0	5,5,5	0.12	0
4	EDO	D	520	-	3,3,3	0.47	0	2,2,2	0.28	0
3	FMT	H	524	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	B	529	-	3,3,3	0.49	0	2,2,2	0.08	0
3	FMT	F	824	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	508	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	H	527	-	0,2,2	0.00	-	0,1,1	0.00	-
7	PZV	F	802	-	24,25,25	1.85	5 (20%)	32,37,37	3.01	7 (21%)
4	EDO	B	526	-	3,3,3	0.48	0	2,2,2	0.26	0
3	FMT	F	803	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	G	304	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	309	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	305	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	302	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	H	514	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	G	308	-	0,2,2	0.00	-	0,1,1	0.00	-
6	MLI	G	311	-	0,6,6	0.00	-	0,7,7	0.00	-
3	FMT	B	528	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FMT	H	526	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	G	306	-	0,2,2	0.00	-	0,1,1	0.00	-
6	MLI	C	307	-	0,6,6	0.00	-	0,7,7	0.00	-
4	EDO	B	510	-	3,3,3	0.51	0	2,2,2	0.15	0
4	EDO	G	312	-	3,3,3	0.59	0	2,2,2	0.19	0
3	FMT	H	519	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	H	512	-	3,3,3	0.52	0	2,2,2	0.02	0
3	FMT	D	508	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	H	516	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	512	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	F	813	-	0,2,2	0.00	-	0,1,1	0.00	-
5	ACT	A	312	-	1,3,3	7.06	1 (100%)	0,3,3	0.00	-
3	FMT	H	503	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	H	523	-	0,2,2	0.00	-	0,1,1	0.00	-
5	ACT	A	310	-	1,3,3	6.69	1 (100%)	0,3,3	0.00	-
3	FMT	D	507	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	519	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	520	-	0,2,2	0.00	-	0,1,1	0.00	-
8	P1T	B	502	-	18,21,21	2.71	1 (5%)	23,30,30	1.37	1 (4%)
8	P1T	D	505	-	18,21,21	2.66	1 (5%)	23,30,30	1.39	1 (4%)
3	FMT	B	522	-	0,2,2	0.00	-	0,1,1	0.00	-

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	H	505	-	-	0/1/1/1	-
7	PZV	F	802	-	-	0/17/26/26	0/3/3/3
4	EDO	B	526	-	-	0/1/1/1	-
6	MLI	F	827	-	-	0/0/4/4	-
4	EDO	B	509	-	-	0/1/1/1	-
4	EDO	D	511	-	-	0/1/1/1	-
13	PGE	F	801	-	-	3/7/7/7	-
4	EDO	C	306	10	-	0/1/1/1	-
9	PEG	H	513	-	-	1/4/4/4	-
4	EDO	F	819	-	-	0/1/1/1	-
4	EDO	F	822	-	-	0/1/1/1	-
4	EDO	H	520	-	-	0/1/1/1	-
4	EDO	B	516	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	EPE	B	527	-	-	5/9/19/19	0/1/1/1
6	MLI	H	530	-	-	0/0/4/4	-
13	PGE	F	809	-	-	6/7/7/7	-
9	PEG	G	309	-	-	0/4/4/4	-
9	PEG	B	506	-	-	0/4/4/4	-
7	PZV	H	502	-	-	0/17/26/26	0/3/3/3
4	EDO	B	510	-	-	0/1/1/1	-
4	EDO	G	312	-	-	0/1/1/1	-
4	EDO	A	304	-	-	0/1/1/1	-
7	PZV	B	501	-	-	0/17/26/26	0/3/3/3
4	EDO	H	512	-	-	0/1/1/1	-
6	MLI	A	311	-	-	0/0/4/4	-
4	EDO	F	812	-	-	0/1/1/1	-
6	MLI	G	311	-	-	0/0/4/4	-
8	P1T	H	504	-	-	3/10/15/15	0/1/1/1
4	EDO	G	310	-	-	1/1/1/1	-
4	EDO	B	511	-	-	0/1/1/1	-
4	EDO	E	305	-	-	0/1/1/1	-
11	EPE	B	530	-	-	3/9/19/19	0/1/1/1
4	EDO	C	301	-	-	0/1/1/1	-
6	MLI	E	302	-	-	0/0/4/4	-
7	PZV	D	501	-	-	0/17/26/26	0/3/3/3
4	EDO	H	533	-	-	1/1/1/1	-
4	EDO	C	303	10	-	0/1/1/1	-
9	PEG	F	829	-	-	1/4/4/4	-
4	EDO	H	521	-	-	1/1/1/1	-
11	EPE	H	532	-	-	6/9/19/19	0/1/1/1
4	EDO	B	503	-	-	0/1/1/1	-
8	P1T	B	502	-	-	3/10/15/15	0/1/1/1
11	EPE	F	830	-	-	2/9/19/19	0/1/1/1
6	MLI	C	307	-	-	0/0/4/4	-
4	EDO	D	520	-	-	0/1/1/1	-
8	P1T	D	505	-	-	3/10/15/15	0/1/1/1
4	EDO	B	529	-	-	0/1/1/1	-
8	P1T	F	805	-	-	3/10/15/15	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	805	P1T	C-CA	-11.96	1.34	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	504	P1T	C-CA	-11.61	1.34	1.52
8	B	502	P1T	C-CA	-11.42	1.34	1.52
8	D	505	P1T	C-CA	-11.21	1.35	1.52
11	F	830	EPE	C10-S	-7.55	1.66	1.77
11	B	527	EPE	C10-S	-7.35	1.67	1.77
5	A	312	ACT	CH3-C	7.06	1.57	1.48
11	H	532	EPE	C10-S	-7.02	1.67	1.77
5	H	506	ACT	CH3-C	6.90	1.57	1.48
5	A	310	ACT	CH3-C	6.69	1.57	1.48
5	F	808	ACT	CH3-C	6.62	1.57	1.48
11	B	530	EPE	C10-S	-6.41	1.68	1.77
5	F	818	ACT	CH3-C	5.77	1.56	1.48
7	H	502	PZV	C15-N12	5.28	1.45	1.36
7	D	501	PZV	C15-N12	5.24	1.45	1.36
7	F	802	PZV	C15-N12	5.10	1.44	1.36
7	B	501	PZV	C15-N12	5.07	1.44	1.36
7	F	802	PZV	C09-N12	4.65	1.48	1.39
7	B	501	PZV	C09-N12	4.48	1.48	1.39
7	D	501	PZV	C09-N12	4.39	1.48	1.39
7	H	502	PZV	C09-N12	4.30	1.48	1.39
7	H	502	PZV	O04-S03	2.96	1.46	1.43
7	B	501	PZV	O04-S03	2.89	1.46	1.43
7	D	501	PZV	O05-S03	2.78	1.46	1.43
7	D	501	PZV	O04-S03	2.70	1.46	1.43
7	F	802	PZV	O05-S03	2.67	1.46	1.43
7	F	802	PZV	O04-S03	2.61	1.46	1.43
7	B	501	PZV	C06-S03	2.33	1.80	1.76
7	H	502	PZV	O05-S03	2.22	1.46	1.43
7	B	501	PZV	O05-S03	2.22	1.46	1.43
7	F	802	PZV	C06-S03	2.19	1.79	1.76
7	B	501	PZV	C13-C14	-2.13	1.50	1.53
7	B	501	PZV	O16-C15	-2.02	1.18	1.22

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	502	PZV	O05-S03-O04	-14.27	102.00	119.55
7	B	501	PZV	O05-S03-O04	-13.02	103.55	119.55
7	F	802	PZV	O05-S03-O04	-12.99	103.58	119.55
7	D	501	PZV	O05-S03-O04	-12.32	104.41	119.55
7	D	501	PZV	O05-S03-N02	6.26	114.14	107.08
7	F	802	PZV	O04-S03-N02	6.15	114.01	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	502	PZV	O04-S03-N02	5.99	113.84	107.08
8	D	505	P1T	CB-CA-N	-5.76	111.93	125.91
7	H	502	PZV	O05-S03-N02	5.64	113.45	107.08
7	B	501	PZV	O05-S03-N02	5.58	113.37	107.08
8	F	805	P1T	CB-CA-N	-5.51	112.54	125.91
8	B	502	P1T	CB-CA-N	-5.51	112.54	125.91
8	H	504	P1T	CB-CA-N	-5.22	113.24	125.91
7	F	802	PZV	O05-S03-N02	5.18	112.93	107.08
7	B	501	PZV	C08-C09-N12	-4.65	107.11	109.66
7	B	501	PZV	O04-S03-N02	4.61	112.28	107.08
7	H	502	PZV	C08-C09-N12	-4.42	107.24	109.66
7	H	502	PZV	C18-C17-C22	4.33	121.59	116.67
7	D	501	PZV	O04-S03-N02	4.31	111.94	107.08
7	B	501	PZV	C18-C17-C22	4.25	121.50	116.67
11	B	530	EPE	O1S-S-C10	4.17	111.93	106.92
7	D	501	PZV	C18-C17-C22	3.91	121.12	116.67
7	D	501	PZV	C08-C09-N12	-3.78	107.59	109.66
7	F	802	PZV	C18-C17-C22	3.75	120.93	116.67
11	B	530	EPE	O3S-S-C10	3.73	111.80	105.77
7	F	802	PZV	C08-C09-N12	-3.46	107.76	109.66
11	F	830	EPE	O1S-S-C10	3.29	110.88	106.92
7	D	501	PZV	C21-C22-C17	-3.16	119.67	123.11
11	B	527	EPE	O2S-S-C10	2.82	110.32	106.92
11	H	532	EPE	O1S-S-C10	2.80	110.29	106.92
11	F	830	EPE	O2S-S-C10	2.70	110.16	106.92
11	F	830	EPE	C2-C3-N4	-2.67	105.17	110.64
7	H	502	PZV	O04-S03-C06	2.63	111.20	107.97
7	D	501	PZV	C07-C08-C09	-2.42	118.83	120.54
11	H	532	EPE	O2S-S-C10	2.30	109.69	106.92
7	H	502	PZV	C21-C22-C17	-2.27	120.64	123.11
7	F	802	PZV	C07-C08-C09	-2.25	118.95	120.54
7	D	501	PZV	C06-S03-N02	2.22	110.62	107.56
7	D	501	PZV	C11-C06-C07	2.14	123.25	120.62
11	H	532	EPE	O3S-S-C10	2.13	109.21	105.77
7	F	802	PZV	C21-C22-C17	-2.13	120.80	123.11
7	B	501	PZV	C21-C22-C17	-2.06	120.87	123.11
11	B	530	EPE	C3-C2-N1	2.05	114.86	110.64
7	H	502	PZV	C11-C06-C07	2.03	123.11	120.62
7	B	501	PZV	C06-S03-N02	2.01	110.34	107.56
7	B	501	PZV	C07-C08-C09	-2.01	119.12	120.54

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	527	EPE	C10-C9-N1-C6
11	B	527	EPE	C8-C7-N4-C3
11	F	830	EPE	C10-C9-N1-C2
8	F	805	P1T	C5-C4-C4A-N
8	H	504	P1T	C5-C4-C4A-N
11	H	532	EPE	C10-C9-N1-C2
11	H	532	EPE	C10-C9-N1-C6
11	H	532	EPE	S-C10-C9-N1
11	H	532	EPE	C9-C10-S-O1S
11	H	532	EPE	C9-C10-S-O3S
8	B	502	P1T	C5-C4-C4A-N
8	D	505	P1T	C5-C4-C4A-N
8	D	505	P1T	C3-C4-C4A-N
13	F	801	PGE	C4-C3-O2-C2
9	H	513	PEG	C4-C3-O2-C2
4	B	516	EDO	O1-C1-C2-O2
11	B	527	EPE	N4-C7-C8-O8
11	F	830	EPE	N4-C7-C8-O8
8	F	805	P1T	C3-C4-C4A-N
13	F	809	PGE	O2-C3-C4-O3
13	F	809	PGE	O3-C5-C6-O4
8	F	805	P1T	C-CA-N-C4A
8	H	504	P1T	C-CA-N-C4A
8	B	502	P1T	C-CA-N-C4A
8	D	505	P1T	C-CA-N-C4A
13	F	809	PGE	O1-C1-C2-O2
11	B	527	EPE	C10-C9-N1-C2
11	B	530	EPE	C10-C9-N1-C6
11	B	530	EPE	N4-C7-C8-O8
4	G	310	EDO	O1-C1-C2-O2
13	F	801	PGE	O2-C3-C4-O3
13	F	801	PGE	O1-C1-C2-O2
13	F	809	PGE	C3-C4-O3-C5
13	F	809	PGE	C4-C3-O2-C2
11	H	532	EPE	C9-C10-S-O2S
13	F	809	PGE	C6-C5-O3-C4
8	H	504	P1T	C3-C4-C4A-N
8	B	502	P1T	C3-C4-C4A-N
11	B	530	EPE	C10-C9-N1-C2
9	F	829	PEG	C4-C3-O2-C2
4	H	533	EDO	O1-C1-C2-O2
4	H	521	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
11	B	527	EPE	C8-C7-N4-C5

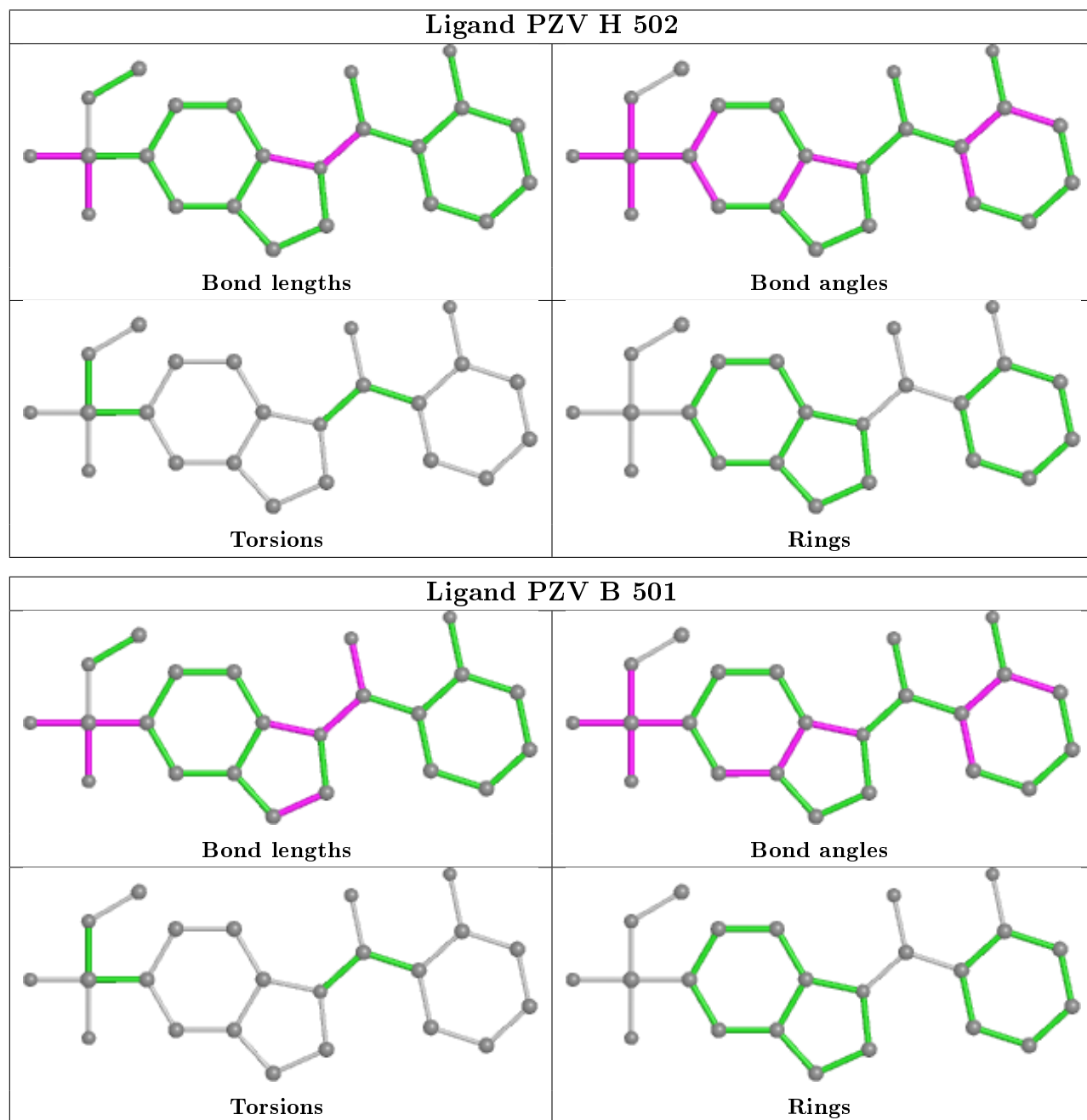
There are no ring outliers.

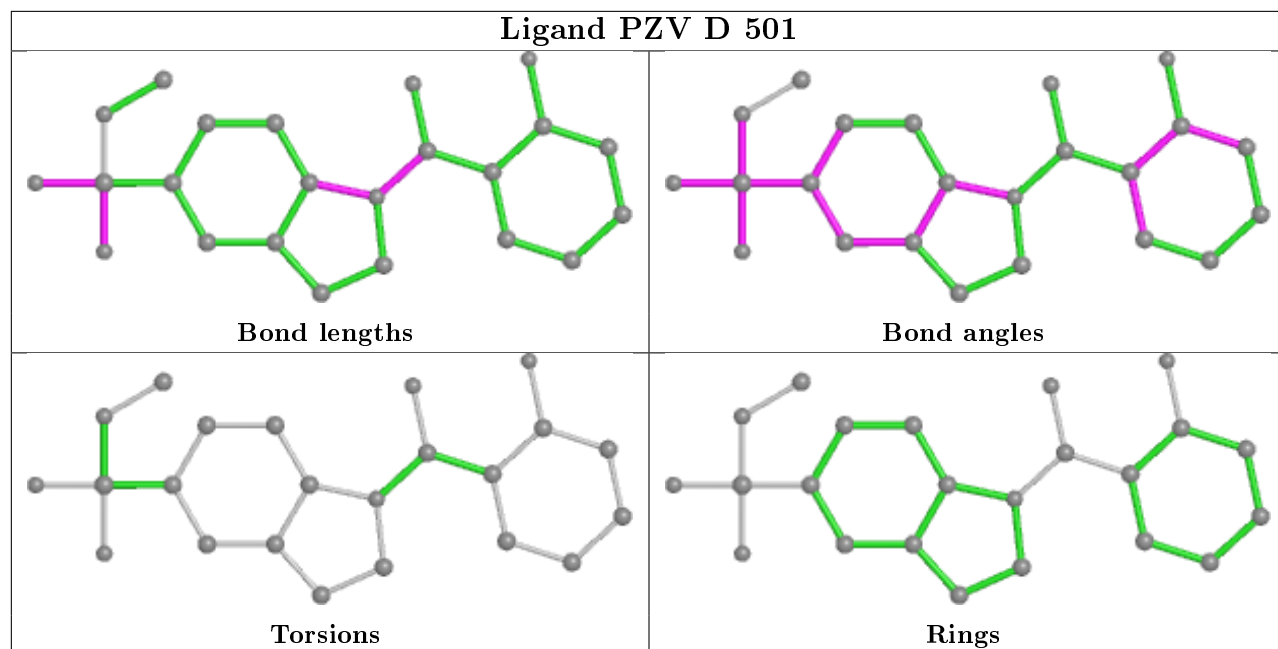
27 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	806	FMT	1	0
3	F	817	FMT	1	0
13	F	809	PGE	3	0
3	C	302	FMT	1	0
4	C	306	EDO	1	0
13	F	801	PGE	5	0
3	F	823	FMT	1	0
9	H	513	PEG	3	0
4	F	812	EDO	1	0
11	B	530	EPE	1	0
11	F	830	EPE	1	0
9	F	829	PEG	1	0
3	H	518	FMT	1	0
8	F	805	P1T	1	0
5	F	818	ACT	2	0
3	H	508	FMT	2	0
11	H	532	EPE	1	0
4	C	303	EDO	1	0
3	D	516	FMT	1	0
4	B	526	EDO	1	0
6	C	307	MLI	1	0
4	G	312	EDO	3	0
4	H	512	EDO	1	0
3	D	512	FMT	1	0
5	A	310	ACT	2	0
8	B	502	P1T	1	0
8	D	505	P1T	2	0

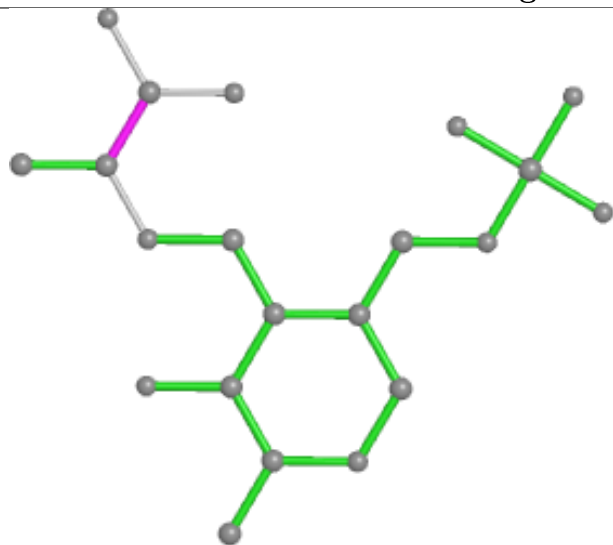
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

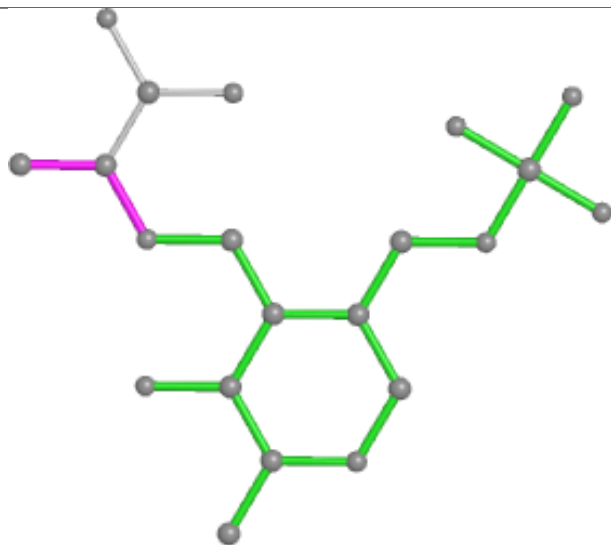




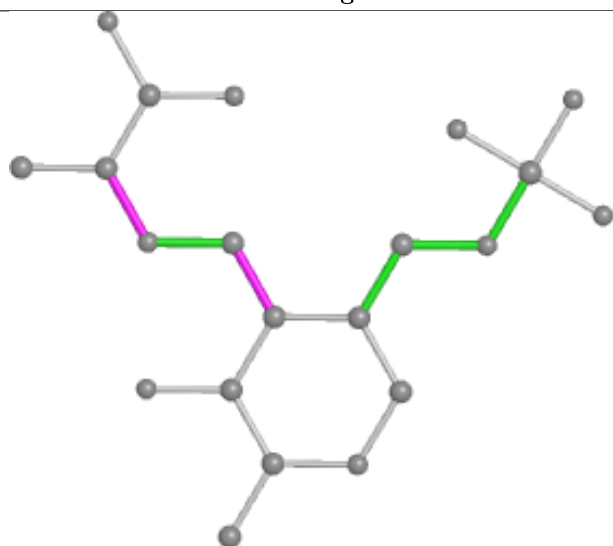
Ligand P1T F 805



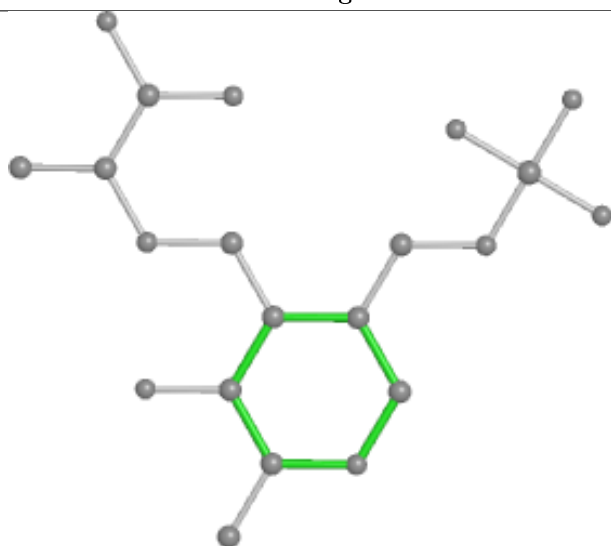
Bond lengths



Bond angles

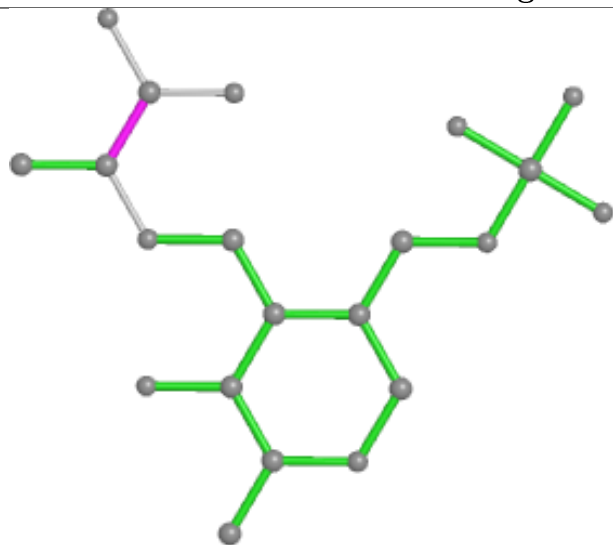


Torsions

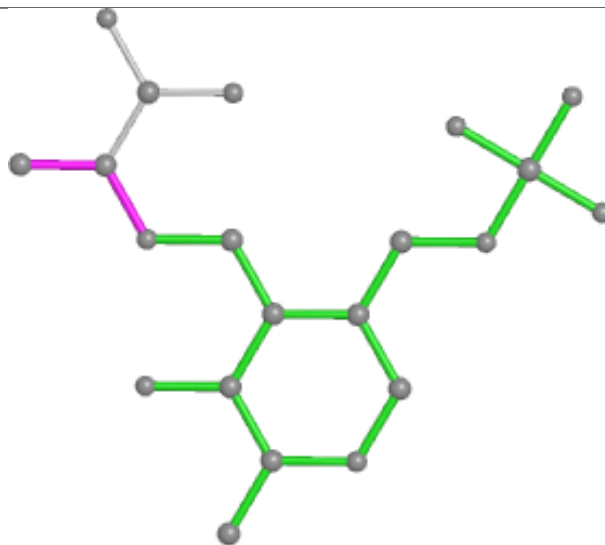


Rings

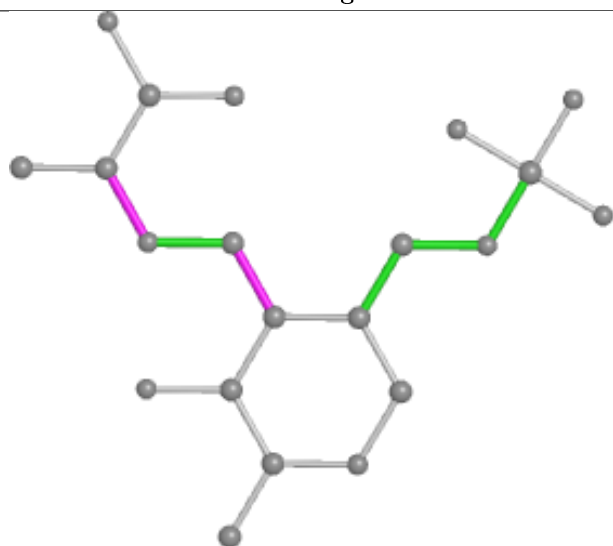
Ligand P1T H 504



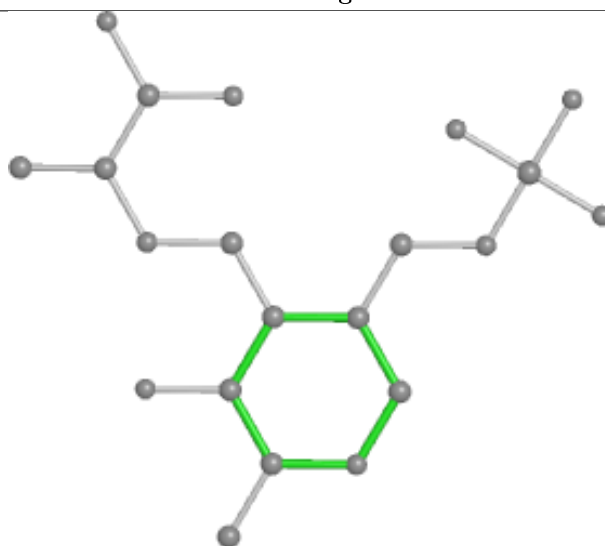
Bond lengths



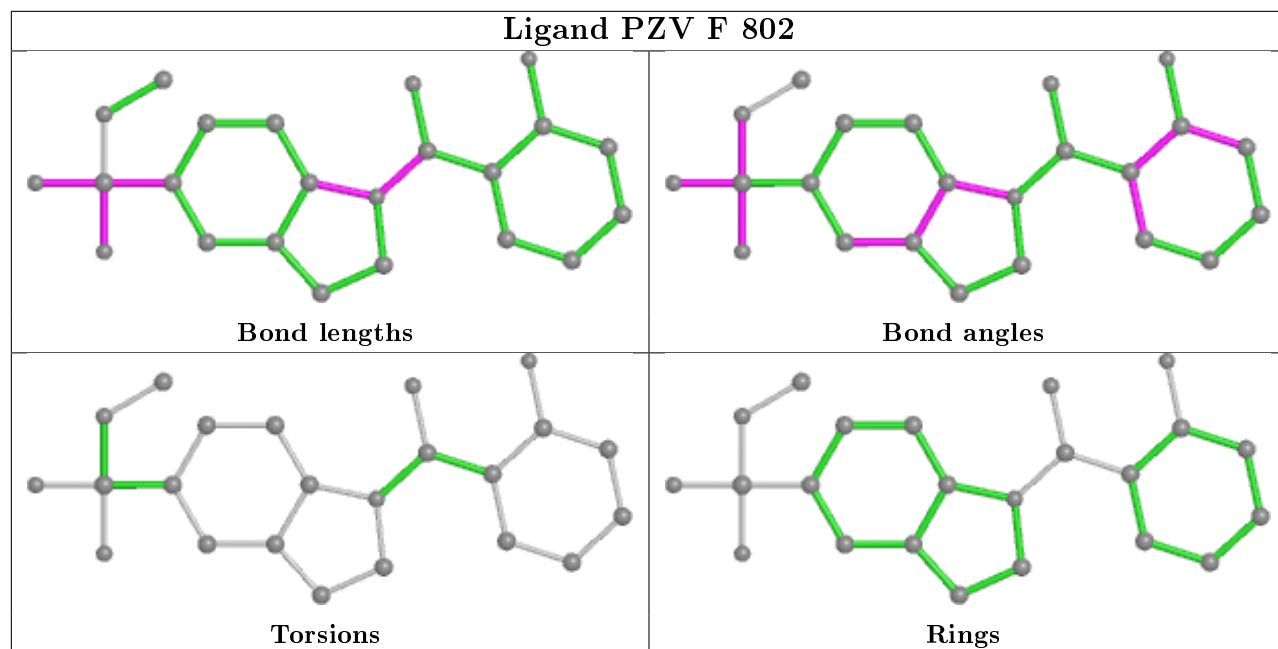
Bond angles



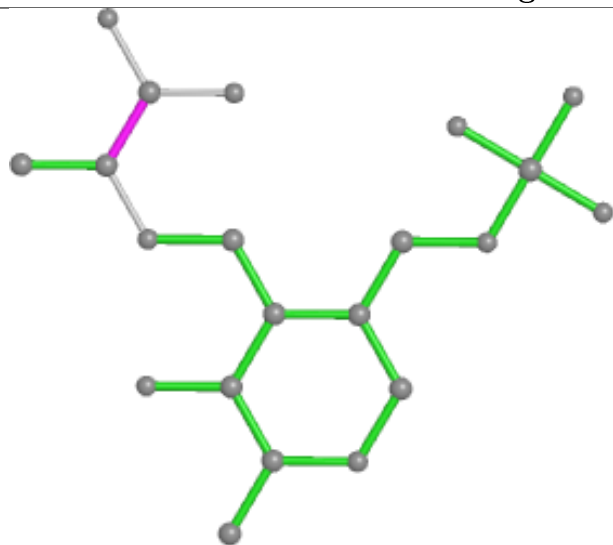
Torsions



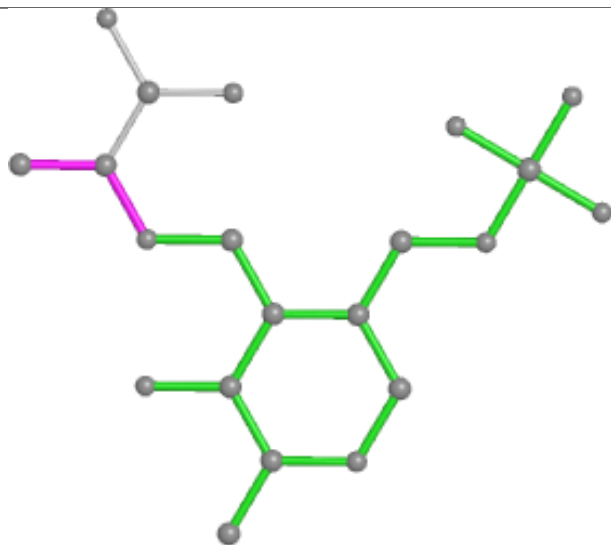
Rings



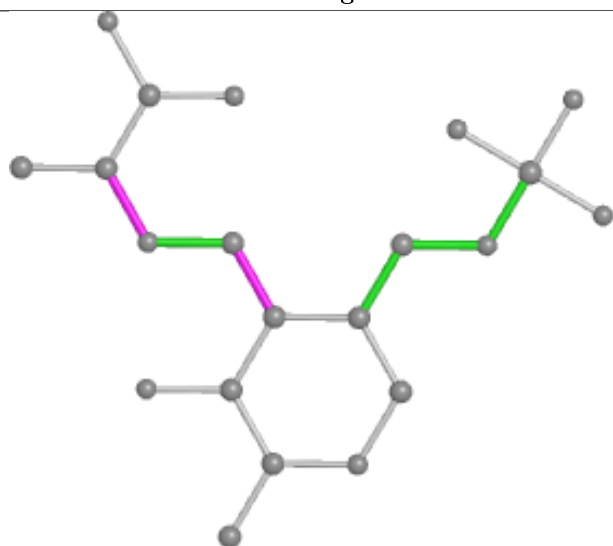
Ligand P1T B 502



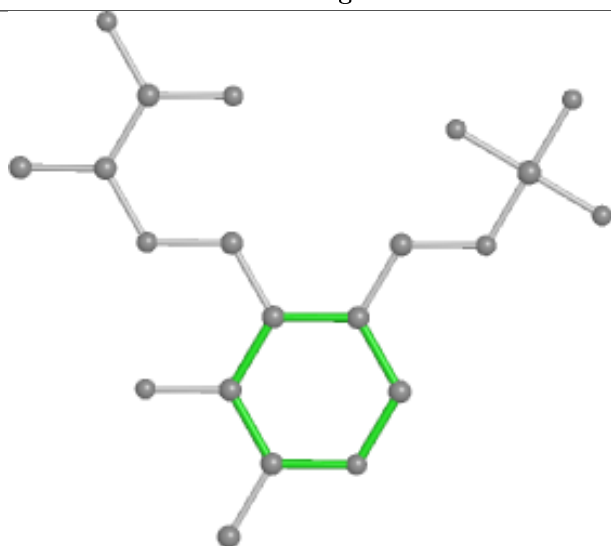
Bond lengths



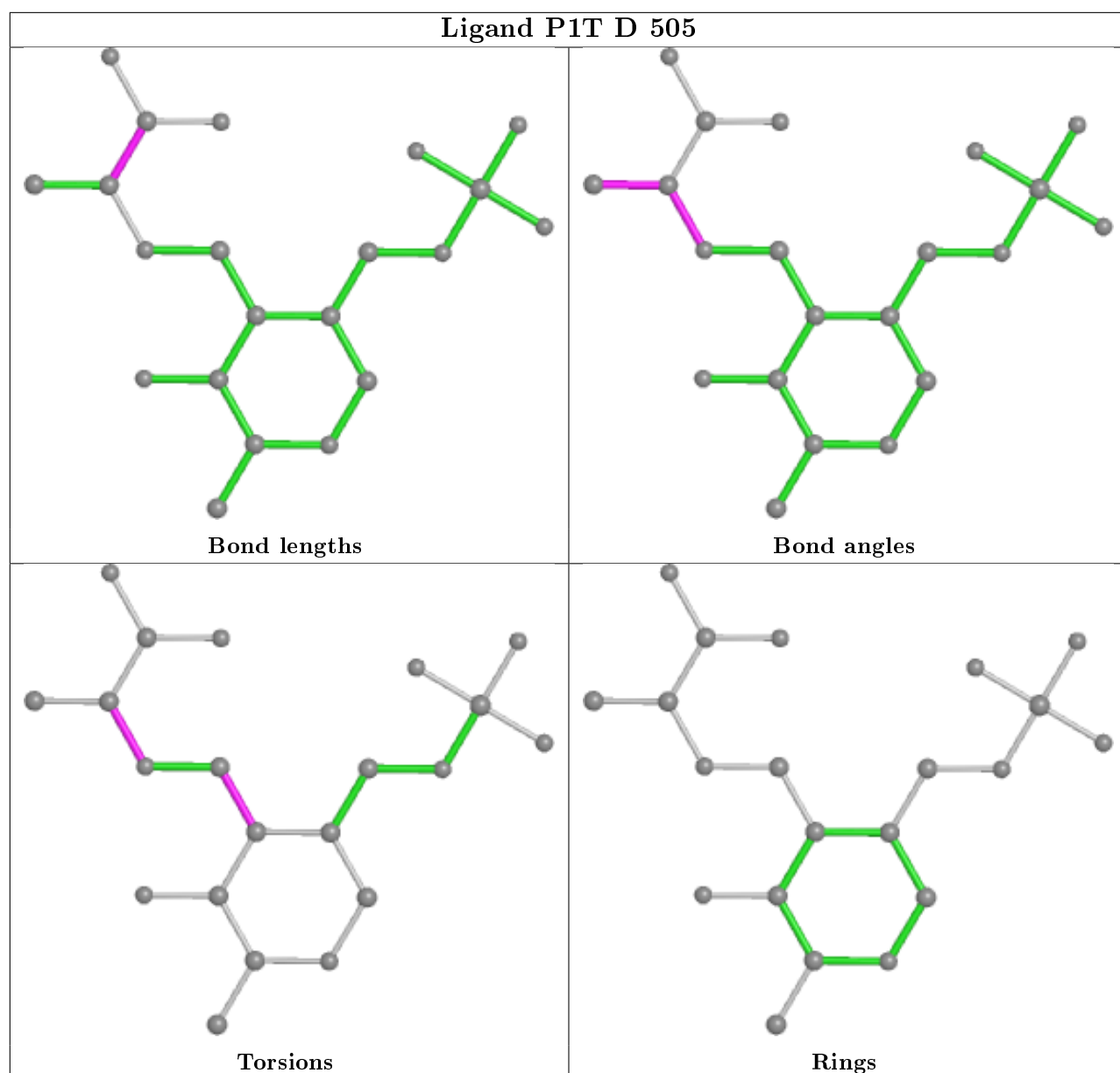
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	249/276 (90%)	-0.51	6 (2%) 59 57	19, 32, 55, 89	0
1	C	249/276 (90%)	-0.39	6 (2%) 59 57	19, 36, 64, 112	0
1	E	245/276 (88%)	-0.22	5 (2%) 65 63	24, 43, 68, 91	0
1	G	249/276 (90%)	-0.61	4 (1%) 72 70	19, 30, 52, 85	0
2	B	405/410 (98%)	-0.77	5 (1%) 79 77	14, 22, 43, 102	0
2	D	404/410 (98%)	-0.72	6 (1%) 73 72	13, 22, 41, 111	0
2	F	404/410 (98%)	-0.75	7 (1%) 70 68	13, 23, 43, 123	0
2	H	404/410 (98%)	-0.75	6 (1%) 73 72	14, 22, 40, 108	0
All	All	2609/2744 (95%)	-0.63	45 (1%) 70 68	13, 26, 56, 123	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	4	ALA	6.3
2	F	6	ALA	5.5
2	F	7	GLU	5.1
1	C	8	GLU	4.9
2	F	5	ILE	4.4
2	H	5	ILE	4.1
2	D	8	PRO	3.3
1	C	267	GLY	3.3
1	G	196	SER	3.3
2	H	9	THR	3.1
2	F	8	PRO	3.1
2	D	6	ALA	3.1
2	B	23	SER	3.0
2	H	6	ALA	3.0
1	A	197	GLN	2.9
1	C	21	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	211	ASP	2.8
1	A	196	SER	2.8
2	B	4	ALA	2.8
2	B	5	ILE	2.8
2	H	4	ALA	2.7
1	C	266	LEU	2.6
1	E	23	ASN	2.6
1	A	23	ASN	2.6
1	G	8	GLU	2.6
2	D	4	ALA	2.6
1	A	267	GLY	2.6
2	F	22	PRO	2.5
1	G	21	ALA	2.5
2	B	8	PRO	2.5
1	C	197	GLN	2.5
2	D	7	GLU	2.4
2	H	7	GLU	2.4
1	E	9	ALA	2.3
1	C	9	ALA	2.3
1	E	21	ALA	2.2
2	D	5	ILE	2.2
1	E	22	ASN	2.2
1	G	23	ASN	2.2
1	A	8	GLU	2.1
2	H	8	PRO	2.1
2	D	22	PRO	2.1
1	A	21	ALA	2.1
2	F	9	THR	2.1
2	B	7	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
3	FMT	G	306	3/3	0.53	0.29	61,61,64,67	0
12	ALA	E	301	5/6	0.54	0.50	73,79,87,88	0
3	FMT	D	504	3/3	0.60	0.38	70,70,74,75	0
9	PEG	F	829	7/7	0.65	0.36	65,75,81,83	0
3	FMT	B	505	3/3	0.67	0.31	60,60,63,64	0
3	FMT	G	307	3/3	0.67	0.42	79,79,81,83	0
4	EDO	B	529	4/4	0.69	0.36	53,61,62,64	0
3	FMT	A	306	3/3	0.69	0.31	56,56,61,61	0
3	FMT	A	301	3/3	0.70	0.43	60,60,66,67	0
4	EDO	B	511	4/4	0.72	0.26	57,60,63,64	0
3	FMT	B	508	3/3	0.72	0.39	68,68,74,75	0
11	EPE	H	532	15/15	0.72	0.27	39,66,99,99	0
4	EDO	B	510	4/4	0.72	0.35	48,60,62,65	0
3	FMT	F	813	3/3	0.72	0.33	44,44,53,56	0
3	FMT	H	511	3/3	0.74	0.41	70,70,70,72	0
13	PGE	F	809	10/10	0.74	0.38	36,57,61,61	10
3	FMT	D	513	3/3	0.75	0.19	67,67,69,70	0
3	FMT	F	821	3/3	0.75	0.28	61,61,66,68	0
3	FMT	G	304	3/3	0.75	0.35	64,64,65,69	0
11	EPE	B	527	15/15	0.76	0.24	48,66,97,98	0
3	FMT	F	816	3/3	0.76	0.23	61,61,66,66	0
9	PEG	G	309	7/7	0.76	0.57	45,62,71,75	0
3	FMT	C	305	3/3	0.77	0.37	69,69,72,73	0
3	FMT	D	503	3/3	0.77	0.24	59,59,62,64	0
13	PGE	F	801	10/10	0.77	0.35	38,70,86,90	0
5	ACT	A	310	4/4	0.77	0.39	66,71,72,75	0
3	FMT	H	526	3/3	0.78	0.45	68,68,68,71	0
3	FMT	H	524	3/3	0.78	0.43	60,60,61,63	0
6	MLI	F	827	7/7	0.78	0.27	66,72,75,77	0
4	EDO	B	516	4/4	0.78	0.21	51,54,55,56	0
9	PEG	B	506	7/7	0.78	0.30	47,56,71,73	0
3	FMT	B	520	3/3	0.78	0.53	72,72,74,77	0
3	FMT	D	517	3/3	0.79	0.27	67,67,67,68	0
3	FMT	H	523	3/3	0.79	0.23	58,58,58,64	0
3	FMT	A	303	3/3	0.79	0.32	53,53,54,59	0
3	FMT	H	516	3/3	0.79	0.36	66,66,67,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	G	312	4/4	0.80	0.29	40,41,46,51	0
3	FMT	H	529	3/3	0.80	0.30	91,91,93,93	0
3	FMT	H	522	3/3	0.80	0.26	57,57,59,62	0
3	FMT	B	521	3/3	0.80	0.28	52,52,56,58	0
3	FMT	F	814	3/3	0.80	0.22	45,45,46,53	0
3	FMT	C	302	3/3	0.80	0.60	74,74,77,79	0
3	FMT	B	519	3/3	0.81	0.23	62,62,65,65	0
3	FMT	C	309	3/3	0.81	0.30	67,67,68,71	0
3	FMT	H	517	3/3	0.81	0.42	54,54,55,61	0
10	K	C	308	1/1	0.81	0.43	108,108,108,108	0
3	FMT	H	508	3/3	0.81	0.34	63,63,65,69	0
4	EDO	H	520	4/4	0.81	0.23	32,48,48,52	0
4	EDO	F	822	4/4	0.81	0.18	50,54,56,58	0
3	FMT	D	514	3/3	0.81	0.19	58,58,58,59	0
3	FMT	G	303	3/3	0.81	0.54	67,67,67,69	0
3	FMT	F	824	3/3	0.81	0.38	62,62,67,68	0
11	EPE	B	530	15/15	0.81	0.30	38,59,81,87	0
4	EDO	E	305	4/4	0.82	0.28	50,57,58,60	0
3	FMT	B	504	3/3	0.82	0.33	46,46,49,55	0
4	EDO	H	512	4/4	0.82	0.27	52,56,58,61	0
3	FMT	B	513	3/3	0.82	0.25	62,62,63,67	0
10	K	D	518	1/1	0.83	0.37	105,105,105,105	0
3	FMT	H	515	3/3	0.83	0.24	44,44,45,51	0
10	K	G	313	1/1	0.83	0.23	87,87,87,87	0
3	FMT	B	517	3/3	0.83	0.24	66,66,68,69	0
3	FMT	H	527	3/3	0.83	0.23	55,55,58,59	0
3	FMT	H	519	3/3	0.84	0.21	68,68,71,72	0
3	FMT	B	531	3/3	0.84	0.28	65,65,69,71	0
3	FMT	B	522	3/3	0.84	0.29	63,63,64,65	0
4	EDO	G	310	4/4	0.85	0.18	30,48,50,52	0
4	EDO	B	526	4/4	0.85	0.34	42,43,51,53	0
3	FMT	G	302	3/3	0.85	0.34	49,49,51,55	0
3	FMT	B	512	3/3	0.85	0.39	76,76,77,78	0
10	K	F	826	1/1	0.85	0.32	84,84,84,84	0
3	FMT	F	817	3/3	0.85	0.24	67,67,68,73	0
3	FMT	A	305	3/3	0.86	0.23	61,61,63,63	0
3	FMT	H	503	3/3	0.86	0.26	57,57,61,63	0
3	FMT	B	524	3/3	0.86	0.21	61,61,65,67	0
6	MLI	H	530	7/7	0.86	0.27	65,69,71,72	0
3	FMT	H	509	3/3	0.86	0.24	50,50,51,54	0
4	EDO	F	819	4/4	0.86	0.20	43,47,52,55	0
3	FMT	F	815	3/3	0.87	0.27	70,70,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FMT	D	512	3/3	0.87	0.25	69,69,70,72	0
3	FMT	E	303	3/3	0.87	0.21	50,50,54,55	0
3	FMT	B	514	3/3	0.87	0.21	67,67,68,70	0
3	FMT	H	518	3/3	0.88	0.37	58,58,62,63	0
3	FMT	H	528	3/3	0.88	0.17	56,56,58,59	0
3	FMT	G	305	3/3	0.88	0.20	60,60,62,63	0
10	K	D	522	1/1	0.88	0.12	87,87,87,87	0
3	FMT	D	521	3/3	0.88	0.35	63,63,63,64	0
4	EDO	A	304	4/4	0.88	0.45	54,56,58,61	0
4	EDO	F	812	4/4	0.89	0.14	57,58,59,64	0
11	EPE	F	830	15/15	0.89	0.26	36,55,70,73	15
3	FMT	F	823	3/3	0.89	0.22	56,56,59,61	0
3	FMT	C	304	3/3	0.89	0.27	61,61,63,64	0
5	ACT	A	312	4/4	0.89	0.22	54,62,63,69	0
3	FMT	F	810	3/3	0.90	0.20	49,49,55,57	0
3	FMT	H	514	3/3	0.90	0.18	48,48,51,54	0
3	FMT	G	308	3/3	0.90	0.45	60,60,64,64	0
3	FMT	D	508	3/3	0.90	0.26	57,57,59,60	0
3	FMT	D	516	3/3	0.90	0.17	52,52,56,60	0
4	EDO	D	511	4/4	0.90	0.15	52,54,59,64	0
4	EDO	H	521	4/4	0.90	0.18	47,48,51,52	0
6	MLI	A	311	7/7	0.91	0.13	43,43,51,53	0
10	K	H	531	1/1	0.91	0.26	73,73,73,73	0
3	FMT	F	811	3/3	0.91	0.27	7,7,17,21	3
3	FMT	A	309	3/3	0.91	0.38	45,45,45,46	0
3	FMT	D	515	3/3	0.91	0.18	39,39,51,51	0
3	FMT	F	828	3/3	0.91	0.20	61,61,61,64	0
6	MLI	G	311	7/7	0.91	0.14	35,43,54,58	0
3	FMT	D	502	3/3	0.91	0.19	25,25,29,38	3
4	EDO	C	301	4/4	0.92	0.24	40,47,47,47	0
3	FMT	H	507	3/3	0.92	0.20	52,52,53,57	0
3	FMT	H	501	3/3	0.92	0.18	50,50,54,58	0
10	K	B	525	1/1	0.92	0.31	75,75,75,75	0
4	EDO	H	533	4/4	0.92	0.17	37,43,46,46	0
3	FMT	H	510	3/3	0.92	0.27	44,44,45,51	0
3	FMT	F	807	3/3	0.92	0.13	43,43,44,48	0
3	FMT	F	804	3/3	0.93	0.19	65,65,66,66	0
3	FMT	A	308	3/3	0.93	0.34	53,53,56,59	0
3	FMT	B	523	3/3	0.93	0.18	42,42,51,53	0
3	FMT	G	301	3/3	0.93	0.25	42,42,46,50	0
3	FMT	F	820	3/3	0.93	0.19	55,55,57,58	0
5	ACT	F	808	4/4	0.93	0.13	45,45,51,60	0

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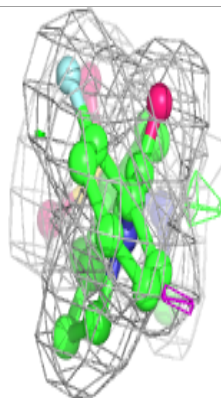
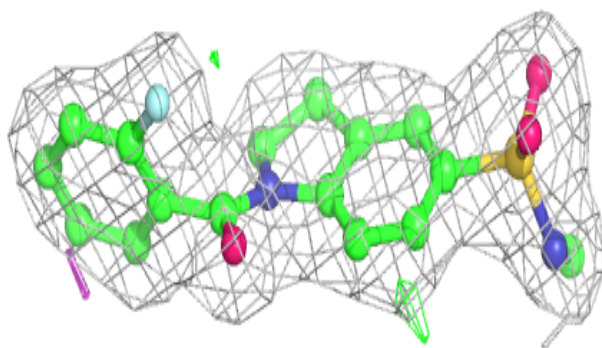
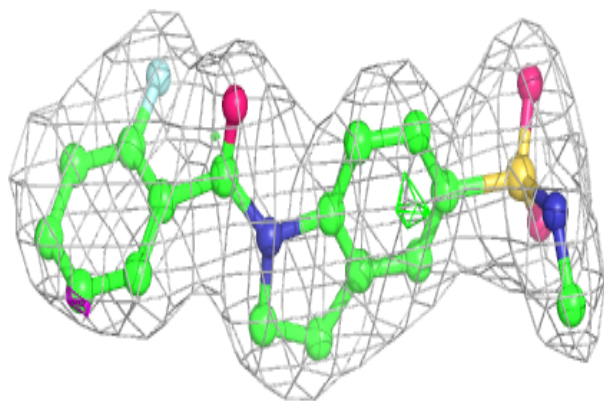
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FMT	B	528	3/3	0.93	0.11	45,45,46,50	0
3	FMT	D	510	3/3	0.93	0.22	55,55,55,57	0
5	ACT	F	818	4/4	0.94	0.16	43,52,54,61	0
3	FMT	A	302	3/3	0.94	0.21	37,37,40,44	0
9	PEG	H	513	7/7	0.94	0.20	7,9,25,33	7
3	FMT	D	506	3/3	0.94	0.11	29,29,31,34	0
6	MLI	E	302	7/7	0.94	0.10	45,51,53,54	0
3	FMT	A	307	3/3	0.94	0.21	56,56,56,59	0
10	K	D	519	1/1	0.94	0.15	75,75,75,75	0
3	FMT	F	803	3/3	0.94	0.15	47,47,48,49	0
6	MLI	C	307	7/7	0.94	0.12	39,45,52,53	0
4	EDO	C	303	4/4	0.94	0.23	39,41,42,47	0
4	EDO	B	503	4/4	0.94	0.26	33,39,41,51	0
4	EDO	B	509	4/4	0.94	0.17	40,41,45,49	0
5	ACT	H	506	4/4	0.95	0.15	39,49,50,59	0
4	EDO	D	520	4/4	0.95	0.17	43,45,46,48	0
3	FMT	H	525	3/3	0.95	0.14	34,34,43,47	0
3	FMT	B	507	3/3	0.95	0.09	52,52,53,54	0
3	FMT	E	304	3/3	0.95	0.37	55,55,56,56	0
3	FMT	F	806	3/3	0.95	0.13	47,47,48,51	0
3	FMT	B	518	3/3	0.96	0.15	33,33,45,49	0
3	FMT	D	507	3/3	0.97	0.08	48,48,49,49	0
14	NA	F	825	1/1	0.97	0.34	61,61,61,61	0
3	FMT	D	509	3/3	0.97	0.10	41,41,43,45	0
4	EDO	H	505	4/4	0.98	0.09	26,29,32,34	0
4	EDO	C	306	4/4	0.98	0.21	36,37,43,52	0
7	PZV	H	502	23/23	0.98	0.14	18,24,29,31	0
7	PZV	B	501	23/23	0.98	0.15	14,23,27,38	0
7	PZV	F	802	23/23	0.98	0.11	20,27,30,33	0
3	FMT	B	515	3/3	0.98	0.21	43,43,51,52	0
8	P1T	D	505	21/21	0.98	0.16	15,21,26,29	0
7	PZV	D	501	23/23	0.98	0.14	15,21,30,31	0
8	P1T	B	502	21/21	0.99	0.18	12,20,25,27	0
8	P1T	H	504	21/21	0.99	0.20	13,20,25,31	0
8	P1T	F	805	21/21	0.99	0.16	12,22,28,34	0

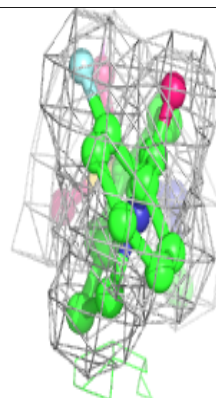
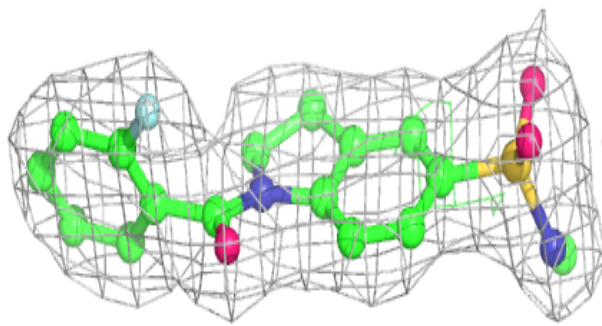
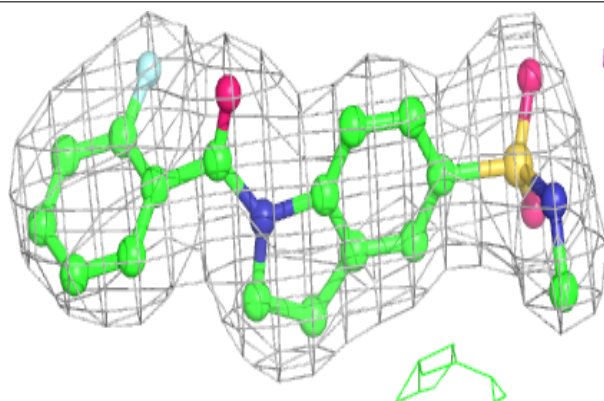
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PZV H 502:

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

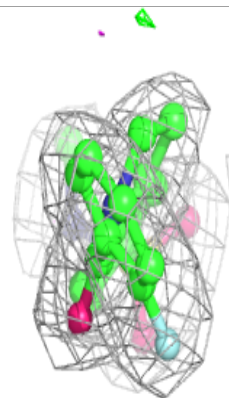
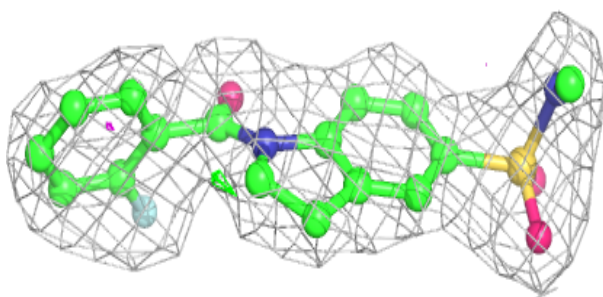
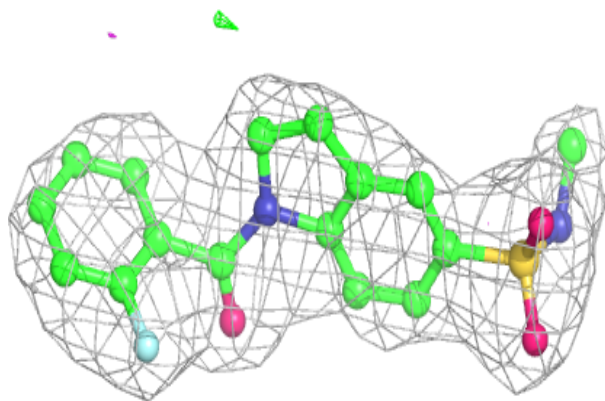
**Electron density around PZV B 501:**

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



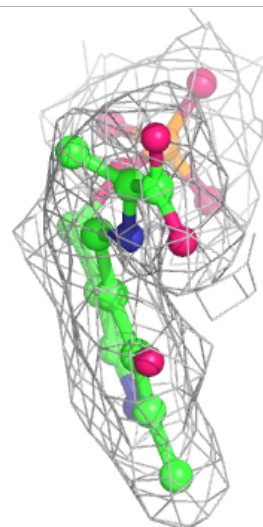
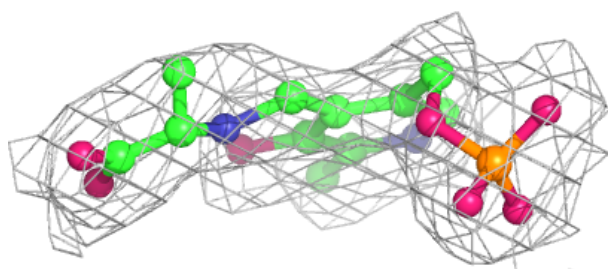
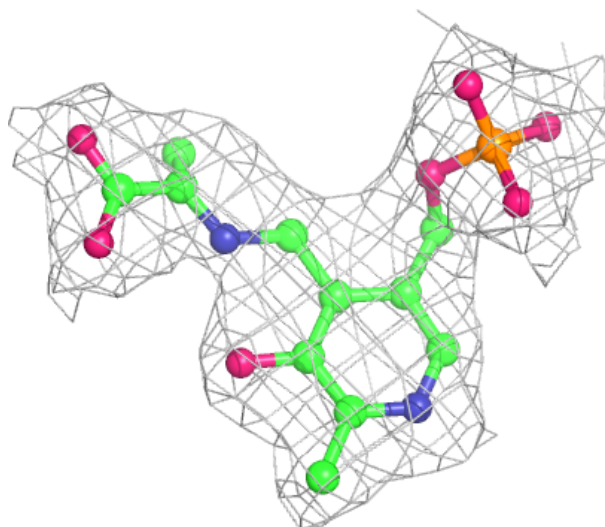
Electron density around PZV F 802:

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



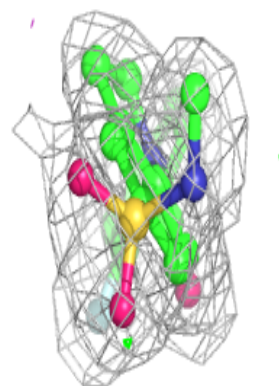
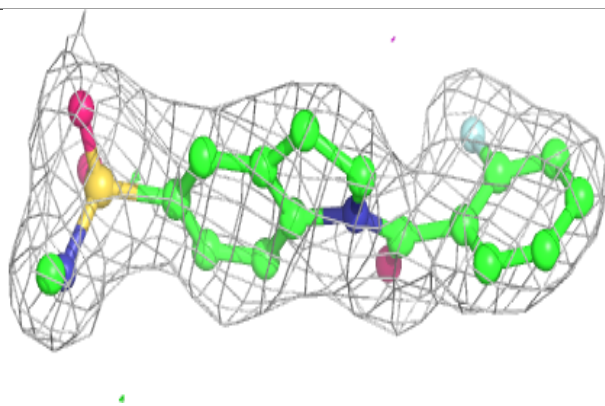
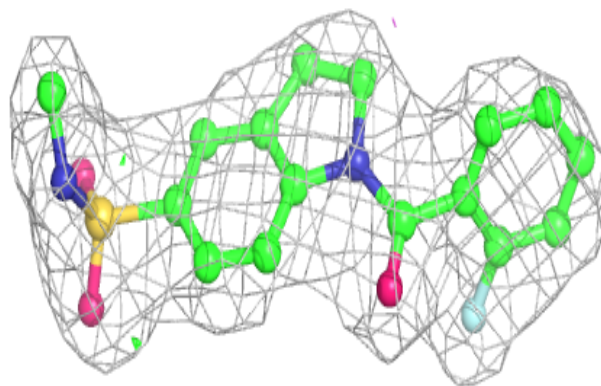
Electron density around P1T D 505:

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



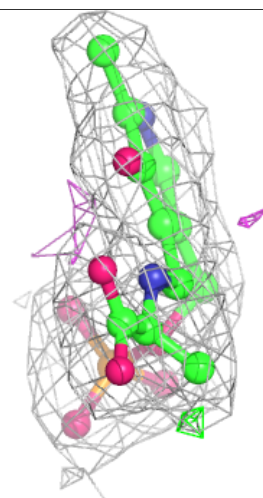
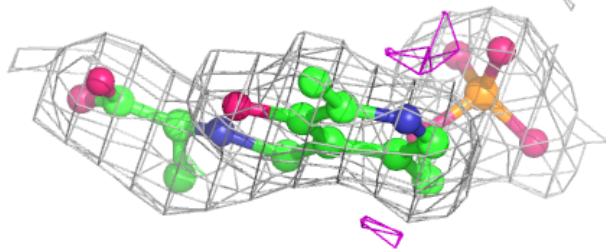
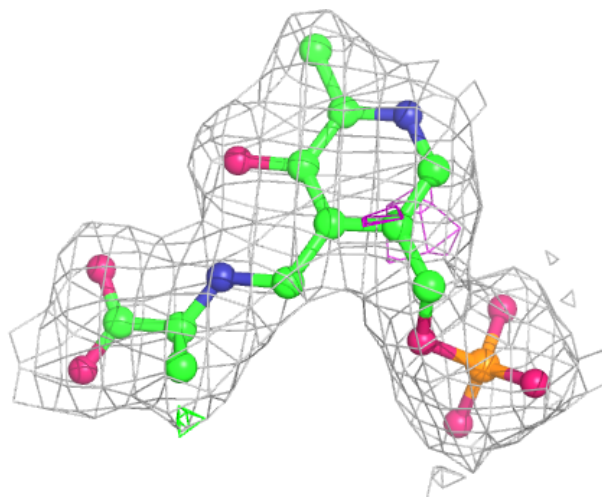
Electron density around PZV D 501:

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



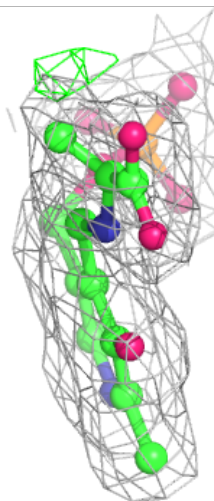
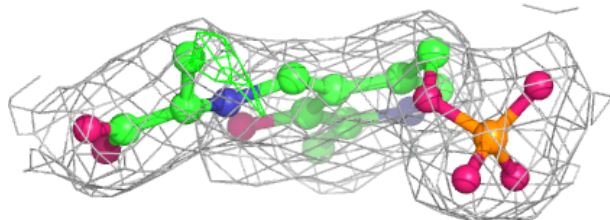
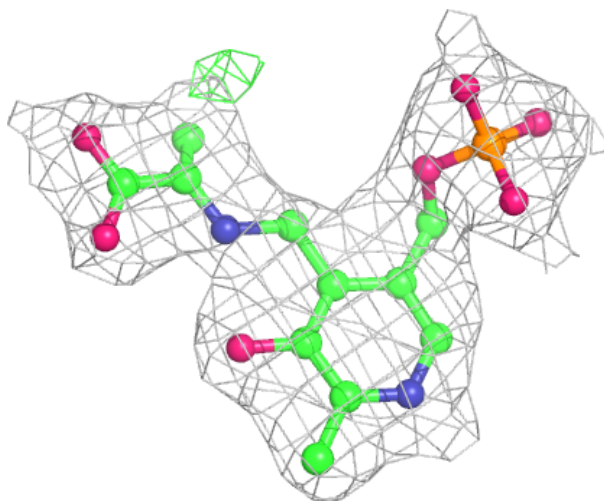
Electron density around P1T B 502:

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



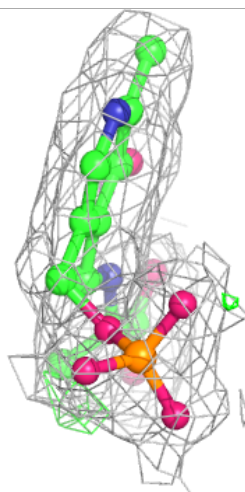
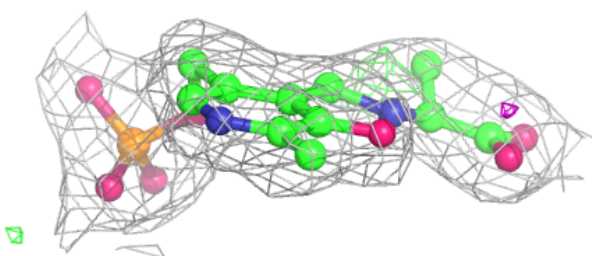
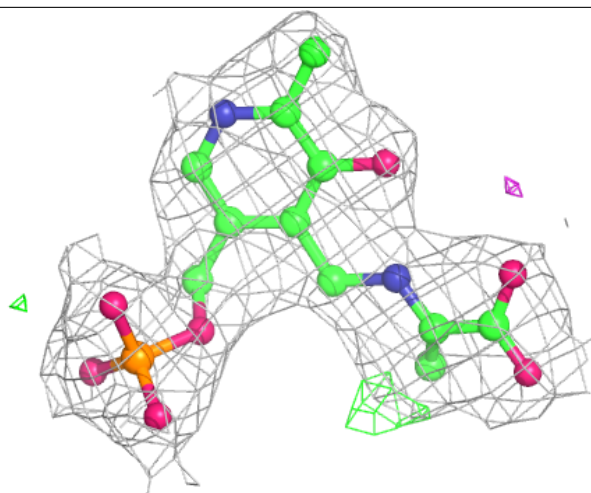
Electron density around P1T H 504:

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



Electron density around P1T F 805:

$2mF_o-DF_c$ (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.