



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 12:14 am BST

PDB ID : 1C7O
Title : CRYSTAL STRUCTURE OF CYSTALYSIN FROM TREPONEMA DENTICOLOA CONTAINS A PYRIDOXAL 5'-PHOSPHATE-L-AMINOETHOXYVINYLGLYCINE COMPLEX
Authors : Krupka, H.I.; Huber, R.; Holt, S.C.; Clausen, T.
Deposited on : 2000-03-16
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

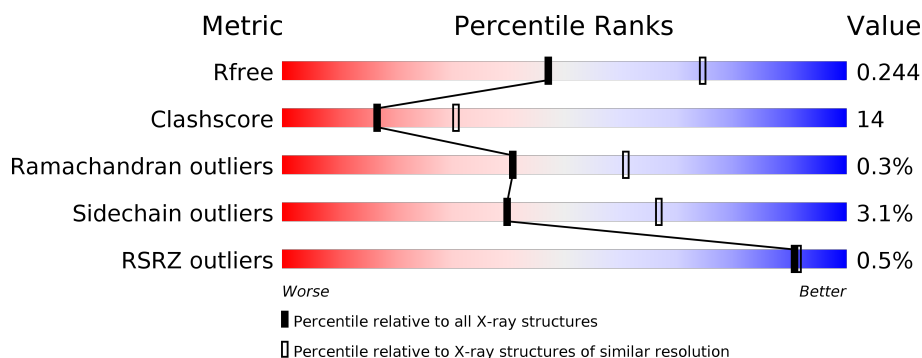
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	399	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>28%</div> <div>..</div> </div> </div>
1	B	399	<div> <div>73%</div> <div>25%</div> <div>..</div> </div>
1	C	399	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>..</div> </div> </div>
1	D	399	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div>..</div> </div> </div>
1	E	399	<div> <div>67%</div> <div>30%</div> <div>..</div> </div>
1	F	399	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	399	<div><div>%</div><div><div></div></div><div>64%33%..</div></div>
1	H	399	<div><div></div><div>67%30%..</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27138 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 CRYSTALYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	B	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	C	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	D	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	E	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	F	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	G	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			
1	H	394	Total	C	N	O	S	0	0	0
			3207	2075	523	590	19			

There are 24 discrepancies between the modelled and reference sequences:

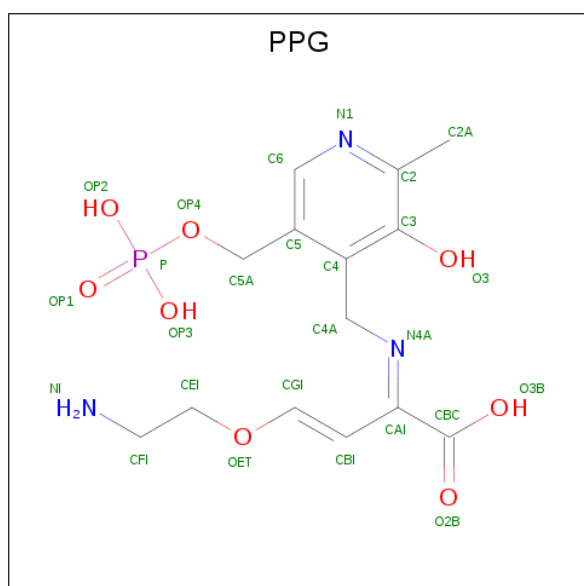
Chain	Residue	Modelled	Actual	Comment	Reference
A	88	GLN	GLU	CONFLICT	UNP Q56257
A	154	GLN	GLU	CONFLICT	UNP Q56257
A	267	ALA	ILE	CONFLICT	UNP Q56257
B	88	GLN	GLU	CONFLICT	UNP Q56257
B	154	GLN	GLU	CONFLICT	UNP Q56257
B	267	ALA	ILE	CONFLICT	UNP Q56257
C	88	GLN	GLU	CONFLICT	UNP Q56257
C	154	GLN	GLU	CONFLICT	UNP Q56257
C	267	ALA	ILE	CONFLICT	UNP Q56257
D	88	GLN	GLU	CONFLICT	UNP Q56257
D	154	GLN	GLU	CONFLICT	UNP Q56257
D	267	ALA	ILE	CONFLICT	UNP Q56257
E	88	GLN	GLU	CONFLICT	UNP Q56257

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	154	GLN	GLU	CONFLICT	UNP Q56257
E	267	ALA	ILE	CONFLICT	UNP Q56257
F	88	GLN	GLU	CONFLICT	UNP Q56257
F	154	GLN	GLU	CONFLICT	UNP Q56257
F	267	ALA	ILE	CONFLICT	UNP Q56257
G	88	GLN	GLU	CONFLICT	UNP Q56257
G	154	GLN	GLU	CONFLICT	UNP Q56257
G	267	ALA	ILE	CONFLICT	UNP Q56257
H	88	GLN	GLU	CONFLICT	UNP Q56257
H	154	GLN	GLU	CONFLICT	UNP Q56257
H	267	ALA	ILE	CONFLICT	UNP Q56257

- Molecule 2 is (2E,3E)-4-(2-aminoethoxy)-2-[(3-hydroxy-2-methyl-5-[(phosphonoxy)methyl]pyridin-4-yl)methyl]imino]but-3-enoic acid (three-letter code: PPG) (formula: C₁₄H₂₀N₃O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	B	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	C	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	D	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	E	1	Total	C	N	O	P	0	0
			26	14	3	8	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	G	1	Total	C	N	O	P	0	0
			26	14	3	8	1		
2	H	1	Total	C	N	O	P	0	0
			26	14	3	8	1		

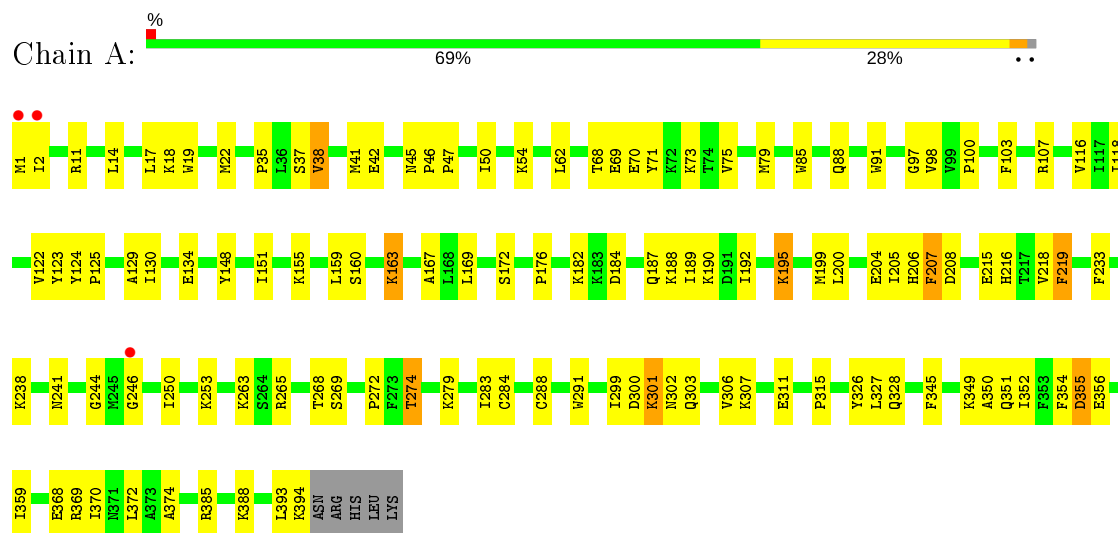
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	175	Total	O	0	0
			175	175		
3	B	181	Total	O	0	0
			181	181		
3	C	167	Total	O	0	0
			167	167		
3	D	139	Total	O	0	0
			139	139		
3	E	142	Total	O	0	0
			142	142		
3	F	180	Total	O	0	0
			180	180		
3	G	161	Total	O	0	0
			161	161		
3	H	129	Total	O	0	0
			129	129		

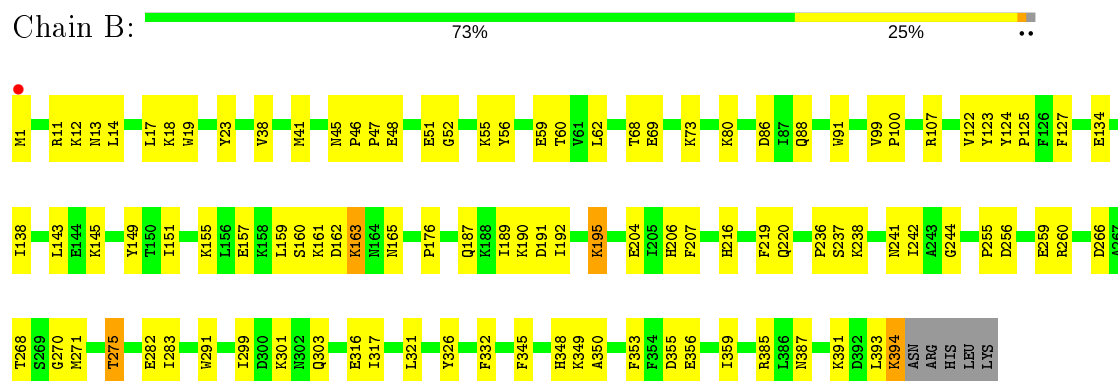
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

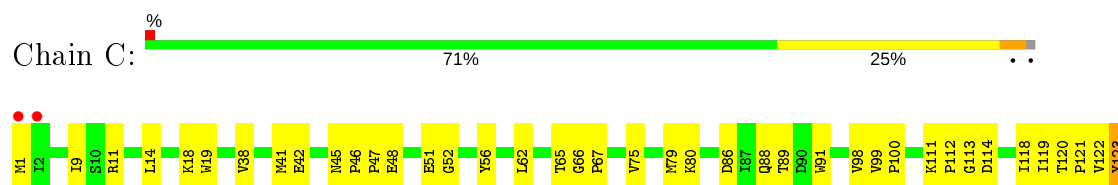
• Molecule 1: CYSTALYSIN

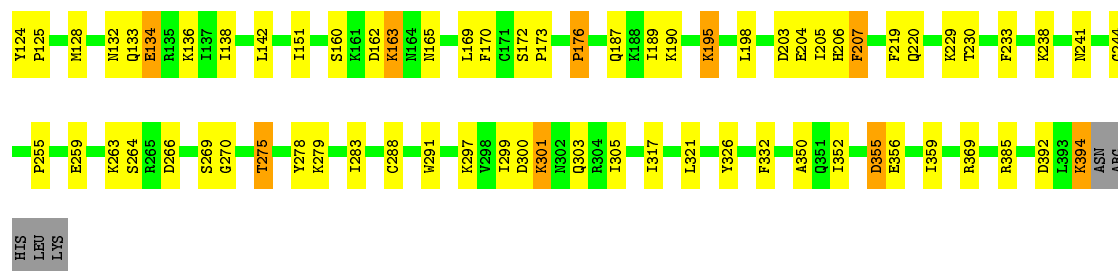


• Molecule 1: CYSTALYSIN

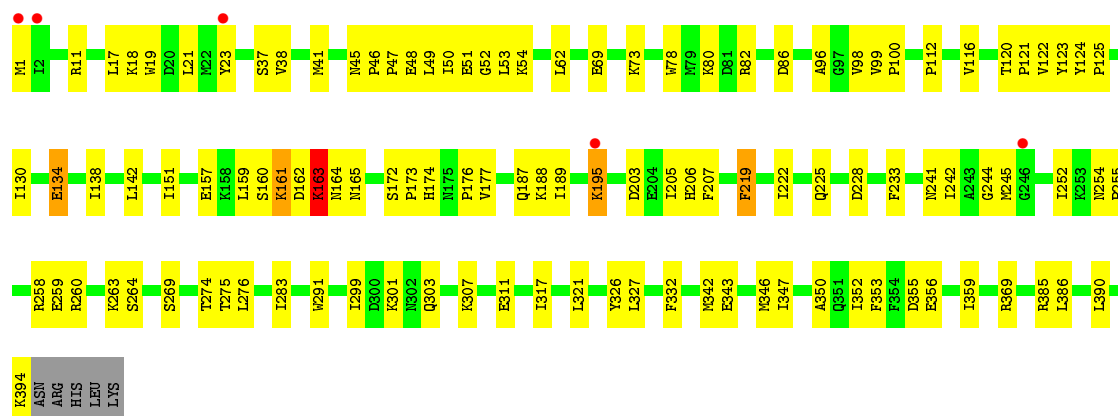


• Molecule 1: CYSTALYSIN

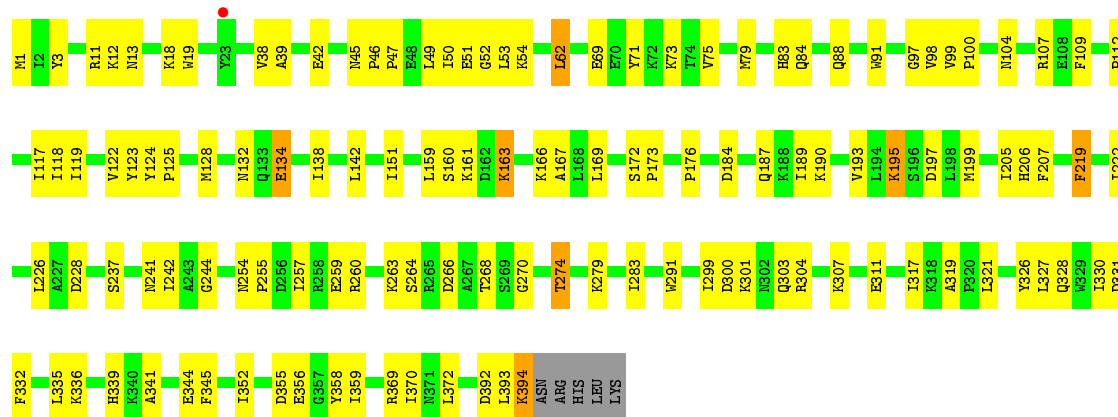




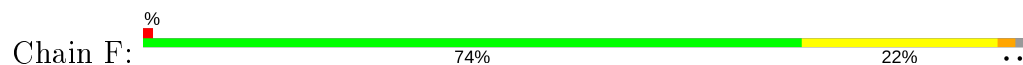
• Molecule 1: CYSTALYSIN

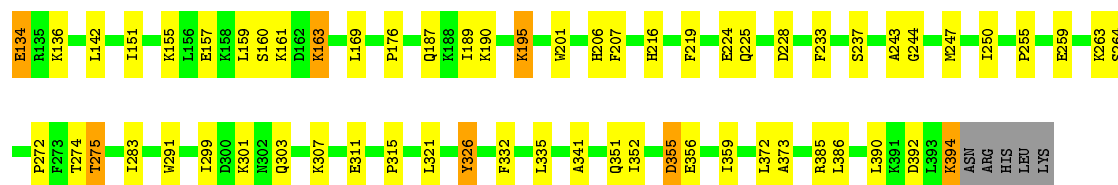


• Molecule 1: CYSTALYSIN

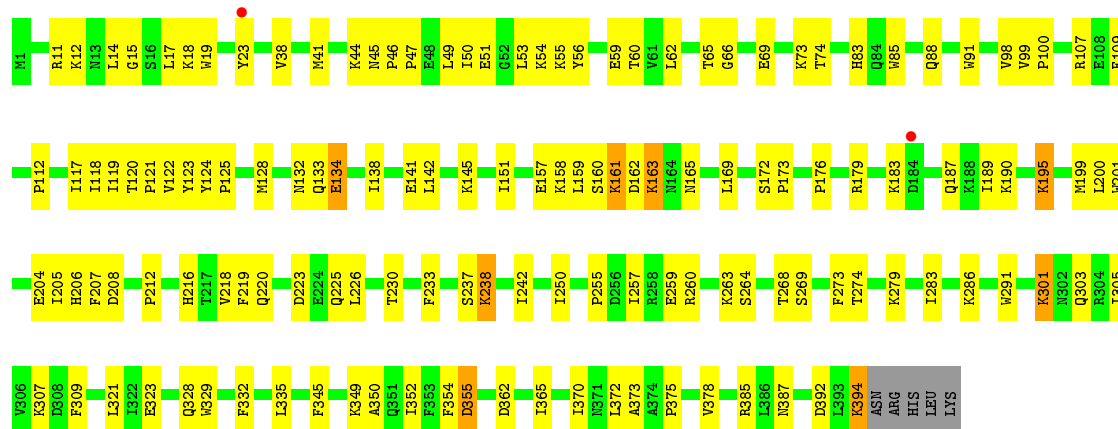


• Molecule 1: CYSTALYSIN

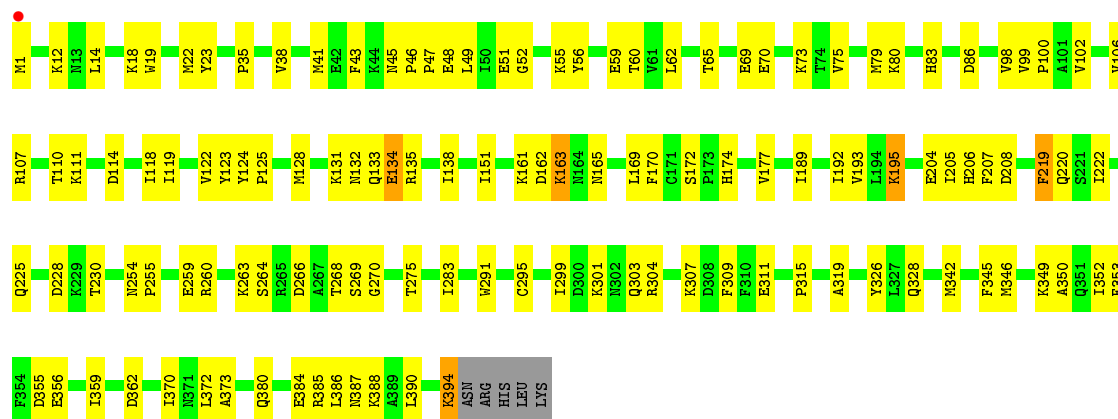




• Molecule 1: CYSTALYSIN



• Molecule 1: CYSTALYSIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.37Å 107.93Å 176.16Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.00-2.50) 91.9 (19.95-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.50Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.193 , 0.260 0.184 , 0.244	Depositor DCC
R_{free} test set	5379 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 21.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.104 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27138	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PPG

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	0.36	0/3283	0.62	0/4429
1	B	0.37	0/3283	0.63	0/4429
1	C	0.35	0/3283	0.62	1/4429 (0.0%)
1	D	0.34	0/3283	0.61	0/4429
1	E	0.35	0/3283	0.61	0/4429
1	F	0.37	0/3283	0.63	1/4429 (0.0%)
1	G	0.36	0/3283	0.61	1/4429 (0.0%)
1	H	0.35	0/3283	0.62	0/4429
All	All	0.36	0/26264	0.62	3/35432 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	355	ASP	N-CA-C	-6.22	94.20	111.00
1	C	355	ASP	N-CA-C	-5.80	95.34	111.00
1	G	355	ASP	N-CA-C	-5.20	96.96	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3207	0	3223	104	0
1	B	3207	0	3223	86	0
1	C	3207	0	3223	91	0
1	D	3207	0	3223	88	0
1	E	3207	0	3223	102	0
1	F	3207	0	3223	74	0
1	G	3207	0	3223	109	0
1	H	3207	0	3223	102	0
2	A	26	0	17	7	0
2	B	26	0	16	4	0
2	C	26	0	16	4	0
2	D	26	0	16	4	0
2	E	26	0	17	3	0
2	F	26	0	16	3	0
2	G	26	0	16	4	0
2	H	26	0	16	3	0
3	A	175	0	0	11	0
3	B	181	0	0	10	0
3	C	167	0	0	5	0
3	D	139	0	0	3	0
3	E	142	0	0	6	0
3	F	180	0	0	8	0
3	G	161	0	0	5	0
3	H	129	0	0	9	0
All	All	27138	0	25914	730	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 14.

The worst 5 of 730 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:163:LYS:H	1:F:163:LYS:HD3	1.03	1.17
1:H:163:LYS:H	1:H:163:LYS:HD3	1.06	1.14
1:G:163:LYS:HD3	1:G:163:LYS:H	1.00	1.13
1:C:163:LYS:HD3	1:C:163:LYS:H	1.01	1.12
1:D:163:LYS:HD3	1:D:163:LYS:H	1.11	1.10

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	392/399 (98%)	368 (94%)	21 (5%)	3 (1%)	19	35
1	B	392/399 (98%)	371 (95%)	21 (5%)	0	100	100
1	C	392/399 (98%)	372 (95%)	19 (5%)	1 (0%)	41	61
1	D	392/399 (98%)	375 (96%)	16 (4%)	1 (0%)	41	61
1	E	392/399 (98%)	374 (95%)	16 (4%)	2 (0%)	29	48
1	F	392/399 (98%)	377 (96%)	15 (4%)	0	100	100
1	G	392/399 (98%)	369 (94%)	22 (6%)	1 (0%)	41	61
1	H	392/399 (98%)	371 (95%)	21 (5%)	0	100	100
All	All	3136/3192 (98%)	2977 (95%)	151 (5%)	8 (0%)	41	61

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	163	LYS
1	A	274	THR
1	E	62	LEU
1	G	141	GLU
1	C	123	TYR

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	353/358 (99%)	344 (98%)	9 (2%)	47	73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	353/358 (99%)	343 (97%)	10 (3%)	43	70
1	C	353/358 (99%)	343 (97%)	10 (3%)	43	70
1	D	353/358 (99%)	343 (97%)	10 (3%)	43	70
1	E	353/358 (99%)	339 (96%)	14 (4%)	31	56
1	F	353/358 (99%)	341 (97%)	12 (3%)	37	63
1	G	353/358 (99%)	340 (96%)	13 (4%)	34	60
1	H	353/358 (99%)	344 (98%)	9 (2%)	47	73
All	All	2824/2864 (99%)	2737 (97%)	87 (3%)	40	67

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1	MET
1	E	207	PHE
1	H	163	LYS
1	E	84	GLN
1	E	176	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	154	GLN
1	E	45	ASN
1	H	25	GLN
1	D	216	HIS
1	E	187	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PPG	E	5500	-	24,26,26	3.94	9 (37%)	22,35,35	2.38	9 (40%)
2	PPG	H	8500	-	24,26,26	3.05	8 (33%)	22,35,35	2.64	8 (36%)
2	PPG	B	2500	-	24,26,26	3.83	7 (29%)	22,35,35	2.61	10 (45%)
2	PPG	G	7500	-	24,26,26	2.91	8 (33%)	22,35,35	2.09	8 (36%)
2	PPG	C	3500	-	24,26,26	2.89	8 (33%)	22,35,35	2.57	9 (40%)
2	PPG	F	6500	-	24,26,26	3.28	5 (20%)	22,35,35	2.48	9 (40%)
2	PPG	A	1500	-	24,26,26	3.40	8 (33%)	22,35,35	1.98	7 (31%)
2	PPG	D	4500	-	24,26,26	2.96	6 (25%)	22,35,35	2.41	9 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PPG	E	5500	-	-	4/16/21/21	0/1/1/1
2	PPG	H	8500	-	-	6/16/21/21	0/1/1/1
2	PPG	B	2500	-	-	5/16/21/21	0/1/1/1
2	PPG	G	7500	-	-	3/16/21/21	0/1/1/1
2	PPG	C	3500	-	-	6/16/21/21	0/1/1/1
2	PPG	F	6500	-	-	4/16/21/21	0/1/1/1
2	PPG	A	1500	-	-	5/16/21/21	0/1/1/1
2	PPG	D	4500	-	-	5/16/21/21	0/1/1/1

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5500	PPG	CAI-N4A	14.48	1.53	1.30
2	B	2500	PPG	CAI-N4A	11.70	1.48	1.30
2	A	1500	PPG	CAI-N4A	11.03	1.47	1.30
2	B	2500	PPG	C5-C4	10.57	1.55	1.40
2	F	6500	PPG	CAI-N4A	10.20	1.46	1.30

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	8500	PPG	C2A-C2-C3	8.03	130.81	120.89
2	C	3500	PPG	C2A-C2-C3	7.82	130.55	120.89
2	B	2500	PPG	C2A-C2-C3	6.15	128.49	120.89
2	E	5500	PPG	C2A-C2-C3	6.14	128.47	120.89
2	D	4500	PPG	C2A-C2-C3	6.09	128.41	120.89

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	5500	PPG	CBI-CAI-N4A-C4A
2	E	5500	PPG	N4A-CAI-CBI-CGI
2	E	5500	PPG	CBC-CAI-CBI-CGI
2	E	5500	PPG	CAI-CBI-CGI-OET
2	H	8500	PPG	CBI-CAI-N4A-C4A

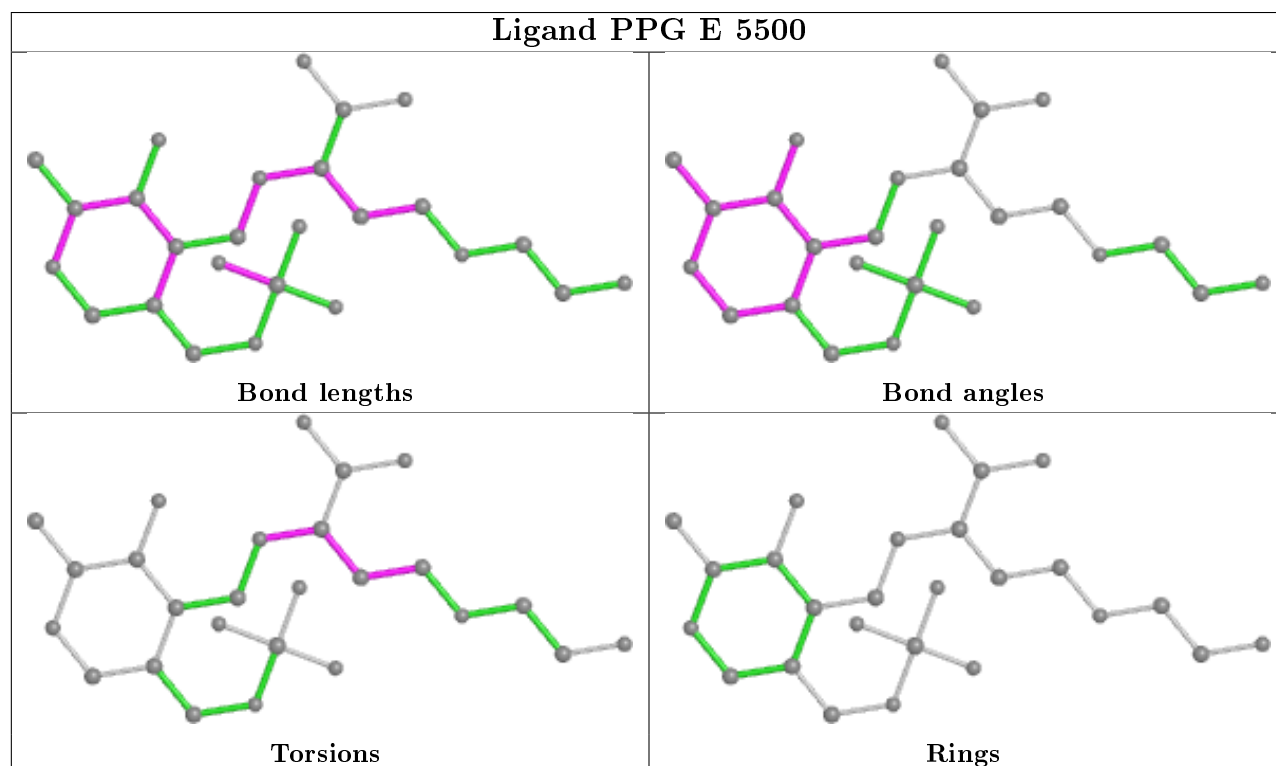
There are no ring outliers.

8 monomers are involved in 32 short contacts:

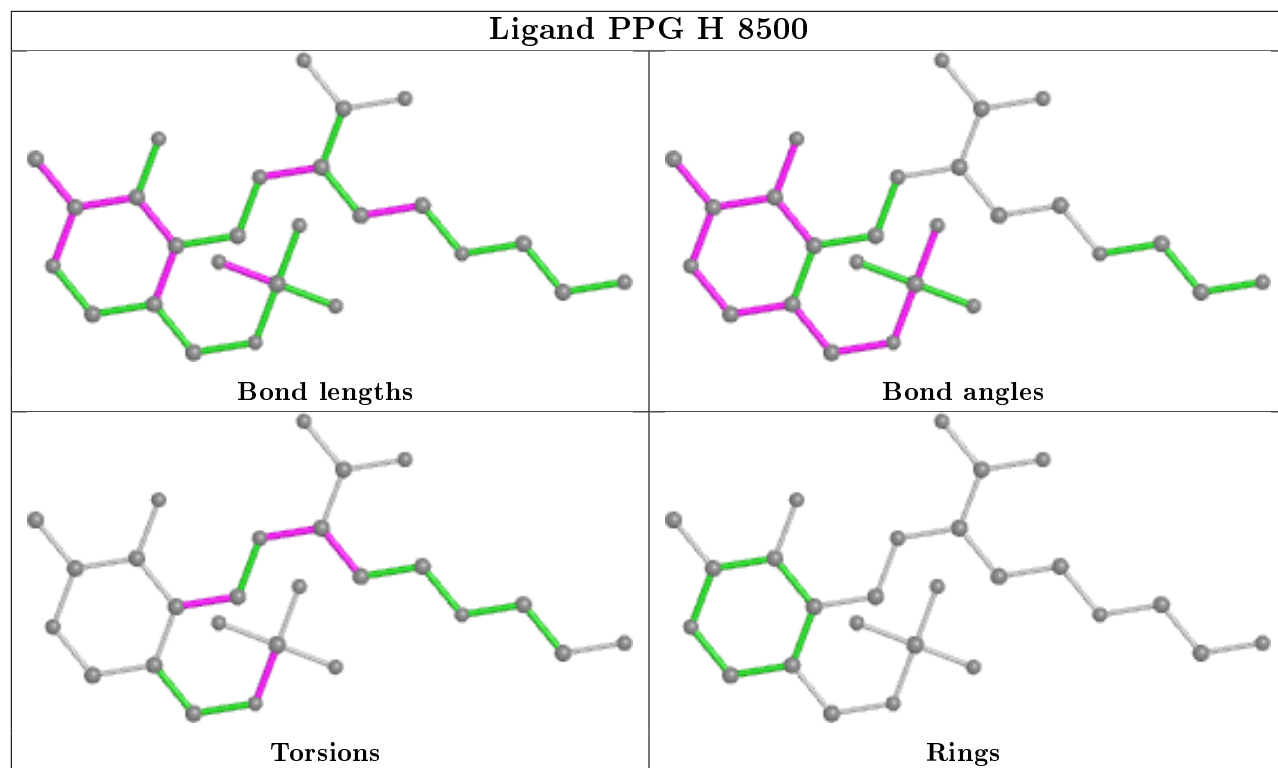
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	5500	PPG	3	0
2	H	8500	PPG	3	0
2	B	2500	PPG	4	0
2	G	7500	PPG	4	0
2	C	3500	PPG	4	0
2	F	6500	PPG	3	0
2	A	1500	PPG	7	0
2	D	4500	PPG	4	0

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

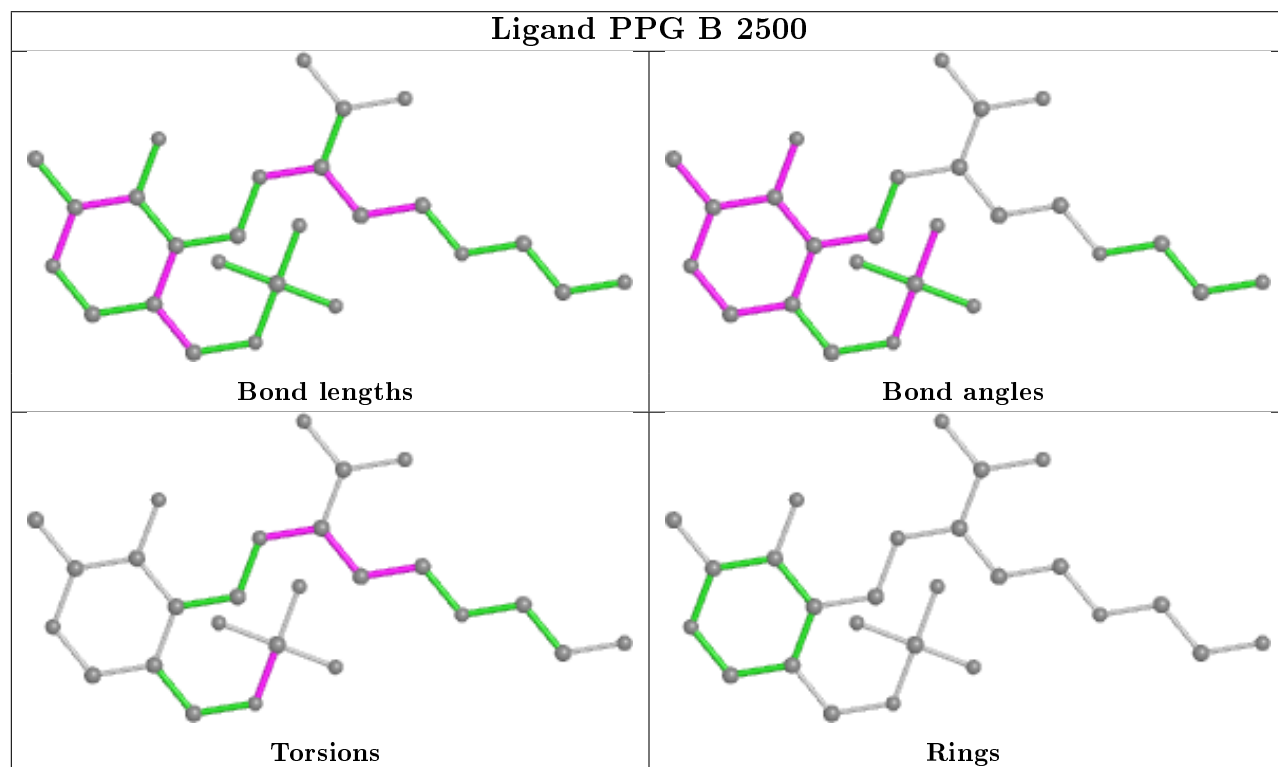
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



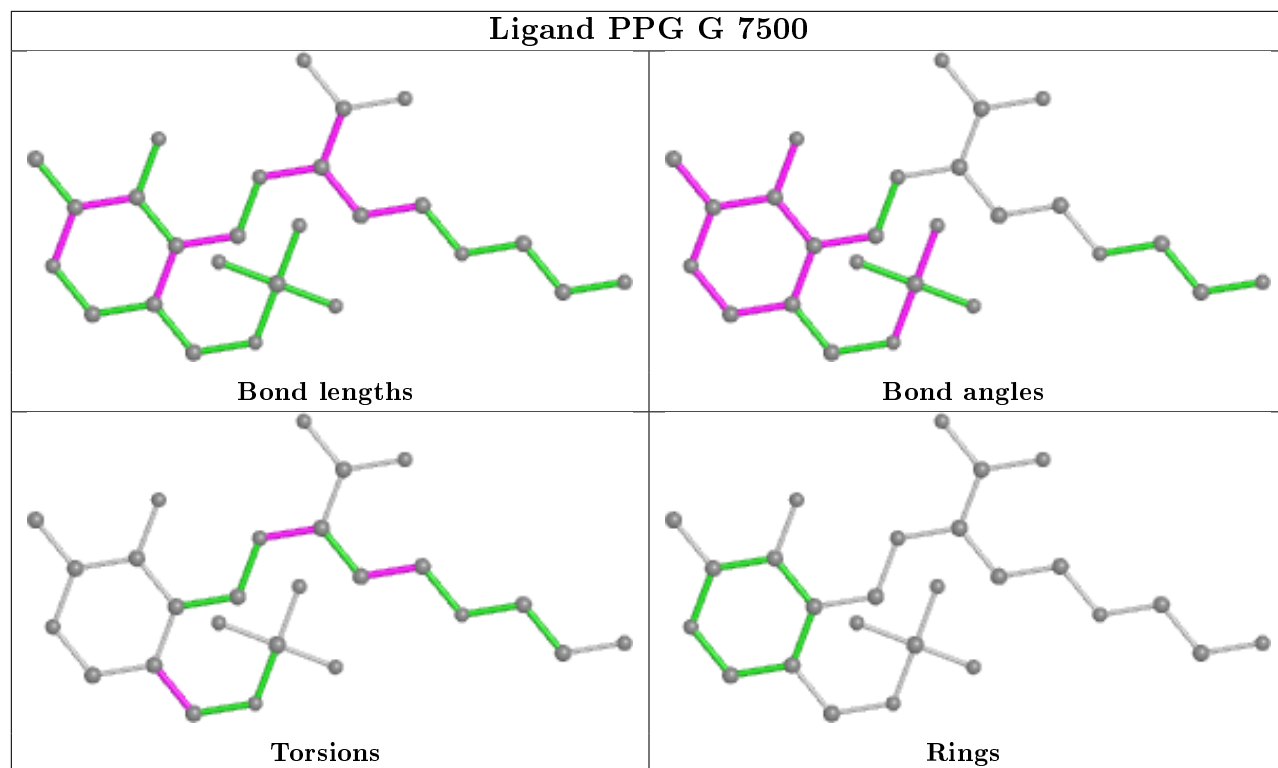
Ligand PPG H 8500



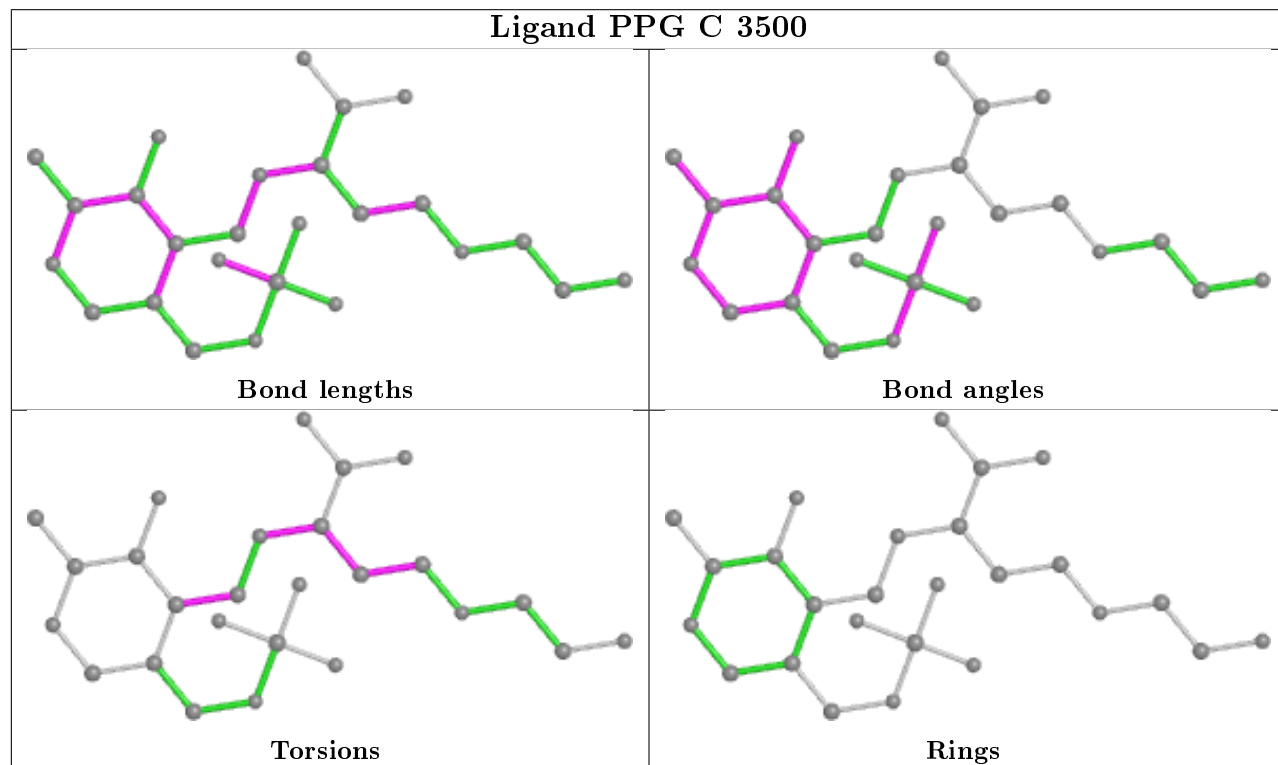
Ligand PPG B 2500



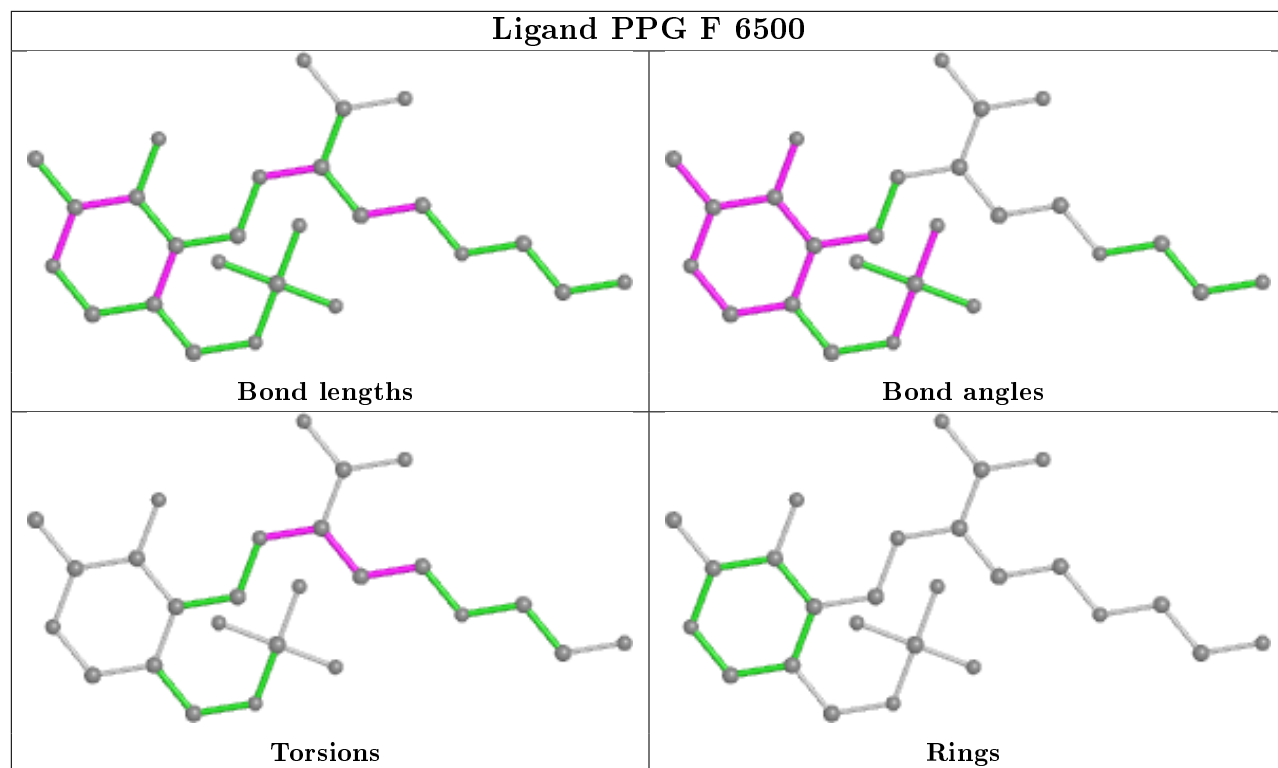
Ligand PPG G 7500



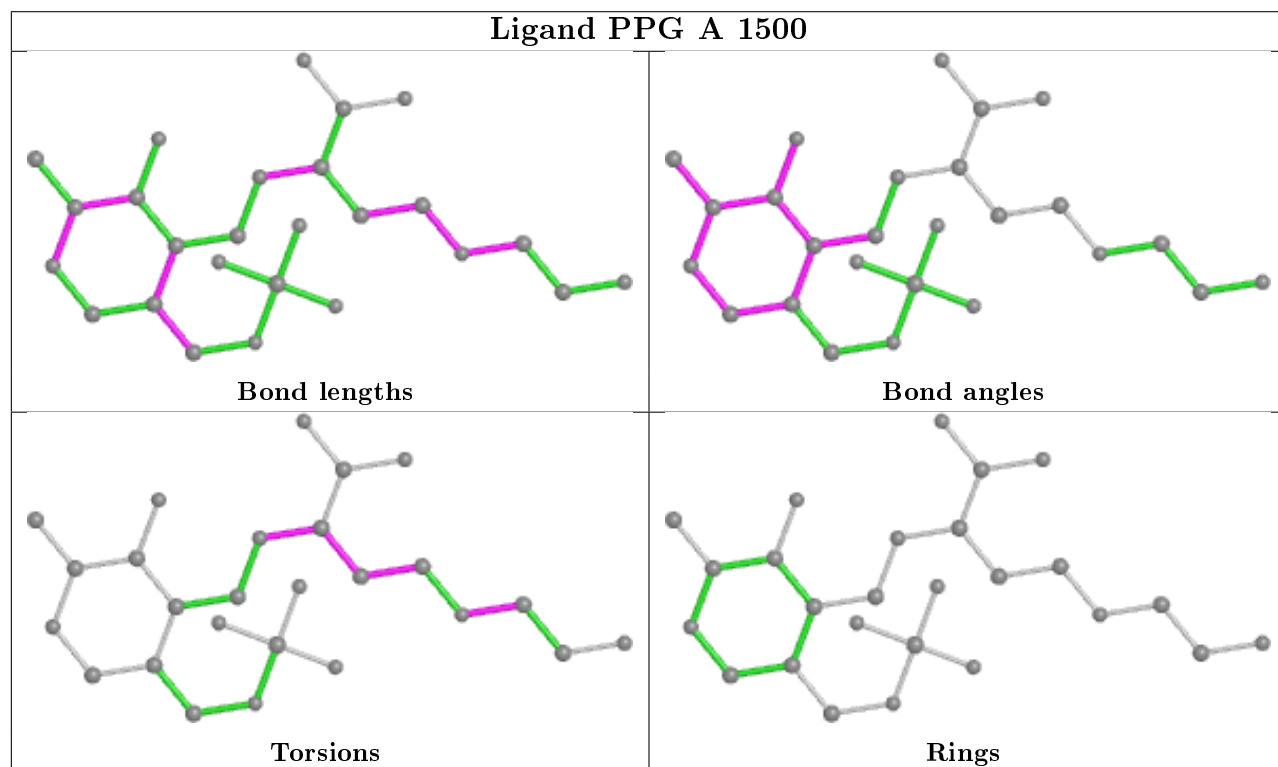
Ligand PPG C 3500

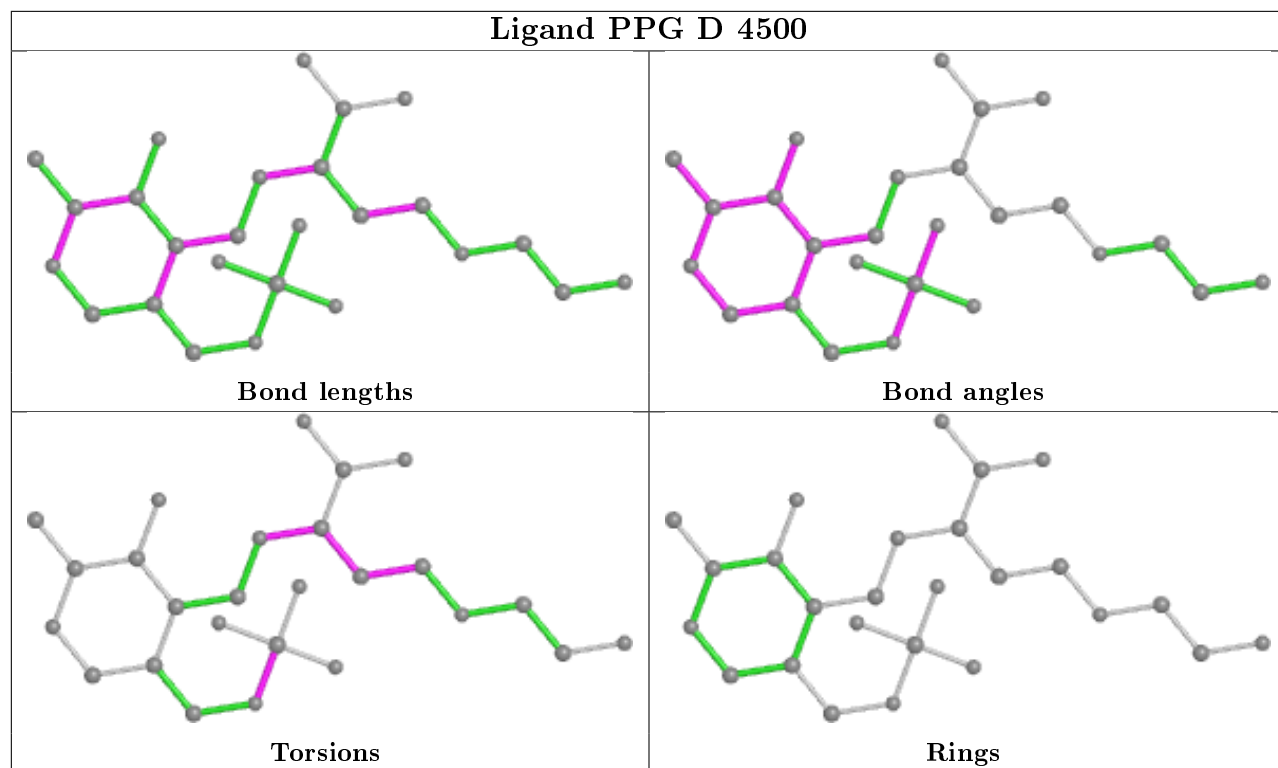


Ligand PPG F 6500



Ligand PPG A 1500





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	394/399 (98%)	-0.54	3 (0%) 86 87	19, 30, 44, 71	0
1	B	394/399 (98%)	-0.69	1 (0%) 94 94	12, 23, 36, 70	0
1	C	394/399 (98%)	-0.61	2 (0%) 91 91	17, 28, 42, 78	0
1	D	394/399 (98%)	-0.48	5 (1%) 77 79	19, 32, 48, 69	0
1	E	394/399 (98%)	-0.52	1 (0%) 94 94	18, 32, 48, 64	0
1	F	394/399 (98%)	-0.67	2 (0%) 91 91	12, 24, 38, 72	0
1	G	394/399 (98%)	-0.49	2 (0%) 91 91	19, 33, 46, 57	0
1	H	394/399 (98%)	-0.51	1 (0%) 94 94	16, 30, 47, 74	0
All	All	3152/3192 (98%)	-0.56	17 (0%) 91 91	12, 29, 45, 78	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	9.3
1	H	1	MET	5.4
1	F	1	MET	5.0
1	B	1	MET	4.7
1	A	2	ILE	4.3

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 carbohydrates in this entry.

6.4 Ligands

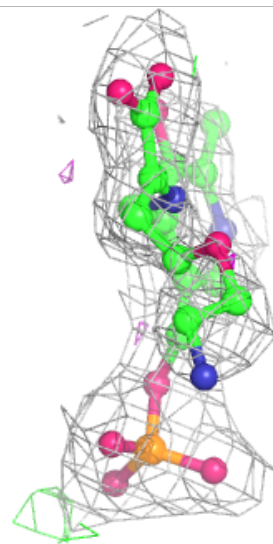
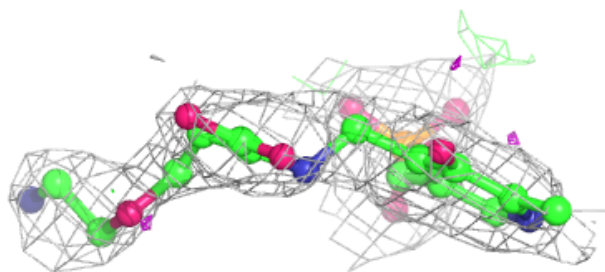
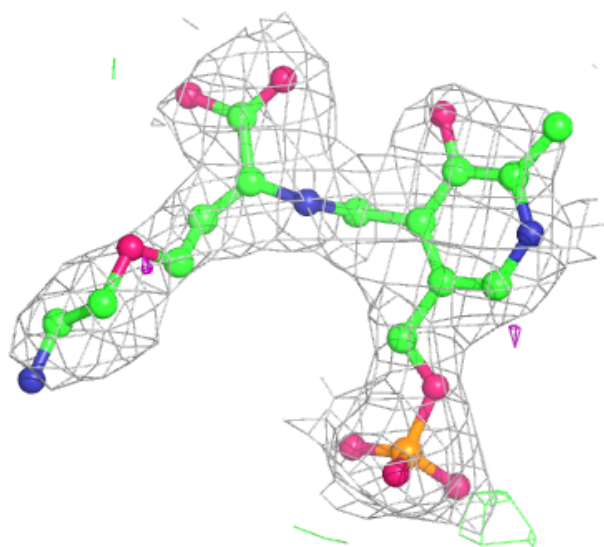
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PPG	G	7500	26/26	0.90	0.19	37,45,56,58	0
2	PPG	E	5500	26/26	0.94	0.15	28,39,52,53	0
2	PPG	D	4500	26/26	0.95	0.14	34,40,49,54	0
2	PPG	H	8500	26/26	0.96	0.14	30,35,55,55	0
2	PPG	C	3500	26/26	0.96	0.11	32,37,54,57	0
2	PPG	B	2500	26/26	0.96	0.13	27,32,47,51	0
2	PPG	A	1500	26/26	0.97	0.11	33,37,50,51	0
2	PPG	F	6500	26/26	0.97	0.12	17,26,44,45	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.

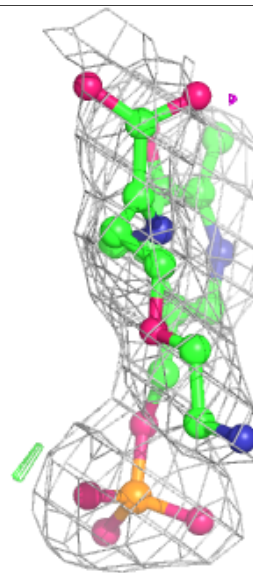
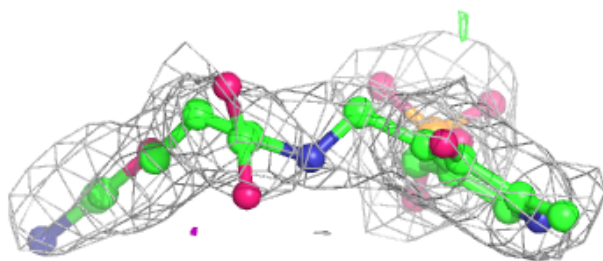
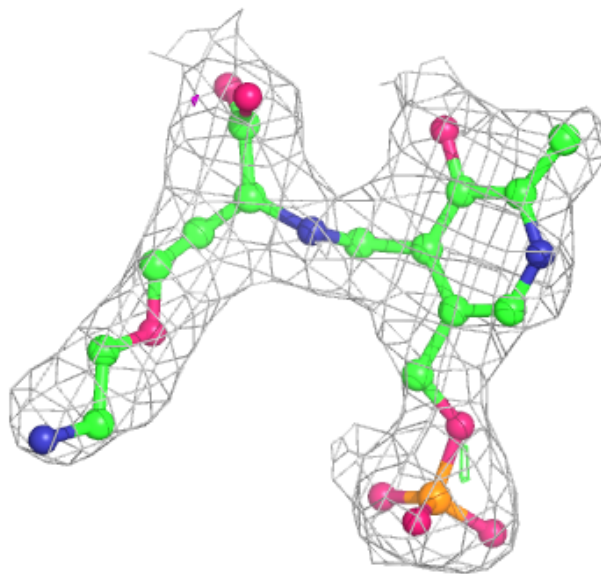
Electron density around PPG G 7500:

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



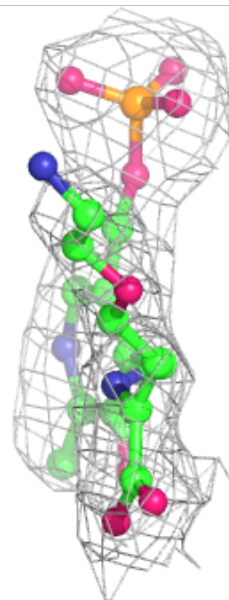
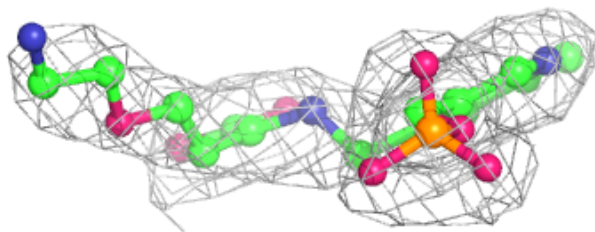
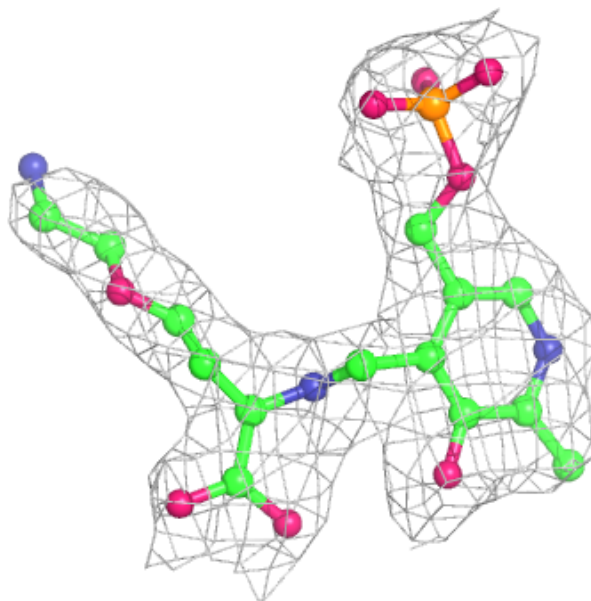
Electron density around PPG E 5500:

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



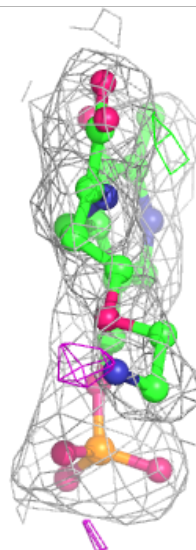
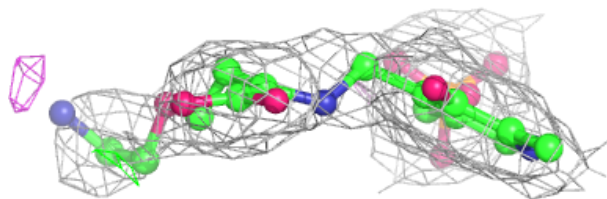
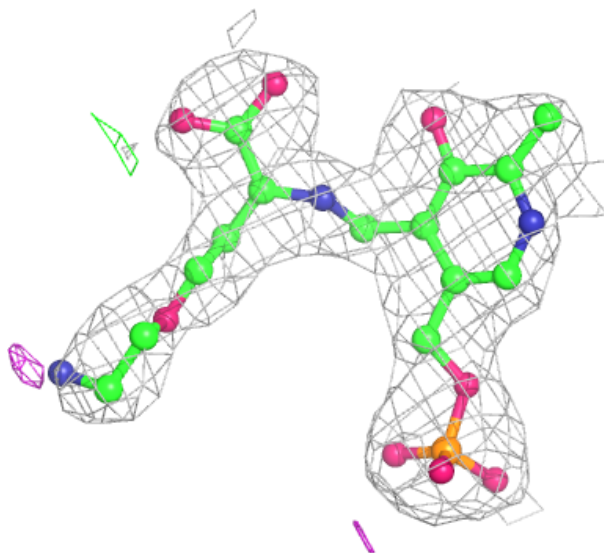
Electron density around PPG D 4500:

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



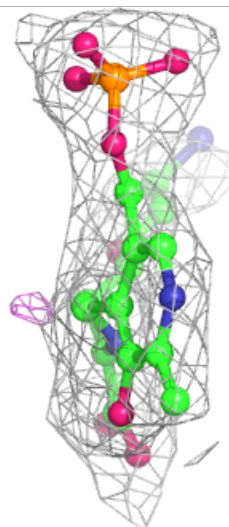
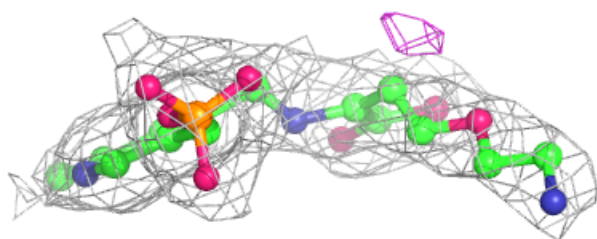
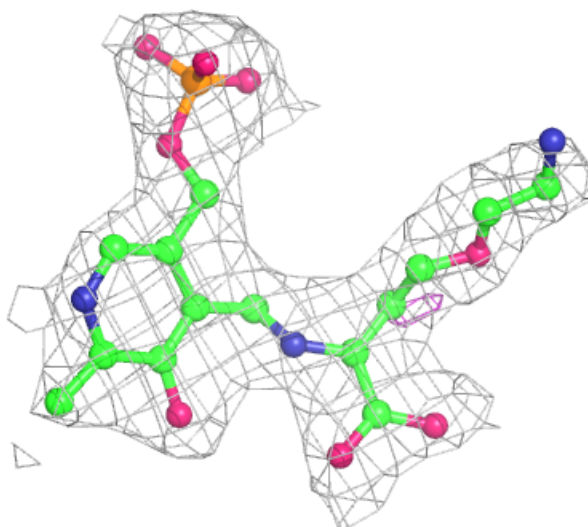
Electron density around PPG H 8500:

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



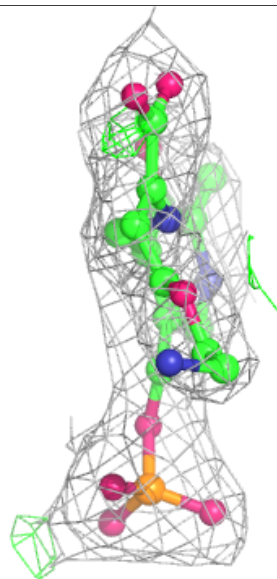
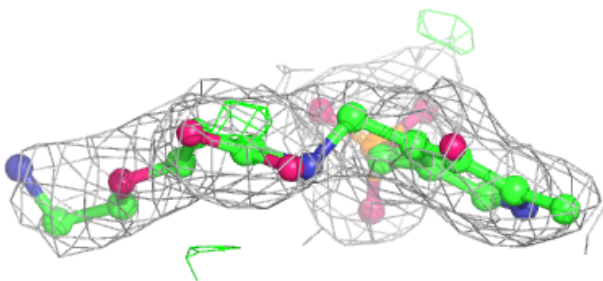
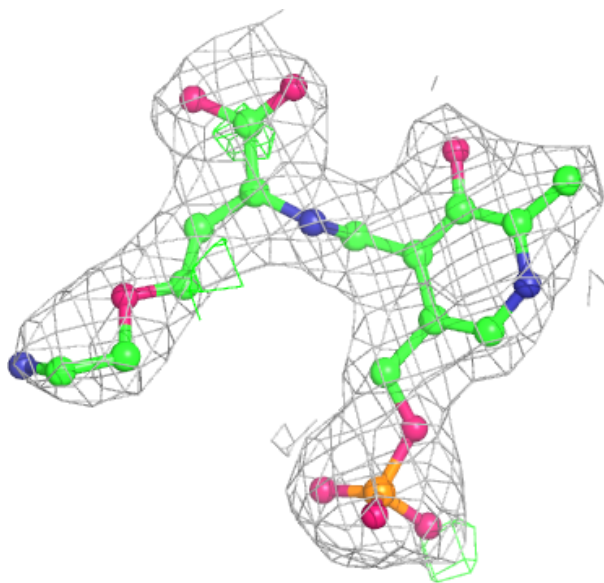
Electron density around PPG C 3500:

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



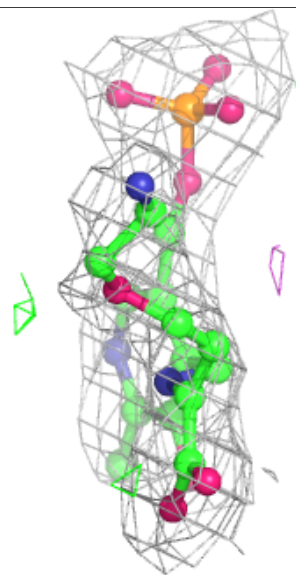
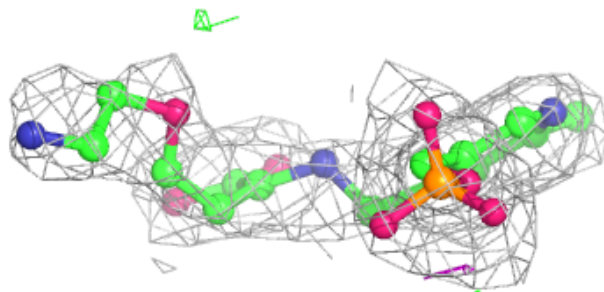
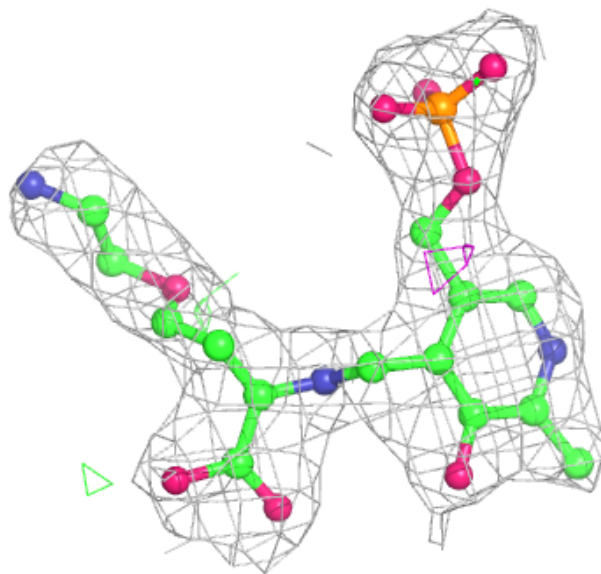
Electron density around PPG B 2500:

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



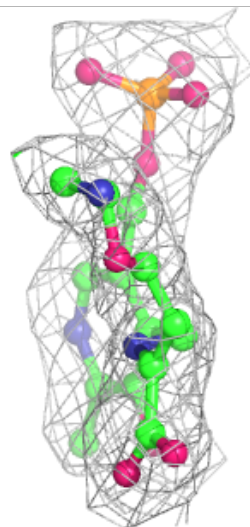
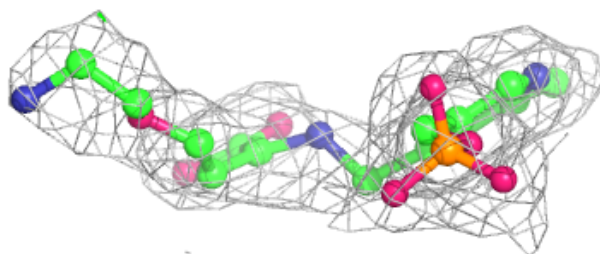
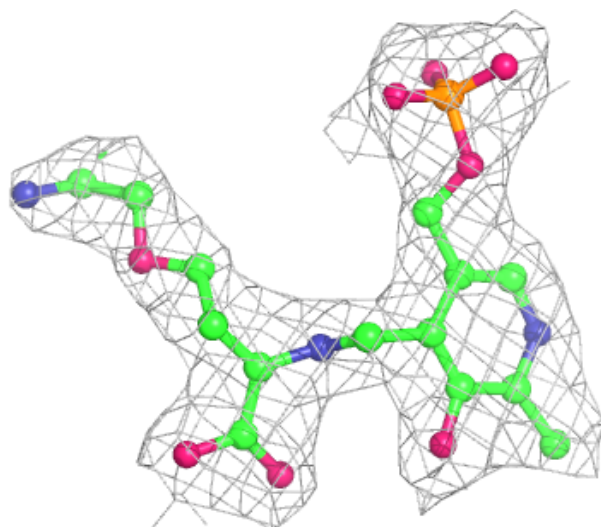
Electron density around PPG A 1500:

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



Electron density around PPG F 6500:

$2mF_o-DF_c$ (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.