



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:01 am BST

PDB ID : 1UPC  
Title : Carboxyethylarginine synthase from *Streptomyces clavuligerus*  
Authors : Caines, M.E.C.; Elkins, J.M.; Hewitson, K.S.; Schofield, C.J.  
Deposited on : 2003-09-29  
Resolution : 2.45 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](mailto: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.

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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

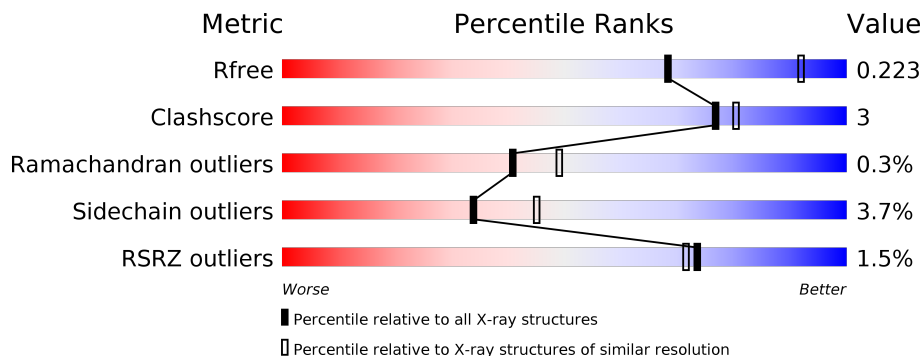
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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  $\geq 3$ , 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	573	 87% 9% ..
1	B	573	 89% 7% ..
1	C	573	 88% 8% ..
1	D	573	 89% 8% ..
1	E	573	 88% 8% ..
1	F	573	 88% 8% ..

## 2 Entry composition [i](#)

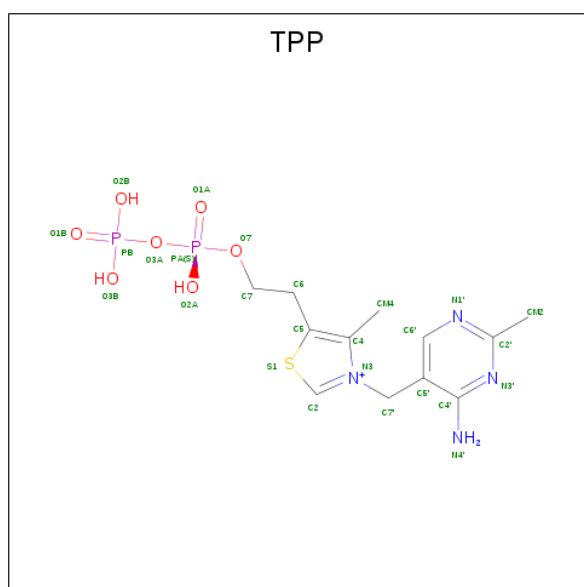
There are 5 unique types of molecules in this entry. The entry contains 26083 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CARBOXYETHYLARGININE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	559	Total 4172	C 2649	N 721	O 789	S 13	0	0	0
1	B	559	Total 4182	C 2653	N 723	O 793	S 13	0	0	0
1	C	557	Total 4149	C 2635	N 718	O 783	S 13	0	0	0
1	D	559	Total 4174	C 2649	N 722	O 790	S 13	0	0	0
1	E	558	Total 4169	C 2646	N 721	O 789	S 13	0	0	0
1	F	558	Total 4163	C 2643	N 718	O 789	S 13	0	0	0

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	E	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	F	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

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

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0

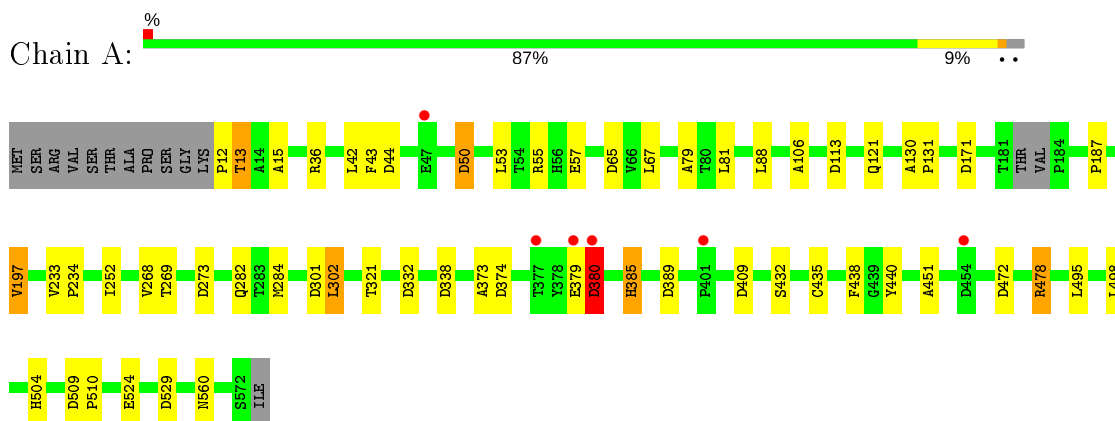
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	139	Total O 139 139	0	0
5	B	185	Total O 185 185	0	0
5	C	118	Total O 118 118	0	0
5	D	157	Total O 157 157	0	0
5	E	117	Total O 117 117	0	0
5	F	136	Total O 136 136	0	0

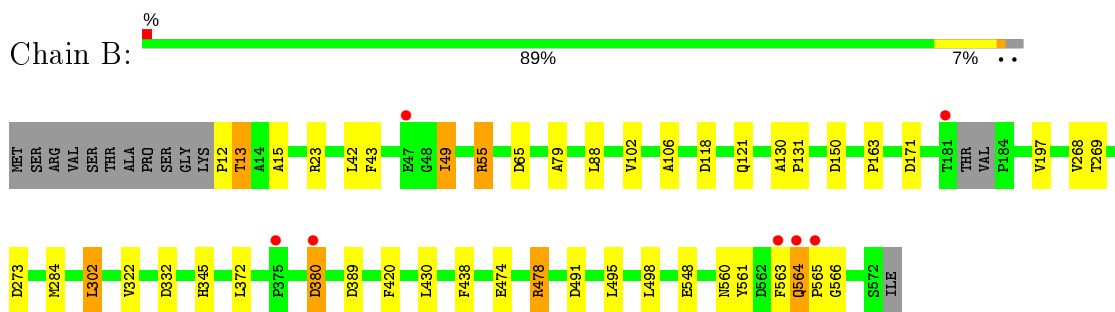
### 3 Residue-property plots [i](#)

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.

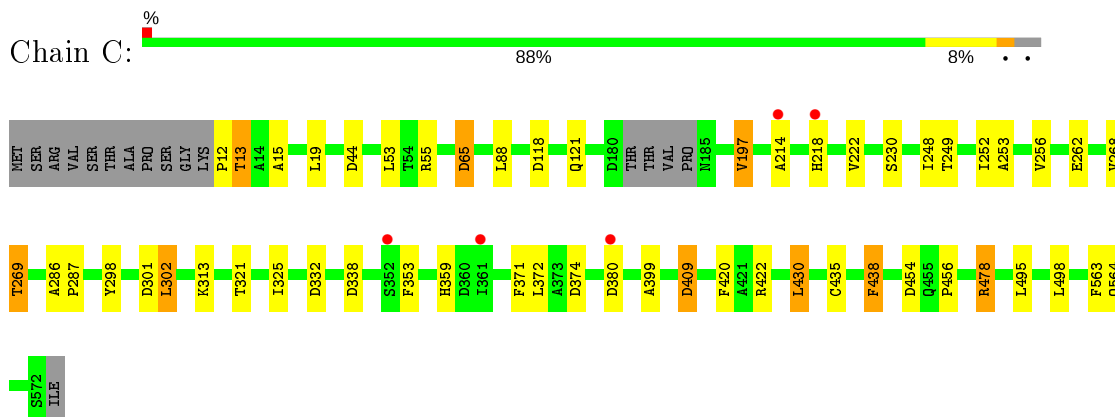
- Molecule 1: CARBOXYETHYLARGININE SYNTHASE



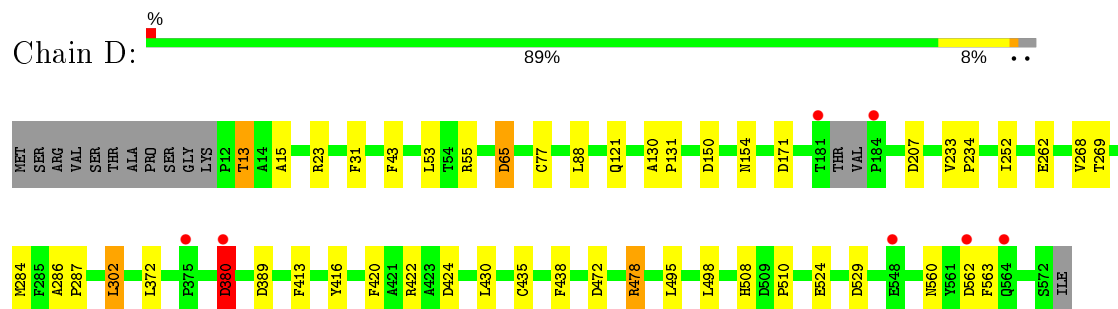
- Molecule 1: CARBOXYETHYLARGININE SYNTHASE



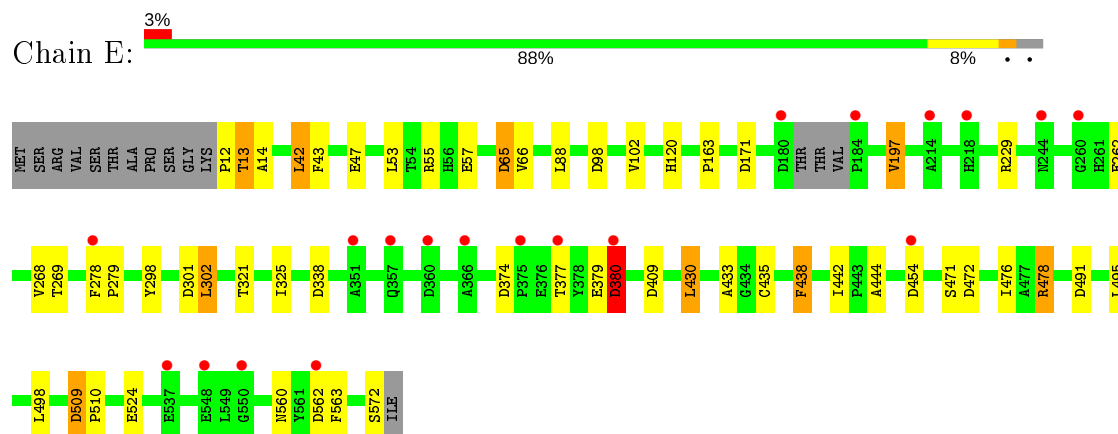
- Molecule 1: CARBOXYETHYLARGININE SYNTHASE



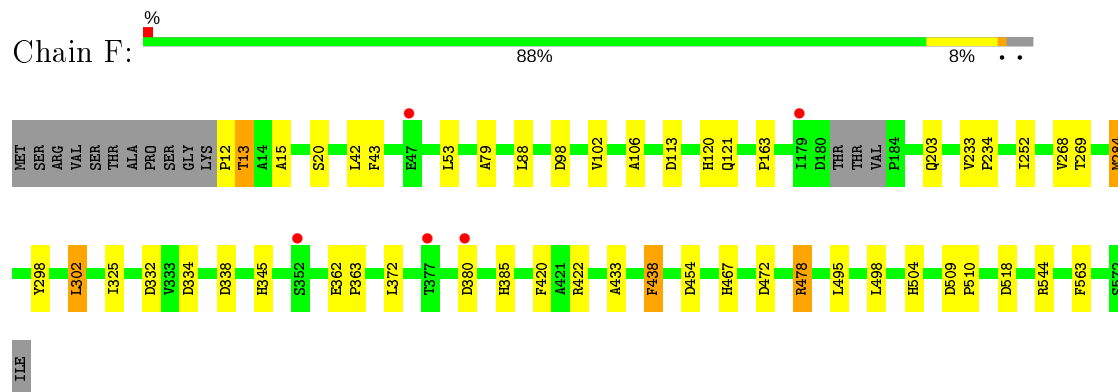
- Molecule 1: CARBOXYETHYLARGININE SYNTHASE



- Molecule 1: CARBOXYETHYLARGININE SYNTHASE



- Molecule 1: CARBOXYETHYLARGININE SYNTHASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.07Å 187.20Å 198.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.00 – 2.45 35.05 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.00-2.45) 99.8 (35.05-2.45)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 2.45Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.176 , 0.216 0.185 , 0.223	Depositor DCC
$R_{free}$ test set	8434 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtrriage
Anisotropy	0.400	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 34.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	26083	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, SO4, TPP

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	0.66	0/4267	0.86	14/5827 (0.2%)
1	B	0.67	0/4277	0.87	12/5840 (0.2%)
1	C	0.68	0/4243	0.83	9/5796 (0.2%)
1	D	0.65	0/4269	0.85	12/5830 (0.2%)
1	E	0.68	0/4264	0.85	15/5823 (0.3%)
1	F	0.66	0/4258	0.83	11/5816 (0.2%)
All	All	0.67	0/25578	0.85	73/34932 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	E	0	1
1	F	0	1
All	All	0	5

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	478	ARG	NE-CZ-NH1	-10.61	115.00	120.30
1	B	478	ARG	NE-CZ-NH2	9.60	125.10	120.30
1	E	301	ASP	CB-CG-OD2	8.97	126.37	118.30
1	D	55	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	D	55	ARG	NE-CZ-NH1	8.20	124.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	478	ARG	NE-CZ-NH1	-8.09	116.25	120.30
1	D	478	ARG	NE-CZ-NH2	7.99	124.30	120.30
1	E	478	ARG	NE-CZ-NH2	7.95	124.28	120.30
1	B	55	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	F	478	ARG	NE-CZ-NH1	-7.55	116.52	120.30
1	F	478	ARG	NE-CZ-NH2	7.25	123.93	120.30
1	A	478	ARG	NE-CZ-NH1	-7.09	116.75	120.30
1	E	478	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	A	478	ARG	NE-CZ-NH2	6.73	123.67	120.30
1	E	338	ASP	CB-CG-OD2	6.67	124.30	118.30
1	C	65	ASP	CB-CG-OD2	6.46	124.11	118.30
1	A	113	ASP	CB-CG-OD2	6.41	124.07	118.30
1	B	65	ASP	CB-CG-OD2	6.40	124.06	118.30
1	C	118	ASP	CB-CG-OD2	6.22	123.90	118.30
1	E	98	ASP	CB-CG-OD2	6.21	123.89	118.30
1	E	562	ASP	CB-CG-OD2	6.17	123.86	118.30
1	C	301	ASP	CB-CG-OD2	6.16	123.84	118.30
1	F	332	ASP	CB-CG-OD2	6.13	123.82	118.30
1	F	98	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	50	ASP	CB-CG-OD2	6.04	123.74	118.30
1	E	472	ASP	CB-CG-OD2	6.04	123.73	118.30
1	E	171	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	338	ASP	CB-CG-OD2	6.02	123.72	118.30
1	E	55	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	171	ASP	CB-CG-OD2	5.99	123.69	118.30
1	D	171	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	118	ASP	CB-CG-OD2	5.98	123.68	118.30
1	C	454	ASP	CB-CG-OD2	5.97	123.67	118.30
1	F	454	ASP	CB-CG-OD2	5.89	123.60	118.30
1	C	332	ASP	CB-CG-OD2	5.88	123.60	118.30
1	C	55	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	E	65	ASP	CB-CG-OD2	5.80	123.52	118.30
1	D	472	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	65	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	332	ASP	CB-CG-OD2	5.69	123.42	118.30
1	F	472	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	273	ASP	CB-CG-OD2	5.67	123.40	118.30
1	D	529	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	389	ASP	CB-CG-OD2	5.61	123.35	118.30
1	E	229	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	F	338	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	332	ASP	CB-CG-OD2	5.52	123.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	454	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	338	ASP	CB-CG-OD2	5.50	123.25	118.30
1	E	374	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	529	ASP	CB-CG-OD2	5.47	123.22	118.30
1	B	491	ASP	CB-CG-OD2	5.45	123.20	118.30
1	F	518	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	409	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	301	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	544	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	273	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	207	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	409	ASP	CB-CG-OD2	5.20	122.98	118.30
1	E	491	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	389	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	36	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	171	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	389	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	55	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	150	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	150	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	478	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	F	334	ASP	CB-CG-OD2	5.06	122.86	118.30
1	E	509	ASP	CB-CG-OD1	5.05	122.84	118.30
1	D	424	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	472	ASP	CB-CG-OD2	5.02	122.82	118.30
1	F	113	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	PRO	Peptide
1	B	12	PRO	Peptide
1	C	12	PRO	Peptide
1	E	12	PRO	Peptide
1	F	12	PRO	Peptide

## 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	4172	0	4110	23	0
1	B	4182	0	4118	20	0
1	C	4149	0	4083	24	0
1	D	4174	0	4108	17	0
1	E	4169	0	4106	22	0
1	F	4163	0	4095	27	0
2	A	26	0	16	5	0
2	B	26	0	16	7	0
2	C	26	0	16	5	0
2	D	26	0	16	4	0
2	E	26	0	16	6	0
2	F	26	0	16	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	10	0	0	1	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	10	0	0	0	0
4	F	10	0	0	0	0
5	A	139	0	0	1	0
5	B	185	0	0	4	0
5	C	118	0	0	3	0
5	D	157	0	0	1	0
5	E	117	0	0	1	0
5	F	136	0	0	2	0
All	All	26083	0	24716	148	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 (148) 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:A:600:TPP:HN42	2:A:600:TPP:C2	1.41	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:600:TPP:HN42	2:F:600:TPP:C2	1.44	1.31
2:B:600:TPP:C2	2:B:600:TPP:HN42	1.45	1.27
2:C:600:TPP:HN42	2:C:600:TPP:C2	1.50	1.24
2:E:600:TPP:C2	2:E:600:TPP:HN42	1.54	1.21
2:D:600:TPP:HN42	2:D:600:TPP:C2	1.52	1.20
2:A:600:TPP:N4'	2:A:600:TPP:C2	2.11	1.14
2:C:600:TPP:H2	2:C:600:TPP:HN42	1.04	1.13
2:E:600:TPP:HN42	2:E:600:TPP:H2	1.03	1.11
2:F:600:TPP:H2	2:F:600:TPP:HN42	1.02	1.10
2:A:600:TPP:H2	2:A:600:TPP:HN42	0.99	1.09
2:B:600:TPP:HN42	2:B:600:TPP:H2	1.12	1.08
2:F:600:TPP:N4'	2:F:600:TPP:C2	2.16	1.08
2:D:600:TPP:HN42	2:D:600:TPP:H2	1.12	1.05
2:C:600:TPP:C2	2:C:600:TPP:N4'	2.17	1.05
2:B:600:TPP:C2	2:B:600:TPP:N4'	2.18	1.04
2:E:600:TPP:N4'	2:E:600:TPP:C2	2.20	1.03
2:D:600:TPP:C2	2:D:600:TPP:N4'	2.22	1.01
1:B:13:THR:HG21	5:B:2007:HOH:O	1.74	0.88
2:C:600:TPP:H2	2:C:600:TPP:N4'	1.87	0.84
2:E:600:TPP:N4'	2:E:600:TPP:H2	1.88	0.84
1:C:13:THR:HG21	5:C:2008:HOH:O	1.83	0.78
2:A:600:TPP:N4'	2:A:600:TPP:H2	1.84	0.78
2:F:600:TPP:H2	2:F:600:TPP:N4'	1.86	0.78
1:F:13:THR:HG21	5:F:2006:HOH:O	1.85	0.77
1:E:13:THR:HG21	5:E:2008:HOH:O	1.87	0.74
2:D:600:TPP:H2	2:D:600:TPP:N4'	1.94	0.71
1:A:385:HIS:H	1:A:385:HIS:CD2	2.09	0.68
2:B:600:TPP:H2	2:B:600:TPP:N4'	1.95	0.67
1:C:252:ILE:HG12	5:C:2076:HOH:O	1.99	0.62
1:F:268:VAL:HB	1:F:302:LEU:HD22	1.82	0.61
1:E:53:LEU:O	1:E:478:ARG:NH1	2.34	0.60
1:F:53:LEU:O	1:F:478:ARG:NH1	2.35	0.59
1:D:380:ASP:HB2	1:D:560:ASN:OD1	2.03	0.58
1:A:79:ALA:O	1:A:106:ALA:HA	2.03	0.57
1:A:268:VAL:HB	1:A:302:LEU:HD22	1.87	0.57
2:E:600:TPP:C4'	2:E:600:TPP:C2	2.82	0.57
1:C:268:VAL:HB	1:C:302:LEU:HD22	1.86	0.57
1:E:438:PHE:CE1	2:E:600:TPP:HM23	2.41	0.56
1:A:560:ASN:ND2	4:A:603:SO4:O2	2.35	0.56
1:B:268:VAL:HB	1:B:302:LEU:HD22	1.88	0.56
1:C:44:ASP:HB3	1:D:508:HIS:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:GLU:OE2	1:B:478:ARG:HD3	2.06	0.55
1:A:233:VAL:HB	1:A:234:PRO:HD3	1.88	0.55
1:F:268:VAL:HG22	1:F:284:MET:CE	2.36	0.54
1:C:218:HIS:ND1	1:C:359:HIS:HB3	2.21	0.54
1:B:345:HIS:CE1	5:B:2128:HOH:O	2.60	0.54
1:E:471:SER:HB3	1:F:467:HIS:CD2	2.42	0.54
1:E:442:ILE:HG23	1:E:476:ILE:HD11	1.90	0.54
1:C:298:TYR:CG	1:C:325:ILE:HD13	2.43	0.54
1:B:561:TYR:OH	2:B:600:TPP:O1B	2.20	0.53
1:D:372:LEU:HD21	1:D:420:PHE:HB3	1.89	0.53
1:E:435:CYS:O	1:F:121:GLN:HG2	2.08	0.53
1:B:564:GLN:O	1:B:566:GLY:N	2.42	0.52
1:A:53:LEU:O	1:A:478:ARG:NH1	2.35	0.51
1:B:322:VAL:HG11	1:D:154:ASN:HB3	1.92	0.51
1:B:102:VAL:O	1:B:163:PRO:HA	2.11	0.50
1:D:508:HIS:CD2	1:D:510:PRO:HD2	2.47	0.50
1:F:372:LEU:HD21	1:F:420:PHE:HB3	1.93	0.50
1:C:222:VAL:HA	1:C:248:ILE:O	2.12	0.50
1:A:385:HIS:H	1:A:385:HIS:HD2	1.57	0.50
1:E:42:LEU:HG	1:F:504:HIS:ND1	2.26	0.50
1:A:435:CYS:O	1:B:121:GLN:HG2	2.12	0.49
1:C:372:LEU:HD21	1:C:420:PHE:HB3	1.95	0.49
1:D:252:ILE:HG12	5:D:2079:HOH:O	2.12	0.49
1:F:509:ASP:N	1:F:510:PRO:CD	2.75	0.49
1:C:399:ALA:HB2	1:C:456:PRO:HG2	1.95	0.49
1:B:372:LEU:HD21	1:B:420:PHE:HB3	1.94	0.48
1:D:268:VAL:HB	1:D:302:LEU:HD22	1.95	0.48
1:C:53:LEU:O	1:C:478:ARG:NH1	2.44	0.48
1:D:53:LEU:O	1:D:478:ARG:NH1	2.37	0.48
1:E:197:VAL:CG2	1:E:321:THR:HA	2.43	0.48
1:C:13:THR:HG22	1:C:15:ALA:HB3	1.96	0.48
1:E:120:HIS:ND1	1:F:433:ALA:O	2.47	0.47
1:E:102:VAL:O	1:E:163:PRO:HA	2.14	0.47
1:D:233:VAL:HB	1:D:234:PRO:HD3	1.96	0.47
1:A:55:ARG:HD2	5:B:2155:HOH:O	2.14	0.47
1:D:13:THR:HG22	1:D:15:ALA:HB3	1.96	0.47
1:A:432:SER:HB2	1:A:440:TYR:CE1	2.50	0.46
1:C:121:GLN:HG2	1:D:435:CYS:O	2.15	0.46
1:E:509:ASP:N	1:E:510:PRO:CD	2.78	0.46
1:F:252:ILE:HG12	5:F:2078:HOH:O	2.15	0.46
1:B:79:ALA:O	1:B:106:ALA:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:LEU:O	1:E:43:PHE:HB2	2.16	0.46
1:C:214:ALA:HB2	1:C:353:PHE:CZ	2.51	0.45
2:B:600:TPP:N4'	2:B:600:TPP:N3	2.59	0.45
1:C:286:ALA:HB3	1:C:287:PRO:HD3	1.98	0.45
1:F:385:HIS:CD2	1:F:385:HIS:H	2.34	0.45
1:D:130:ALA:N	1:D:131:PRO:CD	2.79	0.45
1:D:13:THR:HG23	1:D:15:ALA:H	1.80	0.45
1:B:380:ASP:N	1:B:380:ASP:OD1	2.49	0.45
1:E:433:ALA:O	1:F:120:HIS:ND1	2.49	0.45
1:C:268:VAL:HG12	1:C:269:THR:N	2.30	0.45
1:F:13:THR:HG23	1:F:15:ALA:H	1.82	0.45
1:E:13:THR:HG23	1:E:14:ALA:N	2.32	0.44
1:F:102:VAL:O	1:F:163:PRO:HA	2.17	0.44
1:E:66:VAL:HG21	1:E:444:ALA:HA	1.99	0.44
1:B:49:ILE:HG22	5:B:2009:HOH:O	2.17	0.44
1:A:67:LEU:HD12	1:A:451:ALA:HB2	2.00	0.44
1:C:253:ALA:O	1:C:256:VAL:HG13	2.17	0.43
1:D:413:PHE:O	1:D:416:TYR:HB2	2.18	0.43
1:A:57:GLU:OE2	2:B:600:TPP:N1'	2.52	0.43
1:E:268:VAL:HB	1:E:302:LEU:HD22	2.01	0.43
1:E:298:TYR:CG	1:E:325:ILE:HD13	2.54	0.43
1:C:13:THR:CG2	1:C:15:ALA:H	2.31	0.43
1:A:42:LEU:O	1:A:43:PHE:HB2	2.18	0.43
1:A:81:LEU:HG	1:A:121:GLN:HB3	2.00	0.43
1:F:362:GLU:N	1:F:363:PRO:CD	2.81	0.43
1:F:42:LEU:O	1:F:43:PHE:HB2	2.19	0.43
1:E:120:HIS:CE1	1:F:433:ALA:O	2.72	0.42
1:C:438:PHE:CE1	2:C:600:TPP:HM23	2.54	0.42
1:F:268:VAL:HG22	1:F:284:MET:HE2	1.99	0.42
1:B:13:THR:HG22	1:B:15:ALA:HB3	2.00	0.42
1:F:298:TYR:CG	1:F:325:ILE:HD13	2.54	0.42
5:A:2114:HOH:O	1:B:55:ARG:HD2	2.19	0.42
1:D:31:PHE:O	1:D:77:CYS:HA	2.20	0.42
1:F:345:HIS:O	1:F:345:HIS:HD2	2.01	0.42
1:E:57:GLU:OE2	2:F:600:TPP:N1'	2.52	0.42
1:F:233:VAL:HB	1:F:234:PRO:HD3	2.01	0.42
1:A:282:GLN:HE21	1:A:282:GLN:HB3	1.70	0.42
1:C:197:VAL:HG22	5:C:2059:HOH:O	2.19	0.42
2:A:600:TPP:C2	2:A:600:TPP:C4'	2.82	0.42
1:F:438:PHE:CE1	2:F:600:TPP:HM23	2.55	0.42
1:A:197:VAL:CG2	1:A:321:THR:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:GLU:O	1:A:380:ASP:O	2.38	0.41
1:B:130:ALA:N	1:B:131:PRO:CD	2.83	0.41
1:C:249:THR:HB	1:C:253:ALA:HB3	2.01	0.41
1:F:13:THR:CG2	1:F:15:ALA:HB3	2.50	0.41
1:F:345:HIS:CD2	1:F:345:HIS:O	2.73	0.41
1:C:19:LEU:HD23	1:C:19:LEU:HA	1.90	0.41
1:C:430:LEU:HA	1:C:430:LEU:HD12	1.93	0.41
1:E:380:ASP:HB2	1:E:560:ASN:OD1	2.20	0.41
1:A:13:THR:HG22	1:A:15:ALA:HB3	2.01	0.41
1:E:278:PHE:CG	1:E:279:PRO:HD2	2.55	0.41
1:A:44:ASP:OD1	1:A:44:ASP:C	2.59	0.41
1:A:509:ASP:N	1:A:510:PRO:CD	2.83	0.41
1:C:197:VAL:CG2	1:C:321:THR:HA	2.50	0.41
1:A:373:ALA:O	1:A:374:ASP:C	2.59	0.41
1:E:430:LEU:HD12	1:E:430:LEU:HA	1.97	0.41
1:A:504:HIS:CG	1:B:42:LEU:HG	2.56	0.41
1:D:286:ALA:N	1:D:287:PRO:CD	2.83	0.41
1:A:130:ALA:N	1:A:131:PRO:CD	2.83	0.40
1:B:42:LEU:O	1:B:43:PHE:HB2	2.21	0.40
1:B:380:ASP:HB2	1:B:560:ASN:OD1	2.21	0.40
1:C:435:CYS:O	1:D:121:GLN:HG2	2.21	0.40
1:F:79:ALA:O	1:F:106:ALA:HA	2.21	0.40
1:F:203:GLN:HB3	1:F:345:HIS:HE1	1.86	0.40
1:B:13:THR:HG23	1:B:15:ALA:H	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	555/573 (97%)	533 (96%)	21 (4%)	1 (0%)	47 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	555/573 (97%)	539 (97%)	15 (3%)	1 (0%)	47	57
1	C	553/573 (96%)	532 (96%)	19 (3%)	2 (0%)	34	41
1	D	555/573 (97%)	539 (97%)	14 (2%)	2 (0%)	34	41
1	E	554/573 (97%)	532 (96%)	19 (3%)	3 (0%)	29	34
1	F	554/573 (97%)	539 (97%)	15 (3%)	0	100	100
All	All	3326/3438 (97%)	3214 (97%)	103 (3%)	9 (0%)	41	49

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	ASP
1	B	565	PRO
1	D	380	ASP
1	E	409	ASP
1	E	379	GLU
1	C	409	ASP
1	D	43	PHE
1	E	380	ASP
1	C	374	ASP

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	434/452 (96%)	418 (96%)	16 (4%)	34	45
1	B	436/452 (96%)	420 (96%)	16 (4%)	34	45
1	C	430/452 (95%)	412 (96%)	18 (4%)	30	39
1	D	434/452 (96%)	417 (96%)	17 (4%)	32	42
1	E	434/452 (96%)	416 (96%)	18 (4%)	30	40
1	F	433/452 (96%)	421 (97%)	12 (3%)	43	56
All	All	2601/2712 (96%)	2504 (96%)	97 (4%)	34	45

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	50	ASP
1	A	65	ASP
1	A	88	LEU
1	A	187	PRO
1	A	197	VAL
1	A	252	ILE
1	A	269	THR
1	A	284	MET
1	A	302	LEU
1	A	380	ASP
1	A	385	HIS
1	A	438	PHE
1	A	495	LEU
1	A	498	LEU
1	A	524	GLU
1	B	13	THR
1	B	23	ARG
1	B	49	ILE
1	B	88	LEU
1	B	197	VAL
1	B	269	THR
1	B	284	MET
1	B	302	LEU
1	B	380	ASP
1	B	430	LEU
1	B	438	PHE
1	B	495	LEU
1	B	498	LEU
1	B	548	GLU
1	B	563	PHE
1	B	564	GLN
1	C	13	THR
1	C	65	ASP
1	C	88	LEU
1	C	197	VAL
1	C	230	SER
1	C	262	GLU
1	C	269	THR
1	C	302	LEU
1	C	313	LYS
1	C	371	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	380	ASP
1	C	422	ARG
1	C	430	LEU
1	C	438	PHE
1	C	495	LEU
1	C	498	LEU
1	C	563	PHE
1	C	564	GLN
1	D	13	THR
1	D	23	ARG
1	D	65	ASP
1	D	88	LEU
1	D	262	GLU
1	D	269	THR
1	D	284	MET
1	D	302	LEU
1	D	380	ASP
1	D	422	ARG
1	D	430	LEU
1	D	438	PHE
1	D	495	LEU
1	D	498	LEU
1	D	524	GLU
1	D	562	ASP
1	D	563	PHE
1	E	13	THR
1	E	42	LEU
1	E	47	GLU
1	E	65	ASP
1	E	88	LEU
1	E	197	VAL
1	E	262	GLU
1	E	269	THR
1	E	302	LEU
1	E	377	THR
1	E	380	ASP
1	E	430	LEU
1	E	438	PHE
1	E	495	LEU
1	E	498	LEU
1	E	524	GLU
1	E	563	PHE

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Mol	Chain	Res	Type
1	E	572	SER
1	F	13	THR
1	F	20	SER
1	F	88	LEU
1	F	269	THR
1	F	284	MET
1	F	302	LEU
1	F	380	ASP
1	F	422	ARG
1	F	438	PHE
1	F	495	LEU
1	F	498	LEU
1	F	563	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	277	ASN
1	A	282	GLN
1	A	308	GLN
1	A	359	HIS
1	A	385	HIS
1	A	504	HIS
1	B	140	GLN
1	B	282	GLN
1	B	308	GLN
1	C	308	GLN
1	C	385	HIS
1	C	504	HIS
1	D	16	HIS
1	D	112	HIS
1	D	282	GLN
1	D	308	GLN
1	D	504	HIS
1	E	282	GLN
1	E	308	GLN
1	E	385	HIS
1	F	282	GLN
1	F	308	GLN
1	F	345	HIS
1	F	385	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	E	602	-	4,4,4	0.34	0	6,6,6	0.77	0
2	TPP	A	600	3	22,27,27	2.10	6 (27%)	29,40,40	2.47	9 (31%)
4	SO4	F	602	-	4,4,4	0.33	0	6,6,6	0.51	0
2	TPP	F	600	3	22,27,27	1.87	6 (27%)	29,40,40	2.24	8 (27%)
4	SO4	D	602	-	4,4,4	0.22	0	6,6,6	0.55	0
2	TPP	D	600	3	22,27,27	1.94	8 (36%)	29,40,40	2.25	7 (24%)
4	SO4	B	602	-	4,4,4	0.23	0	6,6,6	0.58	0
4	SO4	A	602	-	4,4,4	0.31	0	6,6,6	0.41	0
4	SO4	C	602	-	4,4,4	0.28	0	6,6,6	0.44	0
4	SO4	E	603	-	4,4,4	0.15	0	6,6,6	0.17	0
4	SO4	F	603	-	4,4,4	0.13	0	6,6,6	0.22	0
4	SO4	C	603	-	4,4,4	0.16	0	6,6,6	0.22	0
4	SO4	A	603	-	4,4,4	0.13	0	6,6,6	0.35	0
4	SO4	B	603	-	4,4,4	0.17	0	6,6,6	0.21	0
2	TPP	E	600	3	22,27,27	2.08	6 (27%)	29,40,40	2.48	10 (34%)
2	TPP	C	600	3	22,27,27	1.89	5 (22%)	29,40,40	2.33	7 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	D	603	-	4,4,4	0.12	0	6,6,6	0.37	0
2	TPP	B	600	3	22,27,27	1.88	6 (27%)	29,40,40	2.20	7 (24%)

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	TPP	F	600	3	-	4/16/17/17	0/2/2/2
2	TPP	D	600	3	-	4/16/17/17	0/2/2/2
2	TPP	B	600	3	-	5/16/17/17	0/2/2/2
2	TPP	E	600	3	-	3/16/17/17	0/2/2/2
2	TPP	C	600	3	-	4/16/17/17	0/2/2/2
2	TPP	A	600	3	-	3/16/17/17	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	600	TPP	C4-N3	-6.24	1.34	1.39
2	A	600	TPP	C4-N3	-5.96	1.34	1.39
2	F	600	TPP	C4-N3	-5.27	1.35	1.39
2	C	600	TPP	C4-N3	-4.93	1.35	1.39
2	B	600	TPP	C4-N3	-4.90	1.35	1.39
2	D	600	TPP	C4-N3	-4.79	1.35	1.39
2	E	600	TPP	C7'-N3	-4.30	1.40	1.48
2	A	600	TPP	C7'-N3	-4.06	1.41	1.48
2	C	600	TPP	C7'-N3	-3.77	1.41	1.48
2	B	600	TPP	C6-C5	-3.38	1.49	1.50
2	D	600	TPP	C4'-N3'	3.38	1.39	1.35
2	F	600	TPP	C7'-N3	-3.24	1.42	1.48
2	A	600	TPP	C2'-N1'	3.16	1.39	1.34
2	A	600	TPP	C4'-N3'	3.13	1.39	1.35
2	D	600	TPP	C7'-N3	-3.11	1.42	1.48
2	C	600	TPP	C2'-N1'	3.07	1.39	1.34
2	E	600	TPP	C4'-N3'	3.06	1.39	1.35
2	F	600	TPP	C2'-N1'	2.81	1.38	1.34
2	B	600	TPP	C6'-N1'	2.75	1.40	1.34
2	B	600	TPP	C2'-N1'	2.70	1.38	1.34
2	E	600	TPP	C2'-N3'	2.65	1.38	1.34
2	D	600	TPP	C6'-N1'	2.56	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	600	TPP	C6'-N1'	2.43	1.39	1.34
2	D	600	TPP	C2'-N1'	2.41	1.38	1.34
2	A	600	TPP	C6'-N1'	2.37	1.39	1.34
2	F	600	TPP	C4'-N3'	2.35	1.38	1.35
2	A	600	TPP	C2'-N3'	2.24	1.38	1.34
2	E	600	TPP	C2'-N1'	2.20	1.37	1.34
2	E	600	TPP	C6'-N1'	2.19	1.39	1.34
2	C	600	TPP	C2'-N3'	2.15	1.37	1.34
2	D	600	TPP	C7'-C5'	2.14	1.55	1.51
2	B	600	TPP	C7'-N3	-2.14	1.44	1.48
2	D	600	TPP	C2'-N3'	2.12	1.37	1.34
2	F	600	TPP	C6-C5	-2.11	1.50	1.50
2	B	600	TPP	C4'-N3'	2.10	1.38	1.35
2	C	600	TPP	C6'-N1'	2.09	1.38	1.34
2	D	600	TPP	C6-C5	2.02	1.51	1.50

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	600	TPP	C5'-C7'-N3	-9.91	96.78	113.28
2	A	600	TPP	C5'-C7'-N3	-9.29	97.81	113.28
2	C	600	TPP	C5'-C7'-N3	-8.59	98.98	113.28
2	F	600	TPP	C5'-C7'-N3	-7.30	101.13	113.28
2	D	600	TPP	C5'-C7'-N3	-7.17	101.34	113.28
2	B	600	TPP	C5'-C7'-N3	-6.23	102.91	113.28
2	B	600	TPP	CM2-C2'-N1'	5.66	123.37	117.14
2	F	600	TPP	CM2-C2'-N1'	5.25	122.91	117.14
2	C	600	TPP	CM2-C2'-N1'	5.05	122.69	117.14
2	A	600	TPP	CM2-C2'-N1'	4.64	122.24	117.14
2	D	600	TPP	CM2-C2'-N1'	4.32	121.89	117.14
2	D	600	TPP	N1'-C2'-N3'	-3.84	118.92	125.54
2	F	600	TPP	C6-C5-C4	3.53	130.26	127.43
2	A	600	TPP	N1'-C2'-N3'	-3.52	119.48	125.54
2	A	600	TPP	PA-O3A-PB	-3.51	120.78	132.83
2	B	600	TPP	CM4-C4-N3	3.38	126.83	122.53
2	B	600	TPP	N1'-C2'-N3'	-3.34	119.79	125.54
2	D	600	TPP	CM4-C4-N3	3.32	126.76	122.53
2	D	600	TPP	PA-O3A-PB	-3.26	121.65	132.83
2	B	600	TPP	PA-O3A-PB	-3.24	121.70	132.83
2	E	600	TPP	CM4-C4-N3	3.12	126.51	122.53
2	C	600	TPP	CM4-C4-N3	3.12	126.51	122.53
2	F	600	TPP	N1'-C2'-N3'	-3.10	120.21	125.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	600	TPP	PA-O3A-PB	-3.07	122.30	132.83
2	C	600	TPP	N1'-C2'-N3'	-2.99	120.40	125.54
2	D	600	TPP	C6'-N1'-C2'	2.90	120.90	115.96
2	E	600	TPP	C6'-N1'-C2'	2.88	120.86	115.96
2	E	600	TPP	C7'-N3-C2	-2.85	120.21	125.35
2	F	600	TPP	CM4-C4-N3	2.84	126.16	122.53
2	A	600	TPP	C6'-N1'-C2'	2.76	120.66	115.96
2	A	600	TPP	CM4-C4-N3	2.63	125.88	122.53
2	F	600	TPP	C6'-N1'-C2'	2.56	120.32	115.96
2	C	600	TPP	PA-O3A-PB	-2.51	124.22	132.83
2	B	600	TPP	C6'-N1'-C2'	2.50	120.22	115.96
2	E	600	TPP	N1'-C2'-N3'	-2.50	121.24	125.54
2	D	600	TPP	C5'-C4'-N4'	-2.45	118.72	122.19
2	E	600	TPP	C5'-C6'-N1'	-2.41	119.80	123.82
2	C	600	TPP	C6'-N1'-C2'	2.37	120.00	115.96
2	E	600	TPP	O3B-PB-O3A	2.36	112.55	104.64
2	A	600	TPP	C7'-N3-C2	-2.32	121.16	125.35
2	F	600	TPP	PA-O3A-PB	-2.31	124.91	132.83
2	C	600	TPP	O3B-PB-O2B	2.28	116.36	107.64
2	E	600	TPP	CM2-C2'-N1'	2.23	119.59	117.14
2	F	600	TPP	O2A-PA-O7	2.20	117.95	107.75
2	A	600	TPP	O3B-PB-O2B	2.19	115.99	107.64
2	B	600	TPP	O3B-PB-O3A	2.14	111.80	104.64
2	A	600	TPP	C6-C5-C4	2.13	129.15	127.43
2	E	600	TPP	C6'-C5'-C4'	2.11	118.59	115.72

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	600	TPP	C4'-C5'-C7'-N3
2	F	600	TPP	PB-O3A-PA-O7
2	D	600	TPP	C4'-C5'-C7'-N3
2	D	600	TPP	PB-O3A-PA-O7
2	A	600	TPP	C4'-C5'-C7'-N3
2	E	600	TPP	C4'-C5'-C7'-N3
2	E	600	TPP	PB-O3A-PA-O7
2	C	600	TPP	C4'-C5'-C7'-N3
2	C	600	TPP	PB-O3A-PA-O7
2	B	600	TPP	C4'-C5'-C7'-N3
2	F	600	TPP	C6-C7-O7-PA
2	D	600	TPP	C6-C7-O7-PA

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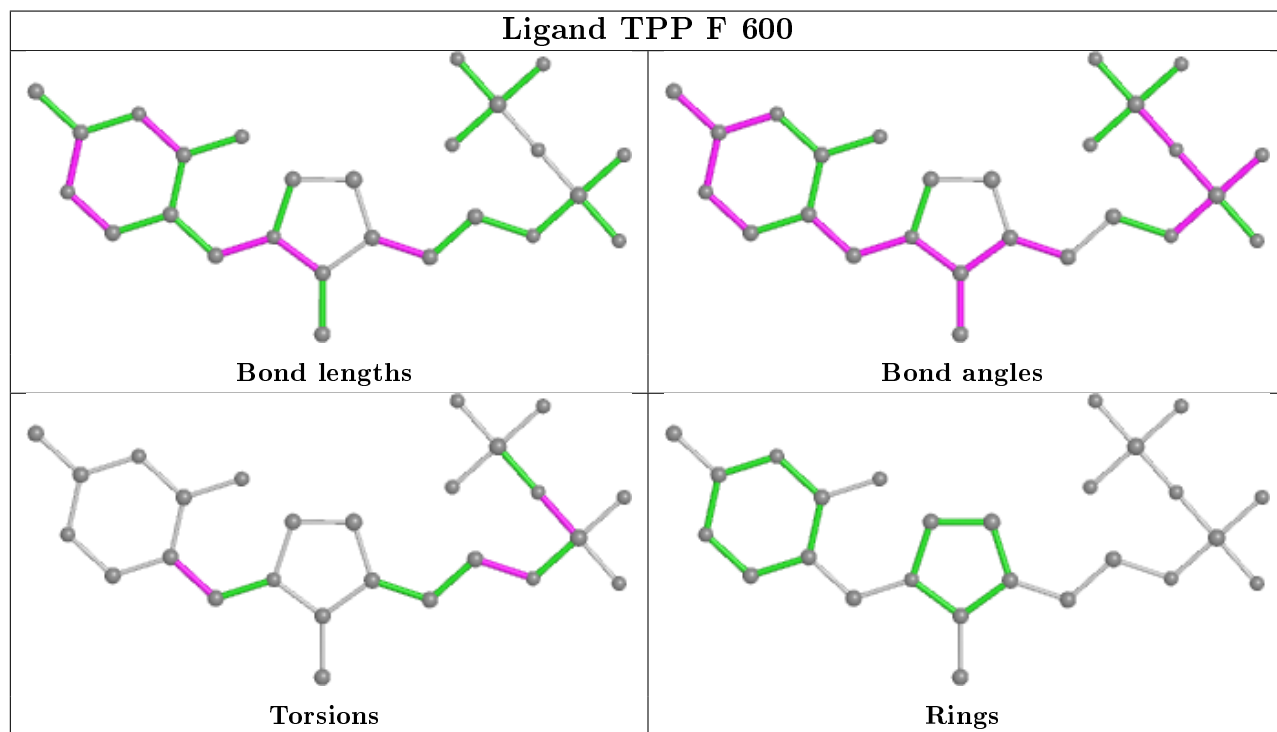
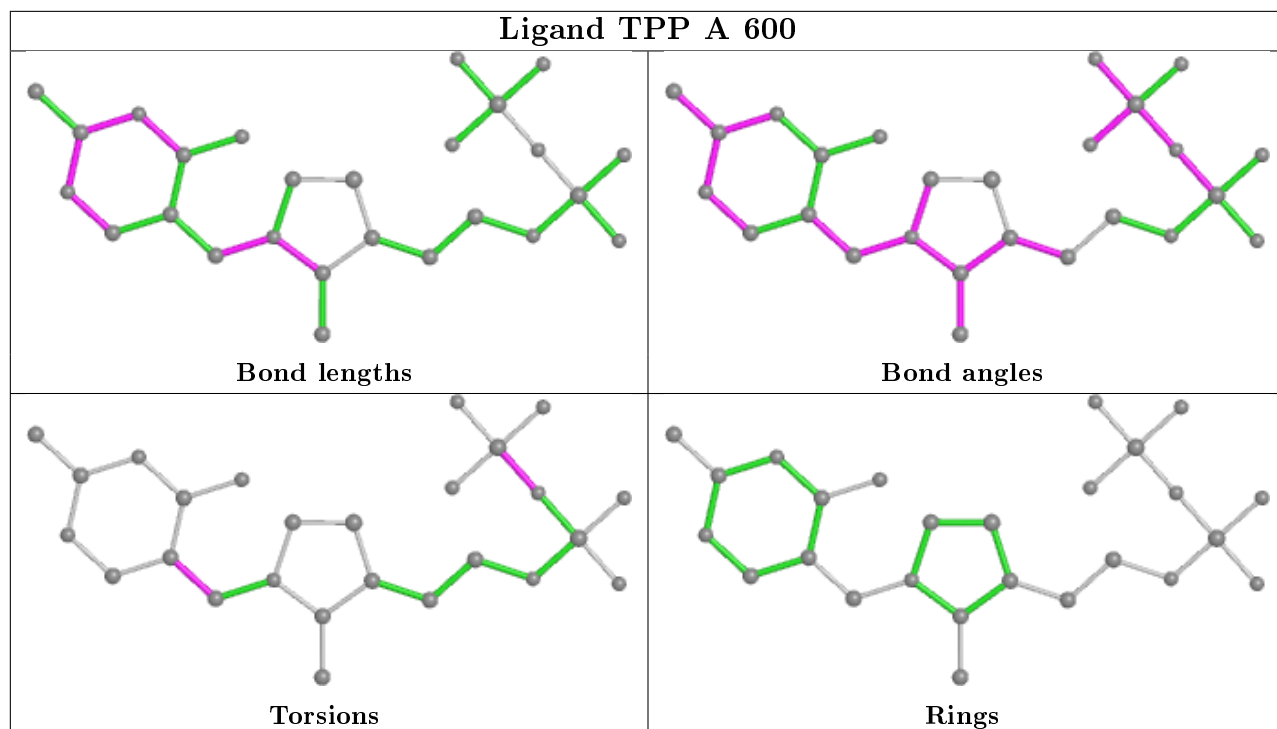
Mol	Chain	Res	Type	Atoms
2	C	600	TPP	C6-C7-O7-PA
2	B	600	TPP	PB-O3A-PA-O7
2	F	600	TPP	C6'-C5'-C7'-N3
2	A	600	TPP	C6'-C5'-C7'-N3
2	B	600	TPP	C6'-C5'-C7'-N3
2	A	600	TPP	PA-O3A-PB-O1B
2	B	600	TPP	PA-O3A-PB-O1B
2	D	600	TPP	C6'-C5'-C7'-N3
2	C	600	TPP	C6'-C5'-C7'-N3
2	E	600	TPP	C6-C7-O7-PA
2	B	600	TPP	C6-C7-O7-PA

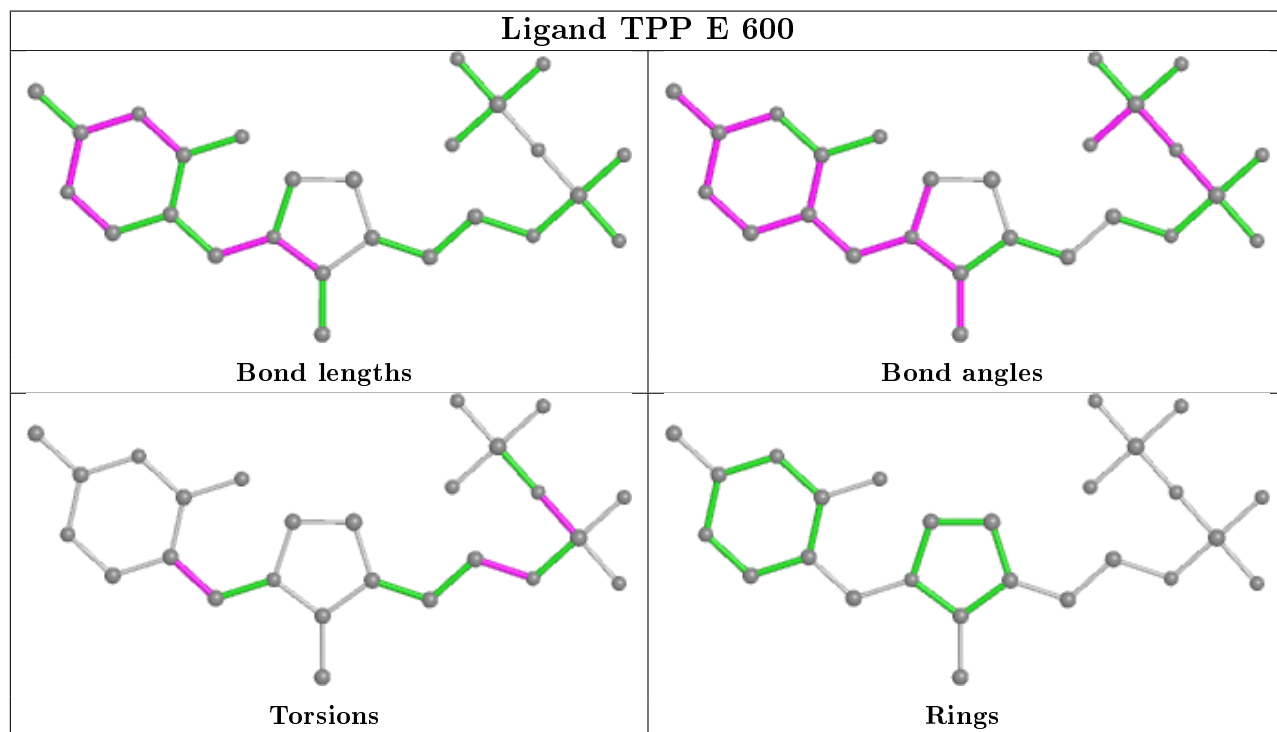
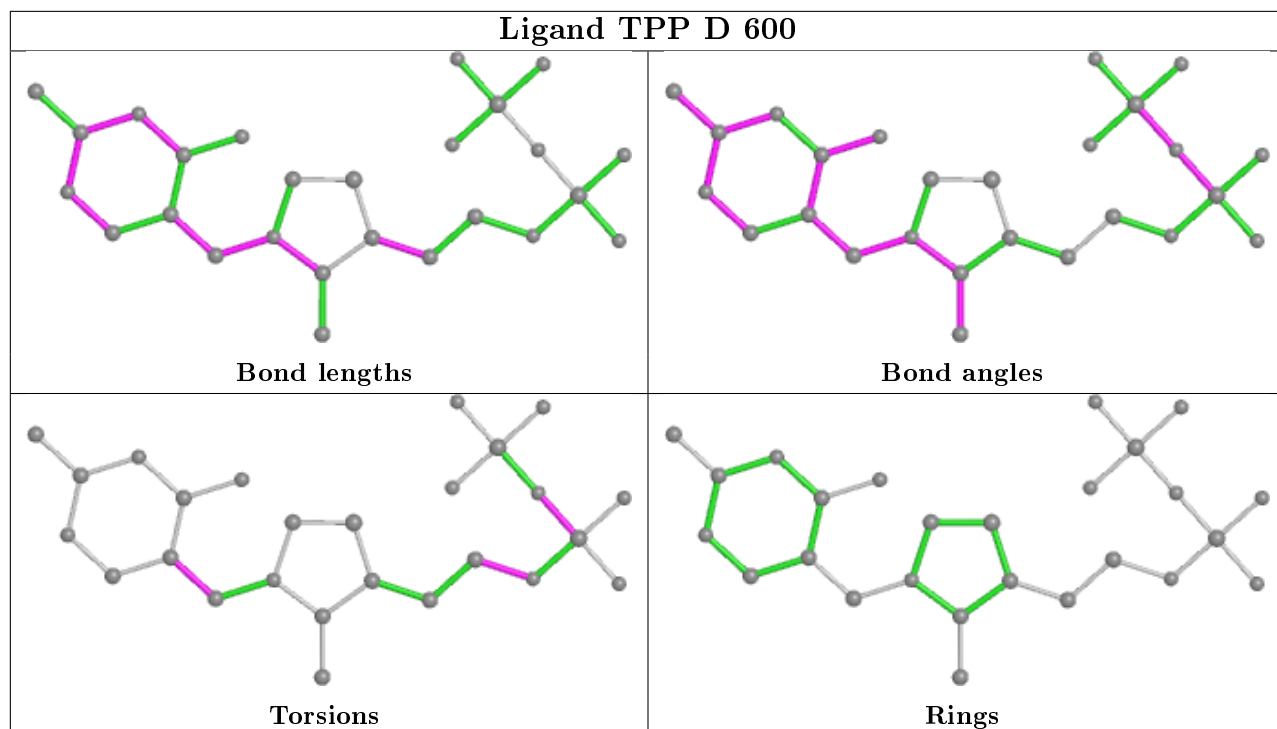
There are no ring outliers.

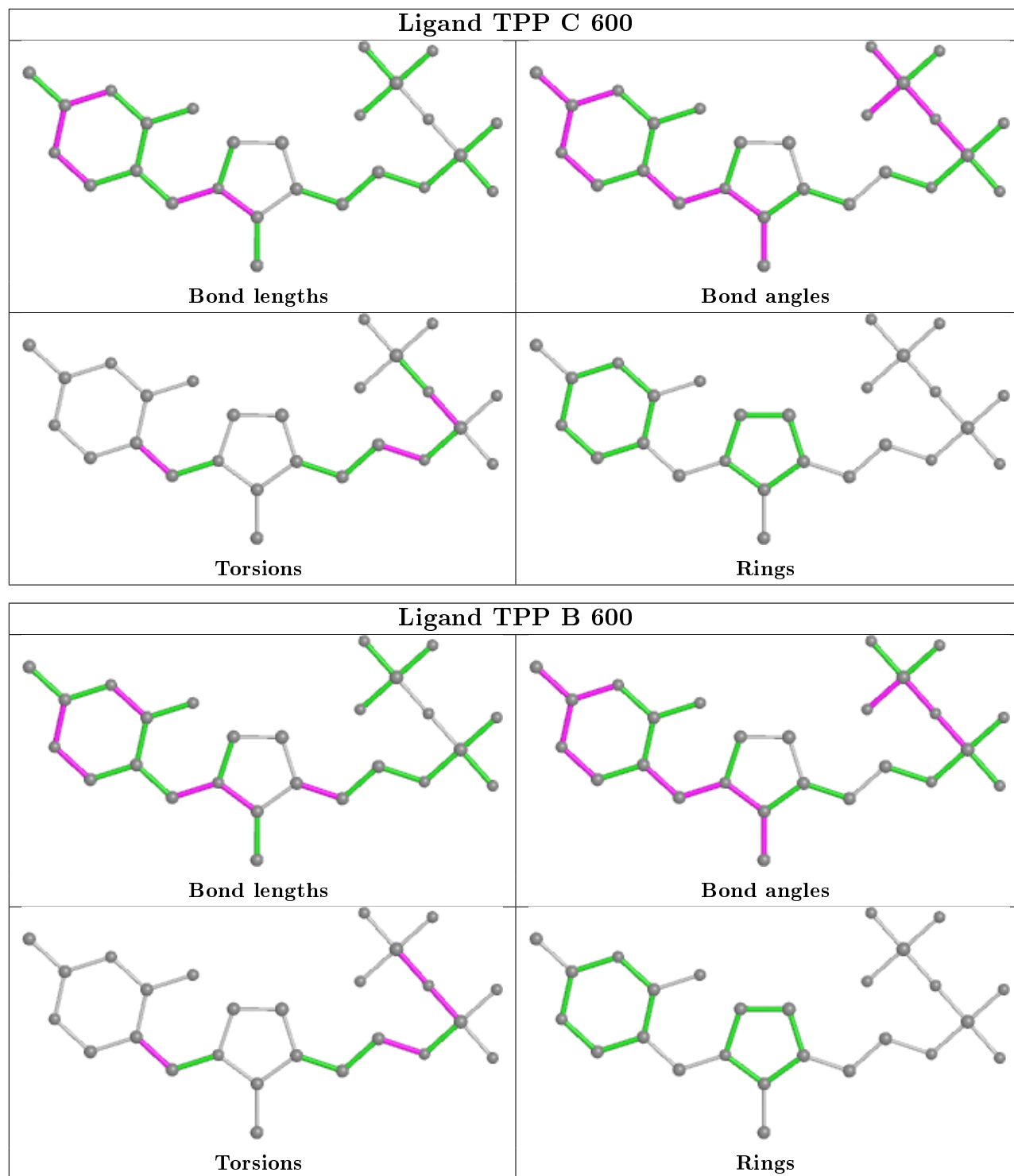
7 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	TPP	5	0
2	F	600	TPP	6	0
2	D	600	TPP	4	0
4	A	603	SO4	1	0
2	E	600	TPP	6	0
2	C	600	TPP	5	0
2	B	600	TPP	7	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.







## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	559/573 (97%)	-0.41	6 (1%) 80 80	20, 31, 46, 59	0
1	B	559/573 (97%)	-0.39	7 (1%) 77 76	19, 30, 45, 62	0
1	C	557/573 (97%)	-0.33	5 (0%) 84 85	19, 31, 45, 58	0
1	D	559/573 (97%)	-0.38	7 (1%) 77 76	18, 30, 45, 58	0
1	E	558/573 (97%)	-0.27	19 (3%) 45 41	19, 31, 45, 57	0
1	F	558/573 (97%)	-0.38	5 (0%) 84 85	19, 30, 45, 57	0
All	All	3350/3438 (97%)	-0.36	49 (1%) 73 71	18, 30, 45, 62	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	380	ASP	4.9
1	B	565	PRO	4.2
1	B	564	GLN	3.8
1	D	380	ASP	3.4
1	F	380	ASP	3.3
1	C	380	ASP	3.2
1	E	357	GLN	3.1
1	B	563	PHE	3.0
1	B	380	ASP	3.0
1	D	184	PRO	3.0
1	C	352	SER	2.9
1	B	181	THR	2.9
1	F	352	SER	2.9
1	E	562	ASP	2.8
1	D	181	THR	2.7
1	A	380	ASP	2.7
1	C	218	HIS	2.7
1	E	537	GLU	2.6
1	A	379	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	351	ALA	2.6
1	C	361	ILE	2.6
1	A	47	GLU	2.6
1	E	260	GLY	2.5
1	E	375	PRO	2.5
1	F	47	GLU	2.4
1	F	179	ILE	2.4
1	E	180	ASP	2.3
1	E	377	THR	2.3
1	E	454	ASP	2.3
1	F	377	THR	2.3
1	D	564	GLN	2.3
1	A	401	PRO	2.3
1	B	47	GLU	2.3
1	A	454	ASP	2.2
1	D	562	ASP	2.2
1	E	244	ASN	2.2
1	B	375	PRO	2.1
1	E	278	PHE	2.1
1	E	366	ALA	2.1
1	A	377	THR	2.1
1	D	548	GLU	2.1
1	C	214	ALA	2.1
1	E	360	ASP	2.1
1	E	218	HIS	2.0
1	E	550	GLY	2.0
1	E	548	GLU	2.0
1	E	214	ALA	2.0
1	D	375	PRO	2.0
1	E	184	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.



## 6.4 Ligands [i](#)

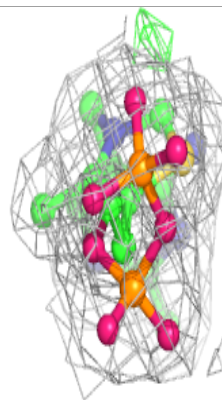
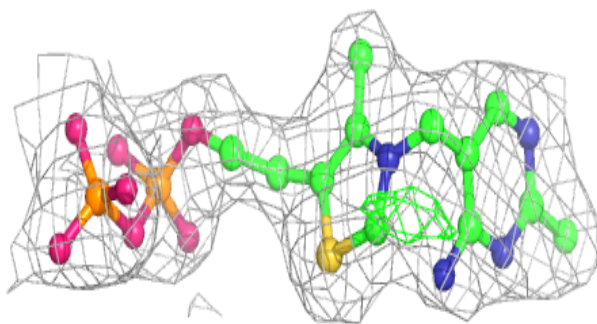
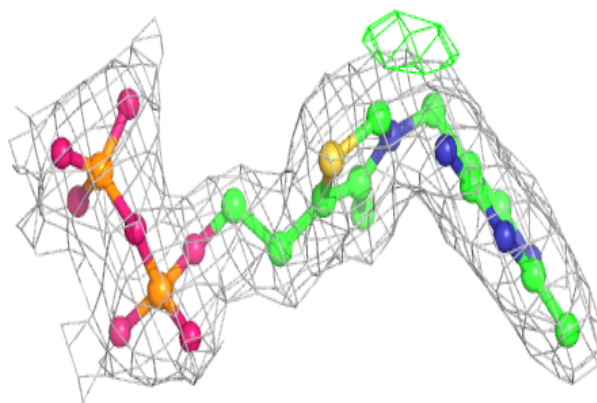
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	D	603	5/5	0.83	0.38	89,91,92,92	0
4	SO4	B	603	5/5	0.85	0.37	91,91,92,92	0
4	SO4	A	603	5/5	0.87	0.19	89,90,91,91	0
4	SO4	F	603	5/5	0.87	0.28	90,91,91,91	0
4	SO4	C	603	5/5	0.91	0.22	89,89,91,91	0
4	SO4	E	603	5/5	0.94	0.31	90,90,91,91	0
2	TPP	A	600	26/26	0.97	0.13	22,26,30,31	0
3	MG	A	601	1/1	0.97	0.13	14,14,14,14	0
3	MG	F	601	1/1	0.97	0.09	15,15,15,15	0
2	TPP	E	600	26/26	0.97	0.13	22,28,31,33	0
2	TPP	F	600	26/26	0.97	0.10	21,26,29,31	0
2	TPP	D	600	26/26	0.98	0.12	22,26,29,30	0
3	MG	E	601	1/1	0.98	0.09	17,17,17,17	0
4	SO4	E	602	5/5	0.98	0.12	32,32,34,35	0
2	TPP	C	600	26/26	0.98	0.12	22,27,30,31	0
2	TPP	B	600	26/26	0.98	0.11	22,27,29,32	0
3	MG	B	601	1/1	0.98	0.12	13,13,13,13	0
3	MG	D	601	1/1	0.98	0.09	15,15,15,15	0
4	SO4	B	602	5/5	0.99	0.12	33,34,35,35	0
4	SO4	F	602	5/5	0.99	0.12	30,31,33,33	0
3	MG	C	601	1/1	0.99	0.09	12,12,12,12	0
4	SO4	D	602	5/5	0.99	0.11	29,30,31,32	0
4	SO4	C	602	5/5	0.99	0.13	30,33,34,35	0
4	SO4	A	602	5/5	1.00	0.12	27,29,30,30	0

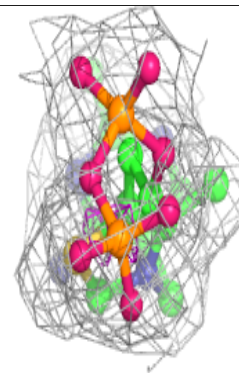
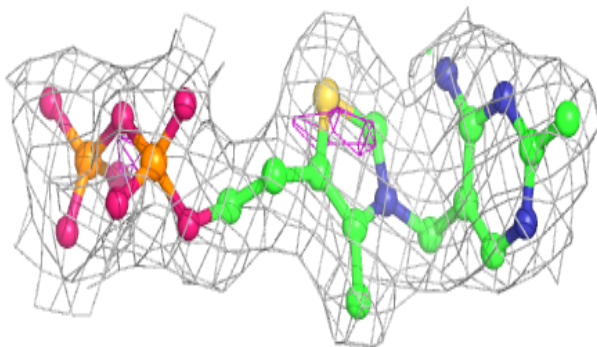
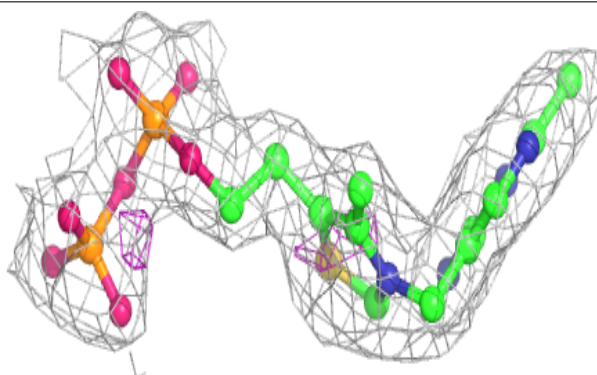
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TPP A 600:**

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

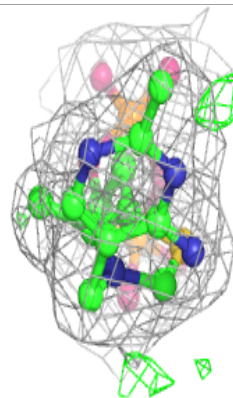
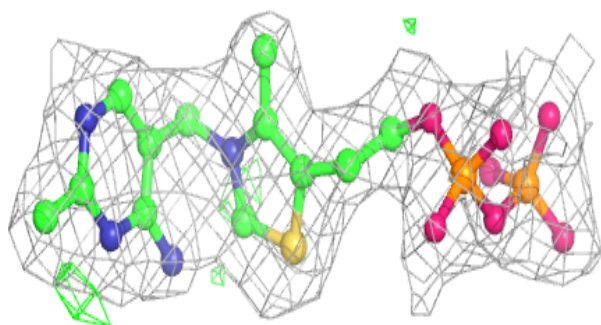
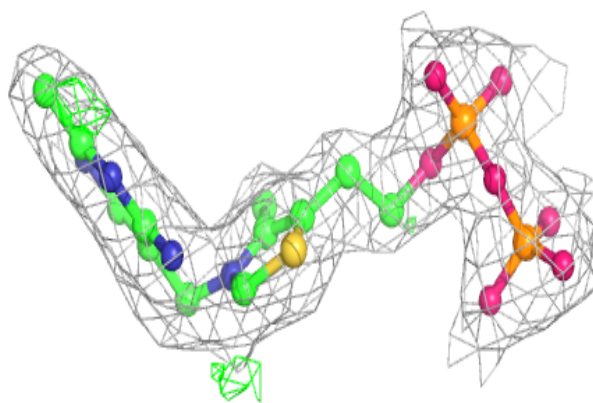
**Electron density around TPP E 600:**

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

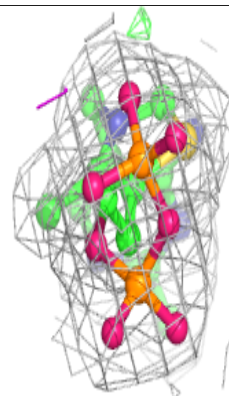
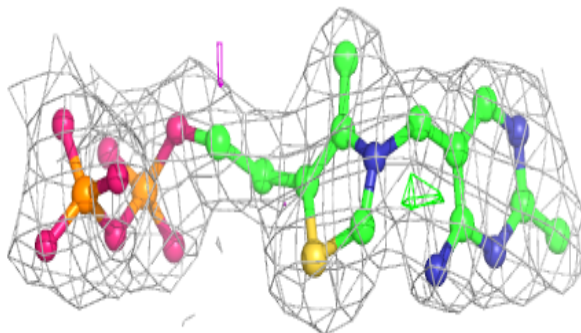
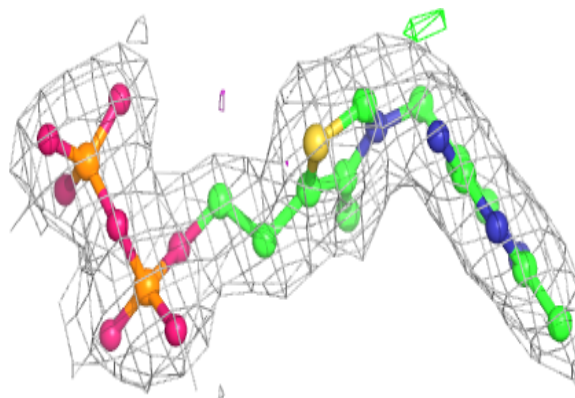


**Electron density around TPP F 600:**

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

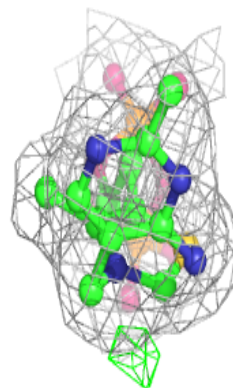
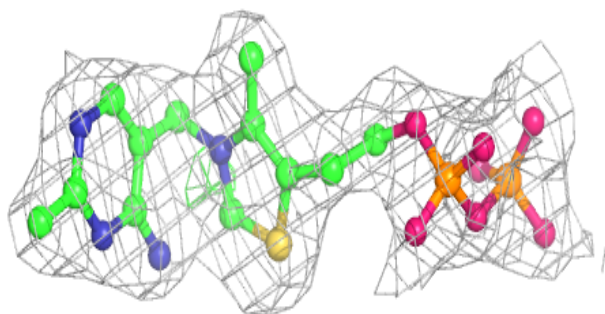
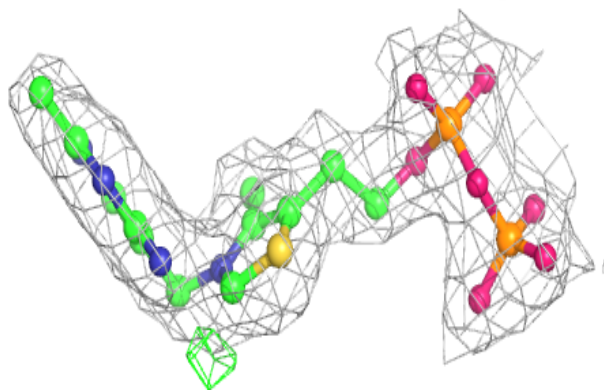
**Electron density around TPP D 600:**

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and green (positive)

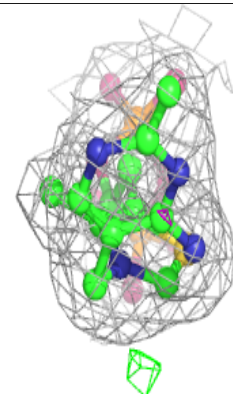
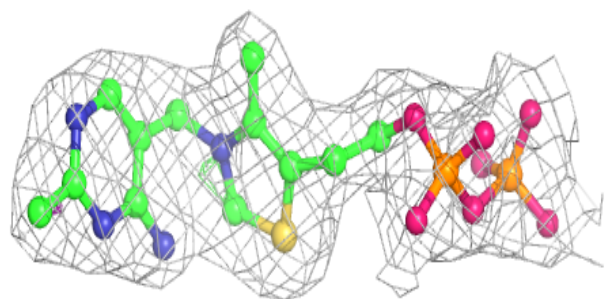
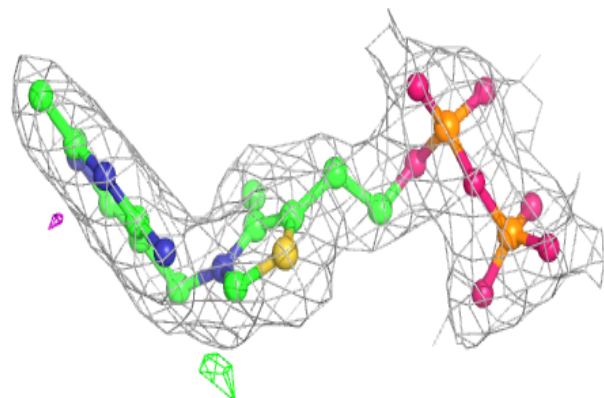


**Electron density around TPP C 600:**

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

**Electron density around TPP B 600:**

$2mF_o-DF_c$  (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.