



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 09:50 am BST

PDB ID : 2C3O
Title : CRYSTAL STRUCTURE OF THE FREE RADICAL INTERMEDIATE
OF PYRUVATE:FERREDOXIN OXIDOREDUCTASE FROM *Desulfovibrio*
africanus
Authors : Cavazza, C.; Contreras-Martel, C.; Pieulle, L.; Chabriere, E.; Hatchikian, E.C.;
Fontecilla-Camps, J.C.
Deposited on : 2005-10-11
Resolution : 2.70 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

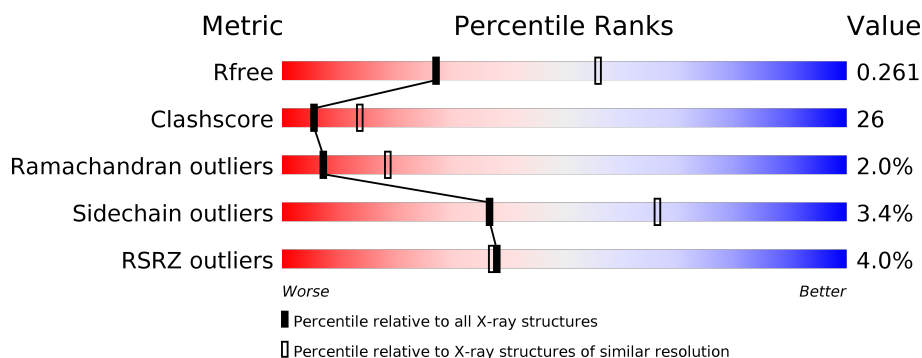
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	1231	<div> <div>5%</div> <div> <div></div> <div>56%</div> <div>41%</div> <div>.</div> </div> </div>
1	B	1231	<div> <div>3%</div> <div> <div></div> <div>57%</div> <div>40%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

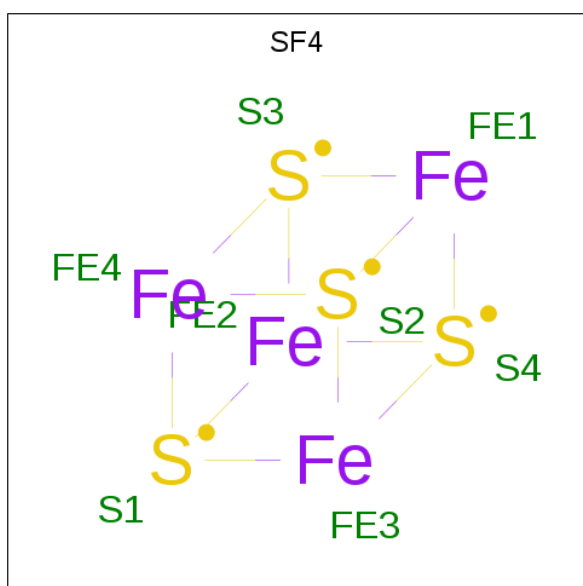
There are 7 unique types of molecules in this entry. The entry contains 19451 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PYRUVATE-FERREDOXIN OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1231	Total	C	N	O	S	0	0	0
			9383	5941	1599	1784	59			
1	B	1231	Total	C	N	O	S	0	0	0
			9383	5941	1599	1784	59			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



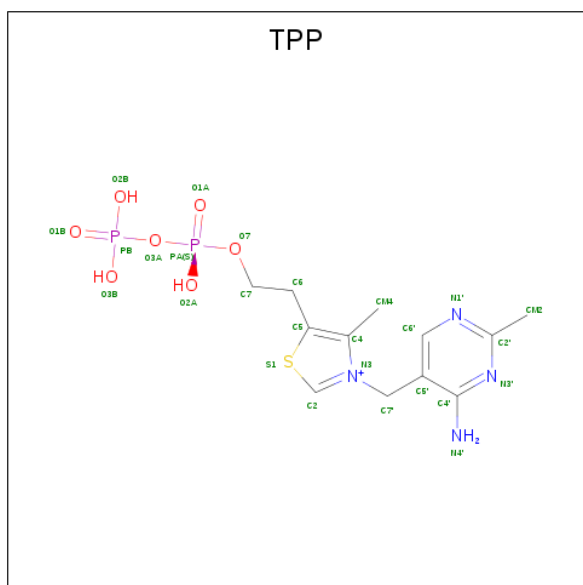
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

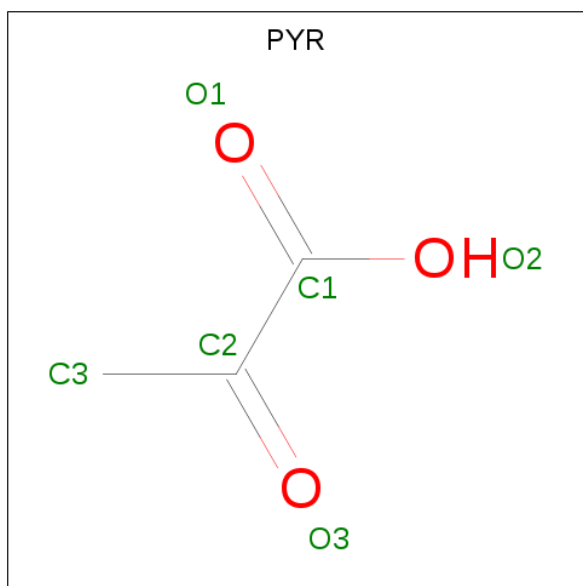
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

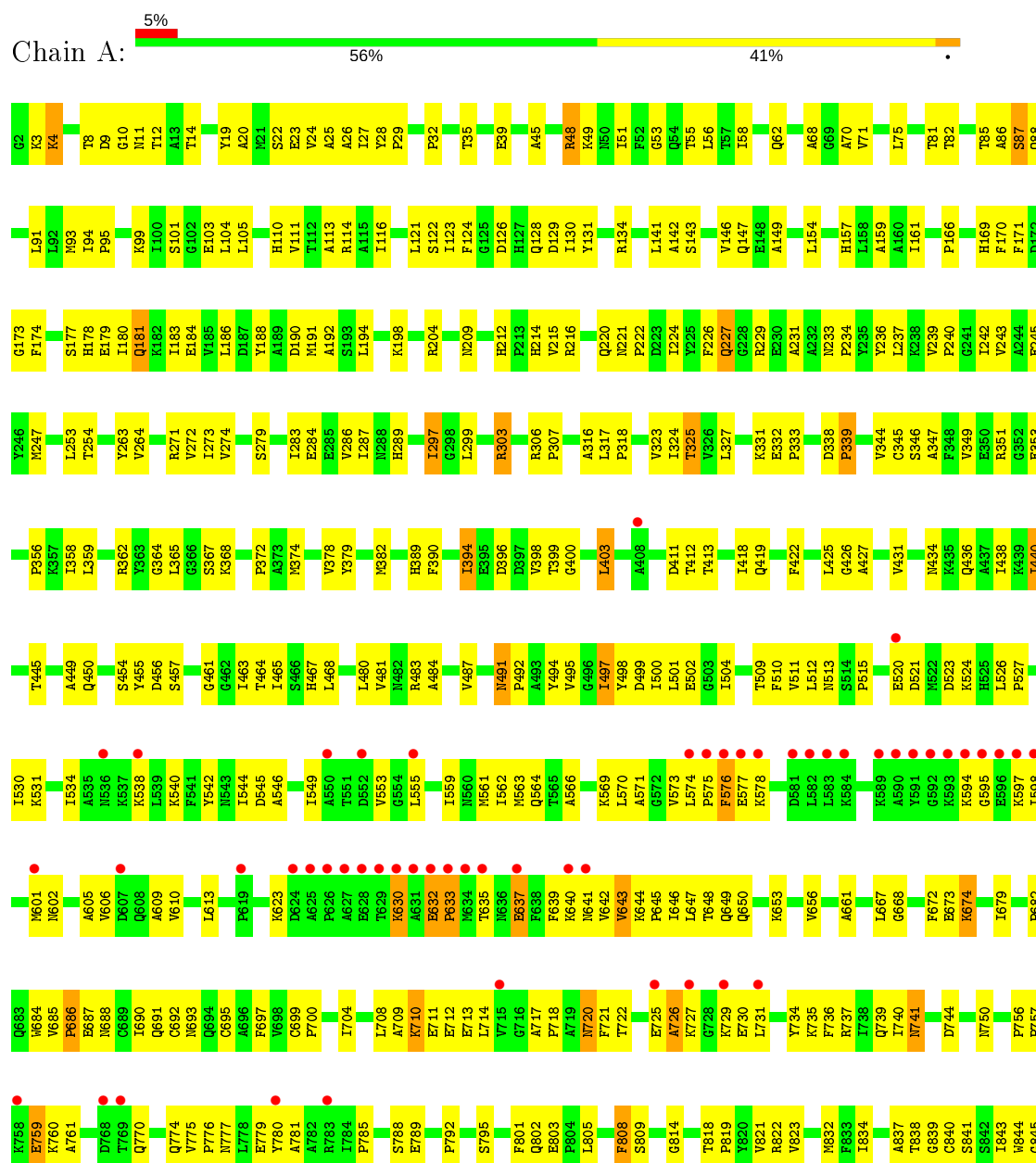
- Molecule 7 is water.

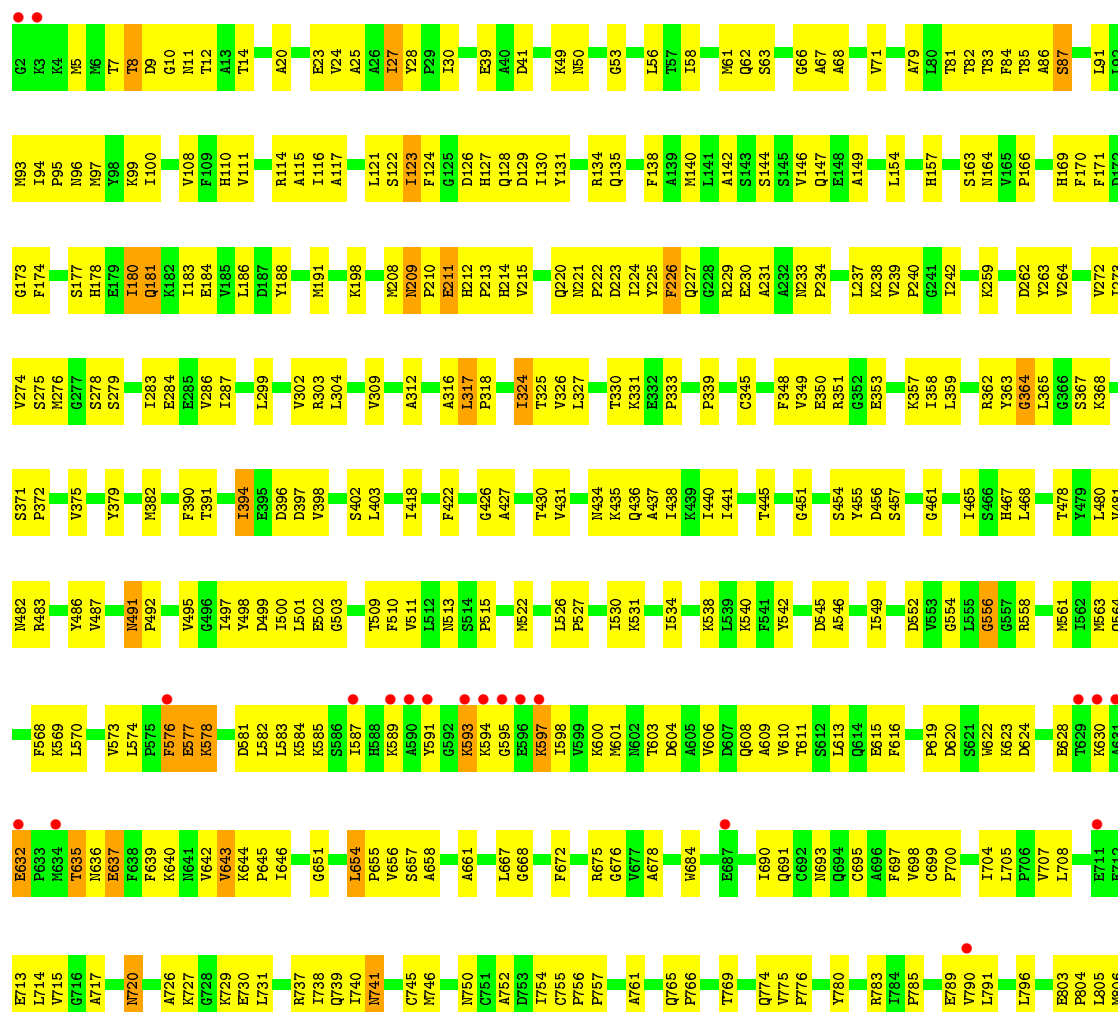
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	262	Total	O	0	0
			262	262		
7	B	307	Total	O	0	0
			307	307		

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: PYRUVATE-FERREDOXIN OXIDOREDUCTASE





E1164	Q1084	Q1000	K896	E807
H1165	D1085	S1001		C812
M1166	V1086	M1002	S903	S813
	M1087	K1003		G814
T1169	M1088	A1004	V906	
F1172	V1091	T1005		E817
	G1094	P1006	L910	T818
A1176		T1007	Q911	P819
P1177		G1008	G912	V820
A1178	F1099	A1009	W913	V821
G1179	R1100		L914	R822
G1180	T1101	K1012		V823
K1181	D1102	F1013		T824
A1182	P1103	A1014	K917	T825
D1183	R1104	A1015		
G1184	L1105		K924	E830
S1185		R1019	E925	
	M1111		V926	A835
D1199		R1027	G927	N836
T1200	Q1114	M1028	D928	A837
P1201	L1115	V1029	K929	T838
M1202		M1030	L930	G839
	K1118		Q937	C840
Q1214	A1119		K938	S841
M1215	P1120	V1037		
R1216		V1040	L941	N844
	S1123	G1043		P849
T1219	V1124	Y1044	I945	S850
S1220	E1125	S1045	S949	P851
E1221	E1126	K1046		P852
Q1222	F1127	Q1047	T952	V853
	L1128	Q1048	G953	K854
L1226		F1049	K954	T855
S1227	M1132		K955	N856
K1228		V1052		R857
A1229	V1136		T959	L858
T1230	D1137	A1056		G859
K1231	L1138		D963	Q860
K1232	R1139	F1059	G964	G861
	E1143	P1060	W965	P862
	D1144	G1061	A966	
	A1145	P1062	V967	G865
	K1146	S1063	D968	N866
	R1147	L1064	I969	S867
	L1148	V1065		L868
		T1066	G973	F869
	Q1151		L974	E870
	V1152	C1071	D975	D871
		Q1074		A872
	E1155		G981	A873
	L1156		V986	E874
	D1157	R1077		
	V1158	K1078		N883
	R1159	G1079	M989	R887
	F1160	M1080		
	K1161	G1081	Y904	
		K1082	N905	S892
	E1162	S1083	W906	L902
	L1163			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.65Å 145.24Å 204.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.11 – 2.70 38.11 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.4 (38.11-2.70) 94.5 (38.11-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.268 0.197 , 0.261	Depositor DCC
R_{free} test set	3476 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19451	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: MG, SF4, PYR, CA, 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	0.28	0/9585	0.52	0/12954
1	B	0.29	0/9585	0.54	0/12954
All	All	0.29	0/19170	0.53	0/25908

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	9383	0	9263	525	0
1	B	9383	0	9262	502	0
2	A	24	0	0	0	0
2	B	24	0	0	1	0
3	A	26	0	16	3	0
3	B	26	0	16	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	6	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	6	0	3	2	0
7	A	262	0	0	13	0
7	B	307	0	0	13	0
All	All	19451	0	18563	960	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 26.

The worst 5 of 960 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:A:1200:THR:HG22	1:A:1202:MET:H	1.19	1.06
1:B:1077:ARG:HB2	1:B:1077:ARG:HH11	1.22	1.02
1:B:239:VAL:HG13	1:B:240:PRO:HD3	1.42	1.02
1:A:198:LYS:H	1:A:198:LYS:HD2	1.24	1.00
1:A:147:GLN:HE22	1:A:184:GLU:H	1.10	0.97

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	1229/1231 (100%)	1105 (90%)	96 (8%)	28 (2%)	6	16
1	B	1229/1231 (100%)	1120 (91%)	89 (7%)	20 (2%)	9	24
All	All	2458/2462 (100%)	2225 (90%)	185 (8%)	48 (2%)	7	19

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1231	LYS

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Mol	Chain	Res	Type
1	B	556	GLY
1	B	577	GLU
1	B	597	LYS
1	A	4	LYS

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	978/978 (100%)	946 (97%)	32 (3%)	38	67
1	B	978/978 (100%)	943 (96%)	35 (4%)	35	64
All	All	1956/1956 (100%)	1889 (97%)	67 (3%)	37	66

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1088	ASN
1	B	180	ILE
1	B	1047	GLN
1	A	1183	ASP
1	B	84	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1108	GLN
1	B	164	ASN
1	B	1048	GLN
1	A	1151	GLN
1	B	46	GLN

5.3.3 RNA ⓘ

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 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SF4	A	2235	1	0,12,12	0.00	-	-		
2	SF4	B	2233	1	0,12,12	0.00	-	-		
6	PYR	B	2239	-	2,5,5	0.81	0	2,6,6	1.42	0
6	PYR	A	2239	-	2,5,5	1.03	0	2,6,6	1.43	0
2	SF4	A	2234	1	0,12,12	0.00	-	-		
2	SF4	A	2233	1	0,12,12	0.00	-	-		
2	SF4	B	2235	1	0,12,12	0.00	-	-		
3	TPP	B	2236	4	22,27,27	3.86	8 (36%)	29,40,40	2.03	8 (27%)
3	TPP	A	2236	4	22,27,27	4.32	9 (40%)	29,40,40	2.03	7 (24%)
2	SF4	B	2234	1	0,12,12	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
2	SF4	A	2235	1	-	-	0/6/5/5
2	SF4	B	2233	1	-	-	0/6/5/5
3	TPP	B	2236	4	-	3/16/17/17	0/2/2/2
3	TPP	A	2236	4	-	6/16/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	A	2234	1	-	-	0/6/5/5
2	SF4	A	2233	1	-	-	0/6/5/5
2	SF4	B	2235	1	-	-	0/6/5/5
6	PYR	B	2239	-	-	0/0/4/4	-
6	PYR	A	2239	-	-	0/0/4/4	-
2	SF4	B	2234	1	-	-	0/6/5/5

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2236	TPP	C4-N3	12.02	1.50	1.39
3	A	2236	TPP	C4-N3	11.67	1.49	1.39
3	A	2236	TPP	C4'-N3'	8.88	1.47	1.35
3	A	2236	TPP	C6-C5	8.13	1.54	1.50
3	B	2236	TPP	C6'-C5'	6.59	1.51	1.37

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2236	TPP	C6-C5-C4	6.33	132.52	127.43
3	A	2236	TPP	C5'-C7'-N3	5.60	122.59	113.28
3	B	2236	TPP	C5'-C7'-N3	5.14	121.83	113.28
3	A	2236	TPP	C6-C5-C4	4.21	130.82	127.43
3	A	2236	TPP	C6'-N1'-C2'	3.51	121.94	115.96

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2236	TPP	C5-C6-C7-O7
3	B	2236	TPP	C7-O7-PA-O1A
3	A	2236	TPP	C5-C6-C7-O7
3	A	2236	TPP	C7-O7-PA-O3A
3	B	2236	TPP	PB-O3A-PA-O7

There are no ring outliers.

4 monomers are involved in 7 short contacts:

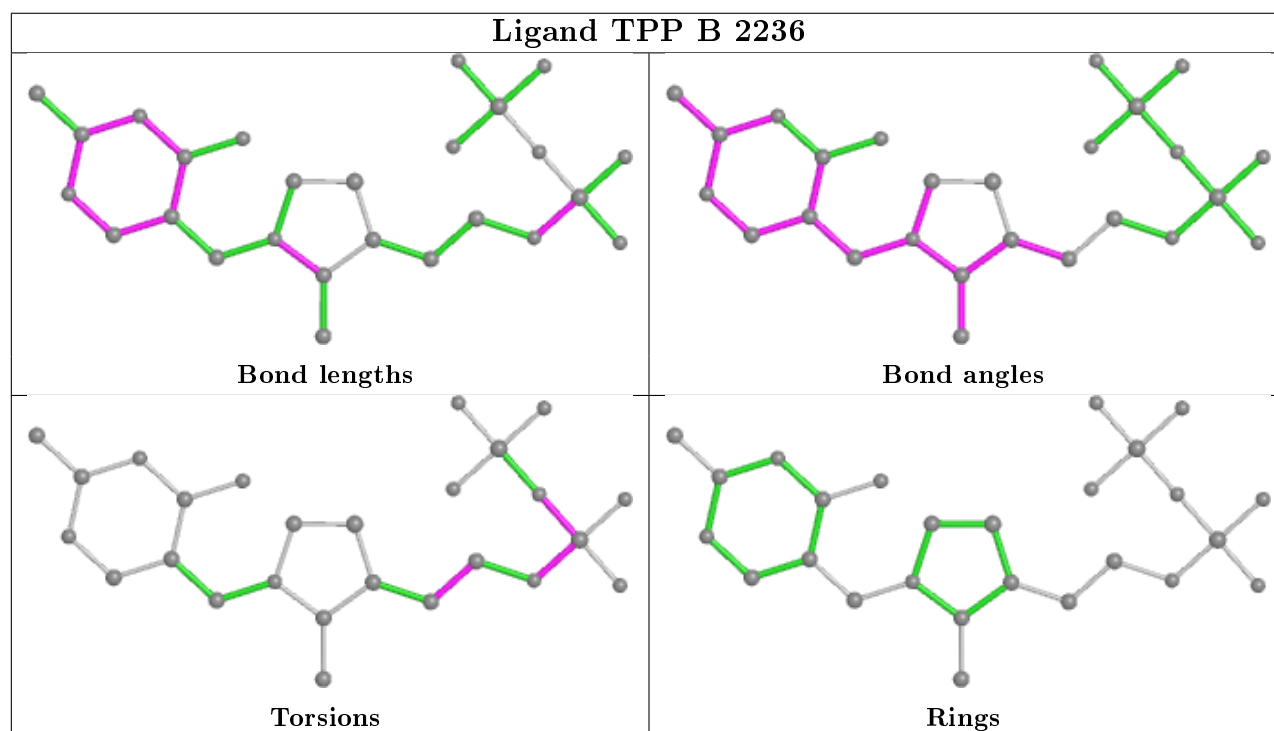
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2233	SF4	1	0
6	B	2239	PYR	2	0

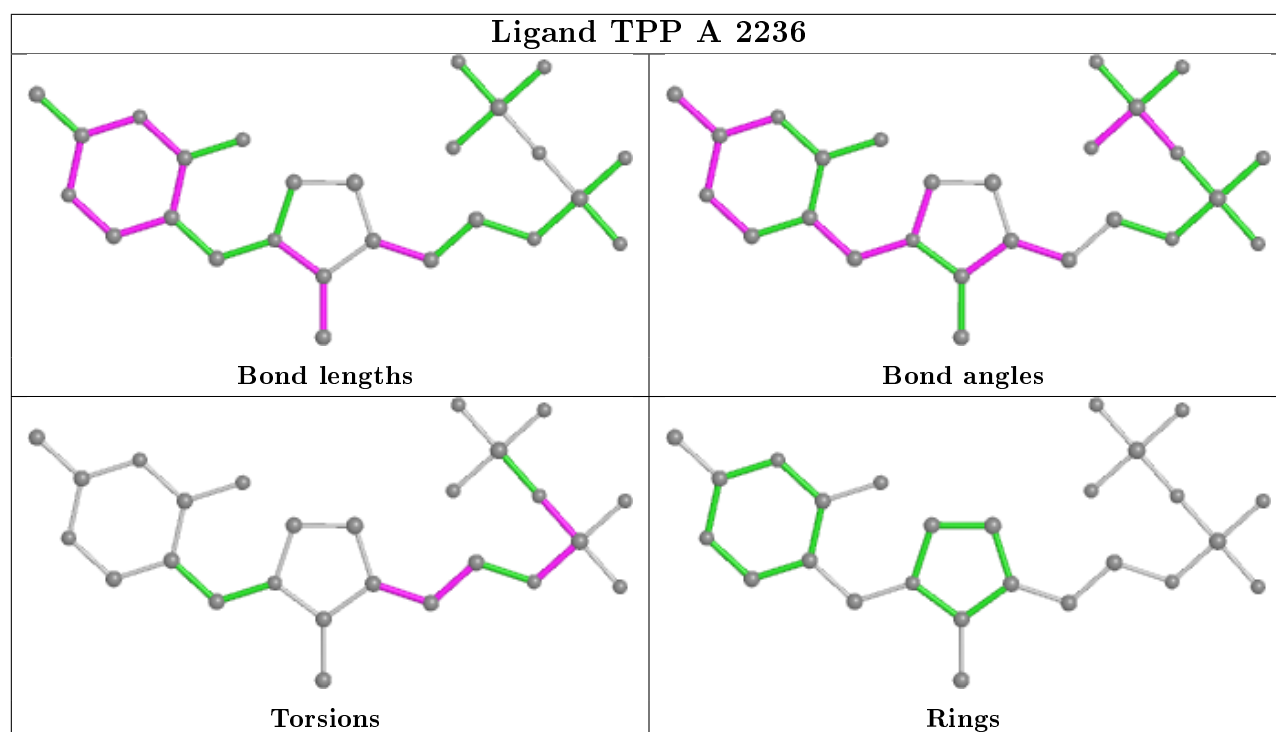
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2236	TPP	1	0
3	A	2236	TPP	3	0

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1231/1231 (100%)	0.08	63 (5%) 28 26	3, 26, 71, 114	0
1	B	1231/1231 (100%)	-0.19	36 (2%) 51 52	2, 18, 55, 117	0
All	All	2462/2462 (100%)	-0.05	99 (4%) 38 37	2, 22, 64, 117	0

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1180	GLY	7.6
1	B	1182	ALA	7.4
1	A	631	ALA	6.6
1	A	595	GLY	6.3
1	A	626	PRO	5.7

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](#)

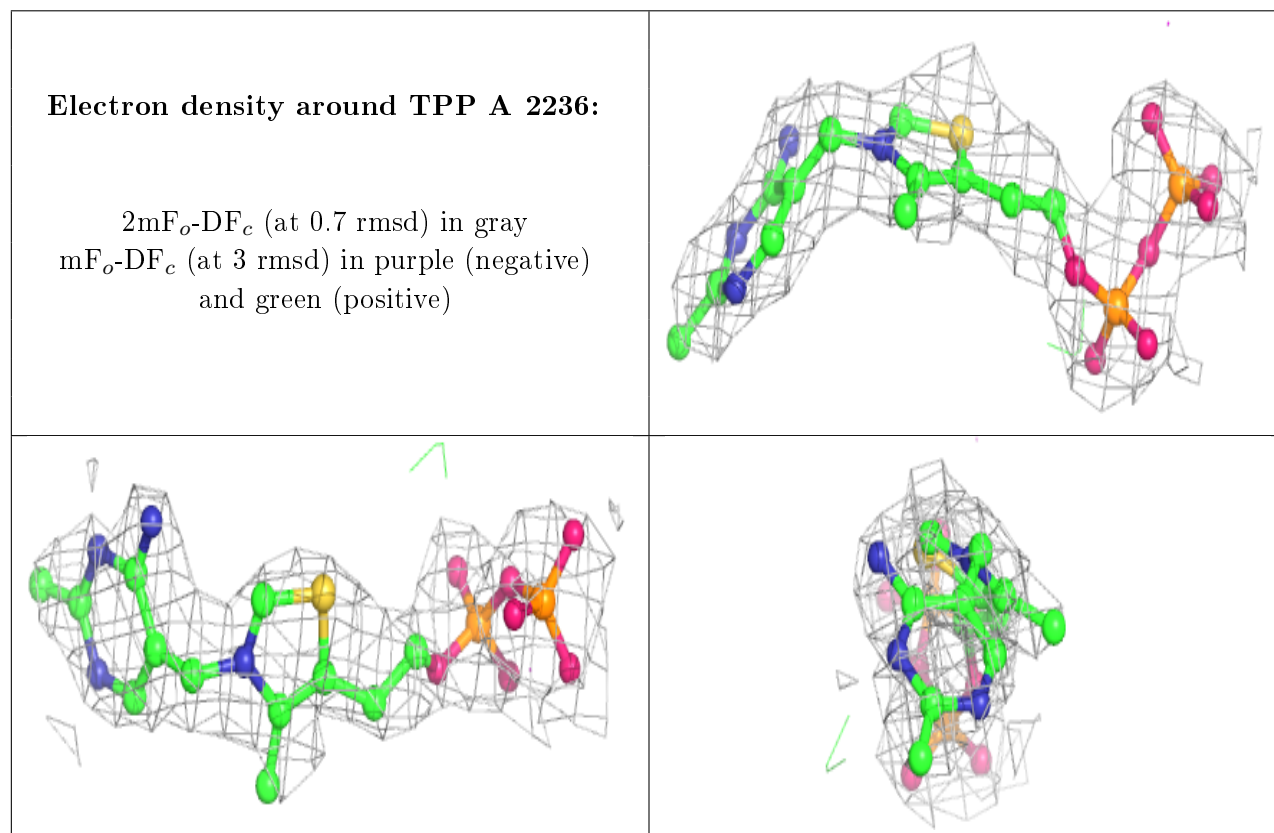
There are no carbohydrates in this entry.

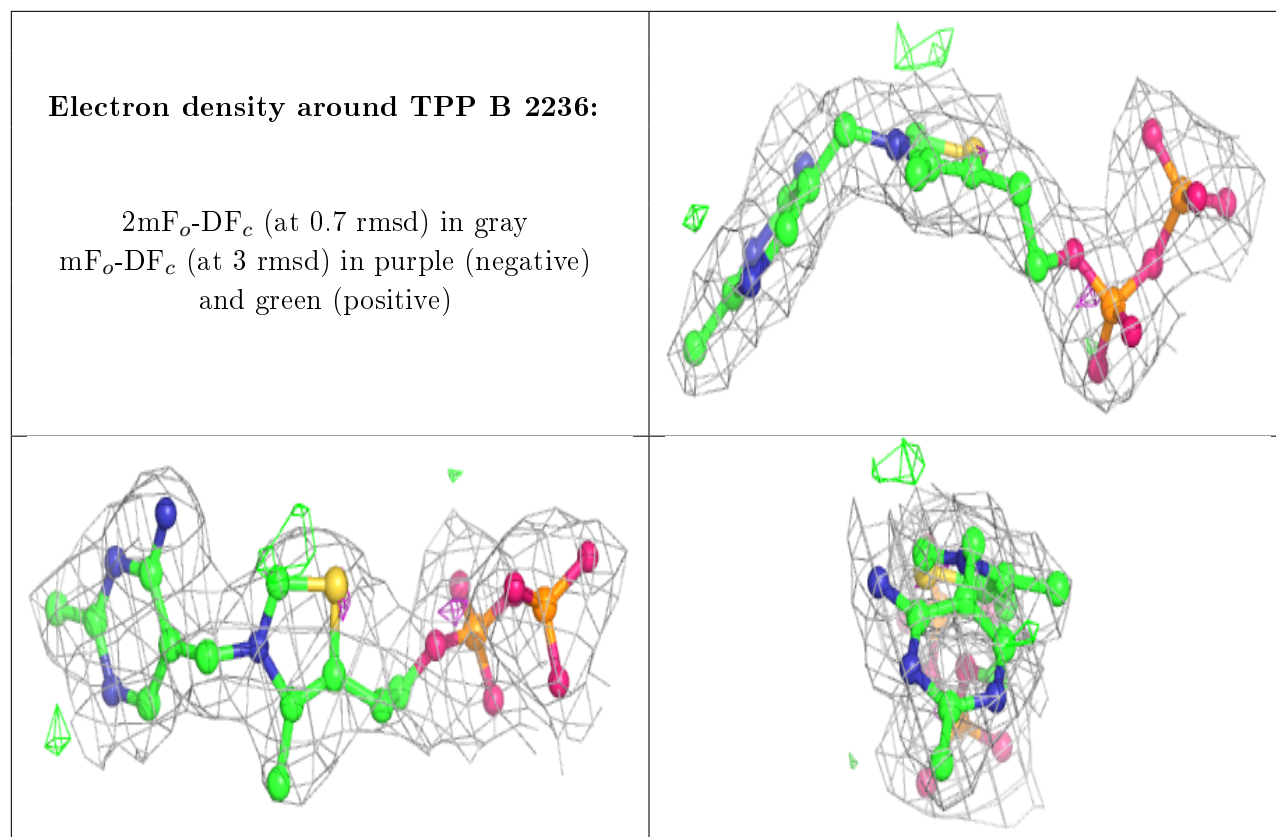
6.4 Ligands [i](#)

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, 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
6	PYR	A	2239	6/6	0.83	0.29	50,55,57,58	0
5	CA	A	2238	1/1	0.92	0.10	61,61,61,61	0
4	MG	A	2237	1/1	0.94	0.07	16,16,16,16	0
6	PYR	B	2239	6/6	0.94	0.17	17,23,25,26	0
2	SF4	A	2235	8/8	0.96	0.07	20,25,26,28	0
3	TPP	A	2236	26/26	0.96	0.14	23,36,48,52	0
2	SF4	A	2233	8/8	0.97	0.10	32,34,36,36	0
5	CA	B	2238	1/1	0.97	0.10	47,47,47,47	0
3	TPP	B	2236	26/26	0.97	0.13	3,14,23,31	0
2	SF4	A	2234	8/8	0.97	0.05	28,29,32,33	0
2	SF4	B	2235	8/8	0.98	0.05	6,11,12,12	0
2	SF4	B	2233	8/8	0.98	0.04	20,22,24,24	0
2	SF4	B	2234	8/8	0.98	0.05	7,10,12,13	0
4	MG	B	2237	1/1	0.99	0.05	3,3,3,3	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.