

wwPDB X-ray Structure Validation Summary Report (i)

Oct 23, 2021 – 04:17 PM EDT

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L. CASEI THYMIDYLATE SYNTHASE MUTANT E60Q TERNARY COM-
PLEX WITH FDUMP AND CB3717
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1996-09-18
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

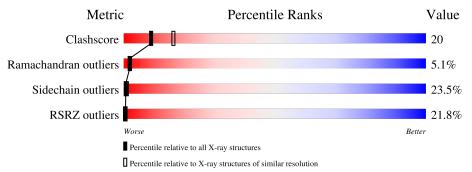
MolProbity		
		1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length		Quality of chain		
			22%			
1	А	316	37%	36%	22%	5%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3561 atoms, of which 789 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.

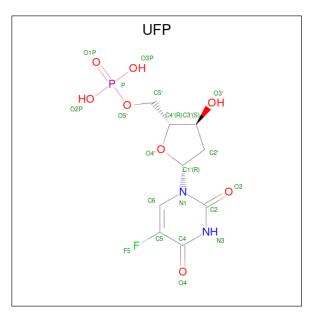
• Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues			Atom	IS			ZeroOcc	AltConf	Trace
1	А	316	Total 3122	C 1677	Н 532	N 439	O 466	S 8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	60	GLN	GLU	engineered mutation	UNP P00469
А	111	ALA	ASP	conflict	UNP P00469

• Molecule 2 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: UFP) (formula: $C_9H_{12}FN_2O_8P$).

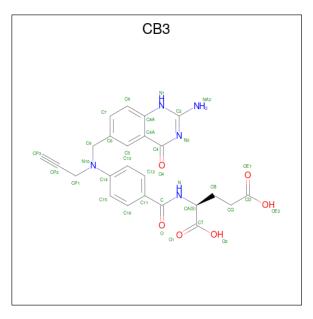


Mol	Chain	Residues			At	oms				ZeroOcc	AltConf
2	А	1	Total 22	•	_		N 2	~	Р 1	0	0

• Molecule 3 is 10-PROPARGYL-5,8-DIDEAZAFOLIC ACID (three-letter code: CB3)



(formula: $C_{24}H_{23}N_5O_6$).



Mol	Chain	Residues		Ato	\mathbf{pms}			ZeroOcc	AltConf
2	٨	1	Total	С	Η	Ν	0	0	0
5	A	1	39	24	4	5	6	0	0

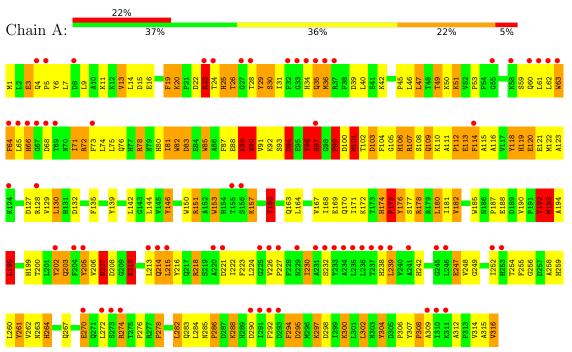
• Molecule 4 is water.

Mol	Chain	Residues	A	toms		ZeroOcc	AltConf
4	А	126	Total 378	Н 252	O 126	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: THYMIDYLATE SYNTHASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants	78.50Å 78.50Å 230.60Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 - 2.50	Depositor
Resolution (A)	67.98 - 2.19	EDS
% Data completeness	(Not available) $(15.00-2.50)$	Depositor
(in resolution range)	45.6(67.98-2.19)	EDS
R _{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.65 (at 2.18 \text{\AA})$	Xtriage
Refinement program	X-PLOR 3.1	Depositor
D D.	0.188 , (Not available)	Depositor
R, R_{free}	0.198 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	10.6	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36 , 850.3	EDS
L-test for twinning ²	$ \langle L \rangle = 0.43, \langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	3561	wwPDB-VP
Average B, all atoms $(Å^2)$	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: UFP, CB3 $\,$

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	Bo	nd lengths	B	ond angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	1.39	4/2674~(0.1%)	2.24	131/3634~(3.6%)

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	А	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	63	TRP	CG-CD2	-5.44	1.34	1.43
1	А	82	TRP	CD1-NE1	-5.34	1.28	1.38
1	А	232	SER	CA-CB	-5.14	1.45	1.52
1	А	286	PRO	CA-CB	-5.08	1.43	1.53

The worst 5 of 131 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	178	ARG	NE-CZ-NH1	17.20	128.90	120.30
1	А	178	ARG	NE-CZ-NH2	-12.21	114.19	120.30
1	А	96	TYR	CA-C-N	-10.74	93.58	117.20
1	А	63	TRP	CD1-CG-CD2	10.15	114.42	106.30
1	А	82	TRP	CD1-CG-CD2	9.60	113.98	106.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	195	LEU	Peptide
1	А	20	LYS	Peptide
1	А	205	TYR	Sidechain
1	А	4	GLN	Peptide
1	А	96	TYR	Sidechain

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	А	2590	532	2501	103	0
2	А	21	1	10	2	0
3	А	35	4	21	3	0
4	А	126	252	0	2	0
All	All	2772	789	2532	104	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 20.

The worst 5 of 104 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:239:LEU:HD23	1:A:284:LEU:HD21	1.39	1.00
1:A:108:SER:HA	1:A:111:ALA:HB2	1.46	0.95
1:A:99:PRO:HB2	1:A:101:MET:HG2	1.55	0.86
1:A:222:ILE:HD11	1:A:258:ALA:HB1	1.66	0.77
1:A:175:PRO:HB3	1:A:206:VAL:HG21	1.67	0.75

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	А	314/316~(99%)	242 (77%)	56 (18%)	16 (5%)	2 2	

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	5	PRO
1	А	94	ASP
1	А	101	MET
1	А	112	PRO
1	А	174	HIS

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	Analysed Rotameric			
1	А	277/277~(100%)	212~(76%)	65 (24%)	1 1	

5 of 65 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	270	GLU
1	А	278	PRO
1	А	97	HIS
1	А	94	ASP
1	А	286	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	35	GLN
1	А	76	GLN
1	А	80	HIS
1	А	207	ASN



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	Turne	Chain	Chain	Chain	Chain	Chain	Chain	Res	Link	B	ond leng	gths	E	ond ang	gles
	Type	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2					
3	CB3	А	318	-	30,37,37	2.60	11 (36%)	38,51,51	2.76	14 (36%)					
2	UFP	А	317	-	19,22,22	2.62	6 (31%)	24,33,33	2.97	5 (20%)					

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
3	CB3	А	318	-	-	14/21/28/28	0/3/3/3
2	UFP	А	317	-	-	7/7/22/22	0/2/2/2

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

Mol	Chain		• •			Observed(Å)	Ideal(Å)
2	А	317	UFP	C4-C5	8.93	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
3	А	318	CB3	O4-C4	5.92	1.39	1.24
3	А	318	CB3	CP1-N10	5.53	1.51	1.46
3	А	318	CB3	C9-N10	5.48	1.54	1.46
3	А	318	CB3	C12-C11	4.49	1.47	1.39

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The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	317	UFP	C4-N3-C2	11.12	124.53	115.14
3	А	318	CB3	C4A-C8A-N1	-8.37	119.06	123.60
2	А	317	UFP	C5-C4-N3	-6.55	115.48	122.39
3	А	318	CB3	C4A-C4-N3	-6.41	119.94	124.40
3	А	318	CB3	CP1-N10-C14	5.29	129.08	119.01

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	317	UFP	O4'-C1'-N1-C6
2	А	317	UFP	C3'-C4'-C5'-O5'
2	А	317	UFP	O4'-C4'-C5'-O5'
2	А	317	UFP	C5'-O5'-P-O1P
2	А	317	UFP	C5'-O5'-P-O2P

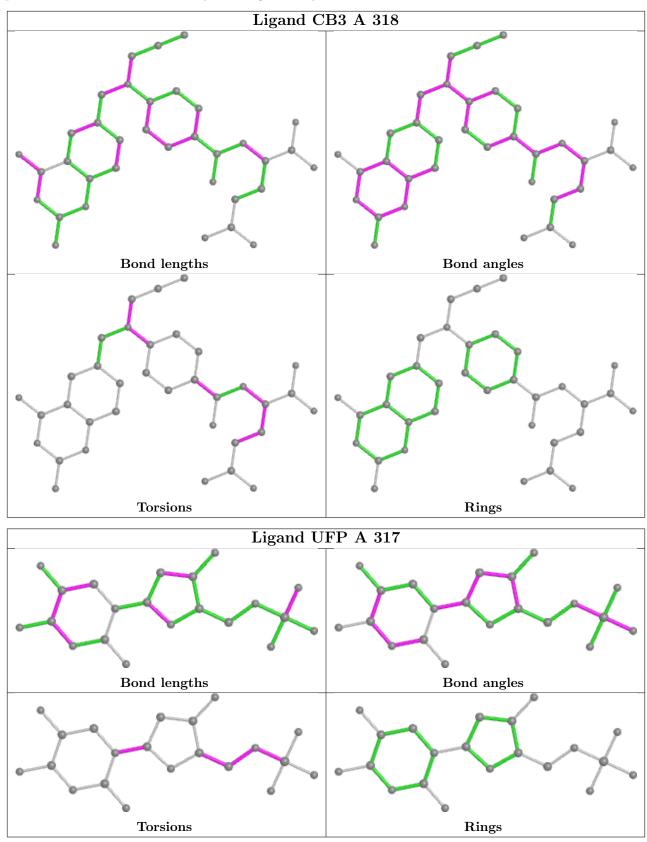
There are no ring outliers.

2 monomers are involved in 5 short contacts:

[Mol	Chain	Res	Type	Clashes	Symm-Clashes
	3	А	318	CB3	3	0
	2	А	317	UFP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient





equivalents in the CSD to analyse the geometry.



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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathbf{A}^2)$	Q < 0.9
1	А	316/316~(100%)	1.12	69 (21%) 0 0	3, 10, 18, 23	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	273	SER	16.5
1	А	233	TYR	12.6
1	А	61	LEU	11.3
1	А	232	SER	11.0
1	А	292	PHE	10.8

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

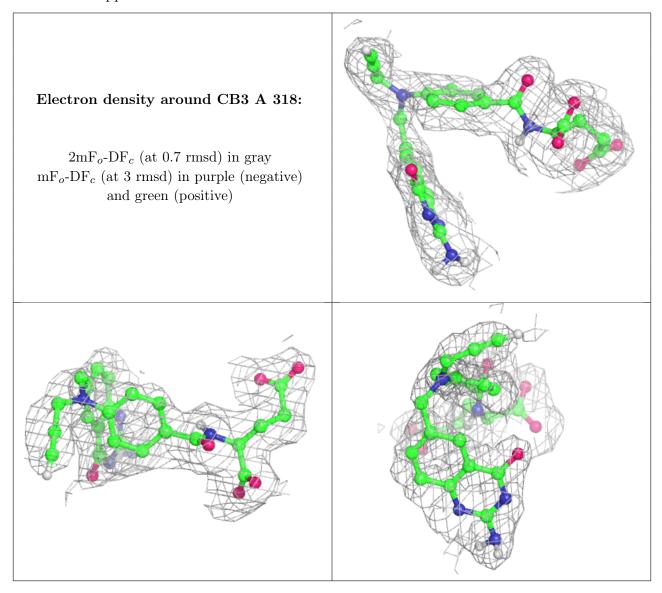
6.4 Ligands (i)

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

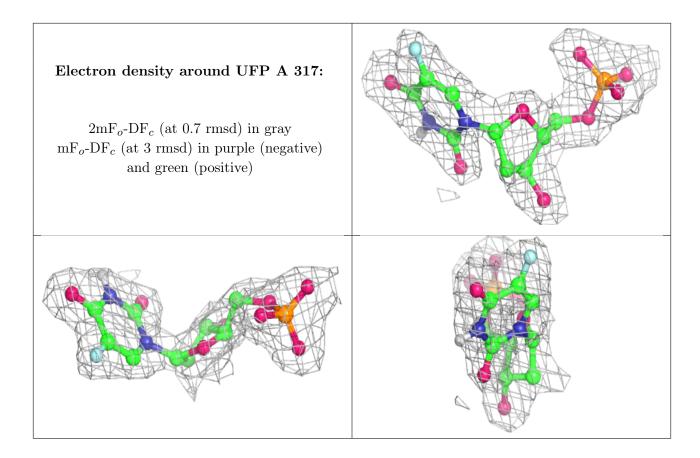
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
3	CB3	А	318	35/35	0.82	0.16	12,20,22,24	0
2	UFP	А	317	21/21	0.93	0.11	12,15,18,22	0



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.

