wwPDB X-ray Structure Validation Summary Report (i)

Jul 26, 2023 – 05:22 AM EDT

PDB ID	:	1AI8
Title	:	HUMAN ALPHA-THROMBIN TERNARY COMPLEX WITH THE EXOSITE INHIBITOR HIRUGEN AND ACTIVE SITE INHIBITOR PHCH 2OCO-D-DPA-PRO-BOROMPG
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Deposited on	:	1997-05-01
Resolution	:	1.85 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

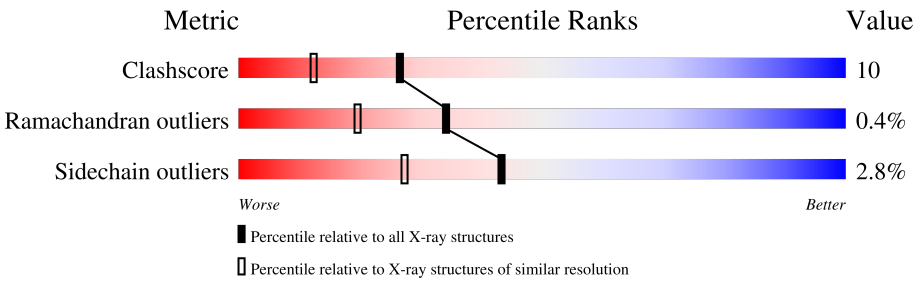
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 1.85 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))
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	53% 19% • 25%
2	H	259	70% 20% 7% •
3	I	12	42% 33% 8% 17%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2671 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 ALPHA-THROMBIN (SMALL SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	27	222	140	36	45	1	0	0	0

- Molecule 2 is a protein called ALPHA-THROMBIN (LARGE SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	251	2017	1288	355	360	14	0	0	0

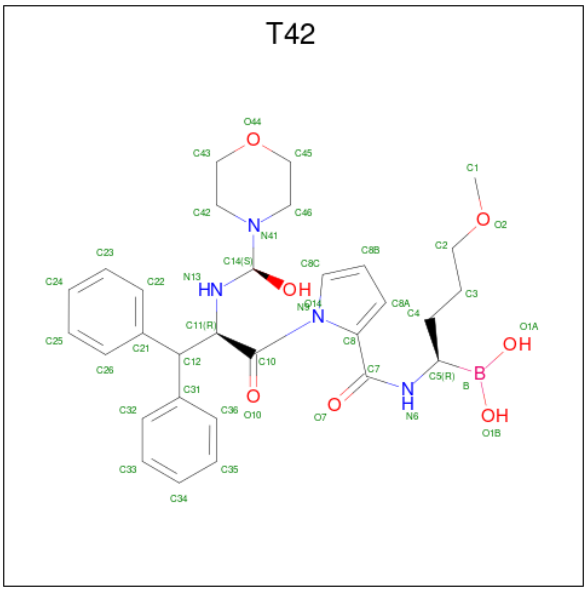
- Molecule 3 is a protein called HIRUDIN IIIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	10	89	56	10	22	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	54	GLU	GLY	conflict	UNP P28501

- Molecule 4 is MORPHOLINO-DIPHENYLALANINE-METHOXYPROPYLBORONIC ACID (three-letter code: T42) (formula: $C_{30}H_{39}BN_4O_7$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	B	C	N	O		
4	H	1	42	1	30	4	7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	L	39	39	39	0	0
			Total	O		
5	H	253	253	253	0	0
			Total	O		
5	I	9	9	9	0	0

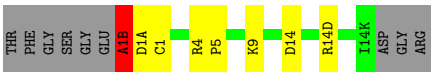
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

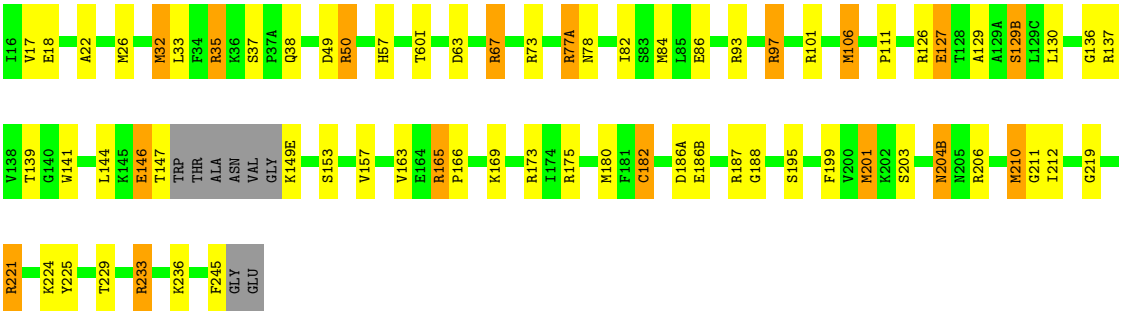
• Molecule 1: ALPHA-THROMBIN (SMALL SUBUNIT)

Chain L:



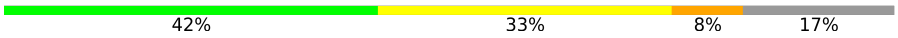
• Molecule 2: ALPHA-THROMBIN (LARGE SUBUNIT)

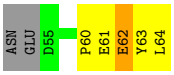
Chain H:



• Molecule 3: HIRUDIN IIIB

Chain I:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	69.71Å 71.46Å 71.65Å 90.00° 99.82° 90.00°	Depositor
Resolution (Å)	20.00 – 1.85	Depositor
% Data completeness (in resolution range)	96.1 (20.00-1.85)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2671	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

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: TYS, T42

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	L	1.31	1/224 (0.4%)	2.06	8/298 (2.7%)
2	H	0.98	1/2069 (0.0%)	1.32	28/2796 (1.0%)
3	I	0.65	0/73	1.57	0/96
All	All	1.01	2/2366 (0.1%)	1.41	36/3190 (1.1%)

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	L	0	2
2	H	0	1
3	I	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	4	ARG	CZ-NH1	6.03	1.40	1.33
2	H	153	SER	CA-CB	5.91	1.61	1.52

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	4	ARG	NE-CZ-NH2	9.96	125.28	120.30
1	L	1(B)	ALA	N-CA-CB	-8.08	98.78	110.10
2	H	187	ARG	NE-CZ-NH2	7.53	124.07	120.30
1	L	14	ASP	CB-CG-OD2	-7.45	111.59	118.30
2	H	50	ARG	NE-CZ-NH2	7.43	124.02	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	224	LYS	Mainchain
3	I	61	GLU	Peptide
1	L	1(B)	ALA	Mainchain
1	L	9	LYS	Mainchain

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	L	222	0	225	1	0
2	H	2017	0	1979	40	0
3	I	89	0	69	3	0
4	H	42	0	39	8	0
5	H	253	0	0	7	3
5	I	9	0	0	1	0
5	L	39	0	0	0	1
All	All	2671	0	2312	48	3

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 10.

The worst 5 of 48 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)
4:H:2:T42:C32	4:H:2:T42:H14	2.05	0.87
3:I:62:GLU:HB3	5:I:250:HOH:O	1.88	0.73
2:H:77(A):ARG:O	5:H:254:HOH:O	2.07	0.72
2:H:219:GLY:O	5:H:252:HOH:O	2.08	0.71
2:H:195:SER:OG	4:H:2:T42:C5	2.43	0.66

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:254:HOH:O	5:H:254:HOH:O[2_656]	1.49	0.71
5:H:345:HOH:O	5:H:345:HOH:O[2_656]	2.04	0.16
5:L:44:HOH:O	5:H:351:HOH:O[4_555]	2.15	0.05

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	L	25/36 (69%)	24 (96%)	1 (4%)	0	100	100
2	H	247/259 (95%)	238 (96%)	9 (4%)	0	100	100
3	I	7/12 (58%)	5 (71%)	1 (14%)	1 (14%)	0	0
All	All	279/307 (91%)	267 (96%)	11 (4%)	1 (0%)	34	19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	62	GLU

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	L	25/31 (81%)	24 (96%)	1 (4%)	31	14
2	H	216/225 (96%)	210 (97%)	6 (3%)	43	27
3	I	8/11 (73%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	249/267 (93%)	242 (97%)	7 (3%)	43 27

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	129(B)	SER
2	H	182	CYS
2	H	233	ARG
2	H	204(B)	ASN
2	H	127	GLU

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

Mol	Chain	Res	Type
2	H	78	ASN
2	H	156	GLN
2	H	204(B)	ASN
2	H	244	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
3	TYS	I	63	3	15,16,17	4.45	2 (13%)	18,22,24	3.00	10 (55%)

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	TYS	I	63	3	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	63	TYS	OH-S	16.88	1.84	1.58
3	I	63	TYS	OH-CZ	-2.55	1.38	1.42

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	63	TYS	O3-S-OH	-5.98	91.44	105.83
3	I	63	TYS	OH-S-O2	-4.75	93.86	107.71
3	I	63	TYS	CE2-CZ-CE1	3.98	126.30	120.18
3	I	63	TYS	CG-CB-CA	-3.91	106.18	114.10
3	I	63	TYS	O2-S-O1	3.67	126.96	112.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
4	T42	H	2	2	35,45,45	5.45	17 (48%)	34,60,60	3.72	17 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	T42	H	2	2	-	3/27/53/53	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	2	T42	C8C-N9	19.74	1.57	1.38
4	H	2	T42	C8A-C8	13.96	1.63	1.40
4	H	2	T42	C8C-C8B	12.92	1.66	1.38
4	H	2	T42	C8B-C8A	10.44	1.73	1.39
4	H	2	T42	C26-C21	5.53	1.48	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	2	T42	C8B-C8C-N9	-15.53	95.63	107.67
4	H	2	T42	C36-C31-C32	5.09	124.64	118.29
4	H	2	T42	C46-N41-C42	4.97	118.16	109.08
4	H	2	T42	C25-C26-C21	-4.59	114.97	120.65
4	H	2	T42	C43-C42-N41	4.22	113.70	109.66

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	2	T42	O7-C7-C8-C8A
4	H	2	T42	C3-C4-C5-B
4	H	2	T42	C10-C11-N13-C14

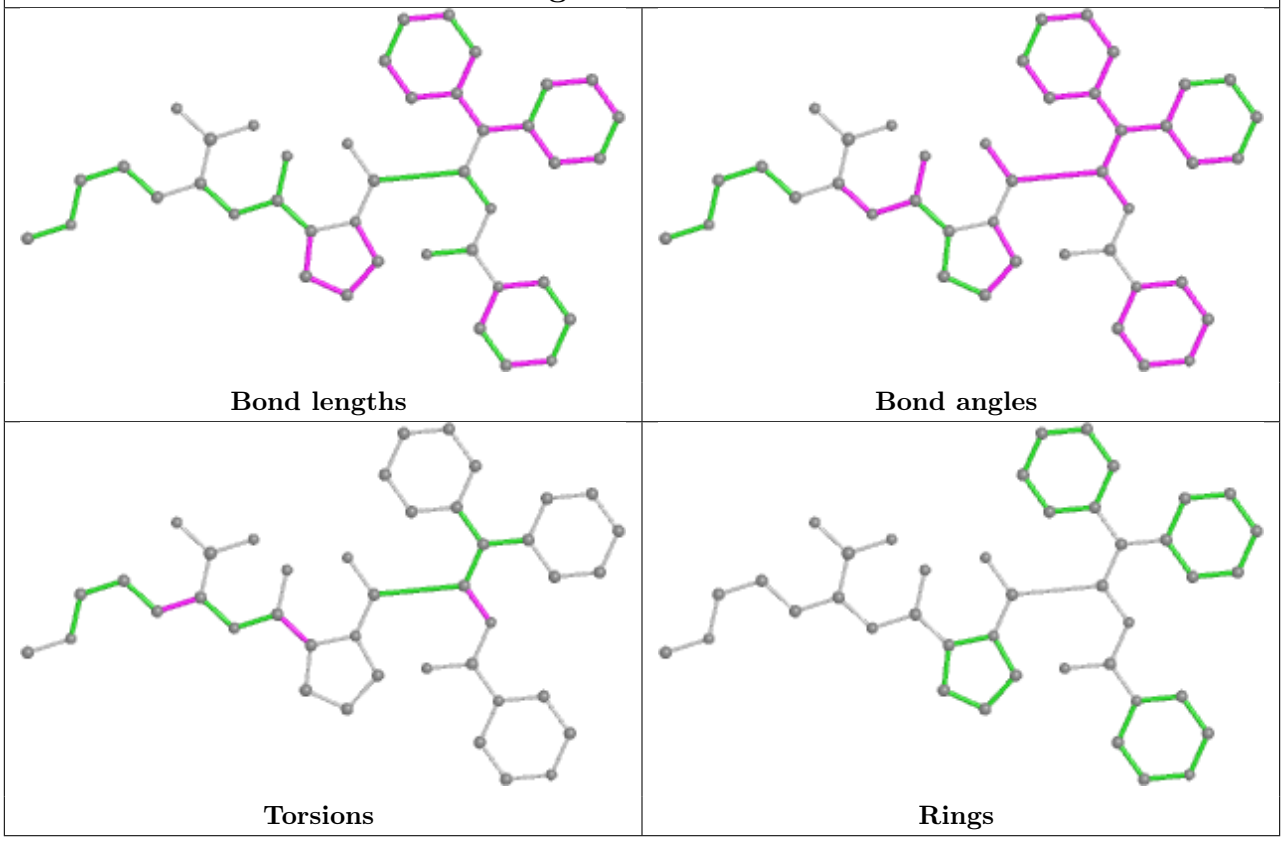
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	2	T42	8	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.

Ligand T42 H 2



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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.