



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 07:45 am BST

PDB ID : 1IB1
Title : CRYSTAL STRUCTURE OF THE 14-3-3 ZETA:SEROTONIN N-ACETYLTRANSFERASE COMPLEX
Authors : Obsil, T.; Ghirlando, R.; Klein, D.C.; Ganguly, S.; Dyda, F.
Deposited on : 2001-03-26
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)	:	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)	:	2.11

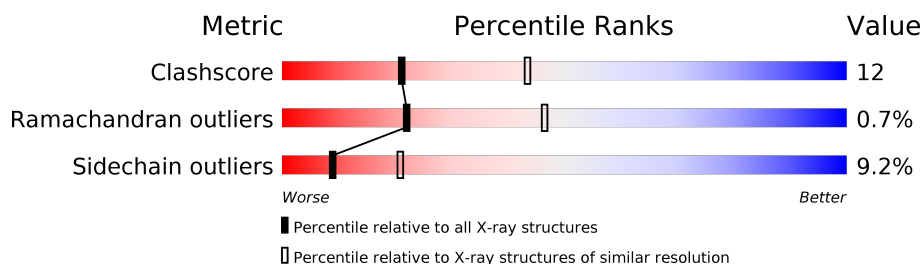
1 Overall quality at a glance

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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	245	
1	B	245	
1	C	245	
1	D	245	
2	E	200	
2	F	200	
2	G	200	
2	H	200	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13407 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 14-3-3 ZETA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1821	1142	306	364	9			
1	B	227	Total	C	N	O	S	0	0	0
			1821	1142	306	364	9			
1	C	227	Total	C	N	O	S	0	0	0
			1821	1142	306	364	9			
1	D	227	Total	C	N	O	S	0	0	0
			1821	1142	306	364	9			

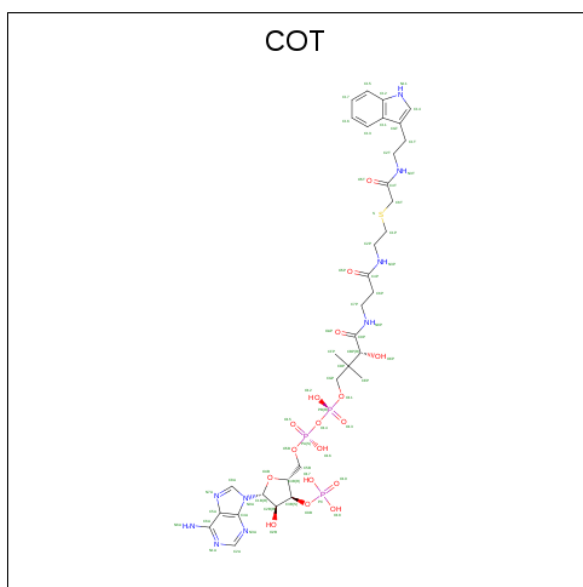
- Molecule 2 is a protein called SEROTONIN N-ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	179	Total	C	N	O	P	S	0	0
			1415	897	263	246	1	8		
2	F	179	Total	C	N	O	P	S	0	0
			1415	897	263	246	1	8		
2	G	179	Total	C	N	O	P	S	0	0
			1415	897	263	246	1	8		
2	H	179	Total	C	N	O	P	S	0	0
			1415	897	263	246	1	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	31	TPO	THR	MODIFIED RESIDUE	UNP Q29495
F	31	TPO	THR	MODIFIED RESIDUE	UNP Q29495
G	31	TPO	THR	MODIFIED RESIDUE	UNP Q29495
H	31	TPO	THR	MODIFIED RESIDUE	UNP Q29495

- Molecule 3 is COA-S-ACETYL TRYPTAMINE (three-letter code: COT) (formula: $C_{33}H_{48}N_9O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	E	1	Total 63	C 33	N 9	O 17	P 3	S 1	0	0
3	F	1	Total 63	C 33	N 9	O 17	P 3	S 1	0	0
3	G	1	Total 63	C 33	N 9	O 17	P 3	S 1	0	0
3	H	1	Total 63	C 33	N 9	O 17	P 3	S 1	0	0

- Molecule 4 is water.

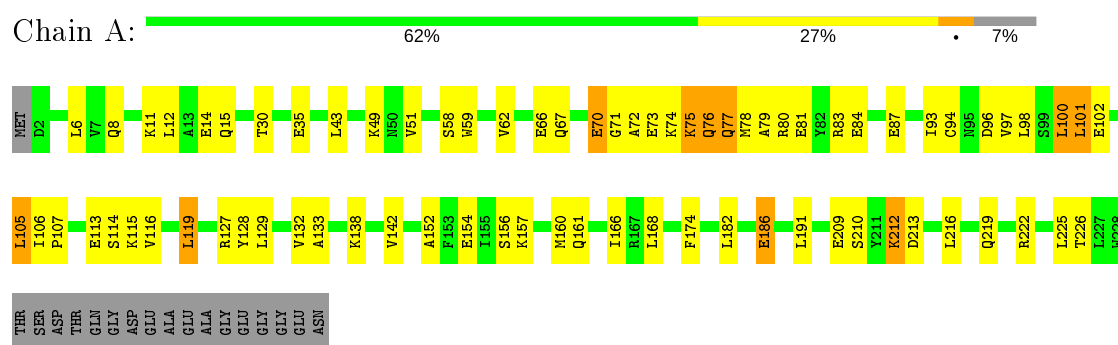
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total	O	0	0
			28	28		
4	B	20	Total	O	0	0
			20	20		
4	C	42	Total	O	0	0
			42	42		
4	D	31	Total	O	0	0
			31	31		
4	E	24	Total	O	0	0
			24	24		
4	F	21	Total	O	0	0
			21	21		
4	G	23	Total	O	0	0
			23	23		
4	H	22	Total	O	0	0
			22	22		

3 Residue-property plots [i](#)

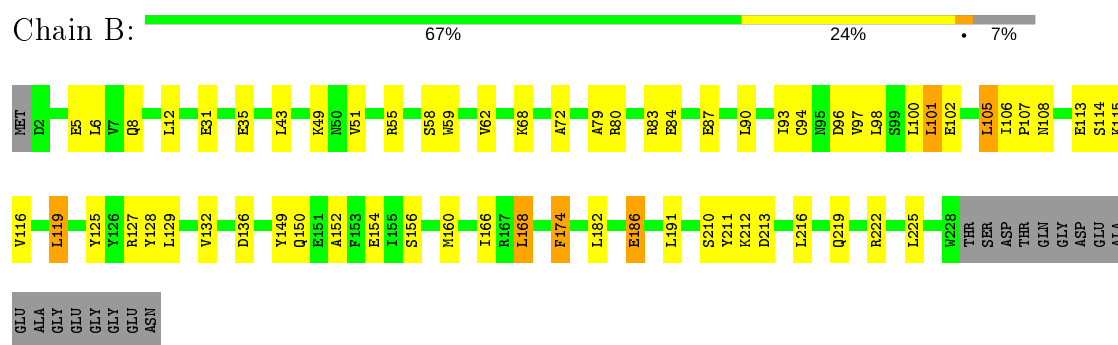
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

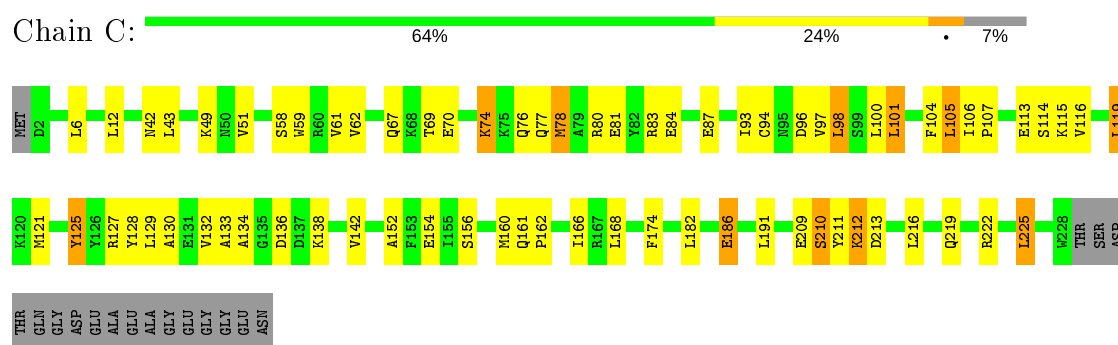
• Molecule 1: 14-3-3 ZETA ISOFORM



• Molecule 1: 14-3-3 ZETA ISOFORM



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• Molecule 1: 14-3-3 ZETA ISOFORM

D213	E113	Met
L216	S114	D2
Q219	K115	L6
R222	V116	K9
L275	L119	A16
R228	Y125	Y19
THR	R127	E35
SER	Y128	E39
ASP	L129	L43
THR	V132	V51
GLN	K138	V52
GLY	K139	G53
ASP	V142	A54
GLU	D143	R55
ALA	Q144	S58
ALA	Y149	W59
GLY	A152	R60
GLU	F153	V61
GLU	E154	V62
ASN	I155	Q67
	S156	K68
	M160	T69
	I166	K74
	R167	A79
	L168	R90
	F174	R83
	S175	E94
	V176	E97
	E180	L90
	I181	I93
	L182	C94
	E186	N95
	L191	D96
	A195	Y97
	A201	L98
	D204	S99
	S207	L100
	E208	L101
	E209	E102
	S210	L105
	Y211	P107
	W212	

L124	SER
Q132	THR
V138	PRO
L139	SER
R142	VAL
Y143	HIS
L144	CYS
H145	LEU
H146	PRO
V147	LEU
Q150	HIS
P151	LEU
R155	PRO
A156	\$18
V157	G19
L158	120
M159	\$23
C160	P24
E161	G25
V165	R28
P166	R29
F167	H30
R170	T31
V183	L32
G184	I33
S185	F33
L186	A34
H192	N35
R196	A46
GLY	B50
HIS	S60
ALA	G61
ALA	N62
LEU	L67
	L76
	C77
	L80
	B87
	G88
	R89
	I94
	L98
	W99
	D100
	H117

899	D100	T105	S108	R115	G116	H117	H122	V138	L139	R142	Y143	V147	Q150	P151	A152	V153	R154	R155	A156	V157	E161	V165	P166	F167	R170	G177	H192	R196	GLY	HIS	ALA	ALA	LEU	SER	THR	PRO	SER	VAL	HIS	CYS	LEU	LYS	PRO	SER	PRO	LEU	HIS	LEU	PRO	G19	L20	P21	G22	S23	P24	G25	R26	R29	H30	T31	L32	P33	A34	N35	D44	V48	E52	R53	I57	S60	P64	L67	T75	L76	C77	L80	E87	G88	R89	T98
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SER	THR	PRO	SER	VAL	HIS	CYS	LEU	LYS	PRO	SER	PRO	LEU	HIS	LEU	PRO	G18	G19	I20	G23	P24	G25	R26	R29	G30	T31	L32	F33	A34	N35	R53	I57	S60	L67	L76	C77	P78	E79	L80	V86	E87	G88	R89	G96	S97	L98	A99	D100	R103
L109	R115	G116	H117	Q132	Q133	G134	K135	V138	L139	R142	Y143	V147	Q150	P151	R155	A156	V157	L158	M159	C160	E161	V165	P166	F167	R170	F173	A180	S185	M191	H192	R196	GLY	HIS	ALA	ALA	LEU												

SER	THR	PRO	SER	SER	VAL	HIS	CYS	LEU	LYS	PRO	PRO	SER	PRO	HIS	LEU	LEU	PRO	S18	G19	I20	S23	R26	Q27	R28	R29	H30	T31	P32	P33	A34	N35	D44	V48	R53	I57	S60	L67	L76	G77	L80	W84	R87	G88	R89	L98	G99	D100
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.72Å 75.08Å 101.78Å 90.14° 90.06° 63.04°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	99.3 (20.00-2.70)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.204 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13407	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: TPO, COT

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	0.42	0/1846	0.67	0/2482
1	B	0.42	0/1846	0.62	0/2482
1	C	0.42	0/1846	0.64	0/2482
1	D	0.41	0/1846	0.65	0/2482
2	E	0.44	0/1443	0.69	1/1956 (0.1%)
2	F	0.46	0/1443	0.71	1/1956 (0.1%)
2	G	0.44	0/1443	0.68	1/1956 (0.1%)
2	H	0.45	0/1443	0.68	0/1956
All	All	0.43	0/13156	0.67	3/17752 (0.0%)

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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	19	GLY	N-CA-C	5.19	126.06	113.10
2	F	19	GLY	N-CA-C	5.18	126.05	113.10
2	E	19	GLY	N-CA-C	5.16	125.99	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	125	TYR	Sidechain
1	C	125	TYR	Sidechain
1	D	125	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1821	0	1809	67	0
1	B	1821	0	1809	40	1
1	C	1821	0	1809	48	0
1	D	1821	0	1809	49	0
2	E	1415	0	1382	32	0
2	F	1415	0	1382	43	1
2	G	1415	0	1382	44	0
2	H	1415	0	1382	34	0
3	E	63	0	44	1	0
3	F	63	0	44	1	0
3	G	63	0	44	1	0
3	H	63	0	44	0	0
4	A	28	0	0	19	0
4	B	20	0	0	5	0
4	C	42	0	0	7	1
4	D	31	0	0	13	1
4	E	24	0	0	2	0
4	F	21	0	0	6	0
4	G	23	0	0	10	0
4	H	22	0	0	2	0
All	All	13407	0	12940	317	2

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 12.

The worst 5 of 317 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:D:80:ARG:HD2	4:D:3635:HOH:O	1.34	1.22
1:D:144:GLN:HG3	4:D:4412:HOH:O	1.37	1.20
1:A:73:GLU:HB2	4:A:2487:HOH:O	1.57	1.03
1:A:75:LYS:HE3	1:B:8:GLN:HG2	1.48	0.94
1:A:226:THR:CB	4:A:3511:HOH:O	2.24	0.86

All (2) 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)
2:F:177:GLY:N	4:C:2713:HOH:O[1_554]	2.05	0.15
1:B:31:GLU:O	4:D:4373:HOH:O[1_464]	2.09	0.11

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/245 (92%)	216 (96%)	8 (4%)	1 (0%)	34	60
1	B	225/245 (92%)	215 (96%)	8 (4%)	2 (1%)	17	40
1	C	225/245 (92%)	218 (97%)	6 (3%)	1 (0%)	34	60
1	D	225/245 (92%)	216 (96%)	9 (4%)	0	100	100
2	E	176/200 (88%)	167 (95%)	7 (4%)	2 (1%)	14	34
2	F	176/200 (88%)	169 (96%)	5 (3%)	2 (1%)	14	34
2	G	176/200 (88%)	169 (96%)	5 (3%)	2 (1%)	14	34
2	H	176/200 (88%)	168 (96%)	6 (3%)	2 (1%)	14	34
All	All	1604/1780 (90%)	1538 (96%)	54 (3%)	12 (1%)	22	46

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	72	ALA
1	C	134	ALA
1	A	75	LYS
2	E	151	PRO
2	F	151	PRO

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	197/209 (94%)	172 (87%)	25 (13%)	4	10
1	B	197/209 (94%)	177 (90%)	20 (10%)	7	17
1	C	197/209 (94%)	174 (88%)	23 (12%)	5	12
1	D	197/209 (94%)	173 (88%)	24 (12%)	5	11
2	E	148/166 (89%)	139 (94%)	9 (6%)	18	41
2	F	148/166 (89%)	140 (95%)	8 (5%)	22	47
2	G	148/166 (89%)	140 (95%)	8 (5%)	22	47
2	H	148/166 (89%)	138 (93%)	10 (7%)	16	36
All	All	1380/1500 (92%)	1253 (91%)	127 (9%)	9	21

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	119	LEU
1	D	68	LYS
2	H	27	GLN
1	C	156	SER
1	C	191	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	219	GLN

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Mol	Chain	Res	Type
2	E	62	ASN
2	H	62	ASN
1	D	108	ASN
1	B	77	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TPO	F	31	2	8,10,11	1.13	0	10,14,16	1.13	0
2	TPO	E	31	2	8,10,11	1.39	2 (25%)	10,14,16	1.13	0
2	TPO	H	31	2	8,10,11	1.44	2 (25%)	10,14,16	1.15	0
2	TPO	G	31	2	8,10,11	1.29	2 (25%)	10,14,16	1.21	0

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	TPO	F	31	2	-	1/9/11/13	-
2	TPO	E	31	2	-	1/9/11/13	-
2	TPO	H	31	2	-	1/9/11/13	-
2	TPO	G	31	2	-	1/9/11/13	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	31	TPO	P-O2P	-2.40	1.45	1.54
2	E	31	TPO	P-O3P	-2.32	1.45	1.54
2	G	31	TPO	P-O2P	-2.32	1.45	1.54
2	E	31	TPO	P-O2P	-2.17	1.46	1.54
2	G	31	TPO	P-O3P	-2.04	1.47	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	31	TPO	O-C-CA-CB
2	E	31	TPO	O-C-CA-CB
2	H	31	TPO	O-C-CA-CB
2	G	31	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	31	TPO	2	0
2	E	31	TPO	2	0
2	H	31	TPO	2	0
2	G	31	TPO	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	COT	E	401	-	58,67,67	0.84	1 (1%)	69,98,98	0.99	4 (5%)
3	COT	G	402	-	58,67,67	0.84	1 (1%)	69,98,98	0.98	3 (4%)
3	COT	H	403	-	58,67,67	0.83	1 (1%)	69,98,98	0.97	3 (4%)
3	COT	F	400	-	58,67,67	0.87	1 (1%)	69,98,98	0.96	2 (2%)

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	COT	E	401	-	-	10/54/74/74	0/5/5/5
3	COT	G	402	-	-	10/54/74/74	0/5/5/5
3	COT	H	403	-	-	10/54/74/74	0/5/5/5
3	COT	F	400	-	-	10/54/74/74	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	COT	O4B-C1B	2.52	1.44	1.41
3	G	402	COT	O4B-C1B	2.40	1.44	1.41
3	H	403	COT	O4B-C1B	2.38	1.44	1.41
3	F	400	COT	O4B-C1B	2.34	1.44	1.41

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	403	COT	N3A-C2A-N1A	-3.42	123.34	128.68
3	F	400	COT	N3A-C2A-N1A	-3.37	123.41	128.68
3	E	401	COT	N3A-C2A-N1A	-3.30	123.52	128.68
3	G	402	COT	N3A-C2A-N1A	-3.17	123.72	128.68
3	G	402	COT	C16-C13-C11	-2.42	117.54	120.89

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	401	COT	CGT-C1T-C2T-N3T
3	E	401	COT	C3B-O3B-PC-O19
3	G	402	COT	CGT-C1T-C2T-N3T

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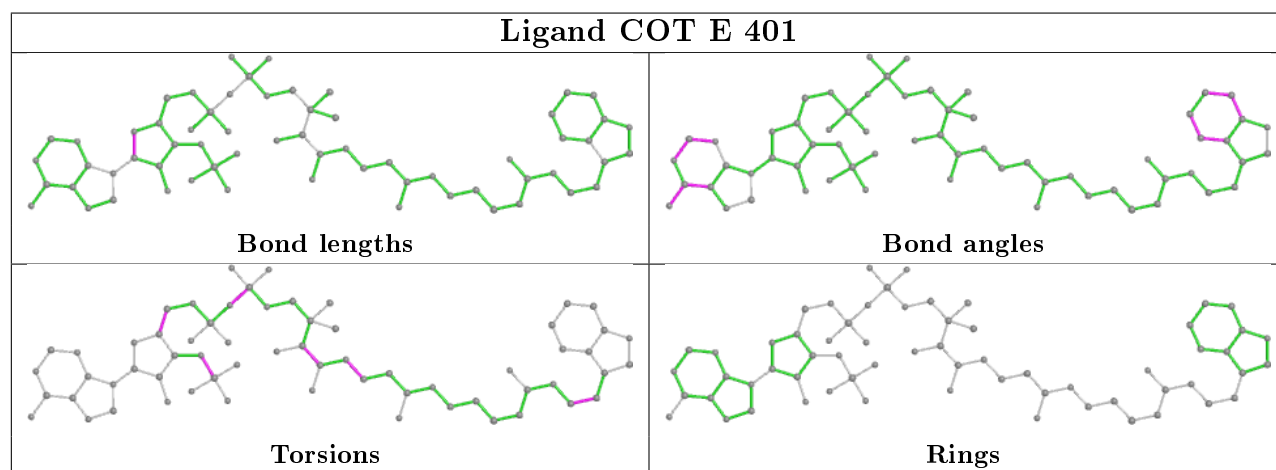
Mol	Chain	Res	Type	Atoms
3	G	402	COT	C3B-O3B-PC-O19
3	H	403	COT	CGT-C1T-C2T-N3T

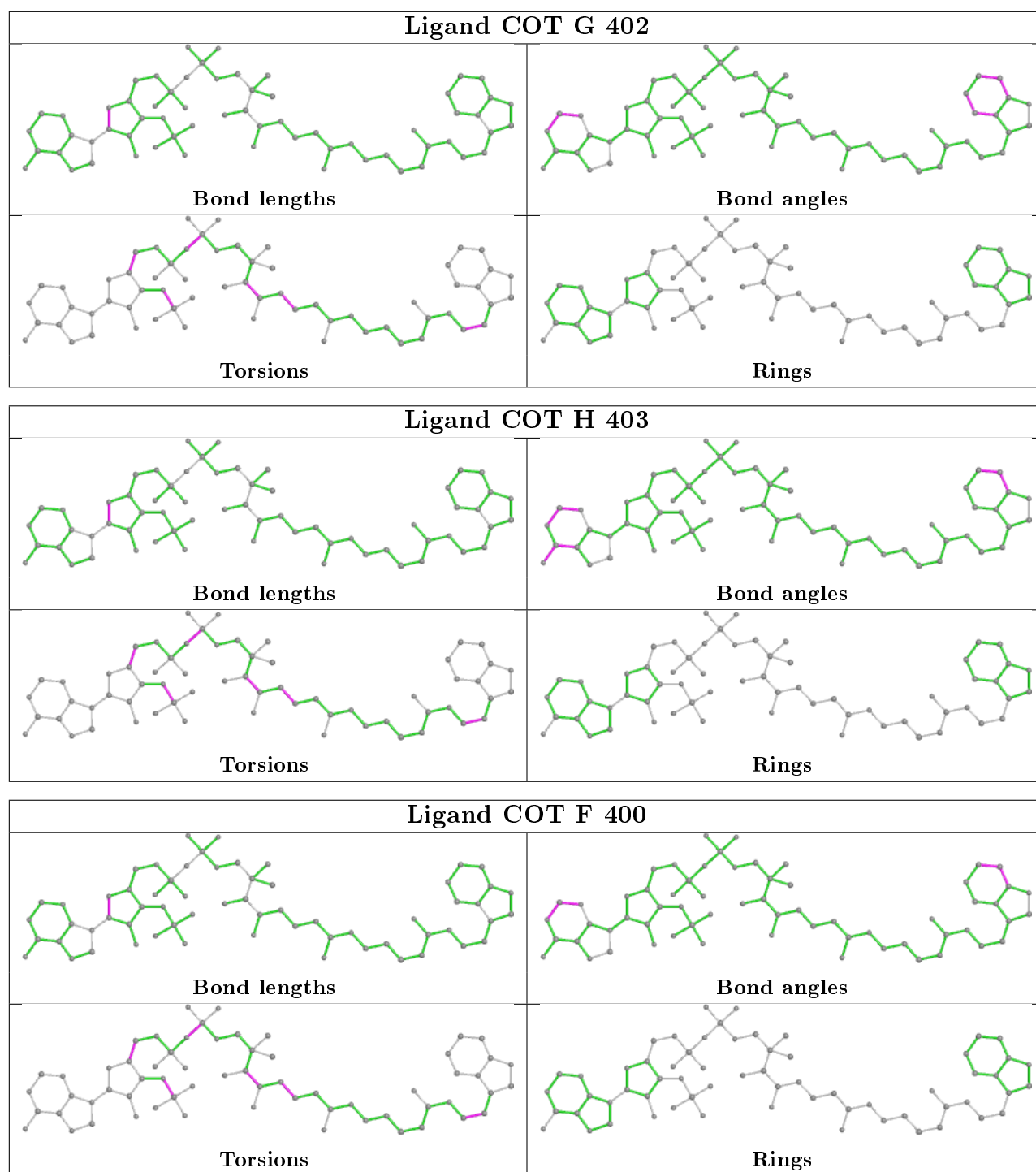
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	401	COT	1	0
3	G	402	COT	1	0
3	F	400	COT	1	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.