



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:14 PM UTC

PDB ID : 1T7Q / pdb_00001t7q
Title : Crystal structure of the F565A mutant of murine carnitine acetyltransferase
in complex with carnitine and CoA
Authors : Hsiao, Y.-S.; Jogl, G.; Tong, L.
Deposited on : 2004-05-10
Resolution : 1.80 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

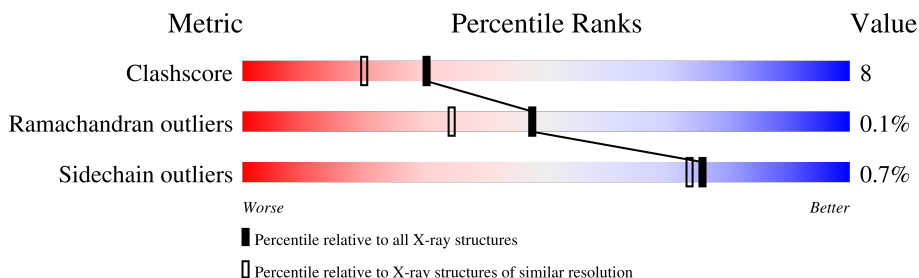
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	618	
1	B	618	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10822 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 Carnitine acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	599	Total	C	N	O	S	0	0	0
			4774	3042	825	878	29			
1	B	599	Total	C	N	O	S	0	0	0
			4774	3042	825	878	29			

There are 44 discrepancies between the modelled and reference sequences:

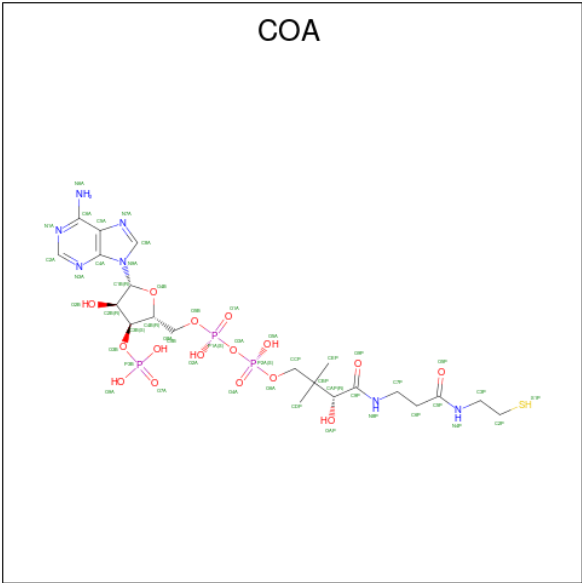
Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	expression tag	UNP P47934
A	10	GLY	-	expression tag	UNP P47934
A	11	SER	-	expression tag	UNP P47934
A	12	SER	-	expression tag	UNP P47934
A	13	HIS	-	expression tag	UNP P47934
A	14	HIS	-	expression tag	UNP P47934
A	15	HIS	-	expression tag	UNP P47934
A	16	HIS	-	expression tag	UNP P47934
A	17	HIS	-	expression tag	UNP P47934
A	18	HIS	-	expression tag	UNP P47934
A	19	SER	-	expression tag	UNP P47934
A	20	SER	-	expression tag	UNP P47934
A	21	GLY	-	expression tag	UNP P47934
A	22	LEU	-	expression tag	UNP P47934
A	23	VAL	-	expression tag	UNP P47934
A	24	PRO	-	expression tag	UNP P47934
A	25	ARG	-	expression tag	UNP P47934
A	26	GLY	-	expression tag	UNP P47934
A	27	SER	-	expression tag	UNP P47934
A	28	HIS	-	expression tag	UNP P47934
A	29	MET	-	expression tag	UNP P47934
A	565	ALA	PHE	engineered mutation	UNP P47934
B	9	MET	-	expression tag	UNP P47934
B	10	GLY	-	expression tag	UNP P47934
B	11	SER	-	expression tag	UNP P47934

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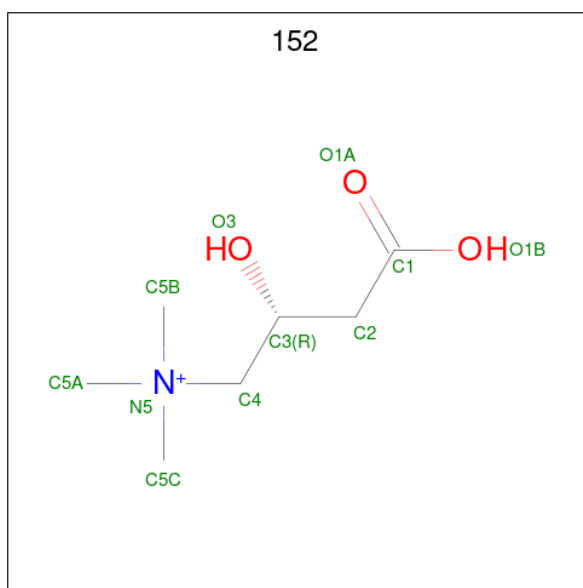
Chain	Residue	Modelled	Actual	Comment	Reference
B	12	SER	-	expression tag	UNP P47934
B	13	HIS	-	expression tag	UNP P47934
B	14	HIS	-	expression tag	UNP P47934
B	15	HIS	-	expression tag	UNP P47934
B	16	HIS	-	expression tag	UNP P47934
B	17	HIS	-	expression tag	UNP P47934
B	18	HIS	-	expression tag	UNP P47934
B	19	SER	-	expression tag	UNP P47934
B	20	SER	-	expression tag	UNP P47934
B	21	GLY	-	expression tag	UNP P47934
B	22	LEU	-	expression tag	UNP P47934
B	23	VAL	-	expression tag	UNP P47934
B	24	PRO	-	expression tag	UNP P47934
B	25	ARG	-	expression tag	UNP P47934
B	26	GLY	-	expression tag	UNP P47934
B	27	SER	-	expression tag	UNP P47934
B	28	HIS	-	expression tag	UNP P47934
B	29	MET	-	expression tag	UNP P47934
B	565	ALA	PHE	engineered mutation	UNP P47934

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



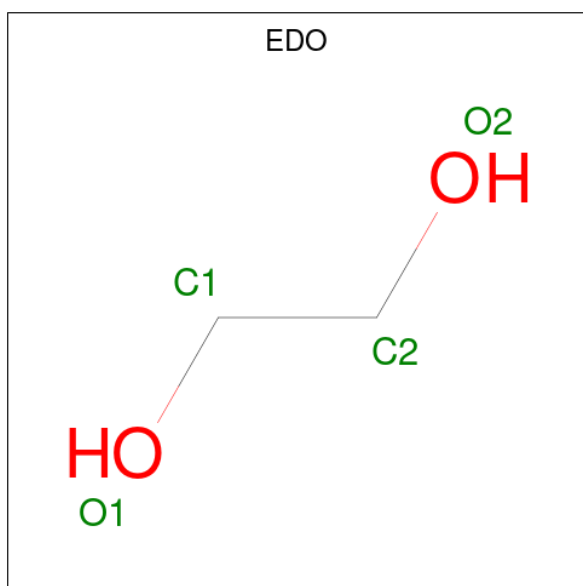
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is CARNITINE (CCD ID: 152) (formula: $C_7H_{16}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	7	1	3		
3	B	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is water.

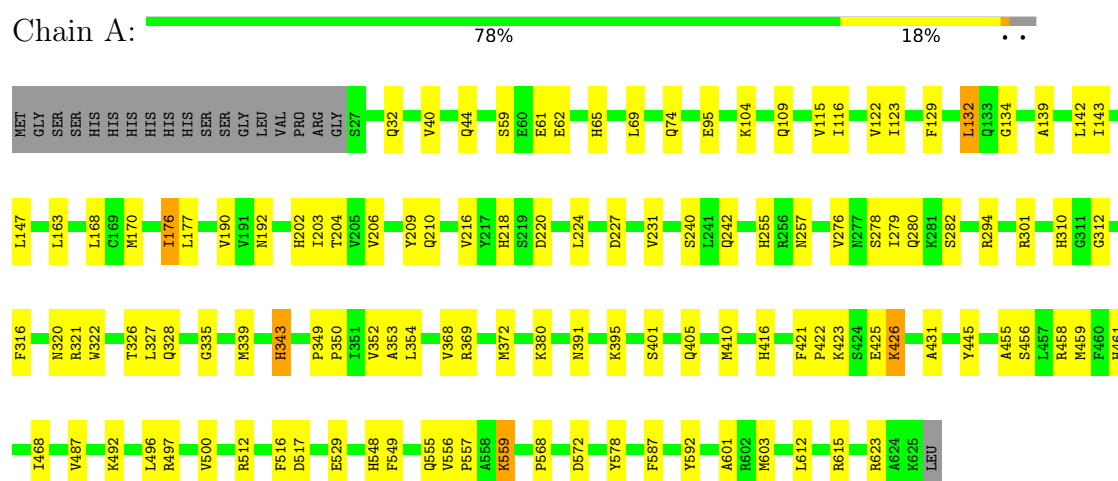
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	503	Total	O	0	0
			503	503		
5	B	645	Total	O	0	0
			645	645		

3 Residue-property plots

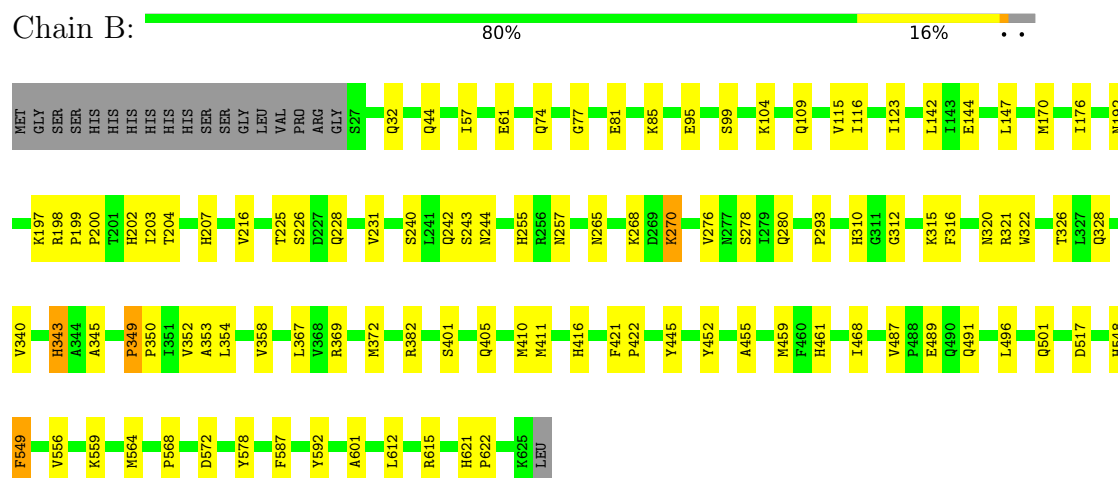
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: Carnitine acetyltransferase



4 Data and refinement statistics

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	165.13Å 89.63Å 123.05Å 90.00° 129.23° 90.00°	Depositor
Resolution (Å)	29.17 – 1.80	Depositor
% Data completeness (in resolution range)	92.7 (29.17-1.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.191 , 0.221	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10822	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 152, COA

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	0.35	1/4889 (0.0%)	0.85	11/6624 (0.2%)
1	B	0.37	0/4889	0.86	13/6624 (0.2%)
All	All	0.36	1/9778 (0.0%)	0.85	24/13248 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	603	MET	SD-CE	-5.06	1.67	1.79

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	HIS	N-CA-C	7.90	122.02	112.38
1	A	343	HIS	N-CA-C	7.00	120.92	112.38
1	B	517	ASP	N-CA-C	6.56	118.09	111.07
1	B	99	SER	N-CA-C	6.41	118.84	111.02
1	A	517	ASP	N-CA-C	6.36	117.87	111.07
1	A	176	ILE	N-CA-C	6.08	119.58	111.44
1	B	57	ILE	N-CA-C	6.05	118.97	113.10
1	B	340	VAL	N-CA-C	-6.03	100.01	108.27
1	B	445	TYR	N-CA-C	5.71	120.41	113.38
1	A	40	VAL	N-CA-C	-5.71	101.22	107.73
1	A	353	ALA	N-CA-C	-5.70	105.07	111.28
1	B	549	PHE	N-CA-C	5.64	118.58	107.98
1	B	459	MET	N-CA-C	-5.41	106.63	113.18
1	A	549	PHE	N-CA-C	5.41	118.18	108.17
1	A	203	ILE	N-CA-C	-5.38	101.65	109.29
1	B	203	ILE	N-CA-C	-5.35	101.36	108.96
1	A	445	TYR	N-CA-C	5.35	119.96	113.38
1	A	459	MET	N-CA-C	-5.29	106.66	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	353	ALA	N-CA-C	-5.09	105.81	111.36
1	B	349	PRO	N-CA-C	5.07	116.89	110.70
1	B	559	LYS	N-CA-C	-5.05	105.96	111.82
1	B	345	ALA	N-CA-C	5.04	117.89	111.69
1	A	316	PHE	N-CA-C	5.03	116.78	108.48
1	A	559	LYS	N-CA-C	-5.00	105.93	112.23

There are no chirality outliers.

There are no planarity outliers.

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	4774	0	4750	84	0
1	B	4774	0	4750	74	0
2	A	48	0	32	2	0
2	B	48	0	32	1	0
3	A	11	0	15	2	0
3	B	11	0	15	2	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	A	503	0	0	7	0
5	B	645	0	0	10	0
All	All	10822	0	9606	162	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 8.

All (162) 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:132:LEU:HD22	1:A:132:LEU:H	1.31	0.96
1:B:81:GLU:O	1:B:85:LYS:HD3	1.66	0.94
1:B:32:GLN:HE22	1:B:170:MET:H	1.23	0.83
1:B:310:HIS:HD2	1:B:312:GLY:H	1.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:GLN:OE1	1:A:557:PRO:HG3	1.86	0.76
1:A:310:HIS:HD2	1:A:312:GLY:H	1.33	0.75
1:A:32:GLN:HE22	1:A:170:MET:H	1.33	0.75
1:B:501:GLN:HG2	5:B:1612:HOH:O	1.88	0.74
1:B:310:HIS:CD2	1:B:312:GLY:H	2.06	0.74
1:B:410:MET:HE3	1:B:411:MET:O	1.88	0.73
1:A:497:ARG:NH2	1:A:623:ARG:HG2	2.03	0.73
1:A:240:SER:HA	1:A:242:GLN:NE2	2.06	0.71
1:B:255:HIS:HD2	1:B:257:ASN:H	1.40	0.69
1:A:310:HIS:CD2	1:A:312:GLY:H	2.14	0.65
1:B:568:PRO:HD2	1:B:592:TYR:CZ	2.33	0.64
1:B:315:LYS:HG2	5:B:1744:HOH:O	1.99	0.63
1:A:349:PRO:HB2	1:A:350:PRO:HD3	1.81	0.62
1:A:132:LEU:H	1:A:132:LEU:CD2	2.09	0.62
1:A:231:VAL:HG21	1:A:372:MET:HE3	1.82	0.62
1:B:231:VAL:HG21	1:B:372:MET:HE3	1.80	0.62
1:A:129:PHE:CZ	1:A:335:GLY:HA2	2.35	0.62
1:B:349:PRO:HB2	1:B:350:PRO:HD3	1.81	0.61
1:B:147:LEU:HD11	1:B:216:VAL:HB	1.83	0.61
1:B:265:ASN:HA	1:B:268:LYS:HE3	1.82	0.61
1:A:349:PRO:HA	1:A:352:VAL:HG22	1.82	0.61
1:B:421:PHE:HB3	1:B:422:PRO:HD3	1.82	0.61
1:A:322:TRP:H	1:A:328:GLN:NE2	1.99	0.60
1:B:255:HIS:CD2	1:B:257:ASN:H	2.18	0.60
1:B:349:PRO:HA	1:B:352:VAL:HG22	1.82	0.60
1:A:391:ASN:O	1:A:395:LYS:HG2	2.02	0.60
1:A:421:PHE:HB3	1:A:422:PRO:HD3	1.83	0.60
3:B:1301:152:O3	3:B:1301:152:H5B3	2.02	0.60
1:B:44:GLN:HG2	1:B:74:GLN:OE1	2.03	0.59
1:B:104:LYS:HG2	1:B:109:GLN:CD	2.28	0.58
1:B:202:HIS:HD2	5:B:1336:HOH:O	1.86	0.58
1:A:227:ASP:CG	1:A:369:ARG:HG3	2.28	0.57
1:A:455:ALA:HB2	1:A:468:ILE:HG13	1.85	0.57
1:B:322:TRP:H	1:B:328:GLN:NE2	2.03	0.57
1:A:61:GLU:H	1:A:61:GLU:CD	2.12	0.57
1:B:489:GLU:HB3	1:B:621:HIS:NE2	2.20	0.56
1:A:227:ASP:OD2	1:A:369:ARG:HG3	2.04	0.56
1:A:255:HIS:NE2	1:A:257:ASN:ND2	2.53	0.56
1:B:242:GLN:HG3	1:B:244:ASN:OD1	2.06	0.55
1:A:548:HIS:HE1	1:A:572:ASP:OD1	1.88	0.55
1:B:548:HIS:HE1	1:B:572:ASP:OD1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:GLN:HE21	1:B:244:ASN:CG	2.14	0.55
1:B:382:ARG:HD3	5:B:1788:HOH:O	2.06	0.55
1:A:206:VAL:HG22	1:A:320:ASN:OD1	2.07	0.55
1:B:401:SER:O	1:B:405:GLN:HG3	2.07	0.55
1:A:255:HIS:CD2	1:A:257:ASN:H	2.25	0.55
3:A:1201:152:H5B3	3:A:1201:152:O3	2.08	0.54
1:A:44:GLN:HG2	1:A:74:GLN:OE1	2.08	0.54
1:A:352:VAL:HG11	1:A:556:VAL:HG12	1.90	0.54
1:A:568:PRO:HD2	1:A:592:TYR:CZ	2.44	0.53
1:A:255:HIS:HD2	1:A:257:ASN:H	1.56	0.53
1:B:123:ILE:HD12	1:B:123:ILE:N	2.24	0.52
1:B:421:PHE:CZ	1:B:615:ARG:HG3	2.44	0.52
1:B:225:THR:H	1:B:228:GLN:NE2	2.08	0.52
1:A:354:LEU:C	1:A:354:LEU:HD23	2.35	0.52
1:A:142:LEU:C	1:A:142:LEU:HD23	2.35	0.52
1:A:122:VAL:HB	1:A:339:MET:HG2	1.90	0.52
1:B:349:PRO:HD3	2:B:1302:COA:H31	1.91	0.52
1:A:147:LEU:HD11	1:A:216:VAL:HB	1.91	0.51
1:A:104:LYS:HG2	1:A:109:GLN:CD	2.34	0.51
1:A:349:PRO:HD3	2:A:1202:COA:H31	1.92	0.51
1:B:95:GLU:OE1	1:B:461:HIS:HE1	1.94	0.51
1:A:163:LEU:HB3	1:A:168:LEU:HD21	1.90	0.51
1:B:352:VAL:HG11	1:B:556:VAL:HG12	1.93	0.51
1:A:512:ARG:HH11	1:A:512:ARG:HG3	1.75	0.50
1:A:497:ARG:HH22	1:A:623:ARG:HG2	1.76	0.50
1:A:59:SER:OG	1:A:62:GLU:HG3	2.11	0.49
1:A:401:SER:O	1:A:405:GLN:HG3	2.13	0.49
1:B:270:LYS:HB2	1:B:270:LYS:NZ	2.28	0.49
1:A:95:GLU:OE1	1:A:461:HIS:HE1	1.95	0.49
1:B:455:ALA:HB2	1:B:468:ILE:HG13	1.95	0.49
1:B:32:GLN:NE2	1:B:170:MET:H	2.02	0.49
1:A:276:VAL:O	1:A:280:GLN:HG3	2.12	0.48
1:B:276:VAL:O	1:B:280:GLN:HG3	2.13	0.48
1:B:202:HIS:HE1	1:B:278:SER:O	1.96	0.48
1:B:548:HIS:HD2	5:B:1752:HOH:O	1.97	0.48
1:A:496:LEU:C	1:A:496:LEU:HD23	2.39	0.48
1:A:487:VAL:O	1:A:492:LYS:HE3	2.13	0.48
1:A:321:ARG:HB3	1:A:328:GLN:HE22	1.79	0.47
1:A:204:THR:HG21	1:A:279:ILE:HA	1.96	0.47
1:B:354:LEU:O	1:B:358:VAL:HG23	2.13	0.47
1:B:198:ARG:O	1:B:198:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASN:C	1:A:321:ARG:HG2	2.39	0.47
1:B:207:HIS:HD2	1:B:240:SER:OG	1.97	0.47
1:B:320:ASN:C	1:B:321:ARG:HG2	2.39	0.47
1:A:176:ILE:HA	1:A:326:THR:HG21	1.97	0.47
1:A:368:VAL:O	1:A:368:VAL:HG23	2.14	0.47
1:A:190:VAL:HG11	5:A:1582:HOH:O	2.15	0.47
1:B:255:HIS:HE1	5:B:1730:HOH:O	1.97	0.47
1:A:204:THR:HG23	1:A:282:SER:HB3	1.96	0.47
1:B:243:SER:HA	5:B:1558:HOH:O	2.13	0.46
1:B:354:LEU:C	1:B:354:LEU:HD23	2.40	0.46
1:A:456:SER:HB2	2:A:1202:COA:H71	1.96	0.46
1:B:61:GLU:H	1:B:61:GLU:CD	2.24	0.46
1:A:431:ALA:HB3	1:A:500:VAL:HG13	1.98	0.46
1:A:310:HIS:HE1	5:A:1526:HOH:O	1.98	0.46
1:A:322:TRP:H	1:A:328:GLN:HE22	1.62	0.46
1:B:310:HIS:HE1	5:B:1726:HOH:O	1.98	0.46
1:A:192:ASN:C	1:A:192:ASN:HD22	2.23	0.46
1:B:352:VAL:CG1	1:B:564:MET:HE3	2.46	0.46
1:B:61:GLU:CD	1:B:61:GLU:N	2.74	0.46
1:B:487:VAL:CG1	1:B:491:GLN:HB3	2.46	0.45
1:A:301:ARG:HG2	1:A:301:ARG:HH11	1.81	0.45
1:B:315:LYS:HG3	1:B:316:PHE:CE1	2.51	0.45
1:A:216:VAL:C	1:A:224:LEU:HD13	2.41	0.45
1:B:322:TRP:H	1:B:328:GLN:HE22	1.62	0.45
1:B:176:ILE:HA	1:B:326:THR:HG21	1.98	0.44
1:B:489:GLU:CB	1:B:621:HIS:NE2	2.80	0.44
1:A:65:HIS:CE1	1:A:69:LEU:HD11	2.52	0.44
1:A:242:GLN:H	1:A:242:GLN:CD	2.26	0.44
1:A:458:ARG:HD3	5:A:1416:HOH:O	2.17	0.44
1:A:294:ARG:HH11	1:A:294:ARG:HG3	1.82	0.44
1:B:192:ASN:HD22	1:B:192:ASN:C	2.25	0.44
1:A:210:GLN:HE21	1:A:380:LYS:CE	2.30	0.44
1:B:85:LYS:NZ	5:B:1734:HOH:O	2.51	0.44
1:A:32:GLN:NE2	1:A:170:MET:H	2.06	0.43
1:A:210:GLN:NE2	1:A:380:LYS:NZ	2.67	0.43
1:A:425:GLU:O	1:A:426:LYS:HB2	2.18	0.43
1:A:516:PHE:CD1	1:A:516:PHE:C	2.96	0.43
1:B:452:TYR:HB2	1:B:549:PHE:CD1	2.53	0.43
1:A:231:VAL:CG2	1:A:372:MET:HE3	2.49	0.43
1:B:410:MET:HG2	1:B:601:ALA:HA	2.01	0.43
1:B:489:GLU:HB3	1:B:621:HIS:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1201:152:H3	3:A:1201:152:H5A2	1.83	0.42
1:A:177:LEU:HD23	1:A:327:LEU:HD12	2.01	0.42
1:A:578:TYR:HB3	1:A:587:PHE:CD1	2.54	0.42
1:B:197:LYS:HG2	5:B:1506:HOH:O	2.19	0.42
1:B:487:VAL:HG13	1:B:491:GLN:HB3	2.01	0.42
1:A:218:HIS:HB2	1:A:220:ASP:OD1	2.19	0.42
1:A:301:ARG:HG2	1:A:301:ARG:NH1	2.35	0.42
1:B:115:VAL:HG12	1:B:116:ILE:HG13	2.02	0.42
1:B:496:LEU:C	1:B:496:LEU:HD23	2.45	0.42
3:B:1301:152:O3	3:B:1301:152:C5B	2.68	0.42
1:A:139:ALA:O	1:A:143:ILE:HG13	2.18	0.42
1:B:416:HIS:CG	1:B:612:LEU:HD21	2.55	0.42
1:B:142:LEU:HD23	1:B:142:LEU:C	2.45	0.41
1:B:293:PRO:HD2	1:B:316:PHE:HE2	1.85	0.41
1:A:512:ARG:HG3	1:A:512:ARG:NH1	2.35	0.41
1:B:578:TYR:HB3	1:B:587:PHE:CD1	2.55	0.41
1:B:77:GLY:H	1:B:81:GLU:CD	2.28	0.41
1:B:242:GLN:HE21	1:B:244:ASN:ND2	2.18	0.41
1:A:202:HIS:HD2	5:A:1341:HOH:O	2.04	0.41
1:A:209:TYR:N	1:A:209:TYR:CD2	2.88	0.41
1:A:416:HIS:CG	1:A:612:LEU:HD21	2.56	0.41
1:A:548:HIS:HD2	5:A:1547:HOH:O	2.03	0.41
1:A:123:ILE:HD12	1:A:123:ILE:N	2.35	0.41
1:A:129:PHE:HB2	1:A:134:GLY:HA3	2.03	0.41
1:A:410:MET:HG2	1:A:601:ALA:HA	2.03	0.41
1:B:199:PRO:HA	1:B:200:PRO:HD3	1.98	0.41
1:B:255:HIS:CD2	1:B:257:ASN:HB2	2.56	0.41
1:A:115:VAL:HG12	1:A:116:ILE:HG13	2.02	0.40
1:B:85:LYS:N	1:B:85:LYS:CD	2.84	0.40
1:A:421:PHE:CZ	1:A:615:ARG:HG3	2.56	0.40
1:A:529:GLU:HG2	5:A:1255:HOH:O	2.21	0.40
1:A:202:HIS:HE1	1:A:278:SER:O	2.03	0.40
1:A:423:LYS:HD2	5:A:1314:HOH:O	2.22	0.40
1:B:144:GLU:OE1	1:B:226:SER:HB3	2.22	0.40
1:B:367:LEU:HB2	1:B:369:ARG:NH1	2.36	0.40

There are no symmetry-related clashes.

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	597/618 (97%)	585 (98%)	12 (2%)	0	100	100
1	B	597/618 (97%)	585 (98%)	11 (2%)	1 (0%)	43	31
All	All	1194/1236 (97%)	1170 (98%)	23 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	622	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	526/542 (97%)	522 (99%)	4 (1%)	73	70
1	B	526/542 (97%)	523 (99%)	3 (1%)	78	77
All	All	1052/1084 (97%)	1045 (99%)	7 (1%)	76	73

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	LEU
1	A	343	HIS
1	A	426	LYS
1	A	559	LYS
1	B	204	THR

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Mol	Chain	Res	Type
1	B	270	LYS
1	B	343	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	44	GLN
1	A	65	HIS
1	A	68	GLN
1	A	74	GLN
1	A	109	GLN
1	A	112	GLN
1	A	135	GLN
1	A	155	ASN
1	A	192	ASN
1	A	202	HIS
1	A	207	HIS
1	A	208	ASN
1	A	210	GLN
1	A	228	GLN
1	A	242	GLN
1	A	307	GLN
1	A	310	HIS
1	A	328	GLN
1	A	357	HIS
1	A	447	GLN
1	A	461	HIS
1	A	503	HIS
1	A	526	GLN
1	A	548	HIS
1	A	550	ASN
1	A	619	GLN
1	A	620	ASN
1	B	32	GLN
1	B	84	GLN
1	B	112	GLN
1	B	135	GLN
1	B	155	ASN
1	B	171	ASN
1	B	192	ASN
1	B	202	HIS

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Mol	Chain	Res	Type
1	B	207	HIS
1	B	210	GLN
1	B	228	GLN
1	B	242	GLN
1	B	255	HIS
1	B	277	ASN
1	B	307	GLN
1	B	310	HIS
1	B	328	GLN
1	B	357	HIS
1	B	461	HIS
1	B	503	HIS
1	B	526	GLN
1	B	548	HIS
1	B	550	ASN
1	B	586	ASN
1	B	619	GLN
1	B	620	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
2	COA	A	1202	-	47,50,50	1.23	6 (12%)	69,75,75	1.52	11 (15%)
3	152	A	1201	-	10,10,10	1.19	1 (10%)	13,14,14	1.13	1 (7%)
3	152	B	1301	-	10,10,10	1.21	1 (10%)	13,14,14	1.15	1 (7%)
4	EDO	B	1303	-	3,3,3	0.62	0	2,2,2	0.41	0
2	COA	B	1302	-	47,50,50	1.23	5 (10%)	69,75,75	1.51	10 (14%)
4	EDO	A	1203	-	3,3,3	0.63	0	2,2,2	0.38	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	COA	A	1202	-	-	2/48/64/64	0/3/3/3
3	152	A	1201	-	-	0/9/9/9	-
3	152	B	1301	-	-	0/9/9/9	-
4	EDO	B	1303	-	-	0/1/1/1	-
2	COA	B	1302	-	-	5/48/64/64	0/3/3/3
4	EDO	A	1203	-	-	0/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1302	COA	P3B-O7A	3.34	1.60	1.50
2	A	1202	COA	P3B-O7A	3.22	1.60	1.50
2	A	1202	COA	C5A-N7A	-3.19	1.33	1.39
2	B	1302	COA	C5A-N7A	-3.11	1.33	1.39
2	B	1302	COA	P1A-O3A	2.69	1.62	1.59
2	A	1202	COA	P2A-O3A	2.63	1.62	1.59
2	A	1202	COA	O4B-C1B	2.38	1.47	1.42
3	A	1201	152	C4-N5	-2.35	1.47	1.52
3	B	1301	152	C4-N5	-2.27	1.47	1.52
2	A	1202	COA	C4A-N9A	-2.20	1.33	1.37
2	A	1202	COA	P1A-O3A	2.17	1.61	1.59
2	B	1302	COA	P2A-O3A	2.06	1.61	1.59
2	B	1302	COA	C4A-N9A	-2.05	1.33	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1202	COA	N3A-C2A-N1A	-5.28	120.59	128.58
2	B	1302	COA	N3A-C2A-N1A	-5.28	120.60	128.58
2	B	1302	COA	C5A-C4A-N3A	-4.99	119.85	126.72
2	A	1202	COA	C5A-C4A-N3A	-4.93	119.93	126.72
2	A	1202	COA	C2A-N3A-C4A	3.68	120.81	111.83
2	B	1302	COA	C2A-N3A-C4A	3.66	120.77	111.83
2	A	1202	COA	N9A-C8A-N7A	-3.49	108.98	113.94
2	B	1302	COA	N9A-C8A-N7A	-3.40	109.12	113.94
2	B	1302	COA	N3A-C4A-N9A	3.37	132.91	127.17
3	A	1201	152	C3-C4-N5	-3.24	110.74	116.70
3	B	1301	152	C3-C4-N5	-3.23	110.75	116.70
2	A	1202	COA	N3A-C4A-N9A	3.20	132.61	127.17
2	B	1302	COA	O9A-P3B-O8A	2.94	118.84	107.80
2	A	1202	COA	O9A-P3B-O8A	2.90	118.67	107.80
2	B	1302	COA	C5A-N7A-C8A	2.81	107.86	103.45
2	A	1202	COA	C5A-N7A-C8A	2.79	107.84	103.45
2	A	1202	COA	C4A-C5A-N7A	-2.47	107.76	110.58
2	B	1302	COA	C4A-C5A-N7A	-2.44	107.79	110.58
2	B	1302	COA	O4B-C1B-N9A	2.41	112.72	108.09
2	A	1202	COA	O4B-C1B-N9A	2.23	112.37	108.09
2	B	1302	COA	C4A-N9A-C8A	2.14	107.98	105.74
2	A	1202	COA	C4A-N9A-C8A	2.12	107.96	105.74
2	A	1202	COA	C5B-C4B-C3B	-2.10	107.37	114.38

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1302	COA	C4B-C3B-O3B-P3B
2	A	1202	COA	C2B-C3B-O3B-P3B
2	B	1302	COA	C2B-C3B-O3B-P3B
2	A	1202	COA	C4B-C3B-O3B-P3B
2	B	1302	COA	P2A-O3A-P1A-O5B
2	B	1302	COA	C3B-O3B-P3B-O9A
2	B	1302	COA	N8P-C9P-CAP-OAP

There are no ring outliers.

4 monomers are involved in 7 short contacts:

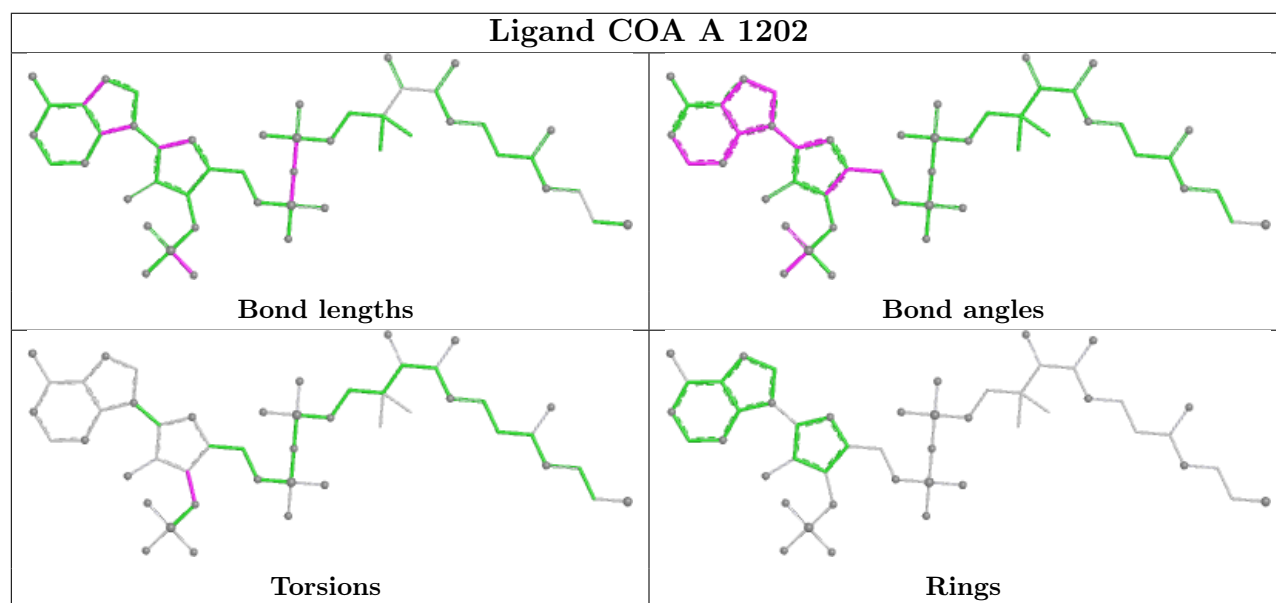
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1202	COA	2	0
3	A	1201	152	2	0

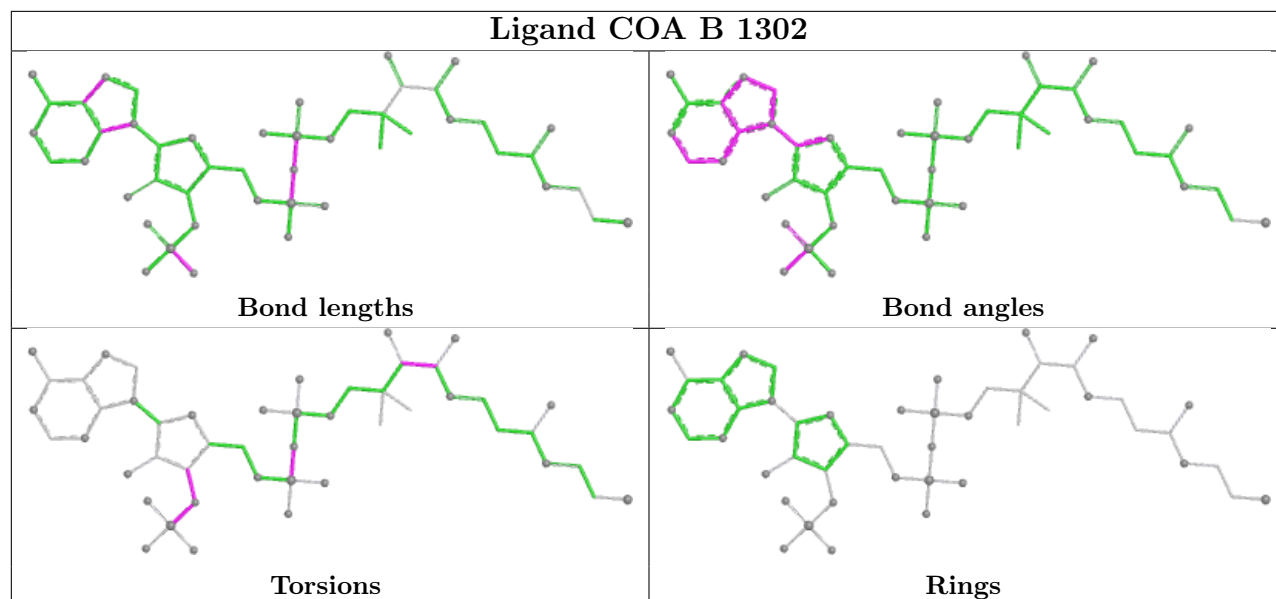
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1301	152	2	0
2	B	1302	COA	1	0

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.