



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:40 PM UTC

PDB ID : 2H3W / pdb_00002h3w
Title : Crystal structure of the S554A/M564G mutant of murine carnitine acetyltransferase in complex with hexanoylcarnitine and CoA
Authors : Hsiao, Y.S.; Jogl, G.; Tong, L.
Deposited on : 2006-05-23
Resolution : 2.10 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

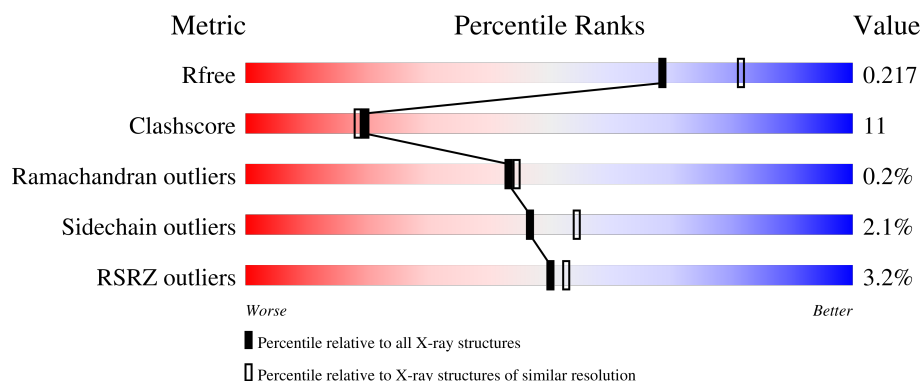
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

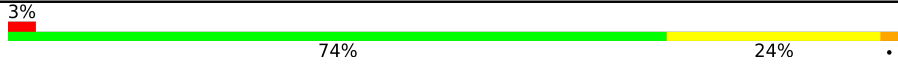
The reported resolution of this entry is 2.10 Å.

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 $\leq 5\%$. 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	599	
1	B	599	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11184 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
			4776	3045	825	878	28			
1	B	599	Total	C	N	O	S	0	0	0
			4776	3045	825	878	28			

There are 10 discrepancies between the modelled and reference sequences:

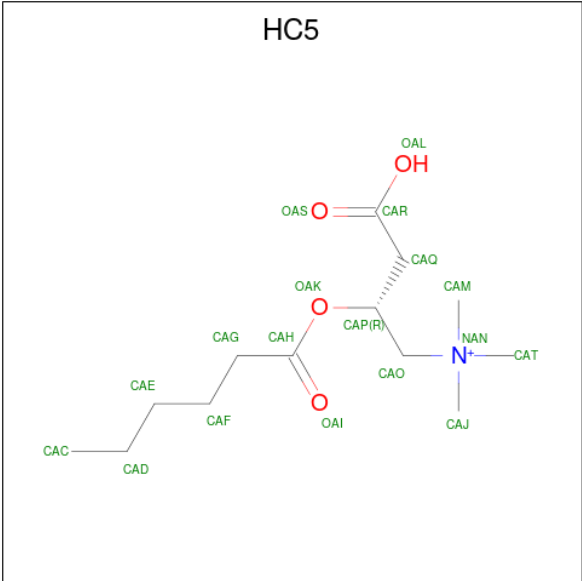
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	SER	-	cloning artifact	UNP Q3V1Y3
A	28	HIS	-	cloning artifact	UNP Q3V1Y3
A	29	MET	-	cloning artifact	UNP Q3V1Y3
A	554	ALA	SER	engineered mutation	UNP Q3V1Y3
A	564	GLY	MET	engineered mutation	UNP Q3V1Y3
B	27	SER	-	cloning artifact	UNP Q3V1Y3
B	28	HIS	-	cloning artifact	UNP Q3V1Y3
B	29	MET	-	cloning artifact	UNP Q3V1Y3
B	554	ALA	SER	engineered mutation	UNP Q3V1Y3
B	564	GLY	MET	engineered mutation	UNP Q3V1Y3

- 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 (R)-3-CARBOXY-2-(HEXANOYLOXY)-N,N,N-TRIMETHYLPROPAN-1-AMINIUM (CCD ID: HC5) (formula: C₁₃H₂₆NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	13	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			18	13	1	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	673	Total	O	0	0
			673	673		
4	B	827	Total	O	0	0
			827	827		

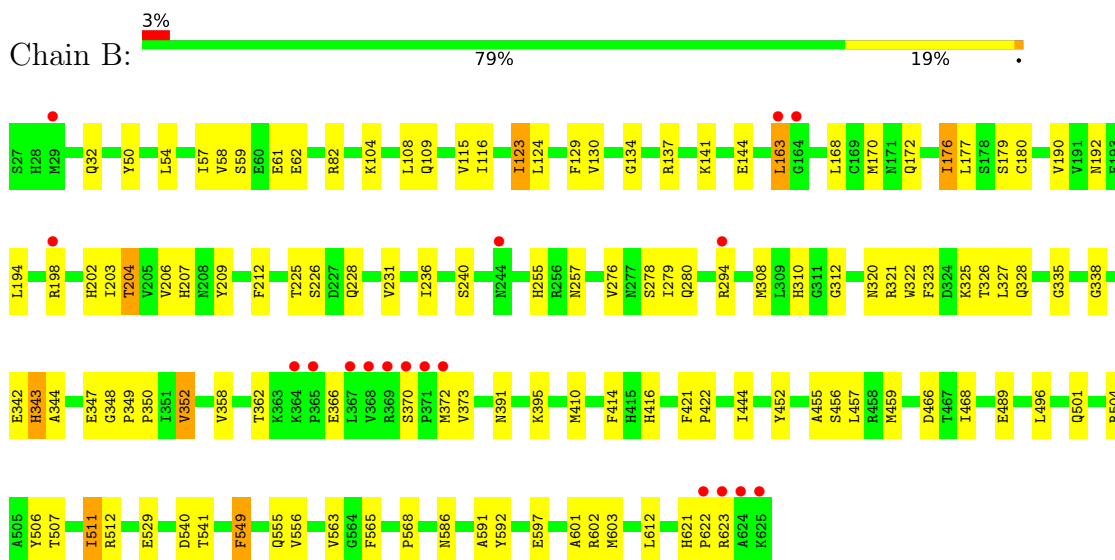
3 Residue-property plots [i](#)

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: carnitine acetyltransferase



- Molecule 1: carnitine acetyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.06Å 89.07Å 122.78Å 90.00° 128.97° 90.00°	Depositor
Resolution (Å)	29.91 – 2.10 29.91 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.3 (29.91-2.10) 94.3 (29.91-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.43 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.177 , 0.219 0.176 , 0.217	Depositor DCC
R_{free} test set	5768 reflections (7.58%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11184	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HC5, 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	0.40	0/4892	0.81	7/6627 (0.1%)
1	B	0.43	1/4892 (0.0%)	0.82	6/6627 (0.1%)
All	All	0.41	1/9784 (0.0%)	0.82	13/13254 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	603	MET	SD-CE	-6.24	1.64	1.79

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	HIS	N-CA-C	6.71	119.43	111.71
1	A	343	HIS	N-CA-C	6.42	119.10	111.71
1	B	323	PHE	N-CA-C	6.04	120.12	112.87
1	B	549	PHE	N-CA-C	5.88	119.05	108.17
1	A	176	ILE	N-CA-C	5.79	117.31	111.00
1	B	176	ILE	N-CA-C	5.62	117.13	111.00
1	A	323	PHE	N-CA-C	5.34	119.28	112.87
1	A	182	VAL	CA-C-N	5.32	125.58	119.83
1	A	182	VAL	C-N-CA	5.32	125.58	119.83
1	A	517	ASP	N-CA-C	5.21	116.64	111.07
1	B	203	ILE	N-CA-C	-5.16	101.64	108.96
1	A	549	PHE	N-CA-C	5.08	117.56	108.17
1	B	57	ILE	N-CA-C	5.04	117.07	112.43

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	4776	0	4748	114	0
1	B	4776	0	4748	96	0
2	A	48	0	32	4	0
2	B	48	0	32	7	0
3	A	18	0	25	7	0
3	B	18	0	25	5	0
4	A	673	0	0	16	0
4	B	827	0	0	23	0
All	All	11184	0	9610	221	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 11.

All (221) 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:B:349:PRO:HD3	2:B:1701:COA:H31	1.56	0.86
1:B:310:HIS:HD2	1:B:312:GLY:H	1.24	0.86
1:A:141:LYS:HD2	1:A:362:THR:HA	1.58	0.85
1:A:457:LEU:HD21	1:A:466:ASP:HB2	1.57	0.85
1:B:325:LYS:HA	4:B:1945:HOH:O	1.77	0.85
1:B:163:LEU:HB2	1:B:168:LEU:HD21	1.62	0.79
1:A:310:HIS:HD2	1:A:312:GLY:H	1.32	0.78
1:A:32:GLN:HE22	1:A:170:MET:H	1.30	0.78
1:B:32:GLN:HE22	1:B:170:MET:H	1.34	0.74
1:B:310:HIS:CD2	1:B:312:GLY:H	2.05	0.74
2:B:1701:COA:H61	4:B:2094:HOH:O	1.86	0.74
1:A:556:VAL:HG11	3:A:1602:HC5:HAE2	1.72	0.72
1:A:349:PRO:HB2	1:A:350:PRO:HD3	1.72	0.71
1:B:372:MET:HB3	4:B:1889:HOH:O	1.91	0.71
1:B:325:LYS:HD2	4:B:1945:HOH:O	1.91	0.70
1:A:321:ARG:HB3	1:A:328:GLN:HE22	1.56	0.68
1:A:556:VAL:CG1	3:A:1602:HC5:HAE2	2.24	0.68
1:B:349:PRO:HB2	1:B:350:PRO:HD3	1.76	0.68
1:B:457:LEU:HD21	1:B:466:ASP:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:HIS:CD2	1:A:312:GLY:H	2.11	0.67
1:B:555:GLN:HB3	4:B:2094:HOH:O	1.95	0.67
1:B:231:VAL:HG11	1:B:372:MET:HE1	1.77	0.66
3:A:1602:HC5:CAH	3:A:1602:HC5:HAJ3	2.26	0.66
1:A:349:PRO:HD3	2:A:1601:COA:H31	1.76	0.66
1:A:320:ASN:O	1:A:321:ARG:HG2	1.96	0.66
1:A:242:GLN:NE2	1:A:244:ASN:HB3	2.12	0.65
1:B:421:PHE:HB3	1:B:422:PRO:HD3	1.78	0.64
1:B:349:PRO:O	1:B:352:VAL:HG22	1.99	0.62
1:B:180:CYS:HA	4:B:1945:HOH:O	1.99	0.62
1:B:556:VAL:HG21	3:B:1702:HC5:HAE2	1.82	0.61
1:A:555:GLN:NE2	1:A:580:PRO:HG2	2.16	0.60
3:B:1702:HC5:HAJ3	3:B:1702:HC5:CAH	2.32	0.60
1:B:141:LYS:HE3	1:B:362:THR:HA	1.83	0.60
1:A:421:PHE:HB3	1:A:422:PRO:HD3	1.83	0.60
2:B:1701:COA:H131	4:B:2094:HOH:O	1.99	0.60
1:A:210:GLN:HE21	1:A:380:LYS:HE3	1.66	0.60
1:A:410:MET:HG2	1:A:601:ALA:HA	1.82	0.59
1:B:348:GLY:O	1:B:352:VAL:HG13	2.01	0.59
1:A:172:GLN:OE1	1:A:350:PRO:HG2	2.03	0.59
1:A:123:ILE:HD12	1:A:411:MET:HE2	1.85	0.58
1:A:32:GLN:NE2	1:A:170:MET:H	2.01	0.57
1:A:204:THR:HG21	1:A:279:ILE:HA	1.86	0.57
1:A:47:LEU:HD12	1:A:74:GLN:HE21	1.69	0.57
1:B:225:THR:HG21	1:B:370:SER:OG	2.04	0.57
2:B:1701:COA:S1P	3:B:1702:HC5:CAH	2.93	0.57
1:A:322:TRP:H	1:A:328:GLN:NE2	2.03	0.56
1:A:555:GLN:HE21	1:A:580:PRO:HG2	1.70	0.56
1:A:131:ASP:OD1	1:A:133:GLN:HG3	2.06	0.56
1:A:482:MET:HA	1:A:492:LYS:HD3	1.88	0.55
1:B:456:SER:HB2	2:B:1701:COA:H71	1.88	0.55
1:B:177:LEU:HD23	1:B:327:LEU:HD12	1.88	0.55
1:A:133:GLN:O	1:A:137:ARG:HB2	2.06	0.55
1:A:255:HIS:CD2	1:A:257:ASN:H	2.25	0.55
1:B:501:GLN:HG2	4:B:2135:HOH:O	2.07	0.55
1:A:192:ASN:ND2	1:A:194:LEU:H	2.05	0.55
1:A:255:HIS:HD2	1:A:257:ASN:H	1.54	0.55
1:A:115:VAL:HG12	1:A:116:ILE:HG13	1.87	0.55
1:A:321:ARG:HG2	1:A:321:ARG:HH11	1.71	0.54
1:A:455:ALA:HB2	1:A:468:ILE:HG13	1.90	0.54
1:B:50:TYR:CZ	1:B:54:LEU:HD11	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:MET:HG3	1:B:373:VAL:N	2.22	0.54
1:A:512:ARG:HG3	1:A:512:ARG:HH11	1.72	0.54
1:A:104:LYS:HG2	1:A:109:GLN:HG3	1.89	0.54
1:A:175:GLN:HG3	4:A:2247:HOH:O	2.08	0.53
1:B:556:VAL:HB	4:B:2108:HOH:O	2.07	0.53
1:B:457:LEU:HD21	1:B:466:ASP:CB	2.39	0.53
1:B:192:ASN:HD22	1:B:192:ASN:C	2.17	0.53
1:A:124:LEU:HG	1:A:338:GLY:HA2	1.91	0.53
1:B:207:HIS:HD2	1:B:240:SER:OG	1.91	0.53
1:A:204:THR:HG23	1:A:282:SER:HB3	1.91	0.52
1:B:504:ARG:HD2	4:B:1862:HOH:O	2.09	0.52
1:B:563:VAL:HB	1:B:586:ASN:HB3	1.90	0.52
1:B:225:THR:H	1:B:228:GLN:NE2	2.08	0.52
2:A:1601:COA:S1P	3:A:1602:HC5:CAH	2.97	0.51
1:A:202:HIS:HD2	4:A:1737:HOH:O	1.92	0.51
1:B:129:PHE:CZ	1:B:335:GLY:HA2	2.45	0.51
1:A:50:TYR:CZ	1:A:54:LEU:HD11	2.46	0.51
1:A:568:PRO:HD2	1:A:592:TYR:CZ	2.46	0.51
1:B:255:HIS:HD2	1:B:257:ASN:H	1.59	0.50
1:A:147:LEU:HD11	1:A:216:VAL:HB	1.93	0.50
1:B:192:ASN:ND2	1:B:194:LEU:H	2.10	0.50
1:B:416:HIS:CG	1:B:612:LEU:HD21	2.47	0.50
1:B:144:GLU:OE1	1:B:226:SER:HB3	2.13	0.49
1:B:179:SER:O	4:B:1945:HOH:O	2.19	0.49
1:B:123:ILE:HB	1:B:565:PHE:HE2	1.78	0.49
1:B:310:HIS:HE1	4:B:2039:HOH:O	1.95	0.49
1:B:529:GLU:HG2	4:B:1817:HOH:O	2.11	0.49
1:A:129:PHE:CZ	1:A:335:GLY:HA2	2.47	0.49
1:A:231:VAL:HG21	1:A:372:MET:SD	2.52	0.49
1:A:261:LYS:HD2	4:A:2188:HOH:O	2.12	0.49
1:B:192:ASN:HD22	1:B:194:LEU:H	1.59	0.49
1:A:456:SER:HB2	2:A:1601:COA:H71	1.94	0.49
1:A:457:LEU:HD21	1:A:466:ASP:CB	2.36	0.49
1:B:190:VAL:HG11	4:B:2273:HOH:O	2.12	0.49
1:B:410:MET:HE2	4:B:2064:HOH:O	2.13	0.48
1:B:129:PHE:HB2	1:B:134:GLY:HA3	1.95	0.48
1:B:366:GLU:HA	4:B:2150:HOH:O	2.12	0.48
1:A:192:ASN:C	1:A:192:ASN:HD22	2.20	0.48
1:B:320:ASN:C	1:B:321:ARG:HG2	2.39	0.48
1:B:444:ILE:HG23	1:B:602:ARG:NH1	2.29	0.48
1:A:47:LEU:HD12	1:A:74:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ASN:O	1:A:395:LYS:HG2	2.14	0.48
1:B:172:GLN:OE1	1:B:350:PRO:HG2	2.13	0.48
1:A:192:ASN:HD22	1:A:193:PHE:N	2.12	0.48
1:B:347:GLU:HG3	4:B:1755:HOH:O	2.14	0.48
1:A:320:ASN:C	1:A:321:ARG:HG2	2.39	0.47
1:B:124:LEU:HG	1:B:338:GLY:HA2	1.95	0.47
1:B:202:HIS:HE1	1:B:278:SER:O	1.97	0.47
1:B:444:ILE:HG23	1:B:602:ARG:HH12	1.78	0.47
1:A:264:ASN:HB2	4:A:1738:HOH:O	2.14	0.47
1:B:204:THR:HG21	1:B:279:ILE:HA	1.95	0.47
1:A:276:VAL:O	1:A:280:GLN:HG3	2.14	0.47
1:A:322:TRP:H	1:A:328:GLN:HE22	1.61	0.47
1:A:59:SER:OG	1:A:62:GLU:HG3	2.14	0.47
1:A:578:TYR:HB3	1:A:587:PHE:CD1	2.50	0.47
2:A:1601:COA:S1P	3:A:1602:HC5:HAQ1	2.55	0.47
1:B:322:TRP:H	1:B:328:GLN:NE2	2.12	0.47
1:A:183:PRO:HG3	1:A:259:TRP:NE1	2.30	0.47
1:A:369:ARG:HD3	4:A:1853:HOH:O	2.15	0.47
1:A:487:VAL:HB	1:A:492:LYS:NZ	2.30	0.47
1:A:163:LEU:HB2	1:A:168:LEU:HD11	1.97	0.47
1:A:177:LEU:HD23	1:A:327:LEU:HD12	1.96	0.46
1:A:296:SER:HB3	1:A:299:VAL:HG22	1.97	0.46
1:A:342:GLU:OE1	1:A:344:ALA:HB3	2.16	0.46
1:A:452:TYR:HB2	1:A:549:PHE:CD1	2.51	0.46
1:B:104:LYS:HG2	1:B:109:GLN:CD	2.40	0.46
1:B:130:VAL:HA	4:B:1808:HOH:O	2.15	0.46
1:B:496:LEU:C	1:B:496:LEU:HD23	2.41	0.46
1:B:512:ARG:HG3	1:B:512:ARG:HH11	1.81	0.46
1:A:416:HIS:CG	1:A:612:LEU:HD21	2.51	0.46
1:A:132:LEU:HD21	1:A:237:TRP:CZ2	2.51	0.45
1:A:133:GLN:HB2	4:A:2026:HOH:O	2.15	0.45
1:A:176:ILE:HA	1:A:326:THR:HG21	1.98	0.45
1:A:41:PRO:HG3	1:A:513:GLY:O	2.16	0.45
1:A:213:GLU:HB2	1:A:381:LEU:HD21	1.98	0.45
1:B:176:ILE:HA	1:B:326:THR:HG21	1.98	0.45
1:A:277:ASN:HD21	1:A:281:LYS:HE3	1.81	0.45
1:A:529:GLU:HG2	4:A:1676:HOH:O	2.15	0.45
1:B:459:MET:HE3	1:B:511:ILE:HG23	1.97	0.45
1:B:54:LEU:O	1:B:58:VAL:HG22	2.17	0.45
1:A:556:VAL:HG23	1:A:556:VAL:O	2.16	0.45
1:B:342:GLU:OE1	1:B:344:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:HD23	1:A:142:LEU:C	2.41	0.45
1:B:326:THR:N	4:B:1945:HOH:O	2.37	0.44
1:B:452:TYR:HB2	1:B:549:PHE:CD1	2.52	0.44
3:B:1702:HC5:HAJ3	3:B:1702:HC5:OAK	2.17	0.44
1:B:59:SER:OG	1:B:62:GLU:HG3	2.18	0.44
1:B:489:GLU:HB3	1:B:621:HIS:NE2	2.32	0.44
1:B:104:LYS:HB2	4:B:2470:HOH:O	2.16	0.44
1:B:410:MET:HG2	1:B:601:ALA:HA	1.98	0.44
1:A:512:ARG:HG3	1:A:512:ARG:NH1	2.32	0.44
1:B:198:ARG:O	1:B:198:ARG:HG3	2.17	0.44
1:A:202:HIS:HE1	1:A:278:SER:O	2.00	0.44
1:B:391:ASN:O	1:B:395:LYS:HG2	2.17	0.44
1:B:115:VAL:HG12	1:B:116:ILE:HG13	2.00	0.44
1:B:352:VAL:HG11	1:B:556:VAL:HG13	2.00	0.44
1:A:410:MET:HE2	4:A:1866:HOH:O	2.17	0.44
1:A:548:HIS:HE1	1:A:572:ASP:OD1	2.01	0.44
1:A:534:MET:O	1:A:539:MET:HE2	2.17	0.44
1:B:104:LYS:HG2	1:B:109:GLN:HG3	1.99	0.43
1:B:255:HIS:CD2	1:B:257:ASN:H	2.35	0.43
1:B:104:LYS:HA	1:B:108:LEU:HB2	1.99	0.43
1:B:255:HIS:HD2	1:B:257:ASN:HB2	1.84	0.43
1:A:142:LEU:O	1:A:146:VAL:HG23	2.18	0.43
1:A:354:LEU:HD23	1:A:354:LEU:C	2.44	0.43
1:B:414:PHE:CE2	1:B:416:HIS:HB2	2.54	0.43
1:A:123:ILE:HG13	1:A:565:PHE:CE2	2.54	0.43
1:A:227:ASP:O	1:A:231:VAL:HG23	2.19	0.43
1:A:555:GLN:C	1:A:557:PRO:HD3	2.44	0.43
1:A:421:PHE:CZ	1:A:615:ARG:HG3	2.54	0.43
3:A:1602:HC5:HAJ3	3:A:1602:HC5:OAK	2.18	0.43
1:B:276:VAL:O	1:B:280:GLN:HG3	2.19	0.43
1:A:374:PRO:HD3	4:A:2184:HOH:O	2.17	0.43
1:A:625:LYS:HB2	1:A:625:LYS:NZ	2.33	0.43
1:A:568:PRO:HG2	1:A:591:ALA:HA	2.01	0.43
1:B:123:ILE:HD13	1:B:124:LEU:N	2.34	0.43
1:B:294:ARG:HD2	4:B:1963:HOH:O	2.18	0.43
1:A:373:VAL:HA	4:A:2184:HOH:O	2.19	0.42
1:A:625:LYS:HD3	1:A:625:LYS:N	2.34	0.42
1:B:123:ILE:HD13	1:B:124:LEU:O	2.19	0.42
1:B:507:THR:HG23	2:B:1701:COA:H143	2.00	0.42
1:A:476:LEU:HA	1:A:479:VAL:HG22	2.02	0.42
2:B:1701:COA:S1P	3:B:1702:HC5:HAQ1	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:LYS:HG2	1:A:109:GLN:CD	2.45	0.42
1:B:622:PRO:HA	4:B:2514:HOH:O	2.19	0.42
1:B:540:ASP:OD2	1:B:541:THR:N	2.53	0.42
1:A:129:PHE:HB2	1:A:134:GLY:HA3	2.02	0.42
1:A:439:LEU:HA	1:A:479:VAL:HG12	2.02	0.42
1:A:55:GLN:N	1:A:56:PRO:HD2	2.35	0.42
1:A:84:GLN:O	1:A:88:GLU:HG3	2.20	0.42
1:B:621:HIS:N	1:B:622:PRO:HD3	2.35	0.42
1:A:184:GLY:HA3	1:A:187:GLN:O	2.20	0.42
1:A:457:LEU:CD2	1:A:466:ASP:HB2	2.39	0.41
1:B:506:TYR:O	1:B:506:TYR:HD2	2.03	0.41
1:B:568:PRO:HD2	1:B:592:TYR:CZ	2.55	0.41
1:B:255:HIS:CD2	1:B:257:ASN:HB2	2.55	0.41
1:A:487:VAL:HA	4:A:1721:HOH:O	2.19	0.41
3:A:1602:HC5:HAJ2	4:A:1663:HOH:O	2.20	0.41
1:A:143:ILE:O	1:A:147:LEU:HG	2.21	0.41
1:A:196:SER:O	1:A:197:LYS:C	2.64	0.41
1:A:349:PRO:HA	1:A:352:VAL:HG22	2.02	0.41
1:B:568:PRO:HG2	1:B:591:ALA:HA	2.02	0.41
1:A:199:PRO:HA	1:A:200:PRO:HD3	1.87	0.41
1:A:209:TYR:N	1:A:209:TYR:CD2	2.88	0.41
1:B:82:ARG:HD2	4:B:2529:HOH:O	2.20	0.41
1:A:118:SER:O	1:A:120:PRO:HD3	2.21	0.41
1:B:322:TRP:H	1:B:328:GLN:HE22	1.69	0.41
1:A:354:LEU:O	1:A:358:VAL:HG23	2.21	0.41
1:A:372:MET:HE1	4:A:1911:HOH:O	2.20	0.41
1:A:489:GLU:O	1:A:617:LEU:HD11	2.21	0.41
1:A:504:ARG:HD2	4:A:1735:HOH:O	2.20	0.41
1:B:455:ALA:HB2	1:B:468:ILE:HG13	2.03	0.41
1:A:451:THR:HG21	1:A:470:SER:HB2	2.03	0.40
1:A:491:GLN:HB2	4:A:2143:HOH:O	2.21	0.40
1:A:563:VAL:HB	1:A:586:ASN:HB3	2.01	0.40
1:A:41:PRO:HA	1:A:42:PRO:HD3	1.98	0.40
1:A:485:SER:HA	4:A:2052:HOH:O	2.21	0.40
1:B:61:GLU:CD	1:B:61:GLU:H	2.28	0.40
1:B:212:PHE:CD1	1:B:236:ILE:HG23	2.56	0.40
1:B:358:VAL:O	1:B:362:THR:HG23	2.22	0.40
1:B:209:TYR:CD2	1:B:209:TYR:N	2.89	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	597/599 (100%)	571 (96%)	24 (4%)	2 (0%)	36	36
1	B	597/599 (100%)	577 (97%)	20 (3%)	0	100	100
All	All	1194/1198 (100%)	1148 (96%)	44 (4%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	MET
1	A	624	ALA

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	525/525 (100%)	514 (98%)	11 (2%)	47	54
1	B	525/525 (100%)	514 (98%)	11 (2%)	47	54
All	All	1050/1050 (100%)	1028 (98%)	22 (2%)	47	54

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ILE
1	A	132	LEU
1	A	133	GLN
1	A	141	LYS

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Mol	Chain	Res	Type
1	A	198	ARG
1	A	206	VAL
1	A	343	HIS
1	A	369	ARG
1	A	372	MET
1	A	517	ASP
1	A	625	LYS
1	B	123	ILE
1	B	137	ARG
1	B	163	LEU
1	B	204	THR
1	B	206	VAL
1	B	308	MET
1	B	343	HIS
1	B	352	VAL
1	B	511	ILE
1	B	597	GLU
1	B	623	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	74	GLN
1	A	84	GLN
1	A	135	GLN
1	A	155	ASN
1	A	192	ASN
1	A	202	HIS
1	A	210	GLN
1	A	242	GLN
1	A	307	GLN
1	A	310	HIS
1	A	328	GLN
1	A	357	HIS
1	A	405	GLN
1	A	447	GLN
1	A	461	HIS
1	A	501	GLN
1	A	526	GLN
1	A	548	HIS
1	A	550	ASN

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Mol	Chain	Res	Type
1	A	586	ASN
1	A	619	GLN
1	A	620	ASN
1	B	32	GLN
1	B	65	HIS
1	B	74	GLN
1	B	84	GLN
1	B	135	GLN
1	B	192	ASN
1	B	202	HIS
1	B	207	HIS
1	B	210	GLN
1	B	228	GLN
1	B	255	HIS
1	B	291	GLN
1	B	307	GLN
1	B	310	HIS
1	B	328	GLN
1	B	357	HIS
1	B	461	HIS
1	B	526	GLN
1	B	548	HIS
1	B	586	ASN
1	B	619	GLN
1	B	620	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	HC5	A	1602	-	17,17,17	1.07	2 (11%)	22,22,22	1.36	3 (13%)
2	COA	B	1701	-	47,50,50	1.22	4 (8%)	69,75,75	1.52	10 (14%)
2	COA	A	1601	-	47,50,50	1.27	5 (10%)	69,75,75	1.52	11 (15%)
3	HC5	B	1702	-	17,17,17	1.04	1 (5%)	22,22,22	1.35	3 (13%)

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	HC5	A	1602	-	-	0/18/18/18	-
2	COA	B	1701	-	-	4/48/64/64	0/3/3/3
2	COA	A	1601	-	-	3/48/64/64	0/3/3/3
3	HC5	B	1702	-	-	0/18/18/18	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1601	COA	C5A-N7A	-3.40	1.32	1.39
2	B	1701	COA	P3B-O7A	3.37	1.61	1.50
2	A	1601	COA	P3B-O7A	3.36	1.60	1.50
2	B	1701	COA	C5A-N7A	-3.30	1.33	1.39
2	A	1601	COA	P2A-O3A	2.72	1.62	1.59
2	A	1601	COA	P1A-O3A	2.72	1.62	1.59
3	B	1702	HC5	OAL-CAR	-2.62	1.22	1.30
3	A	1602	HC5	OAL-CAR	-2.56	1.22	1.30
3	A	1602	HC5	CAO-NAN	-2.26	1.47	1.52
2	A	1601	COA	C4A-N9A	-2.09	1.33	1.37
2	B	1701	COA	P2A-O3A	2.08	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1701	COA	C4A-N9A	-2.05	1.33	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	COA	N3A-C2A-N1A	-5.39	120.42	128.58
2	B	1701	COA	N3A-C2A-N1A	-5.34	120.50	128.58
2	B	1701	COA	C5A-C4A-N3A	-5.00	119.83	126.72
2	A	1601	COA	C5A-C4A-N3A	-4.95	119.90	126.72
3	B	1702	HC5	OAK-CAH-CAG	3.97	120.07	111.48
3	A	1602	HC5	OAK-CAH-CAG	3.79	119.67	111.48
2	A	1601	COA	C2A-N3A-C4A	3.78	121.07	111.83
2	B	1701	COA	C2A-N3A-C4A	3.78	121.07	111.83
2	A	1601	COA	N9A-C8A-N7A	-3.54	108.91	113.94
2	B	1701	COA	N3A-C4A-N9A	3.45	133.04	127.17
2	B	1701	COA	N9A-C8A-N7A	-3.45	109.04	113.94
2	A	1601	COA	N3A-C4A-N9A	3.36	132.88	127.17
2	A	1601	COA	O9A-P3B-O8A	3.02	119.12	107.80
2	B	1701	COA	O9A-P3B-O8A	3.00	119.05	107.80
2	B	1701	COA	O4B-C1B-N9A	2.94	113.73	108.09
2	A	1601	COA	C5A-N7A-C8A	2.85	107.93	103.45
2	B	1701	COA	C5A-N7A-C8A	2.82	107.88	103.45
2	A	1601	COA	O4B-C1B-N9A	2.76	113.39	108.09
3	A	1602	HC5	CAP-OAK-CAH	-2.61	111.55	117.80
2	B	1701	COA	C4A-C5A-N7A	-2.29	107.96	110.58
3	B	1702	HC5	CAP-OAK-CAH	-2.28	112.35	117.80
2	A	1601	COA	C4A-C5A-N7A	-2.25	108.01	110.58
3	A	1602	HC5	OAL-CAR-CAQ	2.19	120.80	114.00
3	B	1702	HC5	OAL-CAR-CAQ	2.14	120.66	114.00
2	B	1701	COA	C4A-N9A-C8A	2.14	107.98	105.74
2	A	1601	COA	C4A-N9A-C8A	2.07	107.92	105.74
2	A	1601	COA	O3B-P3B-O7A	-2.03	102.11	109.33

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1601	COA	P2A-O3A-P1A-O5B
2	B	1701	COA	P2A-O3A-P1A-O5B
2	A	1601	COA	C3B-O3B-P3B-O7A
2	B	1701	COA	C3B-O3B-P3B-O7A
2	A	1601	COA	C4B-C3B-O3B-P3B

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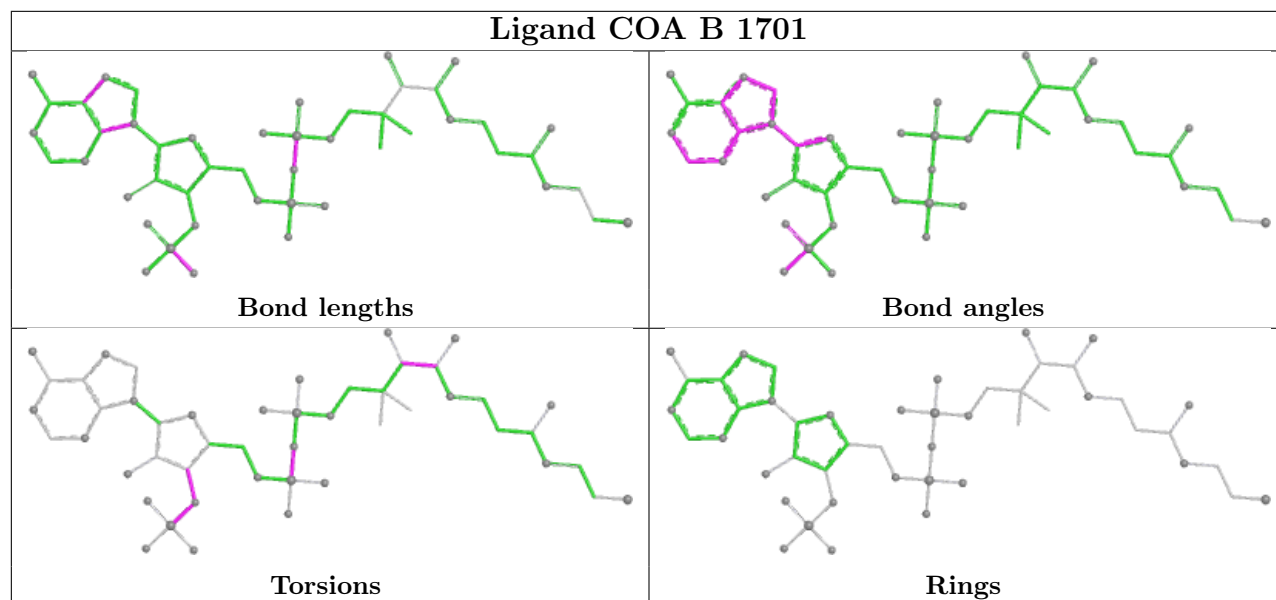
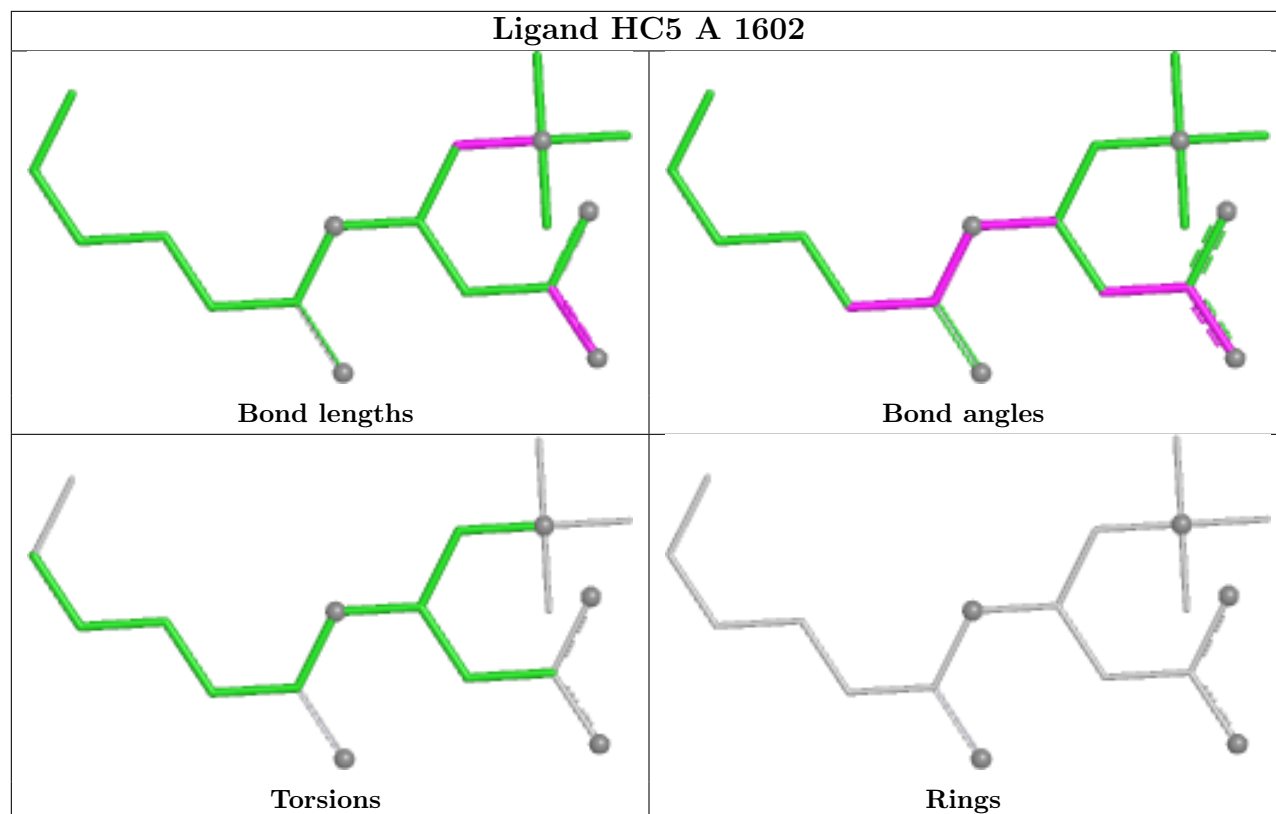
Mol	Chain	Res	Type	Atoms
2	B	1701	COA	C4B-C3B-O3B-P3B
2	B	1701	COA	N8P-C9P-CAP-OAP

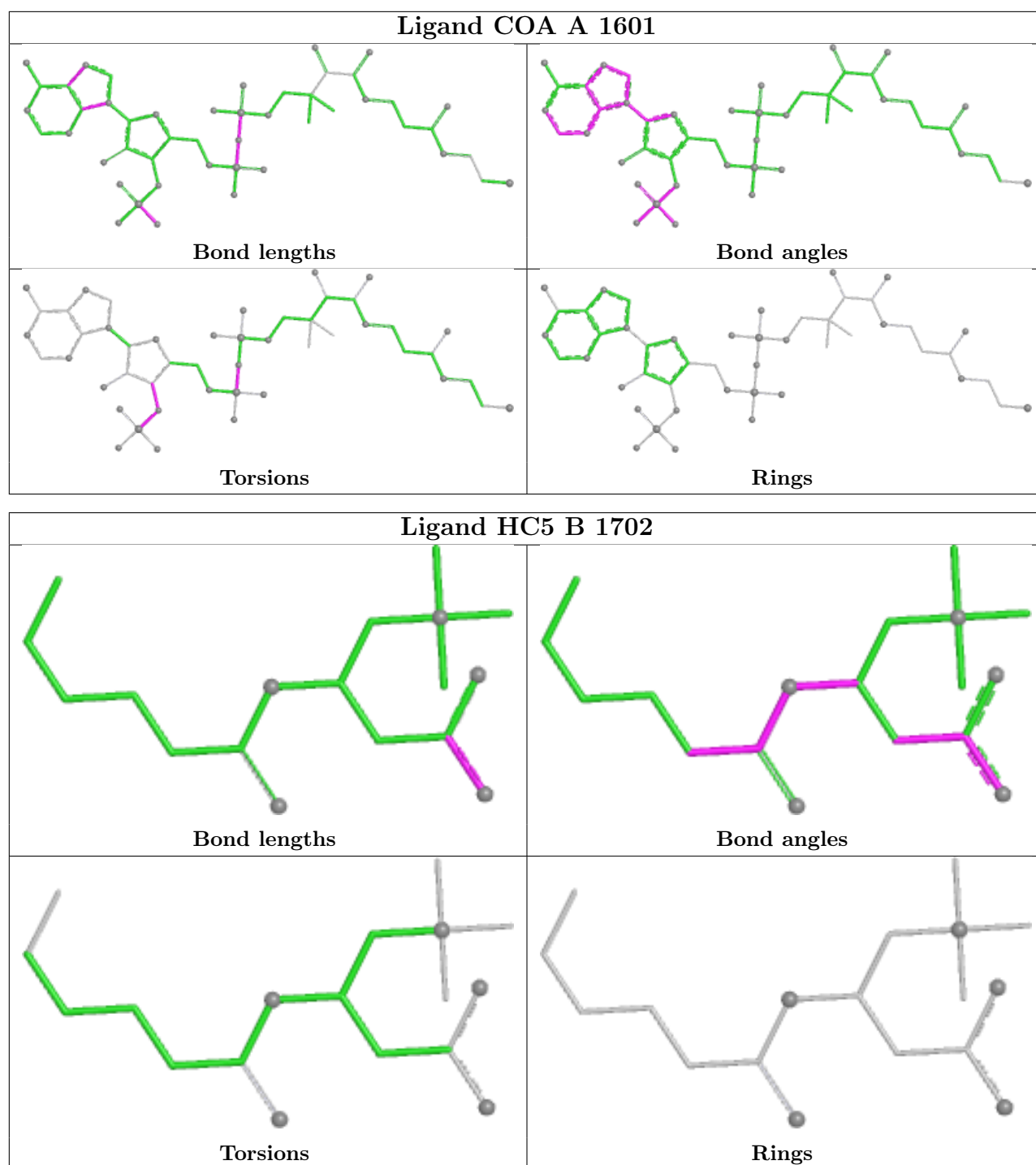
There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1602	HC5	7	0
2	B	1701	COA	7	0
2	A	1601	COA	4	0
3	B	1702	HC5	5	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

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	599/599 (100%)	-0.02	20 (3%)	49	51	9, 21, 45, 73	0
1	B	599/599 (100%)	-0.27	18 (3%)	52	55	7, 16, 36, 71	0
All	All	1198/1198 (100%)	-0.14	38 (3%)	50	53	7, 18, 40, 73	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	VAL	6.7
1	A	624	ALA	6.4
1	B	367	LEU	5.0
1	B	370	SER	4.9
1	A	27	SER	4.8
1	A	371	PRO	4.6
1	B	368	VAL	4.2
1	A	373	VAL	4.0
1	B	624	ALA	3.9
1	B	623	ARG	3.5
1	A	29	MET	3.4
1	A	367	LEU	3.3
1	B	244	ASN	3.3
1	B	163	LEU	3.3
1	B	369	ARG	3.3
1	B	371	PRO	3.1
1	B	622	PRO	3.1
1	A	369	ARG	2.8
1	B	29	MET	2.8
1	A	296	SER	2.8
1	A	372	MET	2.8
1	A	298	ASP	2.7
1	A	625	LYS	2.6
1	B	294	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	219	SER	2.6
1	A	370	SER	2.6
1	A	297	ASP	2.5
1	B	372	MET	2.5
1	B	198	ARG	2.4
1	B	625	LYS	2.4
1	A	242	GLN	2.4
1	A	556	VAL	2.3
1	A	374	PRO	2.3
1	B	365	PRO	2.3
1	B	164	GLY	2.3
1	A	132	LEU	2.1
1	A	345	ALA	2.1
1	B	364	LYS	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

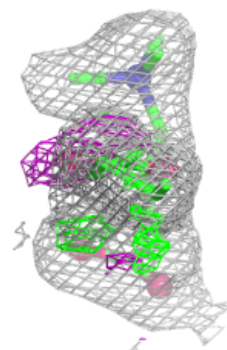
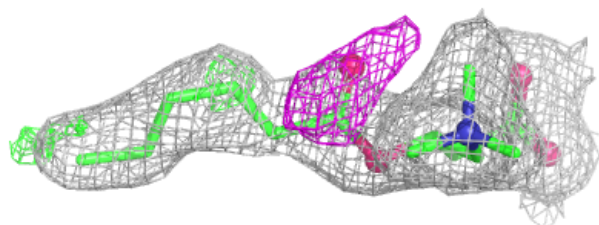
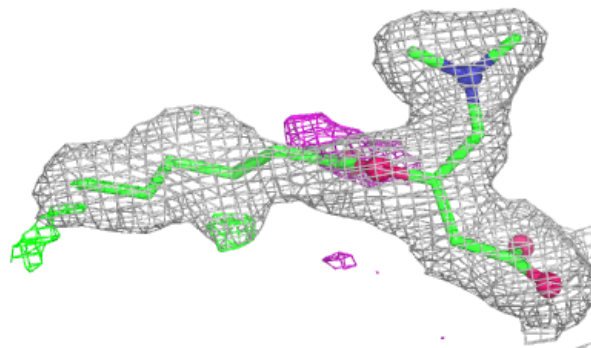
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HC5	A	1602	18/18	0.88	0.13	16,22,34,37	0
2	COA	B	1701	48/48	0.89	0.11	29,34,46,55	0
2	COA	A	1601	48/48	0.89	0.11	28,35,44,49	0
3	HC5	B	1702	18/18	0.92	0.10	14,19,30,31	0

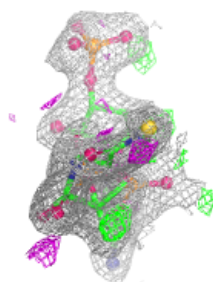
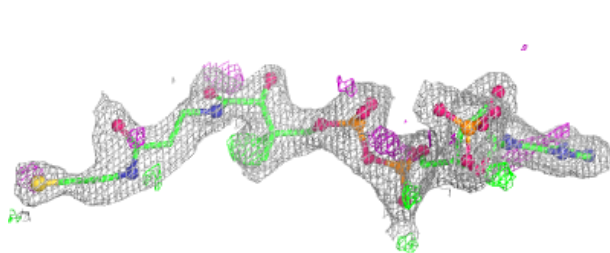
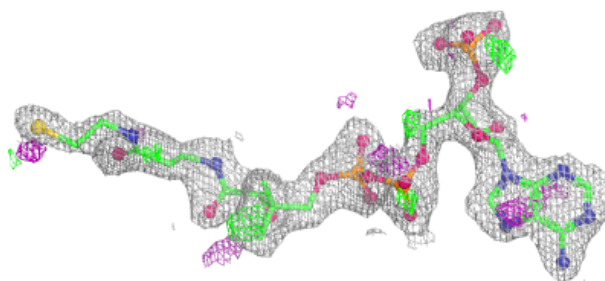
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HC5 A 1602:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

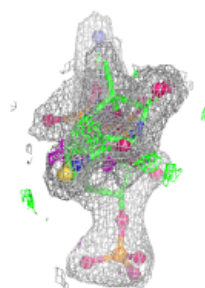
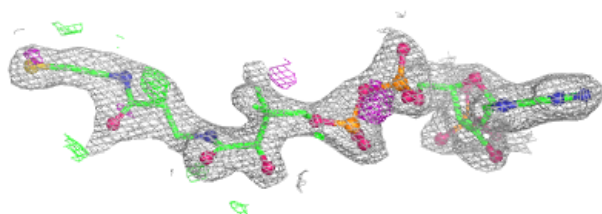
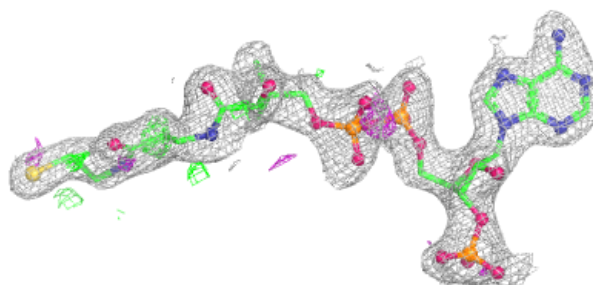
**Electron density around COA B 1701:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

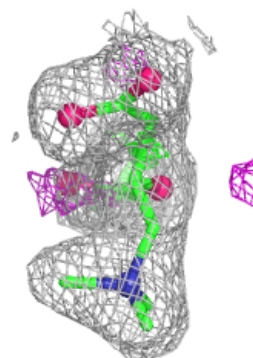
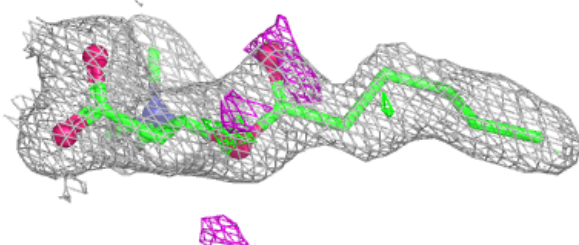
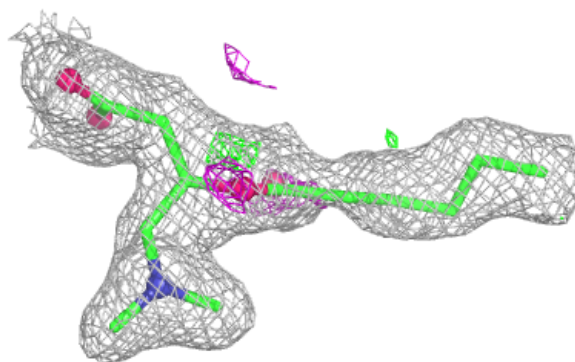


Electron density around COA A 1601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around HC5 B 1702:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.