



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:43 AM UTC

PDB ID : 2H3U / pdb_00002h3u
Title : Crystal structure of murine carnitine acetyltransferase in complex with carnitine and CoA
Authors : Hsiao, Y.S.; Jogl, G.; Tong, L.
Deposited on : 2006-05-23
Resolution : 1.90 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

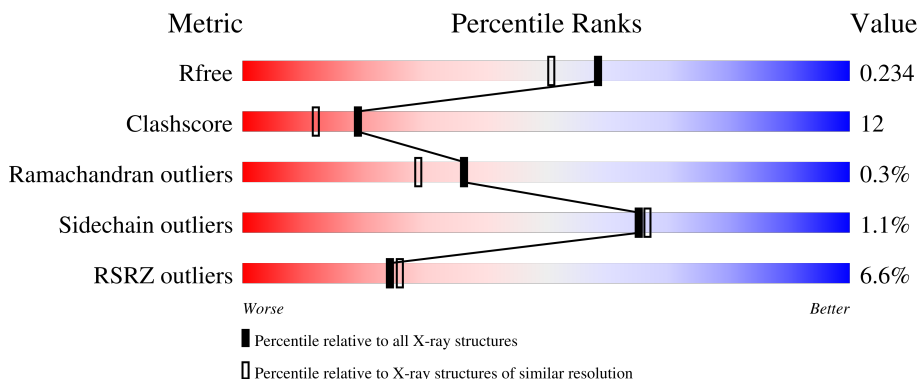
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	9% 75% 23% .
1	B	599	4% 80% 19% .

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 11366 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.

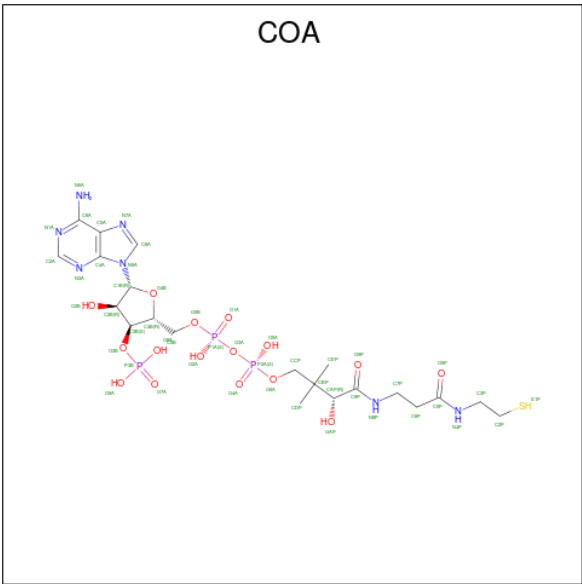
- Molecule 1 is a protein called carnitine acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	599	Total	C	N	O	S	0	0	0
			4781	3048	825	879	29			
1	B	599	Total	C	N	O	S	0	0	0
			4781	3048	825	879	29			

There are 6 discrepancies between the modelled and reference sequences:

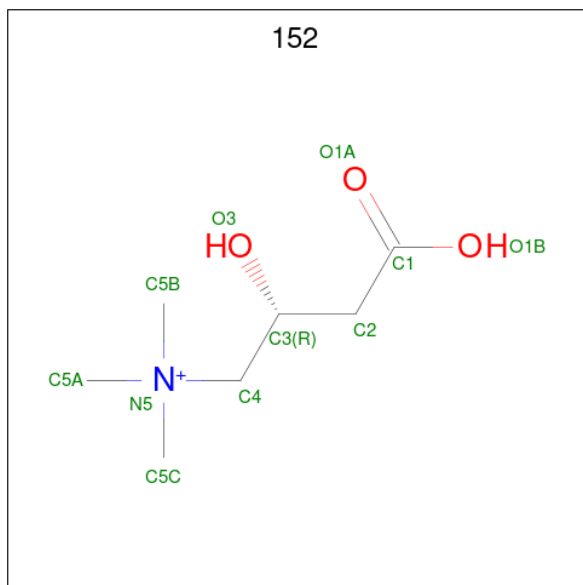
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	SER	-	cloning artifact	UNP Q3V1Y3
A	28	HIS	-	cloning artifact	UNP Q3V1Y3
A	29	MET	-	cloning artifact	UNP Q3V1Y3
B	27	SER	-	cloning artifact	UNP Q3V1Y3
B	28	HIS	-	cloning artifact	UNP Q3V1Y3
B	29	MET	-	cloning artifact	UNP Q3V1Y3

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



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

- 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		

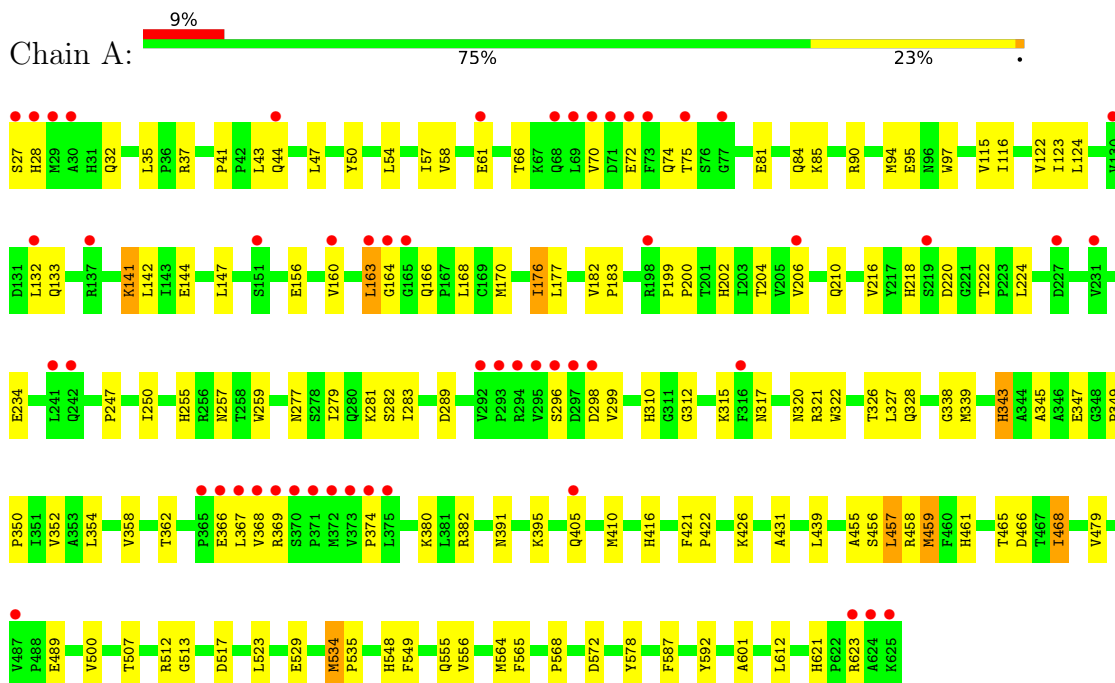
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	737	Total	O	0	0
			737	737		
4	B	949	Total	O	0	0
			949	949		

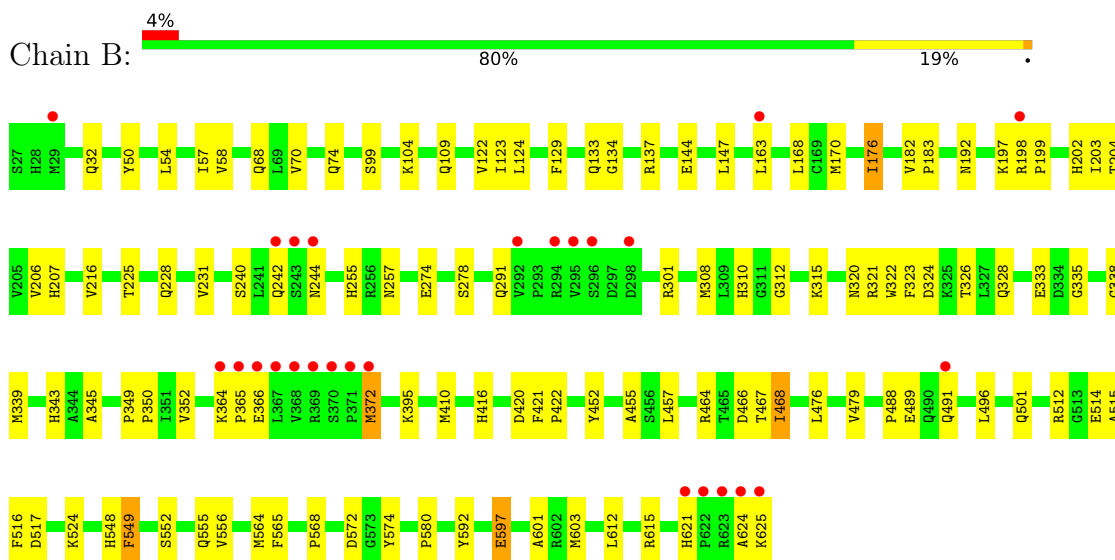
3 Residue-property plots [i](#)

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	164.51Å 89.74Å 122.95Å 90.00° 128.96° 90.00°	Depositor
Resolution (Å)	29.21 – 1.90 29.21 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.5 (29.21-1.90) 92.6 (29.21-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.193 , 0.235 0.193 , 0.234	Depositor DCC
R_{free} test set	8036 reflections (7.52%)	wwPDB-VP
Wilson B-factor (Å ²)	16.1	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11366	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: COA, 152

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	0.36	0/4897	0.82	9/6633 (0.1%)
1	B	0.41	0/4897	0.87	12/6633 (0.2%)
All	All	0.38	0/9794	0.85	21/13266 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	HIS	N-CA-C	6.71	120.56	112.38
1	A	182	VAL	CA-C-N	6.24	126.19	119.76
1	A	182	VAL	C-N-CA	6.24	126.19	119.76
1	B	343	HIS	N-CA-C	6.18	119.91	112.38
1	A	345	ALA	N-CA-C	6.15	118.06	111.36
1	A	549	PHE	N-CA-C	6.05	119.36	108.17
1	B	345	ALA	N-CA-C	5.69	117.56	111.36
1	B	176	ILE	N-CA-C	5.68	119.05	111.44
1	B	57	ILE	N-CA-C	5.55	118.49	113.10
1	B	323	PHE	N-CA-C	5.48	119.45	112.87
1	A	468	ILE	N-CA-C	-5.38	100.66	108.36
1	B	517	ASP	N-CA-C	5.35	116.80	111.07
1	A	176	ILE	N-CA-C	5.32	118.57	111.44
1	B	549	PHE	N-CA-C	5.32	117.98	107.98
1	A	465	THR	N-CA-C	5.28	116.83	108.96
1	A	459	MET	N-CA-C	-5.28	106.67	113.01
1	B	468	ILE	N-CA-C	-5.25	100.32	107.99
1	B	467	THR	N-CA-C	5.22	117.75	109.24
1	B	515	ALA	N-CA-C	-5.09	103.33	110.35
1	B	203	ILE	N-CA-C	-5.04	101.81	108.96
1	B	324	ASP	N-CA-C	-5.02	106.66	112.89

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	4781	0	4754	135	0
1	B	4781	0	4754	90	0
2	A	48	0	32	4	0
2	B	48	0	32	2	0
3	A	11	0	15	1	0
3	B	11	0	15	2	0
4	A	737	0	0	46	0
4	B	949	0	0	26	0
All	All	11366	0	9602	228	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 12.

All (228) 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:141:LYS:HD2	1:A:362:THR:HA	1.46	0.96
3:B:1901:152:H5A1	4:B:2511:HOH:O	1.70	0.92
1:A:457:LEU:HD13	4:A:2014:HOH:O	1.68	0.92
1:A:534:MET:HE2	1:A:535:PRO:HD2	1.50	0.90
1:A:90:ARG:HG2	4:A:2038:HOH:O	1.76	0.84
1:B:310:HIS:HD2	1:B:312:GLY:H	1.26	0.84
1:A:289:ASP:HA	4:A:2047:HOH:O	1.77	0.83
1:A:556:VAL:HG21	1:A:564:MET:HE2	1.62	0.81
1:A:310:HIS:HD2	1:A:312:GLY:H	1.28	0.80
1:A:457:LEU:HD11	1:A:466:ASP:HB2	1.64	0.80
1:B:315:LYS:HG2	4:B:2683:HOH:O	1.81	0.80
1:B:291:GLN:HA	4:B:2747:HOH:O	1.83	0.79
1:A:320:ASN:HB3	4:A:2217:HOH:O	1.82	0.78
1:B:32:GLN:HE22	1:B:170:MET:H	1.33	0.76
1:A:457:LEU:CD1	1:A:466:ASP:HB2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:PRO:HB2	1:A:350:PRO:HD3	1.68	0.76
1:A:461:HIS:HB2	4:A:2045:HOH:O	1.86	0.75
1:B:310:HIS:CD2	1:B:312:GLY:H	2.05	0.74
1:A:200:PRO:HB2	4:A:2157:HOH:O	1.87	0.74
1:B:501:GLN:HG2	4:B:2397:HOH:O	1.90	0.71
1:B:349:PRO:HD3	2:B:1902:COA:H31	1.70	0.71
1:B:333:GLU:HB3	4:B:2747:HOH:O	1.90	0.71
1:A:32:GLN:HE22	1:A:170:MET:H	1.36	0.70
1:B:349:PRO:HB2	1:B:350:PRO:HD3	1.73	0.69
1:A:426:LYS:HG2	1:A:623:ARG:HH22	1.57	0.69
1:B:556:VAL:HG21	1:B:564:MET:HE2	1.75	0.68
1:A:349:PRO:HD3	2:A:1802:COA:H31	1.75	0.68
1:A:283:ILE:HG12	4:A:2157:HOH:O	1.92	0.68
1:B:464:ARG:HD3	4:B:2553:HOH:O	1.93	0.68
1:B:207:HIS:HD2	1:B:240:SER:OG	1.78	0.67
1:A:459:MET:HG2	4:A:2176:HOH:O	1.95	0.67
1:A:426:LYS:HB2	1:A:623:ARG:HH12	1.59	0.66
1:A:310:HIS:CD2	1:A:312:GLY:H	2.12	0.66
1:A:317:ASN:HB3	4:A:2217:HOH:O	1.96	0.66
1:A:457:LEU:HD23	4:A:2176:HOH:O	1.95	0.65
1:B:255:HIS:HD2	1:B:257:ASN:H	1.44	0.65
1:A:534:MET:HE3	1:A:534:MET:HA	1.78	0.65
1:A:97:TRP:HA	4:A:2038:HOH:O	1.95	0.65
1:A:391:ASN:O	1:A:395:LYS:HG2	1.97	0.65
1:A:43:LEU:HD13	4:A:2015:HOH:O	1.96	0.64
1:B:322:TRP:H	1:B:328:GLN:NE2	1.96	0.64
1:A:534:MET:CE	1:A:535:PRO:HD2	2.27	0.63
1:A:321:ARG:HG2	1:A:321:ARG:HH11	1.63	0.63
1:B:491:GLN:HG3	4:B:2552:HOH:O	1.98	0.62
1:B:556:VAL:HG22	2:B:1902:COA:H32	1.82	0.62
1:A:50:TYR:CZ	1:A:54:LEU:HD11	2.35	0.62
1:A:320:ASN:O	1:A:321:ARG:HG2	2.00	0.62
1:A:421:PHE:HB3	1:A:422:PRO:HD3	1.80	0.61
1:A:321:ARG:HB3	1:A:328:GLN:HE22	1.67	0.60
1:A:72:GLU:O	1:A:75:THR:HG22	2.01	0.60
1:B:421:PHE:HB3	1:B:422:PRO:HD3	1.83	0.60
1:A:322:TRP:H	1:A:328:GLN:NE2	2.00	0.59
1:A:90:ARG:CZ	1:A:94:MET:HE1	2.33	0.59
1:A:366:GLU:HA	1:A:369:ARG:HH21	1.68	0.59
1:B:68:GLN:HG2	4:B:2344:HOH:O	2.01	0.58
1:A:132:LEU:HD22	1:A:132:LEU:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LEU:HD11	1:B:216:VAL:HB	1.85	0.58
1:A:84:GLN:CD	4:A:2039:HOH:O	2.46	0.58
1:A:43:LEU:N	4:A:2039:HOH:O	2.35	0.57
1:B:372:MET:HA	4:B:2351:HOH:O	2.04	0.57
1:B:163:LEU:HB3	1:B:168:LEU:HD21	1.86	0.57
1:B:122:VAL:HB	1:B:339:MET:HG2	1.87	0.57
1:B:123:ILE:HG13	1:B:565:PHE:CE2	2.40	0.57
1:A:568:PRO:HD2	1:A:592:TYR:CZ	2.40	0.57
1:B:133:GLN:HE21	1:B:137:ARG:HH11	1.51	0.56
1:A:133:GLN:HG2	4:A:2000:HOH:O	2.06	0.56
1:A:512:ARG:HH11	1:A:512:ARG:HG3	1.70	0.56
1:A:366:GLU:HB3	1:A:369:ARG:HE	1.70	0.55
1:B:410:MET:HE2	4:B:2371:HOH:O	2.05	0.55
1:B:395:LYS:HD3	4:B:2826:HOH:O	2.05	0.55
1:A:177:LEU:HD23	1:A:327:LEU:HD12	1.87	0.55
1:B:555:GLN:NE2	1:B:580:PRO:HG2	2.22	0.54
1:A:489:GLU:HB3	1:A:621:HIS:HE2	1.71	0.54
1:A:322:TRP:H	1:A:328:GLN:HE22	1.55	0.54
1:A:455:ALA:HB2	1:A:468:ILE:HG13	1.89	0.54
1:A:210:GLN:NE2	1:A:380:LYS:HE3	2.23	0.54
1:A:85:LYS:HD3	4:A:1985:HOH:O	2.08	0.53
1:A:44:GLN:HB2	4:A:2200:HOH:O	2.08	0.53
1:B:104:LYS:HG2	1:B:109:GLN:CD	2.34	0.52
1:B:457:LEU:HD21	1:B:466:ASP:HB2	1.91	0.52
1:A:296:SER:HB2	1:A:298:ASP:OD1	2.10	0.52
1:B:568:PRO:HD2	1:B:592:TYR:CZ	2.45	0.52
1:A:176:ILE:HA	1:A:326:THR:HG21	1.91	0.52
1:B:322:TRP:H	1:B:328:GLN:HE22	1.56	0.52
1:A:255:HIS:CD2	1:A:257:ASN:H	2.27	0.52
1:A:28:HIS:HA	1:A:156:GLU:OE1	2.10	0.52
1:B:496:LEU:C	1:B:496:LEU:HD23	2.34	0.52
1:A:320:ASN:ND2	4:A:2047:HOH:O	2.43	0.51
1:B:225:THR:H	1:B:228:GLN:NE2	2.08	0.51
1:B:244:ASN:HB2	4:B:2330:HOH:O	2.08	0.51
1:A:529:GLU:HG2	4:A:1962:HOH:O	2.09	0.51
1:A:84:GLN:NE2	4:A:2015:HOH:O	2.44	0.51
1:A:84:GLN:NE2	4:A:2039:HOH:O	2.43	0.51
1:A:58:VAL:HG21	4:A:2017:HOH:O	2.10	0.51
1:A:32:GLN:NE2	1:A:170:MET:H	2.08	0.51
1:A:457:LEU:HD12	1:A:466:ASP:HB2	1.92	0.51
1:A:548:HIS:HE1	1:A:572:ASP:OD1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ARG:HD3	4:B:2612:HOH:O	2.11	0.50
1:B:176:ILE:HA	1:B:326:THR:HG21	1.93	0.50
3:A:1801:152:O3	3:A:1801:152:H5B3	2.12	0.49
1:A:368:VAL:HG22	4:A:2020:HOH:O	2.12	0.49
1:A:218:HIS:HA	4:A:2396:HOH:O	2.13	0.49
1:A:277:ASN:OD1	1:A:281:LYS:HE2	2.12	0.49
1:A:328:GLN:O	1:A:339:MET:HB2	2.13	0.49
1:B:255:HIS:CD2	1:B:257:ASN:H	2.27	0.49
1:A:41:PRO:HG3	1:A:513:GLY:O	2.11	0.49
1:B:32:GLN:NE2	1:B:170:MET:H	2.08	0.49
1:B:242:GLN:HB2	4:B:2583:HOH:O	2.13	0.49
3:B:1901:152:O3	3:B:1901:152:H5B3	2.12	0.49
1:A:456:SER:HB2	2:A:1802:COA:H71	1.94	0.48
1:B:310:HIS:HE1	4:B:2252:HOH:O	1.95	0.48
1:B:122:VAL:HG22	1:B:564:MET:HG2	1.94	0.48
1:B:349:PRO:HA	1:B:352:VAL:HG22	1.95	0.48
1:B:320:ASN:C	1:B:321:ARG:HG2	2.39	0.48
1:B:123:ILE:HG13	1:B:565:PHE:HE2	1.78	0.48
1:B:574:TYR:CE1	1:B:603:MET:HE3	2.48	0.48
1:A:354:LEU:C	1:A:354:LEU:HD23	2.38	0.48
1:A:367:LEU:HD12	4:A:2196:HOH:O	2.14	0.48
1:B:99:SER:HB3	4:B:2538:HOH:O	2.12	0.48
1:A:163:LEU:HB2	1:A:168:LEU:HD21	1.95	0.48
1:A:296:SER:OG	1:A:299:VAL:HG22	2.14	0.48
1:B:70:VAL:O	1:B:74:GLN:HG2	2.14	0.48
1:A:352:VAL:HG11	1:A:556:VAL:HG12	1.96	0.48
1:A:405:GLN:HG3	4:A:2388:HOH:O	2.13	0.48
1:B:488:PRO:HD2	1:B:491:GLN:CD	2.38	0.48
1:A:122:VAL:HB	1:A:339:MET:HG2	1.96	0.47
1:A:426:LYS:CB	1:A:623:ARG:HH12	2.23	0.47
1:B:452:TYR:HB2	1:B:549:PHE:CD1	2.49	0.47
1:B:197:LYS:C	1:B:199:PRO:HD3	2.40	0.47
1:A:416:HIS:CG	1:A:612:LEU:HD21	2.50	0.47
1:B:198:ARG:O	1:B:198:ARG:HG3	2.14	0.47
1:A:166:GLN:HB2	4:A:2249:HOH:O	2.15	0.47
1:A:321:ARG:NH1	4:A:2217:HOH:O	2.48	0.47
1:B:333:GLU:HB2	4:B:2338:HOH:O	2.13	0.47
1:A:132:LEU:HD22	1:A:132:LEU:N	2.28	0.47
1:A:426:LYS:CG	1:A:623:ARG:HH12	2.27	0.46
1:A:183:PRO:HG3	1:A:259:TRP:NE1	2.30	0.46
1:B:129:PHE:CZ	1:B:335:GLY:HA2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:GLU:HG3	4:B:2378:HOH:O	2.14	0.46
1:A:507:THR:HG23	2:A:1802:COA:H143	1.97	0.46
1:B:192:ASN:HD22	1:B:192:ASN:C	2.22	0.46
1:A:439:LEU:HA	1:A:479:VAL:HG12	1.98	0.46
1:B:410:MET:HG2	1:B:601:ALA:HA	1.99	0.46
1:A:489:GLU:HB3	1:A:621:HIS:NE2	2.31	0.45
1:B:202:HIS:HD2	4:B:1914:HOH:O	1.99	0.45
1:A:255:HIS:HE1	4:A:1986:HOH:O	1.98	0.45
1:B:197:LYS:O	1:B:199:PRO:HD3	2.17	0.45
1:B:512:ARG:HG3	1:B:512:ARG:HH11	1.81	0.45
1:A:124:LEU:HG	1:A:338:GLY:HA2	1.98	0.45
1:B:476:LEU:HA	1:B:479:VAL:HG22	1.98	0.45
1:A:320:ASN:C	1:A:321:ARG:HG2	2.42	0.45
1:A:458:ARG:HD3	4:A:1935:HOH:O	2.17	0.45
1:A:204:THR:HG23	1:A:282:SER:HB3	1.97	0.45
1:B:124:LEU:HG	1:B:338:GLY:HA2	1.98	0.45
1:A:354:LEU:O	1:A:358:VAL:HG23	2.17	0.45
1:A:366:GLU:CA	1:A:369:ARG:HH21	2.29	0.45
1:B:548:HIS:HD2	4:B:2258:HOH:O	2.00	0.45
1:A:35:LEU:C	4:A:2045:HOH:O	2.60	0.44
1:A:144:GLU:HG3	4:A:1953:HOH:O	2.17	0.44
1:B:207:HIS:CD2	1:B:240:SER:OG	2.64	0.44
1:B:420:ASP:OD1	1:B:421:PHE:N	2.50	0.44
1:A:160:VAL:HG13	4:A:2018:HOH:O	2.18	0.44
1:B:50:TYR:CZ	1:B:54:LEU:HD11	2.53	0.44
1:B:182:VAL:HA	1:B:183:PRO:HD3	1.88	0.44
1:A:347:GLU:HB3	1:A:349:PRO:HD2	2.00	0.44
1:B:548:HIS:HE1	1:B:572:ASP:OD1	2.01	0.44
1:B:514:GLU:HG2	4:B:2375:HOH:O	2.17	0.44
1:A:512:ARG:HG3	1:A:512:ARG:NH1	2.31	0.44
1:A:27:SER:OG	1:A:32:GLN:NE2	2.51	0.43
1:A:81:GLU:HG3	4:A:2026:HOH:O	2.18	0.43
1:A:37:ARG:HG3	1:A:95:GLU:O	2.17	0.43
1:A:61:GLU:H	1:A:61:GLU:CD	2.26	0.43
1:B:54:LEU:O	1:B:58:VAL:HG22	2.18	0.43
1:A:47:LEU:HD13	1:A:70:VAL:HG13	2.00	0.43
1:B:310:HIS:HD2	1:B:312:GLY:N	2.06	0.43
1:A:142:LEU:C	1:A:142:LEU:HD23	2.43	0.43
1:A:255:HIS:HD2	1:A:257:ASN:H	1.66	0.43
1:A:115:VAL:HG12	1:A:116:ILE:HG13	2.00	0.43
1:A:204:THR:HG21	1:A:279:ILE:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:TYR:HB3	1:A:587:PHE:CD1	2.54	0.43
1:A:57:ILE:HG13	1:A:58:VAL:HG13	1.99	0.43
1:A:123:ILE:HG13	1:A:565:PHE:CE2	2.54	0.43
1:B:129:PHE:HB2	1:B:134:GLY:HA3	2.00	0.43
1:B:552:SER:C	4:B:2511:HOH:O	2.62	0.43
1:A:147:LEU:HD11	1:A:216:VAL:HB	2.01	0.43
1:A:461:HIS:N	4:A:2045:HOH:O	2.49	0.43
1:A:47:LEU:HD12	1:A:74:GLN:NE2	2.34	0.42
1:A:199:PRO:HA	1:A:200:PRO:HD3	1.93	0.42
1:A:431:ALA:HB3	1:A:500:VAL:HG13	2.00	0.42
1:A:220:ASP:OD1	1:A:222:THR:HG23	2.19	0.42
1:A:523:LEU:HD21	4:A:2015:HOH:O	2.18	0.42
1:B:421:PHE:CZ	1:B:615:ARG:HG3	2.55	0.42
1:B:516:PHE:C	1:B:516:PHE:CD1	2.98	0.42
1:B:597:GLU:HG2	4:B:2522:HOH:O	2.18	0.42
1:A:132:LEU:H	1:A:132:LEU:CD2	2.30	0.42
1:B:489:GLU:HB3	1:B:621:HIS:NE2	2.35	0.42
1:A:202:HIS:HD2	4:A:2069:HOH:O	2.02	0.42
1:B:364:LYS:HA	1:B:365:PRO:HD3	1.94	0.42
1:A:61:GLU:CD	1:A:61:GLU:N	2.78	0.42
1:A:321:ARG:HG2	1:A:321:ARG:NH1	2.32	0.41
1:A:426:LYS:HB2	1:A:623:ARG:NH1	2.32	0.41
1:A:382:ARG:HG3	4:A:2031:HOH:O	2.19	0.41
1:A:234:GLU:HB3	4:A:2140:HOH:O	2.19	0.41
1:B:621:HIS:HB3	4:B:2282:HOH:O	2.19	0.41
1:B:416:HIS:CG	1:B:612:LEU:HD21	2.56	0.41
1:B:455:ALA:HB2	1:B:468:ILE:HG13	2.02	0.41
1:B:144:GLU:HG3	4:B:2087:HOH:O	2.20	0.41
1:A:85:LYS:HE3	4:A:2026:HOH:O	2.20	0.41
1:A:315:LYS:HE3	4:A:2022:HOH:O	2.20	0.41
1:A:556:VAL:HG22	2:A:1802:COA:H32	2.02	0.41
1:B:524:LYS:HD3	4:B:2322:HOH:O	2.21	0.41
1:A:216:VAL:C	1:A:224:LEU:HD13	2.46	0.41
1:A:457:LEU:HA	4:A:2176:HOH:O	2.21	0.41
1:A:564:MET:HE1	4:A:2485:HOH:O	2.20	0.41
1:A:66:THR:O	1:A:70:VAL:HG23	2.21	0.41
1:A:410:MET:HG2	1:A:601:ALA:HA	2.02	0.41
1:A:548:HIS:HD2	4:A:2181:HOH:O	2.03	0.41
1:B:163:LEU:CB	1:B:168:LEU:HD21	2.51	0.41
1:B:202:HIS:HE1	1:B:278:SER:O	2.04	0.41
1:A:374:PRO:HA	4:A:2004:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:GLU:H	1:B:366:GLU:CD	2.29	0.41
1:B:163:LEU:HB2	1:B:168:LEU:HD11	2.02	0.40
1:B:512:ARG:HG3	1:B:512:ARG:NH1	2.37	0.40
1:A:555:GLN:NE2	4:A:1885:HOH:O	2.53	0.40
1:B:231:VAL:HG21	1:B:372:MET:SD	2.61	0.40
1:B:489:GLU:HB3	1:B:621:HIS:HE2	1.86	0.40
1:A:247:PRO:O	1:A:250:ILE:HG22	2.22	0.40
1:B:225:THR:H	1:B:228:GLN:HE21	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	597/599 (100%)	578 (97%)	18 (3%)	1 (0%)	43	36
1	B	597/599 (100%)	580 (97%)	15 (2%)	2 (0%)	36	29
All	All	1194/1198 (100%)	1158 (97%)	33 (3%)	3 (0%)	36	29

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	GLY
1	B	372	MET
1	B	624	ALA

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	A	527/527 (100%)	520 (99%)	7 (1%)	61	61
1	B	527/527 (100%)	522 (99%)	5 (1%)	70	73
All	All	1054/1054 (100%)	1042 (99%)	12 (1%)	65	67

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	LYS
1	A	163	LEU
1	A	206	VAL
1	A	343	HIS
1	A	457	LEU
1	A	517	ASP
1	A	534	MET
1	B	204	THR
1	B	206	VAL
1	B	308	MET
1	B	597	GLU
1	B	625	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	74	GLN
1	A	84	GLN
1	A	109	GLN
1	A	155	ASN
1	A	192	ASN
1	A	202	HIS
1	A	210	GLN
1	A	228	GLN
1	A	255	HIS
1	A	307	GLN
1	A	310	HIS
1	A	328	GLN
1	A	357	HIS
1	A	461	HIS

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Mol	Chain	Res	Type
1	A	490	GLN
1	A	501	GLN
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	55	GLN
1	B	65	HIS
1	B	74	GLN
1	B	84	GLN
1	B	109	GLN
1	B	133	GLN
1	B	135	GLN
1	B	155	ASN
1	B	171	ASN
1	B	192	ASN
1	B	202	HIS
1	B	207	HIS
1	B	228	GLN
1	B	255	HIS
1	B	307	GLN
1	B	310	HIS
1	B	328	GLN
1	B	357	HIS
1	B	405	GLN
1	B	461	HIS
1	B	491	GLN
1	B	503	HIS
1	B	526	GLN
1	B	548	HIS
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	152	B	1901	-	10,10,10	1.12	1 (10%)	13,14,14	1.16	1 (7%)
2	COA	A	1802	-	47,50,50	1.30	6 (12%)	69,75,75	1.50	10 (14%)
2	COA	B	1902	-	47,50,50	1.22	5 (10%)	69,75,75	1.51	10 (14%)
3	152	A	1801	-	10,10,10	1.21	1 (10%)	13,14,14	0.94	1 (7%)

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	152	B	1901	-	-	0/9/9/9	-
2	COA	A	1802	-	-	5/48/64/64	0/3/3/3
2	COA	B	1902	-	-	4/48/64/64	0/3/3/3
3	152	A	1801	-	-	0/9/9/9	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1802	COA	P3B-O7A	3.48	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1802	COA	P1A-O3A	3.37	1.63	1.59
2	B	1902	COA	P3B-O7A	3.29	1.60	1.50
2	A	1802	COA	C5A-N7A	-3.18	1.33	1.39
2	B	1902	COA	C5A-N7A	-3.17	1.33	1.39
2	A	1802	COA	P2A-O3A	2.85	1.62	1.59
2	B	1902	COA	P2A-O3A	2.43	1.62	1.59
2	A	1802	COA	O4B-C1B	2.43	1.47	1.42
2	B	1902	COA	P1A-O3A	2.25	1.61	1.59
3	A	1801	152	C4-N5	-2.22	1.47	1.52
2	B	1902	COA	O4B-C1B	2.12	1.46	1.42
2	A	1802	COA	C4A-N9A	-2.07	1.33	1.37
3	B	1901	152	C4-N5	-2.00	1.48	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1902	COA	N3A-C2A-N1A	-5.38	120.44	128.58
2	A	1802	COA	N3A-C2A-N1A	-5.26	120.61	128.58
2	B	1902	COA	C5A-C4A-N3A	-5.00	119.84	126.72
2	A	1802	COA	C5A-C4A-N3A	-4.99	119.85	126.72
2	A	1802	COA	C2A-N3A-C4A	3.65	120.75	111.83
2	B	1902	COA	C2A-N3A-C4A	3.64	120.72	111.83
2	B	1902	COA	N9A-C8A-N7A	-3.48	109.00	113.94
2	A	1802	COA	N9A-C8A-N7A	-3.45	109.03	113.94
2	B	1902	COA	N3A-C4A-N9A	3.30	132.78	127.17
2	A	1802	COA	N3A-C4A-N9A	3.29	132.77	127.17
3	B	1901	152	C3-C4-N5	-3.09	111.01	116.70
2	A	1802	COA	O9A-P3B-O8A	2.96	118.91	107.80
2	B	1902	COA	O9A-P3B-O8A	2.93	118.78	107.80
2	B	1902	COA	C5A-N7A-C8A	2.83	107.89	103.45
2	A	1802	COA	C5A-N7A-C8A	2.78	107.81	103.45
3	A	1801	152	C3-C4-N5	-2.60	111.91	116.70
2	B	1902	COA	O4B-C1B-N9A	2.37	112.64	108.09
2	B	1902	COA	C4A-C5A-N7A	-2.36	107.88	110.58
2	A	1802	COA	C4A-C5A-N7A	-2.32	107.93	110.58
2	A	1802	COA	O4B-C1B-N9A	2.05	112.02	108.09
2	B	1902	COA	C4A-N9A-C8A	2.03	107.87	105.74
2	A	1802	COA	C4A-N9A-C8A	2.00	107.84	105.74

There are no chirality outliers.

All (9) torsion outliers are listed below:

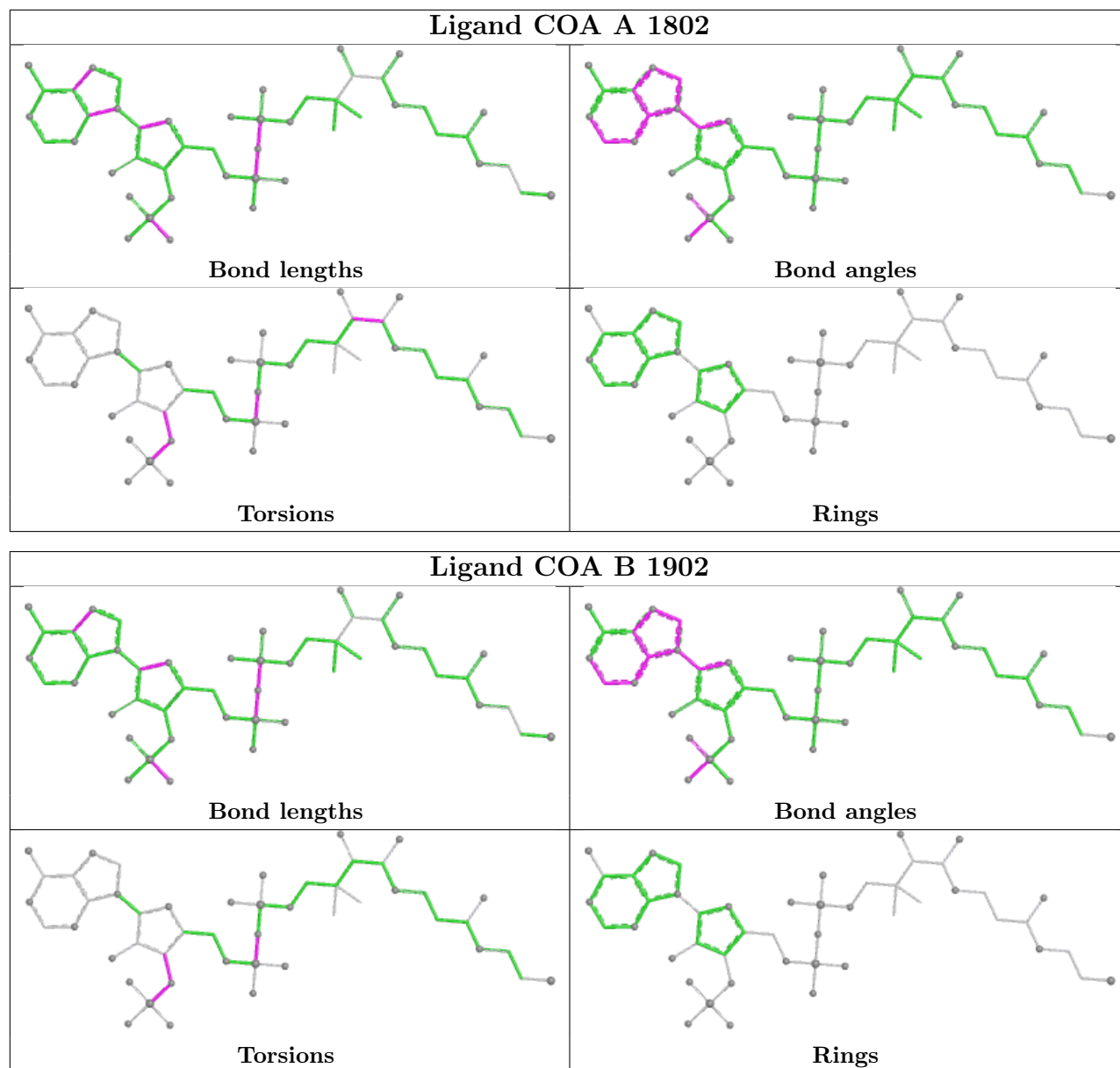
Mol	Chain	Res	Type	Atoms
2	A	1802	COA	C4B-C3B-O3B-P3B
2	A	1802	COA	C2B-C3B-O3B-P3B
2	B	1902	COA	C2B-C3B-O3B-P3B
2	A	1802	COA	P2A-O3A-P1A-O5B
2	B	1902	COA	P2A-O3A-P1A-O5B
2	B	1902	COA	C4B-C3B-O3B-P3B
2	A	1802	COA	C3B-O3B-P3B-O9A
2	B	1902	COA	C3B-O3B-P3B-O9A
2	A	1802	COA	N8P-C9P-CAP-OAP

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1901	152	2	0
2	A	1802	COA	4	0
2	B	1902	COA	2	0
3	A	1801	152	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 ⓘ

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%)	0.62	53 (8%)	15 16	11, 22, 47, 75	0
1	B	599/599 (100%)	0.07	26 (4%)	40 42	7, 15, 36, 75	0
All	All	1198/1198 (100%)	0.35	79 (6%)	24 26	7, 19, 43, 75	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	368	VAL	7.9
1	B	367	LEU	6.8
1	A	624	ALA	6.4
1	B	624	ALA	6.2
1	B	372	MET	6.0
1	A	163	LEU	5.6
1	A	368	VAL	5.2
1	A	367	LEU	5.2
1	A	30	ALA	5.0
1	B	371	PRO	5.0
1	A	27	SER	4.9
1	A	373	VAL	4.7
1	B	369	ARG	4.5
1	A	371	PRO	4.4
1	A	132	LEU	4.4
1	A	625	LYS	4.3
1	B	625	LYS	3.9
1	A	623	ARG	3.9
1	B	370	SER	3.9
1	A	372	MET	3.8
1	A	75	THR	3.8
1	B	622	PRO	3.7
1	A	227	ASP	3.7
1	A	293	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	69	LEU	3.6
1	A	369	ARG	3.6
1	B	163	LEU	3.6
1	A	374	PRO	3.5
1	A	165	GLY	3.5
1	A	298	ASP	3.5
1	B	623	ARG	3.4
1	A	295	VAL	3.4
1	B	244	ASN	3.3
1	A	164	GLY	3.3
1	A	70	VAL	3.3
1	A	296	SER	3.3
1	B	296	SER	3.2
1	B	294	ARG	3.2
1	A	68	GLN	3.1
1	A	375	LEU	3.1
1	B	292	VAL	3.1
1	A	29	MET	3.1
1	B	198	ARG	3.1
1	A	297	ASP	3.0
1	A	292	VAL	3.0
1	A	366	GLU	2.9
1	B	243	SER	2.9
1	A	160	VAL	2.9
1	B	295	VAL	2.8
1	A	28	HIS	2.8
1	A	370	SER	2.7
1	B	364	LYS	2.7
1	A	137	ARG	2.7
1	A	365	PRO	2.7
1	A	294	ARG	2.6
1	B	29	MET	2.6
1	B	366	GLU	2.6
1	A	77	GLY	2.6
1	A	61	GLU	2.6
1	A	72	GLU	2.6
1	A	130	VAL	2.6
1	A	242	GLN	2.5
1	A	206	VAL	2.5
1	B	621	HIS	2.4
1	B	298	ASP	2.3
1	B	242	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	491	GLN	2.3
1	A	241	LEU	2.3
1	B	365	PRO	2.2
1	A	44	GLN	2.2
1	A	405	GLN	2.2
1	A	151	SER	2.2
1	A	73	PHE	2.1
1	A	71	ASP	2.1
1	A	198	ARG	2.1
1	A	219	SER	2.0
1	A	316	PHE	2.0
1	A	231	VAL	2.0
1	A	487	VAL	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](#)

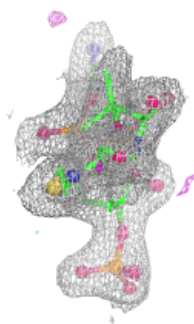
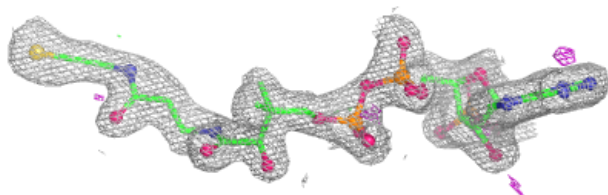
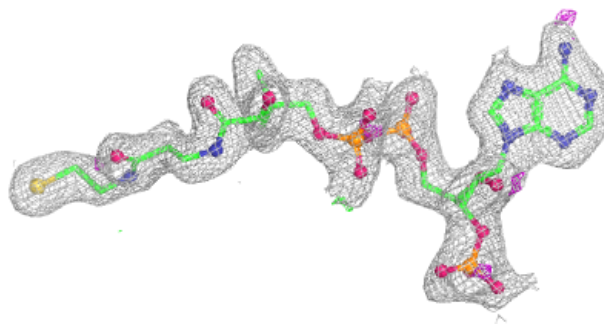
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	152	A	1801	11/11	0.91	0.08	13,15,17,18	0
2	COA	A	1802	48/48	0.93	0.09	19,24,33,35	0
2	COA	B	1902	48/48	0.94	0.08	14,24,31,32	0
3	152	B	1901	11/11	0.95	0.06	8,9,11,13	0

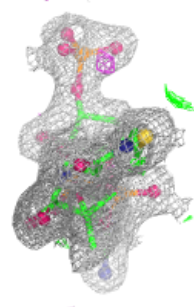
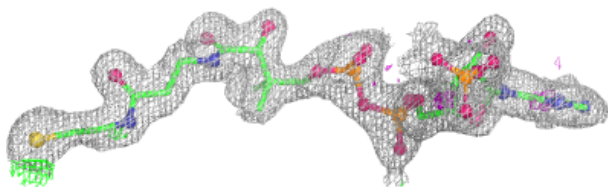
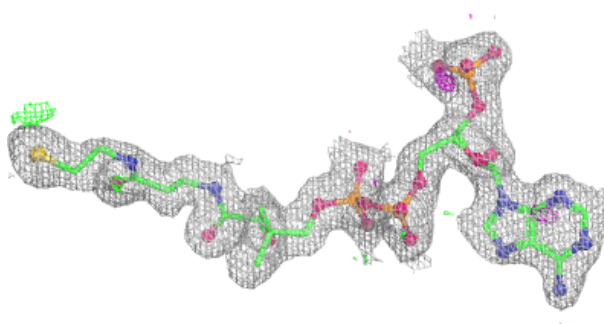
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA A 1802:

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

**Electron density around COA B 1902:**

$2mF_o-DF_c$ (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.