



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2017 – 11:50 AM EDT

PDB ID : 2H3U  
Title : Crystal structure of murine carnitine acetyltransferase in complex with carnitine and CoA  
Authors : Hsiao, Y.S.; Jogl, G.; Tong, L.  
Deposited on : unknown  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

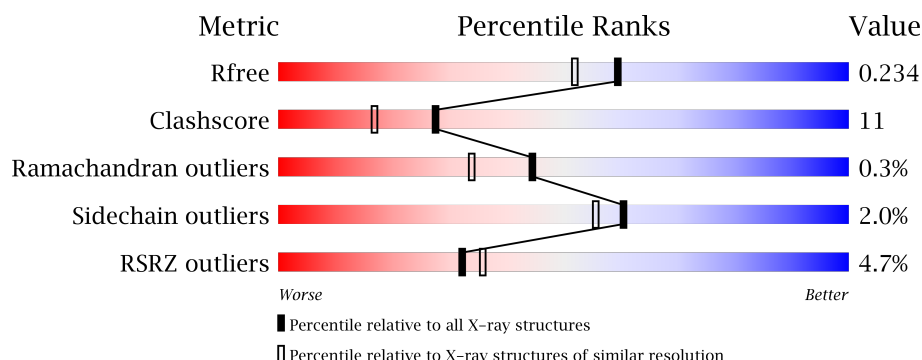
# 1 Overall quality at a glance

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))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>23%</div> <div>.</div> </div> </div>
1	B	599	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>18%</div> <div>.</div> </div> </div>

## 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.

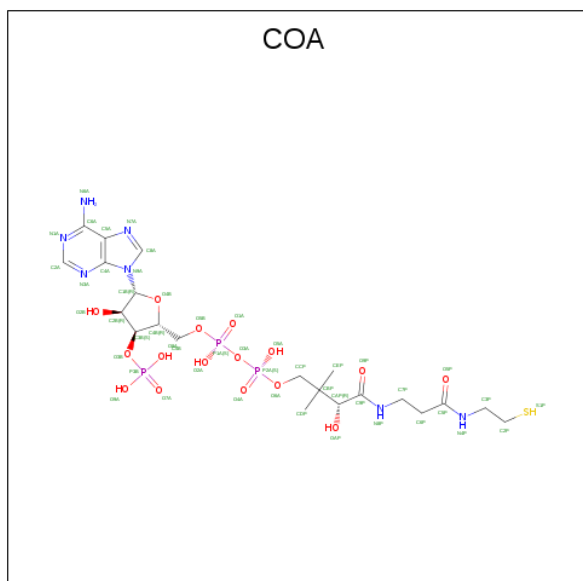
- Molecule 1 is a protein called carnitine acetyltransferase.

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:

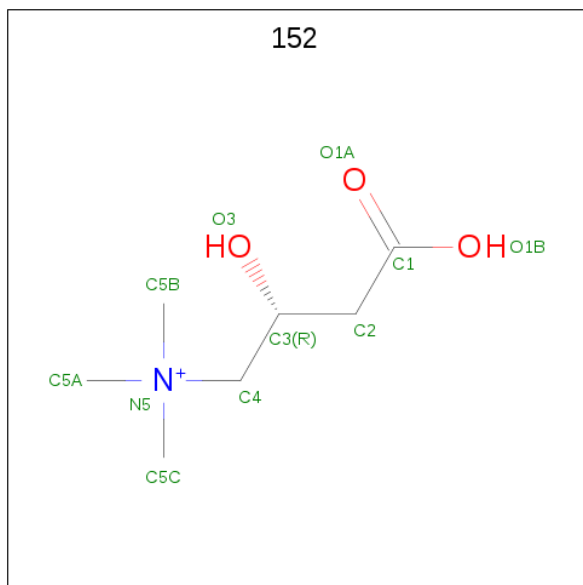
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	SER	-	CLONING ARTIFACT	UNP Q3V1Y3
A	28	HIS	-	CLONING ARTIFACT	UNP Q3V1Y3
A	29	MET	-	CLONING ARTIFACT	UNP Q3V1Y3
B	27	SER	-	CLONING ARTIFACT	UNP Q3V1Y3
B	28	HIS	-	CLONING ARTIFACT	UNP Q3V1Y3
B	29	MET	-	CLONING ARTIFACT	UNP Q3V1Y3

- Molecule 2 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



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

- Molecule 3 is CARNITINE (three-letter code: 152) (formula:  $C_7H_{16}NO_3$ ).



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

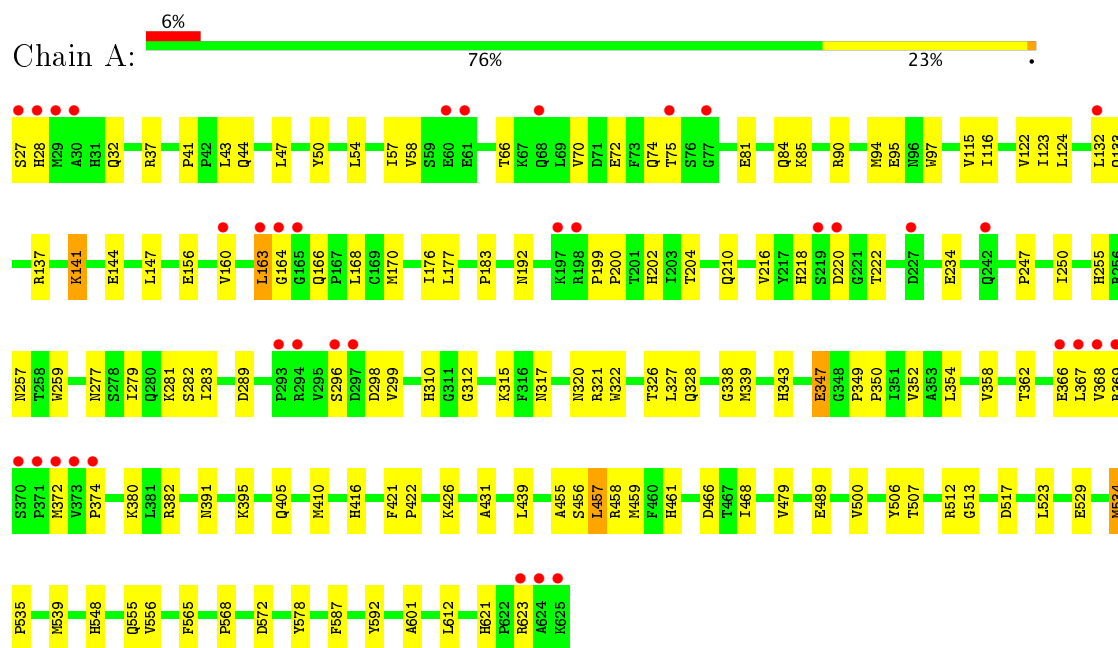
- Molecule 4 is water.

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

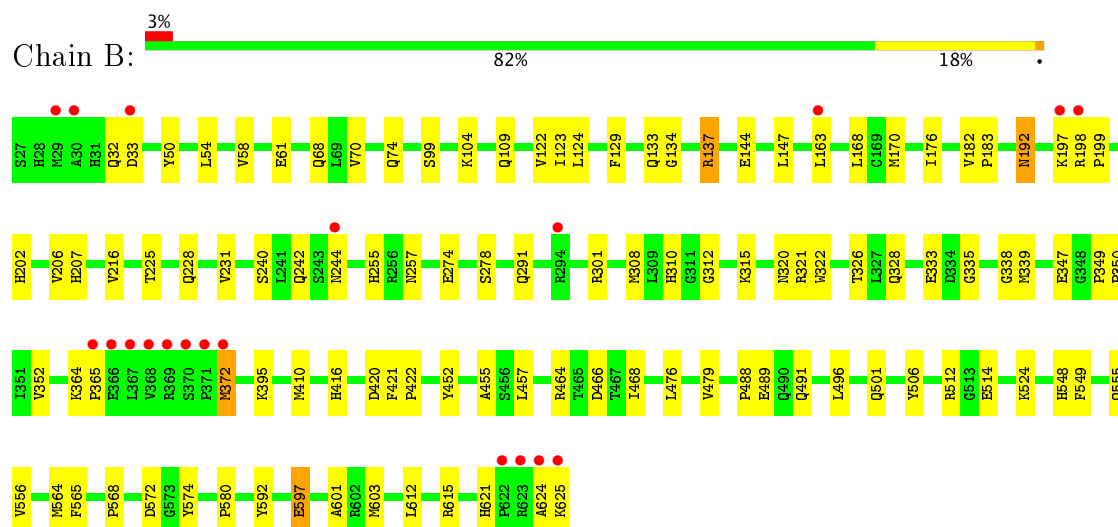
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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, $\alpha$ , $\beta$ , $\gamma$	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) 92.7 (29.21-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	7625 reflections (7.53%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.1	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.31	0/4897	0.53	0/6633
1	B	0.35	0/4897	0.58	0/6633
All	All	0.33	0/9794	0.55	0/13266

There are no bond length outliers.

There are no bond angle outliers.

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	128	0
1	B	4781	0	4754	86	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	24	0
All	All	11366	0	9602	217	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 (217) 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	1.48	0.91
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: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
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: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: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:HH11	1:A:321:ARG:HG2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:MET:HA	1:A:534:MET:HE3	1.80	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: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
1:B:147:LEU:HD11	1:B:216:VAL:HB	1.85	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: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:84:GLN:CD	4:A:2039:HOH:O	2.46	0.53
1:A:85:LYS:HD3	4:A:1985:HOH:O	2.08	0.53
1:A:539:MET:HE1	4:A:2538:HOH:O	2.07	0.53
1:A:44:GLN:HB2	4:A:2200:HOH:O	2.08	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:HIS:HA	1:A:156:GLU:OE1	2.10	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
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
3:B:1901:152:O3	3:B:1901:152:H5B3	2.12	0.49
1:B:242:GLN:HB2	4:B:2583:HOH:O	2.13	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:349:PRO:HA	1:B:352:VAL:HG22	1.95	0.48
1:B:122:VAL:HG22	1:B:564:MET:HG2	1.94	0.48
1:B:123:ILE:HG13	1:B:565:PHE:HE2	1.78	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:104:LYS:HG2	1:B:109:GLN:CD	2.34	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: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:496:LEU:HD23	1:B:496:LEU:C	2.34	0.47
1:B:452:TYR:HB2	1:B:549:PHE:CD1	2.49	0.47
1:A:416:HIS:CG	1:A:612:LEU:HD21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ARG:HG3	1:B:198:ARG:O	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:N	1:A:132:LEU:HD22	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
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: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: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: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:182:VAL:HA	1:B:183:PRO:HD3	1.88	0.44
1:B:50:TYR:CZ	1:B:54:LEU:HD11	2.53	0.44
1:A:347:GLU:HB3	1:A:349:PRO:HD2	2.00	0.44
1:A:94:MET:HE2	4:A:2144:HOH:O	2.17	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:NH1	1:A:512:ARG:HG3	2.31	0.44
1:B:320:ASN:C	1:B:321:ARG:HG2	2.39	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:B:574:TYR:CE1	1:B:603:MET:HE3	2.52	0.43
1:A:354:LEU:C	1:A:354:LEU:HD23	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ARG:HG3	1:A:95:GLU:O	2.17	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: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
1:B:488:PRO:HD2	1:B:491:GLN:CD	2.38	0.43
1:A:578:TYR:HB3	1:A:587:PHE:CD1	2.54	0.43
1:A:123:ILE:HG13	1:A:565:PHE:CE2	2.54	0.43
1:A:57:ILE:HG13	1:A:58:VAL:HG13	1.99	0.43
1:B:129:PHE:HB2	1:B:134:GLY:HA3	2.00	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: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:47:LEU:HD12	1:A:74:GLN:NE2	2.34	0.42
1:B:197:LYS:C	1:B:199:PRO:HD3	2.40	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:597:GLU:HG2	4:B:2522:HOH:O	2.18	0.42
1:A:132:LEU:CD2	1:A:132:LEU:H	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:B:556:VAL:HG21	1:B:564:MET:HE2	2.02	0.42
1:A:321:ARG:NH1	1:A:321:ARG:HG2	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:B:192:ASN:C	1:B:192:ASN:HD22	2.22	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:A:85:LYS:HE3	4:A:2026:HOH:O	2.20	0.41
1:B:524:LYS:HD3	4:B:2322:HOH:O	2.21	0.41
1:A:457:LEU:HA	4:A:2176:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:HIS:HD2	4:A:2181:HOH:O	2.03	0.41
1:B:202:HIS:HE1	1:B:278:SER:O	2.04	0.41
1:A:410:MET:HG2	1:A:601:ALA:HA	2.02	0.41
1:A:66:THR:O	1:A:70:VAL:HG23	2.21	0.41
1:B:163:LEU:CB	1:B:168:LEU:HD21	2.51	0.41
1:A:374:PRO:HA	4:A:2004:HOH:O	2.21	0.41
1:B:163:LEU:HB2	1:B:168:LEU:HD11	2.02	0.40
1:B:512:ARG:NH1	1:B:512:ARG:HG3	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%)	51	41
1	B	597/599 (100%)	580 (97%)	15 (2%)	2 (0%)	44	34
All	All	1194/1198 (100%)	1158 (97%)	33 (3%)	3 (0%)	44	34

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 ⓘ

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%)	516 (98%)	11 (2%)	59	53
1	B	527/527 (100%)	517 (98%)	10 (2%)	62	57
All	All	1054/1054 (100%)	1033 (98%)	21 (2%)	60	55

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ARG
1	A	141	LYS
1	A	163	LEU
1	A	192	ASN
1	A	343	HIS
1	A	347	GLU
1	A	372	MET
1	A	457	LEU
1	A	506	TYR
1	A	517	ASP
1	A	534	MET
1	B	33	ASP
1	B	61	GLU
1	B	137	ARG
1	B	192	ASN
1	B	206	VAL
1	B	308	MET
1	B	347	GLU
1	B	506	TYR
1	B	597	GLU
1	B	625	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN

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Mol	Chain	Res	Type
1	A	74	GLN
1	A	84	GLN
1	A	109	GLN
1	A	135	GLN
1	A	155	ASN
1	A	192	ASN
1	A	202	HIS
1	A	207	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	447	GLN
1	A	461	HIS
1	A	503	HIS
1	A	548	HIS
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	133	GLN
1	B	135	GLN
1	B	155	ASN
1	B	187	GLN
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	490	GLN
1	B	501	GLN

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Mol	Chain	Res	Type
1	B	503	HIS
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 carbohydrates 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	A	1801	-	7,10,10	1.25	1 (14%)	10,14,14	0.92	1 (10%)
2	COA	A	1802	-	43,50,50	1.14	2 (4%)	48,75,75	1.61	2 (4%)
3	152	B	1901	-	7,10,10	1.23	1 (14%)	10,14,14	1.09	1 (10%)
2	COA	B	1902	-	43,50,50	1.11	2 (4%)	48,75,75	1.63	2 (4%)

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	A	1801	-	-	0/7/9/9	0/0/0/0
2	COA	A	1802	-	-	0/44/64/64	0/3/3/3
3	152	B	1901	-	-	0/7/9/9	0/0/0/0
2	COA	B	1902	-	-	0/44/64/64	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1801	152	C4-N5	-2.34	1.47	1.51
3	B	1901	152	C4-N5	-2.10	1.48	1.51
2	B	1902	COA	P3B-O7A	2.92	1.60	1.50
2	A	1802	COA	P3B-O7A	3.10	1.61	1.50
2	B	1902	COA	O4B-C1B	4.08	1.46	1.41
2	A	1802	COA	O4B-C1B	4.59	1.47	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1902	COA	N3A-C2A-N1A	-9.67	120.44	128.86
2	A	1802	COA	N3A-C2A-N1A	-9.47	120.61	128.86
3	B	1901	152	C3-C4-N5	-3.17	111.01	117.17
3	A	1801	152	C3-C4-N5	-2.71	111.91	117.17
2	B	1902	COA	O9A-P3B-O8A	2.77	118.78	107.61
2	A	1802	COA	O9A-P3B-O8A	2.80	118.91	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1801	152	1	0
2	A	1802	COA	4	0
3	B	1901	152	2	0
2	B	1902	COA	2	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	599/599 (100%)	0.28	36 (6%) 23 26	11, 22, 47, 75	0
1	B	599/599 (100%)	-0.11	20 (3%) 47 50	7, 15, 36, 75	0
All	All	1198/1198 (100%)	0.09	56 (4%) 32 36	7, 19, 43, 75	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	368	VAL	14.0
1	B	367	LEU	10.8
1	A	368	VAL	10.0
1	A	367	LEU	9.7
1	B	370	SER	8.2
1	B	371	PRO	8.2
1	A	625	LYS	8.0
1	A	624	ALA	7.9
1	B	369	ARG	7.8
1	B	624	ALA	7.3
1	A	371	PRO	6.5
1	A	370	SER	6.4
1	A	374	PRO	5.6
1	B	625	LYS	5.5
1	A	369	ARG	5.5
1	A	163	LEU	4.8
1	B	372	MET	4.8
1	A	623	ARG	4.5
1	A	30	ALA	4.3
1	B	623	ARG	4.2
1	A	373	VAL	4.2
1	B	366	GLU	4.1
1	B	294	ARG	4.0
1	B	244	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	77	GLY	3.9
1	A	132	LEU	3.8
1	B	29	MET	3.7
1	A	366	GLU	3.7
1	A	198	ARG	3.5
1	A	29	MET	3.5
1	A	372	MET	3.3
1	A	27	SER	3.3
1	A	197	LYS	3.3
1	A	28	HIS	3.0
1	A	165	GLY	3.0
1	A	294	ARG	2.9
1	A	68	GLN	2.9
1	A	220	ASP	2.9
1	B	622	PRO	2.9
1	A	61	GLU	2.8
1	A	227	ASP	2.8
1	B	198	ARG	2.7
1	A	164	GLY	2.6
1	A	160	VAL	2.6
1	A	293	PRO	2.5
1	A	297	ASP	2.5
1	B	30	ALA	2.5
1	A	296	SER	2.5
1	A	219	SER	2.3
1	A	75	THR	2.3
1	A	60	GLU	2.3
1	B	33	ASP	2.2
1	B	163	LEU	2.1
1	B	197	LYS	2.1
1	A	242	GLN	2.0
1	B	365	PRO	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	152	A	1801	11/11	0.93	0.12	1.87	13,15,17,18	0
2	COA	B	1902	48/48	0.92	0.11	0.14	14,24,31,32	0
2	COA	A	1802	48/48	0.94	0.11	-0.13	19,24,33,35	0
3	152	B	1901	11/11	0.96	0.10	-0.29	8,9,11,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.