



# Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:59 pm BST

PDB ID : 1NDF  
Title : Carnitine Acetyltransferase in Complex with Carnitine  
Authors : Jogl, G.; Tong, L.  
Deposited on : 2002-12-09  
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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

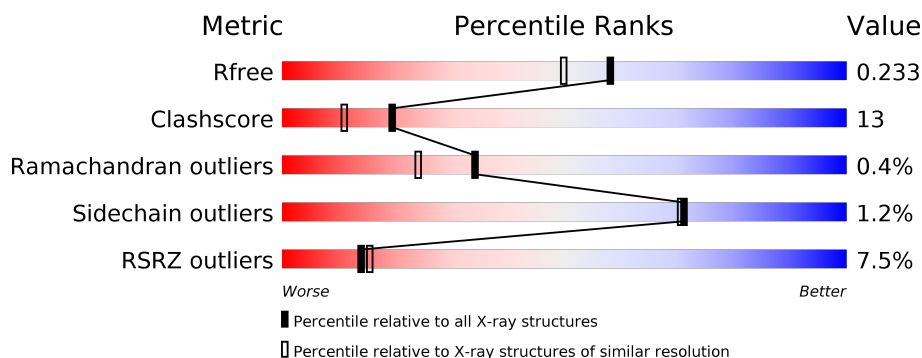
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 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	596	<div> <div>11%</div> <div> <div></div> <div>74%</div> <div>26%</div> </div> <div></div> </div>
1	B	596	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>21%</div> </div> <div></div> </div>

## 2 Entry composition [i](#)

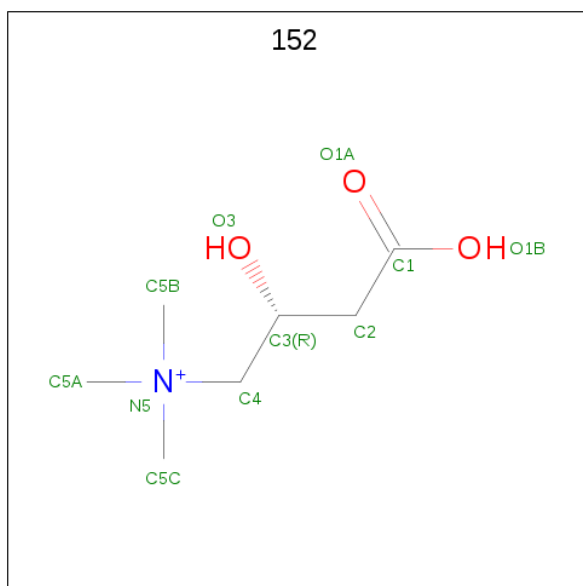
There are 3 unique types of molecules in this entry. The entry contains 10606 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	596	Total	C	N	O	S	0	0	0
			4757	3034	820	875	28			
1	B	596	Total	C	N	O	S	0	0	0
			4757	3034	820	875	28			

- Molecule 2 is CARNITINE (three-letter code: 152) (formula:  $C_7H_{16}NO_3$ ).



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

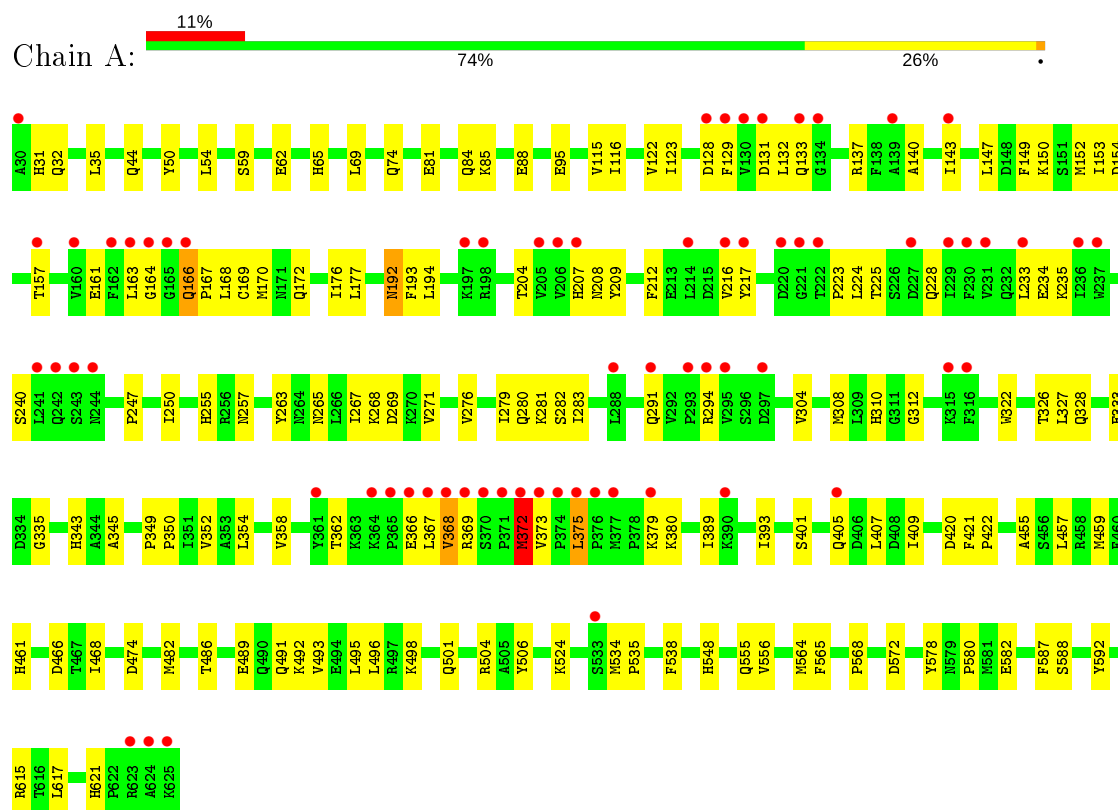
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	469	Total 469	O 469	0	0
3	B	601	Total 601	O 601	0	0

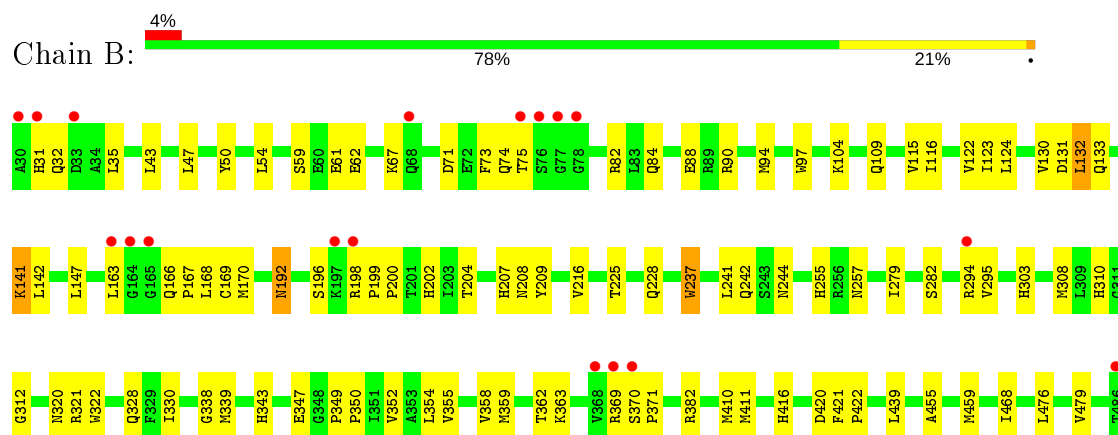
### 3 Residue-property plots [i](#)

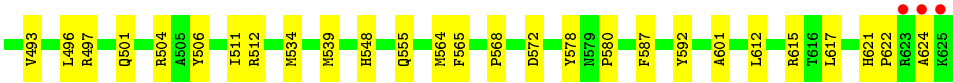
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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, $\alpha$ , $\beta$ , $\gamma$	160.68 Å   91.67 Å   122.61 Å 90.00°   128.84°   90.00°	Depositor
Resolution (Å)	19.95 – 1.90 19.94 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.95-1.90) 96.3 (19.94-1.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.16 (at 1.89 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.200 , 0.241 0.193 , 0.233	Depositor DCC
$R_{free}$ test set	7946 reflections (7.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.9	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10606	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 3.80% 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: 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	0/4872	0.55	0/6600
1	B	0.33	0/4872	0.58	0/6600
All	All	0.32	0/9744	0.56	0/13200

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	4757	0	4733	134	0
1	B	4757	0	4733	108	0
2	A	11	0	15	2	0
2	B	11	0	15	1	0
3	A	469	0	0	8	0
3	B	601	0	0	10	0
All	All	10606	0	9496	244	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 13.

All (244) 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:161:GLU:H	1:A:170:MET:HE3	1.20	1.06
1:B:132:LEU:H	1:B:132:LEU:HD22	1.29	0.96
1:B:308:MET:HE3	1:B:330:ILE:HD12	1.48	0.96
1:B:94:MET:CE	1:B:97:TRP:HA	2.09	0.83
1:A:310:HIS:HD2	1:A:312:GLY:H	1.25	0.82
1:B:310:HIS:HD2	1:B:312:GLY:H	1.29	0.79
1:B:308:MET:HE1	1:B:330:ILE:HB	1.64	0.79
1:A:489:GLU:O	1:A:493:VAL:HG23	1.83	0.78
1:A:504:ARG:HB3	1:A:504:ARG:HH11	1.49	0.78
1:B:90:ARG:NE	1:B:94:MET:HE1	1.98	0.77
1:B:141:LYS:HD2	1:B:362:THR:HA	1.68	0.75
1:A:534:MET:CE	1:A:535:PRO:HD2	2.17	0.72
1:B:31:HIS:HE1	1:B:167:PRO:HB3	1.54	0.72
1:A:161:GLU:N	1:A:170:MET:HE3	2.02	0.72
1:B:493:VAL:HG22	1:B:617:LEU:HG	1.73	0.70
1:A:122:VAL:HG22	1:A:564:MET:HG2	1.74	0.70
1:B:32:GLN:HE22	1:B:170:MET:H	1.38	0.70
1:B:534:MET:HB3	1:B:539:MET:HE2	1.74	0.69
1:A:228:GLN:HB3	1:A:375:LEU:HD11	1.74	0.69
1:B:310:HIS:CD2	1:B:312:GLY:H	2.09	0.69
1:A:493:VAL:HG22	1:A:617:LEU:HG	1.75	0.68
1:B:349:PRO:O	1:B:352:VAL:HG22	1.94	0.68
1:A:457:LEU:HG	3:A:5100:HOH:O	1.94	0.68
1:B:555:GLN:HE21	1:B:580:PRO:HG2	1.59	0.68
1:A:265:ASN:HA	1:A:268:LYS:HE3	1.77	0.67
1:A:310:HIS:CD2	1:A:312:GLY:H	2.11	0.67
1:B:131:ASP:OD1	1:B:133:GLN:HG3	1.94	0.66
1:A:504:ARG:NH1	1:A:504:ARG:HB3	2.10	0.66
1:A:32:GLN:HE22	1:A:170:MET:H	1.44	0.66
1:A:482:MET:HE2	1:A:492:LYS:HD3	1.78	0.66
1:A:204:THR:HG23	1:A:282:SER:HB3	1.78	0.65
1:A:534:MET:HE2	1:A:535:PRO:HD2	1.77	0.65
1:A:255:HIS:HD2	1:A:257:ASN:H	1.44	0.65
1:B:497:ARG:O	1:B:501:GLN:HG2	1.97	0.65
1:B:94:MET:HE3	1:B:97:TRP:HA	1.78	0.64
1:B:308:MET:HE2	1:B:339:MET:N	2.13	0.64
1:B:47:LEU:HD12	1:B:74:GLN:HB3	1.78	0.64
1:A:482:MET:CE	1:A:492:LYS:HB3	2.28	0.63
1:B:308:MET:CE	1:B:330:ILE:HD12	2.26	0.63
1:A:349:PRO:HB2	1:A:350:PRO:HD3	1.80	0.62
1:A:491:GLN:HE21	1:A:495:LEU:HG	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:MET:HB3	1:B:539:MET:CE	2.29	0.62
1:A:247:PRO:O	1:A:250:ILE:HG22	1.99	0.62
1:A:407:LEU:HD21	1:A:409:ILE:HD11	1.79	0.62
1:A:31:HIS:HE1	1:A:167:PRO:HB3	1.64	0.61
1:A:421:PHE:HB3	1:A:422:PRO:HD3	1.82	0.61
1:A:482:MET:CE	1:A:482:MET:HA	2.31	0.61
1:B:132:LEU:H	1:B:132:LEU:CD2	2.06	0.60
1:B:90:ARG:HG2	1:B:94:MET:HE2	1.83	0.60
1:A:225:THR:H	1:A:228:GLN:HE21	1.50	0.60
1:B:370:SER:HB3	1:B:371:PRO:CD	2.31	0.59
1:A:482:MET:HE2	1:A:492:LYS:HB3	1.85	0.59
1:B:47:LEU:CD1	1:B:74:GLN:HB3	2.31	0.59
1:A:225:THR:OG1	1:A:228:GLN:HG3	2.03	0.59
1:A:276:VAL:O	1:A:280:GLN:HG3	2.03	0.59
1:A:216:VAL:C	1:A:224:LEU:HD13	2.23	0.59
1:A:493:VAL:HG22	1:A:617:LEU:CG	2.32	0.58
1:B:369:ARG:N	3:B:6100:HOH:O	2.36	0.58
1:A:84:GLN:O	1:A:88:GLU:HG3	2.04	0.57
1:B:322:TRP:H	1:B:328:GLN:NE2	2.02	0.57
1:B:512:ARG:HG3	1:B:512:ARG:HH11	1.68	0.57
1:B:421:PHE:HB3	1:B:422:PRO:HD3	1.86	0.57
1:A:524:LYS:HG3	1:A:534:MET:HE1	1.86	0.57
1:A:123:ILE:HG13	1:A:565:PHE:CE2	2.40	0.57
1:B:255:HIS:HD2	1:B:257:ASN:H	1.51	0.57
1:B:294:ARG:HG3	3:B:6232:HOH:O	2.04	0.57
1:B:94:MET:HE2	1:B:97:TRP:HA	1.87	0.57
2:A:5001:152:H5B3	2:A:5001:152:O3	2.05	0.56
1:B:59:SER:OG	1:B:62:GLU:HG3	2.05	0.56
1:A:163:LEU:HB3	1:A:166:GLN:OE1	2.05	0.56
1:A:131:ASP:OD1	1:A:133:GLN:HG3	2.05	0.56
1:A:163:LEU:O	1:A:163:LEU:HD13	2.06	0.55
1:B:504:ARG:HB3	1:B:504:ARG:HH11	1.71	0.55
1:A:482:MET:HA	1:A:482:MET:HE2	1.89	0.55
1:A:493:VAL:HG22	1:A:617:LEU:CD1	2.36	0.55
1:B:207:HIS:HE1	3:B:6426:HOH:O	1.90	0.55
1:B:568:PRO:HD2	1:B:592:TYR:CZ	2.42	0.55
1:B:294:ARG:HG3	1:B:294:ARG:HH11	1.72	0.55
1:B:382:ARG:NH1	1:B:382:ARG:HB2	2.21	0.55
1:A:534:MET:HE3	1:A:535:PRO:HD2	1.89	0.55
1:B:370:SER:HB3	1:B:371:PRO:HD2	1.88	0.55
1:A:498:LYS:HD3	3:A:5054:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:GLN:HE21	1:A:580:PRO:HG2	1.72	0.54
1:B:90:ARG:HG2	1:B:94:MET:CE	2.38	0.54
1:A:132:LEU:HD22	1:A:132:LEU:H	1.73	0.54
1:A:352:VAL:HG11	1:A:556:VAL:HG12	1.90	0.54
1:B:358:VAL:O	1:B:362:THR:HG23	2.07	0.54
1:A:50:TYR:CZ	1:A:54:LEU:HD11	2.43	0.54
1:A:228:GLN:HG2	1:A:372:MET:HB3	1.90	0.54
1:A:501:GLN:NE2	3:A:5287:HOH:O	2.42	0.53
1:A:129:PHE:CZ	1:A:335:GLY:HA2	2.43	0.53
1:B:347:GLU:O	1:B:350:PRO:HD2	2.09	0.53
1:A:294:ARG:HG3	3:A:5409:HOH:O	2.08	0.53
1:A:255:HIS:CD2	1:A:257:ASN:H	2.25	0.53
1:B:548:HIS:HE1	1:B:572:ASP:OD1	1.91	0.52
1:A:349:PRO:HA	1:A:352:VAL:HG22	1.91	0.52
1:B:410:MET:HE3	1:B:411:MET:O	2.09	0.52
1:A:269:ASP:OD2	1:A:271:VAL:HB	2.10	0.52
1:A:486:THR:HG21	1:B:196:SER:HB3	1.91	0.52
1:A:568:PRO:HD2	1:A:592:TYR:CZ	2.45	0.52
1:A:193:PHE:CE2	1:A:281:LYS:HG2	2.45	0.52
1:A:115:VAL:HG12	1:A:116:ILE:HG13	1.90	0.52
1:A:132:LEU:HD22	1:A:132:LEU:N	2.25	0.52
1:A:291:GLN:HB2	1:A:333:GLU:HG3	1.92	0.52
1:B:308:MET:CE	1:B:330:ILE:HB	2.37	0.51
1:B:35:LEU:HD11	1:B:169:CYS:HA	1.93	0.51
1:B:132:LEU:HD22	1:B:132:LEU:N	2.11	0.51
1:A:152:MET:HA	1:A:157:THR:OG1	2.11	0.51
1:A:44:GLN:HA	1:A:74:GLN:HE22	1.76	0.51
1:A:455:ALA:HB2	1:A:468:ILE:HG13	1.93	0.51
1:B:90:ARG:HE	1:B:94:MET:HE1	1.74	0.51
1:A:225:THR:HG23	1:A:228:GLN:HE21	1.75	0.51
1:B:539:MET:HE3	3:B:6211:HOH:O	2.10	0.51
1:B:104:LYS:HD2	1:B:109:GLN:OE1	2.12	0.50
2:B:6001:152:O3	2:B:6001:152:H5B3	2.10	0.50
1:B:115:VAL:HG12	1:B:116:ILE:HG13	1.94	0.50
1:A:177:LEU:HD23	1:A:327:LEU:HD12	1.93	0.50
1:A:368:VAL:HG23	1:A:368:VAL:O	2.12	0.50
1:A:132:LEU:CD2	1:A:132:LEU:H	2.25	0.49
1:A:457:LEU:HD21	1:A:466:ASP:HB2	1.94	0.49
1:B:202:HIS:HD2	3:B:6406:HOH:O	1.95	0.49
1:B:204:THR:HG21	1:B:279:ILE:HA	1.93	0.49
1:A:326:THR:HG23	1:A:345:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:PHE:CZ	1:B:615:ARG:HG3	2.46	0.49
1:B:82:ARG:HB3	3:B:6590:HOH:O	2.11	0.49
1:A:234:GLU:HB3	3:A:5184:HOH:O	2.13	0.49
1:A:59:SER:OG	1:A:62:GLU:HG3	2.12	0.49
1:A:123:ILE:HG13	1:A:565:PHE:HE2	1.78	0.49
1:A:81:GLU:O	1:A:85:LYS:HG2	2.11	0.49
1:A:163:LEU:HB2	1:A:168:LEU:HD21	1.94	0.49
1:A:322:TRP:H	1:A:328:GLN:HE22	1.59	0.49
1:B:339:MET:CE	1:B:355:VAL:HG22	2.43	0.49
1:A:366:GLU:HG2	1:A:369:ARG:NH2	2.29	0.48
1:B:493:VAL:HG12	1:B:497:ARG:NH1	2.28	0.48
1:B:142:LEU:C	1:B:142:LEU:HD23	2.34	0.48
1:A:366:GLU:HA	1:A:369:ARG:HH21	1.79	0.48
1:B:122:VAL:HG22	1:B:564:MET:HG2	1.94	0.48
1:A:35:LEU:HD11	1:A:169:CYS:HA	1.96	0.48
1:A:204:THR:HG21	1:A:279:ILE:HA	1.95	0.48
1:A:366:GLU:CB	1:A:369:ARG:HH21	2.26	0.48
1:A:95:GLU:OE1	1:A:461:HIS:HE1	1.96	0.48
1:A:493:VAL:HG22	1:A:617:LEU:HD11	1.96	0.48
1:A:578:TYR:HB3	1:A:587:PHE:CD1	2.48	0.48
1:B:192:ASN:C	1:B:192:ASN:HD22	2.17	0.48
1:B:84:GLN:O	1:B:88:GLU:HG3	2.14	0.48
1:A:217:TYR:CE1	1:A:223:PRO:HB3	2.49	0.47
1:A:32:GLN:NE2	1:A:170:MET:H	2.12	0.47
1:A:496:LEU:C	1:A:496:LEU:HD23	2.34	0.47
1:B:382:ARG:CZ	1:B:382:ARG:HB2	2.44	0.47
1:B:455:ALA:HB2	1:B:468:ILE:HG13	1.96	0.47
1:B:308:MET:CE	1:B:339:MET:N	2.77	0.47
1:A:548:HIS:HE1	1:A:572:ASP:OD1	1.97	0.47
1:A:176:ILE:HB	1:A:327:LEU:HD11	1.97	0.46
1:B:496:LEU:HD23	1:B:496:LEU:C	2.35	0.46
1:B:416:HIS:CG	1:B:612:LEU:HD21	2.50	0.46
1:B:166:GLN:HA	1:B:167:PRO:HD3	1.84	0.46
1:A:225:THR:HG23	1:A:228:GLN:NE2	2.31	0.46
1:B:568:PRO:HB2	1:B:592:TYR:CE2	2.51	0.46
1:A:380:LYS:HD2	3:A:5425:HOH:O	2.14	0.46
1:A:143:ILE:O	1:A:147:LEU:HG	2.16	0.46
1:B:578:TYR:HB3	1:B:587:PHE:CD1	2.51	0.46
1:A:207:HIS:NE2	1:A:208:ASN:ND2	2.64	0.46
1:A:367:LEU:O	1:A:369:ARG:HG2	2.16	0.45
1:B:349:PRO:HB2	1:B:350:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LEU:O	1:B:47:LEU:HG	2.16	0.45
1:B:130:VAL:HA	3:B:6223:HOH:O	2.16	0.45
1:B:73:PHE:C	1:B:75:THR:H	2.18	0.45
1:A:263:TYR:O	1:A:267:ILE:HG12	2.17	0.45
1:A:326:THR:HG23	1:A:345:ALA:CB	2.47	0.45
1:A:140:ALA:HB2	1:A:233:LEU:HD12	1.99	0.45
1:A:322:TRP:H	1:A:328:GLN:NE2	2.15	0.45
1:A:401:SER:O	1:A:405:GLN:HG3	2.17	0.45
1:B:410:MET:HG2	1:B:601:ALA:HA	1.97	0.45
1:A:166:GLN:N	1:A:166:GLN:NE2	2.65	0.45
1:B:255:HIS:CD2	1:B:257:ASN:H	2.33	0.45
1:B:354:LEU:HD23	1:B:354:LEU:C	2.38	0.44
1:A:421:PHE:CZ	1:A:615:ARG:HG3	2.52	0.44
1:A:349:PRO:O	1:A:352:VAL:HG22	2.16	0.44
1:A:225:THR:N	1:A:228:GLN:HE21	2.14	0.44
1:A:172:GLN:OE1	1:A:350:PRO:HG2	2.18	0.44
1:A:65:HIS:CE1	1:A:69:LEU:HD11	2.53	0.44
1:A:150:LYS:HE3	1:A:283:ILE:HD13	2.00	0.44
1:A:150:LYS:HG2	1:A:154:ASP:OD2	2.18	0.44
1:A:166:GLN:HG3	1:A:459:MET:HE1	2.00	0.44
1:B:124:LEU:HD11	1:B:339:MET:CE	2.47	0.44
1:A:294:ARG:HH11	1:A:294:ARG:HG3	1.83	0.43
1:B:295:VAL:HG11	1:B:303:HIS:CD2	2.54	0.43
1:A:176:ILE:HA	1:A:326:THR:HG21	2.00	0.43
1:A:534:MET:HE1	1:A:538:PHE:CD1	2.54	0.43
1:B:320:ASN:C	1:B:321:ARG:HG2	2.38	0.43
1:B:512:ARG:NH1	1:B:512:ARG:HG3	2.31	0.43
1:B:539:MET:HE1	3:B:6523:HOH:O	2.18	0.43
1:B:439:LEU:HA	1:B:479:VAL:HG12	2.01	0.43
1:B:242:GLN:HB3	1:B:244:ASN:OD1	2.19	0.43
1:B:459:MET:HE3	1:B:511:ILE:HG22	2.00	0.43
1:B:204:THR:HG23	1:B:282:SER:HB3	2.00	0.43
1:A:489:GLU:HB3	1:A:621:HIS:NE2	2.33	0.42
1:A:474:ASP:OD1	1:A:498:LYS:HE2	2.19	0.42
1:B:123:ILE:HG13	1:B:565:PHE:CE2	2.55	0.42
1:B:50:TYR:CZ	1:B:54:LEU:HD11	2.55	0.42
1:B:61:GLU:H	1:B:61:GLU:CD	2.22	0.42
1:A:565:PHE:HB3	1:A:588:SER:HB2	2.01	0.42
1:B:163:LEU:HB2	1:B:168:LEU:HD11	2.02	0.42
1:B:147:LEU:HD11	1:B:216:VAL:HB	2.02	0.42
1:B:322:TRP:H	1:B:328:GLN:HE22	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:MET:CE	1:B:338:GLY:C	2.88	0.42
1:B:82:ARG:HD2	3:B:6590:HOH:O	2.18	0.42
1:A:304:VAL:O	1:A:308:MET:HG2	2.20	0.42
1:A:358:VAL:O	1:A:362:THR:HG23	2.20	0.42
1:B:310:HIS:HE1	3:B:6396:HOH:O	2.03	0.42
1:B:208:ASN:O	1:B:209:TYR:HB2	2.19	0.42
1:A:534:MET:HE2	1:A:535:PRO:CD	2.47	0.42
1:B:32:GLN:NE2	1:B:170:MET:H	2.11	0.42
1:A:235:LYS:NZ	1:A:375:LEU:O	2.53	0.41
1:A:192:ASN:HD22	1:A:192:ASN:C	2.22	0.41
1:A:212:PHE:CZ	1:A:240:SER:HB3	2.54	0.41
1:B:225:THR:H	1:B:228:GLN:NE2	2.17	0.41
1:A:354:LEU:C	1:A:354:LEU:HD23	2.41	0.41
1:A:482:MET:HE1	1:A:492:LYS:HB3	1.98	0.41
2:A:5001:152:H5A2	2:A:5001:152:H3	1.82	0.41
1:A:482:MET:HB2	1:A:482:MET:HE3	1.93	0.41
1:A:128:ASP:O	1:A:129:PHE:C	2.59	0.41
1:A:166:GLN:HA	1:A:167:PRO:HD3	1.89	0.41
1:A:209:TYR:CD2	1:A:209:TYR:N	2.89	0.41
1:A:420:ASP:HB3	1:A:582:GLU:OE2	2.21	0.41
1:B:420:ASP:OD1	1:B:421:PHE:N	2.54	0.41
1:B:67:LYS:HE2	1:B:71:ASP:OD2	2.20	0.41
1:B:82:ARG:HH11	1:B:82:ARG:HG3	1.86	0.41
1:A:310:HIS:HE1	3:A:5315:HOH:O	2.02	0.41
1:B:621:HIS:N	1:B:622:PRO:HD3	2.35	0.41
1:A:192:ASN:ND2	1:A:194:LEU:H	2.18	0.40
1:B:308:MET:HE1	1:B:338:GLY:C	2.41	0.40
1:A:255:HIS:CD2	1:A:257:ASN:HB2	2.56	0.40
1:A:372:MET:HB2	1:A:373:VAL:H	1.64	0.40
1:A:389:ILE:O	1:A:393:ILE:HG13	2.22	0.40
1:B:294:ARG:HG3	1:B:294:ARG:NH1	2.35	0.40
1:A:373:VAL:O	1:A:375:LEU:N	2.44	0.40
1:A:149:PHE:HE1	1:A:153:ILE:HD11	1.87	0.40
1:A:379:LYS:HG3	3:A:5451:HOH:O	2.22	0.40
1:A:421:PHE:CE1	1:A:615:ARG:HG3	2.57	0.40
1:B:199:PRO:HA	1:B:200:PRO:HD3	1.93	0.40
1:B:237:TRP:CE2	1:B:241:LEU:HD21	2.57	0.40
1:B:359:MET:O	1:B:363:LYS:HG2	2.21	0.40
1:B:476:LEU:HA	1:B:479:VAL:HG22	2.03	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	594/596 (100%)	569 (96%)	21 (4%)	4 (1%)	22	12
1	B	594/596 (100%)	575 (97%)	18 (3%)	1 (0%)	47	38
All	All	1188/1192 (100%)	1144 (96%)	39 (3%)	5 (0%)	34	24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	372	MET
1	B	624	ALA
1	A	164	GLY
1	A	375	LEU
1	A	368	VAL

### 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	524/524 (100%)	518 (99%)	6 (1%)	73	73
1	B	524/524 (100%)	517 (99%)	7 (1%)	69	68
All	All	1048/1048 (100%)	1035 (99%)	13 (1%)	71	70

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ARG

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Mol	Chain	Res	Type
1	A	166	GLN
1	A	192	ASN
1	A	343	HIS
1	A	372	MET
1	A	506	TYR
1	B	132	LEU
1	B	141	LYS
1	B	192	ASN
1	B	198	ARG
1	B	237	TRP
1	B	343	HIS
1	B	506	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	32	GLN
1	A	74	GLN
1	A	84	GLN
1	A	112	GLN
1	A	135	GLN
1	A	187	GLN
1	A	192	ASN
1	A	202	HIS
1	A	208	ASN
1	A	210	GLN
1	A	228	GLN
1	A	255	HIS
1	A	277	ASN
1	A	307	GLN
1	A	310	HIS
1	A	328	GLN
1	A	461	HIS
1	A	491	GLN
1	A	503	HIS
1	A	548	HIS
1	A	550	ASN
1	A	555	GLN
1	A	586	ASN
1	A	619	GLN
1	A	620	ASN

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Mol	Chain	Res	Type
1	B	32	GLN
1	B	44	GLN
1	B	68	GLN
1	B	84	GLN
1	B	109	GLN
1	B	112	GLN
1	B	135	GLN
1	B	166	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	461	HIS
1	B	503	HIS
1	B	548	HIS
1	B	550	ASN
1	B	555	GLN
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

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	152	A	5001	-	7,10,10	1.17	1 (14%)	10,14,14	1.17	1 (10%)
2	152	B	6001	-	7,10,10	1.16	1 (14%)	10,14,14	1.03	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	152	A	5001	-	-	0/7/9/9	-
2	152	B	6001	-	-	0/7/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6001	152	C4-N5	-2.10	1.47	1.52
2	A	5001	152	C4-N5	-2.05	1.47	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5001	152	C3-C4-N5	-3.55	110.75	116.83
2	B	6001	152	C3-C4-N5	-3.12	111.49	116.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5001	152	2	0
2	B	6001	152	1	0

## 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, 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	596/596 (100%)	0.45	68 (11%) 5 5	9, 23, 57, 90	0
1	B	596/596 (100%)	-0.08	21 (3%) 44 47	7, 17, 39, 73	0
All	All	1192/1192 (100%)	0.18	89 (7%) 14 15	7, 19, 53, 90	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	624	ALA	16.9
1	A	368	VAL	11.3
1	A	625	LYS	10.8
1	A	367	LEU	9.9
1	A	373	VAL	9.3
1	A	370	SER	8.8
1	B	77	GLY	8.5
1	B	76	SER	8.1
1	B	625	LYS	7.4
1	A	624	ALA	7.1
1	A	198	ARG	5.7
1	A	371	PRO	5.7
1	A	369	ARG	5.5
1	A	237	TRP	5.4
1	B	78	GLY	5.2
1	A	163	LEU	5.2
1	A	165	GLY	5.1
1	A	375	LEU	5.0
1	A	372	MET	4.9
1	A	365	PRO	4.7
1	A	366	GLU	4.7
1	B	33	ASP	4.6
1	B	370	SER	4.3
1	A	227	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	294	ARG	4.2
1	A	374	PRO	3.9
1	B	198	ARG	3.7
1	A	166	GLN	3.7
1	A	130	VAL	3.7
1	B	30	ALA	3.6
1	A	128	ASP	3.5
1	B	31	HIS	3.5
1	B	369	ARG	3.5
1	A	220	ASP	3.5
1	A	231	VAL	3.5
1	B	75	THR	3.5
1	B	623	ARG	3.4
1	A	242	GLN	3.3
1	A	293	PRO	3.3
1	A	243	SER	3.2
1	A	316	PHE	3.2
1	A	197	LYS	3.2
1	B	164	GLY	3.1
1	B	165	GLY	3.0
1	A	229	ILE	3.0
1	A	390	LYS	3.0
1	A	216	VAL	3.0
1	A	221	GLY	3.0
1	A	214	LEU	2.9
1	A	233	LEU	2.9
1	A	30	ALA	2.9
1	A	160	VAL	2.9
1	A	162	PHE	2.9
1	A	217	TYR	2.8
1	A	222	THR	2.8
1	A	139	ALA	2.8
1	A	134	GLY	2.8
1	A	379	LYS	2.7
1	A	623	ARG	2.7
1	A	241	LEU	2.7
1	B	197	LYS	2.6
1	A	236	ILE	2.6
1	A	129	PHE	2.6
1	A	157	THR	2.5
1	A	143	ILE	2.5
1	A	376	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	361	TYR	2.4
1	B	163	LEU	2.4
1	B	368	VAL	2.4
1	A	377	MET	2.4
1	B	486	THR	2.4
1	A	405	GLN	2.4
1	A	533	SER	2.3
1	A	133	GLN	2.3
1	A	291	GLN	2.3
1	A	131	ASP	2.3
1	A	297	ASP	2.3
1	A	164	GLY	2.2
1	A	364	LYS	2.2
1	A	244	ASN	2.2
1	A	288	LEU	2.2
1	A	315	LYS	2.2
1	A	207	HIS	2.1
1	A	206	VAL	2.1
1	A	295	VAL	2.1
1	B	294	ARG	2.1
1	A	230	PHE	2.1
1	B	68	GLN	2.0
1	A	205	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 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. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	152	A	5001	11/11	0.96	0.08	9,14,18,18	0
2	152	B	6001	11/11	0.96	0.07	12,14,17,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.