



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:25 AM GMT

PDB ID : 2H3P  
Title : Crystal structure of murine carnitine acetyltransferase in complex with carnitine and acetyl-CoA  
Authors : Hsiao, Y.S.; Jogl, G.; Tong, L.  
Deposited on : 2006-05-22  
Resolution : 2.20 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

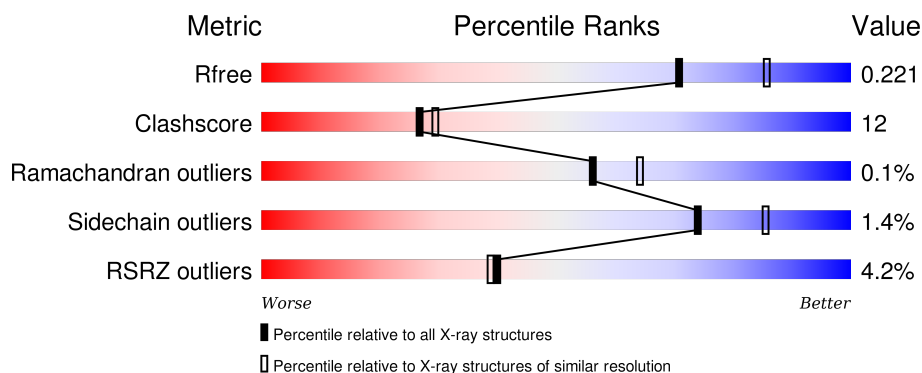
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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>5%</div> <div>72%</div> <div>27%</div> </div>
1	B	599	<div> <div>3%</div> <div>77%</div> <div>22%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11109 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.

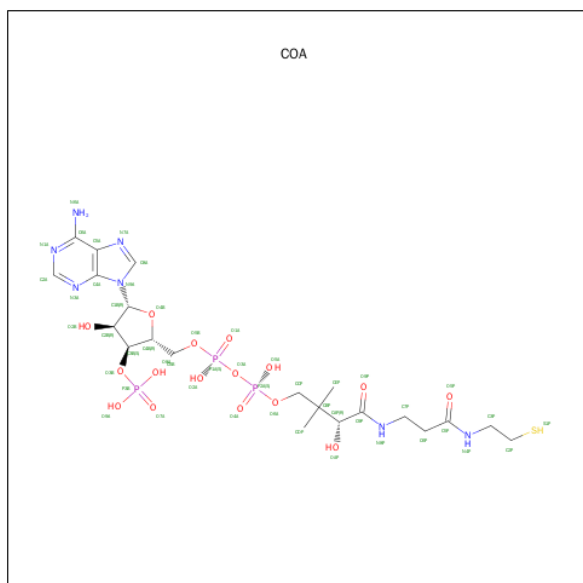
- Molecule 1 is a protein called carnitine acetyltransferase.

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:

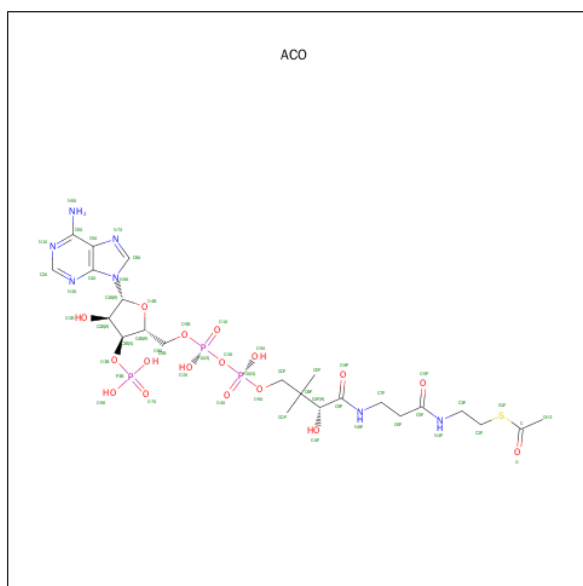
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	SER	-	CLONING ARTIFACT	UNP Q3V1Y3
A	28	HIS	-	CLONING ARTIFACT	UNP Q3V1Y3
A	29	MET	-	CLONING ARTIFACT	UNP Q3V1Y3
B	27	SER	-	CLONING ARTIFACT	UNP Q3V1Y3
B	28	HIS	-	CLONING ARTIFACT	UNP Q3V1Y3
B	29	MET	-	CLONING ARTIFACT	UNP Q3V1Y3

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



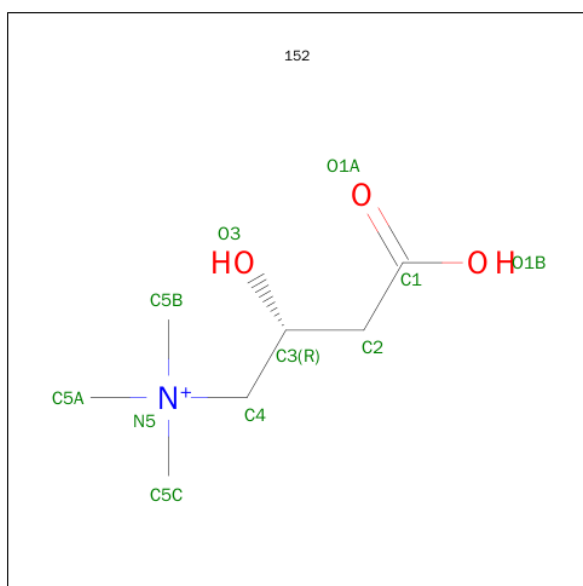
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is ACETYL COENZYME \*A (three-letter code: ACO) (formula:  $C_{23}H_{38}N_7O_{17}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 4 is CARNITINE (three-letter code: 152) (formula:  $C_7H_{16}NO_3$ ).



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

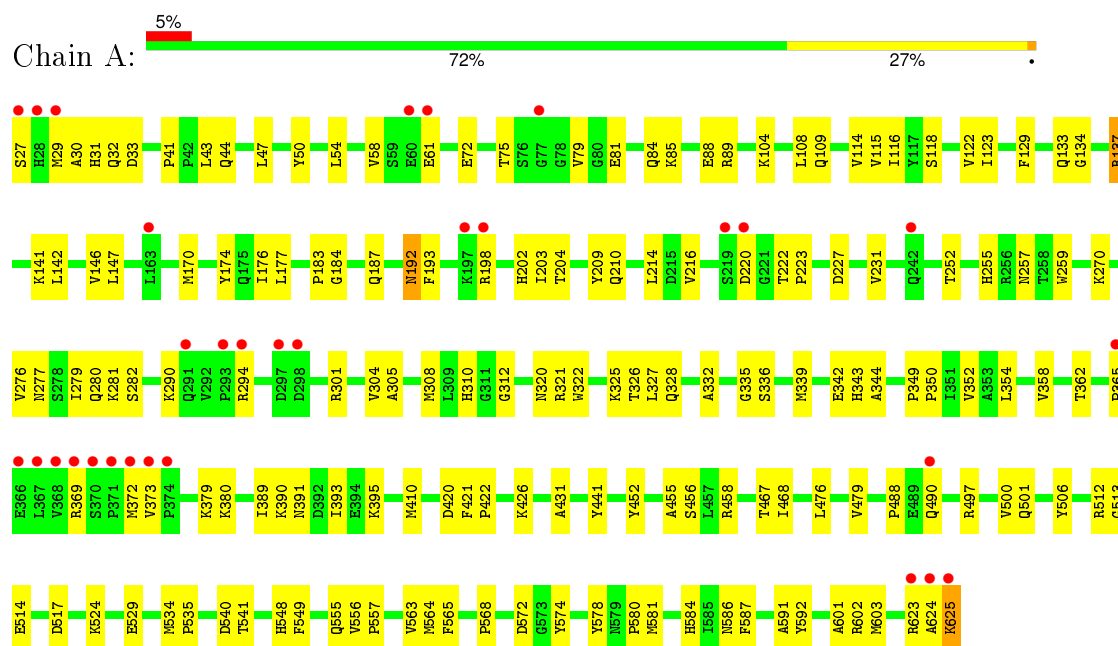
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	639	Total	O	0	0
			639	639		
5	B	787	Total	O	0	0
			787	787		

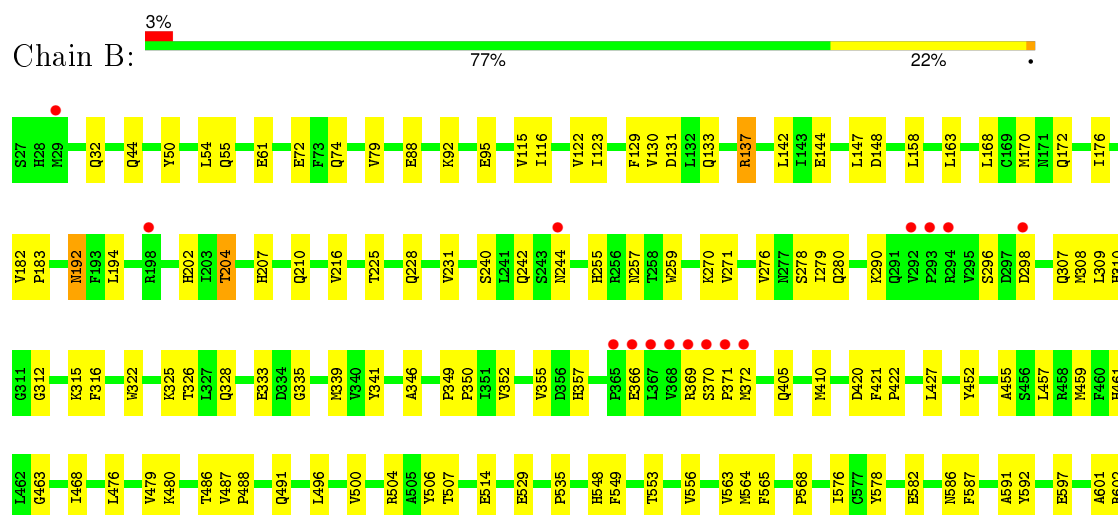
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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, $\alpha$ , $\beta$ , $\gamma$	163.90 Å   89.24 Å   122.64 Å 90.00°   128.96°   90.00°	Depositor
Resolution (Å)	29.92 – 2.20 29.92 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.9 (29.92-2.20) 95.0 (29.92-2.20)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.96 (at 2.20 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.170 , 0.223 0.169 , 0.221	Depositor DCC
$R_{free}$ test set	5039 reflections (7.64%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.6	EDS
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 65954 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11109	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, ACO

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	0.32	0/4897	0.52	0/6633
1	B	0.36	0/4897	0.57	0/6633
All	All	0.34	0/9794	0.54	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	104	0
2	A	48	0	32	3	0
3	B	51	0	34	4	0
4	A	11	0	15	1	0
4	B	11	0	15	1	0
5	A	639	0	0	23	0
5	B	787	0	0	25	0
All	All	11109	0	9604	234	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 (234) 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:457:LEU:HG	5:B:2044:HOH:O	1.71	0.90
1:A:534:MET:HE2	1:A:535:PRO:HD2	1.61	0.82
1:B:310:HIS:HD2	1:B:312:GLY:H	1.29	0.80
1:B:32:GLN:HE22	1:B:170:MET:H	1.33	0.77
1:A:349:PRO:HB2	1:A:350:PRO:HD3	1.67	0.77
1:B:144:GLU:HG2	5:B:1941:HOH:O	1.86	0.75
1:B:310:HIS:CD2	1:B:312:GLY:H	2.05	0.75
1:A:524:LYS:HG3	1:A:534:MET:HE1	1.70	0.73
1:A:534:MET:CE	1:A:535:PRO:HD2	2.18	0.73
1:B:349:PRO:HB2	1:B:350:PRO:HD3	1.72	0.71
1:B:163:LEU:HB2	1:B:168:LEU:HD11	1.73	0.70
1:A:290:LYS:HB3	5:A:1753:HOH:O	1.92	0.70
1:B:514:GLU:HG2	5:B:2137:HOH:O	1.92	0.70
1:A:322:TRP:H	1:A:328:GLN:HE22	1.41	0.68
1:B:244:ASN:HB2	5:B:1823:HOH:O	1.93	0.68
1:A:349:PRO:HD3	2:A:1502:COA:H31	1.76	0.67
1:A:122:VAL:HG22	1:A:564:MET:HG2	1.76	0.67
1:B:349:PRO:HD3	3:B:1602:ACO:H31	1.75	0.66
1:A:227:ASP:HB2	1:A:369:ARG:NH1	2.11	0.66
1:A:497:ARG:NH2	1:A:623:ARG:HG2	2.10	0.66
1:B:405:GLN:HG3	5:B:2371:HOH:O	1.95	0.65
1:A:455:ALA:HB2	1:A:468:ILE:HG13	1.80	0.64
1:A:322:TRP:H	1:A:328:GLN:NE2	1.96	0.64
1:A:602:ARG:HD2	5:A:2012:HOH:O	1.97	0.63
1:B:131:ASP:OD1	1:B:133:GLN:HG3	1.98	0.63
1:B:225:THR:H	1:B:228:GLN:NE2	1.96	0.63
1:A:220:ASP:OD2	1:A:222:THR:HG22	1.98	0.63
1:B:421:PHE:HB3	1:B:422:PRO:HD3	1.81	0.62
1:B:370:SER:HB2	1:B:371:PRO:HD2	1.82	0.62
1:A:32:GLN:HE22	1:A:170:MET:H	1.46	0.62
1:A:310:HIS:CD2	1:A:312:GLY:H	2.19	0.60
1:B:488:PRO:HD2	5:B:2365:HOH:O	2.02	0.60
1:A:204:THR:HG21	1:A:279:ILE:HA	1.85	0.59
1:B:487:VAL:HG13	1:B:491:GLN:HG2	1.86	0.58
1:B:341:TYR:HE2	1:B:564:MET:HE1	1.69	0.58
1:A:44:GLN:HG3	5:A:1752:HOH:O	2.04	0.58
1:A:391:ASN:O	1:A:395:LYS:HG2	2.04	0.58
1:B:122:VAL:HG22	1:B:564:MET:HG2	1.85	0.57
1:B:255:HIS:HD2	1:B:257:ASN:H	1.53	0.57
1:A:310:HIS:HD2	1:A:312:GLY:H	1.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:MET:HG2	1:A:601:ALA:HA	1.85	0.57
1:B:315:LYS:HG2	5:B:1930:HOH:O	2.05	0.57
1:A:514:GLU:HG2	5:A:1927:HOH:O	2.05	0.56
1:A:129:PHE:HB2	1:A:134:GLY:HA3	1.87	0.56
1:B:133:GLN:O	1:B:137:ARG:HB2	2.04	0.56
1:B:410:MET:HG2	1:B:601:ALA:HA	1.87	0.56
1:B:123:ILE:HG13	1:B:565:PHE:CE2	2.40	0.56
1:A:358:VAL:O	1:A:362:THR:HG23	2.06	0.56
1:A:183:PRO:HG3	1:A:259:TRP:NE1	2.21	0.56
1:A:227:ASP:HB2	1:A:369:ARG:HH11	1.70	0.55
1:A:257:ASN:HB3	5:A:2007:HOH:O	2.06	0.55
1:A:142:LEU:O	1:A:146:VAL:HG23	2.07	0.55
1:A:147:LEU:HD11	1:A:216:VAL:HB	1.89	0.54
1:A:379:LYS:HD3	5:A:1770:HOH:O	2.07	0.54
1:A:30:ALA:HB3	5:A:1913:HOH:O	2.08	0.54
1:A:555:GLN:OE1	1:A:557:PRO:HG3	2.07	0.54
1:A:421:PHE:HB3	1:A:422:PRO:HD3	1.90	0.54
1:A:203:ILE:HD11	1:A:214:LEU:HD23	1.89	0.54
1:B:163:LEU:HB3	1:B:168:LEU:HD21	1.89	0.54
1:B:366:GLU:HB3	1:B:369:ARG:HG3	1.90	0.54
1:A:129:PHE:CZ	1:A:335:GLY:HA2	2.42	0.53
1:B:366:GLU:HA	5:B:2311:HOH:O	2.07	0.53
1:B:322:TRP:H	1:B:328:GLN:NE2	2.06	0.53
1:A:255:HIS:CD2	1:A:257:ASN:H	2.27	0.53
1:B:609:LYS:HE2	1:B:613:ASP:OD1	2.09	0.53
1:A:255:HIS:HD2	1:A:257:ASN:H	1.54	0.53
1:A:84:GLN:O	1:A:88:GLU:HG3	2.09	0.53
1:A:270:LYS:HD3	5:A:1723:HOH:O	2.08	0.53
1:B:123:ILE:HG13	1:B:565:PHE:HE2	1.74	0.53
1:A:426:LYS:HG3	1:A:623:ARG:HH22	1.74	0.52
1:B:147:LEU:HD11	1:B:216:VAL:HB	1.90	0.52
1:A:512:ARG:HH11	1:A:512:ARG:HG3	1.74	0.52
1:B:122:VAL:HB	1:B:339:MET:HG2	1.92	0.52
1:A:501:GLN:HG2	5:A:1717:HOH:O	2.09	0.52
1:A:555:GLN:NE2	1:A:580:PRO:HG2	2.25	0.52
1:B:476:LEU:HD11	1:B:480:LYS:HE3	1.91	0.52
1:B:563:VAL:HB	1:B:586:ASN:HB3	1.90	0.52
1:A:227:ASP:O	1:A:231:VAL:HG23	2.10	0.52
1:A:29:MET:HG2	1:A:33:ASP:OD2	2.10	0.52
1:A:456:SER:HB2	2:A:1502:COA:H71	1.91	0.51
1:B:137:ARG:HD3	5:B:1902:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG12	1:A:116:ILE:HG13	1.91	0.51
1:B:455:ALA:HB2	1:B:468:ILE:HG13	1.93	0.51
1:A:294:ARG:HH11	1:A:294:ARG:HG3	1.76	0.51
1:A:133:GLN:O	1:A:137:ARG:HB2	2.11	0.51
1:B:420:ASP:HB3	1:B:582:GLU:OE2	2.11	0.51
1:A:122:VAL:HB	1:A:339:MET:HG2	1.94	0.50
1:B:578:TYR:HB3	1:B:587:PHE:CD1	2.47	0.50
1:A:27:SER:HA	1:A:174:TYR:CE1	2.47	0.50
1:A:625:LYS:NZ	1:A:625:LYS:HB2	2.27	0.50
1:A:556:VAL:HG22	2:A:1502:COA:H32	1.93	0.50
1:B:459:MET:HG2	5:B:1628:HOH:O	2.12	0.50
1:A:104:LYS:HA	1:A:108:LEU:HB2	1.93	0.49
1:B:568:PRO:HD2	1:B:592:TYR:CZ	2.47	0.49
1:B:463:GLY:HA2	5:B:1831:HOH:O	2.13	0.49
1:B:183:PRO:HG3	1:B:259:TRP:NE1	2.28	0.49
1:A:123:ILE:HD11	1:A:305:ALA:HA	1.93	0.49
1:B:548:HIS:HD2	5:B:1938:HOH:O	1.95	0.49
1:B:50:TYR:CZ	1:B:54:LEU:HD11	2.48	0.49
1:A:27:SER:HB2	5:A:2010:HOH:O	2.13	0.48
1:A:210:GLN:HE21	1:A:380:LYS:CE	2.26	0.48
1:A:177:LEU:HD23	1:A:327:LEU:HD12	1.95	0.48
1:B:163:LEU:CB	1:B:168:LEU:HD21	2.44	0.48
1:B:130:VAL:HA	5:B:1785:HOH:O	2.12	0.48
1:B:421:PHE:CZ	1:B:615:ARG:HG3	2.49	0.48
1:A:61:GLU:H	1:A:61:GLU:CD	2.17	0.48
1:B:115:VAL:HG12	1:B:116:ILE:HG13	1.95	0.48
1:B:452:TYR:HB2	1:B:549:PHE:CD1	2.49	0.48
1:A:332:ALA:HB3	1:A:336:SER:O	2.13	0.48
1:B:176:ILE:HA	1:B:326:THR:HG21	1.95	0.48
1:B:202:HIS:HD2	5:B:1623:HOH:O	1.95	0.47
1:A:89:ARG:HD3	5:A:1666:HOH:O	2.12	0.47
1:B:621:HIS:N	1:B:622:PRO:HD3	2.29	0.47
1:A:123:ILE:HD11	1:A:305:ALA:CA	2.43	0.47
1:A:44:GLN:HB2	5:A:1726:HOH:O	2.15	0.47
1:A:72:GLU:O	1:A:75:THR:HG22	2.14	0.47
1:A:202:HIS:HD2	5:A:1746:HOH:O	1.96	0.47
1:B:296:SER:HB2	1:B:298:ASP:OD1	2.15	0.47
1:B:255:HIS:CD2	1:B:257:ASN:H	2.32	0.47
1:A:210:GLN:HE21	1:A:380:LYS:NZ	2.13	0.47
1:A:555:GLN:HG3	1:A:578:TYR:CE2	2.50	0.46
1:A:452:TYR:HB2	1:A:549:PHE:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HH11	1:A:198:ARG:HG3	1.81	0.46
1:B:44:GLN:HA	1:B:74:GLN:HE22	1.81	0.46
1:B:322:TRP:H	1:B:328:GLN:HE22	1.63	0.46
1:A:328:GLN:O	1:A:339:MET:HB2	2.15	0.46
1:B:88:GLU:O	1:B:92:LYS:HG2	2.16	0.46
1:A:431:ALA:HB3	1:A:500:VAL:HG13	1.98	0.46
1:A:420:ASP:OD1	1:A:421:PHE:N	2.48	0.46
1:A:193:PHE:CD1	1:A:281:LYS:HG2	2.51	0.46
1:A:222:THR:OG1	1:A:223:PRO:HD2	2.16	0.46
1:B:309:LEU:HB2	1:B:565:PHE:HE1	1.79	0.45
1:B:307:GLN:HG3	5:B:1819:HOH:O	2.16	0.45
1:B:290:LYS:HE2	1:B:316:PHE:O	2.16	0.45
1:B:172:GLN:OE1	1:B:346:ALA:HB1	2.16	0.45
1:B:341:TYR:OH	3:B:1602:ACO:HH32	2.16	0.45
1:A:352:VAL:HG13	1:A:564:MET:HE1	1.98	0.45
1:A:458:ARG:HD3	5:A:1750:HOH:O	2.16	0.45
1:A:276:VAL:O	1:A:280:GLN:HG3	2.17	0.45
1:A:204:THR:HG23	1:A:282:SER:HB3	1.98	0.45
1:A:184:GLY:HA3	1:A:187:GLN:O	2.16	0.45
1:B:556:VAL:HG22	3:B:1602:ACO:H32	1.98	0.45
1:A:529:GLU:HG2	5:A:1700:HOH:O	2.14	0.45
1:A:277:ASN:OD1	1:A:281:LYS:HE2	2.16	0.45
4:A:1501:152:H3	4:A:1501:152:H5A2	1.74	0.45
1:B:504:ARG:HD2	5:B:1698:HOH:O	2.16	0.45
1:B:270:LYS:HG3	1:B:271:VAL:N	2.31	0.45
1:A:54:LEU:O	1:A:58:VAL:HG22	2.16	0.45
1:B:79:VAL:HB	5:B:2202:HOH:O	2.17	0.45
1:A:352:VAL:HG13	1:A:564:MET:CE	2.47	0.44
1:B:553:THR:HG22	1:B:576:ILE:HB	1.99	0.44
1:A:548:HIS:HE1	1:A:572:ASP:OD1	2.01	0.44
1:A:192:ASN:HD22	1:A:193:PHE:N	2.15	0.44
1:B:79:VAL:HG11	1:B:535:PRO:HG3	2.00	0.44
1:B:476:LEU:HA	1:B:479:VAL:HG22	1.99	0.44
1:A:476:LEU:HA	1:A:479:VAL:HG22	2.00	0.44
1:B:142:LEU:HD23	1:B:142:LEU:C	2.38	0.44
1:B:210:GLN:HG2	5:B:1961:HOH:O	2.16	0.44
1:A:81:GLU:O	1:A:85:LYS:HG2	2.18	0.44
1:B:568:PRO:HG2	1:B:591:ALA:HA	1.99	0.43
1:A:354:LEU:O	1:A:358:VAL:HG23	2.17	0.43
1:B:192:ASN:C	1:B:192:ASN:HD22	2.22	0.43
1:B:129:PHE:CZ	1:B:335:GLY:HA2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:THR:HG23	5:B:1874:HOH:O	2.18	0.43
1:A:390:LYS:HB3	1:A:390:LYS:HE2	1.85	0.43
1:B:204:THR:HG21	1:B:279:ILE:HA	1.99	0.43
1:A:568:PRO:HD2	1:A:592:TYR:CZ	2.53	0.43
1:A:304:VAL:O	1:A:308:MET:HG2	2.18	0.43
1:A:252:THR:HG22	1:A:259:TRP:CZ2	2.53	0.43
1:A:255:HIS:CD2	1:A:257:ASN:HD22	2.37	0.43
1:B:290:LYS:HD3	5:B:2352:HOH:O	2.18	0.43
1:A:365:PRO:HD3	5:A:2111:HOH:O	2.19	0.43
1:A:568:PRO:HG2	1:A:591:ALA:HA	2.01	0.43
4:B:1601:152:H5B3	4:B:1601:152:O3	2.19	0.43
1:A:373:VAL:HB	5:A:2099:HOH:O	2.18	0.43
1:A:142:LEU:C	1:A:142:LEU:HD23	2.39	0.43
1:A:109:GLN:NE2	5:A:1810:HOH:O	2.51	0.43
1:A:141:LYS:HD2	1:A:362:THR:HA	2.01	0.43
1:A:41:PRO:HG3	1:A:513:GLY:O	2.19	0.42
1:A:497:ARG:HB3	5:A:1717:HOH:O	2.18	0.42
1:B:225:THR:H	1:B:228:GLN:HE21	1.62	0.42
1:A:578:TYR:HD2	1:A:580:PRO:HG3	1.83	0.42
1:B:192:ASN:ND2	1:B:194:LEU:H	2.17	0.42
1:B:602:ARG:HD2	5:B:1905:HOH:O	2.19	0.42
1:B:202:HIS:HE1	1:B:278:SER:O	2.02	0.42
1:A:79:VAL:HG21	5:A:2135:HOH:O	2.20	0.42
1:B:72:GLU:HB2	5:B:1711:HOH:O	2.19	0.42
1:A:301:ARG:NH2	5:A:1787:HOH:O	2.51	0.42
1:A:467:THR:HB	1:A:517:ASP:HB2	2.02	0.42
1:A:301:ARG:HH11	1:A:301:ARG:HG3	1.85	0.42
1:A:50:TYR:O	1:A:54:LEU:HG	2.19	0.42
1:B:207:HIS:HD2	1:B:240:SER:OG	2.02	0.42
1:A:389:ILE:O	1:A:393:ILE:HG13	2.19	0.42
1:B:231:VAL:HG21	1:B:372:MET:SD	2.59	0.42
1:B:50:TYR:CE1	1:B:54:LEU:HD21	2.55	0.42
1:B:427:LEU:HD22	1:B:500:VAL:HG11	2.01	0.42
1:B:276:VAL:O	1:B:280:GLN:HG3	2.19	0.42
1:A:441:TYR:HD1	1:A:603:MET:HE1	1.85	0.42
1:B:349:PRO:HA	1:B:352:VAL:HG22	2.02	0.42
1:B:55:GLN:NE2	5:B:1895:HOH:O	2.50	0.41
1:A:123:ILE:HG13	1:A:565:PHE:CZ	2.55	0.41
1:A:255:HIS:HD2	1:A:257:ASN:HB2	1.86	0.41
1:A:563:VAL:HB	1:A:586:ASN:HB3	2.03	0.41
1:B:194:LEU:HD22	5:B:1662:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:GLN:O	1:B:339:MET:HB2	2.21	0.41
1:A:43:LEU:O	1:A:47:LEU:HG	2.21	0.41
1:A:209:TYR:CD2	1:A:209:TYR:N	2.87	0.41
1:B:242:GLN:HB3	1:B:244:ASN:ND2	2.35	0.41
1:A:578:TYR:HB3	1:A:587:PHE:CD1	2.56	0.41
1:B:158:LEU:HD12	1:B:158:LEU:HA	1.96	0.41
1:B:529:GLU:HG2	5:B:1693:HOH:O	2.19	0.41
1:B:352:VAL:HG11	1:B:556:VAL:HG12	2.02	0.41
1:A:574:TYR:CE1	1:A:603:MET:HE2	2.56	0.41
1:B:325:LYS:HA	1:B:325:LYS:HD2	1.88	0.41
1:A:540:ASP:OD2	1:A:541:THR:N	2.53	0.41
1:B:148:ASP:OD2	1:B:357:HIS:HE1	2.03	0.41
1:A:192:ASN:HD22	1:A:192:ASN:C	2.24	0.41
1:A:325:LYS:HA	1:A:325:LYS:HD2	1.95	0.41
1:A:342:GLU:OE1	1:A:344:ALA:HB3	2.21	0.41
1:A:50:TYR:CZ	1:A:54:LEU:HD11	2.55	0.40
1:A:114:VAL:HA	1:A:118:SER:HB3	2.02	0.40
1:B:95:GLU:OE1	1:B:461:HIS:HE1	2.03	0.40
1:B:507:THR:HG23	3:B:1602:ACO:H143	2.03	0.40
1:B:564:MET:HE2	1:B:564:MET:HB3	1.84	0.40
1:A:32:GLN:NE2	1:A:170:MET:H	2.17	0.40
1:A:488:PRO:HD3	5:A:1760:HOH:O	2.21	0.40
1:A:320:ASN:C	1:A:321:ARG:HG2	2.42	0.40
1:A:176:ILE:HA	1:A:326:THR:HG21	2.02	0.40
1:B:32:GLN:NE2	1:B:170:MET:H	2.09	0.40
1:A:581:MET:HB2	1:A:584:HIS:O	2.21	0.40
1:A:31:HIS:HB2	5:A:1777:HOH:O	2.21	0.40
1:B:182:VAL:HA	1:B:183:PRO:HD3	1.91	0.40
1:B:496:LEU:HD23	1:B:496:LEU:C	2.42	0.40
1:B:352:VAL:HA	1:B:355:VAL:HB	2.03	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%)	576 (96%)	20 (3%)	1 (0%)	52	59
1	B	597/599 (100%)	573 (96%)	24 (4%)	0	100	100
All	All	1194/1198 (100%)	1149 (96%)	44 (4%)	1 (0%)	56	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	527/527 (100%)	520 (99%)	7 (1%)	76	87
1	B	527/527 (100%)	519 (98%)	8 (2%)	72	84
All	All	1054/1054 (100%)	1039 (99%)	15 (1%)	74	85

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ARG
1	A	192	ASN
1	A	343	HIS
1	A	372	MET
1	A	490	GLN
1	A	506	TYR
1	A	625	LYS
1	B	61	GLU
1	B	137	ARG
1	B	192	ASN
1	B	204	THR
1	B	308	MET

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Mol	Chain	Res	Type
1	B	333	GLU
1	B	506	TYR
1	B	597	GLU

Some 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	65	HIS
1	A	74	GLN
1	A	84	GLN
1	A	109	GLN
1	A	112	GLN
1	A	135	GLN
1	A	166	GLN
1	A	187	GLN
1	A	192	ASN
1	A	202	HIS
1	A	207	HIS
1	A	210	GLN
1	A	307	GLN
1	A	310	HIS
1	A	328	GLN
1	A	405	GLN
1	A	461	HIS
1	A	501	GLN
1	A	548	HIS
1	A	550	ASN
1	A	586	ASN
1	A	619	GLN
1	A	620	ASN
1	B	32	GLN
1	B	74	GLN
1	B	84	GLN
1	B	112	GLN
1	B	135	GLN
1	B	155	ASN
1	B	192	ASN
1	B	202	HIS
1	B	207	HIS
1	B	210	GLN
1	B	228	GLN

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Mol	Chain	Res	Type
1	B	244	ASN
1	B	255	HIS
1	B	265	ASN
1	B	307	GLN
1	B	310	HIS
1	B	328	GLN
1	B	357	HIS
1	B	399	ASN
1	B	405	GLN
1	B	461	HIS
1	B	501	GLN
1	B	548	HIS
1	B	550	ASN
1	B	586	ASN
1	B	620	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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
4	152	A	1501	-	7,10,10	1.22	1 (14%)	9,14,14	1.04	1 (11%)
2	COA	A	1502	-	40,50,50	1.18	2 (5%)	50,75,75	1.83	3 (6%)
4	152	B	1601	-	7,10,10	1.12	0	9,14,14	1.08	1 (11%)
3	ACO	B	1602	-	43,53,53	1.23	2 (4%)	55,79,79	1.95	6 (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
4	152	A	1501	-	-	0/7/9/9	0/0/0/0
2	COA	A	1502	-	-	0/44/64/64	0/3/3/3
4	152	B	1601	-	-	0/7/9/9	0/0/0/0
3	ACO	B	1602	-	-	0/47/67/67	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1501	152	C4-N5	-2.40	1.47	1.51
2	A	1502	COA	P3B-O7A	2.97	1.60	1.51
3	B	1602	ACO	P3B-O7A	3.11	1.61	1.51
2	A	1502	COA	O4B-C1B	4.65	1.47	1.41
3	B	1602	ACO	O4B-C1B	4.95	1.47	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1602	ACO	N3A-C2A-N1A	-11.10	120.39	128.89
2	A	1502	COA	N3A-C2A-N1A	-10.72	120.69	128.89
3	B	1602	ACO	O-C-CH3	-4.06	103.48	122.83
3	B	1602	ACO	P2A-O3A-P1A	-3.79	122.08	132.73
2	A	1502	COA	P2A-O3A-P1A	-3.67	122.43	132.73
4	B	1601	152	C3-C4-N5	-3.01	111.25	117.24
4	A	1501	152	C3-C4-N5	-2.93	111.41	117.24
3	B	1602	ACO	O4B-C1B-N9A	2.27	112.85	108.10
2	A	1502	COA	O9A-P3B-O8A	3.01	118.83	107.38
3	B	1602	ACO	O9A-P3B-O8A	3.12	119.26	107.38
3	B	1602	ACO	O-C-S1P	3.71	141.93	122.43

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
4	A	1501	152	1	0
2	A	1502	COA	3	0
4	B	1601	152	1	0
3	B	1602	ACO	4	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	599/599 (100%)	-0.06	31 (5%) 31 30	12, 24, 51, 83	0
1	B	599/599 (100%)	-0.31	19 (3%) 51 50	9, 18, 37, 79	0
All	All	1198/1198 (100%)	-0.19	50 (4%) 40 39	9, 21, 46, 83	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	367	LEU	10.8
1	A	368	VAL	8.9
1	B	370	SER	8.2
1	B	368	VAL	8.1
1	A	367	LEU	6.9
1	B	369	ARG	6.7
1	B	371	PRO	6.0
1	B	625	LYS	5.8
1	A	625	LYS	5.7
1	A	624	ALA	5.6
1	A	374	PRO	5.1
1	B	624	ALA	4.9
1	A	371	PRO	4.8
1	A	373	VAL	4.7
1	B	294	ARG	4.1
1	B	366	GLU	4.1
1	A	370	SER	4.1
1	A	197	LYS	4.0
1	A	219	SER	3.8
1	A	369	ARG	3.8
1	A	366	GLU	3.7
1	A	623	ARG	3.5
1	B	29	MET	3.3
1	A	27	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	244	ASN	3.2
1	A	198	ARG	3.2
1	A	220	ASP	3.2
1	A	372	MET	3.1
1	A	242	GLN	2.9
1	A	29	MET	2.9
1	B	298	ASP	2.8
1	B	622	PRO	2.7
1	A	294	ARG	2.6
1	B	365	PRO	2.6
1	A	293	PRO	2.6
1	B	372	MET	2.6
1	A	60	GLU	2.6
1	B	623	ARG	2.5
1	A	298	ASP	2.5
1	A	297	ASP	2.5
1	A	365	PRO	2.4
1	B	198	ARG	2.3
1	A	163	LEU	2.2
1	B	293	PRO	2.2
1	A	490	GLN	2.2
1	A	61	GLU	2.1
1	B	292	VAL	2.1
1	A	77	GLY	2.0
1	A	291	GLN	2.0
1	A	28	HIS	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
4	152	A	1501	11/11	0.96	0.13	0.87	16,17,18,19	0
3	ACO	B	1602	51/51	0.93	0.13	0.28	17,23,28,31	0
2	COA	A	1502	48/48	0.94	0.11	-0.21	16,23,31,34	0
4	152	B	1601	11/11	0.97	0.11	-0.50	8,13,14,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.