



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:42 PM UTC

PDB ID : 2H3P / pdb_00002h3p
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

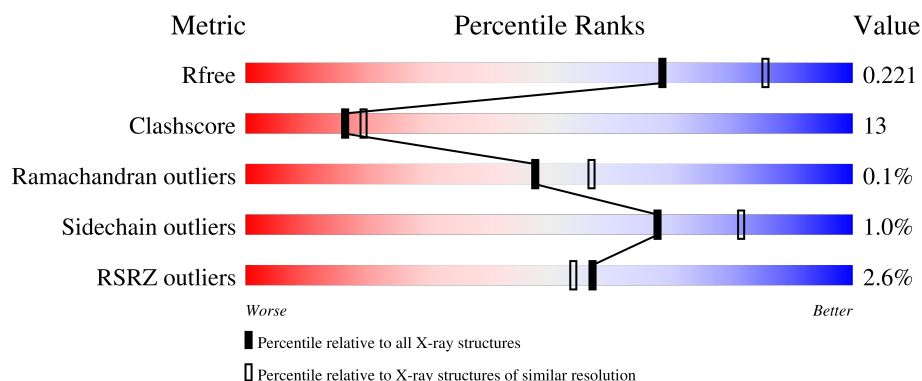
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	3% 71% 28% .
1	B	599	3% 76% 23% .

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.

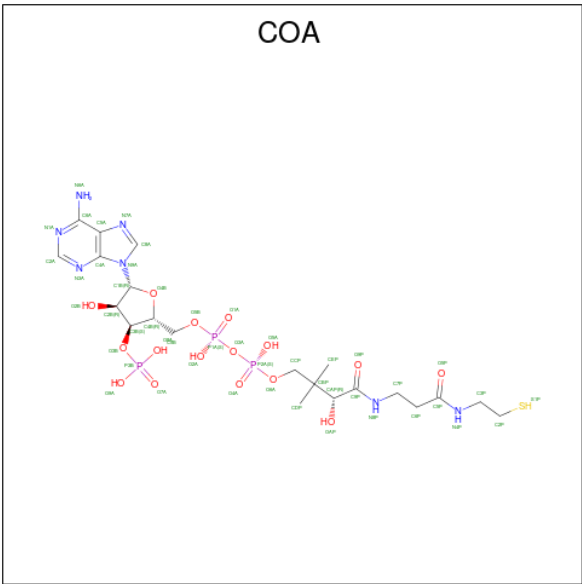
- Molecule 1 is a protein called carnitine acetyltransferase.

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:

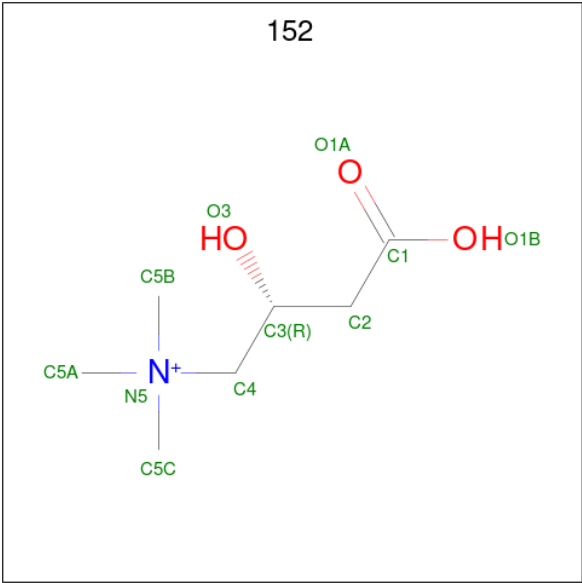
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	SER	-	cloning artifact	UNP Q3V1Y3
A	28	HIS	-	cloning artifact	UNP Q3V1Y3
A	29	MET	-	cloning artifact	UNP Q3V1Y3
B	27	SER	-	cloning artifact	UNP Q3V1Y3
B	28	HIS	-	cloning artifact	UNP Q3V1Y3
B	29	MET	-	cloning artifact	UNP Q3V1Y3

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



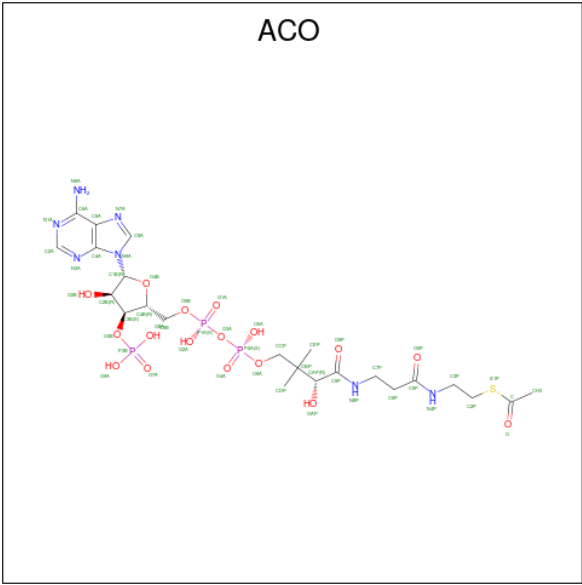
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is CARNITINE (CCD ID: 152) (formula: C₇H₁₆NO₃).



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 ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



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

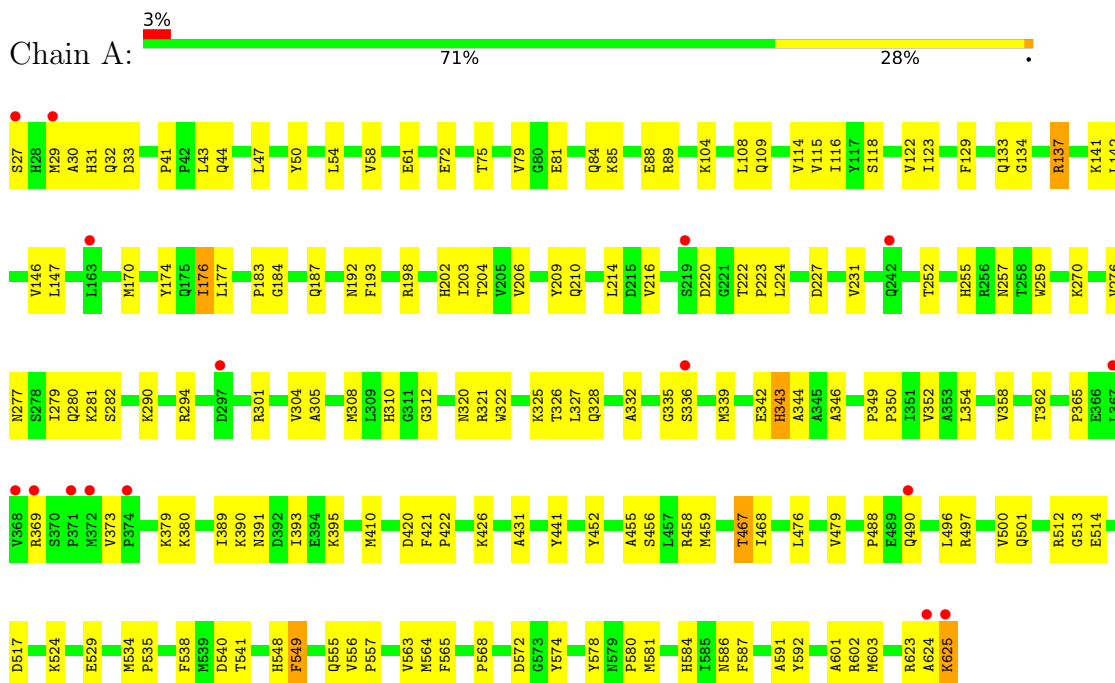
- Molecule 5 is water.

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

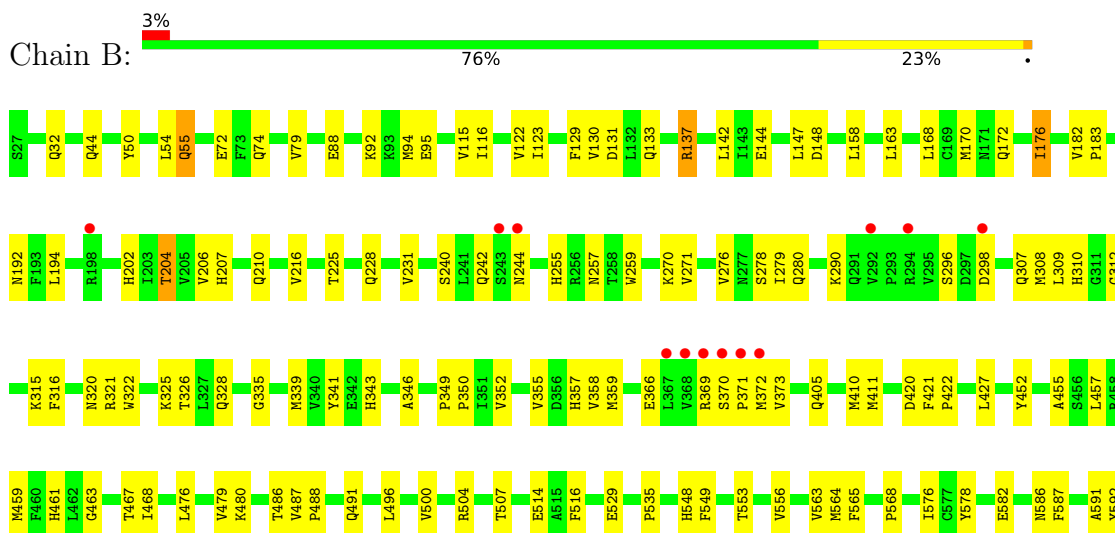
3 Residue-property plots

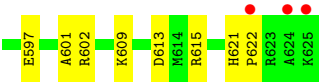
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	163.90Å 89.24Å 122.64Å 90.00° 128.96° 90.00°	Depositor
Resolution (Å)	29.92 – 2.20 29.92 – 2.21	Depositor EDS
% Data completeness (in resolution range)	94.9 (29.92-2.20) 95.0 (29.92-2.21)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.96 (at 2.20Å)	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%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11109	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 152, COA, 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	0.37	0/4897	0.83	6/6633 (0.1%)
1	B	0.41	0/4897	0.86	3/6633 (0.0%)
All	All	0.39	0/9794	0.84	9/13266 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ILE	N-CA-C	8.23	119.04	110.72
1	B	343	HIS	N-CA-C	6.38	120.17	112.38
1	A	343	HIS	N-CA-C	5.92	119.60	112.38
1	B	176	ILE	N-CA-C	5.91	117.44	111.00
1	B	467	THR	N-CA-C	5.61	118.38	109.24
1	A	467	THR	N-CA-C	5.59	118.08	109.07
1	A	459	MET	N-CA-C	-5.47	106.44	113.01
1	A	549	PHE	N-CA-C	5.26	117.91	108.17
1	A	346	ALA	N-CA-C	5.10	115.08	107.88

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	139	0
1	B	4781	0	4754	110	0
2	A	48	0	32	3	0
3	A	11	0	15	1	0
3	B	11	0	15	1	0
4	B	51	0	34	4	0
5	A	639	0	0	24	0
5	B	787	0	0	27	0
All	All	11109	0	9604	251	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 (251) 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: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:534:MET:CE	1:A:535:PRO:HD2	2.18	0.74
1:A:534:MET:HE3	1:A:535:PRO:HD2	1.72	0.71
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	4: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:A:352:VAL:HG13	1:A:564:MET:HE3	1.78	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:B:341:TYR:HE2	1:B:564:MET:HE1	1.63	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:129:PHE:HB2	1:A:134:GLY:HA3	1.87	0.56
1:A:514:GLU:HG2	5:A:1927:HOH:O	2.05	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:183:PRO:HG3	1:A:259:TRP:NE1	2.21	0.56
1:A:358:VAL:O	1:A:362:THR:HG23	2.06	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:524:LYS:HG3	1:A:534:MET:HE1	1.89	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:30:ALA:HB3	5:A:1913:HOH:O	2.08	0.54
1:A:379:LYS:HD3	5:A:1770:HOH:O	2.07	0.54
1:A:534:MET:HE2	1:A:538:PHE:HD1	1.72	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:A:255:HIS:CD2	1:A:257:ASN:H	2.27	0.53
1:B:322:TRP:H	1:B:328:GLN:NE2	2.06	0.53
1:B:609:LYS:HE2	1:B:613:ASP:OD1	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLN:O	1:A:88:GLU:HG3	2.09	0.53
1:A:255:HIS:HD2	1:A:257:ASN:H	1.54	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:61:GLU:H	1:A:61:GLU:CD	2.17	0.52
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:HG3	1:A:512:ARG:HH11	1.74	0.52
1:A:534:MET:HE3	1:A:535:PRO:CD	2.39	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:29:MET:HG2	1:A:33:ASP:OD2	2.10	0.52
1:A:227:ASP:O	1:A:231:VAL:HG23	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
1:A:115:VAL:HG12	1:A:116:ILE:HG13	1.91	0.51
1:A:294:ARG:HG3	1:A:294:ARG:HH11	1.76	0.51
1:A:534:MET:HE3	1:A:534:MET:HA	1.92	0.51
1:B:455:ALA:HB2	1:B:468:ILE:HG13	1.93	0.51
1:A:534:MET:HE2	1:A:535:PRO:HD2	1.93	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:372:MET:HE3	1:B:373:VAL:O	2.11	0.50
1:A:27:SER:HA	1:A:174:TYR:CE1	2.47	0.50
1:B:578:TYR:HB3	1:B:587:PHE:CD1	2.47	0.50
1:A:625:LYS:HB2	1:A:625:LYS:NZ	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:A:123:ILE:HD11	1:A:305:ALA:HA	1.93	0.49
1:B:183:PRO:HG3	1:B:259:TRP:NE1	2.28	0.49
1:B:50:TYR:CZ	1:B:54:LEU:HD11	2.48	0.49
1:B:548:HIS:HD2	5:B:1938:HOH:O	1.95	0.49
1:A:352:VAL:CG1	1:A:564:MET:HE3	2.41	0.48
1:A:27:SER:HB2	5:A:2010:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:94:MET:HE2	5:B:1851:HOH:O	2.12	0.48
1:B:130:VAL:HA	5:B:1785:HOH:O	2.12	0.48
1:B:115:VAL:HG12	1:B:116:ILE:HG13	1.95	0.48
1:B:142:LEU:C	1:B:142:LEU:HD23	2.38	0.48
1:B:421:PHE:CZ	1:B:615:ARG:HG3	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:452:TYR:HB2	1:B:549:PHE:CD1	2.49	0.48
1:A:89:ARG:HD3	5:A:1666:HOH:O	2.12	0.47
1:B:202:HIS:HD2	5:B:1623:HOH:O	1.95	0.47
1:B:621:HIS:N	1:B:622:PRO:HD3	2.29	0.47
1:A:142:LEU:HD23	1:A:142:LEU:C	2.39	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:192:ASN:HD22	1:B:192:ASN:C	2.22	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:452:TYR:HB2	1:A:549:PHE:CD1	2.50	0.46
1:A:555:GLN:HG3	1:A:578:TYR:CE2	2.50	0.46
1:A:198:ARG:HG3	1:A:198:ARG:HH11	1.81	0.46
1:B:44:GLN:HA	1:B:74:GLN:HE22	1.81	0.46
1:A:328:GLN:O	1:A:339:MET:HB2	2.15	0.46
1:B:322:TRP:H	1:B:328:GLN:HE22	1.63	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:192:ASN:C	1:A:192:ASN:HD22	2.24	0.46
1:A:193:PHE:CD1	1:A:281:LYS:HG2	2.51	0.46
1:A:420:ASP:OD1	1:A:421:PHE:N	2.48	0.46
1:A:222:THR:OG1	1:A:223:PRO:HD2	2.16	0.46
1:A:534:MET:HE2	1:A:538:PHE:CD1	2.51	0.45
1:B:172:GLN:OE1	1:B:346:ALA:HB1	2.16	0.45
1:B:290:LYS:HE2	1:B:316:PHE:O	2.16	0.45
1:B:307:GLN:HG3	5:B:1819:HOH:O	2.16	0.45
1:B:309:LEU:HB2	1:B:565:PHE:HE1	1.79	0.45
1:A:281:LYS:NZ	5:A:2020:HOH:O	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:TYR:OH	4:B:1602:ACO:HH32	2.16	0.45
1:A:276:VAL:O	1:A:280:GLN:HG3	2.17	0.45
1:A:320:ASN:C	1:A:321:ARG:HG2	2.42	0.45
1:A:458:ARG:HD3	5:A:1750:HOH:O	2.16	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:A:282:SER:O	1:A:325:LYS:NZ	2.50	0.45
1:A:529:GLU:HG2	5:A:1700:HOH:O	2.14	0.45
1:B:556:VAL:HG22	4:B:1602:ACO:H32	1.98	0.45
1:A:277:ASN:OD1	1:A:281:LYS:HE2	2.16	0.45
3:A:1501:152:H5A2	3:A:1501:152:H3	1.74	0.45
1:B:504:ARG:HD2	5:B:1698:HOH:O	2.16	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:B:270:LYS:HG3	1:B:271:VAL:N	2.31	0.45
1:A:352:VAL:HG13	1:A:564:MET:CE	2.47	0.44
1:B:410:MET:HE2	5:B:2052:HOH:O	2.17	0.44
1:B:496:LEU:C	1:B:496:LEU:HD23	2.42	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:A:476:LEU:HA	1:A:479:VAL:HG22	2.00	0.44
1:B:210:GLN:HG2	5:B:1961:HOH:O	2.16	0.44
1:B:476:LEU:HA	1:B:479:VAL:HG22	1.99	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:129:PHE:CZ	1:B:335:GLY:HA2	2.53	0.43
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:A:568:PRO:HD2	1:A:592:TYR:CZ	2.53	0.43
1:B:204:THR:HG21	1:B:279:ILE:HA	1.99	0.43
1:A:304:VAL:O	1:A:308:MET:HG2	2.18	0.43
1:B:320:ASN:C	1:B:321:ARG:HG2	2.44	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:A:365:PRO:HD3	5:A:2111:HOH:O	2.19	0.43
1:B:290:LYS:HD3	5:B:2352:HOH:O	2.18	0.43
1:A:568:PRO:HG2	1:A:591:ALA:HA	2.01	0.43
1:A:373:VAL:HB	5:A:2099:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1601:152:O3	3:B:1601:152:H5B3	2.19	0.43
1:A:109:GLN:NE2	5:A:1810:HOH:O	2.51	0.43
1:A:216:VAL:C	1:A:224:LEU:HD13	2.44	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:574:TYR:CE1	1:A:603:MET:HE2	2.54	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:A:79:VAL:HG21	5:A:2135:HOH:O	2.20	0.42
1:A:301:ARG:NH2	5:A:1787:HOH:O	2.51	0.42
1:A:354:LEU:HD23	1:A:354:LEU:C	2.44	0.42
1:A:467:THR:HB	1:A:517:ASP:HB2	2.02	0.42
1:B:72:GLU:HB2	5:B:1711:HOH:O	2.19	0.42
1:B:202:HIS:HE1	1:B:278:SER:O	2.02	0.42
1:A:301:ARG:HG3	1:A:301:ARG:HH11	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:358:VAL:HG12	1:B:359:MET:HE2	2.01	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: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
1:B:516:PHE:CD1	1:B:516:PHE:C	2.98	0.41
1:A:43:LEU:O	1:A:47:LEU:HG	2.21	0.41
1:A:209:TYR:N	1:A:209:TYR:CD2	2.87	0.41
1:B:328:GLN:O	1:B:339:MET:HB2	2.21	0.41
1:A:496:LEU:HD23	1:A:496:LEU:C	2.45	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:242:GLN:HB3	1:B:244:ASN:ND2	2.35	0.41
1:B:529:GLU:HG2	5:B:1693:HOH:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:325:LYS:HD2	1:B:325:LYS:HA	1.88	0.41
1:B:352:VAL:HG11	1:B:556:VAL:HG12	2.02	0.41
1:A:325:LYS:HA	1:A:325:LYS:HD2	1.95	0.41
1:B:123:ILE:HD12	1:B:411:MET:HE2	2.03	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:A:32:GLN:NE2	1:A:170:MET:H	2.17	0.40
1:A:176:ILE:HA	1:A:326:THR:HG21	2.02	0.40
1:A:488:PRO:HD3	5:A:1760:HOH:O	2.21	0.40
1:B:507:THR:HG23	4:B:1602:ACO:H143	2.03	0.40
1:A:31:HIS:HB2	5:A:1777:HOH:O	2.21	0.40
1:A:581:MET:HB2	1:A:584:HIS:O	2.21	0.40
1:B:32:GLN:NE2	1:B:170:MET:H	2.09	0.40
1:B:182:VAL:HA	1:B:183:PRO:HD3	1.91	0.40
1:A:441:TYR:HD1	1:A:603:MET:HE1	1.87	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%)	43	51
1	B	597/599 (100%)	573 (96%)	24 (4%)	0	100	100
All	All	1194/1198 (100%)	1149 (96%)	44 (4%)	1 (0%)	48	57

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%)	522 (99%)	5 (1%)	70	84
1	B	527/527 (100%)	521 (99%)	6 (1%)	65	79
All	All	1054/1054 (100%)	1043 (99%)	11 (1%)	68	81

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ARG
1	A	206	VAL
1	A	343	HIS
1	A	490	GLN
1	A	625	LYS
1	B	55	GLN
1	B	137	ARG
1	B	204	THR
1	B	206	VAL
1	B	308	MET
1	B	597	GLU

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	135	GLN
1	A	155	ASN
1	A	166	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	175	GLN
1	A	192	ASN
1	A	207	HIS
1	A	210	GLN
1	A	242	GLN
1	A	307	GLN
1	A	310	HIS
1	A	328	GLN
1	A	357	HIS
1	A	405	GLN
1	A	461	HIS
1	A	501	GLN
1	A	526	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	44	GLN
1	B	74	GLN
1	B	135	GLN
1	B	155	ASN
1	B	192	ASN
1	B	202	HIS
1	B	207	HIS
1	B	228	GLN
1	B	242	GLN
1	B	244	ASN
1	B	255	HIS
1	B	277	ASN
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	501	GLN
1	B	526	GLN
1	B	548	HIS
1	B	586	ASN
1	B	619	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 oligosaccharides 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	$\# Z > 2$
3	152	B	1601	-	10,10,10	1.14	0	13,14,14	1.14	1 (7%)
4	ACO	B	1602	-	51,53,53	1.25	6 (11%)	73,79,79	1.68	11 (15%)
2	COA	A	1502	-	47,50,50	1.24	6 (12%)	69,75,75	1.51	10 (14%)
3	152	A	1501	-	10,10,10	1.19	1 (10%)	13,14,14	1.02	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	1601	-	-	0/9/9/9	-
4	ACO	B	1602	-	-	6/51/67/67	0/3/3/3
2	COA	A	1502	-	-	4/48/64/64	0/3/3/3
3	152	A	1501	-	-	1/9/9/9	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1602	ACO	P3B-O7A	3.51	1.61	1.50
2	A	1502	COA	P3B-O7A	3.36	1.60	1.50
2	A	1502	COA	C5A-N7A	-3.22	1.33	1.39
4	B	1602	ACO	C5A-N7A	-3.21	1.33	1.39
2	A	1502	COA	P2A-O3A	2.85	1.62	1.59
4	B	1602	ACO	P1A-O3A	2.68	1.62	1.59
2	A	1502	COA	P1A-O3A	2.50	1.62	1.59
4	B	1602	ACO	P2A-O3A	2.44	1.62	1.59
4	B	1602	ACO	O4B-C1B	2.36	1.47	1.42
3	A	1501	152	C4-N5	-2.30	1.47	1.52
2	A	1502	COA	O4B-C1B	2.20	1.47	1.42
2	A	1502	COA	C4A-N9A	-2.05	1.33	1.37
4	B	1602	ACO	C4A-N9A	-2.04	1.33	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1602	ACO	N3A-C2A-N1A	-5.41	120.39	128.58
2	A	1502	COA	N3A-C2A-N1A	-5.22	120.69	128.58
4	B	1602	ACO	O-C-CH3	-5.07	103.48	123.12
2	A	1502	COA	C5A-C4A-N3A	-5.05	119.77	126.72
4	B	1602	ACO	C5A-C4A-N3A	-5.00	119.83	126.72
4	B	1602	ACO	O-C-S1P	4.77	141.93	122.65
4	B	1602	ACO	C2A-N3A-C4A	3.73	120.94	111.83
2	A	1502	COA	C2A-N3A-C4A	3.66	120.77	111.83
2	A	1502	COA	N9A-C8A-N7A	-3.55	108.90	113.94
2	A	1502	COA	N3A-C4A-N9A	3.40	132.95	127.17
4	B	1602	ACO	N3A-C4A-N9A	3.30	132.77	127.17
4	B	1602	ACO	N9A-C8A-N7A	-3.29	109.27	113.94
4	B	1602	ACO	O9A-P3B-O8A	3.06	119.26	107.80
3	B	1601	152	C3-C4-N5	-2.96	111.25	116.70
2	A	1502	COA	O9A-P3B-O8A	2.94	118.83	107.80
3	A	1501	152	C3-C4-N5	-2.87	111.41	116.70
2	A	1502	COA	C5A-N7A-C8A	2.86	107.95	103.45
4	B	1602	ACO	C5A-N7A-C8A	2.69	107.67	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1602	ACO	O4B-C1B-N9A	2.48	112.85	108.09
2	A	1502	COA	C4A-C5A-N7A	-2.39	107.84	110.58
4	B	1602	ACO	C4A-C5A-N7A	-2.26	108.00	110.58
2	A	1502	COA	C4A-N9A-C8A	2.19	108.04	105.74
2	A	1502	COA	O4B-C1B-N9A	2.17	112.26	108.09

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1501	152	C1-C2-C3-C4
4	B	1602	ACO	O-C-S1P-C2P
4	B	1602	ACO	CH3-C-S1P-C2P
4	B	1602	ACO	P2A-O3A-P1A-O5B
2	A	1502	COA	C2B-C3B-O3B-P3B
2	A	1502	COA	C4B-C3B-O3B-P3B
4	B	1602	ACO	C2B-C3B-O3B-P3B
4	B	1602	ACO	C4B-C3B-O3B-P3B
2	A	1502	COA	C3B-O3B-P3B-O7A
4	B	1602	ACO	C3B-O3B-P3B-O7A
2	A	1502	COA	N8P-C9P-CAP-OAP

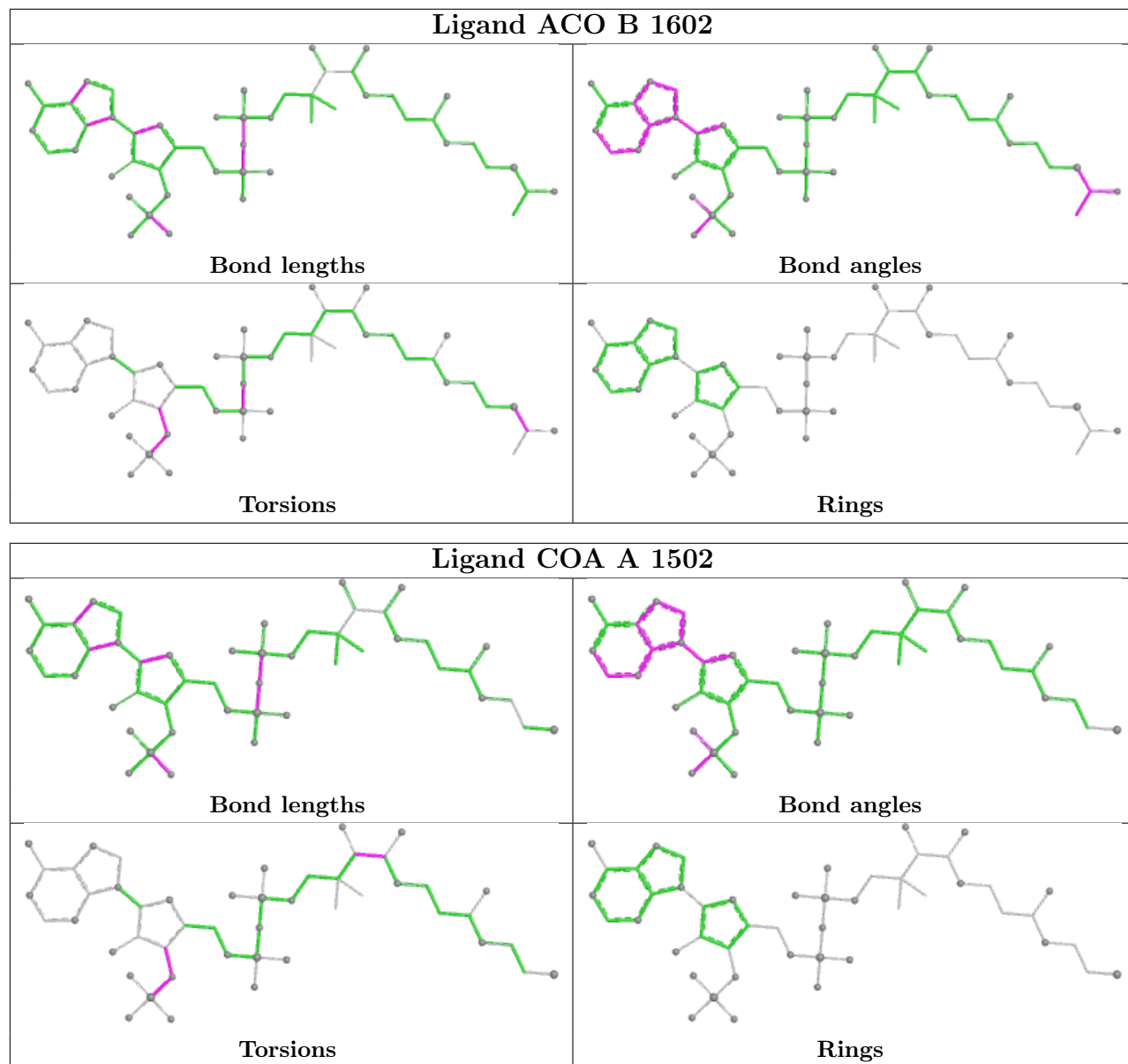
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1601	152	1	0
4	B	1602	ACO	4	0
2	A	1502	COA	3	0
3	A	1501	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%)	-0.08	16 (2%)	56	53	12, 24, 51, 83	0
1	B	599/599 (100%)	-0.37	15 (2%)	58	55	9, 18, 37, 79	0
All	All	1198/1198 (100%)	-0.22	31 (2%)	57	54	9, 21, 46, 83	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	SER	4.4
1	B	371	PRO	4.4
1	B	370	SER	4.4
1	B	368	VAL	4.1
1	B	372	MET	4.0
1	B	367	LEU	4.0
1	B	369	ARG	3.7
1	A	624	ALA	3.7
1	B	624	ALA	3.5
1	A	367	LEU	3.3
1	A	368	VAL	3.1
1	A	371	PRO	3.1
1	B	298	ASP	3.0
1	B	294	ARG	2.9
1	B	625	LYS	2.7
1	A	297	ASP	2.7
1	A	625	LYS	2.5
1	A	336	SER	2.5
1	B	292	VAL	2.4
1	A	372	MET	2.4
1	A	163	LEU	2.4
1	A	369	ARG	2.4
1	A	374	PRO	2.4
1	A	490	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	219	SER	2.3
1	B	622	PRO	2.2
1	B	244	ASN	2.2
1	B	198	ARG	2.1
1	A	242	GLN	2.1
1	B	243	SER	2.0
1	A	29	MET	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](#)

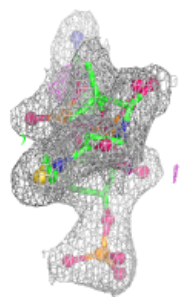
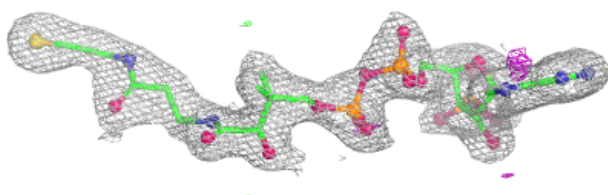
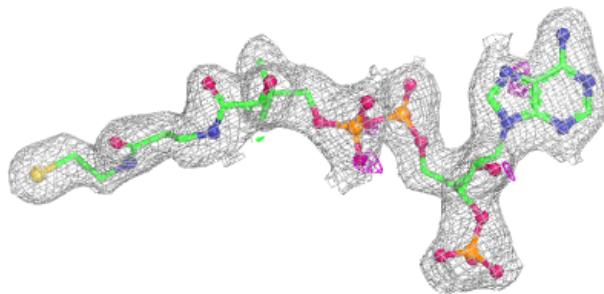
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	COA	A	1502	48/48	0.95	0.07	16,23,31,34	0
3	152	A	1501	11/11	0.95	0.07	16,17,18,19	0
4	ACO	B	1602	51/51	0.96	0.07	17,23,28,31	0
3	152	B	1601	11/11	0.97	0.05	8,13,14,15	0

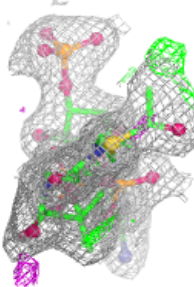
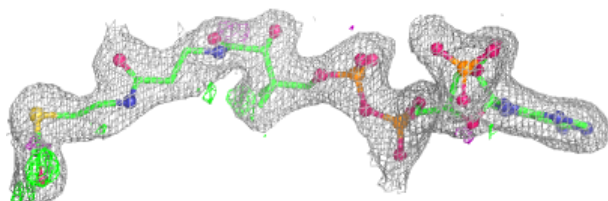
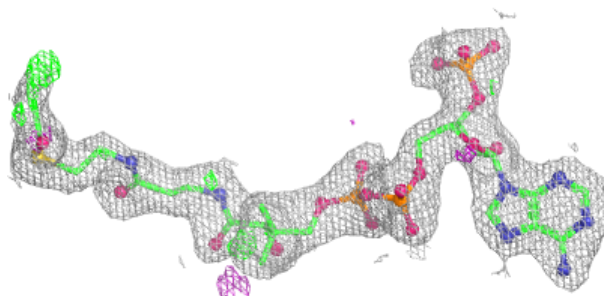
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA A 1502:

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

**Electron density around ACO B 1602:**

$2mF_o-DF_c$ (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.