Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2022 – 04:32 PM EDT

PDB ID	:	5CSL
Title	:	Crystal structure of the 500 kD yeast acetyl-CoA carboxylase holoenzyme dimer
Authors	:	Wei, J.; Tong, L.
Deposited on	:	2015-07-23
Resolution	:	3.20 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 following versions of software and data (see references ⓘ) were used in the production of this report:

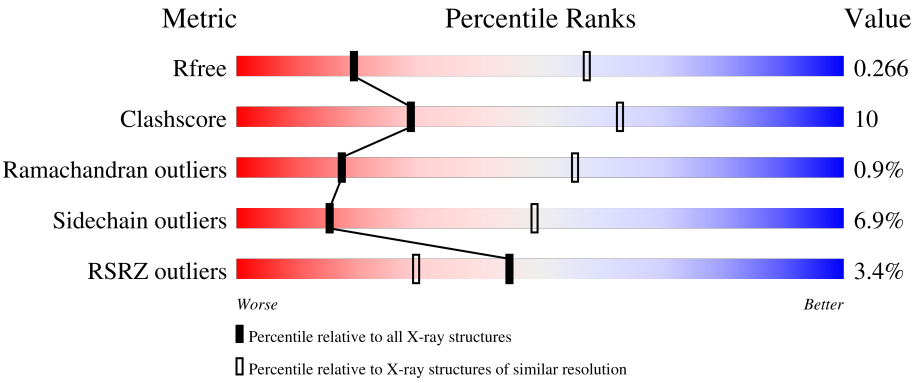
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=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	2218	2% 70% 20% · 8%
1	B	2218	4% 69% 22% · 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 32777 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.

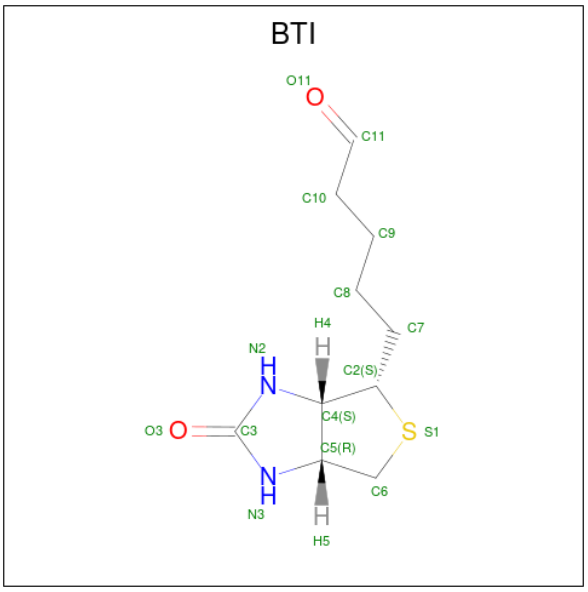
- Molecule 1 is a protein called Acetyl-CoA carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2050	Total	C	N	O	S	0	0	0
			16249	10332	2798	3062	57			
1	B	2072	Total	C	N	O	S	0	0	0
			16402	10428	2835	3085	54			

There are 12 discrepancies between the modelled and reference sequences:

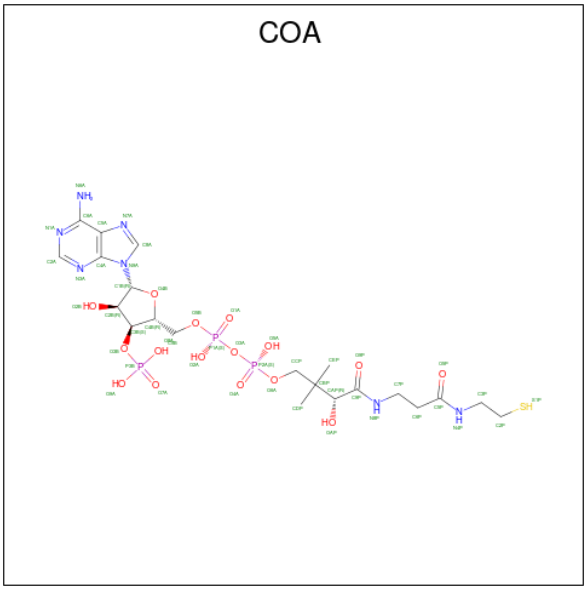
Chain	Residue	Modelled	Actual	Comment	Reference
A	2234	HIS	-	expression tag	UNP Q00955
A	2235	HIS	-	expression tag	UNP Q00955
A	2236	HIS	-	expression tag	UNP Q00955
A	2237	HIS	-	expression tag	UNP Q00955
A	2238	HIS	-	expression tag	UNP Q00955
A	2239	HIS	-	expression tag	UNP Q00955
B	2234	HIS	-	expression tag	UNP Q00955
B	2235	HIS	-	expression tag	UNP Q00955
B	2236	HIS	-	expression tag	UNP Q00955
B	2237	HIS	-	expression tag	UNP Q00955
B	2238	HIS	-	expression tag	UNP Q00955
B	2239	HIS	-	expression tag	UNP Q00955

- Molecule 2 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: $C_{10}H_{16}N_2O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
2	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



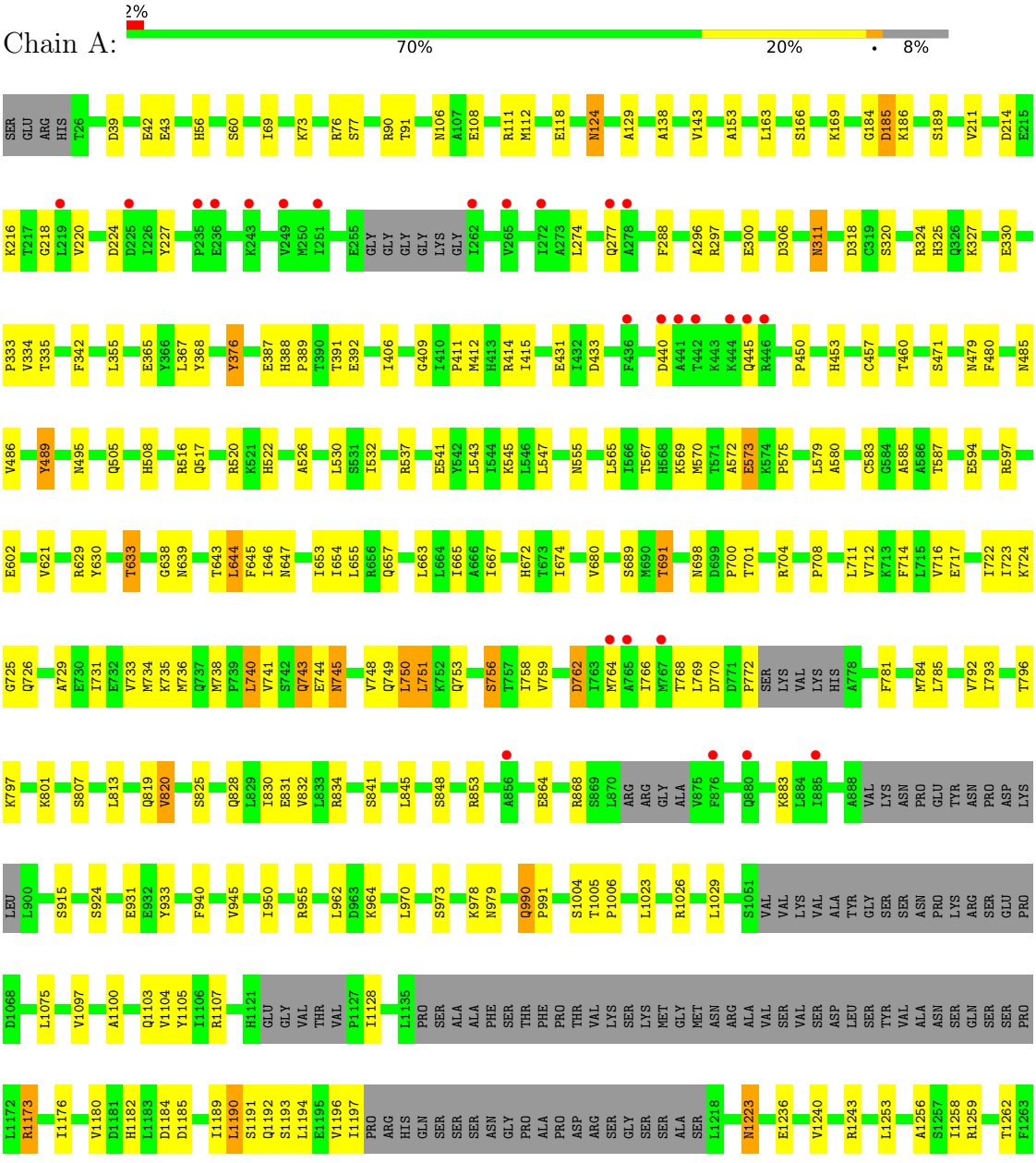
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

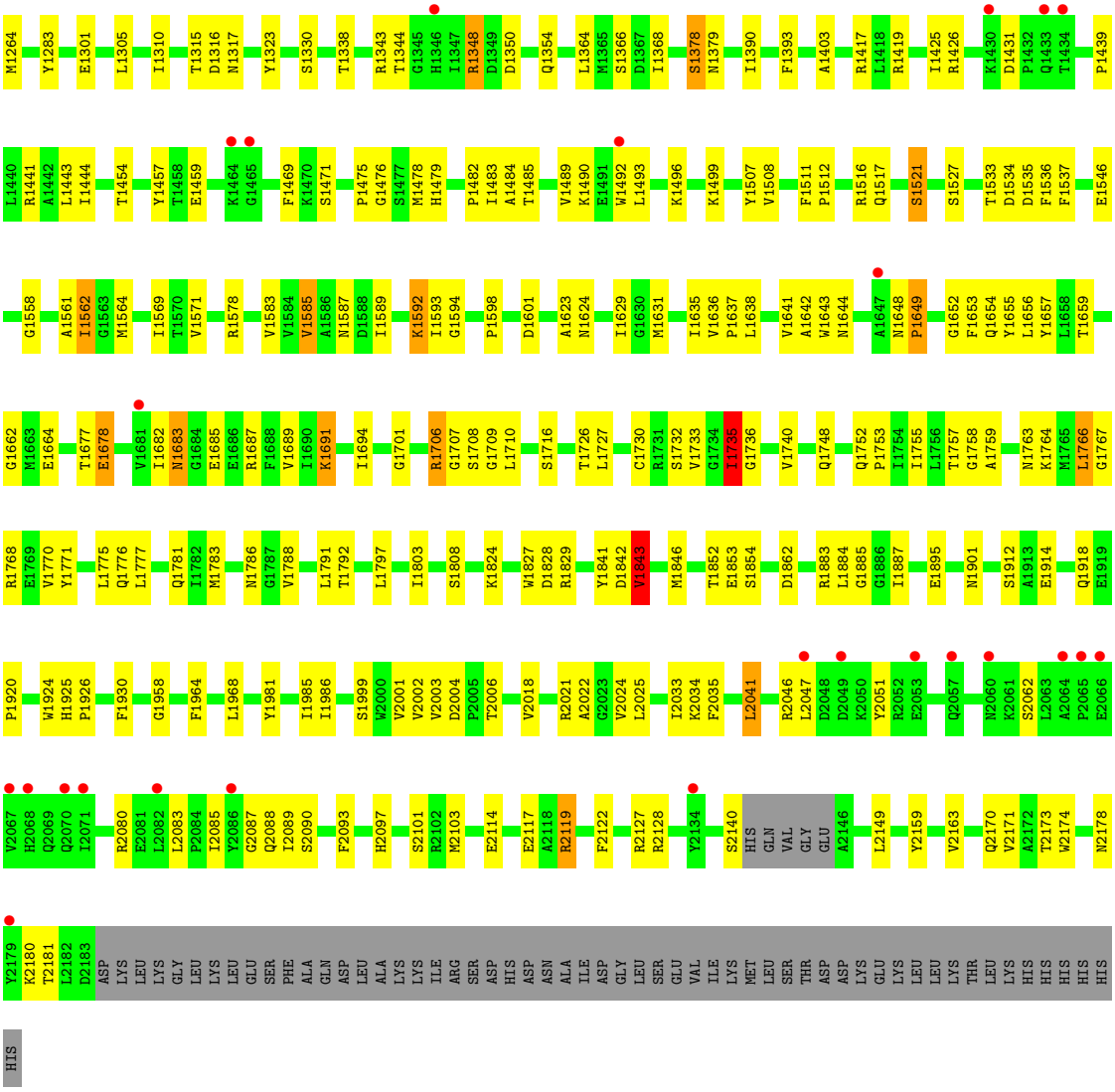
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Acetyl-CoA carboxylase

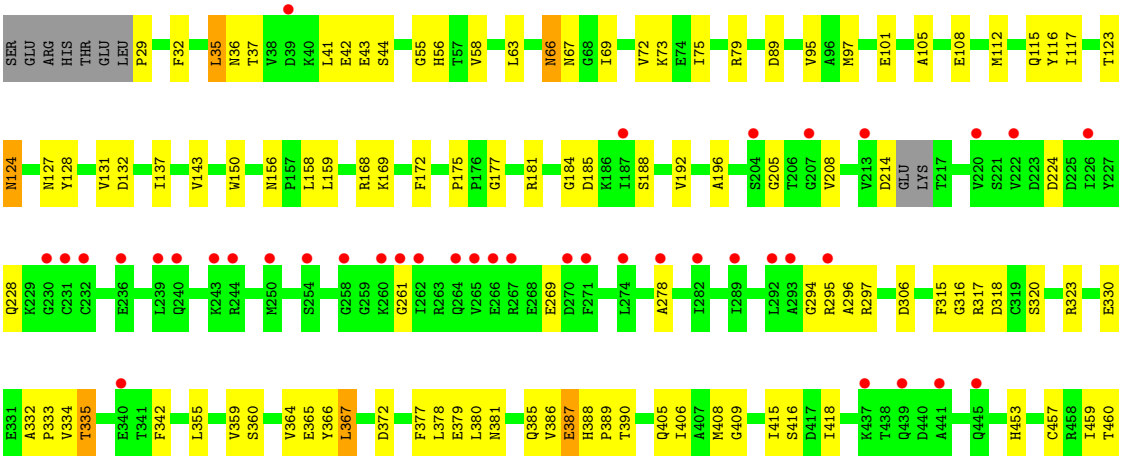
Chain A:

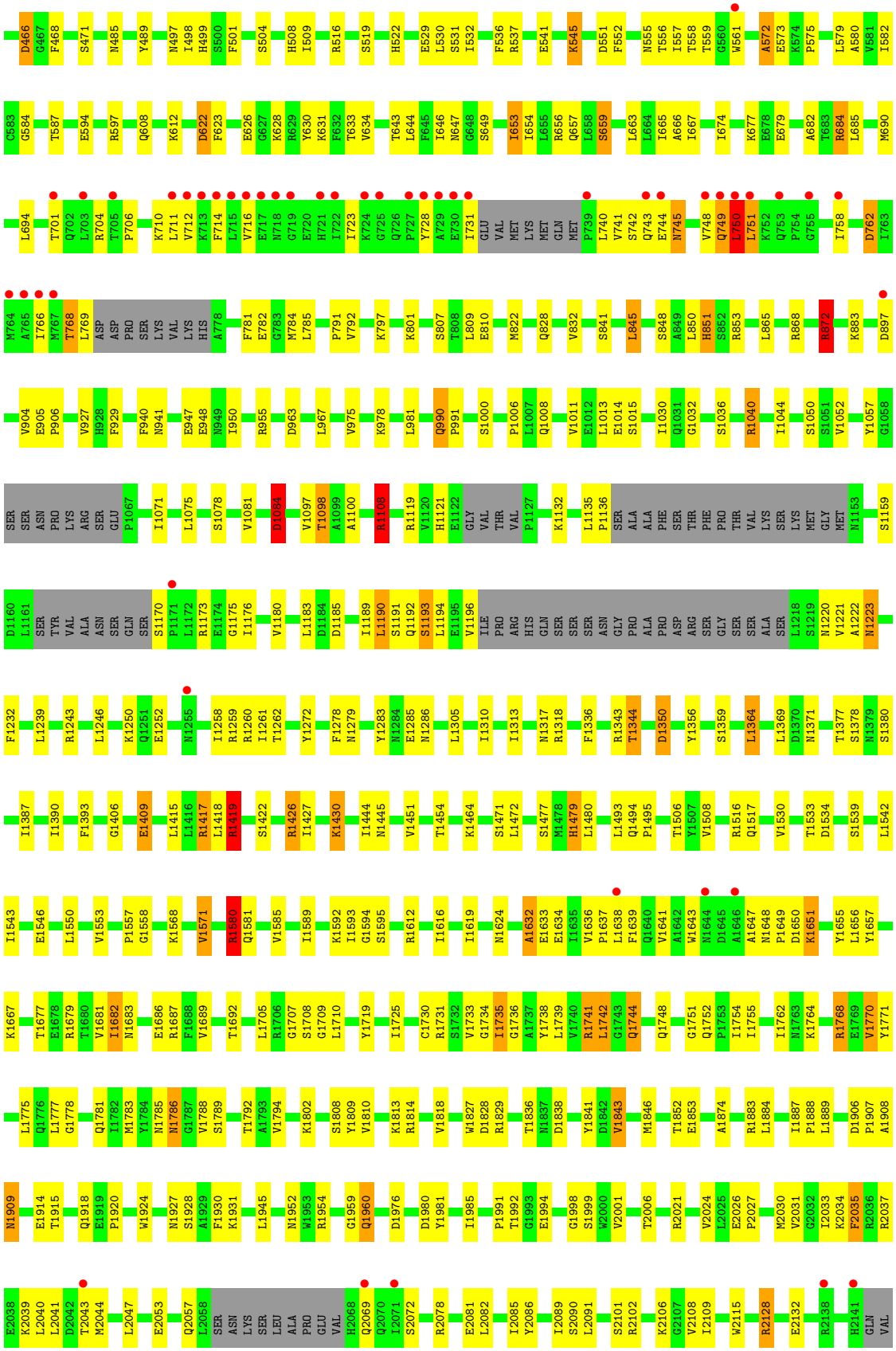


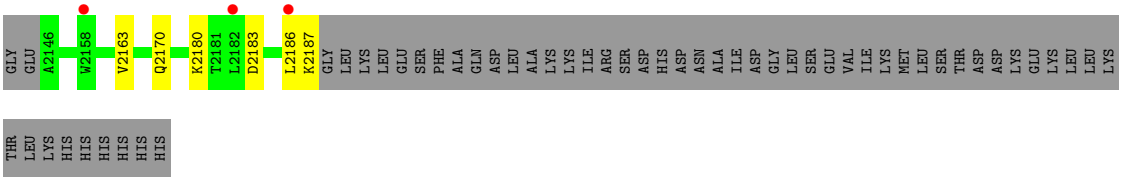


• Molecule 1: Acetyl-CoA carboxylase

Chain B:




D466 G467 F468 S471 N485 Y489 N497 I498 H499 S500 F501 S504 H508 I509 R516 S519 H522 E529 L530 S531 I532 F536 R537 E541 K545 D551 F552 N555 T556 I557 T558 T559 G560 W561 A572 E573 K574 P575 L579 A580 V581 I582
C583 G584 T587 E594 R597 Q608 K612 D622 F623 E626 G627 K628 R629 Y630 K631 F632 T633 V634 T643 L644 F645 I646 N647 G648 S649 I653 I654 L655 R656 Q657 L658 S659 L663 L664 I665 A666 I667 I674 K677 E678 E679 A682 T683 R684 L685 M690
L694 T701 Q702 L703 R704 T705 P706 K710 L711 V712 K713 F714 L715 V716 E717 N718 G719 E720 H721 I722 I723 K724 G725 Q726 P727 Y728 A729 E730 I731 GLU VAL MET LYS MET GLN MET P739 L740 V741 S742 Q743 E744 N745 V748 Q749 L750 L751 K752 Q753 P754 G755 I758 D762 I763
M764 A765 I766 M767 T768 L769 ASP ASP PRO SER LYS VAL LYS HIS A778 F781 E782 G783 M784 L785 P791 V792 K797 K801 S807 T808 L809 E810 M822 Q828 V832 S841 L845 S848 A849 L850 H851 S852 R853 L865 R868 R872 K883 D897
V904 E905 P906 V927 H928 F929 F940 N941 E947 E948 N949 I950 R955 D963 L967 V975 K978 L981 Q990 P991 S1000 P1006 L1007 Q1008 V1011 E1012 L1013 E1014 S1015 I1030 Q1031 G1032 S1036 R1040 I1044 S1050 S1051 V1052 Y1057 G1058
SER SER ASN PRO LYS ARG SER GLU P1067 I1071 L1075 S1078 V1081 D1084 V1097 T1098 A1099 A1100 R1108 R1119 V1120 H1121 E1122 GLY VAL THR VAL P1127 K1132 L1135 P1136 SER ALA ALA PHE SER THR PHE PRO THR VAL LYS SER LYS MET GLY MET N1153 S1159
D1160 L1161 SER TYR VAL ALA ASN SER GLN SER S1170 P1171 L1172 R1173 E1174 G1175 I1176 V1180 L1183 D1184 D1185 I1189 L1190 S1191 Q1192 S1193 L1194 E1195 V1196 ILE PRO ARG HIS GLN SER SER SER ASN GLY PRO ALA PRO ASP ARG SER GLY SER SER ALA SER L1218 S1219 N1220 V1221 A1222 N1223
F1232 L1239 R1243 L1246 K1250 Q1251 E1252 N1255 I1258 R1259 R1260 I1261 T1262 Y1272 F1278 N1279 Y1283 N1284 E1285 N1286 L1305 I1310 I1313 N1317 R1318 F1336 R1343 T1344 D1350 Y1356 S1359 L1364 L1369 D1370 N1371 T1377 S1378 N1379 S1380
I1387 I1390 F1393 G1406 E1409 L1415 L1416 R1417 L1418 R1419 S1422 R1426 I1427 K1430 I1444 N1445 V1451 T1454 K1464 S1471 L1472 S1477 M1478 H1479 L1480 L1493 Q1494 P1495 T1506 Y1507 V1508 R1516 Q1517 V1530 T1533 D1534 S1539 L1542
I1543 E1546 L1550 V1553 P1557 G1558 K1568 R1580 Q1581 V1585 I1589 K1592 I1593 G1594 S1595 R1612 I1616 I1619 N1624 A1632 E1633 E1634 I1635 V1636 P1637 L1638 F1639 Q1640 V1641 A1642 W1643 N1644 D1645 A1646 A1647 N1648 P1649 D1650 K1651 Y1655 L1656 Y1657
K1667 T1677 E1678 R1679 T1680 V1681 I1682 N1683 E1686 R1687 F1688 V1689 T1692 L1705 R1706 G1707 S1708 G1709 L1710 Y1719 I1725 C1730 R1731 S1732 V1733 G1734 I1735 G1736 A1737 Y1738 L1739 Y1740 R1741 L1742 G1743 Q1744 Q1748 G1751 Q1752 P1753 I1754 I1755 I1762 N1763 K1764 R1768 E1769 V1770 Y1771
L1775 Q1776 L1777 G1778 Q1781 I1782 M1783 Y1784 N1785 N1786 G1787 V1788 S1789 T1792 A1793 V1794 K1802 S1808 Y1809 V1810 K1813 R1814 V1818 W1827 D1828 R1829 T1836 N1837 D1838 Y1841 D1842 V1843 M1846 T1852 E1853 A1874 R1883 L1884 I1887 P1888 L1889 D1906 P1907 A1908
N1909 E1914 T1915 Q1918 E1919 P1920 W1924 N1927 S1928 A1929 F1930 K1931 L1945 N1952 W1953 R1954 G1959 Q1960 D1976 D1980 Y1981 I1985 P1991 T1992 G1993 E1994 G1998 S1999 W2000 V2001 T2006 R2021 V2024 L2025 E2026 P2027 M2030 V2031 G2032 I2033 K2034 P2035 R2036 R2037
E2038 K2039 L2040 L2041 D2042 T2043 M2044 L2047 E2053 Q2057 L2058 SER ASN LYS SER LEU ALA PRO GLU VAL H2068 Q2069 Q2070 I2071 S2072 R2078 E2081 L2082 I2085 Y2086 I2089 S2090 L2091 S2101 R2102 K2106 G2107 V2108 I2109 W2115 R2128 E2132 R2138 H2141 GLN VAL


GLY GLU A2146 W2158 V2163 Q2170 K2180 T2181 L2182 D2183 L2186 K2187 GLY LEU LYS LEU GLU SER PHE ALA GLN ASP LEU ALA LYS LYS ILE ARG SER ASP HIS ASP ASN ALA ILE ASP GLY LEU SER GLU VAL ILE LYS MET LEU SER THR ASP ASP LYS GLU LYS LEU LEU LYS
THR LEU LYS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	159.87Å 159.87Å 614.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.93 – 3.20 49.88 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.93-3.20) 97.2 (49.88-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.219 , 0.266 0.220 , 0.266	Depositor DCC
R_{free} test set	6460 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	84.6	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	32777	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, BTI

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	0.56	0/16580	0.76	1/22444 (0.0%)
1	B	0.56	1/16738 (0.0%)	0.77	10/22654 (0.0%)
All	All	0.56	1/33318 (0.0%)	0.77	11/45098 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2187	LYS	C-O	6.45	1.35	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1419	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	1108	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	1084	ASP	CB-CG-OD1	6.32	123.98	118.30
1	B	1580	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	B	1638	LEU	CA-CB-CG	5.86	128.77	115.30
1	B	872	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	1108	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	B	1571	VAL	CB-CA-C	-5.63	100.69	111.40
1	B	1419	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	1843	VAL	CB-CA-C	-5.40	101.15	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1735	ILE	CB-CA-C	-5.06	101.48	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	768	THR	Peptide

5.2 Too-close contacts (i)

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	16249	0	16225	309	1
1	B	16402	0	16387	359	1
2	A	30	0	31	6	0
3	A	48	0	32	5	0
3	B	48	0	32	3	0
All	All	32777	0	32707	634	2

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 10.

All (634) 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:297:ARG:NH2	1:B:555:ASN:O	1.71	1.22
1:B:723:ILE:HA	1:B:745:ASN:HB3	1.37	1.05
1:B:466:ASP:O	1:B:466:ASP:OD1	1.82	0.98
1:A:1243:ARG:NH1	1:A:1283:TYR:O	2.00	0.93
1:A:1493:LEU:HD11	1:A:1507:TYR:CE1	2.03	0.93
1:B:710:LYS:O	1:B:731:ILE:HG23	1.73	0.89
1:B:868:ARG:O	1:B:872:ARG:HB2	1.75	0.86
1:A:297:ARG:NH2	1:A:555:ASN:O	2.09	0.86
1:A:723:ILE:HA	1:A:745:ASN:HB3	1.58	0.85
1:B:1135:LEU:HB3	1:B:1136:PRO:HD2	1.59	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:PHE:HA	1:B:557:ILE:HD11	1.58	0.85
1:A:853:ARG:NH2	1:B:123:THR:OG1	2.09	0.85
1:A:211:VAL:HG13	1:A:220:VAL:HG13	1.59	0.84
1:A:1657:TYR:CD2	1:A:1687:ARG:HG2	2.16	0.81
1:B:1189:ILE:O	1:B:1192:GLN:HG2	1.80	0.81
1:B:1730:CYS:HA	1:B:1752:GLN:OE1	1.80	0.80
1:B:1040:ARG:NH1	1:B:1081:VAL:O	2.15	0.80
1:A:1593:ILE:HD11	3:A:2303:COA:C4A	2.13	0.79
1:B:2044:MET:SD	1:B:2082:LEU:HD23	2.23	0.79
1:A:945:VAL:HG11	1:A:950:ILE:HD11	1.64	0.79
1:B:2082:LEU:HG	1:B:2086:TYR:CE2	2.18	0.79
1:A:220:VAL:HG21	1:A:355:LEU:HG	1.66	0.78
1:A:1735:ILE:HD13	1:A:1735:ILE:H	1.45	0.78
1:B:1344:THR:HG21	1:B:1393:PHE:HZ	1.49	0.78
1:B:1317:ASN:HB3	1:B:1371:ASN:HD21	1.50	0.77
1:A:324:ARG:O	1:A:325:HIS:HB2	1.83	0.76
1:B:1783:MET:HA	1:B:1786:ASN:HB2	1.68	0.76
1:A:1643:TRP:CE3	1:A:1649:PRO:HB2	2.21	0.75
1:A:1981:TYR:CD2	1:A:1985:ILE:HD11	2.22	0.75
1:A:211:VAL:CG1	1:A:220:VAL:HG13	2.16	0.75
1:A:1643:TRP:CZ3	1:B:2085:ILE:HG12	2.22	0.75
1:A:744:GLU:HB3	1:A:769:LEU:CD2	2.16	0.74
1:A:2085:ILE:HD11	1:B:1650:ASP:OD1	1.87	0.74
1:A:2163:VAL:HA	1:A:2170:GLN:NE2	2.02	0.74
1:B:387:GLU:O	1:B:390:THR:OG1	2.04	0.74
1:A:864:GLU:OE1	1:A:868:ARG:NH1	2.22	0.73
1:B:2163:VAL:HA	1:B:2170:GLN:OE1	1.88	0.73
1:A:585:ALA:HA	1:A:621:VAL:HG11	1.71	0.72
1:A:1643:TRP:HZ3	1:B:2085:ILE:HG12	1.52	0.72
1:B:1422:SER:HB3	1:B:1445:ASN:OD1	1.91	0.71
1:B:1593:ILE:HD11	3:B:2301:COA:C4A	2.20	0.71
1:B:556:THR:C	1:B:557:ILE:HG13	2.11	0.71
1:A:1441:ARG:HG3	1:A:1469:PHE:HE1	1.55	0.71
1:A:2004:ASP:OD2	1:A:2006:THR:HG22	1.91	0.71
1:B:537:ARG:NH2	1:B:679:GLU:OE2	2.23	0.71
1:B:365:GLU:OE2	1:B:381:ASN:OD1	2.08	0.70
1:B:557:ILE:HG23	1:B:561:TRP:CG	2.26	0.70
1:A:1981:TYR:CG	1:A:1985:ILE:HD11	2.26	0.70
1:B:1841:TYR:CE1	1:B:1846:MET:HE2	2.27	0.70
1:B:2031:VAL:HG21	1:B:2091:LEU:HD23	1.72	0.70
1:A:744:GLU:HB3	1:A:769:LEU:HD21	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:HD23	1:B:169:LYS:HD2	1.75	0.69
1:B:1222:ALA:O	1:B:1261:ILE:HA	1.92	0.69
1:A:517:GLN:OE1	1:A:520:ARG:NH2	2.26	0.69
1:B:587:THR:HG22	1:B:663:LEU:HD12	1.74	0.69
1:B:1647:ALA:O	1:B:1649:PRO:HD3	1.94	0.68
1:A:711:LEU:HB2	1:A:758:ILE:HD11	1.76	0.68
1:B:1243:ARG:NH1	1:B:1283:TYR:O	2.26	0.68
1:A:630:TYR:CE1	1:A:781:PHE:CE1	2.83	0.67
1:A:1841:TYR:CE1	1:A:1846:MET:CE	2.78	0.67
1:B:2044:MET:CG	1:B:2082:LEU:HD23	2.25	0.67
1:B:2128:ARG:NE	1:B:2132:GLU:OE1	2.21	0.67
1:B:124:ASN:HA	1:B:127:ASN:OD1	1.95	0.67
1:A:1678:GLU:O	1:A:1689:VAL:HG12	1.94	0.66
1:A:579:LEU:HD11	1:A:672:HIS:CD2	2.31	0.66
1:B:1909:ASN:C	1:B:1909:ASN:HD22	1.97	0.66
1:B:156:ASN:OD1	1:B:158:LEU:N	2.28	0.66
1:A:541:GLU:OE1	1:A:691:THR:OG1	2.13	0.66
1:A:723:ILE:N	1:A:726:GLN:OE1	2.30	0.65
1:B:318:ASP:OD1	1:B:320:SER:OG	2.14	0.65
1:B:1223:ASN:HB3	1:B:1262:THR:HB	1.79	0.65
1:B:2082:LEU:HG	1:B:2086:TYR:HE2	1.62	0.65
1:A:108:GLU:O	1:A:112:MET:HG3	1.97	0.65
1:B:545:LYS:HG3	1:B:572:ALA:O	1.98	0.64
1:A:1641:VAL:HG21	1:B:2089:ILE:HD13	1.80	0.64
1:A:1197:ILE:HD12	1:A:1256:ALA:HB1	1.80	0.64
1:A:1643:TRP:HZ3	1:B:2085:ILE:CG1	2.11	0.64
1:A:657:GLN:HA	1:A:663:LEU:HD23	1.81	0.63
1:B:1135:LEU:HB3	1:B:1136:PRO:CD	2.29	0.63
1:B:1719:TYR:CE2	1:B:1744:GLN:HG3	2.33	0.63
1:B:822:MET:SD	1:B:981:LEU:HA	2.37	0.63
1:B:1841:TYR:CE1	1:B:1846:MET:CE	2.81	0.63
1:A:1593:ILE:HD11	3:A:2303:COA:C5A	2.28	0.63
1:A:1643:TRP:CZ3	1:B:2085:ILE:CG1	2.82	0.63
1:B:657:GLN:HA	1:B:663:LEU:HD23	1.81	0.63
1:B:716:VAL:HG23	1:B:728:TYR:HA	1.81	0.62
1:B:1991:PRO:HG3	1:B:2115:TRP:HB2	1.81	0.62
1:A:318:ASP:OD1	1:A:320:SER:OG	2.18	0.62
1:A:69:ILE:HG23	1:A:489:TYR:CE1	2.35	0.62
1:A:1005:THR:HB	1:A:1006:PRO:HD3	1.82	0.62
1:A:1493:LEU:HD11	1:A:1507:TYR:CZ	2.35	0.62
1:B:2040:LEU:O	1:B:2043:THR:HG22	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1643:TRP:CE3	1:B:1649:PRO:HB3	2.35	0.62
2:A:2301:BTI:C3	1:B:1998:GLY:HA3	2.29	0.62
1:A:725:GLY:HA2	1:A:741:VAL:HG13	1.82	0.62
1:A:1652:GLY:HA2	1:B:2085:ILE:HD13	1.81	0.62
1:A:587:THR:HG22	1:A:663:LEU:HD12	1.81	0.61
1:A:300:GLU:OE2	1:A:327:LYS:NZ	2.32	0.61
1:A:1338:THR:HG21	1:A:1368:ILE:HG23	1.82	0.61
1:A:646:ILE:HG21	1:A:785:LEU:HG	1.81	0.61
1:B:2078:ARG:HA	1:B:2081:GLU:OE1	2.01	0.61
1:A:334:VAL:HG21	1:A:342:PHE:CE1	2.36	0.61
1:A:751:LEU:CD1	1:A:766:ILE:HG13	2.31	0.61
1:B:711:LEU:HB2	1:B:758:ILE:HD11	1.81	0.61
1:A:735:LYS:HG2	1:B:1954:ARG:NH1	2.15	0.60
1:B:1444:ILE:HG23	1:B:1454:THR:HG22	1.83	0.60
1:A:453:HIS:CD2	1:A:516:ARG:HA	2.37	0.60
1:A:1655:TYR:CD1	1:A:1689:VAL:HG23	2.36	0.60
1:A:2093:PHE:O	1:A:2097:HIS:CD2	2.54	0.60
1:A:1841:TYR:CE1	1:A:1846:MET:HE3	2.35	0.60
1:B:316:GLY:O	1:B:333:PRO:HA	2.01	0.60
1:A:955:ARG:HG3	1:A:962:LEU:HD21	1.84	0.60
1:A:2178:ASN:HB3	1:A:2181:THR:CG2	2.30	0.60
1:B:1194:LEU:HD12	1:B:1252:GLU:HB3	1.83	0.60
1:B:1344:THR:HG21	1:B:1393:PHE:CZ	2.35	0.60
1:B:1078:SER:O	1:B:1108:ARG:NH2	2.35	0.60
1:B:35:LEU:HG	1:B:168:ARG:O	2.02	0.59
1:A:1192:GLN:HG3	1:A:1193:SER:N	2.16	0.59
1:A:736:MET:HE1	1:B:1918:GLN:HB3	1.84	0.59
1:A:1643:TRP:CZ2	1:B:2089:ILE:HD11	2.37	0.59
1:A:744:GLU:CB	1:A:769:LEU:HD21	2.32	0.59
1:A:1694:ILE:HA	1:B:2102:ARG:HD3	1.84	0.59
1:B:1272:TYR:CE1	1:B:1318:ARG:HD2	2.37	0.59
1:A:945:VAL:CG1	1:A:950:ILE:HD11	2.33	0.59
1:A:330:GLU:OE2	1:A:387:GLU:HB3	2.03	0.58
1:A:2093:PHE:O	1:A:2097:HIS:HD2	1.86	0.58
1:B:654:ILE:HD12	1:B:792:VAL:CG2	2.33	0.58
1:A:1716:SER:OG	1:B:1976:ASP:OD2	2.20	0.58
1:B:295:ARG:HB3	1:B:558:THR:HG21	1.84	0.58
1:A:1593:ILE:CD1	3:A:2303:COA:C4A	2.81	0.58
1:B:1927:ASN:OD1	1:B:1928:SER:N	2.37	0.58
1:A:1808:SER:O	1:A:1883:ARG:NH2	2.36	0.57
1:B:584:GLY:HA2	1:B:685:LEU:HD11	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1751:GLY:HA2	1:B:1775:LEU:HD21	1.86	0.57
1:A:1735:ILE:HD13	1:A:1735:ILE:N	2.17	0.57
1:A:1378:SER:HB3	1:A:1379:ASN:OD1	2.04	0.57
1:A:1691:LYS:HA	1:A:1691:LYS:HE2	1.86	0.57
1:A:594:GLU:OE2	1:A:597:ARG:NH2	2.38	0.57
1:A:1564:MET:CE	1:A:1585:VAL:HG12	2.35	0.57
1:B:1643:TRP:CZ3	1:B:1649:PRO:HB3	2.39	0.57
1:B:1084:ASP:OD2	1:B:1318:ARG:HD3	2.05	0.56
1:A:106:ASN:HB2	1:B:659:SER:HB3	1.87	0.56
1:B:701:THR:O	1:B:766:ILE:HG23	2.05	0.56
1:B:744:GLU:HG3	1:B:769:LEU:CD2	2.35	0.56
1:B:556:THR:O	1:B:557:ILE:HG13	2.05	0.56
1:B:117:ILE:HD13	1:B:137:ILE:HG23	1.88	0.56
1:B:537:ARG:HD2	1:B:537:ARG:N	2.20	0.56
1:B:665:ILE:HD12	1:B:674:ILE:CD1	2.36	0.56
1:B:1050:SER:O	1:B:1071:ILE:HD13	2.06	0.56
1:A:665:ILE:HG13	1:A:674:ILE:HD12	1.88	0.56
1:A:704:ARG:HA	1:A:762:ASP:O	2.05	0.56
1:A:734:MET:HA	1:A:1766:LEU:HB3	1.87	0.55
1:A:124:ASN:OD1	1:A:129:ALA:HB2	2.07	0.55
1:A:1652:GLY:HA2	1:B:2085:ILE:CD1	2.35	0.55
1:A:708:PRO:O	1:A:733:VAL:HG22	2.07	0.55
1:A:734:MET:O	1:A:735:LYS:HB2	2.07	0.55
1:A:1441:ARG:HG3	1:A:1469:PHE:CE1	2.39	0.55
1:A:185:ASP:OD2	1:A:227:TYR:OH	2.25	0.55
1:A:646:ILE:CG2	1:A:785:LEU:HG	2.36	0.55
1:A:1641:VAL:CG1	1:A:1653:PHE:HB2	2.36	0.55
1:B:1176:ILE:HD11	1:B:1196:VAL:HB	1.89	0.55
1:A:106:ASN:OD1	1:A:111:ARG:NH1	2.39	0.55
1:A:1753:PRO:HB3	1:A:1775:LEU:HD23	1.88	0.55
1:B:1994:GLU:HA	1:B:2021:ARG:O	2.07	0.55
1:A:1348:ARG:HG3	1:A:1350:ASP:OD1	2.08	0.54
1:B:1451:VAL:HG22	1:B:1517:GLN:CG	2.37	0.54
1:B:1272:TYR:CD1	1:B:1318:ARG:HD2	2.42	0.54
1:B:1651:LYS:HE3	1:B:1651:LYS:HA	1.89	0.54
1:A:306:ASP:HA	1:A:406:ILE:HG23	1.88	0.54
1:A:751:LEU:HD11	1:A:766:ILE:HG13	1.89	0.54
1:A:2088:GLN:O	1:A:2089:ILE:C	2.46	0.54
1:B:32:PHE:CZ	1:B:359:VAL:HG21	2.43	0.54
1:A:73:LYS:HE3	1:A:389:PRO:HG3	1.88	0.54
1:A:583:CYS:SG	1:A:674:ILE:HD11	2.48	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:941:ASN:HD21	1:B:1013:LEU:HA	1.73	0.54
1:A:56:HIS:CD2	1:A:409:GLY:HA3	2.42	0.54
1:B:72:VAL:HA	1:B:112:MET:HE1	1.89	0.54
1:B:630:TYR:CE1	1:B:781:PHE:CD1	2.96	0.54
1:A:1641:VAL:HG12	1:A:1653:PHE:HB2	1.90	0.54
1:B:156:ASN:OD1	1:B:156:ASN:C	2.45	0.53
1:B:1119:ARG:HB3	1:B:1121:HIS:CE1	2.42	0.53
1:B:297:ARG:HH22	1:B:555:ASN:C	2.12	0.53
1:A:1180:VAL:HG22	1:A:1189:ILE:CD1	2.38	0.53
1:A:1706:ARG:NH1	1:B:2006:THR:CG2	2.71	0.53
1:A:646:ILE:HG23	1:A:647:ASN:H	1.74	0.53
1:A:1517:GLN:O	1:A:1521:SER:HB2	2.08	0.53
1:B:372:ASP:OD1	1:B:372:ASP:N	2.39	0.53
1:B:1735:ILE:HD12	1:B:1735:ILE:N	2.23	0.53
1:B:1580:ARG:NH2	1:B:1810:VAL:O	2.41	0.53
1:B:1841:TYR:HE1	1:B:1846:MET:HE3	1.74	0.53
1:B:177:GLY:O	1:B:181:ARG:HG3	2.09	0.53
1:B:297:ARG:NH2	1:B:555:ASN:C	2.58	0.53
1:B:1783:MET:CA	1:B:1786:ASN:HB2	2.38	0.52
1:A:1128:ILE:HG21	1:A:1196:VAL:HG21	1.90	0.52
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.07	0.52
1:A:1767:GLY:O	1:A:1768:ARG:HG3	2.07	0.52
1:B:196:ALA:HB2	1:B:355:LEU:HD22	1.91	0.52
1:B:63:LEU:HB2	1:B:143:VAL:HG11	1.92	0.52
1:A:76:ARG:HD3	1:B:529:GLU:OE2	2.10	0.52
1:B:453:HIS:CD2	1:B:516:ARG:HA	2.44	0.52
1:A:545:LYS:HD2	1:A:572:ALA:O	2.09	0.52
1:A:1354:GLN:HG3	1:A:1403:ALA:HB2	1.92	0.52
1:B:101:GLU:HB3	1:B:499:HIS:CD2	2.44	0.52
1:B:1451:VAL:HG22	1:B:1517:GLN:HG3	1.92	0.52
1:A:333:PRO:HG3	1:A:450:PRO:HB3	1.92	0.52
1:A:1223:ASN:HB3	1:A:1262:THR:HB	1.91	0.52
1:B:1748:GLN:NE2	1:B:1789:SER:OG	2.43	0.52
1:A:828:GLN:O	1:A:832:VAL:HG23	2.10	0.52
1:A:1176:ILE:CD1	1:A:1197:ILE:HG13	2.40	0.52
1:B:1044:ILE:HD13	1:B:1075:LEU:CD2	2.39	0.52
1:A:1176:ILE:HD12	1:A:1197:ILE:HG13	1.92	0.52
1:A:1958:GLY:H	2:A:2302:BTI:HN3	1.58	0.51
1:B:334:VAL:HG21	1:B:342:PHE:CE1	2.45	0.51
1:B:579:LEU:CD1	1:B:667:ILE:HD12	2.40	0.51
1:B:1619:ILE:HG13	1:B:1725:ILE:CG2	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2033:ILE:HG22	1:B:2034:LYS:CD	2.41	0.51
1:A:2178:ASN:HB3	1:A:2181:THR:HG22	1.92	0.51
1:A:1655:TYR:OH	1:A:1682:ILE:HD11	2.10	0.51
1:B:69:ILE:HG23	1:B:489:TYR:CE1	2.45	0.51
1:B:1369:LEU:HD21	1:B:1415:LEU:HD23	1.93	0.51
1:B:1841:TYR:HE1	1:B:1846:MET:CE	2.22	0.51
1:A:108:GLU:HG2	1:A:111:ARG:NH2	2.25	0.51
1:A:1176:ILE:HD12	1:A:1197:ILE:CG1	2.41	0.51
1:A:1533:THR:OG1	1:A:1535:ASP:OD2	2.28	0.51
1:A:1642:ALA:HB3	1:A:1654:GLN:HB3	1.92	0.51
1:B:990:GLN:HG3	1:B:991:PRO:CD	2.40	0.51
1:B:1633:GLU:HA	1:B:1636:VAL:HG23	1.92	0.51
1:A:1180:VAL:HG13	1:A:1185:ASP:HB2	1.92	0.51
1:A:1757:THR:OG1	2:A:2301:BTI:H4	2.11	0.51
1:A:1103:GLN:O	1:A:1107:ARG:HG2	2.11	0.51
1:A:1301:GLU:OE2	1:A:1441:ARG:NH2	2.44	0.51
1:B:646:ILE:HG23	1:B:647:ASN:N	2.25	0.51
1:A:311:ASN:N	1:A:311:ASN:HD22	2.09	0.51
1:A:1443:LEU:HD12	1:A:1443:LEU:N	2.25	0.51
1:B:744:GLU:CG	1:B:769:LEU:CD2	2.89	0.51
1:B:1735:ILE:HD12	1:B:1735:ILE:H	1.76	0.51
1:B:1344:THR:HB	1:B:1356:TYR:OH	2.11	0.51
1:A:1315:THR:O	1:A:1317:ASN:N	2.44	0.50
1:B:56:HIS:CD2	1:B:409:GLY:HA3	2.46	0.50
1:B:865:LEU:HD12	1:B:868:ARG:NH2	2.26	0.50
1:B:1317:ASN:C	1:B:1317:ASN:OD1	2.48	0.50
1:A:214:ASP:O	1:A:218:GLY:N	2.41	0.50
1:B:1580:ARG:HG3	1:B:1580:ARG:HH11	1.76	0.50
1:A:1682:ILE:O	1:A:1685:GLU:HG2	2.10	0.50
1:A:2004:ASP:OD2	1:A:2006:THR:CG2	2.59	0.50
1:B:306:ASP:HA	1:B:406:ILE:HG23	1.92	0.50
1:B:388:HIS:N	1:B:389:PRO:CD	2.74	0.50
1:A:389:PRO:HA	1:A:392:GLU:HB2	1.93	0.50
1:B:927:VAL:HG13	1:B:1006:PRO:HG3	1.93	0.50
1:B:1097:VAL:O	1:B:1098:THR:C	2.50	0.50
1:B:323:ARG:O	1:B:323:ARG:HG3	2.12	0.50
1:B:1350:ASP:N	1:B:1350:ASP:OD1	2.45	0.50
1:A:565:LEU:HD13	1:A:570:MET:HE3	1.93	0.50
1:A:1636:VAL:N	1:A:1637:PRO:CD	2.74	0.50
1:B:1044:ILE:HD13	1:B:1075:LEU:HD21	1.93	0.50
1:A:300:GLU:HG2	1:A:365:GLU:HG2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1763:ASN:ND2	1:A:1770:VAL:H	2.10	0.50
1:A:2041:LEU:HD13	1:A:2051:TYR:OH	2.12	0.50
1:A:2046:ARG:NH1	1:B:1637:PRO:HA	2.26	0.50
1:B:541:GLU:HG2	1:B:572:ALA:CB	2.41	0.50
1:B:666:ALA:O	1:B:791:PRO:HB3	2.12	0.50
1:B:1883:ARG:HA	1:B:1887:ILE:O	2.12	0.50
1:A:723:ILE:HG22	1:A:724:LYS:N	2.27	0.50
1:A:1631:MET:HE1	1:B:2035:PHE:HD2	1.76	0.50
1:B:1406:GLY:HA2	1:B:1409:GLU:CG	2.42	0.49
1:A:1827:TRP:CE3	1:A:1828:ASP:HA	2.47	0.49
1:B:1783:MET:HA	1:B:1786:ASN:CB	2.40	0.49
1:A:716:VAL:HG11	1:A:722:ILE:HD11	1.94	0.49
1:A:1493:LEU:HD11	1:A:1507:TYR:HE1	1.68	0.49
1:B:1192:GLN:HG3	1:B:1193:SER:N	2.26	0.49
1:B:1471:SER:HB2	1:B:1479:HIS:HD2	1.77	0.49
1:B:1594:GLY:HA3	1:B:1624:ASN:HA	1.94	0.49
1:A:770:ASP:C	1:A:772:PRO:HD3	2.33	0.49
1:B:105:ALA:HB1	1:B:497:ASN:O	2.12	0.49
1:B:557:ILE:CG2	1:B:561:TRP:CG	2.94	0.49
1:B:626:GLU:O	1:B:628:LYS:N	2.44	0.49
1:B:723:ILE:HA	1:B:745:ASN:CB	2.26	0.49
1:B:1180:VAL:HG13	1:B:1185:ASP:HB2	1.93	0.49
1:A:701:THR:O	1:A:766:ILE:HG23	2.13	0.49
1:B:1305:LEU:HB3	1:B:1310:ILE:HD11	1.95	0.49
1:A:1457:TYR:OH	1:A:1476:GLY:HA3	2.12	0.49
1:B:751:LEU:HD13	1:B:766:ILE:HG13	1.95	0.49
1:B:1479:HIS:ND1	1:B:1480:LEU:HG	2.28	0.49
1:B:2030:MET:O	1:B:2033:ILE:N	2.42	0.49
1:A:485:ASN:OD1	1:A:522:HIS:CD2	2.66	0.49
1:A:1701:GLY:HA2	1:B:2024:VAL:HG23	1.93	0.49
1:B:1906:ASP:OD2	1:B:1908:ALA:HB3	2.13	0.49
1:B:579:LEU:HD12	1:B:667:ILE:HD12	1.95	0.49
1:B:828:GLN:O	1:B:832:VAL:HG23	2.12	0.49
1:B:1426:ARG:C	1:B:1427:ILE:HG13	2.33	0.49
1:A:118:GLU:OE1	1:B:656:ARG:NH2	2.46	0.49
1:A:296:ALA:HB3	1:A:367:LEU:HD11	1.94	0.49
1:A:2087:GLY:O	1:A:2090:SER:OG	2.26	0.49
1:B:904:VAL:O	1:B:905:GLU:C	2.51	0.49
1:B:1278:PHE:CE1	1:B:1285:GLU:HB2	2.48	0.49
1:A:933:TYR:OH	1:A:979:ASN:ND2	2.45	0.48
2:A:2301:BTI:O3	1:B:1998:GLY:HA3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:VAL:HG22	1:B:380:LEU:HD12	1.95	0.48
1:B:682:ALA:HB1	1:B:694:LEU:O	2.12	0.48
1:A:1852:THR:HG22	1:A:1853:GLU:N	2.29	0.48
1:A:2047:LEU:HD13	1:B:1641:VAL:HG23	1.94	0.48
3:A:2303:COA:HO1	3:A:2303:COA:C8A	2.26	0.48
1:B:1679:ARG:NH1	1:B:1686:GLU:OE1	2.45	0.48
1:A:296:ALA:HB1	1:A:368:TYR:O	2.13	0.48
1:B:185:ASP:OD1	1:B:188:SER:HB3	2.13	0.48
1:B:537:ARG:HD2	1:B:537:ARG:H	1.78	0.48
1:B:940:PHE:HA	1:B:950:ILE:HD13	1.95	0.48
1:B:2026:GLU:O	1:B:2027:PRO:C	2.50	0.48
1:B:2031:VAL:HG22	1:B:2090:SER:HB2	1.95	0.48
1:A:630:TYR:CE1	1:A:781:PHE:CD1	3.01	0.48
1:B:498:ILE:HD12	1:B:536:PHE:CE2	2.48	0.48
1:A:990:GLN:HG3	1:A:991:PRO:CD	2.44	0.48
1:A:1569:ILE:HG22	1:A:1571:VAL:CG2	2.43	0.48
1:B:1418:LEU:O	1:B:1419:ARG:HB2	2.12	0.48
1:B:1530:VAL:HG23	1:B:1530:VAL:O	2.13	0.48
1:A:90:ARG:O	1:A:91:THR:C	2.51	0.48
1:B:66:ASN:HD22	1:B:67:ASN:H	1.61	0.48
1:B:744:GLU:CG	1:B:769:LEU:HD22	2.42	0.48
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	1.96	0.48
1:A:411:PRO:HG2	1:A:414:ARG:HG2	1.95	0.48
1:B:224:ASP:O	1:B:228:GLN:HG2	2.14	0.48
1:B:405:GLN:O	1:B:408:MET:N	2.37	0.48
1:B:1841:TYR:CZ	1:B:1846:MET:HE2	2.49	0.48
1:A:1103:GLN:O	1:A:1107:ARG:CG	2.61	0.48
1:A:1182:HIS:CD2	1:A:1184:ASP:H	2.32	0.48
1:A:665:ILE:HG22	1:A:667:ILE:HG13	1.96	0.48
1:B:36:ASN:HB3	1:B:41:LEU:HD22	1.96	0.48
1:B:261:GLY:O	1:B:278:ALA:HB1	2.14	0.48
1:B:334:VAL:HG12	1:B:335:THR:N	2.29	0.48
1:B:545:LYS:CG	1:B:572:ALA:O	2.61	0.48
1:A:711:LEU:HD22	1:A:764:MET:CE	2.43	0.47
1:A:2033:ILE:HG22	1:A:2034:LYS:CD	2.42	0.47
1:B:1741:ARG:O	1:B:1741:ARG:HD3	2.14	0.47
1:B:594:GLU:OE1	1:B:597:ARG:NH2	2.47	0.47
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.61	0.47
1:B:1827:TRP:CE3	1:B:1828:ASP:HA	2.49	0.47
1:B:2044:MET:HG3	1:B:2082:LEU:HD23	1.96	0.47
1:B:1612:ARG:O	1:B:1814:ARG:NH2	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ARG:CZ	1:B:123:THR:OG1	2.63	0.47
1:A:970:LEU:O	1:A:973:SER:OG	2.24	0.47
1:A:1659:THR:O	1:A:1662:GLY:N	2.48	0.47
1:B:809:LEU:O	1:B:810:GLU:C	2.51	0.47
1:B:1239:LEU:O	1:B:1243:ARG:HG2	2.14	0.47
1:A:186:LYS:HD3	1:A:288:PHE:HZ	1.78	0.47
1:A:751:LEU:HD13	1:A:766:ILE:HG13	1.96	0.47
1:A:753:GLN:O	1:A:756:SER:OG	2.31	0.47
1:B:941:ASN:ND2	1:B:1013:LEU:HA	2.29	0.47
1:A:486:VAL:HG11	1:A:526:ALA:CB	2.45	0.47
1:A:1173:ARG:HH21	1:A:1259:ARG:NH1	2.13	0.47
1:A:1344:THR:HG21	1:A:1393:PHE:HZ	1.79	0.47
1:B:29:PRO:HD2	1:B:32:PHE:CD2	2.49	0.47
1:B:485:ASN:HB2	1:B:522:HIS:HD2	1.79	0.47
1:B:649:SER:HB3	1:B:784:MET:HB3	1.97	0.47
1:B:744:GLU:HG3	1:B:769:LEU:HD22	1.95	0.47
1:B:1377:THR:O	1:B:1380:SER:OG	2.27	0.47
1:B:1616:ILE:HD12	1:B:1813:LYS:HB3	1.96	0.47
1:B:2108:VAL:HG23	1:B:2109:ILE:HG23	1.97	0.47
1:A:743:GLN:HA	1:A:743:GLN:HE21	1.80	0.47
1:A:1786:ASN:HB3	1:A:1788:VAL:HG23	1.97	0.47
1:B:990:GLN:HG3	1:B:991:PRO:HD3	1.96	0.47
1:B:1827:TRP:O	1:B:1829:ARG:N	2.43	0.47
1:A:1708:SER:HB3	1:A:1735:ILE:HD12	1.97	0.47
1:A:1709:GLY:O	1:A:1710:LEU:C	2.53	0.47
1:A:1516:ARG:HG3	1:A:1537:PHE:CD1	2.50	0.46
1:A:1918:GLN:O	1:A:1920:PRO:HD3	2.14	0.46
1:A:2033:ILE:HG22	1:A:2034:LYS:HD3	1.96	0.46
1:A:433:ASP:H	1:A:445:GLN:HE22	1.62	0.46
1:A:480:PHE:HD1	1:A:530:LEU:HD13	1.79	0.46
1:A:1758:GLY:O	1:A:1759:ALA:C	2.53	0.46
1:B:1189:ILE:HG22	1:B:1193:SER:OG	2.16	0.46
1:A:69:ILE:CG2	1:A:489:TYR:CE1	2.98	0.46
1:A:412:MET:HA	1:A:415:ILE:HD12	1.96	0.46
1:A:1682:ILE:HG22	1:A:1683:ASN:ND2	2.30	0.46
1:A:1730:CYS:O	1:A:1752:GLN:NE2	2.48	0.46
1:B:845:LEU:O	1:B:848:SER:HB2	2.16	0.46
1:A:716:VAL:HG12	1:A:717:GLU:N	2.30	0.46
1:A:1496:LYS:O	1:A:1499:LYS:HB3	2.16	0.46
1:B:385:GLN:HB3	1:B:387:GLU:OE1	2.15	0.46
1:B:530:LEU:HD21	1:B:532:ILE:HD12	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:ILE:HG22	1:B:649:SER:OG	2.15	0.46
1:B:905:GLU:HB3	1:B:906:PRO:HD3	1.97	0.46
1:B:1286:ASN:C	1:B:1286:ASN:OD1	2.54	0.46
1:A:376:TYR:CD2	1:A:376:TYR:N	2.83	0.46
1:A:1829:ARG:CZ	1:A:2119:ARG:HE	2.28	0.46
1:A:1862:ASP:OD1	1:A:1885:GLY:N	2.42	0.46
1:B:172:PHE:HE2	1:B:175:PRO:HD2	1.79	0.46
1:B:955:ARG:NH1	1:B:1914:GLU:OE1	2.48	0.46
1:B:1189:ILE:O	1:B:1190:LEU:C	2.54	0.46
1:B:1735:ILE:O	1:B:1739:LEU:N	2.36	0.46
1:A:1253:LEU:HD23	1:A:1258:ILE:HD12	1.98	0.46
1:A:1594:GLY:O	1:A:1624:ASN:HA	2.14	0.46
1:A:1643:TRP:CH2	1:B:2085:ILE:HG13	2.50	0.46
1:B:868:ARG:HB3	1:B:872:ARG:HH21	1.81	0.46
1:B:1422:SER:CB	1:B:1445:ASN:OD1	2.62	0.46
1:B:1657:TYR:CE2	1:B:1687:ARG:HG2	2.51	0.46
1:A:759:VAL:O	1:A:762:ASP:HB2	2.16	0.46
1:A:1592:LYS:O	1:A:1593:ILE:CG1	2.64	0.46
1:A:2024:VAL:HG22	1:B:1705:LEU:HD13	1.97	0.46
1:B:2035:PHE:HE1	1:B:2043:THR:HG21	1.80	0.46
1:B:1783:MET:HE3	1:B:1788:VAL:HG11	1.98	0.46
1:A:1643:TRP:CH2	1:B:2089:ILE:HD11	2.50	0.45
1:A:1843:VAL:CG2	1:A:1895:GLU:HA	2.46	0.45
1:B:2031:VAL:HG13	1:B:2090:SER:HB2	1.98	0.45
1:A:714:PHE:CD2	1:A:750:LEU:HD13	2.50	0.45
1:B:72:VAL:O	1:B:75:ILE:N	2.49	0.45
1:B:317:ARG:HG2	1:B:332:ALA:HB2	1.99	0.45
1:B:1194:LEU:CD1	1:B:1252:GLU:HB3	2.46	0.45
1:B:1909:ASN:C	1:B:1909:ASN:ND2	2.64	0.45
1:A:334:VAL:HG21	1:A:342:PHE:HE1	1.81	0.45
1:A:1644:ASN:OD1	1:A:1652:GLY:O	2.35	0.45
1:B:623:PHE:CD1	1:B:694:LEU:HD22	2.52	0.45
1:B:1260:ARG:HA	1:B:1278:PHE:O	2.16	0.45
1:B:1809:TYR:O	1:B:1945:LEU:HD11	2.16	0.45
1:B:2033:ILE:HG22	1:B:2034:LYS:HD3	1.98	0.45
1:A:1173:ARG:NH2	1:A:1259:ARG:HD2	2.31	0.45
1:A:1635:ILE:HG22	1:A:1635:ILE:O	2.16	0.45
1:B:1981:TYR:CD2	1:B:1985:ILE:HD11	2.52	0.45
1:A:711:LEU:HA	1:A:731:ILE:HG22	1.99	0.45
1:B:214:ASP:OD1	1:B:214:ASP:C	2.55	0.45
1:B:1220:ASN:O	1:B:1258:ILE:HA	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1959:GLY:O	1:B:1960:GLN:C	2.55	0.45
1:A:532:ILE:O	1:A:532:ILE:HG22	2.16	0.45
1:A:819:GLN:O	1:A:820:VAL:C	2.54	0.45
1:A:1305:LEU:HB3	1:A:1310:ILE:HD11	1.99	0.45
1:A:1964:PHE:O	1:B:1786:ASN:ND2	2.50	0.45
1:B:460:THR:HA	1:B:504:SER:O	2.17	0.45
1:B:575:PRO:HG2	1:B:580:ALA:HB2	1.98	0.45
1:B:1581:GLN:HB2	1:B:1616:ILE:HD11	1.98	0.45
1:A:520:ARG:HD2	1:A:547:LEU:O	2.16	0.45
1:A:2173:THR:O	1:A:2174:TRP:C	2.54	0.45
1:B:541:GLU:OE2	1:B:690:MET:HA	2.16	0.45
1:B:704:ARG:HA	1:B:762:ASP:O	2.16	0.45
1:B:1180:VAL:CG1	1:B:1185:ASP:HB2	2.47	0.45
1:B:2053:GLU:O	1:B:2057:GLN:HG3	2.17	0.45
1:A:1489:VAL:HG12	1:A:1490:LYS:H	1.81	0.45
1:A:1516:ARG:HG3	1:A:1537:PHE:CG	2.52	0.45
1:A:1685:GLU:HG3	1:A:1685:GLU:O	2.15	0.45
1:B:366:TYR:O	1:B:378:LEU:CD1	2.65	0.45
1:B:1655:TYR:CE1	1:B:1689:VAL:HG22	2.52	0.45
1:B:1783:MET:CE	1:B:1788:VAL:HG11	2.47	0.45
1:A:1097:VAL:O	1:A:1100:ALA:N	2.50	0.45
1:A:1736:GLY:O	1:A:1740:VAL:HG23	2.17	0.45
1:B:2034:LYS:O	1:B:2039:LYS:HD2	2.16	0.45
1:A:575:PRO:HG2	1:A:580:ALA:HB2	1.99	0.44
1:B:67:ASN:ND2	1:B:128:TYR:CE2	2.80	0.44
1:A:2159:TYR:CE1	1:A:2171:VAL:HG13	2.52	0.44
2:A:2301:BTI:N3	1:B:1998:GLY:CA	2.80	0.44
1:B:131:VAL:HG13	1:B:159:LEU:HA	2.00	0.44
1:B:205:GLY:O	1:B:208:VAL:HG23	2.17	0.44
1:B:646:ILE:HG23	1:B:647:ASN:H	1.81	0.44
1:B:1682:ILE:HG22	1:B:1683:ASN:N	2.32	0.44
1:B:1754:ILE:O	1:B:1778:GLY:HA3	2.17	0.44
1:A:638:GLY:O	1:A:639:ASN:C	2.55	0.44
1:B:55:GLY:HA2	1:B:409:GLY:O	2.16	0.44
1:B:2183:ASP:HA	1:B:2186:LEU:HD12	1.99	0.44
1:A:129:ALA:HA	1:A:153:ALA:HB2	1.98	0.44
1:A:644:LEU:HD21	1:A:653:ILE:HD12	1.99	0.44
1:A:42:GLU:HG2	1:A:43:GLU:N	2.31	0.44
1:B:296:ALA:O	1:B:559:THR:HG23	2.18	0.44
1:B:1493:LEU:HD21	1:B:1558:GLY:HA3	2.00	0.44
1:B:1707:GLY:O	1:B:1710:LEU:HB3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:947:GLU:O	1:B:948:GLU:C	2.55	0.44
1:B:1738:TYR:O	1:B:1742:LEU:HD22	2.17	0.44
1:A:698:ASN:O	1:A:700:PRO:HD3	2.18	0.44
1:A:1883:ARG:HA	1:A:1887:ILE:O	2.18	0.44
2:A:2302:BTI:H5	1:B:1762:ILE:HD13	1.99	0.44
1:B:1175:GLY:HA2	1:B:1221:VAL:O	2.17	0.44
1:B:1708:SER:O	1:B:1709:GLY:C	2.56	0.44
1:B:2037:ARG:O	1:B:2041:LEU:HG	2.18	0.44
1:A:722:ILE:HG13	1:A:748:VAL:HG21	2.00	0.44
1:A:793:ILE:HD13	1:B:117:ILE:HG12	2.00	0.44
1:A:848:SER:OG	1:B:132:ASP:HB2	2.18	0.43
1:A:1706:ARG:HE	1:B:2108:VAL:HA	1.82	0.43
1:A:1771:TYR:HD2	1:A:1776:GLN:OE1	2.01	0.43
1:B:42:GLU:HG2	1:B:43:GLU:N	2.33	0.43
1:B:711:LEU:HB2	1:B:758:ILE:CD1	2.48	0.43
1:B:809:LEU:HD12	1:B:929:PHE:CE2	2.53	0.43
1:B:1493:LEU:HD11	1:B:1557:PRO:HB2	2.00	0.43
1:A:457:CYS:HB3	1:A:543:LEU:HD13	1.99	0.43
1:A:729:ALA:O	1:A:740:LEU:HB2	2.18	0.43
1:A:1707:GLY:O	1:A:1710:LEU:HB3	2.18	0.43
1:B:73:LYS:HE3	1:B:389:PRO:HG3	1.99	0.43
1:B:377:PHE:CZ	1:B:379:GLU:HA	2.52	0.43
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.83	0.43
1:A:565:LEU:HD22	1:A:570:MET:CE	2.48	0.43
1:A:1236:GLU:O	1:A:1240:VAL:HG23	2.18	0.43
1:B:1369:LEU:HD21	1:B:1415:LEU:CD2	2.48	0.43
1:B:2078:ARG:HG3	1:B:2082:LEU:HD13	2.00	0.43
1:A:744:GLU:HB3	1:A:769:LEU:HD23	2.00	0.43
1:A:830:ILE:HG22	1:A:834:ARG:HD2	1.99	0.43
1:A:1176:ILE:CD1	1:A:1197:ILE:CG1	2.97	0.43
1:B:557:ILE:CG2	1:B:561:TRP:CB	2.96	0.43
1:B:582:ILE:CG2	1:B:653:ILE:HD11	2.49	0.43
1:B:1770:VAL:CG1	1:B:1771:TYR:CD1	3.02	0.43
1:A:734:MET:HA	1:A:1766:LEU:CB	2.47	0.43
1:A:1471:SER:H	1:A:1479:HIS:HD2	1.66	0.43
1:B:459:ILE:HD11	1:B:509:ILE:HD12	2.00	0.43
1:B:2043:THR:O	1:B:2047:LEU:HD13	2.19	0.43
1:A:722:ILE:HG22	1:A:723:ILE:N	2.33	0.43
1:A:1425:ILE:HG22	1:A:1426:ARG:N	2.34	0.43
1:A:1708:SER:HB2	1:B:2001:VAL:HG12	2.00	0.43
1:B:975:VAL:HA	1:B:978:LYS:HD3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1592:LYS:C	1:B:1593:ILE:HG12	2.39	0.43
1:A:711:LEU:HD22	1:A:764:MET:HE2	2.00	0.43
1:A:813:LEU:HA	1:A:978:LYS:HG2	2.00	0.43
1:A:2006:THR:HG23	1:B:1710:LEU:HA	2.00	0.43
1:B:608:GLN:NE2	1:B:1907:PRO:HA	2.34	0.43
1:B:1279:ASN:O	1:B:1283:TYR:HA	2.18	0.43
1:B:1313:ILE:HD12	1:B:1336:PHE:HE1	1.84	0.43
1:A:1190:LEU:O	1:A:1194:LEU:HG	2.19	0.43
1:B:850:LEU:O	1:B:851:HIS:C	2.56	0.43
1:B:1014:GLU:OE2	1:B:1417:ARG:NH1	2.52	0.43
1:B:1494:GLN:N	1:B:1495:PRO:CD	2.81	0.43
1:B:1952:ASN:CG	1:B:1952:ASN:O	2.57	0.43
1:A:655:LEU:CD2	1:A:665:ILE:HG12	2.49	0.43
1:A:1925:HIS:HB3	1:A:1926:PRO:HD2	2.01	0.43
1:A:2101:SER:HB2	1:B:1692:THR:HG21	1.99	0.43
1:B:297:ARG:O	1:B:367:LEU:HD12	2.19	0.43
1:B:499:HIS:CD2	1:B:501:PHE:H	2.37	0.43
1:A:1104:VAL:O	1:A:1105:TYR:C	2.58	0.42
1:A:2002:VAL:HG23	1:A:2003:VAL:HG13	2.01	0.42
1:B:1246:LEU:O	1:B:1250:LYS:N	2.52	0.42
1:B:1097:VAL:O	1:B:1100:ALA:N	2.52	0.42
1:B:1194:LEU:HD23	1:B:1194:LEU:HA	1.89	0.42
1:A:138:ALA:HB1	1:A:143:VAL:CG2	2.50	0.42
1:A:714:PHE:CG	1:A:750:LEU:HD13	2.54	0.42
3:A:2303:COA:O9P	3:A:2303:COA:H141	2.19	0.42
1:B:714:PHE:CG	1:B:750:LEU:HD13	2.54	0.42
1:B:1741:ARG:HD3	1:B:1741:ARG:C	2.40	0.42
1:B:646:ILE:CG2	1:B:649:SER:OG	2.67	0.42
1:B:1733:VAL:HA	1:B:1755:ILE:O	2.19	0.42
1:B:1632:ALA:HB1	1:B:1634:GLU:OE1	2.20	0.42
1:A:541:GLU:CD	1:A:691:THR:HG1	2.23	0.42
1:B:665:ILE:HG13	1:B:674:ILE:HD12	2.01	0.42
1:B:1852:THR:HG22	1:B:1853:GLU:N	2.35	0.42
1:A:274:LEU:HD23	1:A:277:GLN:NE2	2.34	0.42
1:A:663:LEU:HD23	1:A:663:LEU:HA	1.92	0.42
1:A:1223:ASN:HB2	1:A:1264:MET:CE	2.50	0.42
1:B:1430:LYS:O	1:B:1430:LYS:HG3	2.18	0.42
1:B:2031:VAL:CG2	1:B:2090:SER:HB2	2.50	0.42
1:A:1443:LEU:HD21	1:A:1478:MET:CE	2.49	0.42
1:B:150:TRP:CZ2	1:B:386:VAL:HG23	2.54	0.42
1:B:714:PHE:HB3	1:B:750:LEU:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:ILE:HA	1:A:726:GLN:OE1	2.20	0.42
1:A:1589:ILE:O	1:A:1589:ILE:HG13	2.20	0.42
1:B:101:GLU:HB3	1:B:499:HIS:CG	2.55	0.42
1:B:1998:GLY:O	1:B:2001:VAL:HG22	2.19	0.42
1:A:485:ASN:OD1	1:A:522:HIS:NE2	2.53	0.41
1:A:1629:ILE:HG13	1:B:2034:LYS:HE3	2.02	0.41
1:B:1243:ARG:HH12	1:B:1283:TYR:C	2.23	0.41
1:A:1180:VAL:CG2	1:A:1189:ILE:HD13	2.51	0.41
1:A:1180:VAL:CG2	1:A:1189:ILE:CD1	2.98	0.41
1:A:1444:ILE:HG23	1:A:1454:THR:HG22	2.02	0.41
1:B:364:VAL:HG11	1:B:366:TYR:CZ	2.55	0.41
1:B:1589:ILE:HG13	1:B:1589:ILE:O	2.18	0.41
1:B:1655:TYR:O	1:B:1656:LEU:HD12	2.21	0.41
1:B:1733:VAL:O	1:B:1736:GLY:N	2.54	0.41
1:A:333:PRO:HG3	1:A:450:PRO:CB	2.50	0.41
1:A:1759:ALA:HB1	1:A:1771:TYR:HB2	2.03	0.41
1:B:95:VAL:HG22	1:B:115:GLN:CG	2.51	0.41
1:B:1768:ARG:O	1:B:1770:VAL:N	2.53	0.41
1:A:1026:ARG:O	1:A:1029:LEU:N	2.54	0.41
1:A:1489:VAL:HG12	1:A:1490:LYS:N	2.36	0.41
1:A:1727:LEU:HB2	1:A:1803:ILE:HD11	2.03	0.41
1:A:1842:ASP:O	1:A:1843:VAL:C	2.58	0.41
1:A:2024:VAL:HG22	1:B:1705:LEU:CD1	2.51	0.41
1:A:2163:VAL:HA	1:A:2170:GLN:HE21	1.84	0.41
1:A:654:ILE:CD1	1:A:792:VAL:HG21	2.51	0.41
1:A:931:GLU:C	1:A:933:TYR:H	2.24	0.41
1:A:1482:PRO:O	1:A:1485:THR:OG1	2.29	0.41
1:A:1496:LYS:O	1:A:1499:LYS:N	2.52	0.41
1:B:665:ILE:HD12	1:B:674:ILE:HD11	2.02	0.41
1:B:1183:LEU:HD23	1:B:1232:PHE:CZ	2.56	0.41
1:B:1874:ALA:HB3	1:B:1931:LYS:HD2	2.01	0.41
1:A:324:ARG:O	1:A:325:HIS:CB	2.61	0.41
1:A:1852:THR:HG22	1:A:1853:GLU:H	1.85	0.41
1:B:557:ILE:CG2	1:B:561:TRP:CD2	3.04	0.41
1:B:622:ASP:OD1	1:B:631:LYS:HA	2.20	0.41
1:B:1194:LEU:HD12	1:B:1252:GLU:CB	2.49	0.41
1:B:1884:LEU:O	1:B:1887:ILE:HG13	2.21	0.41
1:A:297:ARG:NH1	1:A:318:ASP:OD2	2.54	0.41
1:A:654:ILE:HD12	1:A:792:VAL:CG2	2.51	0.41
1:A:722:ILE:HG12	1:A:748:VAL:HG23	2.01	0.41
1:B:485:ASN:CB	1:B:522:HIS:HD2	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1593:ILE:CD1	3:B:2301:COA:C4A	2.95	0.41
1:B:1762:ILE:HG21	1:B:1771:TYR:HE1	1.85	0.41
1:A:1075:LEU:HD12	1:A:1075:LEU:HA	1.94	0.41
1:A:1483:ILE:HG13	1:A:1484:ALA:N	2.36	0.41
1:B:634:VAL:HG22	1:B:644:LEU:HD22	2.02	0.41
1:B:1119:ARG:HH22	1:B:1132:LYS:HG3	1.85	0.41
1:B:1677:THR:HA	1:B:1689:VAL:O	2.21	0.41
1:A:734:MET:SD	1:A:1766:LEU:HB2	2.61	0.41
1:A:1492:TRP:HZ3	1:A:1558:GLY:O	2.03	0.41
1:A:1564:MET:HE1	1:A:1585:VAL:HG12	2.03	0.41
1:A:1587:ASN:HB2	1:A:1623:ALA:O	2.21	0.41
1:B:58:VAL:O	1:B:58:VAL:HG12	2.19	0.41
1:B:97:MET:HG2	1:B:137:ILE:HD13	2.02	0.41
1:B:415:ILE:O	1:B:418:ILE:N	2.54	0.41
1:B:731:ILE:HD12	1:B:740:LEU:HD21	2.03	0.41
1:B:741:VAL:HG12	1:B:742:SER:O	2.20	0.41
1:B:1180:VAL:CG2	1:B:1189:ILE:CD1	2.98	0.41
1:B:1364:LEU:HD13	1:B:1387:ILE:HG12	2.03	0.41
1:B:1472:LEU:HD23	1:B:1472:LEU:HA	1.88	0.41
1:B:1734:GLY:HA3	3:B:2301:COA:S1P	2.61	0.41
1:A:646:ILE:HG23	1:A:647:ASN:N	2.36	0.41
1:A:940:PHE:HA	1:A:950:ILE:HD13	2.03	0.41
1:A:1310:ILE:CG2	1:A:1323:TYR:CD1	3.04	0.41
1:A:1986:ILE:HD13	1:A:2122:PHE:CD2	2.56	0.41
1:B:684:ARG:CB	1:B:684:ARG:HH11	2.34	0.41
1:B:1960:GLN:HE21	1:B:1960:GLN:HB2	1.67	0.41
1:A:460:THR:HA	1:A:505:GLN:HA	2.03	0.40
1:A:633:THR:HG23	1:A:645:PHE:HB2	2.03	0.40
1:A:1128:ILE:HD11	1:A:1192:GLN:NE2	2.36	0.40
1:A:1511:PHE:N	1:A:1512:PRO:CD	2.84	0.40
1:A:1561:ALA:O	1:A:1562:ILE:HD12	2.21	0.40
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.87	0.40
1:B:330:GLU:CG	1:B:387:GLU:HG2	2.51	0.40
1:B:744:GLU:OE2	1:B:744:GLU:HA	2.21	0.40
1:B:1008:GLN:HA	1:B:1011:VAL:HB	2.03	0.40
1:B:1543:ILE:HD11	1:B:1553:VAL:HG11	2.02	0.40
1:A:1598:PRO:O	1:A:1601:ASP:HB2	2.21	0.40
1:A:1901:ASN:OD1	1:A:1901:ASN:C	2.58	0.40
1:B:541:GLU:HG2	1:B:572:ALA:HB1	2.03	0.40
1:A:73:LYS:NZ	1:A:77:SER:OG	2.51	0.40
1:B:748:VAL:HG12	1:B:749:GLN:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1030:ILE:C	1:B:1032:GLY:H	2.24	0.40
1:A:163:LEU:O	1:A:166:SER:HB3	2.22	0.40
1:A:388:HIS:N	1:A:389:PRO:CD	2.84	0.40
1:A:1439:PRO:HB2	1:A:1459:GLU:HB2	2.02	0.40
1:A:1706:ARG:HH12	1:B:2006:THR:HG22	1.85	0.40
1:B:79:ARG:HG2	1:B:89:ASP:O	2.21	0.40
1:A:714:PHE:HB3	1:A:750:LEU:HD11	2.03	0.40
1:A:2022:ALA:HB3	1:A:2103:MET:CE	2.50	0.40
1:B:188:SER:O	1:B:192:VAL:HG23	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:ASP:OD1	1:A:440:ASP:OD1[7_555]	2.14	0.06
1:B:1170:SER:O	1:B:2180:LYS:NZ[7_645]	2.14	0.06

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	2030/2218 (92%)	1810 (89%)	201 (10%)	19 (1%)	17	56
1	B	2050/2218 (92%)	1836 (90%)	197 (10%)	17 (1%)	19	58
All	All	4080/4436 (92%)	3646 (89%)	398 (10%)	36 (1%)	17	56

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1316	ASP
1	B	712	VAL
1	A	573	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	820	VAL
1	B	572	ALA
1	B	750	LEU
1	B	851	HIS
1	A	169	LYS
1	A	216	LYS
1	A	831	GLU
1	A	1378	SER
1	A	1683	ASN
1	A	2080	ARG
1	B	1098	THR
1	B	1464	LYS
1	B	1632	ALA
1	B	1682	ILE
1	A	431	GLU
1	A	1914	GLU
1	B	315	PHE
1	B	1378	SER
1	B	1479	HIS
1	B	1595	SER
1	A	184	GLY
1	A	569	LYS
1	A	712	VAL
1	A	1004	SER
1	B	184	GLY
1	B	706	PRO
1	B	1052	VAL
1	B	1744	GLN
1	A	1843	VAL
1	A	680	VAL
1	A	1475	PRO
1	A	1649	PRO
1	B	294	GLY

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	1769/1912 (92%)	1652 (93%)	117 (7%)	16 51
1	B	1782/1912 (93%)	1654 (93%)	128 (7%)	14 47
All	All	3551/3824 (93%)	3306 (93%)	245 (7%)	15 49

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	60	SER
1	A	124	ASN
1	A	185	ASP
1	A	189	SER
1	A	224	ASP
1	A	311	ASN
1	A	335	THR
1	A	376	TYR
1	A	391	THR
1	A	471	SER
1	A	479	ASN
1	A	489	TYR
1	A	495	ASN
1	A	508	HIS
1	A	537	ARG
1	A	567	THR
1	A	573	GLU
1	A	602	GLU
1	A	629	ARG
1	A	633	THR
1	A	643	THR
1	A	644	LEU
1	A	689	SER
1	A	691	THR
1	A	738	MET
1	A	740	LEU
1	A	743	GLN
1	A	745	ASN
1	A	749	GLN
1	A	750	LEU
1	A	751	LEU
1	A	756	SER
1	A	762	ASP
1	A	768	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	784	MET
1	A	796	THR
1	A	797	LYS
1	A	801	LYS
1	A	807	SER
1	A	825	SER
1	A	841	SER
1	A	845	LEU
1	A	883	LYS
1	A	915	SER
1	A	924	SER
1	A	964	LYS
1	A	990	GLN
1	A	1023	LEU
1	A	1173	ARG
1	A	1190	LEU
1	A	1191	SER
1	A	1223	ASN
1	A	1330	SER
1	A	1343	ARG
1	A	1348	ARG
1	A	1364	LEU
1	A	1366	SER
1	A	1390	ILE
1	A	1417	ARG
1	A	1419	ARG
1	A	1431	ASP
1	A	1508	VAL
1	A	1521	SER
1	A	1527	SER
1	A	1534	ASP
1	A	1536	PHE
1	A	1546	GLU
1	A	1562	ILE
1	A	1578	ARG
1	A	1583	VAL
1	A	1585	VAL
1	A	1592	LYS
1	A	1638	LEU
1	A	1648	ASN
1	A	1656	LEU
1	A	1664	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1677	THR
1	A	1678	GLU
1	A	1691	LYS
1	A	1706	ARG
1	A	1726	THR
1	A	1732	SER
1	A	1735	ILE
1	A	1755	ILE
1	A	1764	LYS
1	A	1766	LEU
1	A	1777	LEU
1	A	1781	GLN
1	A	1791	LEU
1	A	1792	THR
1	A	1797	LEU
1	A	1824	LYS
1	A	1843	VAL
1	A	1854	SER
1	A	1884	LEU
1	A	1912	SER
1	A	1924	TRP
1	A	1930	PHE
1	A	1968	LEU
1	A	1999	SER
1	A	2001	VAL
1	A	2018	VAL
1	A	2021	ARG
1	A	2025	LEU
1	A	2035	PHE
1	A	2041	LEU
1	A	2062	SER
1	A	2083	LEU
1	A	2114	GLU
1	A	2117	GLU
1	A	2119	ARG
1	A	2127	ARG
1	A	2128	ARG
1	A	2140	SER
1	A	2149	LEU
1	A	2180	LYS
1	B	35	LEU
1	B	37	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	44	SER
1	B	66	ASN
1	B	108	GLU
1	B	116	TYR
1	B	124	ASN
1	B	269	GLU
1	B	335	THR
1	B	360	SER
1	B	367	LEU
1	B	387	GLU
1	B	416	SER
1	B	457	CYS
1	B	466	ASP
1	B	468	PHE
1	B	471	SER
1	B	508	HIS
1	B	519	SER
1	B	531	SER
1	B	545	LYS
1	B	551	ASP
1	B	573	GLU
1	B	612	LYS
1	B	622	ASP
1	B	633	THR
1	B	643	THR
1	B	653	ILE
1	B	659	SER
1	B	677	LYS
1	B	684	ARG
1	B	743	GLN
1	B	745	ASN
1	B	749	GLN
1	B	750	LEU
1	B	751	LEU
1	B	762	ASP
1	B	768	THR
1	B	782	GLU
1	B	785	LEU
1	B	797	LYS
1	B	801	LYS
1	B	807	SER
1	B	841	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	845	LEU
1	B	853	ARG
1	B	872	ARG
1	B	883	LYS
1	B	897	ASP
1	B	963	ASP
1	B	967	LEU
1	B	990	GLN
1	B	1000	SER
1	B	1015	SER
1	B	1036	SER
1	B	1040	ARG
1	B	1057	TYR
1	B	1084	ASP
1	B	1108	ARG
1	B	1159	SER
1	B	1173	ARG
1	B	1190	LEU
1	B	1191	SER
1	B	1193	SER
1	B	1223	ASN
1	B	1259	ARG
1	B	1343	ARG
1	B	1344	THR
1	B	1350	ASP
1	B	1359	SER
1	B	1364	LEU
1	B	1390	ILE
1	B	1409	GLU
1	B	1417	ARG
1	B	1419	ARG
1	B	1426	ARG
1	B	1430	LYS
1	B	1477	SER
1	B	1506	THR
1	B	1508	VAL
1	B	1516	ARG
1	B	1533	THR
1	B	1534	ASP
1	B	1539	SER
1	B	1542	LEU
1	B	1546	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1550	LEU
1	B	1568	LYS
1	B	1571	VAL
1	B	1580	ARG
1	B	1585	VAL
1	B	1639	PHE
1	B	1648	ASN
1	B	1651	LYS
1	B	1667	LYS
1	B	1681	VAL
1	B	1731	ARG
1	B	1735	ILE
1	B	1741	ARG
1	B	1742	LEU
1	B	1764	LYS
1	B	1768	ARG
1	B	1770	VAL
1	B	1777	LEU
1	B	1781	GLN
1	B	1785	ASN
1	B	1786	ASN
1	B	1792	THR
1	B	1794	VAL
1	B	1802	LYS
1	B	1808	SER
1	B	1843	VAL
1	B	1889	LEU
1	B	1909	ASN
1	B	1915	THR
1	B	1920	PRO
1	B	1924	TRP
1	B	1930	PHE
1	B	1960	GLN
1	B	1980	ASP
1	B	1992	THR
1	B	1999	SER
1	B	2035	PHE
1	B	2069	GLN
1	B	2072	SER
1	B	2101	SER
1	B	2106	LYS
1	B	2128	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	GLN
1	A	280	ASN
1	A	370	HIS
1	A	381	ASN
1	A	445	GLN
1	A	453	HIS
1	A	479	ASN
1	A	515	ASN
1	A	743	GLN
1	A	921	HIS
1	A	979	ASN
1	A	988	HIS
1	A	990	GLN
1	A	1121	HIS
1	A	1182	HIS
1	A	1321	HIS
1	A	1384	HIS
1	A	1479	HIS
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1648	ASN
1	A	1748	GLN
1	A	1763	ASN
1	A	1815	ASN
1	A	1937	ASN
1	A	1941	ASN
1	A	2045	ASN
1	A	2060	ASN
1	A	2097	HIS
1	A	2170	GLN
1	B	66	ASN
1	B	228	GLN
1	B	280	ASN
1	B	298	HIS
1	B	343	HIS
1	B	370	HIS
1	B	381	ASN
1	B	445	GLN
1	B	453	HIS
1	B	499	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	522	HIS
1	B	835	ASN
1	B	979	ASN
1	B	988	HIS
1	B	1134	GLN
1	B	1182	HIS
1	B	1319	ASN
1	B	1371	ASN
1	B	1479	HIS
1	B	1522	GLN
1	B	1560	ASN
1	B	1587	ASN
1	B	1605	ASN
1	B	1648	ASN
1	B	1748	GLN
1	B	1774	ASN
1	B	1781	GLN
1	B	1786	ASN
1	B	1909	ASN
1	B	1925	HIS
1	B	1960	GLN
1	B	2011	GLN
1	B	2057	GLN
1	B	2074	GLN

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 monosaccharides 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	COA	B	2301	-	41,50,50	1.14	4 (9%)	52,75,75	1.53	9 (17%)
2	BTI	A	2302	-	16,16,16	0.83	0	21,21,21	2.67	9 (42%)
3	COA	A	2303	-	41,50,50	0.96	3 (7%)	52,75,75	1.42	7 (13%)
2	BTI	A	2301	1	16,16,16	0.95	1 (6%)	21,21,21	2.27	8 (38%)

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	COA	B	2301	-	-	14/44/64/64	0/3/3/3
2	BTI	A	2302	-	-	2/5/27/27	0/2/2/2
3	COA	A	2303	-	-	10/44/64/64	0/3/3/3
2	BTI	A	2301	1	-	4/5/27/27	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2301	COA	O4B-C1B	2.74	1.44	1.41
3	A	2303	COA	C5A-C4A	2.65	1.47	1.40
3	A	2303	COA	O4B-C1B	2.63	1.44	1.41
3	B	2301	COA	C5A-C4A	2.55	1.47	1.40
2	A	2301	BTI	C3-N2	-2.51	1.31	1.35
3	B	2301	COA	C4A-N3A	2.45	1.39	1.35
3	A	2303	COA	C2A-N3A	2.15	1.35	1.32
3	B	2301	COA	C2B-C1B	-2.01	1.50	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2302	BTI	C2-C4-N2	7.13	119.52	113.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2302	BTI	C6-C5-C4	5.57	113.49	108.66
2	A	2301	BTI	C2-C4-N2	-5.45	108.24	113.13
3	B	2301	COA	N3A-C2A-N1A	-5.33	120.35	128.68
3	A	2303	COA	C2P-C3P-N4P	4.37	122.29	112.31
2	A	2302	BTI	C6-S1-C2	4.10	98.31	89.89
2	A	2301	BTI	C2-C4-C5	3.90	113.47	108.94
3	A	2303	COA	N3A-C2A-N1A	-3.55	123.14	128.68
3	B	2301	COA	N6A-C6A-N1A	3.28	125.38	118.57
2	A	2302	BTI	C6-C5-N3	3.22	117.12	113.03
3	B	2301	COA	C2A-N1A-C6A	3.06	123.99	118.75
2	A	2301	BTI	O3-C3-N3	2.94	130.16	125.94
2	A	2301	BTI	O3-C3-N2	-2.94	121.72	125.94
2	A	2301	BTI	C7-C2-C4	-2.78	106.62	114.73
2	A	2302	BTI	C5-N3-C3	2.71	115.99	112.46
2	A	2302	BTI	N2-C3-N3	-2.63	106.29	108.76
3	A	2303	COA	C4A-C5A-N7A	-2.59	106.70	109.40
3	B	2301	COA	C5A-C6A-N6A	-2.58	116.43	120.35
3	A	2303	COA	O5P-C5P-C6P	-2.53	117.40	122.02
3	B	2301	COA	C2B-C3B-C4B	2.51	107.67	103.22
2	A	2301	BTI	C5-C6-S1	2.49	108.44	106.31
2	A	2302	BTI	C4-C2-S1	2.44	107.53	105.20
3	A	2303	COA	O5P-C5P-N4P	2.41	127.56	123.01
3	B	2301	COA	C1B-N9A-C4A	-2.38	122.45	126.64
3	B	2301	COA	C2P-C3P-N4P	2.29	117.53	112.31
3	B	2301	COA	P2A-O3A-P1A	-2.26	125.08	132.83
3	A	2303	COA	O5A-P2A-O4A	2.23	123.29	112.24
2	A	2301	BTI	C8-C9-C10	-2.22	104.10	113.79
3	B	2301	COA	C3B-C2B-C1B	2.18	104.72	99.89
2	A	2301	BTI	C4-C2-S1	2.15	107.26	105.20
3	A	2303	COA	O3B-P3B-O7A	-2.14	101.13	109.39
2	A	2302	BTI	C5-C6-S1	2.08	108.08	106.31
2	A	2302	BTI	C4-C5-N3	-2.02	100.28	102.43

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2301	BTI	C11-C10-C9-C8
2	A	2301	BTI	S1-C2-C7-C8
2	A	2301	BTI	C4-C2-C7-C8
2	A	2302	BTI	C11-C10-C9-C8
3	A	2303	COA	CCP-O6A-P2A-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	2303	COA	CDP-CBP-CCP-O6A
3	A	2303	COA	CAP-CBP-CCP-O6A
3	A	2303	COA	S1P-C2P-C3P-N4P
3	B	2301	COA	C5B-O5B-P1A-O1A
3	B	2301	COA	CCP-O6A-P2A-O3A
3	B	2301	COA	CCP-O6A-P2A-O4A
3	B	2301	COA	CCP-O6A-P2A-O5A
3	B	2301	COA	CDP-CBP-CCP-O6A
3	B	2301	COA	CAP-CBP-CCP-O6A
3	B	2301	COA	C5P-C6P-C7P-N8P
3	B	2301	COA	S1P-C2P-C3P-N4P
3	B	2301	COA	C3B-C4B-C5B-O5B
3	B	2301	COA	O4B-C4B-C5B-O5B
3	A	2303	COA	CEP-CBP-CCP-O6A
3	B	2301	COA	CEP-CBP-CCP-O6A
2	A	2301	BTI	C7-C8-C9-C10
3	B	2301	COA	O9P-C9P-CAP-OAP
3	A	2303	COA	C5P-C6P-C7P-N8P
3	A	2303	COA	CCP-O6A-P2A-O5A
3	B	2301	COA	C2B-C3B-O3B-P3B
2	A	2302	BTI	C2-C7-C8-C9
3	A	2303	COA	C5B-O5B-P1A-O3A
3	B	2301	COA	C5B-O5B-P1A-O3A
3	A	2303	COA	C5B-O5B-P1A-O1A
3	A	2303	COA	CCP-O6A-P2A-O4A

There are no ring outliers.

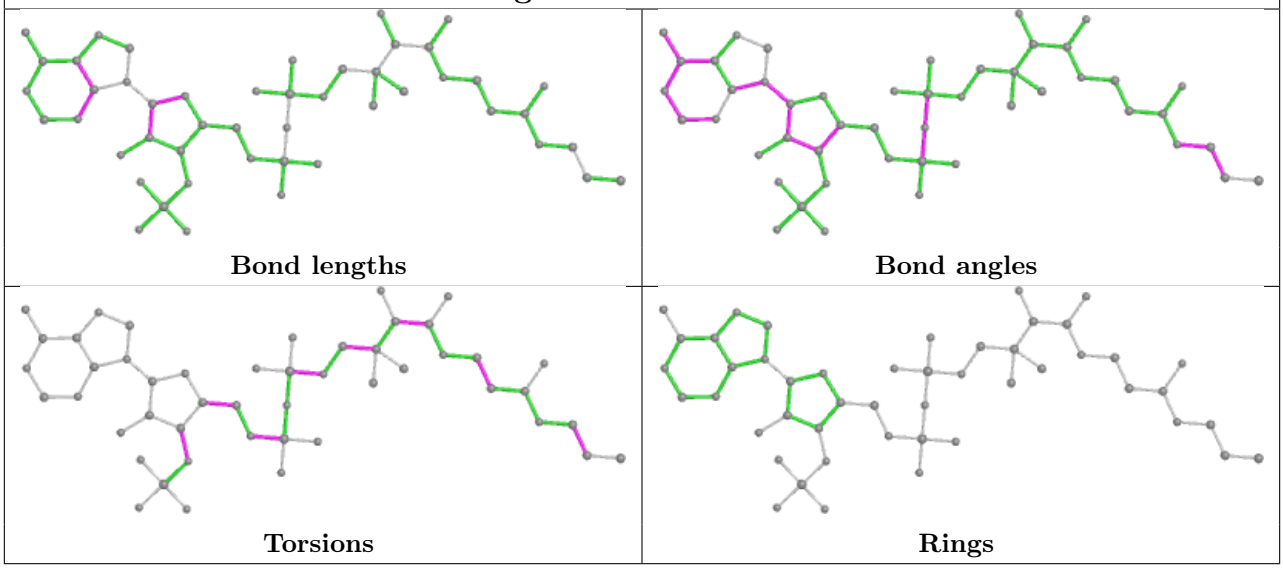
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2301	COA	3	0
2	A	2302	BTI	2	0
3	A	2303	COA	5	0
2	A	2301	BTI	4	0

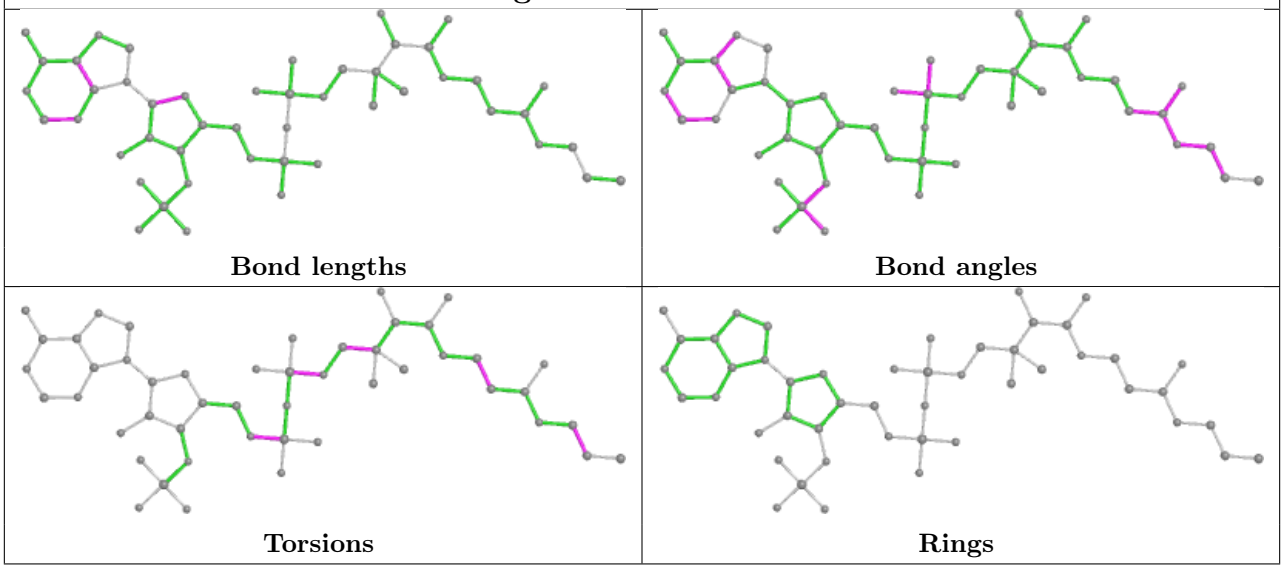
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand COA B 2301



Ligand COA A 2303



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^{th} 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	2050/2218 (92%)	-0.05	51 (2%) 57 43	46, 89, 147, 228	0
1	B	2072/2218 (93%)	0.01	90 (4%) 35 22	43, 88, 170, 239	0
All	All	4122/4436 (92%)	-0.02	141 (3%) 45 29	43, 89, 159, 239	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	441	ALA	5.8
1	B	292	LEU	5.5
1	B	748	VAL	5.3
1	B	2182	LEU	5.3
1	B	226	ILE	5.1
1	B	289	ILE	4.8
1	A	225	ASP	4.7
1	B	750	LEU	4.6
1	A	440	ASP	4.4
1	B	274	LEU	4.4
1	B	282	ILE	4.4
1	B	715	LEU	4.3
1	B	764	MET	4.3
1	B	765	ALA	4.2
1	B	264	GLN	4.1
1	B	39	ASP	4.1
1	B	260	LYS	4.1
1	B	561	TRP	4.0
1	A	262	ILE	4.0
1	B	266	GLU	4.0
1	A	445	GLN	4.0
1	B	267	ARG	3.9
1	B	712	VAL	3.8
1	A	442	THR	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	235	PRO	3.7
1	A	2066	GLU	3.7
1	B	278	ALA	3.6
1	B	705	THR	3.6
1	B	293	ALA	3.6
1	B	261	GLY	3.6
1	B	262	ILE	3.5
1	B	716	VAL	3.5
1	A	1464	LYS	3.5
1	B	1255	ASN	3.4
1	A	1434	THR	3.4
1	A	278	ALA	3.4
1	A	856	ALA	3.4
1	A	2060	ASN	3.4
1	A	1433	GLN	3.3
1	B	204	SER	3.3
1	B	258	GLY	3.2
1	B	767	MET	3.2
1	B	240	GLN	3.2
1	B	717	GLU	3.1
1	B	722	ILE	3.1
1	B	751	LEU	3.1
1	B	749	GLN	3.1
1	A	2067	VAL	3.0
1	B	254	SER	3.0
1	A	1430	LYS	3.0
1	B	755	GLY	2.9
1	B	728	TYR	2.9
1	B	2043	THR	2.9
1	B	437	LYS	2.9
1	A	2057	GLN	2.9
1	A	236	GLU	2.9
1	B	2071	ILE	2.8
1	A	2071	ILE	2.8
1	B	2141	HIS	2.8
1	A	446	ARG	2.8
1	B	744	GLU	2.8
1	B	703	LEU	2.7
1	A	1492	TRP	2.7
1	B	719	GLY	2.7
1	B	714	PHE	2.7
1	A	765	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	207	GLY	2.7
1	B	711	LEU	2.7
1	B	701	THR	2.7
1	B	445	GLN	2.6
1	B	295	ARG	2.6
1	A	444	LYS	2.6
1	B	243	LYS	2.6
1	B	1638	LEU	2.6
1	B	271	PHE	2.5
1	A	2070	GLN	2.5
1	A	1465	GLY	2.5
1	B	2138	ARG	2.5
1	A	2134	TYR	2.5
1	B	213	VAL	2.5
1	B	230	GLY	2.5
1	B	232	CYS	2.5
1	B	727	PRO	2.5
1	B	220	VAL	2.5
1	B	739	PRO	2.5
1	B	340	GLU	2.5
1	B	753	GLN	2.4
1	B	1646	ALA	2.4
1	A	2065	PRO	2.4
1	A	2082	LEU	2.4
1	B	250	MET	2.4
1	A	2086	TYR	2.4
1	B	724	LYS	2.4
1	B	721	HIS	2.4
1	A	1647	ALA	2.4
1	A	249	VAL	2.4
1	B	244	ARG	2.4
1	B	2158	TRP	2.3
1	B	222	VAL	2.3
1	A	2047	LEU	2.3
1	A	277	GLN	2.3
1	A	1681	VAL	2.3
1	A	265	VAL	2.3
1	B	897	ASP	2.3
1	B	743	GLN	2.3
1	B	236	GLU	2.3
1	B	758	ILE	2.3
1	A	885	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	239	LEU	2.2
1	A	876	PHE	2.2
1	B	730	GLU	2.2
1	B	713	LYS	2.2
1	A	2064	ALA	2.2
1	A	272	ILE	2.2
1	B	2069	GLN	2.2
1	A	436	PHE	2.2
1	A	767	MET	2.2
1	A	880	GLN	2.2
1	B	2186	LEU	2.2
1	A	1346	HIS	2.2
1	B	725	GLY	2.2
1	A	219	LEU	2.2
1	B	1644	ASN	2.2
1	A	764	MET	2.1
1	B	718	ASN	2.1
1	B	729	ALA	2.1
1	B	1171	PRO	2.1
1	A	243	LYS	2.1
1	B	439	GLN	2.1
1	B	231	CYS	2.1
1	A	2179	TYR	2.1
1	B	270	ASP	2.1
1	B	731	ILE	2.1
1	B	441	ALA	2.1
1	A	2049	ASP	2.1
1	A	2068	HIS	2.1
1	B	265	VAL	2.0
1	A	251	ILE	2.0
1	B	187	ILE	2.0
1	B	766	ILE	2.0
1	A	2053	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

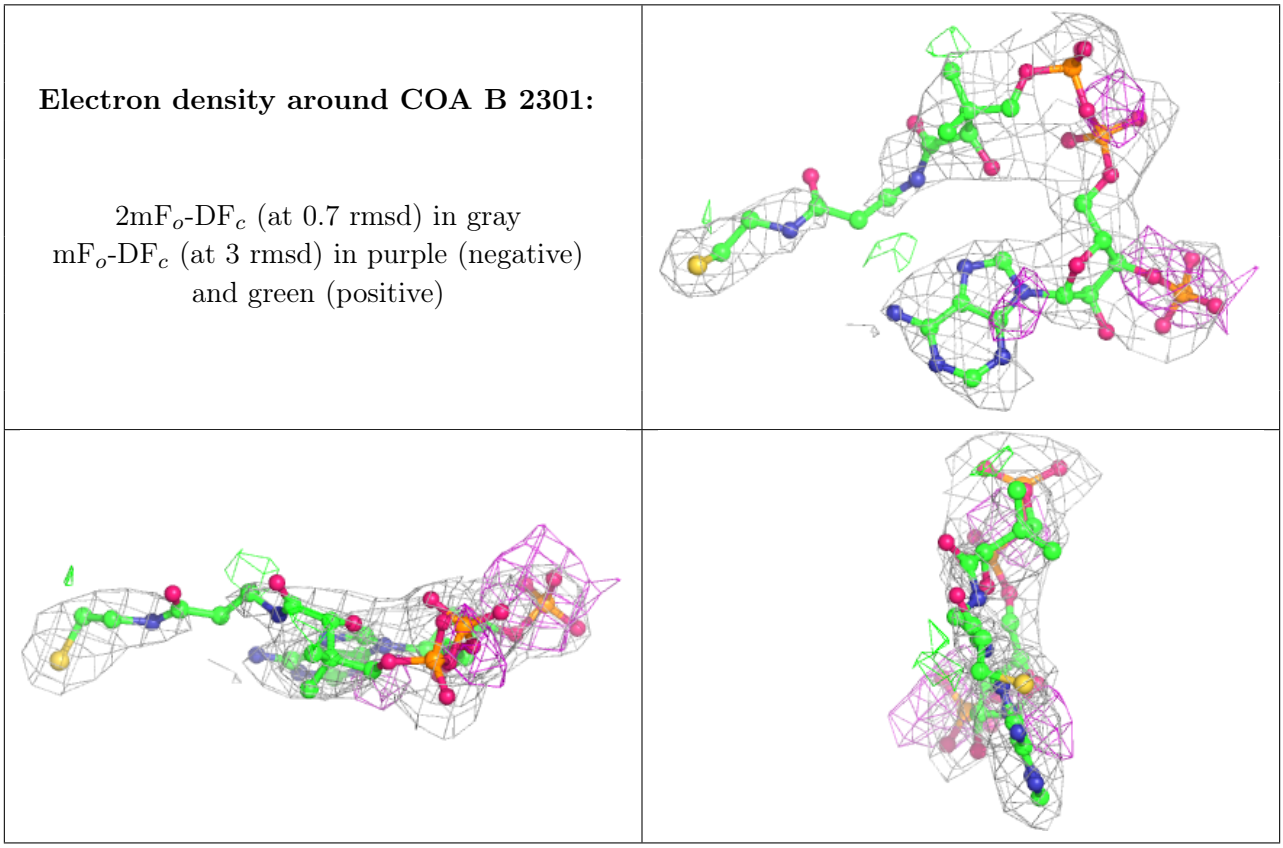
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BTI	A	2302	15/15	0.86	0.28	70,80,93,100	0
3	COA	B	2301	48/48	0.87	0.22	71,128,148,158	0
2	BTI	A	2301	15/15	0.91	0.26	66,74,78,82	0
3	COA	A	2303	48/48	0.92	0.21	74,104,123,129	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.

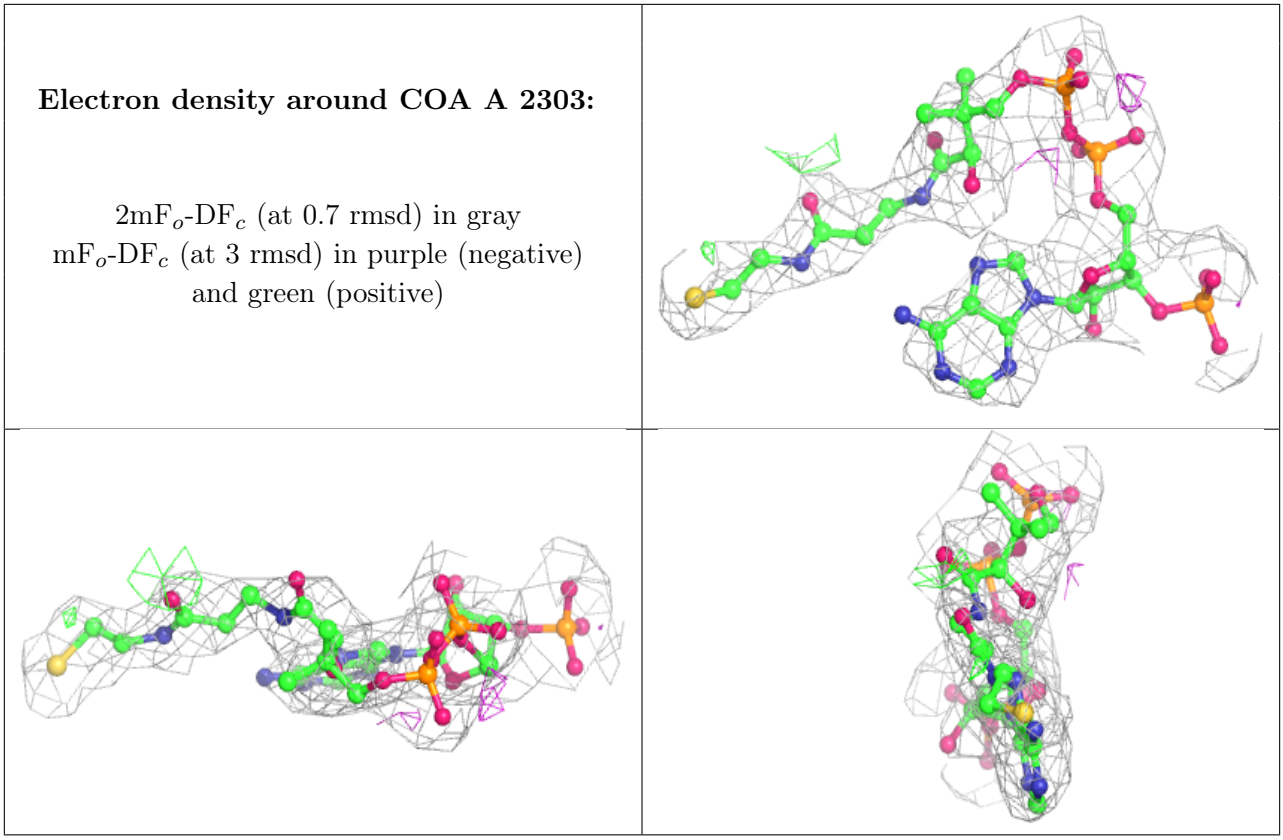
Electron density around COA B 2301:

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



Electron density around COA A 2303:

$2mF_o$-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.