



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 02:42 PM GMT

PDB ID : 1W2X
Title : CRYSTAL STRUCTURE OF THE CARBOXYLTRANSFERASE DOMAIN
OF ACETYL-COENZYME A CARBOXYLASE IN COMPLEX WITH CP-
640186
Authors : Zhang, H.; Tweel, B.; Li, J.; Tong, L.
Deposited on : 2004-07-09
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

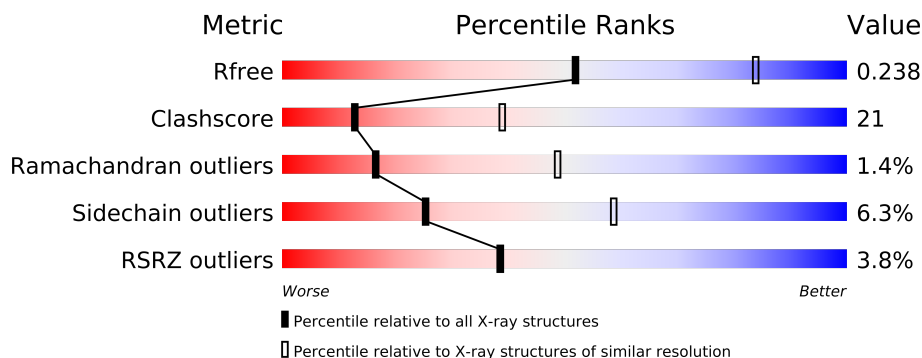
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	758	
1	B	758	
1	C	758	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	RCP	C	3000	-	X

2 Entry composition i

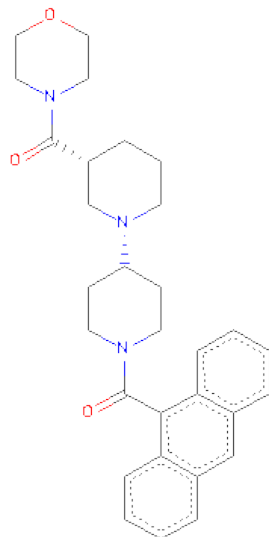
There are 3 unique types of molecules in this entry. The entry contains 16588 atoms, of which 0 are hydrogen and 0 are deuterium.

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	682	Total	C	N	O	S	0	0	1
			5425	3459	931	1016	19			
1	B	676	Total	C	N	O	S	0	0	1
			5377	3427	924	1007	19			
1	C	666	Total	C	N	O	S	0	0	1
			5299	3374	913	993	19			

- Molecule 2 is (3R)-1'-(9-ANTHRYLCARBONYL)-3-(MORPHOLIN-4-YLCARBONYL)-1,4'-BIPIPERIDINE (three-letter code: RCP) (formula: C₃₀H₃₅N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			36	30	3	3		
2	B	1	Total	C	N	O	0	0
			36	30	3	3		
2	C	1	Total	C	N	O	0	0
			36	30	3	3		

- Molecule 3 is water.

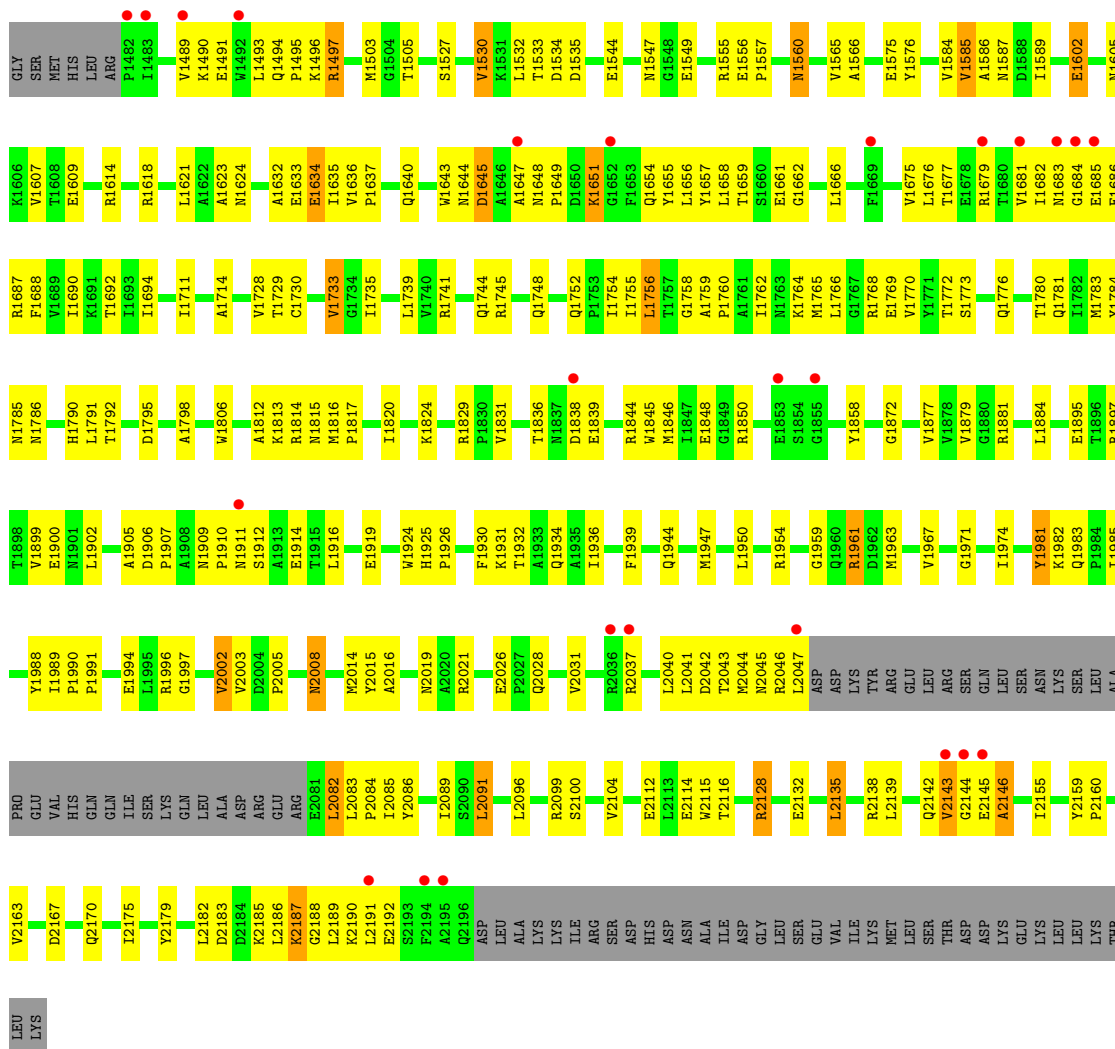
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	147	Total 147	O 147	0	0
3	B	128	Total 128	O 128	0	0
3	C	104	Total 104	O 104	0	0

3 Residue-property plots

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

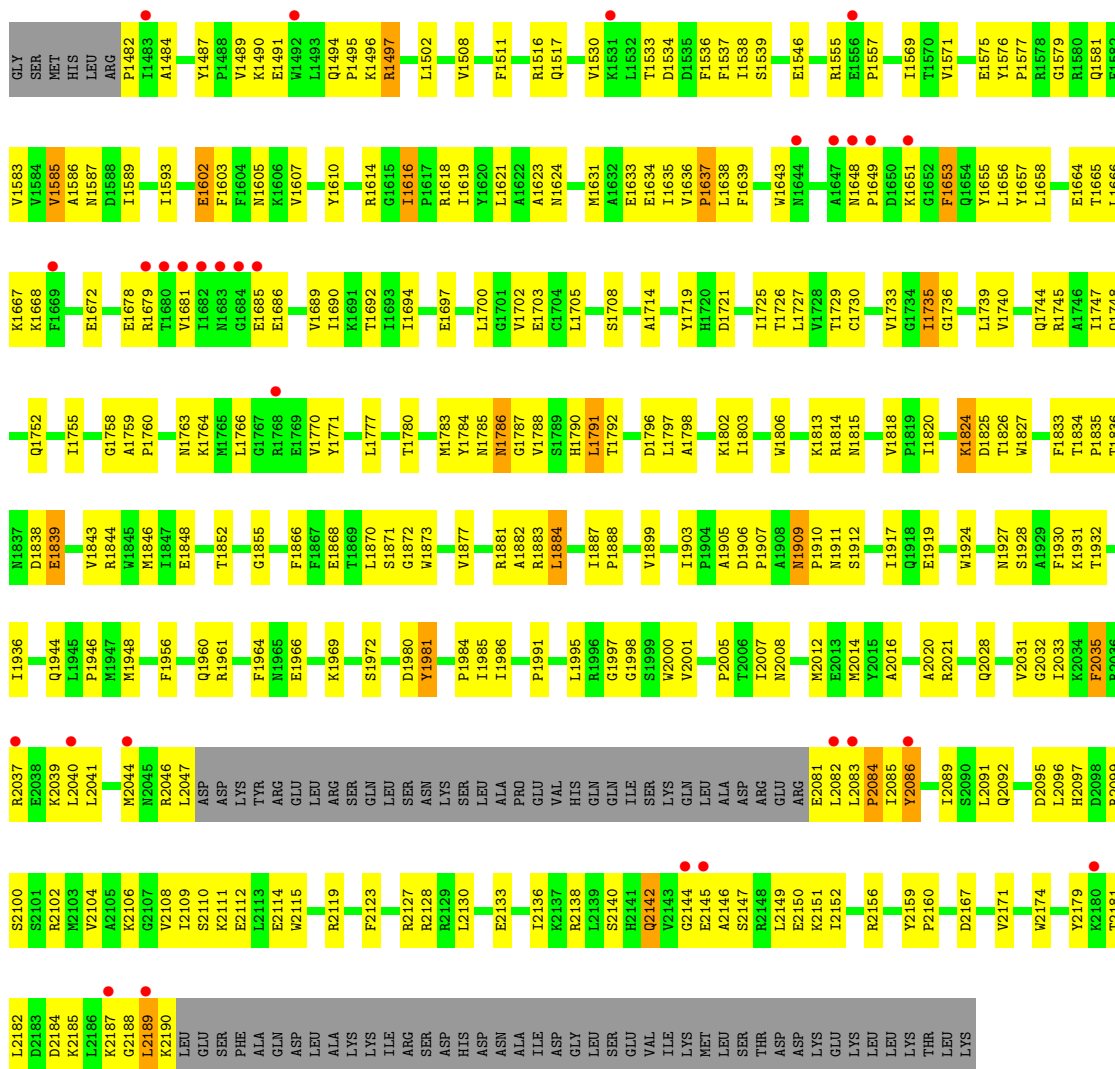
• Molecule 1: ACETYL-COA CARBOXYLASE

Chain A: 



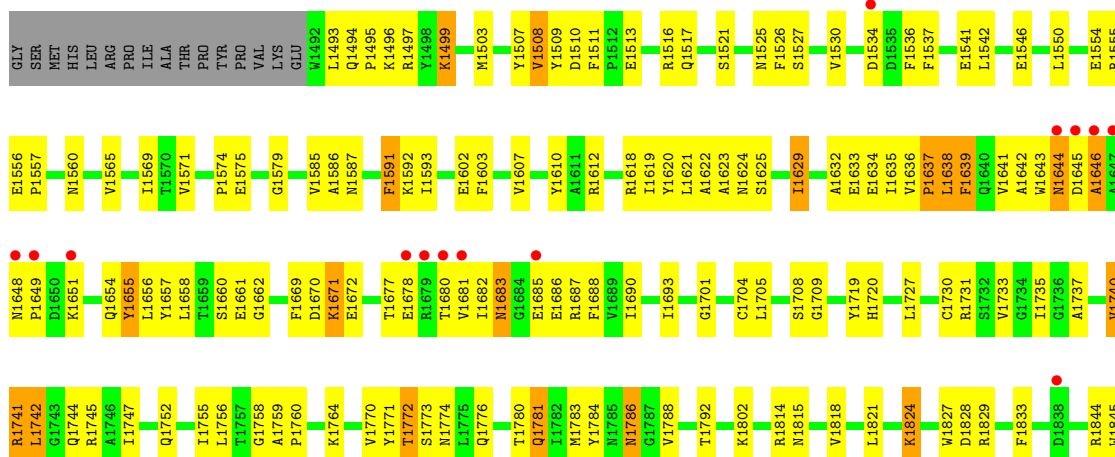
• Molecule 1: ACETYL-COA CARBOXYLASE

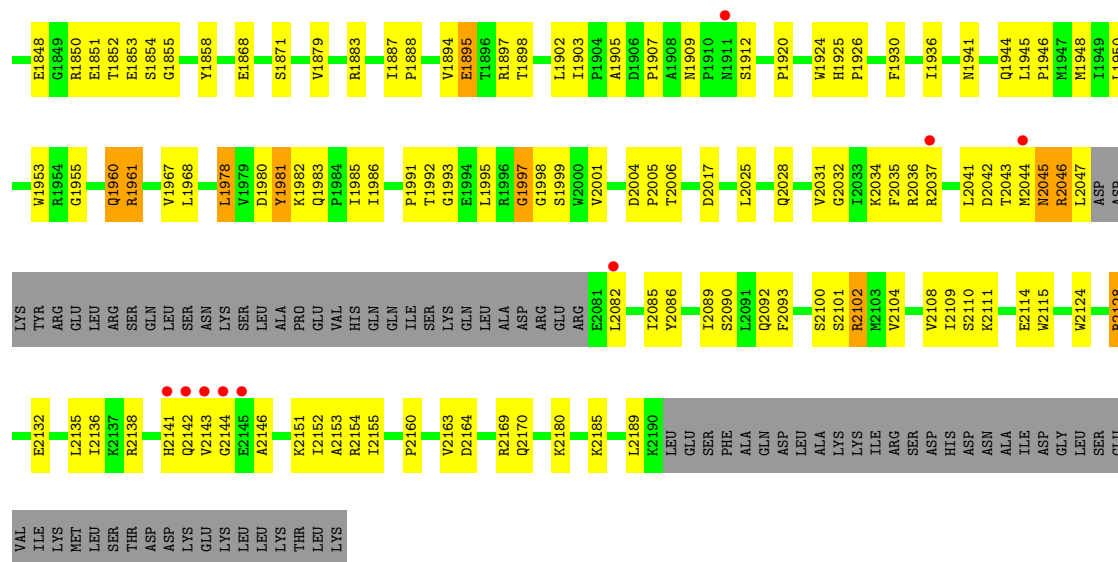
Chain B: 



- Molecule 1: ACETYL-COA CARBOXYLASE

Chain C:





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	246.59Å 124.60Å 145.60Å 90.00° 93.85° 90.00°	Depositor
Resolution (Å)	29.66 – 2.80 29.66 – 2.78	Depositor EDS
% Data completeness (in resolution range)	85.7 (29.66-2.80) 88.7 (29.66-2.78)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.76Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.234 0.202 , 0.238	Depositor DCC
R_{free} test set	9770 reflections (11.04%)	DCC
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 102708 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16588	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RCP

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	0.39	0/5547	0.61	0/7516
1	B	0.39	0/5498	0.62	0/7451
1	C	0.39	0/5416	0.60	0/7337
All	All	0.39	0/16461	0.61	0/22304

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5425	0	5365	209	0
1	B	5377	0	5316	236	0
1	C	5299	0	5234	248	0
2	A	36	0	35	4	0
2	B	36	0	35	2	0
2	C	36	0	35	3	0
3	A	147	0	0	4	0
3	B	128	0	0	7	0
3	C	104	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16588	0	16020	669	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (669) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.21	1.05
1:A:1936:ILE:HG12	1:A:1947:MET:HE1	1.41	1.02
1:C:1772:THR:H	1:C:1776:GLN:NE2	1.59	1.01
1:C:1773:SER:H	1:C:1776:GLN:HE21	1.09	1.00
1:B:1815:ASN:H	1:B:1944:GLN:HE22	0.98	0.98
1:A:1773:SER:H	1:A:1776:GLN:HE21	1.13	0.96
1:A:1813:LYS:HG2	1:A:1816:MET:HE2	1.50	0.93
1:A:1772:THR:H	1:A:1776:GLN:HE22	0.95	0.92
1:C:1637:PRO:HG2	1:C:1638:LEU:HD23	1.49	0.92
1:B:2181:THR:HG22	1:B:2185:LYS:HE2	1.51	0.91
1:B:2031:VAL:HG21	1:B:2091:LEU:HD23	1.54	0.91
1:C:1772:THR:H	1:C:1776:GLN:HE22	0.90	0.89
1:A:1772:THR:N	1:A:1776:GLN:HE22	1.71	0.87
1:B:1764:LYS:HD2	2:B:3000:RCP:H5	1.57	0.86
1:B:1511:PHE:HZ	1:B:1729:THR:HG21	1.42	0.85
1:A:1772:THR:H	1:A:1776:GLN:NE2	1.76	0.84
1:B:1638:LEU:HD23	1:B:1638:LEU:H	1.42	0.84
1:C:1648:ASN:HB2	1:C:1651:LYS:HD3	1.58	0.84
1:A:1813:LYS:HG2	1:A:1816:MET:CE	2.08	0.84
1:A:1733:VAL:HG13	1:A:1755:ILE:HG13	1.61	0.83
1:B:1877:VAL:HG13	1:B:1931:LYS:HD3	1.60	0.82
1:C:1772:THR:N	1:C:1776:GLN:HE22	1.75	0.80
1:B:1836:THR:HB	1:B:1839:GLU:HB3	1.62	0.80
1:A:1633:GLU:O	1:A:1636:VAL:HG12	1.81	0.80
1:B:2147:SER:HB3	1:B:2150:GLU:HG3	1.62	0.80
1:B:1494:GLN:HB3	1:B:1497:ARG:HH21	1.46	0.78
1:B:1692:THR:HG21	1:C:2101:SER:HB2	1.64	0.78
1:C:1646:ALA:HB3	1:C:1651:LYS:HG2	1.63	0.78
1:C:2031:VAL:HG23	1:C:2035:PHE:HB3	1.65	0.78
1:C:1493:LEU:HB2	1:C:1497:ARG:NH1	1.99	0.78
1:B:1494:GLN:NE2	1:B:1496:LYS:HG3	1.99	0.78
1:C:2160:PRO:HD2	1:C:2163:VAL:HG21	1.65	0.77
1:B:2044:MET:SD	1:B:2082:LEU:HD21	2.24	0.77
1:C:1773:SER:N	1:C:1776:GLN:HE21	1.81	0.77
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.50	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1773:SER:H	1:A:1776:GLN:NE2	1.83	0.76
1:A:1812:ALA:HB3	1:A:1816:MET:HE1	1.67	0.76
1:B:2140:SER:O	1:B:2144:GLY:HA3	1.87	0.75
1:B:1827:TRP:HA	1:B:2119:ARG:NH1	2.01	0.75
1:A:1533:THR:HB	1:A:1535:ASP:OD1	1.86	0.74
1:C:1773:SER:H	1:C:1776:GLN:NE2	1.84	0.74
1:B:1511:PHE:CZ	1:B:1729:THR:HG21	2.22	0.74
1:A:1657:TYR:CE2	1:A:1687:ARG:HD2	2.23	0.74
1:A:2135:LEU:HB3	1:A:2155:ILE:HD13	1.69	0.74
1:B:1827:TRP:HA	1:B:2119:ARG:HH12	1.53	0.74
1:C:1625:SER:HB3	1:C:1731:ARG:NH2	2.02	0.74
1:B:2007:ILE:HB	1:B:2012:MET:HE3	1.70	0.74
1:C:1638:LEU:H	1:C:1638:LEU:HD23	1.52	0.74
1:B:1763:ASN:ND2	1:B:1770:VAL:H	1.86	0.74
1:C:1759:ALA:H	1:C:1774:ASN:ND2	1.86	0.73
1:B:1667:LYS:HG2	1:B:1672:GLU:HB3	1.70	0.73
1:A:2183:ASP:HB2	1:B:1482:PRO:HG3	1.71	0.73
1:C:1786:ASN:HB3	1:C:1788:VAL:HG23	1.71	0.72
1:C:2138:ARG:HB3	1:C:2138:ARG:HH11	1.55	0.71
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.37	0.71
1:A:1991:PRO:HG3	1:A:2115:TRP:HB2	1.72	0.71
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	1.88	0.71
1:C:1783:MET:HA	1:C:1786:ASN:HB2	1.72	0.71
1:C:1764:LYS:HD2	2:C:3000:RCP:H5	1.71	0.71
1:C:1772:THR:N	1:C:1776:GLN:NE2	2.35	0.70
1:C:1815:ASN:ND2	1:C:1944:GLN:HE22	1.89	0.70
1:B:2108:VAL:HG23	1:B:2109:ILE:HG23	1.74	0.70
1:C:1759:ALA:H	1:C:1774:ASN:HD21	1.38	0.69
1:C:1909:ASN:HD22	1:C:1912:SER:HB2	1.57	0.69
1:C:1641:VAL:HG12	1:C:1642:ALA:H	1.57	0.69
1:C:2036:ARG:NH1	1:C:2036:ARG:HB3	2.07	0.69
1:C:1550:LEU:HD21	1:C:1607:VAL:HG22	1.74	0.69
1:A:1899:VAL:HB	1:A:1919:GLU:HB2	1.74	0.69
1:B:2100:SER:O	1:B:2104:VAL:HG23	1.93	0.69
1:C:1903:ILE:N	1:C:1903:ILE:HD12	2.08	0.69
1:C:1998:GLY:O	1:C:2001:VAL:HG12	1.92	0.69
1:B:1852:THR:HG22	1:B:1855:GLY:O	1.93	0.68
1:C:1991:PRO:HG2	1:C:2115:TRP:HB2	1.75	0.68
1:A:1585:VAL:HG13	1:A:1607:VAL:HG11	1.75	0.68
1:B:1658:LEU:HD13	1:B:1690:ILE:HD11	1.76	0.68
1:B:1638:LEU:HD11	1:B:1666:LEU:CD1	2.24	0.68
1:B:1763:ASN:HD21	1:B:1771:TYR:H	1.42	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1936:ILE:HD13	1:C:1978:LEU:HD13	1.76	0.67
1:B:1998:GLY:O	1:B:2001:VAL:HG12	1.95	0.67
1:B:1815:ASN:H	1:B:1944:GLN:NE2	1.82	0.67
1:B:2189:LEU:H	1:B:2189:LEU:HD23	1.59	0.67
1:C:2138:ARG:NH1	1:C:2138:ARG:HB3	2.10	0.67
1:B:2082:LEU:HD23	1:B:2082:LEU:H	1.58	0.67
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.42	0.67
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	1.94	0.67
1:B:1815:ASN:N	1:B:1944:GLN:HE22	1.82	0.67
1:C:2160:PRO:HB2	1:C:2163:VAL:HG23	1.75	0.67
1:C:1658:LEU:HG	1:C:1690:ILE:HD11	1.76	0.66
1:A:2041:LEU:HA	1:A:2044:MET:HG2	1.75	0.66
1:A:1677:THR:HG22	1:A:1690:ILE:HA	1.77	0.66
1:A:2037:ARG:O	1:A:2041:LEU:HG	1.96	0.66
1:A:1836:THR:HG22	1:A:1838:ASP:H	1.60	0.66
1:A:1836:THR:HB	1:A:1839:GLU:HB2	1.79	0.65
1:C:2164:ASP:H	1:C:2170:GLN:NE2	1.93	0.65
1:C:2036:ARG:HB3	1:C:2036:ARG:HH11	1.61	0.65
1:B:1735:ILE:HD13	1:B:1739:LEU:HG	1.79	0.65
1:A:1547:ASN:HB2	1:A:1549:GLU:HG2	1.78	0.65
1:C:2100:SER:O	1:C:2104:VAL:HG23	1.97	0.65
1:A:2160:PRO:HD2	1:A:2163:VAL:HG21	1.78	0.64
1:B:2047:LEU:HD21	1:C:1649:PRO:HG3	1.78	0.64
1:A:1632:ALA:HB1	1:A:1634:GLU:OE2	1.97	0.64
1:A:2040:LEU:HD21	1:A:2086:TYR:HB3	1.79	0.64
1:B:1735:ILE:O	1:B:1735:ILE:HD13	1.96	0.64
1:C:1772:THR:HG23	1:C:1776:GLN:NE2	2.12	0.64
1:A:1905:ALA:O	1:A:1907:PRO:HD3	1.98	0.64
1:A:1909:ASN:ND2	1:A:1911:ASN:H	1.96	0.64
1:C:1909:ASN:ND2	1:C:1912:SER:HB2	2.13	0.64
1:A:2044:MET:SD	1:A:2082:LEU:HD11	2.38	0.64
1:B:2008:ASN:N	1:B:2012:MET:CE	2.62	0.63
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.47	0.63
1:A:1812:ALA:HB3	1:A:1816:MET:CE	2.28	0.63
1:B:1745:ARG:NH2	3:B:4057:HOH:O	2.31	0.63
1:C:1772:THR:HG23	1:C:1776:GLN:HE22	1.64	0.62
1:C:1585:VAL:HG22	1:C:1607:VAL:HG11	1.81	0.62
1:C:1936:ILE:HD13	1:C:1978:LEU:CD1	2.29	0.62
1:A:2096:LEU:HD23	1:A:2099:ARG:NH1	2.15	0.62
1:C:1781:GLN:H	1:C:1781:GLN:HE21	1.47	0.62
1:C:2045:ASN:C	1:C:2045:ASN:HD22	2.03	0.62
1:C:1660:SER:HB2	1:C:1686:GLU:HB2	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1747:ILE:HD13	1:C:1802:LYS:HB2	1.82	0.62
1:B:1909:ASN:HB3	1:B:1912:SER:HB2	1.82	0.61
1:A:2046:ARG:O	1:A:2047:LEU:HG	1.99	0.61
1:A:2190:LYS:C	1:A:2192:GLU:H	2.02	0.61
1:C:1745:ARG:NH2	3:C:4033:HOH:O	2.33	0.61
1:C:1554:GLU:O	1:C:1554:GLU:HG3	1.99	0.61
1:B:2037:ARG:HD2	1:B:2083:LEU:HD21	1.83	0.61
1:C:1991:PRO:CG	1:C:2115:TRP:HB2	2.30	0.61
1:B:1909:ASN:HD21	1:B:1911:ASN:ND2	1.99	0.61
1:B:1681:VAL:HA	1:B:1685:GLU:O	2.01	0.61
1:A:2085:ILE:O	1:A:2089:ILE:HG13	2.01	0.61
1:B:1729:THR:HG22	1:B:1796:ASP:OD1	2.00	0.60
1:B:1637:PRO:HG2	1:B:1638:LEU:HD23	1.82	0.60
1:A:1824:LYS:HE2	1:A:1824:LYS:H	1.65	0.60
1:C:1960:GLN:HG3	1:C:1961:ARG:N	2.12	0.60
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	2.16	0.60
1:B:2000:TRP:CD1	1:C:1705:LEU:HB3	2.36	0.60
1:A:1686:GLU:O	1:A:1686:GLU:HG3	2.01	0.59
1:A:1991:PRO:O	1:A:2019:ASN:O	2.19	0.59
1:B:2110:SER:O	1:B:2111:LYS:HG3	2.01	0.59
1:C:1509:TYR:HE2	1:C:1541:GLU:OE1	1.85	0.59
1:B:1824:LYS:HG3	1:B:1825:ASP:H	1.67	0.59
1:A:2143:VAL:HG13	1:A:2144:GLY:H	1.66	0.59
1:C:1493:LEU:HB2	1:C:1497:ARG:HH12	1.66	0.59
1:B:2008:ASN:N	1:B:2012:MET:HE2	2.17	0.59
1:C:1755:ILE:HD12	1:C:1758:GLY:HA2	1.84	0.59
1:A:1490:LYS:HD2	1:A:1497:ARG:NH2	2.17	0.59
1:A:1605:ASN:O	1:A:1609:GLU:HG3	2.03	0.59
1:A:1656:LEU:HB2	1:A:1690:ILE:HD11	1.85	0.58
1:A:1959:GLY:O	1:A:1963:MET:HB2	2.02	0.58
1:A:1813:LYS:CG	1:A:1816:MET:HE2	2.29	0.58
1:A:1560:ASN:HD22	1:A:1560:ASN:H	1.51	0.58
1:B:1491:GLU:O	1:B:1495:PRO:HA	2.02	0.58
1:B:2086:TYR:HA	1:B:2089:ILE:HD12	1.86	0.58
1:A:1936:ILE:HG12	1:A:1947:MET:CE	2.27	0.58
1:C:1555:ARG:NH2	1:C:1560:ASN:HA	2.17	0.58
1:B:2147:SER:HB3	1:B:2150:GLU:CG	2.33	0.58
1:C:1655:TYR:OH	1:C:1687:ARG:HD3	2.04	0.58
1:C:2041:LEU:HA	1:C:2044:MET:CG	2.33	0.58
1:B:1755:ILE:HD12	1:B:1758:GLY:HA2	1.85	0.58
1:C:2082:LEU:O	1:C:2085:ILE:HG22	2.05	0.57
1:C:1677:THR:HG22	1:C:1690:ILE:HD13	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1660:SER:HB2	1:C:1686:GLU:CB	2.34	0.57
1:C:1824:LYS:HE2	1:C:1824:LYS:H	1.69	0.57
1:A:2041:LEU:O	1:A:2044:MET:N	2.37	0.57
1:A:2138:ARG:HB3	1:A:2186:LEU:HD13	1.86	0.57
1:B:1694:ILE:HA	1:C:2102:ARG:HD3	1.86	0.57
1:A:1676:LEU:HD13	1:A:1694:ILE:HD13	1.86	0.57
1:A:1932:THR:O	1:A:1936:ILE:HG13	2.04	0.57
1:C:1655:TYR:O	1:C:1656:LEU:HD12	2.05	0.57
1:B:1585:VAL:HG13	1:B:1607:VAL:HG11	1.86	0.57
1:B:1708:SER:CB	1:B:1735:ILE:HG13	2.35	0.57
1:C:2041:LEU:HA	1:C:2044:MET:HG2	1.85	0.57
1:A:2003:VAL:HG12	1:A:2003:VAL:O	2.03	0.57
1:C:1607:VAL:O	1:C:1610:TYR:HB3	2.04	0.57
1:B:1785:ASN:HA	1:B:1872:GLY:O	2.05	0.57
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.53	0.57
1:B:1634:GLU:O	1:B:1638:LEU:HD21	2.05	0.56
1:C:2164:ASP:H	1:C:2170:GLN:HE22	1.52	0.56
1:A:1758:GLY:O	1:A:1762:ILE:HG13	2.05	0.56
1:C:1612:ARG:O	1:C:1814:ARG:NH2	2.38	0.56
1:B:1984:PRO:HD3	1:B:2133:GLU:HG3	1.87	0.56
1:A:2100:SER:O	1:A:2104:VAL:HG23	2.05	0.56
1:B:1624:ASN:ND2	1:B:1733:VAL:H	2.04	0.56
1:B:1490:LYS:HG3	1:B:1497:ARG:NH1	2.21	0.56
1:A:1654:GLN:O	1:A:1655:TYR:HB3	2.06	0.56
1:C:1546:GLU:CD	1:C:1546:GLU:H	2.09	0.56
1:B:2085:ILE:O	1:B:2089:ILE:HG13	2.05	0.56
1:A:2183:ASP:CB	1:B:1482:PRO:HG3	2.36	0.56
1:A:2186:LEU:C	1:A:2188:GLY:H	2.07	0.56
1:B:1616:ILE:HD11	3:B:4022:HOH:O	2.06	0.56
1:C:1883:ARG:HA	1:C:1887:ILE:O	2.05	0.56
1:C:1587:ASN:ND2	1:C:1624:ASN:HD22	2.03	0.56
1:A:2128:ARG:HE	1:A:2132:GLU:CD	2.08	0.56
1:A:2179:TYR:HD1	1:B:1489:VAL:HA	1.71	0.56
1:C:1586:ALA:HB2	1:C:1621:LEU:HB2	1.88	0.55
1:B:1991:PRO:HG2	1:B:2115:TRP:HB2	1.88	0.55
1:B:2081:GLU:HB3	1:B:2083:LEU:HD13	1.88	0.55
1:B:2008:ASN:HB3	1:B:2012:MET:HE2	1.88	0.55
1:C:1555:ARG:HH22	1:C:1560:ASN:HA	1.71	0.55
1:A:1902:LEU:HD11	1:A:1914:GLU:CG	2.36	0.55
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.36	0.55
1:B:1494:GLN:HE21	1:B:1496:LYS:HG3	1.69	0.55
1:C:2028:GLN:O	1:C:2031:VAL:HG12	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2185:LYS:O	1:A:2189:LEU:HD13	2.07	0.55
1:B:1530:VAL:HG13	1:B:1530:VAL:O	2.06	0.55
1:A:1645:ASP:OD2	1:A:1647:ALA:HB3	2.06	0.55
1:C:1641:VAL:HG12	1:C:1642:ALA:N	2.22	0.55
1:A:1909:ASN:HB3	1:A:1912:SER:HB3	1.87	0.55
1:B:1991:PRO:CG	1:B:2115:TRP:HB2	2.37	0.55
1:B:1637:PRO:HG2	1:B:1638:LEU:CD2	2.36	0.55
1:A:1902:LEU:HD11	1:A:1914:GLU:HG2	1.88	0.55
1:B:2188:GLY:O	1:B:2190:LYS:N	2.40	0.55
1:C:2180:LYS:NZ	1:C:2180:LYS:HB3	2.22	0.55
1:B:2007:ILE:HB	1:B:2012:MET:CE	2.37	0.54
1:A:1527:SER:O	1:A:1530:VAL:HG22	2.07	0.54
1:B:2021:ARG:NH2	1:B:2099:ARG:NE	2.55	0.54
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.26	0.54
1:B:1786:ASN:HB3	1:B:1788:VAL:HG23	1.89	0.54
1:B:1719:TYR:CE2	1:B:1744:GLN:HG3	2.42	0.54
1:C:1629:ILE:HD12	1:C:1629:ILE:H	1.72	0.54
1:B:1636:VAL:N	1:B:1637:PRO:HD2	2.22	0.54
1:B:2008:ASN:H	1:B:2012:MET:HE2	1.73	0.54
1:B:2008:ASN:H	1:B:2012:MET:CE	2.20	0.54
1:C:1681:VAL:HG13	1:C:1685:GLU:O	2.07	0.54
1:C:1733:VAL:HA	1:C:1755:ILE:O	2.08	0.54
1:B:1624:ASN:HD21	1:B:1733:VAL:H	1.55	0.54
1:C:1670:ASP:C	1:C:1672:GLU:H	2.11	0.54
1:A:1982:LYS:HB2	1:A:1983:GLN:OE1	2.08	0.54
1:C:1719:TYR:CE2	1:C:1744:GLN:HG3	2.42	0.54
1:A:1503:MET:HG2	1:A:1589:ILE:HG12	1.89	0.54
1:C:2146:ALA:O	1:C:2151:LYS:HE3	2.07	0.54
1:B:2146:ALA:O	1:B:2151:LYS:HE3	2.07	0.54
1:A:1636:VAL:N	1:A:1637:PRO:HD2	2.22	0.54
1:A:1768:ARG:HG2	1:A:1769:GLU:N	2.23	0.54
1:B:1730:CYS:HA	1:B:1752:GLN:NE2	2.06	0.54
1:C:1682:ILE:HG21	1:C:1687:ARG:NH1	2.22	0.54
1:C:1648:ASN:CB	1:C:1651:LYS:HD3	2.36	0.53
1:A:1764:LYS:HG2	2:A:3000:RCP:H7	1.89	0.53
1:C:1991:PRO:HG3	1:C:2017:ASP:CG	2.29	0.53
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.57	0.53
1:A:1489:VAL:O	1:A:1493:LEU:HG	2.09	0.53
1:A:2044:MET:HE3	1:A:2082:LEU:HD11	1.91	0.53
1:C:1682:ILE:HG21	1:C:1687:ARG:HH11	1.74	0.53
1:C:2041:LEU:O	1:C:2044:MET:HB2	2.08	0.53
1:B:1616:ILE:HD12	1:B:1813:LYS:HB3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1946:PRO:HG3	1:B:2130:LEU:HD21	1.90	0.53
1:A:2183:ASP:OD1	1:A:2187:LYS:HE3	2.09	0.53
1:A:2189:LEU:O	1:A:2192:GLU:HB2	2.09	0.53
1:B:1631:MET:HE2	1:C:2034:LYS:HB3	1.91	0.53
1:C:1720:HIS:HA	1:C:1941:ASN:HD22	1.74	0.53
1:A:2028:GLN:O	1:A:2031:VAL:HG22	2.09	0.53
1:A:1636:VAL:N	1:A:1637:PRO:CD	2.72	0.52
1:C:1655:TYR:C	1:C:1656:LEU:HD12	2.29	0.52
1:C:1770:VAL:HG13	1:C:1771:TYR:CD1	2.44	0.52
1:A:1635:ILE:HG22	1:A:1635:ILE:O	2.10	0.52
1:B:1866:PHE:CE1	1:B:1868:GLU:HB2	2.44	0.52
1:A:2143:VAL:HB	1:A:2192:GLU:OE2	2.09	0.52
1:C:1633:GLU:HA	1:C:1636:VAL:HG23	1.91	0.52
1:C:2185:LYS:O	1:C:2189:LEU:HD13	2.09	0.52
1:B:1927:ASN:OD1	1:B:1928:SER:N	2.43	0.52
1:A:2041:LEU:HA	1:A:2044:MET:CG	2.40	0.52
1:C:2085:ILE:HG23	1:C:2086:TYR:HD1	1.74	0.52
1:A:2008:ASN:HD22	1:A:2008:ASN:C	2.10	0.52
1:C:1730:CYS:HA	1:C:1752:GLN:OE1	2.09	0.52
1:B:1932:THR:O	1:B:1936:ILE:HG13	2.09	0.52
1:C:2004:ASP:OD2	1:C:2006:THR:HG23	2.10	0.52
3:B:4128:HOH:O	1:C:1925:HIS:HE1	1.92	0.52
1:B:1820:ILE:HD12	1:B:1887:ILE:HG12	1.92	0.52
1:A:1544:GLU:OE1	1:A:1602:GLU:OE2	2.28	0.52
1:C:1645:ASP:O	1:C:1646:ALA:HB2	2.10	0.52
1:B:1877:VAL:CG1	1:B:1931:LYS:HD3	2.36	0.52
1:B:2028:GLN:H	1:B:2028:GLN:CD	2.14	0.51
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.75	0.51
1:B:1633:GLU:HA	1:B:1636:VAL:HG23	1.92	0.51
1:A:1657:TYR:O	1:A:1658:LEU:HD23	2.11	0.51
1:B:1694:ILE:N	1:B:1694:ILE:HD12	2.25	0.51
1:B:1678:GLU:O	1:B:1689:VAL:HG12	2.09	0.51
1:C:1556:GLU:HG3	1:C:1557:PRO:HD2	1.92	0.51
1:A:2160:PRO:HD2	1:A:2163:VAL:CG2	2.41	0.51
1:A:1906:ASP:H	1:A:1912:SER:HB2	1.75	0.51
1:C:1585:VAL:CG2	1:C:1607:VAL:HG11	2.40	0.51
1:A:1648:ASN:O	1:A:1651:LYS:HB2	2.11	0.51
1:C:1494:GLN:N	1:C:1495:PRO:HD2	2.26	0.51
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.10	0.51
1:B:2102:ARG:NH1	1:B:2106:LYS:HG3	2.25	0.51
1:B:2182:LEU:HA	1:B:2185:LYS:HD3	1.92	0.51
1:B:1745:ARG:HG2	1:B:1806:TRP:CZ2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2114:GLU:HB3	3:A:4135:HOH:O	2.09	0.51
1:C:1657:TYR:CG	1:C:1687:ARG:HG3	2.46	0.51
1:C:1661:GLU:HG3	1:C:1662:GLY:N	2.26	0.51
1:C:2136:ILE:HD11	1:C:2152:ILE:CG2	2.41	0.50
1:B:1638:LEU:CD2	1:B:1638:LEU:H	2.19	0.50
1:C:1903:ILE:CD1	1:C:1903:ILE:N	2.73	0.50
1:C:1507:TYR:HB3	1:C:1510:ASP:OD2	2.12	0.50
1:B:2037:ARG:HA	1:B:2040:LEU:HB3	1.93	0.50
1:B:1581:GLN:O	1:B:1616:ILE:HG13	2.12	0.50
1:A:1560:ASN:ND2	1:A:1560:ASN:H	2.08	0.50
1:A:1493:LEU:C	1:A:1494:GLN:HG3	2.31	0.50
1:B:2016:ALA:O	1:B:2112:GLU:HA	2.12	0.50
1:C:1759:ALA:HB3	1:C:1760:PRO:HD3	1.92	0.50
1:C:2138:ARG:HA	1:C:2141:HIS:CD2	2.46	0.50
1:C:2044:MET:HA	1:C:2086:TYR:CE2	2.46	0.50
1:B:1697:GLU:O	1:B:1700:LEU:HD13	2.11	0.50
1:B:1605:ASN:ND2	1:B:1714:ALA:HB2	2.26	0.50
1:B:2167:ASP:O	1:B:2171:VAL:HG23	2.12	0.50
1:B:1780:THR:O	1:B:1784:TYR:HB3	2.12	0.50
1:B:1814:ARG:O	1:B:1815:ASN:HB2	2.12	0.50
1:B:1490:LYS:HG3	1:B:1497:ARG:CZ	2.42	0.50
1:B:1909:ASN:HD22	1:B:1910:PRO:CD	2.25	0.50
1:C:1643:TRP:O	1:C:1645:ASP:N	2.44	0.50
1:C:1780:THR:O	1:C:1784:TYR:HB3	2.11	0.50
1:B:2005:PRO:HD3	1:B:2014:MET:CE	2.42	0.50
1:C:2045:ASN:C	1:C:2045:ASN:ND2	2.64	0.49
1:B:1638:LEU:HD11	1:B:1666:LEU:HD13	1.93	0.49
1:C:1646:ALA:CB	1:C:1651:LYS:HG2	2.38	0.49
1:A:1605:ASN:ND2	1:A:1714:ALA:HB2	2.26	0.49
1:A:1936:ILE:HA	1:A:1947:MET:HE3	1.94	0.49
1:B:1909:ASN:HD22	1:B:1910:PRO:HD2	1.78	0.49
1:A:1755:ILE:HD12	1:A:1758:GLY:HA2	1.93	0.49
1:C:1981:TYR:CB	1:C:1985:ILE:HD11	2.42	0.49
1:A:1682:ILE:O	1:A:1683:ASN:C	2.49	0.49
1:A:1576:TYR:CZ	1:A:1812:ALA:HB2	2.48	0.49
1:B:1835:PRO:HG2	1:B:1846:MET:SD	2.51	0.49
1:A:1614:ARG:HH11	1:A:1614:ARG:HG3	1.77	0.49
1:C:1852:THR:HG22	1:C:1853:GLU:N	2.27	0.49
1:C:1493:LEU:HD12	1:C:1497:ARG:HH12	1.76	0.49
1:A:2143:VAL:HG22	1:A:2144:GLY:N	2.28	0.49
1:C:1586:ALA:CB	1:C:1621:LEU:HB2	2.42	0.49
1:B:2005:PRO:HD3	1:B:2014:MET:HE3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:1829:ARG:NH1	1:C:1858:TYR:HB3	2.28	0.49
1:B:1575:GLU:H	1:B:1575:GLU:CD	2.16	0.49
1:C:1955:GLY:HA2	1:C:1999:SER:OG	2.13	0.49
1:B:1736:GLY:O	1:B:1740:VAL:HG23	2.13	0.49
1:B:1907:PRO:HD2	1:C:1960:GLN:HG2	1.95	0.49
1:A:1681:VAL:HG23	1:A:1681:VAL:O	2.13	0.49
1:C:1636:VAL:O	1:C:1639:PHE:HD2	1.95	0.48
1:A:1814:ARG:O	1:A:1815:ASN:HB2	2.13	0.48
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB3	2.47	0.48
1:B:2156:ARG:HD3	1:B:2159:TYR:CE1	2.48	0.48
1:C:1818:VAL:HG11	1:C:1946:PRO:HD3	1.95	0.48
1:B:2044:MET:HA	1:B:2086:TYR:CE2	2.48	0.48
1:B:1679:ARG:HG3	1:B:1679:ARG:O	2.12	0.48
1:B:1546:GLU:H	1:B:1546:GLU:CD	2.16	0.48
1:B:1766:LEU:HD13	1:B:1770:VAL:HG21	1.94	0.48
1:B:1665:THR:O	1:B:1668:LYS:HB3	2.13	0.48
1:B:1538:ILE:HG22	1:B:1539:SER:N	2.29	0.48
1:A:1759:ALA:HB3	1:A:1760:PRO:HD3	1.95	0.48
1:A:1961:ARG:HH11	1:A:1961:ARG:HB3	1.78	0.48
1:A:2135:LEU:HD21	1:A:2182:LEU:HD13	1.96	0.48
1:C:1657:TYR:CD2	1:C:1687:ARG:HG3	2.49	0.48
1:A:1768:ARG:HE	1:A:1770:VAL:HG22	1.79	0.48
1:B:2096:LEU:HB3	1:C:1693:ILE:HG13	1.96	0.47
1:A:1692:THR:HG22	1:A:1694:ILE:HD12	1.95	0.47
1:A:1824:LYS:H	1:A:1824:LYS:CE	2.27	0.47
1:B:1884:LEU:HD22	1:B:2123:PHE:HB2	1.97	0.47
1:A:1735:ILE:O	1:A:1739:LEU:HG	2.14	0.47
1:C:1527:SER:O	1:C:1530:VAL:HG13	2.13	0.47
1:B:1824:LYS:HG3	1:B:1825:ASP:N	2.28	0.47
1:A:1728:VAL:HG21	1:A:1754:ILE:HD11	1.96	0.47
1:C:1619:ILE:N	1:C:1619:ILE:HD12	2.28	0.47
1:C:1670:ASP:O	1:C:1672:GLU:N	2.45	0.47
1:B:2020:ALA:O	1:B:2021:ARG:HD2	2.14	0.47
1:B:1631:MET:HE1	1:C:2034:LYS:O	2.14	0.47
1:A:2016:ALA:O	1:A:2112:GLU:HA	2.15	0.47
1:A:2044:MET:CE	1:A:2082:LEU:HD11	2.44	0.47
1:C:1575:GLU:CD	1:C:1575:GLU:H	2.18	0.47
1:A:1772:THR:N	1:A:1776:GLN:NE2	2.47	0.47
1:B:2082:LEU:CD2	1:B:2082:LEU:H	2.27	0.47
1:B:1657:TYR:O	1:B:1658:LEU:HD12	2.14	0.47
1:A:2002:VAL:HG13	1:A:2003:VAL:HG23	1.97	0.47
1:A:1783:MET:HA	1:A:1786:ASN:HB2	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1640:GLN:NE2	1:A:1640:GLN:HA	2.30	0.47
1:B:1969:LYS:HG2	1:C:1741:ARG:CZ	2.45	0.47
1:A:2003:VAL:CG1	1:A:2003:VAL:O	2.63	0.47
1:C:1845:TRP:CE2	1:C:1850:ARG:HD3	2.49	0.47
1:C:1513:GLU:O	1:C:1517:GLN:HG3	2.15	0.47
1:A:1547:ASN:ND2	1:A:1547:ASN:N	2.63	0.47
1:B:1587:ASN:HB2	1:B:1623:ALA:O	2.14	0.46
1:A:2190:LYS:C	1:A:2192:GLU:N	2.68	0.46
1:B:2136:ILE:HD11	1:B:2152:ILE:HG12	1.96	0.46
1:C:1909:ASN:O	1:C:1912:SER:HB3	2.15	0.46
1:C:1852:THR:HG22	1:C:1854:SER:H	1.79	0.46
1:B:1619:ILE:N	1:B:1619:ILE:HD12	2.31	0.46
1:B:1727:LEU:HB2	1:B:1803:ILE:HD11	1.96	0.46
1:C:1643:TRP:C	1:C:1645:ASP:H	2.19	0.46
1:B:1679:ARG:HH21	1:B:1681:VAL:HG23	1.81	0.46
1:B:2046:ARG:NH1	1:C:1639:PHE:O	2.49	0.46
1:C:1981:TYR:CG	1:C:1985:ILE:HD11	2.50	0.46
1:C:1635:ILE:HG22	1:C:1635:ILE:O	2.15	0.46
1:C:1510:ASP:O	1:C:1513:GLU:HB3	2.16	0.46
1:B:2040:LEU:HD11	1:B:2086:TYR:O	2.15	0.46
1:A:1497:ARG:HB2	1:A:1497:ARG:HH11	1.80	0.46
1:B:1786:ASN:HD22	1:B:1786:ASN:HA	1.47	0.46
1:C:1682:ILE:HG23	1:C:1682:ILE:O	2.16	0.46
1:B:1665:THR:HA	1:B:1668:LYS:HE3	1.97	0.46
1:C:1868:GLU:HG2	1:C:1871:SER:HB3	1.97	0.46
1:C:2042:ASP:O	1:C:2045:ASN:ND2	2.49	0.46
1:A:1711:ILE:HD12	1:A:1739:LEU:HD11	1.96	0.46
1:A:2005:PRO:HG3	1:A:2014:MET:HB2	1.97	0.46
1:C:1569:ILE:HG22	1:C:1571:VAL:HG23	1.98	0.46
1:C:1634:GLU:O	1:C:1638:LEU:HD21	2.15	0.46
2:B:3000:RCP:O15	1:C:2025:LEU:HB3	2.16	0.46
1:A:1762:ILE:O	1:A:1766:LEU:HD13	2.15	0.46
1:B:1826:THR:O	1:B:2119:ARG:NH1	2.41	0.46
1:B:1906:ASP:N	1:B:1912:SER:OG	2.46	0.46
1:C:2136:ILE:HD11	1:C:2152:ILE:HG22	1.98	0.46
1:B:1610:TYR:CE1	1:B:1614:ARG:CZ	2.99	0.46
1:B:1537:PHE:CD1	1:B:1537:PHE:C	2.89	0.46
1:C:1497:ARG:HA	1:C:1507:TYR:HB2	1.98	0.46
1:C:1730:CYS:O	1:C:1731:ARG:C	2.54	0.46
1:B:1881:ARG:HG2	1:B:1881:ARG:HH11	1.81	0.46
1:B:1633:GLU:O	1:B:1636:VAL:HG23	2.15	0.46
1:C:1646:ALA:C	1:C:1648:ASN:H	2.19	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2160:PRO:HD2	1:C:2163:VAL:CG2	2.41	0.46
1:C:1587:ASN:HB2	1:C:1623:ALA:O	2.15	0.46
1:C:1669:PHE:O	1:C:1670:ASP:HB2	2.16	0.46
1:A:1845:TRP:CE2	1:A:1850:ARG:HD3	2.51	0.46
1:A:1846:MET:HE1	1:A:1990:PRO:HB3	1.97	0.46
1:C:1991:PRO:C	1:C:1992:THR:HG23	2.36	0.45
1:B:1658:LEU:CD1	1:B:1690:ILE:HD11	2.44	0.45
1:B:2102:ARG:HD3	3:B:4116:HOH:O	2.16	0.45
1:B:1966:GLU:HB3	1:B:1969:LYS:HD2	1.99	0.45
1:C:1591:PHE:CD2	1:C:1591:PHE:C	2.89	0.45
1:A:1785:ASN:HA	1:A:1872:GLY:O	2.16	0.45
1:C:1783:MET:CA	1:C:1786:ASN:HB2	2.43	0.45
1:A:1605:ASN:HD22	1:A:1714:ALA:HB2	1.81	0.45
1:C:1701:GLY:O	1:C:1704:CYS:HB2	2.16	0.45
1:A:1988:TYR:HA	1:A:2015:TYR:O	2.16	0.45
1:A:1656:LEU:CB	1:A:1690:ILE:HD11	2.45	0.45
1:C:1654:GLN:O	1:C:1655:TYR:HB3	2.15	0.45
1:A:1676:LEU:HD13	1:A:1694:ILE:CD1	2.46	0.45
1:B:1883:ARG:HA	1:B:1887:ILE:O	2.17	0.45
1:B:2156:ARG:HH11	1:B:2156:ARG:HG3	1.81	0.45
1:B:1571:VAL:O	1:B:1579:GLY:HA2	2.17	0.45
1:A:1820:ILE:HD13	1:B:1487:TYR:CZ	2.52	0.45
1:C:1708:SER:HB3	1:C:1735:ILE:HD13	1.98	0.45
1:A:1662:GLY:O	1:A:1666:LEU:HD23	2.16	0.45
1:C:2143:VAL:HG23	1:C:2143:VAL:O	2.17	0.45
1:C:2092:GLN:HA	1:C:2092:GLN:NE2	2.31	0.45
1:B:2138:ARG:O	1:B:2142:GLN:HG2	2.16	0.45
1:C:1727:LEU:HD12	1:C:1747:ILE:O	2.16	0.45
1:C:1741:ARG:O	1:C:1741:ARG:HD3	2.16	0.45
1:C:1991:PRO:C	1:C:1993:GLY:H	2.20	0.45
1:A:1838:ASP:O	1:A:1839:GLU:HG3	2.16	0.45
1:C:1850:ARG:CG	1:C:1851:GLU:N	2.80	0.45
1:C:1620:TYR:CE1	1:C:1622:ALA:HB2	2.51	0.45
1:A:2041:LEU:C	1:A:2043:THR:N	2.70	0.45
1:C:2037:ARG:O	1:C:2041:LEU:HG	2.16	0.45
1:B:1664:GLU:O	1:B:1668:LYS:HB2	2.17	0.45
1:C:2135:LEU:HB3	1:C:2155:ILE:HD13	1.99	0.45
1:B:1848:GLU:HB2	3:B:4081:HOH:O	2.17	0.45
1:B:1903:ILE:HD11	1:B:1917:ILE:HD12	1.98	0.45
1:A:1555:ARG:HH22	1:A:1560:ASN:HA	1.82	0.45
1:C:1644:ASN:HD21	1:C:1687:ARG:HH12	1.65	0.45
1:A:1676:LEU:HB2	1:A:1692:THR:HB	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1747:ILE:HD12	1:B:1803:ILE:HG13	1.98	0.45
1:B:2184:ASP:O	1:B:2187:LYS:HB3	2.16	0.45
1:C:1526:PHE:CD1	1:C:1574:PRO:HB3	2.52	0.45
1:A:1926:PRO:HD3	1:A:1967:VAL:HB	1.99	0.45
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.52	0.45
1:C:1493:LEU:HB2	1:C:1497:ARG:HH11	1.80	0.44
1:B:2096:LEU:HD13	1:C:1690:ILE:CG2	2.47	0.44
1:C:1894:VAL:HG22	1:C:1953:TRP:CZ2	2.52	0.44
1:C:1844:ARG:HH11	1:C:1844:ARG:HG3	1.82	0.44
1:B:1956:PHE:HB2	1:C:1756:LEU:HD13	1.99	0.44
1:B:2021:ARG:NH2	1:B:2095:ASP:OD1	2.48	0.44
1:B:1637:PRO:HG2	1:B:1638:LEU:H	1.82	0.44
1:B:2083:LEU:N	1:B:2084:PRO:CD	2.81	0.44
1:C:1685:GLU:HB3	1:C:1686:GLU:H	1.58	0.44
1:A:2186:LEU:C	1:A:2188:GLY:N	2.71	0.44
1:A:1493:LEU:O	1:A:1494:GLN:HG3	2.17	0.44
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	2.14	0.44
1:C:1833:PHE:CZ	1:C:1845:TRP:HE3	2.36	0.44
1:A:2159:TYR:OH	1:A:2175:ILE:HD11	2.17	0.44
1:B:2147:SER:CB	1:B:2150:GLU:HG3	2.42	0.44
1:B:1763:ASN:HD21	1:B:1770:VAL:H	1.63	0.44
1:B:1703:GLU:OE2	1:C:2102:ARG:NH2	2.51	0.44
1:C:1786:ASN:HD22	1:C:1786:ASN:HA	1.55	0.44
1:B:2033:ILE:HD11	2:C:3000:RCP:H3	1.99	0.44
1:C:1603:PHE:O	1:C:1607:VAL:HG23	2.16	0.44
2:A:3000:RCP:H291	2:A:3000:RCP:H25	1.81	0.44
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.82	0.44
1:C:2135:LEU:CB	1:C:2155:ILE:HD13	2.48	0.44
1:A:1981:TYR:CB	1:A:1985:ILE:HD11	2.48	0.44
1:B:1798:ALA:O	1:B:1802:LYS:HG3	2.18	0.44
1:B:2085:ILE:O	1:B:2085:ILE:HG22	2.17	0.44
1:C:1625:SER:HB3	1:C:1731:ARG:CZ	2.47	0.44
1:A:1623:ALA:HB2	1:A:1729:THR:HG23	2.00	0.44
1:B:1616:ILE:HD12	1:B:1616:ILE:HA	1.83	0.44
1:A:1817:PRO:HD3	1:B:1484:ALA:HB1	1.99	0.44
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.15	0.44
1:C:1493:LEU:HD11	1:C:1557:PRO:HB2	2.00	0.44
1:A:1741:ARG:HH22	1:A:1934:GLN:HE22	1.63	0.44
1:C:1814:ARG:O	1:C:1815:ASN:HB2	2.18	0.44
1:C:1982:LYS:HB2	1:C:1983:GLN:OE1	2.18	0.44
1:C:1905:ALA:O	1:C:1907:PRO:HD3	2.18	0.44
1:B:1787:GLY:HA3	1:B:1873:TRP:CE3	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1619:ILE:HG13	1:B:1725:ILE:CG2	2.48	0.43
1:C:1591:PHE:CE2	1:C:1592:LYS:HG3	2.53	0.43
1:B:1643:TRP:CZ3	1:B:1649:PRO:HB2	2.53	0.43
1:B:1960:GLN:HG3	1:C:1776:GLN:O	2.18	0.43
1:B:2102:ARG:O	1:B:2106:LYS:HG2	2.18	0.43
1:B:1981:TYR:CB	1:B:1985:ILE:HD11	2.49	0.43
1:A:1844:ARG:HG3	1:A:1844:ARG:HH11	1.82	0.43
1:C:2189:LEU:N	1:C:2189:LEU:HD12	2.34	0.43
1:A:1981:TYR:CG	1:A:1985:ILE:HD11	2.52	0.43
1:A:1954:ARG:HD2	1:A:2026:GLU:OE1	2.18	0.43
1:C:1895:GLU:OE2	1:C:1897:ARG:NH2	2.51	0.43
1:A:2186:LEU:O	1:A:2188:GLY:N	2.52	0.43
2:A:3000:RCP:H281	3:A:4045:HOH:O	2.17	0.43
1:A:2031:VAL:HG11	1:A:2091:LEU:HD12	2.00	0.43
1:B:1576:TYR:N	1:B:1577:PRO:HD3	2.34	0.43
1:A:2043:THR:C	1:A:2045:ASN:N	2.72	0.43
1:A:1925:HIS:O	1:A:1926:PRO:C	2.57	0.43
1:B:1870:LEU:HD22	1:B:1873:TRP:HE3	1.83	0.43
1:C:2154:ARG:HG3	1:C:2154:ARG:HH11	1.83	0.43
1:A:1790:HIS:HD2	3:A:4078:HOH:O	2.01	0.43
1:A:1829:ARG:HG3	1:A:1829:ARG:HH11	1.84	0.43
1:A:1494:GLN:HB3	1:A:1496:LYS:HE3	2.00	0.43
1:C:1844:ARG:O	1:C:1848:GLU:HG2	2.18	0.43
1:B:2035:PHE:CD1	1:B:2039:LYS:HE3	2.54	0.43
1:C:1678:GLU:OE2	1:C:1678:GLU:HA	2.19	0.43
1:C:1747:ILE:HD13	1:C:1802:LYS:CB	2.48	0.43
1:C:1509:TYR:HE1	1:C:1560:ASN:ND2	2.16	0.43
1:A:1682:ILE:HG22	1:A:1685:GLU:O	2.19	0.43
1:C:1571:VAL:O	1:C:1579:GLY:HA2	2.19	0.43
1:A:1745:ARG:NH2	3:A:4035:HOH:O	2.42	0.43
1:C:1737:ALA:O	1:C:1740:VAL:HG22	2.19	0.43
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.67	0.43
1:B:1964:PHE:O	1:C:1786:ASN:ND2	2.47	0.43
1:C:2004:ASP:HA	1:C:2005:PRO:HD3	1.91	0.43
1:A:1566:ALA:HA	1:A:1584:VAL:O	2.18	0.43
1:B:1589:ILE:O	1:B:1593:ILE:HA	2.18	0.43
1:C:1496:LYS:O	1:C:1497:ARG:C	2.57	0.43
1:C:1660:SER:HB2	1:C:1686:GLU:HG3	2.00	0.43
1:B:1868:GLU:HG2	1:B:1871:SER:HB3	2.00	0.43
1:A:1651:LYS:O	1:A:1651:LYS:HE3	2.19	0.43
1:A:1954:ARG:O	1:A:1996:ARG:HB2	2.19	0.43
1:A:1877:VAL:CG2	1:A:1931:LYS:HD3	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2045:ASN:ND2	1:C:2045:ASN:O	2.51	0.42
1:A:1494:GLN:NE2	1:A:1557:PRO:HB2	2.33	0.42
1:B:1790:HIS:O	1:B:1791:LEU:HD13	2.18	0.42
1:B:1702:VAL:CG2	1:C:2108:VAL:HG21	2.49	0.42
1:A:1971:GLY:O	1:A:1974:ILE:HB	2.19	0.42
1:B:2083:LEU:O	1:B:2085:ILE:N	2.52	0.42
1:C:1677:THR:HB	1:C:1688:PHE:HB3	2.01	0.42
1:C:1682:ILE:CG2	1:C:1687:ARG:HD2	2.50	0.42
1:A:1644:ASN:ND2	1:A:1651:LYS:O	2.53	0.42
1:C:1521:SER:O	1:C:1525:ASN:ND2	2.52	0.42
1:A:1780:THR:O	1:A:1784:TYR:HB3	2.19	0.42
1:C:1948:MET:HA	1:C:1986:ILE:O	2.18	0.42
1:B:2000:TRP:C	1:B:2000:TRP:CD1	2.93	0.42
1:B:1833:PHE:HE2	1:B:1835:PRO:HG3	1.85	0.42
1:C:2090:SER:O	1:C:2093:PHE:HB3	2.18	0.42
1:C:2110:SER:O	1:C:2111:LYS:HB2	2.18	0.42
1:A:1677:THR:CG2	1:A:1690:ILE:HG22	2.48	0.42
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.68	0.42
1:C:1894:VAL:HG22	1:C:1953:TRP:CE2	2.54	0.42
1:C:1926:PRO:HG3	1:C:1967:VAL:HB	2.00	0.42
1:B:1636:VAL:N	1:B:1637:PRO:CD	2.82	0.42
1:A:1733:VAL:HA	1:A:1755:ILE:O	2.19	0.42
1:C:1759:ALA:N	1:C:1760:PRO:CD	2.82	0.42
1:B:1972:SER:HB3	1:C:1742:LEU:HD13	2.01	0.42
1:C:1995:LEU:HD12	1:C:1995:LEU:HA	1.91	0.42
1:A:1813:LYS:HG2	1:A:1816:MET:HE3	1.94	0.42
1:A:1675:VAL:HG21	1:A:1690:ILE:HG22	2.02	0.42
1:A:2139:LEU:O	1:A:2143:VAL:HG12	2.20	0.42
1:C:2124:TRP:CZ3	1:C:2169:ARG:HG3	2.54	0.42
1:B:1494:GLN:NE2	1:B:1496:LYS:CG	2.77	0.42
1:B:2156:ARG:HD3	1:B:2159:TYR:HE1	1.84	0.42
1:A:1659:THR:C	1:A:1661:GLU:N	2.72	0.42
1:B:1651:LYS:HB2	3:B:4038:HOH:O	2.19	0.42
1:A:1679:ARG:NE	1:A:1686:GLU:OE1	2.50	0.42
1:C:1669:PHE:C	1:C:1671:LYS:H	2.22	0.42
1:C:2152:ILE:HG13	1:C:2153:ALA:N	2.35	0.42
1:C:1591:PHE:HD2	1:C:1591:PHE:C	2.23	0.42
1:B:1844:ARG:O	1:B:1848:GLU:HG2	2.19	0.42
1:B:1882:ALA:O	1:B:1888:PRO:HA	2.19	0.42
1:B:2149:LEU:HD13	1:B:2149:LEU:O	2.20	0.42
1:C:2043:THR:O	1:C:2043:THR:HG22	2.19	0.42
1:B:1497:ARG:HE	1:B:1497:ARG:HB2	1.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2040:LEU:O	1:A:2043:THR:HB	2.19	0.42
1:A:1677:THR:HG22	1:A:1690:ILE:HG22	2.01	0.42
1:C:1850:ARG:HG2	1:C:1851:GLU:N	2.34	0.42
1:C:1821:LEU:HD23	1:C:1821:LEU:O	2.20	0.42
1:C:1516:ARG:HA	1:C:1537:PHE:CD2	2.55	0.42
1:A:2083:LEU:N	1:A:2084:PRO:CD	2.83	0.42
1:B:2008:ASN:HB3	1:B:2012:MET:CE	2.49	0.41
1:A:1895:GLU:OE2	1:A:1897:ARG:NH1	2.53	0.41
1:B:1708:SER:HB3	1:B:1735:ILE:HG13	2.01	0.41
1:B:1833:PHE:C	1:B:1833:PHE:CD2	2.93	0.41
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	2.02	0.41
1:B:2114:GLU:HB3	3:B:4118:HOH:O	2.20	0.41
1:B:1633:GLU:C	1:B:1635:ILE:H	2.23	0.41
1:C:2031:VAL:HG13	1:C:2032:GLY:N	2.35	0.41
2:C:3000:RCP:H172	2:C:3000:RCP:H211	1.86	0.41
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	2.02	0.41
1:C:2128:ARG:HE	1:C:2132:GLU:CD	2.23	0.41
1:A:2170:GLN:HG3	1:B:1517:GLN:NE2	2.35	0.41
1:A:1881:ARG:CZ	1:A:1939:PHE:HE2	2.32	0.41
1:A:1623:ALA:HB2	1:A:1729:THR:CG2	2.50	0.41
1:B:1605:ASN:HD22	1:B:1714:ALA:HB2	1.84	0.41
1:B:1569:ILE:HG22	1:B:1571:VAL:HG22	2.01	0.41
1:A:1795:ASP:O	1:A:1798:ALA:HB3	2.21	0.41
1:A:1657:TYR:CD2	1:A:1687:ARG:HB3	2.56	0.41
1:B:2008:ASN:CB	1:B:2012:MET:HE2	2.49	0.41
1:B:1763:ASN:ND2	1:B:1770:VAL:N	2.63	0.41
1:B:1995:LEU:HD23	1:B:2000:TRP:CE3	2.56	0.41
1:C:1852:THR:HB	1:C:1855:GLY:O	2.21	0.41
1:C:1818:VAL:HB	1:C:1888:PRO:HG2	2.02	0.41
1:A:1900:GLU:OE2	1:A:1916:LEU:HD21	2.19	0.41
1:B:1586:ALA:HB2	1:B:1621:LEU:HB2	2.01	0.41
1:A:2086:TYR:HA	1:A:2089:ILE:HD12	2.01	0.41
1:A:1909:ASN:HD22	1:A:1910:PRO:CD	2.34	0.41
1:B:1681:VAL:HG22	1:B:1686:GLU:HA	2.01	0.41
1:A:1989:ILE:HA	1:A:1990:PRO:HD3	1.79	0.41
1:A:1790:HIS:O	1:A:1791:LEU:HD23	2.21	0.41
1:C:1991:PRO:HG2	1:C:2115:TRP:CB	2.47	0.41
2:A:3000:RCP:H242	2:A:3000:RCP:H191	1.86	0.41
1:A:1556:GLU:HA	1:A:1557:PRO:HD3	1.93	0.41
1:B:1653:PHE:CD1	1:B:1653:PHE:N	2.88	0.41
1:C:1643:TRP:C	1:C:1645:ASP:N	2.74	0.41
1:C:1648:ASN:O	1:C:1651:LYS:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1494:GLN:CB	1:B:1497:ARG:HH21	2.24	0.41
1:B:1694:ILE:HA	1:C:2102:ARG:CD	2.50	0.41
1:B:2021:ARG:NH2	1:B:2099:ARG:HE	2.18	0.41
1:B:1881:ARG:HG2	1:B:1881:ARG:NH1	2.36	0.41
1:C:1592:LYS:O	1:C:1593:ILE:HG12	2.20	0.41
1:A:1844:ARG:O	1:A:1848:GLU:HG2	2.20	0.41
1:A:1505:THR:HB	1:A:1730:CYS:HB2	2.01	0.41
1:C:2041:LEU:HA	1:C:2044:MET:HG3	2.03	0.41
1:A:2145:GLU:O	1:A:2146:ALA:HB2	2.21	0.41
1:B:1998:GLY:O	1:B:2001:VAL:CG1	2.67	0.41
1:B:1905:ALA:O	1:B:1907:PRO:HD3	2.21	0.41
1:A:1752:GLN:NE2	1:A:1752:GLN:HA	2.35	0.41
1:C:1682:ILE:HG22	1:C:1687:ARG:HD2	2.03	0.41
1:A:1565:VAL:HG12	1:A:1566:ALA:N	2.36	0.41
1:A:2167:ASP:HB3	1:A:2170:GLN:HB3	2.02	0.41
1:A:1756:LEU:HA	1:A:1756:LEU:HD12	1.90	0.41
1:B:1721:ASP:OD2	1:B:1814:ARG:NH1	2.54	0.41
1:A:1784:TYR:CD1	1:A:1792:THR:HG23	2.56	0.41
1:A:1575:GLU:CD	1:A:1575:GLU:H	2.25	0.41
1:C:1637:PRO:HG2	1:C:1638:LEU:H	1.86	0.40
1:A:2190:LYS:O	1:A:2192:GLU:N	2.54	0.40
1:B:1820:ILE:CD1	1:B:1887:ILE:HA	2.51	0.40
1:B:2160:PRO:HD3	1:B:2174:TRP:CZ2	2.56	0.40
1:B:1602:GLU:HG3	1:B:1603:PHE:N	2.36	0.40
1:A:1831:VAL:HB	1:A:2116:THR:HA	2.02	0.40
1:B:1655:TYR:O	1:B:1656:LEU:HD23	2.22	0.40
1:B:2185:LYS:H	1:B:2185:LYS:HD2	1.85	0.40
1:A:2044:MET:HA	1:A:2086:TYR:CE2	2.56	0.40
1:A:1679:ARG:HB2	1:A:1688:PHE:CE2	2.56	0.40
1:C:1920:PRO:HD2	1:C:1925:HIS:CE1	2.56	0.40
1:B:1834:THR:HA	1:B:1835:PRO:HD3	1.86	0.40
1:C:1827:TRP:CG	1:C:1828:ASP:N	2.89	0.40
1:A:1491:GLU:O	1:A:1495:PRO:HA	2.22	0.40
1:A:1772:THR:HB	1:A:1776:GLN:NE2	2.36	0.40
1:C:1680:THR:O	1:C:1687:ARG:HB3	2.21	0.40
1:C:1591:PHE:CD2	1:C:1592:LYS:HG3	2.57	0.40
1:C:2108:VAL:HG23	1:C:2109:ILE:HG23	2.03	0.40
1:C:2043:THR:O	1:C:2046:ARG:HB2	2.22	0.40
1:B:1948:MET:HA	1:B:1986:ILE:O	2.21	0.40
1:B:1899:VAL:HB	1:B:1919:GLU:HB2	2.02	0.40
1:C:1682:ILE:O	1:C:1683:ASN:C	2.59	0.40
1:C:2085:ILE:O	1:C:2089:ILE:HG13	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1586:ALA:HB2	1:A:1621:LEU:HB2	2.02	0.40
1:B:2001:VAL:HG23	1:C:1709:GLY:HA2	2.04	0.40
1:B:1705:LEU:HD21	1:C:1997:GLY:HA2	2.04	0.40
1:C:1499:LYS:O	1:C:1503:MET:HG2	2.22	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	678/758 (89%)	618 (91%)	52 (8%)	8 (1%)	19	54
1	B	672/758 (89%)	611 (91%)	51 (8%)	10 (2%)	15	46
1	C	662/758 (87%)	588 (89%)	64 (10%)	10 (2%)	15	46
All	All	2012/2274 (88%)	1817 (90%)	167 (8%)	28 (1%)	16	49

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2145	GLU
1	B	2189	LEU
1	C	1644	ASN
1	A	1684	GLY
1	A	1997	GLY
1	A	2146	ALA
1	B	1997	GLY
1	B	2142	GLN
1	C	1508	VAL
1	C	1534	ASP
1	C	1671	LYS
1	C	1997	GLY
1	A	2187	LYS
1	B	1839	GLU
1	C	1646	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1655	TYR
1	C	1683	ASN
1	C	2144	GLY
1	A	1530	VAL
1	A	1645	ASP
1	A	2191	LEU
1	B	1533	THR
1	A	1744	GLN
1	B	2084	PRO
1	B	1637	PRO
1	B	2032	GLY
1	C	1637	PRO
1	B	1557	PRO

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	577/648 (89%)	548 (95%)	29 (5%)	34	70
1	B	572/648 (88%)	534 (93%)	38 (7%)	24	56
1	C	563/648 (87%)	522 (93%)	41 (7%)	20	49
All	All	1712/1944 (88%)	1604 (94%)	108 (6%)	25	59

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1497	ARG
1	A	1532	LEU
1	A	1534	ASP
1	A	1560	ASN
1	A	1585	VAL
1	A	1602	GLU
1	A	1618	ARG
1	A	1634	GLU
1	A	1651	LYS
1	A	1733	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1756	LEU
1	A	1765	MET
1	A	1781	GLN
1	A	1879	VAL
1	A	1884	LEU
1	A	1924	TRP
1	A	1930	PHE
1	A	1950	LEU
1	A	1961	ARG
1	A	1981	TYR
1	A	2002	VAL
1	A	2008	ASN
1	A	2042	ASP
1	A	2082	LEU
1	A	2091	LEU
1	A	2128	ARG
1	A	2135	LEU
1	A	2142	GLN
1	A	2143	VAL
1	B	1497	ARG
1	B	1502	LEU
1	B	1508	VAL
1	B	1516	ARG
1	B	1534	ASP
1	B	1536	PHE
1	B	1555	ARG
1	B	1583	VAL
1	B	1585	VAL
1	B	1602	GLU
1	B	1616	ILE
1	B	1618	ARG
1	B	1639	PHE
1	B	1648	ASN
1	B	1653	PHE
1	B	1726	THR
1	B	1735	ILE
1	B	1777	LEU
1	B	1786	ASN
1	B	1791	LEU
1	B	1792	THR
1	B	1797	LEU
1	B	1824	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1843	VAL
1	B	1884	LEU
1	B	1909	ASN
1	B	1924	TRP
1	B	1930	PHE
1	B	1961	ARG
1	B	1980	ASP
1	B	1981	TYR
1	B	2035	PHE
1	B	2041	LEU
1	B	2086	TYR
1	B	2092	GLN
1	B	2127	ARG
1	B	2128	ARG
1	B	2179	TYR
1	C	1499	LYS
1	C	1508	VAL
1	C	1511	PHE
1	C	1536	PHE
1	C	1542	LEU
1	C	1565	VAL
1	C	1591	PHE
1	C	1602	GLU
1	C	1618	ARG
1	C	1629	ILE
1	C	1638	LEU
1	C	1639	PHE
1	C	1740	VAL
1	C	1741	ARG
1	C	1742	LEU
1	C	1772	THR
1	C	1781	GLN
1	C	1786	ASN
1	C	1792	THR
1	C	1824	LYS
1	C	1879	VAL
1	C	1895	GLU
1	C	1898	THR
1	C	1902	LEU
1	C	1924	TRP
1	C	1930	PHE
1	C	1945	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1950	LEU
1	C	1960	GLN
1	C	1961	ARG
1	C	1968	LEU
1	C	1978	LEU
1	C	1980	ASP
1	C	1981	TYR
1	C	2045	ASN
1	C	2046	ARG
1	C	2047	LEU
1	C	2102	ARG
1	C	2114	GLU
1	C	2128	ARG
1	C	2142	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1494	GLN
1	A	1522	GLN
1	A	1547	ASN
1	A	1560	ASN
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1640	GLN
1	A	1644	ASN
1	A	1748	GLN
1	A	1752	GLN
1	A	1776	GLN
1	A	1781	GLN
1	A	1790	HIS
1	A	1815	ASN
1	A	1909	ASN
1	A	1925	HIS
1	A	1934	GLN
1	A	1960	GLN
1	A	2008	ASN
1	A	2088	GLN
1	A	2092	GLN
1	A	2097	HIS
1	A	2131	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2170	GLN
1	B	1494	GLN
1	B	1517	GLN
1	B	1525	ASN
1	B	1587	ASN
1	B	1605	ASN
1	B	1624	ASN
1	B	1644	ASN
1	B	1648	ASN
1	B	1654	GLN
1	B	1683	ASN
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1786	ASN
1	B	1815	ASN
1	B	1909	ASN
1	B	1911	ASN
1	B	1941	ASN
1	B	1944	GLN
1	B	2028	GLN
1	B	2045	ASN
1	B	2097	HIS
1	B	2131	ASN
1	C	1517	GLN
1	C	1522	GLN
1	C	1525	ASN
1	C	1560	ASN
1	C	1587	ASN
1	C	1605	ASN
1	C	1640	GLN
1	C	1644	ASN
1	C	1654	GLN
1	C	1683	ASN
1	C	1748	GLN
1	C	1774	ASN
1	C	1776	GLN
1	C	1781	GLN
1	C	1786	ASN
1	C	1815	ASN
1	C	1909	ASN
1	C	1911	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1918	GLN
1	C	1922	GLN
1	C	1925	HIS
1	C	1934	GLN
1	C	1941	ASN
1	C	1960	GLN
1	C	1965	ASN
1	C	2011	GLN
1	C	2045	ASN
1	C	2092	GLN
1	C	2141	HIS
1	C	2142	GLN
1	C	2170	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	RCP	A	3000	-	41,41,41	1.00	1 (2%)	58,58,58	1.36	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	RCP	B	3000	-	41,41,41	1.00	1 (2%)	58,58,58	1.34	7 (12%)
2	RCP	C	3000	-	41,41,41	1.00	1 (2%)	58,58,58	1.37	7 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RCP	A	3000	-	-	0/20/48/48	0/3/6/6
2	RCP	B	3000	-	-	0/20/48/48	0/3/6/6
2	RCP	C	3000	-	-	0/20/48/48	0/3/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3000	RCP	C14-C15	3.77	1.53	1.50
2	B	3000	RCP	C14-C15	3.69	1.53	1.50
2	A	3000	RCP	C14-C15	3.66	1.53	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3000	RCP	C27-N26-C29	4.40	120.92	112.52
2	B	3000	RCP	C27-N26-C29	4.09	120.31	112.52
2	A	3000	RCP	C16-N15-C18	3.81	119.78	112.52
2	A	3000	RCP	C27-N26-C29	3.80	119.76	112.52
2	A	3000	RCP	C25-C26-N26	3.75	121.34	118.05
2	B	3000	RCP	C16-N15-C18	3.69	119.56	112.52
2	C	3000	RCP	C16-N15-C18	3.62	119.41	112.52
2	C	3000	RCP	C25-C26-N26	3.47	121.08	118.05
2	C	3000	RCP	C14-C15-N15	3.41	121.15	117.89
2	A	3000	RCP	C14-C15-N15	3.36	121.11	117.89
2	B	3000	RCP	C25-C26-N26	3.25	120.89	118.05
2	B	3000	RCP	C14-C15-N15	3.03	120.79	117.89
2	C	3000	RCP	C12-C13-C14	-2.28	120.71	123.02
2	B	3000	RCP	O26-C26-N26	-2.27	118.94	121.65
2	B	3000	RCP	C12-C13-C14	-2.25	120.73	123.02
2	B	3000	RCP	C2-C1-C14	-2.25	120.74	123.02
2	C	3000	RCP	O26-C26-N26	-2.23	118.99	121.65
2	A	3000	RCP	C2-C1-C14	-2.22	120.76	123.02
2	A	3000	RCP	O26-C26-N26	-2.22	119.00	121.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3000	RCP	C12-C13-C14	-2.19	120.80	123.02
2	C	3000	RCP	C2-C1-C14	-2.15	120.83	123.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	682/758 (89%)	-0.25	25 (3%)	39 39	22, 47, 98, 99	0
1	B	676/758 (89%)	-0.22	29 (4%)	34 34	24, 49, 99, 99	0
1	C	666/758 (87%)	-0.29	23 (3%)	42 42	22, 49, 99, 99	0
All	All	2024/2274 (89%)	-0.25	77 (3%)	38 38	22, 48, 99, 99	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2082	LEU	6.8
1	C	1644	ASN	5.8
1	B	1680	THR	5.2
1	B	1492	TRP	5.2
1	B	1683	ASN	5.1
1	A	1483	ILE	4.9
1	A	1492	TRP	4.9
1	C	2143	VAL	4.6
1	C	2037	ARG	4.4
1	B	1682	ILE	4.1
1	B	2083	LEU	4.0
1	A	1681	VAL	3.9
1	B	2189	LEU	3.8
1	C	2144	GLY	3.7
1	B	1649	PRO	3.7
1	B	1669	PHE	3.6
1	B	2037	ARG	3.5
1	B	1685	GLU	3.4
1	C	1645	ASP	3.3
1	C	1647	ALA	3.2
1	A	2047	LEU	3.2
1	B	1679	ARG	3.2
1	B	1531	LYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1684	GLY	3.1
1	A	1489	VAL	3.1
1	C	1685	GLU	3.0
1	B	1681	VAL	3.0
1	B	2086	TYR	3.0
1	C	1680	THR	2.9
1	A	2037	ARG	2.9
1	C	1649	PRO	2.8
1	A	1683	ASN	2.8
1	B	1648	ASN	2.8
1	A	1482	PRO	2.8
1	A	1679	ARG	2.7
1	A	2195	ALA	2.7
1	C	2141	HIS	2.7
1	C	1911	ASN	2.7
1	B	2187	LYS	2.6
1	C	2142	GLN	2.6
1	A	2144	GLY	2.6
1	B	1768	ARG	2.6
1	A	1911	ASN	2.6
1	B	1556	GLU	2.5
1	B	2044	MET	2.5
1	C	1648	ASN	2.4
1	A	1685	GLU	2.4
1	C	1678	GLU	2.4
1	A	1647	ALA	2.4
1	A	1684	GLY	2.4
1	A	1669	PHE	2.4
1	C	1838	ASP	2.3
1	C	2044	MET	2.3
1	C	1679	ARG	2.3
1	A	2194	PHE	2.3
1	B	1483	ILE	2.2
1	B	2040	LEU	2.2
1	A	1853	GLU	2.2
1	B	2145	GLU	2.2
1	C	1651	LYS	2.2
1	C	2082	LEU	2.2
1	A	2145	GLU	2.2
1	A	2191	LEU	2.2
1	B	1647	ALA	2.1
1	A	1855	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1646	ALA	2.1
1	B	2180	LYS	2.1
1	C	2145	GLU	2.1
1	A	1652	GLY	2.1
1	A	2143	VAL	2.1
1	B	1644	ASN	2.1
1	A	1838	ASP	2.0
1	B	2144	GLY	2.0
1	B	1651	LYS	2.0
1	C	1681	VAL	2.0
1	A	2036	ARG	2.0
1	C	1534	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	RCP	C	3000	36/36	0.23	2.29	73,87,94,95	0
2	RCP	B	3000	36/36	0.19	0.77	58,63,71,71	0
2	RCP	A	3000	36/36	0.18	0.46	60,68,69,70	0

6.5 Other polymers ⓘ

There are no such residues in this entry.