

Full wwPDB X-ray Structure Validation Report (i)

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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)
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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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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.



Motria	Whole archive	Similar resolution		
wietric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R_{free}	130704	3140 (2.80-2.80)		
Clashscore	141614	3569 (2.80-2.80)		
Ramachandran outliers	138981	3498 (2.80-2.80)		
Sidechain outliers	138945	3500 (2.80-2.80)		
RSRZ outliers	127900	3078 (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 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	А	758	3% 57%	31%	• 10%		
1	В	758	4% 52%	35%	• 11%		
1	С	758	53%	31%	12%		



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16588 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1 A	682	Total	С	Ν	Ο	S	0	0	1	
		5425	3459	931	1016	19				
1	1 D	676	Total	С	Ν	Ο	S	0	0	1
I D	070	5377	3427	924	1007	19	0	0		
1	С	666	Total	С	Ν	Ο	S	0	0	1
	000	5299	3374	913	993	19	0	0	1	

• Molecule 1 is a protein called ACETYL-COA CARBOXYLASE.

• 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	Δ	1	Total	С	Ν	0	0	0
	1	36	30	3	3	0	0	
9	В	1	Total	С	Ν	Ο	0	0
	1	36	30	3	3	0	0	
0	С	1	Total	С	Ν	Ο	0	0
	U		36	30	3	3	0	0



• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	147	Total O 147 147	0	0
3	В	128	Total O 128 128	0	0
3	С	104	Total O 104 104	0	0



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











4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	246.59Å 124.60Å 145.60Å	Depositor
a, b, c, α , β , γ	90.00° 93.85° 90.00°	Depositor
Resolution(A)	29.66 - 2.80	Depositor
Resolution (A)	29.66 - 2.78	EDS
% Data completeness	85.7 (29.66-2.80)	Depositor
(in resolution range)	88.7 (29.66-2.78)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.61 (at 2.76 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
P. P.	0.197 , 0.234	Depositor
n, n_{free}	0.200 , 0.238	DCC
R_{free} test set	10186 reflections (9.92%)	wwPDB-VP
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 , 58.7	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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).

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.39	0/5547	0.61	0/7516	
1	В	0.39	0/5498	0.62	0/7451	
1	С	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 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	А	5425	0	5365	209	0
1	В	5377	0	5316	236	0
1	С	5299	0	5234	248	0
2	А	36	0	35	4	0
2	В	36	0	35	2	0
2	С	36	0	35	3	0
3	А	147	0	0	4	0
3	В	128	0	0	7	0
3	С	104	0	0	1	0
All	All	16588	0	16020	669	0



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (669) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom_2	Interatomic	Clash
Atom-1	At0111-2	distance $(Å)$	overlap (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:B:1836:THR:HB	1:B:1839:GLU:HB3	1.62	0.80
1:C:1772:THR:N	1:C:1776:GLN:HE22	1.75	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:1493:LEU:HB2	1:C:1497:ARG:NH1	1.99	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: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
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



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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:B:1511:PHE:CZ	1:B:1729:THR:HG21	2.22	0.74
1:C:1773:SER:H	1:C:1776:GLN:NE2	1.84	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:B:2007:ILE:HB	1:B:2012:MET:HE3	1.70	0.74
1:C:1625:SER:HB3	1:C:1731:ARG:NH2	2.02	0.74
1:C:1638:LEU:HD23	1:C:1638:LEU:H	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:HH11	1:C:2138:ARG:HB3	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:1764:LYS:HD2	2:C:3000:RCP:H5	1.71	0.71
1:C:1783:MET:HA	1:C:1786:ASN:HB2	1.72	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:HB3	1:C:2036:ARG:NH1	2.07	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:1550:LEU:HD21	1:C:1607:VAL:HG22	1.74	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
1:B:1998:GLY:O	1:B:2001:VAL:HG12	1.95	0.67



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:1936:ILE:HD13	1:C:1978:LEU:HD13	1.76	0.67
1:B:1815:ASN:H	1:B:1944:GLN:NE2	1.82	0.67
1:B:2189:LEU:HD23	1:B:2189:LEU:H	1.59	0.67
1:C:2138:ARG:HB3	1:C:2138:ARG:NH1	2.10	0.67
1:B:2082:LEU:HD23	1:B:2082:LEU:H	1.58	0.67
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	1.94	0.67
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.42	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:1677:THR:HG22	1:A:1690:ILE:HA	1.77	0.66
1:A:2041:LEU:HA	1:A:2044:MET:HG2	1.75	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:B:1735:ILE:HD13	1:B:1739:LEU:HG	1.79	0.65
1:C:2036:ARG:HB3	1:C:2036:ARG:HH11	1.61	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:A:1632:ALA:HB1	1:A:1634:GLU:OE2	1.97	0.64
1:B:2047:LEU:HD21	1:C:1649:PRO:HG3	1.78	0.64
1:A:2040:LEU:HD21	1:A:2086:TYR:HB3	1.79	0.64
1:B:1735:ILE:HD13	1:B:1735:ILE:O	1.96	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:1772:THR:HG23	1:C:1776:GLN:NE2	2.12	0.64
1:A:2044:MET:SD	1:A:2082:LEU:HD11	2.38	0.64
1:C:1909:ASN:ND2	1:C:1912:SER:HB2	2.13	0.64
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.47	0.63
1:B:2008:ASN:N	1:B:2012:MET:CE	2.62	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:1660:SER:HB2	1:C:1686:GLU:HB2	1.82	0.62
1:C:2045:ASN:C	1:C:2045:ASN:HD22	2.03	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (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:1681:VAL:HA	1:B:1685:GLU:O	2.01	0.61
1:B:1909:ASN:HD21	1:B:1911:ASN:ND2	1.99	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:A:1824:LYS:HE2	1:A:1824:LYS:H	1.65	0.60
1:B:1637:PRO:HG2	1:B:1638:LEU:HD23	1.82	0.60
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	2.16	0.60
1:C:1960:GLN:HG3	1:C:1961:ARG:N	2.12	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:1560:ASN:H	1:A:1560:ASN:HD22	1.51	0.58
1:A:1813:LYS:CG	1:A:1816:MET:HE2	2.29	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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:1660:SER:HB2	1:C:1686:GLU:CB	2.34	0.57
1:C:1677:THR:HG22	1:C:1690:ILE:HD13	1.85	0.57
1:C:1824:LYS:H	1:C:1824:LYS:HE2	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:B:1585:VAL:HG13	1:B:1607:VAL:HG11	1.86	0.57
1:C:1655:TYR:O	1:C:1656:LEU:HD12	2.05	0.57
1:A:2003:VAL:HG12	1:A:2003:VAL:O	2.03	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:B:1785:ASN:HA	1:B:1872:GLY:O	2.05	0.57
1:C:1607:VAL:O	1:C:1610:TYR:HB3	2.04	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: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:1984:PRO:HD3	1:B:2133:GLU:HG3	1.87	0.56
1:A:1654:GLN:O	1:A:1655:TYR:HB3	2.06	0.56
1:B:1490:LYS:HG3	1:B:1497:ARG:NH1	2.21	0.56
1:C:1546:GLU:CD	1:C:1546:GLU:H	2.09	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:B:2085:ILE:O	1:B:2089:ILE:HG13	2.05	0.56
1:C:1883:ARG:HA	1:C:1887:ILE:O	2.05	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:1587:ASN:ND2	1:C:1624:ASN:HD22	2.03	0.56
1:B:1991:PRO:HG2	1:B:2115:TRP:HB2	1.88	0.55
1:C:1586:ALA:HB2	1:C:1621:LEU:HB2	1.88	0.55
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.36	0.55
1:A:1902:LEU:HD11	1:A:1914:GLU:CG	2.36	0.55
1:B:2008:ASN:HB3	1:B:2012:MET:HE2	1.88	0.55
1:B:2081:GLU:HB3	1:B:2083:LEU:HD13	1.88	0.55
1:C:1555:ARG:HH22	1:C:1560:ASN:HA	1.71	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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
1:A:2185:LYS:O	1:A:2189:LEU:HD13	2.07	0.55
1:B:1530:VAL:O	1:B:1530:VAL:HG13	2.06	0.55
1:A:1645:ASP:OD2	1:A:1647:ALA:HB3	2.06	0.55
1:A:1909:ASN:HB3	1:A:1912:SER:HB3	1.87	0.55
1:C:1641:VAL:HG12	1:C:1642:ALA:N	2.22	0.55
1:B:1991:PRO:CG	1:B:2115:TRP:HB2	2.37	0.55
1:A:1902:LEU:HD11	1:A:1914:GLU:HG2	1.88	0.55
1:B:1637:PRO:HG2	1:B:1638:LEU:CD2	2.36	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:A:1527:SER:O	1:A:1530:VAL:HG22	2.07	0.54
1:B:2007:ILE:HB	1:B:2012:MET:CE	2.37	0.54
1:B:2021:ARG:NH2	1:B:2099:ARG:NE	2.55	0.54
1:B:1786:ASN:HB3	1:B:1788:VAL:HG23	1.89	0.54
1:B:2097:HIS:CE1	1:C:1632:ALA:H	2.26	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:1624:ASN:HD21	1:B:1733:VAL:H	1.55	0.54
1:B:2008:ASN:H	1:B:2012:MET:CE	2.20	0.54
1:C:1670:ASP:C	1:C:1672:GLU:H	2.11	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:A:1503:MET:HG2	1:A:1589:ILE:HG12	1.89	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:B:2146:ALA:O	1:B:2151:LYS:HE3	2.07	0.54
1:C:2146:ALA:O	1:C: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:A:1764:LYS:HG2	2:A:3000:RCP:H7	1.89	0.53
1:C:1648:ASN:CB	1:C:1651:LYS:HD3	2.36	0.53
1:B:2097:HIS:HE1	1:C:1632:ALA:H	1.57	0.53
1:C:1991:PRO:HG3	1:C:2017:ASP:CG	2.29	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



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:1616:ILE:HD12	1:B:1813:LYS:HB3	1.91	0.53
1:B:1946:PRO:HG3	1:B:2130:LEU:HD21	1.90	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: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:A:2028:GLN:O	1:A:2031:VAL:HG22	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:1635:ILE:HG22	1:A:1635:ILE:O	2.10	0.52
1:A:1636:VAL:N	1:A:1637:PRO:CD	2.72	0.52
1:B:1866:PHE:CE1	1:B:1868:GLU:HB2	2.44	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: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:2008:ASN:C	1:A:2008:ASN:HD22	2.10	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:B:1932:THR:O	1:B:1936:ILE:HG13	2.09	0.52
1:C:1730:CYS:HA	1:C:1752:GLN:OE1	2.09	0.52
3:B:4128:HOH:O	1:C:1925:HIS:HE1	1.92	0.52
1:C:2004:ASP:OD2	1:C:2006:THR:HG23	2.10	0.52
1:A:1544:GLU:OE1	1:A:1602:GLU:OE2	2.28	0.52
1:B:1820:ILE:HD12	1:B:1887:ILE:HG12	1.92	0.52
1:B:1877:VAL:CG1	1:B:1931:LYS:HD3	2.36	0.52
1:C:1645:ASP:O	1:C:1646:ALA:HB2	2.10	0.52
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.75	0.51
1:B:2028:GLN:H	1:B:2028:GLN:CD	2.14	0.51
1:A:1657:TYR:O	1:A:1658:LEU:HD23	2.11	0.51
1:B:1633:GLU:HA	1:B:1636:VAL:HG23	1.92	0.51
1:B:1678:GLU:O	1:B:1689:VAL:HG12	2.09	0.51
1:B:1694:ILE:N	1:B:1694:ILE:HD12	2.25	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: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:C:1585:VAL:CG2	1:C:1607:VAL:HG11	2.40	0.51



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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:A:2114:GLU:HB3	3:A:4135:HOH:O	2.09	0.51
1:B:1745:ARG:HG2	1:B:1806:TRP:CZ2	2.46	0.51
1:B:2182:LEU:HA	1:B:2185:LYS:HD3	1.92	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:H	1:B:1638:LEU:CD2	2.19	0.50
1:C:1903:ILE:N	1:C:1903:ILE:CD1	2.73	0.50
1:B:1581:GLN:O	1:B:1616:ILE:HG13	2.12	0.50
1:B:2037:ARG:HA	1:B:2040:LEU:HB3	1.93	0.50
1:C:1507:TYR:HB3	1:C:1510:ASP:OD2	2.12	0.50
1:A:1493:LEU:C	1:A:1494:GLN:HG3	2.31	0.50
1:A:1560:ASN:H	1:A:1560:ASN:ND2	2.08	0.50
1:B:2016:ALA:O	1:B:2112:GLU:HA	2.12	0.50
1:B:1605:ASN:ND2	1:B:1714:ALA:HB2	2.26	0.50
1:B:1697:GLU:O	1:B:1700:LEU:HD13	2.11	0.50
1:C:1759:ALA:HB3	1:C:1760:PRO:HD3	1.92	0.50
1:C:2044:MET:HA	1:C:2086:TYR:CE2	2.46	0.50
1:C:2138:ARG:HA	1:C:2141:HIS:CD2	2.46	0.50
1:B:1780:THR:O	1:B:1784:TYR:HB3	2.12	0.50
1:B:2167:ASP:O	1:B:2171:VAL:HG23	2.12	0.50
1:B:1490:LYS:HG3	1:B:1497:ARG:CZ	2.42	0.50
1:B:1814:ARG:O	1:B:1815:ASN:HB2	2.12	0.50
1:B:1909:ASN:HD22	1:B:1910:PRO:CD	2.25	0.50
1:B:2005:PRO:HD3	1:B:2014:MET:CE	2.42	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:C:2045:ASN:C	1:C:2045:ASN:ND2	2.64	0.49
1:A:1605:ASN:ND2	1:A:1714:ALA:HB2	2.26	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: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:1682:ILE:O	1:A:1683:ASN:C	2.49	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:1576:TYR:CZ	1:A:1812:ALA:HB2	2.48	0.49
1:A:1614:ARG:HG3	1:A:1614:ARG:HH11	1.77	0.49
1:B:1835:PRO:HG2	1:B:1846:MET:SD	2.51	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:1852:THR:HG22	1:C:1853:GLU:N	2.27	0.49
1:A:2143:VAL:HG22	1:A:2144:GLY:N	2.28	0.49
1:B:2005:PRO:HD3	1:B:2014:MET:HE3	1.93	0.49
1:C:1493:LEU:HD12	1:C:1497:ARG:HH12	1.76	0.49
1:C:1586:ALA:CB	1:C:1621:LEU:HB2	2.42	0.49
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:B:1736:GLY:O	1:B:1740:VAL:HG23	2.13	0.49
1:C:1955:GLY:HA2	1:C:1999:SER:OG	2.13	0.49
1:A:1681:VAL:HG23	1:A:1681:VAL:O	2.13	0.49
1:B:1907:PRO:HD2	1:C:1960:GLN:HG2	1.95	0.49
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB3	2.47	0.48
1:A:1814:ARG:O	1:A:1815:ASN:HB2	2.13	0.48
1:B:2156:ARG:HD3	1:B:2159:TYR:CE1	2.48	0.48
1:C:1636:VAL:O	1:C:1639:PHE:HD2	1.95	0.48
1:C:1818:VAL:HG11	1:C:1946:PRO:HD3	1.95	0.48
1:B:1546:GLU:H	1:B:1546:GLU:CD	2.16	0.48
1:B:1679:ARG:O	1:B:1679:ARG:HG3	2.12	0.48
1:B:2044:MET:HA	1:B:2086:TYR:CE2	2.48	0.48
1:B:1766:LEU:HD13	1:B:1770:VAL:HG21	1.94	0.48
1:B:1538:ILE:HG22	1:B:1539:SER:N	2.29	0.48
1:B:1665:THR:O	1:B:1668:LYS:HB3	2.13	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:1768:ARG:HE	1:A:1770:VAL:HG22	1.79	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:1692:THR:HG22	1:A:1694:ILE:HD12	1.95	0.47
1:B:2096:LEU:HB3	1:C:1693:ILE:HG13	1.96	0.47
1:A:1735:ILE:O	1:A:1739:LEU:HG	2.14	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:C:1527:SER:O	1:C:1530:VAL:HG13	2.13	0.47
1:A:1728:VAL:HG21	1:A:1754:ILE:HD11	1.96	0.47
1:B:1824:LYS:HG3	1:B:1825:ASP:N	2.28	0.47
1:C:1619:ILE:HD12	1:C:1619:ILE:N	2.28	0.47
1:C:1670:ASP:O	1:C:1672:GLU:N	2.45	0.47
1:A:2016:ALA:O	1:A:2112:GLU:HA	2.15	0.47
1:B:1631:MET:HE1	1:C:2034:LYS:O	2.14	0.47
1:B:2020:ALA:O	1:B:2021:ARG:HD2	2.14	0.47
1:A:2044:MET:CE	1:A:2082:LEU:HD11	2.44	0.47



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:1575:GLU:CD	1:C:1575:GLU:H	2.18	0.47
1:A:1640:GLN:HA	1:A:1640:GLN:NE2	2.30	0.47
1:A:1772:THR:N	1:A:1776:GLN:NE2	2.47	0.47
1:A:1783:MET:HA	1:A:1786:ASN:HB2	1.95	0.47
1:A:2002:VAL:HG13	1:A:2003:VAL:HG23	1.97	0.47
1:B:1657:TYR:O	1:B:1658:LEU:HD12	2.14	0.47
1:B:1969:LYS:HG2	1:C:1741:ARG:CZ	2.45	0.47
1:B:2082:LEU:H	1:B:2082:LEU:CD2	2.27	0.47
1:A:2003:VAL:O	1:A:2003:VAL:CG1	2.63	0.47
1:C:1845:TRP:CE2	1:C:1850:ARG:HD3	2.49	0.47
1:A:1547:ASN:N	1:A:1547:ASN:ND2	2.63	0.47
1:C:1513:GLU:O	1:C:1517:GLN:HG3	2.15	0.47
1:A:2190:LYS:C	1:A:2192:GLU:N	2.68	0.46
1:B:1587:ASN:HB2	1:B:1623:ALA:O	2.14	0.46
1:B:2136:ILE:HD11	1:B:2152:ILE:HG12	1.96	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:1852:THR:HG22	1:C:1854:SER:H	1.79	0.46
1:C:1909:ASN:O	1:C:1912:SER:HB3	2.15	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:1635:ILE:HG22	1:C:1635:ILE:O	2.15	0.46
1:C:1643:TRP:C	1:C:1645:ASP:H	2.19	0.46
1:C:1981:TYR:CG	1:C:1985:ILE:HD11	2.50	0.46
1:A:1497:ARG:HH11	1:A:1497:ARG:HB2	1.80	0.46
1:B:1786:ASN:HD22	1:B:1786:ASN:HA	1.47	0.46
1:B:2040:LEU:HD11	1:B:2086:TYR:O	2.15	0.46
1:C:1510:ASP:O	1:C:1513:GLU:HB3	2.16	0.46
1:B:1665:THR:HA	1:B:1668:LYS:HE3	1.97	0.46
1:C:1682:ILE:HG23	1:C:1682:ILE:O	2.16	0.46
1:C:1868:GLU:HG2	1:C:1871:SER:HB3	1.97	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:2042:ASP:O	1:C:2045:ASN:ND2	2.49	0.46
1:A:1762:ILE:O	1:A:1766:LEU:HD13	2.15	0.46
1:B:1537:PHE:CD1	1:B:1537:PHE:C	2.89	0.46
1:B:1610:TYR:CE1	1:B:1614:ARG:CZ	2.99	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
2:B:3000:RCP:O15	1:C:2025:LEU:HB3	2.16	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:1634:GLU:O	1:C:1638:LEU:HD21	2.15	0.46
1:C:2136:ILE:HD11	1:C:2152:ILE:HG22	1.98	0.46
1:B:1881:ARG:HH11	1:B:1881:ARG:HG2	1.81	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: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:B:1633:GLU:O	1:B:1636:VAL:HG23	2.15	0.46
1:C:1587:ASN:HB2	1:C:1623:ALA:O	2.15	0.46
1:C:1646:ALA:C	1:C:1648:ASN:H	2.19	0.46
1:C:1669:PHE:O	1:C:1670:ASP:HB2	2.16	0.46
1:C:2160:PRO:HD2	1:C:2163:VAL:CG2	2.41	0.46
1:A:1785:ASN:HA	1:A:1872:GLY:O	2.16	0.45
1:B:1658:LEU:CD1	1:B:1690:ILE:HD11	2.44	0.45
1:B:1966:GLU:HB3	1:B:1969:LYS:HD2	1.99	0.45
1:B:2102:ARG:HD3	3:B:4116:HOH:O	2.16	0.45
1:C:1591:PHE:C	1:C:1591:PHE:CD2	2.89	0.45
1:C:1991:PRO:C	1:C:1992:THR:HG23	2.36	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:C:1783:MET:CA	1:C:1786:ASN:HB2	2.43	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:A:1662:GLY:O	1:A:1666:LEU:HD23	2.16	0.45
1:A:1676:LEU:HD13	1:A:1694:ILE:CD1	2.46	0.45
1:A:1820:ILE:HD13	1:B:1487:TYR:CZ	2.52	0.45
1:B:1571:VAL:O	1:B:1579:GLY:HA2	2.17	0.45
1:B:1883:ARG:HA	1:B:1887:ILE:O	2.17	0.45
1:B:2138:ARG:O	1:B:2142:GLN:HG2	2.16	0.45
1:B:2156:ARG:HG3	1:B:2156:ARG:HH11	1.81	0.45
1:C:1654:GLN:O	1:C:1655:TYR:HB3	2.15	0.45
1:C:1708:SER:HB3	1:C:1735:ILE:HD13	1.98	0.45
1:C:2092:GLN:NE2	1:C:2092:GLN:HA	2.31	0.45
1:C:2143:VAL:HG23	1:C:2143:VAL:O	2.17	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:A:1838:ASP:O	1:A:1839:GLU:HG3	2.16	0.45
1:C:1620:TYR:CE1	1:C:1622:ALA:HB2	2.51	0.45
1:C:1850:ARG:CG	1:C:1851:GLU:N	2.80	0.45
1:C:1991:PRO:C	1:C:1993:GLY:H	2.20	0.45
1:A:2041:LEU:C	1:A:2043:THR:N	2.70	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:1664:GLU:O	1:B:1668:LYS:HB2	2.17	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:C:2037:ARG:O	1:C:2041:LEU:HG	2.16	0.45
1:C:2135:LEU:HB3	1:C:2155:ILE:HD13	1.99	0.45
1:A:1555:ARG:HH22	1:A:1560:ASN:HA	1.82	0.45
1:A:1676:LEU:HB2	1:A:1692:THR:HB	1.99	0.45
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.52	0.45
1:A:1926:PRO:HD3	1:A:1967:VAL:HB	1.99	0.45
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:C:1644:ASN:HD21	1:C:1687:ARG:HH12	1.65	0.45
1:B:1956:PHE:HB2	1:C:1756:LEU:HD13	1.99	0.44
1:B:2096:LEU:HD13	1:C:1690:ILE:CG2	2.47	0.44
1:C:1493:LEU:HB2	1:C:1497:ARG:HH11	1.80	0.44
1:C:1844:ARG:HH11	1:C:1844:ARG:HG3	1.82	0.44
1:C:1894:VAL:HG22	1:C:1953:TRP:CZ2	2.52	0.44
1:B:2021:ARG:NH2	1:B:2095:ASP:OD1	2.48	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:A:2159:TYR:OH	1:A:2175:ILE:HD11	2.17	0.44
1:A:2186:LEU:C	1:A:2188:GLY:N	2.71	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:C:1833:PHE:CZ	1:C:1845:TRP:HE3	2.36	0.44
1:B:1763:ASN:HD21	1:B:1770:VAL:H	1.63	0.44
1:B:2147:SER:CB	1:B:2150:GLU:HG3	2.42	0.44
1:B:1703:GLU:OE2	1:C:2102:ARG:NH2	2.51	0.44
1:A:1748:GLN:HE22	1:A:1783:MET:HB2	1.82	0.44
2:A:3000:RCP:H25	2:A:3000:RCP:H291	1.81	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
1:C:1786:ASN:HD22	1:C:1786:ASN:HA	1.55	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:A:1623:ALA:HB2	1:A:1729:THR:HG23	2.00	0.44
1:A:1817:PRO:HD3	1:B:1484:ALA:HB1	1.99	0.44
1:B:1616:ILE:HD12	1:B:1616:ILE:HA	1.83	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
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:1624:ASN:ND2	1:A:1733:VAL:H	2.15	0.44
1:A:1741:ARG:HH22	1:A:1934:GLN:HE22	1.63	0.44
1:B:1787:GLY:HA3	1:B:1873:TRP:CE3	2.53	0.44
1:C:1493:LEU:HD11	1:C:1557:PRO:HB2	2.00	0.44
1:C:1814:ARG:O	1:C:1815:ASN:HB2	2.18	0.44
1:C:1905:ALA:O	1:C:1907:PRO:HD3	2.18	0.44
1:C:1982:LYS:HB2	1:C:1983:GLN:OE1	2.18	0.44
1:B:1619:ILE:HG13	1:B:1725:ILE:CG2	2.48	0.43
1:B:1643:TRP:CZ3	1:B:1649:PRO:HB2	2.53	0.43
1:C:1591:PHE:CE2	1:C:1592:LYS:HG3	2.53	0.43
1:A:1844:ARG:HG3	1:A:1844:ARG:HH11	1.82	0.43
1:B:1960:GLN:HG3	1:C:1776:GLN:O	2.18	0.43
1:B:1981:TYR:CB	1:B:1985:ILE:HD11	2.49	0.43
1:B:2102:ARG:O	1:B:2106:LYS:HG2	2.18	0.43
1:A:1954:ARG:HD2	1:A:2026:GLU:OE1	2.18	0.43
1:A:1981:TYR:CG	1:A:1985:ILE:HD11	2.52	0.43
1:C:1895:GLU:OE2	1:C:1897:ARG:NH2	2.51	0.43
1:C:2189:LEU:HD12	1:C:2189:LEU:N	2.34	0.43
1:A:2031:VAL:HG11	1:A:2091:LEU:HD12	2.00	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:B:1576:TYR:N	1:B:1577:PRO:HD3	2.34	0.43
1:A:1790:HIS:HD2	3:A:4078:HOH:O	2.01	0.43
1:A:1925:HIS:O	1:A:1926:PRO:C	2.57	0.43
1:A:2043:THR:C	1:A:2045:ASN:N	2.72	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:1494:GLN:HB3	1:A:1496:LYS:HE3	2.00	0.43
1:A:1829:ARG:HG3	1:A:1829:ARG:HH11	1.84	0.43
1:B:2035:PHE:CD1	1:B:2039:LYS:HE3	2.54	0.43
1:C:1678:GLU:HA	1:C:1678:GLU:OE2	2.19	0.43
1:C:1844:ARG:O	1:C:1848:GLU:HG2	2.18	0.43
1:A:1682:ILE:HG22	1:A:1685:GLU:O	2.19	0.43
1:A:1745:ARG:NH2	3:A:4035:HOH:O	2.42	0.43
1:C:1509:TYR:HE1	1:C:1560:ASN:ND2	2.16	0.43
1:C:1571:VAL:O	1:C:1579:GLY:HA2	2.19	0.43
1:C:1737:ALA:O	1:C:1740:VAL:HG22	2.19	0.43
1:C:1747:ILE:HD13	1:C:1802:LYS:CB	2.48	0.43
1:A:1566:ALA:HA	1:A:1584:VAL:O	2.18	0.43



	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.67	0.43
1:B:1589:ILE:O	1:B:1593:ILE:HA	2.18	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:1651:LYS:HE3	1:A:1651:LYS:O	2.19	0.43
1:A:1877:VAL:CG2	1:A:1931:LYS:HD3	2.49	0.43
1:A:1954:ARG:O	1:A:1996:ARG:HB2	2.19	0.43
1:B:1868:GLU:HG2	1:B:1871:SER:HB3	2.00	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:A:1494:GLN:NE2	1:A:1557:PRO:HB2	2.33	0.42
1:A:1971:GLY:O	1:A:1974:ILE:HB	2.19	0.42
1:B:1702:VAL:CG2	1:C:2108:VAL:HG21	2.49	0.42
1:B:1790:HIS:O	1:B:1791:LEU:HD13	2.18	0.42
1:C:2045:ASN:ND2	1:C:2045:ASN:O	2.51	0.42
1:A:1644:ASN:ND2	1:A:1651:LYS:O	2.53	0.42
1:A:1780:THR:O	1:A:1784:TYR:HB3	2.19	0.42
1:B:2083:LEU:O	1:B:2085:ILE:N	2.52	0.42
1:C:1521:SER:O	1:C:1525:ASN:ND2	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:C:1948:MET:HA	1:C:1986:ILE:O	2.18	0.42
1:B:1833:PHE:HE2	1:B:1835:PRO:HG3	1.85	0.42
1:B:2000:TRP:CD1	1:B:2000:TRP:C	2.93	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:A:1733:VAL:HA	1:A:1755:ILE:O	2.19	0.42
1:B:1636:VAL:N	1:B:1637:PRO:CD	2.82	0.42
1:B:1972:SER:HB3	1:C:1742:LEU:HD13	2.01	0.42
1:C:1759:ALA:N	1:C:1760:PRO:CD	2.82	0.42
1:C:1995:LEU:HD12	1:C:1995:LEU:HA	1.91	0.42
1:A:1675:VAL:HG21	1:A:1690:ILE:HG22	2.02	0.42
1:A:1813:LYS:HG2	1:A:1816:MET:HE3	1.94	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:A:1659:THR:C	1:A:1661:GLU:N	2.72	0.42
1:B:1494:GLN:NE2	1:B:1496:LYS:CG	2.77	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:1651:LYS:HB2	3:B:4038:HOH:O	2.19	0.42
1:B:2156:ARG:HD3	1:B:2159:TYR:HE1	1.84	0.42
1:A:1679:ARG:NE	1:A:1686:GLU:OE1	2.50	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:1591:PHE:C	1:C:1591:PHE:HD2	2.23	0.42
1:C:1669:PHE:C	1:C:1671:LYS:H	2.22	0.42
1:C:2043:THR:HG22	1:C:2043:THR:O	2.19	0.42
1:C:2152:ILE:HG13	1:C:2153:ALA:N	2.35	0.42
1:A:1677:THR:HG22	1:A:1690:ILE:HG22	2.01	0.42
1:A:2040:LEU:O	1:A:2043:THR:HB	2.19	0.42
1:B:1497:ARG:HE	1:B:1497:ARG:HB2	1.53	0.42
1:C:1821:LEU:HD23	1:C:1821:LEU:O	2.20	0.42
1:C:1850:ARG:HG2	1:C:1851:GLU:N	2.34	0.42
1:A:2083:LEU:N	1:A:2084:PRO:CD	2.83	0.42
1:C:1516:ARG:HA	1:C:1537:PHE:CD2	2.55	0.42
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:1759:ALA:HB3	1:B:1760:PRO:HD3	2.02	0.41
1:B:1833:PHE:CD2	1:B:1833:PHE:C	2.93	0.41
1:B:2008:ASN:HB3	1:B:2012:MET:CE	2.49	0.41
1:B:2114:GLU:HB3	3:B:4118:HOH:O	2.20	0.41
1:A:1881:ARG:CZ	1:A:1939:PHE:HE2	2.32	0.41
1:A:2170:GLN:HG3	1:B:1517:GLN:NE2	2.35	0.41
1:B:1633:GLU:C	1:B:1635:ILE:H	2.23	0.41
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	2.02	0.41
1:C:2031:VAL:HG13	1:C:2032:GLY:N	2.35	0.41
1:C:2128:ARG:HE	1:C:2132:GLU:CD	2.23	0.41
2:C:3000:RCP:H172	2:C:3000:RCP:H211	1.86	0.41
1:A:1623:ALA:HB2	1:A:1729:THR:CG2	2.50	0.41
1:A:1795:ASP:O	1:A:1798:ALA:HB3	2.21	0.41
1:B:1569:ILE:HG22	1:B:1571:VAL:HG22	2.01	0.41
1:B:1605:ASN:HD22	1:B:1714:ALA:HB2	1.84	0.41
1:A:1657:TYR:CD2	1:A:1687:ARG:HB3	2.56	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: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:B:2008:ASN:CB	1:B:2012:MET:HE2	2.49	0.41
1:C:1818:VAL:HB	1:C:1888:PRO:HG2	2.02	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:1852:THR:HB	1:C:1855:GLY:O	2.21	0.41
1:A:1790:HIS:O	1:A:1791:LEU:HD23	2.21	0.41
1:A:1909:ASN:HD22	1:A:1910:PRO:CD	2.34	0.41
1:A:1989:ILE:HA	1:A:1990:PRO:HD3	1.79	0.41
1:A:2086:TYR:HA	1:A:2089:ILE:HD12	2.01	0.41
1:B:1681:VAL:HG22	1:B:1686:GLU:HA	2.01	0.41
1:A:1556:GLU:HA	1:A:1557:PRO:HD3	1.93	0.41
2:A:3000:RCP:H242	2:A:3000:RCP:H191	1.86	0.41
1:B:1653:PHE:CD1	1:B:1653:PHE:N	2.88	0.41
1:C:1991:PRO:HG2	1:C:2115:TRP:CB	2.47	0.41
1:A:1844:ARG:O	1:A:1848:GLU:HG2	2.20	0.41
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:1881:ARG:HG2	1:B:1881:ARG:NH1	2.36	0.41
1:B:2021:ARG:NH2	1:B:2099:ARG:HE	2.18	0.41
1:C:1592:LYS:O	1:C:1593:ILE:HG12	2.20	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
1:A:1505:THR:HB	1:A:1730:CYS:HB2	2.01	0.41
1:A:2145:GLU:O	1:A:2146:ALA:HB2	2.21	0.41
1:C:2041:LEU:HA	1:C:2044:MET:HG3	2.03	0.41
1:A:1565:VAL:HG12	1:A:1566:ALA:N	2.36	0.41
1:A:1752:GLN:NE2	1:A:1752:GLN:HA	2.35	0.41
1:A:1756:LEU:HD12	1:A:1756:LEU:HA	1.90	0.41
1:A:2167:ASP:HB3	1:A:2170:GLN:HB3	2.02	0.41
1:B:1905:ALA:O	1:B:1907:PRO:HD3	2.21	0.41
1:B:1998:GLY:O	1:B:2001:VAL:CG1	2.67	0.41
1:C:1682:ILE:HG22	1:C:1687:ARG:HD2	2.03	0.41
1:A:1575:GLU:CD	1:A:1575:GLU:H	2.25	0.41
1:A:1784:TYR:CD1	1:A:1792:THR:HG23	2.56	0.41
1:B:1721:ASP:OD2	1:B:1814:ARG:NH1	2.54	0.41
1:A:1831:VAL:HB	1:A:2116:THR:HA	2.02	0.40
1:A:2190:LYS:O	1:A:2192:GLU:N	2.54	0.40
1:B:1602:GLU:HG3	1:B:1603:PHE:N	2.36	0.40
1:B:1655:TYR:O	1:B:1656:LEU:HD23	2.22	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:C:1637:PRO:HG2	1:C:1638:LEU:H	1.86	0.40
1:A:1491:GLU:O	1:A:1495:PRO:HA	2.22	0.40
1:A:1679:ARG:HB2	1:A:1688:PHE:CE2	2.56	0.40
1:A:2044:MET:HA	1:A:2086:TYR:CE2	2.56	0.40



Atom-1	Atom-2	Interatomic	Clash
	1100111 2	distance $(Å)$	overlap (Å)
1:B:1834:THR:HA	1:B:1835:PRO:HD3	1.86	0.40
1:B:2185:LYS:H	1:B:2185:LYS:HD2	1.85	0.40
1:C:1827:TRP:CG	1:C:1828:ASP:N	2.89	0.40
1:C:1920:PRO:HD2	1:C:1925:HIS:CE1	2.56	0.40
1:A:1772:THR:HB	1:A:1776:GLN:NE2	2.36	0.40
1:B:1899:VAL:HB	1:B:1919:GLU:HB2	2.02	0.40
1:B:1948:MET:HA	1:B:1986:ILE:O	2.21	0.40
1:C:1591:PHE:CD2	1:C:1592:LYS:HG3	2.57	0.40
1:C:1680:THR:O	1:C:1687:ARG:HB3	2.21	0.40
1:C:2043:THR:O	1:C:2046:ARG:HB2	2.22	0.40
1:C:2108:VAL:HG23	1:C:2109:ILE:HG23	2.03	0.40
1:A:1586:ALA:HB2	1:A:1621:LEU: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
1:B:1705:LEU:HD21	1:C:1997:GLY:HA2	2.04	0.40
1:B:2001:VAL:HG23	1:C:1709: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 (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	Perc	entiles
1	А	678/758~(89%)	618 (91%)	52 (8%)	8 (1%)	13	39
1	В	672/758~(89%)	611 (91%)	51 (8%)	10 (2%)	10	33
1	С	662/758~(87%)	588 (89%)	64 (10%)	10 (2%)	10	33
All	All	2012/2274 (88%)	1817 (90%)	167 (8%)	28 (1%)	11	34

All (28) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	В	2145	GLU
1	В	2189	LEU
1	С	1644	ASN
1	А	1684	GLY
1	А	1997	GLY
1	А	2146	ALA
1	В	1997	GLY
1	В	2142	GLN
1	С	1508	VAL
1	С	1534	ASP
1	С	1671	LYS
1	С	1997	GLY
1	А	2187	LYS
1	В	1839	GLU
1	С	1646	ALA
1	С	1655	TYR
1	С	1683	ASN
1	С	2144	GLY
1	А	1530	VAL
1	А	1645	ASP
1	А	2191	LEU
1	В	1533	THR
1	А	1744	GLN
1	В	2084	PRO
1	В	1637	PRO
1	В	2032	GLY
1	С	1637	PRO
1	В	1557	PRO

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	А	577/648~(89%)	548~(95%)	29~(5%)	24 56
1	В	572/648~(88%)	534 (93%)	38 (7%)	16 44
1	С	563/648~(87%)	522 (93%)	41 (7%)	14 38



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Mol	Chain	Analysed	Rotameric	Outliers	Percen	tiles
All	All	1712/1944 (88%)	1604 (94%)	108 (6%)	18	46

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

Mol	Chain	Res	Type
1	А	1497	ARG
1	А	1532	LEU
1	А	1534	ASP
1	А	1560	ASN
1	А	1585	VAL
1	А	1602	GLU
1	А	1618	ARG
1	А	1634	GLU
1	А	1651	LYS
1	А	1733	VAL
1	А	1756	LEU
1	А	1765	MET
1	А	1781	GLN
1	А	1879	VAL
1	А	1884	LEU
1	А	1924	TRP
1	А	1930	PHE
1	А	1950	LEU
1	А	1961	ARG
1	А	1981	TYR
1	А	2002	VAL
1	А	2008	ASN
1	А	2042	ASP
1	А	2082	LEU
1	А	2091	LEU
1	A	2128	ARG
1	А	2135	LEU
1	А	2142	GLN
1	A	2143	VAL
1	В	1497	ARG
1	В	1502	LEU
1	В	1508	VAL
1	В	1516	ARG
1	В	1534	ASP
1	В	1536	PHE
1	В	1555	ARG
1	В	1583	VAL



Mol	Chain	Res	Type
1	В	1585	VAL
1	В	1602	GLU
1	В	1616	ILE
1	В	1618	ARG
1	В	1639	PHE
1	В	1648	ASN
1	В	1653	PHE
1	В	1726	THR
1	В	1735	ILE
1	В	1777	LEU
1	В	1786	ASN
1	В	1791	LEU
1	В	1792	THR
1	В	1797	LEU
1	В	1824	LYS
1	В	1843	VAL
1	В	1884	LEU
1	В	1909	ASN
1	В	1924	TRP
1	В	1930	PHE
1	В	1961	ARG
1	В	1980	ASP
1	В	1981	TYR
1	В	2035	PHE
1	В	2041	LEU
1	В	2086	TYR
1	В	2092	GLN
1	В	2127	ARG
1	В	2128	ARG
1	В	2179	TYR
1	С	1499	LYS
1	C	1508	VAL
1	С	1511	PHE
1	С	1536	PHE
1	С	1542	LEU
1	С	1565	VAL
1	С	1591	PHE
1	С	1602	GLU
1	С	1618	ARG
1	С	1629	ILE
1	С	1638	LEU
1	С	1639	PHE



Mol	Chain	Res	Type
1	С	1740	VAL
1	С	1741	ARG
1	С	1742	LEU
1	С	1772	THR
1	С	1781	GLN
1	С	1786	ASN
1	С	1792	THR
1	С	1824	LYS
1	С	1879	VAL
1	С	1895	GLU
1	С	1898	THR
1	С	1902	LEU
1	С	1924	TRP
1	С	1930	PHE
1	С	1945	LEU
1	С	1950	LEU
1	С	1960	GLN
1	С	1961	ARG
1	С	1968	LEU
1	С	1978	LEU
1	С	1980	ASP
1	С	1981	TYR
1	С	2045	ASN
1	С	2046	ARG
1	С	2047	LEU
1	С	2102	ARG
1	С	2114	GLU
1	С	2128	ARG
1	С	2142	GLN

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

Mol	Chain	\mathbf{Res}	Type
1	А	1494	GLN
1	А	1522	GLN
1	А	1547	ASN
1	А	1560	ASN
1	А	1587	ASN
1	А	1605	ASN
1	А	1624	ASN
1	А	1640	GLN
1	А	1644	ASN



Mol	Chain	Res	Type
1	А	1748	GLN
1	А	1752	GLN
1	А	1776	GLN
1	А	1781	GLN
1	А	1790	HIS
1	А	1815	ASN
1	А	1909	ASN
1	А	1925	HIS
1	А	1934	GLN
1	А	1960	GLN
1	А	2008	ASN
1	А	2088	GLN
1	А	2092	GLN
1	А	2097	HIS
1	A	2131	ASN
1	A	2170	GLN
1	В	1494	GLN
1	В	1517	GLN
1	В	1525	ASN
1	В	1587	ASN
1	В	1605	ASN
1	В	1624	ASN
1	В	1644	ASN
1	В	1648	ASN
1	В	1654	GLN
1	В	1683	ASN
1	В	1748	GLN
1	В	1752	GLN
1	В	1763	ASN
1	В	1786	ASN
1	В	1815	ASN
1	В	1909	ASN
1	В	1911	ASN
1	В	1941	ASN
1	В	1944	GLN
1	В	2028	GLN
1	В	2045	ASN
1	В	2097	HIS
1	В	2131	ASN
1	С	1517	GLN
1	С	1522	GLN
1	С	1525	ASN



Mol	Chain	Res	Type
1	С	1560	ASN
1	С	1587	ASN
1	С	1605	ASN
1	С	1640	GLN
1	С	1644	ASN
1	С	1654	GLN
1	С	1683	ASN
1	С	1748	GLN
1	С	1774	ASN
1	С	1776	GLN
1	С	1781	GLN
1	С	1786	ASN
1	С	1815	ASN
1	С	1909	ASN
1	С	1911	ASN
1	С	1918	GLN
1	С	1922	GLN
1	С	1925	HIS
1	С	1934	GLN
1	С	1941	ASN
1	С	1960	GLN
1	С	1965	ASN
1	С	2011	GLN
1	С	2045	ASN
1	С	2092	GLN
1	С	2141	HIS
1	С	2142	GLN
1	С	2170	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



5.6 Ligand geometry (i)

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 Turno Chain Pog		Tink	Bond lengths			Bond angles				
MOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	RCP	А	3000	-	40,41,41	0.85	0	52,58,58	1.25	5 (9%)
2	RCP	С	3000	-	40,41,41	0.84	1 (2%)	52,58,58	1.28	4 (7%)
2	RCP	В	3000	-	40,41,41	0.83	0	52,58,58	1.25	4 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RCP	А	3000	-	-	0/20/48/48	0/6/6/6
2	RCP	С	3000	-	-	4/20/48/48	0/6/6/6
2	RCP	В	3000	-	-	4/20/48/48	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	С	3000	RCP	C7-C6	-2.02	1.39	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	С	3000	RCP	C27-N26-C29	4.31	120.92	112.62
2	В	3000	RCP	C27-N26-C29	3.99	120.31	112.62
2	А	3000	RCP	C16-N15-C18	3.72	119.78	112.62
2	А	3000	RCP	C27-N26-C29	3.71	119.76	112.62
2	В	3000	RCP	C16-N15-C18	3.60	119.56	112.62
2	С	3000	RCP	C16-N15-C18	3.53	119.41	112.62
2	В	3000	RCP	O26-C26-N26	-2.33	118.94	121.67
2	С	3000	RCP	O26-C26-N26	-2.29	118.99	121.67



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	А	3000	RCP	O26-C26-N26	-2.28	119.00	121.67
2	С	3000	RCP	O15-C15-N15	-2.23	119.12	122.67
2	А	3000	RCP	O15-C15-N15	-2.23	119.12	122.67
2	А	3000	RCP	C25-C26-N26	2.21	121.34	118.80
2	В	3000	RCP	O15-C15-N15	-2.11	119.30	122.67

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
2	В	3000	RCP	O26-C26-N26-C29
2	В	3000	RCP	C25-C26-N26-C29
2	С	3000	RCP	O26-C26-N26-C29
2	С	3000	RCP	C25-C26-N26-C29
2	В	3000	RCP	O26-C26-N26-C27
2	С	3000	RCP	O26-C26-N26-C27
2	В	3000	RCP	C25-C26-N26-C27
2	С	3000	RCP	C25-C26-N26-C27

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	3000	RCP	4	0
2	С	3000	RCP	3	0
2	В	3000	RCP	2	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.









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 (i)

6.1 Protein, DNA and RNA chains (i)

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 $>$	#RS	$\mathbf{RZ}>$	$\cdot 2$	$OWAB(Å^2)$	Q<0.9
1	А	682/758~(89%)	-0.24	21 (3%)	49	39	22, 47, 98, 99	0
1	В	676/758~(89%)	-0.20	28 (4%)	37	27	24, 49, 98, 99	0
1	С	666/758~(87%)	-0.27	21 (3%)	47	37	22, 49, 99, 99	0
All	All	2024/2274 (89%)	-0.23	70 (3%)	44	34	22, 48, 99, 99	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	2082	LEU	6.2
1	С	1644	ASN	5.8
1	В	1492	TRP	5.2
1	В	1680	THR	5.2
1	В	1683	ASN	4.7
1	А	1492	TRP	4.5
1	С	2037	ARG	4.1
1	А	1483	ILE	4.0
1	С	2143	VAL	3.9
1	В	2189	LEU	3.8
1	В	1682	ILE	3.7
1	В	2083	LEU	3.6
1	В	2037	ARG	3.5
1	А	1681	VAL	3.4
1	В	1649	PRO	3.2
1	В	1685	GLU	3.2
1	С	2144	GLY	3.2
1	В	1669	PHE	3.1
1	С	1647	ALA	3.1
1	С	1645	ASP	3.1
1	В	1679	ARG	3.1
1	В	1681	VAL	3.0
1	В	2086	TYR	3.0



1W2	Х
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Mol	Chain	Res	Type	RSRZ
1	A	1683	ASN	3.0
1	С	1685	GLU	2.9
1	А	2195	ALA	2.9
1	В	1648	ASN	2.9
1	С	2141	HIS	2.9
1	В	1531	LYS	2.8
1	С	1680	THR	2.8
1	В	2044	MET	2.8
1	В	1684	GLY	2.8
1	В	2187	LYS	2.8
1	С	1911	ASN	2.7
1	А	1489	VAL	2.7
1	А	2037	ARG	2.7
1	С	1649	PRO	2.7
1	А	2047	LEU	2.7
1	А	1911	ASN	2.5
1	А	2144	GLY	2.5
1	С	1648	ASN	2.5
1	А	1685	GLU	2.4
1	В	1556	GLU	2.4
1	А	1679	ARG	2.4
1	А	1669	PHE	2.4
1	А	1482	PRO	2.4
1	С	2044	MET	2.3
1	А	1684	GLY	2.3
1	В	2040	LEU	2.3
1	А	1855	GLY	2.3
1	С	1681	VAL	2.2
1	С	2142	GLN	2.2
1	В	2038	GLU	2.2
1	С	2082	LEU	2.2
1	А	2194	PHE	2.2
1	С	1678	GLU	2.2
1	В	1483	ILE	2.2
1	A	2191	LEU	2.2
1	А	1838	ASP	2.2
1	В	1647	ALA	2.1
1	С	1534	ASP	2.1
1	В	1644	ASN	2.1
1	А	1853	GLU	2.1
1	В	2145	GLU	2.1
1	С	1651	LYS	2.1



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Mol	Chain	Res	Type	RSRZ
1	С	1838	ASP	2.1
1	С	1652	GLY	2.1
1	В	2041	LEU	2.1
1	В	1768	ARG	2.0
1	А	1647	ALA	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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	RCP	С	3000	36/36	0.90	0.24	73,87,94,95	0
2	RCP	В	3000	36/36	0.94	0.20	58,63,71,71	0
2	RCP	А	3000	36/36	0.94	0.17	60,68,69,70	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.









6.5 Other polymers (i)

There are no such residues in this entry.

