Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:59 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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

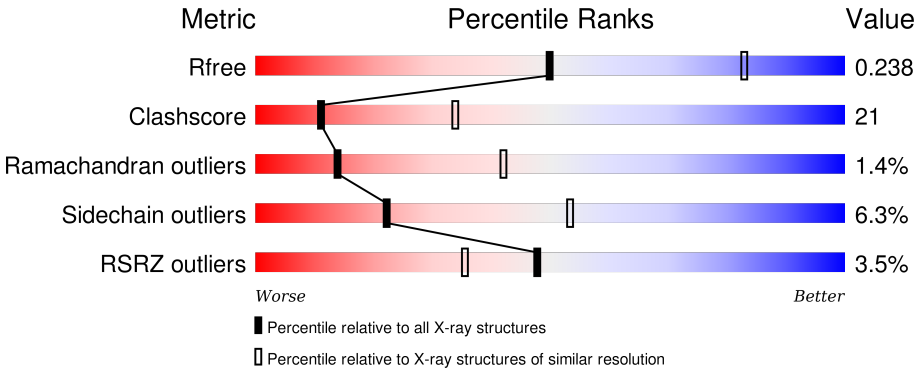
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	758	3% 57% 31% • 10%
1	B	758	4% 52% 35% • 11%
1	C	758	3% 53% 31% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition

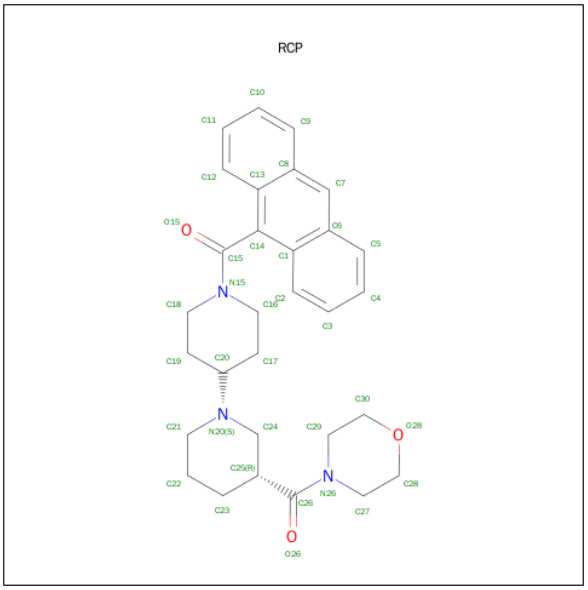
There are 3 unique types of molecules in this entry. The entry contains 16588 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

- 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: $C_{30}H_{35}N_3O_3$).



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.

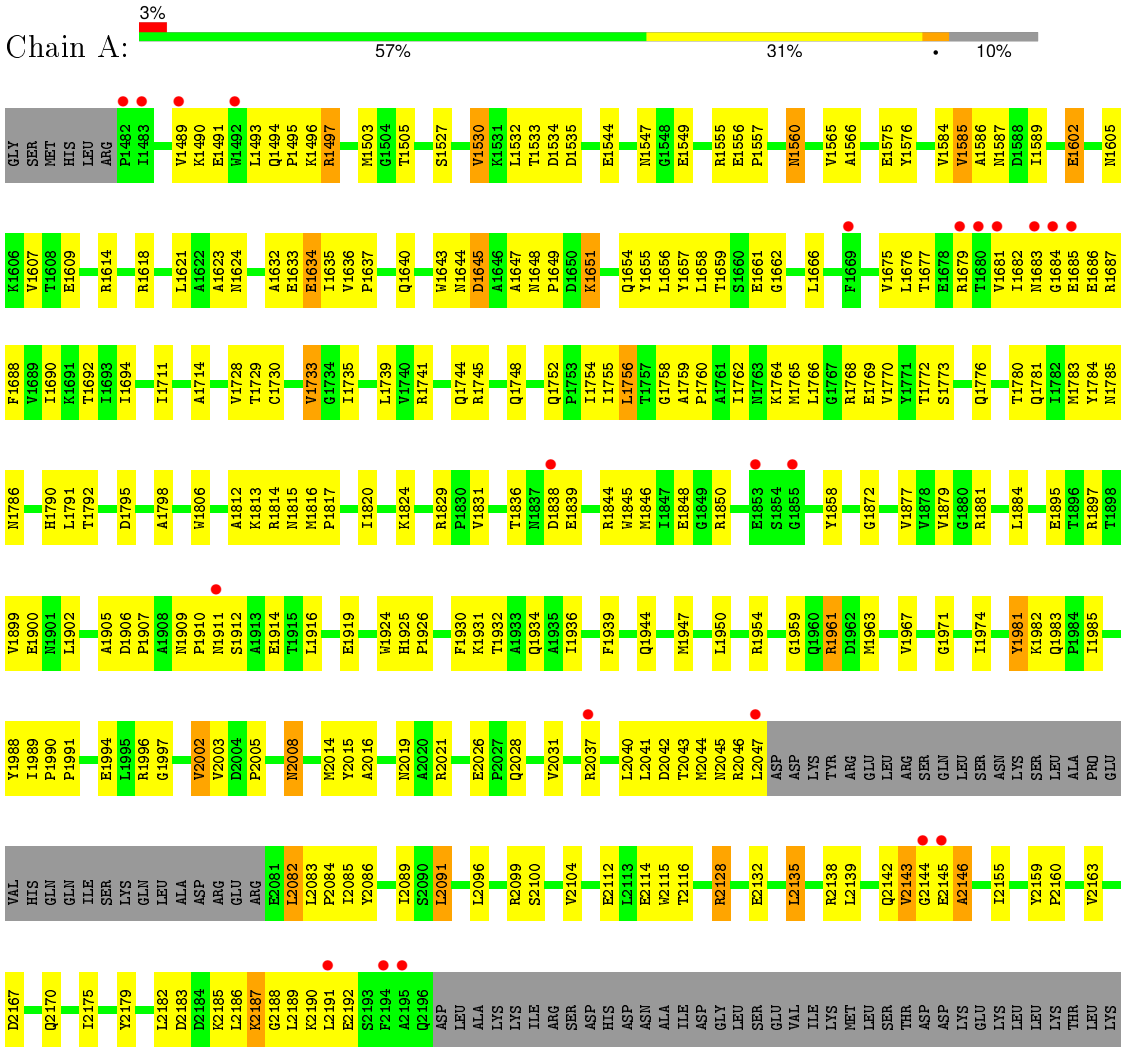
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	147	Total O 147 147	0	0
3	B	128	Total O 128 128	0	0
3	C	104	Total O 104 104	0	0

3 Residue-property plots (i)

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

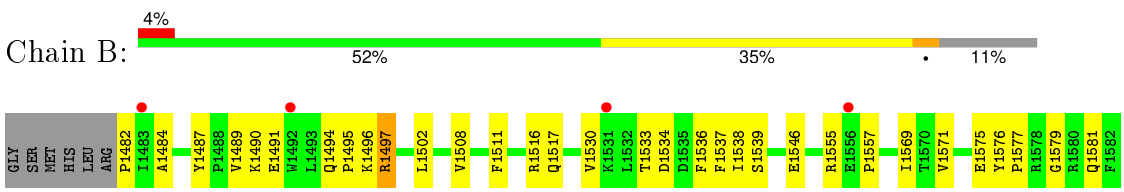
- Molecule 1: ACETYL-COA CARBOXYLASE

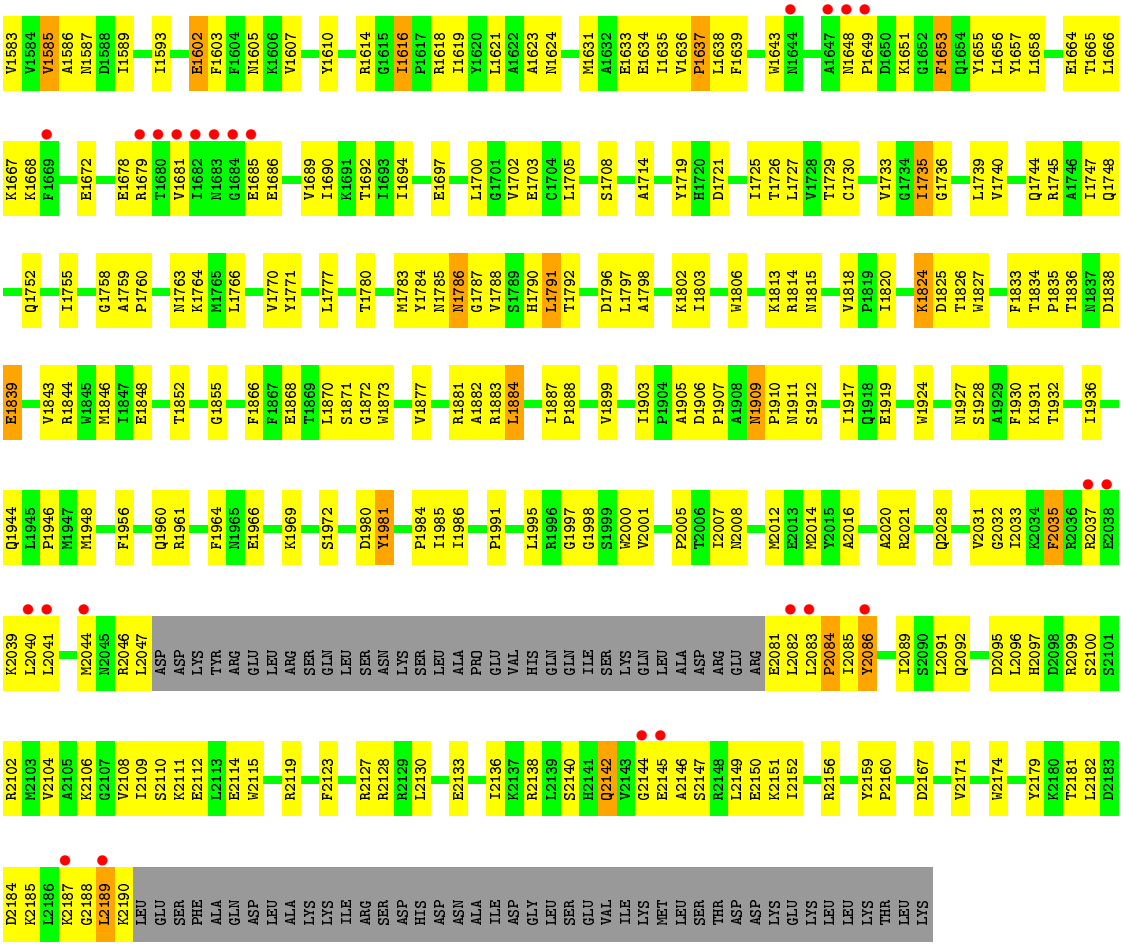
Chain A:



- Molecule 1: ACETYL-COA CARBOXYLASE

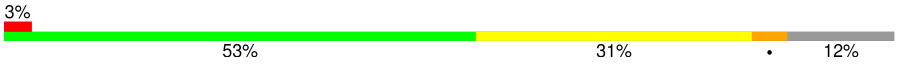
Chain B:

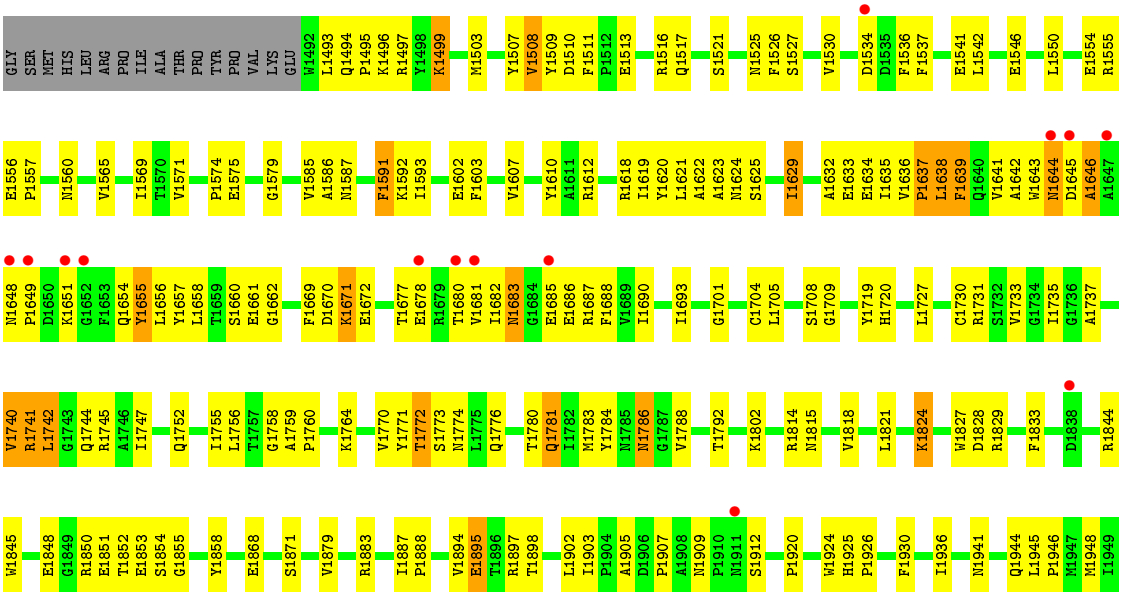


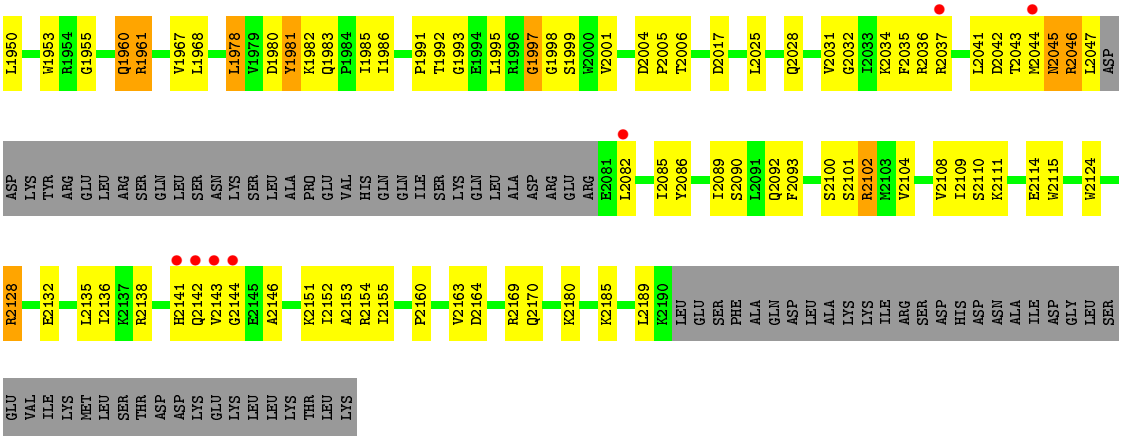


• Molecule 1: ACETYL-COA CARBOXYLASE

Chain C:






L1950 W1953 R1954 G1955 Q1960 R1961 V1967 L1968 L1978 V1979 D1980 Y1981 K1982 Q1983 P1984 I1985 I1986 P1991 T1992 G1993 E1994 L1995 R1996 G1997 G1998 S1999 W2000 V2001 D2004 P2005 T2006 D2017 L2025 Q2028 V2031 G2032 I2033 K2034 F2035 R2036 R2037 L2041 D2042 T2043 M2044 N2045 R2046 L2047 ASP
ASP LYS TYR ARG GLU LEU ARG SER GLN LEU SER ASN LYS SER LEU ALA PRO GLU VAL HIS GLN GLN ILE SER LYS GLN LEU ALA ASP ARG GLU ARG E2081 L2082 I2085 Y2086 I2089 S2090 L2091 Q2092 F2093 S2100 S2101 R2102 M2103 V2104 V2108 I2109 S2110 K2111 E2114 W2115 W2124
R2128 E2132 L2135 I2136 R2137 R2138 H2141 Q2142 V2143 G2144 E2145 A2146 K2151 I2152 A2153 R2154 I2155 P2160 V2163 D2164 R2169 Q2170 K2180 K2185 L2189 K2190 LEU GLU SER PHE ALA GLN ASP LEU ALA LYS LYS ILE ARG SER ASP HIS ASP ASN ALA ILE ASP GLY LEU SER
GLU VAL ILE LYS MET LEU SER THR ASP ASP LYS GLU LYS LEU LEU LYS THR LEU LYS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.61 (at 2.76Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.234 0.201 , 0.238	Depositor DCC
R_{free} test set	10186 reflections (11.65%)	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 , 58.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
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 distance (Å)	Clash 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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
1:C:1936:ILE:HD13	1:C:1978:LEU:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1677:THR:HG22	1:C:1690:ILE:HD13	1.85	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	678/758 (89%)	618 (91%)	52 (8%)	8 (1%)	16	47
1	B	672/758 (89%)	611 (91%)	51 (8%)	10 (2%)	13	40
1	C	662/758 (87%)	588 (89%)	64 (10%)	10 (2%)	13	40
All	All	2012/2274 (88%)	1817 (90%)	167 (8%)	28 (1%)	14	42

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
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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	577/648 (89%)	548 (95%)	29 (5%)	30	64
1	B	572/648 (88%)	534 (93%)	38 (7%)	21	51
1	C	563/648 (87%)	522 (93%)	41 (7%)	17	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1712/1944 (88%)	1604 (94%)	108 (6%)	22 53

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	RCP	A	3000	-	41,41,41	1.01	1 (2%)	58,58,58	1.32	8 (13%)
2	RCP	B	3000	-	41,41,41	1.01	1 (2%)	58,58,58	1.31	6 (10%)
2	RCP	C	3000	-	41,41,41	1.01	1 (2%)	58,58,58	1.34	8 (13%)

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	0/6/6/6
2	RCP	B	3000	-	-	0/20/48/48	0/6/6/6
2	RCP	C	3000	-	-	0/20/48/48	0/6/6/6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3000	RCP	C14-C15	3.67	1.53	1.50
2	B	3000	RCP	C14-C15	3.70	1.53	1.50
2	C	3000	RCP	C14-C15	3.78	1.53	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3000	RCP	C12-C13-C14	-2.33	120.71	123.02
2	B	3000	RCP	C12-C13-C14	-2.31	120.73	123.02
2	B	3000	RCP	C2-C1-C14	-2.30	120.74	123.02
2	A	3000	RCP	C2-C1-C14	-2.28	120.76	123.02
2	A	3000	RCP	C12-C13-C14	-2.24	120.80	123.02
2	C	3000	RCP	C2-C1-C14	-2.21	120.83	123.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3000	RCP	O26-C26-N26	-2.18	118.94	121.66
2	C	3000	RCP	O26-C26-N26	-2.14	118.99	121.66
2	A	3000	RCP	O26-C26-N26	-2.13	119.00	121.66
2	C	3000	RCP	O15-C15-N15	-2.08	119.12	122.42
2	A	3000	RCP	O15-C15-N15	-2.08	119.12	122.42
2	C	3000	RCP	C25-C26-N26	2.14	121.08	119.06
2	A	3000	RCP	C25-C26-N26	2.41	121.34	119.06
2	B	3000	RCP	C14-C15-N15	2.98	120.79	117.75
2	A	3000	RCP	C14-C15-N15	3.28	121.11	117.75
2	C	3000	RCP	C14-C15-N15	3.33	121.15	117.75
2	C	3000	RCP	C16-N15-C18	3.70	119.41	112.56
2	B	3000	RCP	C16-N15-C18	3.77	119.56	112.56
2	A	3000	RCP	C27-N26-C29	3.88	119.76	112.56
2	A	3000	RCP	C16-N15-C18	3.89	119.78	112.56
2	B	3000	RCP	C27-N26-C29	4.18	120.31	112.56
2	C	3000	RCP	C27-N26-C29	4.51	120.92	112.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3000	RCP	4	0
2	B	3000	RCP	2	0
2	C	3000	RCP	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	682/758 (89%)	-0.23	22 (3%)	51	39	22, 47, 98, 99	0
1	B	676/758 (89%)	-0.19	28 (4%)	41	29	24, 49, 99, 99	0
1	C	666/758 (87%)	-0.26	21 (3%)	51	39	22, 49, 99, 99	0
All	All	2024/2274 (89%)	-0.22	71 (3%)	48	35	22, 48, 99, 99	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2082	LEU	6.3
1	C	1644	ASN	6.0
1	B	1492	TRP	5.4
1	B	1680	THR	5.3
1	B	1683	ASN	4.8
1	A	1492	TRP	4.7
1	A	1483	ILE	4.1
1	C	2143	VAL	3.9
1	C	2037	ARG	3.9
1	B	2189	LEU	3.9
1	B	1682	ILE	3.7
1	B	2083	LEU	3.7
1	A	1681	VAL	3.5
1	B	2037	ARG	3.4
1	B	1649	PRO	3.4
1	B	1685	GLU	3.3
1	C	1645	ASP	3.2
1	B	1669	PHE	3.2
1	C	2144	GLY	3.2
1	B	2086	TYR	3.1
1	C	1647	ALA	3.1
1	A	1683	ASN	3.1
1	B	1681	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	1685	GLU	3.0
1	B	1648	ASN	3.0
1	C	1680	THR	3.0
1	B	1679	ARG	2.9
1	B	1531	LYS	2.9
1	C	2141	HIS	2.9
1	B	2044	MET	2.9
1	C	1911	ASN	2.9
1	B	2187	LYS	2.8
1	A	2195	ALA	2.8
1	B	1684	GLY	2.8
1	C	1649	PRO	2.8
1	A	1489	VAL	2.8
1	A	2047	LEU	2.7
1	A	2037	ARG	2.6
1	A	1911	ASN	2.6
1	C	1648	ASN	2.6
1	A	1685	GLU	2.5
1	A	2144	GLY	2.5
1	A	1482	PRO	2.5
1	B	1556	GLU	2.5
1	C	2044	MET	2.4
1	A	1669	PHE	2.4
1	A	1684	GLY	2.4
1	B	2040	LEU	2.3
1	C	2142	GLN	2.3
1	C	1681	VAL	2.3
1	A	1855	GLY	2.3
1	A	1679	ARG	2.3
1	B	2038	GLU	2.3
1	C	1678	GLU	2.3
1	A	2194	PHE	2.3
1	A	1838	ASP	2.2
1	A	2191	LEU	2.2
1	C	2082	LEU	2.2
1	C	1534	ASP	2.2
1	B	1483	ILE	2.2
1	B	1644	ASN	2.2
1	B	2145	GLU	2.2
1	C	1838	ASP	2.2
1	A	1853	GLU	2.2
1	C	1651	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	2041	LEU	2.1
1	B	1647	ALA	2.1
1	C	1652	GLY	2.1
1	A	2145	GLU	2.0
1	A	1680	THR	2.0
1	B	2144	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	LLDF	B-factors(Å^2)	Q<0.9
2	RCP	C	3000	36/36	0.90	0.24	2.00	73,87,94,95	0
2	RCP	B	3000	36/36	0.94	0.20	0.89	58,63,71,71	0
2	RCP	A	3000	36/36	0.94	0.17	0.37	60,68,69,70	0

6.5 Other polymers (i)

There are no such residues in this entry.