



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:44 PM GMT

PDB ID : 1UYS  
Title : Acetyl-CoA carboxylase carboxyltransferase domain in complex with inhibitor haloxyfop  
Authors : Zhang, H.; Tweel, B.; Tong, L.  
Deposited on : 2004-03-02  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

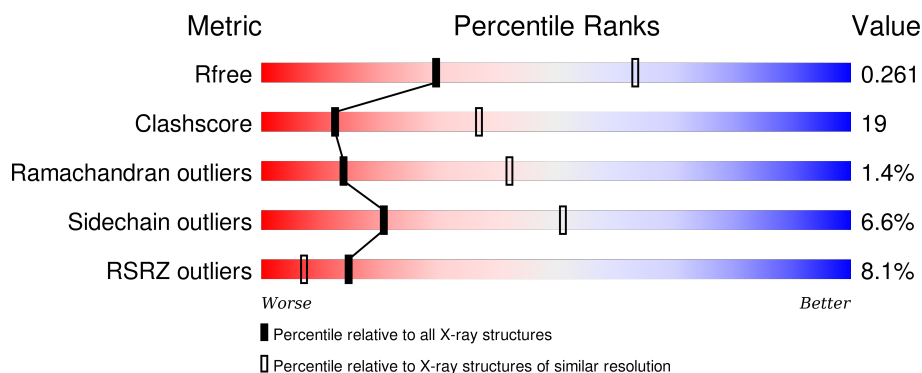
# 1 Overall quality at a glance

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	737	<div> <div>6%</div> <div>56%</div> <div>32%</div> <div>9%</div> </div>
1	B	737	<div> <div>8%</div> <div>54%</div> <div>33%</div> <div>9%</div> </div>
1	C	737	<div> <div>7%</div> <div>53%</div> <div>33%</div> <div>10%</div> </div>

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	H1L	B	3000	-	-	-	X
2	H1L	C	3000	-	-	-	X

## 2 Entry composition [i](#)

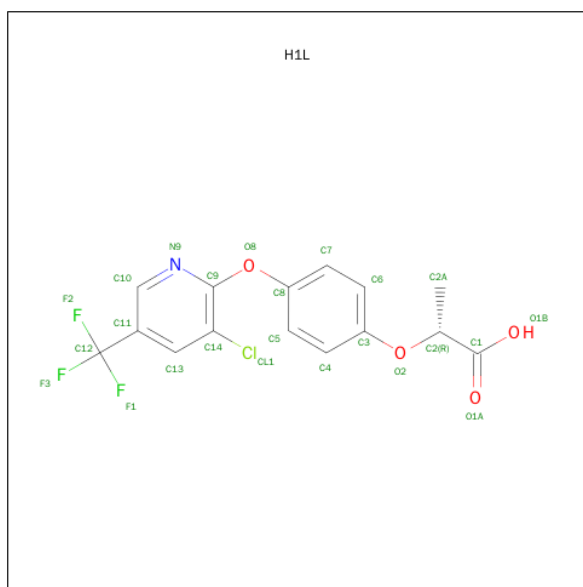
There are 3 unique types of molecules in this entry. The entry contains 16130 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	670	Total	C	N	O	S	Se	0	0	1
			5326	3396	914	998	2	16			
1	B	670	Total	C	N	O	S	Se	0	0	1
			5326	3396	914	998	2	16			
1	C	660	Total	C	N	O	S	Se	0	0	1
			5248	3343	903	984	2	16			

- Molecule 2 is (2R)-2-(4-{[3-CHLORO-5-(TRIFLUOROMETHYL)PYRIDIN-2-YL]OXY}PHENOXY)PROPANOIC ACID (three-letter code: H1L) (formula: C<sub>15</sub>H<sub>11</sub>ClF<sub>3</sub>NO<sub>4</sub>).



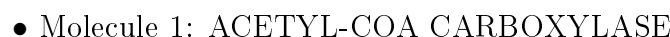
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			24	15	1	3	1	4		
2	B	1	Total	C	Cl	F	N	O	0	0
			24	15	1	3	1	4		
2	C	1	Total	C	Cl	F	N	O	0	0
			24	15	1	3	1	4		

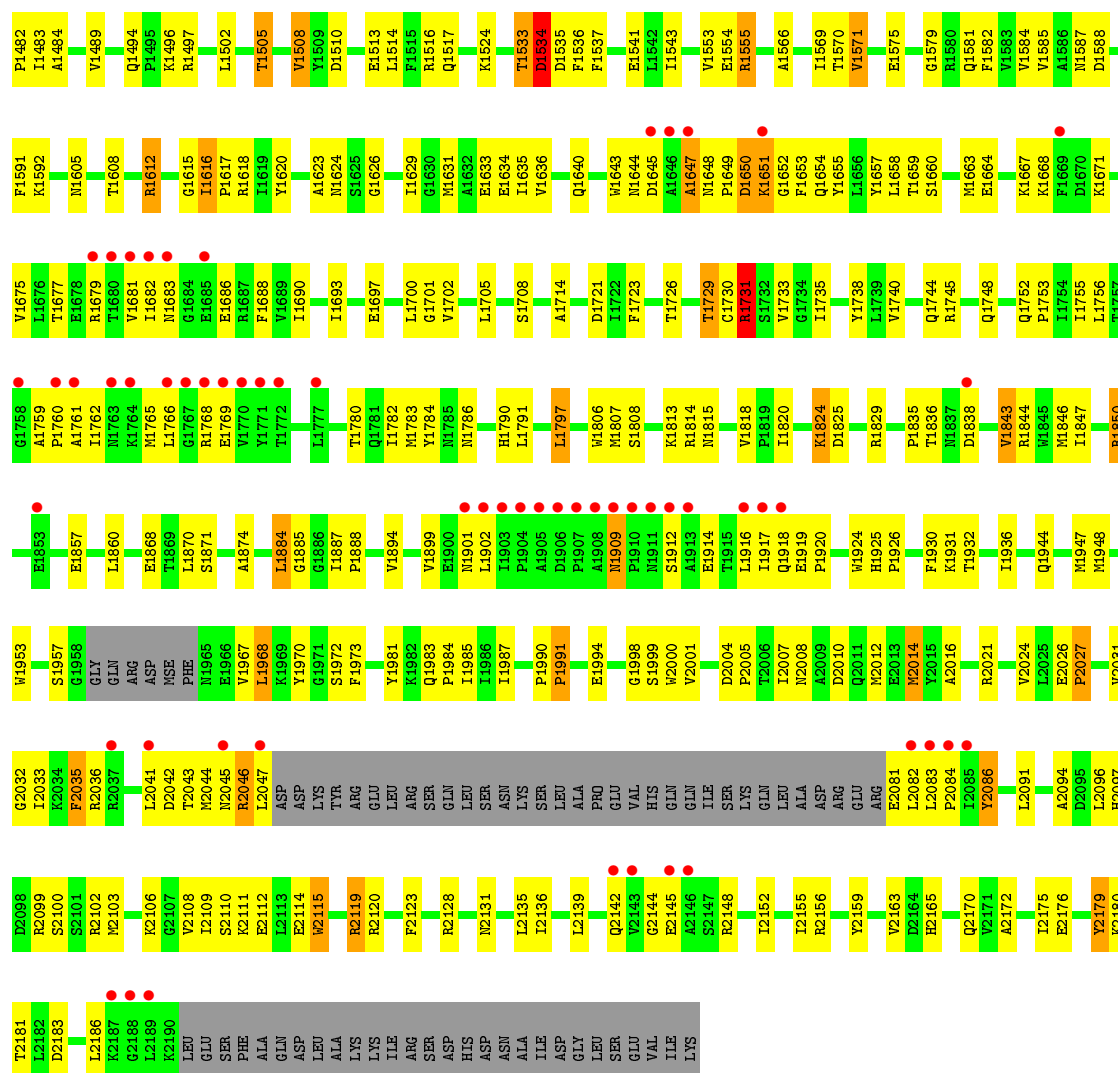
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total 69	O 69	0	0
3	B	50	Total 50	O 50	0	0
3	C	39	Total 39	O 39	0	0

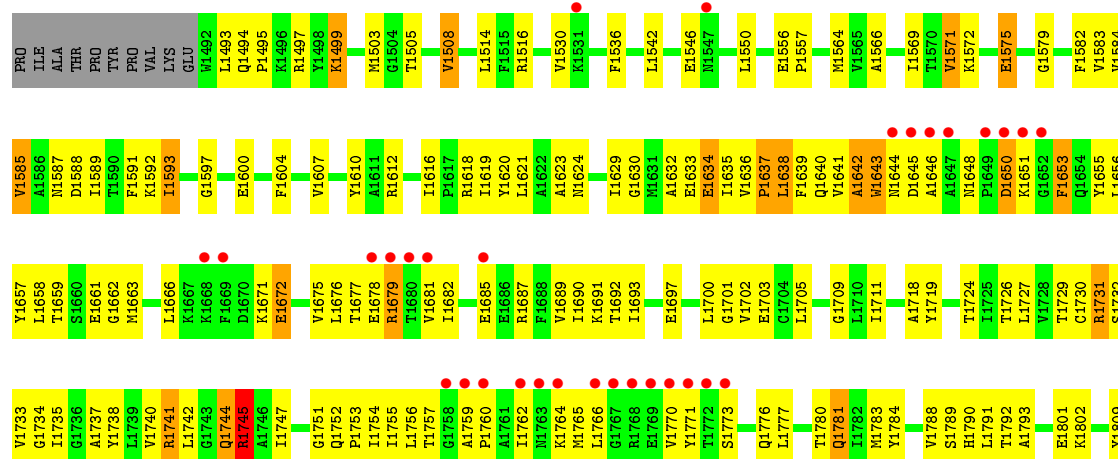


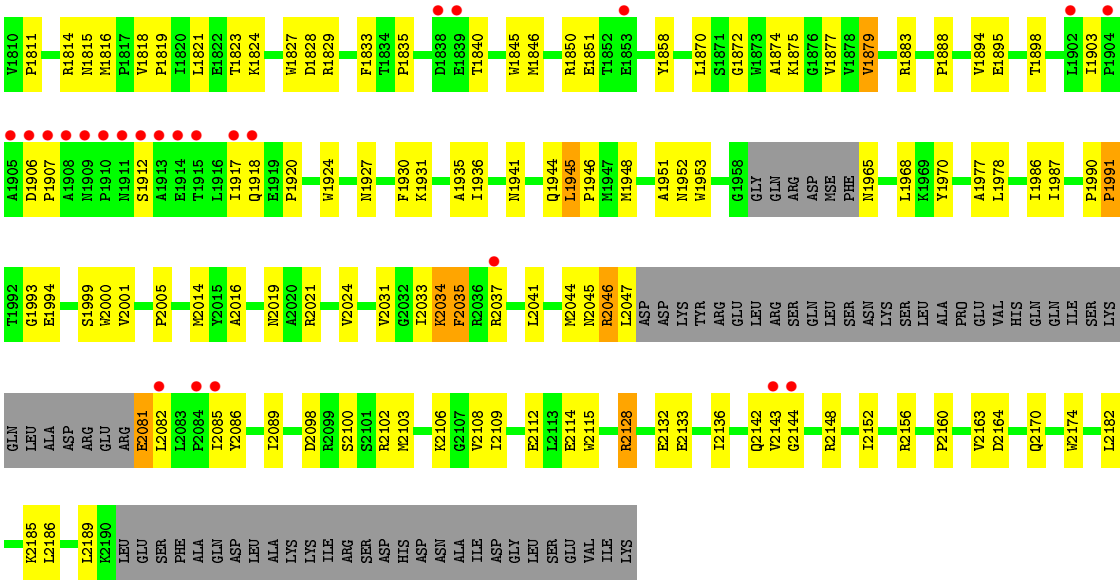
● Molecule 1: ACETYL-COA CARBOXYLASE





● Molecule 1: ACETYL-COA CARBOXYLASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	246.21Å 125.58Å 146.88Å 90.00° 94.08° 90.00°	Depositor
Resolution (Å)	27.42 – 2.80 29.68 – 2.79	Depositor EDS
% Data completeness (in resolution range)	87.6 (27.42-2.80) 93.9 (29.68-2.79)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 2.80Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.218 , 0.252 0.230 , 0.261	Depositor DCC
$R_{free}$ test set	10734 reflections (11.51%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.4	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 107973 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	16130	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 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: H1L

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	0.51	0/5429	0.67	4/7332 (0.1%)
1	B	0.47	0/5429	0.61	0/7332
1	C	0.46	0/5347	0.63	3/7218 (0.0%)
All	All	0.48	0/16205	0.64	7/21882 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1745	ARG	NE-CZ-NH1	-12.57	114.02	120.30
1	C	1745	ARG	NE-CZ-NH2	11.36	125.98	120.30
1	A	1618	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	C	1745	ARG	CD-NE-CZ	-5.82	115.46	123.60
1	A	1618	ARG	NH1-CZ-NH2	-5.23	113.65	119.40
1	A	2174	TRP	CG-CD2-CE3	5.21	138.59	133.90
1	A	2120	ARG	NE-CZ-NH1	5.17	122.89	120.30

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	A	5326	0	5269	199	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5326	0	5269	215	0
1	C	5248	0	5187	231	0
2	A	24	0	10	0	0
2	B	24	0	10	4	0
2	C	24	0	10	6	0
3	A	69	0	0	4	0
3	B	50	0	0	3	0
3	C	39	0	0	4	0
All	All	16130	0	15755	618	1

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 19.

All (618) 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:C:1618:ARG:HG2	1:C:1618:ARG:HH11	1.25	1.01
1:C:1637:PRO:HG2	1:C:1638:LEU:HD23	1.40	1.00
1:C:1823:THR:HG22	1:C:1824:LYS:H	1.33	0.93
1:A:2045:ASN:HB2	1:A:2046:ARG:CZ	1.99	0.92
1:A:1582:PHE:HA	1:A:1616:ILE:HG23	1.54	0.90
1:C:1754:ILE:HD12	1:C:1783:MSE:HG2	1.54	0.88
1:A:2135:LEU:HB3	1:A:2155:ILE:HD13	1.57	0.87
1:A:1624:ASN:ND2	1:A:1733:VAL:H	1.74	0.86
1:A:2045:ASN:HB2	1:A:2046:ARG:NH2	1.90	0.86
1:B:1899:VAL:HB	1:B:1919:GLU:HB2	1.58	0.85
1:B:2031:VAL:HG21	1:B:2091:LEU:HD23	1.59	0.85
1:A:1874:ALA:HB3	1:A:1931:LYS:HD2	1.60	0.84
1:B:1508:VAL:HG21	1:B:1588:ASP:HA	1.61	0.82
1:C:2045:ASN:HB2	1:C:2046:ARG:NH2	1.95	0.81
1:B:1708:SER:HB3	1:B:1735:ILE:HD13	1.63	0.81
1:C:1493:LEU:HB2	1:C:1497:ARG:NH1	1.96	0.80
1:A:1948:MSE:HE2	1:A:1950:LEU:CD1	2.11	0.79
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.32	0.78
1:C:1754:ILE:HB	1:C:1783:MSE:HE3	1.65	0.77
1:A:2183:ASP:HB2	1:B:1482:PRO:HG3	1.67	0.77
1:B:1756:LEU:HD21	1:C:1968:LEU:HD13	1.66	0.77
1:C:1737:ALA:O	1:C:1740:VAL:HG22	1.85	0.77
1:C:2081:GLU:HG2	1:C:2082:LEU:H	1.49	0.76
1:B:1677:THR:HG22	1:B:1690:ILE:HA	1.68	0.76
1:A:1965:ASN:N	1:A:1965:ASN:HD22	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2031:VAL:HG23	1:A:2035:PHE:HB3	1.68	0.75
1:C:1618:ARG:HG2	1:C:1618:ARG:NH1	1.93	0.75
1:B:1730:CYS:HA	1:B:1752:GLN:HG3	1.67	0.74
1:A:2140:SER:OG	1:A:2151:LYS:HE2	1.88	0.74
1:B:1702:VAL:HA	1:B:1705:LEU:HD12	1.68	0.74
1:B:1733:VAL:HG12	1:B:1755:ILE:HB	1.71	0.73
1:A:1899:VAL:HB	1:A:1919:GLU:HB2	1.71	0.73
1:A:1948:MSE:HE2	1:A:1950:LEU:HD13	1.69	0.73
1:A:1750:GLU:HA	1:A:1780:THR:HG21	1.71	0.73
1:C:2047:LEU:HD13	1:C:2082:LEU:HD11	1.70	0.73
1:A:1939:PHE:CD1	1:A:1947:MSE:HE3	2.24	0.73
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.52	0.72
1:B:2135:LEU:HB3	1:B:2155:ILE:HD13	1.70	0.72
1:C:2031:VAL:HG23	1:C:2035:PHE:HB3	1.72	0.72
1:B:1679:ARG:HH21	1:B:1681:VAL:HG21	1.54	0.71
1:C:1658:LEU:HG	1:C:1690:ILE:HD11	1.71	0.71
1:C:1676:LEU:HD12	1:C:1692:THR:HB	1.72	0.71
1:A:1906:ASP:HB3	1:A:1912:SER:OG	1.90	0.71
1:B:1681:VAL:HA	1:B:1686:GLU:HA	1.73	0.70
1:C:1638:LEU:H	1:C:1638:LEU:HD23	1.56	0.70
1:C:1991:PRO:HG3	1:C:2115:TRP:HB2	1.72	0.70
1:C:1672:GLU:H	1:C:1672:GLU:CD	1.95	0.70
1:C:2148:ARG:CZ	1:C:2152:ILE:HD11	2.22	0.70
1:B:1640:GLN:HG3	1:B:1659:THR:HG23	1.73	0.70
1:C:1759:ALA:HB3	1:C:1760:PRO:HD3	1.74	0.70
1:B:1968:LEU:HA	2:C:3000:H1L:CL1	2.29	0.70
1:A:1682:ILE:HD13	1:A:1682:ILE:H	1.56	0.69
1:B:1623:ALA:HB2	1:B:1729:THR:HG23	1.74	0.69
1:C:2045:ASN:HB2	1:C:2046:ARG:CZ	2.22	0.69
2:B:3000:H1L:CL1	1:C:1968:LEU:HA	2.30	0.69
1:B:1762:ILE:HG22	1:B:1766:LEU:HD12	1.75	0.69
1:C:1592:LYS:C	1:C:1593:ILE:HG13	2.12	0.68
1:B:2024:VAL:HG23	1:C:1701:GLY:HA2	1.75	0.68
1:B:1644:ASN:HB3	1:B:1654:GLN:HE21	1.58	0.68
1:C:1747:ILE:HD13	1:C:1802:LYS:HB2	1.75	0.68
1:A:1560:ASN:HD22	1:A:1560:ASN:H	1.40	0.67
1:A:1936:ILE:HG12	1:A:1947:MSE:HE1	1.76	0.67
1:A:1766:LEU:CD2	1:A:1770:VAL:HG11	2.25	0.67
1:A:1948:MSE:HE3	1:A:1988:TYR:HB3	1.75	0.67
1:A:2086:TYR:HA	1:A:2089:ILE:HD12	1.78	0.66
1:C:1651:LYS:HD2	1:C:1651:LYS:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1656:LEU:HB2	1:A:1690:ILE:HD11	1.77	0.66
1:A:1560:ASN:ND2	1:A:1560:ASN:H	1.94	0.66
1:B:1582:PHE:HA	1:B:1616:ILE:HG23	1.77	0.66
1:B:1790:HIS:HA	1:B:1870:LEU:HD23	1.77	0.66
1:A:1846:MSE:HE1	1:A:1991:PRO:HD2	1.76	0.66
1:A:1936:ILE:HA	1:A:1947:MSE:HE1	1.78	0.66
1:B:1663:MSE:O	1:B:1667:LYS:HG3	1.95	0.66
1:B:1494:GLN:HE21	1:B:1496:LYS:H	1.44	0.66
1:A:1766:LEU:HD22	1:A:1770:VAL:HG11	1.78	0.66
1:B:2108:VAL:HG23	1:B:2109:ILE:HG23	1.77	0.66
1:A:1572:LYS:HA	1:A:1579:GLY:HA2	1.78	0.66
1:B:2082:LEU:HD23	1:B:2082:LEU:H	1.60	0.65
1:A:1939:PHE:HD1	1:A:1947:MSE:HE3	1.60	0.65
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.44	0.65
1:C:1493:LEU:HD12	1:C:1497:ARG:HH12	1.62	0.65
1:B:1843:VAL:HG21	1:B:1894:VAL:O	1.97	0.65
1:B:2045:ASN:HB2	1:B:2046:ARG:CZ	2.27	0.65
1:A:1682:ILE:HG12	1:A:1684:GLY:H	1.63	0.64
1:A:1614:ARG:HH11	1:A:1614:ARG:HG3	1.63	0.64
1:C:1846:MSE:HE1	1:C:1990:PRO:HB3	1.79	0.64
1:A:2037:ARG:HB2	1:A:2037:ARG:NH1	2.12	0.64
1:B:1730:CYS:CA	1:B:1752:GLN:HG3	2.26	0.64
1:B:1643:TRP:HA	1:B:1653:PHE:HA	1.79	0.64
1:A:1623:ALA:HB2	1:A:1729:THR:CG2	2.27	0.63
1:C:1877:VAL:HG23	1:C:1931:LYS:HE2	1.79	0.63
1:C:1636:VAL:N	1:C:1637:PRO:HD2	2.13	0.63
1:B:1617:PRO:HB3	1:B:1723:PHE:HB3	1.80	0.63
1:C:1726:THR:HG21	1:C:1740:VAL:HG12	1.81	0.63
1:B:1970:TYR:O	1:B:1973:PHE:HB2	1.99	0.62
1:B:1998:GLY:HA2	1:B:2001:VAL:HG12	1.79	0.62
1:C:2148:ARG:NH1	1:C:2152:ILE:HD11	2.14	0.62
1:C:1637:PRO:HG2	1:C:1638:LEU:H	1.65	0.62
1:B:1902:LEU:HD12	1:B:1916:LEU:HD13	1.82	0.62
1:C:1783:MSE:HG3	1:C:1788:VAL:HB	1.81	0.62
1:A:1748:GLN:HE22	1:A:1783:MSE:HB2	1.65	0.62
1:A:1605:ASN:O	1:A:1609:GLU:HG2	2.00	0.62
1:B:1868:GLU:HG2	1:B:1871:SER:HB3	1.81	0.62
1:C:1793:ALA:HA	3:C:4012:HOH:O	1.99	0.62
1:B:2094:ALA:HA	1:B:2097:HIS:HD2	1.64	0.61
1:A:1530:VAL:HG23	1:A:1530:VAL:O	2.01	0.61
1:B:1483:ILE:HD12	1:B:1484:ALA:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1818:VAL:HG12	1:C:1945:LEU:HD12	1.82	0.61
1:A:1948:MSE:HE2	1:A:1950:LEU:HD11	1.81	0.61
1:B:2001:VAL:HG11	2:C:3000:H1L:C6	2.30	0.61
1:B:1645:ASP:OD2	1:B:1651:LYS:HB2	2.00	0.61
1:A:2028:GLN:HE21	1:A:2091:LEU:HD21	1.65	0.61
1:B:1884:LEU:HD13	1:B:2123:PHE:HA	1.82	0.61
1:A:2180:LYS:HA	1:B:1482:PRO:HD3	1.82	0.61
1:C:2182:LEU:O	1:C:2186:LEU:HD23	2.00	0.61
1:B:1814:ARG:HA	1:B:1944:GLN:HE22	1.65	0.61
1:B:1829:ARG:HH11	1:B:1829:ARG:HG3	1.66	0.61
1:A:1578:ARG:N	1:A:1578:ARG:HD2	2.16	0.60
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	2.16	0.60
1:C:1682:ILE:HG21	1:C:1687:ARG:HD2	1.82	0.60
1:A:2095:ASP:O	1:A:2099:ARG:NH1	2.34	0.60
1:C:2108:VAL:HG23	1:C:2109:ILE:HG23	1.84	0.60
1:C:1508:VAL:HG21	1:C:1588:ASP:HA	1.84	0.60
1:A:1759:ALA:HB3	1:A:1760:PRO:HD3	1.83	0.60
1:C:1874:ALA:HB3	1:C:1931:LYS:HD3	1.83	0.59
1:C:1818:VAL:HG11	1:C:1946:PRO:HD3	1.83	0.59
1:C:1757:THR:HB	1:C:1762:ILE:HD11	1.83	0.59
1:A:2180:LYS:HG2	1:B:1482:PRO:HD3	1.84	0.59
1:B:1745:ARG:HG2	1:B:1806:TRP:CZ2	2.38	0.58
1:A:2044:MSE:SE	1:A:2082:LEU:HD11	2.53	0.58
1:B:2036:ARG:HG2	1:B:2036:ARG:HH11	1.68	0.58
1:A:1682:ILE:HD12	1:A:1687:ARG:HG3	1.86	0.58
1:A:1811:PRO:HG3	1:A:1818:VAL:HA	1.85	0.58
1:C:1898:THR:HG22	1:C:1920:PRO:HA	1.84	0.58
1:A:1623:ALA:HB2	1:A:1729:THR:HG23	1.84	0.58
1:A:1724:THR:H	1:A:1745:ARG:HH21	1.50	0.58
1:B:1790:HIS:HD2	3:B:4039:HOH:O	1.85	0.58
1:A:2028:GLN:NE2	1:A:2091:LEU:HD21	2.19	0.58
1:B:1733:VAL:HA	1:B:1755:ILE:O	2.04	0.58
1:A:2164:ASP:H	1:A:2170:GLN:HE22	1.49	0.58
1:C:1737:ALA:HB3	1:C:1756:LEU:HD12	1.86	0.58
1:A:1809:TYR:O	1:A:1945:LEU:HD21	2.04	0.58
1:C:1823:THR:HB	3:C:4016:HOH:O	2.04	0.57
1:A:1996:ARG:HG3	1:A:1996:ARG:HH11	1.69	0.57
1:B:2031:VAL:HG13	1:B:2035:PHE:HB3	1.85	0.57
1:B:1679:ARG:HH21	1:B:1681:VAL:CG2	2.17	0.57
1:C:1823:THR:HG22	1:C:1824:LYS:N	2.12	0.57
1:B:2142:GLN:HG3	1:B:2186:LEU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1572:LYS:HA	1:C:1579:GLY:HA2	1.87	0.57
1:B:1608:THR:O	1:B:1612:ARG:HG2	2.04	0.57
1:B:2096:LEU:HB3	1:C:1693:ILE:HG13	1.87	0.57
1:A:1894:VAL:HG11	1:A:1952:ASN:O	2.05	0.57
1:A:2136:ILE:HD11	1:A:2152:ILE:HD13	1.87	0.57
1:A:1846:MSE:HE2	1:A:2115:TRP:CH2	2.40	0.57
1:C:2160:PRO:HD2	1:C:2163:VAL:HG21	1.85	0.57
1:A:1582:PHE:HA	1:A:1616:ILE:CG2	2.33	0.57
1:B:2136:ILE:HD11	1:B:2152:ILE:HG12	1.87	0.56
1:A:1922:GLN:HB3	1:A:1954:ARG:HG3	1.87	0.56
1:B:1874:ALA:HB3	1:B:1931:LYS:HD3	1.86	0.56
1:B:1582:PHE:CB	1:B:1617:PRO:HG2	2.35	0.56
1:B:1818:VAL:HB	1:B:1888:PRO:HG2	1.88	0.56
1:B:1846:MSE:HE1	1:B:1990:PRO:HB2	1.87	0.56
1:A:1624:ASN:HD21	1:A:1733:VAL:N	2.00	0.56
1:B:1874:ALA:HB3	1:B:1931:LYS:CD	2.36	0.56
1:B:1748:GLN:HE22	1:B:1783:MSE:HB2	1.70	0.56
1:B:1782:ILE:HG22	1:B:1783:MSE:HE2	1.87	0.56
1:C:1677:THR:HG22	1:C:1690:ILE:HD13	1.88	0.56
1:C:1623:ALA:HB2	1:C:1729:THR:HG23	1.87	0.56
1:C:1612:ARG:HD3	1:C:1718:ALA:HA	1.88	0.56
1:A:2147:SER:HB3	1:A:2150:GLU:HG3	1.88	0.56
1:A:1592:LYS:O	1:A:1593:ILE:HG12	2.06	0.55
1:B:1730:CYS:O	1:B:1731:ARG:C	2.45	0.55
1:C:2086:TYR:HA	1:C:2089:ILE:HD12	1.89	0.55
1:A:1747:ILE:HD13	1:A:1802:LYS:HB3	1.89	0.55
1:B:1605:ASN:ND2	1:B:1714:ALA:HB2	2.22	0.55
1:B:1768:ARG:HG2	1:B:1768:ARG:HH11	1.71	0.55
1:B:1991:PRO:HG3	1:B:2115:TRP:HB2	1.87	0.55
1:C:1815:ASN:HD22	1:C:1944:GLN:HE22	1.54	0.55
1:B:2001:VAL:HG11	2:C:3000:H1L:H6	1.89	0.55
1:C:1724:THR:O	1:C:1745:ARG:HG2	2.06	0.55
1:B:2156:ARG:HD3	1:B:2159:TYR:HE1	1.72	0.55
1:B:1582:PHE:HB3	1:B:1617:PRO:HG2	1.89	0.55
1:A:1948:MSE:HE3	1:A:1988:TYR:CB	2.37	0.55
1:B:1987:ILE:HG22	1:B:2014:MSE:HE3	1.89	0.55
1:B:1824:LYS:HE2	1:B:1825:ASP:N	2.22	0.55
1:A:1585:VAL:HG13	1:A:1607:VAL:HG11	1.89	0.55
1:C:1505:THR:HB	1:C:1730:CYS:HB2	1.90	0.54
1:C:1681:VAL:HG13	1:C:1685:GLU:O	2.08	0.54
1:B:2102:ARG:O	1:B:2106:LYS:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2106:LYS:HA	1:A:2106:LYS:HE2	1.89	0.54
1:A:1508:VAL:HG23	3:A:4018:HOH:O	2.05	0.54
1:A:1948:MSE:CE	1:A:1988:TYR:HD1	2.20	0.54
1:B:1968:LEU:HD22	1:C:1741:ARG:HG3	1.90	0.54
1:A:1970:TYR:O	1:A:1973:PHE:HB2	2.07	0.54
1:A:1790:HIS:HA	1:A:1870:LEU:HD23	1.88	0.54
1:C:2041:LEU:HD23	1:C:2044:MSE:HE3	1.89	0.54
1:A:1758:GLY:O	1:A:1762:ILE:HG13	2.07	0.54
1:B:1651:LYS:HA	1:B:1651:LYS:HE3	1.90	0.54
1:C:1874:ALA:HA	1:C:1927:ASN:HD22	1.73	0.54
1:A:2029:GLY:O	1:A:2033:ILE:HG12	2.07	0.54
1:C:1618:ARG:NH1	1:C:1620:TYR:HB2	2.22	0.54
1:B:2047:LEU:HD22	1:B:2082:LEU:HD22	1.90	0.54
1:B:1947:MSE:HE2	1:B:1985:ILE:HG12	1.90	0.54
1:C:1630:GLY:HA3	1:C:1700:LEU:HA	1.89	0.54
1:B:1860:LEU:O	1:B:2119:ARG:HG3	2.07	0.54
1:B:1987:ILE:CG2	1:B:2014:MSE:HE3	2.38	0.54
1:B:1824:LYS:HZ3	1:B:1825:ASP:H	1.56	0.54
1:B:2081:GLU:HB3	1:B:2083:LEU:HD13	1.88	0.54
1:C:1587:ASN:HD22	1:C:1623:ALA:H	1.56	0.53
1:A:1895:GLU:OE1	1:A:1897:ARG:HD3	2.09	0.53
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.71	0.53
1:A:1633:GLU:O	1:A:1636:VAL:HG12	2.07	0.53
1:B:1820:ILE:HD12	1:B:1887:ILE:HG12	1.90	0.53
1:B:1629:ILE:HG22	1:C:2024:VAL:HG11	1.90	0.53
1:B:1566:ALA:HA	1:B:1584:VAL:O	2.08	0.53
1:B:1972:SER:HB3	1:C:1742:LEU:HD12	1.90	0.53
1:C:1765:MSE:HE2	1:C:1766:LEU:HG	1.91	0.53
1:B:1681:VAL:HG22	1:B:1686:GLU:HB2	1.90	0.53
1:A:2085:ILE:HG23	1:A:2086:TYR:N	2.24	0.53
1:A:2002:VAL:HG13	1:A:2003:VAL:HG13	1.89	0.53
1:C:2016:ALA:O	1:C:2112:GLU:HA	2.07	0.53
1:A:1965:ASN:N	1:A:1965:ASN:ND2	2.56	0.53
1:C:1645:ASP:OD2	1:C:1651:LYS:HB2	2.08	0.53
1:C:1755:ILE:N	1:C:1755:ILE:HD12	2.23	0.53
1:B:1721:ASP:OD2	1:B:1814:ARG:NH1	2.41	0.53
1:A:2032:GLY:O	1:A:2033:ILE:HD13	2.09	0.53
1:B:1909:ASN:HB3	1:B:1912:SER:OG	2.09	0.53
1:C:1918:GLN:O	1:C:1920:PRO:HD3	2.08	0.53
1:C:1991:PRO:O	1:C:2019:ASN:O	2.27	0.53
1:A:1667:LYS:HG3	1:A:1672:GLU:OE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1733:VAL:HA	1:A:1755:ILE:O	2.09	0.53
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.58	0.52
1:A:1635:ILE:O	1:A:1639:PHE:HB3	2.08	0.52
1:B:1655:TYR:HE1	1:B:1657:TYR:HB3	1.74	0.52
1:A:1780:THR:O	1:A:1784:TYR:HB3	2.09	0.52
1:C:1894:VAL:HG11	1:C:1952:ASN:O	2.08	0.52
1:C:1569:ILE:HG22	1:C:1571:VAL:HG22	1.92	0.52
1:C:1823:THR:CG2	1:C:1824:LYS:H	2.14	0.52
1:C:1702:VAL:HA	1:C:1705:LEU:HD12	1.90	0.52
1:B:1932:THR:O	1:B:1936:ILE:HG13	2.09	0.52
1:C:1642:ALA:HB2	1:C:1657:TYR:CE1	2.45	0.52
1:C:1638:LEU:O	1:C:1658:LEU:HD21	2.10	0.52
1:A:1807:MSE:O	1:A:1810:VAL:HG22	2.09	0.52
1:C:1781:GLN:H	1:C:1781:GLN:NE2	2.06	0.52
1:B:2001:VAL:HG23	1:C:1709:GLY:N	2.25	0.52
1:B:1902:LEU:HD21	1:B:1914:GLU:CG	2.39	0.52
1:A:2119:ARG:HB3	3:A:4041:HOH:O	2.09	0.52
1:A:1614:ARG:NH1	1:A:1614:ARG:HG3	2.24	0.51
1:B:1664:GLU:O	1:B:1668:LYS:HG3	2.10	0.51
1:A:1836:THR:HG22	1:A:1838:ASP:H	1.75	0.51
1:C:2081:GLU:CD	1:C:2081:GLU:N	2.64	0.51
1:A:2164:ASP:H	1:A:2170:GLN:NE2	2.09	0.51
1:B:1605:ASN:HD22	1:B:1714:ALA:HB2	1.74	0.51
1:C:2100:SER:HA	1:C:2103:MSE:HE3	1.93	0.51
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.40	0.51
1:A:1948:MSE:HE1	1:A:1988:TYR:HD1	1.75	0.51
1:B:1738:TYR:CG	2:B:3000:H1L:H7	2.46	0.51
1:B:1860:LEU:HD21	1:B:1948:MSE:HE1	1.92	0.51
1:B:2156:ARG:HD3	1:B:2159:TYR:CE1	2.46	0.51
1:B:2008:ASN:HB3	1:B:2012:MSE:HG3	1.91	0.51
1:A:1751:GLY:O	1:A:1775:LEU:HD21	2.11	0.51
1:B:1660:SER:O	1:B:1664:GLU:HG2	2.11	0.50
1:C:1633:GLU:C	1:C:1635:ILE:H	2.14	0.50
1:B:1494:GLN:NE2	1:B:1496:LYS:HG2	2.26	0.50
1:C:1809:TYR:O	1:C:1945:LEU:HD11	2.10	0.50
1:C:1883:ARG:HH11	1:C:1883:ARG:HG3	1.75	0.50
1:C:2160:PRO:HB2	1:C:2163:VAL:HG23	1.92	0.50
1:B:1605:ASN:HD22	1:B:1714:ALA:CB	2.24	0.50
1:C:1814:ARG:O	1:C:1815:ASN:HB2	2.12	0.50
1:A:2005:PRO:HG3	1:A:2014:MSE:HB2	1.93	0.50
1:A:1918:GLN:O	1:A:1920:PRO:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1608:THR:O	1:A:1612:ARG:HG3	2.12	0.50
1:B:1705:LEU:HB3	1:C:2000:TRP:CD1	2.45	0.50
1:C:1835:PRO:HG2	1:C:1991:PRO:HB2	1.93	0.50
1:B:1649:PRO:O	1:B:1651:LYS:N	2.44	0.50
1:C:1818:VAL:HB	1:C:1888:PRO:HG2	1.93	0.50
1:B:1981:TYR:CG	1:B:1985:ILE:HD11	2.47	0.50
1:A:2179:TYR:HD1	1:B:1489:VAL:HA	1.75	0.50
1:B:1753:PRO:HB2	1:B:1755:ILE:HD11	1.93	0.50
1:B:1733:VAL:CG1	1:B:1755:ILE:HB	2.39	0.50
1:A:1936:ILE:HA	1:A:1947:MSE:CE	2.42	0.50
1:C:1987:ILE:HB	1:C:2014:MSE:HG3	1.93	0.50
1:C:1719:TYR:CE2	1:C:1744:GLN:HG3	2.46	0.50
1:C:1493:LEU:HB2	1:C:1497:ARG:HH11	1.73	0.50
1:C:1737:ALA:CB	1:C:1756:LEU:HD12	2.42	0.50
1:A:2093:PHE:HA	1:A:2096:LEU:HD12	1.94	0.50
1:C:1780:THR:O	1:C:1784:TYR:HB3	2.12	0.50
1:B:1697:GLU:O	1:B:1700:LEU:HD13	2.12	0.50
1:C:1621:LEU:HD22	1:C:1727:LEU:HD23	1.94	0.50
1:C:1659:THR:OG1	1:C:1661:GLU:HG3	2.12	0.50
1:B:1634:GLU:HG3	1:B:1671:LYS:HD3	1.93	0.50
1:C:1629:ILE:O	1:C:1629:ILE:HG13	2.09	0.50
1:C:1582:PHE:CD1	1:C:1619:ILE:HD13	2.47	0.50
1:A:2037:ARG:HB2	1:A:2037:ARG:CZ	2.42	0.49
1:A:1719:TYR:CE2	1:A:1744:GLN:HG3	2.47	0.49
1:B:2031:VAL:C	1:B:2033:ILE:H	2.16	0.49
1:B:1918:GLN:O	1:B:1920:PRO:HD3	2.12	0.49
1:B:1570:THR:HG23	1:B:1581:GLN:HG2	1.93	0.49
1:B:2045:ASN:HB2	1:B:2046:ARG:NH2	2.27	0.49
1:A:1636:VAL:N	1:A:1637:PRO:HD2	2.27	0.49
1:A:1564:MSE:HE3	1:A:1604:PHE:HB2	1.93	0.49
1:C:2021:ARG:HA	1:C:2098:ASP:O	2.12	0.49
1:C:1493:LEU:HD12	1:C:1497:ARG:NH1	2.28	0.49
1:C:1697:GLU:HB3	1:C:1700:LEU:HD11	1.94	0.49
1:A:1636:VAL:CG1	1:A:1637:PRO:HD3	2.42	0.49
1:B:1998:GLY:O	1:B:2001:VAL:HG12	2.12	0.49
1:B:2100:SER:HA	1:B:2103:MSE:HE3	1.94	0.49
1:B:1569:ILE:HG22	1:B:1571:VAL:HG22	1.93	0.49
1:A:1619:ILE:N	1:A:1619:ILE:HD12	2.27	0.49
1:B:1983:GLN:HB3	1:B:1984:PRO:HD2	1.94	0.49
1:B:2001:VAL:HG23	1:C:1709:GLY:CA	2.42	0.49
1:B:2099:ARG:HB2	1:C:1692:THR:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1652:GLY:HA2	1:C:2085:ILE:HD11	1.94	0.49
1:A:2041:LEU:O	1:A:2044:MSE:HB2	2.13	0.49
1:A:1636:VAL:N	1:A:1637:PRO:CD	2.76	0.49
1:C:1811:PRO:HA	1:C:1819:PRO:HD3	1.95	0.49
1:A:2170:GLN:HG3	1:B:1517:GLN:NE2	2.28	0.49
1:B:1533:THR:OG1	1:B:1534:ASP:N	2.46	0.49
1:A:2135:LEU:HB3	1:A:2155:ILE:CD1	2.37	0.49
1:B:1686:GLU:HG3	1:B:1686:GLU:O	2.12	0.48
1:A:1572:LYS:HG2	1:A:1577:PRO:O	2.13	0.48
1:C:1655:TYR:C	1:C:1656:LEU:HD12	2.33	0.48
1:B:1780:THR:O	1:B:1784:TYR:HB3	2.13	0.48
1:B:2103:MSE:HG2	1:C:1702:VAL:HG11	1.95	0.48
1:A:1660:SER:HB2	1:A:1686:GLU:OE2	2.12	0.48
1:C:1641:VAL:HG12	1:C:1653:PHE:HB3	1.94	0.48
1:C:1592:LYS:O	1:C:1593:ILE:HG13	2.12	0.48
1:A:2044:MSE:HG3	1:A:2086:TYR:CE2	2.48	0.48
1:A:1487:TYR:HB3	1:A:1488:PRO:HD2	1.95	0.48
1:B:2120:ARG:HG3	3:B:4035:HOH:O	2.11	0.48
1:B:1631:MSE:HE2	1:C:2034:LYS:HB3	1.96	0.48
1:C:1651:LYS:HD2	1:C:1651:LYS:N	2.26	0.48
1:C:1550:LEU:HD11	1:C:1607:VAL:HA	1.95	0.48
1:A:1948:MSE:HA	1:A:1986:ILE:O	2.14	0.48
1:C:1951:ALA:O	1:C:1990:PRO:HD2	2.12	0.48
1:C:2133:GLU:HA	1:C:2136:ILE:HD12	1.93	0.48
1:C:2142:GLN:O	1:C:2144:GLY:N	2.46	0.48
1:A:1754:ILE:HD12	1:A:1783:MSE:HG3	1.95	0.48
1:B:2036:ARG:NH1	1:B:2036:ARG:HG2	2.28	0.48
1:A:2005:PRO:CG	1:A:2014:MSE:HB2	2.43	0.48
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.13	0.48
1:B:1829:ARG:HG3	1:B:1829:ARG:NH1	2.27	0.48
1:A:1987:ILE:HB	1:A:2014:MSE:HG3	1.96	0.48
1:C:2164:ASP:H	1:C:2170:GLN:HE22	1.60	0.48
1:C:1879:VAL:CG1	1:C:1931:LYS:HE3	2.43	0.48
1:C:2081:GLU:OE1	1:C:2081:GLU:N	2.47	0.48
1:B:1755:ILE:HD12	1:B:1755:ILE:N	2.28	0.48
1:C:1650:ASP:HB2	1:C:1651:LYS:HD2	1.96	0.48
1:A:1503:MSE:HB3	1:A:1505:THR:HG22	1.95	0.48
1:B:2044:MSE:HA	1:B:2086:TYR:CE2	2.49	0.48
1:C:2185:LYS:O	1:C:2189:LEU:HD13	2.13	0.48
1:A:1798:ALA:O	1:A:1802:LYS:HD3	2.13	0.48
1:C:1499:LYS:O	1:C:1503:MSE:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1994:GLU:HA	1:B:2021:ARG:O	2.13	0.48
1:C:1643:TRP:C	1:C:1645:ASP:H	2.16	0.47
1:C:1948:MSE:HA	1:C:1986:ILE:O	2.13	0.47
1:C:2044:MSE:HG2	1:C:2086:TYR:CE2	2.49	0.47
1:C:1784:TYR:HA	1:C:1789:SER:HB2	1.95	0.47
1:A:1932:THR:O	1:A:1936:ILE:HG13	2.14	0.47
1:A:1682:ILE:HD13	1:A:1682:ILE:N	2.25	0.47
1:A:2000:TRP:C	1:A:2000:TRP:CD1	2.86	0.47
1:B:2131:ASN:HB3	1:B:2175:ILE:HG21	1.96	0.47
1:B:2001:VAL:O	1:B:2007:ILE:HD11	2.14	0.47
1:A:1830:PRO:HG3	1:A:2120:ARG:HH12	1.79	0.47
1:C:1546:GLU:CD	1:C:1546:GLU:H	2.18	0.47
2:B:3000:H1L:H2A1	1:C:2001:VAL:CG2	2.45	0.47
1:A:2085:ILE:O	1:A:2089:ILE:HG13	2.14	0.47
1:A:2178:ASN:HB3	1:A:2181:THR:HB	1.96	0.47
1:C:1738:TYR:CG	2:C:3000:H1L:H7	2.49	0.47
1:B:1868:GLU:CG	1:B:1871:SER:HB3	2.45	0.47
1:B:1537:PHE:HD2	1:B:1571:VAL:HG13	1.80	0.47
1:C:1566:ALA:HA	1:C:1584:VAL:O	2.15	0.47
1:B:1925:HIS:CE1	1:B:1957:SER:HB3	2.49	0.47
1:C:1636:VAL:N	1:C:1637:PRO:CD	2.77	0.47
1:B:1682:ILE:HG22	1:B:1683:ASN:H	1.80	0.47
1:C:2152:ILE:O	1:C:2156:ARG:HG3	2.15	0.47
1:B:1846:MSE:HE1	1:B:1990:PRO:CB	2.44	0.47
1:C:1681:VAL:HG22	1:C:1685:GLU:O	2.14	0.47
1:B:2001:VAL:HG23	1:C:1709:GLY:HA2	1.95	0.47
1:C:1623:ALA:HB2	1:C:1729:THR:CG2	2.44	0.47
1:A:1844:ARG:HA	1:A:1847:ILE:HD12	1.96	0.47
1:B:1635:ILE:HG22	1:B:1635:ILE:O	2.14	0.47
1:A:1582:PHE:CD1	1:A:1619:ILE:HD13	2.50	0.47
1:A:2135:LEU:HD21	1:A:2182:LEU:HD13	1.97	0.47
1:A:1875:LYS:HB2	1:A:1899:VAL:CG1	2.45	0.47
1:A:2179:TYR:HB2	1:B:1489:VAL:HG13	1.97	0.47
1:C:1790:HIS:HA	1:C:1870:LEU:HD23	1.97	0.47
1:B:1786:ASN:OD1	1:C:1965:ASN:HB3	2.15	0.47
1:B:1681:VAL:O	1:B:1682:ILE:HD13	2.14	0.46
1:B:1759:ALA:HA	1:B:1762:ILE:HD12	1.97	0.46
1:C:2160:PRO:HD3	1:C:2174:TRP:CE2	2.49	0.46
1:B:1991:PRO:CG	1:B:2115:TRP:HB2	2.45	0.46
1:A:1894:VAL:HG11	1:A:1922:GLN:HA	1.97	0.46
1:C:2164:ASP:H	1:C:2170:GLN:NE2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1663:MSE:HG3	1:B:1688:PHE:CD2	2.49	0.46
1:A:1542:LEU:CD2	1:A:1552:GLU:HG2	2.46	0.46
1:C:1906:ASP:HB2	1:C:1912:SER:HB3	1.97	0.46
1:C:1827:TRP:CD2	1:C:1828:ASP:N	2.83	0.46
1:B:2163:VAL:HG13	1:B:2170:GLN:HG2	1.98	0.46
1:C:1672:GLU:N	1:C:1672:GLU:CD	2.66	0.46
1:B:1835:PRO:HG2	1:B:1846:MSE:SE	2.65	0.46
1:C:1872:GLY:HA2	1:C:1875:LYS:HE3	1.97	0.46
1:B:1658:LEU:O	1:B:1688:PHE:HB2	2.15	0.46
1:C:2148:ARG:O	1:C:2152:ILE:HG13	2.15	0.46
1:B:1624:ASN:ND2	1:B:1733:VAL:H	2.13	0.46
1:B:1768:ARG:NH1	1:B:1768:ARG:HG2	2.31	0.46
1:A:1675:VAL:HG22	1:A:1676:LEU:N	2.31	0.46
1:B:2000:TRP:CD1	1:C:1705:LEU:HB3	2.51	0.45
1:B:1571:VAL:O	1:B:1579:GLY:HA2	2.16	0.45
1:A:1990:PRO:HG2	1:A:1993:GLY:HA3	1.98	0.45
1:A:1583:VAL:HG21	1:A:1611:ALA:HB2	1.98	0.45
2:B:3000:H1L:CL1	1:C:1968:LEU:HD12	2.53	0.45
1:A:1760:PRO:HA	1:A:1763:ASN:HD22	1.81	0.45
1:C:1733:VAL:HA	1:C:1755:ILE:O	2.16	0.45
1:A:2160:PRO:HD2	1:A:2163:VAL:HG21	1.97	0.45
1:B:1759:ALA:N	1:B:1760:PRO:CD	2.79	0.45
1:B:2024:VAL:HG11	1:C:1629:ILE:HG22	1.98	0.45
1:B:1616:ILE:HG13	1:B:1617:PRO:HD2	1.97	0.45
1:C:1550:LEU:HD12	1:C:1610:TYR:HB2	1.98	0.45
1:A:2021:ARG:HA	1:A:2098:ASP:O	2.16	0.45
1:B:1514:LEU:HD22	1:B:1797:LEU:HG	1.99	0.45
1:A:1801:GLU:HG2	3:A:4006:HOH:O	2.16	0.45
1:A:1813:LYS:HA	3:A:4033:HOH:O	2.15	0.45
1:A:1494:GLN:HG3	1:A:1497:ARG:NH1	2.31	0.45
1:A:1770:VAL:HG13	1:A:1771:TYR:CD1	2.51	0.45
1:A:1872:GLY:HA2	1:A:1875:LYS:HE2	1.98	0.45
1:B:1885:GLY:HA3	1:B:2123:PHE:CE1	2.52	0.45
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.51	0.45
1:C:1730:CYS:O	1:C:1731:ARG:C	2.55	0.45
1:C:1642:ALA:HB2	1:C:1657:TYR:CD1	2.51	0.45
1:A:2188:GLY:O	1:A:2189:LEU:HD12	2.17	0.45
1:C:2102:ARG:O	1:C:2106:LYS:HG2	2.16	0.45
1:B:1682:ILE:HG22	1:B:1683:ASN:N	2.31	0.45
1:B:2046:ARG:HD2	1:B:2046:ARG:N	2.32	0.45
1:B:1647:ALA:C	1:B:1649:PRO:HD3	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1766:LEU:HD13	1:C:1770:VAL:HG11	1.99	0.45
1:C:1883:ARG:NH1	1:C:1883:ARG:HG3	2.32	0.45
1:B:2110:SER:O	1:B:2111:LYS:HB3	2.17	0.45
1:C:2082:LEU:O	1:C:2086:TYR:HB2	2.16	0.45
1:C:1591:PHE:CD2	1:C:1592:LYS:HG3	2.52	0.45
1:B:2094:ALA:HA	1:B:2097:HIS:CD2	2.49	0.45
1:B:1797:LEU:HB2	3:B:4029:HOH:O	2.17	0.45
1:B:1761:ALA:O	1:B:1765:MSE:HG3	2.16	0.45
1:B:1494:GLN:NE2	1:B:1496:LYS:H	2.12	0.45
1:A:1527:SER:O	1:A:1530:VAL:HG22	2.16	0.45
1:B:1615:GLY:HA2	1:B:1814:ARG:NH1	2.32	0.45
1:C:1875:LYS:O	1:C:1895:GLU:HG3	2.17	0.45
1:B:1675:VAL:HG12	1:B:1693:ILE:HA	1.98	0.45
1:C:1682:ILE:CG2	1:C:1687:ARG:HD2	2.46	0.45
1:B:2179:TYR:HB2	1:B:2180:LYS:NZ	2.31	0.45
1:B:1534:ASP:C	1:B:1536:PHE:H	2.20	0.45
1:C:1564:MSE:HE3	1:C:1604:PHE:HB2	1.98	0.45
1:A:1750:GLU:HA	1:A:1780:THR:CG2	2.45	0.44
1:B:1633:GLU:HA	1:B:1636:VAL:HG23	1.99	0.44
1:A:2081:GLU:OE1	1:A:2081:GLU:N	2.50	0.44
1:C:1663:MSE:HE3	1:C:1666:LEU:HD12	1.99	0.44
1:A:1578:ARG:HD2	1:A:1578:ARG:H	1.83	0.44
1:B:1541:GLU:CD	1:B:1555:ARG:HH11	2.21	0.44
1:C:2031:VAL:CG2	1:C:2035:PHE:HB3	2.45	0.44
1:C:1990:PRO:HG2	1:C:1993:GLY:HA3	1.98	0.44
1:C:1879:VAL:HG12	1:C:1931:LYS:HE3	1.99	0.44
1:B:1730:CYS:HA	1:B:1752:GLN:HE21	1.82	0.44
1:C:1655:TYR:O	1:C:1656:LEU:HD12	2.18	0.44
1:B:1901:ASN:ND2	1:B:1917:ILE:HD12	2.33	0.44
1:A:1492:TRP:CE3	1:A:1493:LEU:HD23	2.53	0.44
1:B:1731:ARG:HA	1:B:1753:PRO:O	2.18	0.44
1:A:1875:LYS:HB2	1:A:1899:VAL:HG11	1.99	0.44
1:B:1649:PRO:C	1:B:1651:LYS:H	2.21	0.44
1:B:2083:LEU:N	1:B:2084:PRO:CD	2.81	0.44
1:B:1953:TRP:HB2	1:B:1999:SER:HB3	2.00	0.44
1:C:1493:LEU:HB2	1:C:1497:ARG:HH12	1.78	0.44
1:B:1582:PHE:CD2	1:B:1807:MSE:HE1	2.52	0.44
1:A:1503:MSE:HG2	1:A:1589:ILE:HG12	1.98	0.44
1:C:1730:CYS:SG	1:C:1731:ARG:N	2.90	0.44
1:A:2125:ARG:O	1:A:2129:ARG:HG3	2.17	0.44
1:C:1903:ILE:HD13	1:C:1917:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1892:ILE:CD1	1:A:1947:MSE:HE2	2.48	0.44
1:A:1656:LEU:CB	1:A:1690:ILE:HD11	2.47	0.44
1:C:1655:TYR:OH	1:C:1687:ARG:NH1	2.51	0.44
1:C:1675:VAL:HG12	1:C:1693:ILE:HG23	1.99	0.44
1:C:1729:THR:O	1:C:1752:GLN:HG3	2.18	0.44
1:C:1745:ARG:HH11	1:C:1745:ARG:HD2	1.31	0.44
1:B:1824:LYS:HE2	1:B:1825:ASP:H	1.83	0.44
1:C:1619:ILE:N	1:C:1619:ILE:HD12	2.33	0.44
1:B:2004:ASP:CG	1:B:2005:PRO:HD2	2.38	0.44
1:C:1703:GLU:N	1:C:1703:GLU:OE1	2.45	0.44
1:C:2128:ARG:HE	1:C:2132:GLU:CD	2.22	0.44
1:A:1690:ILE:O	1:A:1690:ILE:HG13	2.17	0.43
1:C:1583:VAL:HG13	1:C:1616:ILE:HD11	1.98	0.43
1:A:2132:GLU:O	1:A:2136:ILE:HG13	2.18	0.43
1:B:1505:THR:HB	1:B:1730:CYS:HB2	2.00	0.43
1:B:1780:THR:C	1:B:1782:ILE:H	2.22	0.43
1:A:1778:GLY:HA2	1:A:1783:MSE:HE3	2.00	0.43
1:C:1879:VAL:HG12	1:C:1931:LYS:CE	2.49	0.43
1:B:2172:ALA:O	1:B:2176:GLU:HG3	2.18	0.43
1:A:1699:GLY:HA2	1:A:1704:CYS:SG	2.59	0.43
1:A:1641:VAL:HG13	1:A:1643:TRP:NE1	2.34	0.43
1:A:1663:MSE:HG3	1:A:1688:PHE:CD1	2.54	0.43
1:C:1494:GLN:HB3	1:C:1495:PRO:CD	2.48	0.43
1:C:1640:GLN:HB2	1:C:1657:TYR:CE1	2.54	0.43
1:A:1983:GLN:HB3	1:A:1984:PRO:HD2	2.00	0.43
1:A:1655:TYR:CE1	1:A:1689:VAL:HG22	2.54	0.43
1:C:1936:ILE:CG2	1:C:1977:ALA:HB1	2.48	0.43
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	2.00	0.43
1:B:1643:TRP:CZ3	1:B:1649:PRO:HB3	2.53	0.43
1:B:1970:TYR:HH	1:C:1970:TYR:HH	1.66	0.43
1:C:1738:TYR:HB2	2:C:3000:H1L:C7	2.49	0.43
1:C:1607:VAL:O	1:C:1610:TYR:HB3	2.19	0.43
1:A:1892:ILE:HD11	1:A:1947:MSE:HE2	2.00	0.43
1:B:1815:ASN:H	1:B:1944:GLN:HE22	1.65	0.43
1:C:1644:ASN:N	1:C:1644:ASN:HD22	2.16	0.43
1:A:1677:THR:HA	1:A:1689:VAL:O	2.19	0.43
1:B:1844:ARG:HA	1:B:1847:ILE:HD12	2.01	0.43
1:A:1584:VAL:HA	1:A:1619:ILE:O	2.19	0.42
1:A:1879:VAL:HG13	1:A:1931:LYS:HE2	2.00	0.42
1:C:1811:PRO:HB2	1:C:1816:MSE:HB2	2.01	0.42
1:C:1827:TRP:CG	1:C:1828:ASP:N	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1677:THR:HA	1:C:1689:VAL:O	2.20	0.42
1:A:2180:LYS:HG2	1:B:1482:PRO:CD	2.48	0.42
1:A:1846:MSE:CE	1:A:1991:PRO:HD2	2.45	0.42
1:A:2128:ARG:C	1:A:2128:ARG:HD3	2.39	0.42
1:A:2180:LYS:CA	1:B:1482:PRO:HD3	2.49	0.42
1:C:1597:GLY:H	1:C:1600:GLU:HB2	1.84	0.42
1:A:1619:ILE:HG13	1:A:1725:ILE:CG2	2.49	0.42
1:C:2037:ARG:O	1:C:2041:LEU:HG	2.19	0.42
1:B:1582:PHE:HB2	1:B:1617:PRO:HG2	2.01	0.42
1:A:1844:ARG:HG3	1:A:1844:ARG:HH11	1.83	0.42
1:C:1634:GLU:HG3	1:C:1671:LYS:HD3	2.01	0.42
1:B:1926:PRO:HG3	1:B:1967:VAL:HG23	2.00	0.42
1:B:1726:THR:HG21	1:B:1740:VAL:HG22	2.02	0.42
1:C:1646:ALA:C	1:C:1648:ASN:H	2.22	0.42
1:C:1756:LEU:HD21	2:C:3000:H1L:CL1	2.57	0.42
1:A:1996:ARG:O	1:A:1999:SER:HB2	2.19	0.42
1:B:2102:ARG:NH1	1:B:2106:LYS:HG3	2.35	0.42
1:C:1773:SER:HB3	1:C:1776:GLN:HG3	2.02	0.42
1:C:1833:PHE:CZ	1:C:1845:TRP:HE3	2.38	0.42
1:A:1953:TRP:HB2	1:A:1999:SER:HB3	2.02	0.42
1:C:1790:HIS:HD2	3:C:4018:HOH:O	2.02	0.42
1:A:2087:GLY:O	1:A:2090:SER:HB2	2.18	0.42
1:B:1543:ILE:HD11	1:B:1553:VAL:HG11	2.01	0.42
1:B:1585:VAL:O	1:B:1620:TYR:HA	2.19	0.42
1:A:1877:VAL:CG2	1:A:1931:LYS:HD3	2.50	0.42
1:C:1792:THR:CG2	1:C:1793:ALA:N	2.83	0.42
1:B:1701:GLY:HA2	1:C:2024:VAL:HG23	2.01	0.42
1:A:1866:PHE:CE1	1:A:1868:GLU:HB2	2.54	0.42
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.68	0.42
1:A:1753:PRO:HA	1:A:1778:GLY:O	2.20	0.42
1:B:2156:ARG:HH11	1:B:2156:ARG:HG3	1.84	0.42
1:C:1751:GLY:O	1:C:1753:PRO:HD3	2.19	0.42
1:B:2010:ASP:OD2	1:B:2148:ARG:HD3	2.20	0.42
1:C:1829:ARG:CZ	1:C:1858:TYR:HB3	2.49	0.42
1:B:1818:VAL:HB	1:B:1888:PRO:CG	2.48	0.42
1:B:2114:GLU:O	1:B:2115:TRP:C	2.57	0.42
1:C:1790:HIS:O	1:C:1791:LEU:HD23	2.20	0.42
1:A:1565:VAL:HG12	1:A:1566:ALA:N	2.34	0.42
1:C:1711:ILE:HD11	1:C:1735:ILE:HG12	2.02	0.42
1:B:1850:ARG:NH1	1:B:1857:GLU:OE2	2.52	0.42
1:B:1494:GLN:NE2	1:B:1496:LYS:CG	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1505:THR:HB	1:A:1730:CYS:HB2	2.02	0.41
1:A:2095:ASP:C	1:A:2099:ARG:NH1	2.73	0.41
1:A:1585:VAL:O	1:A:1620:TYR:HA	2.20	0.41
1:B:1537:PHE:CD2	1:B:1571:VAL:HG13	2.55	0.41
1:A:2083:LEU:N	1:A:2084:PRO:CD	2.82	0.41
1:B:2027:PRO:O	1:B:2031:VAL:HG23	2.19	0.41
1:C:1753:PRO:CG	1:C:1755:ILE:HD11	2.50	0.41
1:A:1807:MSE:HA	1:A:1810:VAL:HG22	2.02	0.41
1:C:1585:VAL:O	1:C:1620:TYR:HA	2.20	0.41
1:A:1616:ILE:HA	1:A:1617:PRO:HD3	1.91	0.41
1:B:2016:ALA:O	1:B:2112:GLU:HA	2.19	0.41
1:C:1678:GLU:OE2	1:C:1691:LYS:HD2	2.20	0.41
1:C:1759:ALA:HB2	1:C:1777:LEU:HD12	2.02	0.41
1:C:1587:ASN:ND2	1:C:1623:ALA:H	2.18	0.41
1:C:2033:ILE:HG22	1:C:2034:LYS:HD2	2.02	0.41
1:A:1655:TYR:CD1	1:A:1689:VAL:HG13	2.55	0.41
1:B:1543:ILE:HD13	1:B:1553:VAL:HG21	2.02	0.41
1:A:1781:GLN:O	1:A:1782:ILE:HD13	2.20	0.41
1:C:1850:ARG:HG2	1:C:1851:GLU:N	2.35	0.41
1:C:2081:GLU:CG	1:C:2082:LEU:H	2.23	0.41
1:A:1542:LEU:HD21	1:A:1552:GLU:HG2	2.02	0.41
1:B:1648:ASN:ND2	1:B:1650:ASP:OD2	2.53	0.41
1:C:1589:ILE:HA	1:C:1589:ILE:HD12	1.95	0.41
1:C:1530:VAL:O	1:C:1530:VAL:HG23	2.21	0.41
1:C:1587:ASN:ND2	1:C:1624:ASN:HD22	2.18	0.41
1:C:1733:VAL:HG12	1:C:1734:GLY:N	2.35	0.41
1:C:1770:VAL:HG13	1:C:1771:TYR:H	1.85	0.41
1:A:1607:VAL:O	1:A:1610:TYR:HB3	2.21	0.41
1:C:1753:PRO:HG2	1:C:1755:ILE:HD11	2.02	0.41
1:C:2005:PRO:HG3	1:C:2014:MSE:HB2	2.03	0.41
1:C:1661:GLU:HG3	1:C:1662:GLY:N	2.35	0.41
1:C:1679:ARG:HH11	1:C:1679:ARG:HB2	1.85	0.41
1:B:1524:LYS:HE2	1:B:1524:LYS:HA	2.03	0.41
1:B:1591:PHE:O	1:B:1592:LYS:C	2.57	0.41
1:C:1818:VAL:CG1	1:C:1945:LEU:HD12	2.50	0.41
1:C:1569:ILE:CG2	1:C:1571:VAL:HG22	2.51	0.41
1:C:1719:TYR:O	1:C:1941:ASN:HB3	2.21	0.41
1:A:1951:ALA:O	1:A:1990:PRO:HD2	2.21	0.41
1:C:1764:LYS:HD2	1:C:1764:LYS:N	2.36	0.41
1:A:1813:LYS:O	1:A:1816:MSE:HB2	2.21	0.40
1:B:1497:ARG:HD3	1:B:1510:ASP:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2139:LEU:HD22	1:B:2155:ILE:HG13	2.03	0.40
1:C:2148:ARG:HH11	1:C:2148:ARG:HG2	1.85	0.40
1:A:1682:ILE:C	1:A:1684:GLY:N	2.73	0.40
1:C:1792:THR:HG22	1:C:1793:ALA:N	2.36	0.40
1:A:1636:VAL:HG12	1:A:1637:PRO:HD3	2.03	0.40
1:A:2131:ASN:ND2	1:A:2179:TYR:OH	2.54	0.40
1:C:1575:GLU:OE1	1:C:1821:LEU:HD22	2.21	0.40
1:C:1754:ILE:HB	1:C:1783:MSE:CE	2.45	0.40
1:A:2004:ASP:HA	1:A:2005:PRO:HD3	1.98	0.40
1:C:1556:GLU:HA	1:C:1557:PRO:HD3	1.92	0.40
1:C:1935:ALA:HA	3:C:4024:HOH:O	2.22	0.40
1:C:1505:THR:CB	1:C:1730:CYS:HB2	2.51	0.40
1:C:1666:LEU:HB3	1:C:1671:LYS:O	2.21	0.40
1:C:1953:TRP:HB2	1:C:1999:SER:HB3	2.04	0.40
1:A:1762:ILE:O	1:A:1766:LEU:HD13	2.22	0.40
1:A:1949:ILE:HD12	1:A:1987:ILE:CD1	2.52	0.40
1:C:1994:GLU:HA	1:C:2021:ARG:O	2.21	0.40
1:B:1575:GLU:OE1	1:B:1808:SER:HB2	2.22	0.40
1:A:1511:PHE:N	1:A:1512:PRO:CD	2.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1970:TYR:OH	1:A:1970:TYR:OH[2_555]	2.19	0.01

## 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	664/737 (90%)	602 (91%)	57 (9%)	5 (1%)	24 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	664/737 (90%)	597 (90%)	57 (9%)	10 (2%)	13	40
1	C	654/737 (89%)	576 (88%)	66 (10%)	12 (2%)	11	34
All	All	1982/2211 (90%)	1775 (90%)	180 (9%)	27 (1%)	14	42

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1991	PRO
1	B	1534	ASP
1	B	1650	ASP
1	B	1731	ARG
1	C	1632	ALA
1	C	2143	VAL
1	A	2036	ARG
1	B	1744	GLN
1	C	1642	ALA
1	C	1744	GLN
1	C	1907	PRO
1	A	1731	ARG
1	A	1744	GLN
1	B	1533	THR
1	C	1634	GLU
1	C	1637	PRO
1	C	1731	ARG
1	A	1819	PRO
1	B	1991	PRO
1	B	2115	TRP
1	C	1508	VAL
1	C	1653	PHE
1	B	1647	ALA
1	B	2144	GLY
1	C	1650	ASP
1	B	2032	GLY
1	C	1991	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	567/611 (93%)	530 (94%)	37 (6%)	21	52
1	B	567/611 (93%)	523 (92%)	44 (8%)	16	41
1	C	558/611 (91%)	527 (94%)	31 (6%)	26	59
All	All	1692/1833 (92%)	1580 (93%)	112 (7%)	21	51

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1494	GLN
1	A	1533	THR
1	A	1534	ASP
1	A	1554	GLU
1	A	1560	ASN
1	A	1585	VAL
1	A	1613	LYS
1	A	1631	MSE
1	A	1638	LEU
1	A	1682	ILE
1	A	1686	GLU
1	A	1697	GLU
1	A	1781	GLN
1	A	1802	LYS
1	A	1814	ARG
1	A	1824	LYS
1	A	1837	ASN
1	A	1838	ASP
1	A	1851	GLU
1	A	1853	GLU
1	A	1884	LEU
1	A	1924	TRP
1	A	1930	PHE
1	A	1965	ASN
1	A	1968	LEU
1	A	1981	TYR
1	A	1996	ARG
1	A	2008	ASN
1	A	2035	PHE
1	A	2046	ARG
1	A	2081	GLU

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Mol	Chain	Res	Type
1	A	2083	LEU
1	A	2098	ASP
1	A	2128	ARG
1	A	2135	LEU
1	A	2139	LEU
1	A	2148	ARG
1	B	1502	LEU
1	B	1505	THR
1	B	1508	VAL
1	B	1513	GLU
1	B	1516	ARG
1	B	1534	ASP
1	B	1535	ASP
1	B	1554	GLU
1	B	1555	ARG
1	B	1571	VAL
1	B	1612	ARG
1	B	1616	ILE
1	B	1618	ARG
1	B	1651	LYS
1	B	1729	THR
1	B	1731	ARG
1	B	1769	GLU
1	B	1791	LEU
1	B	1797	LEU
1	B	1813	LYS
1	B	1824	LYS
1	B	1843	VAL
1	B	1850	ARG
1	B	1884	LEU
1	B	1909	ASN
1	B	1924	TRP
1	B	1930	PHE
1	B	1968	LEU
1	B	2014	MSE
1	B	2026	GLU
1	B	2027	PRO
1	B	2035	PHE
1	B	2041	LEU
1	B	2042	ASP
1	B	2043	THR
1	B	2046	ARG

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Mol	Chain	Res	Type
1	B	2086	TYR
1	B	2119	ARG
1	B	2128	ARG
1	B	2145	GLU
1	B	2165	HIS
1	B	2179	TYR
1	B	2181	THR
1	B	2183	ASP
1	C	1499	LYS
1	C	1514	LEU
1	C	1516	ARG
1	C	1536	PHE
1	C	1542	LEU
1	C	1571	VAL
1	C	1575	GLU
1	C	1585	VAL
1	C	1593	ILE
1	C	1638	LEU
1	C	1639	PHE
1	C	1643	TRP
1	C	1672	GLU
1	C	1679	ARG
1	C	1732	SER
1	C	1741	ARG
1	C	1745	ARG
1	C	1781	GLN
1	C	1801	GLU
1	C	1840	THR
1	C	1879	VAL
1	C	1924	TRP
1	C	1930	PHE
1	C	1945	LEU
1	C	1978	LEU
1	C	2034	LYS
1	C	2035	PHE
1	C	2046	ARG
1	C	2081	GLU
1	C	2114	GLU
1	C	2128	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1522	GLN
1	A	1525	ASN
1	A	1540	ASN
1	A	1547	ASN
1	A	1560	ASN
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1644	ASN
1	A	1744	GLN
1	A	1748	GLN
1	A	1752	GLN
1	A	1815	ASN
1	A	2008	ASN
1	A	2028	GLN
1	A	2045	ASN
1	A	2092	GLN
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	1654	GLN
1	B	1720	HIS
1	B	1748	GLN
1	B	1752	GLN
1	B	1763	ASN
1	B	1790	HIS
1	B	1815	ASN
1	B	1901	ASN
1	B	1909	ASN
1	B	1941	ASN
1	B	1944	GLN
1	B	2019	ASN
1	B	2045	ASN
1	B	2097	HIS
1	B	2178	ASN
1	C	1517	GLN
1	C	1522	GLN
1	C	1560	ASN

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Mol	Chain	Res	Type
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	1781	GLN
1	C	1786	ASN
1	C	1790	HIS
1	C	1815	ASN
1	C	1922	GLN
1	C	1934	GLN
1	C	2011	GLN
1	C	2092	GLN
1	C	2142	GLN
1	C	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 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	H1L	A	3000	-	21,25,25	1.01	0	28,36,36	1.49	6 (21%)
2	H1L	B	3000	-	21,25,25	1.29	3 (14%)	28,36,36	1.60	8 (28%)
2	H1L	C	3000	-	21,25,25	0.93	0	28,36,36	1.53	6 (21%)

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	H1L	A	3000	-	-	0/14/18/18	0/2/2/2
2	H1L	B	3000	-	-	0/14/18/18	0/2/2/2
2	H1L	C	3000	-	-	0/14/18/18	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3000	H1L	C12-C11	2.22	1.54	1.49
2	B	3000	H1L	C5-C8	2.22	1.43	1.38
2	B	3000	H1L	C7-C6	2.50	1.43	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3000	H1L	C11-C10-N9	-3.63	119.73	123.61
2	B	3000	H1L	C11-C10-N9	-3.22	120.16	123.61
2	B	3000	H1L	C8-O8-C9	-3.16	112.14	118.81
2	C	3000	H1L	C11-C10-N9	-3.10	120.29	123.61
2	B	3000	H1L	C2A-C2-C1	-2.97	109.37	113.18
2	B	3000	H1L	F3-C12-C11	-2.85	106.86	112.95
2	A	3000	H1L	C3-O2-C2	-2.69	114.25	118.41
2	C	3000	H1L	C8-O8-C9	-2.68	113.16	118.81
2	C	3000	H1L	C2A-C2-C1	-2.55	109.91	113.18
2	C	3000	H1L	C3-O2-C2	-2.43	114.64	118.41
2	A	3000	H1L	C8-O8-C9	-2.36	113.83	118.81
2	A	3000	H1L	F2-C12-C11	-2.24	108.16	112.95
2	B	3000	H1L	C3-O2-C2	-2.13	115.11	118.41
2	B	3000	H1L	C14-C13-C11	-2.12	117.05	119.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3000	H1L	C10-N9-C9	2.18	121.39	116.51
2	B	3000	H1L	O8-C9-N9	2.19	122.45	119.81
2	A	3000	H1L	C13-C14-CL1	2.21	121.90	118.50
2	A	3000	H1L	C10-N9-C9	2.48	122.08	116.51
2	C	3000	H1L	C10-N9-C9	2.88	122.96	116.51
2	C	3000	H1L	O8-C9-N9	3.10	123.56	119.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3000	H1L	4	0
2	C	3000	H1L	6	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	654/737 (88%)	-0.05	47 (7%) 18 10	13, 32, 98, 100	0
1	B	654/737 (88%)	0.03	57 (8%) 13 6	15, 37, 99, 100	0
1	C	644/737 (87%)	0.01	55 (8%) 13 6	14, 37, 100, 100	0
All	All	1952/2211 (88%)	-0.01	159 (8%) 15 7	13, 36, 100, 100	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1685	GLU	6.8
1	B	1911	ASN	6.5
1	B	1904	PRO	6.5
1	B	2082	LEU	5.9
1	A	1771	TYR	5.7
1	C	1908	ALA	5.7
1	C	1770	VAL	5.4
1	A	1766	LEU	5.4
1	A	1770	VAL	5.4
1	C	1681	VAL	5.3
1	B	1910	PRO	5.3
1	C	1758	GLY	5.2
1	B	1770	VAL	5.1
1	A	2145	GLU	5.0
1	A	1838	ASP	5.0
1	A	1911	ASN	4.8
1	C	1772	THR	4.8
1	A	1907	PRO	4.8
1	C	1771	TYR	4.5
1	A	1905	ALA	4.5
1	C	1766	LEU	4.5
1	B	1903	ILE	4.4
1	C	1913	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	2143	VAL	4.3
1	B	1766	LEU	4.3
1	C	1906	ASP	4.2
1	C	1909	ASN	4.2
1	B	1680	THR	4.2
1	B	1907	PRO	4.2
1	B	1905	ALA	4.2
1	C	1907	PRO	4.2
1	C	1838	ASP	4.2
1	B	1908	ALA	4.1
1	B	1912	SER	4.1
1	C	1904	PRO	4.0
1	A	1758	GLY	4.0
1	C	1767	GLY	4.0
1	B	1761	ALA	4.0
1	C	1769	GLU	4.0
1	A	1683	ASN	3.9
1	C	1669	PHE	3.9
1	B	1838	ASP	3.9
1	C	1645	ASP	3.9
1	A	1913	ALA	3.9
1	A	1768	ARG	3.9
1	C	1762	ILE	3.9
1	B	2145	GLU	3.8
1	B	1647	ALA	3.8
1	B	1683	ASN	3.7
1	A	1904	PRO	3.7
1	A	1912	SER	3.6
1	C	1911	ASN	3.6
1	C	2144	GLY	3.6
1	A	1915	THR	3.6
1	C	1651	LYS	3.6
1	C	1644	ASN	3.6
1	B	1909	ASN	3.5
1	C	1759	ALA	3.5
1	B	1768	ARG	3.5
1	A	2143	VAL	3.5
1	B	1760	PRO	3.4
1	B	1902	LEU	3.4
1	A	1681	VAL	3.4
1	C	1760	PRO	3.4
1	C	1679	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	1764	LYS	3.4
1	B	2084	PRO	3.4
1	C	1680	THR	3.4
1	A	1769	GLU	3.3
1	B	2037	ARG	3.3
1	A	1767	GLY	3.3
1	C	1768	ARG	3.3
1	C	1912	SER	3.3
1	B	1682	ILE	3.3
1	A	1916	LEU	3.3
1	A	1772	THR	3.3
1	B	1681	VAL	3.2
1	C	1650	ASP	3.2
1	B	1679	ARG	3.2
1	B	1917	ILE	3.2
1	B	2146	ALA	3.2
1	C	1914	GLU	3.1
1	B	2085	ILE	3.1
1	C	1902	LEU	3.1
1	B	2187	LYS	3.1
1	A	1760	PRO	3.0
1	A	2082	LEU	3.0
1	A	1685	GLU	3.0
1	A	1647	ALA	3.0
1	C	1763	ASN	3.0
1	B	1906	ASP	2.9
1	B	1913	ALA	2.9
1	A	1906	ASP	2.9
1	C	1531	LYS	2.9
1	C	1905	ALA	2.9
1	B	1669	PHE	2.9
1	B	1772	THR	2.9
1	C	1646	ALA	2.8
1	A	1908	ALA	2.8
1	C	1915	THR	2.8
1	B	1771	TYR	2.8
1	B	1769	GLU	2.8
1	B	1646	ALA	2.8
1	B	1916	LEU	2.7
1	C	1917	ILE	2.7
1	B	1918	GLN	2.7
1	B	2041	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	1767	GLY	2.7
1	B	1853	GLU	2.7
1	A	1684	GLY	2.7
1	C	1853	GLU	2.6
1	A	1761	ALA	2.6
1	B	1758	GLY	2.6
1	C	1647	ALA	2.6
1	A	1679	ARG	2.6
1	B	1764	LYS	2.6
1	A	2036	ARG	2.5
1	C	2037	ARG	2.5
1	C	1668	LYS	2.5
1	B	2142	GLN	2.5
1	A	1909	ASN	2.5
1	B	2045	ASN	2.4
1	C	1652	GLY	2.4
1	B	2143	VAL	2.4
1	A	1903	ILE	2.4
1	B	1777	LEU	2.4
1	A	1531	LYS	2.4
1	A	2144	GLY	2.4
1	C	2085	ILE	2.4
1	B	1685	GLU	2.3
1	C	1910	PRO	2.3
1	A	1680	THR	2.3
1	B	2083	LEU	2.3
1	A	2046	ARG	2.3
1	C	2084	PRO	2.3
1	A	1643	TRP	2.3
1	C	1649	PRO	2.3
1	A	1917	ILE	2.3
1	B	1645	ASP	2.3
1	C	1918	GLN	2.3
1	A	1914	GLU	2.2
1	A	1762	ILE	2.2
1	C	1773	SER	2.2
1	B	2189	LEU	2.2
1	B	1763	ASN	2.2
1	B	1901	ASN	2.2
1	A	1757	THR	2.2
1	B	2047	LEU	2.2
1	B	1651	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1839	GLU	2.1
1	A	1902	LEU	2.1
1	C	1678	GLU	2.1
1	A	1764	LYS	2.1
1	C	2082	LEU	2.1
1	B	2188	GLY	2.0
1	A	1645	ASP	2.0
1	C	1839	GLU	2.0
1	A	1763	ASN	2.0
1	C	1547	ASN	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	H1L	B	3000	24/24	0.92	0.22	2.72	44,49,59,71	0
2	H1L	C	3000	24/24	0.92	0.21	2.13	52,55,60,71	0
2	H1L	A	3000	24/24	0.93	0.20	1.66	29,38,45,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.