



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:18 PM GMT

PDB ID : 1OD2  
Title : ACETYL-COA CARBOXYLASE CARBOXYLTRANSFERASE DOMAIN  
Authors : Zhang, H.; Yang, Z.; Shen, Y.; Tong, L.  
Deposited on : 2003-02-12  
Resolution : 2.70 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

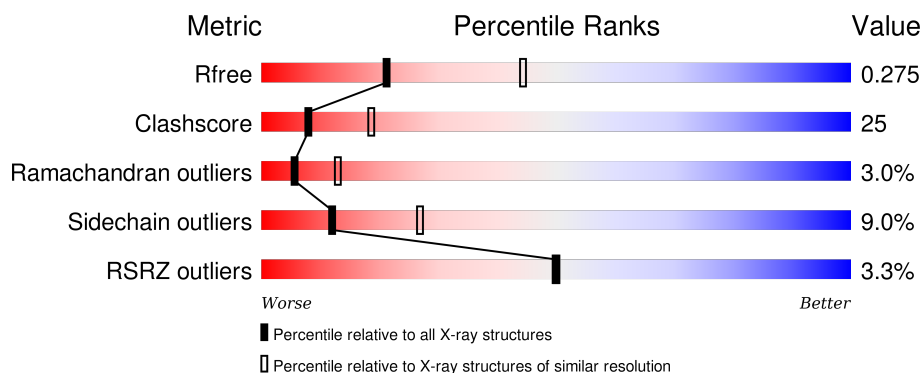
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	805	<div> <div>3%</div> <div>52%</div> <div>32%</div> <div>5%</div> <div>11%</div> </div>
1	B	805	<div> <div>2%</div> <div>44%</div> <div>37%</div> <div>5%</div> <div>14%</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
3	ADE	B	3190	-	-	-	X

## 2 Entry composition [i](#)

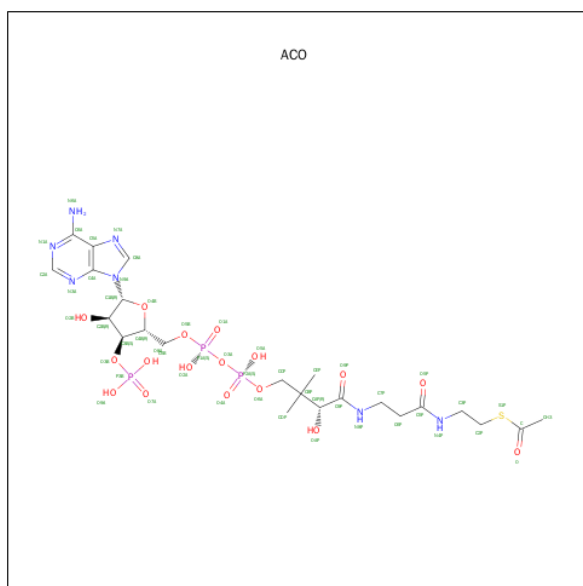
There are 4 unique types of molecules in this entry. The entry contains 11433 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-COENZYME A CARBOXYLASE.

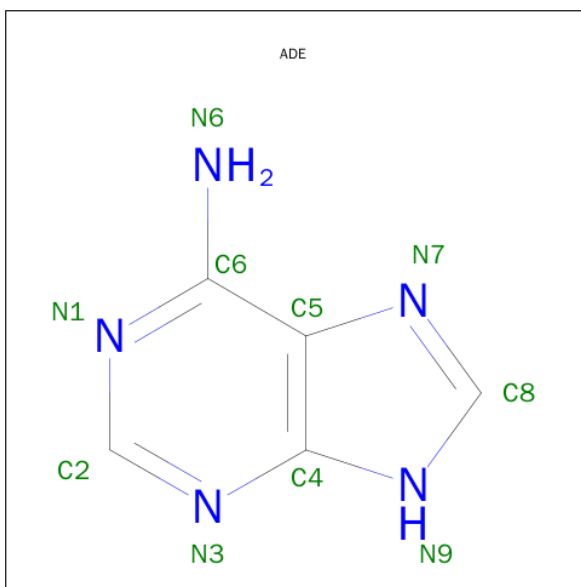
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	720	Total	C	N	O	S	Se	0	0	1
			5742	3650	994	1079	2	17			
1	B	696	Total	C	N	O	S	Se	0	0	1
			5544	3518	963	1044	2	17			

- Molecule 2 is ACETYL COENZYME \*A (three-letter code: ACO) (formula:  $C_{23}H_{38}N_7O_{17}P_3S$ ).



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

- Molecule 3 is ADENINE (three-letter code: ADE) (formula:  $C_5H_5N_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			10	5	5		

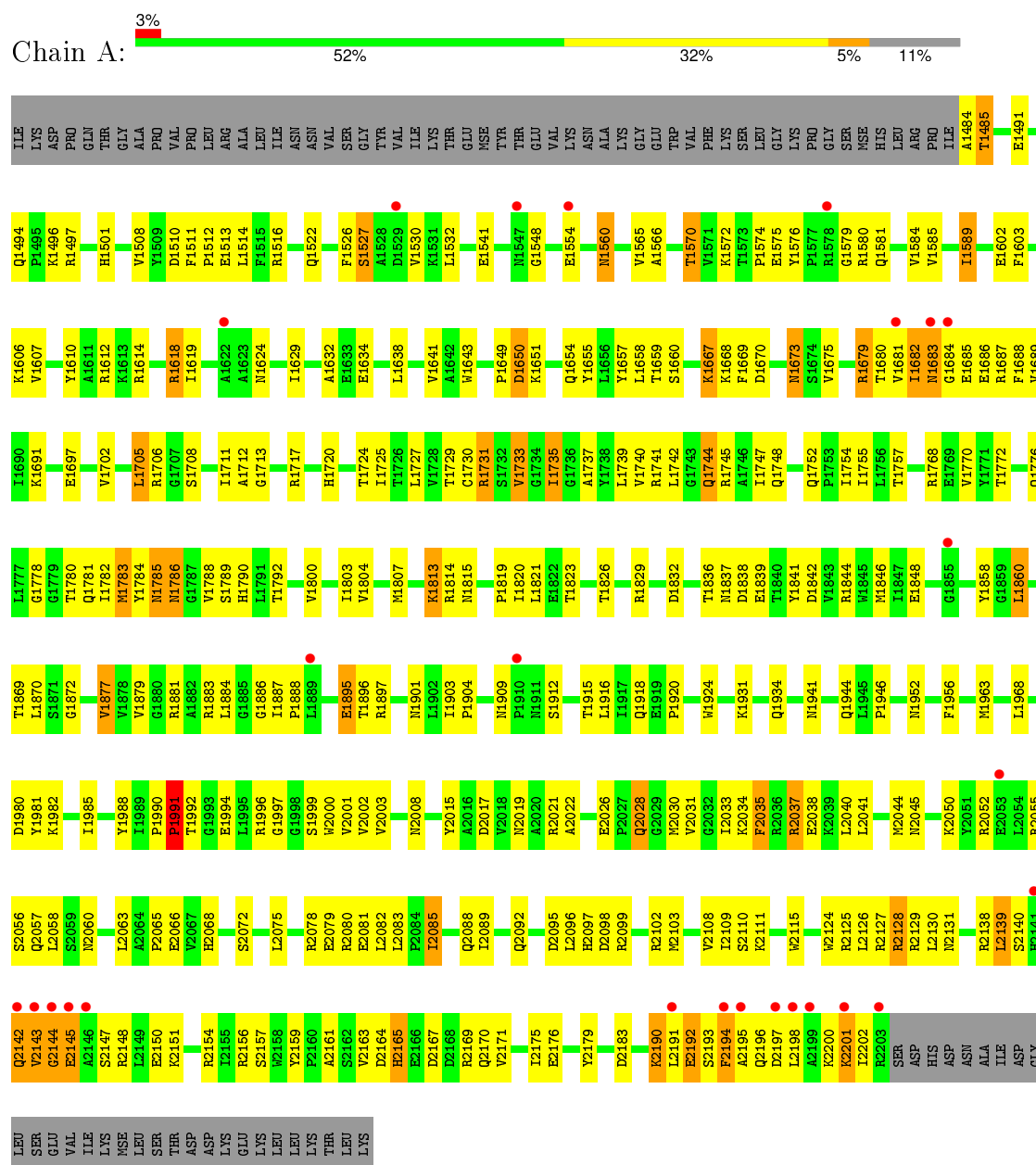
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		
4	B	42	Total	O	0	0
			42	42		

### 3 Residue-property plots

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

- Molecule 1: ACETYL-COENZYME A CARBOXYLASE



- Molecule 1: ACETYL-COENZYME A CARBOXYLASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.87Å 138.13Å 101.40Å 90.00° 114.42° 90.00°	Depositor
Resolution (Å)	28.85 – 2.70 28.85 – 2.69	Depositor EDS
% Data completeness (in resolution range)	93.2 (28.85-2.70) 92.7 (28.85-2.69)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.54 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.226 , 0.279 0.224 , 0.275	Depositor DCC
$R_{free}$ test set	6032 reflections (11.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.8	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.4	EDS
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 60061 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11433	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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

### 5.1 Standard geometry

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

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	0.45	0/5850	0.66	0/7893
1	B	0.45	0/5646	0.67	0/7615
All	All	0.45	0/11496	0.66	0/15508

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	5742	0	5688	271	0
1	B	5544	0	5483	318	0
2	A	48	0	31	4	0
3	B	10	0	4	0	0
4	A	47	0	0	1	0
4	B	42	0	0	2	0
All	All	11433	0	11206	558	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 25.

All (558) 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:A:2085:ILE:HD12	1:A:2085:ILE:H	1.17	1.06
1:A:2085:ILE:HG12	1:B:1650:ASP:HA	1.38	1.01
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.18	0.99
1:A:2034:LYS:HB2	1:B:1631:MSE:HE3	1.48	0.96
1:B:1940:ASN:HD22	1:B:1983:GLN:HE22	1.07	0.94
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	1.82	0.93
1:A:1560:ASN:HD22	1:A:1560:ASN:H	1.11	0.89
1:A:1570:THR:HB	1:A:1581:GLN:HG2	1.52	0.87
1:B:1772:THR:H	1:B:1776:GLN:NE2	1.73	0.87
1:B:1940:ASN:HD22	1:B:1983:GLN:NE2	1.75	0.85
1:B:1860:LEU:CD2	1:B:1948:MSE:HE1	2.06	0.85
1:A:2065:PRO:HG2	1:A:2066:GLU:OE2	1.75	0.84
1:B:1991:PRO:O	1:B:1993:GLY:N	2.09	0.84
1:A:2037:ARG:HB3	1:A:2037:ARG:HH11	1.39	0.84
1:A:1629:ILE:HG22	1:B:2024:VAL:HG11	1.60	0.84
1:B:1772:THR:H	1:B:1776:GLN:HE22	1.25	0.83
1:A:1679:ARG:HG2	1:A:1680:THR:N	1.93	0.83
1:A:2034:LYS:CB	1:B:1631:MSE:HE3	2.10	0.81
1:A:1782:ILE:O	1:A:1786:ASN:HB2	1.81	0.81
1:B:1505:THR:HB	1:B:1730:CYS:HB2	1.62	0.81
1:B:1829:ARG:CZ	1:B:2119:ARG:HE	1.93	0.81
1:B:2070:GLN:HE21	1:B:2074:GLN:HE21	1.29	0.81
1:A:2092:GLN:O	1:A:2096:LEU:HD23	1.81	0.81
1:A:2085:ILE:H	1:A:2085:ILE:CD1	1.94	0.81
1:B:1499:LYS:HE2	1:B:1590:THR:HB	1.60	0.81
1:B:1644:ASN:HD21	1:B:1654:GLN:HE21	1.25	0.80
1:A:1783:MSE:HE1	1:B:1963:MSE:HE3	1.62	0.79
1:A:1560:ASN:ND2	1:A:1560:ASN:H	1.80	0.79
1:B:1940:ASN:ND2	1:B:1983:GLN:HE22	1.81	0.79
1:B:2106:LYS:HA	1:B:2106:LYS:HE2	1.66	0.78
1:A:2031:VAL:HG13	1:A:2035:PHE:HB3	1.66	0.77
2:A:3203:ACO:O4A	2:A:3203:ACO:H10	1.84	0.77
1:B:2146:ALA:HB1	1:B:2150:GLU:OE2	1.84	0.77
1:B:2142:GLN:HE22	1:B:2144:GLY:N	1.84	0.75
1:A:1786:ASN:ND2	1:B:1966:GLU:HG3	2.00	0.75
1:B:1725:ILE:HD11	1:B:1747:ILE:HD11	1.69	0.75
1:B:2077:ASP:O	1:B:2081:GLU:HG3	1.85	0.74
1:B:1860:LEU:HD21	1:B:1948:MSE:HE1	1.68	0.74
1:A:1785:ASN:HD22	1:A:1785:ASN:N	1.85	0.74
1:B:1657:TYR:CD2	1:B:1687:ARG:HB2	2.23	0.73
1:B:1836:THR:HG22	1:B:1838:ASP:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2070:GLN:HE21	1:B:2074:GLN:NE2	1.86	0.73
1:A:2142:GLN:HB3	1:A:2190:LYS:CE	2.19	0.73
1:A:1679:ARG:HG2	1:A:1680:THR:H	1.54	0.72
1:A:1667:LYS:C	1:A:1669:PHE:H	1.91	0.72
1:A:2079:GLU:O	1:A:2083:LEU:HB2	1.89	0.72
1:B:1790:HIS:HA	1:B:1870:LEU:HD23	1.70	0.72
1:B:1508:VAL:HG21	1:B:1588:ASP:HA	1.70	0.72
1:B:1499:LYS:HG2	1:B:1590:THR:HG22	1.71	0.71
1:B:1658:LEU:HG	1:B:1690:ILE:HD11	1.70	0.71
1:B:1921:GLY:O	1:B:1923:VAL:HG12	1.91	0.71
1:A:1815:ASN:ND2	1:A:1944:GLN:HE22	1.89	0.71
1:B:1766:LEU:O	1:B:1768:ARG:HG2	1.91	0.71
1:B:2046:ARG:CZ	1:B:2047:LEU:HD11	2.21	0.71
1:B:1954:ARG:HG3	1:B:1954:ARG:HH11	1.55	0.70
1:A:2080:ARG:O	1:A:2080:ARG:HG2	1.92	0.70
1:A:2142:GLN:HB3	1:A:2190:LYS:HE3	1.74	0.69
1:B:1539:SER:C	1:B:1540:ASN:HD22	1.95	0.69
1:B:2070:GLN:NE2	1:B:2074:GLN:HE21	1.91	0.69
1:A:1838:ASP:HB2	1:A:1839:GLU:OE1	1.91	0.69
1:A:1731:ARG:HH12	2:A:3203:ACO:H121	1.58	0.69
1:A:1815:ASN:HD22	1:A:1944:GLN:HE22	1.40	0.68
1:B:2167:ASP:O	1:B:2171:VAL:HG23	1.93	0.68
1:B:1773:SER:H	1:B:1776:GLN:HE21	1.42	0.68
1:B:2142:GLN:HE22	1:B:2144:GLY:CA	2.06	0.68
1:B:2125:ARG:NH1	1:B:2168:ASP:OD1	2.27	0.68
1:A:2033:ILE:HG22	1:A:2034:LYS:HG3	1.75	0.67
1:B:1634:GLU:O	1:B:1638:LEU:HD22	1.94	0.67
1:B:1768:ARG:HB2	1:B:1768:ARG:HH11	1.58	0.67
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB3	2.29	0.67
1:A:1733:VAL:HG13	1:A:1755:ILE:HG13	1.76	0.67
1:A:1735:ILE:HD12	1:A:1735:ILE:H	1.60	0.67
1:B:1701:GLY:O	1:B:1704:CYS:HB2	1.95	0.67
1:A:1731:ARG:NH1	2:A:3203:ACO:H121	2.09	0.66
1:A:1513:GLU:OE2	1:A:1516:ARG:NH1	2.28	0.66
1:B:2039:LYS:HB2	1:B:2039:LYS:NZ	2.10	0.66
1:A:2147:SER:OG	1:A:2150:GLU:HG3	1.95	0.66
1:B:1540:ASN:HD22	1:B:1540:ASN:N	1.94	0.65
1:B:1733:VAL:HG22	1:B:1755:ILE:HD11	1.79	0.65
1:A:1650:ASP:OD2	1:A:1650:ASP:N	2.30	0.65
1:A:1733:VAL:HA	1:A:1755:ILE:O	1.97	0.65
1:B:1685:GLU:HG2	1:B:1686:GLU:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1637:PRO:HG2	1:B:1638:LEU:HD13	1.80	0.64
1:B:1836:THR:HB	1:B:1839:GLU:OE2	1.97	0.64
1:A:2096:LEU:HD12	1:B:1692:THR:HA	1.80	0.64
1:B:2010:ASP:CG	1:B:2148:ARG:HG3	2.18	0.64
1:B:2055:ARG:HG3	1:B:2055:ARG:HH11	1.63	0.64
1:A:2191:LEU:C	1:A:2191:LEU:HD23	2.18	0.64
1:B:1541:GLU:HG3	1:B:1567:PHE:HE2	1.63	0.64
1:B:2142:GLN:NE2	1:B:2144:GLY:N	2.46	0.64
1:A:1679:ARG:HG3	1:A:1679:ARG:HH11	1.62	0.64
1:A:2089:ILE:HD13	1:B:1641:VAL:HG21	1.80	0.63
1:A:1603:PHE:O	1:A:1607:VAL:HG23	1.99	0.63
1:A:1680:THR:HG22	1:A:1687:ARG:HB2	1.80	0.63
1:A:1682:ILE:C	1:A:1684:GLY:H	2.01	0.63
1:B:2188:GLY:O	1:B:2189:LEU:HD23	1.99	0.62
1:A:2041:LEU:HD12	1:A:2044:MSE:HE3	1.81	0.62
1:B:1780:THR:O	1:B:1784:TYR:HB3	1.97	0.62
1:A:2138:ARG:HB3	1:A:2138:ARG:HH11	1.64	0.62
1:A:1790:HIS:HB3	1:A:1869:THR:HG23	1.80	0.62
1:B:1749:VAL:O	1:B:1752:GLN:HB2	1.99	0.62
1:A:1641:VAL:HG21	1:B:2089:ILE:HD13	1.82	0.62
1:B:1755:ILE:HD13	1:B:1755:ILE:H	1.64	0.62
1:B:1813:LYS:HG3	1:B:1816:MSE:HG3	1.80	0.62
1:A:2200:LYS:HZ1	1:A:2202:ILE:HB	1.64	0.62
1:B:1552:GLU:O	1:B:1553:VAL:HG13	2.00	0.62
1:B:2064:ALA:HB3	1:B:2067:VAL:HG23	1.80	0.62
1:A:1629:ILE:HG22	1:B:2024:VAL:CG1	2.28	0.61
1:A:2200:LYS:HE2	1:A:2202:ILE:HD12	1.82	0.61
1:A:1712:ALA:O	1:A:1742:LEU:HD13	2.00	0.61
1:B:1779:GLY:HA3	1:B:1781:GLN:OE1	2.00	0.61
1:B:1813:LYS:HG3	1:B:1816:MSE:CG	2.31	0.61
1:B:1543:ILE:HD12	1:B:1544:GLU:O	2.00	0.61
1:B:1860:LEU:HD23	1:B:1948:MSE:HE1	1.82	0.61
1:A:2142:GLN:HB3	1:A:2190:LYS:NZ	2.15	0.61
1:A:2057:GLN:O	1:A:2063:LEU:HD11	2.01	0.61
1:A:2139:LEU:O	1:A:2151:LYS:HD3	2.00	0.60
1:A:1820:ILE:HD12	1:A:1886:GLY:C	2.21	0.60
1:A:1589:ILE:HD13	1:A:1589:ILE:O	2.02	0.60
1:B:1966:GLU:HG2	1:B:1969:LYS:HE3	1.82	0.60
1:B:1572:LYS:HA	1:B:1579:GLY:HA2	1.83	0.60
1:B:2139:LEU:HD11	1:B:2154:ARG:NH1	2.17	0.59
1:A:2097:HIS:HE1	1:B:1632:ALA:H	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2099:ARG:HH11	1:A:2099:ARG:HG3	1.67	0.59
1:B:1810:VAL:HG23	1:B:1811:PRO:HD2	1.84	0.59
1:B:1990:PRO:O	1:B:1991:PRO:O	2.20	0.59
1:A:2045:ASN:HD22	1:A:2055:ARG:HG3	1.68	0.59
1:A:1585:VAL:HG22	1:A:1607:VAL:HG11	1.84	0.59
1:A:1491:GLU:OE2	1:A:1501:HIS:HD2	1.86	0.59
1:B:1991:PRO:C	1:B:1993:GLY:H	2.03	0.59
1:B:1772:THR:N	1:B:1776:GLN:NE2	2.49	0.59
1:B:1516:ARG:HH22	1:B:1534:ASP:HA	1.68	0.59
1:B:1589:ILE:O	1:B:1589:ILE:HG13	2.03	0.59
1:A:2035:PHE:HB2	1:B:1631:MSE:HE1	1.84	0.58
1:A:2200:LYS:HA	1:A:2200:LYS:HZ3	1.67	0.58
1:A:1572:LYS:HA	1:A:1579:GLY:HA2	1.85	0.58
1:B:1679:ARG:CZ	1:B:1686:GLU:OE1	2.51	0.58
1:B:2025:LEU:HD12	1:B:2029:GLY:HA3	1.84	0.58
1:A:1682:ILE:O	1:A:1684:GLY:N	2.34	0.58
1:A:1527:SER:O	1:A:1530:VAL:HG22	2.04	0.58
1:B:2125:ARG:NH1	1:B:2128:ARG:HD2	2.19	0.58
1:B:1755:ILE:HD13	1:B:1755:ILE:N	2.18	0.58
1:A:2085:ILE:N	1:A:2085:ILE:HD12	2.02	0.58
1:B:2180:LYS:HB3	1:B:2180:LYS:NZ	2.19	0.58
1:B:2050:LYS:HD2	1:B:2078:ARG:CZ	2.33	0.58
1:B:2135:LEU:HB3	1:B:2155:ILE:HD13	1.86	0.58
1:A:2193:SER:C	1:A:2195:ALA:H	2.07	0.58
1:A:1786:ASN:HD21	1:B:1966:GLU:HG3	1.65	0.57
1:B:1925:HIS:HD2	4:B:5025:HOH:O	1.86	0.57
1:B:1541:GLU:HG3	1:B:1567:PHE:CE2	2.39	0.57
1:A:1848:GLU:HB2	4:A:5031:HOH:O	2.03	0.57
1:B:2010:ASP:OD1	1:B:2148:ARG:HG3	2.04	0.57
1:B:1917:ILE:HD12	1:B:1961:ARG:NH2	2.19	0.57
1:B:2119:ARG:HH11	1:B:2119:ARG:HG2	1.68	0.57
1:B:1711:ILE:HD12	1:B:1739:LEU:HD21	1.86	0.57
1:B:1948:MSE:HE3	1:B:1950:LEU:HD21	1.87	0.57
1:A:2037:ARG:O	1:A:2040:LEU:N	2.37	0.57
1:A:1560:ASN:HD22	1:A:1560:ASN:N	1.93	0.57
1:A:2142:GLN:HB3	1:A:2190:LYS:HG3	1.87	0.57
1:A:2052:ARG:HG3	1:A:2052:ARG:NH1	2.20	0.57
1:B:1786:ASN:OD1	1:B:1788:VAL:HG23	2.06	0.56
1:A:1741:ARG:CZ	1:A:1744:GLN:HE22	2.18	0.56
1:A:1813:LYS:HB2	1:A:1813:LYS:NZ	2.19	0.56
1:A:1730:CYS:CA	1:A:1752:GLN:HE21	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2142:GLN:CD	1:A:2143:VAL:H	2.09	0.56
1:B:1527:SER:O	1:B:1530:VAL:HG22	2.06	0.56
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.53	0.56
1:B:1654:GLN:O	1:B:1655:TYR:HB3	2.06	0.56
1:A:2200:LYS:NZ	1:A:2200:LYS:HA	2.21	0.56
1:A:2148:ARG:HG2	1:A:2148:ARG:HH11	1.71	0.56
1:B:1948:MSE:HE3	1:B:1950:LEU:HG	1.87	0.56
1:B:1657:TYR:HA	1:B:1690:ILE:HG12	1.87	0.56
1:A:1903:ILE:HB	1:A:1915:THR:HG23	1.87	0.56
1:B:1560:ASN:HD22	1:B:1560:ASN:H	1.54	0.56
1:B:1948:MSE:HE3	1:B:1950:LEU:CD2	2.36	0.56
1:A:2142:GLN:CD	1:A:2143:VAL:N	2.59	0.56
1:A:2164:ASP:OD1	1:A:2167:ASP:HB2	2.06	0.56
1:B:2061:LYS:O	1:B:2061:LYS:HD3	2.06	0.56
1:B:2164:ASP:O	1:B:2166:GLU:N	2.39	0.56
1:B:1730:CYS:CA	1:B:1752:GLN:HG3	2.36	0.56
1:A:1632:ALA:H	1:B:2097:HIS:HE1	1.53	0.56
1:B:1877:VAL:HG23	1:B:1928:SER:HB2	1.88	0.56
1:B:2082:LEU:N	1:B:2082:LEU:HD12	2.21	0.55
1:A:1776:GLN:O	1:B:1960:GLN:HG3	2.05	0.55
1:A:1980:ASP:O	1:A:1982:LYS:HD2	2.06	0.55
1:B:1940:ASN:HD21	1:B:1982:LYS:H	1.54	0.55
1:B:1955:GLY:HA2	1:B:1999:SER:HB3	1.88	0.55
1:A:2140:SER:HB3	1:A:2151:LYS:HE2	1.88	0.55
1:B:1516:ARG:NH2	1:B:1534:ASP:HA	2.22	0.55
1:B:2132:GLU:O	1:B:2136:ILE:HG12	2.07	0.55
1:A:1860:LEU:HD23	1:A:2115:TRP:CZ3	2.41	0.55
1:B:1643:TRP:CE3	1:B:1649:PRO:HB3	2.41	0.55
1:B:1556:GLU:O	1:B:1558:GLY:N	2.38	0.55
1:A:2142:GLN:HG2	1:A:2190:LYS:HZ1	1.71	0.55
1:B:2148:ARG:NH2	1:B:2152:ILE:HD11	2.22	0.55
1:A:1667:LYS:C	1:A:1669:PHE:N	2.59	0.55
1:B:2148:ARG:CZ	1:B:2152:ILE:HD11	2.37	0.55
1:A:2142:GLN:HG2	1:A:2190:LYS:NZ	2.22	0.55
1:B:1560:ASN:ND2	1:B:1560:ASN:H	2.05	0.55
1:B:2139:LEU:O	1:B:2141:HIS:N	2.40	0.54
1:B:2100:SER:HA	1:B:2103:MSE:HE3	1.88	0.54
1:A:2034:LYS:HB2	1:B:1631:MSE:CE	2.32	0.54
1:B:1948:MSE:HE3	1:B:1950:LEU:CG	2.37	0.54
1:B:1593:ILE:HB	1:B:1625:SER:OG	2.08	0.54
1:B:1987:ILE:HB	1:B:2014:MSE:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1620:TYR:HB3	1:B:1726:THR:HB	1.88	0.54
1:A:1968:LEU:HD21	1:B:1756:LEU:HD11	1.90	0.54
1:B:1829:ARG:NH2	1:B:2119:ARG:HE	2.06	0.54
1:B:2039:LYS:HZ2	1:B:2039:LYS:HB2	1.71	0.54
1:B:1505:THR:CB	1:B:1730:CYS:HB2	2.35	0.54
1:B:1922:GLN:HB2	1:B:1954:ARG:NH1	2.22	0.54
1:B:2037:ARG:NE	1:B:2083:LEU:HD11	2.21	0.54
1:A:2097:HIS:O	1:A:2102:ARG:HD3	2.08	0.54
1:A:1624:ASN:ND2	1:A:1733:VAL:H	2.05	0.54
1:B:2037:ARG:HE	1:B:2083:LEU:HD11	1.72	0.54
1:A:2050:LYS:NZ	1:A:2078:ARG:HD3	2.23	0.54
1:B:2158:TRP:NE1	1:B:2185:LYS:HE3	2.23	0.54
1:A:1918:GLN:O	1:A:1920:PRO:HD3	2.08	0.53
1:B:1594:GLY:O	1:B:1624:ASN:HB2	2.08	0.53
1:A:2196:GLN:NE2	1:A:2196:GLN:HA	2.22	0.53
1:B:1680:THR:HG22	1:B:1681:VAL:N	2.23	0.53
1:B:1730:CYS:C	1:B:1752:GLN:HG3	2.29	0.53
1:A:1735:ILE:HD12	1:A:1735:ILE:N	2.22	0.53
1:B:2164:ASP:C	1:B:2166:GLU:H	2.11	0.53
1:A:1946:PRO:HG3	1:A:2130:LEU:HD21	1.90	0.53
1:B:1741:ARG:HH22	1:B:1934:GLN:NE2	2.05	0.53
1:B:2075:LEU:O	1:B:2079:GLU:HG3	2.09	0.53
1:B:1966:GLU:HG2	1:B:1969:LYS:CE	2.38	0.53
1:B:2131:ASN:ND2	1:B:2179:TYR:OH	2.42	0.53
1:B:1592:LYS:O	1:B:1593:ILE:HG13	2.08	0.52
1:B:2046:ARG:C	1:B:2047:LEU:HD12	2.29	0.52
1:A:2167:ASP:OD1	1:A:2170:GLN:HB2	2.09	0.52
1:A:1883:ARG:HA	1:A:1887:ILE:O	2.08	0.52
1:B:1783:MSE:SE	1:B:1786:ASN:HD21	2.42	0.52
1:A:1860:LEU:HD23	1:A:2115:TRP:CH2	2.45	0.52
1:A:1655:TYR:CE1	1:A:1689:VAL:HG12	2.44	0.52
1:B:1922:GLN:CD	1:B:1954:ARG:HH12	2.12	0.52
1:A:2052:ARG:HH11	1:A:2052:ARG:HG3	1.73	0.52
1:B:2139:LEU:O	1:B:2140:SER:C	2.47	0.52
1:B:1545:ASP:OD1	1:B:1549:GLU:N	2.42	0.52
1:B:2147:SER:O	1:B:2148:ARG:C	2.48	0.52
1:A:1820:ILE:HD12	1:A:1886:GLY:O	2.10	0.52
1:A:1548:GLY:O	1:A:1606:LYS:HE2	2.09	0.52
1:B:1537:PHE:CZ	1:B:1569:ILE:HD12	2.45	0.52
1:B:1952:ASN:OD1	1:B:1993:GLY:HA2	2.09	0.52
1:B:2148:ARG:O	1:B:2149:LEU:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2082:LEU:CD1	1:B:2082:LEU:N	2.72	0.52
1:A:2028:GLN:H	1:A:2028:GLN:CD	2.13	0.52
1:A:2124:TRP:CZ3	1:A:2169:ARG:HG3	2.45	0.52
1:B:2160:PRO:HD2	1:B:2163:VAL:HG21	1.90	0.52
1:A:1657:TYR:CE2	1:A:1687:ARG:HD2	2.44	0.52
1:A:2142:GLN:HB3	1:A:2190:LYS:HZ2	1.74	0.52
1:A:1727:LEU:HB2	1:A:1803:ILE:HD11	1.91	0.52
1:A:1724:THR:H	1:A:1745:ARG:HH21	1.56	0.52
1:A:1877:VAL:HG23	1:A:1931:LYS:HD3	1.91	0.52
1:A:1655:TYR:CD1	1:A:1689:VAL:HG12	2.45	0.51
1:A:2127:ARG:NH2	1:A:2176:GLU:OE2	2.43	0.51
1:A:1508:VAL:HG21	1:A:1565:VAL:CG2	2.40	0.51
1:A:1511:PHE:CZ	1:A:1729:THR:HG21	2.46	0.51
1:A:1846:MSE:HE2	1:A:2115:TRP:CH2	2.45	0.51
1:A:1881:ARG:HH11	1:A:1881:ARG:HG2	1.76	0.51
1:A:1673:ASN:N	1:A:1673:ASN:OD1	2.42	0.51
1:B:2139:LEU:HD21	1:B:2154:ARG:NH1	2.25	0.51
1:B:2035:PHE:CE2	1:B:2039:LYS:HG2	2.45	0.51
1:A:2099:ARG:NH1	1:A:2099:ARG:HG3	2.26	0.51
1:B:1940:ASN:ND2	1:B:1982:LYS:H	2.08	0.51
1:A:1679:ARG:HG3	1:A:1679:ARG:NH1	2.25	0.51
1:A:2143:VAL:HG12	1:A:2144:GLY:N	2.25	0.51
1:B:1954:ARG:NH1	1:B:1954:ARG:HG3	2.24	0.51
1:B:2010:ASP:OD2	1:B:2148:ARG:HG3	2.08	0.51
1:B:1917:ILE:HD12	1:B:1961:ARG:HH22	1.74	0.51
1:B:1528:ALA:O	1:B:1530:VAL:N	2.44	0.51
1:B:1713:GLY:O	1:B:1717:ARG:HG3	2.11	0.51
1:A:1963:MSE:HE3	1:B:1783:MSE:HE2	1.93	0.51
1:A:1754:ILE:HD12	1:A:1783:MSE:HG2	1.92	0.51
1:A:1667:LYS:O	1:A:1669:PHE:N	2.43	0.51
1:B:2055:ARG:HG3	1:B:2055:ARG:NH1	2.25	0.51
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	1.91	0.51
1:A:2191:LEU:HD23	1:A:2191:LEU:O	2.11	0.51
1:A:1991:PRO:HG3	1:A:2115:TRP:HB2	1.91	0.51
1:A:2022:ALA:HB3	1:A:2103:MSE:HE2	1.92	0.51
1:A:1705:LEU:HB3	1:B:2000:TRP:CD1	2.46	0.51
1:A:1790:HIS:HB3	1:A:1869:THR:CG2	2.41	0.50
1:A:1785:ASN:ND2	1:A:1785:ASN:N	2.56	0.50
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	2.09	0.50
1:B:1856:PHE:CD2	1:B:1863:LYS:HE2	2.45	0.50
1:B:2119:ARG:HH11	1:B:2119:ARG:CG	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2131:ASN:HD22	1:A:2175:ILE:CG2	2.24	0.50
1:B:1785:ASN:HD22	1:B:1785:ASN:N	2.09	0.50
1:B:1661:GLU:O	1:B:1664:GLU:N	2.44	0.50
1:B:1584:VAL:HG22	1:B:1619:ILE:HB	1.91	0.50
1:A:1988:TYR:HA	1:A:2015:TYR:O	2.12	0.50
1:B:1772:THR:HG23	1:B:1776:GLN:HE22	1.76	0.50
1:A:1682:ILE:CG1	1:A:1683:ASN:N	2.74	0.50
1:B:1663:MSE:HB2	1:B:1688:PHE:CE1	2.47	0.50
1:A:2085:ILE:O	1:A:2088:GLN:HB2	2.12	0.50
1:A:2102:ARG:HH11	1:B:1694:ILE:HG23	1.76	0.50
1:A:2167:ASP:HB3	1:A:2170:GLN:HB2	1.94	0.50
1:B:1936:ILE:HG12	1:B:1947:MSE:SE	2.61	0.50
1:A:1778:GLY:HA2	1:A:1783:MSE:HE2	1.93	0.50
1:A:2192:GLU:O	1:A:2196:GLN:HB2	2.11	0.49
1:B:1624:ASN:HD22	1:B:1626:GLY:H	1.59	0.49
1:B:1730:CYS:O	1:B:1731:ARG:HB3	2.13	0.49
1:B:1660:SER:HA	1:B:1688:PHE:HE1	1.77	0.49
1:B:1513:GLU:O	1:B:1517:GLN:HG3	2.11	0.49
1:A:1737:ALA:O	1:A:1740:VAL:CG1	2.60	0.49
1:A:2097:HIS:CE1	1:B:1632:ALA:H	2.30	0.49
1:A:2193:SER:O	1:A:2195:ALA:N	2.46	0.49
1:A:2017:ASP:OD2	1:A:2115:TRP:HB2	2.12	0.49
1:A:1654:GLN:O	1:A:1655:TYR:HB3	2.12	0.49
1:A:1837:ASN:OD1	1:A:1992:THR:HG22	2.12	0.49
1:B:1966:GLU:HG2	1:B:1969:LYS:HD2	1.94	0.49
1:B:1747:ILE:HD12	1:B:1747:ILE:N	2.27	0.49
1:B:1711:ILE:HD11	1:B:1735:ILE:HG12	1.95	0.49
1:A:1497:ARG:HD3	1:A:1510:ASP:OD2	2.12	0.49
1:A:1682:ILE:HG23	1:A:1687:ARG:HG3	1.94	0.49
1:B:1836:THR:HG22	1:B:1838:ASP:N	2.26	0.49
1:A:2058:LEU:HD22	1:A:2068:HIS:CE1	2.46	0.49
1:A:1768:ARG:HD2	1:A:1770:VAL:HG22	1.94	0.49
1:B:1772:THR:HG23	1:B:1776:GLN:NE2	2.27	0.49
1:A:2041:LEU:HD12	1:A:2044:MSE:CE	2.42	0.49
1:A:1494:GLN:OE1	1:A:1496:LYS:HG2	2.13	0.49
1:A:1744:GLN:HA	1:A:1744:GLN:NE2	2.28	0.49
1:B:2160:PRO:HD2	1:B:2163:VAL:CG2	2.43	0.49
1:A:1711:ILE:HD12	1:A:1739:LEU:HD11	1.94	0.49
1:A:1511:PHE:HZ	1:A:1729:THR:HG21	1.77	0.49
1:A:2125:ARG:HH12	1:A:2128:ARG:HH21	1.61	0.49
1:B:1748:GLN:O	1:B:1792:THR:HA	2.13	0.49

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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:B:1495:PRO:HG2	1:B:1496:LYS:H	1.78	0.48
1:A:1803:ILE:HG22	1:A:1807:MSE:CE	2.44	0.48
1:A:1629:ILE:HG12	2:A:3203:ACO:C6A	2.43	0.48
1:A:1963:MSE:HE1	1:B:1755:ILE:HA	1.94	0.48
1:A:1968:LEU:HD12	1:B:1783:MSE:HE1	1.96	0.48
1:B:1643:TRP:HA	1:B:1653:PHE:HA	1.95	0.48
1:B:1883:ARG:HA	1:B:1887:ILE:O	2.13	0.48
1:A:1841:TYR:CZ	1:A:1896:THR:HG21	2.48	0.48
1:B:1575:GLU:H	1:B:1575:GLU:CD	2.17	0.48
1:B:1676:LEU:HD12	1:B:1692:THR:HG21	1.95	0.48
1:B:1682:ILE:HG13	1:B:1685:GLU:O	2.14	0.48
1:B:1975:VAL:O	1:B:1979:VAL:HG23	2.12	0.48
1:A:1735:ILE:H	1:A:1735:ILE:CD1	2.22	0.48
1:A:2156:ARG:HG2	1:A:2159:TYR:CE1	2.49	0.48
1:B:1600:GLU:N	1:B:1600:GLU:OE1	2.45	0.48
1:A:2083:LEU:HA	1:A:2083:LEU:HD12	1.72	0.48
1:A:1748:GLN:O	1:A:1792:THR:HA	2.13	0.48
1:B:1625:SER:OG	1:B:1731:ARG:NH2	2.45	0.48
1:A:1508:VAL:HG21	1:A:1565:VAL:HG21	1.96	0.48
1:A:1651:LYS:HG3	1:A:1651:LYS:O	2.14	0.48
1:B:1645:ASP:O	1:B:1647:ALA:O	2.32	0.47
1:A:2082:LEU:HA	1:A:2085:ILE:HD13	1.96	0.47
1:A:1682:ILE:C	1:A:1684:GLY:N	2.68	0.47
1:B:1766:LEU:O	1:B:1767:GLY:C	2.52	0.47
1:A:1720:HIS:HD2	1:A:1941:ASN:ND2	2.13	0.47
1:A:1842:ASP:HA	1:A:1897:ARG:HH11	1.79	0.47
1:A:1484:ALA:O	1:A:1485:THR:O	2.32	0.47
1:B:2058:LEU:HD21	1:B:2071:ILE:HB	1.96	0.47
1:A:1624:ASN:HD21	1:A:1733:VAL:H	1.62	0.47
1:B:1966:GLU:HG2	1:B:1969:LYS:CD	2.44	0.47
1:A:1909:ASN:HB3	1:A:1912:SER:HB2	1.96	0.47
1:B:2138:ARG:HH11	1:B:2138:ARG:HG3	1.79	0.47
1:B:2164:ASP:C	1:B:2166:GLU:N	2.68	0.47
1:B:1985:ILE:HD12	1:B:2012:MSE:HG2	1.96	0.47
1:A:2197:ASP:O	1:A:2201:LYS:HB3	2.15	0.47
1:A:1689:VAL:HG23	1:A:1691:LYS:HE2	1.97	0.47
1:B:1598:PRO:HG2	1:B:1698:ASP:OD1	2.15	0.47
1:A:1522:GLN:NE2	1:A:1574:PRO:HD2	2.30	0.47
1:A:1508:VAL:CG2	1:A:1565:VAL:HG21	2.44	0.47
1:B:1583:VAL:HG22	1:B:1584:VAL:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1842:ASP:OD1	1:A:1844:ARG:NH1	2.43	0.47
1:A:1667:LYS:NZ	1:A:1670:ASP:HA	2.29	0.47
1:A:2138:ARG:HB3	1:A:2138:ARG:NH1	2.29	0.47
1:B:2180:LYS:HZ2	1:B:2180:LYS:HB3	1.80	0.47
1:A:2128:ARG:HD3	1:A:2171:VAL:HG11	1.97	0.47
1:B:1797:LEU:O	1:B:1801:GLU:HG3	2.15	0.47
1:B:2041:LEU:HA	1:B:2044:MSE:HG3	1.97	0.47
1:B:1852:THR:C	1:B:1854:SER:H	2.18	0.46
1:B:1810:VAL:HG23	1:B:1811:PRO:CD	2.45	0.46
1:B:1523:TRP:HB3	1:B:1530:VAL:HG21	1.98	0.46
1:A:2002:VAL:HG23	1:A:2003:VAL:HG13	1.97	0.46
1:B:2078:ARG:CZ	1:B:2082:LEU:HD11	2.45	0.46
1:B:1682:ILE:HD12	1:B:1682:ILE:C	2.35	0.46
1:B:1940:ASN:ND2	1:B:1983:GLN:NE2	2.50	0.46
1:B:2064:ALA:HB3	1:B:2067:VAL:CG2	2.45	0.46
1:A:1881:ARG:NH1	1:A:1881:ARG:HG2	2.31	0.46
1:A:1681:VAL:HA	1:A:1685:GLU:O	2.15	0.46
1:A:2191:LEU:C	1:A:2191:LEU:CD2	2.83	0.46
1:B:1499:LYS:NZ	1:B:1499:LYS:HB2	2.31	0.46
1:B:2139:LEU:HD11	1:B:2154:ARG:HH11	1.81	0.46
1:A:2143:VAL:O	1:A:2145:GLU:N	2.49	0.46
1:B:1917:ILE:O	1:B:1917:ILE:HG12	2.14	0.46
1:A:2196:GLN:NE2	1:A:2196:GLN:CA	2.77	0.46
1:B:1759:ALA:N	1:B:1760:PRO:CD	2.79	0.46
1:B:1514:LEU:HD22	1:B:1797:LEU:HD13	1.97	0.46
1:B:1729:THR:HG22	1:B:1796:ASP:OD1	2.16	0.46
1:A:1657:TYR:HB2	1:A:1688:PHE:O	2.16	0.46
1:A:1963:MSE:CE	1:B:1755:ILE:HA	2.46	0.46
1:B:1906:ASP:H	1:B:1912:SER:HB2	1.80	0.46
1:A:1730:CYS:O	1:A:1731:ARG:HB3	2.16	0.45
1:A:2102:ARG:NH2	1:B:1700:LEU:HB2	2.31	0.45
1:A:2110:SER:O	1:A:2111:LYS:HG3	2.16	0.45
1:B:1733:VAL:HG22	1:B:1755:ILE:CD1	2.44	0.45
1:B:1906:ASP:H	1:B:1912:SER:CB	2.29	0.45
1:A:2037:ARG:CB	1:A:2037:ARG:HH11	2.20	0.45
1:B:1901:ASN:HB3	1:B:1917:ILE:HG23	1.99	0.45
1:A:2148:ARG:HG2	1:A:2148:ARG:NH1	2.32	0.45
1:A:1575:GLU:HG2	1:A:1576:TYR:CD1	2.51	0.45
1:B:1985:ILE:HD12	1:B:2012:MSE:CG	2.47	0.45
1:A:1619:ILE:HD12	1:A:1725:ILE:CG2	2.45	0.45
1:B:1671:LYS:C	1:B:1673:ASN:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1903:ILE:HD12	1:A:1903:ILE:N	2.32	0.45
1:B:2108:VAL:HG23	1:B:2109:ILE:HG23	1.99	0.45
1:A:2030:MSE:HG3	1:B:1631:MSE:HE2	1.99	0.45
1:B:2044:MSE:HB3	1:B:2044:MSE:HE3	1.84	0.45
1:B:2126:LEU:HD22	1:B:2130:LEU:HD13	1.99	0.45
1:A:2129:ARG:HG3	1:A:2129:ARG:HH11	1.82	0.45
1:A:2021:ARG:HE	1:A:2095:ASP:CG	2.20	0.45
1:B:2188:GLY:C	1:B:2189:LEU:HD23	2.36	0.45
1:A:1901:ASN:O	1:A:1916:LEU:HD12	2.16	0.45
1:A:1720:HIS:HD2	1:A:1941:ASN:HD21	1.63	0.45
1:A:1612:ARG:O	1:A:1814:ARG:NH2	2.37	0.45
1:A:1610:TYR:CE1	1:A:1614:ARG:CZ	3.00	0.45
1:A:1667:LYS:HD3	1:A:1667:LYS:O	2.17	0.45
1:A:1784:TYR:CD1	1:A:1792:THR:HG23	2.51	0.45
1:B:1951:ALA:O	1:B:1990:PRO:HD2	2.18	0.44
1:B:1593:ILE:HB	1:B:1625:SER:HG	1.82	0.44
1:B:2142:GLN:C	1:B:2142:GLN:CD	2.75	0.44
1:A:1956:PHE:HB2	1:B:1756:LEU:HD23	1.99	0.44
1:B:1903:ILE:HA	1:B:1904:PRO:HD3	1.77	0.44
1:B:1744:GLN:O	1:B:1790:HIS:CE1	2.70	0.44
1:B:1874:ALA:HB2	1:B:1927:ASN:HB2	1.98	0.44
1:A:1708:SER:OG	1:A:1735:ILE:HG12	2.18	0.44
1:A:1803:ILE:HG22	1:A:1807:MSE:HE2	2.00	0.44
1:B:1657:TYR:HB2	1:B:1688:PHE:O	2.18	0.44
1:A:1991:PRO:O	1:A:2019:ASN:O	2.34	0.44
1:B:2126:LEU:CD2	1:B:2130:LEU:HD13	2.48	0.44
1:A:1996:ARG:NE	1:A:2026:GLU:HG2	2.32	0.44
1:B:1818:VAL:O	1:B:1820:ILE:HD12	2.17	0.44
1:B:1877:VAL:HG12	1:B:1878:VAL:N	2.33	0.44
1:A:1713:GLY:O	1:A:1717:ARG:HG3	2.18	0.44
1:B:2082:LEU:HB3	1:B:2086:TYR:CD1	2.53	0.44
1:B:1496:LYS:HB3	1:B:1507:TYR:CE2	2.53	0.44
1:A:2000:TRP:CD1	1:B:1705:LEU:HB3	2.53	0.44
1:B:1532:LEU:HD13	1:B:1536:PHE:CE1	2.52	0.44
1:A:2066:GLU:H	1:A:2066:GLU:CD	2.21	0.44
1:B:1657:TYR:CD2	1:B:1687:ARG:CB	2.99	0.44
1:B:1783:MSE:HA	1:B:1786:ASN:ND2	2.33	0.44
1:A:2144:GLY:O	1:A:2145:GLU:C	2.55	0.43
1:B:2047:LEU:N	1:B:2047:LEU:HD12	2.32	0.43
1:B:1640:GLN:O	1:B:1656:LEU:HA	2.17	0.43
1:B:1669:PHE:N	1:B:1669:PHE:CD2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1735:ILE:O	1:A:1739:LEU:HG	2.18	0.43
1:B:2100:SER:CA	1:B:2103:MSE:HE3	2.48	0.43
1:B:1594:GLY:O	1:B:1624:ASN:CB	2.66	0.43
1:A:2072:SER:O	1:A:2075:LEU:HB3	2.18	0.43
1:B:1844:ARG:HH11	1:B:1844:ARG:HG3	1.82	0.43
1:B:2070:GLN:HG3	1:B:2074:GLN:NE2	2.33	0.43
1:B:1607:VAL:O	1:B:1610:TYR:HB3	2.17	0.43
1:B:1644:ASN:OD1	1:B:1651:LYS:O	2.37	0.43
1:B:1602:GLU:O	1:B:1606:LYS:HB2	2.18	0.43
1:B:1676:LEU:HD12	1:B:1692:THR:CG2	2.48	0.43
1:A:1903:ILE:HA	1:A:1904:PRO:HD3	1.86	0.43
1:B:1829:ARG:CZ	1:B:2119:ARG:NE	2.74	0.43
1:A:1829:ARG:CZ	1:A:1858:TYR:HB3	2.48	0.43
1:B:1827:TRP:CD2	1:B:1828:ASP:N	2.87	0.43
1:B:1644:ASN:ND2	1:B:1654:GLN:HE21	2.03	0.43
1:A:2197:ASP:O	1:A:2200:LYS:O	2.36	0.43
1:A:1990:PRO:HB2	1:A:1991:PRO:HD2	2.01	0.43
1:B:1895:GLU:OE2	1:B:1897:ARG:NH2	2.35	0.43
1:A:1895:GLU:HA	1:A:1895:GLU:OE2	2.18	0.43
1:A:1735:ILE:HG23	1:B:2001:VAL:HG21	2.00	0.43
1:A:2138:ARG:C	1:A:2140:SER:H	2.22	0.43
1:A:1566:ALA:HA	1:A:1584:VAL:O	2.19	0.43
1:A:2165:HIS:ND1	1:A:2165:HIS:N	2.65	0.43
1:B:1881:ARG:HH11	1:B:1881:ARG:HG3	1.83	0.43
1:A:1511:PHE:N	1:A:1512:PRO:CD	2.82	0.43
1:B:1617:PRO:HG2	1:B:1807:MSE:HE3	2.00	0.43
1:A:2198:LEU:C	1:A:2198:LEU:HD23	2.37	0.43
1:B:1865:SER:O	1:B:1882:ALA:HA	2.18	0.43
1:B:1660:SER:HA	1:B:1688:PHE:CE1	2.53	0.43
1:A:1702:VAL:HA	1:A:1705:LEU:HD22	2.01	0.43
1:A:1747:ILE:HD12	1:A:1803:ILE:HG13	2.02	0.42
1:B:1785:ASN:HA	1:B:1872:GLY:O	2.19	0.42
1:B:1541:GLU:HA	1:B:1567:PHE:HD2	1.84	0.42
1:B:1728:VAL:HG12	1:B:1752:GLN:HB3	2.01	0.42
1:B:2070:GLN:OE1	1:B:2070:GLN:HA	2.19	0.42
1:A:1783:MSE:HB3	1:A:1789:SER:OG	2.20	0.42
1:B:1786:ASN:C	1:B:1786:ASN:OD1	2.57	0.42
1:A:2154:ARG:O	1:A:2157:SER:OG	2.38	0.42
1:B:1765:MSE:C	1:B:1766:LEU:HD12	2.39	0.42
1:B:2082:LEU:O	1:B:2083:LEU:C	2.58	0.42
1:A:1702:VAL:HA	1:A:1705:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1681:VAL:O	1:B:1681:VAL:HG22	2.20	0.42
1:A:2052:ARG:HH11	1:A:2052:ARG:CG	2.32	0.42
1:B:2179:TYR:O	1:B:2183:ASP:HB2	2.20	0.42
1:B:1644:ASN:HD21	1:B:1654:GLN:NE2	2.05	0.42
1:B:1836:THR:O	1:B:1838:ASP:N	2.52	0.42
1:B:2083:LEU:HA	1:B:2083:LEU:HD23	1.90	0.42
1:A:2108:VAL:HG11	1:B:1702:VAL:HG23	2.01	0.42
1:A:1638:LEU:CD1	1:A:1658:LEU:HD22	2.50	0.41
1:B:1831:VAL:HG22	1:B:2119:ARG:HB2	2.02	0.41
1:A:1901:ASN:ND2	1:A:1903:ILE:HD11	2.35	0.41
1:A:1819:PRO:O	1:A:1888:PRO:HG3	2.20	0.41
1:A:1981:TYR:CG	1:A:1985:ILE:HD11	2.55	0.41
1:A:1952:ASN:HA	1:A:1994:GLU:O	2.20	0.41
1:B:1766:LEU:N	1:B:1766:LEU:CD1	2.84	0.41
1:B:1998:GLY:O	1:B:2001:VAL:CG1	2.68	0.41
1:B:2148:ARG:NE	1:B:2152:ILE:HD11	2.36	0.41
1:B:1813:LYS:HG3	1:B:1816:MSE:HG2	2.02	0.41
1:B:1702:VAL:HA	1:B:1705:LEU:HD12	2.01	0.41
1:B:1881:ARG:HG3	1:B:1881:ARG:NH1	2.36	0.41
1:A:1659:THR:O	1:A:1660:SER:C	2.57	0.41
1:A:1686:GLU:C	1:A:1687:ARG:HG2	2.40	0.41
1:A:1785:ASN:HA	1:A:1872:GLY:O	2.20	0.41
1:A:1737:ALA:O	1:A:1740:VAL:HG13	2.20	0.41
1:A:1800:VAL:O	1:A:1804:VAL:HG23	2.20	0.41
1:A:1680:THR:CG2	1:A:1681:VAL:N	2.82	0.41
1:A:1680:THR:HB	1:A:1687:ARG:O	2.21	0.41
1:B:1643:TRP:CZ3	1:B:1649:PRO:HB3	2.56	0.41
1:A:1686:GLU:O	1:A:1687:ARG:HG2	2.21	0.41
1:A:1643:TRP:CH2	1:A:1649:PRO:HB3	2.55	0.41
1:A:2078:ARG:HA	1:A:2081:GLU:HG2	2.02	0.41
1:B:1702:VAL:HG23	1:B:1703:GLU:N	2.36	0.41
1:A:1836:THR:O	1:A:1838:ASP:N	2.46	0.41
1:B:1671:LYS:C	1:B:1673:ASN:N	2.74	0.41
1:B:1842:ASP:OD1	1:B:1844:ARG:HG3	2.20	0.41
1:B:1834:THR:HA	1:B:1835:PRO:HD3	1.83	0.41
1:B:1755:ILE:N	1:B:1755:ILE:CD1	2.83	0.41
1:A:2102:ARG:NH1	1:B:1694:ILE:HG23	2.36	0.41
1:A:2022:ALA:O	1:A:2098:ASP:HA	2.21	0.41
1:B:1619:ILE:N	1:B:1619:ILE:HD12	2.36	0.41
1:A:2108:VAL:HG23	1:A:2109:ILE:HG23	2.03	0.41
1:B:1615:GLY:HA2	1:B:1814:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1526:PHE:C	1:A:1526:PHE:CD1	2.94	0.41
1:B:1968:LEU:HB2	4:B:5028:HOH:O	2.20	0.41
1:A:1783:MSE:HG3	1:A:1788:VAL:HB	2.02	0.41
1:B:2140:SER:O	1:B:2142:GLN:N	2.54	0.40
1:B:2136:ILE:HD13	1:B:2155:ILE:HD12	2.03	0.40
1:B:2061:LYS:O	1:B:2062:SER:HB3	2.21	0.40
1:B:1852:THR:O	1:B:1854:SER:N	2.49	0.40
1:A:1832:ASP:HB2	1:A:1858:TYR:N	2.35	0.40
1:B:2091:LEU:HA	1:B:2091:LEU:HD12	1.90	0.40
1:B:1728:VAL:O	1:B:1749:VAL:HG23	2.21	0.40
1:B:2144:GLY:O	1:B:2145:GLU:C	2.59	0.40
1:A:1968:LEU:HD12	1:B:1783:MSE:CE	2.52	0.40
1:A:1869:THR:HG22	1:A:1870:LEU:N	2.36	0.40
1:A:2167:ASP:CG	1:A:2170:GLN:HB2	2.42	0.40
1:A:2125:ARG:HH12	1:A:2128:ARG:NH2	2.20	0.40
1:A:2056:SER:O	1:A:2060:ASN:N	2.54	0.40
1:B:1668:LYS:HA	1:B:1668:LYS:HD3	1.91	0.40
1:A:1618:ARG:C	1:A:1618:ARG:HE	2.24	0.40
1:B:2187:LYS:C	1:B:2189:LEU:H	2.24	0.40
1:A:1803:ILE:CG2	1:A:1807:MSE:HE2	2.51	0.40
1:B:1902:LEU:HD21	1:B:1914:GLU:CD	2.42	0.40
1:A:1530:VAL:HG23	1:A:1530:VAL:O	2.20	0.40
1:B:1545:ASP:O	1:B:1548:GLY:N	2.45	0.40
1:B:2178:ASN:HD22	1:B:2181:THR:CB	2.34	0.40
1:B:2052:ARG:HH11	1:B:2052:ARG:HG2	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	718/805 (89%)	640 (89%)	61 (8%)	17 (2%)	7 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	694/805 (86%)	608 (88%)	61 (9%)	25 (4%)	4	9
All	All	1412/1610 (88%)	1248 (88%)	122 (9%)	42 (3%)	5	13

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1683	ASN
1	A	1991	PRO
1	A	2144	GLY
1	A	2194	PHE
1	B	1838	ASP
1	B	1991	PRO
1	B	1992	THR
1	A	1679	ARG
1	A	1997	GLY
1	A	2142	GLN
1	B	1529	ASP
1	B	1683	ASN
1	B	1684	GLY
1	B	2140	SER
1	B	2141	HIS
1	B	2143	VAL
1	B	2165	HIS
1	A	1485	THR
1	A	1668	LYS
1	A	1744	GLN
1	B	1526	PHE
1	B	2061	LYS
1	B	2084	PRO
1	B	2148	ARG
1	A	1527	SER
1	A	1826	THR
1	A	2161	ALA
1	B	1558	GLY
1	B	1837	ASN
1	A	1731	ARG
1	A	2139	LEU
1	B	1731	ARG
1	B	1853	GLU
1	A	1682	ILE
1	B	1508	VAL
1	B	1534	ASP

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Mol	Chain	Res	Type
1	B	2038	GLU
1	B	2145	GLU
1	A	2143	VAL
1	B	1843	VAL
1	B	2144	GLY
1	B	1557	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	612/668 (92%)	556 (91%)	56 (9%)	11	25
1	B	591/668 (88%)	539 (91%)	52 (9%)	12	28
All	All	1203/1336 (90%)	1095 (91%)	108 (9%)	12	27

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

Mol	Chain	Res	Type
1	A	1514	LEU
1	A	1532	LEU
1	A	1541	GLU
1	A	1554	GLU
1	A	1560	ASN
1	A	1570	THR
1	A	1580	ARG
1	A	1589	ILE
1	A	1602	GLU
1	A	1618	ARG
1	A	1634	GLU
1	A	1650	ASP
1	A	1667	LYS
1	A	1673	ASN
1	A	1675	VAL
1	A	1697	GLU
1	A	1705	LEU

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Mol	Chain	Res	Type
1	A	1706	ARG
1	A	1733	VAL
1	A	1735	ILE
1	A	1757	THR
1	A	1772	THR
1	A	1780	THR
1	A	1781	GLN
1	A	1783	MSE
1	A	1785	ASN
1	A	1786	ASN
1	A	1813	LYS
1	A	1821	LEU
1	A	1823	THR
1	A	1860	LEU
1	A	1877	VAL
1	A	1879	VAL
1	A	1884	LEU
1	A	1895	GLU
1	A	1924	TRP
1	A	1991	PRO
1	A	1999	SER
1	A	2001	VAL
1	A	2008	ASN
1	A	2028	GLN
1	A	2035	PHE
1	A	2037	ARG
1	A	2038	GLU
1	A	2085	ILE
1	A	2126	LEU
1	A	2128	ARG
1	A	2145	GLU
1	A	2163	VAL
1	A	2165	HIS
1	A	2179	TYR
1	A	2183	ASP
1	A	2190	LYS
1	A	2192	GLU
1	A	2194	PHE
1	A	2201	LYS
1	B	1499	LYS
1	B	1513	GLU
1	B	1527	SER

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Mol	Chain	Res	Type
1	B	1534	ASP
1	B	1540	ASN
1	B	1553	VAL
1	B	1555	ARG
1	B	1560	ASN
1	B	1568	LYS
1	B	1575	GLU
1	B	1602	GLU
1	B	1618	ARG
1	B	1621	LEU
1	B	1638	LEU
1	B	1675	VAL
1	B	1726	THR
1	B	1739	LEU
1	B	1755	ILE
1	B	1757	THR
1	B	1768	ARG
1	B	1772	THR
1	B	1781	GLN
1	B	1810	VAL
1	B	1839	GLU
1	B	1891	VAL
1	B	1902	LEU
1	B	1910	PRO
1	B	1917	ILE
1	B	1923	VAL
1	B	1924	TRP
1	B	1980	ASP
1	B	1981	TYR
1	B	1991	PRO
1	B	1996	ARG
1	B	2001	VAL
1	B	2026	GLU
1	B	2027	PRO
1	B	2035	PHE
1	B	2037	ARG
1	B	2044	MSE
1	B	2055	ARG
1	B	2063	LEU
1	B	2088	GLN
1	B	2091	LEU
1	B	2092	GLN

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Mol	Chain	Res	Type
1	B	2125	ARG
1	B	2126	LEU
1	B	2128	ARG
1	B	2130	LEU
1	B	2142	GLN
1	B	2166	GLU
1	B	2182	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1501	HIS
1	A	1560	ASN
1	A	1599	GLN
1	A	1624	ASN
1	A	1640	GLN
1	A	1654	GLN
1	A	1720	HIS
1	A	1744	GLN
1	A	1748	GLN
1	A	1785	ASN
1	A	1786	ASN
1	A	1790	HIS
1	A	1815	ASN
1	A	1901	ASN
1	A	1909	ASN
1	A	1934	GLN
1	A	1941	ASN
1	A	1983	GLN
1	A	2008	ASN
1	A	2011	GLN
1	A	2045	ASN
1	A	2060	ASN
1	A	2097	HIS
1	A	2131	ASN
1	A	2178	ASN
1	A	2196	GLN
1	B	1525	ASN
1	B	1540	ASN
1	B	1560	ASN
1	B	1581	GLN
1	B	1587	ASN

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Mol	Chain	Res	Type
1	B	1605	ASN
1	B	1624	ASN
1	B	1644	ASN
1	B	1744	GLN
1	B	1748	GLN
1	B	1776	GLN
1	B	1785	ASN
1	B	1925	HIS
1	B	1934	GLN
1	B	1940	ASN
1	B	2057	GLN
1	B	2074	GLN
1	B	2097	HIS
1	B	2131	ASN
1	B	2141	HIS
1	B	2178	ASN

### 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](#)

2 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	ACO	A	3203	-	40,50,53	1.18	5 (12%)	50,75,79	1.87	9 (18%)
3	ADE	B	3190	-	8,11,11	1.47	2 (25%)	4,15,15	1.25	1 (25%)

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	ACO	A	3203	-	-	0/44/64/67	0/3/3/3
3	ADE	B	3190	-	-	0/0/0/0	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3203	ACO	C8A-N7A	-2.13	1.30	1.34
2	A	3203	ACO	CDP-CBP	2.01	1.58	1.53
2	A	3203	ACO	C9P-N8P	2.16	1.38	1.33
3	B	3190	ADE	C4-N9	2.36	1.39	1.34
2	A	3203	ACO	C4A-N3A	2.69	1.39	1.35
2	A	3203	ACO	C2A-N3A	2.73	1.37	1.32
3	B	3190	ADE	C2-N3	2.95	1.37	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3203	ACO	N3A-C2A-N1A	-4.25	125.64	128.89
2	A	3203	ACO	P2A-O3A-P1A	-4.15	121.08	132.73
2	A	3203	ACO	C2P-C3P-N4P	-3.92	104.64	112.37
2	A	3203	ACO	CDP-CBP-CCP	-2.30	105.52	108.50
3	B	3190	ADE	N3-C2-N1	-2.21	127.20	128.89
2	A	3203	ACO	O9A-P3B-O8A	2.03	115.10	107.38
2	A	3203	ACO	O2B-C2B-C3B	2.05	117.09	111.16
2	A	3203	ACO	C4B-O4B-C1B	4.07	114.20	109.72
2	A	3203	ACO	C3P-N4P-C5P	5.24	133.10	122.79
2	A	3203	ACO	O6A-CCP-CBP	5.46	119.33	110.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3203	ACO	4	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	703/805 (87%)	0.02	26 (3%) 45 45	22, 37, 58, 74	0
1	B	679/805 (84%)	-0.01	19 (2%) 56 57	20, 38, 59, 69	0
All	All	1382/1610 (85%)	0.01	45 (3%) 50 50	20, 38, 59, 74	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2143	VAL	8.0
1	A	2194	PHE	5.2
1	A	2146	ALA	4.5
1	A	2203	ARG	4.4
1	A	2201	LYS	4.3
1	B	1529	ASP	4.2
1	A	2198	LEU	4.0
1	B	1681	VAL	3.8
1	B	2144	GLY	3.6
1	A	2145	GLU	3.5
1	B	1527	SER	3.5
1	B	1839	GLU	3.4
1	A	2191	LEU	3.3
1	B	2190	LYS	3.3
1	B	1682	ILE	3.0
1	A	2199	ALA	3.0
1	A	2143	VAL	2.9
1	A	2195	ALA	2.9
1	B	1498	TYR	2.9
1	A	1683	ASN	2.9
1	B	1726	THR	2.8
1	A	1855	GLY	2.7
1	A	1547	ASN	2.6
1	A	1578	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	2144	GLY	2.5
1	A	2197	ASP	2.5
1	B	1621	LEU	2.5
1	A	1681	VAL	2.5
1	A	1684	GLY	2.5
1	B	1547	ASN	2.3
1	B	1502	LEU	2.3
1	B	1585	VAL	2.3
1	B	1497	ARG	2.2
1	A	2141	HIS	2.2
1	A	1889	LEU	2.2
1	A	1529	ASP	2.2
1	B	1556	GLU	2.2
1	B	1852	THR	2.2
1	B	1620	TYR	2.1
1	B	1584	VAL	2.1
1	A	1910	PRO	2.1
1	A	2053	GLU	2.1
1	A	2142	GLN	2.0
1	A	1554	GLU	2.0
1	A	1622	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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(Å <sup>2</sup> )	Q<0.9
3	ADE	B	3190	10/10	0.85	0.28	2.28	61,63,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ACO	A	3203	48/51	0.91	0.17	-0.34	56,68,77,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.