Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:44 PM GMT

PDB ID	:	1UYR
Title	:	ACETYL-COA CARBOXYLASE CARBOXYLTRANSFERASE DOMAIN IN COMPLEX WITH INHIBITOR DICLOFOP
Authors	:	Zhang, H.; Tweel, B.; Tong, L.
Deposited on	:	2004-03-02
Resolution	:	2.50 Å(reported)

The following versions of software and data (see references (i)) 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 2.50 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	Percentile Ranks	Value
Rfree		0.250
Clashscore		14
Ramachandran outliers		1.2%
Sidechain outliers		5.1%
RSRZ outliers		12.2%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
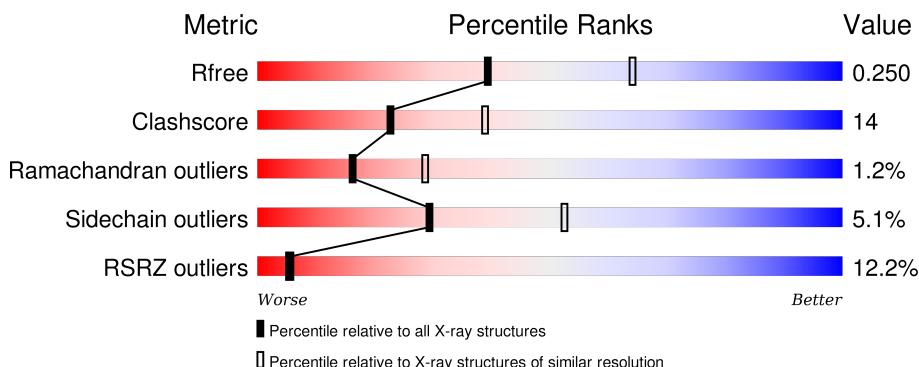
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	737	12% 69% 23% • 5%
1	B	737	12% 66% 26% • 6%
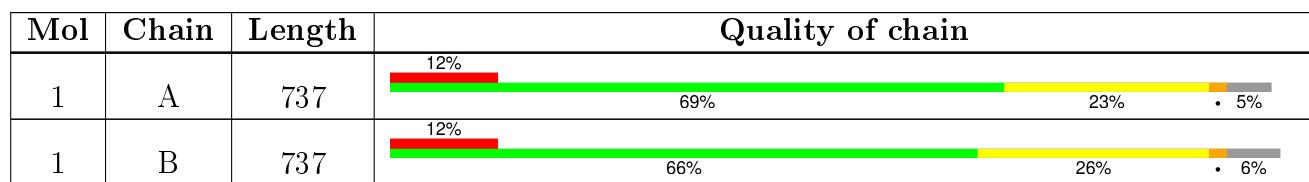
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	D1L	A	3219	-	-	-	X
2	D1L	B	3219	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11229 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	698	Total 5515	C 3514	N 949	O 1034	S 18	0	0	0
1	B	695	Total 5495	C 3498	N 947	O 1032	S 18	0	0	0

- Molecule 2 is 2-[4-(2,4-DICHLOROPHENOXY)PHENOXY]PROPANOIC ACID (three-letter code: D1L) (formula: $C_{15}H_{12}Cl_2O_4$).
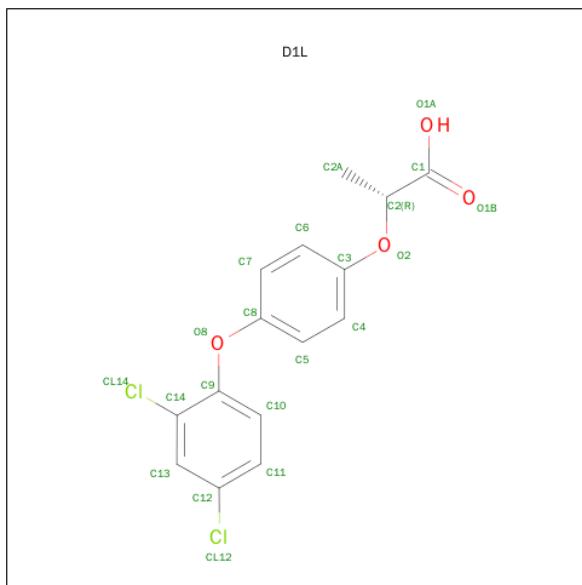
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 21	C 15	Cl 2	O 4	0	0
2	B	1	Total 21	C 15	Cl 2	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total 92	O 92	0	0
3	B	85	Total 85	O 85	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: ACETYL-COA CARBOXYLASE
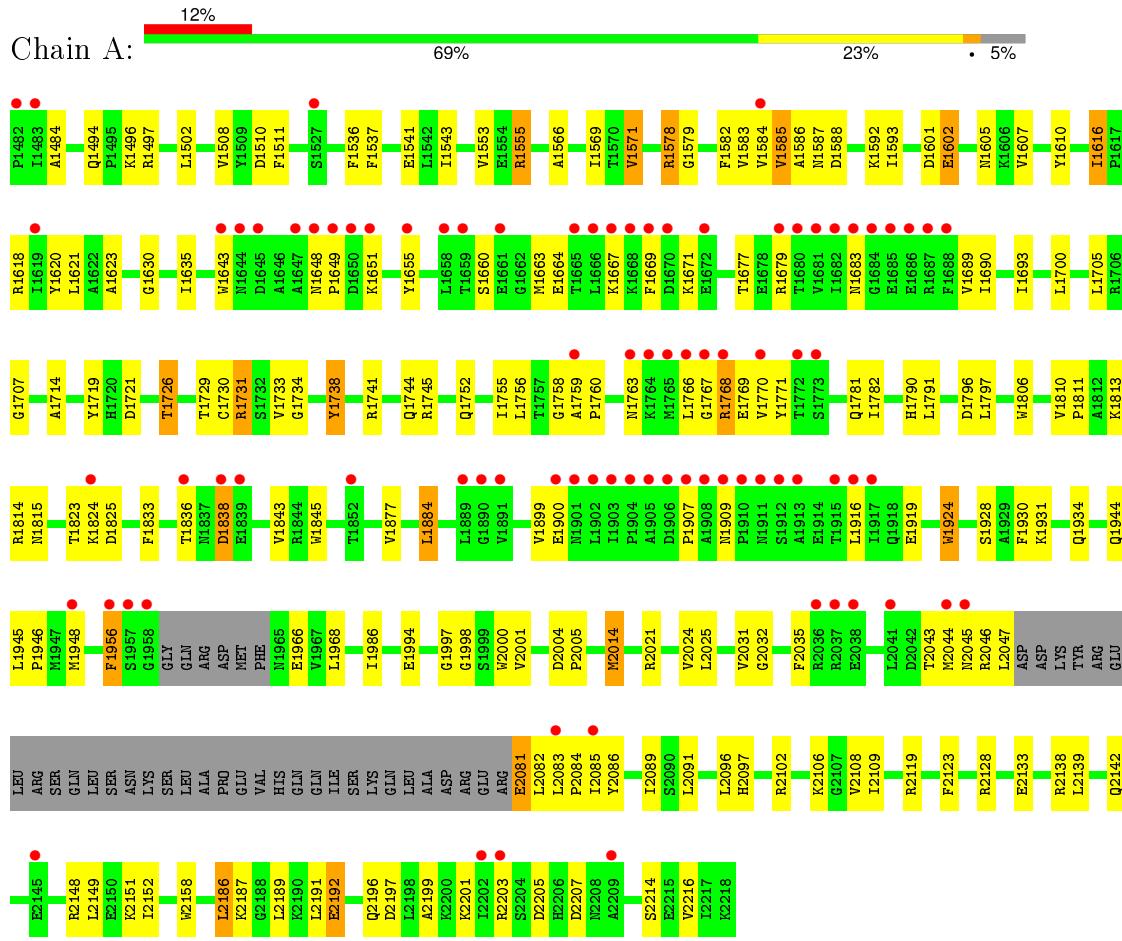
- Molecule 1: ACETYL-COA CARBOXYLASE
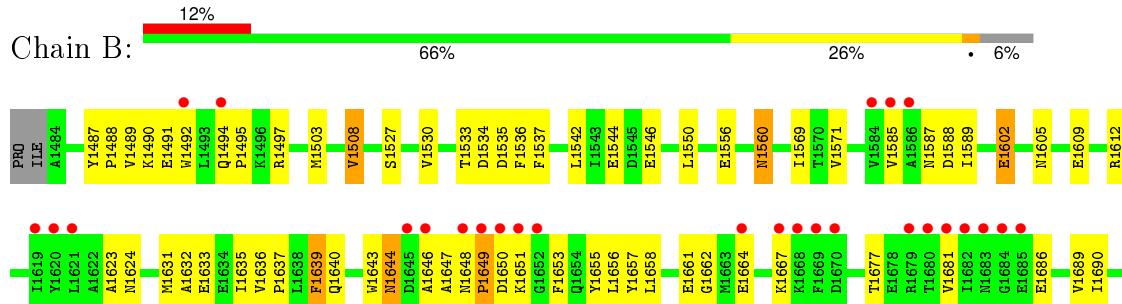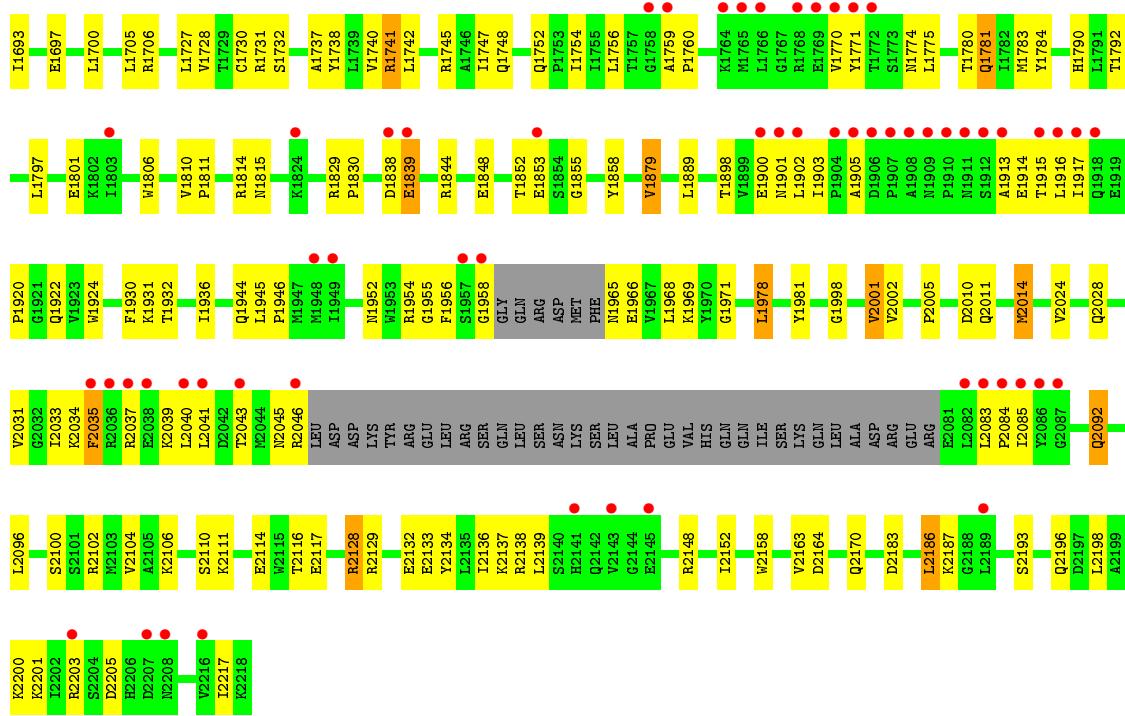
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.78Å 136.78Å 244.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.58 – 2.50 29.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.58-2.50) 98.5 (29.84-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.30 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.248 0.219 , 0.250	Depositor DCC
R_{free} test set	9060 reflections (10.00%)	DCC
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.2	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning [2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 90614 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11229	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: D1L

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	0.37	0/5635	0.59	0/7634
1	B	0.37	0/5614	0.60	1/7605 (0.0%)
All	All	0.37	0/11249	0.59	1/15239 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1647	ALA	N-CA-C	-5.36	96.54	111.00

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	5515	0	5430	141	0
1	B	5495	0	5404	168	0
2	A	21	0	11	6	0
2	B	21	0	11	6	0
3	A	92	0	0	3	0
3	B	85	0	0	5	0
All	All	11229	0	10856	297	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 14.

All (297) 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:1494:GLN:HE21	1:A:1496:LYS:H	1.11	0.98
1:A:2014:MET:HG2	1:A:2109:ILE:HG22	1.45	0.98
1:A:1815:ASN:H	1:A:1944:GLN:HE22	1.06	0.97
1:B:1681:VAL:HA	1:B:1686:GLU:HA	1.51	0.90
1:A:2082:LEU:H	1:A:2082:LEU:HD23	1.38	0.88
1:B:1759:ALA:H	1:B:1774:ASN:HD21	1.20	0.87
1:B:1646:ALA:HB1	1:B:1648:ASN:O	1.77	0.85
1:A:2031:VAL:HG21	1:A:2091:LEU:HD23	1.60	0.84
2:A:3219:D1L:H13	1:B:1971:GLY:HA3	1.59	0.83
1:A:1585:VAL:HG13	1:A:1607:VAL:HG11	1.60	0.83
1:A:1660:SER:O	1:A:1664:GLU:HG2	1.79	0.83
1:A:1781:GLN:HE21	1:A:1782:ILE:HG13	1.46	0.81
1:B:1658:LEU:HG	1:B:1690:ILE:HD11	1.64	0.80
1:A:1587:ASN:HD22	1:A:1623:ALA:H	1.29	0.79
1:A:1836:THR:HG22	1:A:1838:ASP:H	1.48	0.79
1:A:1677:THR:HG22	1:A:1690:ILE:HA	1.66	0.78
1:B:2164:ASP:H	1:B:2170:GLN:NE2	1.82	0.77
1:B:1560:ASN:HD22	1:B:1560:ASN:H	1.34	0.76
1:A:1508:VAL:HG21	1:A:1588:ASP:HA	1.68	0.75
1:B:1681:VAL:HG22	1:B:1686:GLU:HB3	1.69	0.74
1:B:2037:ARG:NH1	1:B:2041:LEU:HD22	2.04	0.72
1:B:2183:ASP:OD1	1:B:2187:LYS:HE3	1.89	0.72
1:A:1738:TYR:CD1	2:A:3219:D1L:H5	2.24	0.72
1:B:1759:ALA:H	1:B:1774:ASN:ND2	1.89	0.71
1:B:1954:ARG:HG3	1:B:1955:GLY:H	1.56	0.70
2:A:3219:D1L:CL14	1:B:1968:LEU:HD12	2.28	0.70
1:A:1738:TYR:OH	1:B:2002:VAL:HG12	1.91	0.70
1:B:2028:GLN:O	1:B:2031:VAL:HG12	1.90	0.70
1:A:1730:CYS:HA	1:A:1752:GLN:HE21	1.57	0.70
1:B:1697:GLU:O	1:B:1700:LEU:HD13	1.92	0.68
1:A:2085:ILE:O	1:A:2089:ILE:HG13	1.94	0.67
1:B:2164:ASP:H	1:B:2170:GLN:HE22	1.41	0.67
1:B:1737:ALA:O	1:B:1740:VAL:HG22	1.95	0.67
1:A:1741:ARG:HH22	1:A:1934:GLN:NE2	1.93	0.66
1:B:1745:ARG:NH2	3:B:4037:HOH:O	2.29	0.66
1:B:1730:CYS:HA	1:B:1752:GLN:OE1	1.96	0.66
1:B:1587:ASN:HD22	1:B:1623:ALA:H	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2197:ASP:OD2	1:A:2201:LYS:HE2	1.96	0.66
1:A:1663:MET:O	1:A:1667:LYS:HG3	1.97	0.64
1:A:2001:VAL:HG21	2:B:3219:D1L:H4	1.79	0.64
1:B:2137:LYS:HE3	3:B:4079:HOH:O	1.97	0.63
1:A:1745:ARG:NH2	3:A:4038:HOH:O	2.31	0.62
1:A:1768:ARG:H	1:A:1768:ARG:HD3	1.65	0.62
1:A:1968:LEU:HD23	2:B:3219:D1L:CL14	2.36	0.62
1:B:2083:LEU:HB3	1:B:2084:PRO:HD3	1.82	0.62
1:A:2083:LEU:HB3	1:A:2084:PRO:HD3	1.82	0.62
1:A:1511:PHE:HZ	1:A:1729:THR:HG21	1.64	0.62
1:A:1956:PHE:CE1	1:A:1998:GLY:HA3	2.34	0.61
1:A:1956:PHE:HE1	1:A:1998:GLY:HA3	1.65	0.61
1:A:2192:GLU:O	1:A:2196:GLN:HG2	2.01	0.61
1:B:1781:GLN:HE21	1:B:1781:GLN:H	1.47	0.60
1:A:2046:ARG:NH1	1:A:2047:LEU:HD11	2.17	0.59
1:B:1902:LEU:HD12	1:B:1915:THR:O	2.02	0.59
1:B:2033:ILE:HG22	1:B:2034:LYS:HD2	1.83	0.59
1:B:1527:SER:O	1:B:1530:VAL:HG22	2.01	0.59
1:A:1571:VAL:O	1:A:1579:GLY:HA2	2.03	0.59
1:B:2110:SER:O	1:B:2111:LYS:HB3	2.02	0.58
1:B:2102:ARG:NH1	1:B:2106:LYS:HG3	2.18	0.58
2:A:3219:D1L:CL14	1:B:1968:LEU:HA	2.40	0.58
1:B:1792:THR:HG23	3:B:4038:HOH:O	2.03	0.58
1:B:1681:VAL:HG22	1:B:1686:GLU:CB	2.34	0.58
1:B:1745:ARG:HG2	1:B:1806:TRP:CZ2	2.39	0.58
2:A:3219:D1L:C4	1:B:2001:VAL:HG11	2.34	0.57
1:A:2046:ARG:C	1:A:2047:LEU:HD12	2.24	0.57
1:B:1901:ASN:HB3	1:B:1917:ILE:HB	1.85	0.57
1:A:1586:ALA:HB2	1:A:1621:LEU:HB2	1.86	0.57
1:B:2136:ILE:HD11	1:B:2152:ILE:HG12	1.84	0.57
1:B:1898:THR:HG22	1:B:1920:PRO:HA	1.85	0.57
1:A:1537:PHE:HD2	1:A:1571:VAL:HG13	1.70	0.57
1:B:1838:ASP:O	1:B:1839:GLU:HB2	2.05	0.57
1:A:2148:ARG:HG3	1:A:2148:ARG:HH11	1.69	0.57
1:B:1905:ALA:HB2	1:B:1913:ALA:C	2.25	0.57
1:B:1560:ASN:ND2	1:B:1560:ASN:H	2.01	0.56
1:A:2082:LEU:N	1:A:2082:LEU:HD23	2.15	0.56
1:A:2001:VAL:HG21	2:B:3219:D1L:C4	2.34	0.56
1:A:1719:TYR:CE2	1:A:1744:GLN:HG3	2.41	0.56
1:A:1763:ASN:HD21	1:A:1771:TYR:H	1.53	0.56
1:B:1569:ILE:HG22	1:B:1571:VAL:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1815:ASN:ND2	1:B:1944:GLN:HE22	2.02	0.56
1:B:1902:LEU:HD11	1:B:1914:GLU:OE1	2.06	0.56
1:A:2097:HIS:NE2	1:B:1631:MET:HG3	2.21	0.56
1:A:2086:TYR:HA	1:A:2089:ILE:HD12	1.87	0.55
1:A:2097:HIS:CE1	1:B:1632:ALA:H	2.25	0.55
1:A:1884:LEU:HD13	1:A:2123:PHE:HA	1.89	0.55
1:A:2142:GLN:NE2	1:A:2151:LYS:HE2	2.22	0.55
1:B:2033:ILE:HG22	1:B:2034:LYS:CD	2.36	0.55
1:B:2100:SER:O	1:B:2104:VAL:HG23	2.06	0.55
1:A:1729:THR:HG22	1:A:1796:ASP:OD1	2.07	0.55
1:B:1903:ILE:HD12	1:B:1903:ILE:N	2.21	0.55
1:B:1966:GLU:OE1	1:B:1966:GLU:HA	2.05	0.54
1:B:1643:TRP:HA	1:B:1653:PHE:HA	1.89	0.54
1:A:1541:GLU:OE1	1:A:1555:ARG:HD3	2.07	0.54
1:A:1756:LEU:HD21	1:B:1968:LEU:HD13	1.90	0.54
1:B:1797:LEU:O	1:B:1801:GLU:HG3	2.08	0.54
1:A:1630:GLY:O	1:A:1700:LEU:HD22	2.08	0.53
1:A:1815:ASN:H	1:A:1944:GLN:NE2	1.90	0.53
1:B:1661:GLU:HG3	1:B:1662:GLY:N	2.23	0.53
1:B:1756:LEU:HD22	2:B:3219:D1L:H7	1.91	0.53
1:B:2193:SER:HA	1:B:2196:GLN:HB2	1.90	0.53
1:A:1630:GLY:C	1:A:1700:LEU:HD22	2.29	0.53
1:B:1922:GLN:HG2	1:B:1952:ASN:O	2.09	0.53
1:A:1630:GLY:O	1:A:1700:LEU:HB3	2.09	0.52
1:B:1900:GLU:OE1	1:B:1916:LEU:HD21	2.10	0.52
1:B:1741:ARG:HD3	1:B:1741:ARG:O	2.09	0.51
1:A:1494:GLN:NE2	1:A:1496:LYS:H	1.94	0.51
1:A:2043:THR:O	1:A:2047:LEU:HD13	2.10	0.51
1:A:2148:ARG:HG3	1:A:2148:ARG:NH1	2.26	0.51
1:B:1781:GLN:H	1:B:1781:GLN:NE2	2.08	0.51
1:A:2139:LEU:HD21	1:A:2189:LEU:HD23	1.93	0.51
1:A:1578:ARG:HH11	1:A:1578:ARG:HG2	1.75	0.51
1:B:1589:ILE:O	1:B:1589:ILE:HG13	2.11	0.51
1:A:1810:VAL:HG13	1:A:1811:PRO:HD2	1.92	0.51
1:B:2010:ASP:OD1	1:B:2148:ARG:HD3	2.11	0.51
1:B:2031:VAL:HG23	1:B:2035:PHE:HB3	1.93	0.51
1:B:1958:GLY:O	1:B:1965:ASN:ND2	2.44	0.51
1:A:1586:ALA:CB	1:A:1621:LEU:HB2	2.41	0.50
1:B:1661:GLU:HG3	1:B:1662:GLY:H	1.76	0.50
1:A:1968:LEU:HA	2:B:3219:D1L:CL14	2.48	0.50
1:B:1643:TRP:CE2	1:B:1649:PRO:HG3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2024:VAL:HG12	1:A:2025:LEU:HD13	1.93	0.50
1:B:2128:ARG:HE	1:B:2132:GLU:CD	2.15	0.50
1:B:1998:GLY:HA2	1:B:2001:VAL:CG1	2.41	0.50
1:B:1635:ILE:O	1:B:1639:PHE:HB3	2.10	0.50
1:A:1824:LYS:HG3	1:A:1825:ASP:N	2.26	0.50
1:A:1781:GLN:NE2	1:A:1782:ILE:HG13	2.23	0.50
1:A:1768:ARG:H	1:A:1768:ARG:CD	2.24	0.50
1:A:1648:ASN:HB3	1:A:1651:LYS:HG2	1.93	0.50
1:B:2136:ILE:CD1	1:B:2152:ILE:HG12	2.42	0.50
1:A:1605:ASN:ND2	1:A:1714:ALA:HB2	2.27	0.50
1:B:2133:GLU:O	1:B:2137:LYS:HG2	2.11	0.49
1:B:1587:ASN:ND2	1:B:1624:ASN:HD22	2.10	0.49
1:B:2005:PRO:HD3	1:B:2014:MET:HG3	1.93	0.49
1:B:1790:HIS:HD2	3:B:4057:HOH:O	1.96	0.49
1:A:1730:CYS:HA	1:A:1752:GLN:NE2	2.24	0.49
1:B:2045:ASN:HD22	1:B:2046:ARG:NH1	2.10	0.49
1:A:2047:LEU:N	1:A:2047:LEU:HD12	2.27	0.49
1:B:1646:ALA:HB1	1:B:1648:ASN:C	2.33	0.49
1:A:2148:ARG:O	1:A:2152:ILE:HG13	2.12	0.49
1:B:1844:ARG:O	1:B:1848:GLU:HG2	2.13	0.49
1:B:1492:TRP:HZ2	1:B:1556:GLU:CG	2.26	0.49
1:B:1636:VAL:N	1:B:1637:PRO:HD2	2.28	0.48
1:A:1602:GLU:HG3	3:A:4023:HOH:O	2.13	0.48
1:B:1544:GLU:OE2	1:B:1602:GLU:OE2	2.31	0.48
1:A:2133:GLU:OE2	1:A:2148:ARG:NH2	2.45	0.48
1:B:1727:LEU:HD12	1:B:1747:ILE:O	2.14	0.48
1:A:1900:GLU:HB3	1:A:1916:LEU:HD11	1.94	0.48
1:B:1741:ARG:HD3	1:B:1741:ARG:C	2.34	0.48
1:A:1705:LEU:HD21	1:B:2024:VAL:HG22	1.95	0.48
1:A:2031:VAL:CG2	1:A:2091:LEU:HD23	2.39	0.48
1:A:1664:GLU:OE2	1:A:1667:LYS:HD2	2.13	0.48
1:B:2043:THR:HG23	1:B:2046:ARG:CZ	2.43	0.48
1:B:1815:ASN:HD22	1:B:1944:GLN:HE22	1.62	0.48
1:A:2086:TYR:HA	1:A:2089:ILE:CD1	2.44	0.47
1:A:2046:ARG:CZ	1:A:2047:LEU:HD11	2.44	0.47
1:B:1646:ALA:C	1:B:1648:ASN:H	2.12	0.47
1:B:1830:PRO:HB2	1:B:2116:THR:HG23	1.95	0.47
1:A:1635:ILE:HG22	1:A:1635:ILE:O	2.14	0.47
1:B:1503:MET:CE	1:B:1731:ARG:HH21	2.28	0.47
1:A:2158:TRP:CZ3	1:A:2186:LEU:HD13	2.50	0.47
1:B:1677:THR:CG2	1:B:1690:ILE:HD13	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2000:TRP:HB3	1:B:1705:LEU:HD13	1.97	0.47
1:B:2198:LEU:O	1:B:2201:LYS:HB2	2.15	0.47
1:B:1664:GLU:O	1:B:1667:LYS:HB2	2.14	0.47
1:B:1508:VAL:HG21	1:B:1588:ASP:HA	1.96	0.47
1:B:1759:ALA:HB3	1:B:1760:PRO:HD3	1.97	0.47
1:B:2043:THR:HG22	1:B:2043:THR:O	2.15	0.47
1:B:2046:ARG:HD2	1:B:2046:ARG:N	2.29	0.47
1:B:1612:ARG:O	1:B:1814:ARG:NH2	2.48	0.47
1:A:1497:ARG:HD3	1:A:1510:ASP:OD1	2.14	0.47
1:B:2035:PHE:HE1	1:B:2040:LEU:HA	1.80	0.47
1:A:1741:ARG:NH2	1:A:1934:GLN:NE2	2.63	0.47
1:A:1745:ARG:HG2	1:A:1806:TRP:CZ2	2.50	0.47
1:A:2082:LEU:CD2	1:A:2082:LEU:H	2.20	0.46
1:B:2200:LYS:HG3	1:B:2203:ARG:NH2	2.30	0.46
1:A:2004:ASP:OD1	1:B:1706:ARG:HA	2.15	0.46
1:A:2001:VAL:HG11	2:B:3219:D1L:H4	1.97	0.46
1:A:2149:LEU:C	1:A:2149:LEU:HD13	2.35	0.46
1:B:1489:VAL:CG1	1:B:1497:ARG:HH12	2.28	0.46
1:A:1592:LYS:O	1:A:1593:ILE:HG12	2.14	0.46
1:B:1494:GLN:HB3	1:B:1495:PRO:CD	2.44	0.46
1:A:1578:ARG:HG2	1:A:1578:ARG:NH1	2.30	0.46
1:A:1620:TYR:HB3	1:A:1726:THR:HB	1.97	0.46
1:B:1646:ALA:C	1:B:1648:ASN:N	2.66	0.46
1:B:1602:GLU:HG3	3:B:4017:HOH:O	2.15	0.46
2:A:3219:D1L:C13	1:B:1971:GLY:HA3	2.39	0.46
1:B:1640:GLN:HB3	1:B:1657:TYR:CZ	2.51	0.46
1:A:1733:VAL:HA	1:A:1755:ILE:O	2.16	0.46
1:B:1852:THR:HG23	1:B:1855:GLY:N	2.31	0.46
1:A:1836:THR:HG22	1:A:1838:ASP:HB2	1.98	0.45
1:A:1511:PHE:CZ	1:A:1729:THR:HG21	2.48	0.45
1:B:1915:THR:HG22	1:B:1916:LEU:N	2.31	0.45
1:B:1491:GLU:HG2	1:B:1492:TRP:HE3	1.81	0.45
1:A:1616:ILE:HD12	1:A:1813:LYS:HB3	1.98	0.45
1:B:1633:GLU:HA	1:B:1636:VAL:HG23	1.96	0.45
1:A:2149:LEU:HD13	1:A:2149:LEU:O	2.15	0.45
1:A:1833:PHE:CZ	1:A:1845:TRP:HE3	2.34	0.45
1:B:1546:GLU:CD	1:B:1546:GLU:H	2.19	0.45
1:B:2092:GLN:HE22	1:B:2096:LEU:HG	1.81	0.45
1:B:2035:PHE:HA	1:B:2039:LYS:HD2	1.98	0.45
1:A:1543:ILE:HD11	1:A:1553:VAL:HG11	1.98	0.45
1:B:1810:VAL:HG13	1:B:1811:PRO:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2097:HIS:HE1	1:B:1632:ALA:H	1.64	0.45
1:B:1643:TRP:CD1	1:B:1649:PRO:HA	2.51	0.45
1:B:1780:THR:O	1:B:1784:TYR:HB3	2.16	0.45
1:A:1994:GLU:HA	1:A:2021:ARG:O	2.17	0.45
1:B:2045:ASN:HB2	1:B:2046:ARG:NH1	2.31	0.45
1:B:1853:GLU:CD	1:B:1853:GLU:H	2.20	0.45
1:A:1966:GLU:HA	1:A:1966:GLU:OE1	2.16	0.45
1:A:1669:PHE:C	1:A:1671:LYS:H	2.20	0.45
1:B:1770:VAL:HG13	1:B:1771:TYR:CD1	2.52	0.45
1:B:2045:ASN:HD22	1:B:2046:ARG:HH12	1.65	0.45
1:B:1605:ASN:O	1:B:1609:GLU:HG3	2.17	0.45
1:B:2158:TRP:HZ3	1:B:2186:LEU:HD13	1.81	0.45
1:B:1494:GLN:HB3	1:B:1495:PRO:HD3	1.98	0.44
1:A:1730:CYS:O	1:A:1731:ARG:C	2.55	0.44
1:B:1537:PHE:CD2	1:B:1571:VAL:HG22	2.52	0.44
1:A:1924:TRP:HD1	1:A:1928:SER:HB2	1.82	0.44
1:A:1566:ALA:HA	1:A:1584:VAL:O	2.17	0.44
1:A:2096:LEU:HB3	1:B:1693:ILE:HG13	2.00	0.44
1:B:1487:TYR:CD2	1:B:1488:PRO:HD2	2.52	0.44
1:B:1491:GLU:HG2	1:B:1492:TRP:CE3	2.53	0.44
1:B:2045:ASN:HB2	1:B:2046:ARG:HH11	1.83	0.44
1:B:1664:GLU:CD	1:B:1667:LYS:HD3	2.38	0.44
1:B:1492:TRP:CZ2	1:B:1556:GLU:CG	3.01	0.44
1:A:1770:VAL:HG13	1:A:1907:PRO:O	2.18	0.44
1:A:1583:VAL:HG11	1:A:1607:VAL:CG1	2.48	0.44
1:B:1492:TRP:CZ2	1:B:1556:GLU:HG2	2.53	0.44
1:B:1635:ILE:O	1:B:1635:ILE:HG22	2.17	0.44
1:B:1655:TYR:C	1:B:1656:LEU:HD12	2.38	0.43
1:A:2187:LYS:O	1:A:2191:LEU:HG	2.18	0.43
1:A:1663:MET:HB3	1:A:1667:LYS:HE2	2.00	0.43
1:B:1643:TRP:NE1	1:B:1649:PRO:HB3	2.32	0.43
1:A:2214:SER:C	1:A:2216:VAL:N	2.72	0.43
1:A:2214:SER:C	1:A:2216:VAL:H	2.22	0.43
1:A:1679:ARG:HG3	1:A:1679:ARG:O	2.18	0.43
1:B:2158:TRP:CZ3	1:B:2186:LEU:HD13	2.54	0.43
1:B:2011:GLN:O	1:B:2129:ARG:NH2	2.51	0.43
1:A:2108:VAL:HG23	1:A:2109:ILE:HG23	2.00	0.43
1:A:1677:THR:HG22	1:A:1689:VAL:O	2.19	0.43
1:B:1508:VAL:CG2	1:B:1588:ASP:HA	2.48	0.43
1:A:1759:ALA:N	1:A:1760:PRO:CD	2.81	0.43
1:A:1649:PRO:O	1:B:2085:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1677:THR:HA	1:B:1689:VAL:O	2.17	0.43
1:B:1487:TYR:HA	1:B:1488:PRO:HD3	1.88	0.43
1:B:2139:LEU:N	1:B:2139:LEU:HD12	2.33	0.43
1:A:1899:VAL:HB	1:A:1919:GLU:HB2	2.01	0.43
1:A:1693:ILE:HG13	1:B:2096:LEU:HB3	2.00	0.43
1:A:1877:VAL:CG1	1:A:1931:LYS:HD3	2.48	0.43
1:B:1748:GLN:HE22	1:B:1783:MET:HB2	1.84	0.43
1:A:2081:GLU:OE1	1:A:2082:LEU:HD23	2.19	0.42
1:B:2005:PRO:HG2	1:B:2014:MET:HB2	2.01	0.42
1:B:1728:VAL:HG21	1:B:1754:ILE:HD11	2.01	0.42
1:B:1889:LEU:HA	1:B:1946:PRO:HD2	2.01	0.42
1:B:1879:VAL:HG13	1:B:1931:LYS:HE2	2.01	0.42
1:B:2045:ASN:C	1:B:2046:ARG:HD2	2.39	0.42
1:A:2199:ALA:O	1:A:2203:ARG:HG2	2.19	0.42
1:B:1533:THR:HG1	1:B:1535:ASP:CG	2.23	0.42
1:A:1537:PHE:CD2	1:A:1571:VAL:HG13	2.52	0.42
1:B:1852:THR:HG23	1:B:1855:GLY:H	1.83	0.42
1:B:1644:ASN:C	1:B:1646:ALA:H	2.23	0.42
1:B:1639:PHE:C	1:B:1639:PHE:CD1	2.91	0.42
1:A:1755:ILE:HD12	1:A:1758:GLY:HA2	2.02	0.42
1:A:1814:ARG:O	1:A:1815:ASN:HB2	2.20	0.42
1:A:1587:ASN:HB2	1:A:1623:ALA:O	2.20	0.42
1:B:1560:ASN:ND2	1:B:1560:ASN:N	2.68	0.42
1:B:1954:ARG:HG3	1:B:1955:GLY:N	2.30	0.42
1:B:1901:ASN:O	1:B:1917:ILE:N	2.53	0.42
1:B:1829:ARG:CZ	1:B:1858:TYR:HB3	2.49	0.42
1:A:1790:HIS:HD2	3:A:4053:HOH:O	2.03	0.42
1:A:2102:ARG:O	1:A:2106:LYS:HG2	2.20	0.42
1:A:1582:PHE:HA	1:A:1616:ILE:HG23	2.02	0.41
1:A:1945:LEU:HA	1:A:1946:PRO:HD3	1.88	0.41
1:B:1775:LEU:HD12	1:B:1775:LEU:N	2.34	0.41
1:A:2005:PRO:HG3	1:A:2014:MET:HB2	2.01	0.41
1:B:1677:THR:HG22	1:B:1689:VAL:O	2.20	0.41
1:A:1569:ILE:HG22	1:A:1571:VAL:HG22	2.02	0.41
1:A:1733:VAL:HG12	1:A:1734:GLY:N	2.34	0.41
1:B:2163:VAL:HG13	1:B:2170:GLN:HE21	1.86	0.41
1:A:1810:VAL:HA	1:A:1811:PRO:HD3	1.94	0.41
1:A:1948:MET:HA	1:A:1986:ILE:O	2.20	0.41
1:A:2000:TRP:C	1:A:2000:TRP:CD1	2.94	0.41
1:B:1664:GLU:OE1	1:B:1667:LYS:HD3	2.20	0.41
1:A:2045:ASN:C	1:A:2047:LEU:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1655:TYR:CD1	1:A:1689:VAL:HG23	2.56	0.41
1:B:1936:ILE:HD13	1:B:1978:LEU:HD13	2.02	0.41
1:A:1601:ASP:OD1	1:A:1707:GLY:HA3	2.21	0.41
1:A:2044:MET:HA	1:A:2086:TYR:CE2	2.56	0.40
1:B:1527:SER:O	1:B:1530:VAL:HG13	2.21	0.40
1:A:1605:ASN:HD22	1:A:1714:ALA:HB2	1.85	0.40
1:A:1643:TRP:CZ3	1:A:1649:PRO:HB3	2.56	0.40
1:A:1741:ARG:CZ	1:B:1969:LYS:HG2	2.51	0.40
1:B:1649:PRO:O	1:B:1651:LYS:N	2.54	0.40
1:B:2116:THR:HG22	1:B:2117:GLU:OE2	2.20	0.40
1:B:1932:THR:O	1:B:1936:ILE:HG13	2.22	0.40
1:A:1607:VAL:O	1:A:1610:TYR:HB3	2.22	0.40
1:B:1697:GLU:HA	1:B:1697:GLU:OE2	2.21	0.40
1:B:2134:TYR:O	1:B:2138:ARG:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	692/737 (94%)	628 (91%)	54 (8%)	10 (1%)	14	24
1	B	689/737 (94%)	619 (90%)	63 (9%)	7 (1%)	19	34
All	All	1381/1474 (94%)	1247 (90%)	117 (8%)	17 (1%)	16	29

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1766	LEU
1	A	2205	ASP
1	A	1683	ASN
1	A	1731	ARG

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Mol	Chain	Res	Type
1	A	1997	GLY
1	A	2207	ASP
1	B	1644	ASN
1	B	1650	ASP
1	B	1839	GLU
1	A	1484	ALA
1	B	1534	ASP
1	A	1838	ASP
1	B	1649	PRO
1	B	2205	ASP
1	A	2032	GLY
1	B	2217	ILE
1	A	1767	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	579/628 (92%)	548 (95%)	31 (5%)	27	49
1	B	577/628 (92%)	549 (95%)	28 (5%)	31	55
All	All	1156/1256 (92%)	1097 (95%)	59 (5%)	29	52

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1502	LEU
1	A	1536	PHE
1	A	1555	ARG
1	A	1571	VAL
1	A	1578	ARG
1	A	1585	VAL
1	A	1602	GLU
1	A	1616	ILE
1	A	1618	ARG
1	A	1721	ASP

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Mol	Chain	Res	Type
1	A	1726	THR
1	A	1738	TYR
1	A	1768	ARG
1	A	1769	GLU
1	A	1791	LEU
1	A	1797	LEU
1	A	1823	THR
1	A	1843	VAL
1	A	1884	LEU
1	A	1909	ASN
1	A	1924	TRP
1	A	1930	PHE
1	A	1956	PHE
1	A	2014	MET
1	A	2035	PHE
1	A	2081	GLU
1	A	2119	ARG
1	A	2128	ARG
1	A	2138	ARG
1	A	2186	LEU
1	A	2192	GLU
1	B	1490	LYS
1	B	1508	VAL
1	B	1536	PHE
1	B	1542	LEU
1	B	1550	LEU
1	B	1560	ASN
1	B	1585	VAL
1	B	1602	GLU
1	B	1639	PHE
1	B	1732	SER
1	B	1738	TYR
1	B	1741	ARG
1	B	1742	LEU
1	B	1781	GLN
1	B	1879	VAL
1	B	1924	TRP
1	B	1930	PHE
1	B	1945	LEU
1	B	1956	PHE
1	B	1978	LEU
1	B	1981	TYR

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Mol	Chain	Res	Type
1	B	2001	VAL
1	B	2014	MET
1	B	2035	PHE
1	B	2092	GLN
1	B	2114	GLU
1	B	2128	ARG
1	B	2186	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1494	GLN
1	A	1517	GLN
1	A	1525	ASN
1	A	1587	ASN
1	A	1605	ASN
1	A	1624	ASN
1	A	1683	ASN
1	A	1748	GLN
1	A	1752	GLN
1	A	1763	ASN
1	A	1781	GLN
1	A	1790	HIS
1	A	1815	ASN
1	A	1909	ASN
1	A	1911	ASN
1	A	1934	GLN
1	A	1944	GLN
1	A	2097	HIS
1	A	2131	ASN
1	A	2142	GLN
1	A	2196	GLN
1	B	1517	GLN
1	B	1522	GLN
1	B	1560	ASN
1	B	1587	ASN
1	B	1605	ASN
1	B	1640	GLN
1	B	1644	ASN
1	B	1648	ASN
1	B	1748	GLN
1	B	1774	ASN

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Mol	Chain	Res	Type
1	B	1781	GLN
1	B	1785	ASN
1	B	1790	HIS
1	B	1815	ASN
1	B	1918	GLN
1	B	2011	GLN
1	B	2045	ASN
1	B	2092	GLN
1	B	2142	GLN
1	B	2170	GLN
1	B	2178	ASN
1	B	2208	ASN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5　Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6　Ligand geometry ⓘ

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	D1L	A	3219	-	19,22,22	0.68	0	26,30,30	0.92	2 (7%)
2	D1L	B	3219	-	19,22,22	0.68	0	26,30,30	0.96	1 (3%)

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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	D1L	A	3219	-	-	0/8/12/12	0/2/2/2
2	D1L	B	3219	-	-	0/8/12/12	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3219	D1L	C2A-C2-C1	-3.62	108.55	113.18
2	A	3219	D1L	C2A-C2-C1	-2.81	109.58	113.18
2	A	3219	D1L	C3-O2-C2	-2.28	114.88	118.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3219	D1L	6	0
2	B	3219	D1L	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	698/737 (94%)	0.44	85 (12%)	5	5	21, 43, 100, 100	0
1	B	695/737 (94%)	0.45	85 (12%)	5	5	21, 44, 100, 100	0
All	All	1393/1474 (94%)	0.44	170 (12%)	5	5	21, 43, 100, 100	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1682	ILE	10.2
1	B	2083	LEU	7.5
1	B	1645	ASP	7.0
1	A	1648	ASN	6.8
1	A	1683	ASN	6.7
1	B	1907	PRO	6.5
1	A	1647	ALA	6.5
1	B	1766	LEU	6.5
1	A	1910	PRO	6.3
1	B	1912	SER	6.1
1	B	1681	VAL	6.0
1	A	1669	PHE	5.7
1	B	1913	ALA	5.6
1	B	1910	PRO	5.4
1	B	1916	LEU	5.4
1	B	1911	ASN	5.3
1	A	1681	VAL	5.3
1	A	1684	GLY	5.1
1	A	1644	ASN	5.1
1	A	2203	ARG	5.0
1	A	1651	LYS	4.8
1	A	1679	ARG	4.8
1	A	1909	ASN	4.8
1	A	1650	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	1908	ALA	4.7
1	A	1905	ALA	4.7
1	A	1685	GLU	4.7
1	A	1908	ALA	4.6
1	A	1911	ASN	4.6
1	A	2037	ARG	4.6
1	B	1769	GLU	4.4
1	B	1905	ALA	4.4
1	B	2084	PRO	4.3
1	B	1648	ASN	4.3
1	B	1651	LYS	4.3
1	B	2041	LEU	4.3
1	B	1669	PHE	4.2
1	B	2145	GLU	4.1
1	A	1680	THR	4.1
1	B	2037	ARG	4.0
1	B	1685	GLU	4.0
1	A	1958	GLY	4.0
1	B	1650	ASP	4.0
1	A	1902	LEU	4.0
1	A	1916	LEU	3.9
1	B	1838	ASP	3.9
1	B	2036	ARG	3.9
1	A	1912	SER	3.9
1	A	1838	ASP	3.9
1	B	1909	ASN	3.9
1	A	1913	ALA	3.8
1	B	2038	GLU	3.8
1	B	1680	THR	3.8
1	B	1649	PRO	3.8
1	B	2203	ARG	3.8
1	A	1645	ASP	3.8
1	A	1904	PRO	3.7
1	B	2082	LEU	3.7
1	B	1770	VAL	3.6
1	B	2085	ILE	3.6
1	A	1773	SER	3.6
1	A	1658	LEU	3.6
1	A	2045	ASN	3.6
1	B	1900	GLU	3.6
1	B	1902	LEU	3.6
1	B	1918	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1767	GLY	3.5
1	B	1652	GLY	3.5
1	A	1667	LYS	3.5
1	B	1679	ARG	3.4
1	B	1904	PRO	3.4
1	B	1682	ILE	3.4
1	A	2085	ILE	3.3
1	B	1901	ASN	3.3
1	A	1665	THR	3.3
1	A	1907	PRO	3.2
1	B	1957	SER	3.2
1	A	1482	PRO	3.2
1	A	1900	GLU	3.2
1	A	1668	LYS	3.2
1	B	1824	LYS	3.2
1	A	2202	ILE	3.2
1	B	2040	LEU	3.1
1	A	1917	ILE	3.1
1	B	2035	PHE	3.1
1	A	1643	TRP	3.1
1	A	1688	PHE	3.0
1	A	1483	ILE	3.0
1	B	1853	GLU	3.0
1	B	1646	ALA	3.0
1	A	1903	ILE	3.0
1	B	1492	TRP	2.9
1	A	2083	LEU	2.9
1	A	1836	THR	2.9
1	B	1765	MET	2.9
1	B	2141	HIS	2.8
1	A	1915	THR	2.8
1	A	1686	GLU	2.8
1	B	1621	LEU	2.8
1	A	1770	VAL	2.8
1	A	1649	PRO	2.8
1	B	1584	VAL	2.7
1	A	2038	GLU	2.7
1	B	2208	ASN	2.7
1	A	2044	MET	2.7
1	B	1906	ASP	2.7
1	A	1766	LEU	2.7
1	A	1672	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1764	LYS	2.6
1	B	1772	THR	2.6
1	B	2087	GLY	2.6
1	B	2046	ARG	2.6
1	A	1824	LYS	2.6
1	A	1906	ASP	2.6
1	A	1661	GLU	2.5
1	B	1668	LYS	2.5
1	B	2216	VAL	2.5
1	A	2041	LEU	2.5
1	A	1839	GLU	2.5
1	A	1889	LEU	2.5
1	A	1852	THR	2.5
1	B	1915	THR	2.5
1	A	2209	ALA	2.5
1	A	1759	ALA	2.5
1	B	1667	LYS	2.4
1	B	1670	ASP	2.4
1	A	1687	ARG	2.4
1	A	1901	ASN	2.4
1	B	2043	THR	2.4
1	A	1772	THR	2.4
1	B	1917	ILE	2.4
1	B	2189	LEU	2.4
1	A	2145	GLU	2.4
1	B	1958	GLY	2.3
1	A	2036	ARG	2.3
1	B	1768	ARG	2.3
1	B	1683	ASN	2.3
1	B	1494	GLN	2.3
1	B	1949	ILE	2.3
1	A	1659	THR	2.3
1	A	1891	VAL	2.3
1	B	1948	MET	2.3
1	A	1655	TYR	2.3
1	B	2143	VAL	2.3
1	A	1527	SER	2.3
1	A	1890	GLY	2.3
1	B	1585	VAL	2.2
1	B	1759	ALA	2.2
1	A	1948	MET	2.2
1	A	1768	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1620	TYR	2.2
1	A	1956	PHE	2.2
1	A	1670	ASP	2.2
1	A	1763	ASN	2.2
1	B	1664	GLU	2.1
1	B	1771	TYR	2.1
1	A	1765	MET	2.1
1	B	1586	ALA	2.1
1	B	1684	GLY	2.1
1	B	1619	ILE	2.1
1	B	1758	GLY	2.1
1	A	1584	VAL	2.1
1	B	1764	LYS	2.1
1	B	1803	ILE	2.1
1	A	1666	LEU	2.1
1	A	1619	ILE	2.0
1	A	1957	SER	2.0
1	B	1839	GLU	2.0
1	B	2207	ASP	2.0
1	B	2086	TYR	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	D1L	B	3219	21/21	0.81	0.27	2.64	73,78,80,89	0
2	D1L	A	3219	21/21	0.84	0.24	2.27	74,79,80,88	0

6.5 Other polymers (i)

There are no such residues in this entry.