



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:46 AM GMT

PDB ID : 3C4T
Title : Structure of RNaseIIIb and dsRNA binding domains of mouse Dicer
Authors : Lee, J.K.; Du, Z.; Tjhen, R.J.; Stroud, R.M.; James, T.L.
Deposited on : 2008-01-30
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

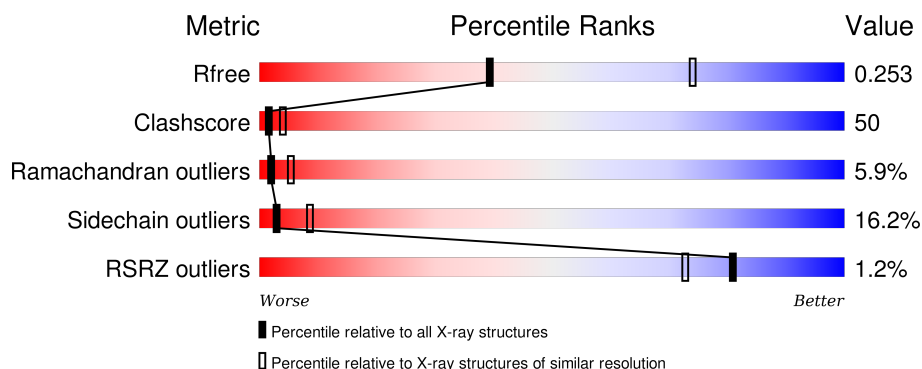
1 Overall quality at a glance

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 ≥ 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	265	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1932 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 Endoribonuclease Dicer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1923	1237	322	357	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1636	GLY	-	EXPRESSION TAG	UNP Q8R418
A	1637	PRO	-	EXPRESSION TAG	UNP Q8R418

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Cd	0	0
			3	3		

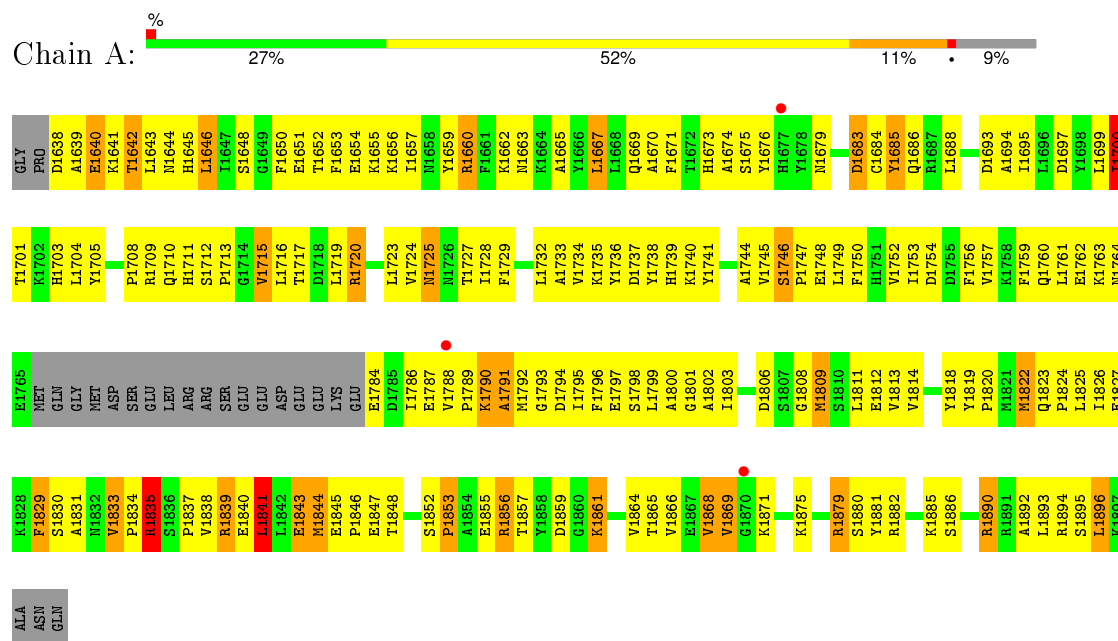
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		

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: Endoribonuclease Dicer



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	70.13 Å 70.13 Å 132.66 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80 39.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.8 (40.00-2.80) 98.0 (39.72-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.51 Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.233 , 0.304 0.235 , 0.253	Depositor DCC
R_{free} test set	407 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 96.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 11818 reflections (0.025%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1932	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: OCS, CD

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	0.92	0/1959	1.06	8/2653 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1700	ILE	CB-CA-C	-7.18	97.25	111.60
1	A	1646	LEU	CA-CB-CG	-7.08	99.01	115.30
1	A	1841	LEU	N-CA-C	6.16	127.64	111.00
1	A	1732	LEU	CA-CB-CG	-5.54	102.56	115.30
1	A	1811	LEU	CB-CG-CD2	-5.54	101.58	111.00
1	A	1803	ILE	CB-CA-C	-5.38	100.84	111.60
1	A	1811	LEU	CA-CB-CG	-5.27	103.17	115.30
1	A	1809	MET	CG-SD-CE	5.03	108.25	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1841	LEU	Peptide

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	1923	0	1854	190	1
2	A	3	0	0	0	1
3	A	6	0	0	0	0
All	All	1932	0	1854	190	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 50.

All (190) 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:1841:LEU:CB	1:A:1844:MET:HG3	1.73	1.16
1:A:1660:ARG:HH11	1:A:1660:ARG:HG3	1.16	1.06
1:A:1700:ILE:HG22	1:A:1700:ILE:O	1.57	1.02
1:A:1841:LEU:CB	1:A:1844:MET:CG	2.39	1.01
1:A:1830:SER:O	1:A:1833:VAL:HG22	1.64	0.97
1:A:1700:ILE:HD12	1:A:1724:VAL:HG22	1.52	0.90
1:A:1787:GLU:HG2	1:A:1788:VAL:H	1.36	0.90
1:A:1753:ILE:O	1:A:1757:VAL:HG23	1.74	0.88
1:A:1841:LEU:CB	1:A:1844:MET:HB2	2.06	0.86
1:A:1837:PRO:HG2	1:A:1886:SER:HB2	1.56	0.85
1:A:1736:TYR:O	1:A:1737:ASP:HB2	1.77	0.83
1:A:1650:PHE:CE1	1:A:1741:TYR:HB3	2.13	0.83
1:A:1746:SER:O	1:A:1750:PHE:HD1	1.60	0.83
1:A:1650:PHE:HE1	1:A:1741:TYR:HB3	1.42	0.82
1:A:1819:TYR:HB3	1:A:1820:PRO:HD3	1.60	0.82
1:A:1659:TYR:OH	1:A:1806:ASP:OD2	1.97	0.82
1:A:1822:MET:C	1:A:1824:PRO:HD2	2.00	0.81
1:A:1700:ILE:O	1:A:1700:ILE:CG2	2.28	0.81
1:A:1760:GLN:O	1:A:1764:ASN:ND2	2.15	0.79
1:A:1660:ARG:NH1	1:A:1660:ARG:HG3	1.97	0.79
1:A:1688:LEU:HD22	1:A:1801:GLY:HA3	1.66	0.77
1:A:1841:LEU:CB	1:A:1844:MET:CB	2.62	0.76
1:A:1840:GLU:O	1:A:1844:MET:HG2	1.84	0.76
1:A:1857:THR:HG23	1:A:1861:LYS:O	1.84	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1835:ARG:HA	1:A:1835:ARG:NE	2.00	0.75
1:A:1643:LEU:HD12	1:A:1643:LEU:O	1.86	0.75
1:A:1684:OCS:OD2	1:A:1686:GLN:HB2	1.87	0.74
1:A:1739:HIS:HB3	1:A:1792:MET:HE2	1.69	0.74
1:A:1787:GLU:HG2	1:A:1788:VAL:N	2.00	0.74
1:A:1685:TYR:C	1:A:1685:TYR:CD2	2.60	0.74
1:A:1739:HIS:HB3	1:A:1792:MET:CE	2.18	0.73
1:A:1848:THR:HB	1:A:1869:VAL:CG2	2.18	0.73
1:A:1673:HIS:HD2	1:A:1675:SER:OG	1.72	0.72
1:A:1725:ASN:HB3	1:A:1728:ILE:HG12	1.69	0.72
1:A:1823:GLN:N	1:A:1824:PRO:HD2	2.05	0.71
1:A:1746:SER:O	1:A:1750:PHE:CD1	2.45	0.70
1:A:1848:THR:HB	1:A:1869:VAL:HG21	1.74	0.69
1:A:1685:TYR:HD2	1:A:1685:TYR:C	1.96	0.68
1:A:1673:HIS:CG	1:A:1674:ALA:H	2.11	0.68
1:A:1709:ARG:NH2	1:A:1830:SER:HB2	2.09	0.67
1:A:1660:ARG:HH11	1:A:1660:ARG:CG	2.01	0.67
1:A:1641:LYS:HA	1:A:1644:ASN:HD22	1.60	0.67
1:A:1808:GLY:O	1:A:1809:MET:HB2	1.93	0.66
1:A:1827:GLU:HA	1:A:1827:GLU:OE1	1.96	0.65
1:A:1673:HIS:CG	1:A:1674:ALA:N	2.64	0.65
1:A:1651:GLU:O	1:A:1655:LYS:HG2	1.96	0.65
1:A:1823:GLN:N	1:A:1824:PRO:CD	2.60	0.65
1:A:1675:SER:O	1:A:1745:VAL:HG23	1.97	0.64
1:A:1657:ILE:CD1	1:A:1659:TYR:HB3	2.28	0.63
1:A:1868:VAL:HG12	1:A:1871:LYS:CB	2.28	0.62
1:A:1819:TYR:HB3	1:A:1820:PRO:CD	2.28	0.62
1:A:1700:ILE:HD12	1:A:1724:VAL:CG2	2.28	0.62
1:A:1795:ILE:HA	1:A:1798:SER:OG	2.00	0.61
1:A:1737:ASP:HA	1:A:1739:HIS:CE1	2.37	0.60
1:A:1727:THR:HG22	1:A:1727:THR:O	2.02	0.59
1:A:1845:GLU:HB3	1:A:1848:THR:OG1	2.02	0.59
1:A:1868:VAL:HG13	1:A:1869:VAL:N	2.18	0.58
1:A:1733:ALA:HB1	1:A:1738:TYR:HB2	1.86	0.58
1:A:1812:GLU:N	1:A:1812:GLU:OE1	2.29	0.58
1:A:1685:TYR:CD2	1:A:1686:GLN:N	2.73	0.57
1:A:1864:VAL:HG12	1:A:1865:THR:N	2.20	0.57
1:A:1693:ASP:OD1	1:A:1797:GLU:OE2	2.21	0.57
1:A:1748:GLU:O	1:A:1752:VAL:HG23	2.05	0.56
1:A:1759:PHE:CG	1:A:1786:ILE:HG13	2.40	0.56
1:A:1711:HIS:HB3	1:A:1715:VAL:CG1	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1705:TYR:CD2	1:A:1705:TYR:O	2.59	0.56
1:A:1704:LEU:HD22	1:A:1719:LEU:HD12	1.86	0.55
1:A:1688:LEU:HD22	1:A:1801:GLY:CA	2.37	0.54
1:A:1745:VAL:O	1:A:1746:SER:HB2	2.08	0.54
1:A:1713:PRO:HD3	1:A:1882:ARG:HH11	1.73	0.54
1:A:1723:LEU:HD22	1:A:1826:ILE:CG1	2.38	0.54
1:A:1667:LEU:HD12	1:A:1667:LEU:O	2.08	0.54
1:A:1723:LEU:HG	1:A:1829:PHE:CD2	2.44	0.53
1:A:1886:SER:O	1:A:1890:ARG:N	2.34	0.53
1:A:1868:VAL:CG1	1:A:1869:VAL:N	2.71	0.53
1:A:1712:SER:O	1:A:1716:LEU:HG	2.08	0.53
1:A:1746:SER:OG	1:A:1749:LEU:CB	2.57	0.53
1:A:1688:LEU:CD2	1:A:1801:GLY:HA3	2.36	0.53
1:A:1864:VAL:HG12	1:A:1865:THR:H	1.75	0.52
1:A:1892:ALA:O	1:A:1893:LEU:C	2.47	0.52
1:A:1673:HIS:CD2	1:A:1675:SER:OG	2.59	0.52
1:A:1657:ILE:HD12	1:A:1659:TYR:HB3	1.91	0.52
1:A:1711:HIS:HB3	1:A:1715:VAL:HG12	1.91	0.52
1:A:1746:SER:CB	1:A:1749:LEU:HB3	2.40	0.51
1:A:1709:ARG:NH1	1:A:1831:ALA:HA	2.25	0.51
1:A:1789:PRO:O	1:A:1790:LYS:C	2.46	0.51
1:A:1819:TYR:CZ	1:A:1823:GLN:HG2	2.45	0.51
1:A:1791:ALA:HA	1:A:1794:ASP:OD2	2.10	0.51
1:A:1819:TYR:CZ	1:A:1823:GLN:CG	2.94	0.51
1:A:1643:LEU:C	1:A:1643:LEU:HD12	2.30	0.51
1:A:1709:ARG:HH21	1:A:1830:SER:HB2	1.75	0.50
1:A:1818:TYR:O	1:A:1819:TYR:C	2.48	0.50
1:A:1688:LEU:O	1:A:1798:SER:HA	2.10	0.50
1:A:1694:ALA:O	1:A:1697:ASP:HB3	2.12	0.50
1:A:1711:HIS:HB2	1:A:1716:LEU:HD21	1.93	0.50
1:A:1839:ARG:O	1:A:1840:GLU:C	2.48	0.50
1:A:1756:PHE:CE2	1:A:1788:VAL:HG22	2.46	0.50
1:A:1746:SER:OG	1:A:1749:LEU:HB3	2.11	0.50
1:A:1841:LEU:CB	1:A:1893:LEU:HD21	2.42	0.49
1:A:1746:SER:HB3	1:A:1749:LEU:HB3	1.92	0.49
1:A:1685:TYR:HD2	1:A:1686:GLN:N	2.08	0.49
1:A:1667:LEU:C	1:A:1667:LEU:HD12	2.33	0.49
1:A:1866:VAL:O	1:A:1866:VAL:HG13	2.12	0.49
1:A:1699:LEU:C	1:A:1701:THR:N	2.66	0.49
1:A:1669:GLN:NE2	1:A:1683:ASP:HB3	2.28	0.49
1:A:1759:PHE:CD2	1:A:1786:ILE:HG13	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1673:HIS:CD2	1:A:1675:SER:H	2.31	0.48
1:A:1741:TYR:N	1:A:1741:TYR:CD2	2.81	0.48
1:A:1819:TYR:CE2	1:A:1823:GLN:HG3	2.47	0.48
1:A:1856:ARG:HG2	1:A:1857:THR:N	2.28	0.48
1:A:1723:LEU:HD22	1:A:1826:ILE:HG12	1.96	0.48
1:A:1646:LEU:HA	1:A:1646:LEU:HD23	1.40	0.48
1:A:1676:TYR:HB2	1:A:1744:ALA:HA	1.96	0.48
1:A:1655:LYS:O	1:A:1656:LYS:C	2.48	0.48
1:A:1723:LEU:HD21	1:A:1826:ILE:HA	1.95	0.48
1:A:1739:HIS:HB3	1:A:1792:MET:HE1	1.95	0.48
1:A:1822:MET:C	1:A:1824:PRO:CD	2.76	0.47
1:A:1713:PRO:HD3	1:A:1882:ARG:NH1	2.29	0.47
1:A:1663:ASN:OD1	1:A:1665:ALA:N	2.44	0.47
1:A:1704:LEU:HD22	1:A:1719:LEU:CD1	2.44	0.47
1:A:1708:PRO:C	1:A:1710:GLN:H	2.17	0.47
1:A:1825:LEU:HD12	1:A:1825:LEU:HA	1.51	0.47
1:A:1723:LEU:HD22	1:A:1826:ILE:HG13	1.97	0.47
1:A:1660:ARG:NH1	1:A:1660:ARG:CG	2.69	0.47
1:A:1670:ALA:HB2	1:A:1802:ALA:HB2	1.97	0.47
1:A:1750:PHE:O	1:A:1754:ASP:N	2.42	0.46
1:A:1752:VAL:O	1:A:1753:ILE:C	2.52	0.46
1:A:1852:SER:C	1:A:1853:PRO:O	2.54	0.46
1:A:1669:GLN:HE21	1:A:1683:ASP:HB3	1.81	0.46
1:A:1695:ILE:HG22	1:A:1699:LEU:HD12	1.97	0.46
1:A:1638:ASP:O	1:A:1642:THR:OG1	2.33	0.46
1:A:1676:TYR:HA	1:A:1745:VAL:HG23	1.98	0.46
1:A:1790:LYS:O	1:A:1792:MET:N	2.49	0.46
1:A:1799:LEU:O	1:A:1802:ALA:HB3	2.16	0.46
1:A:1747:PRO:HG2	1:A:1748:GLU:H	1.80	0.46
1:A:1716:LEU:HD23	1:A:1716:LEU:HA	1.65	0.46
1:A:1837:PRO:HD2	1:A:1838:VAL:H	1.80	0.46
1:A:1727:THR:CG2	1:A:1727:THR:O	2.64	0.46
1:A:1812:GLU:CD	1:A:1812:GLU:H	2.17	0.45
1:A:1685:TYR:HD2	1:A:1686:GLN:HA	1.81	0.45
1:A:1868:VAL:HG13	1:A:1869:VAL:H	1.82	0.45
1:A:1799:LEU:O	1:A:1800:ALA:C	2.55	0.45
1:A:1808:GLY:O	1:A:1809:MET:CB	2.56	0.45
1:A:1843:GLU:O	1:A:1844:MET:C	2.55	0.45
1:A:1639:ALA:O	1:A:1641:LYS:N	2.50	0.45
1:A:1643:LEU:O	1:A:1646:LEU:N	2.48	0.45
1:A:1792:MET:HE3	1:A:1792:MET:HB3	1.76	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1652:THR:O	1:A:1656:LYS:N	2.41	0.44
1:A:1675:SER:O	1:A:1745:VAL:CG2	2.63	0.44
1:A:1819:TYR:N	1:A:1820:PRO:HD2	2.32	0.44
1:A:1701:THR:C	1:A:1703:HIS:N	2.68	0.44
1:A:1734:VAL:C	1:A:1736:TYR:N	2.69	0.44
1:A:1736:TYR:O	1:A:1737:ASP:CB	2.53	0.44
1:A:1830:SER:O	1:A:1833:VAL:CG2	2.51	0.44
1:A:1756:PHE:HE2	1:A:1788:VAL:HG22	1.83	0.43
1:A:1881:TYR:O	1:A:1882:ARG:C	2.57	0.43
1:A:1708:PRO:C	1:A:1710:GLN:N	2.72	0.43
1:A:1729:PHE:HB3	1:A:1793:GLY:HA2	1.99	0.43
1:A:1868:VAL:CG1	1:A:1871:LYS:CB	2.96	0.43
1:A:1650:PHE:O	1:A:1654:GLU:HG3	2.19	0.43
1:A:1723:LEU:HG	1:A:1829:PHE:HD2	1.83	0.43
1:A:1638:ASP:OD2	1:A:1638:ASP:C	2.57	0.43
1:A:1653:PHE:HB2	1:A:1741:TYR:CE1	2.54	0.43
1:A:1835:ARG:HA	1:A:1835:ARG:CZ	2.46	0.43
1:A:1679:ASN:OD1	1:A:1679:ASN:C	2.57	0.43
1:A:1705:TYR:C	1:A:1705:TYR:CD2	2.92	0.43
1:A:1663:ASN:OD1	1:A:1665:ALA:HB3	2.19	0.42
1:A:1859:ASP:OD1	1:A:1861:LYS:HD3	2.19	0.42
1:A:1669:GLN:O	1:A:1685:TYR:HB3	2.20	0.42
1:A:1841:LEU:CA	1:A:1844:MET:HB2	2.50	0.41
1:A:1818:TYR:HB3	1:A:1822:MET:HE2	2.01	0.41
1:A:1796:PHE:CE2	1:A:1818:TYR:HE1	2.38	0.41
1:A:1892:ALA:O	1:A:1894:ARG:N	2.54	0.41
1:A:1719:LEU:O	1:A:1720:ARG:C	2.57	0.41
1:A:1814:VAL:HG12	1:A:1814:VAL:O	2.18	0.41
1:A:1796:PHE:CZ	1:A:1818:TYR:CE1	3.09	0.41
1:A:1699:LEU:C	1:A:1701:THR:H	2.23	0.41
1:A:1734:VAL:O	1:A:1735:LYS:C	2.59	0.41
1:A:1746:SER:HA	1:A:1747:PRO:HD2	1.43	0.41
1:A:1750:PHE:HA	1:A:1753:ILE:HB	2.02	0.41
1:A:1737:ASP:OD2	1:A:1740:LYS:HD2	2.21	0.41
1:A:1641:LYS:C	1:A:1643:LEU:N	2.72	0.41
1:A:1813:VAL:O	1:A:1814:VAL:C	2.58	0.41
1:A:1754:ASP:C	1:A:1756:PHE:N	2.72	0.40
1:A:1866:VAL:CG1	1:A:1866:VAL:O	2.69	0.40
1:A:1879:ARG:HH11	1:A:1879:ARG:HD3	1.76	0.40
1:A:1669:GLN:C	1:A:1671:PHE:N	2.75	0.40
1:A:1797:GLU:O	1:A:1800:ALA:HB3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1693:ASP:HB3	1:A:1694:ALA:H	1.77	0.40
1:A:1759:PHE:CD1	1:A:1786:ILE:HG13	2.57	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:1762:GLU:OE1	2:A:2:CD:CD[5_445]	2.16	0.04

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	237/265 (89%)	178 (75%)	45 (19%)	14 (6%)	2 5

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1640	GLU
1	A	1700	ILE
1	A	1763	LYS
1	A	1844	MET
1	A	1846	PRO
1	A	1869	VAL
1	A	1725	ASN
1	A	1791	ALA
1	A	1835	ARG
1	A	1843	GLU
1	A	1896	LEU
1	A	1746	SER
1	A	1834	PRO
1	A	1853	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	198 / 230 (86%)	166 (84%)	32 (16%)	3 8

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1640	GLU
1	A	1642	THR
1	A	1645	HIS
1	A	1648	SER
1	A	1660	ARG
1	A	1662	LYS
1	A	1667	LEU
1	A	1683	ASP
1	A	1685	TYR
1	A	1715	VAL
1	A	1717	THR
1	A	1720	ARG
1	A	1761	LEU
1	A	1784	GLU
1	A	1790	LYS
1	A	1822	MET
1	A	1829	PHE
1	A	1833	VAL
1	A	1835	ARG
1	A	1839	ARG
1	A	1847	GLU
1	A	1855	GLU
1	A	1856	ARG
1	A	1861	LYS
1	A	1868	VAL
1	A	1875	LYS
1	A	1879	ARG
1	A	1880	SER
1	A	1885	LYS
1	A	1890	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1895	SER
1	A	1896	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1644	ASN
1	A	1669	GLN
1	A	1673	HIS
1	A	1760	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	OCS	A	1684	1	7,8,9	1.46	1 (14%)	7,11,13	2.24	2 (28%)

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
1	OCS	A	1684	1	-	0/4/7/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1684	OCS	CB-SG	3.15	1.82	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1684	OCS	OD3-SG-CB	3.77	110.12	106.94
1	A	1684	OCS	OD1-SG-CB	3.89	110.22	106.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1684	OCS	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	241/265 (90%)	-0.17	3 (1%) 81 73	58, 98, 126, 149	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1788	VAL	2.4
1	A	1677	HIS	2.3
1	A	1870	GLY	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OCS	A	1684	9/10	0.94	0.17	-	96,97,98,100	0

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(\AA^2)	Q<0.9
2	CD	A	2	1/1	0.96	0.10	-	162,162,162,162	0
2	CD	A	1	1/1	0.79	0.12	-	209,209,209,209	0
2	CD	A	3	1/1	0.94	0.09	-	144,144,144,144	0

6.5 Other polymers [i](#)

There are no such residues in this entry.