



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 08:47 AM EDT

PDB ID : 3K16 / pdb_00003k16
Title : Crystal Structure of BRCA1 BRCT D1840T in complex with a minimal recognition tetrapeptide with a free carboxy C-terminus
Authors : Campbell, S.J.; Edwards, R.A.; Glover, J.N.
Deposited on : 2009-09-25
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

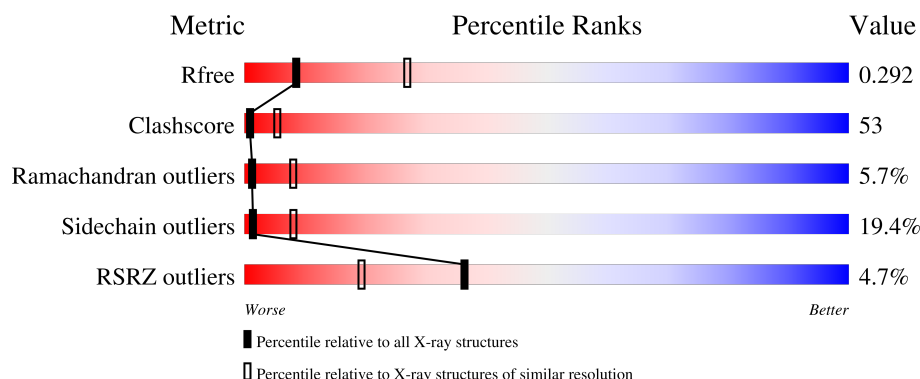
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	215	
2	B	4	

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	SEP	B	1	-	-	X	-
4	CL	B	5	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1738 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 Breast cancer type 1 susceptibility protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1694	1082	289	309	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1645	MET	-	expression tag	UNP P38398
A	1840	THR	ASP	engineered mutation	UNP P38398

- Molecule 2 is a protein called phospho peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	4	Total	C	N	O	P	0	0	0
			36	21	4	10	1			

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

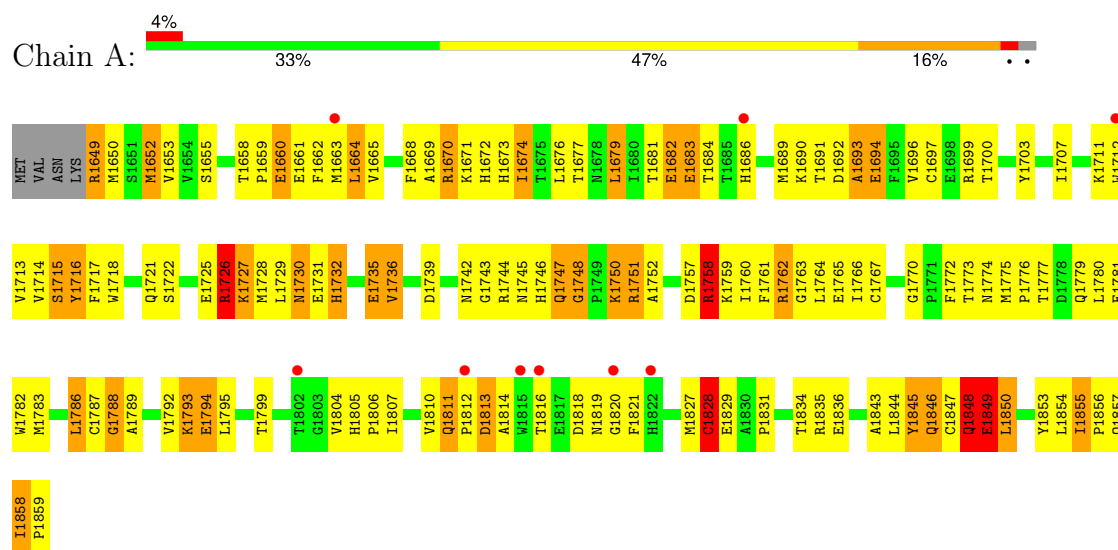
- Molecule 5 is water.

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

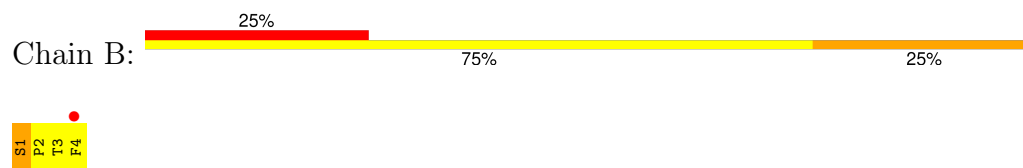
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Breast cancer type 1 susceptibility protein



- Molecule 2: phospho peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	114.34Å 114.34Å 123.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.66 – 3.00 38.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.66-3.00) 99.9 (38.66-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.288 0.228 , 0.292	Depositor DCC
R_{free} test set	480 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	82.7	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	1738	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: SEP, CL, NI

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	0.49	0/1735	0.83	2/2354 (0.1%)
2	B	0.33	0/27	0.67	0/34
All	All	0.49	0/1762	0.83	2/2388 (0.1%)

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	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1748	GLY	CA-C-N	7.20	127.05	119.05
1	A	1748	GLY	C-N-CA	7.20	127.05	119.05

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1652	MET	Peptide
1	A	1726	ARG	Peptide
1	A	1788	GLY	Peptide
1	A	1828	CYS	Peptide
1	A	1849	GLU	Peptide
1	A	1858	ILE	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	1694	0	1674	177	1
2	B	36	0	28	12	0
3	A	1	0	0	0	0
4	B	1	0	0	6	0
5	A	6	0	0	6	1
All	All	1738	0	1702	183	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 53.

All (183) 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:1804:VAL:HG12	1:A:1805:HIS:H	1.01	1.15
1:A:1857:GLN:O	1:A:1859:PRO:HD3	1.54	1.05
2:B:1:SEP:N	4:B:5:CL:CL	2.29	1.03
1:A:1804:VAL:HG12	1:A:1805:HIS:N	1.72	1.02
1:A:1804:VAL:CG1	1:A:1805:HIS:H	1.73	1.01
1:A:1805:HIS:CE1	5:A:3:HOH:O	2.16	0.99
1:A:1850:LEU:N	1:A:1850:LEU:HD12	1.78	0.96
1:A:1758:ARG:O	1:A:1758:ARG:HG3	1.70	0.91
1:A:1855:ILE:HG23	1:A:1856:PRO:HD2	1.56	0.87
1:A:1726:ARG:HG2	1:A:1726:ARG:HH11	1.38	0.86
1:A:1700:THR:O	1:A:1703:TYR:HB3	1.76	0.86
1:A:1649:ARG:HA	1:A:1649:ARG:HE	1.42	0.85
1:A:1725:GLU:C	1:A:1726:ARG:HG3	2.01	0.85
2:B:1:SEP:O	4:B:5:CL:CL	2.32	0.85
1:A:1658:THR:OG1	1:A:1661:GLU:HG3	1.77	0.84
1:A:1650:MET:HE3	1:A:1686:HIS:CE1	2.13	0.84
1:A:1805:HIS:CE1	5:A:4:HOH:O	2.32	0.83
1:A:1816:THR:HG22	1:A:1816:THR:O	1.79	0.83
1:A:1827:MET:O	1:A:1828:CYS:HB3	1.79	0.81
1:A:1699:ARG:HH11	1:A:1742:ASN:HD21	1.25	0.81
1:A:1850:LEU:N	1:A:1850:LEU:CD1	2.44	0.81
1:A:1699:ARG:HB2	2:B:4:PHE:OXT	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1805:HIS:HE1	5:A:4:HOH:O	1.64	0.79
1:A:1726:ARG:HG2	1:A:1726:ARG:NH1	1.98	0.77
1:A:1758:ARG:O	1:A:1758:ARG:CG	2.29	0.77
1:A:1849:GLU:CA	1:A:1850:LEU:HD12	2.15	0.76
1:A:1858:ILE:HG22	1:A:1859:PRO:O	1.86	0.76
1:A:1649:ARG:HA	1:A:1649:ARG:NE	2.02	0.74
1:A:1848:GLN:N	1:A:1848:GLN:HE21	1.86	0.73
1:A:1730:ASN:ND2	1:A:1732:HIS:HB2	2.03	0.73
1:A:1730:ASN:HD22	1:A:1732:HIS:CB	2.02	0.73
1:A:1700:THR:HB	5:A:1860:HOH:O	1.89	0.72
1:A:1672:HIS:HB2	1:A:1674:ILE:HD12	1.72	0.71
1:A:1848:GLN:NE2	1:A:1848:GLN:CA	2.55	0.70
1:A:1691:THR:CG2	1:A:1715:SER:HB2	2.21	0.70
1:A:1712:TRP:HZ3	1:A:1735:GLU:HG3	1.57	0.69
1:A:1811:GLN:OE1	1:A:1835:ARG:CZ	2.40	0.69
1:A:1855:ILE:CG2	1:A:1856:PRO:HD2	2.22	0.69
1:A:1672:HIS:CB	1:A:1674:ILE:HD12	2.23	0.69
1:A:1750:LYS:O	1:A:1751:ARG:C	2.37	0.67
1:A:1805:HIS:HE1	5:A:3:HOH:O	1.67	0.66
1:A:1761:PHE:HB2	1:A:1787:CYS:O	1.97	0.65
1:A:1767:CYS:HB2	1:A:1792:VAL:HB	1.79	0.64
1:A:1684:THR:O	1:A:1711:LYS:HD2	1.98	0.64
1:A:1662:PHE:HE1	1:A:1676:LEU:HD21	1.63	0.64
1:A:1846:GLN:O	1:A:1848:GLN:N	2.31	0.64
1:A:1700:THR:HG22	2:B:2:PRO:O	1.98	0.64
1:A:1813:ASP:OD1	1:A:1813:ASP:N	2.31	0.63
1:A:1696:VAL:HG13	1:A:1739:ASP:HA	1.80	0.63
1:A:1730:ASN:HD22	1:A:1732:HIS:HB2	1.61	0.63
1:A:1776:PRO:HG2	1:A:1779:GLN:HG2	1.80	0.63
1:A:1848:GLN:HE21	1:A:1848:GLN:CA	2.10	0.63
1:A:1713:VAL:HG12	1:A:1736:VAL:CG1	2.29	0.63
1:A:1850:LEU:CD1	1:A:1850:LEU:H	2.10	0.62
1:A:1696:VAL:HG13	1:A:1739:ASP:CA	2.30	0.62
1:A:1662:PHE:CE1	1:A:1676:LEU:HD21	2.35	0.62
1:A:1848:GLN:NE2	1:A:1848:GLN:HA	2.15	0.61
1:A:1712:TRP:CZ3	1:A:1735:GLU:HG3	2.36	0.61
1:A:1649:ARG:HD3	1:A:1650:MET:N	2.16	0.61
1:A:1699:ARG:NH1	1:A:1742:ASN:HD21	1.99	0.61
1:A:1691:THR:HG21	1:A:1715:SER:HB2	1.83	0.60
1:A:1855:ILE:HG23	1:A:1856:PRO:CD	2.31	0.60
1:A:1849:GLU:HA	1:A:1850:LEU:HD12	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1776:PRO:HG2	1:A:1779:GLN:CG	2.31	0.59
1:A:1722:SER:CA	1:A:1729:LEU:HD12	2.33	0.59
1:A:1726:ARG:O	1:A:1727:LYS:HG2	2.03	0.58
1:A:1742:ASN:HD22	1:A:1843:ALA:CB	2.16	0.58
1:A:1811:GLN:OE1	1:A:1835:ARG:NH2	2.37	0.58
1:A:1696:VAL:HG21	1:A:1744:ARG:NH1	2.19	0.58
1:A:1849:GLU:C	1:A:1850:LEU:HD12	2.29	0.58
2:B:1:SEP:CA	4:B:5:CL:CL	2.89	0.58
1:A:1766:ILE:HD12	1:A:1789:ALA:CB	2.33	0.57
1:A:1681:THR:O	1:A:1682:GLU:C	2.47	0.57
1:A:1681:THR:O	1:A:1683:GLU:N	2.37	0.57
1:A:1649:ARG:CG	1:A:1650:MET:H	2.16	0.57
1:A:1650:MET:HE1	1:A:1718:TRP:HH2	1.69	0.56
1:A:1742:ASN:ND2	1:A:1843:ALA:CB	2.68	0.56
1:A:1722:SER:HA	1:A:1729:LEU:HD12	1.86	0.56
1:A:1730:ASN:HD22	1:A:1732:HIS:HB3	1.69	0.56
1:A:1707:ILE:HG23	1:A:1752:ALA:CB	2.36	0.55
1:A:1773:THR:C	1:A:1775:MET:H	2.14	0.55
1:A:1816:THR:O	1:A:1816:THR:CG2	2.51	0.55
1:A:1649:ARG:HD3	1:A:1649:ARG:C	2.31	0.55
1:A:1692:ASP:OD2	1:A:1696:VAL:HB	2.06	0.55
1:A:1849:GLU:CB	1:A:1850:LEU:HD12	2.38	0.54
1:A:1730:ASN:C	1:A:1732:HIS:N	2.63	0.54
1:A:1700:THR:O	1:A:1703:TYR:N	2.42	0.53
2:B:1:SEP:C	4:B:5:CL:CL	2.94	0.53
1:A:1649:ARG:NE	1:A:1649:ARG:CA	2.72	0.53
1:A:1846:GLN:O	1:A:1848:GLN:NE2	2.41	0.53
1:A:1742:ASN:O	1:A:1746:HIS:HD2	1.91	0.53
1:A:1744:ARG:HG2	1:A:1744:ARG:HH11	1.74	0.53
2:B:1:SEP:HB3	4:B:5:CL:CL	2.46	0.52
1:A:1730:ASN:O	1:A:1731:GLU:C	2.50	0.52
1:A:1660:GLU:H	1:A:1660:GLU:CD	2.17	0.52
1:A:1700:THR:O	1:A:1703:TYR:CB	2.54	0.52
1:A:1668:PHE:HE1	1:A:1722:SER:HB3	1.75	0.51
1:A:1655:SER:HB2	2:B:1:SEP:OI1P	2.10	0.51
1:A:1725:GLU:O	1:A:1726:ARG:C	2.53	0.51
1:A:1672:HIS:O	1:A:1673:HIS:HB2	2.11	0.51
1:A:1699:ARG:HG2	1:A:1703:TYR:CE2	2.46	0.51
1:A:1690:LYS:HE2	5:A:5:HOH:O	2.09	0.51
1:A:1681:THR:OG1	1:A:1683:GLU:HG3	2.11	0.51
1:A:1689:MET:HE3	1:A:1697:CYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1713:VAL:HG12	1:A:1736:VAL:HG13	1.93	0.50
1:A:1726:ARG:NH1	1:A:1726:ARG:CG	2.70	0.50
1:A:1653:VAL:HG12	1:A:1677:THR:O	2.11	0.50
1:A:1761:PHE:O	1:A:1788:GLY:O	2.30	0.50
1:A:1763:GLY:O	1:A:1764:LEU:HD23	2.12	0.50
1:A:1747:GLN:N	1:A:1747:GLN:OE1	2.45	0.49
1:A:1773:THR:C	1:A:1775:MET:N	2.69	0.49
1:A:1722:SER:OG	1:A:1729:LEU:HD12	2.12	0.49
1:A:1850:LEU:HD12	1:A:1850:LEU:H	1.64	0.49
1:A:1672:HIS:HB3	1:A:1674:ILE:HD12	1.94	0.49
1:A:1844:LEU:C	1:A:1846:GLN:N	2.71	0.48
1:A:1682:GLU:HB2	1:A:1683:GLU:HG2	1.95	0.48
1:A:1699:ARG:HA	1:A:1703:TYR:CD2	2.48	0.48
1:A:1652:MET:HG3	1:A:1674:ILE:CG2	2.43	0.48
1:A:1760:ILE:HG21	1:A:1845:TYR:O	2.14	0.48
1:A:1806:PRO:O	1:A:1831:PRO:HD2	2.13	0.47
1:A:1795:LEU:HD12	1:A:1827:MET:HE2	1.97	0.47
1:A:1681:THR:C	1:A:1683:GLU:H	2.23	0.47
1:A:1743:GLY:C	1:A:1745:ASN:H	2.23	0.47
2:B:1:SEP:CB	4:B:5:CL:CL	3.00	0.47
1:A:1761:PHE:HB3	1:A:1789:ALA:HB2	1.97	0.47
1:A:1844:LEU:C	1:A:1846:GLN:H	2.21	0.47
1:A:1696:VAL:CG1	1:A:1739:ASP:HA	2.44	0.46
1:A:1684:THR:O	1:A:1711:LYS:CD	2.63	0.46
1:A:1665:VAL:O	1:A:1668:PHE:HB3	2.15	0.46
1:A:1681:THR:C	1:A:1683:GLU:N	2.72	0.46
1:A:1857:GLN:O	1:A:1859:PRO:CD	2.45	0.46
1:A:1658:THR:O	1:A:1659:PRO:C	2.59	0.46
1:A:1692:ASP:O	1:A:1693:ALA:C	2.58	0.46
1:A:1655:SER:CB	2:B:1:SEP:O1P	2.63	0.45
1:A:1699:ARG:HH11	1:A:1742:ASN:ND2	2.03	0.45
1:A:1773:THR:HG23	1:A:1814:ALA:HB2	1.99	0.45
1:A:1848:GLN:HE21	1:A:1848:GLN:H	1.61	0.45
1:A:1722:SER:HA	1:A:1729:LEU:CD1	2.46	0.45
1:A:1707:ILE:HG23	1:A:1752:ALA:HB2	1.98	0.45
1:A:1770:GLY:O	1:A:1772:PHE:CE1	2.69	0.45
1:A:1715:SER:O	1:A:1717:PHE:N	2.49	0.45
1:A:1679:LEU:HD23	1:A:1679:LEU:HA	1.44	0.45
1:A:1799:THR:O	1:A:1799:THR:HG22	2.17	0.45
1:A:1829:GLU:HA	1:A:1829:GLU:OE1	2.16	0.45
1:A:1650:MET:HE3	1:A:1686:HIS:NE2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1759:LYS:H	1:A:1759:LYS:HG2	1.62	0.44
1:A:1652:MET:HG3	1:A:1674:ILE:HG21	2.00	0.44
1:A:1747:GLN:OE1	1:A:1747:GLN:CA	2.66	0.44
1:A:1793:LYS:HA	1:A:1793:LYS:HD3	1.52	0.44
1:A:1669:ALA:O	1:A:1670:ARG:C	2.59	0.44
1:A:1759:LYS:O	1:A:1762:ARG:HG3	2.17	0.44
1:A:1855:ILE:CG2	1:A:1856:PRO:CD	2.93	0.44
1:A:1742:ASN:HD22	1:A:1843:ALA:HB1	1.81	0.44
1:A:1804:VAL:CG1	1:A:1805:HIS:N	2.43	0.44
1:A:1658:THR:H	1:A:1661:GLU:HB2	1.83	0.44
1:A:1664:LEU:HA	1:A:1664:LEU:HD23	1.59	0.44
1:A:1649:ARG:C	1:A:1649:ARG:CD	2.90	0.43
1:A:1775:MET:HE3	2:B:4:PHE:CE1	2.53	0.43
1:A:1811:GLN:HA	1:A:1812:PRO:HD3	1.82	0.43
1:A:1806:PRO:O	1:A:1807:ILE:HG13	2.18	0.43
1:A:1777:THR:O	1:A:1781:GLU:HG3	2.18	0.43
1:A:1692:ASP:OD1	1:A:1692:ASP:C	2.62	0.43
1:A:1649:ARG:HG3	1:A:1650:MET:H	1.82	0.42
1:A:1697:CYS:SG	1:A:1736:VAL:HG21	2.58	0.42
1:A:1783:MET:O	1:A:1786:LEU:HB2	2.18	0.42
1:A:1782:TRP:CE2	1:A:1786:LEU:HD11	2.54	0.42
1:A:1853:TYR:O	1:A:1854:LEU:C	2.61	0.42
1:A:1692:ASP:O	1:A:1694:GLU:N	2.52	0.42
1:A:1855:ILE:HG22	1:A:1857:GLN:NE2	2.35	0.42
1:A:1689:MET:HE2	1:A:1697:CYS:SG	2.60	0.42
1:A:1715:SER:O	1:A:1716:TYR:C	2.63	0.42
1:A:1671:LYS:HE3	1:A:1672:HIS:CE1	2.56	0.41
1:A:1848:GLN:N	1:A:1848:GLN:NE2	2.61	0.41
1:A:1699:ARG:O	2:B:4:PHE:N	2.53	0.41
1:A:1811:GLN:OE1	1:A:1835:ARG:NH1	2.53	0.41
1:A:1810:VAL:O	1:A:1834:THR:HA	2.20	0.41
1:A:1818:ASP:C	1:A:1820:GLY:H	2.27	0.41
1:A:1821:PHE:CD1	1:A:1821:PHE:C	2.98	0.41
1:A:1765:GLU:HG2	1:A:1792:VAL:CG2	2.51	0.41
1:A:1713:VAL:HG12	1:A:1736:VAL:HG11	2.00	0.40
1:A:1717:PHE:O	1:A:1718:TRP:C	2.64	0.40
1:A:1794:GLU:H	1:A:1794:GLU:HG2	1.72	0.40
1:A:1725:GLU:O	1:A:1726:ARG:HG3	2.21	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:1673:HIS:NE2	5:A:3:HOH:O[6_555]	1.89	0.31

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	209/215 (97%)	172 (82%)	25 (12%)	12 (6%)	1	8
2	B	2/4 (50%)	2 (100%)	0	0	100	100
All	All	211/219 (96%)	174 (82%)	25 (12%)	12 (6%)	1	8

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1693	ALA
1	A	1716	TYR
1	A	1828	CYS
1	A	1845	TYR
1	A	1847	CYS
1	A	1682	GLU
1	A	1758	ARG
1	A	1750	LYS
1	A	1774	ASN
1	A	1848	GLN
1	A	1762	ARG
1	A	1748	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	188/192 (98%)	152 (81%)	36 (19%)	1	8
2	B	3/3 (100%)	2 (67%)	1 (33%)	0	1
All	All	191/195 (98%)	154 (81%)	37 (19%)	1	8

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1649	ARG
1	A	1660	GLU
1	A	1663	MET
1	A	1664	LEU
1	A	1670	ARG
1	A	1674	ILE
1	A	1679	LEU
1	A	1683	GLU
1	A	1694	GLU
1	A	1714	VAL
1	A	1715	SER
1	A	1721	GLN
1	A	1726	ARG
1	A	1727	LYS
1	A	1728	MET
1	A	1730	ASN
1	A	1732	HIS
1	A	1735	GLU
1	A	1736	VAL
1	A	1747	GLN
1	A	1751	ARG
1	A	1757	ASP
1	A	1758	ARG
1	A	1780	LEU
1	A	1786	LEU
1	A	1793	LYS
1	A	1794	GLU
1	A	1811	GLN
1	A	1813	ASP
1	A	1819	ASN
1	A	1836	GLU
1	A	1846	GLN
1	A	1848	GLN
1	A	1849	GLU

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Mol	Chain	Res	Type
1	A	1850	LEU
1	A	1855	ILE
2	B	3	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1678	ASN
1	A	1730	ASN
1	A	1742	ASN
1	A	1774	ASN
1	A	1822	HIS
1	A	1846	GLN
1	A	1848	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
2	SEP	B	1	2	8,9,10	1.56	1 (12%)	7,12,14	2.08	3 (42%)

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	SEP	B	1	2	-	5/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	SEP	P-O1P	3.40	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	SEP	OG-CB-CA	2.77	110.84	108.14
2	B	1	SEP	OG-P-O1P	2.57	113.40	106.44
2	B	1	SEP	O2P-P-OG	-2.24	100.83	106.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	SEP	N-CA-CB-OG
2	B	1	SEP	C-CA-CB-OG
2	B	1	SEP	CB-OG-P-O2P
2	B	1	SEP	CB-OG-P-O3P
2	B	1	SEP	CB-OG-P-O1P

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	SEP	8	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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

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	211/215 (98%)	0.47	9 (4%) 40 21	37, 55, 73, 96	1 (0%)
2	B	3/4 (75%)	1.54	1 (33%) 1 1	53, 53, 53, 56	3 (100%)
All	All	214/219 (97%)	0.48	10 (4%) 36 19	37, 55, 73, 96	4 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1816	THR	4.7
1	A	1820	GLY	2.6
1	A	1663	MET	2.5
1	A	1802	THR	2.5
1	A	1815	TRP	2.5
2	B	4	PHE	2.4
1	A	1686	HIS	2.3
1	A	1822	HIS	2.3
1	A	1812	PRO	2.2
1	A	1712	TRP	2.1

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. 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	B-factors(Å ²)	Q<0.9
2	SEP	B	1	10/11	0.85	0.21	54,58,63,64	10

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	B	5	1/1	0.84	0.35	57,57,57,57	1
3	NI	A	1	1/1	0.86	0.17	89,89,89,89	1

6.5 Other polymers [i](#)

There are no such residues in this entry.