



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:06 PM UTC

PDB ID : 1T29 / pdb_00001t29
Title : Crystal structure of the BRCA1 BRCT repeats bound to a phosphorylated BACH1 peptide
Authors : Shiozaki, E.N.; Gu, L.; Yan, N.; Shi, Y.
Deposited on : 2004-04-20
Resolution : 2.30 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

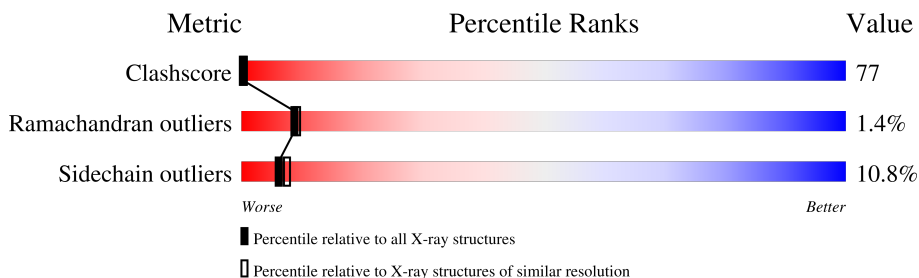
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	
2	B	14	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2009 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
			1675	1071	288	302	14			

- Molecule 2 is a protein called BACH1 phosphorylated peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	P	0	0	0
			99	58	18	22	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	SEP	SER	modified residue	UNP Q9BX63

- Molecule 3 is water.

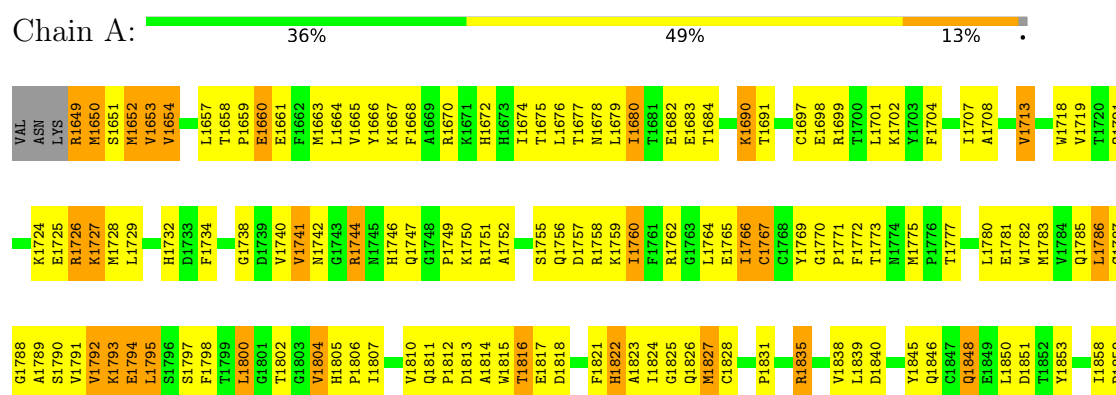
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	216	Total	O	0	0
			216	216		
3	B	19	Total	O	0	0
			19	19		

3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

- Molecule 1: Breast cancer type 1 susceptibility protein



- Molecule 2: BACH1 phosphorylated peptide



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	63.18Å 63.18Å 105.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2009	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.54	0/1715	1.14	11/2323 (0.5%)
2	B	0.68	0/89	1.30	0/116
All	All	0.55	0/1804	1.15	11/2439 (0.5%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1822	HIS	N-CA-C	-13.77	96.50	113.02
1	A	1818	ASP	N-CA-C	-9.65	94.40	109.07
1	A	1802	THR	N-CA-C	9.25	122.77	112.97
1	A	1800	LEU	N-CA-C	8.88	123.94	113.20
1	A	1792	VAL	CB-CA-C	-6.10	101.14	110.95
1	A	1713	VAL	N-CA-C	-5.73	98.71	106.85
1	A	1652	MET	N-CA-C	5.71	118.98	110.52
1	A	1766	ILE	N-CA-C	5.63	116.22	108.12
1	A	1690	LYS	N-CA-C	-5.50	101.71	109.96
1	A	1802	THR	CB-CA-C	-5.23	103.16	111.17
1	A	1741	VAL	N-CA-C	5.09	115.94	111.56

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	1675	0	1646	256	0
2	B	99	0	97	19	0
3	A	216	0	0	152	0
3	B	19	0	0	2	0
All	All	2009	0	1743	271	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 77.

All (271) 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)
2:B:11:LYS:O	2:B:12:GLN:HG2	1.28	1.33
1:A:1804:VAL:HG12	3:A:137:HOH:O	1.56	1.05
1:A:1814:ALA:HB3	3:A:222:HOH:O	1.56	1.05
1:A:1740:VAL:HG23	3:A:219:HOH:O	1.64	0.98
1:A:1665:VAL:HG22	3:A:147:HOH:O	1.65	0.96
1:A:1660:GLU:O	1:A:1663:MET:HG2	1.67	0.95
1:A:1751:ARG:HB2	3:A:203:HOH:O	1.67	0.94
1:A:1851:ASP:HB2	3:A:163:HOH:O	1.68	0.94
1:A:1813:ASP:HB3	3:A:99:HOH:O	1.68	0.93
1:A:1668:PHE:CZ	3:A:112:HOH:O	2.23	0.92
1:A:1728:MET:SD	3:A:142:HOH:O	2.30	0.90
1:A:1683:GLU:HG3	3:A:188:HOH:O	1.72	0.89
1:A:1795:LEU:HD21	1:A:1824:ILE:HG23	1.55	0.88
2:B:11:LYS:O	2:B:12:GLN:CG	2.19	0.88
1:A:1760:ILE:HG13	3:A:81:HOH:O	1.73	0.88
1:A:1826:GLN:HG3	3:A:215:HOH:O	1.73	0.88
1:A:1793:LYS:HD3	3:A:53:HOH:O	1.75	0.85
1:A:1650:MET:HE1	1:A:1728:MET:HE1	1.59	0.84
1:A:1724:LYS:HE2	3:A:217:HOH:O	1.77	0.84
1:A:1728:MET:HB2	3:A:142:HOH:O	1.78	0.84
1:A:1806:PRO:HG2	3:A:141:HOH:O	1.78	0.84
1:A:1814:ALA:HB2	3:A:202:HOH:O	1.78	0.83
1:A:1850:LEU:HD12	3:A:201:HOH:O	1.79	0.83
1:A:1665:VAL:HG13	3:A:84:HOH:O	1.78	0.83
1:A:1672:HIS:CG	3:A:142:HOH:O	2.31	0.83
1:A:1798:PHE:HB3	3:A:224:HOH:O	1.77	0.82
1:A:1771:PRO:HD2	3:A:222:HOH:O	1.77	0.82
1:A:1800:LEU:HB3	3:A:129:HOH:O	1.79	0.81
1:A:1650:MET:SD	3:A:150:HOH:O	2.38	0.81
1:A:1800:LEU:HD23	1:A:1800:LEU:H	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1719:VAL:HG11	3:A:147:HOH:O	1.82	0.80
1:A:1680:ILE:HG22	3:A:151:HOH:O	1.82	0.79
1:A:1746:HIS:HB2	3:A:181:HOH:O	1.83	0.79
1:A:1770:GLY:HA3	3:A:80:HOH:O	1.82	0.78
1:A:1816:THR:CB	1:A:1817:GLU:N	2.48	0.76
1:A:1806:PRO:HD3	3:A:137:HOH:O	1.85	0.76
1:A:1679:LEU:HA	3:A:116:HOH:O	1.86	0.75
1:A:1755:SER:HB3	3:A:176:HOH:O	1.87	0.75
1:A:1816:THR:HA	1:A:1817:GLU:N	2.01	0.75
1:A:1708:ALA:HB2	3:A:78:HOH:O	1.86	0.74
1:A:1707:ILE:HD12	1:A:1749:PRO:HA	1.66	0.74
1:A:1690:LYS:HE2	3:A:11:HOH:O	1.87	0.74
1:A:1707:ILE:HD11	1:A:1749:PRO:HG3	1.70	0.73
1:A:1665:VAL:HA	3:A:84:HOH:O	1.88	0.73
1:A:1677:THR:HB	3:A:136:HOH:O	1.87	0.73
1:A:1821:PHE:C	1:A:1823:ALA:H	1.97	0.73
1:A:1828:CYS:SG	3:A:140:HOH:O	2.47	0.73
1:A:1858:ILE:HG22	1:A:1859:PRO:CD	2.17	0.73
1:A:1772:PHE:HA	3:A:202:HOH:O	1.88	0.72
1:A:1825:GLY:HA3	3:A:161:HOH:O	1.87	0.72
2:B:11:LYS:C	2:B:12:GLN:HG2	2.13	0.72
1:A:1726:ARG:HD2	3:A:179:HOH:O	1.90	0.72
1:A:1707:ILE:HD13	1:A:1713:VAL:HG21	1.72	0.72
2:B:10:ASN:C	2:B:10:ASN:HD22	1.97	0.72
1:A:1815:TRP:CH2	3:A:153:HOH:O	2.42	0.72
1:A:1660:GLU:HA	1:A:1663:MET:HE3	1.72	0.71
1:A:1747:GLN:HG3	3:A:105:HOH:O	1.89	0.71
1:A:1815:TRP:CD1	3:A:171:HOH:O	2.44	0.71
1:A:1773:THR:N	3:A:202:HOH:O	2.23	0.71
1:A:1660:GLU:HG2	3:A:170:HOH:O	1.90	0.70
1:A:1649:ARG:HG2	1:A:1650:MET:H	1.56	0.70
1:A:1752:ALA:HB3	3:A:83:HOH:O	1.90	0.70
1:A:1814:ALA:CB	3:A:202:HOH:O	2.36	0.69
1:A:1783:MET:HE3	1:A:1838:VAL:HG12	1.73	0.69
1:A:1699:ARG:HD3	2:B:9:PHE:O	1.93	0.69
1:A:1800:LEU:H	1:A:1800:LEU:CD2	2.05	0.68
1:A:1798:PHE:N	3:A:162:HOH:O	2.26	0.68
1:A:1777:THR:O	1:A:1781:GLU:HG3	1.94	0.68
1:A:1816:THR:CA	1:A:1817:GLU:N	2.56	0.68
1:A:1792:VAL:HG12	1:A:1793:LYS:N	2.09	0.67
1:A:1858:ILE:HG22	1:A:1859:PRO:HD2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1666:TYR:HD2	3:A:227:HOH:O	1.77	0.67
1:A:1815:TRP:HB3	3:A:89:HOH:O	1.95	0.67
1:A:1827:MET:HG2	3:A:215:HOH:O	1.95	0.67
1:A:1853:TYR:CD2	3:A:182:HOH:O	2.48	0.67
1:A:1690:LYS:HD3	3:A:225:HOH:O	1.93	0.66
1:A:1783:MET:HE3	1:A:1838:VAL:CG1	2.26	0.66
1:A:1816:THR:HB	1:A:1817:GLU:N	2.09	0.66
1:A:1815:TRP:HH2	3:A:153:HOH:O	1.77	0.66
1:A:1690:LYS:CD	3:A:225:HOH:O	2.44	0.66
1:A:1726:ARG:CD	3:A:179:HOH:O	2.43	0.65
1:A:1757:ASP:HB2	3:A:6:HOH:O	1.95	0.65
1:A:1661:GLU:HA	3:A:91:HOH:O	1.96	0.64
1:A:1741:VAL:CG2	3:A:219:HOH:O	2.45	0.64
3:A:11:HOH:O	2:B:3:ARG:HG3	1.97	0.64
1:A:1699:ARG:HH21	1:A:1742:ASN:HD21	1.45	0.64
1:A:1772:PHE:C	3:A:167:HOH:O	2.41	0.64
1:A:1652:MET:HE1	1:A:1668:PHE:CD2	2.32	0.64
1:A:1805:HIS:O	3:A:71:HOH:O	2.15	0.63
1:A:1649:ARG:NH2	1:A:1650:MET:SD	2.71	0.63
1:A:1741:VAL:HG21	2:B:10:ASN:HA	1.81	0.63
1:A:1665:VAL:CG2	3:A:147:HOH:O	2.36	0.63
1:A:1650:MET:CE	1:A:1728:MET:HE1	2.28	0.63
1:A:1794:GLU:CA	3:A:138:HOH:O	2.48	0.62
1:A:1668:PHE:HD2	3:A:84:HOH:O	1.83	0.62
3:A:219:HOH:O	2:B:10:ASN:CB	2.47	0.62
2:B:10:ASN:HB3	3:B:20:HOH:O	1.99	0.62
1:A:1766:ILE:HD12	1:A:1789:ALA:CB	2.29	0.62
1:A:1770:GLY:CA	3:A:80:HOH:O	2.45	0.61
1:A:1795:LEU:HD23	1:A:1827:MET:HB2	1.82	0.61
1:A:1650:MET:HE1	1:A:1728:MET:CE	2.29	0.61
1:A:1815:TRP:CD1	1:A:1816:THR:N	2.68	0.61
1:A:1741:VAL:HG22	3:A:219:HOH:O	2.00	0.60
1:A:1649:ARG:HG2	1:A:1650:MET:N	2.15	0.60
1:A:1806:PRO:CG	3:A:141:HOH:O	2.43	0.60
1:A:1679:LEU:CD1	3:A:148:HOH:O	2.48	0.60
1:A:1667:LYS:HD2	3:A:152:HOH:O	2.02	0.59
1:A:1821:PHE:CD1	1:A:1824:ILE:HD11	2.38	0.59
1:A:1848:GLN:HG2	3:A:18:HOH:O	2.02	0.59
3:A:219:HOH:O	2:B:10:ASN:HB2	2.03	0.59
1:A:1760:ILE:HD11	1:A:1787:CYS:HB3	1.84	0.59
1:A:1760:ILE:HG21	3:A:81:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1751:ARG:HD2	1:A:1845:TYR:O	2.02	0.58
1:A:1783:MET:CG	3:A:78:HOH:O	2.52	0.58
1:A:1800:LEU:HD23	1:A:1800:LEU:N	2.17	0.58
1:A:1756:GLN:HB2	3:A:33:HOH:O	2.04	0.57
1:A:1670:ARG:HB2	3:A:190:HOH:O	2.04	0.57
1:A:1764:LEU:HB3	3:A:71:HOH:O	2.03	0.57
1:A:1667:LYS:HB2	3:A:152:HOH:O	2.05	0.57
1:A:1821:PHE:HB2	3:A:134:HOH:O	2.05	0.57
1:A:1758:ARG:HG3	3:A:176:HOH:O	2.03	0.57
1:A:1675:THR:HG22	3:A:136:HOH:O	2.05	0.57
1:A:1777:THR:HG21	3:A:216:HOH:O	2.04	0.57
1:A:1668:PHE:CD2	3:A:84:HOH:O	2.51	0.56
1:A:1764:LEU:HD22	3:A:71:HOH:O	2.05	0.56
1:A:1813:ASP:OD2	2:B:12:GLN:OE1	2.24	0.56
1:A:1815:TRP:HD1	1:A:1816:THR:N	2.04	0.56
1:A:1665:VAL:CA	3:A:84:HOH:O	2.52	0.55
1:A:1797:SER:HB2	3:A:95:HOH:O	2.06	0.55
1:A:1701:LEU:HD13	1:A:1775:MET:HG3	1.88	0.55
2:B:10:ASN:HD22	2:B:11:LYS:N	2.05	0.55
1:A:1682:GLU:CB	3:A:154:HOH:O	2.54	0.55
1:A:1806:PRO:O	1:A:1831:PRO:HD2	2.06	0.55
1:A:1751:ARG:CZ	3:A:203:HOH:O	2.54	0.54
1:A:1677:THR:HG21	3:A:75:HOH:O	2.06	0.54
1:A:1831:PRO:HG3	3:A:201:HOH:O	2.06	0.54
1:A:1677:THR:CG2	3:A:136:HOH:O	2.55	0.54
1:A:1783:MET:HG2	3:A:78:HOH:O	2.08	0.53
1:A:1828:CYS:CB	3:A:140:HOH:O	2.55	0.53
1:A:1718:TRP:HZ2	1:A:1728:MET:HE3	1.72	0.53
1:A:1759:LYS:HE3	3:A:158:HOH:O	2.06	0.53
1:A:1759:LYS:O	1:A:1762:ARG:HB2	2.09	0.53
1:A:1677:THR:CB	3:A:136:HOH:O	2.53	0.53
1:A:1653:VAL:HG13	1:A:1702:LYS:HD3	1.90	0.53
1:A:1780:LEU:HD12	1:A:1783:MET:HE2	1.89	0.53
1:A:1821:PHE:CZ	3:A:80:HOH:O	2.62	0.53
1:A:1680:ILE:CG2	3:A:151:HOH:O	2.50	0.53
1:A:1845:TYR:HA	3:A:81:HOH:O	2.07	0.53
1:A:1850:LEU:CD1	3:A:201:HOH:O	2.49	0.53
1:A:1791:VAL:HB	3:A:88:HOH:O	2.09	0.53
1:A:1769:TYR:CD1	1:A:1795:LEU:HD13	2.44	0.53
1:A:1772:PHE:CA	3:A:202:HOH:O	2.53	0.53
1:A:1821:PHE:C	1:A:1823:ALA:N	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1795:LEU:HD21	1:A:1824:ILE:CG2	2.36	0.52
1:A:1792:VAL:HG11	3:A:45:HOH:O	2.09	0.52
1:A:1718:TRP:CD2	3:A:112:HOH:O	2.62	0.52
1:A:1652:MET:HE1	1:A:1668:PHE:HD2	1.73	0.52
1:A:1775:MET:HB3	1:A:1835:ARG:NH2	2.25	0.52
1:A:1699:ARG:HD2	1:A:1741:VAL:CG2	2.39	0.52
1:A:1650:MET:HB3	1:A:1674:ILE:HG23	1.92	0.51
1:A:1760:ILE:HD13	1:A:1760:ILE:N	2.25	0.51
1:A:1787:CYS:SG	3:A:78:HOH:O	2.59	0.51
1:A:1649:ARG:NE	3:A:135:HOH:O	2.42	0.51
1:A:1795:LEU:HD23	1:A:1827:MET:CB	2.41	0.51
1:A:1701:LEU:HD13	1:A:1775:MET:HE2	1.91	0.51
1:A:1804:VAL:CG2	3:A:122:HOH:O	2.59	0.50
1:A:1746:HIS:CB	3:A:181:HOH:O	2.50	0.50
1:A:1783:MET:HG3	3:A:78:HOH:O	2.11	0.50
1:A:1668:PHE:HB3	3:A:84:HOH:O	2.11	0.50
1:A:1659:PRO:O	3:A:165:HOH:O	2.20	0.50
1:A:1699:ARG:HD2	1:A:1741:VAL:HG21	1.94	0.50
1:A:1858:ILE:CG2	1:A:1859:PRO:CD	2.88	0.50
1:A:1823:ALA:O	1:A:1826:GLN:HG2	2.12	0.50
1:A:1762:ARG:NH2	1:A:1788:GLY:HA2	2.26	0.49
1:A:1660:GLU:HG3	3:A:91:HOH:O	2.11	0.49
1:A:1652:MET:HE1	1:A:1668:PHE:CE2	2.48	0.49
1:A:1665:VAL:CG1	3:A:84:HOH:O	2.46	0.49
1:A:1699:ARG:NH2	1:A:1840:ASP:OD1	2.45	0.49
1:A:1760:ILE:HD12	1:A:1845:TYR:CE1	2.46	0.49
1:A:1667:LYS:CB	3:A:152:HOH:O	2.60	0.49
1:A:1758:ARG:HG2	3:A:169:HOH:O	2.12	0.49
1:A:1792:VAL:CG1	1:A:1793:LYS:N	2.76	0.49
1:A:1775:MET:HB3	1:A:1835:ARG:HH21	1.78	0.49
1:A:1858:ILE:HG22	1:A:1859:PRO:N	2.27	0.49
1:A:1699:ARG:NH2	1:A:1742:ASN:HD21	2.10	0.48
1:A:1787:CYS:HA	3:A:30:HOH:O	2.13	0.48
1:A:1728:MET:HE2	3:A:22:HOH:O	2.13	0.48
1:A:1782:TRP:NE1	1:A:1786:LEU:HD11	2.29	0.48
1:A:1691:THR:HG22	1:A:1697:CYS:HB3	1.96	0.47
1:A:1665:VAL:HG12	1:A:1676:LEU:HD22	1.96	0.47
1:A:1769:TYR:CD2	1:A:1824:ILE:HD13	2.49	0.47
1:A:1807:ILE:CD1	3:A:71:HOH:O	2.63	0.47
1:A:1827:MET:CG	3:A:215:HOH:O	2.58	0.47
1:A:1744:ARG:HD2	3:A:36:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:THR:CG2	2:B:5:THR:O	2.63	0.47
3:A:219:HOH:O	2:B:10:ASN:HB3	2.12	0.47
1:A:1811:GLN:CD	3:A:202:HOH:O	2.57	0.46
2:B:5:THR:O	2:B:5:THR:HG22	2.15	0.46
1:A:1767:CYS:HB2	1:A:1792:VAL:HB	1.97	0.46
1:A:1658:THR:HB	3:A:8:HOH:O	2.15	0.46
1:A:1651:SER:O	1:A:1684:THR:HG23	2.16	0.46
1:A:1746:HIS:CG	3:A:181:HOH:O	2.69	0.46
1:A:1719:VAL:CB	3:A:147:HOH:O	2.64	0.46
1:A:1651:SER:HB3	1:A:1684:THR:HA	1.97	0.46
1:A:1704:PHE:HB3	1:A:1783:MET:SD	2.55	0.46
1:A:1760:ILE:HD12	1:A:1845:TYR:CZ	2.50	0.46
1:A:1781:GLU:O	1:A:1785:GLN:HG3	2.17	0.46
1:A:1825:GLY:CA	3:A:161:HOH:O	2.57	0.46
1:A:1667:LYS:CG	3:A:152:HOH:O	2.63	0.45
1:A:1807:ILE:HG13	3:A:71:HOH:O	2.16	0.45
1:A:1657:LEU:CD2	3:A:225:HOH:O	2.65	0.45
1:A:1791:VAL:C	3:A:53:HOH:O	2.58	0.45
1:A:1652:MET:HG3	1:A:1674:ILE:HG21	1.99	0.45
1:A:1769:TYR:HE2	1:A:1821:PHE:CE1	2.35	0.45
2:B:9:PHE:CD1	2:B:9:PHE:N	2.85	0.45
1:A:1793:LYS:CD	3:A:53:HOH:O	2.50	0.45
1:A:1650:MET:SD	1:A:1728:MET:HE1	2.56	0.45
1:A:1659:PRO:HD2	3:A:8:HOH:O	2.17	0.44
1:A:1672:HIS:CD2	3:A:142:HOH:O	2.65	0.44
1:A:1682:GLU:CA	3:A:154:HOH:O	2.65	0.44
1:A:1690:LYS:HE3	3:B:24:HOH:O	2.17	0.44
1:A:1822:HIS:O	1:A:1858:ILE:HG13	2.17	0.44
1:A:1751:ARG:NE	3:A:203:HOH:O	2.51	0.44
1:A:1771:PRO:HD2	3:A:90:HOH:O	2.17	0.44
1:A:1851:ASP:CB	3:A:163:HOH:O	2.42	0.44
1:A:1785:GLN:HG2	1:A:1791:VAL:CG2	2.48	0.44
1:A:1762:ARG:HA	1:A:1762:ARG:HD2	1.43	0.43
1:A:1690:LYS:HD2	3:A:225:HOH:O	2.11	0.43
1:A:1719:VAL:CG1	3:A:147:HOH:O	2.51	0.43
1:A:1765:GLU:OE2	1:A:1804:VAL:HG11	2.18	0.43
1:A:1800:LEU:CB	3:A:233:HOH:O	2.67	0.43
1:A:1657:LEU:HA	1:A:1661:GLU:OE1	2.18	0.43
1:A:1670:ARG:HG3	3:A:114:HOH:O	2.18	0.43
1:A:1769:TYR:O	1:A:1810:VAL:HG12	2.19	0.43
1:A:1758:ARG:HA	3:A:39:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1762:ARG:NH2	1:A:1788:GLY:CA	2.81	0.43
1:A:1654:VAL:HG11	1:A:1657:LEU:HD12	2.01	0.42
1:A:1758:ARG:HG3	1:A:1758:ARG:O	2.17	0.42
1:A:1759:LYS:HB3	1:A:1787:CYS:O	2.19	0.42
1:A:1846:GLN:HG3	3:A:211:HOH:O	2.19	0.42
2:B:10:ASN:C	2:B:10:ASN:ND2	2.68	0.42
1:A:1721:GLN:HG2	1:A:1729:LEU:HD11	2.01	0.42
1:A:1750:LYS:HD2	3:A:57:HOH:O	2.19	0.42
1:A:1846:GLN:CD	3:A:211:HOH:O	2.62	0.42
1:A:1835:ARG:NH2	3:A:65:HOH:O	2.37	0.42
1:A:1657:LEU:HB3	1:A:1661:GLU:HB2	2.01	0.42
1:A:1800:LEU:HB3	3:A:233:HOH:O	2.19	0.42
1:A:1744:ARG:HD2	1:A:1744:ARG:HH11	1.68	0.42
1:A:1725:GLU:O	1:A:1727:LYS:N	2.52	0.42
1:A:1762:ARG:HH22	1:A:1788:GLY:HA2	1.85	0.42
1:A:1794:GLU:CA	3:A:103:HOH:O	2.67	0.42
1:A:1825:GLY:O	1:A:1828:CYS:O	2.38	0.42
1:A:1708:ALA:CB	3:A:78:HOH:O	2.57	0.42
1:A:1785:GLN:CG	1:A:1791:VAL:CG2	2.98	0.41
1:A:1815:TRP:HZ2	3:A:29:HOH:O	2.03	0.41
1:A:1707:ILE:HD12	1:A:1749:PRO:CA	2.43	0.41
1:A:1853:TYR:CE2	3:A:182:HOH:O	2.71	0.41
1:A:1652:MET:CE	1:A:1668:PHE:CE2	3.03	0.41
1:A:1721:GLN:O	1:A:1724:LYS:HB3	2.21	0.41
1:A:1792:VAL:CG1	3:A:45:HOH:O	2.66	0.41
1:A:1810:VAL:O	1:A:1812:PRO:HD3	2.20	0.41
1:A:1835:ARG:HD3	1:A:1839:LEU:HD11	2.01	0.41
1:A:1698:GLU:HG3	2:B:1:ILE:HB	2.01	0.41
1:A:1816:THR:HG1	1:A:1817:GLU:N	2.18	0.41
1:A:1721:GLN:NE2	1:A:1734:PHE:CE2	2.89	0.41
1:A:1792:VAL:CA	3:A:53:HOH:O	2.70	0.40
2:B:10:ASN:HD22	2:B:11:LYS:HB2	1.86	0.40
1:A:1785:GLN:HG2	1:A:1791:VAL:HG23	2.02	0.40
1:A:1664:LEU:HD23	1:A:1664:LEU:HA	1.97	0.40
1:A:1721:GLN:NE2	1:A:1734:PHE:HE2	2.19	0.40
1:A:1738:GLY:HA2	1:A:1746:HIS:CE1	2.57	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	207/214 (97%)	189 (91%)	15 (7%)	3 (1%)	9	9
2	B	9/14 (64%)	8 (89%)	1 (11%)	0	100	100
All	All	216/228 (95%)	197 (91%)	16 (7%)	3 (1%)	9	9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1650	MET
1	A	1794	GLU
1	A	1726	ARG

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	183/191 (96%)	163 (89%)	20 (11%)	6	7
2	B	11/13 (85%)	10 (91%)	1 (9%)	9	11
All	All	194/204 (95%)	173 (89%)	21 (11%)	6	7

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1649	ARG
1	A	1653	VAL
1	A	1654	VAL

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Mol	Chain	Res	Type
1	A	1660	GLU
1	A	1678	ASN
1	A	1680	ILE
1	A	1727	LYS
1	A	1732	HIS
1	A	1744	ARG
1	A	1760	ILE
1	A	1767	CYS
1	A	1786	LEU
1	A	1790	SER
1	A	1793	LYS
1	A	1795	LEU
1	A	1804	VAL
1	A	1816	THR
1	A	1827	MET
1	A	1835	ARG
1	A	1848	GLN
2	B	10	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1721	GLN
1	A	1732	HIS
1	A	1742	ASN
1	A	1745	ASN
2	B	10	ASN

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	6	2	8,9,10	1.02	0	7,12,14	1.60	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
2	SEP	B	6	2	-	0/6/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	SEP	O3P-P-O1P	2.70	121.35	110.83
2	B	6	SEP	O2P-P-OG	2.16	112.31	106.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1816:THR	C	1817:GLU	N	3.29

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.