Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 08:41 AM EDT

PDB ID	:	1T2V
Title	:	Structural basis of phospho-peptide recognition by the BRCT domain of BRCA1, structure with phosphopeptide
Authors	:	Williams, R.S.; Lee, M.S.; Hau, D.D.; Glover, J.N.M.
Deposited on	:	2004-04-22
Resolution	:	3.30 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 (i) 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 (i)) were used in the production of this report:

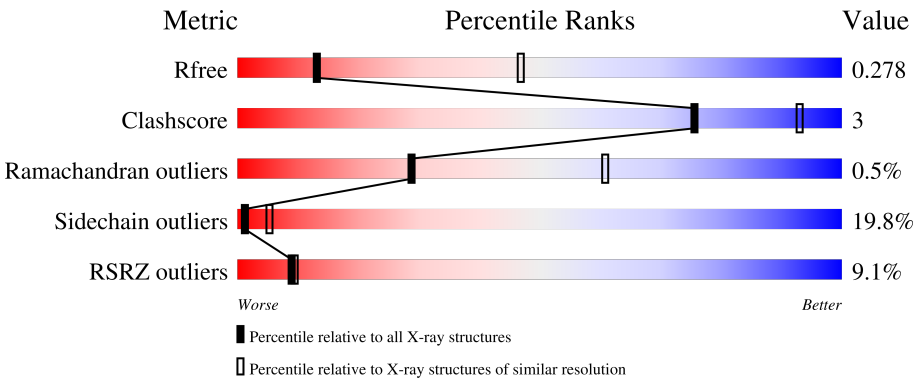
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 <=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	214	7% 72% 23% • •
1	B	214	10% 75% 21% • •
1	C	214	13% 70% 23% • 6%
1	D	214	12% 73% 21% • •
1	E	214	4% 77% 20% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	16	6%, 56%, 31%, 12%
2	G	16	6%, 62%, 12%, 12%, 12%
2	H	16	62%, 25%, 12%
2	I	16	6%, 50%, 19%, 31%
2	J	16	6%, 38%, 25%, 12%, 25%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8380 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
			Total	C	N	O	S			
1	A	208	1601	1030	264	293	14	0	0	0
1	B	210	1605	1026	271	295	13	0	0	0
1	C	202	1532	988	249	282	13	0	0	0
1	D	205	1523	982	252	276	13	0	0	0
1	E	211	1620	1041	267	298	14	0	0	0

- Molecule 2 is a protein called BRCTide-7PS.

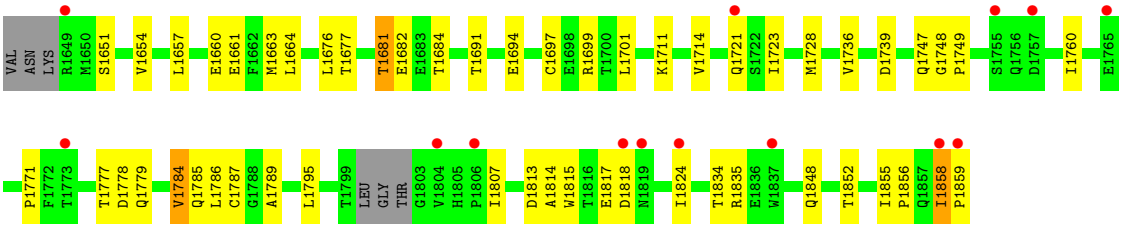
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	F	14	107	69	15	22	1	0	0	0
2	G	14	101	63	15	22	1	0	0	0
2	H	14	107	69	15	22	1	0	0	0
2	I	11	86	54	12	19	1	0	0	0
2	J	12	98	64	13	20	1	0	0	0

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 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.

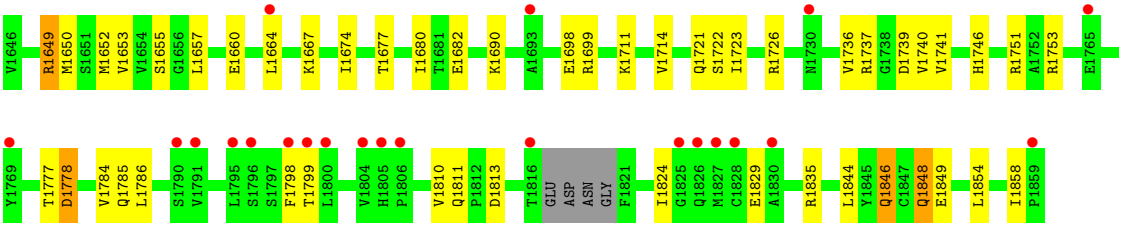
• Molecule 1: Breast cancer type 1 susceptibility protein

Chain A:



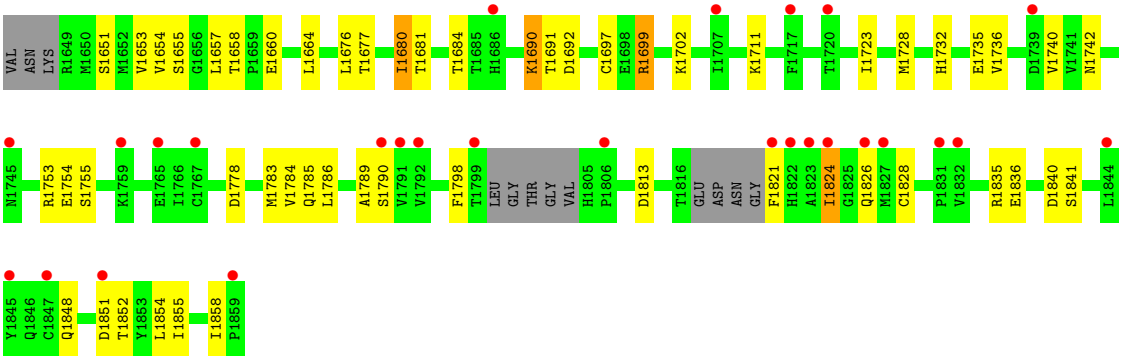
• Molecule 1: Breast cancer type 1 susceptibility protein

Chain B:



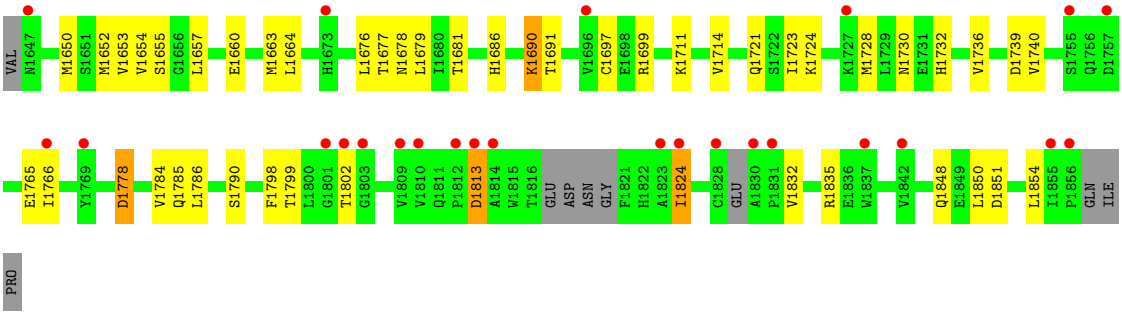
• Molecule 1: Breast cancer type 1 susceptibility protein

Chain C:



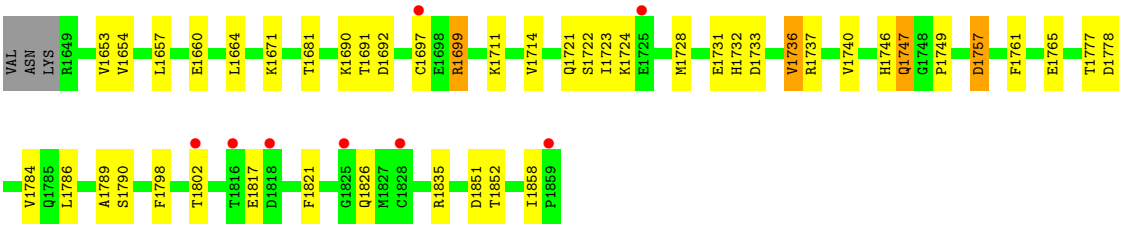
• Molecule 1: Breast cancer type 1 susceptibility protein

Chain D:



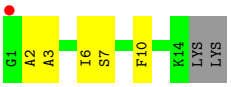
- Molecule 1: Breast cancer type 1 susceptibility protein

Chain E:



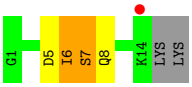
- Molecule 2: BRCTide-7PS

Chain F:



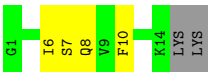
- Molecule 2: BRCTide-7PS

Chain G:



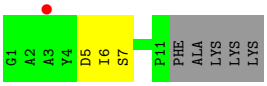
- Molecule 2: BRCTide-7PS

Chain H:



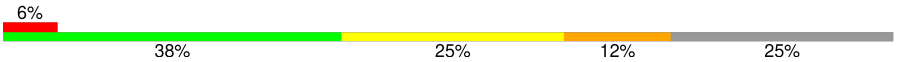
- Molecule 2: BRCTide-7PS

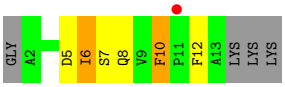
Chain I:



- Molecule 2: BRCTide-7PS

Chain J:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	97.12Å 138.36Å 198.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 49.57 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-3.30) 99.3 (49.57-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.258 , 0.301 0.232 , 0.278	Depositor DCC
R_{free} test set	1016 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	64.3	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 90.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8380	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.38	0/1641	0.68	4/2238 (0.2%)
1	B	0.37	0/1642	0.67	3/2238 (0.1%)
1	C	0.39	0/1569	0.67	3/2144 (0.1%)
1	D	0.35	0/1558	0.66	2/2126 (0.1%)
1	E	0.40	0/1661	0.71	5/2266 (0.2%)
2	F	0.52	0/99	0.80	0/133
2	G	0.52	0/92	0.85	1/124 (0.8%)
2	H	0.54	0/99	0.76	0/133
2	I	0.49	0/77	0.79	1/103 (1.0%)
2	J	0.88	0/90	1.65	2/121 (1.7%)
All	All	0.39	0/8528	0.70	21/11626 (0.2%)

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	E	0	1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	10	PHE	CA-C-N	6.58	135.51	117.10
1	B	1739	ASP	CB-CG-OD2	5.99	123.69	118.30
1	D	1739	ASP	CB-CG-OD2	5.86	123.57	118.30
2	J	5	ASP	CB-CG-OD2	5.84	123.55	118.30
1	A	1818	ASP	CB-CG-OD2	5.76	123.48	118.30
2	G	5	ASP	CB-CG-OD2	5.67	123.40	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1778	ASP	CB-CG-OD2	5.54	123.28	118.30
1	C	1692	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	1778	ASP	CB-CG-OD2	5.40	123.16	118.30
1	E	1733	ASP	CB-CG-OD2	5.36	123.13	118.30
1	A	1739	ASP	CB-CG-OD2	5.36	123.12	118.30
1	E	1757	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	1813	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	1813	ASP	CB-CG-OD2	5.14	122.93	118.30
1	D	1778	ASP	CB-CG-OD2	5.13	122.92	118.30
1	E	1692	ASP	CB-CG-OD2	5.10	122.89	118.30
1	E	1778	ASP	CB-CG-OD2	5.09	122.89	118.30
1	B	1778	ASP	CB-CG-OD2	5.06	122.85	118.30
1	C	1813	ASP	CB-CG-OD2	5.05	122.84	118.30
2	I	5	ASP	CB-CG-OD2	5.03	122.83	118.30
1	E	1851	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	1817	GLU	Peptide

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	1601	0	1516	14	0
1	B	1605	0	1520	8	0
1	C	1532	0	1433	11	0
1	D	1523	0	1425	7	0
1	E	1620	0	1536	10	0
2	F	107	0	92	3	0
2	G	101	0	85	3	0
2	H	107	0	92	2	0
2	I	86	0	76	0	0
2	J	98	0	84	2	0
All	All	8380	0	7859	51	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 3.

All (51) 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:E:1777:THR:HG21	2:F:3:ALA:HB1	1.47	0.95
1:B:1751:ARG:NH1	1:B:1844:LEU:O	2.20	0.74
1:D:1691:THR:HG22	1:D:1697:CYS:HB3	1.71	0.70
1:A:1691:THR:HG22	1:A:1697:CYS:HB3	1.82	0.61
1:E:1691:THR:HG22	1:E:1697:CYS:HB3	1.84	0.60
1:C:1691:THR:HG22	1:C:1697:CYS:HB3	1.84	0.59
1:E:1777:THR:HG21	2:F:3:ALA:CB	2.28	0.59
1:B:1657:LEU:HD23	1:B:1690:LYS:HB2	1.85	0.58
1:E:1765:GLU:HG3	1:E:1790:SER:HB3	1.86	0.57
1:A:1760:ILE:HG13	1:A:1787:CYS:HB3	1.91	0.52
2:G:8:GLN:NE2	2:H:8:GLN:HE22	2.06	0.52
1:A:1651:SER:HB3	1:A:1684:THR:HA	1.91	0.52
1:D:1824:ILE:HD12	1:D:1832:VAL:HG11	1.93	0.50
1:E:1699:ARG:NH1	2:J:10:PHE:O	2.46	0.49
1:E:1761:PHE:HB3	1:E:1789:ALA:HB2	1.95	0.49
1:A:1814:ALA:HB1	2:J:6:ILE:HD11	1.95	0.48
1:A:1701:LEU:HD21	1:A:1779:GLN:HE21	1.79	0.48
1:C:1821:PHE:HA	1:C:1824:ILE:HD11	1.96	0.48
1:B:1846:GLN:O	1:B:1848:GLN:NE2	2.47	0.48
1:C:1742:ASN:HD21	1:C:1840:ASP:HA	1.77	0.48
2:G:6:ILE:HD13	2:G:6:ILE:HA	1.72	0.48
1:C:1824:ILE:H	1:C:1824:ILE:HG12	1.58	0.47
1:D:1813:ASP:OD1	1:D:1813:ASP:N	2.37	0.46
1:D:1678:ASN:OD1	1:D:1678:ASN:N	2.41	0.46
1:A:1795:LEU:HD11	1:A:1824:ILE:HG23	1.98	0.45
1:E:1747:GLN:HE21	1:E:1747:GLN:HB2	1.63	0.45
1:B:1699:ARG:HD2	1:B:1741:VAL:HB	1.98	0.45
1:D:1657:LEU:HD23	1:D:1690:LYS:HB2	1.98	0.45
1:A:1771:PRO:HD2	1:A:1815:TRP:CE2	2.53	0.44
1:A:1736:VAL:HG22	1:A:1749:PRO:HG2	1.98	0.44
1:C:1680:ILE:HD12	1:C:1702:LYS:HG2	1.99	0.44
1:D:1652:MET:HG2	1:D:1686:HIS:HB2	1.99	0.44
1:A:1855:ILE:HA	1:A:1856:PRO:HD2	1.88	0.44
1:A:1858:ILE:HA	1:A:1859:PRO:HD3	1.92	0.43
1:B:1650:MET:HB3	1:B:1674:ILE:HG23	2.00	0.43
1:A:1784:VAL:HG13	1:A:1789:ALA:HB3	1.99	0.43
1:E:1657:LEU:HD23	1:E:1690:LYS:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1746:HIS:O	1:B:1746:HIS:CG	2.73	0.42
1:C:1655:SER:HB2	1:C:1702:LYS:HD2	2.01	0.42
1:D:1851:ASP:HA	1:D:1854:LEU:HD12	2.02	0.42
1:E:1736:VAL:HG22	1:E:1749:PRO:HG2	2.02	0.42
1:A:1681:THR:OG1	1:A:1682:GLU:N	2.52	0.42
1:A:1699:ARG:NH1	2:F:10:PHE:O	2.53	0.42
1:C:1699:ARG:NH1	2:H:10:PHE:O	2.53	0.42
1:C:1651:SER:HB3	1:C:1684:THR:HA	2.03	0.41
1:B:1649:ARG:HG3	1:E:1746:HIS:HB3	2.02	0.41
1:A:1657:LEU:HD13	1:A:1661:GLU:HB3	2.03	0.41
1:C:1784:VAL:HG13	1:C:1789:ALA:HB3	2.01	0.41
1:C:1735:GLU:OE2	1:C:1753:ARG:NE	2.49	0.41
1:B:1655:SER:HA	2:G:7:SEP:O2P	2.21	0.40
1:C:1657:LEU:HD23	1:C:1690:LYS:HB2	2.03	0.40

There are no symmetry-related clashes.

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	204/214 (95%)	194 (95%)	9 (4%)	1 (0%)	29	61
1	B	206/214 (96%)	196 (95%)	9 (4%)	1 (0%)	29	61
1	C	196/214 (92%)	187 (95%)	8 (4%)	1 (0%)	29	61
1	D	199/214 (93%)	190 (96%)	8 (4%)	1 (0%)	29	61
1	E	209/214 (98%)	204 (98%)	5 (2%)	0	100	100
2	F	11/16 (69%)	10 (91%)	0	1 (9%)	1	4
2	G	11/16 (69%)	10 (91%)	1 (9%)	0	100	100
2	H	11/16 (69%)	10 (91%)	1 (9%)	0	100	100
2	I	8/16 (50%)	8 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	9/16 (56%)	8 (89%)	1 (11%)	0	100	100
All	All	1064/1150 (92%)	1017 (96%)	42 (4%)	5 (0%)	29	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1851	ASP
2	F	2	ALA
1	D	1802	THR
1	A	1748	GLY
1	B	1726	ARG

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	169/191 (88%)	144 (85%)	25 (15%)	3	13
1	B	168/191 (88%)	132 (79%)	36 (21%)	1	4
1	C	159/191 (83%)	124 (78%)	35 (22%)	1	3
1	D	154/191 (81%)	117 (76%)	37 (24%)	0	2
1	E	171/191 (90%)	141 (82%)	30 (18%)	2	8
2	F	8/11 (73%)	7 (88%)	1 (12%)	4	19
2	G	7/11 (64%)	6 (86%)	1 (14%)	3	15
2	H	8/11 (73%)	7 (88%)	1 (12%)	4	19
2	I	7/11 (64%)	6 (86%)	1 (14%)	3	15
2	J	8/11 (73%)	5 (62%)	3 (38%)	0	0
All	All	859/1010 (85%)	689 (80%)	170 (20%)	1	5

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1654	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1660	GLU
1	A	1663	MET
1	A	1664	LEU
1	A	1676	LEU
1	A	1677	THR
1	A	1681	THR
1	A	1694	GLU
1	A	1711	LYS
1	A	1714	VAL
1	A	1721	GLN
1	A	1723	ILE
1	A	1728	MET
1	A	1747	GLN
1	A	1777	THR
1	A	1784	VAL
1	A	1785	GLN
1	A	1786	LEU
1	A	1807	ILE
1	A	1817	GLU
1	A	1834	THR
1	A	1835	ARG
1	A	1848	GLN
1	A	1852	THR
1	A	1858	ILE
1	B	1649	ARG
1	B	1652	MET
1	B	1653	VAL
1	B	1660	GLU
1	B	1664	LEU
1	B	1667	LYS
1	B	1677	THR
1	B	1680	ILE
1	B	1682	GLU
1	B	1698	GLU
1	B	1711	LYS
1	B	1714	VAL
1	B	1721	GLN
1	B	1722	SER
1	B	1723	ILE
1	B	1736	VAL
1	B	1737	ARG
1	B	1740	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1753	ARG
1	B	1777	THR
1	B	1778	ASP
1	B	1784	VAL
1	B	1785	GLN
1	B	1786	LEU
1	B	1798	PHE
1	B	1799	THR
1	B	1810	VAL
1	B	1811	GLN
1	B	1824	ILE
1	B	1829	GLU
1	B	1835	ARG
1	B	1846	GLN
1	B	1848	GLN
1	B	1849	GLU
1	B	1854	LEU
1	B	1858	ILE
1	C	1653	VAL
1	C	1654	VAL
1	C	1658	THR
1	C	1660	GLU
1	C	1664	LEU
1	C	1676	LEU
1	C	1677	THR
1	C	1680	ILE
1	C	1681	THR
1	C	1690	LYS
1	C	1699	ARG
1	C	1711	LYS
1	C	1723	ILE
1	C	1728	MET
1	C	1732	HIS
1	C	1736	VAL
1	C	1740	VAL
1	C	1754	GLU
1	C	1755	SER
1	C	1783	MET
1	C	1785	GLN
1	C	1786	LEU
1	C	1790	SER
1	C	1798	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1824	ILE
1	C	1826	GLN
1	C	1828	CYS
1	C	1835	ARG
1	C	1836	GLU
1	C	1841	SER
1	C	1848	GLN
1	C	1852	THR
1	C	1854	LEU
1	C	1855	ILE
1	C	1858	ILE
1	D	1650	MET
1	D	1653	VAL
1	D	1654	VAL
1	D	1655	SER
1	D	1660	GLU
1	D	1663	MET
1	D	1664	LEU
1	D	1676	LEU
1	D	1677	THR
1	D	1679	LEU
1	D	1681	THR
1	D	1690	LYS
1	D	1699	ARG
1	D	1711	LYS
1	D	1714	VAL
1	D	1721	GLN
1	D	1723	ILE
1	D	1724	LYS
1	D	1728	MET
1	D	1730	ASN
1	D	1732	HIS
1	D	1736	VAL
1	D	1740	VAL
1	D	1765	GLU
1	D	1766	ILE
1	D	1778	ASP
1	D	1784	VAL
1	D	1785	GLN
1	D	1786	LEU
1	D	1790	SER
1	D	1798	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1799	THR
1	D	1813	ASP
1	D	1824	ILE
1	D	1835	ARG
1	D	1848	GLN
1	D	1850	LEU
1	E	1653	VAL
1	E	1654	VAL
1	E	1660	GLU
1	E	1664	LEU
1	E	1671	LYS
1	E	1681	THR
1	E	1699	ARG
1	E	1711	LYS
1	E	1714	VAL
1	E	1721	GLN
1	E	1722	SER
1	E	1723	ILE
1	E	1724	LYS
1	E	1728	MET
1	E	1731	GLU
1	E	1732	HIS
1	E	1736	VAL
1	E	1737	ARG
1	E	1740	VAL
1	E	1747	GLN
1	E	1757	ASP
1	E	1784	VAL
1	E	1786	LEU
1	E	1798	PHE
1	E	1802	THR
1	E	1821	PHE
1	E	1826	GLN
1	E	1835	ARG
1	E	1852	THR
1	E	1858	ILE
2	F	6	ILE
2	G	6	ILE
2	H	6	ILE
2	I	6	ILE
2	J	6	ILE
2	J	8	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	12	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1672	HIS
1	A	1721	GLN
1	A	1742	ASN
1	A	1779	GLN
1	A	1785	GLN
1	B	1721	GLN
1	B	1742	ASN
1	B	1746	HIS
1	B	1785	GLN
1	B	1826	GLN
1	C	1721	GLN
1	C	1742	ASN
1	C	1746	HIS
1	C	1848	GLN
1	D	1746	HIS
1	D	1848	GLN
1	E	1746	HIS
1	E	1747	GLN
1	E	1785	GLN
2	G	8	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	SEP	F	7	2	8,9,10	1.54	1 (12%)	7,12,14	1.68	1 (14%)
2	SEP	G	7	2	8,9,10	1.61	1 (12%)	7,12,14	1.53	1 (14%)
2	SEP	H	7	2	8,9,10	1.61	1 (12%)	7,12,14	2.05	1 (14%)
2	SEP	I	7	2	8,9,10	1.57	1 (12%)	7,12,14	1.48	2 (28%)
2	SEP	J	7	2	8,9,10	1.69	1 (12%)	7,12,14	1.64	1 (14%)

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	F	7	2	-	2/6/8/10	-
2	SEP	G	7	2	-	5/6/8/10	-
2	SEP	H	7	2	-	2/6/8/10	-
2	SEP	I	7	2	-	3/6/8/10	-
2	SEP	J	7	2	-	2/6/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	7	SEP	P-O1P	3.57	1.61	1.50
2	H	7	SEP	P-O1P	3.57	1.61	1.50
2	G	7	SEP	P-O1P	3.53	1.61	1.50
2	I	7	SEP	P-O1P	3.45	1.61	1.50
2	F	7	SEP	P-O1P	3.40	1.61	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	7	SEP	OG-CB-CA	5.00	113.01	108.14
2	F	7	SEP	OG-CB-CA	3.76	111.81	108.14
2	J	7	SEP	OG-CB-CA	3.55	111.60	108.14
2	G	7	SEP	OG-CB-CA	3.41	111.47	108.14
2	I	7	SEP	OG-CB-CA	2.87	110.94	108.14
2	I	7	SEP	OG-P-O1P	2.32	112.71	106.44

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	7	SEP	N-CA-CB-OG
2	F	7	SEP	C-CA-CB-OG
2	G	7	SEP	N-CA-CB-OG
2	G	7	SEP	C-CA-CB-OG
2	G	7	SEP	CB-OG-P-O1P
2	G	7	SEP	CB-OG-P-O2P
2	H	7	SEP	N-CA-CB-OG
2	H	7	SEP	C-CA-CB-OG
2	I	7	SEP	N-CA-CB-OG
2	I	7	SEP	C-CA-CB-OG
2	J	7	SEP	N-CA-CB-OG
2	J	7	SEP	C-CA-CB-OG
2	I	7	SEP	CB-OG-P-O2P
2	G	7	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	7	SEP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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 (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	208/214 (97%)	0.62	14 (6%)	17	17	69, 69, 69, 69	0
1	B	210/214 (98%)	0.76	22 (10%)	6	6	69, 69, 69, 69	0
1	C	202/214 (94%)	0.89	27 (13%)	3	3	69, 69, 69, 69	0
1	D	205/214 (95%)	0.98	25 (12%)	4	3	69, 69, 69, 69	0
1	E	211/214 (98%)	0.39	8 (3%)	40	37	69, 69, 69, 69	0
2	F	13/16 (81%)	0.59	1 (7%)	13	12	69, 69, 69, 69	0
2	G	13/16 (81%)	0.95	1 (7%)	13	12	69, 69, 69, 69	0
2	H	13/16 (81%)	0.60	0	100	100	69, 69, 69, 69	0
2	I	10/16 (62%)	0.83	1 (10%)	7	7	69, 69, 69, 69	0
2	J	11/16 (68%)	0.82	1 (9%)	9	9	69, 69, 69, 69	0
All	All	1096/1150 (95%)	0.73	100 (9%)	9	9	69, 69, 69, 69	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1824	ILE	6.3
1	B	1796	SER	5.8
1	D	1755	SER	5.3
1	D	1828	CYS	5.3
1	A	1806	PRO	5.3
1	D	1803	GLY	5.0
1	D	1802	THR	4.5
1	B	1795	LEU	4.5
2	G	14	LYS	4.2
1	A	1858	ILE	4.1
1	C	1791	VAL	4.1
1	A	1859	PRO	3.9
1	C	1765	GLU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1757	ASP	3.6
1	D	1647	ASN	3.5
1	C	1806	PRO	3.4
1	D	1757	ASP	3.3
1	C	1847	CYS	3.3
1	C	1826	GLN	3.2
1	C	1844	LEU	3.1
1	C	1859	PRO	3.1
1	D	1801	GLY	3.1
1	D	1855	ILE	3.1
1	A	1649	ARG	3.0
1	E	1859	PRO	3.0
1	D	1696	VAL	3.0
1	D	1856	PRO	2.9
1	C	1821	PHE	2.9
1	A	1773	THR	2.9
1	E	1818	ASP	2.9
1	C	1745	ASN	2.8
1	A	1755	SER	2.8
1	B	1805	HIS	2.8
1	C	1717	PHE	2.8
1	B	1790	SER	2.8
1	C	1827	MET	2.7
1	B	1826	GLN	2.7
1	C	1832	VAL	2.7
1	D	1837	TRP	2.7
1	C	1792	VAL	2.7
1	B	1830	ALA	2.7
1	C	1739	ASP	2.6
1	A	1721	GLN	2.6
1	C	1824	ILE	2.6
1	D	1769	TYR	2.6
1	D	1813	ASP	2.6
1	C	1790	SER	2.6
1	A	1804	VAL	2.6
1	C	1767	CYS	2.6
1	D	1823	ALA	2.6
1	B	1828	CYS	2.6
1	D	1812	PRO	2.6
1	D	1831	PRO	2.5
1	C	1823	ALA	2.5
2	F	1	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	1727	LYS	2.5
1	B	1798	PHE	2.5
1	E	1816	THR	2.5
1	B	1799	THR	2.4
1	E	1697	CYS	2.4
1	C	1851	ASP	2.4
1	B	1730	ASN	2.4
1	D	1810	VAL	2.4
1	B	1769	TYR	2.4
1	B	1816	THR	2.3
1	C	1686	HIS	2.3
1	C	1822	HIS	2.3
1	E	1802	THR	2.3
1	C	1707	ILE	2.3
1	D	1830	ALA	2.3
1	B	1859	PRO	2.3
1	D	1809	VAL	2.3
1	D	1814	ALA	2.3
1	A	1818	ASP	2.3
1	A	1837	TRP	2.3
1	D	1842	VAL	2.2
2	I	3	ALA	2.2
1	E	1828	CYS	2.2
1	C	1759	LYS	2.2
2	J	11	PRO	2.2
1	B	1791	VAL	2.2
1	B	1693	ALA	2.2
1	E	1825	GLY	2.2
1	B	1800	LEU	2.2
1	B	1804	VAL	2.2
1	E	1725	GLU	2.2
1	C	1799	THR	2.1
1	B	1825	GLY	2.1
1	A	1824	ILE	2.1
1	C	1831	PRO	2.1
1	A	1765	GLU	2.1
1	B	1664	LEU	2.1
1	D	1673	HIS	2.1
1	B	1806	PRO	2.1
1	B	1765	GLU	2.1
1	D	1766	ILE	2.1
1	A	1819	ASN	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1720	THR	2.0
1	B	1827	MET	2.0
1	C	1845	TYR	2.0

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	J	7	10/11	0.91	0.19	69,69,69,69	0
2	SEP	I	7	10/11	0.93	0.16	69,69,69,69	0
2	SEP	H	7	10/11	0.93	0.20	69,69,69,69	0
2	SEP	G	7	10/11	0.94	0.23	69,69,69,69	0
2	SEP	F	7	10/11	0.96	0.20	69,69,69,69	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.