wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 – 11:29 AM EDT

PDB ID	:	3COJ
Title	:	Crystal Structure of the BRCT Domains of Human BRCA1 in Complex with a Phosphorylated Peptide from Human Acetyl-CoA Carboxylase 1
Authors	:	Shen, Y.; Tong, L.
Deposited on	:	2008-03-28
Resolution	:	3.21 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

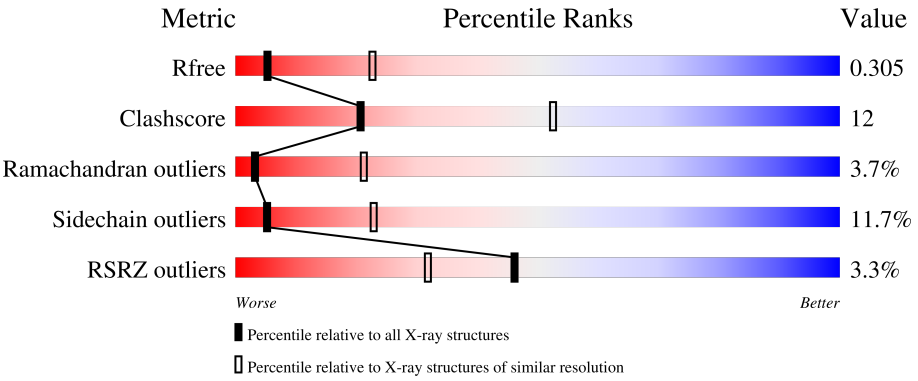
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.21 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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	235	.% 52% 31% 6% 11%
1	B	235	57% 23% 8% 11%
1	C	235	56% 26% 6% 11%
1	D	235	6% 58% 26% . 12%
1	E	235	2% 58% 26% . . 12%

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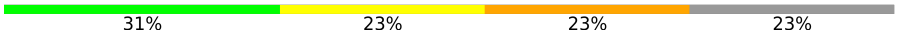
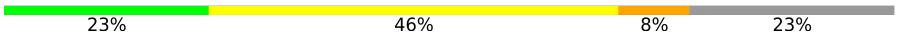
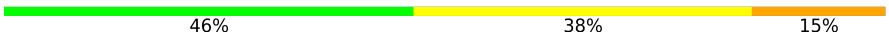
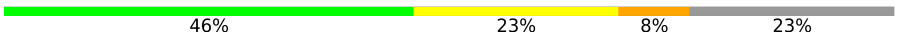
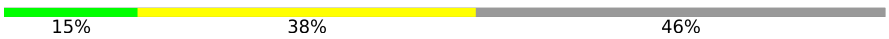
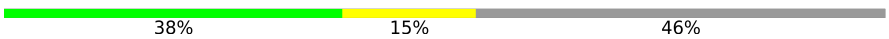
Mol	Chain	Length	Quality of chain
1	F	235	
1	G	235	
1	X	235	
2	H	13	
2	I	13	
2	J	13	
2	K	13	
2	L	13	
2	M	13	
2	N	13	
2	O	13	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13867 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	X	208	Total	C	N	O	S	0	0	0
			1670	1070	286	300	14			
1	A	208	Total	C	N	O	S	0	0	0
			1670	1070	286	300	14			
1	B	208	Total	C	N	O	S	0	0	0
			1670	1070	286	300	14			
1	C	208	Total	C	N	O	S	0	0	0
			1670	1070	286	300	14			
1	D	207	Total	C	N	O	S	0	0	0
			1661	1064	284	299	14			
1	E	207	Total	C	N	O	S	0	0	0
			1661	1064	284	299	14			
1	F	207	Total	C	N	O	S	0	0	0
			1654	1057	284	299	14			
1	G	206	Total	C	N	O	S	0	0	0
			1650	1055	283	298	14			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1625	MET	-	expression tag	UNP P38398
X	1626	GLY	-	expression tag	UNP P38398
X	1627	SER	-	expression tag	UNP P38398
X	1628	SER	-	expression tag	UNP P38398
X	1629	HIS	-	expression tag	UNP P38398
X	1630	HIS	-	expression tag	UNP P38398
X	1631	HIS	-	expression tag	UNP P38398
X	1632	HIS	-	expression tag	UNP P38398
X	1633	HIS	-	expression tag	UNP P38398
X	1634	HIS	-	expression tag	UNP P38398
X	1635	SER	-	expression tag	UNP P38398
X	1636	SER	-	expression tag	UNP P38398
X	1637	GLY	-	expression tag	UNP P38398

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Chain	Residue	Modelled	Actual	Comment	Reference
X	1638	LEU	-	expression tag	UNP P38398
X	1639	VAL	-	expression tag	UNP P38398
X	1640	PRO	-	expression tag	UNP P38398
X	1641	ARG	-	expression tag	UNP P38398
X	1642	GLY	-	expression tag	UNP P38398
X	1643	SER	-	expression tag	UNP P38398
X	1644	HIS	-	expression tag	UNP P38398
X	1645	MET	-	expression tag	UNP P38398
A	1625	MET	-	expression tag	UNP P38398
A	1626	GLY	-	expression tag	UNP P38398
A	1627	SER	-	expression tag	UNP P38398
A	1628	SER	-	expression tag	UNP P38398
A	1629	HIS	-	expression tag	UNP P38398
A	1630	HIS	-	expression tag	UNP P38398
A	1631	HIS	-	expression tag	UNP P38398
A	1632	HIS	-	expression tag	UNP P38398
A	1633	HIS	-	expression tag	UNP P38398
A	1634	HIS	-	expression tag	UNP P38398
A	1635	SER	-	expression tag	UNP P38398
A	1636	SER	-	expression tag	UNP P38398
A	1637	GLY	-	expression tag	UNP P38398
A	1638	LEU	-	expression tag	UNP P38398
A	1639	VAL	-	expression tag	UNP P38398
A	1640	PRO	-	expression tag	UNP P38398
A	1641	ARG	-	expression tag	UNP P38398
A	1642	GLY	-	expression tag	UNP P38398
A	1643	SER	-	expression tag	UNP P38398
A	1644	HIS	-	expression tag	UNP P38398
A	1645	MET	-	expression tag	UNP P38398
B	1625	MET	-	expression tag	UNP P38398
B	1626	GLY	-	expression tag	UNP P38398
B	1627	SER	-	expression tag	UNP P38398
B	1628	SER	-	expression tag	UNP P38398
B	1629	HIS	-	expression tag	UNP P38398
B	1630	HIS	-	expression tag	UNP P38398
B	1631	HIS	-	expression tag	UNP P38398
B	1632	HIS	-	expression tag	UNP P38398
B	1633	HIS	-	expression tag	UNP P38398
B	1634	HIS	-	expression tag	UNP P38398
B	1635	SER	-	expression tag	UNP P38398
B	1636	SER	-	expression tag	UNP P38398
B	1637	GLY	-	expression tag	UNP P38398

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1638	LEU	-	expression tag	UNP P38398
B	1639	VAL	-	expression tag	UNP P38398
B	1640	PRO	-	expression tag	UNP P38398
B	1641	ARG	-	expression tag	UNP P38398
B	1642	GLY	-	expression tag	UNP P38398
B	1643	SER	-	expression tag	UNP P38398
B	1644	HIS	-	expression tag	UNP P38398
B	1645	MET	-	expression tag	UNP P38398
C	1625	MET	-	expression tag	UNP P38398
C	1626	GLY	-	expression tag	UNP P38398
C	1627	SER	-	expression tag	UNP P38398
C	1628	SER	-	expression tag	UNP P38398
C	1629	HIS	-	expression tag	UNP P38398
C	1630	HIS	-	expression tag	UNP P38398
C	1631	HIS	-	expression tag	UNP P38398
C	1632	HIS	-	expression tag	UNP P38398
C	1633	HIS	-	expression tag	UNP P38398
C	1634	HIS	-	expression tag	UNP P38398
C	1635	SER	-	expression tag	UNP P38398
C	1636	SER	-	expression tag	UNP P38398
C	1637	GLY	-	expression tag	UNP P38398
C	1638	LEU	-	expression tag	UNP P38398
C	1639	VAL	-	expression tag	UNP P38398
C	1640	PRO	-	expression tag	UNP P38398
C	1641	ARG	-	expression tag	UNP P38398
C	1642	GLY	-	expression tag	UNP P38398
C	1643	SER	-	expression tag	UNP P38398
C	1644	HIS	-	expression tag	UNP P38398
C	1645	MET	-	expression tag	UNP P38398
D	1625	MET	-	expression tag	UNP P38398
D	1626	GLY	-	expression tag	UNP P38398
D	1627	SER	-	expression tag	UNP P38398
D	1628	SER	-	expression tag	UNP P38398
D	1629	HIS	-	expression tag	UNP P38398
D	1630	HIS	-	expression tag	UNP P38398
D	1631	HIS	-	expression tag	UNP P38398
D	1632	HIS	-	expression tag	UNP P38398
D	1633	HIS	-	expression tag	UNP P38398
D	1634	HIS	-	expression tag	UNP P38398
D	1635	SER	-	expression tag	UNP P38398
D	1636	SER	-	expression tag	UNP P38398
D	1637	GLY	-	expression tag	UNP P38398

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1638	LEU	-	expression tag	UNP P38398
D	1639	VAL	-	expression tag	UNP P38398
D	1640	PRO	-	expression tag	UNP P38398
D	1641	ARG	-	expression tag	UNP P38398
D	1642	GLY	-	expression tag	UNP P38398
D	1643	SER	-	expression tag	UNP P38398
D	1644	HIS	-	expression tag	UNP P38398
D	1645	MET	-	expression tag	UNP P38398
E	1625	MET	-	expression tag	UNP P38398
E	1626	GLY	-	expression tag	UNP P38398
E	1627	SER	-	expression tag	UNP P38398
E	1628	SER	-	expression tag	UNP P38398
E	1629	HIS	-	expression tag	UNP P38398
E	1630	HIS	-	expression tag	UNP P38398
E	1631	HIS	-	expression tag	UNP P38398
E	1632	HIS	-	expression tag	UNP P38398
E	1633	HIS	-	expression tag	UNP P38398
E	1634	HIS	-	expression tag	UNP P38398
E	1635	SER	-	expression tag	UNP P38398
E	1636	SER	-	expression tag	UNP P38398
E	1637	GLY	-	expression tag	UNP P38398
E	1638	LEU	-	expression tag	UNP P38398
E	1639	VAL	-	expression tag	UNP P38398
E	1640	PRO	-	expression tag	UNP P38398
E	1641	ARG	-	expression tag	UNP P38398
E	1642	GLY	-	expression tag	UNP P38398
E	1643	SER	-	expression tag	UNP P38398
E	1644	HIS	-	expression tag	UNP P38398
E	1645	MET	-	expression tag	UNP P38398
F	1625	MET	-	expression tag	UNP P38398
F	1626	GLY	-	expression tag	UNP P38398
F	1627	SER	-	expression tag	UNP P38398
F	1628	SER	-	expression tag	UNP P38398
F	1629	HIS	-	expression tag	UNP P38398
F	1630	HIS	-	expression tag	UNP P38398
F	1631	HIS	-	expression tag	UNP P38398
F	1632	HIS	-	expression tag	UNP P38398
F	1633	HIS	-	expression tag	UNP P38398
F	1634	HIS	-	expression tag	UNP P38398
F	1635	SER	-	expression tag	UNP P38398
F	1636	SER	-	expression tag	UNP P38398
F	1637	GLY	-	expression tag	UNP P38398

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1638	LEU	-	expression tag	UNP P38398
F	1639	VAL	-	expression tag	UNP P38398
F	1640	PRO	-	expression tag	UNP P38398
F	1641	ARG	-	expression tag	UNP P38398
F	1642	GLY	-	expression tag	UNP P38398
F	1643	SER	-	expression tag	UNP P38398
F	1644	HIS	-	expression tag	UNP P38398
F	1645	MET	-	expression tag	UNP P38398
G	1625	MET	-	expression tag	UNP P38398
G	1626	GLY	-	expression tag	UNP P38398
G	1627	SER	-	expression tag	UNP P38398
G	1628	SER	-	expression tag	UNP P38398
G	1629	HIS	-	expression tag	UNP P38398
G	1630	HIS	-	expression tag	UNP P38398
G	1631	HIS	-	expression tag	UNP P38398
G	1632	HIS	-	expression tag	UNP P38398
G	1633	HIS	-	expression tag	UNP P38398
G	1634	HIS	-	expression tag	UNP P38398
G	1635	SER	-	expression tag	UNP P38398
G	1636	SER	-	expression tag	UNP P38398
G	1637	GLY	-	expression tag	UNP P38398
G	1638	LEU	-	expression tag	UNP P38398
G	1639	VAL	-	expression tag	UNP P38398
G	1640	PRO	-	expression tag	UNP P38398
G	1641	ARG	-	expression tag	UNP P38398
G	1642	GLY	-	expression tag	UNP P38398
G	1643	SER	-	expression tag	UNP P38398
G	1644	HIS	-	expression tag	UNP P38398
G	1645	MET	-	expression tag	UNP P38398

- Molecule 2 is a protein called Acetyl-CoA carboxylase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	10	Total	C	N	O	P	0	0	0
			76	46	11	18	1			
2	I	10	Total	C	N	O	P	0	0	0
			76	46	11	18	1			
2	J	10	Total	C	N	O	P	0	0	0
			76	46	11	18	1			
2	K	13	Total	C	N	O	P	0	0	0
			97	58	14	24	1			
2	L	10	Total	C	N	O	P	0	0	0
			76	46	11	18	1			

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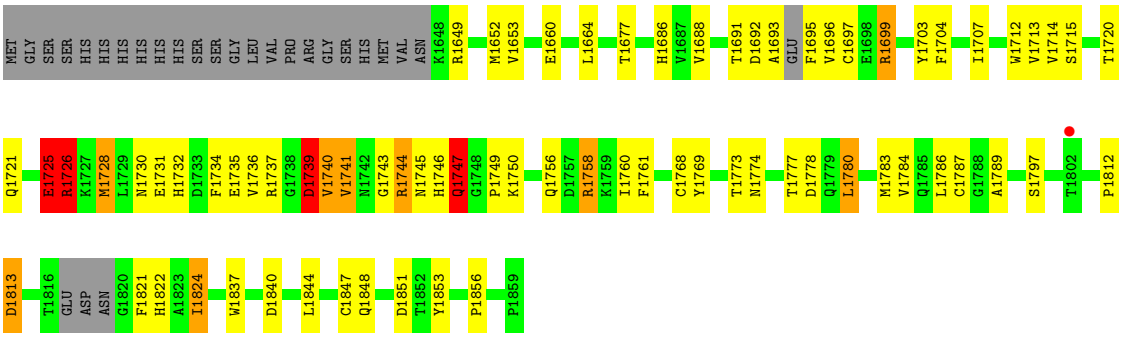
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	7	Total	C	N	O	P	0	0	0
			58	36	8	13	1			
2	N	5	Total	C	N	O	P	0	0	0
			44	26	6	11	1			
2	O	7	Total	C	N	O	P	0	0	0
			58	36	8	13	1			

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.

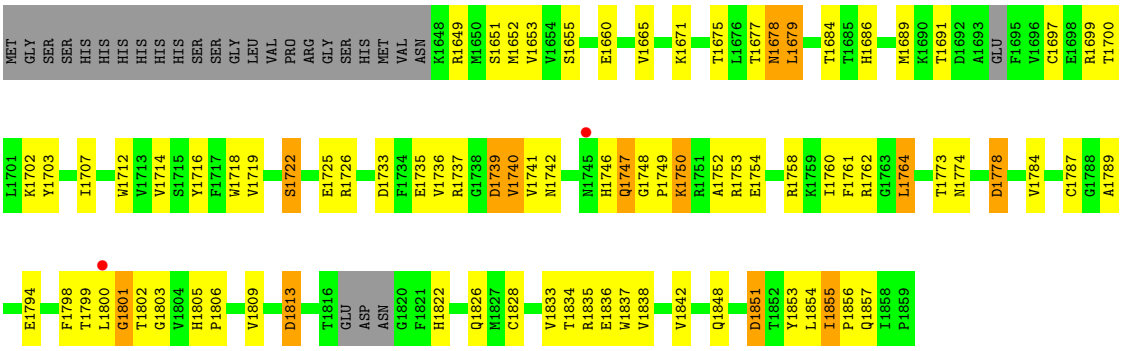
• Molecule 1: Breast cancer type 1 susceptibility protein

Chain X:



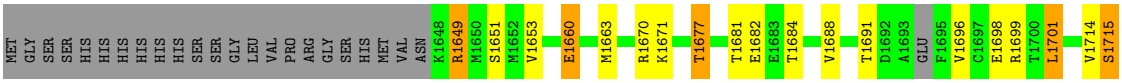
• Molecule 1: Breast cancer type 1 susceptibility protein

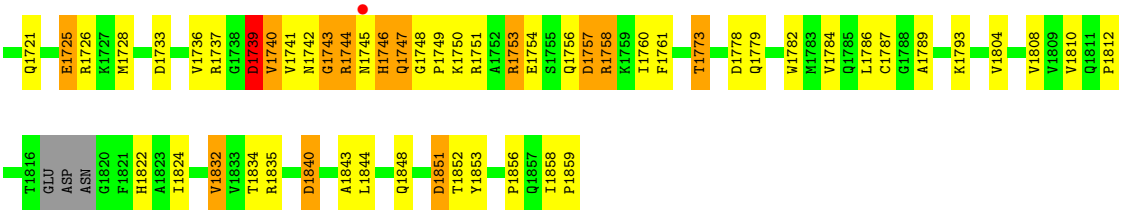
Chain A:



• Molecule 1: Breast cancer type 1 susceptibility protein

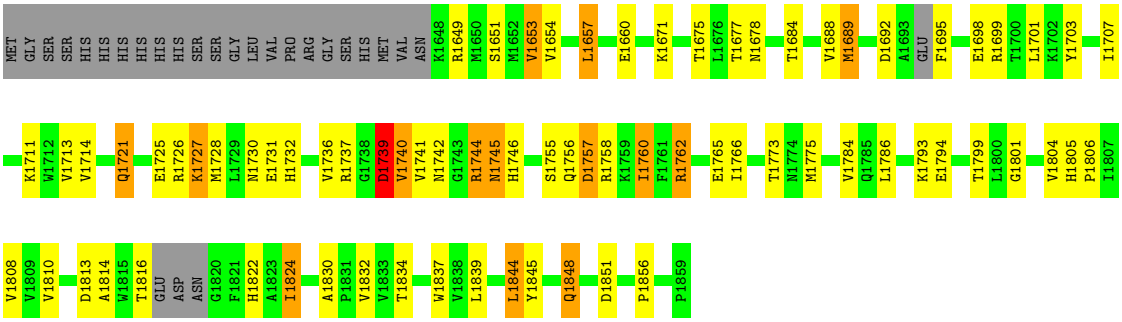
Chain B:





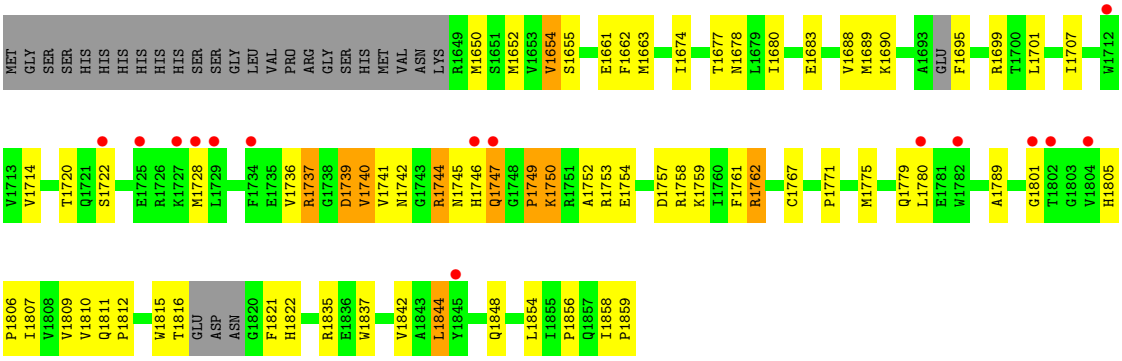
• Molecule 1: Breast cancer type 1 susceptibility protein

Chain C:



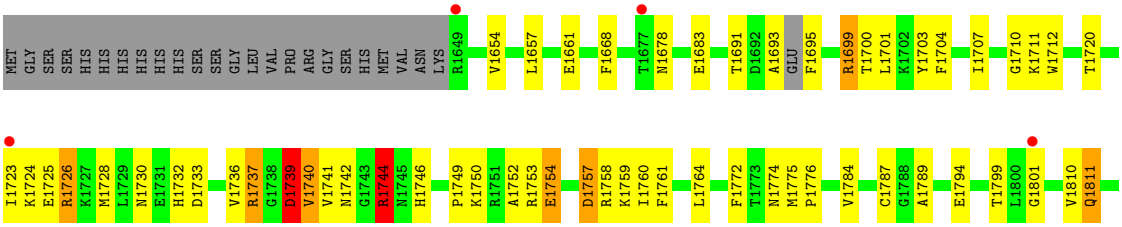
• Molecule 1: Breast cancer type 1 susceptibility protein

Chain D:

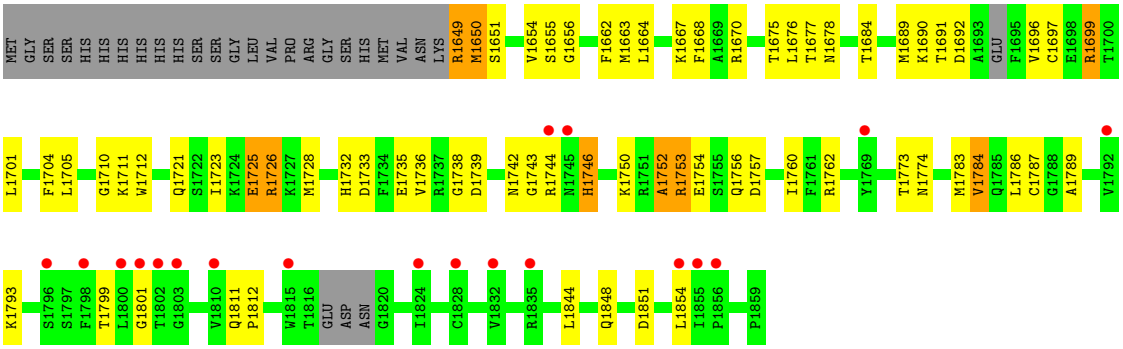


• Molecule 1: Breast cancer type 1 susceptibility protein

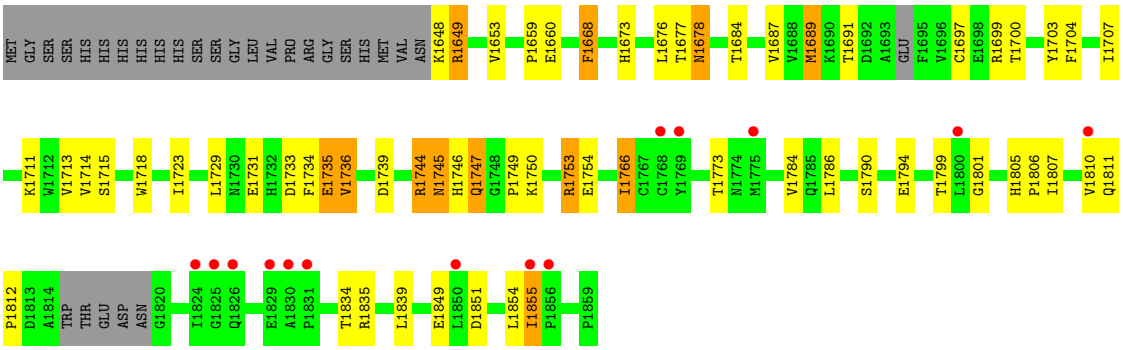
Chain E:



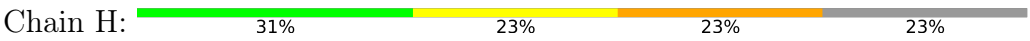
• Molecule 1: Breast cancer type 1 susceptibility protein



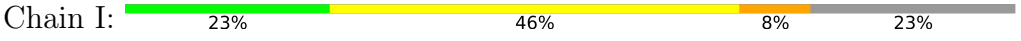
• Molecule 1: Breast cancer type 1 susceptibility protein



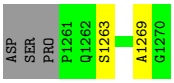
• Molecule 2: Acetyl-CoA carboxylase 1



• Molecule 2: Acetyl-CoA carboxylase 1



• Molecule 2: Acetyl-CoA carboxylase 1

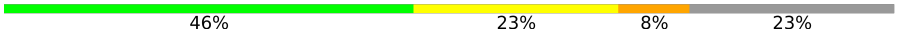


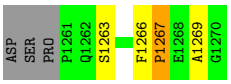
• Molecule 2: Acetyl-CoA carboxylase 1

Chain K:

• Molecule 2: Acetyl-CoA carboxylase 1

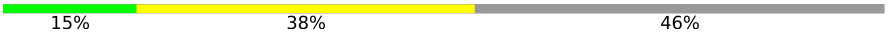
Chain L:





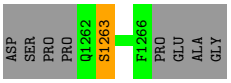
• Molecule 2: Acetyl-CoA carboxylase 1

Chain M:



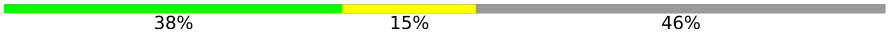
• Molecule 2: Acetyl-CoA carboxylase 1

Chain N:



• Molecule 2: Acetyl-CoA carboxylase 1

Chain O:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.33Å 181.51Å 194.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.89 – 3.21 29.89 – 3.21	Depositor EDS
% Data completeness (in resolution range)	91.6 (29.89-3.21) 75.1 (29.89-3.21)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 3.24Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.257 , 0.307 0.254 , 0.305	Depositor DCC
R_{free} test set	2249 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	84.8	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 92.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	13867	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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

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	0.42	0/1709	0.74	5/2314 (0.2%)
1	B	0.42	0/1709	0.74	5/2314 (0.2%)
1	C	0.40	0/1709	0.75	2/2314 (0.1%)
1	D	0.38	0/1700	0.68	1/2303 (0.0%)
1	E	0.37	0/1700	0.67	3/2303 (0.1%)
1	F	0.37	0/1692	0.69	3/2292 (0.1%)
1	G	0.37	0/1687	0.70	3/2281 (0.1%)
1	X	0.42	0/1709	0.75	5/2314 (0.2%)
2	H	0.44	0/68	0.77	0/90
2	I	0.57	0/68	0.80	0/90
2	J	0.44	0/68	0.65	0/90
2	K	0.49	0/90	0.91	1/122 (0.8%)
2	L	0.38	0/68	0.70	0/90
2	M	0.38	0/50	0.60	0/66
2	N	0.60	0/34	0.68	0/43
2	O	0.50	0/50	0.65	0/66
All	All	0.40	0/14111	0.72	28/19092 (0.1%)

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1840	ASP	CB-CG-OD2	6.40	124.06	118.30
1	X	1739	ASP	CB-CG-OD2	6.12	123.81	118.30
1	G	1733	ASP	CB-CG-OD2	6.11	123.80	118.30
1	E	1757	ASP	CB-CG-OD2	6.11	123.80	118.30
1	B	1739	ASP	CB-CG-OD2	5.92	123.63	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1670	0	1660	47	0
1	B	1670	0	1660	41	0
1	C	1670	0	1660	50	0
1	D	1661	0	1647	40	0
1	E	1661	0	1647	40	0
1	F	1654	0	1639	42	0
1	G	1650	0	1643	33	0
1	X	1670	0	1660	45	0
2	H	76	0	62	3	0
2	I	76	0	63	6	0
2	J	76	0	63	1	0
2	K	97	0	78	3	0
2	L	76	0	63	3	0
2	M	58	0	49	3	0
2	N	44	0	33	1	0
2	O	58	0	48	2	0
All	All	13867	0	13675	338	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 12.

The worst 5 of 338 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:B:1741:VAL:HG13	1:B:1742:ASN:H	1.20	1.05
1:B:1696:VAL:HG21	1:B:1744:ARG:HD2	1.46	0.93
1:C:1742:ASN:HB2	1:C:1746:HIS:HB2	1.47	0.93
1:C:1742:ASN:HB2	1:C:1746:HIS:CB	2.01	0.90
1:G:1766:ILE:HD11	1:G:1784:VAL:HG11	1.63	0.79

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	202/235 (86%)	176 (87%)	18 (9%)	8 (4%)	3 20
1	B	202/235 (86%)	169 (84%)	22 (11%)	11 (5%)	2 13
1	C	202/235 (86%)	178 (88%)	17 (8%)	7 (4%)	3 23
1	D	201/235 (86%)	179 (89%)	16 (8%)	6 (3%)	4 27
1	E	201/235 (86%)	186 (92%)	11 (6%)	4 (2%)	7 36
1	F	201/235 (86%)	174 (87%)	22 (11%)	5 (2%)	5 31
1	G	200/235 (85%)	172 (86%)	24 (12%)	4 (2%)	7 36
1	X	202/235 (86%)	164 (81%)	28 (14%)	10 (5%)	2 15
2	H	7/13 (54%)	4 (57%)	1 (14%)	2 (29%)	0 0
2	I	7/13 (54%)	4 (57%)	1 (14%)	2 (29%)	0 0
2	J	7/13 (54%)	4 (57%)	3 (43%)	0	100 100
2	K	10/13 (77%)	7 (70%)	2 (20%)	1 (10%)	0 3
2	L	7/13 (54%)	5 (71%)	0	2 (29%)	0 0
2	M	4/13 (31%)	3 (75%)	1 (25%)	0	100 100
2	N	2/13 (15%)	1 (50%)	1 (50%)	0	100 100
2	O	4/13 (31%)	4 (100%)	0	0	100 100
All	All	1659/1984 (84%)	1430 (86%)	167 (10%)	62 (4%)	3 21

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	1740	VAL
1	X	1824	ILE
1	A	1762	ARG
1	B	1745	ASN
1	B	1851	ASP

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	185/209 (88%)	164 (89%)	21 (11%)	5 24
1	B	185/209 (88%)	156 (84%)	29 (16%)	2 11
1	C	185/209 (88%)	162 (88%)	23 (12%)	4 20
1	D	184/209 (88%)	162 (88%)	22 (12%)	5 21
1	E	184/209 (88%)	160 (87%)	24 (13%)	4 18
1	F	183/209 (88%)	164 (90%)	19 (10%)	7 28
1	G	183/209 (88%)	162 (88%)	21 (12%)	5 23
1	X	185/209 (88%)	167 (90%)	18 (10%)	8 31
2	H	7/10 (70%)	6 (86%)	1 (14%)	3 14
2	I	7/10 (70%)	7 (100%)	0	100 100
2	J	7/10 (70%)	7 (100%)	0	100 100
2	K	10/10 (100%)	10 (100%)	0	100 100
2	L	7/10 (70%)	7 (100%)	0	100 100
2	M	6/10 (60%)	5 (83%)	1 (17%)	2 10
2	N	4/10 (40%)	4 (100%)	0	100 100
2	O	6/10 (60%)	6 (100%)	0	100 100
All	All	1528/1752 (87%)	1349 (88%)	179 (12%)	5 23

5 of 179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1683	GLU
1	F	1711	LYS
1	E	1728	MET
1	E	1794	GLU
1	F	1753	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1774	ASN
1	E	1848	GLN
1	D	1822	HIS
1	E	1746	HIS
1	F	1721	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)

8 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	O	1263	2	8,9,10	1.58	1 (12%)	8,12,14	1.55	2 (25%)
2	SEP	I	1263	2	8,9,10	1.47	1 (12%)	8,12,14	2.20	2 (25%)
2	SEP	L	1263	2	8,9,10	1.56	1 (12%)	8,12,14	1.21	2 (25%)
2	SEP	H	1263	2	8,9,10	1.55	1 (12%)	8,12,14	1.43	1 (12%)
2	SEP	M	1263	2	8,9,10	1.51	1 (12%)	8,12,14	1.63	2 (25%)
2	SEP	N	1263	2	8,9,10	1.56	1 (12%)	8,12,14	1.55	2 (25%)
2	SEP	K	1263	2	8,9,10	1.56	1 (12%)	8,12,14	1.77	2 (25%)
2	SEP	J	1263	2	8,9,10	1.45	1 (12%)	8,12,14	1.78	2 (25%)

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	O	1263	2	-	0/5/8/10	-
2	SEP	I	1263	2	-	1/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	L	1263	2	-	1/5/8/10	-
2	SEP	H	1263	2	-	1/5/8/10	-
2	SEP	M	1263	2	-	1/5/8/10	-
2	SEP	N	1263	2	-	1/5/8/10	-
2	SEP	K	1263	2	-	1/5/8/10	-
2	SEP	J	1263	2	-	1/5/8/10	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	1263	SEP	P-O1P	3.44	1.61	1.50
2	K	1263	SEP	P-O1P	3.42	1.61	1.50
2	H	1263	SEP	P-O1P	3.42	1.61	1.50
2	L	1263	SEP	P-O1P	3.41	1.61	1.50
2	N	1263	SEP	P-O1P	3.39	1.61	1.50

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1263	SEP	OG-CB-CA	4.46	112.49	108.14
2	K	1263	SEP	OG-CB-CA	3.88	111.92	108.14
2	I	1263	SEP	P-OG-CB	-3.65	108.23	118.30
2	J	1263	SEP	OG-CB-CA	3.44	111.50	108.14
2	M	1263	SEP	P-OG-CB	-3.22	109.41	118.30

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1263	SEP	N-CA-CB-OG
2	I	1263	SEP	N-CA-CB-OG
2	J	1263	SEP	N-CA-CB-OG
2	K	1263	SEP	N-CA-CB-OG
2	M	1263	SEP	N-CA-CB-OG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1263	SEP	1	0
2	N	1263	SEP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1263	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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	208/235 (88%)	0.10	2 (0%) 82 73	85, 88, 90, 92	0
1	B	208/235 (88%)	0.08	1 (0%) 91 86	84, 88, 90, 92	0
1	C	208/235 (88%)	0.02	0 100 100	84, 88, 90, 92	0
1	D	207/235 (88%)	0.33	15 (7%) 15 9	85, 88, 90, 92	0
1	E	207/235 (88%)	0.28	5 (2%) 59 45	85, 88, 90, 92	0
1	F	207/235 (88%)	0.41	19 (9%) 9 5	85, 88, 90, 92	0
1	G	206/235 (87%)	0.50	14 (6%) 17 10	83, 88, 90, 92	0
1	X	208/235 (88%)	0.04	1 (0%) 91 86	84, 88, 90, 92	0
2	H	9/13 (69%)	0.50	0 100 100	81, 84, 86, 86	0
2	I	9/13 (69%)	0.14	0 100 100	85, 86, 87, 87	0
2	J	9/13 (69%)	0.99	0 100 100	82, 83, 85, 85	0
2	K	12/13 (92%)	0.36	0 100 100	83, 85, 85, 86	0
2	L	9/13 (69%)	0.38	0 100 100	84, 85, 85, 86	0
2	M	6/13 (46%)	0.33	0 100 100	85, 85, 85, 86	0
2	N	4/13 (30%)	-0.15	0 100 100	85, 85, 85, 86	0
2	O	6/13 (46%)	0.44	0 100 100	85, 85, 86, 86	0
All	All	1723/1984 (86%)	0.23	57 (3%) 46 32	81, 88, 90, 92	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	1830	ALA	7.0
1	F	1803	GLY	5.4
1	G	1829	GLU	4.9
1	D	1802	THR	4.5
1	G	1768	CYS	4.4

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, 95^{th} 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	M	1263	10/11	0.74	0.25	84,84,85,85	0
2	SEP	J	1263	10/11	0.81	0.38	82,83,84,84	0
2	SEP	I	1263	10/11	0.87	0.26	83,84,85,85	0
2	SEP	L	1263	10/11	0.89	0.14	84,84,85,85	0
2	SEP	H	1263	10/11	0.90	0.27	83,84,85,85	0
2	SEP	O	1263	10/11	0.90	0.12	84,84,85,85	0
2	SEP	N	1263	10/11	0.93	0.16	84,84,85,85	0
2	SEP	K	1263	10/11	0.94	0.20	83,84,85,85	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.