Full wwPDB X-ray Structure Validation Report ⓘ

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 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:

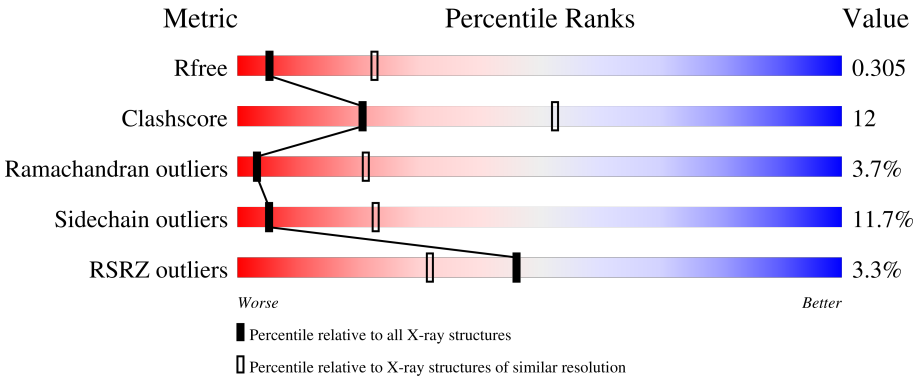
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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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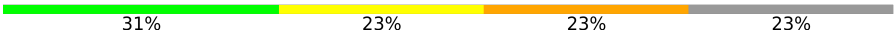
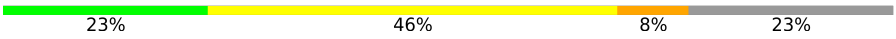
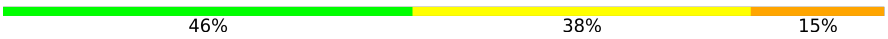
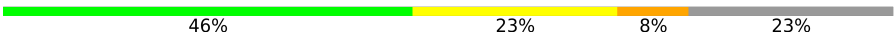
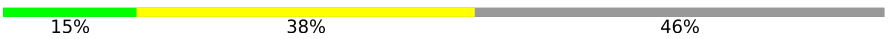
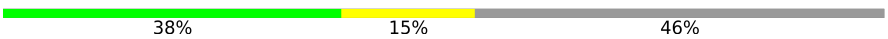
Mol	Chain	Length	Quality of chain
1	F	235	
1	G	235	
1	X	235	
2	H	13	
2	I	13	
2	J	13	
2	K	13	
2	L	13	
2	M	13	
2	N	13	
2	O	13	

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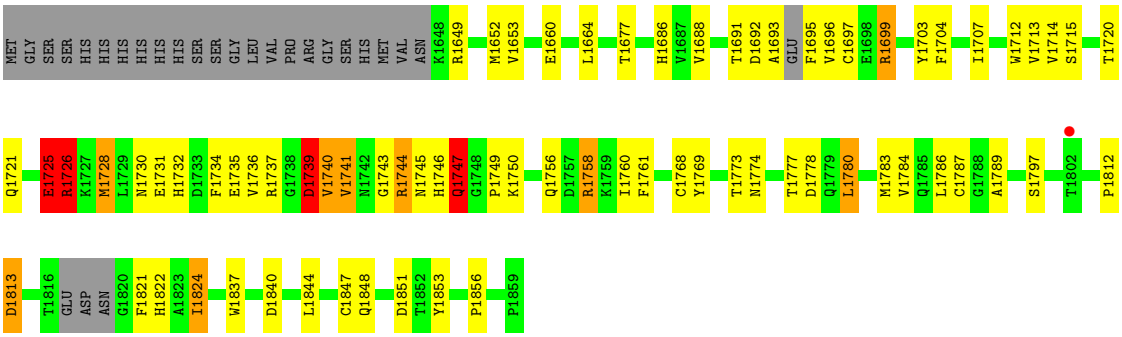
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	7	Total	C	N	O	P	0	0	0
			58	36	8	13	1			
2	N	5	Total	C	N	O	P	0	0	0
			44	26	6	11	1			
2	O	7	Total	C	N	O	P	0	0	0
			58	36	8	13	1			

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.

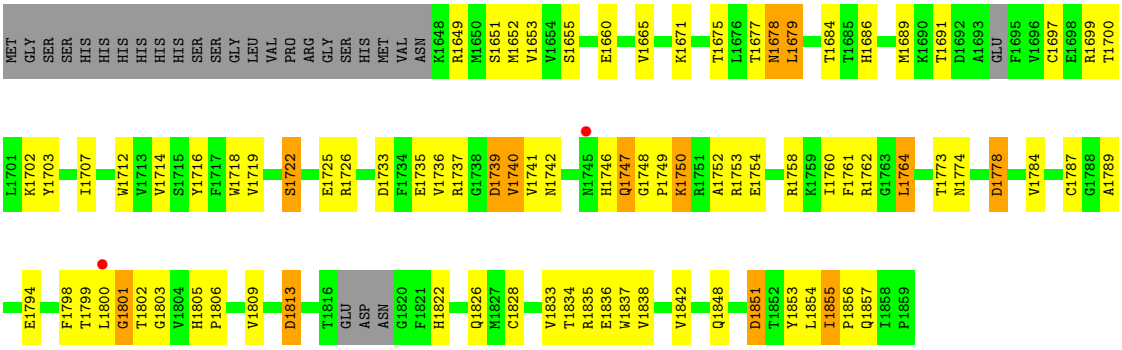
• Molecule 1: Breast cancer type 1 susceptibility protein

Chain X:



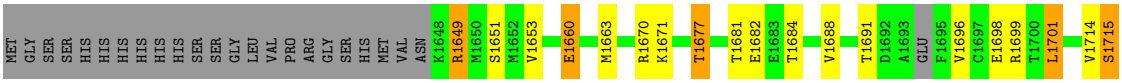
• Molecule 1: Breast cancer type 1 susceptibility protein

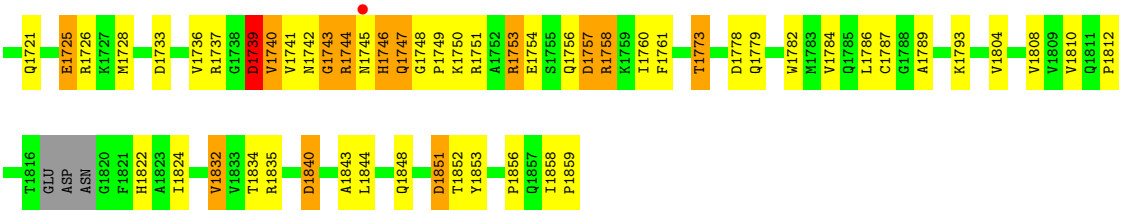
Chain A:



• Molecule 1: Breast cancer type 1 susceptibility protein

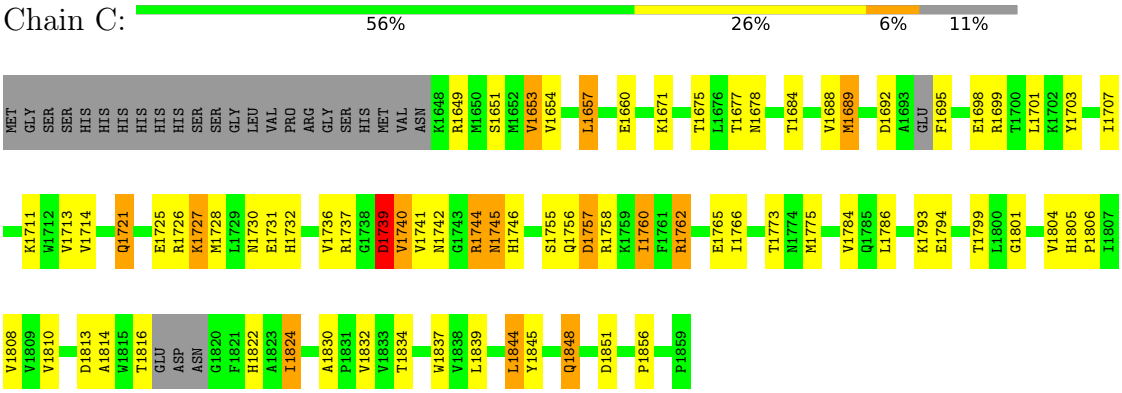
Chain B:





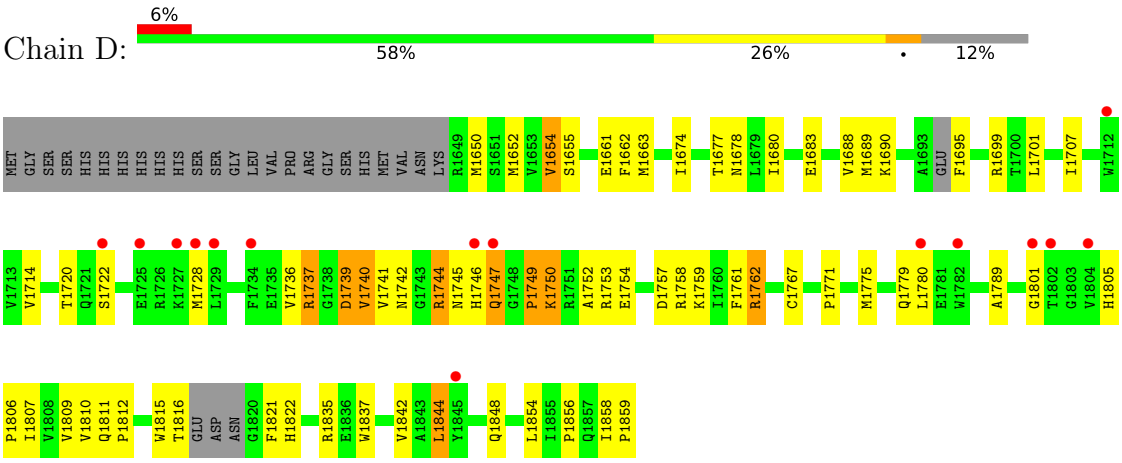
• Molecule 1: Breast cancer type 1 susceptibility protein

Chain C:



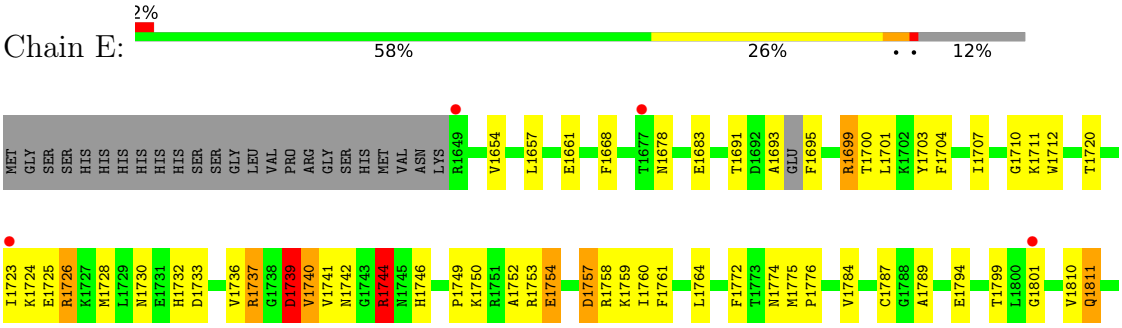
• Molecule 1: Breast cancer type 1 susceptibility protein

Chain D:

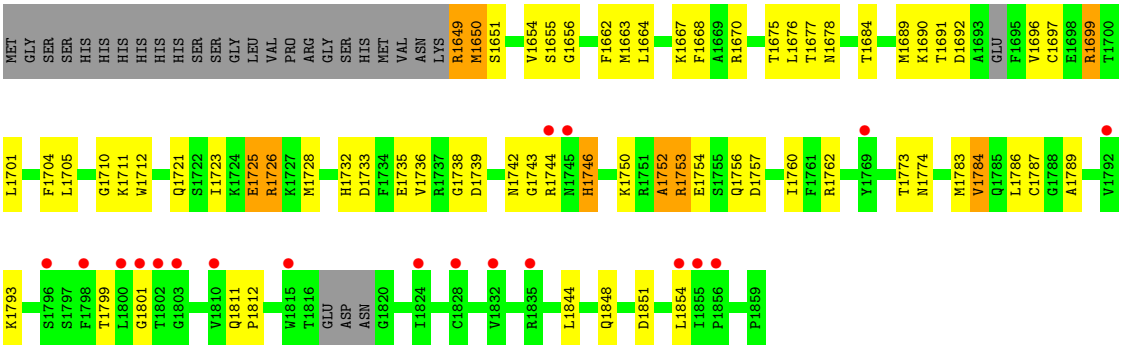


• Molecule 1: Breast cancer type 1 susceptibility protein

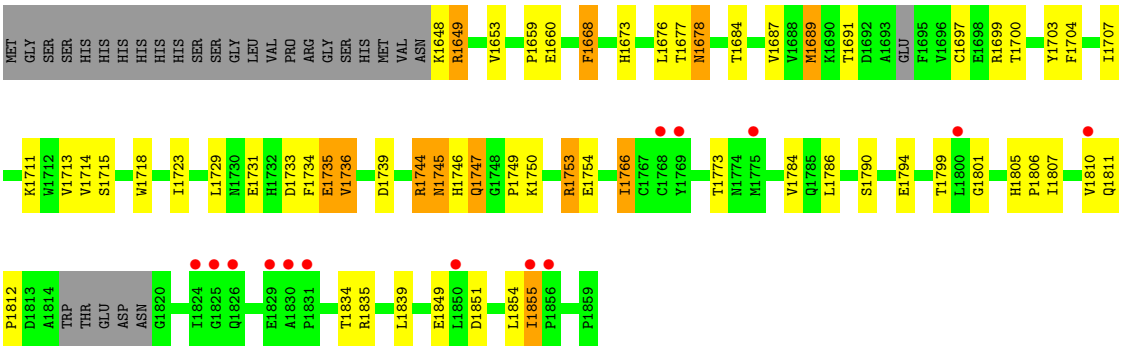
Chain E:



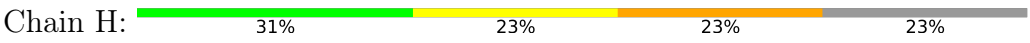
• Molecule 1: Breast cancer type 1 susceptibility protein



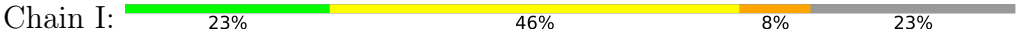
• Molecule 1: Breast cancer type 1 susceptibility protein



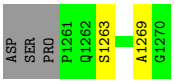
• Molecule 2: Acetyl-CoA carboxylase 1



• Molecule 2: Acetyl-CoA carboxylase 1



• Molecule 2: Acetyl-CoA carboxylase 1

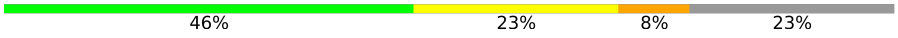


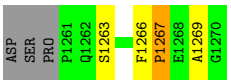
• Molecule 2: Acetyl-CoA carboxylase 1

Chain K:

• Molecule 2: Acetyl-CoA carboxylase 1

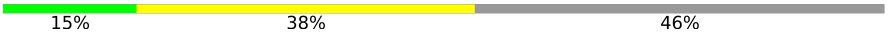
Chain L:





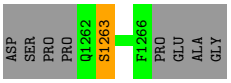
• Molecule 2: Acetyl-CoA carboxylase 1

Chain M:



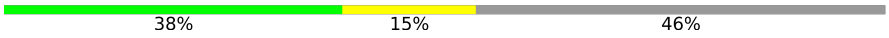
• Molecule 2: Acetyl-CoA carboxylase 1

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.

All (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
1	C	1757	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	1733	ASP	CB-CG-OD2	5.83	123.55	118.30
1	E	1851	ASP	CB-CG-OD2	5.81	123.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	1739	ASP	CB-CG-OD2	5.76	123.49	118.30
1	G	1851	ASP	CB-CG-OD2	5.75	123.48	118.30
1	F	1733	ASP	CB-CG-OD2	5.72	123.45	118.30
1	F	1851	ASP	CB-CG-OD2	5.64	123.37	118.30
1	C	1692	ASP	CB-CG-OD2	5.61	123.35	118.30
1	F	1757	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	1739	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	1733	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	1851	ASP	CB-CG-OD2	5.50	123.25	118.30
1	X	1813	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	1778	ASP	CB-CG-OD2	5.38	123.15	118.30
1	D	1739	ASP	CB-CG-OD2	5.37	123.14	118.30
1	X	1840	ASP	CB-CG-OD2	5.32	123.09	118.30
1	E	1739	ASP	CB-CG-OD2	5.31	123.08	118.30
2	K	1258	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	1778	ASP	CB-CG-OD2	5.21	122.99	118.30
1	X	1851	ASP	CB-CG-OD2	5.13	122.92	118.30
1	X	1778	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	1757	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	1813	ASP	CB-CG-OD2	5.07	122.86	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:D:1699:ARG:HH11	1:D:1741:VAL:HG22	1.48	0.79
1:B:1742:ASN:HB3	1:B:1844:LEU:CD2	2.13	0.78
1:G:1689:MET:HE1	1:G:1703:TYR:HB2	1.66	0.77
2:I:1266:PHE:HB3	2:I:1267:PRO:HD2	1.66	0.77
1:X:1784:VAL:HG13	1:X:1789:ALA:HB3	1.66	0.77
1:B:1741:VAL:HG13	1:B:1742:ASN:N	1.99	0.77
1:C:1714:VAL:HG21	1:C:1731:GLU:HB3	1.68	0.74
1:A:1655:SER:OG	1:A:1700:THR:HG21	1.88	0.74
1:E:1657:LEU:HD12	1:E:1661:GLU:HB3	1.70	0.73
1:B:1741:VAL:CG1	1:B:1742:ASN:H	1.99	0.73
1:D:1699:ARG:HH11	1:D:1741:VAL:CG2	2.03	0.72
1:G:1689:MET:CE	1:G:1703:TYR:HB2	2.19	0.72
1:X:1743:GLY:C	1:X:1745:ASN:H	1.94	0.71
1:B:1761:PHE:HB3	1:B:1789:ALA:HB2	1.70	0.71
1:B:1691:THR:OG1	1:B:1715:SER:HB2	1.91	0.71
1:A:1838:VAL:O	1:A:1842:VAL:HG23	1.91	0.70
1:B:1739:ASP:OD1	1:B:1741:VAL:HG12	1.92	0.70
1:C:1654:VAL:HG11	1:C:1657:LEU:HD11	1.74	0.69
1:D:1811:GLN:CD	1:D:1835:ARG:HH21	1.95	0.69
1:X:1736:VAL:HG13	1:X:1749:PRO:HG2	1.75	0.69
1:E:1750:LYS:O	1:E:1754:GLU:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1735:GLU:OE2	1:G:1753:ARG:NH2	2.27	0.68
1:C:1766:ILE:HD13	1:C:1784:VAL:HG21	1.76	0.68
1:F:1784:VAL:HG13	1:F:1789:ALA:HB3	1.75	0.68
1:E:1784:VAL:HG13	1:E:1789:ALA:HB3	1.76	0.67
1:D:1737:ARG:HB2	1:D:1744:ARG:O	1.95	0.67
1:E:1849:GLU:H	1:E:1849:GLU:CD	1.95	0.67
1:G:1714:VAL:HA	1:G:1735:GLU:HA	1.77	0.66
1:D:1699:ARG:CD	1:D:1741:VAL:HG23	2.27	0.65
1:B:1742:ASN:HB3	1:B:1844:LEU:HD22	1.79	0.64
1:B:1742:ASN:HB2	1:B:1746:HIS:HB2	1.80	0.64
1:F:1799:THR:HG22	1:F:1801:GLY:H	1.64	0.63
1:B:1739:ASP:O	1:B:1740:VAL:HG23	1.99	0.63
1:D:1695:PHE:HB2	1:D:1737:ARG:HG2	1.81	0.63
1:A:1857:GLN:H	1:F:1649:ARG:N	1.96	0.63
1:C:1742:ASN:HB2	1:C:1746:HIS:HB3	1.80	0.63
1:C:1766:ILE:HD13	1:C:1784:VAL:CG2	2.29	0.62
1:F:1756:GLN:HA	1:F:1756:GLN:OE1	1.99	0.62
1:B:1739:ASP:O	1:B:1740:VAL:CG2	2.47	0.62
1:G:1745:ASN:HD22	1:G:1746:HIS:H	1.46	0.61
1:E:1699:ARG:HE	1:E:1741:VAL:CG2	2.13	0.61
1:X:1731:GLU:CD	1:X:1731:GLU:H	2.03	0.61
1:A:1799:THR:HG22	1:A:1801:GLY:H	1.65	0.61
1:D:1699:ARG:HD3	1:D:1741:VAL:HG23	1.81	0.61
1:G:1653:VAL:HG23	1:G:1677:THR:HG23	1.83	0.61
1:X:1688:VAL:HA	1:X:1714:VAL:O	2.02	0.60
1:D:1699:ARG:NH1	1:D:1741:VAL:HG22	2.15	0.60
1:G:1648:LYS:O	1:G:1649:ARG:HB2	2.00	0.60
1:A:1718:TRP:O	1:A:1722:SER:HB2	2.02	0.60
1:E:1699:ARG:HD2	1:E:1704:PHE:CZ	2.36	0.60
1:F:1692:ASP:HB2	1:F:1696:VAL:H	1.67	0.60
1:C:1684:THR:O	1:C:1711:LYS:HD3	2.01	0.59
1:F:1760:ILE:HG12	1:F:1787:CYS:HB3	1.84	0.59
1:C:1699:ARG:HH21	1:C:1839:LEU:HB3	1.67	0.59
1:B:1682:GLU:HG3	1:B:1782:TRP:HZ2	1.68	0.59
1:F:1678:ASN:OD1	1:G:1676:LEU:HB3	2.03	0.59
1:D:1742:ASN:HD22	1:D:1844:LEU:HD23	1.67	0.58
1:X:1696:VAL:CG2	1:X:1744:ARG:HB3	2.33	0.58
1:G:1766:ILE:HG22	1:G:1807:ILE:HB	1.84	0.58
1:A:1735:GLU:CD	1:A:1753:ARG:HH21	2.06	0.58
1:A:1700:THR:HG22	1:A:1702:LYS:H	1.69	0.57
1:E:1799:THR:HG22	1:E:1801:GLY:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1707:ILE:HG23	1:D:1752:ALA:HB2	1.85	0.57
1:C:1727:LYS:HD3	1:C:1728:MET:H	1.69	0.57
1:D:1650:MET:SD	1:D:1674:ILE:HG21	2.44	0.57
1:C:1713:VAL:O	1:C:1736:VAL:HG12	2.04	0.57
1:G:1691:THR:HG22	1:G:1697:CYS:HB3	1.86	0.57
1:C:1742:ASN:CB	1:C:1746:HIS:HB3	2.34	0.57
1:E:1742:ASN:HD22	1:E:1746:HIS:HD2	1.53	0.56
1:X:1713:VAL:O	1:X:1736:VAL:HG12	2.04	0.56
1:E:1725:GLU:O	1:E:1726:ARG:HB2	2.06	0.56
1:G:1799:THR:HG22	1:G:1801:GLY:H	1.70	0.56
1:A:1712:TRP:HB3	1:A:1714:VAL:HG23	1.87	0.56
1:F:1654:VAL:HG21	1:F:1662:PHE:HD1	1.70	0.56
1:A:1750:LYS:HD3	1:A:1754:GLU:OE2	2.06	0.56
1:E:1849:GLU:CD	1:E:1849:GLU:N	2.59	0.56
1:C:1742:ASN:HB3	1:C:1844:LEU:HD23	1.88	0.56
1:C:1727:LYS:HD3	1:C:1728:MET:N	2.20	0.56
1:E:1668:PHE:HB2	1:E:1723:ILE:HD11	1.88	0.56
1:F:1670:ARG:HG2	2:O:1261:PRO:HB3	1.88	0.55
1:X:1784:VAL:HG13	1:X:1789:ALA:CB	2.36	0.55
1:X:1691:THR:HA	1:X:1696:VAL:O	2.07	0.55
1:A:1747:GLN:NE2	1:A:1750:LYS:HE2	2.22	0.55
1:A:1651:SER:HA	1:A:1675:THR:HB	1.88	0.55
1:B:1651:SER:HB2	1:B:1684:THR:HA	1.89	0.55
1:E:1736:VAL:HG13	1:E:1749:PRO:HG2	1.89	0.55
1:A:1652:MET:HB3	1:A:1686:HIS:HB2	1.87	0.55
1:C:1730:ASN:ND2	1:C:1732:HIS:HB2	2.21	0.55
1:C:1806:PRO:HB2	1:C:1830:ALA:HB2	1.88	0.54
1:C:1758:ARG:NE	1:C:1762:ARG:HH21	2.05	0.54
1:A:1691:THR:HG21	1:A:1736:VAL:HG12	1.89	0.54
1:C:1651:SER:HA	1:C:1675:THR:HB	1.89	0.54
1:X:1730:ASN:HB2	1:D:1821:PHE:HE2	1.72	0.54
1:X:1760:ILE:HB	1:X:1847:CYS:HB2	1.90	0.53
1:F:1844:LEU:HD12	1:F:1848:GLN:HE22	1.72	0.53
1:B:1750:LYS:HG2	1:B:1753:ARG:HH21	1.73	0.53
1:X:1704:PHE:HB3	1:X:1783:MET:SD	2.49	0.53
1:F:1663:MET:HE1	1:G:1659:PRO:O	2.08	0.53
1:G:1766:ILE:HA	1:G:1807:ILE:O	2.09	0.53
1:E:1822:HIS:HB3	1:E:1858:ILE:HG13	1.90	0.53
1:C:1799:THR:HG22	1:C:1801:GLY:H	1.73	0.53
1:F:1750:LYS:HG2	1:F:1753:ARG:HH12	1.73	0.53
1:A:1653:VAL:HG23	1:A:1677:THR:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1747:GLN:HE22	1:A:1750:LYS:HE2	1.73	0.53
1:A:1813:ASP:HB3	1:F:1732:HIS:CD2	2.44	0.53
1:D:1761:PHE:HB3	1:D:1789:ALA:HB2	1.91	0.53
1:F:1655:SER:HB3	1:F:1689:MET:SD	2.49	0.53
1:C:1742:ASN:CB	1:C:1746:HIS:CB	2.82	0.53
1:D:1736:VAL:HG13	1:D:1749:PRO:HG2	1.91	0.53
1:F:1667:LYS:HG3	2:O:1261:PRO:HG3	1.91	0.52
1:D:1771:PRO:HD2	1:D:1815:TRP:NE1	2.24	0.52
1:E:1693:ALA:O	1:E:1695:PHE:N	2.42	0.52
1:A:1678:ASN:HD22	1:A:1679:LEU:N	2.08	0.52
1:C:1742:ASN:HB3	1:C:1844:LEU:CD2	2.40	0.51
1:E:1699:ARG:HH21	1:E:1741:VAL:HG22	1.75	0.51
1:F:1742:ASN:ND2	1:F:1746:HIS:O	2.43	0.51
1:F:1844:LEU:HD12	1:F:1848:GLN:NE2	2.25	0.51
1:C:1695:PHE:O	1:C:1736:VAL:HG23	2.11	0.51
1:E:1699:ARG:HE	1:E:1741:VAL:HG23	1.74	0.51
1:F:1651:SER:HA	1:F:1675:THR:O	2.09	0.51
1:D:1699:ARG:HH21	2:L:1266:PHE:HB3	1.74	0.51
1:E:1742:ASN:HB2	1:E:1746:HIS:HB3	1.93	0.51
1:E:1759:LYS:HB3	1:E:1787:CYS:O	2.09	0.51
1:X:1741:VAL:HG12	1:X:1844:LEU:HD21	1.92	0.51
1:A:1856:PRO:CB	1:F:1650:MET:HB3	2.40	0.51
1:C:1713:VAL:HG12	1:C:1736:VAL:HG11	1.92	0.51
1:G:1714:VAL:HG21	1:G:1731:GLU:HB3	1.92	0.51
1:D:1699:ARG:HD2	1:D:1741:VAL:HG23	1.93	0.51
1:A:1725:GLU:O	1:A:1726:ARG:HB2	2.11	0.50
1:F:1704:PHE:HB3	1:F:1783:MET:SD	2.52	0.50
1:X:1768:CYS:SG	1:X:1780:LEU:HG	2.51	0.50
1:D:1701:LEU:HD13	1:D:1775:MET:HG3	1.94	0.50
1:E:1761:PHE:HB3	1:E:1789:ALA:HB2	1.94	0.50
1:A:1689:MET:O	1:A:1716:TYR:N	2.45	0.50
1:C:1699:ARG:HD2	1:C:1741:VAL:HG23	1.93	0.50
1:X:1699:ARG:NE	1:X:1741:VAL:HG23	2.26	0.50
1:F:1664:LEU:HD22	1:F:1723:ILE:HD13	1.92	0.50
1:C:1737:ARG:HB3	1:C:1745:ASN:HA	1.93	0.50
1:E:1707:ILE:HG23	1:E:1752:ALA:HB2	1.93	0.50
1:C:1701:LEU:HD13	1:C:1775:MET:HG3	1.93	0.50
2:K:1268:GLU:CD	2:K:1269:ALA:H	2.15	0.50
1:B:1784:VAL:HG13	1:B:1789:ALA:HB3	1.94	0.49
1:D:1688:VAL:HA	1:D:1714:VAL:O	2.12	0.49
1:C:1824:ILE:HB	1:C:1832:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1772:PHE:HD2	1:E:1811:GLN:HB2	1.77	0.49
1:E:1772:PHE:CD2	1:E:1811:GLN:HB2	2.48	0.49
1:F:1754:GLU:HB3	2:I:1268:GLU:CG	2.42	0.49
1:X:1761:PHE:HB2	1:X:1789:ALA:HB2	1.95	0.49
1:B:1834:THR:HG22	1:B:1853:TYR:HB3	1.95	0.49
1:E:1737:ARG:HB2	1:E:1744:ARG:O	2.13	0.49
1:F:1760:ILE:CG1	1:F:1787:CYS:HB3	2.42	0.49
1:A:1742:ASN:HB2	1:A:1746:HIS:HB2	1.95	0.49
1:G:1653:VAL:O	1:G:1687:VAL:HA	2.13	0.49
1:F:1691:THR:HG22	1:F:1697:CYS:HB3	1.94	0.48
1:B:1808:VAL:HG11	1:B:1824:ILE:HG21	1.94	0.48
1:C:1688:VAL:HA	1:C:1714:VAL:O	2.13	0.48
1:E:1699:ARG:HB3	2:M:1266:PHE:HB2	1.94	0.48
1:E:1720:THR:O	1:E:1724:LYS:HB2	2.13	0.48
1:E:1761:PHE:CD1	1:E:1787:CYS:HB2	2.48	0.48
1:D:1654:VAL:HG11	1:D:1662:PHE:HD1	1.78	0.48
1:D:1722:SER:OG	1:D:1728:MET:HA	2.13	0.48
1:X:1837:TRP:HB2	1:X:1853:TYR:CG	2.49	0.48
1:A:1697:CYS:SG	1:A:1703:TYR:CE1	3.05	0.48
1:D:1699:ARG:HD2	1:D:1741:VAL:CG2	2.44	0.48
1:X:1653:VAL:HG23	1:X:1677:THR:O	2.13	0.48
1:B:1688:VAL:HA	1:B:1714:VAL:O	2.14	0.48
1:C:1755:SER:OG	2:J:1269:ALA:HB1	2.14	0.48
1:E:1760:ILE:HG13	1:E:1787:CYS:HB3	1.95	0.48
1:X:1714:VAL:HA	1:X:1735:GLU:HA	1.94	0.48
1:X:1712:TRP:CZ2	1:X:1732:HIS:CE1	3.02	0.48
1:X:1736:VAL:HG22	1:X:1737:ARG:N	2.28	0.48
1:X:1692:ASP:O	1:X:1693:ALA:HB3	2.14	0.47
1:E:1761:PHE:CB	1:E:1789:ALA:HB2	2.44	0.47
1:X:1703:TYR:CE1	1:X:1707:ILE:HD11	2.49	0.47
1:X:1824:ILE:HD13	1:X:1824:ILE:H	1.79	0.47
1:C:1822:HIS:HD2	1:C:1856:PRO:O	1.97	0.47
1:C:1742:ASN:HD22	1:C:1844:LEU:HD23	1.78	0.47
1:E:1772:PHE:HB3	1:E:1835:ARG:HH21	1.78	0.47
1:X:1699:ARG:HD2	1:X:1739:ASP:OD1	2.15	0.47
1:A:1699:ARG:O	2:I:1265:THR:HA	2.15	0.47
1:D:1807:ILE:HD13	1:D:1837:TRP:CH2	2.49	0.47
1:B:1822:HIS:HD2	1:B:1856:PRO:O	1.97	0.47
1:F:1710:GLY:HA2	1:F:1752:ALA:HB1	1.95	0.47
1:G:1747:GLN:HB3	1:G:1750:LYS:HB3	1.97	0.47
1:A:1699:ARG:HD2	1:A:1741:VAL:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1808:VAL:HG11	1:C:1824:ILE:HG21	1.96	0.47
1:C:1745:ASN:C	1:C:1745:ASN:HD22	2.19	0.47
1:X:1739:ASP:O	1:X:1740:VAL:HB	2.14	0.46
1:B:1696:VAL:HG21	1:B:1744:ARG:CD	2.32	0.46
1:C:1824:ILE:HG13	1:C:1832:VAL:HG11	1.98	0.46
1:A:1856:PRO:HB2	1:F:1650:MET:HB3	1.97	0.46
1:F:1699:ARG:HG2	1:F:1704:PHE:CZ	2.50	0.46
1:A:1822:HIS:HD2	1:A:1856:PRO:O	1.99	0.46
1:B:1701:LEU:HD21	1:B:1779:GLN:HE21	1.79	0.46
1:B:1728:MET:O	1:B:1728:MET:HG3	2.15	0.46
1:C:1760:ILE:HG21	1:C:1845:TYR:O	2.15	0.46
1:X:1756:GLN:C	1:X:1758:ARG:H	2.19	0.46
1:C:1810:VAL:O	1:C:1834:THR:HA	2.16	0.46
1:G:1713:VAL:HB	1:G:1749:PRO:HB3	1.97	0.46
1:D:1812:PRO:HB3	1:D:1821:PHE:CE1	2.51	0.46
1:B:1742:ASN:O	1:B:1743:GLY:C	2.55	0.45
1:F:1750:LYS:HA	1:F:1753:ARG:NH1	2.31	0.45
1:G:1805:HIS:HA	1:G:1806:PRO:HD3	1.81	0.45
1:F:1705:LEU:HD23	1:F:1783:MET:HG3	1.96	0.45
1:B:1840:ASP:O	1:B:1844:LEU:HG	2.17	0.45
1:C:1689:MET:HE1	1:C:1703:TYR:HB2	1.98	0.45
1:X:1697:CYS:SG	1:X:1736:VAL:HG21	2.56	0.45
1:D:1652:MET:O	1:D:1677:THR:HG22	2.16	0.45
1:F:1696:VAL:HG13	1:F:1738:GLY:O	2.17	0.45
1:D:1858:ILE:HA	1:D:1859:PRO:HD3	1.86	0.45
1:X:1697:CYS:O	1:X:1739:ASP:HA	2.17	0.45
1:X:1728:MET:HE3	1:X:1728:MET:HB3	1.68	0.45
1:X:1736:VAL:CG2	1:X:1737:ARG:N	2.79	0.45
1:X:1769:TYR:CE2	1:X:1824:ILE:HD12	2.51	0.45
1:X:1822:HIS:CD2	1:X:1856:PRO:O	2.70	0.45
1:A:1784:VAL:CG1	1:A:1789:ALA:HB3	2.47	0.45
1:X:1743:GLY:O	1:X:1745:ASN:N	2.50	0.45
1:C:1765:GLU:HB2	1:C:1804:VAL:HG22	1.99	0.45
1:F:1656:GLY:N	2:N:1263:SEP:O2P	2.50	0.44
1:G:1653:VAL:HB	1:G:1684:THR:HG21	1.98	0.44
1:C:1653:VAL:HG23	1:C:1677:THR:O	2.17	0.44
1:C:1813:ASP:O	1:C:1814:ALA:HB3	2.18	0.44
1:A:1760:ILE:HG13	1:A:1787:CYS:HB3	1.98	0.44
1:A:1805:HIS:HA	1:A:1806:PRO:HD3	1.73	0.44
1:E:1691:THR:HB	1:E:1695:PHE:HA	1.98	0.44
1:F:1668:PHE:HZ	1:F:1728:MET:HG3	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1741:VAL:CG1	1:B:1742:ASN:N	2.67	0.44
1:D:1742:ASN:CG	1:D:1746:HIS:NE2	2.71	0.44
1:G:1715:SER:HB3	1:G:1734:PHE:O	2.17	0.44
1:A:1678:ASN:ND2	1:A:1679:LEU:N	2.66	0.44
1:E:1710:GLY:O	1:E:1753:ARG:HB3	2.18	0.44
2:I:1266:PHE:HB3	2:I:1267:PRO:CD	2.40	0.44
1:F:1690:LYS:O	1:F:1697:CYS:HB2	2.18	0.44
1:G:1810:VAL:O	1:G:1834:THR:HA	2.18	0.44
1:X:1760:ILE:HG12	1:X:1787:CYS:HB3	2.00	0.44
1:A:1784:VAL:HG13	1:A:1789:ALA:HB3	1.99	0.44
1:X:1652:MET:HB3	1:X:1686:HIS:HB2	2.00	0.44
2:I:1268:GLU:O	2:I:1270:GLY:N	2.47	0.43
1:A:1855:ILE:HG23	1:A:1857:GLN:NE2	2.33	0.43
1:B:1748:GLY:H	1:B:1749:PRO:HD2	1.83	0.43
1:D:1810:VAL:O	1:D:1812:PRO:HD3	2.18	0.43
1:X:1743:GLY:C	1:X:1745:ASN:N	2.61	0.43
1:A:1754:GLU:HB3	2:H:1268:GLU:HB3	1.99	0.43
1:D:1750:LYS:O	1:D:1754:GLU:HB2	2.18	0.43
1:E:1826:GLN:NE2	1:E:1859:PRO:O	2.50	0.43
1:B:1810:VAL:O	1:B:1812:PRO:HD3	2.18	0.43
1:E:1742:ASN:HD22	1:E:1746:HIS:CD2	2.34	0.43
1:X:1703:TYR:CZ	1:X:1707:ILE:HD11	2.53	0.43
1:C:1805:HIS:HA	1:C:1806:PRO:HD3	1.79	0.43
1:C:1806:PRO:HB2	1:C:1830:ALA:CB	2.48	0.43
1:B:1741:VAL:HG21	1:B:1840:ASP:HA	2.00	0.43
1:D:1707:ILE:HG21	1:D:1842:VAL:O	2.19	0.43
1:G:1689:MET:HB2	1:G:1736:VAL:HG11	1.98	0.43
1:G:1703:TYR:CZ	1:G:1707:ILE:HD11	2.54	0.43
1:C:1762:ARG:HB2	1:C:1762:ARG:NH1	2.33	0.43
1:F:1735:GLU:OE1	1:F:1753:ARG:NH1	2.52	0.43
1:C:1689:MET:CE	1:C:1703:TYR:HB2	2.48	0.43
1:D:1775:MET:SD	1:D:1780:LEU:HD13	2.59	0.43
1:G:1718:TRP:NE1	1:G:1729:LEU:O	2.49	0.43
1:B:1808:VAL:HB	1:B:1832:VAL:HG13	2.00	0.42
1:F:1754:GLU:HB3	2:I:1268:GLU:HG3	2.00	0.42
1:G:1684:THR:O	1:G:1711:LYS:HD3	2.19	0.42
1:G:1745:ASN:ND2	1:G:1746:HIS:H	2.16	0.42
2:K:1266:PHE:HA	2:K:1267:PRO:HD2	1.88	0.42
1:A:1833:VAL:HA	1:A:1853:TYR:O	2.20	0.42
1:A:1856:PRO:HB3	1:F:1650:MET:HB3	2.01	0.42
1:X:1747:GLN:H	1:X:1747:GLN:HG3	1.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1837:TRP:NE1	1:C:1848:GLN:O	2.43	0.42
1:E:1774:ASN:HB3	2:M:1264:PRO:HB3	2.01	0.42
2:L:1266:PHE:HA	2:L:1267:PRO:HD3	1.75	0.42
1:A:1655:SER:HB3	1:A:1689:MET:SD	2.59	0.42
1:B:1649:ARG:O	1:E:1856:PRO:HB3	2.19	0.42
1:C:1699:ARG:NH2	1:C:1839:LEU:HB3	2.33	0.42
1:D:1655:SER:HB3	1:D:1689:MET:SD	2.59	0.42
1:E:1712:TRP:CH2	1:E:1732:HIS:HA	2.54	0.42
1:G:1704:PHE:CZ	1:G:1839:LEU:HB3	2.54	0.42
2:H:1263:SEP:HA	2:H:1264:PRO:HD3	1.92	0.42
1:X:1725:GLU:HB3	1:X:1726:ARG:H	1.64	0.42
1:G:1812:PRO:HG3	1:G:1855:ILE:HD13	2.01	0.42
2:K:1263:SEP:HA	2:K:1264:PRO:HD3	1.94	0.42
1:X:1747:GLN:HB2	1:X:1750:LYS:HG3	2.02	0.42
1:E:1775:MET:HA	1:E:1776:PRO:HD3	1.92	0.42
1:F:1712:TRP:CH2	1:F:1732:HIS:CE1	3.08	0.42
1:A:1736:VAL:HG23	1:A:1749:PRO:HG2	2.02	0.41
1:B:1747:GLN:HE21	1:B:1747:GLN:HB3	1.61	0.41
1:B:1760:ILE:HG13	1:B:1787:CYS:HB3	2.02	0.41
1:D:1746:HIS:CG	1:D:1747:GLN:N	2.88	0.41
1:G:1773:THR:H	1:G:1811:GLN:HE22	1.67	0.41
1:A:1758:ARG:HE	1:A:1758:ARG:HB3	1.55	0.41
1:C:1721:GLN:O	1:C:1725:GLU:HB2	2.20	0.41
1:A:1798:PHE:CD2	1:A:1806:PRO:HB3	2.56	0.41
1:C:1703:TYR:OH	1:C:1739:ASP:OD2	2.24	0.41
1:F:1738:GLY:HA3	1:F:1743:GLY:O	2.20	0.41
1:B:1653:VAL:HG23	1:B:1677:THR:O	2.20	0.41
1:B:1858:ILE:HA	1:B:1859:PRO:HD2	1.93	0.41
1:G:1731:GLU:CD	1:G:1731:GLU:H	2.23	0.41
1:A:1809:VAL:CG1	1:A:1835:ARG:HA	2.51	0.41
1:A:1707:ILE:HG23	1:A:1752:ALA:HB2	2.03	0.41
1:X:1731:GLU:O	1:X:1734:PHE:N	2.48	0.41
1:A:1665:VAL:HG22	1:A:1719:VAL:HG21	2.03	0.41
1:A:1834:THR:HG23	1:A:1836:GLU:HB3	2.03	0.41
1:D:1822:HIS:HD2	1:D:1856:PRO:O	2.04	0.41
2:M:1266:PHE:HA	2:M:1267:PRO:HD2	1.95	0.41
1:B:1742:ASN:O	1:B:1743:GLY:O	2.38	0.41
1:E:1821:PHE:CE1	1:E:1822:HIS:CE1	3.09	0.41
1:X:1693:ALA:O	1:X:1695:PHE:N	2.54	0.41
1:B:1660:GLU:O	1:B:1663:MET:HB2	2.21	0.41
1:B:1740:VAL:O	1:B:1740:VAL:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1758:ARG:NH2	1:B:1758:ARG:HB2	2.36	0.41
1:C:1756:GLN:C	1:C:1758:ARG:H	2.24	0.41
1:E:1695:PHE:O	1:E:1736:VAL:HG23	2.21	0.41
1:F:1676:LEU:HB3	1:G:1678:ASN:OD1	2.21	0.41
1:F:1811:GLN:HA	1:F:1812:PRO:HD3	1.95	0.41
2:H:1266:PHE:HA	2:H:1267:PRO:HD3	1.79	0.41
1:D:1661:GLU:OE2	1:D:1690:LYS:HE2	2.20	0.41
1:D:1747:GLN:NE2	1:D:1750:LYS:HE2	2.36	0.41
1:G:1668:PHE:CD1	1:G:1668:PHE:C	2.94	0.40
1:A:1761:PHE:O	1:A:1764:LEU:HG	2.21	0.40
1:A:1855:ILE:HG23	1:A:1857:GLN:HE21	1.85	0.40
1:X:1812:PRO:HB3	1:X:1821:PHE:CZ	2.56	0.40
1:A:1748:GLY:N	1:A:1749:PRO:CD	2.84	0.40
1:D:1699:ARG:HH21	2:L:1266:PHE:CB	2.35	0.40
1:D:1761:PHE:CB	1:D:1789:ALA:HB2	2.51	0.40
1:F:1691:THR:HB	1:F:1692:ASP:H	1.56	0.40
1:B:1651:SER:CB	1:B:1684:THR:HA	2.51	0.40
1:D:1805:HIS:HA	1:D:1806:PRO:HD3	1.87	0.40
1:F:1696:VAL:CG2	1:F:1744:ARG:HG3	2.51	0.40
1:X:1691:THR:OG1	1:X:1715:SER:HB2	2.22	0.40
1:A:1837:TRP:HB2	1:A:1853:TYR:CG	2.57	0.40
1:B:1741:VAL:HG11	1:B:1843:ALA:HB3	2.02	0.40
1:C:1703:TYR:CZ	1:C:1707:ILE:HD11	2.57	0.40
1:D:1809:VAL:CG1	1:D:1835:ARG:HA	2.52	0.40
1:E:1700:THR:O	1:E:1703:TYR:HB3	2.22	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	202/235 (86%)	176 (87%)	18 (9%)	8 (4%)	3 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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

All (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
1	C	1757	ASP
1	C	1762	ARG
1	C	1851	ASP
1	D	1801	GLY
1	E	1726	ARG
1	F	1726	ARG
1	G	1649	ARG
1	G	1678	ASN
2	H	1267	PRO
2	I	1267	PRO
2	I	1269	ALA
1	X	1725	GLU

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Mol	Chain	Res	Type
1	X	1741	VAL
1	X	1744	ARG
1	X	1747	GLN
1	X	1813	ASP
1	A	1740	VAL
1	A	1802	THR
1	A	1851	ASP
1	B	1740	VAL
1	B	1743	GLY
1	B	1757	ASP
1	C	1740	VAL
1	D	1762	ARG
1	E	1740	VAL
1	F	1762	ARG
1	F	1773	THR
1	G	1790	SER
2	K	1269	ALA
1	X	1773	THR
1	B	1698	GLU
1	B	1699	ARG
1	B	1739	ASP
1	C	1739	ASP
1	D	1745	ASN
1	E	1744	ARG
2	H	1269	ALA
2	L	1267	PRO
2	L	1269	ALA
1	A	1774	ASN
1	B	1725	GLU
1	D	1739	ASP
1	E	1739	ASP
1	F	1752	ALA
1	X	1726	ARG
1	A	1739	ASP
1	B	1773	THR
1	C	1744	ARG
1	F	1725	GLU
1	G	1744	ARG
1	X	1739	ASP
1	B	1746	HIS
1	C	1773	THR
1	A	1801	GLY

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Mol	Chain	Res	Type
1	D	1740	VAL
1	D	1749	PRO
1	A	1803	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	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

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	1649	ARG

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Mol	Chain	Res	Type
1	X	1660	GLU
1	X	1664	LEU
1	X	1699	ARG
1	X	1720	THR
1	X	1721	GLN
1	X	1725	GLU
1	X	1726	ARG
1	X	1728	MET
1	X	1746	HIS
1	X	1747	GLN
1	X	1758	ARG
1	X	1774	ASN
1	X	1777	THR
1	X	1780	LEU
1	X	1786	LEU
1	X	1797	SER
1	X	1848	GLN
1	A	1649	ARG
1	A	1660	GLU
1	A	1671	LYS
1	A	1678	ASN
1	A	1679	LEU
1	A	1684	THR
1	A	1722	SER
1	A	1737	ARG
1	A	1740	VAL
1	A	1747	GLN
1	A	1750	LYS
1	A	1764	LEU
1	A	1773	THR
1	A	1778	ASP
1	A	1794	GLU
1	A	1800	LEU
1	A	1826	GLN
1	A	1828	CYS
1	A	1848	GLN
1	A	1854	LEU
1	A	1855	ILE
1	B	1649	ARG
1	B	1660	GLU
1	B	1670	ARG
1	B	1671	LYS

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Mol	Chain	Res	Type
1	B	1677	THR
1	B	1681	THR
1	B	1701	LEU
1	B	1715	SER
1	B	1721	GLN
1	B	1725	GLU
1	B	1726	ARG
1	B	1736	VAL
1	B	1737	ARG
1	B	1744	ARG
1	B	1747	GLN
1	B	1751	ARG
1	B	1753	ARG
1	B	1754	GLU
1	B	1756	GLN
1	B	1758	ARG
1	B	1773	THR
1	B	1786	LEU
1	B	1793	LYS
1	B	1804	VAL
1	B	1832	VAL
1	B	1835	ARG
1	B	1848	GLN
1	B	1851	ASP
1	B	1852	THR
1	C	1649	ARG
1	C	1653	VAL
1	C	1657	LEU
1	C	1660	GLU
1	C	1671	LYS
1	C	1678	ASN
1	C	1689	MET
1	C	1698	GLU
1	C	1721	GLN
1	C	1726	ARG
1	C	1727	LYS
1	C	1739	ASP
1	C	1740	VAL
1	C	1744	ARG
1	C	1745	ASN
1	C	1760	ILE
1	C	1786	LEU

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Mol	Chain	Res	Type
1	C	1793	LYS
1	C	1794	GLU
1	C	1816	THR
1	C	1824	ILE
1	C	1844	LEU
1	C	1848	GLN
1	D	1654	VAL
1	D	1663	MET
1	D	1678	ASN
1	D	1680	ILE
1	D	1683	GLU
1	D	1720	THR
1	D	1737	ARG
1	D	1740	VAL
1	D	1744	ARG
1	D	1747	GLN
1	D	1750	LYS
1	D	1753	ARG
1	D	1757	ASP
1	D	1758	ARG
1	D	1759	LYS
1	D	1762	ARG
1	D	1767	CYS
1	D	1779	GLN
1	D	1816	THR
1	D	1844	LEU
1	D	1848	GLN
1	D	1854	LEU
1	E	1654	VAL
1	E	1678	ASN
1	E	1683	GLU
1	E	1699	ARG
1	E	1701	LEU
1	E	1711	LYS
1	E	1728	MET
1	E	1730	ASN
1	E	1733	ASP
1	E	1737	ARG
1	E	1739	ASP
1	E	1740	VAL
1	E	1744	ARG
1	E	1754	GLU

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Mol	Chain	Res	Type
1	E	1757	ASP
1	E	1758	ARG
1	E	1764	LEU
1	E	1794	GLU
1	E	1810	VAL
1	E	1811	GLN
1	E	1841	SER
1	E	1848	GLN
1	E	1849	GLU
1	E	1854	LEU
1	F	1649	ARG
1	F	1650	MET
1	F	1677	THR
1	F	1684	THR
1	F	1699	ARG
1	F	1701	LEU
1	F	1711	LYS
1	F	1721	GLN
1	F	1725	GLU
1	F	1726	ARG
1	F	1736	VAL
1	F	1739	ASP
1	F	1746	HIS
1	F	1753	ARG
1	F	1774	ASN
1	F	1784	VAL
1	F	1786	LEU
1	F	1793	LYS
1	F	1854	LEU
1	G	1660	GLU
1	G	1668	PHE
1	G	1673	HIS
1	G	1689	MET
1	G	1699	ARG
1	G	1700	THR
1	G	1723	ILE
1	G	1735	GLU
1	G	1736	VAL
1	G	1744	ARG
1	G	1745	ASN
1	G	1747	GLN
1	G	1753	ARG

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Mol	Chain	Res	Type
1	G	1754	GLU
1	G	1766	ILE
1	G	1786	LEU
1	G	1794	GLU
1	G	1835	ARG
1	G	1849	GLU
1	G	1854	LEU
1	G	1855	ILE
2	H	1268	GLU
2	M	1265	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	1747	GLN
1	X	1822	HIS
1	X	1846	GLN
1	X	1848	GLN
1	A	1672	HIS
1	A	1678	ASN
1	A	1747	GLN
1	A	1785	GLN
1	A	1822	HIS
1	A	1826	GLN
1	A	1848	GLN
1	B	1721	GLN
1	B	1742	ASN
1	B	1747	GLN
1	B	1822	HIS
1	B	1848	GLN
1	C	1672	HIS
1	C	1678	ASN
1	C	1730	ASN
1	C	1745	ASN
1	C	1756	GLN
1	C	1779	GLN
1	C	1785	GLN
1	C	1822	HIS
1	D	1672	HIS
1	D	1678	ASN
1	D	1742	ASN
1	D	1747	GLN

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Mol	Chain	Res	Type
1	D	1774	ASN
1	D	1822	HIS
1	D	1848	GLN
1	E	1721	GLN
1	E	1746	HIS
1	E	1747	GLN
1	E	1822	HIS
1	E	1848	GLN
1	F	1672	HIS
1	F	1721	GLN
1	F	1732	HIS
1	G	1745	ASN
1	G	1785	GLN
1	G	1846	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	-
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	-

All (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
2	M	1263	SEP	P-O1P	3.32	1.61	1.50
2	I	1263	SEP	P-O1P	3.25	1.61	1.50
2	J	1263	SEP	P-O1P	3.24	1.61	1.50

All (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
2	H	1263	SEP	P-OG-CB	-3.09	109.79	118.30
2	N	1263	SEP	OG-CB-CA	2.99	111.06	108.14
2	O	1263	SEP	OG-CB-CA	2.88	110.95	108.14
2	O	1263	SEP	P-OG-CB	-2.74	110.76	118.30
2	J	1263	SEP	P-OG-CB	-2.72	110.79	118.30
2	N	1263	SEP	P-OG-CB	-2.53	111.34	118.30
2	M	1263	SEP	OG-CB-CA	2.47	110.55	108.14
2	K	1263	SEP	P-OG-CB	-2.46	111.53	118.30
2	L	1263	SEP	P-OG-CB	-2.08	112.57	118.30
2	L	1263	SEP	OG-CB-CA	2.07	110.16	108.14

There are no chirality outliers.

All (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
2	L	1263	SEP	N-CA-CB-OG
2	N	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
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

All (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

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Mol	Chain	Res	Type	RSRZ
1	G	1855	ILE	4.3
1	G	1850	LEU	4.3
1	G	1824	ILE	4.1
1	G	1810	VAL	3.6
1	F	1802	THR	3.6
1	G	1825	GLY	3.5
1	F	1855	ILE	3.5
1	F	1745	ASN	3.4
1	G	1856	PRO	3.4
1	F	1769	TYR	3.3
1	F	1796	SER	3.3
1	F	1792	VAL	3.1
1	F	1824	ILE	3.1
1	G	1769	TYR	3.1
1	A	1800	LEU	3.0
1	F	1800	LEU	2.8
1	G	1775	MET	2.8
1	B	1745	ASN	2.7
1	D	1734	PHE	2.6
1	E	1801	GLY	2.6
1	A	1745	ASN	2.6
1	F	1856	PRO	2.6
1	G	1800	LEU	2.5
1	D	1804	VAL	2.5
1	E	1850	LEU	2.5
1	E	1649	ARG	2.5
1	D	1729	LEU	2.4
1	D	1725	GLU	2.4
1	E	1723	ILE	2.4
1	F	1815	TRP	2.4
1	F	1835	ARG	2.4
1	D	1845	TYR	2.4
1	D	1727	LYS	2.3
1	F	1798	PHE	2.3
1	F	1810	VAL	2.3
1	F	1801	GLY	2.3
1	D	1782	TRP	2.3
1	G	1826	GLN	2.3
1	G	1831	PRO	2.2
1	D	1746	HIS	2.2
1	F	1854	LEU	2.2
1	D	1747	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	1832	VAL	2.1
1	D	1728	MET	2.1
1	D	1712	TRP	2.1
1	D	1722	SER	2.1
1	D	1780	LEU	2.1
1	E	1677	THR	2.1
1	X	1802	THR	2.1
1	F	1828	CYS	2.1
1	D	1801	GLY	2.0
1	F	1744	ARG	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, 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.