Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 06:18 PM EDT

PDB ID	:	3PXE
Title	:	Impact of BRCA1 BRCT domain missense substitutions on phospho-peptide recognition: E1836K
Authors	:	Coquelle, N.; Green, R.; Glover, J.N.M.
Deposited on	:	2010-12-09
Resolution	:	2.85 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:

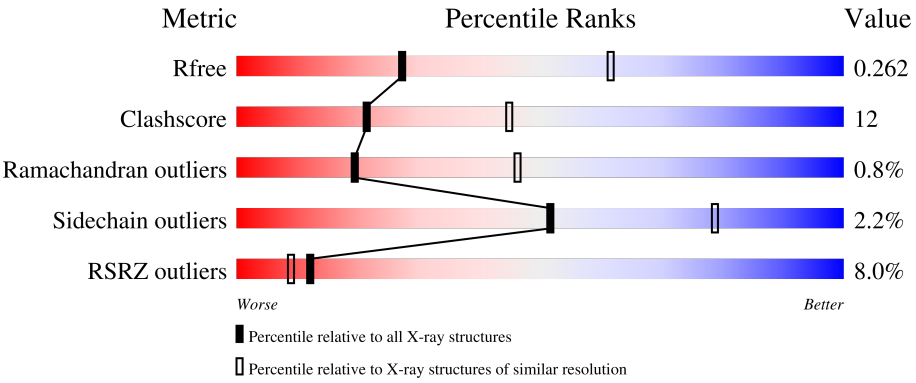
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	71% 27%
1	B	214	2% 78% 21%
1	C	214	5% 69% 29%
1	D	214	24% 70% 25%
2	E	10	50% 20% 30%

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Mol	Chain	Length	Quality of chain
2	F	10	
2	G	10	
2	H	10	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6831 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Breast cancer type 1 susceptibility protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1672	1073	283	302	14			
1	B	213	Total	C	N	O	S	0	0	0
			1672	1071	280	307	14			
1	C	211	Total	C	N	O	S	0	0	0
			1660	1064	275	307	14			
1	D	206	Total	C	N	O	S	0	0	0
			1612	1033	268	297	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1836	LYS	GLU	engineered mutation	UNP P38398
B	1836	LYS	GLU	engineered mutation	UNP P38398
C	1836	LYS	GLU	engineered mutation	UNP P38398
D	1836	LYS	GLU	engineered mutation	UNP P38398

- Molecule 2 is a protein called phospho peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	P	0	0	0
			56	32	8	15	1			
2	F	5	Total	C	N	O	P	0	0	0
			43	25	6	11	1			
2	G	6	Total	C	N	O	P	0	0	0
			50	29	7	13	1			
2	H	6	Total	C	N	O	P	0	0	0
			50	29	7	13	1			

- Molecule 3 is water.

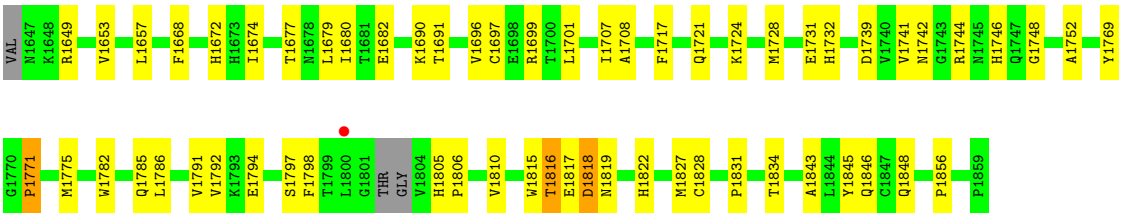
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	8	Total O 8 8	0	0
3	E	2	Total O 2 2	0	0
3	F	1	Total O 1 1	0	0

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.

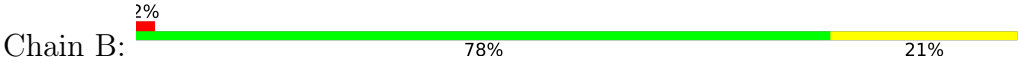
• Molecule 1: Breast cancer type 1 susceptibility protein

Chain A:



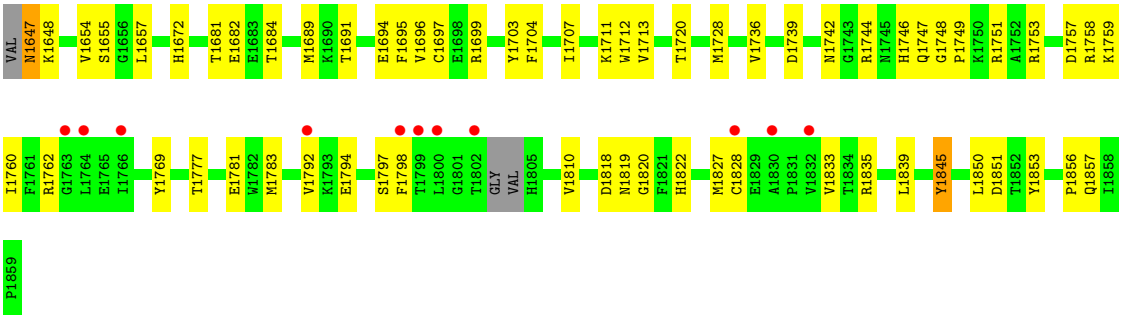
• Molecule 1: Breast cancer type 1 susceptibility protein

Chain B:



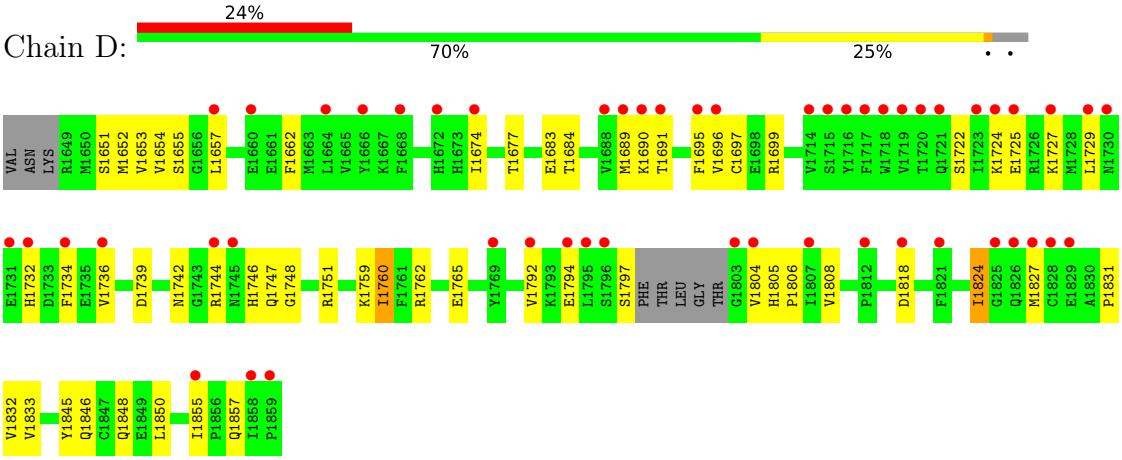
• Molecule 1: Breast cancer type 1 susceptibility protein

Chain C:



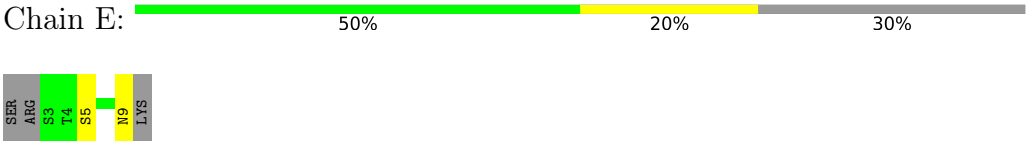
• Molecule 1: Breast cancer type 1 susceptibility protein

Chain D:



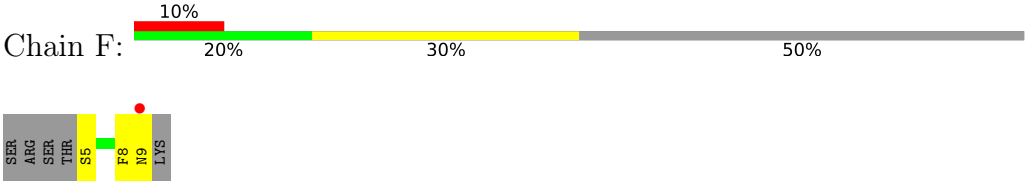
• Molecule 2: phospho peptide

Chain E:



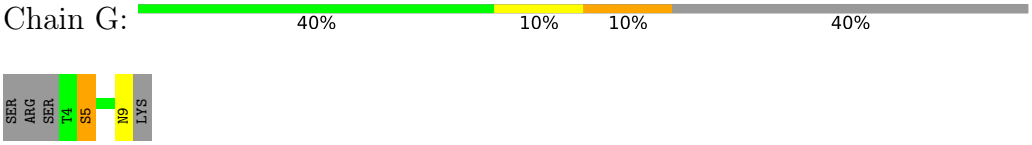
• Molecule 2: phospho peptide

Chain F:



• Molecule 2: phospho peptide

Chain G:



• Molecule 2: phospho peptide

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	115.82Å 131.05Å 180.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.36 – 2.85 44.36 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.1 (44.36-2.85) 96.2 (44.36-2.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.3_473)	Depositor
R, R_{free}	0.220 , 0.266 0.221 , 0.262	Depositor DCC
R_{free} test set	1561 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	66.4	Xtriage
Anisotropy	0.671	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 59.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6831	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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	0/1712	0.60	0/2323
1	B	0.42	0/1713	0.58	0/2330
1	C	0.35	0/1700	0.52	0/2311
1	D	0.30	0/1651	0.50	0/2246
2	E	0.60	0/46	0.53	0/60
2	F	0.46	0/34	0.50	0/45
2	G	0.48	0/40	0.64	0/52
2	H	0.45	0/40	0.46	0/52
All	All	0.38	0/6936	0.55	0/9419

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1672	0	1643	45	0
1	B	1672	0	1623	36	0
1	C	1660	0	1605	45	0
1	D	1612	0	1555	41	0
2	E	56	0	44	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	43	0	34	2	0
2	G	50	0	39	1	0
2	H	50	0	39	0	0
3	A	5	0	0	0	0
3	B	8	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
All	All	6831	0	6582	161	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 (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1746:HIS:HD2	1:A:1748:GLY:H	1.19	0.85
1:D:1792:VAL:HG13	1:D:1797:SER:HB2	1.61	0.79
1:B:1759:LYS:O	1:B:1762:ARG:HD3	1.83	0.79
1:A:1785:GLN:HE21	1:A:1791:VAL:HG21	1.49	0.78
1:C:1759:LYS:O	1:C:1762:ARG:HD3	1.83	0.77
1:A:1696:VAL:HG21	1:A:1744:ARG:HG3	1.66	0.77
1:B:1699:ARG:NH1	1:B:1742:ASN:HD21	1.82	0.76
1:B:1699:ARG:HH11	1:B:1742:ASN:HD21	1.30	0.76
1:D:1765:GLU:HG3	1:D:1804:VAL:HG11	1.66	0.76
1:C:1691:THR:HG22	1:C:1697:CYS:HB3	1.66	0.75
1:B:1746:HIS:CD2	1:B:1748:GLY:H	2.04	0.75
1:C:1746:HIS:CD2	1:C:1748:GLY:H	2.04	0.73
1:D:1696:VAL:HG21	1:D:1744:ARG:HG3	1.69	0.73
1:B:1818:ASP:HB3	1:B:1820:GLY:H	1.54	0.73
1:A:1746:HIS:CD2	1:A:1748:GLY:H	2.04	0.71
1:C:1696:VAL:HG21	1:C:1744:ARG:HG3	1.71	0.71
1:D:1747:GLN:O	1:D:1751:ARG:HG2	1.91	0.70
1:C:1746:HIS:HD2	1:C:1748:GLY:H	1.40	0.68
1:C:1736:VAL:HG13	1:C:1749:PRO:HG2	1.76	0.66
1:D:1806:PRO:O	1:D:1831:PRO:HD2	1.95	0.66
1:C:1747:GLN:O	1:C:1751:ARG:HG3	1.98	0.64
1:D:1746:HIS:HD2	1:D:1748:GLY:H	1.46	0.64
1:D:1832:VAL:HG12	1:D:1855:ILE:HD12	1.79	0.64
1:B:1746:HIS:HD2	1:B:1748:GLY:H	1.43	0.63
1:C:1739:ASP:OD2	1:C:1746:HIS:HE1	1.81	0.63
1:D:1699:ARG:HH11	1:D:1742:ASN:HD21	1.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1746:HIS:HD2	1:C:1748:GLY:N	1.96	0.62
1:A:1691:THR:HG22	1:A:1697:CYS:HB3	1.81	0.61
1:C:1647:ASN:HD22	1:C:1648:LYS:N	1.98	0.61
1:D:1833:VAL:HG11	1:D:1850:LEU:HD22	1.83	0.61
1:B:1759:LYS:O	1:B:1762:ARG:CD	2.48	0.60
1:B:1769:TYR:HB3	1:B:1810:VAL:HG12	1.83	0.60
1:C:1695:PHE:O	1:C:1736:VAL:HG23	2.02	0.59
1:B:1724:LYS:O	1:B:1724:LYS:HG2	2.02	0.59
1:D:1846:GLN:HE21	1:D:1848:GLN:HE22	1.48	0.59
1:A:1653:VAL:HG21	1:A:1680:ILE:HG12	1.84	0.58
1:A:1746:HIS:HD2	1:A:1748:GLY:N	1.95	0.58
1:C:1647:ASN:HD22	1:C:1648:LYS:H	1.52	0.57
1:B:1741:VAL:HG21	2:F:9:ASN:HA	1.86	0.57
1:C:1713:VAL:O	1:C:1736:VAL:HG12	2.06	0.56
1:D:1696:VAL:CG2	1:D:1744:ARG:HG3	2.35	0.56
1:D:1699:ARG:NH1	1:D:1742:ASN:HD21	2.04	0.56
1:B:1722:SER:HA	1:B:1729:LEU:HD13	1.88	0.55
1:A:1674:ILE:HD11	1:A:1728:MET:HE3	1.87	0.55
1:A:1721:GLN:NE2	1:A:1724:LYS:HD3	2.22	0.55
1:A:1682:GLU:H	1:A:1682:GLU:CD	2.09	0.55
1:A:1699:ARG:NH1	1:A:1742:ASN:HD21	2.05	0.54
1:A:1846:GLN:HG3	1:A:1848:GLN:NE2	2.23	0.54
1:D:1759:LYS:O	1:D:1762:ARG:HD3	2.07	0.54
1:C:1792:VAL:HG13	1:C:1797:SER:HB2	1.90	0.54
1:C:1818:ASP:C	1:C:1820:GLY:H	2.11	0.54
1:D:1655:SER:HB3	1:D:1689:MET:SD	2.48	0.54
1:B:1806:PRO:O	1:B:1831:PRO:HD2	2.08	0.53
1:D:1746:HIS:CD2	1:D:1748:GLY:H	2.26	0.53
1:D:1657:LEU:HD23	1:D:1690:LYS:HB2	1.90	0.53
1:D:1739:ASP:OD2	1:D:1746:HIS:HE1	1.90	0.53
1:C:1684:THR:O	1:C:1711:LYS:HD3	2.08	0.53
1:D:1651:SER:HB3	1:D:1684:THR:HA	1.91	0.52
1:C:1712:TRP:CH2	1:C:1753:ARG:CZ	2.92	0.52
1:C:1833:VAL:HG11	1:C:1850:LEU:HD22	1.93	0.51
1:A:1769:TYR:HB3	1:A:1810:VAL:HG12	1.93	0.51
1:C:1694:GLU:OE1	1:C:1744:ARG:HD3	2.11	0.51
1:C:1672:HIS:CG	1:C:1728:MET:HE3	2.46	0.51
1:D:1722:SER:HA	1:D:1729:LEU:HD23	1.92	0.51
1:A:1794:GLU:HA	1:A:1794:GLU:OE1	2.11	0.51
1:B:1751:ARG:HD2	1:B:1844:LEU:O	2.10	0.51
1:A:1810:VAL:O	1:A:1834:THR:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1724:LYS:O	1:D:1724:LYS:HG2	2.10	0.50
1:A:1827:MET:O	1:A:1828:CYS:HB3	2.12	0.50
1:D:1794:GLU:HA	1:D:1794:GLU:OE1	2.11	0.50
1:D:1760:ILE:HG23	1:D:1845:TYR:CE2	2.46	0.50
1:D:1792:VAL:CG1	1:D:1797:SER:HB2	2.38	0.50
1:A:1741:VAL:HG21	2:E:9:ASN:HA	1.94	0.50
1:D:1832:VAL:HB	1:D:1857:GLN:HE21	1.77	0.49
1:C:1681:THR:HG22	1:C:1682:GLU:N	2.27	0.49
1:C:1769:TYR:HB3	1:C:1810:VAL:HG12	1.93	0.49
1:C:1759:LYS:O	1:C:1762:ARG:CD	2.58	0.49
1:A:1657:LEU:HD23	1:A:1690:LYS:HB2	1.94	0.49
1:A:1846:GLN:HG3	1:A:1848:GLN:HE22	1.76	0.49
1:B:1691:THR:HG22	1:B:1697:CYS:HB3	1.95	0.49
1:A:1752:ALA:HB2	1:A:1845:TYR:CD1	2.48	0.49
1:B:1746:HIS:HD2	1:B:1748:GLY:N	2.11	0.49
1:D:1846:GLN:O	1:D:1846:GLN:HG3	2.13	0.48
1:D:1691:THR:HG21	1:D:1736:VAL:HG22	1.96	0.48
1:A:1696:VAL:HG13	1:A:1739:ASP:HA	1.95	0.47
1:A:1822:HIS:HD2	1:A:1856:PRO:O	1.97	0.47
1:C:1760:ILE:HG23	1:C:1845:TYR:CE2	2.49	0.47
1:D:1808:VAL:HG11	1:D:1824:ILE:HG21	1.95	0.47
1:C:1655:SER:HA	2:G:5:SEP:O2P	2.14	0.47
1:C:1777:THR:O	1:C:1781:GLU:HG3	2.14	0.47
1:C:1689:MET:O	1:C:1691:THR:HG23	2.15	0.46
1:C:1819:ASN:OD1	1:C:1822:HIS:CD2	2.68	0.46
1:A:1674:ILE:HD11	1:A:1728:MET:CE	2.45	0.46
1:A:1728:MET:CE	1:B:1819:ASN:ND2	2.78	0.46
1:A:1696:VAL:CG2	1:A:1744:ARG:HG3	2.40	0.46
1:A:1771:PRO:HD2	1:A:1815:TRP:NE1	2.30	0.46
1:B:1805:HIS:HA	1:B:1806:PRO:HD3	1.74	0.45
1:D:1695:PHE:CE1	1:D:1734:PHE:HA	2.51	0.45
1:D:1804:VAL:CG1	1:D:1805:HIS:N	2.79	0.45
1:A:1728:MET:HB3	1:B:1819:ASN:HD22	1.81	0.45
1:B:1695:PHE:CE1	1:B:1734:PHE:HA	2.51	0.45
1:A:1728:MET:CE	1:B:1819:ASN:HD22	2.30	0.45
1:C:1699:ARG:HH11	1:C:1742:ASN:HD21	1.63	0.45
1:C:1672:HIS:CG	1:C:1728:MET:CE	3.00	0.45
1:C:1704:PHE:HB3	1:C:1783:MET:SD	2.57	0.45
1:A:1816:THR:HG22	1:A:1817:GLU:N	2.32	0.45
1:C:1827:MET:O	1:C:1828:CYS:HB3	2.17	0.45
1:B:1792:VAL:HG13	1:B:1797:SER:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1774:ASN:O	2:F:8:PHE:HZ	2.00	0.44
1:D:1654:VAL:HG21	1:D:1662:PHE:HD1	1.82	0.44
1:A:1771:PRO:HD2	1:A:1815:TRP:CD1	2.52	0.44
1:C:1699:ARG:NH1	1:C:1742:ASN:HD21	2.14	0.44
1:D:1746:HIS:HD2	1:D:1748:GLY:N	2.14	0.44
1:A:1822:HIS:CD2	1:A:1856:PRO:O	2.71	0.44
1:A:1798:PHE:CD2	1:A:1806:PRO:HB3	2.53	0.43
1:C:1794:GLU:OE1	1:C:1794:GLU:HA	2.18	0.43
1:B:1747:GLN:HE21	1:B:1747:GLN:HB3	1.61	0.43
1:D:1652:MET:HE3	1:D:1674:ILE:HG21	2.00	0.43
1:B:1699:ARG:HH11	1:B:1742:ASN:ND2	2.07	0.43
1:B:1760:ILE:HG13	1:B:1761:PHE:CD2	2.54	0.43
1:C:1833:VAL:HA	1:C:1853:TYR:O	2.19	0.43
1:A:1792:VAL:HG13	1:A:1797:SER:HB2	2.01	0.43
1:B:1701:LEU:HD21	1:B:1779:GLN:HG3	2.01	0.43
1:D:1691:THR:HG22	1:D:1697:CYS:HB3	2.00	0.43
1:D:1805:HIS:HA	1:D:1806:PRO:HD3	1.86	0.43
1:A:1732:HIS:CE1	1:B:1812:PRO:HB2	2.54	0.42
1:A:1748:GLY:HA3	1:A:1843:ALA:O	2.19	0.42
1:C:1751:ARG:HH11	1:C:1751:ARG:HB3	1.84	0.42
1:C:1757:ASP:OD1	1:C:1757:ASP:N	2.45	0.42
1:A:1701:LEU:HD13	1:A:1775:MET:HG3	2.00	0.42
1:A:1707:ILE:O	1:A:1708:ALA:C	2.58	0.42
1:B:1760:ILE:HG23	1:B:1845:TYR:CE2	2.54	0.42
1:D:1832:VAL:CG1	1:D:1855:ILE:HD12	2.47	0.42
1:D:1827:MET:HB3	1:D:1827:MET:HE2	1.90	0.42
1:B:1805:HIS:ND1	1:B:1805:HIS:N	2.68	0.42
1:D:1759:LYS:O	1:D:1762:ARG:CD	2.68	0.42
1:A:1668:PHE:CE1	1:A:1672:HIS:CD2	3.08	0.42
1:B:1647:ASN:HD21	1:C:1857:GLN:HG2	1.85	0.42
1:C:1835:ARG:HE	1:C:1835:ARG:HB3	1.65	0.42
1:A:1792:VAL:CG1	1:A:1797:SER:HB2	2.50	0.41
1:C:1758:ARG:C	1:C:1762:ARG:HD2	2.40	0.41
1:A:1806:PRO:O	1:A:1831:PRO:HD2	2.19	0.41
1:B:1721:GLN:HA	1:B:1721:GLN:OE1	2.21	0.41
1:D:1683:GLU:H	1:D:1683:GLU:CD	2.23	0.41
1:A:1815:TRP:HE3	1:A:1818:ASP:HB3	1.84	0.41
1:B:1655:SER:HB3	1:B:1689:MET:SD	2.60	0.41
1:C:1654:VAL:HB	1:C:1657:LEU:CD1	2.50	0.41
1:B:1747:GLN:NE2	1:B:1750:LYS:HD3	2.36	0.41
1:B:1648:LYS:HB2	1:C:1856:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1759:LYS:N	1:B:1762:ARG:HD2	2.36	0.41
1:C:1759:LYS:N	1:C:1762:ARG:HD2	2.36	0.41
1:C:1835:ARG:O	1:C:1839:LEU:HG	2.21	0.41
1:A:1782:TRP:CE2	1:A:1786:LEU:HD11	2.56	0.40
1:A:1819:ASN:ND2	1:A:1822:HIS:ND1	2.70	0.40
1:D:1653:VAL:HG12	1:D:1677:THR:O	2.21	0.40
1:D:1695:PHE:HB3	1:D:1736:VAL:HA	2.03	0.40
1:A:1717:PHE:O	1:A:1721:GLN:HB2	2.21	0.40
1:B:1696:VAL:HG21	1:B:1744:ARG:HH11	1.87	0.40
1:C:1703:TYR:CZ	1:C:1707:ILE:HD11	2.57	0.40
1:A:1805:HIS:HA	1:A:1806:PRO:HD3	1.83	0.40
1:D:1725:GLU:C	1:D:1727:LYS:H	2.25	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	207/214 (97%)	191 (92%)	15 (7%)	1 (0%)	29	57
1	B	211/214 (99%)	200 (95%)	9 (4%)	2 (1%)	17	43
1	C	207/214 (97%)	195 (94%)	10 (5%)	2 (1%)	15	40
1	D	202/214 (94%)	189 (94%)	11 (5%)	2 (1%)	15	40
2	E	4/10 (40%)	4 (100%)	0	0	100	100
2	F	3/10 (30%)	3 (100%)	0	0	100	100
2	G	3/10 (30%)	3 (100%)	0	0	100	100
2	H	3/10 (30%)	3 (100%)	0	0	100	100
All	All	840/896 (94%)	788 (94%)	45 (5%)	7 (1%)	19	46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1760	ILE
1	B	1802	THR
1	C	1845	TYR
1	B	1820	GLY
1	A	1816	THR
1	C	1851	ASP
1	D	1824	ILE

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	183/191 (96%)	177 (97%)	6 (3%)	38 68
1	B	182/191 (95%)	178 (98%)	4 (2%)	52 79
1	C	181/191 (95%)	178 (98%)	3 (2%)	60 83
1	D	175/191 (92%)	173 (99%)	2 (1%)	73 90
2	E	6/9 (67%)	6 (100%)	0	100 100
2	F	4/9 (44%)	4 (100%)	0	100 100
2	G	5/9 (56%)	4 (80%)	1 (20%)	1 3
2	H	5/9 (56%)	5 (100%)	0	100 100
All	All	741/800 (93%)	725 (98%)	16 (2%)	52 79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1649	ARG
1	A	1677	THR
1	A	1679	LEU
1	A	1731	GLU
1	A	1771	PRO
1	A	1818	ASP
1	B	1731	GLU
1	B	1732	HIS
1	B	1753	ARG

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Mol	Chain	Res	Type
1	B	1816	THR
1	C	1647	ASN
1	C	1720	THR
1	C	1798	PHE
1	D	1732	HIS
1	D	1818	ASP
2	G	9	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1672	HIS
1	A	1721	GLN
1	A	1732	HIS
1	A	1742	ASN
1	A	1746	HIS
1	A	1747	GLN
1	A	1785	GLN
1	A	1848	GLN
1	B	1647	ASN
1	B	1678	ASN
1	B	1742	ASN
1	B	1746	HIS
1	B	1747	GLN
1	B	1779	GLN
1	B	1848	GLN
1	C	1647	ASN
1	C	1678	ASN
1	C	1732	HIS
1	C	1742	ASN
1	C	1746	HIS
1	C	1747	GLN
1	C	1848	GLN
1	D	1742	ASN
1	D	1746	HIS
1	D	1747	GLN
1	D	1822	HIS
1	D	1848	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)

4 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	G	5	2	8,9,10	1.63	1 (12%)	8,12,14	1.80	2 (25%)
2	SEP	E	5	2	8,9,10	1.62	2 (25%)	8,12,14	1.36	2 (25%)
2	SEP	H	5	2	8,9,10	1.63	1 (12%)	8,12,14	1.39	2 (25%)
2	SEP	F	5	2	8,9,10	1.59	1 (12%)	8,12,14	1.69	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	G	5	2	-	0/5/8/10	-
2	SEP	E	5	2	-	2/5/8/10	-
2	SEP	H	5	2	-	2/5/8/10	-
2	SEP	F	5	2	-	2/5/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	5	SEP	P-O1P	3.68	1.62	1.50
2	H	5	SEP	P-O1P	3.48	1.61	1.50
2	F	5	SEP	P-O1P	3.23	1.61	1.50
2	E	5	SEP	P-O1P	3.22	1.60	1.50
2	E	5	SEP	P-O3P	2.10	1.62	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	5	SEP	OG-CB-CA	3.97	112.00	108.14
2	G	5	SEP	OG-CB-CA	3.88	111.92	108.14
2	G	5	SEP	P-OG-CB	-2.62	111.08	118.30
2	H	5	SEP	OG-P-O1P	2.43	113.29	106.47
2	H	5	SEP	OG-CB-CA	2.43	110.51	108.14
2	E	5	SEP	OG-CB-CA	2.37	110.45	108.14
2	F	5	SEP	P-OG-CB	-2.05	112.66	118.30
2	E	5	SEP	OG-P-O1P	2.00	112.08	106.47

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	5	SEP	CB-OG-P-O2P
2	E	5	SEP	CB-OG-P-O3P
2	F	5	SEP	N-CA-CB-OG
2	H	5	SEP	N-CA-CB-OG
2	F	5	SEP	CB-OG-P-O1P
2	H	5	SEP	CB-OG-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	5	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	211/214 (98%)	0.09	1 (0%) 91 90	47, 72, 116, 162	0
1	B	213/214 (99%)	0.07	4 (1%) 66 64	53, 72, 110, 152	0
1	C	211/214 (98%)	0.29	11 (5%) 27 22	66, 91, 133, 169	0
1	D	206/214 (96%)	1.19	52 (25%) 0 0	80, 130, 192, 276	0
2	E	6/10 (60%)	0.10	0 100 100	65, 76, 85, 104	0
2	F	4/10 (40%)	0.60	1 (25%) 0 0	106, 106, 116, 124	0
2	G	5/10 (50%)	0.17	0 100 100	84, 89, 95, 110	0
2	H	5/10 (50%)	0.28	0 100 100	115, 126, 135, 137	0
All	All	861/896 (96%)	0.40	69 (8%) 12 9	47, 88, 168, 276	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1668	PHE	7.7
1	D	1859	PRO	6.7
1	D	1796	SER	5.3
1	D	1731	GLU	5.2
1	D	1826	GLN	5.1
1	B	1803	GLY	4.2
1	D	1714	VAL	4.2
1	D	1795	LEU	4.1
1	B	1802	THR	4.1
1	D	1674	ILE	4.0
1	D	1732	HIS	3.8
1	D	1723	ILE	3.8
1	D	1724	LYS	3.7
1	C	1800	LEU	3.6
1	D	1718	TRP	3.5
1	C	1764	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	1730	ASN	3.4
1	D	1804	VAL	3.4
1	D	1734	PHE	3.4
1	D	1803	GLY	3.4
1	D	1729	LEU	3.3
1	D	1657	LEU	3.2
1	D	1664	LEU	3.2
1	D	1721	GLN	3.1
1	D	1794	GLU	3.1
1	D	1719	VAL	3.0
1	D	1818	ASP	3.0
1	D	1696	VAL	3.0
1	D	1744	ARG	2.9
1	D	1825	GLY	2.9
1	D	1821	PHE	2.9
1	D	1689	MET	2.8
1	D	1769	TYR	2.8
1	D	1716	TYR	2.8
1	D	1666	TYR	2.7
1	D	1688	VAL	2.7
1	D	1736	VAL	2.7
1	D	1855	ILE	2.6
1	C	1798	PHE	2.6
1	D	1807	ILE	2.6
1	D	1672	HIS	2.5
1	D	1720	THR	2.5
1	C	1802	THR	2.4
1	D	1792	VAL	2.4
1	D	1717	PHE	2.4
1	D	1725	GLU	2.4
1	C	1830	ALA	2.3
1	D	1858	ILE	2.3
1	D	1690	LYS	2.3
1	D	1812	PRO	2.3
1	D	1828	CYS	2.3
1	C	1766	ILE	2.3
1	C	1763	GLY	2.2
1	A	1800	LEU	2.2
1	D	1691	THR	2.2
1	D	1829	GLU	2.2
2	F	9	ASN	2.2
1	D	1660	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	1827	MET	2.1
1	D	1727	LYS	2.1
1	D	1745	ASN	2.1
1	C	1828	CYS	2.1
1	C	1792	VAL	2.1
1	C	1832	VAL	2.1
1	B	1800	LEU	2.1
1	D	1695	PHE	2.1
1	D	1715	SER	2.0
1	B	1801	GLY	2.0
1	C	1799	THR	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	F	5	10/11	0.89	0.25	83,83,137,137	0
2	SEP	G	5	10/11	0.93	0.18	93,98,98,98	0
2	SEP	H	5	10/11	0.93	0.15	106,106,137,137	0
2	SEP	E	5	10/11	0.97	0.16	57,57,62,62	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.