



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:53 AM UTC

PDB ID : 4Y18 / pdb_00004y18
Title : Structure of BRCA1 BRCT domains in complex with Abraxas double phosphorylated peptide
Authors : Wu, Q.; Blundell, T.L.
Deposited on : 2015-02-06
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

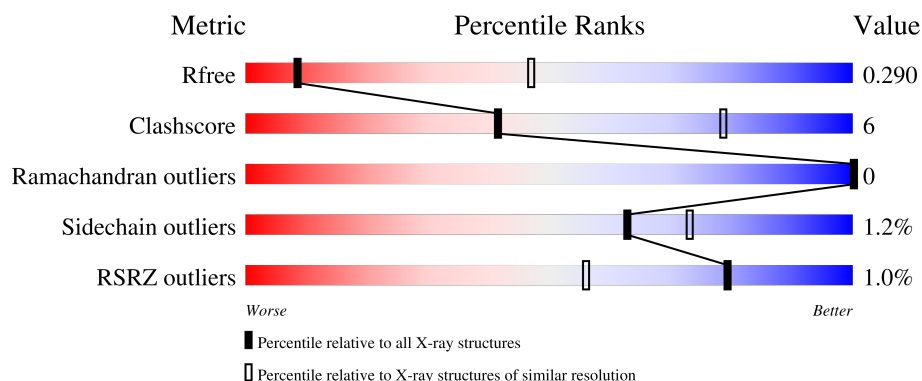
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	224	% 75% 20% • •
1	B	224	84% 11% •
1	C	224	84% 11% •
1	D	224	% 79% 15% • 5%
1	E	224	81% 14% •

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Mol	Chain	Length	Quality of chain
1	F	224	
1	G	224	
1	H	224	
2	I	11	
2	J	11	
2	K	11	
2	L	11	
2	M	11	
2	N	11	
2	O	11	
2	P	11	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SEP	P	406	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13976 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	214	Total	C	N	O	S	0	0	0
			1699	1084	289	312	14			
1	B	214	Total	C	N	O	S	0	0	0
			1696	1083	286	313	14			
1	C	214	Total	C	N	O	S	0	0	0
			1695	1082	288	311	14			
1	D	213	Total	C	N	O	S	0	0	0
			1677	1073	282	308	14			
1	E	214	Total	C	N	O	S	0	0	0
			1682	1074	282	312	14			
1	F	214	Total	C	N	O	S	0	0	0
			1679	1075	281	309	14			
1	G	211	Total	C	N	O	S	0	0	0
			1664	1063	283	306	12			
1	H	211	Total	C	N	O	S	0	0	0
			1623	1032	275	304	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1636	MET	-	initiating methionine	UNP P38398
A	1637	SER	-	expression tag	UNP P38398
A	1638	HIS	-	expression tag	UNP P38398
A	1639	HIS	-	expression tag	UNP P38398
A	1640	HIS	-	expression tag	UNP P38398
A	1641	HIS	-	expression tag	UNP P38398
A	1642	HIS	-	expression tag	UNP P38398
A	1643	HIS	-	expression tag	UNP P38398
A	1644	SER	-	expression tag	UNP P38398
A	1645	MET	-	expression tag	UNP P38398
B	1636	MET	-	initiating methionine	UNP P38398
B	1637	SER	-	expression tag	UNP P38398
B	1638	HIS	-	expression tag	UNP P38398

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1639	HIS	-	expression tag	UNP P38398
B	1640	HIS	-	expression tag	UNP P38398
B	1641	HIS	-	expression tag	UNP P38398
B	1642	HIS	-	expression tag	UNP P38398
B	1643	HIS	-	expression tag	UNP P38398
B	1644	SER	-	expression tag	UNP P38398
B	1645	MET	-	expression tag	UNP P38398
C	1636	MET	-	initiating methionine	UNP P38398
C	1637	SER	-	expression tag	UNP P38398
C	1638	HIS	-	expression tag	UNP P38398
C	1639	HIS	-	expression tag	UNP P38398
C	1640	HIS	-	expression tag	UNP P38398
C	1641	HIS	-	expression tag	UNP P38398
C	1642	HIS	-	expression tag	UNP P38398
C	1643	HIS	-	expression tag	UNP P38398
C	1644	SER	-	expression tag	UNP P38398
C	1645	MET	-	expression tag	UNP P38398
D	1636	MET	-	initiating methionine	UNP P38398
D	1637	SER	-	expression tag	UNP P38398
D	1638	HIS	-	expression tag	UNP P38398
D	1639	HIS	-	expression tag	UNP P38398
D	1640	HIS	-	expression tag	UNP P38398
D	1641	HIS	-	expression tag	UNP P38398
D	1642	HIS	-	expression tag	UNP P38398
D	1643	HIS	-	expression tag	UNP P38398
D	1644	SER	-	expression tag	UNP P38398
D	1645	MET	-	expression tag	UNP P38398
E	1636	MET	-	initiating methionine	UNP P38398
E	1637	SER	-	expression tag	UNP P38398
E	1638	HIS	-	expression tag	UNP P38398
E	1639	HIS	-	expression tag	UNP P38398
E	1640	HIS	-	expression tag	UNP P38398
E	1641	HIS	-	expression tag	UNP P38398
E	1642	HIS	-	expression tag	UNP P38398
E	1643	HIS	-	expression tag	UNP P38398
E	1644	SER	-	expression tag	UNP P38398
E	1645	MET	-	expression tag	UNP P38398
F	1636	MET	-	initiating methionine	UNP P38398
F	1637	SER	-	expression tag	UNP P38398
F	1638	HIS	-	expression tag	UNP P38398
F	1639	HIS	-	expression tag	UNP P38398
F	1640	HIS	-	expression tag	UNP P38398

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1641	HIS	-	expression tag	UNP P38398
F	1642	HIS	-	expression tag	UNP P38398
F	1643	HIS	-	expression tag	UNP P38398
F	1644	SER	-	expression tag	UNP P38398
F	1645	MET	-	expression tag	UNP P38398
G	1636	MET	-	initiating methionine	UNP P38398
G	1637	SER	-	expression tag	UNP P38398
G	1638	HIS	-	expression tag	UNP P38398
G	1639	HIS	-	expression tag	UNP P38398
G	1640	HIS	-	expression tag	UNP P38398
G	1641	HIS	-	expression tag	UNP P38398
G	1642	HIS	-	expression tag	UNP P38398
G	1643	HIS	-	expression tag	UNP P38398
G	1644	SER	-	expression tag	UNP P38398
G	1645	MET	-	expression tag	UNP P38398
H	1636	MET	-	initiating methionine	UNP P38398
H	1637	SER	-	expression tag	UNP P38398
H	1638	HIS	-	expression tag	UNP P38398
H	1639	HIS	-	expression tag	UNP P38398
H	1640	HIS	-	expression tag	UNP P38398
H	1641	HIS	-	expression tag	UNP P38398
H	1642	HIS	-	expression tag	UNP P38398
H	1643	HIS	-	expression tag	UNP P38398
H	1644	SER	-	expression tag	UNP P38398
H	1645	MET	-	expression tag	UNP P38398

- Molecule 2 is a protein called BRCA1-A complex subunit Abraxas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	9	Total	C	N	O	P	0	0	0
			76	43	9	22	2			
2	J	9	Total	C	N	O	P	0	0	0
			76	43	9	22	2			
2	K	9	Total	C	N	O	P	0	0	0
			76	43	9	22	2			
2	L	8	Total	C	N	O	P	0	0	0
			72	41	8	21	2			
2	M	8	Total	C	N	O	P	0	0	0
			78	44	11	21	2			
2	N	7	Total	C	N	O	P	0	0	0
			63	36	7	18	2			
2	O	7	Total	C	N	O	P	0	0	0
			56	30	7	17	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	P	0	0	0
			63	36	7	18	2			

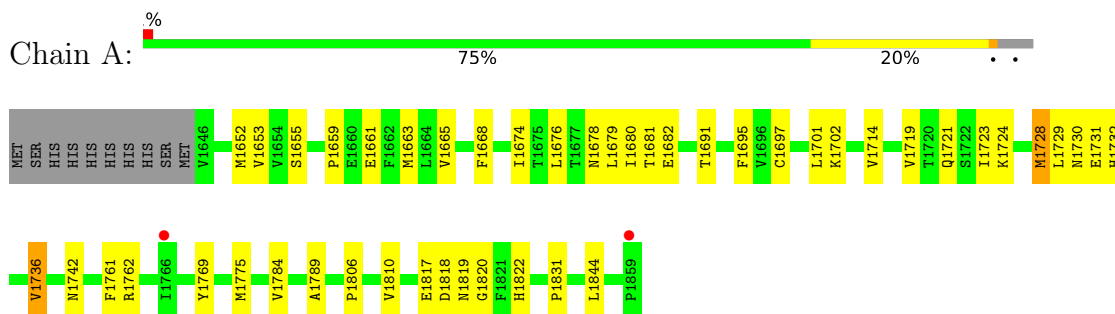
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	O	0	0
			1	1		

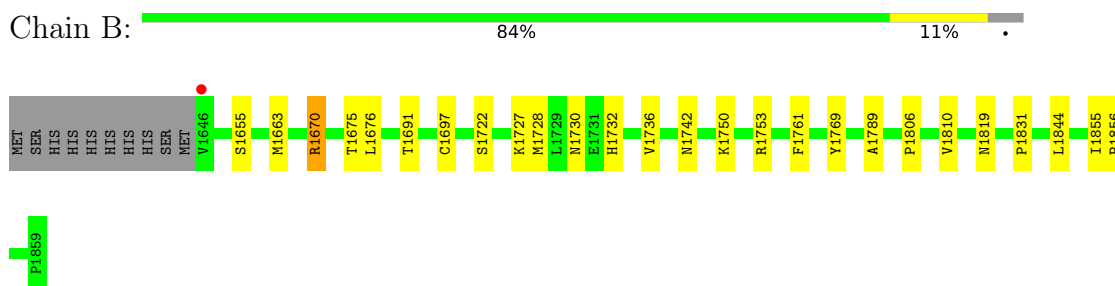
3 Residue-property plots

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.

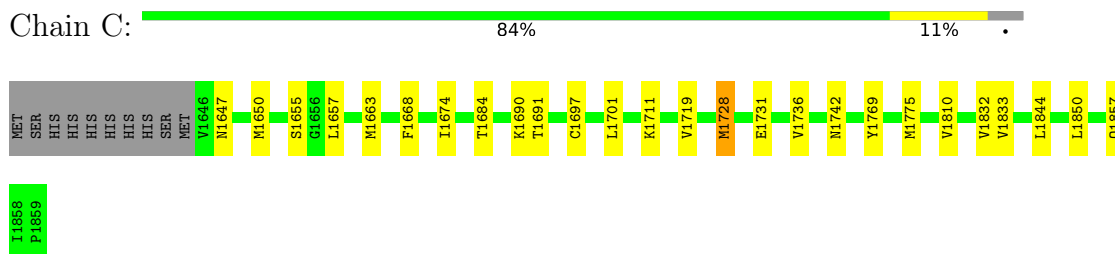
- Molecule 1: Breast cancer type 1 susceptibility protein



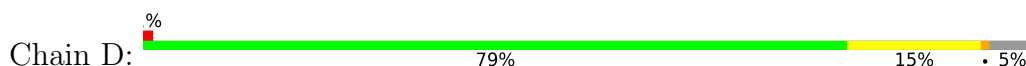
- Molecule 1: Breast cancer type 1 susceptibility protein

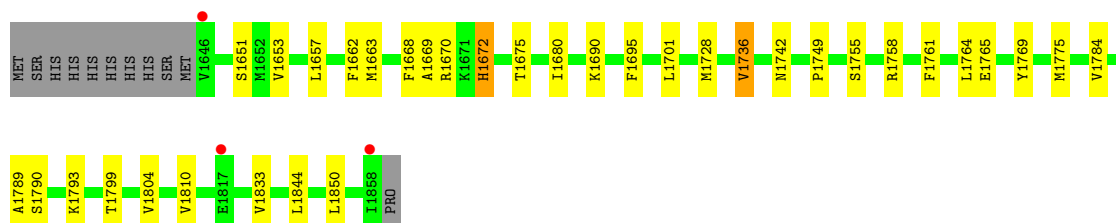


- Molecule 1: Breast cancer type 1 susceptibility protein



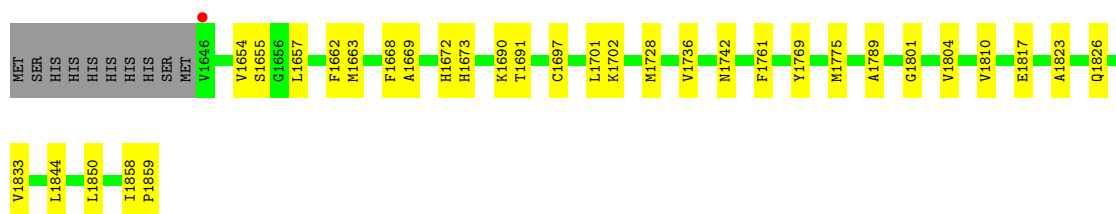
- Molecule 1: Breast cancer type 1 susceptibility protein





- Molecule 1: Breast cancer type 1 susceptibility protein

Chain E: 81% 14% .



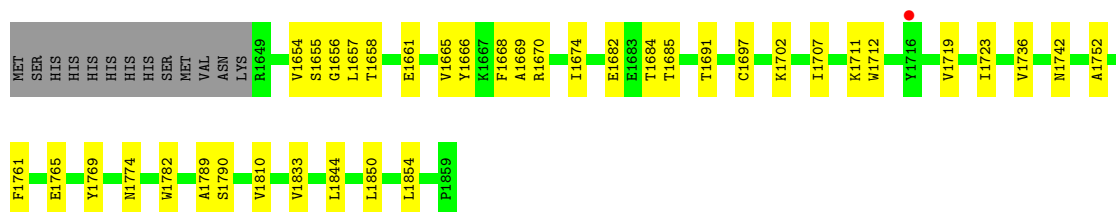
- Molecule 1: Breast cancer type 1 susceptibility protein

Chain F: 2% 83% 12% .



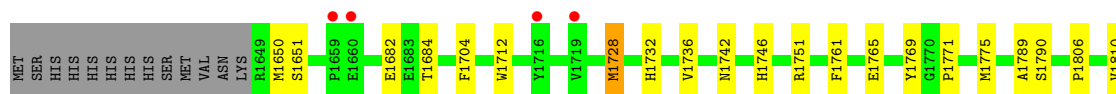
- Molecule 1: Breast cancer type 1 susceptibility protein

Chain G: 77% 17% 6%



- Molecule 1: Breast cancer type 1 susceptibility protein

Chain H: 2% 83% 11% 6%

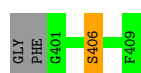




- Molecule 2: BRCA1-A complex subunit Abraxas



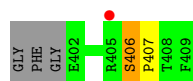
- Molecule 2: BRCA1-A complex subunit Abraxas



- Molecule 2: BRCA1-A complex subunit Abraxas



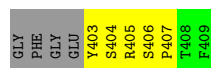
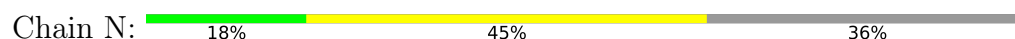
- Molecule 2: BRCA1-A complex subunit Abraxas



- Molecule 2: BRCA1-A complex subunit Abraxas



- Molecule 2: BRCA1-A complex subunit Abraxas

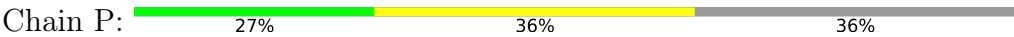


- Molecule 2: BRCA1-A complex subunit Abraxas



GLY	PHE	GLY	GLU	Y403	S404	R405	S406	P407	T408	F409
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- Molecule 2: BRCA1-A complex subunit Abraxas



GLY	PHE	GLY	GLU	Y403	S404	R405	S406	P407	T408	F409
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.82Å 183.73Å 190.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.25 – 3.50 95.25 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (95.25-3.50) 95.8 (95.25-3.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.49Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.233 , 0.297 0.238 , 0.290	Depositor DCC
R_{free} test set	1961 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	103.9	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.048 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13976	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.31	0/1740	0.79	1/2364 (0.0%)
1	B	0.29	0/1737	0.75	0/2360
1	C	0.31	0/1736	0.76	0/2359
1	D	0.33	0/1716	0.78	1/2332 (0.0%)
1	E	0.32	0/1723	0.76	0/2345
1	F	0.30	0/1720	0.78	0/2341
1	G	0.30	0/1704	0.75	0/2317
1	H	0.32	0/1661	0.78	0/2266
2	I	0.21	0/56	0.39	0/70
2	J	0.16	0/56	0.45	0/70
2	K	0.24	0/56	0.45	0/70
2	L	0.20	0/52	0.48	0/65
2	M	0.16	0/58	0.40	0/72
2	N	0.18	0/43	0.35	0/53
2	O	0.18	0/35	0.35	0/42
2	P	0.20	0/43	0.28	0/53
All	All	0.31	0/14136	0.76	2/19179 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1820	GLY	N-CA-C	5.55	120.88	114.16
1	D	1672	HIS	N-CA-C	-5.15	100.34	108.73

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	1699	0	1655	32	0
1	B	1696	0	1651	17	0
1	C	1695	0	1649	15	4
1	D	1677	0	1633	17	2
1	E	1682	0	1620	27	4
1	F	1679	0	1623	15	0
1	G	1664	0	1622	37	0
1	H	1623	0	1540	15	0
2	I	76	0	50	6	0
2	J	76	0	50	1	0
2	K	76	0	49	2	0
2	L	72	0	46	1	0
2	M	78	0	58	1	0
2	N	63	0	40	4	2
2	O	56	0	33	4	0
2	P	63	0	40	19	0
3	E	1	0	0	0	0
All	All	13976	0	13359	174	6

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 6.

All (174) 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:H:1651:SER:OG	1:H:1684:THR:HA	1.38	1.21
1:G:1670:ARG:NH2	2:P:407:PRO:HD3	1.62	1.14
1:G:1670:ARG:NH2	2:P:407:PRO:CD	2.23	1.00
1:G:1670:ARG:HH22	2:P:407:PRO:CD	1.76	0.97
1:D:1669:ALA:O	1:D:1672:HIS:O	1.88	0.92
1:H:1650:MET:HE1	1:H:1728:MET:HE1	1.54	0.89
1:E:1672:HIS:CG	1:E:1728:MET:CE	2.60	0.85
1:F:1824:ILE:HB	1:F:1857:GLN:HE22	1.44	0.83
1:H:1651:SER:HG	1:H:1684:THR:HA	1.45	0.82
1:E:1672:HIS:CE1	1:E:1728:MET:HE3	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1670:ARG:HH22	2:P:407:PRO:HD2	1.48	0.79
1:G:1670:ARG:HH21	2:P:407:PRO:HD3	1.49	0.78
1:E:1672:HIS:CD2	1:E:1728:MET:CE	2.68	0.77
2:P:404:SEP:O2P	2:P:404:SEP:HA	1.87	0.74
1:C:1691:THR:HG22	1:C:1697:CYS:HB3	1.70	0.73
1:E:1672:HIS:CG	1:E:1728:MET:HE3	2.23	0.73
1:E:1672:HIS:CD2	1:E:1728:MET:HE3	2.26	0.71
1:G:1774:ASN:HB3	2:O:407:PRO:HB3	1.74	0.70
1:G:1670:ARG:HH22	2:P:406:SEP:HA	1.57	0.70
1:G:1769:TYR:HB3	1:G:1810:VAL:HG12	1.75	0.69
1:E:1769:TYR:HB3	1:E:1810:VAL:HG12	1.75	0.69
1:A:1691:THR:HG22	1:A:1697:CYS:HB3	1.77	0.66
1:B:1819:ASN:HB2	1:C:1728:MET:HB3	1.78	0.66
1:E:1691:THR:HG22	1:E:1697:CYS:HB3	1.77	0.65
1:A:1729:LEU:CD2	1:E:1817:GLU:HA	2.26	0.65
1:G:1670:ARG:NH2	2:P:407:PRO:HD2	2.05	0.65
1:C:1769:TYR:HB3	1:C:1810:VAL:HG12	1.79	0.64
1:F:1769:TYR:HB3	1:F:1810:VAL:HG12	1.77	0.64
1:G:1656:GLY:N	2:O:406:SEP:O3P	2.31	0.62
1:H:1765:GLU:HG2	1:H:1790:SER:HB3	1.81	0.62
1:E:1657:LEU:HD23	1:E:1690:LYS:HB2	1.82	0.62
1:G:1670:ARG:NH2	2:P:406:SEP:HA	2.14	0.62
1:E:1672:HIS:ND1	1:E:1728:MET:HE3	2.15	0.61
1:H:1858:ILE:HD12	1:H:1859:PRO:HD2	1.82	0.61
1:A:1775:MET:HE3	2:I:409:PHE:HE2	1.65	0.61
1:A:1729:LEU:HD23	1:E:1817:GLU:HA	1.83	0.60
1:D:1662:PHE:HD2	1:D:1663:MET:HE2	1.68	0.59
1:B:1769:TYR:HB3	1:B:1810:VAL:HG12	1.85	0.59
1:C:1657:LEU:HD23	1:C:1690:LYS:HB2	1.83	0.59
1:B:1722:SER:OG	1:B:1727:LYS:O	2.16	0.58
1:A:1663:MET:HG3	1:B:1663:MET:HE2	1.86	0.58
1:G:1655:SER:HB2	1:G:1702:LYS:HD2	1.86	0.58
2:O:404:SEP:O3P	2:O:404:SEP:HA	2.04	0.57
1:E:1833:VAL:HG11	1:E:1850:LEU:HD22	1.86	0.57
1:G:1691:THR:HG22	1:G:1697:CYS:HB3	1.87	0.56
1:H:1742:ASN:HB3	1:H:1844:LEU:HD21	1.85	0.56
1:E:1672:HIS:NE2	1:E:1728:MET:HE3	2.21	0.56
1:B:1691:THR:HG22	1:B:1697:CYS:HB3	1.87	0.56
1:H:1769:TYR:HB3	1:H:1810:VAL:HG12	1.88	0.56
1:F:1761:PHE:HB3	1:F:1789:ALA:HB2	1.88	0.56
1:G:1666:TYR:OH	2:P:406:SEP:O1P	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1742:ASN:HB3	1:G:1844:LEU:HD21	1.88	0.54
1:C:1655:SER:OG	2:K:406:SEP:O1P	2.24	0.54
1:G:1655:SER:HA	2:O:406:SEP:O3P	2.07	0.54
1:D:1668:PHE:CE1	1:D:1672:HIS:CE1	2.96	0.54
1:D:1769:TYR:HB3	1:D:1810:VAL:HG12	1.89	0.54
2:I:404:SEP:O2P	2:I:404:SEP:HA	2.08	0.53
1:B:1670:ARG:NH1	2:I:406:SEP:O2P	2.41	0.53
1:C:1832:VAL:HG21	1:C:1857:GLN:NE2	2.23	0.53
1:A:1652:MET:HE3	1:A:1676:LEU:HD13	1.91	0.53
1:B:1670:ARG:NH2	2:I:404:SEP:O	2.41	0.53
1:B:1655:SER:HA	2:J:406:SEP:O2P	2.08	0.53
1:E:1672:HIS:C	1:E:1673:HIS:CG	2.86	0.53
1:E:1672:HIS:CG	1:E:1728:MET:HE1	2.43	0.52
1:A:1769:TYR:HB3	1:A:1810:VAL:HG12	1.92	0.52
1:G:1670:ARG:NH1	2:P:406:SEP:OG	2.41	0.52
1:A:1659:PRO:HD3	2:I:403:TYR:CE2	2.45	0.51
1:D:1657:LEU:HD23	1:D:1690:LYS:HB2	1.92	0.51
1:G:1707:ILE:HG23	1:G:1752:ALA:HB2	1.91	0.51
1:E:1672:HIS:CD2	1:E:1728:MET:HE2	2.44	0.51
1:B:1730:ASN:HD21	1:B:1732:HIS:HD2	1.58	0.50
1:C:1833:VAL:HG11	1:C:1850:LEU:HD22	1.93	0.49
1:A:1701:LEU:HD13	1:A:1775:MET:HE2	1.95	0.49
1:B:1831:PRO:HA	1:C:1647:ASN:OD1	2.12	0.49
1:D:1653:VAL:HG21	1:D:1680:ILE:HB	1.94	0.49
1:D:1765:GLU:HG2	1:D:1790:SER:HB3	1.95	0.49
1:G:1682:GLU:HG3	1:G:1782:TRP:HZ2	1.78	0.49
1:D:1736:VAL:HG22	1:D:1749:PRO:HG2	1.94	0.49
1:G:1684:THR:O	1:G:1711:LYS:HD3	2.12	0.48
1:H:1682:GLU:H	1:H:1682:GLU:CD	2.21	0.48
1:A:1655:SER:HB2	1:A:1702:LYS:HD2	1.96	0.48
1:A:1695:PHE:HB3	1:A:1736:VAL:HA	1.94	0.48
1:A:1819:ASN:ND2	1:A:1822:HIS:HD2	2.11	0.48
1:D:1784:VAL:HB	1:D:1789:ALA:HB3	1.94	0.48
1:F:1653:VAL:HG21	1:F:1680:ILE:HB	1.95	0.48
1:G:1761:PHE:HB3	1:G:1789:ALA:HB2	1.95	0.48
1:H:1746:HIS:O	1:H:1751:ARG:NH2	2.38	0.48
1:G:1685:THR:O	1:G:1712:TRP:HB2	2.13	0.47
1:C:1650:MET:HE3	1:C:1674:ILE:HG23	1.97	0.47
1:C:1742:ASN:HB3	1:C:1844:LEU:HD21	1.96	0.47
1:F:1784:VAL:HB	1:F:1789:ALA:HB3	1.95	0.47
1:C:1775:MET:HE3	2:K:409:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1799:THR:HB	1:D:1804:VAL:HG11	1.97	0.47
1:D:1833:VAL:HG11	1:D:1850:LEU:HD22	1.97	0.47
1:G:1669:ALA:HA	1:G:1674:ILE:HB	1.97	0.47
1:A:1761:PHE:HB3	1:A:1789:ALA:HB2	1.96	0.46
1:D:1701:LEU:HD13	1:D:1775:MET:HG3	1.96	0.46
1:F:1808:VAL:HB	1:F:1832:VAL:HG22	1.97	0.46
1:E:1701:LEU:HD13	1:E:1775:MET:HE2	1.98	0.46
1:G:1833:VAL:HG11	1:G:1850:LEU:HD22	1.98	0.46
2:M:402:GLU:N	2:M:402:GLU:OE1	2.49	0.46
2:N:403:TYR:O	2:N:404:SEP:CB	2.62	0.46
1:A:1678:ASN:OD1	1:B:1676:LEU:N	2.47	0.46
1:A:1817:GLU:HG2	1:A:1818:ASP:HB2	1.98	0.46
1:H:1775:MET:HE3	2:P:409:PHE:CE2	2.51	0.46
1:B:1750:LYS:HG3	1:B:1753:ARG:NH2	2.30	0.46
1:A:1719:VAL:O	1:A:1723:ILE:HG13	2.16	0.46
1:H:1761:PHE:HB3	1:H:1789:ALA:HB2	1.98	0.46
1:H:1806:PRO:O	1:H:1831:PRO:HD2	2.16	0.45
1:G:1670:ARG:HH12	2:P:406:SEP:HA	1.82	0.45
1:D:1651:SER:HA	1:D:1675:THR:HB	1.97	0.45
1:H:1712:TRP:HH2	1:H:1732:HIS:NE2	2.14	0.45
1:F:1821:PHE:O	1:F:1857:GLN:NE2	2.39	0.45
1:C:1668:PHE:CD2	1:C:1719:VAL:HG13	2.52	0.45
1:A:1784:VAL:HB	1:A:1789:ALA:HB3	1.99	0.45
1:A:1819:ASN:HD21	1:A:1822:HIS:HD2	1.65	0.45
1:F:1656:GLY:N	2:N:406:SEP:O2P	2.43	0.45
1:E:1823:ALA:O	1:E:1826:GLN:HG2	2.17	0.45
1:G:1654:VAL:HB	1:G:1657:LEU:HD12	1.99	0.44
1:F:1765:GLU:HG2	1:F:1790:SER:HB3	1.99	0.44
1:F:1768:CYS:HB3	1:F:1772:PHE:HE1	1.83	0.44
1:G:1670:ARG:HH21	2:P:407:PRO:CD	2.17	0.44
1:A:1674:ILE:HD11	1:A:1728:MET:HE1	1.99	0.44
1:B:1742:ASN:HB3	1:B:1844:LEU:HD21	1.98	0.44
1:E:1761:PHE:HB3	1:E:1789:ALA:HB2	1.99	0.44
1:A:1819:ASN:HB2	1:F:1728:MET:O	2.18	0.44
1:D:1695:PHE:HB3	1:D:1736:VAL:HA	2.00	0.44
1:E:1672:HIS:O	1:E:1673:HIS:ND1	2.51	0.44
1:G:1670:ARG:NH1	2:P:406:SEP:HA	2.33	0.44
1:D:1742:ASN:HB3	1:D:1844:LEU:HD21	1.99	0.43
1:E:1654:VAL:HG21	1:E:1662:PHE:HD1	1.83	0.43
1:G:1682:GLU:H	1:G:1682:GLU:CD	2.26	0.43
1:H:1704:PHE:HE1	2:P:409:PHE:HD2	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1742:ASN:HB3	1:A:1844:LEU:HD21	2.00	0.43
1:D:1755:SER:HB3	1:D:1758:ARG:HG3	1.99	0.43
1:E:1668:PHE:CE1	1:E:1672:HIS:CD2	3.07	0.43
1:G:1670:ARG:HH12	2:P:406:SEP:CA	2.32	0.43
1:A:1668:PHE:CD2	1:A:1719:VAL:HG13	2.54	0.43
1:B:1806:PRO:O	1:B:1831:PRO:HD2	2.19	0.43
1:F:1730:ASN:OD1	1:F:1732:HIS:HB2	2.19	0.43
1:E:1655:SER:HB2	1:E:1702:LYS:HD2	2.01	0.42
1:G:1668:PHE:CD1	1:G:1723:ILE:HG12	2.54	0.42
1:G:1658:THR:N	1:G:1661:GLU:OE1	2.48	0.42
1:B:1855:ILE:HA	1:B:1856:PRO:HD3	1.90	0.42
1:G:1850:LEU:O	1:G:1854:LEU:HG	2.19	0.42
2:L:406:SEP:HA	2:L:407:PRO:HD3	1.83	0.42
1:A:1730:ASN:OD1	1:A:1732:HIS:HB2	2.19	0.42
1:E:1742:ASN:HB3	1:E:1844:LEU:HD21	2.01	0.42
1:C:1684:THR:O	1:C:1711:LYS:HD3	2.20	0.42
1:F:1659:PRO:HG3	2:N:403:TYR:CZ	2.55	0.42
1:D:1761:PHE:HA	1:D:1764:LEU:HD12	2.01	0.42
1:A:1714:VAL:HG11	1:A:1731:GLU:HB3	2.01	0.42
1:A:1775:MET:HE3	2:I:409:PHE:CE2	2.51	0.42
1:H:1771:PRO:HD2	1:H:1815:TRP:CD1	2.55	0.41
1:A:1806:PRO:O	1:A:1831:PRO:HD2	2.20	0.41
1:A:1653:VAL:HG21	1:A:1680:ILE:HB	2.03	0.41
1:A:1762:ARG:HE	1:A:1762:ARG:HB3	1.73	0.41
1:B:1761:PHE:HB3	1:B:1789:ALA:HB2	2.03	0.41
1:C:1701:LEU:HD13	1:C:1775:MET:HE2	2.03	0.41
1:G:1665:VAL:HG22	1:G:1719:VAL:HG11	2.03	0.41
1:A:1679:LEU:HD12	1:B:1675:THR:OG1	2.21	0.41
1:A:1681:THR:OG1	1:A:1682:GLU:N	2.54	0.40
1:E:1669:ALA:O	1:E:1673:HIS:N	2.54	0.40
1:A:1721:GLN:OE1	1:A:1724:LYS:HD3	2.21	0.40
1:C:1731:GLU:H	1:C:1731:GLU:HG2	1.70	0.40
1:F:1858:ILE:HA	1:F:1859:PRO:HD2	1.95	0.40
1:E:1801:GLY:O	1:E:1804:VAL:HG22	2.22	0.40
1:G:1670:ARG:HH22	2:P:406:SEP:CA	2.28	0.40
1:F:1742:ASN:HB3	1:F:1844:LEU:HD21	2.03	0.40
2:N:406:SEP:HA	2:N:407:PRO:HD2	1.94	0.40
1:A:1661:GLU:O	1:A:1665:VAL:HG23	2.21	0.40
1:E:1858:ILE:HA	1:E:1859:PRO:HD3	1.88	0.40
1:G:1670:ARG:CZ	2:P:406:SEP:HA	2.51	0.40
1:G:1765:GLU:HG2	1:G:1790:SER:HB3	2.03	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1663:MET:SD	1:E:1663:MET:SD[4_445]	1.03	1.17
1:C:1663:MET:SD	1:E:1663:MET:CG[4_445]	1.80	0.40
1:C:1663:MET:SD	1:E:1663:MET:CE[4_445]	1.91	0.29
1:C:1663:MET:CE	1:E:1663:MET:CG[4_445]	1.94	0.26
1:D:1670:ARG:NH2	2:N:406:SEP:O1P[3_544]	2.06	0.14
1:D:1670:ARG:NH2	2:N:405:ARG:O[3_544]	2.11	0.09

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	212/224 (95%)	206 (97%)	6 (3%)	0	100	100
1	B	212/224 (95%)	207 (98%)	5 (2%)	0	100	100
1	C	212/224 (95%)	207 (98%)	5 (2%)	0	100	100
1	D	211/224 (94%)	205 (97%)	6 (3%)	0	100	100
1	E	212/224 (95%)	205 (97%)	7 (3%)	0	100	100
1	F	212/224 (95%)	206 (97%)	6 (3%)	0	100	100
1	G	209/224 (93%)	203 (97%)	6 (3%)	0	100	100
1	H	209/224 (93%)	202 (97%)	7 (3%)	0	100	100
2	I	5/11 (46%)	5 (100%)	0	0	100	100
2	J	5/11 (46%)	5 (100%)	0	0	100	100
2	K	5/11 (46%)	5 (100%)	0	0	100	100
2	L	4/11 (36%)	4 (100%)	0	0	100	100
2	M	4/11 (36%)	4 (100%)	0	0	100	100
2	N	3/11 (27%)	2 (67%)	1 (33%)	0	100	100
2	O	3/11 (27%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	3/11 (27%)	3 (100%)	0	0	100	100
All	All	1721/1880 (92%)	1672 (97%)	49 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/201 (92%)	184 (99%)	2 (1%)	65	74
1	B	186/201 (92%)	183 (98%)	3 (2%)	55	70
1	C	185/201 (92%)	183 (99%)	2 (1%)	65	74
1	D	182/201 (90%)	179 (98%)	3 (2%)	55	70
1	E	183/201 (91%)	182 (100%)	1 (0%)	81	80
1	F	182/201 (90%)	179 (98%)	3 (2%)	55	70
1	G	181/201 (90%)	180 (99%)	1 (1%)	78	79
1	H	172/201 (86%)	170 (99%)	2 (1%)	63	73
2	I	5/7 (71%)	5 (100%)	0	100	100
2	J	5/7 (71%)	5 (100%)	0	100	100
2	K	5/7 (71%)	5 (100%)	0	100	100
2	L	5/7 (71%)	5 (100%)	0	100	100
2	M	6/7 (86%)	5 (83%)	1 (17%)	2	13
2	N	4/7 (57%)	4 (100%)	0	100	100
2	O	3/7 (43%)	3 (100%)	0	100	100
2	P	4/7 (57%)	4 (100%)	0	100	100
All	All	1494/1664 (90%)	1476 (99%)	18 (1%)	63	73

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1728	MET
1	A	1736	VAL
1	B	1670	ARG
1	B	1728	MET
1	B	1736	VAL
1	C	1728	MET
1	C	1736	VAL
1	D	1728	MET
1	D	1736	VAL
1	D	1793	LYS
1	E	1736	VAL
1	F	1728	MET
1	F	1736	VAL
1	F	1855	ILE
1	G	1736	VAL
1	H	1728	MET
1	H	1736	VAL
2	M	405	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1672	HIS
1	B	1730	ASN
1	B	1848	GLN
1	C	1672	HIS
1	C	1732	HIS
1	C	1848	GLN
1	D	1673	HIS
1	D	1730	ASN
1	E	1672	HIS
1	E	1779	GLN
1	E	1848	GLN
1	F	1730	ASN
1	G	1672	HIS
1	H	1672	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 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	M	404	2	8,9,10	0.90	0	7,12,14	1.09	0
2	SEP	O	404	2	8,9,10	0.83	0	7,12,14	1.00	0
2	SEP	N	404	2	8,9,10	0.78	0	7,12,14	1.11	0
2	SEP	I	406	2	8,9,10	0.83	0	7,12,14	1.26	0
2	SEP	O	406	2	8,9,10	0.77	0	7,12,14	1.48	1 (14%)
2	SEP	J	406	2	8,9,10	0.85	0	7,12,14	1.82	1 (14%)
2	SEP	L	406	2	8,9,10	0.81	0	7,12,14	1.34	1 (14%)
2	SEP	M	406	2	8,9,10	0.89	0	7,12,14	1.37	0
2	SEP	I	404	2	8,9,10	0.88	0	7,12,14	1.19	0
2	SEP	P	404	2	8,9,10	0.85	0	7,12,14	1.02	0
2	SEP	N	406	2	8,9,10	0.85	0	7,12,14	1.21	0
2	SEP	J	404	2	8,9,10	0.83	0	7,12,14	1.17	0
2	SEP	L	404	2	8,9,10	0.80	0	7,12,14	1.22	0
2	SEP	K	406	2	8,9,10	0.83	0	7,12,14	1.19	0
2	SEP	K	404	2	8,9,10	0.87	0	7,12,14	1.08	0
2	SEP	P	406	2	8,9,10	0.75	0	7,12,14	1.10	0

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	M	404	2	-	0/6/8/10	-
2	SEP	O	404	2	-	1/6/8/10	-
2	SEP	N	404	2	-	3/6/8/10	-
2	SEP	I	406	2	-	5/6/8/10	-
2	SEP	O	406	2	-	0/6/8/10	-
2	SEP	J	406	2	-	4/6/8/10	-
2	SEP	L	406	2	-	3/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	M	406	2	-	2/6/8/10	-
2	SEP	I	404	2	-	3/6/8/10	-
2	SEP	P	404	2	-	3/6/8/10	-
2	SEP	N	406	2	-	2/6/8/10	-
2	SEP	J	404	2	-	2/6/8/10	-
2	SEP	L	404	2	-	1/6/8/10	-
2	SEP	K	406	2	-	2/6/8/10	-
2	SEP	K	404	2	-	0/6/8/10	-
2	SEP	P	406	2	-	2/6/8/10	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	406	SEP	OG-CB-CA	3.89	111.93	108.14
2	O	406	SEP	OG-CB-CA	2.85	110.92	108.14
2	L	406	SEP	OG-CB-CA	2.24	110.32	108.14

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	404	SEP	N-CA-CB-OG
2	I	404	SEP	C-CA-CB-OG
2	I	406	SEP	N-CA-CB-OG
2	I	406	SEP	C-CA-CB-OG
2	I	406	SEP	CB-OG-P-O1P
2	I	406	SEP	CB-OG-P-O2P
2	I	406	SEP	CB-OG-P-O3P
2	J	404	SEP	N-CA-CB-OG
2	J	404	SEP	C-CA-CB-OG
2	J	406	SEP	N-CA-CB-OG
2	J	406	SEP	CB-OG-P-O2P
2	K	406	SEP	N-CA-CB-OG
2	K	406	SEP	C-CA-CB-OG
2	L	404	SEP	CA-CB-OG-P
2	L	406	SEP	CB-OG-P-O2P
2	L	406	SEP	CB-OG-P-O3P
2	M	406	SEP	N-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
2	M	406	SEP	C-CA-CB-OG
2	N	404	SEP	N-CA-CB-OG
2	N	404	SEP	CA-CB-OG-P
2	N	406	SEP	N-CA-CB-OG
2	N	406	SEP	C-CA-CB-OG
2	P	404	SEP	N-CA-CB-OG
2	P	404	SEP	C-CA-CB-OG
2	P	406	SEP	N-CA-CB-OG
2	L	406	SEP	CB-OG-P-O1P
2	I	404	SEP	CA-CB-OG-P
2	O	404	SEP	CA-CB-OG-P
2	J	406	SEP	CB-OG-P-O1P
2	J	406	SEP	CB-OG-P-O3P
2	P	404	SEP	CA-CB-OG-P
2	N	404	SEP	C-CA-CB-OG
2	P	406	SEP	C-CA-CB-OG

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	404	SEP	1	0
2	N	404	SEP	1	0
2	I	406	SEP	1	0
2	O	406	SEP	2	0
2	J	406	SEP	1	0
2	L	406	SEP	1	0
2	I	404	SEP	2	0
2	P	404	SEP	1	0
2	N	406	SEP	2	1
2	K	406	SEP	1	0
2	P	406	SEP	9	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	214/224 (95%)	-0.11	2 (0%) 81 58	75, 96, 126, 152	0
1	B	214/224 (95%)	-0.14	1 (0%) 87 68	67, 88, 115, 146	0
1	C	214/224 (95%)	-0.02	0 100 100	64, 96, 125, 160	0
1	D	213/224 (95%)	0.03	3 (1%) 73 48	77, 109, 151, 173	0
1	E	214/224 (95%)	-0.12	1 (0%) 87 68	68, 88, 115, 153	0
1	F	214/224 (95%)	0.07	4 (1%) 66 41	81, 111, 169, 181	0
1	G	211/224 (94%)	0.08	1 (0%) 87 68	92, 153, 191, 203	0
1	H	211/224 (94%)	0.23	4 (1%) 66 41	89, 161, 200, 220	0
2	I	7/11 (63%)	0.27	0 100 100	96, 101, 150, 151	0
2	J	7/11 (63%)	-0.10	0 100 100	81, 90, 121, 127	0
2	K	7/11 (63%)	0.30	0 100 100	96, 100, 136, 153	0
2	L	6/11 (54%)	0.27	1 (16%) 4 4	95, 99, 131, 141	0
2	M	6/11 (54%)	0.05	0 100 100	86, 89, 118, 150	0
2	N	5/11 (45%)	0.29	0 100 100	105, 106, 113, 113	0
2	O	5/11 (45%)	0.06	0 100 100	138, 139, 141, 145	0
2	P	5/11 (45%)	0.19	0 100 100	140, 146, 155, 155	0
All	All	1753/1880 (93%)	0.01	17 (0%) 79 56	64, 105, 180, 220	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1858	ILE	3.4
1	H	1660	GLU	3.0
1	H	1719	VAL	2.8
1	H	1716	TYR	2.6
1	F	1817	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1859	PRO	2.5
1	F	1646	VAL	2.4
1	F	1806	PRO	2.4
1	D	1646	VAL	2.4
1	A	1766	ILE	2.3
1	G	1716	TYR	2.2
1	H	1659	PRO	2.2
2	L	405	ARG	2.2
1	F	1818	ASP	2.2
1	B	1646	VAL	2.1
1	E	1646	VAL	2.1
1	D	1817	GLU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SEP	I	404	10/11	0.63	0.10	133,149,166,180	0
2	SEP	P	404	10/11	0.65	0.09	146,164,171,171	0
2	SEP	L	404	10/11	0.66	0.10	132,138,157,157	0
2	SEP	O	404	10/11	0.71	0.08	142,152,163,166	0
2	SEP	M	404	10/11	0.71	0.10	111,127,152,158	0
2	SEP	K	404	10/11	0.72	0.09	127,138,159,163	0
2	SEP	J	404	10/11	0.78	0.08	102,122,142,146	0
2	SEP	P	406	10/11	0.81	0.10	149,153,171,171	0
2	SEP	N	404	10/11	0.82	0.07	117,124,144,145	0
2	SEP	O	406	10/11	0.83	0.08	143,149,163,171	0
2	SEP	K	406	10/11	0.87	0.10	84,92,98,109	0
2	SEP	M	406	10/11	0.88	0.09	79,88,92,94	0
2	SEP	N	406	10/11	0.90	0.08	84,98,108,112	0
2	SEP	I	406	10/11	0.92	0.08	78,94,103,107	0
2	SEP	L	406	10/11	0.92	0.09	89,98,104,108	0
2	SEP	J	406	10/11	0.94	0.09	83,91,95,99	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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.