



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:15 AM UTC

PDB ID : 5U6K / pdb_00005u6k
Title : Crystal structure of TopBP1 BRCT4/5 in complex with a BLM phosphopeptide
Authors : Glover, J.N.M.; Sun, L.; Edwards, R.A.
Deposited on : 2016-12-08
Resolution : 2.60 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

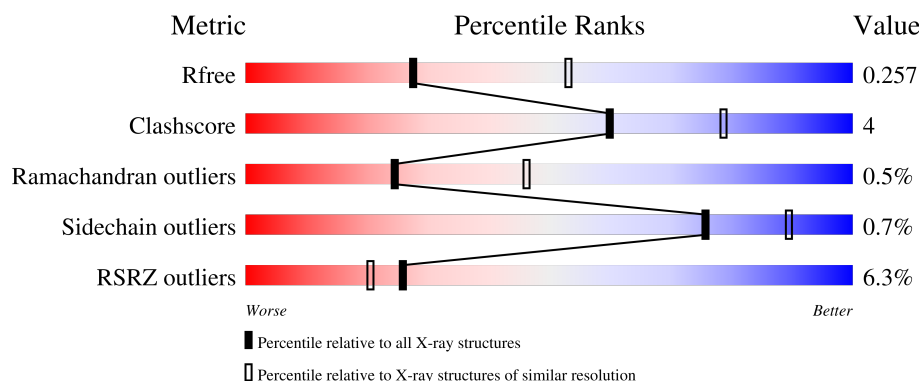
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	200	4% 82% 12% 5%
1	B	200	4% 86% 9% 5%
1	C	200	2% 82% 12% 5%
1	D	200	2% 85% 10% 5%
1	E	200	2% 86% 9% 5%

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Mol	Chain	Length	Quality of chain
1	F	200	14% 87% 6%
1	G	200	8% 84% 11%
1	H	200	12% 84% 12%
2	L	13	23% 15% 8% 54%
2	M	13	8% 31% 15% 54%
2	N	13	8% 23% 8% 8% 62%
2	O	13	62% 8% 8% 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11899 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 DNA topoisomerase 2-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1455	931	245	272	7			
1	B	190	Total	C	N	O	S	0	0	0
			1455	931	245	272	7			
1	C	190	Total	C	N	O	S	0	0	0
			1455	931	245	272	7			
1	D	190	Total	C	N	O	S	0	0	0
			1455	931	245	272	7			
1	E	191	Total	C	N	O	S	0	0	0
			1464	936	246	275	7			
1	F	191	Total	C	N	O	S	0	0	0
			1464	936	246	275	7			
1	G	191	Total	C	N	O	S	0	0	0
			1464	936	246	275	7			
1	H	191	Total	C	N	O	S	0	0	0
			1464	936	246	275	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	547	GLY	-	expression tag	UNP Q6ZQF0
A	548	PRO	-	expression tag	UNP Q6ZQF0
A	549	LEU	-	expression tag	UNP Q6ZQF0
A	550	GLY	-	expression tag	UNP Q6ZQF0
A	551	SER	-	expression tag	UNP Q6ZQF0
A	552	MET	-	expression tag	UNP Q6ZQF0
B	547	GLY	-	expression tag	UNP Q6ZQF0
B	548	PRO	-	expression tag	UNP Q6ZQF0
B	549	LEU	-	expression tag	UNP Q6ZQF0
B	550	GLY	-	expression tag	UNP Q6ZQF0
B	551	SER	-	expression tag	UNP Q6ZQF0
B	552	MET	-	expression tag	UNP Q6ZQF0
C	547	GLY	-	expression tag	UNP Q6ZQF0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	548	PRO	-	expression tag	UNP Q6ZQF0
C	549	LEU	-	expression tag	UNP Q6ZQF0
C	550	GLY	-	expression tag	UNP Q6ZQF0
C	551	SER	-	expression tag	UNP Q6ZQF0
C	552	MET	-	expression tag	UNP Q6ZQF0
D	547	GLY	-	expression tag	UNP Q6ZQF0
D	548	PRO	-	expression tag	UNP Q6ZQF0
D	549	LEU	-	expression tag	UNP Q6ZQF0
D	550	GLY	-	expression tag	UNP Q6ZQF0
D	551	SER	-	expression tag	UNP Q6ZQF0
D	552	MET	-	expression tag	UNP Q6ZQF0
E	547	GLY	-	expression tag	UNP Q6ZQF0
E	548	PRO	-	expression tag	UNP Q6ZQF0
E	549	LEU	-	expression tag	UNP Q6ZQF0
E	550	GLY	-	expression tag	UNP Q6ZQF0
E	551	SER	-	expression tag	UNP Q6ZQF0
E	552	MET	-	expression tag	UNP Q6ZQF0
F	547	GLY	-	expression tag	UNP Q6ZQF0
F	548	PRO	-	expression tag	UNP Q6ZQF0
F	549	LEU	-	expression tag	UNP Q6ZQF0
F	550	GLY	-	expression tag	UNP Q6ZQF0
F	551	SER	-	expression tag	UNP Q6ZQF0
F	552	MET	-	expression tag	UNP Q6ZQF0
G	547	GLY	-	expression tag	UNP Q6ZQF0
G	548	PRO	-	expression tag	UNP Q6ZQF0
G	549	LEU	-	expression tag	UNP Q6ZQF0
G	550	GLY	-	expression tag	UNP Q6ZQF0
G	551	SER	-	expression tag	UNP Q6ZQF0
G	552	MET	-	expression tag	UNP Q6ZQF0
H	547	GLY	-	expression tag	UNP Q6ZQF0
H	548	PRO	-	expression tag	UNP Q6ZQF0
H	549	LEU	-	expression tag	UNP Q6ZQF0
H	550	GLY	-	expression tag	UNP Q6ZQF0
H	551	SER	-	expression tag	UNP Q6ZQF0
H	552	MET	-	expression tag	UNP Q6ZQF0

- Molecule 2 is a protein called Bloom Syndrome recQ helicase like protein (BLM).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	6	Total 49	C 32	N 6	O 10	P 1	0	0	0
2	M	6	Total 49	C 32	N 6	O 10	P 1	0	0	0

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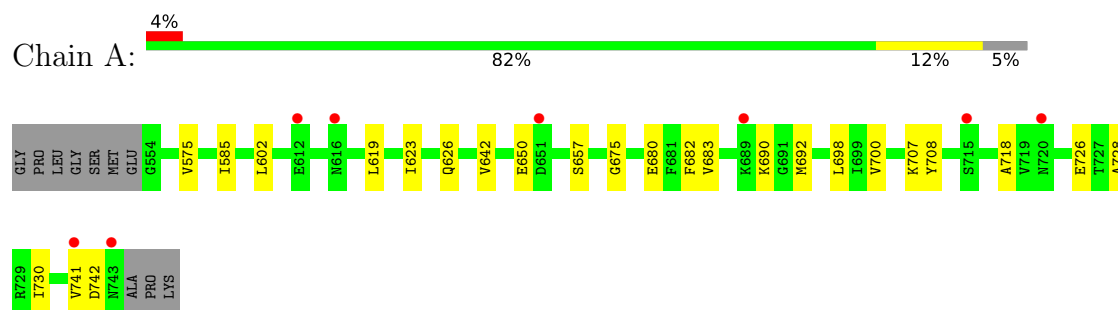
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	5	Total	C	N	O	P	0	0	0
			42	27	5	9	1			
2	O	10	Total	C	N	O	P	0	0	0
			83	54	10	18	1			

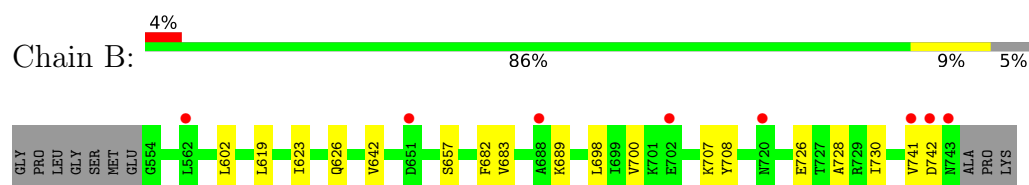
3 Residue-property plots [i](#)

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.

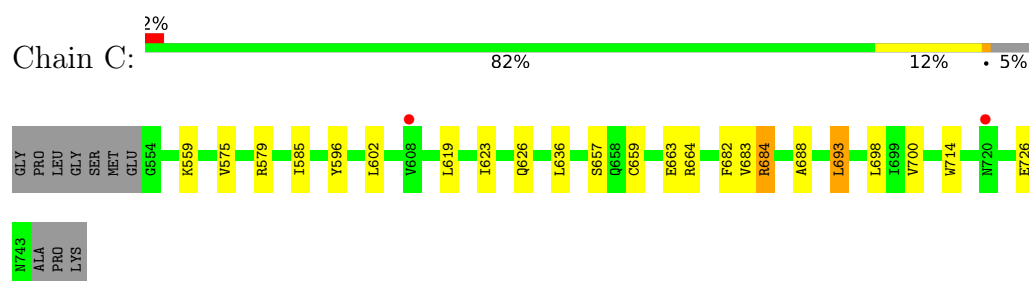
- Molecule 1: DNA topoisomerase 2-binding protein 1



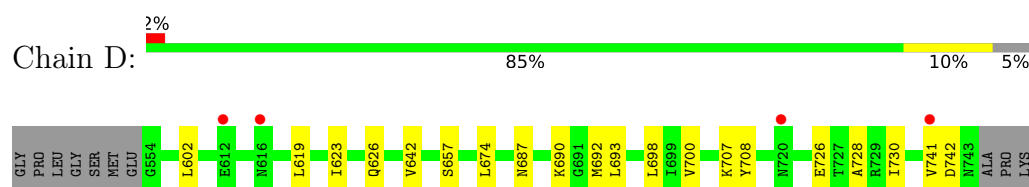
- Molecule 1: DNA topoisomerase 2-binding protein 1



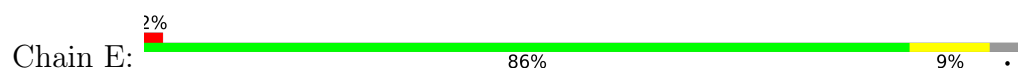
- Molecule 1: DNA topoisomerase 2-binding protein 1



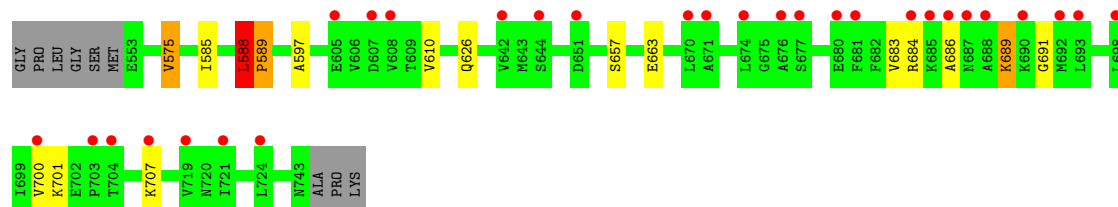
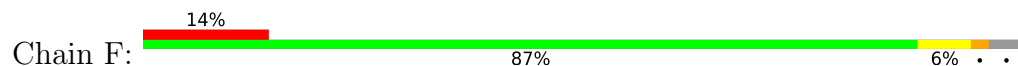
- Molecule 1: DNA topoisomerase 2-binding protein 1



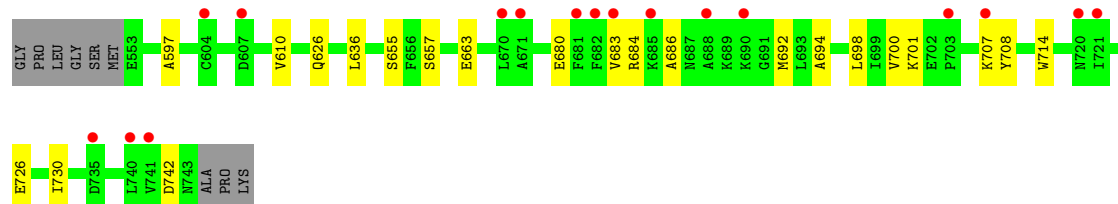
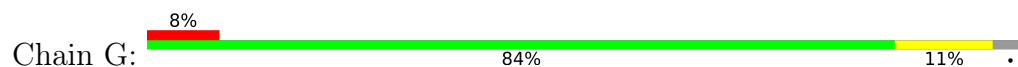
- Molecule 1: DNA topoisomerase 2-binding protein 1



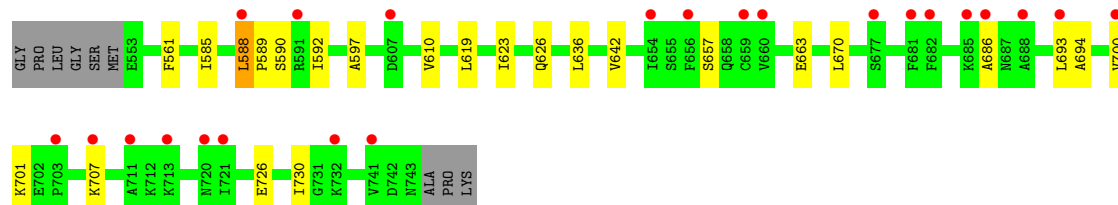
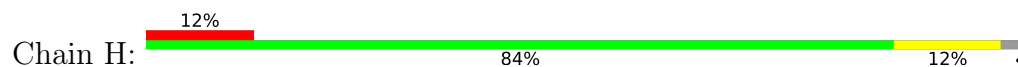
- Molecule 1: DNA topoisomerase 2-binding protein 1



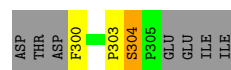
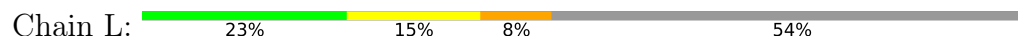
- Molecule 1: DNA topoisomerase 2-binding protein 1



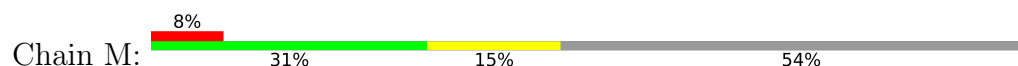
- Molecule 1: DNA topoisomerase 2-binding protein 1

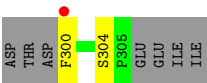


- Molecule 2: Bloom Syndrome recQ helicase like protein (BLM)

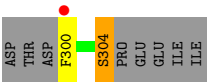


- Molecule 2: Bloom Syndrome recQ helicase like protein (BLM)

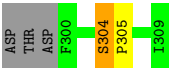




● Molecule 2: Bloom Syndrome recQ helicase like protein (BLM)



● Molecule 2: Bloom Syndrome recQ helicase like protein (BLM)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.16Å 96.82Å 127.05Å 90.00° 94.25° 90.00°	Depositor
Resolution (Å)	47.87 – 2.60 47.87 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (47.87-2.60) 98.2 (47.87-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.61Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.219 , 0.256 0.221 , 0.257	Depositor DCC
R_{free} test set	3646 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtrriage
Anisotropy	0.965	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 72.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11899	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2054e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.19	0/1483	0.37	0/2017
1	B	0.15	0/1483	0.32	0/2017
1	C	0.18	0/1483	0.35	0/2017
1	D	0.14	0/1483	0.31	0/2017
1	E	0.16	0/1492	0.32	0/2029
1	F	0.14	0/1492	0.33	0/2029
1	G	0.16	0/1492	0.35	0/2029
1	H	0.11	0/1492	0.29	0/2029
2	L	0.10	0/41	0.24	0/55
2	M	0.11	0/41	0.25	0/55
2	N	0.13	0/34	0.24	0/47
2	O	0.17	0/75	0.31	0/101
All	All	0.16	0/12091	0.33	0/16442

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	588	LEU	Peptide

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	1455	0	1480	17	0
1	B	1455	0	1480	12	0
1	C	1455	0	1480	17	0
1	D	1455	0	1480	14	0
1	E	1464	0	1486	14	0
1	F	1464	0	1486	9	0
1	G	1464	0	1486	13	0
1	H	1464	0	1486	12	0
2	L	49	0	42	3	0
2	M	49	0	42	1	0
2	N	42	0	35	2	0
2	O	83	0	76	3	0
All	All	11899	0	12059	104	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 4.

All (104) 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:C:657:SER:HB3	1:C:700:VAL:HG12	1.55	0.89
1:D:657:SER:HB3	1:D:700:VAL:HG12	1.57	0.86
1:C:659:CYS:O	1:C:664:ARG:NH1	2.08	0.86
1:E:713:LYS:HZ3	2:O:305:PRO:HD2	1.41	0.83
1:B:657:SER:HB3	1:B:700:VAL:HG12	1.58	0.83
1:A:657:SER:HB3	1:A:700:VAL:HG12	1.60	0.82
1:G:680:GLU:OE2	1:G:707:LYS:NZ	2.16	0.76
1:F:663:GLU:OE2	1:F:701:LYS:NZ	2.22	0.70
1:C:683:VAL:HG23	2:N:300:PHE:HB3	1.75	0.69
1:D:690:LYS:NZ	1:D:692:MET:HE2	2.10	0.65
1:D:657:SER:HB2	1:D:707:LYS:HD2	1.80	0.64
1:E:657:SER:HB3	1:E:700:VAL:HG13	1.78	0.64
1:F:689:LYS:HD3	1:F:691:GLY:H	1.63	0.63
1:E:708:TYR:OH	1:E:742:ASP:OD1	2.14	0.62
1:H:597:ALA:HB2	1:H:610:VAL:HG11	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:713:LYS:NZ	2:O:305:PRO:HD2	2.13	0.60
1:A:602:LEU:HG	1:E:626:GLN:OE1	2.02	0.60
1:C:602:LEU:HG	1:G:626:GLN:OE1	2.04	0.58
1:G:663:GLU:OE2	1:G:701:LYS:NZ	2.37	0.57
1:E:713:LYS:NZ	2:O:304:SEP:OG	2.37	0.57
1:D:690:LYS:HZ2	1:D:692:MET:HE2	1.70	0.55
1:H:588:LEU:HB3	1:H:589:PRO:HD2	1.89	0.55
1:B:623:ILE:O	1:B:626:GLN:NE2	2.39	0.55
1:F:597:ALA:HB2	1:F:610:VAL:HG11	1.90	0.54
1:D:602:LEU:HG	1:H:626:GLN:OE1	2.09	0.53
1:G:657:SER:HB2	1:G:707:LYS:HD2	1.90	0.53
1:C:657:SER:OG	2:N:304:SEP:O1P	2.23	0.52
1:A:619:LEU:O	1:A:623:ILE:HD12	2.09	0.52
1:A:726:GLU:OE2	1:A:730:ILE:HD11	2.10	0.52
1:A:683:VAL:HA	2:L:300:PHE:HA	1.92	0.52
1:H:726:GLU:OE2	1:H:730:ILE:HD11	2.10	0.52
1:H:657:SER:HB2	1:H:707:LYS:HD2	1.92	0.52
1:A:680:GLU:HG2	2:L:303:PRO:HB3	1.91	0.51
1:B:683:VAL:HA	2:M:300:PHE:HA	1.93	0.51
1:E:597:ALA:HB2	1:E:610:VAL:HG11	1.90	0.51
1:C:726:GLU:OE2	1:C:730:ILE:HD11	2.11	0.51
1:G:683:VAL:HA	1:G:714:TRP:CH2	2.46	0.50
1:G:726:GLU:OE2	1:G:730:ILE:HD11	2.12	0.50
1:F:657:SER:HB2	1:F:707:LYS:HD2	1.93	0.50
1:D:674:LEU:HD11	1:D:728:ALA:HB2	1.93	0.50
1:B:726:GLU:OE2	1:B:730:ILE:HD11	2.12	0.50
1:D:642:VAL:HG22	1:D:728:ALA:HB1	1.93	0.50
1:A:708:TYR:OH	1:A:742:ASP:OD1	2.19	0.49
1:B:698:LEU:HG	1:B:700:VAL:HG13	1.94	0.49
1:C:693:LEU:H	1:C:693:LEU:HD12	1.76	0.49
1:C:619:LEU:O	1:C:623:ILE:HD12	2.13	0.49
1:B:708:TYR:OH	1:B:742:ASP:OD1	2.27	0.48
1:G:636:LEU:HD12	1:G:663:GLU:HG3	1.95	0.48
1:A:642:VAL:HG22	1:A:728:ALA:HB1	1.95	0.47
1:D:726:GLU:OE2	1:D:730:ILE:HD11	2.14	0.47
1:D:708:TYR:OH	1:D:742:ASP:OD1	2.17	0.47
1:E:674:LEU:HD11	1:E:728:ALA:HB2	1.97	0.47
1:C:698:LEU:HG	1:C:700:VAL:HG13	1.96	0.47
1:G:683:VAL:HG12	1:G:684:ARG:HE	1.80	0.47
1:A:698:LEU:HG	1:A:700:VAL:HG13	1.97	0.47
1:E:698:LEU:HG	1:E:700:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:619:LEU:O	1:H:623:ILE:HD12	2.15	0.46
1:E:726:GLU:OE2	1:E:730:ILE:HD11	2.15	0.46
1:C:623:ILE:O	1:C:626:GLN:NE2	2.48	0.46
1:C:636:LEU:HD12	1:C:663:GLU:HG3	1.97	0.46
1:A:657:SER:HB2	1:A:707:LYS:HD2	1.98	0.45
1:C:575:VAL:HG13	1:C:585:ILE:CD1	2.46	0.45
1:D:700:VAL:CG2	1:D:741:VAL:HG21	2.47	0.45
1:C:684:ARG:HG2	1:C:714:TRP:CD2	2.52	0.45
1:A:657:SER:OG	2:L:304:SEP:O3P	2.23	0.45
1:G:597:ALA:HB2	1:G:610:VAL:HG11	1.98	0.45
1:D:698:LEU:HG	1:D:700:VAL:HG13	1.99	0.45
1:B:619:LEU:O	1:B:623:ILE:HD12	2.17	0.45
1:F:683:VAL:HG21	1:F:686:ALA:HB2	1.99	0.44
1:C:682:PHE:CE1	1:C:698:LEU:HB2	2.51	0.44
1:A:650:GLU:HA	1:A:675:GLY:O	2.17	0.44
1:A:682:PHE:CE1	1:A:698:LEU:HB2	2.52	0.44
1:A:718:ALA:O	1:A:741:VAL:HG23	2.18	0.44
1:G:683:VAL:HA	1:G:714:TRP:HH2	1.82	0.44
1:B:657:SER:HB2	1:B:707:LYS:HD2	2.00	0.44
1:B:642:VAL:HG22	1:B:728:ALA:HB1	1.99	0.44
1:H:561:PHE:HB2	1:H:585:ILE:HD13	2.00	0.44
1:H:663:GLU:OE2	1:H:701:LYS:NZ	2.43	0.44
1:D:623:ILE:O	1:D:626:GLN:NE2	2.50	0.43
1:C:700:VAL:CG2	1:C:741:VAL:HG21	2.48	0.43
1:H:590:SER:C	1:H:592:ILE:H	2.26	0.43
1:A:623:ILE:O	1:A:626:GLN:NE2	2.50	0.43
1:G:708:TYR:OH	1:G:742:ASP:OD1	2.28	0.43
1:E:657:SER:HB2	1:E:707:LYS:HD2	2.01	0.43
1:A:690:LYS:HD2	1:A:692:MET:HE2	2.00	0.42
1:H:642:VAL:HG21	1:H:670:LEU:HD21	2.02	0.42
1:F:588:LEU:HB3	1:F:589:PRO:CD	2.50	0.42
1:A:575:VAL:HG13	1:A:585:ILE:CD1	2.50	0.42
1:D:619:LEU:O	1:D:623:ILE:HD12	2.19	0.42
1:F:575:VAL:HG13	1:F:585:ILE:CD1	2.50	0.42
1:E:650:GLU:HA	1:E:675:GLY:O	2.20	0.42
1:B:700:VAL:CG2	1:B:741:VAL:HG21	2.50	0.42
1:B:682:PHE:CE1	1:B:698:LEU:HB2	2.55	0.41
1:C:579:ARG:NE	1:C:585:ILE:HD12	2.35	0.41
1:E:642:VAL:HG21	1:E:670:LEU:HD21	2.03	0.41
1:H:636:LEU:HD12	1:H:663:GLU:HG3	2.02	0.41
1:G:655:SER:O	1:G:698:LEU:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:686:ALA:N	1:G:694:ALA:HB2	2.36	0.41
1:H:686:ALA:HB2	1:H:694:ALA:HB2	2.03	0.41
1:B:602:LEU:HG	1:F:626:GLN:OE1	2.21	0.41
1:C:559:LYS:HD2	1:C:596:TYR:HE2	1.86	0.40
1:E:643:MET:HE3	1:E:643:MET:HB2	1.97	0.40
1:F:575:VAL:HG22	1:F:585:ILE:HD13	2.03	0.40
1:D:687:ASN:HD22	1:D:692:MET:HE3	1.86	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	188/200 (94%)	185 (98%)	3 (2%)	0	100	100
1	B	188/200 (94%)	182 (97%)	5 (3%)	1 (0%)	24	46
1	C	188/200 (94%)	182 (97%)	4 (2%)	2 (1%)	11	25
1	D	188/200 (94%)	182 (97%)	6 (3%)	0	100	100
1	E	189/200 (94%)	187 (99%)	2 (1%)	0	100	100
1	F	189/200 (94%)	177 (94%)	9 (5%)	3 (2%)	7	16
1	G	189/200 (94%)	182 (96%)	7 (4%)	0	100	100
1	H	189/200 (94%)	180 (95%)	8 (4%)	1 (0%)	24	46
2	L	3/13 (23%)	3 (100%)	0	0	100	100
2	M	3/13 (23%)	3 (100%)	0	0	100	100
2	N	3/13 (23%)	3 (100%)	0	0	100	100
2	O	7/13 (54%)	7 (100%)	0	0	100	100
All	All	1524/1652 (92%)	1473 (97%)	44 (3%)	7 (0%)	24	46

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	684	ARG
1	F	588	LEU
1	F	589	PRO
1	H	588	LEU
1	F	684	ARG
1	B	689	LYS
1	C	688	ALA

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	165/172 (96%)	165 (100%)	0	100	100
1	B	165/172 (96%)	165 (100%)	0	100	100
1	C	165/172 (96%)	164 (99%)	1 (1%)	78	91
1	D	165/172 (96%)	164 (99%)	1 (1%)	78	91
1	E	166/172 (96%)	165 (99%)	1 (1%)	78	91
1	F	166/172 (96%)	163 (98%)	3 (2%)	51	76
1	G	166/172 (96%)	164 (99%)	2 (1%)	63	83
1	H	166/172 (96%)	164 (99%)	2 (1%)	63	83
2	L	5/12 (42%)	5 (100%)	0	100	100
2	M	5/12 (42%)	5 (100%)	0	100	100
2	N	4/12 (33%)	4 (100%)	0	100	100
2	O	9/12 (75%)	9 (100%)	0	100	100
All	All	1347/1424 (95%)	1337 (99%)	10 (1%)	76	89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	693	LEU
1	D	693	LEU
1	E	700	VAL
1	F	575	VAL

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Mol	Chain	Res	Type
1	F	689	LYS
1	F	700	VAL
1	G	692	MET
1	G	700	VAL
1	H	693	LEU
1	H	700	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	687	ASN
1	D	687	ASN
1	E	558	GLN
1	E	720	ASN
1	G	720	ASN
1	H	720	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	O	304	2	8,9,10	1.64	1 (12%)	7,12,14	1.29	1 (14%)
2	SEP	M	304	2	8,9,10	1.60	1 (12%)	7,12,14	1.38	1 (14%)
2	SEP	L	304	2	8,9,10	1.59	1 (12%)	7,12,14	1.18	1 (14%)
2	SEP	N	304	2	8,9,10	1.61	1 (12%)	7,12,14	1.28	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SEP	O	304	2	-	4/6/8/10	-
2	SEP	M	304	2	-	3/6/8/10	-
2	SEP	L	304	2	-	3/6/8/10	-
2	SEP	N	304	2	-	0/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	304	SEP	P-O1P	3.55	1.61	1.50
2	N	304	SEP	P-O1P	3.53	1.61	1.50
2	M	304	SEP	P-O1P	3.52	1.61	1.50
2	L	304	SEP	P-O1P	3.48	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	304	SEP	OG-CB-CA	3.03	111.09	108.14
2	N	304	SEP	OG-CB-CA	2.82	110.89	108.14
2	O	304	SEP	OG-CB-CA	2.74	110.81	108.14
2	L	304	SEP	OG-CB-CA	2.44	110.52	108.14

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	304	SEP	CB-OG-P-O1P
2	L	304	SEP	CB-OG-P-O3P
2	M	304	SEP	CB-OG-P-O1P
2	M	304	SEP	CB-OG-P-O3P
2	O	304	SEP	CB-OG-P-O1P
2	O	304	SEP	CB-OG-P-O3P
2	O	304	SEP	CA-CB-OG-P
2	L	304	SEP	CB-OG-P-O2P
2	M	304	SEP	CB-OG-P-O2P
2	O	304	SEP	CB-OG-P-O2P

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	304	SEP	1	0
2	L	304	SEP	1	0
2	N	304	SEP	1	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(Å²)	Q<0.9
1	A	190/200 (95%)	0.14	8 (4%)	40	35	36, 71, 136, 162	0
1	B	190/200 (95%)	0.35	8 (4%)	40	35	60, 88, 142, 189	0
1	C	190/200 (95%)	0.04	3 (1%)	70	66	48, 75, 129, 182	0
1	D	190/200 (95%)	0.29	4 (2%)	63	58	58, 90, 141, 196	0
1	E	191/200 (95%)	0.25	4 (2%)	63	58	44, 93, 160, 192	0
1	F	191/200 (95%)	0.89	29 (15%)	5	4	62, 146, 232, 275	0
1	G	191/200 (95%)	0.72	17 (8%)	15	12	59, 131, 211, 242	0
1	H	191/200 (95%)	0.82	23 (12%)	9	7	63, 153, 264, 301	0
2	L	5/13 (38%)	1.46	0	100	100	139, 144, 151, 164	0
2	M	5/13 (38%)	1.29	1 (20%)	3	2	130, 154, 162, 171	1 (20%)
2	N	4/13 (30%)	1.78	1 (25%)	2	1	117, 143, 172, 204	1 (25%)
2	O	9/13 (69%)	0.79	0	100	100	93, 111, 132, 160	3 (33%)
All	All	1547/1652 (93%)	0.45	98 (6%)	26	20	36, 93, 218, 301	5 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	720	ASN	5.6
1	G	683	VAL	4.5
1	F	681	PHE	4.5
1	F	671	ALA	4.2
1	H	681	PHE	4.1
1	H	588	LEU	4.0
1	H	607	ASP	3.9
1	H	654	ILE	3.7
1	G	682	PHE	3.6
1	A	720	ASN	3.5
1	F	670	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	686	ALA	3.3
1	F	674	LEU	3.3
1	G	690	LYS	3.2
2	N	300	PHE	3.2
1	F	685	LYS	3.1
1	B	651	ASP	3.0
1	D	616	ASN	3.0
1	B	743	ASN	2.9
1	H	591	ARG	2.9
1	A	651	ASP	2.9
1	H	686	ALA	2.9
1	G	707	LYS	2.8
1	B	741	VAL	2.8
1	F	698	LEU	2.8
1	G	685	LYS	2.8
1	C	720	ASN	2.8
1	G	607	ASP	2.8
1	G	671	ALA	2.8
1	F	707	LYS	2.7
1	A	743	ASN	2.7
1	H	685	LYS	2.7
1	H	732	LYS	2.7
1	A	616	ASN	2.7
1	H	741	VAL	2.6
1	F	724	LEU	2.6
1	F	687	ASN	2.6
1	G	688	ALA	2.6
1	H	707	LYS	2.5
1	B	688	ALA	2.5
1	A	689	LYS	2.5
1	G	721	ILE	2.5
1	H	721	ILE	2.5
1	B	702	GLU	2.5
1	F	608	VAL	2.5
1	F	676	ALA	2.5
1	F	693	LEU	2.4
1	F	703	PRO	2.4
1	F	642	VAL	2.4
1	H	682	PHE	2.4
1	E	607	ASP	2.4
1	A	741	VAL	2.4
1	F	688	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	656	PHE	2.4
1	G	720	ASN	2.4
1	F	692	MET	2.4
1	E	684	ARG	2.4
1	H	720	ASN	2.3
1	F	651	ASP	2.3
1	H	677	SER	2.3
1	H	703	PRO	2.3
1	G	740	LEU	2.3
1	H	693	LEU	2.3
1	F	721	ILE	2.3
1	B	742	ASP	2.3
1	F	700	VAL	2.3
1	H	659	CYS	2.3
1	G	681	PHE	2.3
1	F	690	LYS	2.3
1	G	703	PRO	2.3
1	D	612	GLU	2.2
1	D	741	VAL	2.2
1	A	715	SER	2.2
1	F	644	SER	2.2
1	B	562	LEU	2.2
1	G	670	LEU	2.2
1	H	660	VAL	2.2
1	A	612	GLU	2.2
1	C	741	VAL	2.2
1	F	680	GLU	2.2
1	F	607	ASP	2.2
1	F	677	SER	2.2
1	G	741	VAL	2.2
1	F	684	ARG	2.1
1	F	704	THR	2.1
1	D	720	ASN	2.1
1	H	700	VAL	2.1
1	G	604	CYS	2.1
1	F	719	VAL	2.1
1	H	688	ALA	2.1
1	F	605	GLU	2.0
1	C	608	VAL	2.0
1	E	553	GLU	2.0
2	M	300	PHE	2.0
1	G	735	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	711	ALA	2.0
1	H	713	LYS	2.0
1	E	693	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SEP	N	304	10/11	0.76	0.14	89,128,139,142	0
2	SEP	M	304	10/11	0.82	0.09	150,153,156,157	0
2	SEP	L	304	10/11	0.85	0.10	133,139,145,146	0
2	SEP	O	304	10/11	0.94	0.07	126,129,132,138	0

6.3 Carbohydrates [i](#)

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.