



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:58 PM UTC

PDB ID : 5AJD / pdb_00005ajd
Title : Not1 C-terminal domain in complex with Not4
Authors : Bhaskar, V.; Basquin, J.; Conti, E.
Deposited on : 2015-02-23
Resolution : 3.62 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
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

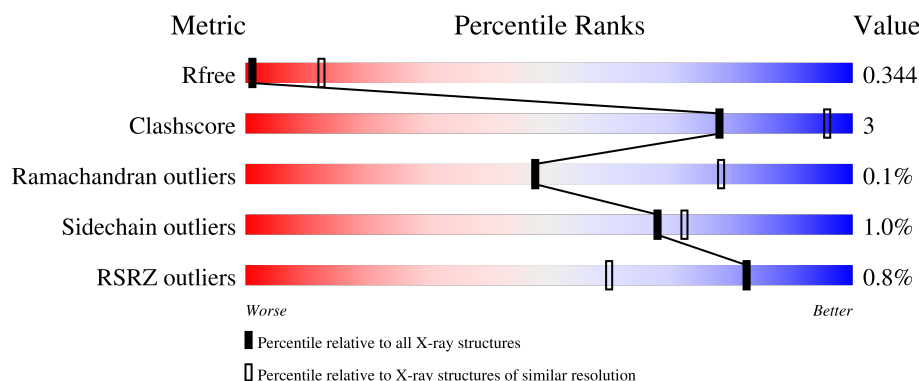
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.62 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	1062 (3.72-3.52)
Clashscore	190562	1092 (3.72-3.52)
Ramachandran outliers	187476	1057 (3.72-3.52)
Sidechain outliers	187428	1055 (3.72-3.52)
RSRZ outliers	180081	1060 (3.72-3.52)

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	556	82% 6% 12%
1	C	556	81% 6% 12%
1	E	556	82% 7% 11%
1	G	556	80% 8% 12%
1	I	556	80% 8% 12%

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Mol	Chain	Length	Quality of chain
1	K	556	% 79%8%12%
2	B	65	66%11%23%
2	D	65	2% 71%5%23%
2	F	65	65%.34%
2	H	65	5% 63%6%31%
2	J	65	72%.26%
2	L	65	2% 63%8%29%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 47509 atoms, of which 22962 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 CDC39P.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	489	Total	C	H	N	O	S	0	0	0
			7349	2487	3584	602	665	11			
1	C	487	Total	C	H	N	O	S	0	0	0
			7279	2461	3541	593	673	11			
1	E	496	Total	C	H	N	O	S	0	0	0
			7357	2498	3563	607	679	10			
1	G	489	Total	C	H	N	O	S	0	0	0
			7150	2442	3448	592	658	10			
1	I	490	Total	C	H	N	O	S	0	0	0
			7299	2473	3543	599	675	9			
1	K	489	Total	C	H	N	O	S	0	0	0
			7164	2439	3465	586	663	11			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1538	ARG	-	expression tag	UNP N1P976
A	1539	SER	-	expression tag	UNP N1P976
A	1540	MET	-	expression tag	UNP N1P976
C	1538	ARG	-	expression tag	UNP N1P976
C	1539	SER	-	expression tag	UNP N1P976
C	1540	MET	-	expression tag	UNP N1P976
E	1538	ARG	-	expression tag	UNP N1P976
E	1539	SER	-	expression tag	UNP N1P976
E	1540	MET	-	expression tag	UNP N1P976
G	1538	ARG	-	expression tag	UNP N1P976
G	1539	SER	-	expression tag	UNP N1P976
G	1540	MET	-	expression tag	UNP N1P976
I	1538	ARG	-	expression tag	UNP N1P976
I	1539	SER	-	expression tag	UNP N1P976
I	1540	MET	-	expression tag	UNP N1P976
K	1538	ARG	-	expression tag	UNP N1P976
K	1539	SER	-	expression tag	UNP N1P976

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Chain	Residue	Modelled	Actual	Comment	Reference
K	1540	MET	-	expression tag	UNP N1P976

- Molecule 2 is a protein called GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	50	Total	C	H	N	O	0	0	0
			704	243	328	63	70			
2	D	50	Total	C	H	N	O	0	0	0
			704	242	325	64	73			
2	F	43	Total	C	H	N	O	0	0	0
			619	212	294	56	57			
2	H	45	Total	C	H	N	O	0	0	0
			616	216	286	54	60			
2	J	48	Total	C	H	N	O	0	0	0
			661	229	304	62	66			
2	L	46	Total	C	H	N	O	0	0	0
			607	210	281	58	58			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	413	GLY	-	expression tag	UNP P34909
B	414	PRO	-	expression tag	UNP P34909
B	415	ASP	-	expression tag	UNP P34909
B	416	SER	-	expression tag	UNP P34909
B	417	MET	-	expression tag	UNP P34909
D	413	GLY	-	expression tag	UNP P34909
D	414	PRO	-	expression tag	UNP P34909
D	415	ASP	-	expression tag	UNP P34909
D	416	SER	-	expression tag	UNP P34909
D	417	MET	-	expression tag	UNP P34909
F	413	GLY	-	expression tag	UNP P34909
F	414	PRO	-	expression tag	UNP P34909
F	415	ASP	-	expression tag	UNP P34909
F	416	SER	-	expression tag	UNP P34909
F	417	MET	-	expression tag	UNP P34909
H	413	GLY	-	expression tag	UNP P34909
H	414	PRO	-	expression tag	UNP P34909
H	415	ASP	-	expression tag	UNP P34909
H	416	SER	-	expression tag	UNP P34909
H	417	MET	-	expression tag	UNP P34909

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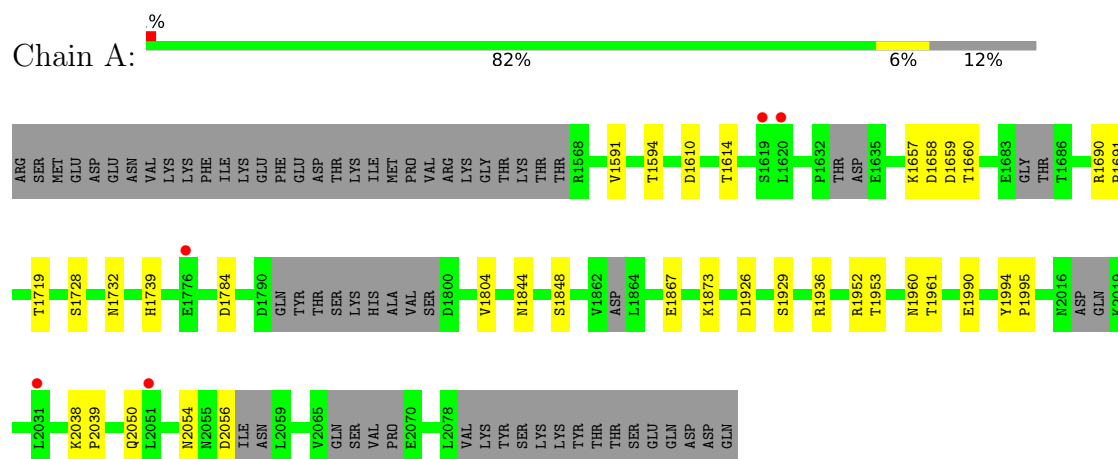
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Chain	Residue	Modelled	Actual	Comment	Reference
J	413	GLY	-	expression tag	UNP P34909
J	414	PRO	-	expression tag	UNP P34909
J	415	ASP	-	expression tag	UNP P34909
J	416	SER	-	expression tag	UNP P34909
J	417	MET	-	expression tag	UNP P34909
L	413	GLY	-	expression tag	UNP P34909
L	414	PRO	-	expression tag	UNP P34909
L	415	ASP	-	expression tag	UNP P34909
L	416	SER	-	expression tag	UNP P34909
L	417	MET	-	expression tag	UNP P34909

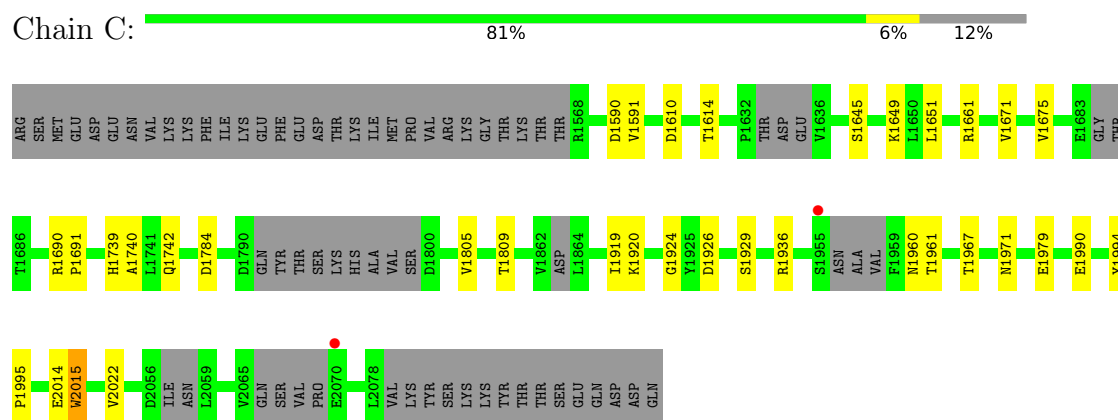
3 Residue-property plots

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.

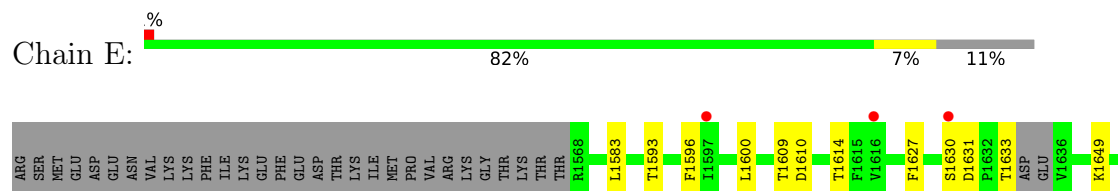
• Molecule 1: CDC39P

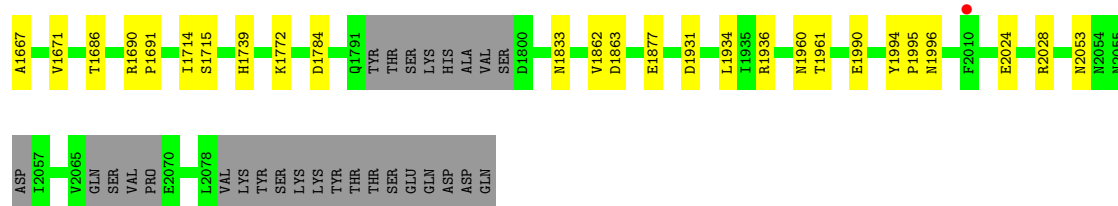


• Molecule 1: CDC39P

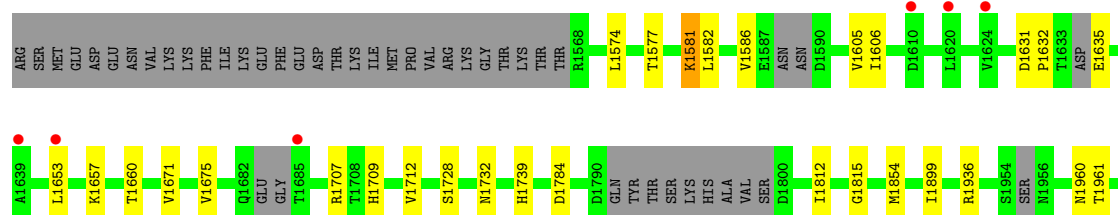
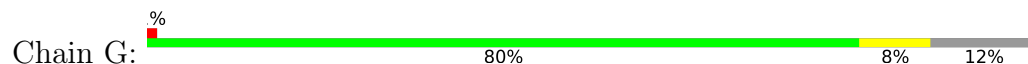


• Molecule 1: CDC39P

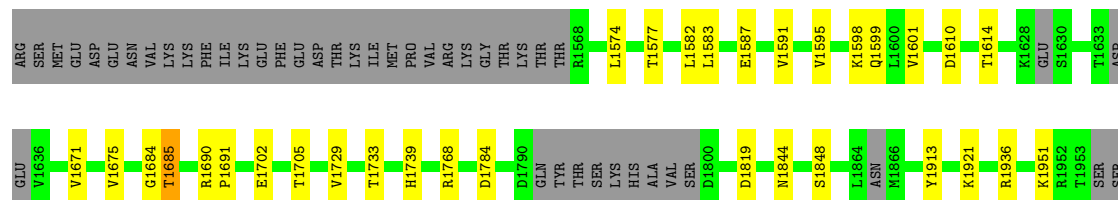
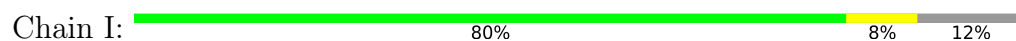




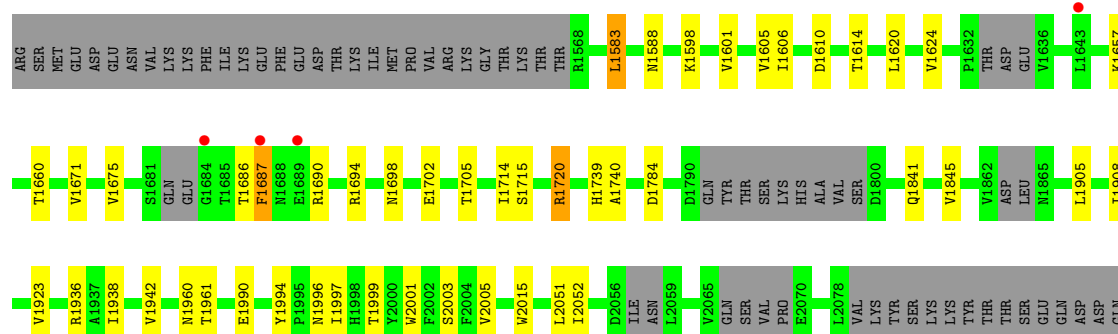
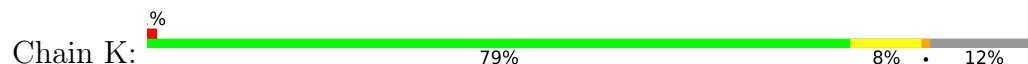
● Molecule 1: CDC39P



● Molecule 1: CDC39P



● Molecule 1: CDC39P



- Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 4

Chain B:  66% 11% 23%



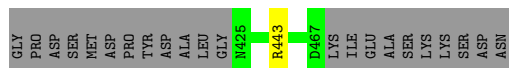
- Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 4

Chain D:  2% 71% 5% 23%



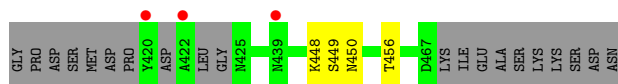
- Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 4

Chain F:  65% 0% 34%



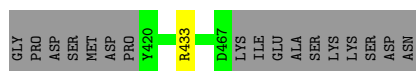
- Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 4

Chain H:  5% 63% 6% 31%



- Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 4

Chain J:  72% 0% 26%



- Molecule 2: GENERAL NEGATIVE REGULATOR OF TRANSCRIPTION SUBUNIT 4

Chain L:  2% 63% 8% 29%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.66Å 173.66Å 262.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.66 – 3.62 75.66 – 3.62	Depositor EDS
% Data completeness (in resolution range)	99.0 (75.66-3.62) 99.5 (75.66-3.62)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.58Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.266 , 0.319 0.296 , 0.344	Depositor DCC
R_{free} test set	2629 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	133.1	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 101.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	47509	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.20 % 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 1.8292e-05. 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

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	0.29	0/3853	0.66	1/5263 (0.0%)
1	C	0.28	0/3824	0.65	0/5223
1	E	0.30	0/3886	0.67	0/5316
1	G	0.30	0/3787	0.67	0/5175
1	I	0.29	0/3843	0.65	0/5246
1	K	0.30	0/3784	0.67	0/5181
2	B	0.35	0/385	0.66	0/527
2	D	0.32	0/388	0.70	0/531
2	F	0.37	0/333	0.70	0/455
2	H	0.35	0/336	0.79	1/458 (0.2%)
2	J	0.28	0/366	0.70	0/500
2	L	0.32	0/333	0.76	0/456
All	All	0.30	0/25118	0.67	2/34331 (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	1719	THR	N-CA-C	-6.44	104.11	112.23
2	H	456	THR	N-CA-C	-5.42	105.40	112.23

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	3765	3584	3581	19	0
1	C	3738	3541	3538	20	0
1	E	3794	3563	3562	20	0
1	G	3702	3448	3444	23	0
1	I	3756	3543	3540	21	0
1	K	3699	3465	3462	28	0
2	B	376	328	328	4	0
2	D	379	325	325	1	0
2	F	325	294	293	1	0
2	H	330	286	284	1	0
2	J	357	304	304	1	0
2	L	326	281	280	3	0
All	All	24547	22962	22941	134	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 3.

All (134) 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:1739:HIS:ND1	1:A:1784:ASP:OD2	2.11	0.83
1:C:1926:ASP:O	1:C:1929:SER:OG	2.06	0.71
1:A:1936:ARG:NH1	1:A:1990:GLU:OE1	2.25	0.70
1:E:1593:THR:OG1	1:E:1649:LYS:NZ	2.25	0.70
1:C:1742:GLN:HG2	1:K:1923:VAL:HG11	1.73	0.69
1:E:1994:TYR:O	1:E:1996:ASN:ND2	2.26	0.68
1:G:1936:ARG:NH1	1:G:1990:GLU:OE1	2.27	0.68
1:C:1967:THR:O	1:C:1971:ASN:ND2	2.28	0.67
1:I:1994:TYR:O	1:I:1996:ASN:ND2	2.29	0.66
1:K:1994:TYR:O	1:K:1996:ASN:ND2	2.29	0.65
1:G:1979:GLU:OE2	2:J:433:ARG:NH1	2.30	0.65
1:C:1740:ALA:HA	1:K:1923:VAL:HG13	1.79	0.64
1:G:2010:PHE:O	1:G:2023:GLN:NE2	2.32	0.62
1:E:1960:ASN:OD1	1:E:1961:THR:N	2.33	0.62
1:E:1772:LYS:NZ	1:E:1877:GLU:OE2	2.26	0.62
1:G:1739:HIS:ND1	1:G:1784:ASP:OD2	2.34	0.61
1:C:2015:TRP:CH2	1:C:2022:VAL:HG11	2.35	0.60
1:A:1926:ASP:O	1:A:1929:SER:OG	2.20	0.59
1:C:1651:LEU:O	1:C:1661:ARG:NH1	2.36	0.58
1:I:1960:ASN:OD1	1:I:1961:THR:N	2.37	0.58
1:C:1739:HIS:ND1	1:C:1784:ASP:OD2	2.37	0.58
1:I:1595:VAL:O	1:I:1599:GLN:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1709:HIS:O	1:G:1712:VAL:HG23	2.05	0.57
1:K:1960:ASN:OD1	1:K:1961:THR:N	2.37	0.56
1:E:1739:HIS:ND1	1:E:1784:ASP:OD2	2.38	0.56
1:G:2052:ILE:O	1:G:2055:ASN:N	2.38	0.56
1:G:1657:LYS:N	1:G:1660:THR:OG1	2.37	0.56
2:B:425:ASN:OD1	2:B:426:ALA:N	2.38	0.55
2:B:450:ASN:OD1	2:B:451:ILE:N	2.39	0.55
1:C:1960:ASN:OD1	1:C:1961:THR:N	2.40	0.55
1:I:1739:HIS:ND1	1:I:1784:ASP:OD2	2.40	0.55
1:E:1863:ASP:OD1	1:E:2053:ASN:ND2	2.40	0.55
1:C:1936:ARG:NH1	1:C:1990:GLU:OE1	2.39	0.54
1:K:1714:ILE:HG21	1:K:1720:ARG:HB2	1.90	0.54
1:A:1844:ASN:O	1:A:1848:SER:N	2.41	0.53
1:A:1960:ASN:OD1	1:A:1961:THR:N	2.42	0.53
1:K:1598:LYS:O	1:K:1601:VAL:HG22	2.09	0.53
1:K:1694:ARG:NH1	1:K:1698:ASN:OD1	2.43	0.52
1:I:1702:GLU:O	1:I:1705:THR:OG1	2.26	0.52
1:C:1590:ASP:OD1	1:C:1591:VAL:N	2.42	0.52
1:I:1729:VAL:O	1:I:1733:THR:OG1	2.25	0.52
1:C:1994:TYR:HB2	1:C:1995:PRO:HD2	1.92	0.51
1:E:1936:ARG:NH1	1:E:1990:GLU:OE1	2.43	0.51
1:I:1913:TYR:OH	1:I:1975:ASN:O	2.29	0.51
1:G:1728:SER:O	1:G:1732:ASN:ND2	2.43	0.51
1:E:1833:ASN:OD1	1:E:1936:ARG:NE	2.44	0.50
1:I:1936:ARG:NH1	1:I:1990:GLU:OE1	2.43	0.50
1:K:1739:HIS:ND1	1:K:1784:ASP:OD2	2.44	0.50
1:E:1630:SER:OG	1:E:1631:ASP:N	2.44	0.50
1:A:1658:ASP:OD1	1:A:1659:ASP:N	2.40	0.49
1:A:1657:LYS:N	1:A:1660:THR:OG1	2.45	0.49
1:E:1931:ASP:OD1	1:E:1934:LEU:N	2.45	0.49
1:K:1657:LYS:N	1:K:1660:THR:OG1	2.46	0.49
2:B:422:ALA:O	2:B:424:GLY:N	2.42	0.48
1:G:1631:ASP:N	1:G:1632:PRO:CD	2.76	0.48
1:A:1591:VAL:O	1:A:1594:THR:OG1	2.24	0.48
1:K:2051:LEU:HD12	1:K:2052:ILE:N	2.29	0.47
1:I:1598:LYS:O	1:I:1601:VAL:HG22	2.15	0.47
1:A:1994:TYR:HB2	1:A:1995:PRO:HD2	1.97	0.47
1:C:1920:LYS:NZ	1:C:1929:SER:O	2.46	0.47
1:I:1768:ARG:NH1	1:I:1819:ASP:OD1	2.48	0.47
1:E:2024:GLU:O	1:E:2028:ARG:N	2.47	0.46
1:K:1905:LEU:HA	1:K:1908:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1582:LEU:O	1:G:1586:VAL:N	2.47	0.46
2:L:451:ILE:HG23	2:L:452:ILE:N	2.30	0.46
1:K:1999:THR:O	1:K:2003:SER:OG	2.32	0.46
1:K:1936:ARG:NH1	1:K:1990:GLU:OE1	2.49	0.46
1:I:1844:ASN:O	1:I:1848:SER:N	2.45	0.45
1:A:1952:ARG:HG2	1:A:1953:THR:N	2.32	0.45
1:K:1610:ASP:O	1:K:1614:THR:OG1	2.29	0.45
1:C:1671:VAL:O	1:C:1675:VAL:HG23	2.16	0.45
2:D:451:ILE:HG13	2:D:452:ILE:H	1.81	0.45
1:G:1960:ASN:OD1	1:G:1961:THR:N	2.50	0.45
1:I:1671:VAL:O	1:I:1675:VAL:HG23	2.17	0.45
1:E:1596:PHE:CE2	1:E:1600:LEU:HD21	2.52	0.44
1:C:1690:ARG:N	1:C:1691:PRO:CD	2.81	0.44
1:K:1702:GLU:O	1:K:1705:THR:OG1	2.27	0.44
1:K:1997:ILE:O	1:K:2001:TRP:N	2.49	0.44
1:C:1979:GLU:OE2	2:L:433:ARG:NH1	2.51	0.44
1:K:2001:TRP:O	1:K:2005:VAL:HG23	2.18	0.44
1:K:1583:LEU:HD13	1:K:1588:ASN:CB	2.47	0.44
1:C:1805:VAL:O	1:C:1809:THR:N	2.51	0.44
1:I:1610:ASP:O	1:I:1614:THR:OG1	2.28	0.44
1:C:1610:ASP:O	1:C:1614:THR:OG1	2.24	0.43
1:C:1924:GLY:N	1:K:1740:ALA:O	2.50	0.43
1:G:2036:VAL:HG13	1:G:2037:ASN:H	1.83	0.43
1:K:1714:ILE:CG2	1:K:1720:ARG:HB2	2.49	0.43
1:A:1610:ASP:O	1:A:1614:THR:OG1	2.29	0.43
1:E:1610:ASP:O	1:E:1614:THR:OG1	2.29	0.43
1:A:1728:SER:O	1:A:1732:ASN:ND2	2.49	0.43
1:G:1999:THR:O	1:G:2003:SER:OG	2.37	0.43
1:K:1620:LEU:O	1:K:1624:VAL:HG23	2.19	0.43
2:L:451:ILE:HG23	2:L:452:ILE:H	1.83	0.43
1:I:1574:LEU:O	1:I:1577:THR:OG1	2.34	0.43
1:A:1867:GLU:O	1:A:1873:LYS:NZ	2.52	0.42
1:I:2036:VAL:O	1:I:2040:HIS:NE2	2.51	0.42
1:A:1804:VAL:HG12	1:E:1686:THR:HG22	2.01	0.42
1:I:1591:VAL:O	1:I:1595:VAL:HG23	2.20	0.42
1:I:2041:THR:HG23	1:I:2044:VAL:HG22	2.02	0.42
1:K:1671:VAL:O	1:K:1675:VAL:HG23	2.20	0.42
1:K:1686:THR:HG23	1:K:1687:PHE:N	2.34	0.42
1:A:1952:ARG:C	1:A:1953:THR:HG22	2.45	0.42
1:A:2050:GLN:O	1:A:2054:ASN:N	2.51	0.42
1:A:1690:ARG:N	1:A:1691:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1667:ALA:O	1:E:1671:VAL:HG23	2.20	0.41
1:I:2001:TRP:O	1:I:2005:VAL:HG23	2.19	0.41
1:E:1690:ARG:N	1:E:1691:PRO:CD	2.84	0.41
1:G:1581:LYS:HD3	1:G:1582:LEU:N	2.35	0.41
1:I:1985:ILE:O	1:I:1989:VAL:HG23	2.20	0.41
1:G:1605:VAL:HG12	1:G:1606:ILE:HG12	2.03	0.41
1:I:1684:GLY:O	1:I:1685:THR:HG22	2.20	0.41
1:K:1841:GLN:O	1:K:1845:VAL:HG23	2.19	0.41
1:G:1635:GLU:OE2	1:K:1690:ARG:NH1	2.51	0.41
1:E:1631:ASP:O	1:E:1633:THR:N	2.53	0.41
1:G:1854:MET:HE1	1:G:1995:PRO:HD2	2.02	0.41
1:G:2036:VAL:HG13	1:G:2037:ASN:N	2.36	0.41
1:K:1605:VAL:HG22	1:K:1606:ILE:HD12	2.03	0.41
2:B:451:ILE:HG13	2:B:452:ILE:N	2.36	0.41
1:C:1645:SER:OG	1:C:1649:LYS:NZ	2.50	0.41
1:C:1919:ILE:HG12	1:C:1920:LYS:H	1.86	0.41
1:E:1714:ILE:HG22	1:E:1715:SER:N	2.36	0.41
2:H:448:LYS:O	2:H:450:ASN:N	2.54	0.41
1:E:1609:THR:OG1	2:F:443:ARG:O	2.26	0.41
1:G:2001:TRP:O	1:G:2005:VAL:HG23	2.21	0.40
1:G:1671:VAL:O	1:G:1675:VAL:HG23	2.21	0.40
1:I:1690:ARG:N	1:I:1691:PRO:CD	2.84	0.40
1:K:1938:ILE:O	1:K:1942:VAL:HG23	2.21	0.40
1:A:1690:ARG:N	1:A:1691:PRO:CD	2.85	0.40
1:E:1994:TYR:HB2	1:E:1995:PRO:HD2	2.03	0.40
1:K:1714:ILE:HG13	1:K:1715:SER:N	2.36	0.40
1:A:2038:LYS:CB	1:A:2039:PRO:HA	2.52	0.40
1:G:2015:TRP:HB3	1:G:2019:LYS:CB	2.52	0.40
1:G:1574:LEU:O	1:G:1577:THR:OG1	2.37	0.40
1:G:1812:ILE:O	1:G:1815:GLY:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	473/556 (85%)	455 (96%)	18 (4%)	0	100	100
1	C	471/556 (85%)	446 (95%)	25 (5%)	0	100	100
1	E	486/556 (87%)	455 (94%)	30 (6%)	1 (0%)	43	71
1	G	471/556 (85%)	448 (95%)	23 (5%)	0	100	100
1	I	472/556 (85%)	449 (95%)	23 (5%)	0	100	100
1	K	475/556 (85%)	448 (94%)	27 (6%)	0	100	100
2	B	48/65 (74%)	40 (83%)	8 (17%)	0	100	100
2	D	48/65 (74%)	41 (85%)	7 (15%)	0	100	100
2	F	41/65 (63%)	34 (83%)	7 (17%)	0	100	100
2	H	41/65 (63%)	33 (80%)	7 (17%)	1 (2%)	4	26
2	J	46/65 (71%)	42 (91%)	4 (9%)	0	100	100
2	L	44/65 (68%)	41 (93%)	3 (7%)	0	100	100
All	All	3116/3726 (84%)	2932 (94%)	182 (6%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	1862	VAL
2	H	449	SER

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	384/525 (73%)	383 (100%)	1 (0%)	86	81
1	C	384/525 (73%)	382 (100%)	2 (0%)	81	78
1	E	383/525 (73%)	381 (100%)	2 (0%)	81	78
1	G	365/525 (70%)	361 (99%)	4 (1%)	65	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	381/525 (73%)	375 (98%)	6 (2%)	55	66
1	K	369/525 (70%)	365 (99%)	4 (1%)	65	71
2	B	34/59 (58%)	34 (100%)	0	100	100
2	D	35/59 (59%)	32 (91%)	3 (9%)	10	32
2	F	30/59 (51%)	30 (100%)	0	100	100
2	H	28/59 (48%)	28 (100%)	0	100	100
2	J	31/59 (52%)	31 (100%)	0	100	100
2	L	27/59 (46%)	25 (93%)	2 (7%)	13	37
All	All	2451/3504 (70%)	2427 (99%)	24 (1%)	68	72

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2056	ASP
1	C	2014	GLU
1	C	2015	TRP
2	D	429	PHE
2	D	441	GLN
2	D	452	ILE
1	E	1583	LEU
1	E	1627	PHE
1	G	1581	LYS
1	G	1653	LEU
1	G	1707	ARG
1	G	1899	ILE
1	I	1582	LEU
1	I	1583	LEU
1	I	1587	GLU
1	I	1685	THR
1	I	1921	LYS
1	I	1951	LYS
1	K	1583	LEU
1	K	1687	PHE
1	K	1720	ARG
1	K	2015	TRP
2	L	430	LEU
2	L	443	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1818	ASN
1	A	1834	ASN
1	A	1902	ASN
1	A	1975	ASN
1	A	2055	ASN
1	C	1710	ASN
1	C	1818	ASN
1	C	1834	ASN
1	E	1654	GLN
1	E	1975	ASN
1	E	2054	ASN
1	G	1834	ASN
1	G	1902	ASN
1	G	1991	GLN
1	I	1682	GLN
1	K	1834	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

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 ⓘ

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	489/556 (87%)	-0.13	5 (1%) 79 55	79, 126, 170, 191	0
1	C	487/556 (87%)	-0.15	2 (0%) 88 71	96, 134, 174, 205	0
1	E	496/556 (89%)	-0.10	4 (0%) 82 60	85, 133, 170, 193	0
1	G	489/556 (87%)	-0.07	7 (1%) 73 47	93, 137, 175, 203	0
1	I	490/556 (88%)	-0.13	0 100 100	89, 134, 171, 207	0
1	K	489/556 (87%)	-0.08	4 (0%) 82 60	92, 141, 174, 202	0
2	B	50/65 (76%)	-0.28	0 100 100	113, 156, 178, 181	0
2	D	50/65 (76%)	-0.18	1 (2%) 65 40	126, 158, 185, 210	0
2	F	43/65 (66%)	-0.24	0 100 100	114, 147, 179, 203	0
2	H	45/65 (69%)	0.21	3 (6%) 24 16	127, 160, 187, 195	0
2	J	48/65 (73%)	-0.21	0 100 100	120, 150, 177, 192	0
2	L	46/65 (70%)	-0.30	1 (2%) 62 38	121, 154, 180, 185	0
All	All	3222/3726 (86%)	-0.12	27 (0%) 82 60	79, 136, 175, 210	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	422	ALA	4.1
1	A	1620	LEU	3.6
1	G	1620	LEU	3.2
1	K	1687	PHE	3.0
1	K	1689	GLU	2.7
2	L	453	ASP	2.5
1	G	1639	ALA	2.5
1	E	1616	VAL	2.4
2	H	420	TYR	2.4
1	C	1955	SER	2.4
1	G	1685	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	1624	VAL	2.3
1	E	1630	SER	2.3
1	A	2031	LEU	2.3
1	G	1653	LEU	2.2
1	E	1597	ILE	2.2
1	G	2070	GLU	2.2
1	A	1619	SER	2.2
1	K	1643	LEU	2.2
2	H	439	ASN	2.1
1	A	1776	GLU	2.1
1	G	1610	ASP	2.0
2	D	428	ASP	2.0
1	C	2070	GLU	2.0
1	A	2051	LEU	2.0
1	K	1684	GLY	2.0
1	E	2010	PHE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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.